Full wwPDB EM Validation Report

Aug 5, 2026 – 07:18 AM EDT

PDB ID	:	9E0J / pdb_00009e0j
EMDB ID	:	EMD-47359
Title	:	Structure and evolution of Photosystem I in the early-branching cyanobacterium Anthocerotibacter panamensis
Authors	:	Gisriel, C.J.; Ho, M.
Deposited on	:	2024-10-18
Resolution	:	2.40 Å(reported)

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

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

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

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

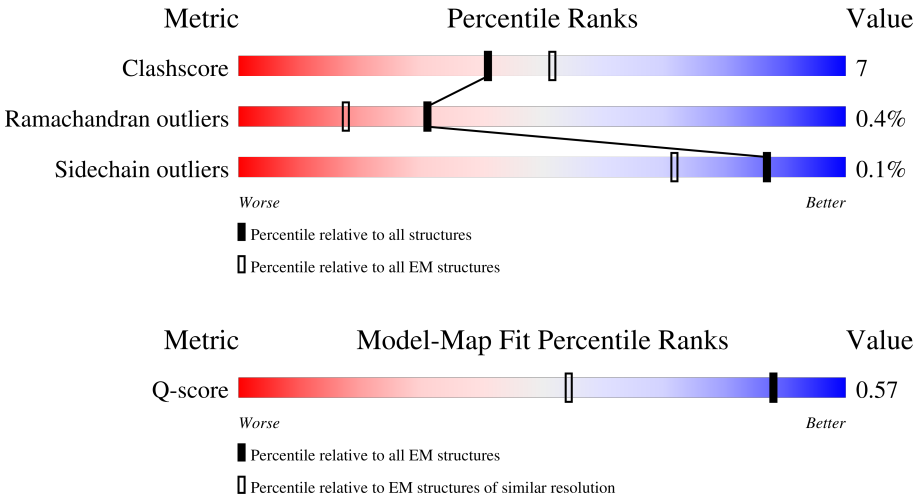
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	A	785	7% 85% 13%
1	G	785	7% 82% 16%
1	a	785	7% 82% 16%
2	M	32	88% 9%

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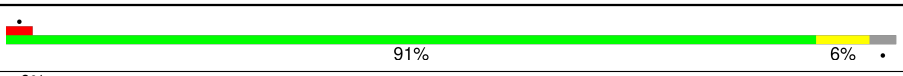
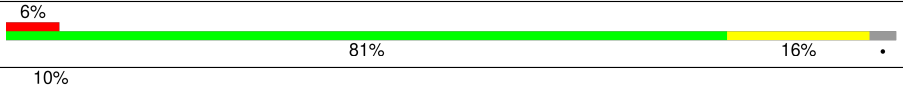
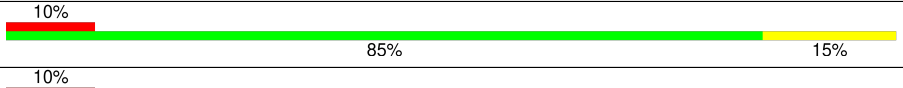
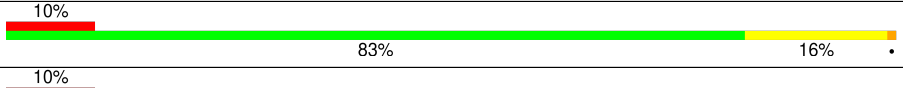
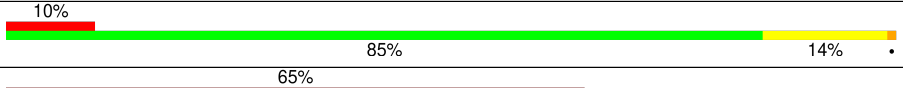
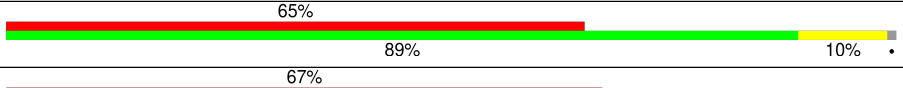
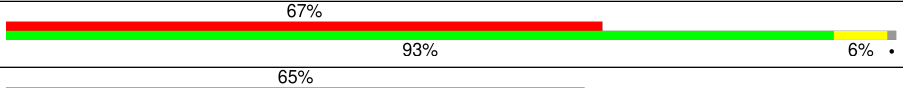
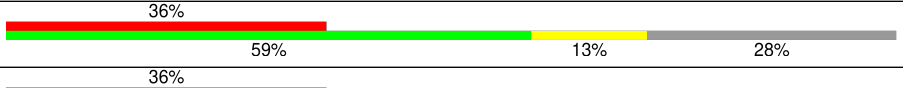
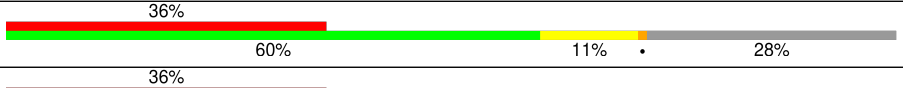
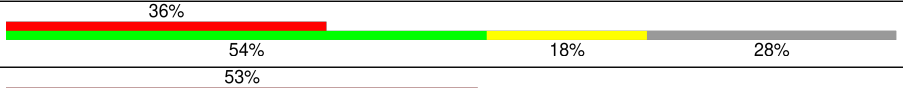
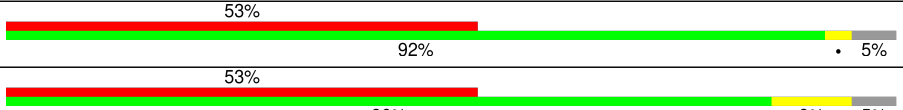
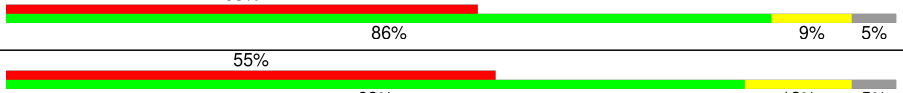
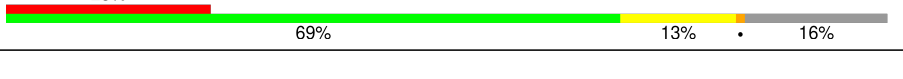
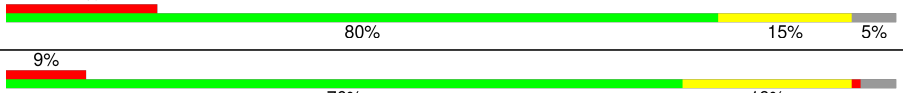
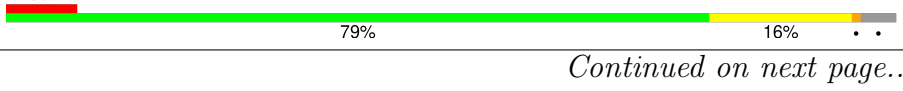
Mol	Chain	Length	Quality of chain
2	T	32	
2	m	32	
3	B	749	
3	H	749	
3	b	749	
4	C	81	
4	K	81	
4	c	81	
5	D	143	
5	N	143	
5	d	143	
6	E	64	
6	O	64	
6	e	64	
7	F	177	
7	P	177	
7	f	177	
8	I	32	
8	Q	32	
8	i	32	
9	J	41	
9	R	41	
9	j	41	
10	L	160	
10	S	160	

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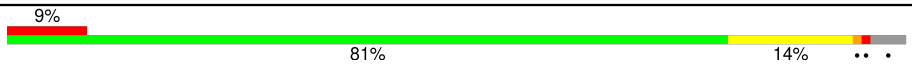
Mol	Chain	Length	Quality of chain
10	l	160	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 69921 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	G	773	Total	C	N	O	S	0	0
			5997	3925	1024	1023	25		
1	a	773	Total	C	N	O	S	0	0
			5997	3925	1024	1023	25		
1	A	773	Total	C	N	O	S	0	0
			5997	3925	1024	1023	25		

- Molecule 2 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	31	Total	C	N	O	S	0	0
			226	152	34	38	2		
2	m	31	Total	C	N	O	S	0	0
			226	152	34	38	2		
2	M	31	Total	C	N	O	S	0	0
			226	152	34	38	2		

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	746	Total	C	N	O	S	0	0
			5866	3864	981	1001	20		
3	b	746	Total	C	N	O	S	0	0
			5866	3864	981	1001	20		
3	B	746	Total	C	N	O	S	0	0
			5866	3864	981	1001	20		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	80	Total	C	N	O	S	0	0
			599	367	105	117	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	80	Total	C	N	O	S	0	0
			599	367	105	117	10		
4	C	80	Total	C	N	O	S	0	0
			599	367	105	117	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	103	Total	C	N	O	S	0	0
			784	500	138	143	3		
5	d	103	Total	C	N	O	S	0	0
			784	500	138	143	3		
5	D	103	Total	C	N	O	S	0	0
			784	500	138	143	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	61	Total	C	N	O	0	0
			489	308	84	97		
6	e	61	Total	C	N	O	0	0
			489	308	84	97		
6	E	61	Total	C	N	O	0	0
			489	308	84	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	148	Total	C	N	O	S	0	0
			1148	738	191	215	4		
7	f	148	Total	C	N	O	S	0	0
			1148	738	191	215	4		
7	F	148	Total	C	N	O	S	0	0
			1148	738	191	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	31	Total	C	N	O	S	0	0
			254	175	36	42	1		
8	i	31	Total	C	N	O	S	0	0
			254	175	36	42	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	31	Total	C	N	O	S	0	0
			254	175	36	42	1		

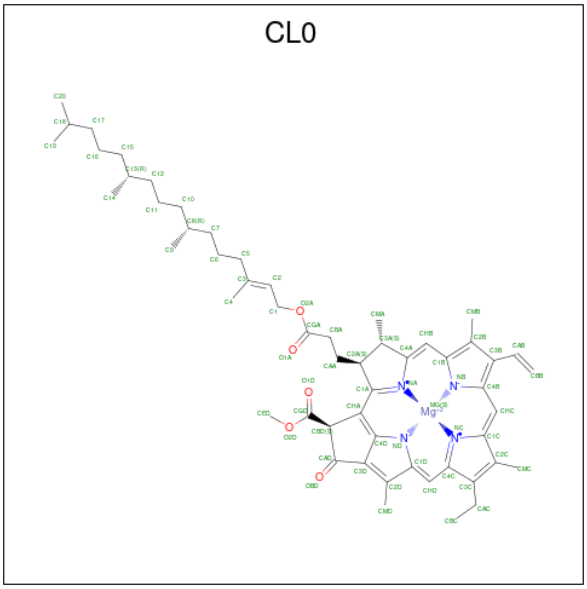
- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	39	Total	C	N	O	0	0
			293	204	44	45		
9	j	39	Total	C	N	O	0	0
			293	204	44	45		
9	J	39	Total	C	N	O	0	0
			293	204	44	45		

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

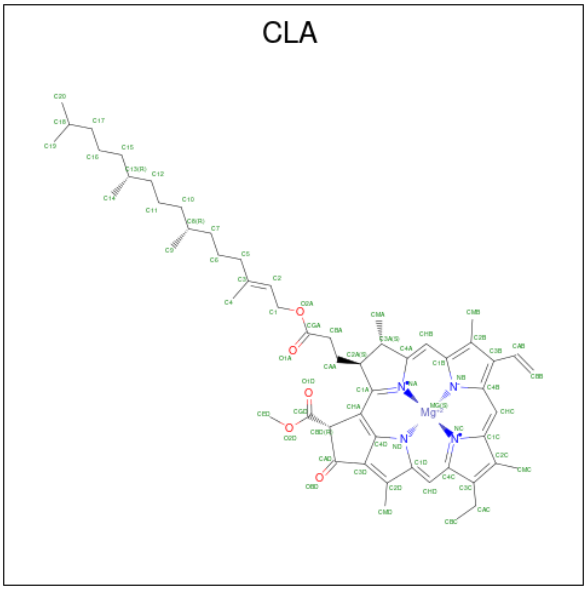
Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		
10	l	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		
10	L	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		

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



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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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

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

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

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

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

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

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

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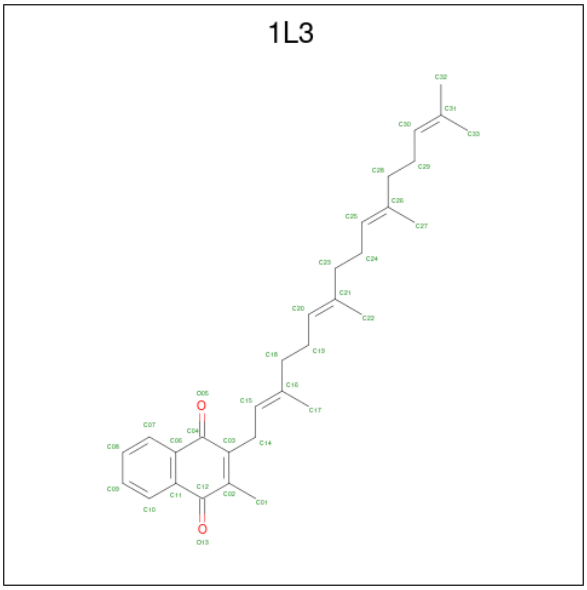
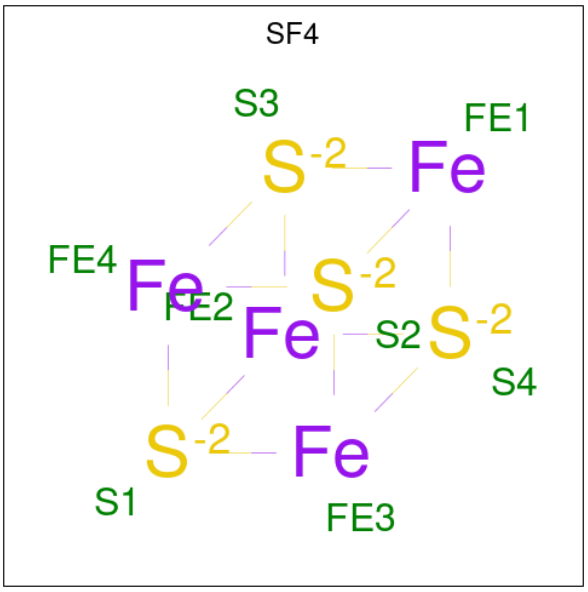
Mol	Chain	Residues	Atoms					AltConf
12	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



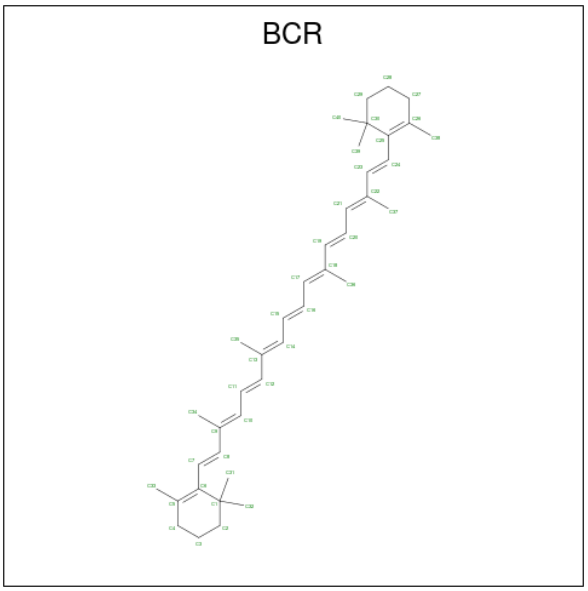
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			33	31	2	
13	H	1	Total	C	O	0
			33	31	2	
13	a	1	Total	C	O	0
			33	31	2	
13	b	1	Total	C	O	0
			33	31	2	
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

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



Mol	Chain	Residues	Atoms	AltConf
14	G	1	Total Fe S 8 4 4	0
14	K	1	Total Fe S 8 4 4	0
14	K	1	Total Fe S 8 4 4	0
14	a	1	Total Fe S 8 4 4	0
14	c	1	Total Fe S 8 4 4	0
14	c	1	Total Fe S 8 4 4	0
14	A	1	Total Fe S 8 4 4	0
14	C	1	Total Fe S 8 4 4	0
14	C	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	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 25 25	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	P	1	Total C 40 40	0
15	P	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 25 25	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 25 25	0
15	B	1	Total C 40 40	0

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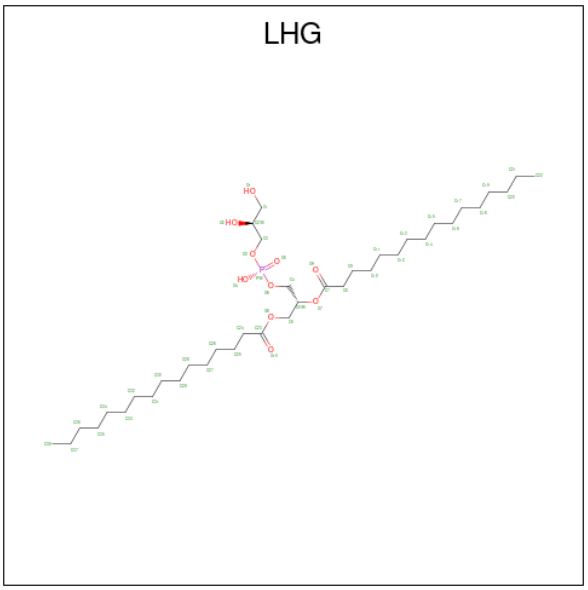
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0

- 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	G	1	Total C O P 49 38 10 1	0

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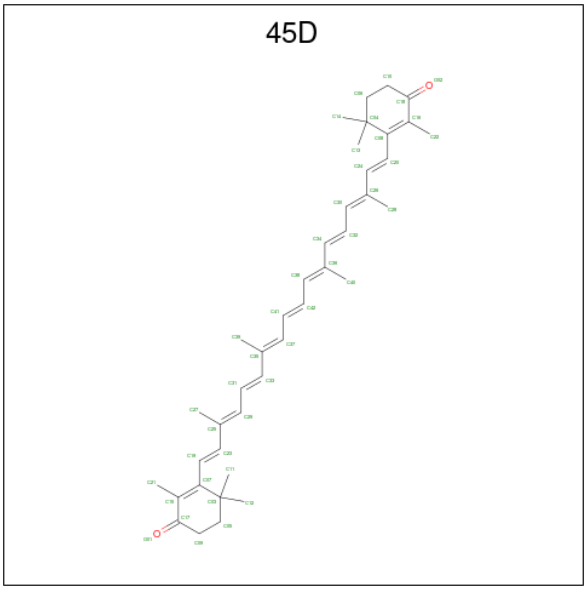
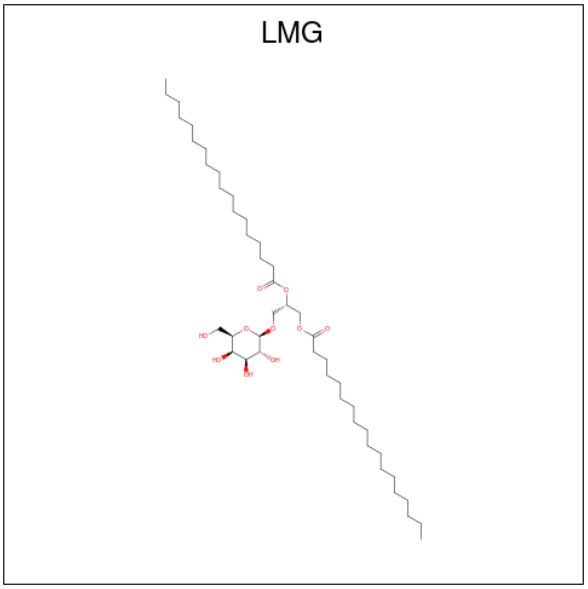
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			27	16	10	1	
16	G	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			27	16	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			27	16	10	1	
16	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 17 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



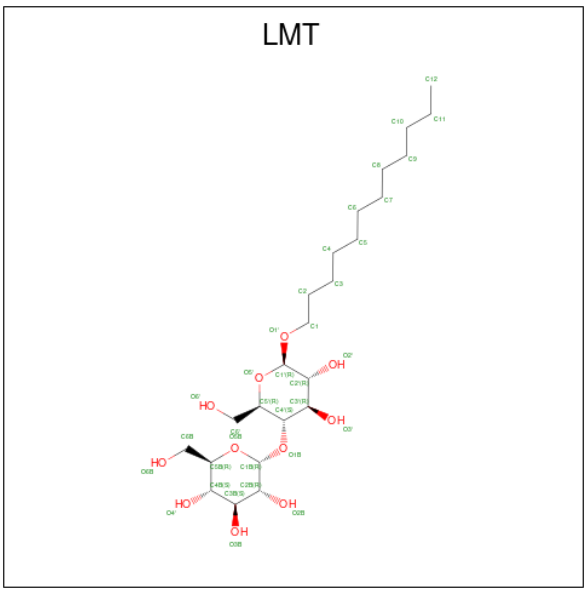
Mol	Chain	Residues	Atoms			AltConf
17	T	1	Total	C	O	0
			42	40	2	
17	m	1	Total	C	O	0
			42	40	2	
17	M	1	Total	C	O	0
			42	40	2	

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



Mol	Chain	Residues	Atoms			AltConf
18	H	1	Total	C	O	0
			55	45	10	
18	b	1	Total	C	O	0
			55	45	10	
18	B	1	Total	C	O	0
			55	45	10	

- Molecule 19 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C O 35 24 11	0
19	b	1	Total C O 35 24 11	0
19	B	1	Total C O 35 24 11	0

- Molecule 20 is water.

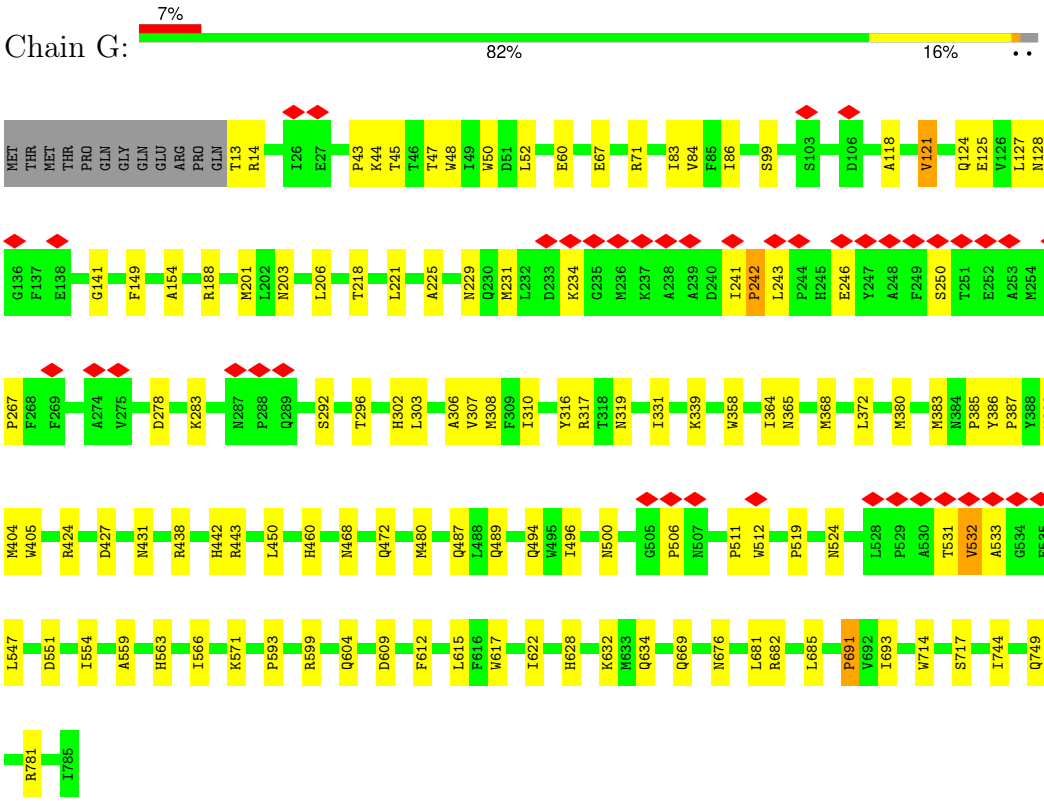
Mol	Chain	Residues	Atoms	AltConf
20	G	58	Total O 58 58	0
20	H	80	Total O 80 80	0
20	K	26	Total O 26 26	0
20	N	15	Total O 15 15	0
20	O	1	Total O 1 1	0
20	S	5	Total O 5 5	0
20	a	57	Total O 57 57	0
20	b	82	Total O 82 82	0
20	c	22	Total O 22 22	0
20	d	17	Total O 17 17	0
20	e	1	Total O 1 1	0
20	l	6	Total O 6 6	0
20	A	56	Total O 56 56	0
20	B	82	Total O 82 82	0
20	C	24	Total O 24 24	0
20	D	16	Total O 16 16	0
20	L	7	Total O 7 7	0

3 Residue-property plots (i)

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

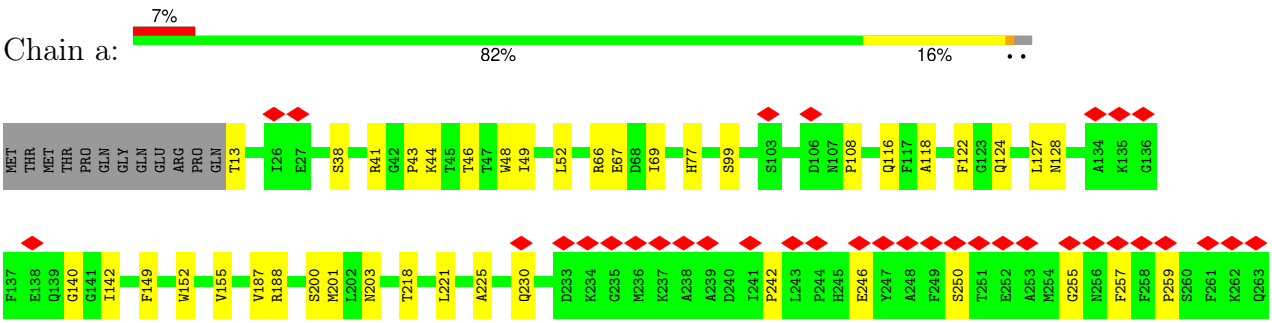
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

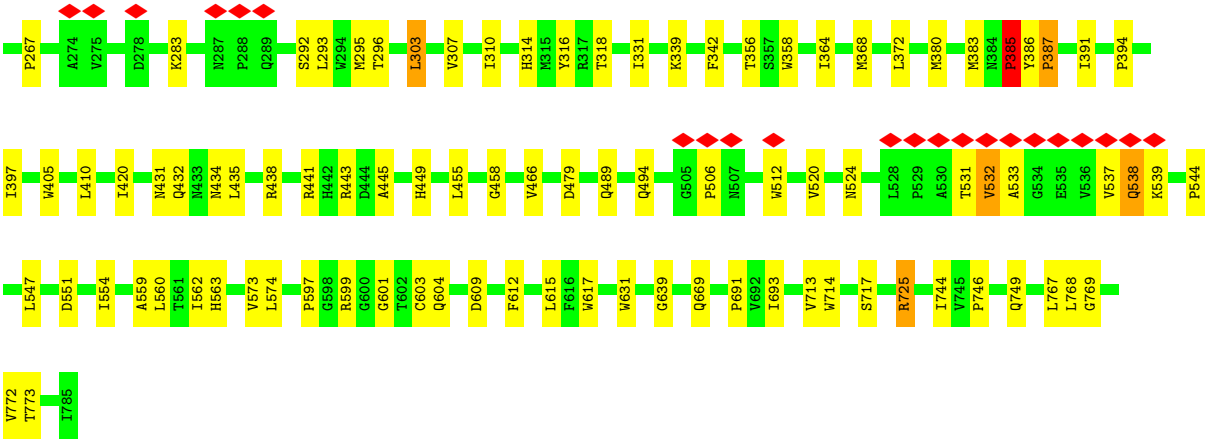
Chain G:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

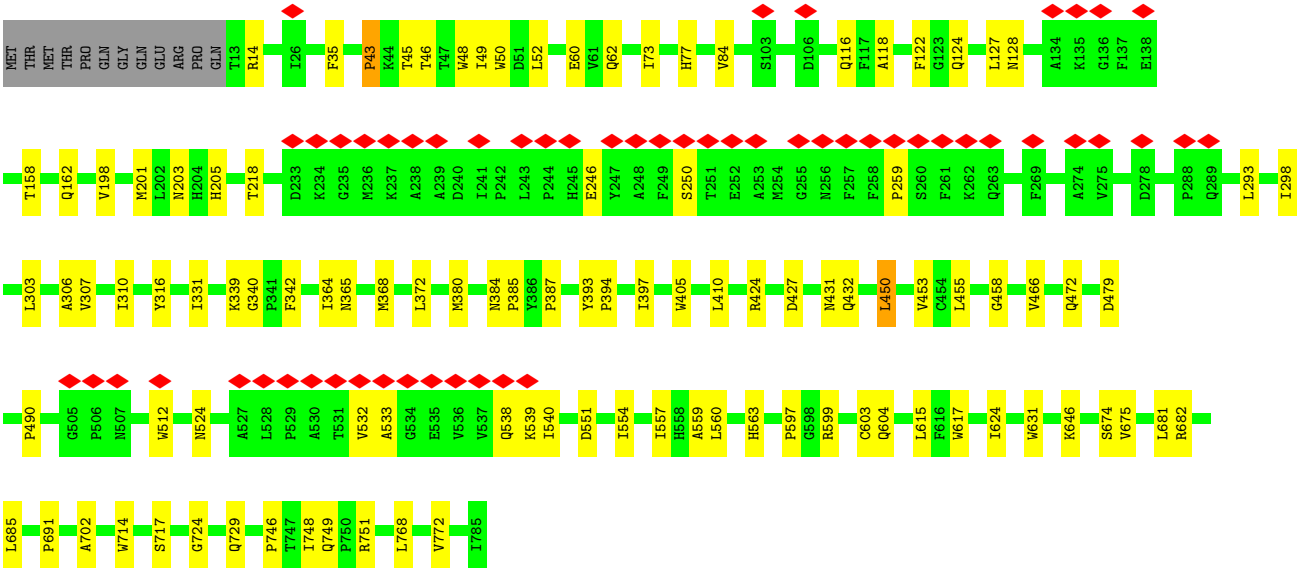
Chain a:





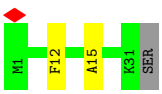
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



• Molecule 2: Photosystem I reaction center subunit XII

Chain T:

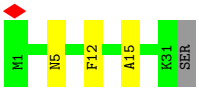


• Molecule 2: Photosystem I reaction center subunit XII

Chain m:

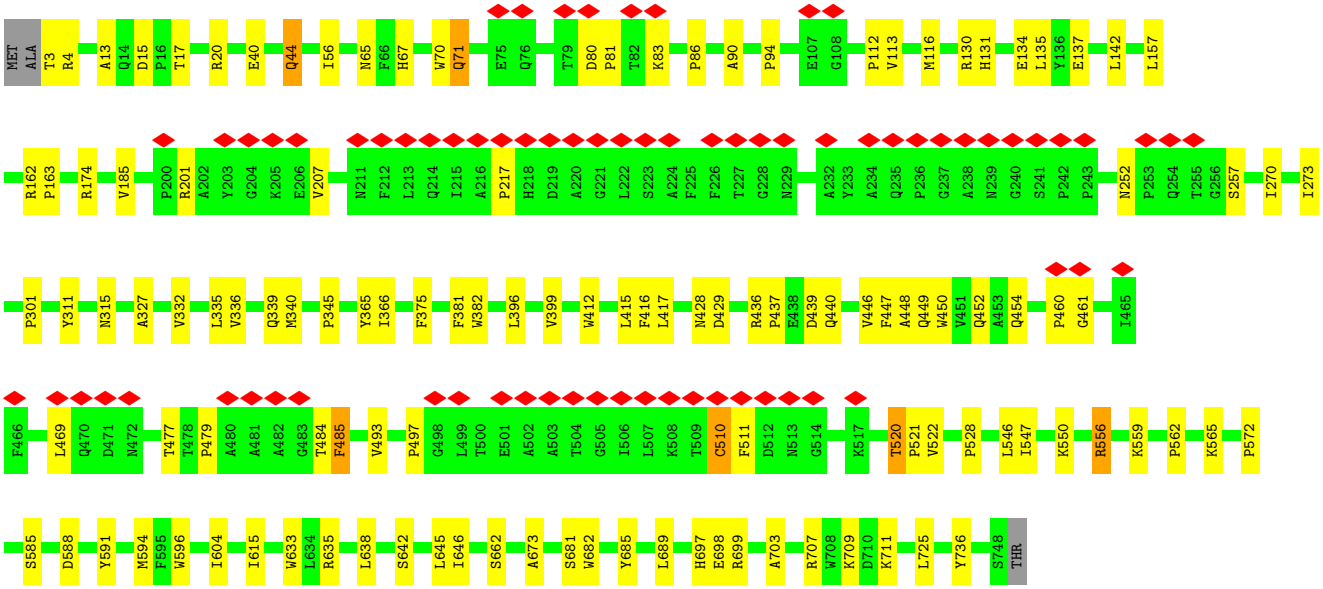
• Molecule 2: Photosystem I reaction center subunit XII

Chain M:



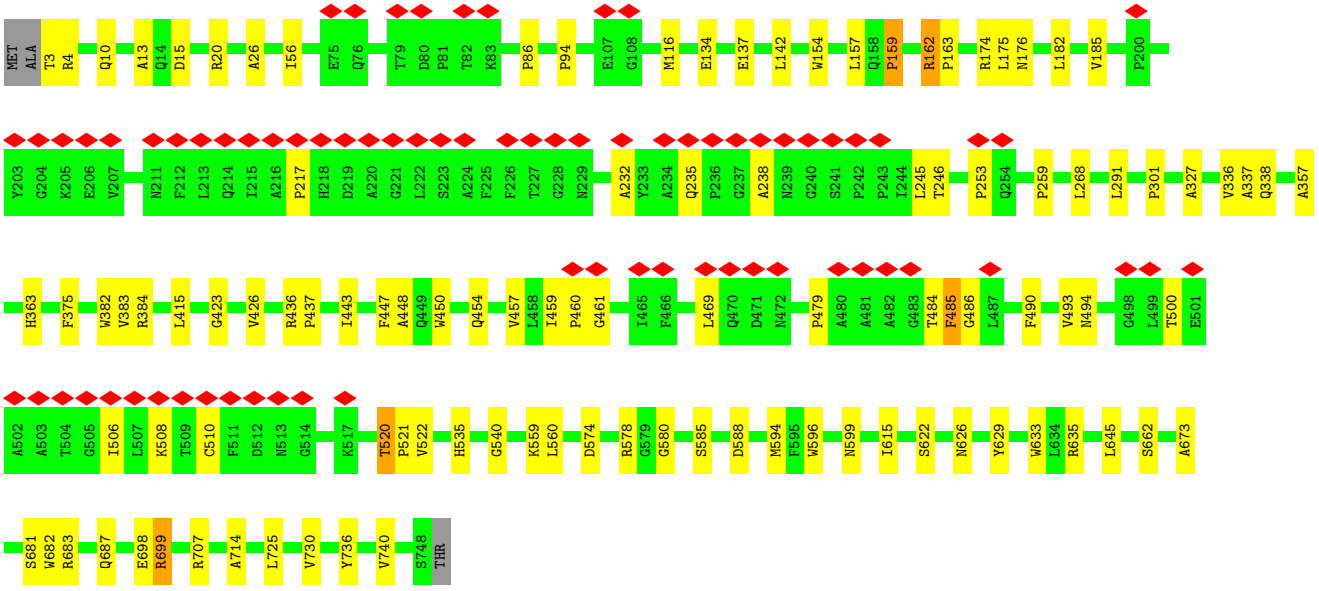
• Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2

Chain H:



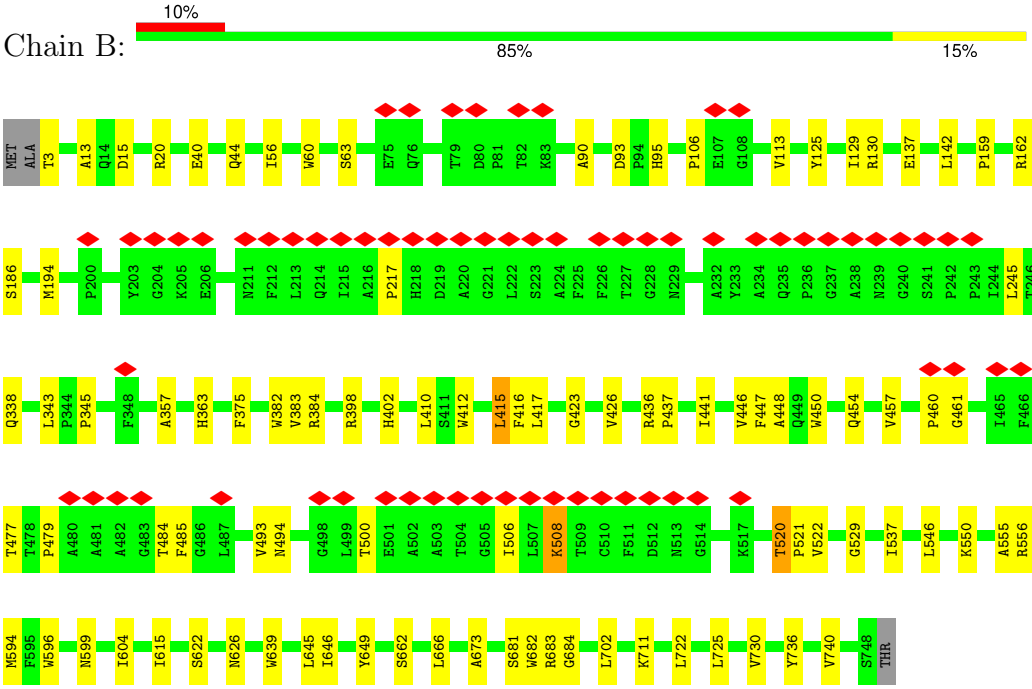
• Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



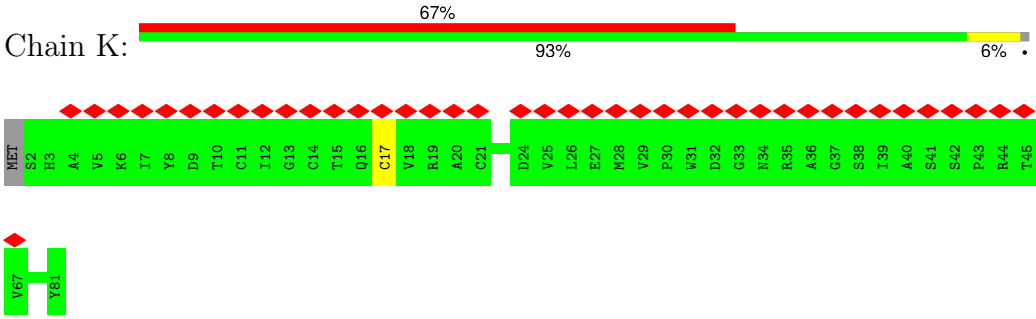
• Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



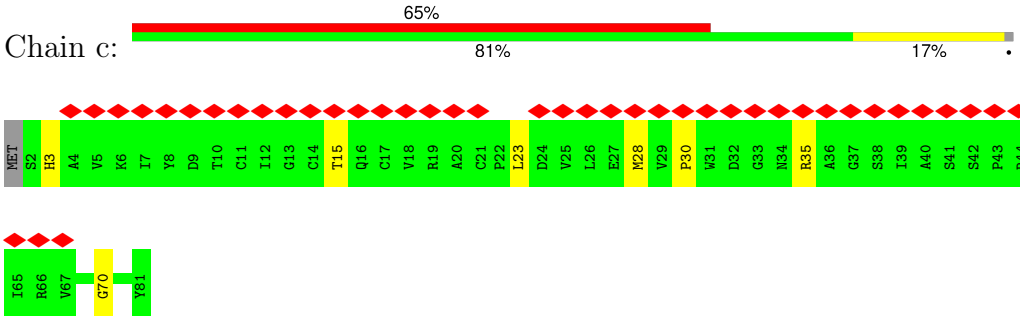
• Molecule 4: Photosystem I iron-sulfur center

Chain K:



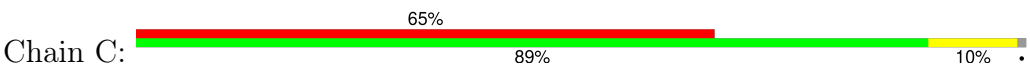
• Molecule 4: Photosystem I iron-sulfur center

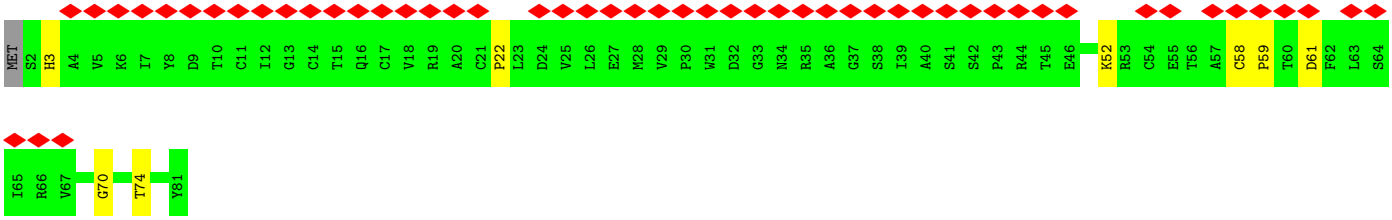
Chain c:



• Molecule 4: Photosystem I iron-sulfur center

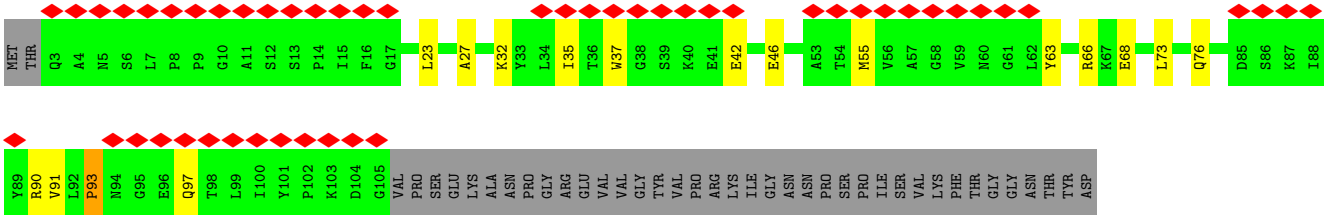
Chain C:





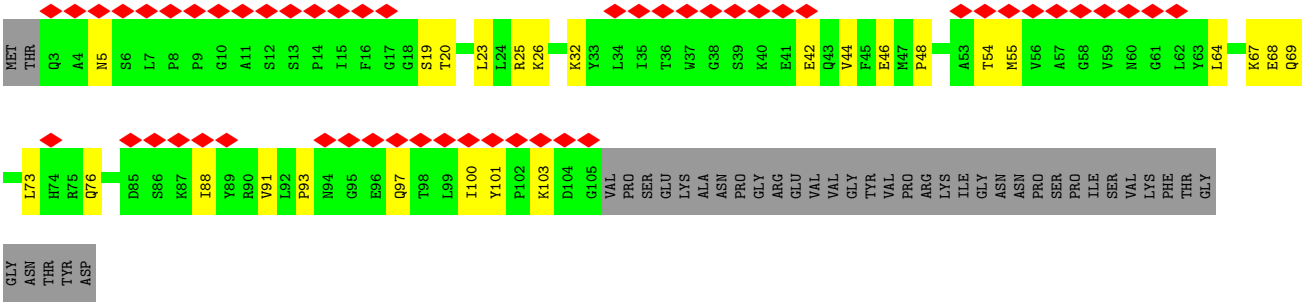
• Molecule 5: Photosystem I reaction center subunit II

Chain N:



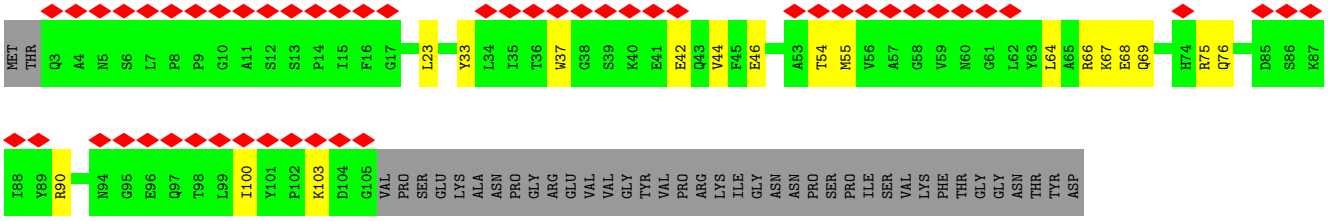
• Molecule 5: Photosystem I reaction center subunit II

Chain d:



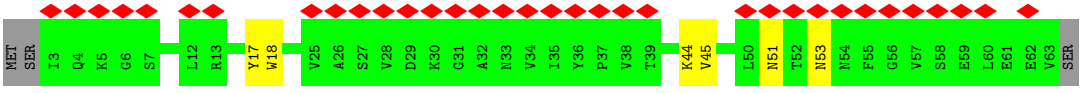
• Molecule 5: Photosystem I reaction center subunit II

Chain D:



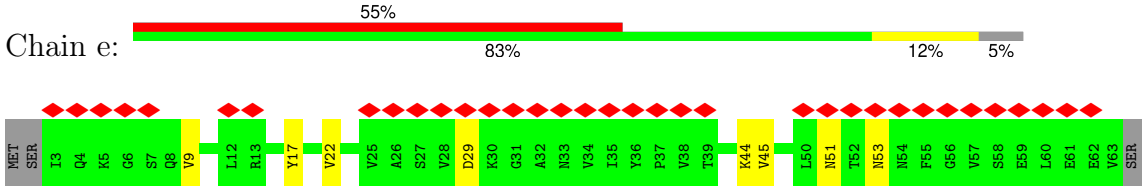
• Molecule 6: Photosystem I reaction center subunit IV

Chain O:



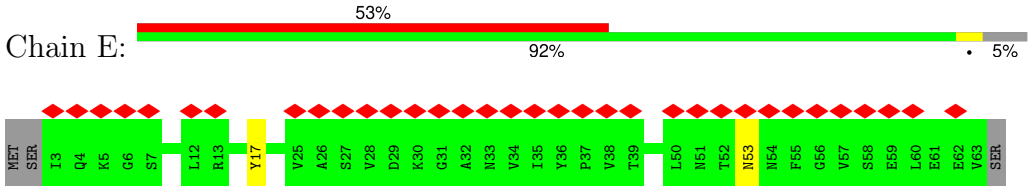
• Molecule 6: Photosystem I reaction center subunit IV

Chain e:



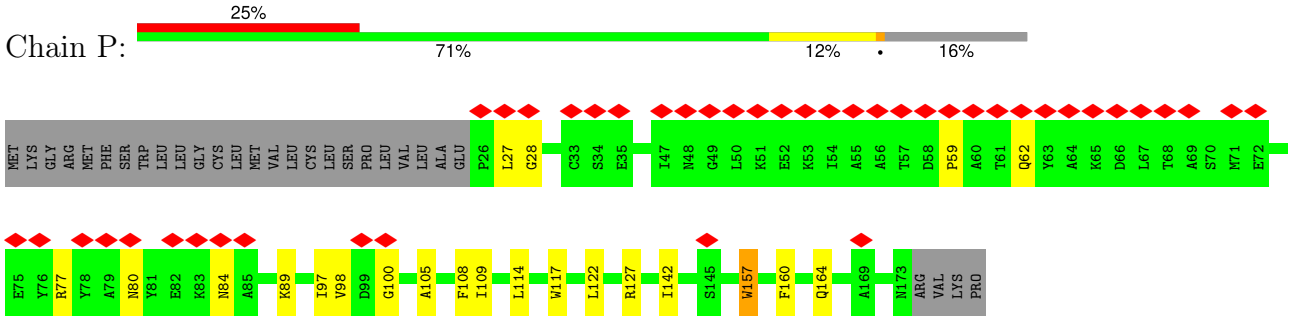
• Molecule 6: Photosystem I reaction center subunit IV

Chain E:



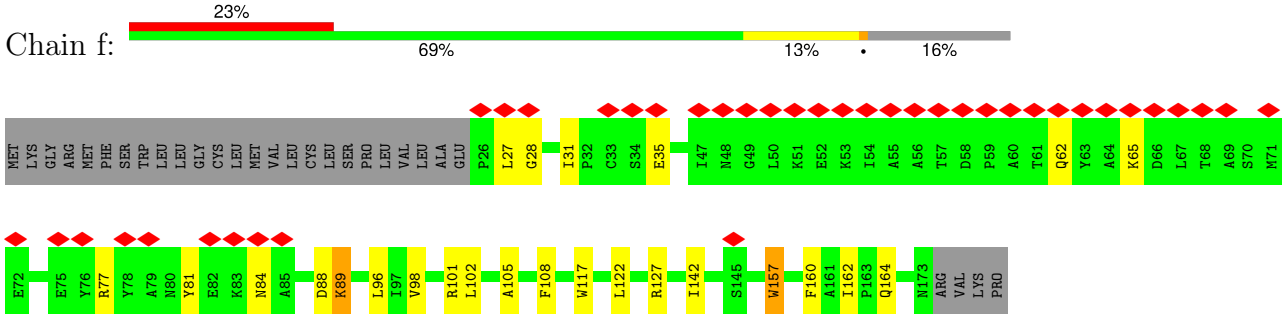
• Molecule 7: Photosystem I reaction center subunit III

Chain P:



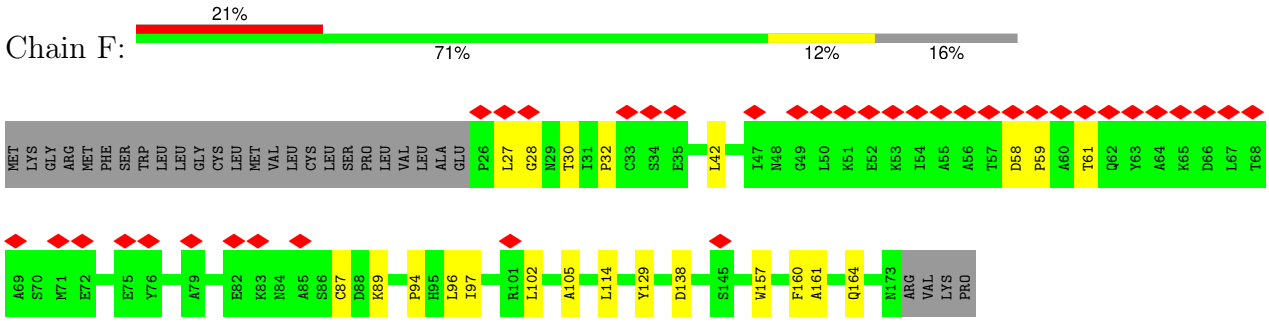
• Molecule 7: Photosystem I reaction center subunit III

Chain f:



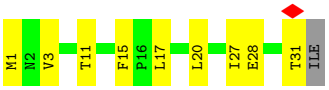
• Molecule 7: Photosystem I reaction center subunit III

Chain F:



• Molecule 8: Photosystem I reaction center subunit VIII

Chain Q:

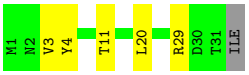


• Molecule 8: Photosystem I reaction center subunit VIII

Chain i:

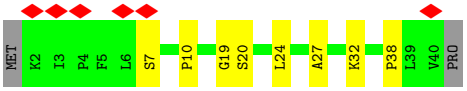
• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



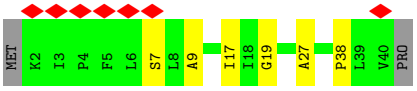
• Molecule 9: Photosystem I reaction center subunit IX

Chain R:



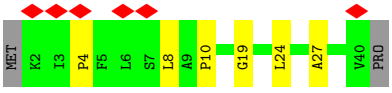
• Molecule 9: Photosystem I reaction center subunit IX

Chain j:



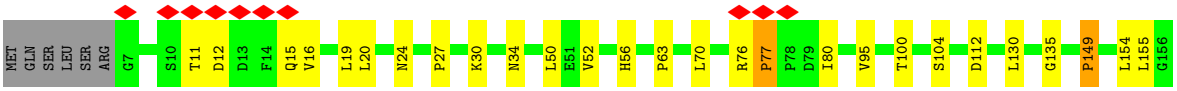
• Molecule 9: Photosystem I reaction center subunit IX

Chain J:



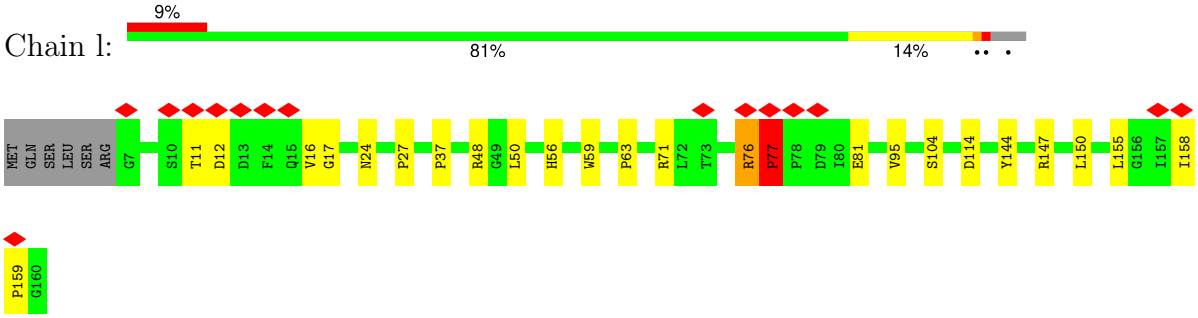
• Molecule 10: Photosystem I reaction center subunit XI

Chain S:



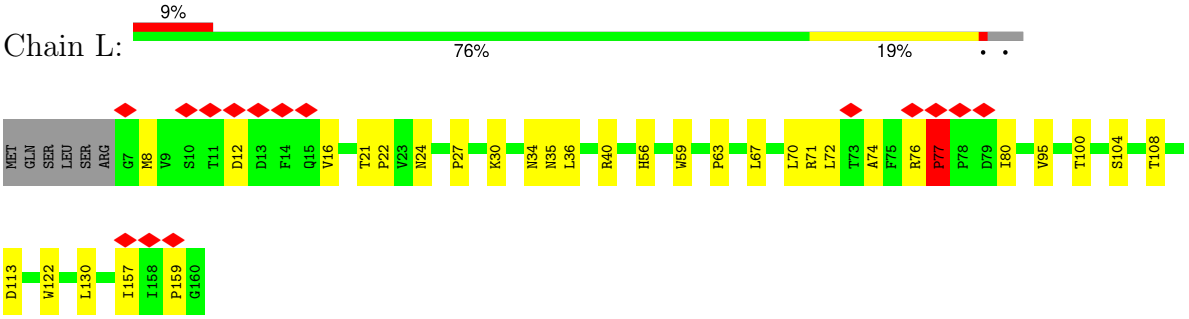
• Molecule 10: Photosystem I reaction center subunit XI

Chain l:



• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	403080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00112	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, SF4, 1L3, LHG, BCR, CLA, 45D, LMT, CL0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.57	3/6200 (0.0%)	1.03	16/8468 (0.2%)
1	G	0.60	6/6200 (0.1%)	1.07	25/8468 (0.3%)
1	a	0.62	9/6200 (0.1%)	1.14	29/8468 (0.3%)
2	M	0.37	0/229	0.79	0/308
2	T	0.40	0/229	0.69	0/308
2	m	0.42	0/229	0.75	0/308
3	B	0.62	7/6079 (0.1%)	1.16	32/8310 (0.4%)
3	H	0.62	7/6079 (0.1%)	1.13	33/8310 (0.4%)
3	b	0.68	9/6079 (0.1%)	1.17	36/8310 (0.4%)
4	C	0.39	0/609	0.81	3/825 (0.4%)
4	K	0.34	0/609	0.74	0/825
4	c	0.41	0/609	0.95	4/825 (0.5%)
5	D	0.40	0/800	0.72	0/1079
5	N	0.40	1/800 (0.1%)	0.76	3/1079 (0.3%)
5	d	0.40	1/800 (0.1%)	0.76	3/1079 (0.3%)
6	E	0.25	0/497	0.54	0/675
6	O	0.32	0/497	0.70	0/675
6	e	0.29	0/497	0.59	0/675
7	F	0.55	2/1175 (0.2%)	1.11	10/1596 (0.6%)
7	P	0.52	1/1175 (0.1%)	1.06	4/1596 (0.3%)
7	f	0.57	2/1175 (0.2%)	1.03	2/1596 (0.1%)
8	I	0.43	0/261	0.82	0/360
8	Q	0.45	0/261	0.91	0/360
8	i	0.52	0/261	0.95	0/360
9	J	0.56	0/301	1.21	2/413 (0.5%)
9	R	1.38	3/301 (1.0%)	1.89	7/413 (1.7%)
9	j	0.58	1/301 (0.3%)	1.02	0/413
10	L	0.59	2/1193 (0.2%)	1.09	6/1628 (0.4%)
10	S	0.56	1/1193 (0.1%)	1.10	7/1628 (0.4%)
10	l	0.72	2/1193 (0.2%)	1.22	14/1628 (0.9%)
All	All	0.59	57/52032 (0.1%)	1.08	236/70986 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
3	B	0	3
3	H	0	5
3	b	0	5
5	D	0	1
8	i	0	1
10	S	0	1
10	l	0	3
All	All	0	20

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	163	PRO	CG-CD	-24.62	0.67	1.50
1	a	387	PRO	CG-CD	-19.52	0.84	1.50
1	A	746	PRO	CG-CD	-17.89	0.90	1.50
9	R	38	PRO	CG-CD	-17.11	0.92	1.50
3	H	528	PRO	CG-CD	-16.43	0.94	1.50
1	G	242	PRO	CB-CG	14.99	2.24	1.49
3	B	163	PRO	CG-CD	-14.27	1.02	1.50
10	l	77	PRO	CG-CD	-13.37	1.05	1.50
3	b	217	PRO	CB-CG	-12.21	0.88	1.49
3	B	521	PRO	CG-CD	-11.81	1.10	1.50
3	B	437	PRO	CG-CD	-11.63	1.11	1.50
3	H	562	PRO	CG-CD	-11.21	1.12	1.50
3	H	217	PRO	CB-CG	-10.77	0.95	1.49
1	G	242	PRO	CG-CD	-10.76	1.14	1.50
3	B	301	PRO	CG-CD	-10.65	1.14	1.50
3	B	217	PRO	CB-CG	-10.25	0.98	1.49
1	G	691	PRO	CG-CD	-9.60	1.18	1.50
1	a	242	PRO	CG-CD	-9.52	1.18	1.50
1	a	387	PRO	CB-CG	9.49	1.97	1.49
9	R	38	PRO	N-CD	9.48	1.61	1.47
1	G	511	PRO	CG-CD	-9.44	1.18	1.50
1	a	746	PRO	CG-CD	-9.30	1.19	1.50
3	H	301	PRO	CG-CD	-9.13	1.19	1.50
3	B	217	PRO	CG-CD	-8.76	1.21	1.50
3	b	163	PRO	N-CD	8.76	1.60	1.47
3	b	521	PRO	CG-CD	-8.70	1.21	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	242	PRO	CB-CG	-8.59	1.06	1.49
3	b	217	PRO	CG-CD	-8.13	1.23	1.50
3	b	163	PRO	CB-CG	8.09	1.90	1.49
7	f	157	TRP	C-N	7.81	1.43	1.34
3	H	217	PRO	CG-CD	-7.56	1.25	1.50
3	B	163	PRO	N-CA	7.39	1.55	1.47
3	b	437	PRO	CG-CD	-7.19	1.26	1.50
3	b	259	PRO	CG-CD	-7.12	1.26	1.50
3	H	521	PRO	CG-CD	-7.03	1.26	1.50
7	f	162	ILE	C-N	6.66	1.41	1.34
1	a	746	PRO	CB-CG	-6.64	1.16	1.49
9	R	38	PRO	CB-CG	6.57	1.82	1.49
10	L	21	THR	C-N	6.19	1.41	1.33
5	N	93	PRO	CG-CD	-6.18	1.29	1.50
1	a	387	PRO	N-CD	6.01	1.56	1.47
7	F	157	TRP	C-N	6.01	1.41	1.34
10	S	149	PRO	CG-CD	-5.98	1.30	1.50
10	L	27	PRO	CG-CD	-5.89	1.30	1.50
1	G	519	PRO	CG-CD	-5.76	1.31	1.50
3	H	437	PRO	CG-CD	-5.73	1.31	1.50
1	a	385	PRO	CG-CD	-5.70	1.31	1.50
7	F	58	ASP	C-N	5.69	1.38	1.33
1	A	490	PRO	N-CD	-5.64	1.39	1.47
3	b	259	PRO	N-CD	5.64	1.55	1.47
1	a	387	PRO	N-CA	5.59	1.54	1.47
1	G	691	PRO	N-CD	5.53	1.55	1.47
9	j	9	ALA	C-N	5.51	1.41	1.34
10	l	27	PRO	CG-CD	-5.48	1.32	1.50
5	d	93	PRO	CG-CD	-5.19	1.33	1.50
1	A	43	PRO	CG-CD	-5.15	1.33	1.50
7	P	59	PRO	CG-CD	-5.14	1.33	1.50

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	163	PRO	N-CD-CG	-28.03	61.15	103.20
1	G	242	PRO	CB-CG-CD	-25.47	24.60	106.10
3	B	163	PRO	N-CD-CG	-25.10	65.55	103.20
1	a	387	PRO	N-CD-CG	-25.02	65.67	103.20
1	A	746	PRO	N-CD-CG	-23.74	67.59	103.20
1	a	746	PRO	CB-CG-CD	23.09	179.98	106.10
1	G	242	PRO	CA-N-CD	-22.76	80.14	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	528	PRO	N-CD-CG	-22.14	69.99	103.20
1	a	242	PRO	CB-CG-CD	21.81	175.91	106.10
3	H	217	PRO	CA-CB-CG	-21.55	63.55	104.50
3	H	217	PRO	N-CD-CG	-21.32	71.21	103.20
3	B	217	PRO	N-CD-CG	-21.12	71.52	103.20
1	a	746	PRO	N-CD-CG	-20.99	71.71	103.20
3	b	217	PRO	CB-CG-CD	20.35	171.21	106.10
1	a	387	PRO	CA-CB-CG	-20.30	65.92	104.50
3	B	217	PRO	CA-CB-CG	-20.19	66.14	104.50
9	R	38	PRO	N-CD-CG	-19.49	73.96	103.20
3	B	163	PRO	CA-CB-CG	-19.16	68.09	104.50
1	a	242	PRO	N-CD-CG	-18.98	74.73	103.20
3	b	163	PRO	CA-CB-CG	-18.09	70.13	104.50
3	b	217	PRO	N-CD-CG	-17.47	76.99	103.20
3	B	163	PRO	CB-CG-CD	17.05	160.66	106.10
3	b	217	PRO	CA-CB-CG	-16.40	73.34	104.50
3	H	562	PRO	N-CD-CG	-16.38	78.63	103.20
1	a	746	PRO	CA-CB-CG	-16.34	73.45	104.50
1	A	746	PRO	CA-CB-CG	-16.25	73.62	104.50
3	B	521	PRO	N-CD-CG	-16.12	79.01	103.20
3	B	437	PRO	N-CD-CG	-15.67	79.70	103.20
3	H	528	PRO	CA-CB-CG	-15.35	75.34	104.50
10	l	77	PRO	N-CD-CG	-15.23	80.36	103.20
1	a	242	PRO	CA-CB-CG	-14.87	76.24	104.50
9	R	38	PRO	CA-CB-CG	-14.47	77.01	104.50
3	B	301	PRO	N-CD-CG	-14.12	82.01	103.20
1	G	511	PRO	N-CD-CG	-14.12	82.02	103.20
3	B	217	PRO	CB-CG-CD	13.45	149.15	106.10
3	b	163	PRO	N-CA-CB	-13.45	87.12	102.72
3	b	521	PRO	N-CD-CG	-13.07	83.59	103.20
1	G	691	PRO	N-CD-CG	-13.03	83.66	103.20
3	H	562	PRO	CA-CB-CG	-12.42	80.89	104.50
1	G	242	PRO	N-CD-CG	12.05	121.27	103.20
3	b	301	PRO	CA-N-CD	-11.25	96.25	112.00
3	b	437	PRO	N-CD-CG	-11.20	86.40	103.20
3	b	259	PRO	N-CD-CG	-11.14	86.50	103.20
1	G	242	PRO	N-CA-CB	-11.03	91.67	103.25
3	H	301	PRO	N-CD-CG	-11.01	86.69	103.20
1	G	387	PRO	CA-N-CD	-11.00	96.60	112.00
9	R	38	PRO	N-CA-CB	-10.99	93.69	103.36
3	H	217	PRO	CB-CG-CD	10.97	141.21	106.10
3	H	521	PRO	N-CD-CG	-10.80	87.00	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	385	PRO	N-CD-CG	-10.78	87.04	103.20
3	b	163	PRO	CA-N-CD	-10.60	97.16	112.00
3	B	437	PRO	CA-CB-CG	-10.47	84.60	104.50
10	L	27	PRO	N-CD-CG	-10.45	87.53	103.20
3	H	528	PRO	N-CA-CB	-10.42	93.51	103.51
4	c	30	PRO	CA-N-CD	-10.37	97.48	112.00
3	H	301	PRO	CA-N-CD	-10.21	97.70	112.00
3	B	521	PRO	CA-CB-CG	-10.08	85.36	104.50
10	l	27	PRO	N-CD-CG	-9.96	88.25	103.20
7	F	59	PRO	CA-N-CD	-9.68	98.45	112.00
1	G	691	PRO	CA-CB-CG	-9.58	86.29	104.50
10	l	77	PRO	CA-CB-CG	-9.57	86.31	104.50
3	H	528	PRO	N-CA-C	9.56	125.81	113.86
1	G	691	PRO	N-CA-CB	-9.47	92.55	102.88
10	l	77	PRO	CA-N-CD	-9.40	98.83	112.00
1	G	511	PRO	CA-CB-CG	-9.34	86.76	104.50
1	G	519	PRO	N-CD-CG	-9.20	89.41	103.20
1	a	506	PRO	CA-N-CD	-9.17	99.17	112.00
7	F	94	PRO	CA-N-CD	-9.11	99.25	112.00
3	H	437	PRO	N-CD-CG	-9.05	89.62	103.20
5	N	93	PRO	N-CD-CG	-9.04	89.64	103.20
3	H	484	THR	CA-C-N	9.03	134.93	122.19
3	H	484	THR	C-N-CA	9.03	134.93	122.19
3	b	163	PRO	CB-CG-CD	-8.97	77.39	106.10
1	a	387	PRO	N-CA-CB	-8.97	93.83	103.25
9	R	38	PRO	N-CA-C	8.90	124.24	110.80
10	L	27	PRO	N-CA-CB	-8.72	95.21	103.41
3	b	163	PRO	N-CA-C	8.62	126.38	111.03
1	A	746	PRO	CB-CG-CD	8.53	133.39	106.10
1	A	490	PRO	CA-N-CD	-8.52	100.07	112.00
3	b	259	PRO	CA-CB-CG	-8.41	88.52	104.50
7	F	94	PRO	N-CA-C	8.41	124.00	110.21
3	B	163	PRO	N-CA-C	8.38	123.62	111.13
10	l	27	PRO	N-CA-CB	-8.25	95.59	103.51
3	B	301	PRO	CA-N-CD	-8.18	100.54	112.00
3	B	484	THR	CA-C-N	8.15	134.47	122.74
3	B	484	THR	C-N-CA	8.15	134.47	122.74
3	H	562	PRO	N-CA-CB	-8.12	95.07	103.19
3	b	163	PRO	CB-CA-C	8.05	121.96	110.20
3	b	259	PRO	N-CA-CB	-8.04	95.86	103.34
7	f	88	ASP	N-CA-C	7.99	123.25	111.34
5	d	93	PRO	N-CD-CG	-7.95	91.28	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	S	11	THR	CA-C-N	7.94	136.71	121.54
10	S	11	THR	C-N-CA	7.94	136.71	121.54
10	S	27	PRO	N-CD-CG	-7.87	91.40	103.20
3	b	484	THR	CA-C-N	7.85	136.54	121.54
3	b	484	THR	C-N-CA	7.85	136.54	121.54
3	b	521	PRO	CA-CB-CG	-7.85	89.59	104.50
1	a	267	PRO	CA-N-CD	-7.83	101.04	112.00
3	b	437	PRO	CA-CB-CG	-7.80	89.69	104.50
1	a	385	PRO	CA-CB-CG	-7.76	89.75	104.50
1	A	43	PRO	N-CD-CG	-7.74	91.60	103.20
10	S	149	PRO	N-CD-CG	-7.71	91.64	103.20
1	A	746	PRO	N-CA-CB	-7.69	96.35	103.27
10	l	77	PRO	CB-CG-CD	7.66	130.60	106.10
3	B	301	PRO	CA-CB-CG	-7.65	89.96	104.50
1	G	506	PRO	CA-N-CD	-7.57	101.41	112.00
3	H	217	PRO	CA-N-CD	-7.46	101.55	112.00
5	N	93	PRO	CA-CB-CG	-7.46	90.32	104.50
1	a	13	THR	CA-C-N	7.39	135.65	121.54
1	a	13	THR	C-N-CA	7.39	135.65	121.54
10	L	27	PRO	CA-CB-CG	-7.38	90.48	104.50
3	b	162	ARG	CA-C-N	-7.33	112.94	120.85
3	b	162	ARG	C-N-CA	-7.33	112.94	120.85
3	H	528	PRO	CB-CG-CD	7.24	129.27	106.10
7	P	59	PRO	N-CD-CG	-7.20	92.39	103.20
7	F	161	ALA	CA-C-N	7.19	124.77	120.24
7	F	161	ALA	C-N-CA	7.19	124.77	120.24
7	P	59	PRO	CA-N-CD	-7.12	102.03	112.00
1	G	545	VAL	N-CA-C	-6.97	101.25	108.15
10	L	157	ILE	N-CA-C	-6.95	105.84	111.81
3	B	217	PRO	CA-N-CD	-6.93	102.29	112.00
1	a	387	PRO	CA-N-CD	-6.92	102.31	112.00
3	B	106	PRO	N-CD-CG	-6.91	92.84	103.20
1	A	387	PRO	CA-N-CD	-6.86	102.40	112.00
3	B	484	THR	CA-CB-CG2	6.83	122.12	110.50
3	b	217	PRO	CA-N-CD	-6.82	102.45	112.00
10	l	27	PRO	CA-CB-CG	-6.76	91.65	104.50
4	c	57	ALA	CA-C-N	-6.73	112.26	121.61
4	c	57	ALA	C-N-CA	-6.73	112.26	121.61
3	b	437	PRO	CA-N-CD	-6.61	102.75	112.00
3	b	484	THR	CA-CB-CG2	6.54	121.62	110.50
5	d	93	PRO	CA-CB-CG	-6.51	92.14	104.50
1	G	511	PRO	N-CA-CB	-6.49	96.99	103.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	385	PRO	N-CA-CB	-6.48	96.45	103.25
4	c	30	PRO	N-CD-CG	-6.45	93.53	103.20
3	H	521	PRO	CA-CB-CG	-6.40	92.34	104.50
3	H	437	PRO	CA-N-CD	-6.39	103.06	112.00
3	B	437	PRO	CA-N-CD	-6.39	103.06	112.00
1	G	243	LEU	N-CA-C	6.33	123.81	109.81
1	a	506	PRO	N-CD-CG	-6.29	93.76	103.20
3	b	253	PRO	CA-N-CD	-6.22	103.29	112.00
1	A	675	VAL	CB-CA-C	6.22	128.01	111.34
1	A	646	LYS	CA-CB-CG	6.21	126.53	114.10
1	A	691	PRO	CA-N-CD	-6.17	103.36	112.00
1	G	519	PRO	CA-CB-CG	-6.16	92.80	104.50
1	a	420	ILE	CG1-CB-CG2	-6.15	92.24	110.70
1	A	384	ASN	N-CA-C	-6.14	101.91	109.65
3	H	485	PHE	CA-CB-CG	6.13	119.93	113.80
3	H	345	PRO	N-CD-CG	-6.13	94.01	103.20
1	a	108	PRO	CA-N-CD	-6.06	103.52	112.00
3	b	162	ARG	C-N-CD	6.06	149.83	125.00
1	A	539	LYS	N-CA-C	6.02	117.96	110.91
1	G	267	PRO	CA-N-CD	-6.02	103.57	112.00
3	B	163	PRO	CA-N-CD	-6.02	103.57	112.00
3	H	572	PRO	N-CD-CG	-6.01	94.19	103.20
10	l	77	PRO	N-CA-C	5.99	118.01	110.70
3	b	506	ILE	CG1-CB-CG2	-5.99	92.73	110.70
1	a	441	ARG	CB-CG-CD	5.98	125.06	111.30
10	L	159	PRO	CA-N-CD	-5.98	103.63	112.00
1	a	691	PRO	CA-N-CD	-5.98	103.63	112.00
3	B	163	PRO	N-CA-CB	-5.96	95.47	103.15
1	A	43	PRO	CA-N-CD	-5.94	103.68	112.00
1	G	130	PRO	CA-N-CD	-5.94	103.69	112.00
1	G	389	MET	CA-CB-CG	5.93	125.96	114.10
10	l	76	ARG	C-N-CD	-5.92	100.74	125.00
1	G	121	VAL	CG1-CB-CG2	-5.90	97.81	110.80
10	S	149	PRO	CA-CB-CG	-5.90	93.29	104.50
3	b	485	PHE	CA-CB-CG	5.89	119.69	113.80
3	H	301	PRO	CA-CB-CG	-5.89	93.30	104.50
3	B	506	ILE	CG1-CB-CG2	-5.88	93.07	110.70
9	R	38	PRO	CB-CA-C	5.84	118.53	111.46
4	C	22	PRO	N-CD-CG	-5.82	94.47	103.20
7	F	157	TRP	N-CA-C	5.79	122.62	109.81
3	b	159	PRO	CA-N-CD	-5.79	103.90	112.00
1	A	691	PRO	N-CD-CG	-5.79	94.52	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	238	ALA	CA-C-N	5.77	132.57	121.54
3	b	238	ALA	C-N-CA	5.77	132.57	121.54
5	N	93	PRO	N-CA-CB	-5.76	97.98	103.51
10	S	77	PRO	N-CA-C	5.74	117.70	110.70
1	G	241	ILE	CB-CA-C	5.73	117.36	110.78
3	b	246	THR	CA-C-N	-5.70	113.97	123.04
3	b	246	THR	C-N-CA	-5.70	113.97	123.04
3	H	81	PRO	CA-N-CD	-5.68	104.05	112.00
3	B	521	PRO	N-CA-CB	-5.67	97.42	103.38
7	F	61	THR	CA-C-N	5.64	132.31	121.54
7	F	61	THR	C-N-CA	5.64	132.31	121.54
1	a	691	PRO	N-CD-CG	-5.63	94.75	103.20
1	A	450	LEU	CB-CG-CD2	-5.59	93.93	110.70
10	L	77	PRO	N-CA-C	5.59	117.52	110.70
10	l	76	ARG	CA-C-N	5.57	126.12	120.38
10	l	76	ARG	C-N-CA	5.57	126.12	120.38
3	B	508	LYS	CA-C-N	5.57	128.01	120.38
3	B	508	LYS	C-N-CA	5.57	128.01	120.38
1	G	691	PRO	CA-N-CD	-5.50	104.29	112.00
1	a	435	LEU	CB-CG-CD2	5.50	127.20	110.70
9	J	4	PRO	CA-C-N	5.46	131.97	121.54
9	J	4	PRO	C-N-CA	5.46	131.97	121.54
7	F	42	LEU	CA-CB-CG	5.44	135.32	116.30
7	P	157	TRP	N-CA-C	5.42	121.79	109.81
3	B	550	LYS	CD-CE-NZ	-5.41	94.60	111.90
3	B	485	PHE	CA-CB-CG	5.39	119.19	113.80
9	R	38	PRO	CA-N-CD	-5.38	104.47	112.00
10	l	159	PRO	CA-N-CD	-5.37	104.48	112.00
1	a	67	GLU	CA-CB-CG	5.36	124.82	114.10
3	B	345	PRO	N-CD-CG	-5.36	95.16	103.20
3	H	345	PRO	CA-CB-CG	-5.34	94.35	104.50
7	P	62	GLN	CA-CB-CG	5.33	124.77	114.10
3	b	415	LEU	CA-CB-CG	5.32	134.90	116.30
3	H	429	ASP	N-CA-C	5.30	116.74	111.07
1	G	241	ILE	C-N-CD	5.27	146.62	125.00
1	a	639	GLY	N-CA-C	5.25	117.14	110.20
3	B	415	LEU	CA-CB-CG	5.25	134.66	116.30
10	l	77	PRO	N-CA-CB	-5.22	98.02	103.08
1	G	387	PRO	N-CD-CG	-5.21	95.38	103.20
5	d	93	PRO	N-CA-CB	-5.18	98.54	103.51
3	H	521	PRO	CA-N-CD	-5.16	104.77	112.00
3	H	437	PRO	CA-CB-CG	-5.14	94.72	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	59	PRO	N-CA-C	5.14	120.03	114.68
3	b	437	PRO	N-CA-CB	-5.13	98.59	103.41
3	H	44	GLN	N-CA-CB	5.10	118.16	110.30
3	H	562	PRO	CA-N-CD	-5.10	104.86	112.00
10	S	76	ARG	C-N-CD	-5.09	104.13	125.00
1	A	14	ARG	N-CA-CB	-5.07	108.39	114.17
4	C	22	PRO	CA-CB-CG	-5.06	94.89	104.50
10	l	77	PRO	CB-CA-C	5.06	117.09	110.92
3	H	497	PRO	CA-N-CD	-5.04	104.94	112.00
7	f	89	LYS	N-CA-C	5.04	121.54	110.80
1	a	303	LEU	CB-CG-CD2	-5.03	95.61	110.70
1	a	537	VAL	CA-C-N	5.03	131.14	121.54
1	a	537	VAL	C-N-CA	5.03	131.14	121.54
3	H	71	GLN	CA-CB-CG	5.02	124.15	114.10
9	R	38	PRO	CA-C-O	5.02	126.75	121.03
3	B	529	GLY	CA-C-N	5.01	127.00	120.28
3	B	529	GLY	C-N-CA	5.01	127.00	120.28
1	G	691	PRO	CB-CA-C	5.01	117.94	110.88
4	C	22	PRO	N-CA-CB	-5.00	98.19	103.19

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	247	PHE	Sidechain
3	B	556	ARG	Sidechain
3	B	682	TRP	Peptide
5	D	75	ARG	Sidechain
3	H	485	PHE	Peptide
3	H	510	CYS	Peptide
3	H	556	ARG	Sidechain
3	H	682	TRP	Peptide
3	H	70	TRP	Peptide
10	S	20	LEU	Peptide
1	a	725	ARG	Sidechain
3	b	459	ILE	Peptide
3	b	485	PHE	Peptide
3	b	510	CYS	Peptide
3	b	682	TRP	Peptide
3	b	699	ARG	Sidechain
8	i	29	ARG	Sidechain
10	l	11	THR	Peptide

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Mol	Chain	Res	Type	Group
10	l	76	ARG	Peptide
10	l	77	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	A	5997	0	5811	69	0
1	G	5997	0	5811	81	0
1	a	5997	0	5811	87	0
2	M	226	0	240	3	0
2	T	226	0	240	2	0
2	m	226	0	240	5	0
3	B	5866	0	5675	75	0
3	H	5866	0	5675	86	0
3	b	5866	0	5675	73	0
4	C	599	0	577	5	0
4	K	599	0	577	4	0
4	c	599	0	577	8	0
5	D	784	0	798	12	0
5	N	784	0	798	12	0
5	d	784	0	798	16	0
6	E	489	0	474	2	0
6	O	489	0	474	6	0
6	e	489	0	474	7	0
7	F	1148	0	1143	10	0
7	P	1148	0	1143	16	0
7	f	1148	0	1143	15	0
8	I	254	0	269	5	0
8	Q	254	0	269	10	0
8	i	254	0	269	9	0
9	J	293	0	327	5	0
9	R	293	0	327	8	0
9	j	293	0	327	5	0
10	L	1159	0	1179	21	0
10	S	1159	0	1179	16	0
10	l	1159	0	1179	15	0
11	A	65	0	72	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	65	0	72	1	0
11	a	65	0	72	0	0
12	A	2375	0	2267	65	0
12	B	2190	0	2162	57	0
12	F	110	0	104	4	0
12	G	2440	0	2339	67	0
12	H	2310	0	2282	68	0
12	J	45	0	32	1	0
12	L	250	0	265	11	0
12	P	110	0	104	5	0
12	R	45	0	32	1	0
12	S	185	0	193	7	0
12	a	2375	0	2270	75	0
12	b	2185	0	2148	66	0
12	f	110	0	104	5	0
12	j	110	0	104	2	0
12	l	250	0	265	12	0
13	A	33	0	0	0	0
13	B	33	0	0	0	0
13	G	33	0	0	0	0
13	H	33	0	0	0	0
13	a	33	0	0	0	0
13	b	33	0	0	0	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
14	G	8	0	0	0	0
14	K	16	0	0	1	0
14	a	8	0	0	0	0
14	c	16	0	0	0	0
15	A	280	0	341	15	0
15	B	225	0	273	13	0
15	F	80	0	98	5	0
15	G	280	0	341	14	0
15	H	265	0	322	21	0
15	I	40	0	49	4	0
15	J	120	0	145	6	0
15	L	120	0	147	5	0
15	P	80	0	98	5	0
15	Q	80	0	98	5	0
15	R	80	0	96	5	0
15	S	80	0	98	5	0
15	a	280	0	341	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b	265	0	322	21	0
15	f	80	0	98	4	0
15	i	80	0	98	3	0
15	j	80	0	96	5	0
15	l	80	0	98	4	0
16	A	125	0	172	3	0
16	G	125	0	172	5	0
16	a	125	0	172	4	0
17	M	42	0	52	3	0
17	T	42	0	52	3	0
17	m	42	0	52	4	0
18	B	55	0	86	4	0
18	H	55	0	86	5	0
18	b	55	0	86	3	0
19	B	35	0	44	2	0
19	H	35	0	45	1	0
19	b	35	0	46	1	0
20	A	56	0	0	1	0
20	B	82	0	0	0	0
20	C	24	0	0	0	0
20	D	16	0	0	0	0
20	G	58	0	0	2	0
20	H	80	0	0	0	0
20	K	26	0	0	0	0
20	L	7	0	0	0	0
20	N	15	0	0	0	0
20	O	1	0	0	0	0
20	S	5	0	0	0	0
20	a	57	0	0	2	0
20	b	82	0	0	0	0
20	c	22	0	0	0	0
20	d	17	0	0	1	0
20	e	1	0	0	0	0
20	l	6	0	0	0	0
All	All	69921	0	68590	949	0

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

All (949) 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)
3:H:67:HIS:O	3:H:71:GLN:HB3	1.71	0.88
5:d:42:GLU:HA	5:d:55:MET:O	1.78	0.83
12:a:839:CLA:HAB	12:a:839:CLA:H111	1.66	0.78
5:N:42:GLU:HA	5:N:55:MET:O	1.84	0.77
12:A:839:CLA:H111	12:A:839:CLA:HAB	1.69	0.74
12:a:832:CLA:H151	12:b:836:CLA:H2	1.72	0.72
5:N:46:GLU:H	5:N:76:GLN:HE22	1.37	0.71
12:G:832:CLA:H151	12:H:838:CLA:H2	1.73	0.70
1:A:405:TRP:CD1	12:A:827:CLA:HAB	2.27	0.70
12:G:839:CLA:HAB	12:G:839:CLA:H111	1.71	0.69
12:A:832:CLA:H151	12:B:837:CLA:H2	1.73	0.69
1:G:405:TRP:CD1	12:G:828:CLA:HAB	2.28	0.68
12:G:821:CLA:H2	12:G:825:CLA:HBB1	1.73	0.68
1:a:405:TRP:CD1	12:a:827:CLA:HAB	2.29	0.68
10:S:30:LYS:O	10:S:34:ASN:HB2	1.93	0.67
5:D:42:GLU:HA	5:D:55:MET:O	1.95	0.67
12:A:803:CLA:HBB2	15:A:852:BCR:H343	1.77	0.67
2:T:12:PHE:HB3	17:T:101:45D:H291	1.78	0.66
3:H:375:PHE:HZ	12:H:823:CLA:HAB	1.60	0.66
1:G:472:GLN:OE1	1:G:676:ASN:ND2	2.29	0.66
12:a:803:CLA:HBB2	15:a:852:BCR:H343	1.75	0.65
12:G:804:CLA:HBB2	15:G:853:BCR:H343	1.77	0.65
1:a:187:VAL:HG12	1:a:188:ARG:HG3	1.79	0.65
2:M:12:PHE:HB3	17:M:101:45D:H291	1.79	0.65
12:B:804:CLA:H162	12:B:825:CLA:HBB2	1.79	0.65
3:b:375:PHE:HZ	12:b:822:CLA:HAB	1.62	0.65
1:A:479:ASP:HA	10:L:71:ARG:HH22	1.61	0.64
1:G:124:GLN:O	1:G:127:LEU:HB2	1.98	0.64
1:a:118:ALA:H	1:a:128:ASN:HD21	1.46	0.64
4:c:15:THR:HA	4:c:28:MET:HE1	1.79	0.64
1:G:744:ILE:HG12	7:P:127:ARG:HG3	1.78	0.64
12:A:820:CLA:H2	12:A:824:CLA:HBB1	1.79	0.64
5:d:88:ILE:HB	5:d:101:TYR:HB3	1.79	0.64
4:c:3:HIS:HD2	4:c:70:GLY:H	1.46	0.63
1:a:713:VAL:HG11	1:a:768:LEU:HD23	1.80	0.63
1:a:431:ASN:HD22	1:a:434:ASN:HD21	1.43	0.63
2:m:12:PHE:HB3	17:m:101:45D:H291	1.80	0.63
3:H:86:PRO:HB2	3:H:116:MET:HB3	1.81	0.63
7:P:80:ASN:OD1	7:P:84:ASN:ND2	2.32	0.62
12:B:805:CLA:HHB	12:B:806:CLA:HMB3	1.81	0.62
3:H:44:GLN:NE2	3:H:163:PRO:O	2.33	0.62
1:a:372:LEU:HD12	12:a:826:CLA:H52	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:820:CLA:H2	12:a:824:CLA:HBB1	1.80	0.62
12:G:808:CLA:H203	15:R:101:BCR:H14C	1.82	0.62
1:G:13:THR:HG23	1:G:14:ARG:HG2	1.82	0.61
12:a:807:CLA:H203	15:j:101:BCR:H14C	1.82	0.61
1:G:339:LYS:H	12:G:842:CLA:HBC2	1.64	0.61
17:T:101:45D:H201	3:H:56:ILE:HD11	1.81	0.61
9:J:8:LEU:HG	9:J:10:PRO:HD2	1.80	0.61
3:B:460:PRO:HD2	7:F:28:GLY:HA2	1.82	0.61
5:d:25:ARG:NH1	10:l:114:ASP:OD1	2.34	0.61
5:N:63:TYR:HB2	10:S:15:GLN:HG2	1.83	0.61
5:D:44:VAL:HG22	5:D:54:THR:HG22	1.83	0.60
1:A:158:THR:H	1:A:162:GLN:HE22	1.48	0.60
5:N:91:VAL:HG22	5:N:97:GLN:HG2	1.83	0.60
1:A:203:ASN:HD21	1:A:316:TYR:H	1.49	0.60
1:G:772:VAL:HG22	15:G:850:BCR:HC21	1.83	0.60
5:N:23:LEU:HB2	10:S:16:VAL:HA	1.83	0.60
12:G:855:CLA:HAB	3:H:596:TRP:CH2	2.37	0.59
3:H:460:PRO:HD2	7:P:28:GLY:HA2	1.85	0.59
1:a:218:THR:HG21	1:a:303:LEU:HB2	1.84	0.59
12:b:848:CLA:HBC2	1:A:339:LYS:H	1.66	0.59
4:C:3:HIS:HD2	4:C:70:GLY:H	1.50	0.59
3:H:90:ALA:HB1	8:Q:1:MET:HE3	1.85	0.59
1:a:617:TRP:CH2	12:a:802:CLA:HAB	2.38	0.59
12:b:822:CLA:HED2	12:b:823:CLA:HBD	1.85	0.59
5:d:23:LEU:HB2	10:l:16:VAL:HA	1.85	0.59
1:A:772:VAL:HG22	15:A:849:BCR:HC21	1.84	0.59
3:B:450:TRP:O	3:B:454:GLN:NE2	2.36	0.59
1:G:617:TRP:CH2	12:G:803:CLA:HAB	2.38	0.58
7:P:114:LEU:HG	12:R:103:CLA:HAB	1.86	0.58
10:L:30:LYS:O	10:L:34:ASN:HB2	2.03	0.58
1:G:118:ALA:H	1:G:128:ASN:HD21	1.51	0.58
3:b:450:TRP:O	3:b:454:GLN:NE2	2.37	0.58
1:a:631:TRP:HE1	1:a:669:GLN:HG2	1.67	0.58
1:G:538:GLN:HG2	1:G:539:LYS:HG2	1.85	0.58
1:a:122:PHE:O	3:b:436:ARG:NH2	2.37	0.58
3:B:375:PHE:HZ	12:B:822:CLA:HAB	1.69	0.57
3:H:698:GLU:OE2	3:H:707:ARG:NH1	2.37	0.57
1:a:307:VAL:HG21	12:a:816:CLA:HAB	1.86	0.57
4:K:17:CYS:HB3	14:K:102:SF4:S4	2.45	0.57
1:G:512:TRP:HB2	12:G:835:CLA:HED3	1.86	0.57
1:A:432:GLN:HE21	5:D:44:VAL:HG21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:479:ASP:HA	10:l:71:ARG:HH22	1.67	0.57
12:G:832:CLA:HBB1	12:G:833:CLA:H2	1.86	0.57
7:F:114:LEU:HG	12:J:103:CLA:HAB	1.87	0.57
3:H:201:ARG:NH2	3:H:207:VAL:O	2.38	0.57
1:a:772:VAL:HG22	15:a:849:BCR:HC21	1.85	0.57
3:b:383:VAL:HG23	3:b:384:ARG:HG3	1.87	0.57
8:Q:11:THR:HA	8:Q:15:PHE:HB3	1.87	0.57
10:l:144:TYR:O	10:l:147:ARG:NH1	2.38	0.57
12:B:837:CLA:HAC2	15:B:845:BCR:H23C	1.87	0.56
10:S:149:PRO:HB3	10:S:154:LEU:HD22	1.86	0.56
15:L:201:BCR:H14C	12:L:206:CLA:H172	1.88	0.56
17:m:101:45D:H201	3:b:56:ILE:HD11	1.87	0.56
1:A:631:TRP:HZ3	1:A:674:SER:HB3	1.71	0.56
12:a:818:CLA:H92	12:a:828:CLA:H91	1.88	0.56
3:H:142:LEU:HD21	15:H:843:BCR:H24C	1.86	0.56
12:H:804:CLA:H162	12:H:826:CLA:HBB2	1.88	0.56
1:A:682:ARG:HG3	3:B:646:ILE:HD12	1.86	0.56
1:a:66:ARG:NH2	1:a:356:THR:O	2.38	0.56
1:a:283:LYS:NZ	1:a:296:THR:OG1	2.37	0.56
1:a:383:MET:HE1	12:a:826:CLA:HAB	1.88	0.56
3:b:4:ARG:HH22	3:b:10:GLN:HE22	1.53	0.56
3:H:450:TRP:O	3:H:454:GLN:NE2	2.39	0.55
3:H:645:LEU:O	3:H:662:SER:OG	2.25	0.55
3:b:461:GLY:HA3	7:f:27:LEU:HA	1.87	0.55
17:M:101:45D:H201	3:B:56:ILE:HD11	1.87	0.55
5:N:27:ALA:HB1	5:N:32:LYS:HE3	1.88	0.55
1:a:394:PRO:HA	1:a:397:ILE:HG22	1.89	0.55
10:l:81:GLU:OE2	10:l:147:ARG:NH2	2.39	0.55
3:B:15:ASP:HB3	3:B:20:ARG:HB2	1.89	0.55
1:G:201:MET:HB2	12:G:813:CLA:HBC2	1.88	0.55
6:O:45:VAL:HG12	6:O:51:ASN:HB3	1.87	0.55
3:b:645:LEU:O	3:b:662:SER:OG	2.23	0.55
1:A:617:TRP:CH2	12:A:802:CLA:HAB	2.42	0.55
12:B:830:CLA:H42	9:J:27:ALA:HB1	1.89	0.55
1:G:218:THR:HG21	1:G:303:LEU:HB2	1.89	0.55
5:d:44:VAL:HG22	5:d:54:THR:HG22	1.88	0.55
10:S:155:LEU:HD23	10:S:158:ILE:HD11	1.89	0.55
10:L:100:THR:HG21	10:L:130:LEU:HD22	1.88	0.55
1:G:682:ARG:HG3	3:H:646:ILE:HD12	1.88	0.55
1:a:201:MET:HE1	12:a:824:CLA:H142	1.89	0.55
12:a:831:CLA:O1A	10:l:24:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:15:ASP:HB3	3:b:20:ARG:HB2	1.89	0.55
5:D:33:TYR:OH	5:D:90:ARG:NH1	2.40	0.55
3:b:142:LEU:HD21	15:b:841:BCR:H24C	1.89	0.54
12:A:832:CLA:HBB1	12:A:833:CLA:H2	1.90	0.54
5:D:66:ARG:NH2	5:D:68:GLU:OE1	2.41	0.54
12:G:855:CLA:HAB	3:H:596:TRP:HH2	1.70	0.54
3:H:638:LEU:O	3:H:642:SER:OG	2.25	0.54
3:B:500:THR:HG22	3:B:508:LYS:HD3	1.89	0.54
1:G:44:LYS:HE3	6:O:45:VAL:HG13	1.90	0.54
2:M:15:ALA:HB1	17:M:101:45D:H421	1.89	0.54
12:b:804:CLA:H162	12:b:825:CLA:HBB2	1.88	0.54
8:I:29:ARG:NH2	10:L:108:THR:OG1	2.40	0.54
12:H:828:CLA:HBC2	15:H:844:BCR:H292	1.90	0.54
3:B:461:GLY:HA3	7:F:27:LEU:HA	1.88	0.54
12:G:802:CLA:HBA2	3:H:415:LEU:HD23	1.88	0.54
5:d:100:ILE:HA	5:d:103:LYS:HE2	1.89	0.54
1:A:307:VAL:HG21	12:A:816:CLA:HAB	1.90	0.54
3:B:137:GLU:HG3	19:B:847:LMT:H91	1.89	0.54
3:B:594:MET:HG3	3:B:725:LEU:HD21	1.90	0.54
1:A:218:THR:HG21	1:A:303:LEU:HB2	1.90	0.54
3:B:245:LEU:HD11	12:B:812:CLA:HBC1	1.90	0.54
5:D:33:TYR:OH	5:D:67:LYS:NZ	2.38	0.54
3:H:157:LEU:O	3:H:162:ARG:NH2	2.41	0.53
3:H:461:GLY:HA3	7:P:27:LEU:HA	1.90	0.53
12:H:804:CLA:H143	12:H:826:CLA:HBB2	1.90	0.53
12:A:818:CLA:H92	12:A:828:CLA:H91	1.89	0.53
5:D:100:ILE:HA	5:D:103:LYS:HZ3	1.73	0.53
1:G:669:GLN:NE2	20:G:902:HOH:O	2.41	0.53
3:H:436:ARG:NH1	3:H:439:ASP:OD2	2.41	0.53
3:H:709:LYS:HG2	12:H:837:CLA:HED3	1.91	0.53
1:G:307:VAL:HG21	12:G:817:CLA:HAB	1.89	0.53
12:H:850:CLA:HBC2	1:a:339:LYS:H	1.72	0.53
12:b:805:CLA:HBB1	12:b:805:CLA:H112	1.90	0.53
12:A:854:CLA:H52	3:B:426:VAL:HG13	1.90	0.53
3:b:629:TYR:OH	3:b:635:ARG:NH2	2.42	0.53
12:b:822:CLA:HBB2	15:b:842:BCR:H381	1.91	0.53
3:B:125:TYR:HA	3:B:130:ARG:HH12	1.74	0.53
5:d:46:GLU:HB3	5:d:76:GLN:HE22	1.73	0.53
1:A:714:TRP:O	1:A:717:SER:OG	2.27	0.53
1:G:487:GLN:HE21	1:G:489:GLN:HE21	1.55	0.53
12:b:804:CLA:H143	12:b:825:CLA:HBB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:807:CLA:H42	16:G:851:LHG:H261	1.90	0.53
1:a:44:LYS:HZ1	6:e:44:LYS:HA	1.74	0.53
12:b:827:CLA:HBC2	15:b:842:BCR:H292	1.90	0.53
3:B:415:LEU:HD23	12:B:801:CLA:HBA2	1.90	0.53
1:G:201:MET:HE1	12:G:825:CLA:H142	1.91	0.53
1:G:283:LYS:NZ	1:G:296:THR:OG1	2.42	0.53
4:K:47:ASP:OD1	5:N:90:ARG:NH2	2.40	0.53
3:H:67:HIS:ND1	3:H:71:GLN:OE1	2.39	0.53
12:b:832:CLA:H62	12:f:203:CLA:HBB2	1.91	0.53
12:B:827:CLA:HAB	12:B:835:CLA:HBB2	1.91	0.53
12:H:805:CLA:HBB1	12:H:805:CLA:H112	1.91	0.52
12:H:823:CLA:H12	12:H:832:CLA:HBB2	1.91	0.52
12:H:829:CLA:HAC1	12:H:836:CLA:HBC3	1.91	0.52
3:B:382:TRP:HE1	15:B:844:BCR:H271	1.74	0.52
1:A:557:ILE:HD12	11:A:801:CL0:H63	1.92	0.52
1:G:628:HIS:O	1:G:632:LYS:HB2	2.09	0.52
4:K:55:GLU:OE1	4:K:66:ARG:NH1	2.43	0.52
1:a:601:GLY:O	3:b:683:ARG:NH1	2.42	0.52
3:b:698:GLU:OE1	3:b:707:ARG:NH1	2.43	0.52
7:f:101:ARG:HH22	12:f:203:CLA:HBC2	1.75	0.52
3:B:337:ALA:HB2	3:B:363:HIS:HB2	1.90	0.52
1:G:599:ARG:NH2	5:N:68:GLU:OE2	2.43	0.52
1:G:714:TRP:O	1:G:717:SER:OG	2.27	0.52
12:G:819:CLA:H92	12:G:829:CLA:H91	1.91	0.52
12:l:202:CLA:H91	12:L:206:CLA:H93	1.90	0.52
3:B:142:LEU:HD21	15:B:842:BCR:H24C	1.92	0.52
12:B:806:CLA:HAB	12:B:807:CLA:HAA2	1.92	0.52
3:H:736:TYR:HB2	12:H:802:CLA:HED3	1.91	0.52
12:H:838:CLA:HAC2	15:H:846:BCR:H23C	1.92	0.52
12:f:201:CLA:H161	9:j:19:GLY:HA3	1.92	0.52
1:a:494:GLN:NE2	1:a:547:LEU:O	2.41	0.52
3:b:137:GLU:HB3	19:b:846:LMT:H41	1.91	0.52
1:G:47:THR:HA	1:G:50:TRP:HD1	1.75	0.52
3:b:469:LEU:HD11	3:b:479:PRO:HA	1.91	0.52
12:b:822:CLA:H12	12:b:830:CLA:HBB2	1.92	0.52
1:A:201:MET:HE1	12:A:824:CLA:H142	1.92	0.52
3:H:137:GLU:HB3	19:H:848:LMT:H41	1.91	0.52
12:H:806:CLA:HAB	12:H:807:CLA:HAA2	1.92	0.52
1:a:603:CYS:HB2	3:b:683:ARG:H	1.75	0.52
3:b:245:LEU:HD11	12:b:812:CLA:HBC1	1.92	0.52
1:G:44:LYS:HZ2	6:O:45:VAL:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:839:CLA:H203	12:P:201:CLA:H51	1.92	0.51
3:b:338:GLN:NE2	12:b:822:CLA:OBD	2.43	0.51
3:b:448:ALA:HB1	12:b:832:CLA:HBD	1.92	0.51
12:b:828:CLA:HAC1	12:b:834:CLA:HBC3	1.90	0.51
12:B:805:CLA:H112	12:B:805:CLA:HBB1	1.93	0.51
12:F:201:CLA:H161	9:J:19:GLY:HA3	1.92	0.51
3:H:428:ASN:HA	3:H:440:GLN:HG2	1.91	0.51
1:a:512:TRP:HB2	12:a:835:CLA:HED3	1.91	0.51
12:a:807:CLA:H2	12:a:827:CLA:H2	1.92	0.51
3:b:699:ARG:NH1	10:l:17:GLY:O	2.36	0.51
3:H:448:ALA:HB1	12:H:834:CLA:HBD	1.92	0.51
12:S:204:CLA:H172	15:S:205:BCR:H14C	1.93	0.51
1:A:201:MET:HB2	12:A:812:CLA:HBC2	1.92	0.51
3:B:645:LEU:O	3:B:662:SER:OG	2.25	0.51
1:G:221:LEU:HA	1:G:225:ALA:HB3	1.93	0.51
1:a:364:ILE:HD11	15:a:847:BCR:HC7	1.92	0.51
1:a:597:PRO:HD2	4:c:52:LYS:HG3	1.91	0.51
3:b:736:TYR:HB2	12:b:802:CLA:HED3	1.92	0.51
5:d:26:LYS:NZ	20:d:202:HOH:O	2.44	0.51
5:N:66:ARG:NH2	5:N:68:GLU:OE1	2.40	0.51
12:a:805:CLA:H152	12:a:828:CLA:H12	1.93	0.51
12:b:805:CLA:HED2	8:i:3:VAL:HG23	1.92	0.51
1:A:364:ILE:HD11	15:A:847:BCR:HC7	1.93	0.51
3:H:174:ARG:HB2	12:H:811:CLA:HBC2	1.92	0.51
12:a:841:CLA:H192	8:i:17:LEU:HD12	1.92	0.51
12:b:824:CLA:H141	12:b:826:CLA:H151	1.92	0.51
7:f:98:VAL:HG12	7:f:108:PHE:HB2	1.91	0.51
1:A:681:LEU:HD12	1:A:685:LEU:HD23	1.93	0.51
3:B:585:SER:OG	3:B:588:ASP:OD1	2.29	0.51
10:S:52:VAL:O	10:S:56:HIS:ND1	2.43	0.51
12:a:818:CLA:HAB	12:a:818:CLA:H8	1.93	0.51
1:A:749:GLN:NE2	20:A:914:HOH:O	2.44	0.51
12:A:825:CLA:HAB	15:A:848:BCR:H311	1.93	0.51
1:a:749:GLN:NE2	20:a:917:HOH:O	2.43	0.50
12:a:832:CLA:HBB1	12:a:833:CLA:H2	1.93	0.50
15:A:845:BCR:H362	15:A:846:BCR:HC8	1.93	0.50
15:F:202:BCR:H332	15:J:101:BCR:H281	1.93	0.50
10:L:35:ASN:HB3	12:L:204:CLA:HAC1	1.93	0.50
3:H:131:HIS:HB2	3:H:134:GLU:HG3	1.94	0.50
1:G:128:ASN:HD22	1:G:141:GLY:HA2	1.77	0.50
1:a:331:ILE:HG21	12:a:824:CLA:HAC1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:368:MET:HG3	12:a:824:CLA:HHB	1.93	0.50
3:H:447:PHE:HB3	12:H:834:CLA:H42	1.93	0.50
3:b:159:PRO:HA	3:b:162:ARG:HG3	1.92	0.50
3:B:457:VAL:HA	3:B:494:ASN:HD21	1.77	0.50
12:B:828:CLA:HAC1	12:B:835:CLA:HBC3	1.92	0.50
3:b:460:PRO:HD2	7:f:28:GLY:HA2	1.94	0.50
9:j:17:ILE:HD13	15:j:103:BCR:H401	1.94	0.50
3:B:711:LYS:NZ	4:C:74:THR:OG1	2.44	0.50
10:L:70:LEU:HD22	10:L:80:ILE:HD11	1.94	0.50
1:G:67:GLU:OE2	1:G:71:ARG:NH2	2.45	0.50
12:G:819:CLA:H8	12:G:819:CLA:HAB	1.93	0.50
3:H:477:THR:HG21	12:H:832:CLA:HMD3	1.94	0.50
12:H:831:CLA:H42	9:R:27:ALA:HB1	1.93	0.50
12:H:837:CLA:H143	10:S:95:VAL:HG13	1.93	0.50
12:b:836:CLA:HAC2	15:b:844:BCR:H23C	1.93	0.50
1:A:365:ASN:ND2	12:A:805:CLA:OBD	2.36	0.50
12:B:822:CLA:HBB2	15:B:843:BCR:H381	1.94	0.50
1:G:118:ALA:HB1	1:G:124:GLN:HG3	1.94	0.50
1:G:278:ASP:OD2	1:G:278:ASP:N	2.43	0.50
3:H:709:LYS:HZ2	10:S:112:ASP:H	1.59	0.49
1:a:432:GLN:HE21	5:d:44:VAL:HG11	1.77	0.49
1:A:50:TRP:HZ2	12:F:201:CLA:HAB	1.77	0.49
1:A:410:LEU:HD21	12:A:806:CLA:H142	1.94	0.49
1:A:512:TRP:HB2	12:A:835:CLA:HED3	1.94	0.49
12:B:827:CLA:HBC2	15:B:843:BCR:H292	1.94	0.49
3:H:412:TRP:O	3:H:416:PHE:HB2	2.13	0.49
1:a:203:ASN:HD21	1:a:316:TYR:H	1.60	0.49
1:a:443:ARG:NH1	20:a:903:HOH:O	2.46	0.49
12:b:833:CLA:H152	15:f:204:BCR:H23C	1.94	0.49
6:e:45:VAL:HG12	6:e:51:ASN:HB3	1.93	0.49
15:H:844:BCR:H371	15:H:845:BCR:H23C	1.94	0.49
12:P:201:CLA:H161	9:R:19:GLY:HA3	1.94	0.49
1:a:604:GLN:HE22	3:b:681:SER:HA	1.77	0.49
3:H:65:ASN:HD22	3:H:135:LEU:HD22	1.77	0.49
12:a:829:CLA:H102	12:a:840:CLA:HAA2	1.95	0.49
5:d:48:PRO:HD3	5:d:73:LEU:HD13	1.94	0.49
7:f:31:ILE:HD12	7:f:35:GLU:HG2	1.95	0.49
1:A:604:GLN:HE22	3:B:681:SER:HA	1.78	0.49
1:A:631:TRP:CZ3	1:A:674:SER:HB3	2.47	0.49
12:B:822:CLA:HED2	12:B:823:CLA:HBD	1.95	0.49
1:G:302:HIS:O	1:G:306:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:365:ASN:ND2	12:G:806:CLA:OBD	2.36	0.49
12:H:823:CLA:HBB2	15:H:844:BCR:H381	1.93	0.49
12:b:806:CLA:HAB	12:b:807:CLA:HAA2	1.94	0.49
3:B:398:ARG:O	3:B:402:HIS:ND1	2.44	0.49
15:F:202:BCR:H333	9:J:24:LEU:HD13	1.93	0.49
1:G:427:ASP:O	1:G:431:ASN:ND2	2.43	0.49
12:G:826:CLA:HAB	15:G:849:BCR:H311	1.94	0.49
2:T:15:ALA:HB1	17:T:101:45D:H421	1.95	0.49
2:m:15:ALA:HB1	17:m:101:45D:H421	1.94	0.49
1:A:603:CYS:O	3:B:684:GLY:N	2.37	0.49
3:H:90:ALA:HA	3:H:113:VAL:HA	1.95	0.49
5:d:19:SER:OG	5:d:20:THR:N	2.45	0.49
12:A:804:CLA:H72	15:A:852:BCR:H313	1.95	0.49
12:A:831:CLA:HAA1	10:L:24:ASN:HD21	1.78	0.49
3:B:137:GLU:HB2	19:B:847:LMT:H41	1.94	0.49
3:B:702:LEU:HB2	15:L:203:BCR:H282	1.93	0.49
1:a:617:TRP:HH2	12:a:802:CLA:HAB	1.76	0.49
12:a:825:CLA:HAB	15:a:848:BCR:H311	1.93	0.49
12:a:854:CLA:HAB	3:b:596:TRP:HH2	1.78	0.49
12:A:829:CLA:H102	12:A:840:CLA:HAA2	1.95	0.49
1:G:203:ASN:HD21	1:G:316:TYR:H	1.61	0.49
9:R:10:PRO:HB3	15:R:101:BCR:H343	1.94	0.49
3:B:417:LEU:HD11	12:B:834:CLA:HMB2	1.93	0.49
1:G:531:THR:OG1	1:G:532:VAL:N	2.46	0.49
12:b:812:CLA:HBB1	15:b:840:BCR:HC21	1.95	0.49
3:B:447:PHE:HB3	12:B:833:CLA:H42	1.93	0.49
3:B:537:ILE:HG21	12:B:833:CLA:HAB	1.95	0.49
7:F:32:PRO:HA	7:F:87:CYS:HA	1.94	0.49
10:S:19:LEU:O	10:S:24:ASN:ND2	2.42	0.48
12:f:201:CLA:H41	12:f:201:CLA:H61	1.69	0.48
3:H:130:ARG:HG2	3:H:201:ARG:HD3	1.94	0.48
3:b:535:HIS:HD2	15:b:847:BCR:HC21	1.77	0.48
3:B:592:LEU:HB3	12:B:801:CLA:HMD1	1.95	0.48
5:D:46:GLU:H	5:D:76:GLN:HE22	1.60	0.48
12:A:807:CLA:H2	12:A:827:CLA:H2	1.94	0.48
12:B:829:CLA:H122	15:F:204:BCR:HC8	1.95	0.48
1:G:292:SER:OG	1:G:386:TYR:O	2.32	0.48
10:S:70:LEU:HD22	10:S:80:ILE:HD11	1.94	0.48
12:b:805:CLA:HHB	12:b:806:CLA:HMB3	1.94	0.48
1:A:617:TRP:CZ2	12:A:802:CLA:HAB	2.48	0.48
1:G:443:ARG:NH1	20:G:901:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:100:THR:HG21	10:S:130:LEU:HD22	1.95	0.48
12:A:828:CLA:H2	15:A:846:BCR:H24C	1.96	0.48
3:B:469:LEU:HD11	3:B:479:PRO:HA	1.95	0.48
10:L:35:ASN:O	10:L:40:ARG:NH2	2.42	0.48
3:H:559:LYS:NZ	6:O:17:TYR:O	2.39	0.48
7:P:77:ARG:HA	9:R:32:LYS:HZ3	1.79	0.48
12:S:204:CLA:H93	12:L:202:CLA:H91	1.95	0.48
1:a:538:GLN:HG2	1:a:539:LYS:HG2	1.94	0.48
15:b:842:BCR:H371	15:b:843:BCR:H23C	1.95	0.48
1:A:124:GLN:O	1:A:127:LEU:HB2	2.13	0.48
1:A:551:ASP:HA	1:A:554:ILE:HG22	1.94	0.48
1:G:221:LEU:HD11	1:G:302:HIS:HD2	1.79	0.48
1:G:364:ILE:HD11	15:G:848:BCR:HC7	1.95	0.48
1:a:342:PHE:O	1:a:438:ARG:NH2	2.45	0.48
1:A:472:GLN:HG2	3:B:649:TYR:HD1	1.79	0.48
12:B:833:CLA:H62	12:F:203:CLA:HBB2	1.95	0.48
12:G:808:CLA:HBA2	12:G:808:CLA:H3A	1.71	0.48
3:H:446:VAL:H	12:H:835:CLA:HMD3	1.79	0.48
12:a:806:CLA:HED1	12:a:829:CLA:H2	1.96	0.48
8:i:29:ARG:HH12	10:L:35:ASN:HD21	1.62	0.48
12:B:828:CLA:HBA2	12:B:828:CLA:H3A	1.73	0.48
1:a:44:LYS:HE3	6:e:45:VAL:HG13	1.95	0.47
12:a:824:CLA:H151	12:a:824:CLA:H18	1.68	0.47
12:b:827:CLA:HAB	12:b:834:CLA:HBB2	1.95	0.47
12:b:835:CLA:H143	10:l:95:VAL:HG13	1.95	0.47
1:G:604:GLN:HE22	3:H:681:SER:HA	1.78	0.47
12:b:823:CLA:H2	15:b:843:BCR:H14C	1.96	0.47
12:A:823:CLA:HBB2	16:A:851:LHG:HC82	1.96	0.47
3:H:439:ASP:OD1	7:P:77:ARG:NH1	2.45	0.47
12:b:804:CLA:H91	18:b:845:LMG:H422	1.95	0.47
12:A:820:CLA:H12	12:A:823:CLA:HBA2	1.96	0.47
3:B:730:VAL:HA	18:B:846:LMG:H442	1.96	0.47
3:H:399:VAL:HG21	15:H:844:BCR:H401	1.96	0.47
12:H:823:CLA:HED2	12:H:824:CLA:HBD	1.97	0.47
10:S:50:LEU:HD21	10:L:130:LEU:HD23	1.96	0.47
1:a:615:LEU:HB3	1:a:767:LEU:HD11	1.96	0.47
3:b:493:VAL:HA	3:b:522:VAL:HB	1.96	0.47
3:B:182:LEU:O	3:B:186:SER:OG	2.32	0.47
3:B:604:ILE:HD13	12:B:833:CLA:HBB2	1.96	0.47
7:P:105:ALA:HA	7:P:109:ILE:HD13	1.96	0.47
3:b:382:TRP:HE1	15:b:843:BCR:H271	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD21	1:A:702:ALA:H	1.79	0.47
3:H:4:ARG:HG3	8:Q:31:THR:H	1.79	0.47
3:H:604:ILE:HD13	12:H:834:CLA:HBB2	1.97	0.47
4:c:23:LEU:O	5:d:67:LYS:NZ	2.38	0.47
1:A:603:CYS:HB2	3:B:683:ARG:H	1.79	0.47
1:a:599:ARG:NH2	5:d:68:GLU:OE1	2.47	0.47
12:a:828:CLA:H2	15:a:846:BCR:H392	1.97	0.47
12:a:831:CLA:H61	12:a:831:CLA:H41	1.68	0.47
12:a:854:CLA:H52	3:b:426:VAL:HG13	1.97	0.47
12:a:855:CLA:HAB	3:b:673:ALA:C	2.40	0.47
1:A:729:GLN:HE22	1:A:751:ARG:HA	1.80	0.47
3:B:520:THR:HG22	3:B:615:ILE:HG21	1.96	0.47
12:B:822:CLA:H12	12:B:831:CLA:HBB2	1.97	0.47
15:B:844:BCR:H371	15:B:844:BCR:H24C	1.71	0.47
12:H:824:CLA:H2	15:H:845:BCR:H14C	1.97	0.47
1:a:66:ARG:HD2	1:a:69:ILE:HD12	1.97	0.47
1:a:714:TRP:O	1:a:717:SER:OG	2.28	0.47
1:a:744:ILE:HG12	7:f:127:ARG:HG3	1.97	0.47
3:b:26:ALA:HA	12:b:826:CLA:H42	1.97	0.47
3:b:594:MET:HG2	3:b:725:LEU:HD21	1.97	0.47
12:b:805:CLA:H92	12:b:805:CLA:HMC1	1.96	0.47
1:A:205:HIS:HB3	12:A:824:CLA:HED3	1.97	0.47
16:G:851:LHG:H281	16:G:851:LHG:H251	1.82	0.47
3:H:417:LEU:HD11	12:H:835:CLA:HMB2	1.96	0.47
1:a:201:MET:HB2	12:a:812:CLA:HBC2	1.97	0.47
15:b:843:BCR:H24C	15:b:843:BCR:H371	1.71	0.47
12:A:841:CLA:HHD	15:B:845:BCR:H383	1.97	0.47
15:B:841:BCR:H351	15:B:841:BCR:H15C	1.71	0.47
10:L:8:MET:HE3	10:L:22:PRO:HG3	1.97	0.47
12:G:807:CLA:HED1	12:G:830:CLA:H2	1.97	0.47
12:H:805:CLA:HHB	12:H:806:CLA:HMB3	1.97	0.47
12:b:848:CLA:H41	12:b:848:CLA:H93	1.97	0.47
1:G:43:PRO:HD3	1:G:48:TRP:CE2	2.50	0.46
3:H:17:THR:HG22	3:H:711:LYS:HB2	1.96	0.46
15:H:843:BCR:H351	15:H:843:BCR:H15C	1.73	0.46
12:a:829:CLA:H111	16:a:850:LHG:H171	1.95	0.46
10:l:147:ARG:HA	10:l:150:LEU:HB3	1.97	0.46
5:D:64:LEU:HD13	5:D:69:GLN:HB3	1.97	0.46
3:H:510:CYS:SG	3:H:511:PHE:N	2.85	0.46
3:H:556:ARG:HA	3:H:565:LYS:HB3	1.97	0.46
12:a:834:CLA:H41	12:a:834:CLA:H62	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:854:CLA:HAB	3:b:596:TRP:CH2	2.50	0.46
12:b:833:CLA:H171	15:f:204:BCR:H23C	1.97	0.46
10:l:37:PRO:O	10:l:48:ARG:NH1	2.44	0.46
3:B:383:VAL:HG23	3:B:384:ARG:HG3	1.98	0.46
12:G:825:CLA:H18	12:G:825:CLA:H151	1.70	0.46
12:P:201:CLA:H41	12:P:201:CLA:H61	1.75	0.46
12:A:821:CLA:HBA2	12:A:821:CLA:H3A	1.76	0.46
3:B:477:THR:HG21	12:B:831:CLA:HMD3	1.96	0.46
8:Q:27:ILE:HG13	8:Q:28:GLU:HG2	1.96	0.46
12:A:807:CLA:H111	12:A:807:CLA:H202	1.96	0.46
12:l:205:CLA:H3A	12:l:205:CLA:HBA2	1.72	0.46
1:G:99:SER:HB2	1:G:149:PHE:HZ	1.80	0.46
1:G:331:ILE:HG21	12:G:825:CLA:HAC1	1.98	0.46
1:G:368:MET:HG3	12:G:825:CLA:HHB	1.97	0.46
1:a:200:SER:HB2	1:a:318:THR:HG21	1.97	0.46
7:f:122:LEU:HD22	15:j:103:BCR:H372	1.97	0.46
3:B:423:GLY:HA3	12:B:830:CLA:HAB	1.96	0.46
1:G:372:LEU:HD11	12:G:819:CLA:H71	1.97	0.46
3:H:469:LEU:HD11	3:H:479:PRO:HA	1.97	0.46
12:H:805:CLA:H12	8:Q:11:THR:HG21	1.97	0.46
1:a:188:ARG:NH1	12:a:809:CLA:OBD	2.49	0.46
15:b:847:BCR:H371	15:b:847:BCR:H24C	1.74	0.46
5:d:5:ASN:HD22	5:d:32:LYS:HE3	1.81	0.46
1:A:394:PRO:HA	1:A:397:ILE:HG22	1.97	0.46
12:A:818:CLA:HAB	12:A:818:CLA:H8	1.96	0.46
12:A:831:CLA:H61	12:A:831:CLA:H41	1.67	0.46
12:G:829:CLA:H2	15:G:847:BCR:H392	1.98	0.46
1:a:246:GLU:O	1:a:250:SER:OG	2.33	0.46
3:B:194:MET:HE3	3:B:194:MET:HB3	1.84	0.46
15:B:844:BCR:H351	15:B:844:BCR:H15C	1.72	0.46
15:Q:102:BCR:H15C	15:Q:102:BCR:H351	1.76	0.46
12:a:833:CLA:HHD	12:b:807:CLA:HBB2	1.98	0.46
12:B:825:CLA:H3A	12:B:825:CLA:HBA2	1.74	0.46
1:G:231:MET:HA	1:G:234:LYS:HG2	1.98	0.46
3:H:270:ILE:HA	3:H:273:ILE:HG22	1.97	0.46
3:H:382:TRP:HE1	15:H:845:BCR:H271	1.81	0.46
1:a:551:ASP:HA	1:a:554:ILE:HG22	1.97	0.46
12:a:835:CLA:HBA2	12:a:835:CLA:H3A	1.66	0.46
15:a:845:BCR:H24C	15:a:845:BCR:H371	1.80	0.46
3:b:559:LYS:NZ	6:e:17:TYR:O	2.40	0.46
3:b:585:SER:OG	3:b:588:ASP:OD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE1	1:A:424:ARG:NH1	2.48	0.46
12:A:804:CLA:HBA2	12:A:804:CLA:H3A	1.85	0.46
12:A:854:CLA:H61	12:A:854:CLA:H41	1.74	0.46
5:D:23:LEU:HB2	10:L:16:VAL:HA	1.97	0.46
1:G:450:LEU:HD21	1:G:566:ILE:HG22	1.98	0.45
12:G:856:CLA:OBD	3:H:685:TYR:OH	2.34	0.45
3:H:185:VAL:HG13	15:H:842:BCR:HC31	1.98	0.45
3:H:594:MET:HG3	3:H:725:LEU:HD21	1.98	0.45
15:H:841:BCR:H351	15:H:841:BCR:H15C	1.73	0.45
1:a:573:VAL:HG12	1:a:574:LEU:HD23	1.97	0.45
3:b:185:VAL:HG11	15:b:840:BCR:HC8	1.97	0.45
12:H:801:CLA:H61	12:H:801:CLA:H41	1.69	0.45
1:A:599:ARG:HE	5:D:66:ARG:HH22	1.65	0.45
12:A:854:CLA:HAB	3:B:596:TRP:HH2	1.80	0.45
12:H:805:CLA:HED2	8:Q:3:VAL:HG13	1.99	0.45
5:N:35:ILE:HG21	5:N:73:LEU:HD23	1.98	0.45
2:m:28:THR:HG21	3:b:154:TRP:HD1	1.81	0.45
15:i:101:BCR:H24C	15:i:101:BCR:H371	1.76	0.45
3:B:493:VAL:HA	3:B:522:VAL:HB	1.99	0.45
12:H:828:CLA:HAB	12:H:836:CLA:HBB2	1.98	0.45
1:a:385:PRO:HB3	12:a:818:CLA:HAA2	1.97	0.45
3:b:500:THR:HG22	3:b:508:LYS:HB3	1.98	0.45
3:B:722:LEU:HD11	18:B:846:LMG:H341	1.98	0.45
15:G:849:BCR:H351	15:G:849:BCR:H15C	1.74	0.45
3:H:134:GLU:HA	3:H:137:GLU:HG2	1.99	0.45
8:Q:17:LEU:HD11	15:Q:101:BCR:H362	1.98	0.45
12:S:202:CLA:OBD	10:L:104:SER:OG	2.32	0.45
12:A:824:CLA:H151	12:A:824:CLA:H18	1.64	0.45
3:B:736:TYR:HB2	12:B:802:CLA:HED3	1.98	0.45
12:B:836:CLA:H143	10:L:95:VAL:HG13	1.97	0.45
12:G:821:CLA:H12	12:G:824:CLA:HBA2	1.99	0.45
12:G:841:CLA:HHD	15:H:846:BCR:H383	1.99	0.45
1:a:230:GLN:HE22	1:a:257:PHE:HA	1.82	0.45
3:b:730:VAL:HA	18:b:845:LMG:H442	1.98	0.45
1:G:460:HIS:HD2	16:G:854:LHG:H191	1.82	0.45
1:G:615:LEU:HD21	12:G:830:CLA:HBC1	1.98	0.45
12:G:803:CLA:H91	12:G:856:CLA:H112	1.99	0.45
3:H:112:PRO:HD2	8:Q:1:MET:HE1	1.98	0.45
3:H:493:VAL:HA	3:H:522:VAL:HB	1.99	0.45
3:H:585:SER:OG	3:H:588:ASP:OD2	2.34	0.45
15:Q:101:BCR:H351	15:Q:101:BCR:H15C	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:77:HIS:ND1	12:a:812:CLA:OBD	2.50	0.45
12:A:807:CLA:H203	15:J:101:BCR:H14C	1.99	0.45
12:A:854:CLA:HBC2	3:B:599:ASN:HB2	1.99	0.45
3:H:332:VAL:HG22	12:H:816:CLA:H71	1.99	0.45
12:H:815:CLA:HBA2	12:H:815:CLA:H3A	1.62	0.45
1:a:410:LEU:HD21	12:a:806:CLA:H142	1.98	0.45
12:a:817:CLA:HAC1	12:a:834:CLA:H42	1.99	0.45
12:b:822:CLA:H13	12:b:822:CLA:H102	1.82	0.45
1:A:116:GLN:NE2	12:A:808:CLA:OBD	2.45	0.45
3:B:343:LEU:HD13	12:B:814:CLA:HAA2	1.99	0.45
1:G:48:TRP:O	1:G:52:LEU:N	2.48	0.45
5:N:37:TRP:NE1	5:N:55:MET:SD	2.77	0.45
1:a:455:LEU:HD23	12:a:855:CLA:HBA2	1.98	0.45
1:a:725:ARG:NH1	3:b:580:GLY:O	2.40	0.45
12:a:806:CLA:H42	16:a:850:LHG:H261	1.99	0.45
3:b:3:THR:OG1	3:b:13:ALA:O	2.29	0.45
12:b:816:CLA:HBB1	12:b:821:CLA:H71	1.98	0.45
1:A:45:THR:HG22	1:A:749:GLN:HB2	1.99	0.45
1:A:466:VAL:HG12	12:A:833:CLA:HBC2	1.99	0.45
12:B:825:CLA:H202	12:B:825:CLA:H161	1.89	0.45
12:B:837:CLA:H41	8:I:20:LEU:HD11	1.98	0.45
5:D:37:TRP:NE1	5:D:55:MET:SD	2.85	0.45
1:G:383:MET:HG2	12:G:818:CLA:HAA2	1.99	0.45
12:G:818:CLA:H62	12:G:818:CLA:H41	1.71	0.45
12:H:850:CLA:H93	12:H:850:CLA:H41	1.99	0.45
12:a:839:CLA:H3A	12:a:839:CLA:HBA2	1.77	0.45
7:f:117:TRP:HA	7:f:157:TRP:HE1	1.82	0.45
10:l:63:PRO:HA	12:l:206:CLA:HMB2	1.99	0.45
1:A:118:ALA:H	1:A:128:ASN:HD21	1.64	0.45
1:A:615:LEU:HD21	12:A:829:CLA:HBC1	1.98	0.45
12:A:806:CLA:HED1	12:A:829:CLA:H2	1.98	0.45
12:A:818:CLA:HAB	12:A:818:CLA:H111	1.99	0.45
3:B:93:ASP:OD2	3:B:95:HIS:ND1	2.36	0.45
15:I:101:BCR:H24C	15:I:101:BCR:H371	1.76	0.45
12:H:808:CLA:H61	12:H:808:CLA:H101	1.77	0.44
15:P:202:BCR:H15C	15:P:202:BCR:H351	1.74	0.44
3:b:176:ASN:HB3	12:b:817:CLA:HMD1	1.99	0.44
12:b:805:CLA:HAA1	8:i:8:VAL:HG22	1.99	0.44
7:f:160:PHE:O	7:f:164:GLN:NE2	2.50	0.44
1:G:681:LEU:HD12	1:G:685:LEU:HD23	1.98	0.44
3:H:446:VAL:HG21	7:P:97:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:807:CLA:H111	12:a:807:CLA:H202	1.99	0.44
18:b:845:LMG:H382	18:b:845:LMG:H351	1.78	0.44
7:f:142:ILE:N	9:j:7:SER:O	2.45	0.44
12:l:202:CLA:H101	12:l:202:CLA:H61	1.72	0.44
12:A:855:CLA:HAB	3:B:673:ALA:C	2.42	0.44
12:B:822:CLA:H72	12:B:833:CLA:H102	1.99	0.44
12:L:205:CLA:H41	12:L:205:CLA:H62	1.79	0.44
1:G:246:GLU:O	1:G:250:SER:OG	2.35	0.44
1:G:308:MET:HE1	12:G:818:CLA:HBC2	1.98	0.44
3:H:71:GLN:HE21	3:H:90:ALA:H	1.65	0.44
12:H:808:CLA:H91	12:l:206:CLA:H93	1.98	0.44
1:a:520:VAL:HA	1:a:544:PRO:HA	1.98	0.44
12:a:818:CLA:HAB	12:a:818:CLA:H111	2.00	0.44
3:b:560:LEU:O	3:b:578:ARG:NE	2.48	0.44
12:b:815:CLA:HBA2	12:b:815:CLA:H3A	1.77	0.44
12:l:205:CLA:H62	12:l:205:CLA:H41	1.78	0.44
3:B:269:ALA:HB3	12:B:814:CLA:HAB	2.00	0.44
10:L:113:ASP:OD2	10:L:122:TRP:NE1	2.45	0.44
1:G:317:ARG:HD2	1:G:319:ASN:HD21	1.82	0.44
3:H:546:LEU:O	3:H:550:LYS:HB2	2.16	0.44
15:S:201:BCR:H15C	15:S:201:BCR:H351	1.75	0.44
15:a:848:BCR:H351	15:a:848:BCR:H15C	1.76	0.44
9:j:27:ALA:HB1	12:j:102:CLA:H42	1.98	0.44
12:A:803:CLA:H112	12:A:803:CLA:H152	1.78	0.44
12:A:817:CLA:H62	12:A:817:CLA:H41	1.72	0.44
12:G:829:CLA:H102	12:G:829:CLA:H62	1.81	0.44
12:G:830:CLA:H72	16:G:851:LHG:H162	2.00	0.44
12:G:856:CLA:HAB	3:H:673:ALA:C	2.43	0.44
3:H:80:ASP:OD2	3:H:83:LYS:NZ	2.49	0.44
10:S:104:SER:OG	12:l:204:CLA:OBD	2.34	0.44
12:S:203:CLA:HBA2	12:S:203:CLA:H3A	1.71	0.44
12:a:818:CLA:HBA2	12:a:818:CLA:H3A	1.91	0.44
12:a:821:CLA:HBA2	12:a:821:CLA:H3A	1.74	0.44
3:b:443:ILE:HD13	7:f:96:LEU:HB2	1.98	0.44
12:b:822:CLA:H72	12:b:832:CLA:H102	1.99	0.44
15:l:203:BCR:H351	15:l:203:BCR:H15C	1.74	0.44
1:A:368:MET:HG3	12:A:824:CLA:HHB	2.00	0.44
3:B:448:ALA:HB1	12:B:833:CLA:HBD	1.98	0.44
15:H:849:BCR:H24C	15:H:849:BCR:H371	1.76	0.44
10:l:104:SER:OG	12:L:204:CLA:OBD	2.33	0.44
12:A:803:CLA:H71	12:B:801:CLA:H143	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:104:BCR:H351	15:J:104:BCR:H15C	1.85	0.44
10:L:63:PRO:HA	12:L:206:CLA:HMB2	1.99	0.44
10:L:72:LEU:HB3	10:L:74:ALA:H	1.83	0.44
15:H:842:BCR:H351	15:H:842:BCR:H15C	1.72	0.44
1:a:48:TRP:O	1:a:52:LEU:N	2.48	0.44
12:a:855:CLA:H111	15:b:844:BCR:H362	1.99	0.44
18:B:846:LMG:H382	18:B:846:LMG:H351	1.77	0.44
12:G:835:CLA:H3A	12:G:835:CLA:HBA2	1.70	0.44
12:G:837:CLA:H92	12:G:837:CLA:H61	1.89	0.44
3:H:65:ASN:HD21	15:H:843:BCR:H281	1.83	0.44
1:a:445:ALA:O	1:a:449:HIS:ND1	2.40	0.44
3:b:338:GLN:NE2	12:b:832:CLA:HBB1	2.33	0.44
3:b:486:GLY:O	3:b:490:PHE:HB2	2.16	0.44
12:b:805:CLA:H43	8:i:11:THR:HG21	2.00	0.44
1:A:768:LEU:HD11	15:A:849:BCR:HC8	1.99	0.44
3:B:357:ALA:HB1	3:B:740:VAL:HG22	1.99	0.44
12:B:807:CLA:H122	12:B:807:CLA:H8	1.87	0.44
1:G:380:MET:HE3	1:G:385:PRO:HG2	2.00	0.44
1:G:559:ALA:O	1:G:563:HIS:ND1	2.46	0.44
3:H:15:ASP:HB3	3:H:20:ARG:HB2	2.00	0.44
12:H:804:CLA:H43	18:H:847:LMG:H312	2.00	0.44
3:b:520:THR:HG22	3:b:615:ILE:HG21	1.99	0.44
12:G:824:CLA:HMD2	12:G:825:CLA:HAB	2.00	0.43
15:H:845:BCR:H371	15:H:845:BCR:H24C	1.74	0.43
12:b:827:CLA:H3A	12:b:827:CLA:HBA2	1.84	0.43
1:A:293:LEU:HB2	1:A:298:ILE:HD11	2.00	0.43
12:B:804:CLA:H91	18:B:846:LMG:H422	2.00	0.43
12:B:804:CLA:H143	12:B:825:CLA:HBB2	1.99	0.43
6:O:18:TRP:NE1	6:O:44:LYS:O	2.42	0.43
3:b:268:LEU:HG	12:b:813:CLA:HAB	1.99	0.43
15:A:845:BCR:H371	15:A:845:BCR:H24C	1.79	0.43
15:A:848:BCR:H15C	15:A:848:BCR:H351	1.74	0.43
12:B:815:CLA:H111	12:B:815:CLA:H72	1.81	0.43
15:L:201:BCR:H15C	15:L:201:BCR:H351	1.73	0.43
15:L:203:BCR:H15C	15:L:203:BCR:H351	1.75	0.43
1:G:83:ILE:HD13	1:G:86:ILE:HD12	1.99	0.43
1:G:496:ILE:O	1:G:500:ASN:ND2	2.51	0.43
12:a:814:CLA:HBB1	15:a:845:BCR:H19C	2.00	0.43
3:b:687:GLN:NE2	3:b:714:ALA:H	2.16	0.43
1:G:551:ASP:HA	1:G:554:ILE:HG22	2.00	0.43
3:H:336:VAL:HG13	3:H:340:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:339:GLN:NE2	12:H:815:CLA:OBD	2.50	0.43
12:a:841:CLA:HHD	15:b:844:BCR:H383	1.99	0.43
17:m:101:45D:H371	17:m:101:45D:H311	1.89	0.43
3:b:574:ASP:OD2	3:b:578:ARG:NH1	2.45	0.43
15:A:849:BCR:H23C	12:B:801:CLA:H112	2.01	0.43
12:A:855:CLA:H122	15:I:101:BCR:H281	1.99	0.43
7:F:102:LEU:HA	7:F:105:ALA:HB2	2.00	0.43
12:L:205:CLA:H3A	12:L:205:CLA:HBA2	1.69	0.43
15:L:207:BCR:H15C	15:L:207:BCR:H351	1.76	0.43
12:G:802:CLA:HMD3	3:H:547:ILE:HG12	2.00	0.43
1:a:38:SER:HA	1:a:41:ARG:HE	1.83	0.43
1:a:714:TRP:HZ3	12:a:854:CLA:HMD3	1.82	0.43
1:a:769:GLY:O	1:a:773:THR:OG1	2.29	0.43
12:a:817:CLA:HBA2	12:a:817:CLA:H3A	1.83	0.43
12:b:828:CLA:HBA2	12:b:828:CLA:H3A	1.70	0.43
15:A:845:BCR:H351	15:A:845:BCR:H15C	1.83	0.43
3:B:60:TRP:O	3:B:63:SER:OG	2.33	0.43
12:B:805:CLA:HED2	8:I:3:VAL:HG23	2.00	0.43
1:G:188:ARG:HD3	12:G:810:CLA:HED2	2.01	0.43
1:G:468:ASN:HD22	1:G:480:MET:HG2	1.83	0.43
12:G:856:CLA:H122	15:Q:101:BCR:H281	1.99	0.43
10:S:135:GLY:C	15:S:205:BCR:H23C	2.44	0.43
1:a:49:ILE:HD13	12:f:201:CLA:HMB3	2.00	0.43
1:A:380:MET:HG2	1:A:385:PRO:HG2	2.00	0.43
4:C:58:CYS:HA	4:C:59:PRO:HD3	1.81	0.43
15:G:846:BCR:H351	15:G:846:BCR:H15C	1.86	0.43
12:H:817:CLA:HBB1	12:H:822:CLA:H71	1.99	0.43
12:a:823:CLA:HBB2	16:a:851:LHG:HC82	2.00	0.43
12:a:833:CLA:H152	15:l:203:BCR:H372	2.01	0.43
1:A:342:PHE:HB2	16:A:851:LHG:HC41	2.00	0.43
12:G:802:CLA:H102	12:G:840:CLA:HMC1	2.00	0.43
12:G:827:CLA:H91	12:G:827:CLA:H112	1.88	0.43
15:G:845:BCR:H24C	15:G:845:BCR:H371	1.78	0.43
12:H:838:CLA:HHD	12:H:838:CLA:HAC1	1.92	0.43
7:P:100:GLY:HA2	7:P:109:ILE:HD11	2.00	0.43
3:b:134:GLU:HA	3:b:137:GLU:HG2	2.01	0.43
3:b:232:ALA:HA	3:b:235:GLN:HG2	2.00	0.43
10:l:155:LEU:HD23	10:l:158:ILE:HD11	2.01	0.43
1:A:35:PHE:HD2	1:A:62:GLN:HG2	1.84	0.43
15:A:846:BCR:H24C	15:A:846:BCR:H371	1.82	0.43
12:B:805:CLA:HMC1	12:B:805:CLA:H92	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:56:HIS:HA	10:L:59:TRP:CD1	2.53	0.43
1:G:50:TRP:HZ2	12:P:201:CLA:HAB	1.84	0.43
1:G:438:ARG:O	1:G:442:HIS:ND1	2.48	0.43
12:H:823:CLA:HBA1	12:H:836:CLA:HAA1	2.01	0.43
12:H:828:CLA:H3A	12:H:828:CLA:HBA2	1.79	0.43
12:b:815:CLA:H111	12:b:815:CLA:H72	1.79	0.43
2:M:5:ASN:ND2	8:I:4:TYR:OH	2.52	0.43
3:B:90:ALA:HA	3:B:113:VAL:HA	2.01	0.43
10:L:36:LEU:HD22	12:L:205:CLA:HBD	2.00	0.43
11:G:801:CL0:H41	11:G:801:CL0:H49	1.89	0.43
12:G:827:CLA:H162	12:G:834:CLA:H111	2.01	0.43
10:S:63:PRO:HA	12:S:204:CLA:HMB2	1.99	0.43
12:S:203:CLA:H41	12:S:203:CLA:H62	1.81	0.43
1:a:310:ILE:O	1:a:314:HIS:ND1	2.52	0.43
3:b:174:ARG:HB2	12:b:810:CLA:HBC2	2.01	0.43
12:b:829:CLA:H2	12:b:829:CLA:H62	1.80	0.43
15:f:202:BCR:H351	15:f:202:BCR:H15C	1.73	0.43
1:A:46:THR:O	1:A:49:ILE:HB	2.19	0.43
7:F:30:THR:HG23	7:F:87:CYS:HB3	2.01	0.43
1:G:593:PRO:HB3	1:G:755:ILE:HB	2.01	0.42
3:H:520:THR:HG22	3:H:615:ILE:HG21	2.01	0.42
1:a:43:PRO:HG3	1:a:48:TRP:CZ3	2.53	0.42
2:m:5:ASN:ND2	8:i:4:TYR:OH	2.52	0.42
12:G:855:CLA:H61	12:G:855:CLA:H41	1.78	0.42
3:H:697:HIS:NE2	3:H:703:ALA:O	2.52	0.42
10:S:130:LEU:HD23	10:l:50:LEU:HD21	2.01	0.42
1:a:609:ASP:HA	1:a:612:PHE:HB3	2.01	0.42
3:b:337:ALA:HB2	3:b:363:HIS:HB2	2.01	0.42
15:b:839:BCR:H15C	15:b:839:BCR:H351	1.65	0.42
4:c:35:ARG:NH2	6:e:29:ASP:OD1	2.51	0.42
1:A:48:TRP:O	1:A:52:LEU:N	2.52	0.42
1:A:393:TYR:OH	1:A:540:ILE:O	2.29	0.42
3:B:185:VAL:HG11	15:B:841:BCR:HC8	2.00	0.42
12:H:807:CLA:H143	18:H:847:LMG:H221	2.00	0.42
16:a:853:LHG:H161	16:a:853:LHG:H132	1.80	0.42
2:m:29:LEU:HD22	12:b:837:CLA:HMA2	2.00	0.42
5:d:91:VAL:HG13	5:d:97:GLN:HE22	1.85	0.42
1:A:331:ILE:HG21	12:A:824:CLA:HAC1	2.00	0.42
12:A:826:CLA:H91	12:A:826:CLA:H112	1.88	0.42
12:A:834:CLA:H41	12:A:834:CLA:H62	1.79	0.42
1:G:84:VAL:HG11	12:G:806:CLA:H41	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:822:CLA:H3A	12:G:822:CLA:HBA2	1.76	0.42
18:H:847:LMG:H261	18:H:847:LMG:H232	1.82	0.42
1:a:221:LEU:HA	1:a:225:ALA:HB3	2.02	0.42
15:a:846:BCR:H371	15:a:846:BCR:H24C	1.81	0.42
12:a:855:CLA:H122	15:i:101:BCR:H281	2.00	0.42
3:b:633:TRP:CD2	12:b:802:CLA:H112	2.54	0.42
1:A:340:GLY:HA3	16:A:851:LHG:HC32	2.01	0.42
1:G:60:GLU:OE1	1:G:424:ARG:NH1	2.46	0.42
12:H:823:CLA:H102	12:H:823:CLA:H13	1.82	0.42
1:a:124:GLN:O	1:a:127:LEU:HB2	2.19	0.42
1:a:531:THR:OG1	1:a:532:VAL:N	2.52	0.42
15:a:847:BCR:H351	15:a:847:BCR:H15C	1.83	0.42
12:b:825:CLA:HBA2	12:b:825:CLA:H3A	1.77	0.42
7:f:102:LEU:HA	7:f:105:ALA:HB2	2.00	0.42
1:A:427:ASP:O	1:A:431:ASN:ND2	2.52	0.42
3:B:446:VAL:HG21	7:F:97:ILE:HG23	2.01	0.42
12:G:823:CLA:HAB	12:G:842:CLA:CBB	2.50	0.42
12:H:831:CLA:H143	12:H:831:CLA:H162	1.97	0.42
18:H:847:LMG:H382	18:H:847:LMG:H351	1.75	0.42
12:P:201:CLA:H92	12:P:201:CLA:H62	1.89	0.42
15:S:205:BCR:H371	15:S:205:BCR:H24C	1.81	0.42
1:a:458:GLY:HA2	1:a:560:LEU:HD22	2.01	0.42
1:a:562:ILE:HD11	12:a:836:CLA:HBB1	2.01	0.42
12:a:805:CLA:H143	12:a:805:CLA:H112	1.81	0.42
3:b:175:LEU:HD12	3:b:291:LEU:HD11	2.01	0.42
15:l:201:BCR:H351	15:l:201:BCR:H15C	1.73	0.42
12:A:818:CLA:H152	12:A:826:CLA:H51	2.02	0.42
12:A:834:CLA:H203	12:A:834:CLA:H161	1.92	0.42
3:B:335:LEU:HD13	12:B:823:CLA:HAA2	2.01	0.42
12:B:822:CLA:H42	12:B:834:CLA:HBA1	2.02	0.42
15:B:845:BCR:H15C	15:B:845:BCR:H351	1.65	0.42
3:H:452:GLN:NE2	12:H:834:CLA:OBD	2.52	0.42
12:H:835:CLA:H152	15:P:204:BCR:H23C	2.01	0.42
8:Q:1:MET:HG2	8:Q:3:VAL:HG23	2.02	0.42
12:a:809:CLA:H3A	12:a:809:CLA:HBA2	1.80	0.42
12:a:854:CLA:HBC2	3:b:599:ASN:HB2	2.00	0.42
3:b:327:ALA:HB2	15:b:843:BCR:H372	2.00	0.42
12:A:832:CLA:H193	12:A:832:CLA:H162	1.90	0.42
3:B:3:THR:OG1	3:B:13:ALA:O	2.35	0.42
3:B:622:SER:O	3:B:626:ASN:ND2	2.53	0.42
1:G:121:VAL:N	1:G:125:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:824:CLA:HBB2	16:G:852:LHG:HC82	2.02	0.42
12:G:829:CLA:H41	12:G:829:CLA:H61	1.89	0.42
12:H:816:CLA:HBA2	12:H:816:CLA:H3A	1.81	0.42
1:a:152:TRP:HA	1:a:155:VAL:HG22	2.01	0.42
1:a:358:TRP:HB3	12:a:805:CLA:HAC1	2.02	0.42
12:a:828:CLA:H2	15:a:846:BCR:H24C	2.02	0.42
12:b:836:CLA:H41	8:i:20:LEU:HD11	2.00	0.42
1:A:43:PRO:HB2	1:A:748:ILE:HG12	2.01	0.42
1:A:624:ILE:HD12	11:A:801:CL0:H53	2.01	0.42
12:F:201:CLA:H41	12:F:201:CLA:H61	1.75	0.42
15:I:101:BCR:H351	15:I:101:BCR:H15C	1.64	0.42
12:G:826:CLA:HAB	15:G:849:BCR:C8	2.50	0.42
12:G:833:CLA:H152	15:S:201:BCR:H372	2.02	0.42
3:H:335:LEU:HD13	12:H:824:CLA:HAA2	2.01	0.42
3:H:381:PHE:HZ	3:H:396:LEU:HD21	1.84	0.42
3:H:633:TRP:CD2	12:H:802:CLA:H112	2.55	0.42
12:H:805:CLA:H111	15:Q:101:BCR:HC31	2.02	0.42
1:a:116:GLN:HG3	1:a:142:ILE:HB	2.01	0.42
15:a:849:BCR:H393	15:j:101:BCR:H403	2.01	0.42
3:b:447:PHE:HB3	12:b:832:CLA:H42	2.02	0.42
4:c:58:CYS:HA	4:c:59:PRO:HD3	1.90	0.42
12:B:805:CLA:H43	8:I:11:THR:HG21	2.01	0.42
12:B:807:CLA:H72	12:B:824:CLA:H193	2.02	0.42
7:F:129:TYR:OH	7:F:138:ASP:OD1	2.34	0.42
15:P:202:BCR:H341	15:R:102:BCR:H373	2.00	0.42
12:a:817:CLA:H62	12:a:817:CLA:H41	1.76	0.42
7:f:77:ARG:NH2	7:f:81:TYR:OH	2.52	0.42
8:i:14:VAL:HG21	12:L:206:CLA:H112	2.02	0.42
10:l:56:HIS:HA	10:l:59:TRP:CD1	2.55	0.42
1:A:198:VAL:HB	12:A:824:CLA:HMD3	2.01	0.42
1:A:246:GLU:O	1:A:250:SER:OG	2.35	0.42
12:A:829:CLA:H201	12:A:840:CLA:H2	2.00	0.42
7:F:160:PHE:O	7:F:164:GLN:NE2	2.53	0.42
12:L:202:CLA:H101	12:L:202:CLA:H61	1.76	0.42
3:H:365:TYR:CD2	12:H:825:CLA:HAB	2.55	0.41
12:H:812:CLA:H3A	15:H:843:BCR:H383	2.02	0.41
15:H:845:BCR:H351	15:H:845:BCR:H15C	1.73	0.41
12:a:832:CLA:H61	12:b:835:CLA:H52	2.02	0.41
3:b:157:LEU:HB3	3:b:162:ARG:HH21	1.84	0.41
3:b:185:VAL:HG13	15:b:840:BCR:HC31	2.02	0.41
12:b:806:CLA:H111	12:b:806:CLA:H2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:64:LEU:HB3	5:d:69:GLN:HE21	1.85	0.41
1:A:122:PHE:O	3:B:436:ARG:NH2	2.51	0.41
3:B:40:GLU:HG2	3:B:44:GLN:HE22	1.85	0.41
3:B:129:ILE:O	3:B:130:ARG:NH1	2.52	0.41
15:J:104:BCR:H24C	15:J:104:BCR:H371	1.84	0.41
1:G:634:GLN:NE2	1:G:781:ARG:HH21	2.19	0.41
3:H:366:ILE:HG21	12:H:826:CLA:HBB1	2.02	0.41
1:a:127:LEU:HD23	1:a:127:LEU:HA	1.90	0.41
1:a:489:GLN:NE2	1:a:494:GLN:HE22	2.17	0.41
15:a:849:BCR:H23C	12:b:801:CLA:H112	2.02	0.41
12:a:855:CLA:HAB	3:b:673:ALA:O	2.20	0.41
3:B:176:ASN:HD21	3:B:281:TYR:H	1.68	0.41
3:B:383:VAL:HG13	3:B:555:ALA:HB1	2.02	0.41
10:L:63:PRO:O	10:L:67:LEU:HB2	2.19	0.41
1:G:154:ALA:HA	1:G:229:ASN:HD21	1.84	0.41
12:G:825:CLA:H2	12:G:825:CLA:H62	1.73	0.41
15:G:850:BCR:H15C	15:G:850:BCR:H351	1.93	0.41
3:H:327:ALA:HB2	15:H:845:BCR:H372	2.03	0.41
12:H:850:CLA:CBB	12:a:822:CLA:HAB	2.50	0.41
15:P:202:BCR:H333	9:R:24:LEU:HD13	2.01	0.41
9:R:20:SER:HB3	15:R:102:BCR:H383	2.01	0.41
1:a:128:ASN:HB3	1:a:140:GLY:HA3	2.02	0.41
1:a:292:SER:OG	1:a:386:TYR:O	2.35	0.41
12:a:826:CLA:H91	12:a:826:CLA:H112	1.88	0.41
15:a:847:BCR:H371	15:a:847:BCR:H24C	1.83	0.41
3:b:357:ALA:HB1	3:b:740:VAL:HG22	2.02	0.41
3:b:622:SER:O	3:b:626:ASN:ND2	2.52	0.41
12:b:803:CLA:H71	12:b:810:CLA:H2	2.02	0.41
15:b:847:BCR:H351	15:b:847:BCR:H15C	1.77	0.41
1:A:84:VAL:HG11	12:A:805:CLA:H41	2.03	0.41
1:A:559:ALA:O	1:A:563:HIS:ND1	2.46	0.41
11:A:801:CL0:H57	11:A:801:CL0:H60	1.89	0.41
3:B:412:TRP:O	3:B:416:PHE:HB2	2.20	0.41
15:B:843:BCR:H371	15:B:844:BCR:H23C	2.02	0.41
1:G:372:LEU:HD21	12:G:819:CLA:H93	2.02	0.41
12:G:829:CLA:H122	15:G:847:BCR:H383	2.02	0.41
12:H:825:CLA:H143	12:H:825:CLA:H162	1.96	0.41
12:H:835:CLA:HBC2	15:H:849:BCR:HC7	2.02	0.41
15:P:202:BCR:H24C	15:P:202:BCR:H371	1.88	0.41
1:a:559:ALA:O	1:a:563:HIS:ND1	2.53	0.41
1:a:693:ILE:O	3:b:635:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:824:CLA:HBA2	12:b:824:CLA:H3A	1.84	0.41
1:A:458:GLY:HA2	1:A:560:LEU:HD22	2.02	0.41
1:A:724:GLY:HA3	3:B:582:CYS:HB2	2.02	0.41
12:A:840:CLA:HMC1	12:B:801:CLA:H102	2.02	0.41
15:A:849:BCR:H351	15:A:849:BCR:H15C	1.86	0.41
3:B:410:LEU:HB3	3:B:546:LEU:HB2	2.02	0.41
1:G:358:TRP:HB3	12:G:806:CLA:HAC1	2.01	0.41
1:G:494:GLN:NE2	1:G:547:LEU:O	2.46	0.41
12:G:821:CLA:H172	12:G:824:CLA:HAC2	2.01	0.41
12:H:802:CLA:H62	12:H:802:CLA:H41	1.81	0.41
12:a:828:CLA:HBC2	15:a:846:BCR:H381	2.03	0.41
12:b:802:CLA:H62	12:b:802:CLA:H41	1.80	0.41
1:A:73:ILE:O	1:A:77:HIS:ND1	2.53	0.41
11:A:801:CL0:H21	3:B:639:TRP:HD1	1.86	0.41
12:A:827:CLA:H2	12:A:827:CLA:H61	1.86	0.41
15:A:849:BCR:H282	15:J:102:BCR:H393	2.02	0.41
3:H:311:TYR:O	3:H:315:ASN:HB2	2.20	0.41
1:a:255:GLY:HA2	1:a:259:PRO:HA	2.01	0.41
3:b:94:PRO:HB2	12:l:202:CLA:H3A	2.01	0.41
3:b:182:LEU:HG	12:b:810:CLA:H52	2.03	0.41
15:G:847:BCR:H24C	15:G:847:BCR:H371	1.75	0.41
12:H:838:CLA:H41	8:Q:20:LEU:HD11	2.02	0.41
7:P:117:TRP:HA	7:P:157:TRP:HE1	1.86	0.41
7:P:122:LEU:HD22	15:R:102:BCR:H372	2.03	0.41
1:a:293:LEU:HD21	1:a:383:MET:HB3	2.02	0.41
1:a:391:ILE:HB	1:a:539:LYS:HE2	2.03	0.41
12:a:807:CLA:H93	12:a:807:CLA:H61	1.89	0.41
3:b:336:VAL:HG21	12:b:825:CLA:HHD	2.01	0.41
12:b:816:CLA:H91	12:b:816:CLA:H111	1.85	0.41
4:C:61:ASP:HB2	6:E:53:ASN:HD22	1.85	0.41
12:H:831:CLA:H142	9:R:24:LEU:HB2	2.02	0.41
1:a:295:MET:HE3	1:a:295:MET:HB3	1.86	0.41
12:b:805:CLA:H111	15:i:101:BCR:HC31	2.03	0.41
1:A:306:ALA:O	1:A:310:ILE:HG13	2.20	0.41
12:B:802:CLA:H41	12:B:802:CLA:H62	1.84	0.41
12:B:806:CLA:H62	12:B:806:CLA:H102	1.80	0.41
1:G:404:MET:HB3	1:G:622:ILE:HG23	2.03	0.41
1:G:571:LYS:HE3	3:H:689:LEU:HB2	2.02	0.41
12:G:802:CLA:H143	12:G:804:CLA:H71	2.03	0.41
12:G:802:CLA:H112	15:G:850:BCR:H23C	2.03	0.41
3:H:94:PRO:HB2	12:H:808:CLA:H3A	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:825:CLA:HBC3	18:H:847:LMG:H432	2.03	0.41
7:P:98:VAL:HG12	7:P:108:PHE:HB2	2.02	0.41
15:b:842:BCR:H392	15:b:843:BCR:H272	2.03	0.41
1:A:455:LEU:HD23	12:A:855:CLA:HBA2	2.03	0.41
12:A:802:CLA:H42	3:B:666:LEU:HB2	2.03	0.41
12:A:840:CLA:H3A	12:A:840:CLA:HBA2	1.85	0.41
12:B:803:CLA:H142	12:B:803:CLA:H112	1.93	0.41
12:G:808:CLA:H93	12:G:808:CLA:H61	1.90	0.41
15:G:848:BCR:H15C	15:G:848:BCR:H351	1.79	0.41
12:H:811:CLA:H143	12:H:811:CLA:H112	1.97	0.41
1:a:380:MET:HE2	1:a:380:MET:HB3	1.81	0.41
1:a:466:VAL:HG12	12:a:833:CLA:HBC2	2.03	0.41
12:a:802:CLA:H91	12:a:855:CLA:H112	2.03	0.41
3:b:540:GLY:HA2	3:b:596:TRP:CZ3	2.55	0.41
15:j:103:BCR:H371	15:j:103:BCR:H24C	1.88	0.41
1:A:372:LEU:HD11	12:A:818:CLA:H51	2.02	0.41
3:B:159:PRO:HA	3:B:162:ARG:HG3	2.03	0.41
12:B:830:CLA:H142	9:J:24:LEU:HB2	2.03	0.41
12:G:818:CLA:HAC1	12:G:834:CLA:H42	2.04	0.40
1:a:46:THR:O	1:a:49:ILE:HB	2.21	0.40
12:a:805:CLA:H91	12:a:805:CLA:H111	1.87	0.40
3:b:423:GLY:HA3	12:j:102:CLA:HAB	2.03	0.40
4:c:61:ASP:HB2	6:e:53:ASN:ND2	2.36	0.40
8:i:13:LEU:HB2	12:l:202:CLA:HAB	2.02	0.40
15:l:201:BCR:H24C	15:l:201:BCR:H371	1.79	0.40
12:l:202:CLA:H143	12:l:202:CLA:H112	1.93	0.40
3:H:3:THR:OG1	3:H:13:ALA:O	2.32	0.40
3:H:588:ASP:HA	3:H:591:TYR:HB3	2.04	0.40
12:H:807:CLA:H72	12:H:825:CLA:H193	2.01	0.40
12:H:822:CLA:H122	12:H:822:CLA:H162	1.83	0.40
15:H:849:BCR:H15C	15:H:849:BCR:H351	1.76	0.40
12:S:203:CLA:H51	12:S:203:CLA:H12	1.84	0.40
1:a:99:SER:HB2	1:a:149:PHE:HZ	1.84	0.40
1:a:116:GLN:HE22	12:a:807:CLA:C4D	2.35	0.40
12:a:828:CLA:H62	12:a:828:CLA:H102	1.75	0.40
3:b:86:PRO:HB2	3:b:116:MET:HB3	2.02	0.40
12:b:836:CLA:H93	12:b:836:CLA:H61	1.90	0.40
15:b:847:BCR:H363	15:f:202:BCR:HC31	2.04	0.40
12:A:825:CLA:H92	12:A:825:CLA:H61	1.92	0.40
15:J:102:BCR:H24C	15:J:102:BCR:H371	1.75	0.40
1:G:609:ASP:HA	1:G:612:PHE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:693:ILE:O	3:H:635:ARG:NH1	2.53	0.40
12:H:816:CLA:H72	12:H:816:CLA:H111	1.82	0.40
4:K:61:ASP:HB2	6:O:53:ASN:ND2	2.36	0.40
5:N:32:LYS:HG3	5:N:91:VAL:HB	2.04	0.40
3:b:291:LEU:HD13	12:b:821:CLA:HAC2	2.04	0.40
12:b:836:CLA:HHD	12:b:836:CLA:HAC1	1.94	0.40
15:b:840:BCR:H15C	15:b:840:BCR:H351	1.70	0.40
4:c:60:THR:OG1	4:c:62:PHE:O	2.37	0.40
7:f:62:GLN:H	7:f:65:LYS:HZ1	1.69	0.40
1:A:450:LEU:HA	1:A:453:VAL:HG12	2.03	0.40
12:A:837:CLA:H92	12:A:837:CLA:H61	1.87	0.40
3:B:185:VAL:HG13	15:B:841:BCR:HC31	2.03	0.40
12:B:810:CLA:H193	12:B:810:CLA:H161	1.93	0.40
3:H:40:GLU:HG3	3:H:44:GLN:HE22	1.87	0.40
3:H:252:ASN:N	3:H:257:SER:O	2.46	0.40
3:H:449:GLN:HA	3:H:452:GLN:HB2	2.03	0.40
12:H:808:CLA:H193	12:H:808:CLA:H161	1.92	0.40
12:H:817:CLA:H41	12:H:817:CLA:H61	1.88	0.40
12:H:825:CLA:H141	12:H:827:CLA:H151	2.04	0.40
12:b:821:CLA:H162	12:b:821:CLA:H122	1.85	0.40
12:b:822:CLA:H202	12:b:822:CLA:H161	1.95	0.40
6:e:9:VAL:O	6:e:22:VAL:HA	2.22	0.40
7:f:84:ASN:HD22	9:j:38:PRO:HB3	1.86	0.40
12:l:204:CLA:CAB	12:l:205:CLA:HAA2	2.51	0.40
12:l:205:CLA:HMA1	12:l:206:CLA:HBC1	2.03	0.40
3:B:537:ILE:HD13	3:B:604:ILE:HG12	2.04	0.40
3:B:559:LYS:NZ	6:E:17:TYR:O	2.46	0.40
12:B:805:CLA:H111	15:I:101:BCR:HC31	2.03	0.40
12:B:830:CLA:H143	12:B:830:CLA:H112	1.92	0.40
15:F:202:BCR:H15C	15:F:202:BCR:H351	1.83	0.40
15:F:204:BCR:H24C	15:F:204:BCR:H371	1.82	0.40
1:G:45:THR:HA	1:G:749:GLN:H	1.85	0.40
1:G:206:LEU:HD23	1:G:206:LEU:HA	1.92	0.40
1:G:306:ALA:O	1:G:310:ILE:HG13	2.21	0.40
1:G:394:PRO:HA	1:G:397:ILE:HG22	2.03	0.40
12:G:827:CLA:H171	12:G:834:CLA:H61	2.02	0.40
3:H:699:ARG:HD3	3:H:699:ARG:HA	1.76	0.40
7:P:122:LEU:HD12	7:P:122:LEU:HA	1.86	0.40
7:P:142:ILE:N	9:R:7:SER:O	2.44	0.40
7:P:160:PHE:O	7:P:164:GLN:NE2	2.54	0.40
3:b:457:VAL:HA	3:b:494:ASN:HD21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PRO:HD2	4:C:52:LYS:HG3	2.03	0.40
12:A:833:CLA:HHD	12:B:807:CLA:HBB2	2.03	0.40
3:B:338:GLN:NE2	12:B:833:CLA:HBB1	2.37	0.40
3:B:441:ILE:HG23	7:F:96:LEU:HD12	2.04	0.40
10:L:76:ARG:HD2	10:L:77:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	771/785 (98%)	720 (93%)	46 (6%)	5 (1%)	21	32
1	G	771/785 (98%)	725 (94%)	40 (5%)	6 (1%)	16	25
1	a	771/785 (98%)	722 (94%)	45 (6%)	4 (0%)	24	37
2	M	29/32 (91%)	29 (100%)	0	0	100	100
2	T	29/32 (91%)	29 (100%)	0	0	100	100
2	m	29/32 (91%)	29 (100%)	0	0	100	100
3	B	744/749 (99%)	707 (95%)	36 (5%)	1 (0%)	48	64
3	H	744/749 (99%)	702 (94%)	41 (6%)	1 (0%)	48	64
3	b	744/749 (99%)	700 (94%)	43 (6%)	1 (0%)	48	64
4	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	K	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
5	D	101/143 (71%)	98 (97%)	3 (3%)	0	100	100
5	N	101/143 (71%)	97 (96%)	4 (4%)	0	100	100
5	d	101/143 (71%)	95 (94%)	6 (6%)	0	100	100
6	E	59/64 (92%)	57 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	O	59/64 (92%)	56 (95%)	3 (5%)	0	100	100
6	e	59/64 (92%)	56 (95%)	3 (5%)	0	100	100
7	F	146/177 (82%)	132 (90%)	13 (9%)	1 (1%)	18	28
7	P	146/177 (82%)	134 (92%)	11 (8%)	1 (1%)	18	28
7	f	146/177 (82%)	135 (92%)	10 (7%)	1 (1%)	18	28
8	I	29/32 (91%)	27 (93%)	2 (7%)	0	100	100
8	Q	29/32 (91%)	29 (100%)	0	0	100	100
8	i	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
9	R	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
9	j	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
10	L	152/160 (95%)	143 (94%)	7 (5%)	2 (1%)	9	14
10	S	152/160 (95%)	145 (95%)	5 (3%)	2 (1%)	9	14
10	l	152/160 (95%)	143 (94%)	7 (5%)	2 (1%)	9	14
All	All	6438/6792 (95%)	6065 (94%)	346 (5%)	27 (0%)	31	43

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	259	PRO
7	P	89	LYS
10	S	12	ASP
10	S	77	PRO
7	f	89	LYS
10	l	77	PRO
1	A	259	PRO
1	A	538	GLN
7	F	89	LYS
10	L	12	ASP
10	L	77	PRO
1	G	538	GLN
1	a	533	ALA
1	a	538	GLN
1	A	532	VAL
1	G	532	VAL
1	G	533	ALA
1	A	533	ALA

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Mol	Chain	Res	Type
1	G	242	PRO
1	G	524	ASN
1	a	524	ASN
3	H	520	THR
1	a	532	VAL
3	b	520	THR
10	l	12	ASP
1	A	524	ASN
3	B	520	THR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/628 (96%)	603 (100%)	0	100 100
1	G	603/628 (96%)	602 (100%)	1 (0%)	87 94
1	a	603/628 (96%)	601 (100%)	2 (0%)	86 93
2	M	22/23 (96%)	22 (100%)	0	100 100
2	T	22/23 (96%)	22 (100%)	0	100 100
2	m	22/23 (96%)	22 (100%)	0	100 100
3	B	591/593 (100%)	591 (100%)	0	100 100
3	H	591/593 (100%)	591 (100%)	0	100 100
3	b	591/593 (100%)	591 (100%)	0	100 100
4	C	67/68 (98%)	67 (100%)	0	100 100
4	K	67/68 (98%)	67 (100%)	0	100 100
4	c	67/68 (98%)	67 (100%)	0	100 100
5	D	81/116 (70%)	81 (100%)	0	100 100
5	N	81/116 (70%)	80 (99%)	1 (1%)	63 81
5	d	81/116 (70%)	81 (100%)	0	100 100
6	E	55/58 (95%)	55 (100%)	0	100 100
6	O	55/58 (95%)	55 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	e	55/58 (95%)	55 (100%)	0	100	100
7	F	120/146 (82%)	120 (100%)	0	100	100
7	P	120/146 (82%)	120 (100%)	0	100	100
7	f	120/146 (82%)	120 (100%)	0	100	100
8	I	29/30 (97%)	29 (100%)	0	100	100
8	Q	29/30 (97%)	29 (100%)	0	100	100
8	i	29/30 (97%)	29 (100%)	0	100	100
9	J	32/34 (94%)	32 (100%)	0	100	100
9	R	32/34 (94%)	32 (100%)	0	100	100
9	j	32/34 (94%)	32 (100%)	0	100	100
10	L	119/125 (95%)	119 (100%)	0	100	100
10	S	119/125 (95%)	119 (100%)	0	100	100
10	l	119/125 (95%)	119 (100%)	0	100	100
All	All	5157/5463 (94%)	5153 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	691	PRO
5	N	93	PRO
1	a	385	PRO
1	a	387	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	116	GLN
1	G	128	ASN
1	G	203	ASN
1	G	272	ASN
1	G	319	ASN
1	G	417	HIS
1	G	451	ASN
1	G	460	HIS
1	G	468	ASN
1	G	487	GLN

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Mol	Chain	Res	Type
1	G	497	GLN
1	G	500	ASN
1	G	524	ASN
1	G	558	HIS
1	G	604	GLN
1	G	749	GLN
3	H	10	GLN
3	H	65	ASN
3	H	131	HIS
3	H	214	GLN
3	H	298	GLN
3	H	316	ASN
3	H	339	GLN
3	H	409	HIS
3	H	427	HIS
3	H	432	GLN
3	H	612	HIS
5	N	71	HIS
5	N	76	GLN
6	O	53	ASN
7	P	84	ASN
7	P	93	GLN
7	P	164	GLN
1	a	20	ASN
1	a	62	GLN
1	a	80	HIS
1	a	128	ASN
1	a	162	GLN
1	a	203	ASN
1	a	204	HIS
1	a	220	HIS
1	a	230	GLN
1	a	302	HIS
1	a	319	ASN
1	a	365	ASN
1	a	431	ASN
1	a	432	GLN
1	a	451	ASN
1	a	489	GLN
1	a	497	GLN
1	a	500	ASN
1	a	524	ASN

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Mol	Chain	Res	Type
1	a	558	HIS
1	a	604	GLN
1	a	634	GLN
1	a	749	GLN
2	m	4	ASN
2	m	5	ASN
3	b	10	GLN
3	b	29	HIS
3	b	50	HIS
3	b	131	HIS
3	b	214	GLN
3	b	218	HIS
3	b	239	ASN
3	b	252	ASN
3	b	298	GLN
3	b	316	ASN
3	b	319	HIS
3	b	339	GLN
3	b	440	GLN
3	b	449	GLN
3	b	494	ASN
3	b	599	ASN
3	b	687	GLN
4	c	3	HIS
5	d	5	ASN
5	d	60	ASN
5	d	69	GLN
5	d	76	GLN
6	e	54	ASN
7	f	62	GLN
7	f	134	GLN
7	f	164	GLN
9	j	28	ASN
10	l	24	ASN
10	l	34	ASN
1	A	128	ASN
1	A	160	GLN
1	A	162	GLN
1	A	186	HIS
1	A	203	ASN
1	A	204	HIS
1	A	272	ASN

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Mol	Chain	Res	Type
1	A	347	HIS
1	A	378	HIS
1	A	396	GLN
1	A	432	GLN
1	A	451	ASN
1	A	468	ASN
1	A	524	ASN
1	A	604	GLN
1	A	665	GLN
1	A	688	GLN
1	A	694	ASN
1	A	729	GLN
1	A	739	HIS
1	A	740	ASN
1	A	749	GLN
2	M	5	ASN
3	B	29	HIS
3	B	44	GLN
3	B	73	ASN
3	B	114	ASN
3	B	132	ASN
3	B	158	GLN
3	B	176	ASN
3	B	214	GLN
3	B	267	HIS
3	B	298	GLN
3	B	316	ASN
3	B	321	GLN
3	B	339	GLN
3	B	363	HIS
3	B	427	HIS
3	B	440	GLN
3	B	494	ASN
3	B	612	HIS
3	B	626	ASN
3	B	719	GLN
5	D	5	ASN
5	D	60	ASN
5	D	69	GLN
5	D	71	HIS
6	E	20	ASN
6	E	54	ASN

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Mol	Chain	Res	Type
7	F	29	ASN
7	F	37	GLN
7	F	93	GLN
7	F	134	GLN
7	F	164	GLN
10	L	15	GLN
10	L	24	ASN
10	L	34	ASN
10	L	82	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

366 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	A	803	1	69,73,73	2.26	23 (33%)	82,113,113	2.53	30 (36%)
12	CLA	G	802	-	64,68,73	2.33	22 (34%)	76,107,113	2.64	30 (39%)
12	CLA	B	810	3	69,73,73	2.21	22 (31%)	82,113,113	2.71	29 (35%)
15	BCR	b	847	-	41,41,41	2.63	6 (14%)	56,56,56	6.61	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	G	842	16	64,68,73	2.29	22 (34%)	76,107,113	2.55	26 (34%)
12	CLA	A	841	20	69,73,73	2.21	21 (30%)	82,113,113	2.41	27 (32%)
12	CLA	B	814	-	59,63,73	2.36	22 (37%)	70,101,113	2.64	25 (35%)
12	CLA	a	804	12	59,63,73	2.41	23 (38%)	70,101,113	2.80	30 (42%)
12	CLA	A	810	12,1	54,58,73	2.48	23 (42%)	64,95,113	2.93	27 (42%)
12	CLA	A	812	-	54,58,73	2.53	24 (44%)	64,95,113	2.90	28 (43%)
12	CLA	A	826	1	69,73,73	2.23	21 (30%)	82,113,113	2.57	29 (35%)
12	CLA	b	802	-	69,73,73	2.15	21 (30%)	82,113,113	2.85	33 (40%)
12	CLA	a	810	12,1	54,58,73	2.49	23 (42%)	64,95,113	2.88	28 (43%)
12	CLA	B	819	-	49,53,73	2.54	22 (44%)	58,89,113	2.84	26 (44%)
12	CLA	H	816	-	64,68,73	2.36	22 (34%)	76,107,113	2.90	28 (36%)
12	CLA	S	204	20	69,73,73	2.23	21 (30%)	82,113,113	2.46	25 (30%)
12	CLA	G	827	-	69,73,73	2.23	23 (33%)	82,113,113	2.54	31 (37%)
12	CLA	A	825	20	59,63,73	2.40	23 (38%)	70,101,113	2.68	28 (40%)
12	CLA	B	835	3	49,53,73	2.49	21 (42%)	58,89,113	2.93	25 (43%)
12	CLA	b	824	3	69,73,73	2.18	23 (33%)	82,113,113	2.53	32 (39%)
12	CLA	a	855	-	69,73,73	2.15	22 (31%)	82,113,113	2.72	29 (35%)
12	CLA	a	811	-	49,53,73	2.56	22 (44%)	58,89,113	2.74	23 (39%)
12	CLA	B	825	-	69,73,73	2.27	22 (31%)	82,113,113	2.12	26 (31%)
15	BCR	b	840	-	41,41,41	2.62	6 (14%)	56,56,56	6.59	25 (44%)
13	1L3	B	839	-	34,34,34	2.67	12 (35%)	43,45,45	1.54	9 (20%)
12	CLA	L	206	20	69,73,73	2.23	21 (30%)	82,113,113	2.44	24 (29%)
12	CLA	B	809	3	49,53,73	2.57	22 (44%)	58,89,113	2.81	25 (43%)
16	LHG	a	850	-	48,48,48	0.92	2 (4%)	51,54,54	0.93	2 (3%)
12	CLA	H	806	-	69,73,73	2.20	21 (30%)	82,113,113	2.72	28 (34%)
12	CLA	A	819	1	49,53,73	2.55	23 (46%)	58,89,113	2.84	25 (43%)
12	CLA	B	833	3	64,68,73	2.28	22 (34%)	76,107,113	2.68	26 (34%)
12	CLA	A	836	1	54,58,73	2.63	23 (42%)	64,95,113	3.26	32 (50%)
12	CLA	B	828	3	49,53,73	2.55	23 (46%)	58,89,113	2.81	26 (44%)
12	CLA	H	829	3	49,53,73	2.55	23 (46%)	58,89,113	2.79	26 (44%)
12	CLA	b	811	-	64,68,73	2.33	23 (35%)	76,107,113	2.59	27 (35%)
12	CLA	J	103	-	49,53,73	2.58	24 (48%)	58,89,113	2.78	23 (39%)
15	BCR	H	849	-	41,41,41	2.57	6 (14%)	56,56,56	6.50	20 (35%)
12	CLA	B	805	3	69,73,73	2.22	23 (33%)	82,113,113	2.56	28 (34%)
12	CLA	B	836	20	69,73,73	2.28	23 (33%)	82,113,113	2.52	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	L	207	-	41,41,41	2.71	6 (14%)	56,56,56	6.75	18 (32%)
12	CLA	b	806	-	69,73,73	2.19	21 (30%)	82,113,113	2.75	29 (35%)
12	CLA	b	813	3	59,63,73	2.42	25 (42%)	70,101,113	2.70	26 (37%)
12	CLA	A	832	1	69,73,73	2.25	22 (31%)	82,113,113	2.35	25 (30%)
15	BCR	G	849	-	41,41,41	2.75	6 (14%)	56,56,56	6.76	21 (37%)
12	CLA	A	818	-	69,73,73	2.19	23 (33%)	82,113,113	2.60	27 (32%)
12	CLA	b	831	3	49,53,73	2.57	22 (44%)	58,89,113	2.85	25 (43%)
12	CLA	a	803	1	69,73,73	2.25	23 (33%)	82,113,113	2.53	32 (39%)
16	LHG	A	851	12	26,26,48	1.25	2 (7%)	29,32,54	1.24	3 (10%)
12	CLA	B	832	3	49,53,73	2.56	22 (44%)	58,89,113	2.82	25 (43%)
12	CLA	B	818	-	49,53,73	2.57	23 (46%)	58,89,113	2.87	23 (39%)
12	CLA	H	831	-	69,73,73	2.22	20 (28%)	82,113,113	2.48	28 (34%)
15	BCR	L	203	-	41,41,41	2.78	6 (14%)	56,56,56	6.44	21 (37%)
18	LMG	H	847	-	55,55,55	1.49	8 (14%)	63,63,63	1.10	4 (6%)
12	CLA	G	812	-	49,53,73	2.54	22 (44%)	58,89,113	2.75	22 (37%)
12	CLA	G	839	1	69,73,73	2.27	24 (34%)	82,113,113	2.47	26 (31%)
12	CLA	A	831	1	59,63,73	2.42	23 (38%)	70,101,113	2.62	29 (41%)
12	CLA	A	809	1	49,53,73	2.57	22 (44%)	58,89,113	2.88	25 (43%)
19	LMT	b	846	-	36,36,36	1.17	4 (11%)	47,47,47	1.01	2 (4%)
12	CLA	B	813	3	59,63,73	2.43	24 (40%)	70,101,113	2.67	25 (35%)
12	CLA	H	809	3	49,53,73	2.55	22 (44%)	58,89,113	2.83	27 (46%)
12	CLA	A	823	-	59,63,73	2.38	22 (37%)	70,101,113	2.68	25 (35%)
12	CLA	b	809	3	49,53,73	2.57	22 (44%)	58,89,113	2.82	25 (43%)
12	CLA	G	820	1	49,53,73	2.51	22 (44%)	58,89,113	2.83	26 (44%)
12	CLA	a	823	-	59,63,73	2.38	22 (37%)	70,101,113	2.70	26 (37%)
12	CLA	G	819	-	69,73,73	2.20	24 (34%)	82,113,113	2.56	30 (36%)
15	BCR	G	848	-	41,41,41	2.65	6 (14%)	56,56,56	6.74	25 (44%)
12	CLA	H	814	3	59,63,73	2.42	24 (40%)	70,101,113	2.64	24 (34%)
12	CLA	a	807	-	69,73,73	2.22	22 (31%)	82,113,113	2.61	29 (35%)
12	CLA	A	835	-	49,53,73	2.53	21 (42%)	58,89,113	2.85	25 (43%)
12	CLA	H	817	-	69,73,73	2.26	24 (34%)	82,113,113	2.33	27 (32%)
12	CLA	G	809	1	54,58,73	2.56	23 (42%)	64,95,113	2.87	27 (42%)
12	CLA	F	201	20	69,73,73	2.27	23 (33%)	82,113,113	2.30	27 (32%)
15	BCR	B	842	-	41,41,41	2.58	6 (14%)	56,56,56	6.62	21 (37%)
12	CLA	a	822	-	54,58,73	2.56	23 (42%)	64,95,113	2.77	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	b	821	20	69,73,73	2.18	22 (31%)	82,113,113	2.53	33 (40%)
12	CLA	H	838	-	69,73,73	2.23	22 (31%)	82,113,113	2.65	32 (39%)
15	BCR	H	845	-	41,41,41	2.64	6 (14%)	56,56,56	6.83	25 (44%)
12	CLA	G	814	1	49,53,73	2.52	22 (44%)	58,89,113	3.00	24 (41%)
19	LMT	B	847	-	36,36,36	1.26	5 (13%)	47,47,47	1.11	3 (6%)
12	CLA	A	816	1	54,58,73	2.51	22 (40%)	64,95,113	2.78	30 (46%)
12	CLA	b	814	3	59,63,73	2.39	21 (35%)	70,101,113	2.61	26 (37%)
12	CLA	B	817	3	49,53,73	2.53	21 (42%)	58,89,113	2.95	23 (39%)
12	CLA	a	838	1	49,53,73	2.55	22 (44%)	58,89,113	2.89	27 (46%)
12	CLA	b	817	3	49,53,73	2.53	21 (42%)	58,89,113	2.85	24 (41%)
17	45D	M	101	-	43,43,43	3.99	19 (44%)	54,60,60	7.88	31 (57%)
17	45D	m	101	-	43,43,43	4.00	19 (44%)	54,60,60	7.90	31 (57%)
12	CLA	B	812	-	49,53,73	2.55	24 (48%)	58,89,113	2.84	24 (41%)
12	CLA	a	831	1	59,63,73	2.44	23 (38%)	70,101,113	2.59	27 (38%)
15	BCR	j	101	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	21 (37%)
12	CLA	B	816	-	69,73,73	2.25	24 (34%)	82,113,113	2.35	29 (35%)
15	BCR	B	843	-	25,25,41	2.18	2 (8%)	33,33,56	7.57	17 (51%)
12	CLA	H	830	3	69,73,73	2.22	23 (33%)	82,113,113	2.59	25 (30%)
13	1L3	a	842	-	34,34,34	2.65	14 (41%)	43,45,45	1.51	11 (25%)
15	BCR	G	847	-	41,41,41	2.70	6 (14%)	56,56,56	6.50	21 (37%)
15	BCR	a	848	-	41,41,41	2.72	6 (14%)	56,56,56	6.78	21 (37%)
15	BCR	b	844	-	41,41,41	2.57	6 (14%)	56,56,56	6.69	22 (39%)
13	1L3	b	838	-	34,34,34	2.67	12 (35%)	43,45,45	1.51	8 (18%)
12	CLA	G	841	20	69,73,73	2.20	21 (30%)	82,113,113	2.39	26 (31%)
15	BCR	G	850	-	41,41,41	2.65	6 (14%)	56,56,56	6.77	25 (44%)
15	BCR	L	201	-	41,41,41	2.67	6 (14%)	56,56,56	6.55	26 (46%)
12	CLA	H	801	1	59,63,73	2.43	24 (40%)	70,101,113	2.61	28 (40%)
12	CLA	A	824	20	69,73,73	2.26	23 (33%)	82,113,113	2.39	26 (31%)
14	SF4	K	102	4	0,12,12	-	-	-		
12	CLA	b	804	-	69,73,73	2.18	21 (30%)	82,113,113	2.63	26 (31%)
12	CLA	H	802	-	69,73,73	2.19	22 (31%)	82,113,113	2.80	34 (41%)
12	CLA	a	808	1	54,58,73	2.56	22 (40%)	64,95,113	2.82	27 (42%)
15	BCR	a	844	-	41,41,41	2.61	6 (14%)	56,56,56	6.65	21 (37%)
12	CLA	P	203	-	49,53,73	2.55	22 (44%)	58,89,113	4.47	25 (43%)
12	CLA	b	830	-	49,53,73	2.54	21 (42%)	58,89,113	2.71	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	LHG	G	852	12	26,26,48	1.24	2 (7%)	29,32,54	1.25	4 (13%)
12	CLA	H	822	20	69,73,73	2.22	21 (30%)	82,113,113	2.41	30 (36%)
12	CLA	A	839	1	69,73,73	2.27	24 (34%)	82,113,113	2.46	29 (35%)
12	CLA	A	829	1	69,73,73	2.19	22 (31%)	82,113,113	2.37	28 (34%)
12	CLA	G	803	20	69,73,73	2.24	20 (28%)	82,113,113	2.23	26 (31%)
12	CLA	S	202	10	59,63,73	2.41	21 (35%)	70,101,113	2.63	27 (38%)
12	CLA	f	203	-	49,53,73	2.57	22 (44%)	58,89,113	4.46	25 (43%)
12	CLA	a	839	1	69,73,73	2.27	24 (34%)	82,113,113	2.49	24 (29%)
15	BCR	B	840	-	41,41,41	2.62	6 (14%)	56,56,56	6.68	20 (35%)
12	CLA	a	827	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	28 (36%)
12	CLA	H	807	3	69,73,73	2.23	22 (31%)	82,113,113	2.45	30 (36%)
12	CLA	a	830	1	54,58,73	2.54	22 (40%)	64,95,113	2.77	29 (45%)
12	CLA	a	834	-	69,73,73	2.23	22 (31%)	82,113,113	2.39	29 (35%)
12	CLA	b	810	3	69,73,73	2.20	21 (30%)	82,113,113	2.71	32 (39%)
12	CLA	A	811	-	49,53,73	2.56	22 (44%)	58,89,113	2.71	22 (37%)
12	CLA	A	822	-	54,58,73	2.57	23 (42%)	64,95,113	2.72	27 (42%)
13	1L3	G	843	-	34,34,34	2.68	15 (44%)	43,45,45	1.48	10 (23%)
15	BCR	S	205	-	41,41,41	2.67	6 (14%)	56,56,56	6.46	25 (44%)
12	CLA	G	828	-	64,68,73	2.30	21 (32%)	76,107,113	2.59	28 (36%)
12	CLA	G	856	-	69,73,73	2.18	23 (33%)	82,113,113	2.55	28 (34%)
12	CLA	G	818	-	59,63,73	2.50	23 (38%)	70,101,113	2.72	33 (47%)
12	CLA	b	808	3	49,53,73	2.53	22 (44%)	58,89,113	2.87	28 (48%)
12	CLA	b	822	20	69,73,73	2.24	24 (34%)	82,113,113	2.61	28 (34%)
12	CLA	B	811	-	64,68,73	2.32	23 (35%)	76,107,113	2.55	26 (34%)
16	LHG	A	850	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
12	CLA	B	802	-	69,73,73	2.18	22 (31%)	82,113,113	2.71	31 (37%)
12	CLA	b	803	-	69,73,73	2.27	22 (31%)	82,113,113	2.56	27 (32%)
12	CLA	a	841	20	69,73,73	2.18	21 (30%)	82,113,113	2.42	28 (34%)
15	BCR	P	204	-	41,41,41	2.61	6 (14%)	56,56,56	6.51	23 (41%)
12	CLA	G	816	-	49,53,73	2.55	23 (46%)	58,89,113	2.85	25 (43%)
12	CLA	S	203	10	69,73,73	2.20	21 (30%)	82,113,113	2.60	27 (32%)
12	CLA	H	837	20	69,73,73	2.29	23 (33%)	82,113,113	2.54	26 (31%)
12	CLA	G	815	-	49,53,73	2.53	22 (44%)	58,89,113	2.85	25 (43%)
15	BCR	J	101	-	41,41,41	2.71	6 (14%)	56,56,56	6.56	22 (39%)
12	CLA	a	840	1	54,58,73	2.54	22 (40%)	64,95,113	2.72	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	a	819	1	49,53,73	2.49	22 (44%)	58,89,113	2.86	26 (44%)
15	BCR	f	204	-	41,41,41	2.61	6 (14%)	56,56,56	6.44	22 (39%)
12	CLA	G	838	1	49,53,73	2.55	22 (44%)	58,89,113	2.90	26 (44%)
12	CLA	b	805	3	69,73,73	2.21	22 (31%)	82,113,113	2.57	29 (35%)
12	CLA	A	820	-	69,73,73	2.23	21 (30%)	82,113,113	2.66	30 (36%)
12	CLA	b	815	-	64,68,73	2.25	22 (34%)	76,107,113	2.73	27 (35%)
15	BCR	J	104	-	41,41,41	2.54	6 (14%)	56,56,56	6.56	23 (41%)
15	BCR	H	841	-	41,41,41	2.62	6 (14%)	56,56,56	6.61	20 (35%)
12	CLA	B	831	-	49,53,73	2.59	22 (44%)	58,89,113	2.71	24 (41%)
12	CLA	G	806	-	69,73,73	2.17	21 (30%)	82,113,113	2.61	26 (31%)
12	CLA	a	820	-	69,73,73	2.27	23 (33%)	82,113,113	2.37	26 (31%)
15	BCR	B	841	-	41,41,41	2.61	6 (14%)	56,56,56	6.61	25 (44%)
17	45D	T	101	-	43,43,43	4.00	19 (44%)	54,60,60	7.84	31 (57%)
12	CLA	H	810	3	49,53,73	2.57	22 (44%)	58,89,113	2.82	24 (41%)
15	BCR	H	844	-	25,25,41	2.21	2 (8%)	33,33,56	7.59	18 (54%)
12	CLA	G	813	1	54,58,73	2.51	23 (42%)	64,95,113	2.91	28 (43%)
12	CLA	b	819	-	49,53,73	2.55	22 (44%)	58,89,113	2.81	23 (39%)
15	BCR	A	849	-	41,41,41	2.63	6 (14%)	56,56,56	6.81	25 (44%)
16	LHG	G	854	-	48,48,48	0.94	2 (4%)	51,54,54	3.78	6 (11%)
12	CLA	A	830	1	54,58,73	2.52	22 (40%)	64,95,113	2.83	30 (46%)
12	CLA	H	825	-	69,73,73	2.18	21 (30%)	82,113,113	2.44	28 (34%)
12	CLA	H	808	3	69,73,73	2.26	21 (30%)	82,113,113	2.41	27 (32%)
12	CLA	B	804	-	69,73,73	2.17	21 (30%)	82,113,113	2.60	26 (31%)
14	SF4	K	101	4	0,12,12	-	-	-		
12	CLA	G	804	1	69,73,73	2.25	23 (33%)	82,113,113	2.50	29 (35%)
15	BCR	J	102	-	41,41,41	2.65	6 (14%)	56,56,56	6.86	19 (33%)
12	CLA	l	204	10	59,63,73	2.41	21 (35%)	70,101,113	2.65	25 (35%)
12	CLA	H	813	-	49,53,73	2.48	22 (44%)	58,89,113	3.02	26 (44%)
12	CLA	B	803	-	69,73,73	2.23	24 (34%)	82,113,113	2.68	28 (34%)
12	CLA	A	837	1	69,73,73	2.21	23 (33%)	82,113,113	2.58	30 (36%)
15	BCR	a	845	-	41,41,41	2.65	6 (14%)	56,56,56	6.65	23 (41%)
12	CLA	G	826	20	59,63,73	2.41	21 (35%)	70,101,113	2.68	32 (45%)
12	CLA	b	832	3	64,68,73	2.31	22 (34%)	76,107,113	2.58	28 (36%)
15	BCR	b	841	-	41,41,41	2.55	6 (14%)	56,56,56	6.66	26 (46%)
12	CLA	G	810	1	49,53,73	2.54	22 (44%)	58,89,113	2.86	25 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	A	847	-	41,41,41	2.71	6 (14%)	56,56,56	6.75	27 (48%)
12	CLA	G	833	1	69,73,73	2.22	21 (30%)	82,113,113	2.42	27 (32%)
12	CLA	a	837	1	69,73,73	2.21	23 (33%)	82,113,113	2.61	30 (36%)
15	BCR	I	101	-	41,41,41	2.61	6 (14%)	56,56,56	6.86	21 (37%)
12	CLA	G	831	1	54,58,73	2.54	22 (40%)	64,95,113	2.70	30 (46%)
12	CLA	b	826	3	69,73,73	2.36	21 (30%)	82,113,113	2.55	30 (36%)
12	CLA	A	828	-	69,73,73	2.28	22 (31%)	82,113,113	2.28	27 (32%)
12	CLA	G	855	20	69,73,73	2.27	23 (33%)	82,113,113	2.57	28 (34%)
12	CLA	H	819	-	49,53,73	2.59	23 (46%)	58,89,113	2.83	24 (41%)
12	CLA	H	805	3	69,73,73	2.24	24 (34%)	82,113,113	2.59	29 (35%)
12	CLA	A	802	20	69,73,73	2.23	21 (30%)	82,113,113	2.26	26 (31%)
12	CLA	A	827	1	64,68,73	2.28	21 (32%)	76,107,113	2.59	29 (38%)
15	BCR	G	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.69	22 (39%)
13	1L3	H	840	-	34,34,34	2.70	13 (38%)	43,45,45	1.46	8 (18%)
12	CLA	A	833	-	69,73,73	2.20	22 (31%)	82,113,113	2.49	28 (34%)
12	CLA	b	834	3	49,53,73	2.50	22 (44%)	58,89,113	2.95	23 (39%)
12	CLA	H	821	-	49,53,73	2.50	21 (42%)	58,89,113	2.83	26 (44%)
12	CLA	A	855	-	69,73,73	2.15	23 (33%)	82,113,113	2.70	30 (36%)
12	CLA	b	825	-	69,73,73	2.29	22 (31%)	82,113,113	2.17	25 (30%)
12	CLA	H	839	-	69,73,73	2.21	23 (33%)	82,113,113	2.59	31 (37%)
12	CLA	G	805	12,1	59,63,73	2.40	24 (40%)	70,101,113	2.80	31 (44%)
12	CLA	G	836	1	54,58,73	2.61	24 (44%)	64,95,113	2.89	27 (42%)
12	CLA	H	834	20	64,68,73	2.30	22 (34%)	76,107,113	2.56	25 (32%)
15	BCR	H	846	-	41,41,41	2.59	6 (14%)	56,56,56	6.68	19 (33%)
12	CLA	A	806	1	69,73,73	2.17	21 (30%)	82,113,113	2.64	25 (30%)
12	CLA	A	821	1	49,53,73	2.55	23 (46%)	58,89,113	2.91	23 (39%)
12	CLA	a	821	-	49,53,73	2.55	23 (46%)	58,89,113	2.91	24 (41%)
12	CLA	H	832	-	49,53,73	2.52	22 (44%)	58,89,113	2.71	24 (41%)
12	CLA	A	813	-	49,53,73	2.60	22 (44%)	58,89,113	2.96	26 (44%)
15	BCR	a	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.76	26 (46%)
16	LHG	G	851	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
12	CLA	L	205	10	69,73,73	2.20	21 (30%)	82,113,113	2.61	27 (32%)
12	CLA	B	806	3	69,73,73	2.19	21 (30%)	82,113,113	2.75	29 (35%)
12	CLA	B	838	-	69,73,73	2.22	23 (33%)	82,113,113	2.59	31 (37%)
12	CLA	G	840	1	54,58,73	2.54	22 (40%)	64,95,113	2.70	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	b	807	-	69,73,73	2.18	22 (31%)	82,113,113	2.52	27 (32%)
15	BCR	a	852	-	41,41,41	2.71	6 (14%)	56,56,56	6.46	20 (35%)
13	1L3	A	842	-	34,34,34	2.63	14 (41%)	43,45,45	1.50	11 (25%)
14	SF4	a	843	3,1	0,12,12	-	-	-		
12	CLA	a	854	20	69,73,73	2.26	24 (34%)	82,113,113	2.55	30 (36%)
15	BCR	b	839	-	41,41,41	2.68	6 (14%)	56,56,56	6.58	20 (35%)
12	CLA	H	820	-	49,53,73	2.54	22 (44%)	58,89,113	2.85	25 (43%)
14	SF4	C	102	4	0,12,12	-	-	-		
15	BCR	b	843	-	41,41,41	2.63	6 (14%)	56,56,56	6.84	24 (42%)
12	CLA	H	803	-	69,73,73	2.26	22 (31%)	82,113,113	2.53	26 (31%)
12	CLA	G	817	1	54,58,73	2.51	23 (42%)	64,95,113	2.79	32 (50%)
12	CLA	A	838	1	49,53,73	2.55	22 (44%)	58,89,113	2.92	27 (46%)
11	CL0	a	801	1	69,73,73	2.32	20 (28%)	82,113,113	2.49	33 (40%)
12	CLA	b	848	16	64,68,73	2.29	21 (32%)	76,107,113	2.57	25 (32%)
12	CLA	a	813	-	49,53,73	2.52	23 (46%)	58,89,113	2.83	26 (44%)
12	CLA	L	202	3	69,73,73	2.25	21 (30%)	82,113,113	2.40	27 (32%)
15	BCR	B	845	-	41,41,41	2.58	6 (14%)	56,56,56	6.68	18 (32%)
12	CLA	G	835	1	49,53,73	2.52	23 (46%)	58,89,113	2.84	25 (43%)
12	CLA	G	823	1	54,58,73	2.56	24 (44%)	64,95,113	2.76	24 (37%)
15	BCR	A	852	-	41,41,41	2.70	6 (14%)	56,56,56	6.43	20 (35%)
12	CLA	a	814	-	49,53,73	2.53	21 (42%)	58,89,113	2.82	24 (41%)
15	BCR	F	202	-	41,41,41	2.79	6 (14%)	56,56,56	6.76	23 (41%)
12	CLA	B	823	3	69,73,73	2.22	21 (30%)	82,113,113	2.50	32 (39%)
15	BCR	l	201	-	41,41,41	2.67	6 (14%)	56,56,56	6.52	24 (42%)
12	CLA	H	835	3	69,73,73	2.19	22 (31%)	82,113,113	2.43	26 (31%)
12	CLA	H	824	3	69,73,73	2.23	21 (30%)	82,113,113	2.51	32 (39%)
12	CLA	H	827	3	69,73,73	2.31	22 (31%)	82,113,113	2.74	34 (41%)
12	CLA	l	205	10	69,73,73	2.19	21 (30%)	82,113,113	2.63	27 (32%)
12	CLA	G	811	12,1	54,58,73	2.49	24 (44%)	64,95,113	2.97	28 (43%)
12	CLA	G	824	-	59,63,73	2.39	23 (38%)	70,101,113	2.65	25 (35%)
12	CLA	a	824	20	69,73,73	2.26	23 (33%)	82,113,113	2.48	32 (39%)
12	CLA	B	827	3	49,53,73	2.58	21 (42%)	58,89,113	2.70	24 (41%)
12	CLA	a	812	-	54,58,73	2.53	23 (42%)	64,95,113	2.87	29 (45%)
12	CLA	B	830	-	69,73,73	2.23	22 (31%)	82,113,113	2.36	27 (32%)
12	CLA	B	834	3	69,73,73	2.19	22 (31%)	82,113,113	2.48	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	a	826	1	69,73,73	2.23	23 (33%)	82,113,113	2.57	28 (34%)
12	CLA	b	823	3	69,73,73	2.22	21 (30%)	82,113,113	2.49	30 (36%)
12	CLA	R	103	-	49,53,73	2.58	23 (46%)	58,89,113	2.78	23 (39%)
15	BCR	A	844	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	21 (37%)
12	CLA	H	828	3	49,53,73	2.56	21 (42%)	58,89,113	2.87	24 (41%)
12	CLA	H	811	3	69,73,73	2.19	22 (31%)	82,113,113	2.61	32 (39%)
12	CLA	G	807	1	69,73,73	2.16	22 (31%)	82,113,113	2.63	24 (29%)
12	CLA	G	825	20	69,73,73	2.28	23 (33%)	82,113,113	2.37	30 (36%)
12	CLA	a	825	20	59,63,73	2.42	23 (38%)	70,101,113	2.68	28 (40%)
12	CLA	A	808	1	54,58,73	2.54	23 (42%)	64,95,113	2.88	25 (39%)
12	CLA	B	824	-	69,73,73	2.18	21 (30%)	82,113,113	2.41	29 (35%)
12	CLA	l	206	20	69,73,73	2.23	21 (30%)	82,113,113	2.46	24 (29%)
15	BCR	R	101	-	41,41,41	2.67	6 (14%)	56,56,56	6.58	23 (41%)
12	CLA	H	818	-	49,53,73	2.54	22 (44%)	58,89,113	2.84	23 (39%)
12	CLA	a	832	1	69,73,73	2.25	22 (31%)	82,113,113	2.33	26 (31%)
12	CLA	a	828	-	69,73,73	2.23	21 (30%)	82,113,113	2.31	30 (36%)
15	BCR	j	103	-	41,41,41	2.65	6 (14%)	56,56,56	6.80	16 (28%)
12	CLA	a	818	-	69,73,73	2.22	24 (34%)	82,113,113	2.54	28 (34%)
12	CLA	A	834	-	69,73,73	2.24	23 (33%)	82,113,113	2.43	27 (32%)
12	CLA	b	835	20	69,73,73	2.28	23 (33%)	82,113,113	2.49	29 (35%)
12	CLA	B	808	3	49,53,73	2.56	23 (46%)	58,89,113	2.84	27 (46%)
12	CLA	B	822	20	69,73,73	2.26	23 (33%)	82,113,113	2.44	27 (32%)
12	CLA	a	802	20	69,73,73	2.23	20 (28%)	82,113,113	2.26	27 (32%)
12	CLA	A	817	-	59,63,73	2.52	22 (37%)	70,101,113	2.66	32 (45%)
12	CLA	A	805	-	69,73,73	2.19	23 (33%)	82,113,113	2.64	28 (34%)
12	CLA	G	822	1	49,53,73	2.56	23 (46%)	58,89,113	2.90	24 (41%)
15	BCR	A	848	-	41,41,41	2.71	6 (14%)	56,56,56	6.77	20 (35%)
12	CLA	a	805	1	69,73,73	2.19	23 (33%)	82,113,113	2.55	27 (32%)
18	LMG	B	846	-	55,55,55	1.48	8 (14%)	63,63,63	1.12	3 (4%)
15	BCR	G	853	-	41,41,41	2.71	6 (14%)	56,56,56	6.40	20 (35%)
12	CLA	b	829	3	69,73,73	2.26	23 (33%)	82,113,113	2.57	27 (32%)
12	CLA	b	833	3	69,73,73	2.21	23 (33%)	82,113,113	2.48	30 (36%)
15	BCR	i	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.97	21 (37%)
15	BCR	H	843	-	41,41,41	2.57	6 (14%)	56,56,56	6.64	24 (42%)
12	CLA	H	804	-	69,73,73	2.18	21 (30%)	82,113,113	2.65	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	b	828	3	49,53,73	2.55	24 (48%)	58,89,113	2.83	26 (44%)
15	BCR	A	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.91	19 (33%)
12	CLA	G	808	1	69,73,73	2.17	22 (31%)	82,113,113	2.60	27 (32%)
12	CLA	a	809	1	49,53,73	2.49	21 (42%)	58,89,113	2.89	25 (43%)
12	CLA	H	826	-	69,73,73	2.29	22 (31%)	82,113,113	2.09	26 (31%)
12	CLA	b	836	-	69,73,73	2.23	22 (31%)	82,113,113	2.67	32 (39%)
12	CLA	b	816	-	69,73,73	2.23	24 (34%)	82,113,113	2.33	28 (34%)
16	LHG	a	851	12	26,26,48	1.25	2 (7%)	29,32,54	1.25	3 (10%)
12	CLA	a	833	-	69,73,73	2.21	22 (31%)	82,113,113	2.49	28 (34%)
12	CLA	G	829	1	69,73,73	2.28	23 (33%)	82,113,113	2.27	26 (31%)
12	CLA	A	814	-	49,53,73	2.54	22 (44%)	58,89,113	2.78	25 (43%)
15	BCR	a	849	-	41,41,41	2.64	6 (14%)	56,56,56	6.77	26 (46%)
12	CLA	a	829	1	69,73,73	2.19	22 (31%)	82,113,113	2.38	26 (31%)
15	BCR	Q	102	-	41,41,41	2.71	6 (14%)	56,56,56	6.73	17 (30%)
12	CLA	H	836	3	49,53,73	2.49	22 (44%)	58,89,113	2.95	23 (39%)
12	CLA	H	815	3	59,63,73	2.39	21 (35%)	70,101,113	2.69	28 (40%)
12	CLA	a	836	1	54,58,73	2.64	24 (44%)	64,95,113	2.95	31 (48%)
15	BCR	P	202	-	41,41,41	2.72	6 (14%)	56,56,56	6.71	23 (41%)
12	CLA	B	837	3	69,73,73	2.20	21 (30%)	82,113,113	2.68	31 (37%)
15	BCR	i	102	-	41,41,41	2.71	6 (14%)	56,56,56	6.73	19 (33%)
15	BCR	A	845	-	41,41,41	2.62	6 (14%)	56,56,56	6.64	22 (39%)
12	CLA	B	829	3	69,73,73	2.26	25 (36%)	82,113,113	2.54	26 (31%)
12	CLA	H	823	20	69,73,73	2.25	23 (33%)	82,113,113	2.47	27 (32%)
12	CLA	b	818	-	49,53,73	2.57	23 (46%)	58,89,113	2.85	24 (41%)
12	CLA	A	840	1	54,58,73	2.54	21 (38%)	64,95,113	2.66	26 (40%)
12	CLA	b	812	-	49,53,73	2.54	21 (42%)	58,89,113	3.01	25 (43%)
11	CL0	G	801	1	69,73,73	2.25	21 (30%)	82,113,113	2.35	28 (34%)
12	CLA	H	812	3	64,68,73	2.33	24 (37%)	76,107,113	2.57	26 (34%)
14	SF4	G	844	3,1	0,12,12	-	-	-		
12	CLA	P	201	20	69,73,73	2.27	21 (30%)	82,113,113	2.34	25 (30%)
18	LMG	b	845	-	55,55,55	1.49	8 (14%)	63,63,63	1.11	3 (4%)
14	SF4	c	101	4	0,12,12	-	-	-		
12	CLA	B	821	20	69,73,73	2.19	22 (31%)	82,113,113	2.54	31 (37%)
15	BCR	R	102	-	41,41,41	2.63	6 (14%)	56,56,56	6.83	17 (30%)
12	CLA	b	837	-	69,73,73	2.20	23 (33%)	82,113,113	2.60	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	G	834	-	69,73,73	2.23	22 (31%)	82,113,113	2.45	28 (34%)
14	SF4	C	101	4	0,12,12	-	-	-		
12	CLA	H	833	-	49,53,73	2.57	22 (44%)	58,89,113	2.82	24 (41%)
12	CLA	A	815	-	49,53,73	2.52	23 (46%)	58,89,113	2.90	25 (43%)
16	LHG	A	853	-	48,48,48	0.93	2 (4%)	51,54,54	3.77	6 (11%)
12	CLA	a	835	1	49,53,73	2.51	23 (46%)	58,89,113	2.85	24 (41%)
12	CLA	j	104	-	49,53,73	2.60	23 (46%)	58,89,113	2.74	24 (41%)
15	BCR	Q	101	-	41,41,41	2.62	6 (14%)	56,56,56	6.90	22 (39%)
15	BCR	H	842	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	25 (44%)
12	CLA	B	815	-	64,68,73	2.30	24 (37%)	76,107,113	2.67	26 (34%)
12	CLA	B	807	3	69,73,73	2.19	21 (30%)	82,113,113	2.44	30 (36%)
14	SF4	c	102	4	0,12,12	-	-	-		
12	CLA	f	201	20	69,73,73	2.27	22 (31%)	82,113,113	2.29	26 (31%)
15	BCR	a	846	-	41,41,41	2.68	6 (14%)	56,56,56	6.62	22 (39%)
12	CLA	j	102	-	69,73,73	2.23	22 (31%)	82,113,113	2.34	29 (35%)
12	CLA	b	827	3	49,53,73	2.58	22 (44%)	58,89,113	2.79	24 (41%)
14	SF4	A	843	3,1	0,12,12	-	-	-		
12	CLA	F	203	-	49,53,73	2.57	23 (46%)	58,89,113	4.48	26 (44%)
12	CLA	B	820	3	49,53,73	2.53	22 (44%)	58,89,113	2.79	25 (43%)
12	CLA	b	820	-	49,53,73	2.51	22 (44%)	58,89,113	2.83	23 (39%)
12	CLA	a	817	-	59,63,73	2.45	25 (42%)	70,101,113	2.75	28 (40%)
12	CLA	G	832	1	69,73,73	2.26	24 (34%)	82,113,113	2.33	27 (32%)
15	BCR	b	842	-	25,25,41	2.19	2 (8%)	33,33,56	7.60	18 (54%)
19	LMT	H	848	-	36,36,36	1.18	4 (11%)	47,47,47	0.96	1 (2%)
12	CLA	A	854	20	69,73,73	2.31	24 (34%)	82,113,113	2.57	33 (40%)
12	CLA	A	807	1	69,73,73	2.20	21 (30%)	82,113,113	2.63	28 (34%)
12	CLA	H	850	16	64,68,73	2.30	22 (34%)	76,107,113	2.53	28 (36%)
12	CLA	a	816	1	54,58,73	2.52	20 (37%)	64,95,113	2.72	31 (48%)
12	CLA	a	815	-	49,53,73	2.56	22 (44%)	58,89,113	2.82	23 (39%)
16	LHG	a	853	-	48,48,48	0.94	2 (4%)	51,54,54	1.09	3 (5%)
15	BCR	G	845	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	21 (37%)
11	CL0	A	801	1	69,73,73	2.23	21 (30%)	82,113,113	2.44	29 (35%)
12	CLA	l	202	3	69,73,73	2.26	23 (33%)	82,113,113	2.41	25 (30%)
12	CLA	L	204	10	59,63,73	2.41	21 (35%)	70,101,113	2.68	24 (34%)
12	CLA	a	806	-	69,73,73	2.16	20 (28%)	82,113,113	2.63	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	G	830	-	69,73,73	2.23	22 (31%)	82,113,113	2.40	25 (30%)
15	BCR	f	202	-	41,41,41	2.80	6 (14%)	56,56,56	6.66	24 (42%)
15	BCR	B	844	-	41,41,41	2.64	6 (14%)	56,56,56	6.82	25 (44%)
15	BCR	S	201	-	41,41,41	2.80	6 (14%)	56,56,56	6.51	23 (41%)
12	CLA	A	804	12	59,63,73	2.42	23 (38%)	70,101,113	2.81	30 (42%)
12	CLA	G	821	-	69,73,73	2.26	23 (33%)	82,113,113	2.41	30 (36%)
15	BCR	l	203	-	41,41,41	2.79	6 (14%)	56,56,56	6.50	22 (39%)
12	CLA	B	826	3	69,73,73	2.33	22 (31%)	82,113,113	2.57	31 (37%)
12	CLA	G	837	1	69,73,73	2.20	23 (33%)	82,113,113	2.59	31 (37%)
12	CLA	B	801	-	64,68,73	2.30	21 (32%)	76,107,113	2.60	27 (35%)
15	BCR	F	204	-	41,41,41	2.63	6 (14%)	56,56,56	6.47	22 (39%)
12	CLA	b	801	-	64,68,73	2.30	22 (34%)	76,107,113	2.58	27 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	803	1	-	14/39/115/115	-
12	CLA	G	802	-	-	7/33/109/115	-
12	CLA	B	810	3	-	27/39/115/115	-
15	BCR	b	847	-	-	7/29/63/63	0/2/2/2
12	CLA	G	842	16	-	13/33/109/115	-
12	CLA	A	841	20	-	17/39/115/115	-
12	CLA	B	814	-	-	9/27/103/115	-
12	CLA	a	804	12	-	13/27/103/115	-
12	CLA	A	810	12,1	-	7/21/97/115	-
12	CLA	A	812	-	-	10/21/97/115	-
12	CLA	A	826	1	-	15/39/115/115	-
12	CLA	b	802	-	-	13/39/115/115	-
12	CLA	a	810	12,1	-	9/21/97/115	-
12	CLA	B	819	-	-	7/15/91/115	-
12	CLA	H	816	-	-	10/33/109/115	-
12	CLA	S	204	20	-	10/39/115/115	-
12	CLA	G	827	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	825	20	-	5/27/103/115	-
12	CLA	B	835	3	-	7/15/91/115	-
12	CLA	b	824	3	-	22/39/115/115	-
12	CLA	a	855	-	-	13/39/115/115	-
12	CLA	a	811	-	-	6/15/91/115	-
12	CLA	B	825	-	-	11/39/115/115	-
15	BCR	b	840	-	-	8/29/63/63	0/2/2/2
13	1L3	B	839	-	-	5/23/43/43	0/2/2/2
12	CLA	L	206	20	-	10/39/115/115	-
12	CLA	B	809	3	-	5/15/91/115	-
16	LHG	a	850	-	-	26/53/53/53	-
12	CLA	H	806	-	-	13/39/115/115	-
12	CLA	A	819	1	-	9/15/91/115	-
12	CLA	B	833	3	-	15/33/109/115	-
12	CLA	A	836	1	-	7/21/97/115	-
12	CLA	B	828	3	-	4/15/91/115	-
12	CLA	H	829	3	-	4/15/91/115	-
12	CLA	b	811	-	-	10/33/109/115	-
12	CLA	J	103	-	-	8/15/91/115	-
15	BCR	H	849	-	-	8/29/63/63	0/2/2/2
12	CLA	B	805	3	-	17/39/115/115	-
12	CLA	B	836	20	-	13/39/115/115	-
15	BCR	L	207	-	-	10/29/63/63	0/2/2/2
12	CLA	b	806	-	-	13/39/115/115	-
12	CLA	b	813	3	-	9/27/103/115	-
12	CLA	A	832	1	-	15/39/115/115	-
15	BCR	G	849	-	-	12/29/63/63	0/2/2/2
12	CLA	A	818	-	-	15/39/115/115	-
12	CLA	b	831	3	-	5/15/91/115	-
12	CLA	a	803	1	-	14/39/115/115	-
16	LHG	A	851	12	-	14/31/31/53	-
12	CLA	B	832	3	-	5/15/91/115	-
12	CLA	B	818	-	-	3/15/91/115	-
12	CLA	H	831	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	L	203	-	-	14/29/63/63	0/2/2/2
18	LMG	H	847	-	-	16/50/70/70	0/1/1/1
12	CLA	G	812	-	-	6/15/91/115	-
12	CLA	G	839	1	-	7/39/115/115	-
12	CLA	A	831	1	-	11/27/103/115	-
12	CLA	A	809	1	-	7/15/91/115	-
19	LMT	b	846	-	-	10/21/61/61	0/2/2/2
12	CLA	B	813	3	-	7/27/103/115	-
12	CLA	H	809	3	-	3/15/91/115	-
12	CLA	A	823	-	-	13/27/103/115	-
12	CLA	b	809	3	-	2/15/91/115	-
12	CLA	G	820	1	-	8/15/91/115	-
12	CLA	a	823	-	-	11/27/103/115	-
12	CLA	G	819	-	-	15/39/115/115	-
15	BCR	G	848	-	-	4/29/63/63	0/2/2/2
12	CLA	H	814	3	-	6/27/103/115	-
12	CLA	a	807	-	-	22/39/115/115	-
12	CLA	A	835	-	-	9/15/91/115	-
12	CLA	H	817	-	-	15/39/115/115	-
12	CLA	G	809	1	-	7/21/97/115	-
12	CLA	F	201	20	-	13/39/115/115	-
15	BCR	B	842	-	-	9/29/63/63	0/2/2/2
12	CLA	a	822	-	-	6/21/97/115	-
12	CLA	b	821	20	-	15/39/115/115	-
12	CLA	H	838	-	-	20/39/115/115	-
15	BCR	H	845	-	-	9/29/63/63	0/2/2/2
12	CLA	G	814	1	-	4/15/91/115	-
19	LMT	B	847	-	-	10/21/61/61	0/2/2/2
12	CLA	A	816	1	-	6/21/97/115	-
12	CLA	b	814	3	-	8/27/103/115	-
12	CLA	B	817	3	-	10/15/91/115	-
12	CLA	a	838	1	-	3/15/91/115	-
12	CLA	b	817	3	-	10/15/91/115	-
17	45D	M	101	-	-	13/29/69/69	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	45D	m	101	-	-	13/29/69/69	0/2/2/2
12	CLA	B	812	-	-	9/15/91/115	-
12	CLA	a	831	1	-	11/27/103/115	-
15	BCR	j	101	-	-	12/29/63/63	0/2/2/2
12	CLA	B	816	-	-	15/39/115/115	-
15	BCR	B	843	-	-	3/18/35/63	0/1/1/2
12	CLA	H	830	3	-	18/39/115/115	-
13	1L3	a	842	-	-	5/23/43/43	0/2/2/2
15	BCR	G	847	-	-	6/29/63/63	0/2/2/2
15	BCR	a	848	-	-	12/29/63/63	0/2/2/2
15	BCR	b	844	-	-	6/29/63/63	0/2/2/2
13	1L3	b	838	-	-	5/23/43/43	0/2/2/2
12	CLA	G	841	20	-	15/39/115/115	-
15	BCR	G	850	-	-	12/29/63/63	0/2/2/2
15	BCR	L	201	-	-	8/29/63/63	0/2/2/2
12	CLA	H	801	1	-	11/27/103/115	-
12	CLA	A	824	20	-	18/39/115/115	-
14	SF4	K	102	4	-	-	0/6/5/5
12	CLA	b	804	-	-	18/39/115/115	-
12	CLA	H	802	-	-	13/39/115/115	-
12	CLA	a	808	1	-	7/21/97/115	-
15	BCR	a	844	-	-	11/29/63/63	0/2/2/2
12	CLA	P	203	-	-	8/15/91/115	-
12	CLA	b	830	-	-	6/15/91/115	-
16	LHG	G	852	12	-	16/31/31/53	-
12	CLA	H	822	20	-	16/39/115/115	-
12	CLA	A	839	1	-	7/39/115/115	-
12	CLA	A	829	1	-	10/39/115/115	-
12	CLA	G	803	20	-	8/39/115/115	-
12	CLA	S	202	10	-	9/27/103/115	-
12	CLA	f	203	-	-	8/15/91/115	-
12	CLA	a	839	1	-	11/39/115/115	-
15	BCR	B	840	-	-	10/29/63/63	0/2/2/2
12	CLA	a	827	-	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	807	3	-	9/39/115/115	-
12	CLA	a	830	1	-	10/21/97/115	-
12	CLA	a	834	-	-	20/39/115/115	-
12	CLA	b	810	3	-	25/39/115/115	-
12	CLA	A	811	-	-	6/15/91/115	-
12	CLA	A	822	-	-	6/21/97/115	-
13	1L3	G	843	-	-	5/23/43/43	0/2/2/2
15	BCR	S	205	-	-	9/29/63/63	0/2/2/2
12	CLA	G	828	-	-	13/33/109/115	-
12	CLA	G	856	-	-	12/39/115/115	-
12	CLA	G	818	-	-	15/27/103/115	-
12	CLA	b	808	3	-	3/15/91/115	-
12	CLA	b	822	20	-	16/39/115/115	-
12	CLA	B	811	-	-	11/33/109/115	-
16	LHG	A	850	-	-	30/53/53/53	-
12	CLA	B	802	-	-	15/39/115/115	-
12	CLA	b	803	-	-	16/39/115/115	-
12	CLA	a	841	20	-	15/39/115/115	-
15	BCR	P	204	-	-	7/29/63/63	0/2/2/2
12	CLA	G	816	-	-	5/15/91/115	-
12	CLA	S	203	10	-	14/39/115/115	-
12	CLA	H	837	20	-	14/39/115/115	-
12	CLA	G	815	-	-	7/15/91/115	-
15	BCR	J	101	-	-	10/29/63/63	0/2/2/2
12	CLA	a	840	1	-	9/21/97/115	-
12	CLA	a	819	1	-	8/15/91/115	-
15	BCR	f	204	-	-	7/29/63/63	0/2/2/2
12	CLA	G	838	1	-	3/15/91/115	-
12	CLA	b	805	3	-	20/39/115/115	-
12	CLA	A	820	-	-	17/39/115/115	-
12	CLA	b	815	-	-	8/33/109/115	-
15	BCR	J	104	-	-	5/29/63/63	0/2/2/2
15	BCR	H	841	-	-	14/29/63/63	0/2/2/2
12	CLA	B	831	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	806	-	-	10/39/115/115	-
12	CLA	a	820	-	-	15/39/115/115	-
15	BCR	B	841	-	-	8/29/63/63	0/2/2/2
17	45D	T	101	-	-	13/29/69/69	0/2/2/2
12	CLA	H	810	3	-	2/15/91/115	-
15	BCR	H	844	-	-	3/18/35/63	0/1/1/2
12	CLA	G	813	1	-	10/21/97/115	-
12	CLA	b	819	-	-	7/15/91/115	-
15	BCR	A	849	-	-	12/29/63/63	0/2/2/2
16	LHG	G	854	-	-	37/53/53/53	-
12	CLA	A	830	1	-	7/21/97/115	-
12	CLA	H	825	-	-	22/39/115/115	-
12	CLA	H	808	3	-	13/39/115/115	-
12	CLA	B	804	-	-	18/39/115/115	-
14	SF4	K	101	4	-	-	0/6/5/5
12	CLA	G	804	1	-	15/39/115/115	-
15	BCR	J	102	-	-	18/29/63/63	0/2/2/2
12	CLA	l	204	10	-	6/27/103/115	-
12	CLA	H	813	-	-	9/15/91/115	-
12	CLA	B	803	-	-	17/39/115/115	-
12	CLA	A	837	1	-	17/39/115/115	-
15	BCR	a	845	-	-	8/29/63/63	0/2/2/2
12	CLA	G	826	20	-	7/27/103/115	-
12	CLA	b	832	3	-	15/33/109/115	-
15	BCR	b	841	-	-	9/29/63/63	0/2/2/2
12	CLA	G	810	1	-	7/15/91/115	-
15	BCR	A	847	-	-	4/29/63/63	0/2/2/2
12	CLA	G	833	1	-	15/39/115/115	-
12	CLA	a	837	1	-	14/39/115/115	-
15	BCR	I	101	-	-	8/29/63/63	0/2/2/2
12	CLA	G	831	1	-	8/21/97/115	-
12	CLA	b	826	3	-	10/39/115/115	-
12	CLA	A	828	-	-	13/39/115/115	-
12	CLA	G	855	20	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	819	-	-	3/15/91/115	-
12	CLA	H	805	3	-	16/39/115/115	-
12	CLA	A	802	20	-	8/39/115/115	-
12	CLA	A	827	1	-	14/33/109/115	-
15	BCR	G	846	-	-	3/29/63/63	0/2/2/2
13	1L3	H	840	-	-	5/23/43/43	0/2/2/2
12	CLA	A	833	-	-	15/39/115/115	-
12	CLA	b	834	3	-	7/15/91/115	-
12	CLA	H	821	-	-	2/15/91/115	-
12	CLA	A	855	-	-	11/39/115/115	-
12	CLA	b	825	-	-	12/39/115/115	-
12	CLA	H	839	-	-	14/39/115/115	-
12	CLA	G	805	12,1	-	13/27/103/115	-
12	CLA	G	836	1	-	5/21/97/115	-
12	CLA	H	834	20	-	15/33/109/115	-
15	BCR	H	846	-	-	9/29/63/63	0/2/2/2
12	CLA	A	806	1	-	13/39/115/115	-
12	CLA	A	821	1	-	9/15/91/115	-
12	CLA	a	821	-	-	9/15/91/115	-
12	CLA	H	832	-	-	6/15/91/115	-
12	CLA	A	813	-	-	2/15/91/115	-
15	BCR	a	847	-	-	4/29/63/63	0/2/2/2
16	LHG	G	851	-	-	31/53/53/53	-
12	CLA	L	205	10	-	14/39/115/115	-
12	CLA	B	806	3	-	13/39/115/115	-
12	CLA	B	838	-	-	19/39/115/115	-
12	CLA	G	840	1	-	7/21/97/115	-
12	CLA	b	807	-	-	10/39/115/115	-
15	BCR	a	852	-	-	13/29/63/63	0/2/2/2
13	1L3	A	842	-	-	5/23/43/43	0/2/2/2
14	SF4	a	843	3,1	-	-	0/6/5/5
12	CLA	a	854	20	-	19/39/115/115	-
15	BCR	b	839	-	-	13/29/63/63	0/2/2/2
12	CLA	H	820	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	C	102	4	-	-	0/6/5/5
15	BCR	b	843	-	-	9/29/63/63	0/2/2/2
12	CLA	H	803	-	-	17/39/115/115	-
12	CLA	G	817	1	-	6/21/97/115	-
12	CLA	A	838	1	-	3/15/91/115	-
11	CL0	a	801	1	-	8/39/115/115	-
12	CLA	b	848	16	-	15/33/109/115	-
12	CLA	a	813	-	-	2/15/91/115	-
12	CLA	L	202	3	-	13/39/115/115	-
15	BCR	B	845	-	-	6/29/63/63	0/2/2/2
12	CLA	G	835	1	-	9/15/91/115	-
12	CLA	G	823	1	-	7/21/97/115	-
15	BCR	A	852	-	-	12/29/63/63	0/2/2/2
12	CLA	a	814	-	-	7/15/91/115	-
15	BCR	F	202	-	-	13/29/63/63	0/2/2/2
12	CLA	B	823	3	-	17/39/115/115	-
15	BCR	l	201	-	-	8/29/63/63	0/2/2/2
12	CLA	H	835	3	-	12/39/115/115	-
12	CLA	H	824	3	-	18/39/115/115	-
12	CLA	H	827	3	-	12/39/115/115	-
12	CLA	l	205	10	-	13/39/115/115	-
12	CLA	G	811	12,1	-	8/21/97/115	-
12	CLA	G	824	-	-	9/27/103/115	-
12	CLA	a	824	20	-	16/39/115/115	-
12	CLA	B	827	3	-	6/15/91/115	-
12	CLA	a	812	-	-	10/21/97/115	-
12	CLA	B	830	-	-	13/39/115/115	-
12	CLA	B	834	3	-	9/39/115/115	-
12	CLA	a	826	1	-	15/39/115/115	-
12	CLA	b	823	3	-	16/39/115/115	-
12	CLA	R	103	-	-	7/15/91/115	-
15	BCR	A	844	-	-	10/29/63/63	0/2/2/2
12	CLA	H	828	3	-	5/15/91/115	-
12	CLA	H	811	3	-	23/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	807	1	-	13/39/115/115	-
12	CLA	G	825	20	-	16/39/115/115	-
12	CLA	a	825	20	-	5/27/103/115	-
12	CLA	A	808	1	-	7/21/97/115	-
12	CLA	B	824	-	-	24/39/115/115	-
12	CLA	l	206	20	-	11/39/115/115	-
15	BCR	R	101	-	-	11/29/63/63	0/2/2/2
12	CLA	H	818	-	-	10/15/91/115	-
12	CLA	a	832	1	-	15/39/115/115	-
12	CLA	a	828	-	-	11/39/115/115	-
15	BCR	j	103	-	-	17/29/63/63	0/2/2/2
12	CLA	a	818	-	-	17/39/115/115	-
12	CLA	A	834	-	-	18/39/115/115	-
12	CLA	b	835	20	-	13/39/115/115	-
12	CLA	B	808	3	-	3/15/91/115	-
12	CLA	B	822	20	-	18/39/115/115	-
12	CLA	a	802	20	-	10/39/115/115	-
12	CLA	A	817	-	-	15/27/103/115	-
12	CLA	A	805	-	-	12/39/115/115	-
12	CLA	G	822	1	-	9/15/91/115	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
12	CLA	a	805	1	-	14/39/115/115	-
18	LMG	B	846	-	-	18/50/70/70	0/1/1/1
15	BCR	G	853	-	-	12/29/63/63	0/2/2/2
12	CLA	b	829	3	-	18/39/115/115	-
12	CLA	b	833	3	-	11/39/115/115	-
15	BCR	i	101	-	-	9/29/63/63	0/2/2/2
15	BCR	H	843	-	-	9/29/63/63	0/2/2/2
12	CLA	H	804	-	-	18/39/115/115	-
12	CLA	b	828	3	-	4/15/91/115	-
15	BCR	A	846	-	-	8/29/63/63	0/2/2/2
12	CLA	G	808	1	-	21/39/115/115	-
12	CLA	a	809	1	-	7/15/91/115	-
12	CLA	H	826	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	836	-	-	18/39/115/115	-
12	CLA	b	816	-	-	15/39/115/115	-
16	LHG	a	851	12	-	18/31/31/53	-
12	CLA	a	833	-	-	15/39/115/115	-
12	CLA	G	829	1	-	14/39/115/115	-
12	CLA	A	814	-	-	7/15/91/115	-
15	BCR	a	849	-	-	12/29/63/63	0/2/2/2
12	CLA	a	829	1	-	10/39/115/115	-
15	BCR	Q	102	-	-	11/29/63/63	0/2/2/2
12	CLA	H	836	3	-	5/15/91/115	-
12	CLA	H	815	3	-	8/27/103/115	-
12	CLA	a	836	1	-	5/21/97/115	-
15	BCR	P	202	-	-	13/29/63/63	0/2/2/2
12	CLA	B	837	3	-	18/39/115/115	-
15	BCR	i	102	-	-	11/29/63/63	0/2/2/2
15	BCR	A	845	-	-	7/29/63/63	0/2/2/2
12	CLA	B	829	3	-	18/39/115/115	-
12	CLA	H	823	20	-	19/39/115/115	-
12	CLA	b	818	-	-	4/15/91/115	-
12	CLA	A	840	1	-	9/21/97/115	-
12	CLA	b	812	-	-	9/15/91/115	-
11	CL0	G	801	1	-	10/39/115/115	-
12	CLA	H	812	3	-	11/33/109/115	-
14	SF4	G	844	3,1	-	-	0/6/5/5
12	CLA	P	201	20	-	16/39/115/115	-
18	LMG	b	845	-	-	18/50/70/70	0/1/1/1
14	SF4	c	101	4	-	-	0/6/5/5
12	CLA	B	821	20	-	17/39/115/115	-
15	BCR	R	102	-	-	19/29/63/63	0/2/2/2
12	CLA	b	837	-	-	14/39/115/115	-
12	CLA	G	834	-	-	21/39/115/115	-
14	SF4	C	101	4	-	-	0/6/5/5
12	CLA	H	833	-	-	7/15/91/115	-
12	CLA	A	815	-	-	5/15/91/115	-
16	LHG	A	853	-	-	39/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	835	1	-	7/15/91/115	-
12	CLA	j	104	-	-	7/15/91/115	-
15	BCR	Q	101	-	-	8/29/63/63	0/2/2/2
15	BCR	H	842	-	-	8/29/63/63	0/2/2/2
12	CLA	B	815	-	-	11/33/109/115	-
12	CLA	B	807	3	-	8/39/115/115	-
14	SF4	c	102	4	-	-	0/6/5/5
12	CLA	f	201	20	-	16/39/115/115	-
15	BCR	a	846	-	-	8/29/63/63	0/2/2/2
12	CLA	j	102	-	-	13/39/115/115	-
12	CLA	b	827	3	-	5/15/91/115	-
14	SF4	A	843	3,1	-	-	0/6/5/5
12	CLA	F	203	-	-	8/15/91/115	-
12	CLA	B	820	3	-	4/15/91/115	-
12	CLA	b	820	-	-	2/15/91/115	-
12	CLA	a	817	-	-	15/27/103/115	-
12	CLA	G	832	1	-	14/39/115/115	-
15	BCR	b	842	-	-	3/18/35/63	0/1/1/2
19	LMT	H	848	-	-	11/21/61/61	0/2/2/2
12	CLA	A	854	20	-	18/39/115/115	-
12	CLA	A	807	1	-	23/39/115/115	-
12	CLA	H	850	16	-	14/33/109/115	-
12	CLA	a	816	1	-	9/21/97/115	-
12	CLA	a	815	-	-	5/15/91/115	-
16	LHG	a	853	-	-	35/53/53/53	-
15	BCR	G	845	-	-	10/29/63/63	0/2/2/2
11	CL0	A	801	1	-	6/39/115/115	-
12	CLA	l	202	3	-	17/39/115/115	-
12	CLA	L	204	10	-	7/27/103/115	-
12	CLA	a	806	-	-	13/39/115/115	-
12	CLA	G	830	-	-	10/39/115/115	-
15	BCR	f	202	-	-	14/29/63/63	0/2/2/2
15	BCR	B	844	-	-	8/29/63/63	0/2/2/2
15	BCR	S	201	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	804	12	-	14/27/103/115	-
12	CLA	G	821	-	-	11/39/115/115	-
15	BCR	l	203	-	-	16/29/63/63	0/2/2/2
12	CLA	B	826	3	-	12/39/115/115	-
12	CLA	G	837	1	-	14/39/115/115	-
12	CLA	B	801	-	-	6/33/109/115	-
15	BCR	F	204	-	-	7/29/63/63	0/2/2/2
12	CLA	b	801	-	-	7/33/109/115	-

All (6515) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	101	45D	C07-C15	13.72	1.54	1.35
17	m	101	45D	C07-C15	13.70	1.54	1.35
17	M	101	45D	C07-C15	13.69	1.54	1.35
17	m	101	45D	C08-C16	13.67	1.54	1.35
17	M	101	45D	C08-C16	13.59	1.54	1.35
17	T	101	45D	C08-C16	13.57	1.54	1.35
15	f	202	BCR	C8-C9	-8.92	1.26	1.46
15	F	202	BCR	C8-C9	-8.83	1.27	1.46
15	G	853	BCR	C8-C9	-8.60	1.27	1.46
15	P	202	BCR	C8-C9	-8.57	1.27	1.46
15	J	101	BCR	C8-C9	-8.54	1.27	1.46
15	S	201	BCR	C8-C9	-8.50	1.27	1.46
15	G	849	BCR	C8-C9	-8.49	1.27	1.46
15	A	848	BCR	C8-C9	-8.48	1.27	1.46
15	b	839	BCR	C8-C9	-8.46	1.27	1.46
15	j	101	BCR	C8-C9	-8.46	1.27	1.46
15	a	852	BCR	C8-C9	-8.44	1.27	1.46
15	A	852	BCR	C8-C9	-8.44	1.27	1.46
15	L	203	BCR	C8-C9	-8.43	1.27	1.46
15	l	203	BCR	C8-C9	-8.42	1.27	1.46
15	A	847	BCR	C8-C9	-8.42	1.27	1.46
15	Q	102	BCR	C8-C9	-8.40	1.28	1.46
15	R	101	BCR	C8-C9	-8.40	1.28	1.46
15	G	849	BCR	C11-C10	-8.39	1.17	1.43
15	a	848	BCR	C8-C9	-8.37	1.28	1.46
15	J	102	BCR	C8-C9	-8.36	1.28	1.46
15	a	848	BCR	C11-C10	-8.35	1.17	1.43
15	i	102	BCR	C8-C9	-8.33	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	201	BCR	C11-C10	-8.33	1.17	1.43
15	A	848	BCR	C11-C10	-8.31	1.17	1.43
15	A	847	BCR	C11-C10	-8.31	1.17	1.43
15	L	203	BCR	C11-C10	-8.30	1.17	1.43
15	l	201	BCR	C8-C9	-8.30	1.28	1.46
15	a	845	BCR	C8-C9	-8.28	1.28	1.46
15	b	847	BCR	C8-C9	-8.28	1.28	1.46
15	G	847	BCR	C11-C10	-8.28	1.17	1.43
15	R	102	BCR	C8-C9	-8.28	1.28	1.46
15	G	845	BCR	C8-C9	-8.27	1.28	1.46
15	S	205	BCR	C8-C9	-8.26	1.28	1.46
15	a	846	BCR	C11-C10	-8.26	1.17	1.43
15	b	839	BCR	C11-C10	-8.26	1.17	1.43
15	l	203	BCR	C11-C10	-8.25	1.17	1.43
15	a	844	BCR	C8-C9	-8.25	1.28	1.46
15	G	853	BCR	C11-C10	-8.24	1.17	1.43
15	B	844	BCR	C8-C9	-8.23	1.28	1.46
15	L	201	BCR	C8-C9	-8.22	1.28	1.46
15	a	847	BCR	C8-C9	-8.22	1.28	1.46
15	L	207	BCR	C8-C9	-8.22	1.28	1.46
15	a	852	BCR	C11-C10	-8.21	1.17	1.43
15	j	103	BCR	C8-C9	-8.20	1.28	1.46
15	L	207	BCR	C11-C10	-8.20	1.17	1.43
15	f	202	BCR	C11-C10	-8.19	1.17	1.43
15	F	204	BCR	C8-C9	-8.19	1.28	1.46
15	B	840	BCR	C8-C9	-8.18	1.28	1.46
15	f	204	BCR	C8-C9	-8.18	1.28	1.46
15	A	844	BCR	C8-C9	-8.18	1.28	1.46
15	J	101	BCR	C11-C10	-8.17	1.17	1.43
13	H	840	1L3	C03-C02	8.17	1.49	1.35
15	a	849	BCR	C8-C9	-8.17	1.28	1.46
15	G	848	BCR	C8-C9	-8.17	1.28	1.46
15	i	102	BCR	C11-C10	-8.16	1.17	1.43
15	a	847	BCR	C11-C10	-8.16	1.17	1.43
15	H	845	BCR	C8-C9	-8.15	1.28	1.46
15	A	845	BCR	C8-C9	-8.15	1.28	1.46
15	A	852	BCR	C11-C10	-8.15	1.17	1.43
15	b	843	BCR	C8-C9	-8.15	1.28	1.46
15	F	202	BCR	C11-C10	-8.15	1.17	1.43
15	j	101	BCR	C11-C10	-8.15	1.17	1.43
15	G	850	BCR	C8-C9	-8.14	1.28	1.46
15	A	849	BCR	C8-C9	-8.14	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	845	BCR	C11-C10	-8.13	1.18	1.43
15	H	841	BCR	C8-C9	-8.13	1.28	1.46
15	Q	102	BCR	C11-C10	-8.12	1.18	1.43
15	G	848	BCR	C11-C10	-8.12	1.18	1.43
15	P	202	BCR	C11-C10	-8.10	1.18	1.43
15	R	101	BCR	C11-C10	-8.09	1.18	1.43
15	G	846	BCR	C8-C9	-8.09	1.28	1.46
15	a	846	BCR	C8-C9	-8.08	1.28	1.46
15	J	102	BCR	C11-C10	-8.07	1.18	1.43
15	b	840	BCR	C11-C10	-8.06	1.18	1.43
15	H	842	BCR	C11-C10	-8.05	1.18	1.43
15	P	204	BCR	C8-C9	-8.05	1.28	1.46
15	Q	101	BCR	C11-C10	-8.04	1.18	1.43
15	B	841	BCR	C11-C10	-8.04	1.18	1.43
15	S	205	BCR	C11-C10	-8.03	1.18	1.43
15	A	846	BCR	C11-C10	-8.03	1.18	1.43
15	l	201	BCR	C11-C10	-8.03	1.18	1.43
15	A	845	BCR	C11-C10	-8.03	1.18	1.43
15	G	846	BCR	C11-C10	-8.02	1.18	1.43
15	i	101	BCR	C11-C10	-8.02	1.18	1.43
15	j	103	BCR	C11-C10	-8.02	1.18	1.43
15	L	201	BCR	C11-C10	-8.01	1.18	1.43
15	a	844	BCR	C11-C10	-8.00	1.18	1.43
15	I	101	BCR	C11-C10	-8.00	1.18	1.43
12	A	836	CLA	MG-NA	8.00	2.25	2.06
15	G	850	BCR	C11-C10	-7.99	1.18	1.43
13	B	839	1L3	C03-C02	7.99	1.49	1.35
15	B	844	BCR	C11-C10	-7.99	1.18	1.43
15	B	840	BCR	C11-C10	-7.99	1.18	1.43
15	G	847	BCR	C8-C9	-7.99	1.28	1.46
15	R	102	BCR	C11-C10	-7.98	1.18	1.43
15	F	204	BCR	C11-C10	-7.98	1.18	1.43
15	b	847	BCR	C11-C10	-7.98	1.18	1.43
15	H	841	BCR	C11-C10	-7.98	1.18	1.43
15	H	845	BCR	C11-C10	-7.97	1.18	1.43
15	A	846	BCR	C8-C9	-7.97	1.28	1.46
12	G	836	CLA	MG-NA	7.97	2.25	2.06
15	P	204	BCR	C11-C10	-7.97	1.18	1.43
12	a	824	CLA	MG-NA	7.96	2.25	2.06
15	a	849	BCR	C11-C10	-7.95	1.18	1.43
13	b	838	1L3	C03-C02	7.95	1.49	1.35
15	A	844	BCR	C11-C10	-7.95	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	846	BCR	C11-C10	-7.95	1.18	1.43
15	a	849	BCR	C20-C21	-7.94	1.18	1.43
15	G	845	BCR	C11-C10	-7.94	1.18	1.43
15	b	840	BCR	C8-C9	-7.93	1.29	1.46
15	b	843	BCR	C11-C10	-7.93	1.18	1.43
15	B	845	BCR	C11-C10	-7.93	1.18	1.43
15	b	844	BCR	C11-C10	-7.92	1.18	1.43
15	f	204	BCR	C11-C10	-7.92	1.18	1.43
15	H	842	BCR	C8-C9	-7.92	1.29	1.46
15	i	101	BCR	C8-C9	-7.91	1.29	1.46
15	H	843	BCR	C11-C10	-7.91	1.18	1.43
15	B	842	BCR	C11-C10	-7.90	1.18	1.43
15	G	850	BCR	C20-C21	-7.90	1.18	1.43
12	a	836	CLA	MG-NA	7.90	2.25	2.06
15	b	841	BCR	C11-C10	-7.89	1.18	1.43
15	l	203	BCR	C20-C21	-7.89	1.18	1.43
15	I	101	BCR	C8-C9	-7.88	1.29	1.46
12	A	824	CLA	MG-NA	7.88	2.25	2.06
15	Q	101	BCR	C8-C9	-7.86	1.29	1.46
15	B	841	BCR	C8-C9	-7.85	1.29	1.46
13	a	842	1L3	C03-C02	7.85	1.49	1.35
12	b	832	CLA	MG-NA	7.84	2.24	2.06
15	A	849	BCR	C11-C10	-7.83	1.18	1.43
12	G	825	CLA	MG-NA	7.83	2.24	2.06
15	H	849	BCR	C11-C10	-7.82	1.18	1.43
15	F	202	BCR	C16-C17	-7.81	1.19	1.43
15	S	201	BCR	C20-C21	-7.79	1.19	1.43
15	A	849	BCR	C20-C21	-7.79	1.19	1.43
13	A	842	1L3	C03-C02	7.79	1.49	1.35
12	B	809	CLA	MG-NA	7.79	2.24	2.06
12	b	809	CLA	MG-NA	7.77	2.24	2.06
15	F	202	BCR	C20-C21	-7.77	1.19	1.43
12	G	818	CLA	MG-NA	7.77	2.24	2.06
15	a	846	BCR	C20-C21	-7.77	1.19	1.43
13	G	843	1L3	C03-C02	7.77	1.49	1.35
12	H	824	CLA	MG-NA	7.77	2.24	2.06
12	B	823	CLA	MG-NA	7.77	2.24	2.06
15	H	843	BCR	C8-C9	-7.76	1.29	1.46
15	J	104	BCR	C11-C10	-7.76	1.19	1.43
12	B	831	CLA	MG-NA	7.75	2.24	2.06
15	B	842	BCR	C8-C9	-7.74	1.29	1.46
12	b	823	CLA	MG-NA	7.74	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	835	CLA	MG-NA	7.74	2.24	2.06
15	G	847	BCR	C20-C21	-7.73	1.19	1.43
12	A	813	CLA	MG-NA	7.73	2.24	2.06
15	b	841	BCR	C8-C9	-7.72	1.29	1.46
12	a	830	CLA	MG-NA	7.72	2.24	2.06
15	L	203	BCR	C20-C21	-7.72	1.19	1.43
12	A	803	CLA	MG-NA	7.72	2.24	2.06
15	f	202	BCR	C20-C21	-7.71	1.19	1.43
15	S	201	BCR	C16-C17	-7.71	1.19	1.43
12	A	811	CLA	MG-NA	7.71	2.24	2.06
12	J	103	CLA	MG-NA	7.71	2.24	2.06
12	a	816	CLA	MG-NA	7.71	2.24	2.06
12	H	819	CLA	MG-NA	7.71	2.24	2.06
12	A	817	CLA	MG-NA	7.71	2.24	2.06
12	j	104	CLA	MG-NA	7.71	2.24	2.06
12	R	103	CLA	MG-NA	7.71	2.24	2.06
12	l	202	CLA	MG-NA	7.70	2.24	2.06
12	H	808	CLA	MG-NA	7.70	2.24	2.06
12	B	812	CLA	MG-NA	7.70	2.24	2.06
15	f	202	BCR	C16-C17	-7.70	1.19	1.43
15	L	207	BCR	C20-C21	-7.69	1.19	1.43
12	A	831	CLA	MG-NA	7.69	2.24	2.06
15	H	849	BCR	C8-C9	-7.69	1.29	1.46
12	H	810	CLA	MG-NA	7.68	2.24	2.06
15	l	203	BCR	C16-C17	-7.68	1.19	1.43
12	f	201	CLA	MG-NA	7.68	2.24	2.06
12	b	818	CLA	MG-NA	7.68	2.24	2.06
12	a	803	CLA	MG-NA	7.68	2.24	2.06
15	L	203	BCR	C16-C17	-7.67	1.19	1.43
12	G	832	CLA	MG-NA	7.67	2.24	2.06
15	H	846	BCR	C8-C9	-7.67	1.29	1.46
12	b	817	CLA	MG-NA	7.67	2.24	2.06
12	B	817	CLA	MG-NA	7.67	2.24	2.06
12	a	811	CLA	MG-NA	7.67	2.24	2.06
12	F	203	CLA	MG-NA	7.66	2.24	2.06
12	G	812	CLA	MG-NA	7.66	2.24	2.06
15	G	849	BCR	C20-C21	-7.65	1.19	1.43
12	G	823	CLA	MG-NA	7.65	2.24	2.06
15	i	102	BCR	C20-C21	-7.65	1.19	1.43
12	A	832	CLA	MG-NA	7.65	2.24	2.06
15	J	104	BCR	C8-C9	-7.65	1.29	1.46
12	b	830	CLA	MG-NA	7.65	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	804	CLA	MG-NA	7.64	2.24	2.06
12	B	818	CLA	MG-NA	7.64	2.24	2.06
15	B	845	BCR	C8-C9	-7.64	1.29	1.46
12	a	835	CLA	MG-NA	7.64	2.24	2.06
12	f	203	CLA	MG-NA	7.63	2.24	2.06
12	A	822	CLA	MG-NA	7.63	2.24	2.06
12	H	834	CLA	MG-NA	7.63	2.24	2.06
12	a	832	CLA	MG-NA	7.62	2.24	2.06
15	P	202	BCR	C20-C21	-7.62	1.19	1.43
12	G	835	CLA	MG-NA	7.62	2.24	2.06
12	a	822	CLA	MG-NA	7.62	2.24	2.06
12	b	812	CLA	MG-NA	7.62	2.24	2.06
12	H	832	CLA	MG-NA	7.61	2.24	2.06
15	Q	102	BCR	C20-C21	-7.61	1.19	1.43
12	G	831	CLA	MG-NA	7.61	2.24	2.06
12	F	201	CLA	MG-NA	7.61	2.24	2.06
12	a	807	CLA	MG-NA	7.61	2.24	2.06
12	a	840	CLA	MG-NA	7.61	2.24	2.06
12	G	824	CLA	MG-NA	7.61	2.24	2.06
12	a	826	CLA	MG-NA	7.60	2.24	2.06
12	G	829	CLA	MG-NA	7.60	2.24	2.06
12	H	801	CLA	MG-NA	7.60	2.24	2.06
12	a	815	CLA	MG-NA	7.59	2.24	2.06
12	L	202	CLA	MG-NA	7.59	2.24	2.06
12	G	805	CLA	MG-NA	7.59	2.24	2.06
12	G	840	CLA	MG-NA	7.59	2.24	2.06
12	B	830	CLA	MG-NA	7.59	2.24	2.06
12	a	821	CLA	MG-NA	7.58	2.24	2.06
12	A	840	CLA	MG-NA	7.58	2.24	2.06
12	H	818	CLA	MG-NA	7.58	2.24	2.06
12	A	812	CLA	MG-NA	7.58	2.24	2.06
12	a	831	CLA	MG-NA	7.57	2.24	2.06
12	G	839	CLA	MG-NA	7.57	2.24	2.06
12	A	830	CLA	MG-NA	7.57	2.24	2.06
12	G	827	CLA	MG-NA	7.57	2.24	2.06
12	A	828	CLA	MG-NA	7.57	2.24	2.06
12	A	816	CLA	MG-NA	7.57	2.24	2.06
15	P	202	BCR	C16-C17	-7.57	1.19	1.43
12	P	201	CLA	MG-NA	7.56	2.24	2.06
12	A	821	CLA	MG-NA	7.56	2.24	2.06
15	A	846	BCR	C20-C21	-7.55	1.19	1.43
12	G	822	CLA	MG-NA	7.55	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	820	CLA	MG-NA	7.55	2.24	2.06
12	A	819	CLA	MG-NA	7.55	2.24	2.06
12	G	816	CLA	MG-NA	7.55	2.24	2.06
15	A	848	BCR	C20-C21	-7.55	1.19	1.43
12	l	204	CLA	MG-NA	7.54	2.24	2.06
12	A	826	CLA	MG-NA	7.54	2.24	2.06
15	j	103	BCR	C20-C21	-7.54	1.19	1.43
12	B	828	CLA	MG-NA	7.54	2.24	2.06
12	A	841	CLA	MG-NA	7.53	2.24	2.06
12	A	839	CLA	MG-NA	7.53	2.24	2.06
12	H	817	CLA	MG-NA	7.53	2.24	2.06
12	a	808	CLA	MG-NA	7.53	2.24	2.06
12	A	804	CLA	MG-NA	7.53	2.24	2.06
12	a	838	CLA	MG-NA	7.52	2.24	2.06
12	b	836	CLA	MG-NA	7.52	2.24	2.06
12	G	826	CLA	MG-NA	7.51	2.24	2.06
12	B	815	CLA	MG-NA	7.51	2.24	2.06
12	P	203	CLA	MG-NA	7.51	2.24	2.06
15	J	102	BCR	C20-C21	-7.51	1.19	1.43
12	a	804	CLA	MG-NA	7.51	2.24	2.06
15	a	848	BCR	C20-C21	-7.51	1.19	1.43
12	G	813	CLA	MG-NA	7.51	2.24	2.06
15	Q	101	BCR	C20-C21	-7.51	1.19	1.43
12	b	819	CLA	MG-NA	7.51	2.24	2.06
12	A	823	CLA	MG-NA	7.50	2.24	2.06
15	b	844	BCR	C8-C9	-7.50	1.29	1.46
15	i	101	BCR	C20-C21	-7.50	1.19	1.43
12	b	831	CLA	MG-NA	7.49	2.24	2.06
12	B	832	CLA	MG-NA	7.49	2.24	2.06
12	A	814	CLA	MG-NA	7.49	2.24	2.06
12	a	820	CLA	MG-NA	7.49	2.24	2.06
12	H	829	CLA	MG-NA	7.49	2.24	2.06
15	i	102	BCR	C16-C17	-7.49	1.20	1.43
12	a	823	CLA	MG-NA	7.48	2.24	2.06
12	S	202	CLA	MG-NA	7.48	2.24	2.06
12	B	833	CLA	MG-NA	7.48	2.24	2.06
12	a	813	CLA	MG-NA	7.48	2.24	2.06
12	B	813	CLA	MG-NA	7.48	2.24	2.06
15	L	201	BCR	C16-C17	-7.48	1.20	1.43
12	G	820	CLA	MG-NA	7.47	2.24	2.06
12	H	833	CLA	MG-NA	7.47	2.24	2.06
15	H	841	BCR	C20-C21	-7.47	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	844	BCR	C20-C21	-7.46	1.20	1.43
12	b	810	CLA	MG-NA	7.46	2.24	2.06
12	B	819	CLA	MG-NA	7.46	2.24	2.06
12	H	838	CLA	MG-NA	7.46	2.24	2.06
12	H	814	CLA	MG-NA	7.46	2.24	2.06
15	R	102	BCR	C20-C21	-7.46	1.20	1.43
12	b	834	CLA	MG-NA	7.46	2.24	2.06
15	b	842	BCR	C20-C21	-7.46	1.20	1.43
15	a	852	BCR	C20-C21	-7.46	1.20	1.43
15	F	204	BCR	C20-C21	-7.45	1.20	1.43
15	J	101	BCR	C16-C17	-7.45	1.20	1.43
12	B	837	CLA	MG-NA	7.45	2.24	2.06
15	A	852	BCR	C20-C21	-7.45	1.20	1.43
15	H	845	BCR	C20-C21	-7.45	1.20	1.43
15	I	101	BCR	C20-C21	-7.45	1.20	1.43
12	A	838	CLA	MG-NA	7.45	2.24	2.06
15	S	205	BCR	C16-C17	-7.45	1.20	1.43
12	j	102	CLA	MG-NA	7.44	2.24	2.06
12	G	817	CLA	MG-NA	7.44	2.24	2.06
12	a	828	CLA	MG-NA	7.44	2.24	2.06
12	B	816	CLA	MG-NA	7.44	2.24	2.06
12	b	813	CLA	MG-NA	7.44	2.23	2.06
12	G	837	CLA	MG-NA	7.44	2.23	2.06
15	b	843	BCR	C20-C21	-7.44	1.20	1.43
12	b	837	CLA	MG-NA	7.44	2.23	2.06
12	A	807	CLA	MG-NA	7.44	2.23	2.06
15	L	201	BCR	C20-C21	-7.44	1.20	1.43
12	b	827	CLA	MG-NA	7.44	2.23	2.06
12	B	838	CLA	MG-NA	7.43	2.23	2.06
15	G	849	BCR	C16-C17	-7.43	1.20	1.43
12	b	848	CLA	MG-NA	7.43	2.23	2.06
15	G	853	BCR	C20-C21	-7.43	1.20	1.43
12	H	828	CLA	MG-NA	7.43	2.23	2.06
12	G	809	CLA	MG-NA	7.43	2.23	2.06
12	a	812	CLA	MG-NA	7.43	2.23	2.06
15	Q	102	BCR	C16-C17	-7.42	1.20	1.43
15	B	840	BCR	C20-C21	-7.42	1.20	1.43
12	G	841	CLA	MG-NA	7.42	2.23	2.06
12	a	839	CLA	MG-NA	7.42	2.23	2.06
12	b	816	CLA	MG-NA	7.42	2.23	2.06
12	b	828	CLA	MG-NA	7.42	2.23	2.06
15	L	207	BCR	C16-C17	-7.42	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	853	BCR	C16-C17	-7.42	1.20	1.43
12	A	837	CLA	MG-NA	7.42	2.23	2.06
12	a	814	CLA	MG-NA	7.41	2.23	2.06
12	H	811	CLA	MG-NA	7.41	2.23	2.06
15	B	844	BCR	C16-C17	-7.41	1.20	1.43
12	H	850	CLA	MG-NA	7.41	2.23	2.06
15	A	852	BCR	C16-C17	-7.41	1.20	1.43
15	J	101	BCR	C20-C21	-7.41	1.20	1.43
15	A	847	BCR	C16-C17	-7.41	1.20	1.43
12	a	819	CLA	MG-NA	7.41	2.23	2.06
15	b	840	BCR	C20-C21	-7.40	1.20	1.43
15	l	201	BCR	C16-C17	-7.40	1.20	1.43
12	b	803	CLA	MG-NA	7.40	2.23	2.06
12	B	810	CLA	MG-NA	7.40	2.23	2.06
15	a	847	BCR	C16-C17	-7.40	1.20	1.43
12	L	204	CLA	MG-NA	7.40	2.23	2.06
15	B	844	BCR	C20-C21	-7.40	1.20	1.43
12	H	839	CLA	MG-NA	7.40	2.23	2.06
12	G	838	CLA	MG-NA	7.40	2.23	2.06
12	a	837	CLA	MG-NA	7.40	2.23	2.06
12	b	826	CLA	MG-NA	7.40	2.23	2.06
12	a	825	CLA	MG-NA	7.40	2.23	2.06
12	G	810	CLA	MG-NA	7.40	2.23	2.06
15	j	101	BCR	C20-C21	-7.40	1.20	1.43
15	a	852	BCR	C16-C17	-7.39	1.20	1.43
12	A	825	CLA	MG-NA	7.39	2.23	2.06
15	j	103	BCR	C16-C17	-7.39	1.20	1.43
15	b	847	BCR	C20-C21	-7.39	1.20	1.43
15	j	101	BCR	C16-C17	-7.39	1.20	1.43
15	B	841	BCR	C20-C21	-7.39	1.20	1.43
12	H	836	CLA	MG-NA	7.38	2.23	2.06
15	H	842	BCR	C20-C21	-7.38	1.20	1.43
12	G	815	CLA	MG-NA	7.38	2.23	2.06
12	A	808	CLA	MG-NA	7.38	2.23	2.06
12	H	813	CLA	MG-NA	7.38	2.23	2.06
15	b	843	BCR	C16-C17	-7.38	1.20	1.43
12	b	829	CLA	MG-NA	7.38	2.23	2.06
15	G	846	BCR	C20-C21	-7.38	1.20	1.43
15	P	204	BCR	C20-C21	-7.38	1.20	1.43
12	a	817	CLA	MG-NA	7.38	2.23	2.06
15	H	846	BCR	C20-C21	-7.37	1.20	1.43
15	H	845	BCR	C16-C17	-7.37	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	845	BCR	C20-C21	-7.37	1.20	1.43
15	b	844	BCR	C20-C21	-7.37	1.20	1.43
12	B	835	CLA	MG-NA	7.37	2.23	2.06
15	R	101	BCR	C16-C17	-7.36	1.20	1.43
15	B	845	BCR	C20-C21	-7.36	1.20	1.43
15	S	205	BCR	C20-C21	-7.36	1.20	1.43
12	B	829	CLA	MG-NA	7.36	2.23	2.06
15	B	843	BCR	C20-C21	-7.36	1.20	1.43
15	A	847	BCR	C20-C21	-7.36	1.20	1.43
15	l	201	BCR	C20-C21	-7.35	1.20	1.43
12	a	809	CLA	MG-NA	7.35	2.23	2.06
15	R	101	BCR	C20-C21	-7.35	1.20	1.43
15	G	848	BCR	C16-C17	-7.35	1.20	1.43
15	Q	101	BCR	C16-C17	-7.34	1.20	1.43
15	b	840	BCR	C16-C17	-7.34	1.20	1.43
15	H	843	BCR	C20-C21	-7.34	1.20	1.43
12	a	841	CLA	MG-NA	7.33	2.23	2.06
15	A	845	BCR	C20-C21	-7.33	1.20	1.43
12	b	822	CLA	MG-NA	7.33	2.23	2.06
15	a	847	BCR	C20-C21	-7.33	1.20	1.43
15	b	839	BCR	C20-C21	-7.33	1.20	1.43
15	F	204	BCR	C16-C17	-7.32	1.20	1.43
15	H	844	BCR	C16-C17	-7.32	1.20	1.43
12	B	826	CLA	MG-NA	7.32	2.23	2.06
12	H	827	CLA	MG-NA	7.32	2.23	2.06
15	G	847	BCR	C16-C17	-7.32	1.20	1.43
12	H	826	CLA	MG-NA	7.32	2.23	2.06
15	B	842	BCR	C20-C21	-7.32	1.20	1.43
12	G	842	CLA	MG-NA	7.31	2.23	2.06
12	B	827	CLA	MG-NA	7.31	2.23	2.06
12	A	809	CLA	MG-NA	7.31	2.23	2.06
15	I	101	BCR	C16-C17	-7.31	1.20	1.43
12	B	822	CLA	MG-NA	7.31	2.23	2.06
15	f	204	BCR	C20-C21	-7.30	1.20	1.43
15	a	846	BCR	C16-C17	-7.30	1.20	1.43
15	G	846	BCR	C16-C17	-7.30	1.20	1.43
15	J	102	BCR	C16-C17	-7.30	1.20	1.43
15	G	845	BCR	C20-C21	-7.30	1.20	1.43
15	a	848	BCR	C16-C17	-7.30	1.20	1.43
15	B	840	BCR	C16-C17	-7.30	1.20	1.43
12	l	205	CLA	MG-NA	7.29	2.23	2.06
15	B	843	BCR	C16-C17	-7.29	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	205	CLA	MG-NA	7.29	2.23	2.06
12	a	810	CLA	MG-NA	7.29	2.23	2.06
12	H	803	CLA	MG-NA	7.29	2.23	2.06
15	A	845	BCR	C16-C17	-7.29	1.20	1.43
15	A	848	BCR	C16-C17	-7.29	1.20	1.43
15	b	841	BCR	C20-C21	-7.29	1.20	1.43
15	G	848	BCR	C20-C21	-7.28	1.20	1.43
15	a	845	BCR	C16-C17	-7.28	1.20	1.43
12	B	820	CLA	MG-NA	7.28	2.23	2.06
12	B	825	CLA	MG-NA	7.27	2.23	2.06
12	S	203	CLA	MG-NA	7.27	2.23	2.06
12	a	818	CLA	MG-NA	7.27	2.23	2.06
12	G	821	CLA	MG-NA	7.27	2.23	2.06
15	B	841	BCR	C16-C17	-7.27	1.20	1.43
12	H	823	CLA	MG-NA	7.26	2.23	2.06
12	b	820	CLA	MG-NA	7.26	2.23	2.06
12	H	831	CLA	MG-NA	7.26	2.23	2.06
15	b	842	BCR	C16-C17	-7.26	1.20	1.43
15	G	845	BCR	C16-C17	-7.26	1.20	1.43
15	A	844	BCR	C20-C21	-7.26	1.20	1.43
12	l	206	CLA	MG-NA	7.26	2.23	2.06
15	H	842	BCR	C16-C17	-7.25	1.20	1.43
15	b	847	BCR	C16-C17	-7.25	1.20	1.43
12	B	824	CLA	MG-NA	7.25	2.23	2.06
15	H	841	BCR	C16-C17	-7.25	1.20	1.43
15	H	849	BCR	C20-C21	-7.25	1.20	1.43
15	A	846	BCR	C16-C17	-7.25	1.20	1.43
12	b	811	CLA	MG-NA	7.25	2.23	2.06
15	H	849	BCR	C16-C17	-7.25	1.20	1.43
15	J	104	BCR	C20-C21	-7.25	1.20	1.43
12	A	810	CLA	MG-NA	7.24	2.23	2.06
15	A	849	BCR	C16-C17	-7.24	1.20	1.43
12	S	204	CLA	MG-NA	7.24	2.23	2.06
12	G	808	CLA	MG-NA	7.24	2.23	2.06
12	A	818	CLA	MG-NA	7.24	2.23	2.06
15	B	842	BCR	C16-C17	-7.24	1.20	1.43
12	B	811	CLA	MG-NA	7.24	2.23	2.06
15	b	839	BCR	C16-C17	-7.24	1.20	1.43
12	G	819	CLA	MG-NA	7.23	2.23	2.06
12	H	805	CLA	MG-NA	7.23	2.23	2.06
15	A	844	BCR	C16-C17	-7.23	1.20	1.43
15	a	844	BCR	C16-C17	-7.23	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	844	BCR	C20-C21	-7.23	1.20	1.43
12	H	837	CLA	MG-NA	7.23	2.23	2.06
12	H	812	CLA	MG-NA	7.23	2.23	2.06
12	a	834	CLA	MG-NA	7.22	2.23	2.06
15	H	846	BCR	C16-C17	-7.22	1.20	1.43
15	f	204	BCR	C16-C17	-7.22	1.20	1.43
12	H	809	CLA	MG-NA	7.22	2.23	2.06
12	H	815	CLA	MG-NA	7.22	2.23	2.06
12	A	815	CLA	MG-NA	7.22	2.23	2.06
12	B	814	CLA	MG-NA	7.22	2.23	2.06
15	P	204	BCR	C16-C17	-7.22	1.20	1.43
12	b	804	CLA	MG-NA	7.22	2.23	2.06
12	A	854	CLA	MG-NA	7.21	2.23	2.06
15	R	102	BCR	C16-C17	-7.20	1.20	1.43
12	H	830	CLA	MG-NA	7.20	2.23	2.06
12	G	855	CLA	MG-NA	7.19	2.23	2.06
12	G	803	CLA	MG-NA	7.19	2.23	2.06
15	B	845	BCR	C16-C17	-7.19	1.20	1.43
12	G	811	CLA	MG-NA	7.19	2.23	2.06
12	b	805	CLA	MG-NA	7.18	2.23	2.06
15	b	844	BCR	C16-C17	-7.18	1.20	1.43
12	B	804	CLA	MG-NA	7.17	2.23	2.06
15	b	841	BCR	C16-C17	-7.17	1.20	1.43
12	L	206	CLA	MG-NA	7.17	2.23	2.06
12	A	833	CLA	MG-NA	7.17	2.23	2.06
15	H	843	BCR	C16-C17	-7.17	1.21	1.43
12	H	835	CLA	MG-NA	7.16	2.23	2.06
11	G	801	CL0	MG-NA	7.16	2.23	2.06
12	H	807	CLA	MG-NA	7.16	2.23	2.06
12	b	833	CLA	MG-NA	7.16	2.23	2.06
12	b	835	CLA	MG-NA	7.16	2.23	2.06
12	B	834	CLA	MG-NA	7.15	2.23	2.06
11	a	801	CL0	MG-NA	7.15	2.23	2.06
12	b	807	CLA	MG-NA	7.15	2.23	2.06
12	G	833	CLA	MG-NA	7.14	2.23	2.06
12	B	805	CLA	MG-NA	7.14	2.23	2.06
12	B	836	CLA	MG-NA	7.13	2.23	2.06
15	J	104	BCR	C16-C17	-7.13	1.21	1.43
15	i	101	BCR	C16-C17	-7.12	1.21	1.43
12	A	834	CLA	MG-NA	7.12	2.23	2.06
12	a	833	CLA	MG-NA	7.11	2.23	2.06
15	a	849	BCR	C16-C17	-7.11	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	804	CLA	MG-NA	7.11	2.23	2.06
12	H	825	CLA	MG-NA	7.11	2.23	2.06
12	a	802	CLA	MG-NA	7.10	2.23	2.06
15	G	850	BCR	C16-C17	-7.10	1.21	1.43
12	B	808	CLA	MG-NA	7.09	2.23	2.06
12	B	807	CLA	MG-NA	7.09	2.23	2.06
12	B	803	CLA	MG-NA	7.09	2.23	2.06
12	A	802	CLA	MG-NA	7.09	2.23	2.06
12	a	854	CLA	MG-NA	7.07	2.23	2.06
12	b	814	CLA	MG-NA	7.06	2.23	2.06
12	H	821	CLA	MG-NA	7.05	2.23	2.06
12	b	808	CLA	MG-NA	7.04	2.23	2.06
12	H	822	CLA	MG-NA	7.03	2.23	2.06
12	b	815	CLA	MG-NA	7.03	2.23	2.06
11	A	801	CL0	MG-NA	7.02	2.22	2.06
12	b	821	CLA	MG-NA	7.00	2.22	2.06
12	G	830	CLA	MG-NA	7.00	2.22	2.06
12	H	806	CLA	MG-NA	7.00	2.22	2.06
12	a	827	CLA	MG-NA	6.99	2.22	2.06
12	B	821	CLA	MG-NA	6.99	2.22	2.06
12	G	828	CLA	MG-NA	6.98	2.22	2.06
12	a	806	CLA	MG-NA	6.97	2.22	2.06
12	A	806	CLA	MG-NA	6.97	2.22	2.06
12	B	806	CLA	MG-NA	6.97	2.22	2.06
12	a	829	CLA	MG-NA	6.96	2.22	2.06
12	G	814	CLA	MG-NA	6.96	2.22	2.06
12	G	834	CLA	MG-NA	6.96	2.22	2.06
12	A	829	CLA	MG-NA	6.94	2.22	2.06
12	G	807	CLA	MG-NA	6.91	2.22	2.06
12	G	806	CLA	MG-NA	6.89	2.22	2.06
12	b	825	CLA	MG-NA	6.89	2.22	2.06
12	H	802	CLA	MG-NA	6.88	2.22	2.06
12	b	806	CLA	MG-NA	6.85	2.22	2.06
12	B	802	CLA	MG-NA	6.83	2.22	2.06
12	b	824	CLA	MG-NA	6.82	2.22	2.06
12	H	816	CLA	MG-NA	6.82	2.22	2.06
17	T	101	45D	C33-C35	6.77	1.60	1.46
12	G	856	CLA	MG-NA	6.77	2.22	2.06
12	A	827	CLA	MG-NA	6.76	2.22	2.06
17	m	101	45D	C33-C35	6.75	1.60	1.46
12	A	820	CLA	MG-NA	6.73	2.22	2.06
17	M	101	45D	C33-C35	6.73	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	801	CLA	MG-NA	6.73	2.22	2.06
12	B	801	CLA	MG-NA	6.72	2.22	2.06
12	G	802	CLA	MG-NA	6.66	2.22	2.06
12	b	802	CLA	MG-NA	6.60	2.22	2.06
12	a	805	CLA	MG-NA	6.58	2.21	2.06
12	A	855	CLA	MG-NA	6.51	2.21	2.06
12	a	855	CLA	MG-NA	6.49	2.21	2.06
12	A	805	CLA	MG-NA	6.40	2.21	2.06
17	T	101	45D	C23-C25	5.81	1.58	1.46
12	G	802	CLA	C1D-ND	-5.79	1.30	1.37
13	G	843	1L3	C06-C04	5.78	1.59	1.48
12	A	854	CLA	O2A-C1	5.75	1.61	1.46
12	G	818	CLA	O2A-C1	5.74	1.61	1.46
17	M	101	45D	C23-C25	5.74	1.58	1.46
17	m	101	45D	C23-C25	5.72	1.58	1.46
12	A	817	CLA	O2A-C1	5.67	1.61	1.46
12	B	806	CLA	O2A-C1	5.66	1.61	1.46
13	a	842	1L3	C06-C04	5.64	1.59	1.48
13	b	838	1L3	C14-C15	5.64	1.59	1.50
13	G	843	1L3	C14-C15	5.60	1.59	1.50
12	A	817	CLA	CHC-C1C	5.58	1.49	1.38
13	A	842	1L3	C06-C04	5.58	1.59	1.48
12	A	809	CLA	O2D-CGD	5.57	1.46	1.33
13	H	840	1L3	C14-C15	5.57	1.59	1.50
12	A	854	CLA	CHC-C1C	5.55	1.49	1.38
12	A	827	CLA	O2A-C1	5.55	1.61	1.46
13	B	839	1L3	C06-C04	5.51	1.58	1.48
13	B	839	1L3	C14-C15	5.50	1.59	1.50
12	b	813	CLA	O2A-C1	5.49	1.60	1.46
11	a	801	CL0	C1D-ND	-5.47	1.30	1.37
12	H	806	CLA	O2A-C1	5.47	1.60	1.46
12	H	823	CLA	O2A-C1	5.46	1.60	1.46
12	B	822	CLA	O2A-C1	5.46	1.60	1.46
12	a	827	CLA	O2A-C1	5.45	1.60	1.46
12	B	813	CLA	O2A-C1	5.45	1.60	1.46
12	H	839	CLA	O2A-C1	5.45	1.60	1.46
12	H	831	CLA	O2A-C1	5.45	1.60	1.46
12	B	801	CLA	C1D-ND	-5.44	1.30	1.37
12	P	201	CLA	O2A-C1	5.44	1.60	1.46
12	A	820	CLA	O2A-C1	5.44	1.60	1.46
12	B	834	CLA	O2A-C1	5.44	1.60	1.46
12	b	826	CLA	C3D-C4D	-5.44	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	836	CLA	O2D-CGD	5.43	1.46	1.33
17	T	101	45D	C24-C26	5.43	1.57	1.46
12	a	840	CLA	O2A-C1	5.43	1.60	1.46
12	b	833	CLA	O2A-C1	5.43	1.60	1.46
12	a	839	CLA	O2A-C1	5.43	1.60	1.46
12	b	822	CLA	O2A-C1	5.43	1.60	1.46
12	a	808	CLA	O2A-C1	5.42	1.60	1.46
12	A	810	CLA	O2A-C1	5.42	1.60	1.46
12	b	835	CLA	O2A-C1	5.42	1.60	1.46
12	b	823	CLA	O2A-C1	5.42	1.60	1.46
12	G	818	CLA	CHC-C1C	5.42	1.49	1.38
17	m	101	45D	C24-C26	5.42	1.57	1.46
12	H	814	CLA	O2A-C1	5.42	1.60	1.46
17	M	101	45D	C24-C26	5.42	1.57	1.46
12	G	811	CLA	O2A-C1	5.41	1.60	1.46
12	B	838	CLA	O2A-C1	5.41	1.60	1.46
13	H	840	1L3	C06-C04	5.41	1.58	1.48
12	G	834	CLA	O2A-C1	5.41	1.60	1.46
12	A	834	CLA	O2A-C1	5.41	1.60	1.46
12	b	825	CLA	O2A-C1	5.41	1.60	1.46
13	G	843	1L3	C11-C12	5.40	1.58	1.48
12	H	835	CLA	O2A-C1	5.40	1.60	1.46
12	a	823	CLA	O2A-C1	5.40	1.60	1.46
12	L	202	CLA	O2A-C1	5.40	1.60	1.46
12	H	816	CLA	C1B-NB	-5.39	1.30	1.37
12	A	808	CLA	O2A-C1	5.39	1.60	1.46
12	B	811	CLA	O2A-C1	5.39	1.60	1.46
12	l	202	CLA	O2A-C1	5.39	1.60	1.46
12	G	840	CLA	O2A-C1	5.39	1.60	1.46
12	H	808	CLA	O2A-C1	5.38	1.60	1.46
12	a	817	CLA	O2A-C1	5.38	1.60	1.46
13	A	842	1L3	C11-C12	5.38	1.58	1.48
12	G	821	CLA	O2A-C1	5.38	1.60	1.46
12	a	834	CLA	O2A-C1	5.38	1.60	1.46
12	a	854	CLA	CHC-C1C	5.38	1.49	1.38
12	H	830	CLA	O2A-C1	5.38	1.60	1.46
12	G	813	CLA	O2A-C1	5.38	1.60	1.46
12	b	837	CLA	O2A-C1	5.37	1.60	1.46
12	A	840	CLA	O2A-C1	5.37	1.60	1.46
12	A	812	CLA	O2A-C1	5.37	1.60	1.46
12	H	834	CLA	O2A-C1	5.37	1.60	1.46
12	A	822	CLA	O2A-C1	5.37	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	812	CLA	O2A-C1	5.37	1.60	1.46
12	b	811	CLA	O2A-C1	5.36	1.60	1.46
12	b	801	CLA	C1D-ND	-5.36	1.30	1.37
12	G	839	CLA	O2A-C1	5.36	1.60	1.46
12	a	806	CLA	O2A-C1	5.35	1.60	1.46
12	b	824	CLA	O2A-C1	5.35	1.60	1.46
12	a	837	CLA	O2A-C1	5.35	1.60	1.46
12	G	809	CLA	O2A-C1	5.35	1.60	1.46
12	B	830	CLA	O2A-C1	5.35	1.60	1.46
12	a	820	CLA	O2A-C1	5.35	1.60	1.46
12	A	837	CLA	O2A-C1	5.35	1.60	1.46
12	j	102	CLA	O2A-C1	5.34	1.60	1.46
12	a	816	CLA	O2A-C1	5.34	1.60	1.46
12	a	822	CLA	O2A-C1	5.34	1.60	1.46
13	H	840	1L3	C11-C12	5.34	1.58	1.48
12	G	823	CLA	O2A-C1	5.34	1.60	1.46
12	A	839	CLA	O2A-C1	5.34	1.60	1.46
12	G	807	CLA	O2A-C1	5.34	1.60	1.46
12	H	822	CLA	O2A-C1	5.34	1.60	1.46
12	A	823	CLA	O2A-C1	5.34	1.60	1.46
12	G	817	CLA	O2A-C1	5.34	1.60	1.46
12	a	809	CLA	O2D-CGD	5.33	1.46	1.33
12	G	828	CLA	O2A-C1	5.33	1.60	1.46
12	H	815	CLA	O2A-C1	5.33	1.60	1.46
12	a	830	CLA	O2A-C1	5.33	1.60	1.46
12	a	812	CLA	O2A-C1	5.32	1.60	1.46
13	a	842	1L3	C14-C15	5.32	1.58	1.50
12	b	806	CLA	O2A-C1	5.32	1.60	1.46
12	b	832	CLA	O2A-C1	5.32	1.60	1.46
12	H	807	CLA	O2A-C1	5.32	1.60	1.46
12	B	823	CLA	O2A-C1	5.32	1.60	1.46
12	a	810	CLA	O2A-C1	5.32	1.60	1.46
12	b	814	CLA	O2A-C1	5.31	1.60	1.46
12	b	821	CLA	O2A-C1	5.31	1.60	1.46
12	B	829	CLA	O2A-C1	5.31	1.60	1.46
12	G	803	CLA	O2A-C1	5.31	1.60	1.46
12	L	205	CLA	O2A-C1	5.31	1.60	1.46
12	G	831	CLA	O2A-C1	5.31	1.60	1.46
12	a	804	CLA	O2A-C1	5.30	1.60	1.46
12	H	837	CLA	O2A-C1	5.30	1.60	1.46
12	B	821	CLA	O2A-C1	5.30	1.60	1.46
12	B	833	CLA	O2A-C1	5.30	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	836	CLA	O2A-C1	5.30	1.60	1.46
12	S	203	CLA	O2A-C1	5.29	1.60	1.46
12	G	855	CLA	O2A-C1	5.29	1.60	1.46
12	G	837	CLA	O2A-C1	5.29	1.60	1.46
12	B	807	CLA	O2A-C1	5.29	1.60	1.46
12	G	855	CLA	CHC-C1C	5.28	1.49	1.38
12	B	824	CLA	O2A-C1	5.28	1.60	1.46
12	G	802	CLA	O2A-C1	5.28	1.60	1.46
12	b	829	CLA	O2A-C1	5.28	1.60	1.46
12	H	826	CLA	O2A-C1	5.28	1.60	1.46
12	A	804	CLA	O2A-C1	5.28	1.60	1.46
13	b	838	1L3	C06-C04	5.28	1.58	1.48
12	A	836	CLA	O2A-C1	5.28	1.60	1.46
12	H	824	CLA	O2A-C1	5.27	1.60	1.46
12	b	810	CLA	O2A-C1	5.26	1.60	1.46
12	a	836	CLA	O2A-C1	5.26	1.60	1.46
12	A	826	CLA	O2A-C1	5.26	1.60	1.46
13	a	842	1L3	C11-C12	5.26	1.58	1.48
12	B	814	CLA	O2A-C1	5.26	1.60	1.46
12	G	805	CLA	O2A-C1	5.25	1.60	1.46
12	b	807	CLA	O2A-C1	5.25	1.60	1.46
11	a	801	CL0	C3D-C4D	-5.24	1.32	1.44
12	A	830	CLA	O2A-C1	5.24	1.60	1.46
12	G	824	CLA	O2A-C1	5.24	1.60	1.46
12	l	205	CLA	O2A-C1	5.24	1.60	1.46
12	G	836	CLA	O2A-C1	5.24	1.60	1.46
12	A	807	CLA	O2A-C1	5.24	1.60	1.46
12	S	202	CLA	O2A-C1	5.24	1.60	1.46
12	G	804	CLA	O2A-C1	5.23	1.60	1.46
12	G	827	CLA	O2A-C1	5.23	1.60	1.46
12	l	204	CLA	O2A-C1	5.22	1.60	1.46
12	G	833	CLA	O2A-C1	5.22	1.60	1.46
12	H	801	CLA	O2A-C1	5.22	1.60	1.46
12	A	816	CLA	O2A-C1	5.22	1.60	1.46
12	H	827	CLA	CHD-C1D	5.22	1.48	1.38
12	f	201	CLA	O2A-C1	5.22	1.60	1.46
17	m	101	45D	C34-C36	5.22	1.57	1.46
12	H	805	CLA	O2A-C1	5.21	1.60	1.46
12	B	837	CLA	O2A-C1	5.21	1.60	1.46
17	M	101	45D	C34-C36	5.21	1.57	1.46
12	L	204	CLA	O2A-C1	5.21	1.60	1.46
12	G	808	CLA	O2A-C1	5.21	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	805	CLA	O2A-C1	5.21	1.60	1.46
12	B	820	CLA	O2D-CGD	5.21	1.46	1.33
12	A	806	CLA	O2A-C1	5.21	1.60	1.46
12	a	831	CLA	O2A-C1	5.21	1.60	1.46
12	b	836	CLA	O2A-C1	5.20	1.60	1.46
12	a	833	CLA	O2A-C1	5.20	1.60	1.46
12	G	815	CLA	O2D-CGD	5.20	1.46	1.33
17	T	101	45D	C34-C36	5.19	1.57	1.46
12	A	802	CLA	O2A-C1	5.19	1.60	1.46
12	A	816	CLA	O2D-CGD	5.19	1.46	1.33
13	A	842	1L3	C14-C15	5.19	1.58	1.50
12	G	806	CLA	O2A-C1	5.19	1.60	1.46
12	G	839	CLA	O2D-CGD	5.19	1.46	1.33
12	b	803	CLA	O2A-C1	5.18	1.60	1.46
12	F	201	CLA	O2A-C1	5.18	1.60	1.46
12	A	827	CLA	O2D-CGD	5.18	1.46	1.33
12	G	842	CLA	O2A-C1	5.17	1.60	1.46
12	a	805	CLA	O2A-C1	5.17	1.60	1.46
12	H	821	CLA	O2D-CGD	5.17	1.45	1.33
12	B	825	CLA	O2A-C1	5.17	1.60	1.46
12	A	828	CLA	O2A-C1	5.17	1.60	1.46
12	B	810	CLA	O2A-C1	5.17	1.60	1.46
12	G	830	CLA	O2A-C1	5.17	1.60	1.46
13	B	839	1L3	C11-C12	5.17	1.58	1.48
12	B	805	CLA	O2A-C1	5.16	1.60	1.46
12	H	838	CLA	O2A-C1	5.16	1.60	1.46
12	a	816	CLA	O2D-CGD	5.16	1.45	1.33
12	a	803	CLA	O2A-C1	5.16	1.60	1.46
12	b	848	CLA	O2A-C1	5.16	1.60	1.46
12	a	854	CLA	O2A-C1	5.16	1.60	1.46
12	H	850	CLA	O2D-CGD	5.16	1.45	1.33
12	b	826	CLA	O2A-C1	5.16	1.60	1.46
12	H	850	CLA	O2A-C1	5.16	1.60	1.46
12	A	831	CLA	O2A-C1	5.15	1.60	1.46
12	A	833	CLA	O2A-C1	5.15	1.60	1.46
12	H	811	CLA	O2A-C1	5.15	1.60	1.46
12	H	801	CLA	O2D-CGD	5.15	1.45	1.33
13	b	838	1L3	C11-C12	5.15	1.58	1.48
12	G	826	CLA	O2A-C1	5.15	1.60	1.46
12	a	815	CLA	O2D-CGD	5.15	1.45	1.33
12	A	803	CLA	O2A-C1	5.15	1.60	1.46
12	a	807	CLA	O2A-C1	5.15	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	839	CLA	O2D-CGD	5.15	1.45	1.33
12	G	822	CLA	O2D-CGD	5.15	1.45	1.33
12	a	826	CLA	O2A-C1	5.15	1.60	1.46
12	b	805	CLA	O2A-C1	5.14	1.60	1.46
12	a	818	CLA	O2A-C1	5.14	1.60	1.46
12	A	817	CLA	O2D-CGD	5.14	1.45	1.33
12	G	817	CLA	O2D-CGD	5.14	1.45	1.33
12	a	827	CLA	O2D-CGD	5.14	1.45	1.33
12	A	824	CLA	O2A-C1	5.14	1.60	1.46
12	F	201	CLA	O2D-CGD	5.14	1.45	1.33
12	A	839	CLA	O2D-CGD	5.13	1.45	1.33
12	H	817	CLA	O2A-C1	5.13	1.59	1.46
12	A	831	CLA	O2D-CGD	5.13	1.45	1.33
12	B	819	CLA	O2D-CGD	5.13	1.45	1.33
12	G	816	CLA	O2D-CGD	5.13	1.45	1.33
12	B	813	CLA	O2D-CGD	5.13	1.45	1.33
12	a	825	CLA	O2A-C1	5.13	1.59	1.46
12	J	103	CLA	O2D-CGD	5.13	1.45	1.33
12	b	820	CLA	O2D-CGD	5.13	1.45	1.33
12	b	831	CLA	O2D-CGD	5.13	1.45	1.33
12	A	815	CLA	O2D-CGD	5.13	1.45	1.33
12	a	831	CLA	O2D-CGD	5.12	1.45	1.33
12	b	828	CLA	O2D-CGD	5.12	1.45	1.33
12	B	816	CLA	O2A-C1	5.12	1.59	1.46
12	f	203	CLA	O2D-CGD	5.12	1.45	1.33
12	A	814	CLA	O2D-CGD	5.12	1.45	1.33
12	j	104	CLA	O2D-CGD	5.12	1.45	1.33
12	G	810	CLA	O2D-CGD	5.12	1.45	1.33
12	B	804	CLA	O2A-C1	5.12	1.59	1.46
12	a	814	CLA	O2D-CGD	5.11	1.45	1.33
12	A	841	CLA	O2A-C1	5.11	1.59	1.46
12	a	821	CLA	O2D-CGD	5.11	1.45	1.33
12	G	825	CLA	O2A-C1	5.11	1.59	1.46
12	A	825	CLA	O2A-C1	5.11	1.59	1.46
11	A	801	CL0	O2A-C1	5.11	1.59	1.46
12	b	836	CLA	O2D-CGD	5.11	1.45	1.33
12	G	828	CLA	O2D-CGD	5.11	1.45	1.33
12	a	818	CLA	O2D-CGD	5.11	1.45	1.33
12	A	818	CLA	O2D-CGD	5.11	1.45	1.33
12	A	818	CLA	O2A-C1	5.11	1.59	1.46
12	H	838	CLA	O2D-CGD	5.11	1.45	1.33
12	B	826	CLA	C3D-C4D	-5.11	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	804	CLA	O2A-C1	5.11	1.59	1.46
12	G	834	CLA	O2D-CGD	5.10	1.45	1.33
12	H	833	CLA	O2D-CGD	5.10	1.45	1.33
12	P	203	CLA	O2D-CGD	5.10	1.45	1.33
11	G	801	CL0	O2A-C1	5.10	1.59	1.46
12	H	820	CLA	O2D-CGD	5.10	1.45	1.33
12	b	813	CLA	O2D-CGD	5.10	1.45	1.33
12	a	841	CLA	O2D-CGD	5.09	1.45	1.33
12	H	825	CLA	O2A-C1	5.09	1.59	1.46
12	b	804	CLA	O2A-C1	5.09	1.59	1.46
12	H	829	CLA	O2D-CGD	5.09	1.45	1.33
12	R	103	CLA	O2D-CGD	5.09	1.45	1.33
12	B	805	CLA	O2D-CGD	5.09	1.45	1.33
12	H	814	CLA	O2D-CGD	5.08	1.45	1.33
12	a	824	CLA	O2A-C1	5.08	1.59	1.46
12	b	819	CLA	O2D-CGD	5.08	1.45	1.33
12	A	832	CLA	O2A-C1	5.08	1.59	1.46
12	G	818	CLA	O2D-CGD	5.07	1.45	1.33
12	B	816	CLA	O2D-CGD	5.07	1.45	1.33
12	A	821	CLA	O2D-CGD	5.07	1.45	1.33
12	a	841	CLA	O2A-C1	5.07	1.59	1.46
12	a	840	CLA	O2D-CGD	5.07	1.45	1.33
12	G	841	CLA	O2A-C1	5.07	1.59	1.46
12	b	804	CLA	O2D-CGD	5.07	1.45	1.33
12	H	815	CLA	O2D-CGD	5.07	1.45	1.33
12	G	811	CLA	O2D-CGD	5.07	1.45	1.33
12	G	841	CLA	O2D-CGD	5.07	1.45	1.33
12	S	204	CLA	O2A-C1	5.07	1.59	1.46
12	b	810	CLA	O2D-CGD	5.06	1.45	1.33
12	B	837	CLA	O2D-CGD	5.06	1.45	1.33
12	B	818	CLA	O2D-CGD	5.06	1.45	1.33
12	L	206	CLA	O2A-C1	5.06	1.59	1.46
12	H	816	CLA	O2A-C1	5.06	1.59	1.46
12	G	823	CLA	O2D-CGD	5.06	1.45	1.33
12	P	201	CLA	O2D-CGD	5.06	1.45	1.33
12	H	826	CLA	O2D-CGD	5.06	1.45	1.33
11	a	801	CL0	O2A-C1	5.05	1.59	1.46
12	A	823	CLA	O2D-CGD	5.05	1.45	1.33
12	F	203	CLA	O2D-CGD	5.05	1.45	1.33
12	G	856	CLA	O2A-C1	5.05	1.59	1.46
12	a	829	CLA	O2A-C1	5.05	1.59	1.46
12	a	822	CLA	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	834	CLA	O2D-CGD	5.05	1.45	1.33
12	G	824	CLA	O2D-CGD	5.05	1.45	1.33
12	G	836	CLA	C3D-C4D	-5.05	1.32	1.44
12	b	818	CLA	O2D-CGD	5.05	1.45	1.33
12	B	814	CLA	O2D-CGD	5.05	1.45	1.33
12	G	832	CLA	O2A-C1	5.05	1.59	1.46
12	a	823	CLA	O2D-CGD	5.04	1.45	1.33
12	b	806	CLA	O2D-CGD	5.04	1.45	1.33
12	B	832	CLA	O2D-CGD	5.04	1.45	1.33
12	B	825	CLA	O2D-CGD	5.04	1.45	1.33
12	a	826	CLA	CHC-C1C	5.04	1.48	1.38
12	B	826	CLA	CHD-C1D	5.04	1.48	1.38
12	b	814	CLA	O2D-CGD	5.04	1.45	1.33
12	a	832	CLA	O2A-C1	5.03	1.59	1.46
12	A	819	CLA	O2D-CGD	5.03	1.45	1.33
12	B	804	CLA	O2D-CGD	5.03	1.45	1.33
12	H	805	CLA	O2D-CGD	5.03	1.45	1.33
12	A	841	CLA	O2D-CGD	5.03	1.45	1.33
12	a	819	CLA	O2D-CGD	5.03	1.45	1.33
12	H	819	CLA	O2D-CGD	5.03	1.45	1.33
12	A	808	CLA	O2D-CGD	5.03	1.45	1.33
12	G	821	CLA	O2D-CGD	5.03	1.45	1.33
12	j	102	CLA	O2D-CGD	5.03	1.45	1.33
12	A	803	CLA	O2D-CGD	5.03	1.45	1.33
12	a	808	CLA	O2D-CGD	5.03	1.45	1.33
12	H	827	CLA	O2A-C1	5.03	1.59	1.46
12	G	804	CLA	O2D-CGD	5.03	1.45	1.33
12	A	813	CLA	O2D-CGD	5.02	1.45	1.33
12	B	801	CLA	O2A-C1	5.02	1.59	1.46
12	A	829	CLA	O2A-C1	5.02	1.59	1.46
12	G	809	CLA	O2D-CGD	5.02	1.45	1.33
12	a	803	CLA	O2D-CGD	5.02	1.45	1.33
12	G	840	CLA	O2D-CGD	5.02	1.45	1.33
12	G	820	CLA	O2D-CGD	5.01	1.45	1.33
12	A	834	CLA	O2D-CGD	5.01	1.45	1.33
12	B	834	CLA	O2D-CGD	5.01	1.45	1.33
12	a	813	CLA	O2D-CGD	5.01	1.45	1.33
12	b	825	CLA	O2D-CGD	5.01	1.45	1.33
12	A	804	CLA	O2D-CGD	5.01	1.45	1.33
12	A	840	CLA	O2D-CGD	5.00	1.45	1.33
12	A	822	CLA	O2D-CGD	5.00	1.45	1.33
12	B	826	CLA	O2A-C1	5.00	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	848	CLA	O2D-CGD	5.00	1.45	1.33
12	b	816	CLA	O2A-C1	5.00	1.59	1.46
12	H	817	CLA	O2D-CGD	4.99	1.45	1.33
12	a	804	CLA	O2D-CGD	4.99	1.45	1.33
12	a	810	CLA	O2D-CGD	4.99	1.45	1.33
12	B	808	CLA	O2D-CGD	4.99	1.45	1.33
12	A	836	CLA	C3D-C4D	-4.99	1.33	1.44
12	G	819	CLA	O2A-C1	4.99	1.59	1.46
12	b	826	CLA	CHD-C1D	4.99	1.48	1.38
12	H	804	CLA	O2D-CGD	4.99	1.45	1.33
12	G	819	CLA	O2D-CGD	4.99	1.45	1.33
12	l	206	CLA	O2A-C1	4.99	1.59	1.46
12	a	802	CLA	O2D-CGD	4.99	1.45	1.33
12	G	842	CLA	O2D-CGD	4.99	1.45	1.33
12	H	807	CLA	O2D-CGD	4.99	1.45	1.33
12	a	811	CLA	O2D-CGD	4.98	1.45	1.33
12	a	828	CLA	O2A-C1	4.98	1.59	1.46
12	b	817	CLA	O2D-CGD	4.98	1.45	1.33
12	B	830	CLA	O2D-CGD	4.98	1.45	1.33
12	B	803	CLA	O2A-C1	4.98	1.59	1.46
12	a	828	CLA	O2D-CGD	4.98	1.45	1.33
12	a	817	CLA	O2D-CGD	4.98	1.45	1.33
15	G	849	BCR	C10-C9	-4.97	1.24	1.35
12	B	815	CLA	O2A-C1	4.97	1.59	1.46
12	B	828	CLA	O2D-CGD	4.97	1.45	1.33
12	j	104	CLA	CHC-C1C	4.97	1.48	1.38
12	b	833	CLA	O2D-CGD	4.96	1.45	1.33
12	H	802	CLA	CHC-C1C	4.96	1.48	1.38
12	G	829	CLA	O2A-C1	4.96	1.59	1.46
12	H	803	CLA	O2D-CGD	4.96	1.45	1.33
12	A	811	CLA	O2D-CGD	4.96	1.45	1.33
12	B	810	CLA	O2D-CGD	4.96	1.45	1.33
12	H	818	CLA	O2D-CGD	4.96	1.45	1.33
12	A	810	CLA	O2D-CGD	4.95	1.45	1.33
12	L	202	CLA	O2D-CGD	4.95	1.45	1.33
12	a	802	CLA	O2A-C1	4.95	1.59	1.46
12	B	823	CLA	O2D-CGD	4.95	1.45	1.33
12	A	830	CLA	O2D-CGD	4.95	1.45	1.33
12	A	809	CLA	CHD-C1D	4.95	1.48	1.38
12	H	817	CLA	CHC-C1C	4.95	1.48	1.38
12	b	825	CLA	C1D-ND	-4.95	1.31	1.37
12	a	824	CLA	O2D-CGD	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	808	CLA	O2D-CGD	4.95	1.45	1.33
12	H	824	CLA	O2D-CGD	4.95	1.45	1.33
15	S	201	BCR	C10-C9	-4.94	1.24	1.35
15	a	848	BCR	C10-C9	-4.94	1.24	1.35
12	a	817	CLA	CHC-C1C	4.93	1.48	1.38
12	a	802	CLA	C3D-C4D	-4.93	1.33	1.44
11	G	801	CL0	C1D-ND	-4.93	1.31	1.37
12	B	827	CLA	O2D-CGD	4.93	1.45	1.33
12	B	836	CLA	CHC-C1C	4.93	1.48	1.38
12	b	816	CLA	O2D-CGD	4.93	1.45	1.33
12	H	812	CLA	O2D-CGD	4.93	1.45	1.33
12	H	825	CLA	O2D-CGD	4.93	1.45	1.33
12	B	811	CLA	O2D-CGD	4.93	1.45	1.33
12	b	805	CLA	O2D-CGD	4.93	1.45	1.33
12	b	803	CLA	O2D-CGD	4.93	1.45	1.33
12	H	813	CLA	O2D-CGD	4.92	1.45	1.33
12	b	823	CLA	O2D-CGD	4.92	1.45	1.33
12	B	802	CLA	O2A-C1	4.92	1.59	1.46
12	G	829	CLA	O2D-CGD	4.92	1.45	1.33
12	l	206	CLA	O2D-CGD	4.92	1.45	1.33
12	S	202	CLA	O2D-CGD	4.92	1.45	1.33
12	G	825	CLA	O2D-CGD	4.92	1.45	1.33
12	B	817	CLA	O2D-CGD	4.92	1.45	1.33
15	a	852	BCR	C10-C9	-4.92	1.24	1.35
12	b	802	CLA	O2A-C1	4.92	1.59	1.46
12	G	814	CLA	O2D-CGD	4.91	1.45	1.33
12	a	802	CLA	CHC-C1C	4.91	1.48	1.38
12	f	201	CLA	O2D-CGD	4.91	1.45	1.33
12	b	815	CLA	O2A-C1	4.91	1.59	1.46
12	H	823	CLA	O2D-CGD	4.91	1.45	1.33
12	A	828	CLA	O2D-CGD	4.91	1.45	1.33
12	A	805	CLA	CHC-C1C	4.91	1.48	1.38
12	A	812	CLA	O2D-CGD	4.91	1.45	1.33
12	R	103	CLA	CHC-C1C	4.91	1.48	1.38
12	G	805	CLA	O2D-CGD	4.90	1.45	1.33
12	A	824	CLA	O2D-CGD	4.90	1.45	1.33
12	b	801	CLA	O2A-C1	4.90	1.59	1.46
12	H	814	CLA	CHC-C1C	4.90	1.48	1.38
12	H	827	CLA	C1B-NB	-4.90	1.31	1.37
12	H	828	CLA	O2D-CGD	4.90	1.45	1.33
12	H	809	CLA	O2D-CGD	4.90	1.45	1.33
12	A	807	CLA	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	815	CLA	O2D-CGD	4.90	1.45	1.33
12	b	836	CLA	C3C-C2C	4.90	1.47	1.36
12	H	838	CLA	C3C-C2C	4.90	1.47	1.36
12	a	825	CLA	O2D-CGD	4.89	1.45	1.33
11	A	801	CL0	C1D-ND	-4.89	1.31	1.37
12	G	808	CLA	O2D-CGD	4.89	1.45	1.33
12	H	803	CLA	O2A-C1	4.89	1.59	1.46
12	b	822	CLA	O2D-CGD	4.89	1.45	1.33
12	A	802	CLA	C3D-C4D	-4.89	1.33	1.44
12	b	827	CLA	CHC-C1C	4.89	1.48	1.38
12	L	204	CLA	O2D-CGD	4.89	1.45	1.33
12	b	812	CLA	O2D-CGD	4.89	1.45	1.33
12	a	855	CLA	O2A-C1	4.89	1.59	1.46
12	b	835	CLA	CHC-C1C	4.89	1.48	1.38
12	G	826	CLA	O2D-CGD	4.89	1.45	1.33
12	A	825	CLA	O2D-CGD	4.88	1.45	1.33
12	H	835	CLA	O2D-CGD	4.88	1.45	1.33
12	H	822	CLA	C1D-ND	-4.88	1.31	1.37
12	H	816	CLA	O2D-CGD	4.88	1.45	1.33
12	A	855	CLA	O2D-CGD	4.88	1.45	1.33
15	l	203	BCR	C10-C9	-4.88	1.24	1.35
12	A	825	CLA	CHC-C1C	4.88	1.48	1.38
12	H	802	CLA	O2A-C1	4.88	1.59	1.46
12	A	855	CLA	O2A-C1	4.88	1.59	1.46
12	B	822	CLA	O2D-CGD	4.87	1.45	1.33
12	H	837	CLA	CHC-C1C	4.87	1.48	1.38
12	G	803	CLA	C3D-C4D	-4.87	1.33	1.44
12	a	805	CLA	CHC-C1C	4.87	1.48	1.38
12	J	103	CLA	CHC-C1C	4.87	1.48	1.38
12	b	827	CLA	O2D-CGD	4.87	1.45	1.33
12	B	829	CLA	C3C-C2C	4.86	1.47	1.36
12	A	833	CLA	O2D-CGD	4.85	1.45	1.33
12	B	813	CLA	CHC-C1C	4.85	1.48	1.38
12	B	824	CLA	O2D-CGD	4.85	1.45	1.33
12	S	204	CLA	O2D-CGD	4.85	1.45	1.33
12	a	820	CLA	O2D-CGD	4.85	1.45	1.33
12	b	811	CLA	O2D-CGD	4.85	1.45	1.33
12	A	830	CLA	C3D-C4D	-4.85	1.33	1.44
12	H	827	CLA	C3D-C4D	-4.85	1.33	1.44
12	a	855	CLA	C1D-ND	-4.85	1.31	1.37
12	B	821	CLA	O2D-CGD	4.85	1.45	1.33
12	H	806	CLA	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	830	CLA	CHC-C1C	4.84	1.48	1.38
12	a	807	CLA	O2D-CGD	4.84	1.45	1.33
12	B	807	CLA	O2D-CGD	4.84	1.45	1.33
12	B	834	CLA	CHC-C1C	4.84	1.48	1.38
12	B	812	CLA	O2D-CGD	4.84	1.45	1.33
15	L	203	BCR	C10-C9	-4.84	1.24	1.35
12	A	830	CLA	CHC-C1C	4.83	1.48	1.38
12	b	821	CLA	O2D-CGD	4.83	1.45	1.33
12	l	204	CLA	O2D-CGD	4.83	1.45	1.33
12	G	831	CLA	CHC-C1C	4.83	1.48	1.38
12	L	205	CLA	O2D-CGD	4.83	1.45	1.33
12	l	202	CLA	O2D-CGD	4.83	1.45	1.33
12	A	820	CLA	O2D-CGD	4.83	1.45	1.33
12	H	809	CLA	CHD-C1D	4.83	1.47	1.38
12	G	856	CLA	O2D-CGD	4.83	1.45	1.33
12	b	816	CLA	CHD-C1D	4.83	1.47	1.38
12	H	822	CLA	O2D-CGD	4.82	1.45	1.33
12	G	831	CLA	O2D-CGD	4.82	1.45	1.33
12	H	837	CLA	C3D-C4D	-4.82	1.33	1.44
12	G	838	CLA	O2D-CGD	4.82	1.45	1.33
12	B	806	CLA	O2D-CGD	4.82	1.45	1.33
12	b	830	CLA	O2D-CGD	4.81	1.45	1.33
12	A	838	CLA	O2D-CGD	4.81	1.45	1.33
11	G	801	CL0	O2D-CGD	4.81	1.45	1.33
12	G	826	CLA	CHC-C1C	4.81	1.48	1.38
12	b	834	CLA	O2D-CGD	4.81	1.45	1.33
12	G	856	CLA	C1D-ND	-4.81	1.31	1.37
12	b	808	CLA	O2D-CGD	4.80	1.45	1.33
12	A	826	CLA	O2D-CGD	4.80	1.45	1.33
12	G	833	CLA	O2D-CGD	4.80	1.45	1.33
12	a	855	CLA	O2D-CGD	4.80	1.45	1.33
12	H	817	CLA	CHD-C1D	4.80	1.47	1.38
12	H	803	CLA	CHC-C1C	4.80	1.48	1.38
12	G	830	CLA	O2D-CGD	4.80	1.45	1.33
12	B	838	CLA	O2D-CGD	4.79	1.45	1.33
15	A	852	BCR	C10-C9	-4.79	1.24	1.35
12	G	827	CLA	CHC-C1C	4.79	1.48	1.38
12	a	820	CLA	CHD-C1D	4.79	1.47	1.38
12	b	809	CLA	O2D-CGD	4.79	1.45	1.33
12	G	809	CLA	CHD-C1D	4.79	1.47	1.38
12	H	837	CLA	O2D-CGD	4.79	1.45	1.33
12	a	838	CLA	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	810	CLA	O2D-CGD	4.79	1.45	1.33
12	B	836	CLA	O2D-CGD	4.79	1.45	1.33
12	A	839	CLA	CHD-C1D	4.78	1.47	1.38
12	b	801	CLA	C1B-NB	-4.78	1.31	1.37
12	H	828	CLA	CHC-C1C	4.78	1.48	1.38
12	G	836	CLA	O2D-CGD	4.78	1.45	1.33
12	B	816	CLA	CHC-C1C	4.78	1.48	1.38
12	b	813	CLA	CHC-C1C	4.78	1.48	1.38
15	G	847	BCR	C10-C9	-4.78	1.24	1.35
12	a	825	CLA	CHC-C1C	4.77	1.48	1.38
12	b	825	CLA	C3D-C4D	-4.77	1.33	1.44
12	A	820	CLA	C3C-C2C	4.77	1.47	1.36
12	B	820	CLA	CHC-C1C	4.77	1.48	1.38
12	A	838	CLA	CHC-C1C	4.77	1.48	1.38
11	a	801	CL0	O2D-CGD	4.77	1.44	1.33
12	G	822	CLA	CHC-C1C	4.76	1.48	1.38
12	b	832	CLA	O2D-CGD	4.76	1.44	1.33
12	b	835	CLA	O2D-CGD	4.76	1.44	1.33
12	B	801	CLA	C1B-NB	-4.76	1.31	1.37
12	B	833	CLA	O2D-CGD	4.76	1.44	1.33
12	b	824	CLA	C1C-NC	-4.76	1.30	1.37
12	L	206	CLA	O2D-CGD	4.76	1.44	1.33
15	A	848	BCR	C10-C9	-4.76	1.24	1.35
12	G	829	CLA	CHC-C1C	4.76	1.48	1.38
12	B	827	CLA	CHC-C1C	4.76	1.48	1.38
12	B	803	CLA	O2D-CGD	4.76	1.44	1.33
12	a	826	CLA	O2D-CGD	4.76	1.44	1.33
12	a	833	CLA	O2D-CGD	4.76	1.44	1.33
12	B	825	CLA	C1D-ND	-4.76	1.31	1.37
12	A	831	CLA	C3D-C4D	-4.75	1.33	1.44
12	b	820	CLA	CHC-C1C	4.75	1.48	1.38
12	G	802	CLA	C1B-NB	-4.75	1.31	1.37
12	H	825	CLA	C3D-C4D	-4.75	1.33	1.44
12	G	838	CLA	C3D-C4D	-4.75	1.33	1.44
12	b	831	CLA	CHD-C1D	4.75	1.47	1.38
12	B	837	CLA	C3C-C2C	4.75	1.47	1.36
12	A	802	CLA	CHC-C1C	4.74	1.48	1.38
12	A	806	CLA	O2D-CGD	4.74	1.44	1.33
11	A	801	CL0	O2D-CGD	4.73	1.44	1.33
12	a	829	CLA	O2D-CGD	4.73	1.44	1.33
15	A	847	BCR	C10-C9	-4.73	1.24	1.35
12	B	835	CLA	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	838	CLA	CHC-C1C	4.73	1.48	1.38
12	b	807	CLA	O2D-CGD	4.73	1.44	1.33
12	B	816	CLA	CHD-C1D	4.73	1.47	1.38
12	G	830	CLA	C3C-C2C	4.73	1.47	1.36
12	G	814	CLA	CHD-C1D	4.72	1.47	1.38
12	B	809	CLA	O2D-CGD	4.72	1.44	1.33
12	H	836	CLA	O2D-CGD	4.72	1.44	1.33
12	B	808	CLA	CHD-C1D	4.72	1.47	1.38
12	G	802	CLA	O2D-CGD	4.72	1.44	1.33
12	H	826	CLA	C3D-C4D	-4.72	1.33	1.44
12	A	819	CLA	CHD-C1D	4.72	1.47	1.38
12	a	832	CLA	CHC-C1C	4.72	1.47	1.38
12	b	815	CLA	O2D-CGD	4.72	1.44	1.33
12	A	808	CLA	CHD-C1D	4.72	1.47	1.38
12	G	806	CLA	O2D-CGD	4.72	1.44	1.33
12	b	837	CLA	O2D-CGD	4.72	1.44	1.33
12	H	819	CLA	CHC-C1C	4.71	1.47	1.38
12	G	813	CLA	O2D-CGD	4.71	1.44	1.33
12	H	839	CLA	O2D-CGD	4.71	1.44	1.33
12	B	822	CLA	CHC-C1C	4.71	1.47	1.38
12	A	835	CLA	O2D-CGD	4.71	1.44	1.33
12	G	807	CLA	O2D-CGD	4.71	1.44	1.33
12	a	836	CLA	CHC-C1C	4.71	1.47	1.38
12	b	822	CLA	CHC-C1C	4.71	1.47	1.38
12	a	831	CLA	C3C-C2C	4.71	1.46	1.36
12	b	808	CLA	CHD-C1D	4.71	1.47	1.38
12	b	835	CLA	CHD-C1D	4.70	1.47	1.38
12	a	838	CLA	C3D-C4D	-4.70	1.33	1.44
12	a	817	CLA	C3C-C2C	4.70	1.46	1.36
12	H	837	CLA	CHD-C1D	4.70	1.47	1.38
12	a	839	CLA	CHD-C1D	4.70	1.47	1.38
12	A	838	CLA	C3D-C4D	-4.70	1.33	1.44
12	H	831	CLA	O2D-CGD	4.70	1.44	1.33
12	A	803	CLA	CHC-C1C	4.70	1.47	1.38
12	H	832	CLA	O2D-CGD	4.70	1.44	1.33
12	G	821	CLA	CHD-C1D	4.70	1.47	1.38
12	f	203	CLA	CHD-C1D	4.70	1.47	1.38
12	H	815	CLA	CHC-C1C	4.70	1.47	1.38
12	A	836	CLA	CHC-C1C	4.69	1.47	1.38
12	G	812	CLA	O2D-CGD	4.69	1.44	1.33
12	F	201	CLA	CHC-C1C	4.69	1.47	1.38
12	b	827	CLA	C3C-C2C	4.69	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	831	CLA	O2D-CGD	4.69	1.44	1.33
12	H	811	CLA	O2D-CGD	4.69	1.44	1.33
12	a	832	CLA	O2D-CGD	4.69	1.44	1.33
12	G	840	CLA	CHC-C1C	4.69	1.47	1.38
12	A	831	CLA	CHC-C1C	4.69	1.47	1.38
12	B	816	CLA	C3C-C2C	4.68	1.46	1.36
12	G	805	CLA	CHC-C1C	4.68	1.47	1.38
12	G	823	CLA	CHC-C1C	4.68	1.47	1.38
12	G	832	CLA	O2D-CGD	4.68	1.44	1.33
12	G	821	CLA	C3C-C2C	4.68	1.46	1.36
12	a	829	CLA	C3C-C2C	4.68	1.46	1.36
12	A	829	CLA	C3C-C2C	4.68	1.46	1.36
12	G	835	CLA	O2D-CGD	4.68	1.44	1.33
12	b	818	CLA	CHC-C1C	4.68	1.47	1.38
12	B	802	CLA	C1D-ND	-4.68	1.31	1.37
12	a	814	CLA	C3C-C2C	4.68	1.46	1.36
12	A	813	CLA	CHC-C1C	4.68	1.47	1.38
12	a	836	CLA	CHD-C1D	4.68	1.47	1.38
12	H	824	CLA	C3D-C4D	-4.68	1.33	1.44
12	H	826	CLA	C1D-ND	-4.68	1.31	1.37
12	H	823	CLA	C3C-C2C	4.68	1.46	1.36
12	G	827	CLA	O2D-CGD	4.68	1.44	1.33
12	H	826	CLA	C3C-C2C	4.68	1.46	1.36
12	B	836	CLA	C3D-C4D	-4.67	1.33	1.44
12	B	832	CLA	CHD-C1D	4.67	1.47	1.38
12	a	827	CLA	CHC-C1C	4.67	1.47	1.38
12	a	803	CLA	CHC-C1C	4.67	1.47	1.38
12	a	830	CLA	C3D-C4D	-4.67	1.33	1.44
12	B	825	CLA	C3C-C2C	4.67	1.46	1.36
12	A	820	CLA	CHD-C1D	4.66	1.47	1.38
12	B	836	CLA	CHD-C1D	4.66	1.47	1.38
12	A	826	CLA	C3C-C2C	4.66	1.46	1.36
12	b	833	CLA	CHC-C1C	4.66	1.47	1.38
12	H	823	CLA	CHC-C1C	4.66	1.47	1.38
12	S	203	CLA	O2D-CGD	4.66	1.44	1.33
12	G	828	CLA	CHC-C1C	4.66	1.47	1.38
12	H	802	CLA	O2D-CGD	4.66	1.44	1.33
12	B	817	CLA	CHC-C1C	4.66	1.47	1.38
12	H	833	CLA	CHD-C1D	4.66	1.47	1.38
12	A	813	CLA	C3D-C4D	-4.66	1.33	1.44
12	a	812	CLA	O2D-CGD	4.66	1.44	1.33
12	l	205	CLA	O2D-CGD	4.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	203	CLA	CHD-C1D	4.66	1.47	1.38
12	B	838	CLA	CHC-C1C	4.66	1.47	1.38
12	b	829	CLA	C3C-C2C	4.66	1.46	1.36
12	a	808	CLA	CHD-C1D	4.66	1.47	1.38
12	b	802	CLA	O2D-CGD	4.65	1.44	1.33
12	b	837	CLA	CHC-C1C	4.65	1.47	1.38
12	a	838	CLA	CHC-C1C	4.65	1.47	1.38
12	A	821	CLA	CHC-C1C	4.65	1.47	1.38
12	a	813	CLA	CHD-C1D	4.65	1.47	1.38
12	G	806	CLA	CHC-C1C	4.65	1.47	1.38
12	a	804	CLA	CHD-C1D	4.65	1.47	1.38
12	H	816	CLA	CHC-C1C	4.65	1.47	1.38
12	A	812	CLA	C3C-C2C	4.65	1.46	1.36
12	P	203	CLA	CHD-C1D	4.65	1.47	1.38
12	G	813	CLA	C3C-C2C	4.65	1.46	1.36
12	a	805	CLA	O2D-CGD	4.65	1.44	1.33
12	H	828	CLA	C3C-C2C	4.65	1.46	1.36
12	a	840	CLA	CHC-C1C	4.65	1.47	1.38
12	b	803	CLA	CHC-C1C	4.64	1.47	1.38
12	A	817	CLA	C3C-C2C	4.64	1.46	1.36
12	H	802	CLA	C1D-ND	-4.64	1.31	1.37
12	A	828	CLA	CHC-C1C	4.64	1.47	1.38
12	G	816	CLA	CHC-C1C	4.64	1.47	1.38
12	b	817	CLA	CHC-C1C	4.64	1.47	1.38
12	a	824	CLA	C3D-C4D	-4.64	1.33	1.44
12	G	815	CLA	C3C-C2C	4.64	1.46	1.36
12	H	818	CLA	CHC-C1C	4.64	1.47	1.38
12	A	832	CLA	CHC-C1C	4.64	1.47	1.38
12	A	834	CLA	C3C-C2C	4.64	1.46	1.36
12	b	848	CLA	CHC-C1C	4.64	1.47	1.38
12	A	805	CLA	O2D-CGD	4.64	1.44	1.33
12	G	833	CLA	C3D-C4D	-4.64	1.33	1.44
12	B	808	CLA	C3C-C2C	4.63	1.46	1.36
12	b	821	CLA	C3D-C4D	-4.63	1.33	1.44
12	b	835	CLA	C3D-C4D	-4.63	1.33	1.44
12	a	821	CLA	CHC-C1C	4.63	1.47	1.38
12	H	835	CLA	CHC-C1C	4.63	1.47	1.38
12	H	839	CLA	CHC-C1C	4.63	1.47	1.38
12	B	810	CLA	C3D-C4D	-4.63	1.33	1.44
12	R	103	CLA	CHD-C1D	4.63	1.47	1.38
12	H	850	CLA	CHC-C1C	4.63	1.47	1.38
12	A	840	CLA	CHC-C1C	4.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	826	CLA	C1D-ND	-4.63	1.31	1.37
12	a	806	CLA	O2D-CGD	4.63	1.44	1.33
12	G	824	CLA	CHD-C1D	4.63	1.47	1.38
12	H	824	CLA	C3C-C2C	4.62	1.46	1.36
12	j	104	CLA	CHD-C1D	4.62	1.47	1.38
12	G	804	CLA	CHC-C1C	4.62	1.47	1.38
12	B	823	CLA	C3D-C4D	-4.62	1.33	1.44
12	B	818	CLA	CHC-C1C	4.62	1.47	1.38
12	G	826	CLA	C3D-C4D	-4.62	1.33	1.44
12	H	801	CLA	C3C-C2C	4.62	1.46	1.36
17	m	101	45D	C42-C38	4.62	1.57	1.43
12	a	820	CLA	CHC-C1C	4.62	1.47	1.38
12	a	815	CLA	CHC-C1C	4.62	1.47	1.38
12	B	827	CLA	C3C-C2C	4.61	1.46	1.36
12	a	837	CLA	O2D-CGD	4.61	1.44	1.33
15	a	845	BCR	C10-C9	-4.61	1.25	1.35
12	b	823	CLA	CHC-C1C	4.61	1.47	1.38
17	M	101	45D	C42-C38	4.61	1.57	1.43
12	G	812	CLA	CHC-C1C	4.61	1.47	1.38
12	a	819	CLA	CHC-C1C	4.61	1.47	1.38
12	H	817	CLA	C3C-C2C	4.61	1.46	1.36
12	b	814	CLA	CHC-C1C	4.61	1.47	1.38
12	A	827	CLA	CHC-C1C	4.61	1.47	1.38
12	H	807	CLA	C1D-ND	-4.61	1.31	1.37
12	b	835	CLA	C3C-C2C	4.61	1.46	1.36
12	J	103	CLA	CHD-C1D	4.61	1.47	1.38
12	a	822	CLA	C3C-C2C	4.60	1.46	1.36
12	b	826	CLA	C3C-C2C	4.60	1.46	1.36
12	H	819	CLA	CHD-C1D	4.60	1.47	1.38
12	G	836	CLA	CHD-C1D	4.60	1.47	1.38
12	H	801	CLA	CHC-C1C	4.60	1.47	1.38
17	T	101	45D	C42-C38	4.60	1.57	1.43
12	A	803	CLA	CHD-C1D	4.60	1.47	1.38
12	G	816	CLA	CHD-C1D	4.60	1.47	1.38
12	G	803	CLA	CHC-C1C	4.60	1.47	1.38
12	G	839	CLA	CHD-C1D	4.60	1.47	1.38
12	G	823	CLA	C3C-C2C	4.60	1.46	1.36
12	G	804	CLA	CHD-C1D	4.60	1.47	1.38
12	B	826	CLA	C3C-C2C	4.60	1.46	1.36
12	A	814	CLA	C3C-C2C	4.60	1.46	1.36
12	A	822	CLA	C3C-C2C	4.60	1.46	1.36
15	J	101	BCR	C10-C9	-4.60	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	820	CLA	C3C-C2C	4.60	1.46	1.36
12	G	831	CLA	C3D-C4D	-4.59	1.33	1.44
12	A	815	CLA	CHD-C1D	4.59	1.47	1.38
12	A	836	CLA	C3C-C2C	4.59	1.46	1.36
12	H	821	CLA	CHC-C1C	4.59	1.47	1.38
12	a	803	CLA	CHD-C1D	4.59	1.47	1.38
12	H	833	CLA	C3C-C2C	4.59	1.46	1.36
12	A	811	CLA	CHC-C1C	4.59	1.47	1.38
12	b	810	CLA	C3D-C4D	-4.59	1.33	1.44
12	B	829	CLA	CHC-C1C	4.59	1.47	1.38
12	b	808	CLA	C3C-C2C	4.59	1.46	1.36
12	A	855	CLA	C1D-ND	-4.59	1.31	1.37
12	H	801	CLA	C3D-C4D	-4.59	1.33	1.44
12	b	816	CLA	CHC-C1C	4.59	1.47	1.38
12	j	104	CLA	C3C-C2C	4.59	1.46	1.36
11	G	801	CL0	C3D-C4D	-4.58	1.33	1.44
12	G	832	CLA	CHC-C1C	4.58	1.47	1.38
12	H	811	CLA	C3D-C4D	-4.58	1.33	1.44
12	b	819	CLA	CHC-C1C	4.58	1.47	1.38
12	H	809	CLA	C3C-C2C	4.58	1.46	1.36
12	A	824	CLA	CHC-C1C	4.58	1.47	1.38
12	A	805	CLA	C3D-C4D	-4.58	1.33	1.44
12	a	805	CLA	C3D-C4D	-4.58	1.33	1.44
12	G	834	CLA	C3C-C2C	4.58	1.46	1.36
12	B	824	CLA	C3D-C4D	-4.58	1.33	1.44
15	G	848	BCR	C10-C9	-4.58	1.25	1.35
12	B	826	CLA	C1B-NB	-4.58	1.31	1.37
12	a	830	CLA	O2D-CGD	4.58	1.44	1.33
15	f	202	BCR	C10-C9	-4.57	1.25	1.35
12	a	824	CLA	CHC-C1C	4.57	1.47	1.38
12	b	829	CLA	CHC-C1C	4.57	1.47	1.38
17	T	101	45D	C41-C37	4.57	1.57	1.43
12	G	832	CLA	CHD-C1D	4.57	1.47	1.38
12	a	815	CLA	CHD-C1D	4.57	1.47	1.38
15	b	839	BCR	C10-C9	-4.57	1.25	1.35
17	M	101	45D	C32-C30	4.57	1.57	1.43
12	a	811	CLA	CHC-C1C	4.57	1.47	1.38
12	B	825	CLA	C3D-C4D	-4.57	1.33	1.44
12	b	826	CLA	O2D-CGD	4.57	1.44	1.33
12	H	805	CLA	CHC-C1C	4.57	1.47	1.38
12	H	831	CLA	C1D-ND	-4.56	1.31	1.37
12	a	812	CLA	C3C-C2C	4.56	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	825	CLA	C1D-ND	-4.56	1.31	1.37
12	A	822	CLA	CHC-C1C	4.56	1.47	1.38
12	a	810	CLA	CHC-C1C	4.56	1.47	1.38
17	M	101	45D	C41-C37	4.56	1.57	1.43
11	A	801	CL0	C3D-C4D	-4.56	1.33	1.44
12	B	802	CLA	O2D-CGD	4.56	1.44	1.33
12	A	827	CLA	C3D-C4D	-4.55	1.33	1.44
12	H	818	CLA	C3C-C2C	4.55	1.46	1.36
12	A	814	CLA	CHC-C1C	4.55	1.47	1.38
12	b	824	CLA	C3D-C4D	-4.55	1.33	1.44
12	B	802	CLA	CHC-C1C	4.55	1.47	1.38
12	A	822	CLA	CHD-C1D	4.55	1.47	1.38
12	a	836	CLA	O2D-CGD	4.55	1.44	1.33
12	A	817	CLA	C3D-C4D	-4.55	1.34	1.44
12	b	822	CLA	C3C-C2C	4.55	1.46	1.36
12	b	825	CLA	C3C-C2C	4.55	1.46	1.36
12	G	818	CLA	C3C-C2C	4.55	1.46	1.36
12	B	801	CLA	O2D-CGD	4.55	1.44	1.33
12	b	834	CLA	CHC-C1C	4.55	1.47	1.38
12	A	854	CLA	CHC-C4B	4.55	1.49	1.39
12	R	103	CLA	C3C-C2C	4.55	1.46	1.36
12	a	808	CLA	C3C-C2C	4.55	1.46	1.36
12	a	854	CLA	C1D-ND	-4.54	1.31	1.37
12	G	856	CLA	CHC-C1C	4.54	1.47	1.38
12	A	832	CLA	O2D-CGD	4.54	1.44	1.33
12	A	815	CLA	CHC-C1C	4.54	1.47	1.38
12	B	812	CLA	CHC-C1C	4.54	1.47	1.38
15	i	102	BCR	C10-C9	-4.54	1.25	1.35
12	a	811	CLA	CHD-C1D	4.54	1.47	1.38
12	a	816	CLA	CHD-C1D	4.54	1.47	1.38
12	H	833	CLA	CHC-C1C	4.54	1.47	1.38
12	a	822	CLA	CHC-C1C	4.54	1.47	1.38
12	G	825	CLA	CHC-C1C	4.54	1.47	1.38
12	A	837	CLA	C3C-C2C	4.54	1.46	1.36
15	a	847	BCR	C10-C9	-4.54	1.25	1.35
12	G	836	CLA	CHC-C1C	4.54	1.47	1.38
12	B	826	CLA	O2D-CGD	4.54	1.44	1.33
12	G	807	CLA	CHC-C1C	4.54	1.47	1.38
12	a	834	CLA	C3C-C2C	4.53	1.46	1.36
17	T	101	45D	C32-C30	4.53	1.57	1.43
12	G	808	CLA	C3C-C2C	4.53	1.46	1.36
12	B	831	CLA	CHC-C1C	4.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	855	CLA	C3C-C2C	4.53	1.46	1.36
17	m	101	45D	C32-C30	4.53	1.57	1.43
12	B	832	CLA	C3C-C2C	4.53	1.46	1.36
12	a	818	CLA	CHD-C1D	4.53	1.47	1.38
12	G	822	CLA	C3C-C2C	4.53	1.46	1.36
12	A	803	CLA	C3C-C2C	4.53	1.46	1.36
12	a	839	CLA	C3C-C2C	4.53	1.46	1.36
12	A	804	CLA	CHD-C1D	4.53	1.47	1.38
12	f	201	CLA	CHC-C1C	4.53	1.47	1.38
15	L	207	BCR	C10-C9	-4.53	1.25	1.35
12	b	817	CLA	C3C-C2C	4.53	1.46	1.36
12	G	809	CLA	CHC-C1C	4.53	1.47	1.38
12	G	816	CLA	C3C-C2C	4.53	1.46	1.36
12	B	822	CLA	C3C-C2C	4.53	1.46	1.36
15	j	101	BCR	C10-C9	-4.52	1.25	1.35
12	B	831	CLA	C3C-C2C	4.52	1.46	1.36
12	a	836	CLA	C3C-C2C	4.52	1.46	1.36
12	A	854	CLA	C1D-ND	-4.52	1.31	1.37
12	G	810	CLA	CHD-C1D	4.52	1.47	1.38
12	G	806	CLA	C3D-C4D	-4.52	1.34	1.44
12	G	836	CLA	C3C-C2C	4.52	1.46	1.36
17	m	101	45D	C41-C37	4.52	1.57	1.43
12	a	806	CLA	CHC-C1C	4.52	1.47	1.38
12	a	839	CLA	CHC-C1C	4.52	1.47	1.38
12	A	815	CLA	C3C-C2C	4.52	1.46	1.36
12	G	837	CLA	C3C-C2C	4.52	1.46	1.36
12	H	834	CLA	C3C-C2C	4.52	1.46	1.36
12	H	830	CLA	C3C-C2C	4.52	1.46	1.36
12	H	804	CLA	CHC-C1C	4.52	1.47	1.38
12	b	818	CLA	CHD-C1D	4.51	1.47	1.38
12	H	837	CLA	C3C-C2C	4.51	1.46	1.36
12	G	828	CLA	C3D-C4D	-4.51	1.34	1.44
12	a	822	CLA	CHD-C1D	4.51	1.47	1.38
12	G	823	CLA	CHD-C1D	4.51	1.47	1.38
12	a	831	CLA	CHD-C1D	4.51	1.47	1.38
12	b	819	CLA	C3C-C2C	4.51	1.46	1.36
12	G	804	CLA	C3C-C2C	4.51	1.46	1.36
12	H	816	CLA	C3D-C4D	-4.51	1.34	1.44
12	A	806	CLA	CHC-C1C	4.51	1.47	1.38
12	G	820	CLA	CHC-C1C	4.51	1.47	1.38
12	A	837	CLA	CHC-C1C	4.51	1.47	1.38
12	H	812	CLA	CHD-C1D	4.51	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	831	CLA	C3C-C2C	4.51	1.46	1.36
12	A	824	CLA	C3D-C4D	-4.51	1.34	1.44
12	a	836	CLA	C3D-C4D	-4.51	1.34	1.44
12	b	812	CLA	C3C-C2C	4.51	1.46	1.36
12	B	817	CLA	C3C-C2C	4.50	1.46	1.36
12	A	812	CLA	CHD-C1D	4.50	1.47	1.38
12	b	831	CLA	CHC-C1C	4.50	1.47	1.38
12	H	827	CLA	O2D-CGD	4.50	1.44	1.33
12	B	832	CLA	CHC-C1C	4.50	1.47	1.38
15	R	101	BCR	C10-C9	-4.50	1.25	1.35
15	P	202	BCR	C10-C9	-4.50	1.25	1.35
12	P	201	CLA	CHD-C1D	4.49	1.47	1.38
12	G	842	CLA	CHC-C1C	4.49	1.47	1.38
12	a	806	CLA	C3D-C4D	-4.49	1.34	1.44
12	G	803	CLA	O2D-CGD	4.49	1.44	1.33
12	f	203	CLA	C3C-C2C	4.49	1.46	1.36
12	H	810	CLA	CHD-C1D	4.49	1.47	1.38
12	B	836	CLA	C3C-C2C	4.49	1.46	1.36
12	b	802	CLA	C3D-C4D	-4.49	1.34	1.44
12	a	832	CLA	CHD-C1D	4.49	1.47	1.38
12	A	817	CLA	CHC-C4B	4.49	1.49	1.39
12	G	802	CLA	CHC-C1C	4.49	1.47	1.38
12	A	812	CLA	CHC-C1C	4.49	1.47	1.38
12	B	819	CLA	CHC-C1C	4.49	1.47	1.38
12	P	201	CLA	CHC-C1C	4.49	1.47	1.38
12	a	855	CLA	CHC-C1C	4.49	1.47	1.38
12	b	811	CLA	C3C-C2C	4.48	1.46	1.36
12	A	811	CLA	C3C-C2C	4.48	1.46	1.36
15	A	845	BCR	C10-C9	-4.48	1.25	1.35
12	b	832	CLA	C3C-C2C	4.48	1.46	1.36
12	b	809	CLA	CHD-C1D	4.48	1.47	1.38
12	a	827	CLA	C3D-C4D	-4.48	1.34	1.44
12	G	812	CLA	C3C-C2C	4.48	1.46	1.36
12	S	204	CLA	CHC-C1C	4.48	1.47	1.38
12	a	823	CLA	CHD-C1D	4.48	1.47	1.38
12	A	839	CLA	C3C-C2C	4.48	1.46	1.36
12	H	829	CLA	CHD-C1D	4.48	1.47	1.38
12	a	803	CLA	C3C-C2C	4.48	1.46	1.36
12	H	836	CLA	CHC-C1C	4.48	1.47	1.38
12	a	815	CLA	C3C-C2C	4.48	1.46	1.36
12	B	828	CLA	C3C-C2C	4.48	1.46	1.36
15	G	846	BCR	C10-C9	-4.48	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	102	BCR	C10-C9	-4.48	1.25	1.35
12	b	805	CLA	CHC-C1C	4.48	1.47	1.38
12	A	811	CLA	CHD-C1D	4.48	1.47	1.38
12	A	802	CLA	O2D-CGD	4.48	1.44	1.33
12	G	832	CLA	C3C-C2C	4.48	1.46	1.36
12	H	806	CLA	CHC-C1C	4.47	1.47	1.38
12	H	829	CLA	C3C-C2C	4.47	1.46	1.36
12	A	821	CLA	C3C-C2C	4.47	1.46	1.36
12	G	817	CLA	CHD-C1D	4.47	1.47	1.38
12	b	811	CLA	CHD-C1D	4.47	1.47	1.38
12	A	806	CLA	C3D-C4D	-4.47	1.34	1.44
12	A	833	CLA	CHC-C1C	4.47	1.47	1.38
12	B	811	CLA	CHD-C1D	4.47	1.47	1.38
12	b	828	CLA	CHD-C1D	4.47	1.47	1.38
12	B	809	CLA	CHC-C1C	4.47	1.47	1.38
12	B	821	CLA	C3D-C4D	-4.47	1.34	1.44
12	b	814	CLA	CHD-C1D	4.47	1.47	1.38
12	J	103	CLA	C3C-C2C	4.47	1.46	1.36
15	S	205	BCR	C10-C9	-4.47	1.25	1.35
12	a	808	CLA	CHC-C1C	4.47	1.47	1.38
12	A	826	CLA	CHC-C1C	4.47	1.47	1.38
12	B	823	CLA	CHC-C1C	4.47	1.47	1.38
12	B	804	CLA	C3D-C4D	-4.47	1.34	1.44
12	H	820	CLA	CHD-C1D	4.47	1.47	1.38
12	H	805	CLA	C3C-C2C	4.46	1.46	1.36
12	A	826	CLA	C3D-C4D	-4.46	1.34	1.44
12	A	816	CLA	CHD-C1D	4.46	1.47	1.38
12	G	837	CLA	CHC-C1C	4.46	1.47	1.38
12	b	818	CLA	C3C-C2C	4.46	1.46	1.36
12	b	828	CLA	C3C-C2C	4.46	1.46	1.36
12	H	812	CLA	C3C-C2C	4.46	1.46	1.36
12	B	821	CLA	CHC-C1C	4.46	1.47	1.38
12	B	818	CLA	CHD-C1D	4.46	1.47	1.38
12	B	819	CLA	CHD-C1D	4.46	1.47	1.38
12	a	833	CLA	C3D-C4D	-4.46	1.34	1.44
12	b	811	CLA	CHC-C1C	4.46	1.47	1.38
12	G	841	CLA	CHD-C1D	4.46	1.47	1.38
12	a	837	CLA	C3C-C2C	4.46	1.46	1.36
12	H	820	CLA	CHC-C1C	4.46	1.47	1.38
12	B	803	CLA	CHC-C1C	4.46	1.47	1.38
12	A	855	CLA	CHC-C1C	4.46	1.47	1.38
12	b	816	CLA	C3C-C2C	4.45	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	813	CLA	C3D-C4D	-4.45	1.34	1.44
12	b	819	CLA	CHD-C1D	4.45	1.47	1.38
12	G	839	CLA	CHC-C1C	4.45	1.47	1.38
12	H	832	CLA	CHC-C1C	4.45	1.47	1.38
12	P	203	CLA	CHC-C1C	4.45	1.47	1.38
12	B	814	CLA	C3D-C4D	-4.45	1.34	1.44
12	G	809	CLA	C3C-C2C	4.45	1.46	1.36
12	a	807	CLA	C3C-C2C	4.45	1.46	1.36
12	a	832	CLA	C3C-C2C	4.45	1.46	1.36
15	F	202	BCR	C10-C9	-4.45	1.25	1.35
12	G	807	CLA	C3D-C4D	-4.45	1.34	1.44
12	b	801	CLA	CHC-C1C	4.45	1.47	1.38
12	b	804	CLA	C3D-C4D	-4.45	1.34	1.44
12	b	827	CLA	C3D-C4D	-4.45	1.34	1.44
12	H	828	CLA	C3D-C4D	-4.45	1.34	1.44
12	a	811	CLA	C3C-C2C	4.45	1.46	1.36
12	a	812	CLA	CHC-C1C	4.45	1.47	1.38
12	a	837	CLA	CHC-C1C	4.45	1.47	1.38
12	H	831	CLA	C3C-C2C	4.45	1.46	1.36
12	b	813	CLA	C3C-C2C	4.45	1.46	1.36
12	H	808	CLA	CHC-C1C	4.44	1.47	1.38
12	l	206	CLA	CHC-C1C	4.44	1.47	1.38
12	B	805	CLA	CHC-C1C	4.44	1.47	1.38
12	G	811	CLA	CHC-C1C	4.44	1.47	1.38
12	a	821	CLA	C3C-C2C	4.44	1.46	1.36
12	a	825	CLA	C3C-C2C	4.44	1.46	1.36
12	B	802	CLA	C3D-C4D	-4.44	1.34	1.44
12	l	202	CLA	CHC-C1C	4.44	1.47	1.38
12	B	819	CLA	C3C-C2C	4.44	1.46	1.36
12	A	804	CLA	CHC-C1C	4.44	1.47	1.38
12	b	809	CLA	C3C-C2C	4.44	1.46	1.36
12	G	830	CLA	CHD-C1D	4.44	1.47	1.38
12	G	838	CLA	C3C-C2C	4.44	1.46	1.36
12	L	202	CLA	CHC-C1C	4.44	1.47	1.38
12	G	810	CLA	CHC-C1C	4.44	1.47	1.38
12	G	821	CLA	CHC-C1C	4.44	1.47	1.38
12	H	820	CLA	C3C-C2C	4.44	1.46	1.36
12	P	203	CLA	C3C-C2C	4.43	1.46	1.36
12	H	830	CLA	CHC-C1C	4.43	1.47	1.38
12	A	825	CLA	C3C-C2C	4.43	1.46	1.36
12	A	832	CLA	C3C-C2C	4.43	1.46	1.36
12	H	836	CLA	C3D-C4D	-4.43	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	824	CLA	CHC-C1C	4.43	1.47	1.38
12	A	835	CLA	CHC-C1C	4.43	1.47	1.38
12	H	819	CLA	C3C-C2C	4.43	1.46	1.36
15	G	853	BCR	C10-C9	-4.43	1.25	1.35
12	b	834	CLA	C3D-C4D	-4.43	1.34	1.44
12	H	810	CLA	CHC-C1C	4.43	1.47	1.38
12	b	809	CLA	CHC-C1C	4.43	1.47	1.38
12	b	832	CLA	CHC-C1C	4.43	1.47	1.38
12	G	826	CLA	C3C-C2C	4.43	1.46	1.36
12	H	810	CLA	C3C-C2C	4.43	1.46	1.36
12	j	102	CLA	C3C-C2C	4.42	1.46	1.36
12	H	812	CLA	CHC-C1C	4.42	1.47	1.38
12	a	854	CLA	CHC-C4B	4.42	1.49	1.39
12	A	807	CLA	C3C-C2C	4.42	1.46	1.36
12	H	815	CLA	C3D-C4D	-4.42	1.34	1.44
12	a	831	CLA	CHC-C1C	4.42	1.47	1.38
12	b	829	CLA	C3D-C4D	-4.42	1.34	1.44
12	a	835	CLA	CHC-C1C	4.42	1.47	1.38
15	f	204	BCR	C10-C9	-4.42	1.25	1.35
12	A	833	CLA	C3D-C4D	-4.42	1.34	1.44
15	a	846	BCR	C10-C9	-4.42	1.25	1.35
12	a	854	CLA	C3C-C2C	4.42	1.46	1.36
12	B	813	CLA	C3C-C2C	4.42	1.46	1.36
12	F	203	CLA	CHC-C1C	4.42	1.47	1.38
16	a	853	LHG	O8-C23	4.42	1.46	1.33
12	G	839	CLA	C3C-C2C	4.42	1.46	1.36
12	B	827	CLA	C3D-C4D	-4.42	1.34	1.44
12	a	826	CLA	C3C-C2C	4.42	1.46	1.36
12	b	803	CLA	C3C-C2C	4.42	1.46	1.36
12	B	809	CLA	C3C-C2C	4.42	1.46	1.36
12	A	823	CLA	CHD-C1D	4.42	1.47	1.38
12	b	814	CLA	C3D-C4D	-4.42	1.34	1.44
12	B	831	CLA	CHD-C1D	4.41	1.47	1.38
12	A	834	CLA	CHD-C1D	4.41	1.47	1.38
12	f	203	CLA	CHC-C1C	4.41	1.47	1.38
12	G	810	CLA	C3C-C2C	4.41	1.46	1.36
12	B	835	CLA	C3D-C4D	-4.41	1.34	1.44
12	B	809	CLA	CHD-C1D	4.41	1.47	1.38
11	a	801	CL0	MG-ND	-4.41	1.97	2.05
12	j	102	CLA	CHC-C1C	4.41	1.47	1.38
12	F	203	CLA	C3C-C2C	4.41	1.46	1.36
12	b	823	CLA	C3D-C4D	-4.41	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	832	CLA	CHD-C1D	4.41	1.47	1.38
12	a	854	CLA	O2D-CGD	4.41	1.44	1.33
12	G	820	CLA	CHD-C1D	4.41	1.47	1.38
12	G	818	CLA	CHC-C4B	4.40	1.49	1.39
12	B	818	CLA	C3C-C2C	4.40	1.46	1.36
12	a	819	CLA	CHD-C1D	4.40	1.47	1.38
12	G	827	CLA	C3D-C4D	-4.40	1.34	1.44
12	a	814	CLA	CHC-C1C	4.40	1.47	1.38
12	B	811	CLA	C3C-C2C	4.40	1.46	1.36
12	b	815	CLA	CHC-C1C	4.40	1.47	1.38
12	G	855	CLA	O2D-CGD	4.40	1.44	1.33
12	G	804	CLA	C3D-C4D	-4.40	1.34	1.44
12	l	202	CLA	C3D-C4D	-4.40	1.34	1.44
12	b	801	CLA	O2D-CGD	4.40	1.44	1.33
12	B	835	CLA	CHC-C1C	4.40	1.47	1.38
12	A	854	CLA	O2D-CGD	4.40	1.44	1.33
12	G	829	CLA	C3C-C2C	4.40	1.46	1.36
12	S	202	CLA	CHC-C1C	4.40	1.47	1.38
12	B	814	CLA	CHC-C1C	4.40	1.47	1.38
16	G	854	LHG	O8-C23	4.40	1.46	1.33
12	b	829	CLA	O2D-CGD	4.39	1.44	1.33
12	A	819	CLA	CHC-C1C	4.39	1.47	1.38
12	a	838	CLA	C3C-C2C	4.39	1.46	1.36
12	G	837	CLA	O2D-CGD	4.39	1.44	1.33
12	a	826	CLA	C3D-C4D	-4.39	1.34	1.44
16	G	852	LHG	O8-C23	4.39	1.46	1.33
12	a	808	CLA	C3D-C4D	-4.39	1.34	1.44
12	G	855	CLA	CHC-C4B	4.39	1.49	1.39
12	G	840	CLA	C3D-C4D	-4.39	1.34	1.44
12	A	809	CLA	C3C-C2C	4.39	1.46	1.36
12	A	838	CLA	C3C-C2C	4.39	1.46	1.36
12	G	833	CLA	CHC-C1C	4.39	1.47	1.38
12	A	839	CLA	CHC-C1C	4.39	1.47	1.38
12	B	828	CLA	CHD-C1D	4.39	1.47	1.38
12	H	803	CLA	C3C-C2C	4.38	1.46	1.36
12	H	834	CLA	O2D-CGD	4.38	1.44	1.33
15	l	201	BCR	C10-C9	-4.38	1.25	1.35
12	L	202	CLA	C3C-C2C	4.38	1.46	1.36
12	B	827	CLA	CHD-C1D	4.38	1.47	1.38
12	b	832	CLA	C3D-C4D	-4.38	1.34	1.44
12	b	804	CLA	CHC-C1C	4.38	1.47	1.38
12	b	821	CLA	CHC-C1C	4.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	833	CLA	C3C-C2C	4.38	1.46	1.36
12	B	801	CLA	CHC-C1C	4.38	1.47	1.38
12	B	823	CLA	C3C-C2C	4.37	1.46	1.36
12	G	815	CLA	CHD-C1D	4.37	1.47	1.38
12	l	205	CLA	CHC-C1C	4.37	1.47	1.38
12	A	835	CLA	CHD-C1D	4.37	1.47	1.38
12	G	835	CLA	CHD-C1D	4.37	1.47	1.38
16	A	851	LHG	O8-C23	4.37	1.46	1.33
12	a	829	CLA	C3D-C4D	-4.37	1.34	1.44
12	B	811	CLA	CHC-C1C	4.37	1.47	1.38
12	B	830	CLA	CHD-C1D	4.37	1.46	1.38
12	A	828	CLA	C3C-C2C	4.37	1.46	1.36
12	A	807	CLA	CHC-C1C	4.37	1.47	1.38
12	a	813	CLA	CHC-C1C	4.37	1.47	1.38
12	a	835	CLA	C3C-C2C	4.37	1.46	1.36
12	F	201	CLA	C3C-C2C	4.37	1.46	1.36
12	b	812	CLA	CHC-C1C	4.37	1.47	1.38
12	A	808	CLA	C3C-C2C	4.37	1.46	1.36
12	G	830	CLA	C3D-C4D	-4.37	1.34	1.44
12	G	813	CLA	CHD-C1D	4.37	1.46	1.38
12	a	809	CLA	CHD-C1D	4.37	1.46	1.38
12	S	204	CLA	C3D-C4D	-4.37	1.34	1.44
12	a	807	CLA	CHC-C1C	4.37	1.47	1.38
12	H	804	CLA	C3D-C4D	-4.36	1.34	1.44
12	H	814	CLA	C3C-C2C	4.36	1.46	1.36
16	A	853	LHG	O8-C23	4.36	1.46	1.33
12	A	825	CLA	C3D-C4D	-4.36	1.34	1.44
12	B	805	CLA	C3D-C4D	-4.36	1.34	1.44
12	L	206	CLA	CHC-C1C	4.36	1.47	1.38
12	H	804	CLA	C3C-C2C	4.36	1.46	1.36
12	G	808	CLA	CHC-C1C	4.36	1.47	1.38
12	H	808	CLA	C3D-C4D	-4.36	1.34	1.44
12	G	842	CLA	C3C-C2C	4.36	1.46	1.36
12	L	206	CLA	C3D-C4D	-4.36	1.34	1.44
12	B	815	CLA	C3C-C2C	4.36	1.46	1.36
12	H	813	CLA	CHC-C1C	4.36	1.47	1.38
12	f	201	CLA	C3D-C4D	-4.36	1.34	1.44
12	a	814	CLA	CHD-C1D	4.36	1.46	1.38
12	H	830	CLA	O2D-CGD	4.36	1.43	1.33
12	b	802	CLA	C1D-ND	-4.36	1.32	1.37
12	b	805	CLA	C3D-C4D	-4.36	1.34	1.44
12	G	818	CLA	C3D-C4D	-4.35	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	816	CLA	C3D-C4D	-4.35	1.34	1.44
15	Q	101	BCR	C10-C9	-4.35	1.25	1.35
12	G	809	CLA	C3D-C4D	-4.35	1.34	1.44
12	H	822	CLA	C3D-C4D	-4.35	1.34	1.44
12	G	814	CLA	C3C-C2C	4.35	1.46	1.36
12	b	827	CLA	CHD-C1D	4.35	1.46	1.38
12	L	202	CLA	C3D-C4D	-4.35	1.34	1.44
12	a	829	CLA	CHD-C1D	4.35	1.46	1.38
12	a	833	CLA	CHC-C1C	4.35	1.47	1.38
12	G	834	CLA	CHD-C1D	4.35	1.46	1.38
12	l	202	CLA	CHD-C1D	4.35	1.46	1.38
12	l	206	CLA	C3D-C4D	-4.35	1.34	1.44
15	G	850	BCR	C10-C9	-4.35	1.25	1.35
15	b	840	BCR	C10-C9	-4.35	1.25	1.35
15	L	201	BCR	C10-C9	-4.35	1.25	1.35
12	b	803	CLA	C3D-C4D	-4.35	1.34	1.44
12	A	854	CLA	C3C-C2C	4.35	1.46	1.36
12	S	203	CLA	C3C-C2C	4.35	1.46	1.36
12	A	841	CLA	CHD-C1D	4.35	1.46	1.38
16	a	851	LHG	O8-C23	4.34	1.46	1.33
12	l	202	CLA	C3C-C2C	4.34	1.46	1.36
15	H	845	BCR	C10-C9	-4.34	1.25	1.35
12	b	836	CLA	C3D-C4D	-4.34	1.34	1.44
12	B	835	CLA	C3C-C2C	4.34	1.46	1.36
12	B	805	CLA	C3C-C2C	4.34	1.46	1.36
12	b	822	CLA	C3D-C4D	-4.34	1.34	1.44
12	H	815	CLA	CHD-C1D	4.34	1.46	1.38
12	f	201	CLA	CHD-C1D	4.34	1.46	1.38
12	a	807	CLA	CHD-C1D	4.34	1.46	1.38
12	B	808	CLA	C3D-C4D	-4.34	1.34	1.44
12	A	818	CLA	CHC-C1C	4.34	1.47	1.38
12	B	830	CLA	C3C-C2C	4.34	1.46	1.36
12	H	804	CLA	C1D-ND	-4.34	1.32	1.37
12	a	828	CLA	CHD-C1D	4.34	1.46	1.38
12	L	204	CLA	C3C-C2C	4.33	1.46	1.36
12	H	802	CLA	C3D-C4D	-4.33	1.34	1.44
12	a	825	CLA	CHD-C1D	4.33	1.46	1.38
12	H	822	CLA	CHC-C1C	4.33	1.47	1.38
12	b	815	CLA	C1B-NB	-4.33	1.32	1.37
12	A	822	CLA	C3D-C4D	-4.33	1.34	1.44
12	L	205	CLA	CHC-C1C	4.33	1.47	1.38
13	B	839	1L3	C23-C21	4.33	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	828	CLA	CHC-C1C	4.33	1.47	1.38
15	I	101	BCR	C10-C9	-4.33	1.25	1.35
12	A	814	CLA	CHD-C1D	4.33	1.46	1.38
12	B	804	CLA	CHC-C1C	4.33	1.47	1.38
12	B	812	CLA	C3C-C2C	4.33	1.46	1.36
15	H	842	BCR	C10-C9	-4.33	1.25	1.35
12	b	808	CLA	C3D-C4D	-4.33	1.34	1.44
12	B	810	CLA	C3C-C2C	4.33	1.46	1.36
12	B	829	CLA	C3D-C4D	-4.33	1.34	1.44
12	B	828	CLA	CHC-C1C	4.32	1.47	1.38
12	A	829	CLA	O2D-CGD	4.32	1.43	1.33
12	b	833	CLA	C3C-C2C	4.32	1.46	1.36
12	S	203	CLA	CHC-C1C	4.32	1.47	1.38
12	A	808	CLA	CHC-C1C	4.32	1.47	1.38
12	G	834	CLA	CHC-C1C	4.32	1.47	1.38
12	G	835	CLA	C3C-C2C	4.32	1.46	1.36
12	a	840	CLA	C3C-C2C	4.32	1.46	1.36
12	b	806	CLA	C3D-C4D	-4.32	1.34	1.44
12	A	803	CLA	C3D-C4D	-4.32	1.34	1.44
12	H	816	CLA	C3C-C2C	4.32	1.46	1.36
15	H	841	BCR	C10-C9	-4.32	1.25	1.35
12	G	814	CLA	CHC-C1C	4.32	1.47	1.38
12	a	837	CLA	CHD-C1D	4.32	1.46	1.38
12	B	830	CLA	CHC-C1C	4.31	1.47	1.38
12	B	837	CLA	C3D-C4D	-4.31	1.34	1.44
12	A	810	CLA	CHC-C1C	4.31	1.47	1.38
12	G	829	CLA	C3D-C4D	-4.31	1.34	1.44
12	b	805	CLA	C3C-C2C	4.31	1.46	1.36
12	A	829	CLA	CHD-C1D	4.31	1.46	1.38
12	b	826	CLA	C1B-NB	-4.31	1.32	1.37
15	i	101	BCR	C10-C9	-4.31	1.25	1.35
12	A	831	CLA	C3C-C2C	4.31	1.46	1.36
12	A	812	CLA	C3D-C4D	-4.31	1.34	1.44
15	J	102	BCR	C10-C9	-4.31	1.25	1.35
12	B	811	CLA	C3D-C4D	-4.31	1.34	1.44
12	A	808	CLA	C3D-C4D	-4.31	1.34	1.44
12	G	840	CLA	C3C-C2C	4.31	1.46	1.36
15	H	846	BCR	C10-C9	-4.31	1.25	1.35
12	a	809	CLA	C3C-C2C	4.31	1.46	1.36
12	A	829	CLA	C3D-C4D	-4.30	1.34	1.44
12	a	817	CLA	C3D-C4D	-4.30	1.34	1.44
12	G	819	CLA	CHD-C1D	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	803	CLA	C3D-C4D	-4.30	1.34	1.44
15	B	844	BCR	C10-C9	-4.30	1.25	1.35
12	A	834	CLA	CHC-C1C	4.30	1.47	1.38
12	l	204	CLA	C3C-C2C	4.30	1.46	1.36
12	H	830	CLA	C3D-C4D	-4.30	1.34	1.44
12	a	820	CLA	C3D-C4D	-4.30	1.34	1.44
12	b	830	CLA	C3C-C2C	4.30	1.46	1.36
12	H	808	CLA	C3C-C2C	4.30	1.46	1.36
15	a	844	BCR	C10-C9	-4.30	1.25	1.35
12	B	812	CLA	CHD-C1D	4.30	1.46	1.38
12	a	828	CLA	C3D-C4D	-4.30	1.34	1.44
12	f	201	CLA	C3C-C2C	4.30	1.46	1.36
12	A	840	CLA	C3D-C4D	-4.30	1.34	1.44
12	A	837	CLA	O2D-CGD	4.30	1.43	1.33
12	H	813	CLA	CHD-C1D	4.30	1.46	1.38
12	B	806	CLA	CHC-C1C	4.30	1.47	1.38
12	H	807	CLA	C3D-C4D	-4.29	1.34	1.44
12	b	825	CLA	C1B-NB	-4.29	1.32	1.37
12	H	836	CLA	C3C-C2C	4.29	1.46	1.36
15	B	841	BCR	C10-C9	-4.29	1.25	1.35
12	G	819	CLA	C3D-C4D	-4.29	1.34	1.44
12	G	814	CLA	C3D-C4D	-4.29	1.34	1.44
12	l	204	CLA	CHC-C1C	4.29	1.47	1.38
12	G	824	CLA	CHC-C1C	4.29	1.47	1.38
15	F	204	BCR	C10-C9	-4.29	1.25	1.35
12	G	812	CLA	CHD-C1D	4.29	1.46	1.38
12	H	814	CLA	CHD-C1D	4.29	1.46	1.38
12	b	802	CLA	CHC-C1C	4.29	1.47	1.38
15	b	843	BCR	C10-C9	-4.29	1.25	1.35
12	a	837	CLA	C3D-C4D	-4.29	1.34	1.44
12	b	834	CLA	C3C-C2C	4.29	1.46	1.36
12	G	827	CLA	C3C-C2C	4.29	1.46	1.36
12	A	810	CLA	C3D-C4D	-4.29	1.34	1.44
12	A	819	CLA	C3C-C2C	4.29	1.46	1.36
13	H	840	1L3	C23-C21	4.29	1.60	1.51
12	a	823	CLA	CHC-C1C	4.29	1.47	1.38
12	P	201	CLA	C3D-C4D	-4.29	1.34	1.44
15	R	102	BCR	C10-C9	-4.29	1.25	1.35
12	A	840	CLA	C3C-C2C	4.29	1.46	1.36
12	G	835	CLA	CHC-C1C	4.28	1.47	1.38
12	a	818	CLA	C3D-C4D	-4.28	1.34	1.44
12	H	838	CLA	C3D-C4D	-4.28	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	201	CLA	CHD-C1D	4.28	1.46	1.38
12	H	805	CLA	C3D-C4D	-4.28	1.34	1.44
12	G	805	CLA	CHD-C1D	4.28	1.46	1.38
12	L	205	CLA	C3C-C2C	4.28	1.46	1.36
12	H	829	CLA	CHC-C1C	4.28	1.47	1.38
12	G	831	CLA	C3C-C2C	4.28	1.46	1.36
12	B	803	CLA	C3C-C2C	4.28	1.46	1.36
12	H	806	CLA	C3D-C4D	-4.28	1.34	1.44
12	a	840	CLA	C3D-C4D	-4.28	1.34	1.44
12	b	803	CLA	CHD-C1D	4.28	1.46	1.38
12	L	202	CLA	CHD-C1D	4.28	1.46	1.38
12	a	813	CLA	C3C-C2C	4.28	1.46	1.36
12	b	831	CLA	C3D-C4D	-4.28	1.34	1.44
12	A	809	CLA	CHC-C1C	4.28	1.47	1.38
15	a	849	BCR	C10-C9	-4.28	1.25	1.35
15	B	840	BCR	C10-C9	-4.28	1.25	1.35
12	A	835	CLA	C3C-C2C	4.27	1.46	1.36
12	l	206	CLA	C3C-C2C	4.27	1.46	1.36
12	a	841	CLA	C3D-C4D	-4.27	1.34	1.44
12	G	815	CLA	CHC-C1C	4.27	1.47	1.38
15	j	103	BCR	C10-C9	-4.27	1.25	1.35
16	G	851	LHG	O7-C7	4.27	1.46	1.34
12	G	811	CLA	CHD-C1D	4.27	1.46	1.38
15	A	846	BCR	C10-C9	-4.27	1.25	1.35
12	G	811	CLA	C3C-C2C	4.27	1.46	1.36
12	b	848	CLA	C3C-C2C	4.27	1.46	1.36
12	A	806	CLA	C3C-C2C	4.27	1.46	1.36
12	a	833	CLA	C3C-C2C	4.27	1.46	1.36
12	L	206	CLA	CHD-C1D	4.27	1.46	1.38
12	H	812	CLA	C3D-C4D	-4.27	1.34	1.44
12	S	204	CLA	CHD-C1D	4.27	1.46	1.38
12	H	827	CLA	CHD-C4C	4.27	1.48	1.39
12	G	817	CLA	C3C-C2C	4.27	1.46	1.36
12	A	828	CLA	C1D-ND	-4.26	1.32	1.37
12	b	824	CLA	O2D-CGD	4.26	1.43	1.33
12	G	832	CLA	C3D-C4D	-4.26	1.34	1.44
12	b	826	CLA	MG-ND	-4.26	1.97	2.05
12	G	821	CLA	C3D-C4D	-4.26	1.34	1.44
12	a	810	CLA	CHD-C1D	4.26	1.46	1.38
13	b	838	1L3	C23-C21	4.26	1.60	1.51
12	A	816	CLA	C3C-C2C	4.26	1.46	1.36
11	a	801	CL0	CHB-C1B	4.26	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	206	CLA	CHD-C1D	4.26	1.46	1.38
12	G	819	CLA	CHC-C1C	4.26	1.47	1.38
12	a	804	CLA	CHC-C1C	4.26	1.47	1.38
12	a	810	CLA	C3C-C2C	4.26	1.46	1.36
12	B	832	CLA	C3D-C4D	-4.26	1.34	1.44
15	G	845	BCR	C10-C9	-4.26	1.26	1.35
12	b	826	CLA	CHD-C4C	4.26	1.48	1.39
12	b	811	CLA	C3D-C4D	-4.26	1.34	1.44
12	a	834	CLA	CHC-C1C	4.26	1.47	1.38
12	B	815	CLA	CHD-C4C	4.26	1.48	1.39
12	a	810	CLA	C3D-C4D	-4.26	1.34	1.44
12	j	102	CLA	C3D-C4D	-4.26	1.34	1.44
12	B	820	CLA	CHD-C1D	4.25	1.46	1.38
12	a	836	CLA	CHD-C4C	4.25	1.48	1.39
12	a	834	CLA	CHD-C1D	4.25	1.46	1.38
12	a	832	CLA	C3D-C4D	-4.25	1.34	1.44
12	b	823	CLA	C3C-C2C	4.25	1.45	1.36
12	H	850	CLA	C3C-C2C	4.25	1.45	1.36
12	H	802	CLA	CHC-C4B	4.25	1.48	1.39
12	B	826	CLA	C1D-ND	-4.25	1.32	1.37
12	A	834	CLA	C3D-C4D	-4.25	1.34	1.44
12	G	817	CLA	C3D-C4D	-4.25	1.34	1.44
12	a	841	CLA	CHD-C1D	4.24	1.46	1.38
12	b	807	CLA	C3D-C4D	-4.24	1.34	1.44
12	b	824	CLA	C4B-NB	-4.24	1.32	1.37
11	G	801	CL0	CHC-C1C	4.24	1.47	1.38
15	A	844	BCR	C10-C9	-4.24	1.26	1.35
12	H	833	CLA	C3D-C4D	-4.24	1.34	1.44
12	b	833	CLA	CHD-C1D	4.24	1.46	1.38
12	F	201	CLA	C3D-C4D	-4.24	1.34	1.44
12	A	810	CLA	CHD-C1D	4.24	1.46	1.38
12	H	832	CLA	C3C-C2C	4.24	1.45	1.36
12	A	832	CLA	C3D-C4D	-4.24	1.34	1.44
12	a	833	CLA	CHD-C1D	4.24	1.46	1.38
12	S	202	CLA	C3C-C2C	4.24	1.45	1.36
12	B	807	CLA	C3D-C4D	-4.24	1.34	1.44
12	A	838	CLA	CHC-C4B	4.24	1.48	1.39
12	A	833	CLA	C3C-C2C	4.24	1.45	1.36
12	a	835	CLA	CHD-C1D	4.24	1.46	1.38
12	A	818	CLA	C3D-C4D	-4.24	1.34	1.44
12	B	814	CLA	CHD-C1D	4.23	1.46	1.38
12	G	817	CLA	CHC-C1C	4.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	810	CLA	C3C-C2C	4.23	1.45	1.36
12	H	801	CLA	CHD-C1D	4.23	1.46	1.38
12	a	816	CLA	C3C-C2C	4.23	1.45	1.36
15	b	847	BCR	C10-C9	-4.23	1.26	1.35
12	G	837	CLA	CHD-C1D	4.23	1.46	1.38
12	b	833	CLA	C3D-C4D	-4.23	1.34	1.44
12	b	830	CLA	CHD-C1D	4.23	1.46	1.38
18	b	845	LMG	O8-C28	4.23	1.45	1.33
12	b	830	CLA	CHC-C1C	4.23	1.47	1.38
12	A	809	CLA	C3D-C4D	-4.23	1.34	1.44
12	H	823	CLA	C1D-ND	-4.23	1.32	1.37
12	B	833	CLA	C3C-C2C	4.22	1.45	1.36
12	S	204	CLA	C3C-C2C	4.22	1.45	1.36
12	G	820	CLA	C3D-C4D	-4.22	1.34	1.44
12	B	829	CLA	O2D-CGD	4.22	1.43	1.33
12	a	807	CLA	C3D-C4D	-4.22	1.34	1.44
12	A	811	CLA	C3D-C4D	-4.22	1.34	1.44
12	A	828	CLA	C3D-C4D	-4.22	1.34	1.44
12	A	841	CLA	C3D-C4D	-4.22	1.34	1.44
15	B	845	BCR	C10-C9	-4.22	1.26	1.35
12	a	819	CLA	C3D-C4D	-4.22	1.34	1.44
12	a	828	CLA	CHC-C1C	4.22	1.46	1.38
12	a	826	CLA	CHC-C4B	4.22	1.48	1.39
12	G	829	CLA	C1D-ND	-4.22	1.32	1.37
18	B	846	LMG	O8-C28	4.22	1.45	1.33
12	b	804	CLA	C3C-C2C	4.22	1.45	1.36
12	H	831	CLA	CHD-C1D	4.22	1.46	1.38
12	G	802	CLA	C3D-C4D	-4.22	1.34	1.44
12	B	817	CLA	C3D-C4D	-4.22	1.34	1.44
12	B	803	CLA	C3D-C4D	-4.22	1.34	1.44
12	G	855	CLA	C1D-ND	-4.21	1.32	1.37
12	A	823	CLA	CHC-C1C	4.21	1.46	1.38
12	A	819	CLA	C3D-C4D	-4.21	1.34	1.44
11	G	801	CL0	C3C-C2C	4.21	1.45	1.36
12	A	830	CLA	C3C-C2C	4.21	1.45	1.36
15	H	849	BCR	C10-C9	-4.21	1.26	1.35
12	P	201	CLA	C3C-C2C	4.21	1.45	1.36
12	B	834	CLA	C3C-C2C	4.21	1.45	1.36
12	B	830	CLA	C3D-C4D	-4.21	1.34	1.44
12	B	833	CLA	C3D-C4D	-4.21	1.34	1.44
12	B	821	CLA	C3C-C2C	4.21	1.45	1.36
12	H	809	CLA	C3D-C4D	-4.21	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	820	CLA	C3D-C4D	-4.20	1.34	1.44
15	B	842	BCR	C10-C9	-4.20	1.26	1.35
12	a	811	CLA	C3D-C4D	-4.20	1.34	1.44
12	b	837	CLA	C3D-C4D	-4.20	1.34	1.44
12	b	814	CLA	C3C-C2C	4.20	1.45	1.36
12	G	811	CLA	C3D-C4D	-4.20	1.34	1.44
12	L	206	CLA	C3C-C2C	4.20	1.45	1.36
12	H	808	CLA	CHD-C1D	4.20	1.46	1.38
12	a	831	CLA	C3D-C4D	-4.20	1.34	1.44
17	T	101	45D	C31-C29	4.20	1.56	1.43
15	P	204	BCR	C10-C9	-4.20	1.26	1.35
12	a	835	CLA	O2D-CGD	4.20	1.43	1.33
12	H	810	CLA	C3D-C4D	-4.20	1.34	1.44
12	A	810	CLA	C3C-C2C	4.20	1.45	1.36
12	A	823	CLA	C3D-C4D	-4.20	1.34	1.44
12	a	804	CLA	C3D-C4D	-4.20	1.34	1.44
12	B	816	CLA	C3D-C4D	-4.19	1.34	1.44
12	l	205	CLA	C3C-C2C	4.19	1.45	1.36
12	G	827	CLA	CHC-C4B	4.19	1.48	1.39
12	R	103	CLA	C3D-C4D	-4.19	1.34	1.44
12	A	802	CLA	C1B-NB	-4.19	1.32	1.37
12	b	806	CLA	CHC-C1C	4.19	1.46	1.38
12	G	825	CLA	C3D-C4D	-4.19	1.34	1.44
12	L	204	CLA	CHC-C1C	4.19	1.46	1.38
12	B	838	CLA	C3D-C4D	-4.19	1.34	1.44
15	b	844	BCR	C10-C9	-4.19	1.26	1.35
12	A	839	CLA	CHD-C4C	4.19	1.48	1.39
12	b	809	CLA	C3D-C4D	-4.18	1.34	1.44
12	A	837	CLA	CHD-C1D	4.18	1.46	1.38
12	a	803	CLA	C3D-C4D	-4.18	1.34	1.44
12	a	825	CLA	C3D-C4D	-4.18	1.34	1.44
12	a	830	CLA	CHC-C4B	4.18	1.48	1.39
12	H	815	CLA	C3C-C2C	4.18	1.45	1.36
12	A	833	CLA	CHD-C1D	4.18	1.46	1.38
12	b	816	CLA	C3D-C4D	-4.18	1.34	1.44
12	H	828	CLA	CHD-C1D	4.18	1.46	1.38
12	G	834	CLA	C3D-C4D	-4.18	1.34	1.44
12	G	808	CLA	C3D-C4D	-4.18	1.34	1.44
12	A	804	CLA	C3D-C4D	-4.18	1.34	1.44
12	A	820	CLA	C1C-NC	-4.18	1.31	1.37
12	H	817	CLA	C3D-C4D	-4.18	1.34	1.44
12	a	820	CLA	CHD-C4C	4.18	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	822	CLA	C3D-C4D	-4.18	1.34	1.44
12	a	812	CLA	CHD-C1D	4.18	1.46	1.38
12	G	824	CLA	C3D-C4D	-4.18	1.34	1.44
12	G	841	CLA	C3D-C4D	-4.17	1.34	1.44
11	G	801	CL0	CHB-C1B	4.17	1.48	1.39
12	B	804	CLA	C3C-C2C	4.17	1.45	1.36
15	H	843	BCR	C10-C9	-4.17	1.26	1.35
12	B	828	CLA	C3D-C4D	-4.17	1.34	1.44
12	A	815	CLA	C3D-C4D	-4.17	1.34	1.44
12	H	835	CLA	C3C-C2C	4.17	1.45	1.36
12	P	203	CLA	C3D-C4D	-4.17	1.34	1.44
12	A	828	CLA	CHD-C1D	4.17	1.46	1.38
12	a	823	CLA	C3D-C4D	-4.17	1.34	1.44
12	j	102	CLA	CHD-C1D	4.17	1.46	1.38
12	H	816	CLA	C4B-NB	-4.17	1.32	1.37
17	m	101	45D	C31-C29	4.17	1.56	1.43
12	F	203	CLA	C3D-C4D	-4.16	1.34	1.44
12	G	823	CLA	C3D-C4D	-4.16	1.34	1.44
12	A	837	CLA	C3D-C4D	-4.16	1.34	1.44
12	H	826	CLA	CHC-C1C	4.16	1.46	1.38
17	M	101	45D	C31-C29	4.16	1.56	1.43
11	A	801	CL0	CHC-C1C	4.16	1.46	1.38
12	H	821	CLA	CHD-C1D	4.16	1.46	1.38
12	H	819	CLA	C3D-C4D	-4.16	1.34	1.44
12	B	834	CLA	C3D-C4D	-4.16	1.34	1.44
18	H	847	LMG	O8-C28	4.16	1.45	1.33
12	H	821	CLA	C3D-C4D	-4.16	1.34	1.44
12	a	824	CLA	C3C-C2C	4.16	1.45	1.36
12	j	104	CLA	C3D-C4D	-4.16	1.34	1.44
12	B	822	CLA	C3D-C4D	-4.16	1.34	1.44
12	B	810	CLA	CHC-C1C	4.16	1.46	1.38
12	H	839	CLA	C3D-C4D	-4.16	1.34	1.44
12	a	830	CLA	C3C-C2C	4.16	1.45	1.36
12	G	803	CLA	CHD-C1D	4.16	1.46	1.38
15	J	104	BCR	C10-C9	-4.15	1.26	1.35
12	B	807	CLA	C1D-ND	-4.15	1.32	1.37
12	A	824	CLA	C1D-ND	-4.15	1.32	1.37
12	b	815	CLA	C3D-C4D	-4.15	1.34	1.44
12	G	805	CLA	C3D-C4D	-4.15	1.34	1.44
12	A	816	CLA	CHC-C1C	4.15	1.46	1.38
12	A	840	CLA	CHD-C1D	4.15	1.46	1.38
12	H	823	CLA	C3D-C4D	-4.15	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	818	CLA	C3D-C4D	-4.15	1.34	1.44
12	b	801	CLA	C3D-C4D	-4.15	1.34	1.44
12	H	834	CLA	C3D-C4D	-4.15	1.34	1.44
15	b	841	BCR	C10-C9	-4.15	1.26	1.35
12	H	829	CLA	C3D-C4D	-4.14	1.34	1.44
12	f	203	CLA	C3D-C4D	-4.14	1.34	1.44
12	a	809	CLA	CHC-C1C	4.14	1.46	1.38
11	a	801	CL0	CHC-C1C	4.14	1.46	1.38
12	G	813	CLA	CHC-C1C	4.14	1.46	1.38
12	H	814	CLA	C3D-C4D	-4.14	1.34	1.44
12	A	813	CLA	C3C-C2C	4.14	1.45	1.36
12	B	809	CLA	C3D-C4D	-4.14	1.34	1.44
11	A	801	CL0	C3C-C2C	4.14	1.45	1.36
12	j	104	CLA	CHC-C4B	4.14	1.48	1.39
12	b	829	CLA	CHD-C4C	4.14	1.48	1.39
12	b	835	CLA	CHD-C4C	4.14	1.48	1.39
12	a	802	CLA	CHD-C1D	4.14	1.46	1.38
12	b	819	CLA	C3D-C4D	-4.14	1.34	1.44
12	B	812	CLA	C3D-C4D	-4.14	1.34	1.44
12	A	830	CLA	CHC-C4B	4.14	1.48	1.39
12	b	813	CLA	C3D-C4D	-4.14	1.34	1.44
11	A	801	CL0	CHB-C1B	4.14	1.48	1.39
12	A	825	CLA	CHD-C1D	4.14	1.46	1.38
12	a	815	CLA	C3D-C4D	-4.13	1.34	1.44
12	b	817	CLA	C3D-C4D	-4.13	1.34	1.44
12	a	818	CLA	CHC-C1C	4.13	1.46	1.38
12	A	807	CLA	C3D-C4D	-4.13	1.34	1.44
12	A	817	CLA	CHD-C4C	4.13	1.48	1.39
12	A	816	CLA	C3D-C4D	-4.13	1.34	1.44
12	H	834	CLA	CHC-C1C	4.13	1.46	1.38
12	b	831	CLA	CHD-C4C	4.13	1.48	1.39
12	A	813	CLA	CHD-C1D	4.13	1.46	1.38
12	a	814	CLA	C3D-C4D	-4.13	1.34	1.44
12	B	816	CLA	CHD-C4C	4.13	1.48	1.39
12	l	204	CLA	C3D-C4D	-4.13	1.34	1.44
12	H	839	CLA	C3C-C2C	4.13	1.45	1.36
12	G	824	CLA	C3C-C2C	4.13	1.45	1.36
12	G	842	CLA	C3D-C4D	-4.13	1.34	1.44
12	G	818	CLA	CHD-C4C	4.12	1.48	1.39
15	A	849	BCR	C10-C9	-4.12	1.26	1.35
12	H	850	CLA	C3D-C4D	-4.12	1.34	1.44
12	G	828	CLA	C3C-C2C	4.12	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	821	CLA	CHD-C4C	4.12	1.48	1.39
12	G	814	CLA	CHD-C4C	4.12	1.48	1.39
12	G	829	CLA	CHD-C1D	4.12	1.46	1.38
12	a	838	CLA	CHC-C4B	4.12	1.48	1.39
12	A	814	CLA	C3D-C4D	-4.12	1.34	1.44
12	G	837	CLA	C3D-C4D	-4.12	1.34	1.44
12	L	205	CLA	C3D-C4D	-4.12	1.34	1.44
12	H	809	CLA	CHC-C1C	4.12	1.46	1.38
12	J	103	CLA	C3D-C4D	-4.12	1.34	1.44
12	b	815	CLA	CHD-C1D	4.12	1.46	1.38
12	G	856	CLA	CHC-C4B	4.12	1.48	1.39
12	B	813	CLA	C3D-C4D	-4.12	1.34	1.44
12	a	828	CLA	C1D-ND	-4.11	1.32	1.37
12	G	816	CLA	C3D-C4D	-4.11	1.34	1.44
12	B	819	CLA	C3D-C4D	-4.11	1.34	1.44
12	G	839	CLA	C3D-C4D	-4.11	1.34	1.44
12	A	807	CLA	CHD-C1D	4.11	1.46	1.38
12	B	807	CLA	C1B-NB	-4.11	1.32	1.37
12	A	808	CLA	CHD-C4C	4.11	1.48	1.39
12	l	204	CLA	CHD-C1D	4.11	1.46	1.38
12	a	813	CLA	C3D-C4D	-4.11	1.34	1.44
12	b	828	CLA	C3D-C4D	-4.11	1.34	1.44
12	b	818	CLA	C3D-C4D	-4.11	1.34	1.44
12	B	806	CLA	CHD-C1D	4.11	1.46	1.38
12	B	820	CLA	C3D-C4D	-4.11	1.34	1.44
12	a	818	CLA	C3C-C2C	4.11	1.45	1.36
12	b	820	CLA	C3D-C4D	-4.11	1.34	1.44
12	G	826	CLA	CHD-C1D	4.11	1.46	1.38
12	a	839	CLA	CHD-C4C	4.10	1.48	1.39
12	H	820	CLA	C3D-C4D	-4.10	1.35	1.44
12	a	812	CLA	C3D-C4D	-4.10	1.35	1.44
12	B	826	CLA	MG-ND	-4.10	1.97	2.05
12	H	806	CLA	C3C-C2C	4.10	1.45	1.36
12	G	839	CLA	CHD-C4C	4.10	1.48	1.39
12	H	835	CLA	C3D-C4D	-4.10	1.35	1.44
12	H	817	CLA	CHD-C4C	4.10	1.48	1.39
12	B	826	CLA	CHD-C4C	4.10	1.48	1.39
12	a	824	CLA	C1D-ND	-4.09	1.32	1.37
12	G	831	CLA	CHC-C4B	4.09	1.48	1.39
12	G	812	CLA	C3D-C4D	-4.09	1.35	1.44
12	B	822	CLA	C1D-ND	-4.09	1.32	1.37
12	a	827	CLA	C3C-C2C	4.09	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	806	CLA	C3C-C2C	4.09	1.45	1.36
12	B	820	CLA	C3C-C2C	4.09	1.45	1.36
12	B	808	CLA	CHC-C1C	4.09	1.46	1.38
12	B	836	CLA	CHD-C4C	4.09	1.48	1.39
12	H	808	CLA	CHC-C4B	4.09	1.48	1.39
12	B	829	CLA	CHD-C4C	4.09	1.48	1.39
12	H	810	CLA	CHC-C4B	4.09	1.48	1.39
12	f	201	CLA	CHC-C4B	4.08	1.48	1.39
12	a	808	CLA	CHD-C4C	4.08	1.48	1.39
12	H	822	CLA	C1B-NB	-4.08	1.32	1.37
12	H	805	CLA	CHD-C1D	4.08	1.46	1.38
12	A	818	CLA	CHD-C1D	4.08	1.46	1.38
12	H	833	CLA	CHD-C4C	4.08	1.48	1.39
12	A	824	CLA	C3C-C2C	4.08	1.45	1.36
12	G	809	CLA	CHD-C4C	4.08	1.48	1.39
12	L	205	CLA	C1D-ND	-4.08	1.32	1.37
12	b	834	CLA	CHC-C4B	4.08	1.48	1.39
12	H	834	CLA	CHD-C1D	4.08	1.46	1.38
12	H	825	CLA	C3C-C2C	4.08	1.45	1.36
12	G	838	CLA	CHC-C4B	4.08	1.48	1.39
12	b	837	CLA	CHD-C1D	4.07	1.46	1.38
12	H	830	CLA	CHD-C4C	4.07	1.48	1.39
12	B	801	CLA	C3D-C4D	-4.07	1.35	1.44
12	B	805	CLA	CHD-C1D	4.07	1.46	1.38
12	j	104	CLA	CHD-C4C	4.07	1.48	1.39
12	H	827	CLA	C1D-ND	-4.07	1.32	1.37
12	H	813	CLA	C3D-C4D	-4.07	1.35	1.44
12	b	812	CLA	C3D-C4D	-4.07	1.35	1.44
12	H	837	CLA	CHD-C4C	4.07	1.48	1.39
12	B	831	CLA	C3D-C4D	-4.07	1.35	1.44
12	S	203	CLA	C1D-ND	-4.07	1.32	1.37
12	a	831	CLA	CHD-C4C	4.07	1.48	1.39
12	b	816	CLA	CHD-C4C	4.07	1.48	1.39
12	G	832	CLA	CHD-C4C	4.07	1.48	1.39
12	b	830	CLA	C3D-C4D	-4.07	1.35	1.44
12	H	818	CLA	C3D-C4D	-4.07	1.35	1.44
12	H	832	CLA	CHD-C1D	4.07	1.46	1.38
12	H	813	CLA	C3C-C2C	4.07	1.45	1.36
12	G	810	CLA	C3D-C4D	-4.07	1.35	1.44
12	a	839	CLA	C3D-C4D	-4.07	1.35	1.44
12	b	807	CLA	C1B-NB	-4.06	1.32	1.37
12	B	815	CLA	CHD-C1D	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	836	CLA	CHD-C1D	4.06	1.46	1.38
12	H	832	CLA	C3D-C4D	-4.06	1.35	1.44
11	a	801	CL0	C3C-C2C	4.06	1.45	1.36
12	H	837	CLA	CHC-C4B	4.06	1.48	1.39
12	b	808	CLA	CHC-C1C	4.06	1.46	1.38
12	L	204	CLA	C3D-C4D	-4.06	1.35	1.44
12	B	817	CLA	CHD-C1D	4.06	1.46	1.38
12	H	818	CLA	CHD-C1D	4.06	1.46	1.38
12	a	809	CLA	C3D-C4D	-4.06	1.35	1.44
12	G	856	CLA	C3D-C4D	-4.06	1.35	1.44
12	a	804	CLA	CHD-C4C	4.05	1.48	1.39
12	B	825	CLA	C1B-NB	-4.05	1.32	1.37
12	b	810	CLA	CHC-C1C	4.05	1.46	1.38
12	H	807	CLA	C3C-C2C	4.05	1.45	1.36
12	A	839	CLA	C3D-C4D	-4.05	1.35	1.44
12	a	828	CLA	C3C-C2C	4.05	1.45	1.36
12	H	811	CLA	C3C-C2C	4.05	1.45	1.36
12	G	835	CLA	C3D-C4D	-4.05	1.35	1.44
12	F	201	CLA	CHC-C4B	4.05	1.48	1.39
12	H	811	CLA	CHD-C1D	4.05	1.46	1.38
12	H	836	CLA	CHC-C4B	4.05	1.48	1.39
12	S	202	CLA	CHD-C1D	4.05	1.46	1.38
13	a	842	1L3	C23-C21	4.05	1.59	1.51
12	G	815	CLA	C3D-C4D	-4.05	1.35	1.44
12	B	836	CLA	CHC-C4B	4.05	1.48	1.39
12	G	833	CLA	CHD-C1D	4.05	1.46	1.38
12	L	204	CLA	CHD-C1D	4.05	1.46	1.38
12	A	803	CLA	CHC-C4B	4.05	1.48	1.39
12	G	825	CLA	C3C-C2C	4.05	1.45	1.36
12	B	806	CLA	C3D-C4D	-4.05	1.35	1.44
12	B	832	CLA	CHD-C4C	4.04	1.48	1.39
12	b	809	CLA	CHC-C4B	4.04	1.48	1.39
12	B	809	CLA	CHC-C4B	4.04	1.48	1.39
12	b	848	CLA	C3D-C4D	-4.04	1.35	1.44
12	b	801	CLA	C3C-C2C	4.04	1.45	1.36
12	H	819	CLA	CHD-C4C	4.04	1.48	1.39
12	B	837	CLA	CHB-C1B	4.04	1.48	1.39
12	G	819	CLA	C3C-C2C	4.04	1.45	1.36
12	H	826	CLA	CHD-C1D	4.03	1.46	1.38
12	G	841	CLA	C3C-C2C	4.03	1.45	1.36
12	G	822	CLA	C3D-C4D	-4.03	1.35	1.44
12	A	835	CLA	C3D-C4D	-4.03	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	850	LHG	O7-C7	4.03	1.45	1.34
12	A	819	CLA	CHD-C4C	4.03	1.48	1.39
12	b	848	CLA	CHD-C1D	4.03	1.46	1.38
12	G	831	CLA	CHD-C1D	4.03	1.46	1.38
12	b	827	CLA	CHD-C4C	4.03	1.48	1.39
12	A	813	CLA	CHD-C4C	4.03	1.48	1.39
12	A	821	CLA	CHD-C4C	4.02	1.48	1.39
12	a	806	CLA	C3C-C2C	4.02	1.45	1.36
12	a	840	CLA	CHD-C1D	4.02	1.46	1.38
12	B	806	CLA	C3C-C2C	4.02	1.45	1.36
12	A	821	CLA	C3D-C4D	-4.02	1.35	1.44
18	H	847	LMG	O7-C10	4.02	1.45	1.34
12	b	807	CLA	C3C-C2C	4.02	1.45	1.36
12	S	202	CLA	C3D-C4D	-4.02	1.35	1.44
12	b	813	CLA	CHD-C1D	4.02	1.46	1.38
12	a	841	CLA	C3C-C2C	4.02	1.45	1.36
12	B	814	CLA	C3C-C2C	4.02	1.45	1.36
12	G	840	CLA	CHD-C1D	4.02	1.46	1.38
12	b	820	CLA	C3C-C2C	4.02	1.45	1.36
12	H	803	CLA	CHD-C1D	4.01	1.46	1.38
12	B	815	CLA	C1D-ND	-4.01	1.32	1.37
12	A	855	CLA	CHC-C4B	4.01	1.48	1.39
12	b	820	CLA	CHD-C1D	4.01	1.46	1.38
12	A	817	CLA	CHD-C1D	4.01	1.46	1.38
12	H	850	CLA	CHD-C1D	4.01	1.46	1.38
12	b	821	CLA	CHD-C1D	4.01	1.46	1.38
16	a	850	LHG	O8-C23	4.01	1.45	1.33
12	b	818	CLA	CHD-C4C	4.01	1.48	1.39
12	A	841	CLA	C3C-C2C	4.01	1.45	1.36
12	b	825	CLA	CHC-C1C	4.00	1.46	1.38
12	B	813	CLA	CHC-C4B	4.00	1.48	1.39
12	a	817	CLA	CHC-C4B	4.00	1.48	1.39
12	H	838	CLA	CHD-C1D	4.00	1.46	1.38
12	A	841	CLA	CHB-C1B	4.00	1.48	1.39
12	A	815	CLA	CHD-C4C	4.00	1.48	1.39
12	B	833	CLA	CHC-C1C	4.00	1.46	1.38
12	f	203	CLA	CHD-C4C	4.00	1.48	1.39
12	G	805	CLA	C3C-C2C	4.00	1.45	1.36
12	B	818	CLA	CHD-C4C	4.00	1.48	1.39
16	G	854	LHG	O7-C7	4.00	1.45	1.34
12	B	801	CLA	C3C-C2C	4.00	1.45	1.36
12	A	804	CLA	CHD-C4C	4.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	803	CLA	CHC-C4B	3.99	1.48	1.39
12	G	822	CLA	CHD-C4C	3.99	1.48	1.39
12	H	822	CLA	MG-ND	-3.99	1.97	2.05
12	H	809	CLA	CHD-C4C	3.99	1.48	1.39
12	a	834	CLA	C3D-C4D	-3.99	1.35	1.44
12	a	835	CLA	C3D-C4D	-3.99	1.35	1.44
12	S	203	CLA	C3D-C4D	-3.99	1.35	1.44
12	a	821	CLA	CHD-C4C	3.99	1.48	1.39
12	H	807	CLA	C1B-NB	-3.99	1.32	1.37
12	A	836	CLA	CHD-C1D	3.99	1.46	1.38
12	B	808	CLA	CHD-C4C	3.99	1.48	1.39
12	B	803	CLA	CHD-C4C	3.99	1.48	1.39
12	l	205	CLA	C3D-C4D	-3.99	1.35	1.44
12	a	854	CLA	C3D-C4D	-3.98	1.35	1.44
12	R	103	CLA	CHD-C4C	3.98	1.48	1.39
12	B	835	CLA	CHC-C4B	3.98	1.48	1.39
12	G	820	CLA	C3C-C2C	3.98	1.45	1.36
12	b	815	CLA	C3C-C2C	3.98	1.45	1.36
12	a	821	CLA	C3D-C4D	-3.97	1.35	1.44
12	b	821	CLA	C1B-NB	-3.97	1.32	1.37
12	G	807	CLA	C3C-C2C	3.97	1.45	1.36
12	a	817	CLA	CHD-C4C	3.97	1.48	1.39
12	A	827	CLA	C3C-C2C	3.97	1.45	1.36
12	B	815	CLA	CHC-C1C	3.97	1.46	1.38
12	A	802	CLA	CHD-C1D	3.97	1.46	1.38
12	A	804	CLA	C3C-C2C	3.97	1.45	1.36
12	H	821	CLA	C3C-C2C	3.96	1.45	1.36
12	b	834	CLA	CHD-C1D	3.96	1.46	1.38
12	H	816	CLA	OBD-CAD	3.96	1.29	1.22
12	H	811	CLA	CHC-C1C	3.96	1.46	1.38
12	G	841	CLA	CHC-C1C	3.96	1.46	1.38
13	G	843	1L3	C23-C21	3.96	1.59	1.51
12	B	813	CLA	CHD-C1D	3.96	1.46	1.38
12	B	803	CLA	CHD-C1D	3.96	1.46	1.38
12	A	805	CLA	CHC-C4B	3.96	1.48	1.39
12	G	840	CLA	CHC-C4B	3.96	1.48	1.39
12	l	202	CLA	CHC-C4B	3.96	1.48	1.39
12	b	824	CLA	MG-ND	-3.96	1.97	2.05
12	G	816	CLA	CHD-C4C	3.96	1.48	1.39
12	B	835	CLA	CHD-C1D	3.96	1.46	1.38
12	a	815	CLA	CHD-C4C	3.96	1.48	1.39
12	H	824	CLA	CHD-C1D	3.96	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	806	CLA	CHB-C1B	3.96	1.48	1.39
12	a	841	CLA	CHC-C1C	3.96	1.46	1.38
12	A	831	CLA	CHD-C1D	3.96	1.46	1.38
12	F	203	CLA	CHD-C4C	3.95	1.48	1.39
13	A	842	1L3	C23-C21	3.95	1.59	1.51
16	A	853	LHG	O7-C7	3.95	1.45	1.34
12	A	820	CLA	C4B-NB	-3.95	1.32	1.37
16	A	850	LHG	O7-C7	3.95	1.45	1.34
12	A	810	CLA	CHD-C4C	3.95	1.48	1.39
12	H	829	CLA	CHD-C4C	3.95	1.48	1.39
12	A	822	CLA	CHD-C4C	3.95	1.48	1.39
12	A	821	CLA	CHD-C1D	3.95	1.46	1.38
12	G	803	CLA	C1B-NB	-3.95	1.32	1.37
12	b	837	CLA	C3C-C2C	3.95	1.45	1.36
12	B	834	CLA	CHD-C1D	3.95	1.46	1.38
12	A	813	CLA	OBD-CAD	3.95	1.29	1.22
12	A	820	CLA	CHD-C4C	3.94	1.48	1.39
12	G	802	CLA	C3C-C2C	3.94	1.45	1.36
12	G	855	CLA	C3D-C4D	-3.94	1.35	1.44
12	B	815	CLA	C3D-C4D	-3.94	1.35	1.44
12	B	838	CLA	CHD-C1D	3.94	1.46	1.38
12	H	826	CLA	C1B-NB	-3.94	1.32	1.37
12	A	805	CLA	CHD-C1D	3.94	1.46	1.38
12	P	203	CLA	CHD-C4C	3.94	1.48	1.39
12	B	813	CLA	CHD-C4C	3.94	1.48	1.39
12	G	811	CLA	CHD-C4C	3.94	1.48	1.39
12	G	842	CLA	CHD-C1D	3.94	1.46	1.38
12	b	805	CLA	CHC-C4B	3.94	1.48	1.39
12	a	823	CLA	C3C-C2C	3.94	1.45	1.36
12	b	805	CLA	CHD-C1D	3.94	1.46	1.38
12	L	202	CLA	CHC-C4B	3.93	1.48	1.39
12	G	804	CLA	CHC-C4B	3.93	1.48	1.39
12	b	807	CLA	CHD-C1D	3.93	1.46	1.38
12	H	831	CLA	CHC-C1C	3.93	1.46	1.38
12	H	825	CLA	C1C-NC	-3.93	1.31	1.37
12	B	823	CLA	CHD-C1D	3.93	1.46	1.38
12	H	822	CLA	C3C-C2C	3.93	1.45	1.36
12	A	805	CLA	C3C-C2C	3.93	1.45	1.36
12	b	821	CLA	C3C-C2C	3.93	1.45	1.36
12	b	808	CLA	CHD-C4C	3.93	1.48	1.39
12	a	816	CLA	CHC-C1C	3.93	1.46	1.38
12	G	836	CLA	CHD-C4C	3.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	855	CLA	C3D-C4D	-3.93	1.35	1.44
12	B	838	CLA	C3C-C2C	3.92	1.45	1.36
12	a	832	CLA	CHD-C4C	3.92	1.48	1.39
12	A	805	CLA	CHD-C4C	3.92	1.48	1.39
12	b	823	CLA	CHC-C4B	3.92	1.48	1.39
12	A	809	CLA	CHD-C4C	3.92	1.48	1.39
12	H	827	CLA	MG-ND	-3.92	1.98	2.05
12	H	820	CLA	CHD-C4C	3.92	1.48	1.39
12	B	825	CLA	CHC-C1C	3.92	1.46	1.38
16	A	850	LHG	O8-C23	3.92	1.44	1.33
12	B	824	CLA	CHC-C1C	3.92	1.46	1.38
12	b	813	CLA	CHD-C4C	3.92	1.48	1.39
12	B	825	CLA	CHD-C1D	3.92	1.46	1.38
12	a	813	CLA	CHD-C4C	3.92	1.48	1.39
12	H	802	CLA	CHB-C1B	3.92	1.48	1.39
12	b	835	CLA	CHC-C4B	3.92	1.48	1.39
12	B	802	CLA	CHC-C4B	3.91	1.48	1.39
12	b	812	CLA	CHD-C1D	3.91	1.46	1.38
12	B	821	CLA	CHD-C1D	3.91	1.46	1.38
12	P	201	CLA	CHC-C4B	3.91	1.48	1.39
12	a	840	CLA	CHC-C4B	3.91	1.48	1.39
12	B	827	CLA	CHC-C4B	3.91	1.48	1.39
16	a	853	LHG	O7-C7	3.91	1.45	1.34
12	H	805	CLA	CHC-C4B	3.91	1.48	1.39
12	a	855	CLA	CHC-C4B	3.91	1.48	1.39
12	J	103	CLA	CHC-C4B	3.91	1.48	1.39
12	a	824	CLA	CHB-C1B	3.91	1.48	1.39
12	B	804	CLA	C1D-ND	-3.91	1.32	1.37
12	H	825	CLA	CHC-C1C	3.91	1.46	1.38
12	a	805	CLA	CHD-C4C	3.91	1.48	1.39
12	b	814	CLA	CHD-C4C	3.91	1.48	1.39
12	A	832	CLA	CHD-C4C	3.90	1.48	1.39
12	J	103	CLA	CHD-C4C	3.90	1.48	1.39
12	A	817	CLA	C1D-ND	-3.90	1.32	1.37
12	A	823	CLA	C3C-C2C	3.90	1.45	1.36
12	G	823	CLA	CHD-C4C	3.90	1.48	1.39
12	l	206	CLA	CHB-C1B	3.90	1.48	1.39
12	B	836	CLA	C1B-NB	-3.90	1.32	1.37
12	B	819	CLA	CHD-C4C	3.90	1.48	1.39
18	b	845	LMG	O7-C10	3.90	1.45	1.34
12	B	830	CLA	CHD-C4C	3.90	1.48	1.39
12	H	828	CLA	CHD-C4C	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	201	BCR	C11-C12	-3.90	1.24	1.34
12	b	828	CLA	CHD-C4C	3.90	1.48	1.39
12	b	817	CLA	CHD-C1D	3.90	1.46	1.38
12	G	806	CLA	CHD-C1D	3.90	1.46	1.38
12	b	813	CLA	CHC-C4B	3.90	1.48	1.39
12	B	824	CLA	C1D-ND	-3.89	1.32	1.37
12	b	824	CLA	C3C-C2C	3.89	1.45	1.36
12	G	810	CLA	CHD-C4C	3.89	1.48	1.39
12	G	830	CLA	C1B-NB	-3.89	1.32	1.37
12	H	814	CLA	CHC-C4B	3.89	1.48	1.39
12	B	828	CLA	CHD-C4C	3.89	1.48	1.39
12	H	803	CLA	CHD-C4C	3.89	1.48	1.39
12	b	804	CLA	C1D-ND	-3.89	1.32	1.37
12	a	841	CLA	CHB-C1B	3.89	1.48	1.39
12	A	840	CLA	CHC-C4B	3.89	1.48	1.39
12	a	809	CLA	CHB-C1B	3.89	1.48	1.39
12	H	806	CLA	CHD-C1D	3.89	1.46	1.38
12	B	820	CLA	CHC-C4B	3.89	1.48	1.39
12	A	836	CLA	CHD-C4C	3.89	1.48	1.39
12	H	805	CLA	CHB-C1B	3.88	1.48	1.39
12	A	809	CLA	CHB-C1B	3.88	1.48	1.39
12	G	814	CLA	OBD-CAD	3.88	1.29	1.22
12	B	807	CLA	C3C-C2C	3.88	1.45	1.36
12	A	838	CLA	CHB-C1B	3.88	1.48	1.39
12	H	817	CLA	CHC-C4B	3.88	1.48	1.39
12	B	831	CLA	CHC-C4B	3.88	1.48	1.39
12	H	801	CLA	CHD-C4C	3.88	1.48	1.39
12	H	836	CLA	CHD-C1D	3.88	1.46	1.38
12	A	854	CLA	C3D-C4D	-3.88	1.35	1.44
12	H	810	CLA	CHD-C4C	3.88	1.48	1.39
12	B	833	CLA	CHD-C1D	3.88	1.46	1.38
12	A	803	CLA	CHD-C4C	3.88	1.48	1.39
12	b	825	CLA	CHD-C1D	3.88	1.46	1.38
12	b	829	CLA	CHD-C1D	3.88	1.46	1.38
12	H	825	CLA	MG-ND	-3.88	1.98	2.05
12	R	103	CLA	CHC-C4B	3.87	1.48	1.39
12	S	204	CLA	CHB-C1B	3.87	1.48	1.39
12	G	835	CLA	CHD-C4C	3.87	1.48	1.39
12	a	829	CLA	C1B-NB	-3.87	1.32	1.37
12	B	837	CLA	CHD-C1D	3.87	1.46	1.38
12	a	822	CLA	CHD-C4C	3.87	1.48	1.39
11	a	801	CL0	C1B-NB	-3.87	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	810	CLA	CHB-C1B	3.87	1.48	1.39
12	a	818	CLA	CHD-C4C	3.87	1.48	1.39
12	A	811	CLA	CHD-C4C	3.87	1.48	1.39
12	L	206	CLA	CHB-C1B	3.87	1.48	1.39
12	G	829	CLA	CHC-C4B	3.87	1.48	1.39
12	A	825	CLA	CHC-C4B	3.86	1.48	1.39
12	b	832	CLA	CHB-C1B	3.86	1.48	1.39
12	H	830	CLA	CHD-C1D	3.86	1.45	1.38
12	a	805	CLA	C3C-C2C	3.86	1.45	1.36
12	S	202	CLA	C1D-ND	-3.86	1.32	1.37
12	a	837	CLA	CHD-C4C	3.86	1.48	1.39
12	A	830	CLA	C1D-ND	-3.86	1.32	1.37
12	B	802	CLA	CHB-C1B	3.86	1.48	1.39
12	a	807	CLA	CHD-C4C	3.86	1.48	1.39
12	b	820	CLA	CHC-C4B	3.86	1.48	1.39
15	l	203	BCR	C11-C12	-3.86	1.24	1.34
15	L	203	BCR	C11-C12	-3.86	1.24	1.34
12	b	832	CLA	CHD-C1D	3.86	1.45	1.38
12	H	824	CLA	CHC-C4B	3.86	1.48	1.39
12	G	821	CLA	C1B-NB	-3.86	1.32	1.37
12	a	805	CLA	CHD-C1D	3.86	1.45	1.38
12	A	837	CLA	CHD-C4C	3.86	1.48	1.39
12	b	824	CLA	CHC-C1C	3.86	1.46	1.38
12	B	829	CLA	C1D-ND	-3.86	1.32	1.37
12	H	831	CLA	CHD-C4C	3.86	1.48	1.39
12	H	838	CLA	C1C-NC	-3.86	1.31	1.37
12	a	819	CLA	C3C-C2C	3.85	1.45	1.36
12	b	803	CLA	CHD-C4C	3.85	1.48	1.39
12	B	824	CLA	C1C-NC	-3.85	1.31	1.37
12	F	203	CLA	CHC-C4B	3.85	1.48	1.39
12	a	811	CLA	CHD-C4C	3.85	1.48	1.39
12	b	809	CLA	CHD-C4C	3.85	1.48	1.39
12	b	835	CLA	C1D-ND	-3.85	1.32	1.37
12	B	824	CLA	C3C-C2C	3.85	1.45	1.36
12	b	819	CLA	CHD-C4C	3.85	1.48	1.39
12	A	836	CLA	CHC-C4B	3.85	1.48	1.39
12	a	830	CLA	CHD-C1D	3.85	1.45	1.38
12	a	810	CLA	CHD-C4C	3.85	1.48	1.39
12	A	830	CLA	CHD-C1D	3.85	1.45	1.38
12	a	802	CLA	C1B-NB	-3.85	1.32	1.37
12	l	205	CLA	C1D-ND	-3.85	1.32	1.37
12	a	804	CLA	C3C-C2C	3.85	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	824	CLA	CHD-C4C	3.85	1.48	1.39
12	B	827	CLA	CHD-C4C	3.85	1.48	1.39
12	H	828	CLA	CHC-C4B	3.85	1.48	1.39
12	a	838	CLA	CHB-C1B	3.85	1.48	1.39
12	G	805	CLA	CHC-C4B	3.84	1.48	1.39
12	H	804	CLA	CHC-C4B	3.84	1.48	1.39
12	G	818	CLA	CHD-C1D	3.84	1.45	1.38
12	H	823	CLA	CHC-C4B	3.84	1.48	1.39
12	H	818	CLA	CHC-C4B	3.84	1.48	1.39
12	A	826	CLA	CHD-C1D	3.84	1.45	1.38
12	b	805	CLA	CHB-C1B	3.84	1.48	1.39
12	G	828	CLA	C1D-ND	-3.84	1.32	1.37
12	b	802	CLA	CHB-C1B	3.84	1.48	1.39
12	A	822	CLA	OBD-CAD	3.84	1.29	1.22
12	B	822	CLA	CHC-C4B	3.84	1.48	1.39
12	a	820	CLA	C1B-NB	-3.84	1.32	1.37
12	B	836	CLA	C1D-ND	-3.84	1.32	1.37
12	H	815	CLA	CHD-C4C	3.84	1.47	1.39
12	a	805	CLA	CHC-C4B	3.83	1.48	1.39
12	B	823	CLA	CHC-C4B	3.83	1.48	1.39
15	G	849	BCR	C11-C12	-3.83	1.24	1.34
12	B	838	CLA	CHC-C4B	3.83	1.48	1.39
12	A	829	CLA	C1B-NB	-3.83	1.32	1.37
12	A	841	CLA	CHC-C1C	3.83	1.46	1.38
12	b	806	CLA	CHD-C1D	3.83	1.45	1.38
12	H	839	CLA	CHC-C4B	3.83	1.48	1.39
12	G	826	CLA	CHC-C4B	3.83	1.48	1.39
12	B	809	CLA	CHD-C4C	3.83	1.47	1.39
12	H	813	CLA	CHD-C4C	3.83	1.47	1.39
12	H	835	CLA	CHD-C1D	3.83	1.45	1.38
12	b	827	CLA	CHC-C4B	3.83	1.48	1.39
12	G	803	CLA	C3C-C2C	3.83	1.45	1.36
12	H	803	CLA	C1D-ND	-3.82	1.32	1.37
12	b	836	CLA	C1C-NC	-3.82	1.31	1.37
12	G	825	CLA	CHB-C1B	3.82	1.48	1.39
12	G	834	CLA	CHC-C4B	3.82	1.48	1.39
12	b	811	CLA	CHD-C4C	3.82	1.47	1.39
12	b	822	CLA	CHC-C4B	3.82	1.48	1.39
12	a	825	CLA	CHC-C4B	3.82	1.48	1.39
12	B	806	CLA	C1B-NB	-3.82	1.32	1.37
12	G	841	CLA	CHB-C1B	3.82	1.48	1.39
12	a	803	CLA	CHD-C4C	3.82	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	812	CLA	CHD-C4C	3.82	1.47	1.39
12	G	822	CLA	CHC-C4B	3.82	1.48	1.39
12	b	818	CLA	CHC-C4B	3.82	1.48	1.39
12	a	827	CLA	C1D-ND	-3.82	1.32	1.37
18	B	846	LMG	O7-C10	3.81	1.45	1.34
12	H	812	CLA	CHD-C4C	3.81	1.47	1.39
12	a	855	CLA	C3D-C4D	-3.81	1.35	1.44
12	A	824	CLA	CHB-C1B	3.81	1.48	1.39
12	b	829	CLA	C1D-ND	-3.81	1.32	1.37
12	f	203	CLA	CHC-C4B	3.81	1.48	1.39
12	a	802	CLA	C1D-ND	-3.81	1.32	1.37
12	b	821	CLA	C1D-ND	-3.81	1.32	1.37
16	a	851	LHG	O7-C7	3.81	1.45	1.34
12	b	825	CLA	MG-ND	-3.81	1.98	2.05
12	a	833	CLA	CHD-C4C	3.81	1.47	1.39
12	A	818	CLA	C3C-C2C	3.81	1.45	1.36
12	G	805	CLA	CHD-C4C	3.81	1.47	1.39
12	A	802	CLA	C1D-ND	-3.81	1.32	1.37
12	b	817	CLA	CHC-C4B	3.81	1.48	1.39
12	a	824	CLA	MG-ND	-3.81	1.98	2.05
12	B	817	CLA	CHC-C4B	3.81	1.48	1.39
16	A	851	LHG	O7-C7	3.81	1.45	1.34
12	b	848	CLA	OBD-CAD	3.81	1.29	1.22
12	G	817	CLA	CHD-C4C	3.81	1.47	1.39
12	G	836	CLA	CHC-C4B	3.80	1.48	1.39
12	b	810	CLA	CHD-C1D	3.80	1.45	1.38
12	L	204	CLA	C1D-ND	-3.80	1.32	1.37
12	B	810	CLA	CHD-C1D	3.80	1.45	1.38
12	A	806	CLA	CHD-C4C	3.80	1.47	1.39
12	a	817	CLA	CHD-C1D	3.80	1.45	1.38
12	a	821	CLA	CHD-C1D	3.80	1.45	1.38
12	l	204	CLA	C1D-ND	-3.80	1.32	1.37
12	G	820	CLA	CHD-C4C	3.80	1.47	1.39
12	B	824	CLA	MG-ND	-3.80	1.98	2.05
12	G	837	CLA	CHD-C4C	3.80	1.47	1.39
12	B	832	CLA	OBD-CAD	3.79	1.29	1.22
12	a	811	CLA	CHC-C4B	3.79	1.47	1.39
12	f	203	CLA	OBD-CAD	3.79	1.29	1.22
12	a	816	CLA	CHD-C4C	3.79	1.47	1.39
12	J	103	CLA	OBD-CAD	3.79	1.29	1.22
12	H	816	CLA	CHD-C4C	3.79	1.47	1.39
12	H	804	CLA	CHD-C4C	3.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	830	CLA	CHB-C1B	3.79	1.47	1.39
12	A	811	CLA	CHC-C4B	3.79	1.47	1.39
12	b	804	CLA	CHC-C4B	3.78	1.47	1.39
12	l	202	CLA	CHD-C4C	3.78	1.47	1.39
12	B	818	CLA	CHC-C4B	3.78	1.47	1.39
12	G	806	CLA	CHD-C4C	3.78	1.47	1.39
12	G	807	CLA	CHD-C4C	3.78	1.47	1.39
12	b	812	CLA	CHD-C4C	3.78	1.47	1.39
12	G	840	CLA	CHB-C1B	3.78	1.47	1.39
12	b	836	CLA	CHB-C1B	3.78	1.47	1.39
15	a	848	BCR	C11-C12	-3.78	1.24	1.34
12	B	811	CLA	CHD-C4C	3.78	1.47	1.39
12	H	839	CLA	CHD-C1D	3.78	1.45	1.38
12	A	835	CLA	CHC-C4B	3.78	1.47	1.39
12	A	839	CLA	OBD-CAD	3.77	1.29	1.22
12	G	806	CLA	CHC-C4B	3.77	1.47	1.39
12	A	828	CLA	OBD-CAD	3.77	1.29	1.22
12	b	829	CLA	CHC-C4B	3.77	1.47	1.39
12	P	203	CLA	OBD-CAD	3.77	1.29	1.22
12	G	825	CLA	CHD-C1D	3.77	1.45	1.38
12	a	830	CLA	C1D-ND	-3.77	1.32	1.37
12	R	103	CLA	OBD-CAD	3.77	1.29	1.22
12	a	815	CLA	OBD-CAD	3.77	1.29	1.22
12	a	828	CLA	OBD-CAD	3.77	1.29	1.22
12	B	805	CLA	CHB-C1B	3.77	1.47	1.39
12	G	823	CLA	CHC-C4B	3.77	1.47	1.39
12	H	814	CLA	CHD-C4C	3.77	1.47	1.39
12	a	806	CLA	CHC-C4B	3.77	1.47	1.39
12	L	206	CLA	CHD-C4C	3.77	1.47	1.39
12	A	826	CLA	CHC-C4B	3.77	1.47	1.39
12	G	808	CLA	CHD-C1D	3.77	1.45	1.38
12	a	821	CLA	CHC-C4B	3.77	1.47	1.39
12	A	833	CLA	CHD-C4C	3.77	1.47	1.39
12	B	804	CLA	C1B-NB	-3.77	1.32	1.37
12	A	834	CLA	CHC-C4B	3.77	1.47	1.39
15	A	847	BCR	C11-C12	-3.77	1.24	1.34
12	A	824	CLA	CHC-C4B	3.77	1.47	1.39
12	B	805	CLA	CHC-C4B	3.76	1.47	1.39
12	a	840	CLA	OBD-CAD	3.76	1.29	1.22
12	a	836	CLA	CHC-C4B	3.76	1.47	1.39
12	A	823	CLA	CHD-C4C	3.76	1.47	1.39
12	H	807	CLA	CHD-C1D	3.76	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	812	CLA	CHC-C4B	3.76	1.47	1.39
12	a	809	CLA	CHD-C4C	3.76	1.47	1.39
11	G	801	CL0	MG-ND	-3.76	1.98	2.05
12	A	816	CLA	CHB-C1B	3.76	1.47	1.39
12	G	816	CLA	CHC-C4B	3.76	1.47	1.39
12	A	831	CLA	CHC-C4B	3.76	1.47	1.39
12	B	837	CLA	CHC-C1C	3.76	1.46	1.38
12	A	813	CLA	CHC-C4B	3.76	1.47	1.39
12	a	813	CLA	C1D-ND	-3.76	1.32	1.37
12	a	827	CLA	CHC-C4B	3.76	1.47	1.39
12	B	829	CLA	CHD-C1D	3.75	1.45	1.38
12	b	817	CLA	CHB-C1B	3.75	1.47	1.39
12	G	815	CLA	CHD-C4C	3.75	1.47	1.39
12	H	803	CLA	CHC-C4B	3.75	1.47	1.39
12	G	822	CLA	CHD-C1D	3.75	1.45	1.38
12	A	828	CLA	CHC-C4B	3.75	1.47	1.39
12	B	820	CLA	CHD-C4C	3.75	1.47	1.39
12	G	828	CLA	CHC-C4B	3.75	1.47	1.39
12	b	812	CLA	CHB-C1B	3.75	1.47	1.39
12	F	203	CLA	OBD-CAD	3.75	1.28	1.22
12	B	821	CLA	C1B-NB	-3.75	1.32	1.37
12	b	837	CLA	CHC-C4B	3.75	1.47	1.39
12	b	831	CLA	OBD-CAD	3.75	1.28	1.22
12	b	822	CLA	CHD-C1D	3.75	1.45	1.38
12	a	815	CLA	CHC-C4B	3.75	1.47	1.39
12	H	819	CLA	CHC-C4B	3.75	1.47	1.39
12	B	814	CLA	CHD-C4C	3.75	1.47	1.39
12	G	827	CLA	CHD-C1D	3.75	1.45	1.38
12	L	202	CLA	CHD-C4C	3.75	1.47	1.39
12	H	827	CLA	C3C-C2C	3.74	1.44	1.36
12	A	827	CLA	C1D-ND	-3.74	1.32	1.37
12	H	832	CLA	CHC-C4B	3.74	1.47	1.39
12	a	824	CLA	CHC-C4B	3.74	1.47	1.39
12	H	819	CLA	OBD-CAD	3.74	1.28	1.22
12	G	816	CLA	OBD-CAD	3.74	1.28	1.22
12	a	823	CLA	CHD-C4C	3.74	1.47	1.39
12	A	806	CLA	CHD-C1D	3.74	1.45	1.38
12	H	837	CLA	C1D-ND	-3.74	1.32	1.37
12	H	820	CLA	CHB-C1B	3.74	1.47	1.39
12	a	822	CLA	OBD-CAD	3.74	1.28	1.22
12	B	826	CLA	OBD-CAD	3.74	1.28	1.22
12	a	825	CLA	CHD-C4C	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	801	CL0	CMD-C2D	-3.74	1.43	1.50
12	B	831	CLA	CHB-C1B	3.74	1.47	1.39
12	A	821	CLA	CHC-C4B	3.74	1.47	1.39
12	A	819	CLA	OBD-CAD	3.74	1.28	1.22
12	H	838	CLA	C1D-ND	-3.74	1.33	1.37
12	L	202	CLA	OBD-CAD	3.74	1.28	1.22
15	A	848	BCR	C11-C12	-3.73	1.24	1.34
12	A	815	CLA	OBD-CAD	3.73	1.28	1.22
12	b	835	CLA	C1B-NB	-3.73	1.33	1.37
12	G	829	CLA	OBD-CAD	3.73	1.28	1.22
12	a	814	CLA	CHD-C4C	3.73	1.47	1.39
15	G	853	BCR	C11-C12	-3.73	1.24	1.34
12	G	838	CLA	CHB-C1B	3.73	1.47	1.39
12	l	204	CLA	CHC-C4B	3.73	1.47	1.39
12	B	803	CLA	C1D-ND	-3.73	1.33	1.37
12	A	820	CLA	CHC-C1C	3.73	1.46	1.38
12	H	809	CLA	CHB-C1B	3.73	1.47	1.39
12	H	838	CLA	CHB-C1B	3.73	1.47	1.39
12	b	819	CLA	CHC-C4B	3.73	1.47	1.39
12	b	802	CLA	C3C-C2C	3.73	1.44	1.36
12	l	206	CLA	CHD-C4C	3.73	1.47	1.39
12	G	815	CLA	OBD-CAD	3.73	1.28	1.22
12	A	835	CLA	CHD-C4C	3.73	1.47	1.39
12	G	809	CLA	OBD-CAD	3.73	1.28	1.22
12	B	808	CLA	OBD-CAD	3.73	1.28	1.22
12	G	830	CLA	CHD-C4C	3.73	1.47	1.39
12	H	834	CLA	CHD-C4C	3.73	1.47	1.39
12	A	821	CLA	OBD-CAD	3.72	1.28	1.22
12	H	833	CLA	OBD-CAD	3.72	1.28	1.22
12	G	835	CLA	CHC-C4B	3.72	1.47	1.39
12	A	824	CLA	CHD-C1D	3.72	1.45	1.38
12	b	834	CLA	CHD-C4C	3.72	1.47	1.39
12	a	834	CLA	CHC-C4B	3.72	1.47	1.39
12	H	825	CLA	C1D-ND	-3.72	1.33	1.37
12	H	838	CLA	CHC-C1C	3.72	1.45	1.38
12	b	818	CLA	OBD-CAD	3.72	1.28	1.22
12	H	809	CLA	OBD-CAD	3.72	1.28	1.22
12	a	805	CLA	C1D-ND	-3.72	1.33	1.37
12	a	838	CLA	C1D-ND	-3.72	1.33	1.37
12	H	820	CLA	OBD-CAD	3.72	1.28	1.22
12	G	835	CLA	OBD-CAD	3.72	1.28	1.22
12	S	204	CLA	CHD-C4C	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	829	CLA	CHC-C4B	3.72	1.47	1.39
12	P	201	CLA	CHD-C4C	3.72	1.47	1.39
12	a	819	CLA	CHD-C4C	3.72	1.47	1.39
12	A	829	CLA	C1C-NC	-3.72	1.32	1.37
12	A	802	CLA	MG-ND	-3.72	1.98	2.05
12	b	804	CLA	CHD-C4C	3.72	1.47	1.39
12	B	811	CLA	OBD-CAD	3.72	1.28	1.22
12	H	814	CLA	OBD-CAD	3.71	1.28	1.22
12	H	820	CLA	CHC-C4B	3.71	1.47	1.39
12	S	202	CLA	CHC-C4B	3.71	1.47	1.39
12	a	835	CLA	CHC-C4B	3.71	1.47	1.39
18	b	845	LMG	C19-C18	-3.71	1.33	1.51
12	a	832	CLA	CHC-C4B	3.71	1.47	1.39
12	b	811	CLA	OBD-CAD	3.71	1.28	1.22
12	A	814	CLA	OBD-CAD	3.71	1.28	1.22
12	G	802	CLA	MG-ND	-3.71	1.98	2.05
12	G	812	CLA	CHD-C4C	3.71	1.47	1.39
12	B	818	CLA	OBD-CAD	3.71	1.28	1.22
18	H	847	LMG	C19-C18	-3.71	1.33	1.51
12	B	815	CLA	CHC-C4B	3.71	1.47	1.39
12	G	807	CLA	CHC-C4B	3.71	1.47	1.39
12	G	822	CLA	OBD-CAD	3.71	1.28	1.22
12	b	836	CLA	CHC-C1C	3.71	1.45	1.38
12	G	825	CLA	CHC-C4B	3.71	1.47	1.39
12	G	804	CLA	CHD-C4C	3.71	1.47	1.39
12	a	805	CLA	CHB-C1B	3.71	1.47	1.39
12	a	821	CLA	OBD-CAD	3.71	1.28	1.22
12	A	840	CLA	OBD-CAD	3.71	1.28	1.22
12	G	842	CLA	CHB-C1B	3.71	1.47	1.39
12	H	818	CLA	CHB-C1B	3.71	1.47	1.39
12	B	817	CLA	CHB-C1B	3.71	1.47	1.39
12	j	104	CLA	OBD-CAD	3.70	1.28	1.22
12	B	813	CLA	OBD-CAD	3.70	1.28	1.22
18	B	846	LMG	C19-C18	-3.70	1.33	1.51
12	a	806	CLA	CHD-C4C	3.70	1.47	1.39
12	A	820	CLA	C1B-NB	-3.70	1.33	1.37
12	H	832	CLA	CHB-C1B	3.70	1.47	1.39
12	b	813	CLA	OBD-CAD	3.70	1.28	1.22
12	H	850	CLA	CHB-C1B	3.70	1.47	1.39
12	a	810	CLA	CHC-C4B	3.70	1.47	1.39
12	L	205	CLA	CHC-C4B	3.70	1.47	1.39
12	G	842	CLA	OBD-CAD	3.70	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	838	CLA	C1D-ND	-3.70	1.33	1.37
12	a	822	CLA	CHC-C4B	3.70	1.47	1.39
12	H	818	CLA	OBD-CAD	3.70	1.28	1.22
12	A	824	CLA	MG-ND	-3.70	1.98	2.05
12	B	835	CLA	CHD-C4C	3.70	1.47	1.39
12	B	819	CLA	CHB-C1B	3.70	1.47	1.39
12	B	819	CLA	CHC-C4B	3.70	1.47	1.39
12	f	201	CLA	C1D-ND	-3.70	1.33	1.37
12	l	206	CLA	OBD-CAD	3.70	1.28	1.22
12	H	815	CLA	CHC-C4B	3.70	1.47	1.39
12	G	815	CLA	CHB-C1B	3.70	1.47	1.39
12	A	815	CLA	CHC-C4B	3.70	1.47	1.39
12	H	831	CLA	C1C-NC	-3.70	1.32	1.37
12	H	838	CLA	OBD-CAD	3.70	1.28	1.22
12	A	835	CLA	CHB-C1B	3.69	1.47	1.39
12	a	819	CLA	CHB-C1B	3.69	1.47	1.39
12	a	829	CLA	CHB-C1B	3.69	1.47	1.39
12	j	102	CLA	CHB-C1B	3.69	1.47	1.39
12	B	818	CLA	CHB-C1B	3.69	1.47	1.39
12	A	804	CLA	OBD-CAD	3.69	1.28	1.22
12	H	807	CLA	CHB-C1B	3.69	1.47	1.39
12	H	816	CLA	CHC-C4B	3.69	1.47	1.39
12	a	812	CLA	OBD-CAD	3.69	1.28	1.22
12	a	835	CLA	OBD-CAD	3.69	1.28	1.22
12	H	826	CLA	MG-ND	-3.69	1.98	2.05
12	H	831	CLA	C3D-C2D	3.69	1.49	1.39
12	A	835	CLA	OBD-CAD	3.69	1.28	1.22
16	G	852	LHG	O7-C7	3.69	1.44	1.34
15	F	202	BCR	C11-C12	-3.69	1.25	1.34
12	A	822	CLA	CHC-C4B	3.69	1.47	1.39
12	B	819	CLA	OBD-CAD	3.69	1.28	1.22
12	B	833	CLA	CHD-C4C	3.69	1.47	1.39
18	B	846	LMG	C22-C21	-3.68	1.33	1.51
12	G	838	CLA	CHD-C4C	3.68	1.47	1.39
11	A	801	CL0	C1B-NB	-3.68	1.33	1.37
12	l	205	CLA	CHD-C4C	3.68	1.47	1.39
15	L	207	BCR	C11-C12	-3.68	1.25	1.34
12	A	806	CLA	CHC-C4B	3.68	1.47	1.39
12	A	807	CLA	CHD-C4C	3.68	1.47	1.39
12	b	811	CLA	CHC-C4B	3.68	1.47	1.39
12	b	807	CLA	CHD-C4C	3.68	1.47	1.39
12	A	838	CLA	CHD-C4C	3.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	816	CLA	CHC-C4B	3.68	1.47	1.39
12	H	836	CLA	CHD-C4C	3.68	1.47	1.39
12	b	808	CLA	OBD-CAD	3.68	1.28	1.22
12	b	819	CLA	OBD-CAD	3.68	1.28	1.22
12	G	803	CLA	C1D-ND	-3.68	1.33	1.37
12	a	826	CLA	CHD-C1D	3.68	1.45	1.38
18	H	847	LMG	C40-C39	-3.68	1.33	1.51
12	G	820	CLA	CHB-C1B	3.68	1.47	1.39
12	A	837	CLA	CHC-C4B	3.68	1.47	1.39
12	a	814	CLA	OBD-CAD	3.68	1.28	1.22
12	a	838	CLA	CHD-C4C	3.68	1.47	1.39
12	B	804	CLA	CHD-C4C	3.68	1.47	1.39
12	a	814	CLA	CHB-C1B	3.67	1.47	1.39
12	B	822	CLA	OBD-CAD	3.67	1.28	1.22
12	b	830	CLA	CHC-C4B	3.67	1.47	1.39
12	B	821	CLA	CHD-C4C	3.67	1.47	1.39
12	b	848	CLA	CHC-C4B	3.67	1.47	1.39
12	A	819	CLA	CHB-C1B	3.67	1.47	1.39
12	b	816	CLA	OBD-CAD	3.67	1.28	1.22
12	G	823	CLA	CHB-C1B	3.67	1.47	1.39
12	b	833	CLA	CHD-C4C	3.67	1.47	1.39
12	H	830	CLA	CHC-C4B	3.67	1.47	1.39
12	G	805	CLA	OBD-CAD	3.67	1.28	1.22
12	b	823	CLA	CHD-C1D	3.67	1.45	1.38
18	H	847	LMG	C22-C21	-3.67	1.33	1.51
12	H	831	CLA	CHB-C1B	3.67	1.47	1.39
12	a	840	CLA	CHB-C1B	3.67	1.47	1.39
12	a	804	CLA	OBD-CAD	3.67	1.28	1.22
12	P	203	CLA	CHB-C1B	3.67	1.47	1.39
18	b	845	LMG	C22-C21	-3.67	1.33	1.51
12	a	809	CLA	OBD-CAD	3.67	1.28	1.22
12	G	835	CLA	CHB-C1B	3.67	1.47	1.39
12	a	834	CLA	OBD-CAD	3.67	1.28	1.22
12	G	820	CLA	CHC-C4B	3.67	1.47	1.39
12	H	835	CLA	C1D-ND	-3.66	1.33	1.37
12	B	802	CLA	C1B-NB	-3.66	1.33	1.37
12	H	821	CLA	CHC-C4B	3.66	1.47	1.39
12	S	204	CLA	CHC-C4B	3.66	1.47	1.39
12	L	206	CLA	OBD-CAD	3.66	1.28	1.22
12	H	821	CLA	CHD-C4C	3.66	1.47	1.39
12	G	855	CLA	OBD-CAD	3.66	1.28	1.22
12	S	203	CLA	CHC-C4B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	806	CLA	C1D-ND	-3.66	1.33	1.37
12	G	840	CLA	OBD-CAD	3.66	1.28	1.22
12	b	831	CLA	CHB-C1B	3.66	1.47	1.39
12	H	850	CLA	CHC-C4B	3.66	1.47	1.39
12	b	803	CLA	CHC-C4B	3.66	1.47	1.39
12	A	808	CLA	OBD-CAD	3.66	1.28	1.22
18	B	846	LMG	C40-C39	-3.66	1.33	1.51
12	a	835	CLA	CHD-C4C	3.66	1.47	1.39
12	b	836	CLA	CHD-C4C	3.66	1.47	1.39
12	B	804	CLA	CHC-C4B	3.66	1.47	1.39
12	L	205	CLA	CHD-C4C	3.66	1.47	1.39
12	b	802	CLA	OBD-CAD	3.66	1.28	1.22
12	H	812	CLA	OBD-CAD	3.66	1.28	1.22
12	b	824	CLA	C1B-NB	-3.66	1.33	1.37
12	b	836	CLA	C1D-ND	-3.66	1.33	1.37
12	A	807	CLA	CHC-C4B	3.66	1.47	1.39
12	B	823	CLA	CHB-C1B	3.66	1.47	1.39
12	H	850	CLA	OBD-CAD	3.66	1.28	1.22
12	B	830	CLA	CHB-C1B	3.66	1.47	1.39
12	a	836	CLA	OBD-CAD	3.65	1.28	1.22
12	b	808	CLA	CHB-C1B	3.65	1.47	1.39
12	B	832	CLA	CHB-C1B	3.65	1.47	1.39
12	G	841	CLA	C1D-ND	-3.65	1.33	1.37
12	H	812	CLA	CHC-C4B	3.65	1.47	1.39
12	b	820	CLA	CHD-C4C	3.65	1.47	1.39
12	L	205	CLA	CHB-C1B	3.65	1.47	1.39
12	B	805	CLA	OBD-CAD	3.65	1.28	1.22
11	A	801	CL0	MG-ND	-3.65	1.98	2.05
12	H	816	CLA	CHD-C1D	3.65	1.45	1.38
12	G	820	CLA	OBD-CAD	3.65	1.28	1.22
12	b	829	CLA	OBD-CAD	3.65	1.28	1.22
12	S	203	CLA	CHD-C4C	3.65	1.47	1.39
12	A	821	CLA	CHB-C1B	3.65	1.47	1.39
18	H	847	LMG	C25-C24	-3.65	1.33	1.51
12	a	819	CLA	CHC-C4B	3.65	1.47	1.39
12	b	826	CLA	OBD-CAD	3.65	1.28	1.22
18	b	845	LMG	C40-C39	-3.65	1.33	1.51
12	B	809	CLA	OBD-CAD	3.65	1.28	1.22
12	A	802	CLA	C4B-NB	-3.65	1.33	1.37
12	H	826	CLA	OBD-CAD	3.65	1.28	1.22
12	G	807	CLA	CHD-C1D	3.64	1.45	1.38
12	H	819	CLA	CHB-C1B	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	819	CLA	OBD-CAD	3.64	1.28	1.22
15	i	102	BCR	C11-C12	-3.64	1.25	1.34
12	b	834	CLA	CHB-C1B	3.64	1.47	1.39
12	b	824	CLA	C1D-ND	-3.64	1.33	1.37
12	A	816	CLA	CHD-C4C	3.64	1.47	1.39
12	H	806	CLA	CHC-C4B	3.64	1.47	1.39
12	G	833	CLA	C1D-ND	-3.64	1.33	1.37
12	H	807	CLA	MG-ND	-3.64	1.98	2.05
12	A	831	CLA	CHD-C4C	3.64	1.47	1.39
12	B	808	CLA	CHB-C1B	3.64	1.47	1.39
12	a	841	CLA	C1D-ND	-3.64	1.33	1.37
12	b	819	CLA	CHB-C1B	3.64	1.47	1.39
15	a	852	BCR	C11-C12	-3.64	1.25	1.34
12	l	202	CLA	OBD-CAD	3.64	1.28	1.22
12	b	832	CLA	CHC-C4B	3.64	1.47	1.39
18	b	845	LMG	C25-C24	-3.64	1.33	1.51
12	a	830	CLA	CHB-C1B	3.64	1.47	1.39
12	l	204	CLA	CHD-C4C	3.64	1.47	1.39
12	G	834	CLA	OBD-CAD	3.63	1.28	1.22
12	H	808	CLA	OBD-CAD	3.63	1.28	1.22
12	A	826	CLA	CHB-C1B	3.63	1.47	1.39
15	Q	102	BCR	C11-C12	-3.63	1.25	1.34
12	A	811	CLA	CHB-C1B	3.63	1.47	1.39
12	a	822	CLA	CHB-C1B	3.63	1.47	1.39
12	G	841	CLA	CHD-C4C	3.63	1.47	1.39
12	b	802	CLA	CHC-C4B	3.63	1.47	1.39
12	G	812	CLA	CHB-C1B	3.63	1.47	1.39
12	G	827	CLA	CHB-C1B	3.63	1.47	1.39
12	b	836	CLA	OBD-CAD	3.63	1.28	1.22
12	H	830	CLA	OBD-CAD	3.63	1.28	1.22
12	b	823	CLA	CHB-C1B	3.63	1.47	1.39
12	H	801	CLA	CHC-C4B	3.63	1.47	1.39
12	H	830	CLA	C1D-ND	-3.63	1.33	1.37
12	a	817	CLA	C1D-ND	-3.63	1.33	1.37
12	B	837	CLA	OBD-CAD	3.63	1.28	1.22
12	A	832	CLA	CHC-C4B	3.63	1.47	1.39
12	S	203	CLA	CHB-C1B	3.63	1.47	1.39
12	j	102	CLA	CHD-C4C	3.63	1.47	1.39
18	B	846	LMG	C43-C42	-3.63	1.33	1.51
15	f	202	BCR	C11-C12	-3.63	1.25	1.34
12	a	808	CLA	OBD-CAD	3.63	1.28	1.22
12	b	815	CLA	C4B-NB	-3.63	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	835	CLA	CHB-C1B	3.62	1.47	1.39
12	G	831	CLA	C1D-ND	-3.62	1.33	1.37
12	F	203	CLA	CHB-C1B	3.62	1.47	1.39
18	b	845	LMG	C43-C42	-3.62	1.33	1.51
12	H	817	CLA	OBD-CAD	3.62	1.28	1.22
12	G	825	CLA	MG-ND	-3.62	1.98	2.05
12	a	829	CLA	CHD-C4C	3.62	1.47	1.39
12	b	818	CLA	CHB-C1B	3.62	1.47	1.39
12	H	831	CLA	OBD-CAD	3.62	1.28	1.22
12	B	801	CLA	CHC-C4B	3.62	1.47	1.39
12	G	810	CLA	OBD-CAD	3.62	1.28	1.22
12	B	834	CLA	CHC-C4B	3.62	1.47	1.39
12	b	805	CLA	OBD-CAD	3.62	1.28	1.22
12	A	854	CLA	OBD-CAD	3.62	1.28	1.22
12	B	833	CLA	CHB-C1B	3.62	1.47	1.39
12	a	837	CLA	CHC-C4B	3.62	1.47	1.39
12	A	814	CLA	CHB-C1B	3.61	1.47	1.39
12	G	832	CLA	CHC-C4B	3.61	1.47	1.39
12	l	206	CLA	CHC-C4B	3.61	1.47	1.39
12	B	807	CLA	CHC-C1C	3.61	1.45	1.38
12	H	805	CLA	OBD-CAD	3.61	1.28	1.22
18	H	847	LMG	C43-C42	-3.61	1.33	1.51
12	f	203	CLA	CHB-C1B	3.61	1.47	1.39
12	H	824	CLA	CHB-C1B	3.61	1.47	1.39
15	G	848	BCR	C11-C12	-3.61	1.25	1.34
12	b	832	CLA	CHD-C4C	3.61	1.47	1.39
12	H	832	CLA	C1D-ND	-3.61	1.33	1.37
12	G	838	CLA	CHD-C1D	3.61	1.45	1.38
12	b	807	CLA	C1D-ND	-3.61	1.33	1.37
12	A	838	CLA	C1D-ND	-3.61	1.33	1.37
12	j	102	CLA	OBD-CAD	3.61	1.28	1.22
12	G	831	CLA	CHD-C4C	3.61	1.47	1.39
12	B	830	CLA	OBD-CAD	3.61	1.28	1.22
12	b	814	CLA	C1B-NB	-3.61	1.33	1.37
12	G	802	CLA	CHC-C4B	3.61	1.47	1.39
12	A	814	CLA	CHD-C4C	3.61	1.47	1.39
12	a	810	CLA	CHB-C1B	3.61	1.47	1.39
12	B	838	CLA	C1D-ND	-3.61	1.33	1.37
12	a	821	CLA	CHB-C1B	3.61	1.47	1.39
12	H	808	CLA	CHD-C4C	3.61	1.47	1.39
12	b	802	CLA	C1B-NB	-3.61	1.33	1.37
15	J	101	BCR	C11-C12	-3.61	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	812	CLA	OBD-CAD	3.61	1.28	1.22
12	f	201	CLA	C1B-NB	-3.61	1.33	1.37
12	G	819	CLA	CHD-C4C	3.61	1.47	1.39
12	A	827	CLA	CHC-C4B	3.61	1.47	1.39
12	a	806	CLA	CHB-C1B	3.60	1.47	1.39
12	B	812	CLA	CHB-C1B	3.60	1.47	1.39
12	b	821	CLA	CHD-C4C	3.60	1.47	1.39
12	G	836	CLA	C1B-NB	-3.60	1.33	1.37
12	H	802	CLA	OBD-CAD	3.60	1.28	1.22
18	B	846	LMG	C25-C24	-3.60	1.33	1.51
12	b	830	CLA	C1D-ND	-3.60	1.33	1.37
12	a	829	CLA	CHC-C1C	3.60	1.45	1.38
12	H	806	CLA	OBD-CAD	3.60	1.28	1.22
12	H	836	CLA	CHB-C1B	3.60	1.47	1.39
12	A	806	CLA	CHB-C1B	3.60	1.47	1.39
12	H	811	CLA	C4B-NB	-3.60	1.33	1.37
12	B	829	CLA	OBD-CAD	3.60	1.28	1.22
12	a	808	CLA	CHC-C4B	3.60	1.47	1.39
12	a	854	CLA	C1B-NB	-3.60	1.33	1.37
12	A	841	CLA	C1D-ND	-3.60	1.33	1.37
12	G	823	CLA	OBD-CAD	3.60	1.28	1.22
12	S	204	CLA	OBD-CAD	3.60	1.28	1.22
12	H	837	CLA	C1B-NB	-3.60	1.33	1.37
12	a	839	CLA	OBD-CAD	3.60	1.28	1.22
12	B	816	CLA	OBD-CAD	3.60	1.28	1.22
12	A	822	CLA	CHB-C1B	3.59	1.47	1.39
15	a	847	BCR	C11-C12	-3.59	1.25	1.34
12	a	828	CLA	CHD-C4C	3.59	1.47	1.39
12	A	814	CLA	CHC-C4B	3.59	1.47	1.39
12	A	854	CLA	C1B-NB	-3.59	1.33	1.37
12	L	206	CLA	CHC-C4B	3.59	1.47	1.39
11	G	801	CL0	OBD-CAD	3.59	1.28	1.22
12	B	807	CLA	CHB-C1B	3.59	1.47	1.39
12	L	204	CLA	CHC-C4B	3.59	1.47	1.39
12	A	829	CLA	CHB-C1B	3.59	1.47	1.39
12	G	830	CLA	CHC-C1C	3.59	1.45	1.38
12	G	837	CLA	CHC-C4B	3.59	1.47	1.39
12	a	820	CLA	CHC-C4B	3.59	1.47	1.39
12	A	840	CLA	CHB-C1B	3.59	1.47	1.39
11	A	801	CL0	OBD-CAD	3.59	1.28	1.22
12	b	801	CLA	CHC-C4B	3.59	1.47	1.39
11	G	801	CL0	CHD-C1D	3.59	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	834	CLA	CHD-C4C	3.58	1.47	1.39
12	H	828	CLA	C1D-ND	-3.58	1.33	1.37
12	B	811	CLA	CHC-C4B	3.58	1.47	1.39
12	B	837	CLA	C1C-NC	-3.58	1.32	1.37
12	b	807	CLA	CHC-C1C	3.58	1.45	1.38
12	H	833	CLA	CHB-C1B	3.58	1.47	1.39
12	A	829	CLA	C1D-ND	-3.58	1.33	1.37
12	G	855	CLA	CHD-C4C	3.58	1.47	1.39
12	a	810	CLA	OBD-CAD	3.58	1.28	1.22
12	H	834	CLA	CHB-C1B	3.58	1.47	1.39
12	G	839	CLA	CHC-C4B	3.58	1.47	1.39
12	b	822	CLA	CHD-C4C	3.58	1.47	1.39
12	B	807	CLA	CHD-C1D	3.58	1.45	1.38
12	G	809	CLA	CHC-C4B	3.58	1.47	1.39
12	G	822	CLA	CHB-C1B	3.58	1.47	1.39
12	a	817	CLA	CHB-C1B	3.58	1.47	1.39
12	a	802	CLA	MG-ND	-3.58	1.98	2.05
12	B	806	CLA	OBD-CAD	3.58	1.28	1.22
12	A	854	CLA	C3D-C2D	3.58	1.48	1.39
12	a	802	CLA	C3C-C2C	3.58	1.44	1.36
12	G	830	CLA	C1D-ND	-3.58	1.33	1.37
12	b	822	CLA	C1D-ND	-3.58	1.33	1.37
12	H	835	CLA	CHC-C4B	3.58	1.47	1.39
12	B	825	CLA	OBD-CAD	3.58	1.28	1.22
12	G	824	CLA	CHB-C1B	3.58	1.47	1.39
12	l	205	CLA	CHB-C1B	3.58	1.47	1.39
12	G	819	CLA	CHC-C4B	3.58	1.47	1.39
12	G	828	CLA	CHD-C1D	3.57	1.45	1.38
12	G	803	CLA	MG-ND	-3.57	1.98	2.05
12	P	201	CLA	C1B-NB	-3.57	1.33	1.37
12	H	823	CLA	OBD-CAD	3.57	1.28	1.22
12	B	801	CLA	MG-ND	-3.57	1.98	2.05
12	G	811	CLA	CHB-C1B	3.57	1.47	1.39
12	H	834	CLA	CHC-C4B	3.57	1.47	1.39
12	G	817	CLA	OBD-CAD	3.57	1.28	1.22
12	a	806	CLA	CHD-C1D	3.57	1.45	1.38
12	A	818	CLA	CHC-C4B	3.57	1.47	1.39
12	b	809	CLA	OBD-CAD	3.57	1.28	1.22
12	J	103	CLA	CHB-C1B	3.57	1.47	1.39
12	a	833	CLA	OBD-CAD	3.57	1.28	1.22
12	G	824	CLA	CHC-C4B	3.57	1.47	1.39
12	a	829	CLA	C1C-NC	-3.57	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	203	CLA	OBD-CAD	3.57	1.28	1.22
12	b	830	CLA	CHD-C4C	3.57	1.47	1.39
12	a	807	CLA	CHC-C4B	3.57	1.47	1.39
12	a	815	CLA	CHB-C1B	3.57	1.47	1.39
12	a	807	CLA	OBD-CAD	3.57	1.28	1.22
12	F	201	CLA	CHD-C4C	3.57	1.47	1.39
12	B	812	CLA	CHC-C4B	3.56	1.47	1.39
12	H	810	CLA	CHB-C1B	3.56	1.47	1.39
12	l	205	CLA	CHC-C4B	3.56	1.47	1.39
12	a	827	CLA	CHD-C1D	3.56	1.45	1.38
12	H	806	CLA	C1B-NB	-3.56	1.33	1.37
12	A	840	CLA	C1D-ND	-3.56	1.33	1.37
12	A	828	CLA	CHB-C1B	3.56	1.47	1.39
12	B	825	CLA	CHB-C1B	3.56	1.47	1.39
12	H	838	CLA	CHD-C4C	3.56	1.47	1.39
12	H	810	CLA	OBD-CAD	3.56	1.28	1.22
12	B	838	CLA	CHB-C1B	3.56	1.47	1.39
12	a	828	CLA	C1B-NB	-3.56	1.33	1.37
15	A	852	BCR	C11-C12	-3.56	1.25	1.34
12	B	835	CLA	CHB-C1B	3.56	1.47	1.39
12	a	823	CLA	CHC-C4B	3.56	1.47	1.39
12	G	817	CLA	CHB-C1B	3.56	1.47	1.39
12	G	825	CLA	MG-NC	3.56	2.14	2.06
12	B	831	CLA	CHD-C4C	3.56	1.47	1.39
12	b	828	CLA	CHC-C4B	3.56	1.47	1.39
12	a	854	CLA	OBD-CAD	3.55	1.28	1.22
12	P	203	CLA	CHC-C4B	3.55	1.47	1.39
12	H	839	CLA	CHB-C1B	3.55	1.47	1.39
12	A	812	CLA	CHD-C4C	3.55	1.47	1.39
12	G	811	CLA	OBD-CAD	3.55	1.28	1.22
12	a	811	CLA	CHB-C1B	3.55	1.47	1.39
12	A	825	CLA	CHD-C4C	3.55	1.47	1.39
16	G	851	LHG	O8-C23	3.55	1.43	1.33
12	A	813	CLA	CHB-C1B	3.55	1.47	1.39
12	G	807	CLA	CHB-C1B	3.55	1.47	1.39
12	B	832	CLA	CHC-C4B	3.55	1.47	1.39
15	j	101	BCR	C11-C12	-3.55	1.25	1.34
12	A	816	CLA	OBD-CAD	3.55	1.28	1.22
12	B	827	CLA	C1D-ND	-3.55	1.33	1.37
12	a	831	CLA	OBD-CAD	3.55	1.28	1.22
12	l	204	CLA	OBD-CAD	3.55	1.28	1.22
12	H	804	CLA	CHB-C1B	3.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	816	CLA	CHC-C4B	3.55	1.47	1.39
12	a	825	CLA	OBD-CAD	3.55	1.28	1.22
12	B	817	CLA	CHD-C4C	3.55	1.47	1.39
12	A	810	CLA	OBD-CAD	3.55	1.28	1.22
12	b	815	CLA	CHD-C4C	3.55	1.47	1.39
12	H	804	CLA	C1B-NB	-3.55	1.33	1.37
12	b	817	CLA	OBD-CAD	3.54	1.28	1.22
12	G	818	CLA	C1D-ND	-3.54	1.33	1.37
18	B	846	LMG	C37-C36	-3.54	1.34	1.51
12	a	824	CLA	MG-NC	3.54	2.14	2.06
12	A	829	CLA	CHD-C4C	3.54	1.47	1.39
12	B	806	CLA	C4B-NB	-3.54	1.33	1.37
12	f	201	CLA	CHD-C4C	3.54	1.47	1.39
12	A	805	CLA	CHB-C1B	3.54	1.47	1.39
12	a	840	CLA	C1D-ND	-3.54	1.33	1.37
12	B	821	CLA	C1D-ND	-3.54	1.33	1.37
15	P	202	BCR	C11-C12	-3.54	1.25	1.34
12	a	823	CLA	OBD-CAD	3.54	1.28	1.22
12	a	838	CLA	CHD-C1D	3.54	1.45	1.38
12	b	828	CLA	OBD-CAD	3.54	1.28	1.22
12	A	810	CLA	CHB-C1B	3.54	1.47	1.39
18	H	847	LMG	C37-C36	-3.53	1.34	1.51
12	A	819	CLA	CHC-C4B	3.53	1.47	1.39
12	H	813	CLA	OBD-CAD	3.53	1.28	1.22
12	A	833	CLA	OBD-CAD	3.53	1.28	1.22
12	G	830	CLA	CHB-C1B	3.53	1.47	1.39
12	G	842	CLA	CHC-C4B	3.53	1.47	1.39
12	a	854	CLA	CHD-C4C	3.53	1.47	1.39
12	B	834	CLA	CHD-C4C	3.53	1.47	1.39
12	a	826	CLA	CHB-C1B	3.53	1.47	1.39
18	b	845	LMG	C37-C36	-3.53	1.34	1.51
12	G	803	CLA	CHD-C4C	3.53	1.47	1.39
12	B	828	CLA	CHB-C1B	3.53	1.47	1.39
12	G	840	CLA	C1D-ND	-3.53	1.33	1.37
12	G	826	CLA	CHD-C4C	3.53	1.47	1.39
12	G	821	CLA	OBD-CAD	3.53	1.28	1.22
12	H	826	CLA	CHD-C4C	3.53	1.47	1.39
12	L	204	CLA	CHD-C4C	3.53	1.47	1.39
12	G	840	CLA	CHD-C4C	3.53	1.47	1.39
12	b	830	CLA	OBD-CAD	3.53	1.28	1.22
12	A	838	CLA	CHD-C1D	3.53	1.45	1.38
12	b	820	CLA	OBD-CAD	3.53	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	806	CLA	C1C-NC	-3.52	1.32	1.37
12	B	837	CLA	C1D-ND	-3.52	1.33	1.37
12	B	814	CLA	CHC-C4B	3.52	1.47	1.39
12	a	828	CLA	CHB-C1B	3.52	1.47	1.39
12	G	808	CLA	CHC-C4B	3.52	1.47	1.39
12	F	201	CLA	C1D-ND	-3.52	1.33	1.37
12	b	809	CLA	CHB-C1B	3.52	1.47	1.39
12	H	818	CLA	CHD-C4C	3.52	1.47	1.39
12	B	831	CLA	OBD-CAD	3.52	1.28	1.22
12	B	826	CLA	CHC-C1C	3.52	1.45	1.38
12	B	827	CLA	OBD-CAD	3.52	1.28	1.22
12	B	836	CLA	OBD-CAD	3.52	1.28	1.22
12	B	803	CLA	CHC-C4B	3.52	1.47	1.39
12	b	827	CLA	C1D-ND	-3.52	1.33	1.37
11	a	801	CL0	CHC-C4B	3.51	1.47	1.39
12	G	811	CLA	CHC-C4B	3.51	1.47	1.39
12	G	834	CLA	CHD-C4C	3.51	1.47	1.39
12	b	825	CLA	CHC-C4B	3.51	1.47	1.39
12	A	836	CLA	MG-NC	3.51	2.14	2.06
12	a	831	CLA	CHB-C1B	3.51	1.47	1.39
12	B	828	CLA	CHC-C4B	3.51	1.47	1.39
12	F	201	CLA	OBD-CAD	3.51	1.28	1.22
12	G	830	CLA	C1C-NC	-3.51	1.32	1.37
12	G	808	CLA	CHD-C4C	3.51	1.47	1.39
12	b	801	CLA	CHD-C4C	3.51	1.47	1.39
12	A	812	CLA	CHC-C4B	3.51	1.47	1.39
12	S	202	CLA	CHD-C4C	3.51	1.47	1.39
12	G	810	CLA	CHC-C4B	3.51	1.47	1.39
12	A	823	CLA	CHB-C1B	3.51	1.47	1.39
12	a	802	CLA	CHC-C4B	3.51	1.47	1.39
12	B	802	CLA	C3C-C2C	3.51	1.44	1.36
12	L	204	CLA	OBD-CAD	3.51	1.28	1.22
12	G	833	CLA	CHD-C4C	3.51	1.47	1.39
12	A	823	CLA	CHC-C4B	3.51	1.47	1.39
12	a	840	CLA	CHD-C4C	3.51	1.47	1.39
12	B	815	CLA	OBD-CAD	3.51	1.28	1.22
12	l	205	CLA	CHD-C1D	3.51	1.45	1.38
12	H	834	CLA	OBD-CAD	3.51	1.28	1.22
12	b	822	CLA	OBD-CAD	3.51	1.28	1.22
12	A	830	CLA	CHB-C1B	3.51	1.47	1.39
12	B	828	CLA	OBD-CAD	3.51	1.28	1.22
12	H	807	CLA	CHC-C1C	3.51	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	818	CLA	CHB-C1B	3.50	1.47	1.39
12	b	831	CLA	CHC-C4B	3.50	1.47	1.39
12	a	807	CLA	CHB-C1B	3.50	1.47	1.39
12	a	802	CLA	CHD-C4C	3.50	1.47	1.39
12	H	839	CLA	OBD-CAD	3.50	1.28	1.22
12	H	829	CLA	CHC-C4B	3.50	1.47	1.39
12	b	812	CLA	CHC-C4B	3.50	1.47	1.39
12	b	806	CLA	CHC-C4B	3.50	1.47	1.39
12	b	803	CLA	C1D-ND	-3.50	1.33	1.37
12	A	839	CLA	CHC-C4B	3.50	1.47	1.39
12	A	823	CLA	OBD-CAD	3.50	1.28	1.22
12	a	813	CLA	OBD-CAD	3.50	1.28	1.22
12	a	855	CLA	OBD-CAD	3.50	1.28	1.22
12	G	832	CLA	C1B-NB	-3.50	1.33	1.37
12	B	801	CLA	CHD-C4C	3.50	1.47	1.39
12	G	806	CLA	C3C-C2C	3.50	1.44	1.36
12	a	818	CLA	OBD-CAD	3.50	1.28	1.22
12	A	840	CLA	CHD-C4C	3.50	1.47	1.39
12	b	804	CLA	CHB-C1B	3.50	1.47	1.39
12	G	829	CLA	CHD-C4C	3.50	1.47	1.39
12	A	807	CLA	CHB-C1B	3.50	1.47	1.39
12	B	803	CLA	OBD-CAD	3.50	1.28	1.22
15	G	850	BCR	C11-C12	-3.50	1.25	1.34
12	G	813	CLA	CHD-C4C	3.49	1.47	1.39
12	B	809	CLA	CHB-C1B	3.49	1.47	1.39
12	G	822	CLA	C1D-ND	-3.49	1.33	1.37
12	B	833	CLA	OBD-CAD	3.49	1.28	1.22
12	H	802	CLA	C3C-C2C	3.49	1.44	1.36
12	B	802	CLA	OBD-CAD	3.49	1.28	1.22
12	B	810	CLA	MG-ND	-3.49	1.98	2.05
12	G	829	CLA	CHB-C1B	3.49	1.47	1.39
12	b	804	CLA	C1B-NB	-3.49	1.33	1.37
12	a	839	CLA	CHC-C4B	3.49	1.47	1.39
12	A	855	CLA	C1C-NC	-3.49	1.32	1.37
12	H	831	CLA	CHC-C4B	3.49	1.47	1.39
12	A	824	CLA	MG-NC	3.49	2.14	2.06
12	H	822	CLA	CHC-C4B	3.49	1.47	1.39
12	b	817	CLA	C1D-ND	-3.49	1.33	1.37
12	A	804	CLA	CHC-C4B	3.49	1.47	1.39
12	H	833	CLA	CHC-C4B	3.49	1.47	1.39
12	A	833	CLA	CHC-C4B	3.48	1.47	1.39
12	H	832	CLA	OBD-CAD	3.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	825	CLA	CHC-C4B	3.48	1.47	1.39
12	b	848	CLA	CHB-C1B	3.48	1.47	1.39
12	B	833	CLA	CHC-C4B	3.48	1.47	1.39
12	H	823	CLA	C1B-NB	-3.48	1.33	1.37
12	b	837	CLA	CHD-C4C	3.48	1.47	1.39
12	G	816	CLA	CHB-C1B	3.48	1.47	1.39
12	a	812	CLA	CHC-C4B	3.48	1.47	1.39
12	a	834	CLA	C1D-ND	-3.48	1.33	1.37
12	B	822	CLA	CHD-C1D	3.48	1.45	1.38
12	B	834	CLA	CHB-C1B	3.48	1.47	1.39
12	F	201	CLA	CHB-C1B	3.48	1.47	1.39
12	A	818	CLA	CHD-C4C	3.48	1.47	1.39
12	A	832	CLA	OBD-CAD	3.48	1.28	1.22
11	G	801	CL0	CHC-C4B	3.48	1.47	1.39
15	G	847	BCR	C11-C12	-3.48	1.25	1.34
12	b	829	CLA	CHB-C1B	3.48	1.47	1.39
12	H	829	CLA	OBD-CAD	3.48	1.28	1.22
12	a	823	CLA	CHB-C1B	3.48	1.47	1.39
12	R	103	CLA	CHB-C1B	3.47	1.47	1.39
17	T	101	45D	C20-C08	3.47	1.56	1.45
15	R	101	BCR	C11-C12	-3.47	1.25	1.34
12	l	205	CLA	OBD-CAD	3.47	1.28	1.22
12	A	818	CLA	OBD-CAD	3.47	1.28	1.22
12	H	816	CLA	MG-ND	-3.47	1.98	2.05
15	b	839	BCR	C11-C12	-3.47	1.25	1.34
12	G	817	CLA	CHC-C4B	3.47	1.47	1.39
15	a	845	BCR	C11-C12	-3.47	1.25	1.34
12	b	821	CLA	OBD-CAD	3.47	1.28	1.22
12	b	825	CLA	OBD-CAD	3.47	1.28	1.22
12	H	808	CLA	CHB-C1B	3.47	1.47	1.39
12	A	832	CLA	C1B-NB	-3.47	1.33	1.37
12	B	831	CLA	C1D-ND	-3.47	1.33	1.37
17	m	101	45D	C20-C08	3.47	1.56	1.45
12	G	842	CLA	CHD-C4C	3.47	1.47	1.39
12	B	821	CLA	OBD-CAD	3.47	1.28	1.22
12	H	826	CLA	CHC-C4B	3.47	1.47	1.39
12	H	839	CLA	C1D-ND	-3.47	1.33	1.37
12	H	825	CLA	CHD-C1D	3.47	1.45	1.38
12	G	831	CLA	CHB-C1B	3.47	1.47	1.39
12	H	835	CLA	CHB-C1B	3.47	1.47	1.39
12	A	828	CLA	CHD-C4C	3.47	1.47	1.39
12	A	841	CLA	CHD-C4C	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	826	CLA	CHB-C1B	3.47	1.47	1.39
12	L	204	CLA	CHB-C1B	3.47	1.47	1.39
17	M	101	45D	C20-C08	3.47	1.56	1.45
12	b	827	CLA	OBD-CAD	3.47	1.28	1.22
15	J	102	BCR	C11-C12	-3.47	1.25	1.34
11	A	801	CL0	CHC-C4B	3.47	1.47	1.39
12	j	102	CLA	CHC-C4B	3.46	1.47	1.39
12	A	805	CLA	C1D-ND	-3.46	1.33	1.37
12	b	806	CLA	OBD-CAD	3.46	1.28	1.22
12	l	204	CLA	CHB-C1B	3.46	1.47	1.39
12	a	812	CLA	CHB-C1B	3.46	1.47	1.39
12	H	805	CLA	CHD-C4C	3.46	1.47	1.39
12	B	820	CLA	OBD-CAD	3.46	1.28	1.22
12	A	827	CLA	MG-ND	-3.46	1.98	2.05
12	G	802	CLA	CHD-C4C	3.46	1.47	1.39
12	b	803	CLA	OBD-CAD	3.46	1.28	1.22
12	H	813	CLA	CHB-C1B	3.46	1.47	1.39
12	b	833	CLA	CHC-C4B	3.46	1.47	1.39
12	B	814	CLA	CHB-C1B	3.46	1.47	1.39
15	I	101	BCR	C11-C12	-3.46	1.25	1.34
12	b	813	CLA	CHB-C1B	3.46	1.47	1.39
12	A	820	CLA	OBD-CAD	3.46	1.28	1.22
15	Q	101	BCR	C11-C12	-3.46	1.25	1.34
12	H	822	CLA	CHD-C1D	3.46	1.45	1.38
12	b	837	CLA	CHB-C1B	3.46	1.47	1.39
12	b	835	CLA	OBD-CAD	3.46	1.28	1.22
12	a	832	CLA	C1B-NB	-3.46	1.33	1.37
12	l	206	CLA	C1D-ND	-3.46	1.33	1.37
12	A	837	CLA	OBD-CAD	3.45	1.28	1.22
12	b	815	CLA	OBD-CAD	3.45	1.28	1.22
12	a	854	CLA	C3D-C2D	3.45	1.48	1.39
12	A	827	CLA	CHD-C1D	3.45	1.45	1.38
12	B	821	CLA	CHC-C4B	3.45	1.47	1.39
12	A	829	CLA	CHC-C1C	3.45	1.45	1.38
12	b	828	CLA	CHB-C1B	3.45	1.47	1.39
12	B	807	CLA	OBD-CAD	3.45	1.28	1.22
12	G	833	CLA	OBD-CAD	3.45	1.28	1.22
12	A	833	CLA	CHB-C1B	3.45	1.47	1.39
12	A	855	CLA	OBD-CAD	3.45	1.28	1.22
12	a	836	CLA	C1B-NB	-3.45	1.33	1.37
12	G	855	CLA	C3D-C2D	3.44	1.48	1.39
12	B	805	CLA	CHD-C4C	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	821	CLA	C1D-ND	-3.44	1.33	1.37
12	a	828	CLA	CHC-C4B	3.44	1.47	1.39
12	A	834	CLA	C1D-ND	-3.44	1.33	1.37
12	b	810	CLA	CHB-C1B	3.44	1.47	1.39
12	B	807	CLA	C1C-NC	-3.44	1.32	1.37
12	B	829	CLA	CHB-C1B	3.44	1.47	1.39
12	b	821	CLA	CHC-C4B	3.44	1.47	1.39
12	G	808	CLA	OBD-CAD	3.44	1.28	1.22
12	H	828	CLA	OBD-CAD	3.44	1.28	1.22
12	H	837	CLA	OBD-CAD	3.44	1.28	1.22
12	B	822	CLA	C1B-NB	-3.44	1.33	1.37
12	H	812	CLA	CHB-C1B	3.44	1.47	1.39
15	S	205	BCR	C11-C12	-3.44	1.25	1.34
12	a	829	CLA	C1D-ND	-3.44	1.33	1.37
12	b	803	CLA	CHB-C1B	3.44	1.47	1.39
12	L	202	CLA	CHB-C1B	3.44	1.47	1.39
12	G	819	CLA	OBD-CAD	3.44	1.28	1.22
15	A	846	BCR	C11-C12	-3.44	1.25	1.34
12	A	836	CLA	MG-ND	-3.44	1.99	2.05
12	S	202	CLA	CHB-C1B	3.44	1.47	1.39
12	A	831	CLA	CHB-C1B	3.44	1.47	1.39
12	H	824	CLA	CHD-C4C	3.44	1.47	1.39
12	H	832	CLA	CHD-C4C	3.44	1.47	1.39
12	l	202	CLA	CHB-C1B	3.43	1.47	1.39
12	B	810	CLA	CHB-C1B	3.43	1.47	1.39
12	b	814	CLA	C1D-ND	-3.43	1.33	1.37
12	A	807	CLA	OBD-CAD	3.43	1.28	1.22
15	B	840	BCR	C11-C12	-3.43	1.25	1.34
12	G	855	CLA	C1B-NB	-3.43	1.33	1.37
12	B	804	CLA	CHB-C1B	3.43	1.47	1.39
12	b	810	CLA	MG-ND	-3.43	1.99	2.05
11	G	801	CL0	C1B-NB	-3.43	1.33	1.37
12	G	833	CLA	CHC-C4B	3.43	1.47	1.39
12	b	810	CLA	C1C-NC	-3.43	1.32	1.37
15	G	846	BCR	C11-C12	-3.43	1.25	1.34
12	b	807	CLA	CHB-C1B	3.43	1.47	1.39
15	L	201	BCR	C11-C12	-3.43	1.25	1.34
12	G	836	CLA	MG-ND	-3.43	1.99	2.05
15	A	845	BCR	C11-C12	-3.43	1.25	1.34
12	B	823	CLA	CHD-C4C	3.43	1.47	1.39
12	H	824	CLA	MG-ND	-3.43	1.99	2.05
12	S	204	CLA	C1D-ND	-3.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	801	CLA	MG-ND	-3.42	1.99	2.05
12	B	801	CLA	OBD-CAD	3.42	1.28	1.22
12	a	818	CLA	CHB-C1B	3.42	1.47	1.39
12	H	827	CLA	OBD-CAD	3.42	1.28	1.22
12	A	816	CLA	CHC-C4B	3.42	1.47	1.39
12	S	202	CLA	C3D-C2D	3.42	1.48	1.39
12	A	810	CLA	CHC-C4B	3.42	1.47	1.39
12	b	821	CLA	MG-ND	-3.42	1.99	2.05
12	G	837	CLA	OBD-CAD	3.42	1.28	1.22
12	G	834	CLA	C1D-ND	-3.42	1.33	1.37
12	b	837	CLA	OBD-CAD	3.42	1.28	1.22
12	H	835	CLA	CHD-C4C	3.42	1.47	1.39
12	B	824	CLA	C1B-NB	-3.41	1.33	1.37
12	a	816	CLA	MG-ND	-3.41	1.99	2.05
15	i	101	BCR	C11-C12	-3.41	1.25	1.34
12	a	834	CLA	CHD-C4C	3.41	1.47	1.39
12	H	801	CLA	CHB-C1B	3.41	1.47	1.39
12	G	839	CLA	OBD-CAD	3.41	1.28	1.22
12	A	809	CLA	CHC-C4B	3.41	1.47	1.39
12	G	804	CLA	OBD-CAD	3.41	1.28	1.22
12	a	814	CLA	CHC-C4B	3.41	1.47	1.39
12	B	806	CLA	CHC-C4B	3.41	1.47	1.39
12	B	837	CLA	CHD-C4C	3.41	1.47	1.39
12	G	824	CLA	OBD-CAD	3.41	1.28	1.22
12	H	803	CLA	OBD-CAD	3.41	1.28	1.22
15	H	842	BCR	C11-C12	-3.41	1.25	1.34
12	a	836	CLA	MG-NC	3.41	2.14	2.06
12	B	817	CLA	OBD-CAD	3.41	1.28	1.22
12	b	815	CLA	CHC-C4B	3.41	1.47	1.39
12	b	810	CLA	C1B-NB	-3.41	1.33	1.37
12	H	821	CLA	OBD-CAD	3.41	1.28	1.22
12	a	841	CLA	CHD-C4C	3.41	1.47	1.39
12	G	807	CLA	C1D-ND	-3.41	1.33	1.37
12	a	831	CLA	CHC-C4B	3.41	1.47	1.39
12	B	811	CLA	CHB-C1B	3.41	1.47	1.39
12	B	810	CLA	C1B-NB	-3.41	1.33	1.37
12	G	821	CLA	CHC-C4B	3.40	1.47	1.39
15	b	840	BCR	C11-C12	-3.40	1.25	1.34
12	b	820	CLA	CHB-C1B	3.40	1.47	1.39
12	a	820	CLA	OBD-CAD	3.40	1.28	1.22
12	P	201	CLA	OBD-CAD	3.40	1.28	1.22
15	j	103	BCR	C11-C12	-3.40	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	836	CLA	CHB-C1B	3.40	1.47	1.39
12	G	818	CLA	CHB-C1B	3.40	1.47	1.39
12	H	829	CLA	CHB-C1B	3.40	1.47	1.39
12	A	808	CLA	CHC-C4B	3.40	1.47	1.39
12	A	836	CLA	CHB-C1B	3.40	1.47	1.39
12	H	813	CLA	CHC-C4B	3.40	1.47	1.39
12	H	823	CLA	MG-ND	-3.40	1.99	2.05
12	H	822	CLA	OBD-CAD	3.40	1.28	1.22
12	H	807	CLA	OBD-CAD	3.40	1.28	1.22
12	H	814	CLA	CHB-C1B	3.40	1.47	1.39
12	b	817	CLA	CHD-C4C	3.40	1.46	1.39
12	a	827	CLA	MG-ND	-3.40	1.99	2.05
15	P	204	BCR	C11-C12	-3.39	1.25	1.34
12	B	807	CLA	MG-ND	-3.39	1.99	2.05
12	a	824	CLA	CHD-C1D	3.39	1.45	1.38
12	H	830	CLA	CHB-C1B	3.39	1.47	1.39
12	B	803	CLA	CHB-C1B	3.39	1.47	1.39
12	B	825	CLA	CHD-C4C	3.39	1.46	1.39
15	a	849	BCR	C11-C12	-3.39	1.25	1.34
15	a	846	BCR	C11-C12	-3.39	1.25	1.34
12	B	824	CLA	CHD-C1D	3.39	1.45	1.38
12	b	811	CLA	CHB-C1B	3.39	1.47	1.39
17	T	101	45D	C19-C07	3.39	1.56	1.45
12	a	804	CLA	CHC-C4B	3.39	1.47	1.39
12	b	833	CLA	CHB-C1B	3.39	1.47	1.39
15	l	201	BCR	C11-C12	-3.39	1.25	1.34
12	A	854	CLA	CHD-C4C	3.39	1.46	1.39
12	B	825	CLA	MG-ND	-3.39	1.99	2.05
15	B	841	BCR	C11-C12	-3.39	1.25	1.34
12	A	809	CLA	OBD-CAD	3.38	1.28	1.22
12	H	806	CLA	C1D-ND	-3.38	1.33	1.37
12	H	850	CLA	CHD-C4C	3.38	1.46	1.39
12	a	803	CLA	OBD-CAD	3.38	1.28	1.22
12	B	810	CLA	C1C-NC	-3.38	1.32	1.37
12	f	201	CLA	OBD-CAD	3.38	1.28	1.22
12	b	814	CLA	CHC-C4B	3.38	1.47	1.39
12	A	834	CLA	OBD-CAD	3.38	1.28	1.22
12	G	833	CLA	MG-ND	-3.38	1.99	2.05
12	B	830	CLA	CHC-C4B	3.38	1.47	1.39
12	G	815	CLA	CHC-C4B	3.38	1.47	1.39
12	G	808	CLA	CHB-C1B	3.38	1.47	1.39
12	B	813	CLA	CHB-C1B	3.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	801	CL0	CHD-C1D	3.38	1.45	1.38
12	a	818	CLA	CHC-C4B	3.38	1.47	1.39
12	L	205	CLA	OBD-CAD	3.37	1.28	1.22
12	H	802	CLA	C1B-NB	-3.37	1.33	1.37
12	G	804	CLA	CHB-C1B	3.37	1.47	1.39
12	G	828	CLA	OBD-CAD	3.37	1.28	1.22
12	b	848	CLA	CHD-C4C	3.37	1.46	1.39
15	R	102	BCR	C11-C12	-3.37	1.25	1.34
12	F	201	CLA	C1B-NB	-3.37	1.33	1.37
12	G	819	CLA	CHB-C1B	3.37	1.47	1.39
12	G	836	CLA	MG-NC	3.37	2.14	2.06
12	A	803	CLA	CHB-C1B	3.37	1.47	1.39
12	G	855	CLA	CHD-C1D	3.37	1.45	1.38
12	B	838	CLA	OBD-CAD	3.37	1.28	1.22
12	b	826	CLA	CHC-C1C	3.37	1.45	1.38
12	a	803	CLA	CHB-C1B	3.37	1.47	1.39
12	b	820	CLA	C1D-ND	-3.37	1.33	1.37
12	G	829	CLA	C1B-NB	-3.37	1.33	1.37
12	B	823	CLA	MG-ND	-3.37	1.99	2.05
12	H	811	CLA	CHD-C4C	3.36	1.46	1.39
12	G	856	CLA	C1C-NC	-3.36	1.32	1.37
12	H	825	CLA	C4B-NB	-3.36	1.33	1.37
12	b	825	CLA	CHD-C4C	3.36	1.46	1.39
12	G	832	CLA	OBD-CAD	3.36	1.28	1.22
12	A	827	CLA	C1C-NC	-3.36	1.32	1.37
12	B	835	CLA	C1D-ND	-3.36	1.33	1.37
12	f	201	CLA	CHB-C1B	3.36	1.47	1.39
12	G	805	CLA	CHB-C1B	3.36	1.47	1.39
12	H	827	CLA	C4C-C3C	3.36	1.50	1.45
15	F	204	BCR	C11-C12	-3.36	1.25	1.34
12	b	806	CLA	CHB-C1B	3.36	1.47	1.39
12	H	806	CLA	CHB-C1B	3.36	1.46	1.39
12	a	836	CLA	CHB-C1B	3.36	1.46	1.39
12	a	855	CLA	C1C-NC	-3.36	1.32	1.37
17	m	101	45D	C19-C07	3.36	1.56	1.45
12	H	811	CLA	MG-ND	-3.36	1.99	2.05
12	B	822	CLA	CHB-C1B	3.36	1.46	1.39
12	a	855	CLA	C1B-NB	-3.36	1.33	1.37
12	a	813	CLA	CHB-C1B	3.35	1.46	1.39
12	A	808	CLA	CHB-C1B	3.35	1.46	1.39
17	M	101	45D	C19-C07	3.35	1.56	1.45
12	b	801	CLA	OBD-CAD	3.35	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	845	BCR	C11-C12	-3.35	1.25	1.34
12	a	825	CLA	C1D-ND	-3.35	1.33	1.37
12	G	831	CLA	OBD-CAD	3.35	1.28	1.22
12	G	825	CLA	OBD-CAD	3.35	1.28	1.22
12	H	826	CLA	CHB-C1B	3.34	1.46	1.39
12	A	831	CLA	MG-ND	-3.34	1.99	2.05
11	A	801	CL0	CHD-C1D	3.34	1.44	1.38
12	G	813	CLA	OBD-CAD	3.34	1.28	1.22
12	B	807	CLA	CHD-C4C	3.34	1.46	1.39
12	H	821	CLA	CHB-C1B	3.34	1.46	1.39
12	j	102	CLA	C3D-C2D	3.34	1.48	1.39
12	a	816	CLA	CHB-C1B	3.34	1.46	1.39
12	G	803	CLA	C4B-NB	-3.34	1.33	1.37
12	a	837	CLA	OBD-CAD	3.34	1.28	1.22
12	a	833	CLA	CHC-C4B	3.34	1.46	1.39
12	B	824	CLA	OBD-CAD	3.34	1.28	1.22
12	B	823	CLA	C1B-NB	-3.34	1.33	1.37
12	A	829	CLA	MG-ND	-3.34	1.99	2.05
15	b	843	BCR	C11-C12	-3.34	1.26	1.34
15	H	841	BCR	C11-C12	-3.33	1.26	1.34
12	H	828	CLA	CHB-C1B	3.33	1.46	1.39
12	A	826	CLA	C1D-ND	-3.33	1.33	1.37
12	a	812	CLA	C1D-ND	-3.33	1.33	1.37
12	B	810	CLA	C4B-NB	-3.33	1.33	1.37
12	B	822	CLA	CHD-C4C	3.33	1.46	1.39
12	B	838	CLA	CHD-C4C	3.33	1.46	1.39
12	B	822	CLA	MG-ND	-3.33	1.99	2.05
12	L	204	CLA	C3D-C2D	3.33	1.48	1.39
12	a	827	CLA	OBD-CAD	3.33	1.28	1.22
12	a	832	CLA	C1D-ND	-3.33	1.33	1.37
12	G	813	CLA	CHB-C1B	3.33	1.46	1.39
12	a	808	CLA	CHB-C1B	3.32	1.46	1.39
12	B	834	CLA	C1D-ND	-3.32	1.33	1.37
12	f	201	CLA	MG-ND	-3.32	1.99	2.05
12	S	203	CLA	CHD-C1D	3.32	1.44	1.38
12	B	831	CLA	MG-NC	3.32	2.14	2.06
12	a	813	CLA	CHC-C4B	3.32	1.46	1.39
12	H	836	CLA	C1D-ND	-3.32	1.33	1.37
12	B	806	CLA	CHB-C1B	3.32	1.46	1.39
12	S	202	CLA	OBD-CAD	3.32	1.28	1.22
12	H	827	CLA	CHB-C1B	3.32	1.46	1.39
12	a	809	CLA	CHC-C4B	3.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	802	CLA	CHD-C4C	3.32	1.46	1.39
12	G	856	CLA	OBD-CAD	3.32	1.28	1.22
12	A	812	CLA	OBD-CAD	3.32	1.28	1.22
12	b	823	CLA	MG-ND	-3.32	1.99	2.05
12	j	104	CLA	CHB-C1B	3.32	1.46	1.39
12	B	820	CLA	CHB-C1B	3.32	1.46	1.39
12	B	820	CLA	C1D-ND	-3.32	1.33	1.37
12	H	823	CLA	CHB-C1B	3.32	1.46	1.39
12	H	838	CLA	CHC-C4B	3.32	1.46	1.39
15	b	847	BCR	C11-C12	-3.32	1.26	1.34
12	b	808	CLA	C1C-NC	-3.31	1.32	1.37
12	a	816	CLA	C1D-ND	-3.31	1.33	1.37
15	G	845	BCR	C11-C12	-3.31	1.26	1.34
12	G	826	CLA	MG-ND	-3.31	1.99	2.05
12	b	823	CLA	C1B-NB	-3.31	1.33	1.37
12	G	856	CLA	MG-ND	-3.31	1.99	2.05
12	H	815	CLA	CHB-C1B	3.31	1.46	1.39
12	G	833	CLA	CHB-C1B	3.31	1.46	1.39
12	G	825	CLA	C1B-NB	-3.31	1.33	1.37
15	B	844	BCR	C11-C12	-3.31	1.26	1.34
12	A	812	CLA	CHB-C1B	3.31	1.46	1.39
12	A	811	CLA	OBD-CAD	3.31	1.28	1.22
12	H	824	CLA	C1B-NB	-3.31	1.33	1.37
12	B	814	CLA	C1D-ND	-3.31	1.33	1.37
12	A	830	CLA	CHD-C4C	3.31	1.46	1.39
12	B	805	CLA	C1C-NC	-3.31	1.32	1.37
12	A	802	CLA	C1C-NC	-3.30	1.32	1.37
12	a	830	CLA	CHD-C4C	3.30	1.46	1.39
15	a	844	BCR	C11-C12	-3.30	1.26	1.34
12	L	206	CLA	C1D-ND	-3.30	1.33	1.37
12	B	826	CLA	C1C-NC	-3.30	1.32	1.37
12	P	201	CLA	C1D-ND	-3.30	1.33	1.37
12	H	819	CLA	MG-NC	3.30	2.14	2.06
12	A	826	CLA	CHD-C4C	3.30	1.46	1.39
12	G	856	CLA	C3C-C2C	3.30	1.43	1.36
12	H	803	CLA	C1B-NB	-3.30	1.33	1.37
12	B	834	CLA	OBD-CAD	3.30	1.28	1.22
12	b	822	CLA	C1B-NB	-3.30	1.33	1.37
12	G	828	CLA	MG-ND	-3.30	1.99	2.05
12	b	805	CLA	C1C-NC	-3.30	1.32	1.37
12	b	833	CLA	OBD-CAD	3.30	1.28	1.22
12	a	830	CLA	MG-ND	-3.30	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	836	CLA	C1B-NB	-3.30	1.33	1.37
12	b	837	CLA	C1D-ND	-3.30	1.33	1.37
12	G	802	CLA	OBD-CAD	3.30	1.28	1.22
12	H	818	CLA	C1D-ND	-3.30	1.33	1.37
12	b	810	CLA	C4B-NB	-3.29	1.33	1.37
12	b	822	CLA	CHB-C1B	3.29	1.46	1.39
12	H	811	CLA	C1C-NC	-3.29	1.32	1.37
12	b	823	CLA	C1D-ND	-3.29	1.33	1.37
12	A	841	CLA	CHC-C4B	3.29	1.46	1.39
12	H	807	CLA	CHD-C4C	3.29	1.46	1.39
12	b	805	CLA	CHD-C4C	3.29	1.46	1.39
12	b	805	CLA	C1D-ND	-3.29	1.33	1.37
12	a	806	CLA	C1D-ND	-3.29	1.33	1.37
12	B	826	CLA	CHB-C1B	3.29	1.46	1.39
12	B	827	CLA	CHB-C1B	3.29	1.46	1.39
12	A	828	CLA	C1B-NB	-3.28	1.33	1.37
12	L	204	CLA	C1B-NB	-3.28	1.33	1.37
12	G	813	CLA	C1C-NC	-3.28	1.32	1.37
12	H	803	CLA	MG-ND	-3.28	1.99	2.05
12	b	834	CLA	OBD-CAD	3.28	1.28	1.22
12	A	855	CLA	C1B-NB	-3.28	1.33	1.37
12	H	823	CLA	CHD-C4C	3.28	1.46	1.39
12	A	817	CLA	OBD-CAD	3.28	1.28	1.22
12	a	832	CLA	OBD-CAD	3.28	1.28	1.22
12	G	806	CLA	C1D-ND	-3.28	1.33	1.37
12	a	812	CLA	CHD-C4C	3.27	1.46	1.39
12	a	816	CLA	C1B-NB	-3.27	1.33	1.37
12	A	803	CLA	OBD-CAD	3.27	1.28	1.22
12	A	837	CLA	CHB-C1B	3.27	1.46	1.39
12	G	830	CLA	MG-ND	-3.27	1.99	2.05
12	A	813	CLA	C1B-C2B	3.27	1.50	1.43
12	H	811	CLA	C1B-NB	-3.27	1.33	1.37
12	G	837	CLA	CHB-C1B	3.27	1.46	1.39
12	G	856	CLA	CHB-C1B	3.27	1.46	1.39
12	A	820	CLA	C3D-C2D	3.27	1.47	1.39
12	H	827	CLA	CHC-C1C	3.27	1.45	1.38
12	G	814	CLA	C1B-NB	-3.27	1.33	1.37
12	a	855	CLA	CHB-C1B	3.27	1.46	1.39
12	G	830	CLA	OBD-CAD	3.27	1.28	1.22
12	B	805	CLA	C1D-ND	-3.27	1.33	1.37
12	A	802	CLA	C3C-C2C	3.27	1.43	1.36
12	H	822	CLA	CHB-C1B	3.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	809	CLA	MG-NC	3.27	2.14	2.06
12	a	836	CLA	C4C-C3C	3.26	1.50	1.45
12	a	834	CLA	C3D-C2D	3.26	1.47	1.39
12	L	202	CLA	C1D-ND	-3.26	1.33	1.37
12	A	810	CLA	C1D-ND	-3.26	1.33	1.37
12	G	834	CLA	CHB-C1B	3.26	1.46	1.39
12	L	205	CLA	CHD-C1D	3.26	1.44	1.38
12	b	808	CLA	C1B-C2B	3.26	1.50	1.43
12	A	831	CLA	C1B-NB	-3.26	1.33	1.37
12	B	803	CLA	C1B-NB	-3.26	1.33	1.37
12	j	102	CLA	C1D-ND	-3.26	1.33	1.37
12	H	829	CLA	C1B-NB	-3.26	1.33	1.37
12	H	807	CLA	C1C-NC	-3.26	1.32	1.37
15	H	843	BCR	C11-C12	-3.26	1.26	1.34
12	H	831	CLA	C3D-C4D	-3.26	1.36	1.44
12	B	810	CLA	C1D-ND	-3.26	1.33	1.37
12	a	816	CLA	CHC-C4B	3.25	1.46	1.39
12	a	833	CLA	CHB-C1B	3.25	1.46	1.39
12	B	837	CLA	CHC-C4B	3.25	1.46	1.39
12	H	825	CLA	C1B-NB	-3.25	1.33	1.37
12	a	830	CLA	OBD-CAD	3.25	1.28	1.22
12	b	834	CLA	C1D-ND	-3.25	1.33	1.37
12	G	809	CLA	CHB-C1B	3.25	1.46	1.39
12	G	841	CLA	C3D-C2D	3.25	1.47	1.39
12	F	201	CLA	MG-NC	3.25	2.14	2.06
12	A	840	CLA	MG-ND	-3.25	1.99	2.05
12	A	832	CLA	C1D-ND	-3.25	1.33	1.37
12	G	828	CLA	CHD-C4C	3.25	1.46	1.39
19	B	847	LMT	O2B-C2B	-3.25	1.34	1.43
12	H	805	CLA	C1C-NC	-3.25	1.32	1.37
12	A	828	CLA	MG-NC	3.25	2.14	2.06
12	b	848	CLA	C4D-CHA	3.25	1.49	1.38
15	b	841	BCR	C11-C12	-3.24	1.26	1.34
12	G	827	CLA	MG-NC	3.24	2.14	2.06
12	G	827	CLA	CHD-C4C	3.24	1.46	1.39
12	A	806	CLA	C1B-NB	-3.24	1.33	1.37
12	b	830	CLA	MG-NC	3.24	2.14	2.06
12	B	835	CLA	OBD-CAD	3.24	1.28	1.22
12	f	201	CLA	MG-NC	3.24	2.14	2.06
12	P	201	CLA	CHB-C1B	3.24	1.46	1.39
15	B	842	BCR	C11-C12	-3.24	1.26	1.34
12	G	828	CLA	CHB-C1B	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	833	CLA	C1D-ND	-3.24	1.33	1.37
15	A	844	BCR	C11-C12	-3.24	1.26	1.34
15	f	204	BCR	C11-C12	-3.24	1.26	1.34
12	H	832	CLA	MG-ND	-3.24	1.99	2.05
12	a	854	CLA	CHD-C1D	3.24	1.44	1.38
12	G	829	CLA	MG-ND	-3.24	1.99	2.05
12	G	803	CLA	CHC-C4B	3.23	1.46	1.39
12	G	818	CLA	OBD-CAD	3.23	1.28	1.22
12	A	833	CLA	C1D-ND	-3.23	1.33	1.37
12	l	202	CLA	C1D-ND	-3.23	1.33	1.37
12	A	837	CLA	C1D-ND	-3.23	1.33	1.37
12	G	803	CLA	CHB-C1B	3.23	1.46	1.39
12	A	855	CLA	C3C-C2C	3.23	1.43	1.36
12	b	806	CLA	CHD-C4C	3.23	1.46	1.39
12	b	826	CLA	C1C-NC	-3.23	1.32	1.37
12	A	806	CLA	C1D-ND	-3.23	1.33	1.37
12	G	839	CLA	CHB-C1B	3.23	1.46	1.39
12	G	813	CLA	C1B-NB	-3.23	1.33	1.37
12	H	835	CLA	C1B-NB	-3.23	1.33	1.37
12	H	807	CLA	C3D-C2D	3.23	1.47	1.39
12	a	816	CLA	OBD-CAD	3.22	1.28	1.22
12	G	828	CLA	C1C-NC	-3.22	1.32	1.37
12	G	856	CLA	C1B-NB	-3.22	1.33	1.37
12	S	202	CLA	C1B-NB	-3.22	1.33	1.37
12	b	830	CLA	C1B-NB	-3.22	1.33	1.37
12	a	827	CLA	CHB-C1B	3.22	1.46	1.39
15	H	846	BCR	C11-C12	-3.22	1.26	1.34
12	a	817	CLA	OBD-CAD	3.22	1.28	1.22
12	j	104	CLA	MG-NC	3.22	2.13	2.06
12	b	830	CLA	MG-ND	-3.22	1.99	2.05
12	a	804	CLA	CHB-C1B	3.22	1.46	1.39
12	G	803	CLA	C1C-NC	-3.22	1.32	1.37
12	A	825	CLA	C1D-ND	-3.22	1.33	1.37
12	G	832	CLA	C1D-ND	-3.22	1.33	1.37
12	H	806	CLA	CHD-C4C	3.22	1.46	1.39
12	A	816	CLA	MG-NC	3.22	2.13	2.06
12	H	836	CLA	OBD-CAD	3.22	1.28	1.22
12	H	835	CLA	OBD-CAD	3.22	1.28	1.22
12	A	824	CLA	CHD-C4C	3.22	1.46	1.39
12	B	809	CLA	MG-NC	3.22	2.13	2.06
12	b	812	CLA	OBD-CAD	3.22	1.28	1.22
12	a	828	CLA	MG-ND	-3.22	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	845	BCR	C11-C12	-3.22	1.26	1.34
12	a	821	CLA	C1D-ND	-3.21	1.33	1.37
12	G	807	CLA	OBD-CAD	3.21	1.28	1.22
12	G	836	CLA	C1D-ND	-3.21	1.33	1.37
12	B	830	CLA	C3D-C2D	3.21	1.47	1.39
12	A	854	CLA	CHD-C1D	3.21	1.44	1.38
12	l	204	CLA	C3D-C2D	3.21	1.47	1.39
12	H	810	CLA	MG-NC	3.21	2.13	2.06
12	B	821	CLA	MG-ND	-3.21	1.99	2.05
12	G	825	CLA	CHD-C4C	3.21	1.46	1.39
12	A	822	CLA	MG-NC	3.21	2.13	2.06
12	B	810	CLA	CHC-C4B	3.21	1.46	1.39
12	G	807	CLA	C1B-NB	-3.21	1.33	1.37
12	A	806	CLA	OBD-CAD	3.21	1.28	1.22
12	b	804	CLA	CHD-C1D	3.21	1.44	1.38
12	B	831	CLA	C1B-NB	-3.21	1.33	1.37
12	B	808	CLA	C1C-NC	-3.21	1.32	1.37
12	B	822	CLA	C3D-C2D	3.21	1.47	1.39
12	H	832	CLA	MG-NC	3.21	2.13	2.06
12	b	825	CLA	CHB-C1B	3.21	1.46	1.39
12	H	803	CLA	CHB-C1B	3.20	1.46	1.39
12	a	826	CLA	CHD-C4C	3.20	1.46	1.39
12	b	832	CLA	MG-NC	3.20	2.13	2.06
15	A	849	BCR	C11-C12	-3.20	1.26	1.34
12	H	825	CLA	CHD-C4C	3.20	1.46	1.39
12	a	811	CLA	OBD-CAD	3.20	1.28	1.22
12	G	808	CLA	C1D-ND	-3.20	1.33	1.37
12	a	826	CLA	MG-NC	3.20	2.13	2.06
12	b	812	CLA	MG-NC	3.20	2.13	2.06
15	H	849	BCR	C11-C12	-3.20	1.26	1.34
12	H	823	CLA	CHD-C1D	3.20	1.44	1.38
12	a	831	CLA	C1B-NB	-3.20	1.33	1.37
12	b	812	CLA	C1D-ND	-3.20	1.33	1.37
12	a	841	CLA	CHC-C4B	3.20	1.46	1.39
12	a	822	CLA	MG-NC	3.20	2.13	2.06
12	H	806	CLA	C4B-NB	-3.20	1.33	1.37
12	A	821	CLA	C1D-ND	-3.20	1.33	1.37
12	B	814	CLA	C1B-NB	-3.20	1.33	1.37
12	H	835	CLA	C3D-C2D	3.20	1.47	1.39
12	G	828	CLA	C4B-NB	-3.19	1.33	1.37
12	A	834	CLA	CHB-C1B	3.19	1.46	1.39
12	G	833	CLA	C1B-NB	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	842	CLA	C1C-NC	-3.19	1.32	1.37
12	B	831	CLA	MG-ND	-3.19	1.99	2.05
12	a	824	CLA	C1B-NB	-3.19	1.33	1.37
12	a	837	CLA	CHB-C1B	3.19	1.46	1.39
12	A	827	CLA	CHD-C4C	3.19	1.46	1.39
12	H	808	CLA	C1D-ND	-3.19	1.33	1.37
12	b	833	CLA	C1B-NB	-3.19	1.33	1.37
12	B	817	CLA	C1D-ND	-3.19	1.33	1.37
12	A	854	CLA	MG-ND	-3.19	1.99	2.05
12	G	837	CLA	C1B-NB	-3.19	1.33	1.37
12	A	804	CLA	CHB-C1B	3.19	1.46	1.39
12	H	801	CLA	C1B-NB	-3.19	1.33	1.37
12	B	823	CLA	C1D-ND	-3.19	1.33	1.37
12	G	812	CLA	MG-NC	3.19	2.13	2.06
12	B	812	CLA	C4D-CHA	3.19	1.49	1.38
12	A	822	CLA	C1D-ND	-3.19	1.33	1.37
12	a	841	CLA	C1C-NC	-3.18	1.32	1.37
12	H	809	CLA	CHC-C4B	3.18	1.46	1.39
12	b	818	CLA	MG-NC	3.18	2.13	2.06
12	b	807	CLA	MG-ND	-3.18	1.99	2.05
12	H	813	CLA	C1B-NB	-3.18	1.33	1.37
12	b	827	CLA	CHB-C1B	3.18	1.46	1.39
12	a	833	CLA	C1D-ND	-3.18	1.33	1.37
12	b	802	CLA	CHD-C4C	3.18	1.46	1.39
12	A	813	CLA	MG-ND	-3.18	1.99	2.05
12	J	103	CLA	MG-NC	3.18	2.13	2.06
12	A	827	CLA	C4B-NB	-3.18	1.33	1.37
12	A	831	CLA	C1D-ND	-3.18	1.33	1.37
12	a	816	CLA	C3D-C2D	3.18	1.47	1.39
12	A	826	CLA	MG-ND	-3.18	1.99	2.05
15	b	844	BCR	C11-C12	-3.18	1.26	1.34
12	G	823	CLA	MG-NC	3.18	2.13	2.06
12	G	813	CLA	MG-ND	-3.18	1.99	2.05
12	H	839	CLA	CHD-C4C	3.18	1.46	1.39
12	b	810	CLA	CHC-C4B	3.17	1.46	1.39
12	G	841	CLA	CHC-C4B	3.17	1.46	1.39
12	a	837	CLA	C1B-NB	-3.17	1.33	1.37
12	B	824	CLA	CHD-C4C	3.17	1.46	1.39
12	A	841	CLA	MG-NC	3.17	2.13	2.06
12	a	810	CLA	C1D-ND	-3.17	1.33	1.37
12	G	837	CLA	C1D-ND	-3.17	1.33	1.37
12	A	816	CLA	C3D-C2D	3.17	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	855	CLA	C3C-C2C	3.17	1.43	1.36
12	B	816	CLA	C3D-C2D	3.17	1.47	1.39
12	b	810	CLA	C1D-ND	-3.17	1.33	1.37
12	G	840	CLA	MG-ND	-3.17	1.99	2.05
12	B	808	CLA	C1B-C2B	3.17	1.50	1.43
12	A	835	CLA	MG-NC	3.17	2.13	2.06
12	b	836	CLA	CHC-C4B	3.17	1.46	1.39
12	B	815	CLA	CHB-C1B	3.17	1.46	1.39
11	a	801	CL0	OBD-CAD	3.17	1.27	1.22
12	A	841	CLA	OBD-CAD	3.17	1.27	1.22
12	B	817	CLA	MG-NC	3.16	2.13	2.06
12	G	827	CLA	C1D-ND	-3.16	1.33	1.37
12	A	811	CLA	MG-NC	3.16	2.13	2.06
12	A	836	CLA	C1D-ND	-3.16	1.33	1.37
12	a	825	CLA	C3D-C2D	3.16	1.47	1.39
12	a	827	CLA	CHD-C4C	3.16	1.46	1.39
12	H	817	CLA	C3D-C2D	3.16	1.47	1.39
12	a	806	CLA	C1B-NB	-3.16	1.33	1.37
12	G	814	CLA	CHC-C4B	3.16	1.46	1.39
12	a	855	CLA	MG-ND	-3.16	1.99	2.05
12	B	806	CLA	CHD-C4C	3.16	1.46	1.39
12	H	823	CLA	C3D-C2D	3.16	1.47	1.39
12	A	855	CLA	CHD-C4C	3.16	1.46	1.39
12	L	205	CLA	MG-ND	-3.16	1.99	2.05
12	H	825	CLA	CHB-C1B	3.16	1.46	1.39
12	B	802	CLA	MG-ND	-3.16	1.99	2.05
12	b	823	CLA	CHD-C4C	3.16	1.46	1.39
12	A	829	CLA	C3D-C2D	3.15	1.47	1.39
12	a	802	CLA	CHB-C1B	3.15	1.46	1.39
12	G	829	CLA	MG-NC	3.15	2.13	2.06
12	B	812	CLA	MG-NC	3.15	2.13	2.06
12	a	807	CLA	MG-NC	3.15	2.13	2.06
12	B	824	CLA	CHB-C1B	3.15	1.46	1.39
12	G	830	CLA	C3D-C2D	3.15	1.47	1.39
12	a	830	CLA	MG-NC	3.15	2.13	2.06
12	H	820	CLA	MG-NC	3.15	2.13	2.06
12	B	818	CLA	MG-NC	3.15	2.13	2.06
12	b	816	CLA	C3D-C2D	3.15	1.47	1.39
12	H	815	CLA	C1B-NB	-3.15	1.33	1.37
12	H	811	CLA	C4D-CHA	3.15	1.49	1.38
12	a	840	CLA	MG-ND	-3.15	1.99	2.05
12	R	103	CLA	MG-NC	3.15	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	809	CLA	C1B-C2B	3.15	1.50	1.43
12	A	823	CLA	C1D-ND	-3.15	1.33	1.37
12	A	827	CLA	CHB-C1B	3.15	1.46	1.39
12	H	806	CLA	C1C-NC	-3.15	1.32	1.37
12	H	824	CLA	C1D-ND	-3.15	1.33	1.37
12	A	839	CLA	CHB-C1B	3.15	1.46	1.39
12	a	834	CLA	CHB-C1B	3.15	1.46	1.39
12	a	854	CLA	MG-ND	-3.15	1.99	2.05
12	b	807	CLA	C1C-NC	-3.15	1.32	1.37
17	m	101	45D	C27-C25	3.15	1.57	1.50
12	A	832	CLA	CHB-C1B	3.14	1.46	1.39
12	B	806	CLA	C1C-NC	-3.14	1.32	1.37
12	B	819	CLA	MG-NC	3.14	2.13	2.06
12	a	839	CLA	CHB-C1B	3.14	1.46	1.39
12	b	817	CLA	MG-NC	3.14	2.13	2.06
12	B	813	CLA	C1D-ND	-3.14	1.33	1.37
12	H	811	CLA	CHB-C1B	3.14	1.46	1.39
12	a	829	CLA	C3D-C2D	3.14	1.47	1.39
12	G	813	CLA	CHC-C4B	3.14	1.46	1.39
12	G	856	CLA	CHD-C4C	3.14	1.46	1.39
12	A	834	CLA	C1B-NB	-3.14	1.33	1.37
12	A	805	CLA	C1B-NB	-3.14	1.33	1.37
12	a	825	CLA	MG-NC	3.13	2.13	2.06
12	G	806	CLA	OBD-CAD	3.13	1.27	1.22
12	a	831	CLA	C3D-C2D	3.13	1.47	1.39
17	M	101	45D	C27-C25	3.13	1.57	1.50
12	A	805	CLA	OBD-CAD	3.13	1.27	1.22
12	b	809	CLA	C4D-CHA	3.13	1.49	1.38
12	G	821	CLA	C3D-C2D	3.13	1.47	1.39
12	a	855	CLA	CHD-C4C	3.13	1.46	1.39
12	A	803	CLA	MG-NC	3.13	2.13	2.06
12	b	803	CLA	C1B-NB	-3.13	1.33	1.37
12	A	855	CLA	CHB-C1B	3.13	1.46	1.39
12	A	840	CLA	C1B-NB	-3.13	1.33	1.37
12	H	834	CLA	MG-NC	3.13	2.13	2.06
12	b	803	CLA	MG-ND	-3.13	1.99	2.05
12	b	833	CLA	C1D-ND	-3.13	1.33	1.37
12	a	820	CLA	C3D-C2D	3.13	1.47	1.39
12	H	818	CLA	MG-NC	3.13	2.13	2.06
12	A	839	CLA	C3D-C2D	3.12	1.47	1.39
12	B	837	CLA	C1B-C2B	3.12	1.50	1.43
12	b	830	CLA	C3D-C2D	3.12	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	822	CLA	C1D-ND	-3.12	1.33	1.37
12	S	203	CLA	MG-ND	-3.12	1.99	2.05
12	b	807	CLA	OBD-CAD	3.12	1.27	1.22
12	H	815	CLA	C1D-ND	-3.12	1.33	1.37
12	a	832	CLA	CHB-C1B	3.12	1.46	1.39
12	b	801	CLA	CHD-C1D	3.12	1.44	1.38
12	B	808	CLA	C3D-C2D	3.12	1.47	1.39
12	G	817	CLA	C3D-C2D	3.12	1.47	1.39
12	G	818	CLA	MG-ND	-3.12	1.99	2.05
12	A	803	CLA	C4D-CHA	3.12	1.49	1.38
12	a	827	CLA	C4B-NB	-3.12	1.33	1.37
12	A	840	CLA	MG-NC	3.12	2.13	2.06
12	l	204	CLA	C1B-NB	-3.12	1.33	1.37
12	A	827	CLA	OBD-CAD	3.12	1.27	1.22
12	A	855	CLA	MG-ND	-3.12	1.99	2.05
12	G	825	CLA	C3D-C2D	3.12	1.47	1.39
12	G	833	CLA	C1C-NC	-3.12	1.33	1.37
12	G	804	CLA	MG-NC	3.12	2.13	2.06
12	G	806	CLA	C1B-C2B	3.12	1.50	1.43
12	b	819	CLA	MG-NC	3.12	2.13	2.06
12	a	841	CLA	MG-ND	-3.11	1.99	2.05
12	A	825	CLA	MG-ND	-3.11	1.99	2.05
12	a	829	CLA	MG-ND	-3.11	1.99	2.05
12	G	811	CLA	C1D-ND	-3.11	1.33	1.37
12	G	812	CLA	C1D-ND	-3.11	1.33	1.37
12	a	837	CLA	C1D-ND	-3.11	1.33	1.37
12	B	809	CLA	C4D-CHA	3.11	1.49	1.38
12	A	809	CLA	C1B-C2B	3.11	1.50	1.43
12	H	829	CLA	C1D-ND	-3.11	1.33	1.37
12	B	830	CLA	C1D-ND	-3.11	1.33	1.37
12	H	838	CLA	C1B-C2B	3.11	1.50	1.43
12	a	804	CLA	C4D-CHA	3.11	1.49	1.38
12	a	826	CLA	C1D-ND	-3.11	1.33	1.37
12	A	830	CLA	MG-ND	-3.11	1.99	2.05
15	J	104	BCR	C11-C12	-3.11	1.26	1.34
12	H	850	CLA	C4D-CHA	3.11	1.49	1.38
12	A	830	CLA	MG-NC	3.11	2.13	2.06
12	b	816	CLA	CHB-C1B	3.11	1.46	1.39
12	a	839	CLA	C1B-NB	-3.11	1.33	1.37
12	B	807	CLA	C3D-C2D	3.11	1.47	1.39
12	H	809	CLA	C1C-NC	-3.11	1.33	1.37
12	H	813	CLA	C4D-CHA	3.11	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	832	CLA	MG-ND	-3.10	1.99	2.05
12	A	829	CLA	C4B-NB	-3.10	1.33	1.37
12	A	828	CLA	MG-ND	-3.10	1.99	2.05
17	T	101	45D	C27-C25	3.10	1.57	1.50
12	b	813	CLA	C1D-ND	-3.10	1.33	1.37
12	A	820	CLA	C4D-CHA	3.10	1.49	1.38
12	H	802	CLA	MG-ND	-3.10	1.99	2.05
12	F	203	CLA	MG-NC	3.10	2.13	2.06
12	A	821	CLA	MG-NC	3.10	2.13	2.06
12	H	821	CLA	C3D-C2D	3.10	1.47	1.39
12	B	816	CLA	CHB-C1B	3.10	1.46	1.39
12	b	822	CLA	C3D-C2D	3.10	1.47	1.39
12	G	809	CLA	C1B-NB	-3.10	1.33	1.37
12	H	834	CLA	C1D-ND	-3.10	1.33	1.37
12	B	831	CLA	C3D-C2D	3.10	1.47	1.39
12	A	804	CLA	C4D-CHA	3.10	1.49	1.38
12	a	841	CLA	C3D-C2D	3.10	1.47	1.39
12	b	832	CLA	C1D-ND	-3.10	1.33	1.37
12	A	825	CLA	C3D-C2D	3.10	1.47	1.39
12	b	830	CLA	C4D-CHA	3.10	1.49	1.38
12	A	817	CLA	MG-ND	-3.10	1.99	2.05
12	B	824	CLA	C4B-NB	-3.10	1.33	1.37
12	B	825	CLA	C1C-NC	-3.10	1.33	1.37
12	G	826	CLA	CHB-C1B	3.10	1.46	1.39
12	j	104	CLA	C3D-C2D	3.10	1.47	1.39
12	G	835	CLA	MG-NC	3.10	2.13	2.06
12	A	825	CLA	CHB-C1B	3.09	1.46	1.39
12	l	204	CLA	C4D-CHA	3.09	1.49	1.38
12	G	830	CLA	CHC-C4B	3.09	1.46	1.39
12	a	818	CLA	C4D-CHA	3.09	1.49	1.38
12	G	827	CLA	OBD-CAD	3.09	1.27	1.22
12	A	818	CLA	C1C-NC	-3.09	1.33	1.37
12	G	826	CLA	C4D-CHA	3.09	1.49	1.38
12	a	811	CLA	MG-NC	3.09	2.13	2.06
12	H	805	CLA	C1D-ND	-3.09	1.33	1.37
12	G	839	CLA	C4D-CHA	3.09	1.49	1.38
11	a	801	CL0	MG-NC	3.09	2.13	2.06
12	A	839	CLA	C4D-CHA	3.09	1.49	1.38
12	A	826	CLA	C1C-NC	-3.09	1.33	1.37
12	B	815	CLA	MG-NC	3.09	2.13	2.06
12	b	848	CLA	C3D-C2D	3.09	1.47	1.39
12	H	827	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	812	CLA	C1B-C2B	3.09	1.50	1.43
12	G	810	CLA	C1B-C2B	3.09	1.50	1.43
12	a	815	CLA	MG-NC	3.09	2.13	2.06
12	A	834	CLA	C3D-C2D	3.09	1.47	1.39
12	a	825	CLA	CHB-C1B	3.08	1.46	1.39
12	b	848	CLA	C1C-NC	-3.08	1.33	1.37
12	b	808	CLA	CHC-C4B	3.08	1.46	1.39
12	B	808	CLA	CHC-C4B	3.08	1.46	1.39
12	H	817	CLA	MG-NC	3.08	2.13	2.06
12	a	821	CLA	MG-NC	3.08	2.13	2.06
12	S	202	CLA	C4D-CHA	3.08	1.48	1.38
12	b	824	CLA	OBD-CAD	3.08	1.27	1.22
12	A	824	CLA	C1B-NB	-3.08	1.33	1.37
12	A	825	CLA	C4D-CHA	3.08	1.48	1.38
12	b	831	CLA	MG-NC	3.08	2.13	2.06
12	a	816	CLA	MG-NC	3.08	2.13	2.06
12	A	811	CLA	C1D-ND	-3.08	1.33	1.37
12	b	802	CLA	CHD-C1D	3.08	1.44	1.38
12	A	817	CLA	CHB-C1B	3.08	1.46	1.39
12	a	839	CLA	C4D-CHA	3.08	1.48	1.38
12	G	822	CLA	MG-NC	3.08	2.13	2.06
12	A	804	CLA	C3D-C2D	3.07	1.47	1.39
12	B	810	CLA	C4D-CHA	3.07	1.48	1.38
12	A	809	CLA	C3D-C2D	3.07	1.47	1.39
12	a	804	CLA	C1B-NB	-3.07	1.33	1.37
12	S	204	CLA	C3D-C2D	3.07	1.47	1.39
12	a	835	CLA	MG-NC	3.07	2.13	2.06
12	b	806	CLA	C4B-NB	-3.07	1.33	1.37
12	A	812	CLA	C4D-CHA	3.07	1.48	1.38
12	b	807	CLA	C3D-C2D	3.07	1.47	1.39
12	B	832	CLA	MG-NC	3.07	2.13	2.06
12	G	804	CLA	C4D-CHA	3.07	1.48	1.38
12	G	832	CLA	C4D-CHA	3.07	1.48	1.38
12	H	838	CLA	MG-ND	-3.07	1.99	2.05
12	A	825	CLA	MG-NC	3.07	2.13	2.06
12	G	832	CLA	CHB-C1B	3.07	1.46	1.39
12	j	102	CLA	C1C-NC	-3.07	1.33	1.37
12	G	832	CLA	MG-ND	-3.07	1.99	2.05
12	A	841	CLA	C1C-NC	-3.07	1.33	1.37
12	A	802	CLA	CHC-C4B	3.07	1.46	1.39
12	B	828	CLA	MG-NC	3.07	2.13	2.06
12	B	819	CLA	C3D-C2D	3.07	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	808	CLA	C4D-CHA	3.07	1.48	1.38
12	J	103	CLA	C4D-CHA	3.07	1.48	1.38
12	a	812	CLA	C1C-NC	-3.07	1.33	1.37
12	a	818	CLA	C1D-ND	-3.07	1.33	1.37
12	H	828	CLA	MG-NC	3.07	2.13	2.06
12	G	826	CLA	C1D-ND	-3.07	1.33	1.37
12	b	812	CLA	C4D-CHA	3.07	1.48	1.38
12	A	835	CLA	C4D-CHA	3.07	1.48	1.38
12	B	834	CLA	C1B-NB	-3.06	1.33	1.37
12	G	831	CLA	MG-NC	3.06	2.13	2.06
12	a	803	CLA	C4D-CHA	3.06	1.48	1.38
12	a	818	CLA	C3D-C2D	3.06	1.47	1.39
12	P	201	CLA	MG-ND	-3.06	1.99	2.05
12	P	201	CLA	MG-NC	3.06	2.13	2.06
12	b	810	CLA	C4D-CHA	3.06	1.48	1.38
12	b	828	CLA	C1D-ND	-3.06	1.33	1.37
12	b	828	CLA	MG-NC	3.06	2.13	2.06
12	b	827	CLA	MG-NC	3.06	2.13	2.06
12	j	104	CLA	C4D-CHA	3.06	1.48	1.38
12	H	850	CLA	C1C-NC	-3.06	1.33	1.37
12	b	828	CLA	C1B-NB	-3.06	1.33	1.37
12	B	804	CLA	CHD-C1D	3.06	1.44	1.38
12	a	836	CLA	C1D-ND	-3.06	1.33	1.37
12	A	841	CLA	C3D-C2D	3.06	1.47	1.39
12	A	838	CLA	MG-NC	3.06	2.13	2.06
12	G	833	CLA	C4B-NB	-3.06	1.33	1.37
12	B	820	CLA	C3D-C2D	3.06	1.47	1.39
12	b	811	CLA	C1D-ND	-3.06	1.33	1.37
12	A	833	CLA	C3D-C2D	3.06	1.47	1.39
12	f	203	CLA	MG-NC	3.06	2.13	2.06
12	A	808	CLA	C1B-NB	-3.06	1.33	1.37
12	a	826	CLA	MG-ND	-3.06	1.99	2.05
12	P	203	CLA	C3D-C2D	3.06	1.47	1.39
12	H	811	CLA	CHC-C4B	3.05	1.46	1.39
11	G	801	CL0	MG-NC	3.05	2.13	2.06
12	G	840	CLA	MG-NC	3.05	2.13	2.06
12	b	823	CLA	C4D-CHA	3.05	1.48	1.38
12	a	833	CLA	C3D-C2D	3.05	1.47	1.39
12	L	204	CLA	C4D-CHA	3.05	1.48	1.38
12	a	823	CLA	C1D-ND	-3.05	1.33	1.37
12	A	839	CLA	MG-NC	3.05	2.13	2.06
12	b	831	CLA	C3D-C2D	3.05	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	805	CLA	C1B-NB	-3.05	1.33	1.37
12	B	819	CLA	C4D-CHA	3.05	1.48	1.38
12	G	810	CLA	C4D-CHA	3.05	1.48	1.38
12	B	831	CLA	C4D-CHA	3.05	1.48	1.38
12	a	838	CLA	MG-NC	3.05	2.13	2.06
12	a	828	CLA	C3D-C2D	3.05	1.47	1.39
12	b	814	CLA	C3D-C2D	3.05	1.47	1.39
12	A	837	CLA	C1B-NB	-3.05	1.33	1.37
12	F	203	CLA	C3D-C2D	3.05	1.47	1.39
12	H	831	CLA	C4D-CHA	3.05	1.48	1.38
12	G	839	CLA	MG-NC	3.05	2.13	2.06
12	B	828	CLA	C1D-ND	-3.05	1.33	1.37
12	a	838	CLA	MG-ND	-3.05	1.99	2.05
12	G	814	CLA	C1D-ND	-3.05	1.33	1.37
12	b	803	CLA	MG-NC	3.05	2.13	2.06
12	B	821	CLA	CHB-C1B	3.05	1.46	1.39
12	G	832	CLA	C3D-C2D	3.04	1.47	1.39
12	b	806	CLA	C1B-NB	-3.04	1.33	1.37
12	H	819	CLA	C4D-CHA	3.04	1.48	1.38
12	B	801	CLA	CHD-C1D	3.04	1.44	1.38
12	H	801	CLA	MG-ND	-3.04	1.99	2.05
12	A	832	CLA	MG-ND	-3.04	1.99	2.05
12	a	833	CLA	C1C-NC	-3.04	1.33	1.37
12	a	827	CLA	C1C-NC	-3.04	1.33	1.37
12	B	812	CLA	C1B-NB	-3.04	1.33	1.37
12	a	831	CLA	C1D-ND	-3.04	1.33	1.37
12	b	829	CLA	MG-NC	3.04	2.13	2.06
12	H	820	CLA	C4D-CHA	3.04	1.48	1.38
12	H	823	CLA	C1C-NC	-3.04	1.33	1.37
12	A	836	CLA	C4C-C3C	3.04	1.50	1.45
12	H	838	CLA	C3D-C2D	3.04	1.47	1.39
12	b	836	CLA	C1B-C2B	3.04	1.50	1.43
12	b	808	CLA	C4B-NB	-3.04	1.33	1.37
12	A	804	CLA	MG-NC	3.04	2.13	2.06
12	a	808	CLA	C4D-CHA	3.04	1.48	1.38
12	b	808	CLA	C3D-C2D	3.04	1.47	1.39
12	G	817	CLA	MG-NC	3.04	2.13	2.06
12	a	803	CLA	MG-NC	3.04	2.13	2.06
12	G	814	CLA	C3D-C2D	3.03	1.47	1.39
12	A	832	CLA	C4D-CHA	3.03	1.48	1.38
12	H	809	CLA	C3D-C2D	3.03	1.47	1.39
12	a	807	CLA	C4D-CHA	3.03	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	818	CLA	C4D-CHA	3.03	1.48	1.38
12	b	828	CLA	C3D-C2D	3.03	1.47	1.39
12	H	832	CLA	C4D-CHA	3.03	1.48	1.38
12	B	822	CLA	MG-NC	3.03	2.13	2.06
12	G	841	CLA	MG-NC	3.03	2.13	2.06
12	H	816	CLA	C1C-NC	-3.03	1.33	1.37
12	b	836	CLA	MG-ND	-3.03	1.99	2.05
12	a	826	CLA	C4D-CHA	3.03	1.48	1.38
12	B	815	CLA	C4D-CHA	3.03	1.48	1.38
12	a	829	CLA	CHC-C4B	3.03	1.46	1.39
12	A	813	CLA	C1D-ND	-3.03	1.33	1.37
12	H	818	CLA	C4D-CHA	3.03	1.48	1.38
12	G	842	CLA	C1D-ND	-3.03	1.33	1.37
12	G	826	CLA	MG-NC	3.03	2.13	2.06
12	b	833	CLA	C3D-C2D	3.03	1.47	1.39
12	G	831	CLA	MG-ND	-3.03	1.99	2.05
12	H	829	CLA	C3D-C2D	3.03	1.47	1.39
12	a	811	CLA	C4D-CHA	3.03	1.48	1.38
12	a	820	CLA	C4D-CHA	3.03	1.48	1.38
12	G	827	CLA	C1B-NB	-3.03	1.33	1.37
12	b	827	CLA	C1B-NB	-3.03	1.33	1.37
12	a	822	CLA	C4D-CHA	3.03	1.48	1.38
12	b	820	CLA	C3D-C2D	3.03	1.47	1.39
12	f	203	CLA	C3D-C2D	3.03	1.47	1.39
12	B	828	CLA	C1B-NB	-3.03	1.33	1.37
12	a	817	CLA	MG-ND	-3.03	1.99	2.05
12	H	835	CLA	MG-ND	-3.02	1.99	2.05
12	G	805	CLA	C4D-CHA	3.02	1.48	1.38
12	a	834	CLA	C1C-NC	-3.02	1.33	1.37
12	A	811	CLA	MG-ND	-3.02	1.99	2.05
12	G	842	CLA	C4D-CHA	3.02	1.48	1.38
12	a	814	CLA	C3D-C2D	3.02	1.47	1.39
12	l	206	CLA	C3D-C2D	3.02	1.47	1.39
12	G	809	CLA	C4D-CHA	3.02	1.48	1.38
12	G	819	CLA	C1C-NC	-3.02	1.33	1.37
12	G	841	CLA	C1C-NC	-3.02	1.33	1.37
12	B	829	CLA	C3D-C2D	3.02	1.47	1.39
12	H	810	CLA	C4D-CHA	3.02	1.48	1.38
12	a	808	CLA	MG-ND	-3.02	1.99	2.05
12	b	836	CLA	C3D-C2D	3.02	1.47	1.39
12	H	823	CLA	MG-NC	3.02	2.13	2.06
12	B	810	CLA	CHD-C4C	3.02	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	815	CLA	C3D-C2D	3.02	1.47	1.39
12	R	103	CLA	C3D-C2D	3.02	1.47	1.39
12	B	814	CLA	C3D-C2D	3.02	1.47	1.39
12	B	830	CLA	C4D-CHA	3.02	1.48	1.38
12	G	824	CLA	MG-NC	3.02	2.13	2.06
12	A	812	CLA	MG-NC	3.02	2.13	2.06
12	b	825	CLA	C1C-NC	-3.02	1.33	1.37
12	G	808	CLA	C4D-CHA	3.02	1.48	1.38
12	B	833	CLA	MG-NC	3.02	2.13	2.06
12	b	828	CLA	C4D-CHA	3.02	1.48	1.38
12	G	814	CLA	C4B-NB	-3.02	1.33	1.37
12	G	839	CLA	C1B-NB	-3.02	1.33	1.37
12	l	206	CLA	C1B-NB	-3.02	1.33	1.37
12	B	818	CLA	C4D-CHA	3.02	1.48	1.38
12	l	205	CLA	MG-ND	-3.02	1.99	2.05
12	A	819	CLA	C3D-C2D	3.02	1.47	1.39
12	B	817	CLA	C4D-CHA	3.02	1.48	1.38
12	B	818	CLA	C3D-C2D	3.02	1.47	1.39
12	a	804	CLA	C3D-C2D	3.02	1.47	1.39
12	G	823	CLA	C4D-CHA	3.01	1.48	1.38
12	S	203	CLA	MG-NC	3.01	2.13	2.06
12	H	812	CLA	C1D-ND	-3.01	1.33	1.37
12	a	832	CLA	C4D-CHA	3.01	1.48	1.38
12	G	855	CLA	MG-ND	-3.01	1.99	2.05
12	a	821	CLA	C3D-C2D	3.01	1.47	1.39
12	B	802	CLA	CHD-C1D	3.01	1.44	1.38
12	H	801	CLA	C1D-ND	-3.01	1.33	1.37
12	G	835	CLA	C4D-CHA	3.01	1.48	1.38
12	H	825	CLA	CHC-C4B	3.01	1.46	1.39
12	L	206	CLA	C3D-C2D	3.01	1.47	1.39
12	B	823	CLA	C4D-CHA	3.01	1.48	1.38
12	b	822	CLA	MG-ND	-3.01	1.99	2.05
12	H	833	CLA	C3D-C2D	3.01	1.47	1.39
12	H	805	CLA	C1B-C2B	3.01	1.50	1.43
12	H	816	CLA	CHB-C1B	3.01	1.46	1.39
12	G	815	CLA	C3D-C2D	3.01	1.47	1.39
12	A	826	CLA	C4D-CHA	3.01	1.48	1.38
12	B	827	CLA	MG-NC	3.01	2.13	2.06
12	A	841	CLA	MG-ND	-3.01	1.99	2.05
12	a	809	CLA	C3D-C2D	3.01	1.47	1.39
12	R	103	CLA	C4D-CHA	3.01	1.48	1.38
12	G	833	CLA	C3D-C2D	3.01	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	806	CLA	MG-ND	-3.01	1.99	2.05
12	S	202	CLA	MG-NC	3.01	2.13	2.06
12	B	810	CLA	MG-NC	3.01	2.13	2.06
12	a	828	CLA	MG-NC	3.01	2.13	2.06
12	G	838	CLA	MG-ND	-3.01	1.99	2.05
12	F	201	CLA	MG-ND	-3.01	1.99	2.05
12	A	807	CLA	C1D-ND	-3.01	1.33	1.37
12	B	815	CLA	C3D-C2D	3.01	1.47	1.39
12	G	834	CLA	C3D-C2D	3.01	1.47	1.39
12	A	809	CLA	C4D-CHA	3.01	1.48	1.38
12	G	816	CLA	MG-NC	3.00	2.13	2.06
12	b	819	CLA	C4D-CHA	3.00	1.48	1.38
12	b	832	CLA	OBD-CAD	3.00	1.27	1.22
12	B	834	CLA	C3D-C2D	3.00	1.47	1.39
12	H	831	CLA	MG-NC	3.00	2.13	2.06
12	b	823	CLA	MG-NC	3.00	2.13	2.06
12	a	835	CLA	C4D-CHA	3.00	1.48	1.38
12	H	820	CLA	C3D-C2D	3.00	1.47	1.39
12	A	815	CLA	C3D-C2D	3.00	1.47	1.39
12	B	832	CLA	C3D-C2D	3.00	1.47	1.39
12	a	812	CLA	C1B-NB	-3.00	1.33	1.37
12	P	203	CLA	C4D-CHA	3.00	1.48	1.38
12	A	807	CLA	C4D-CHA	3.00	1.48	1.38
12	a	825	CLA	C4D-CHA	3.00	1.48	1.38
12	a	805	CLA	C1B-NB	-3.00	1.33	1.37
12	G	829	CLA	C3D-C2D	3.00	1.47	1.39
12	A	804	CLA	MG-ND	-3.00	1.99	2.05
12	H	808	CLA	C3D-C2D	3.00	1.47	1.39
12	a	807	CLA	C1D-ND	-3.00	1.33	1.37
12	G	810	CLA	MG-NC	3.00	2.13	2.06
12	H	817	CLA	CHB-C1B	3.00	1.46	1.39
12	L	206	CLA	C1B-NB	-3.00	1.33	1.37
12	H	833	CLA	MG-NC	3.00	2.13	2.06
12	G	827	CLA	C4D-CHA	3.00	1.48	1.38
12	b	819	CLA	C3D-C2D	3.00	1.47	1.39
11	G	801	CL0	CHD-C4C	3.00	1.46	1.39
12	A	826	CLA	MG-NC	3.00	2.13	2.06
12	J	103	CLA	C3D-C2D	3.00	1.47	1.39
12	A	821	CLA	C4D-CHA	3.00	1.48	1.38
12	B	838	CLA	MG-NC	3.00	2.13	2.06
12	G	813	CLA	C4D-CHA	3.00	1.48	1.38
12	a	806	CLA	OBD-CAD	3.00	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	803	CLA	MG-ND	-3.00	1.99	2.05
12	H	824	CLA	MG-NC	3.00	2.13	2.06
12	A	819	CLA	MG-NC	3.00	2.13	2.06
11	A	801	CL0	CHD-C4C	3.00	1.46	1.39
12	G	819	CLA	C3D-C2D	2.99	1.47	1.39
12	a	841	CLA	MG-NC	2.99	2.13	2.06
12	B	811	CLA	C1B-NB	-2.99	1.33	1.37
12	A	838	CLA	MG-ND	-2.99	1.99	2.05
12	a	815	CLA	C3D-C2D	2.99	1.47	1.39
12	a	834	CLA	MG-ND	-2.99	1.99	2.05
12	P	201	CLA	C4D-CHA	2.99	1.48	1.38
12	a	833	CLA	MG-ND	-2.99	1.99	2.05
12	l	202	CLA	MG-NC	2.99	2.13	2.06
12	L	204	CLA	MG-NC	2.99	2.13	2.06
12	B	828	CLA	C4D-CHA	2.99	1.48	1.38
12	G	824	CLA	C3D-C2D	2.99	1.47	1.39
12	H	829	CLA	MG-NC	2.99	2.13	2.06
12	P	203	CLA	MG-NC	2.99	2.13	2.06
12	H	828	CLA	MG-ND	-2.99	1.99	2.05
12	G	810	CLA	C3D-C2D	2.99	1.47	1.39
12	b	824	CLA	CHD-C1D	2.99	1.44	1.38
12	G	827	CLA	MG-ND	-2.99	1.99	2.05
12	G	814	CLA	MG-ND	-2.99	1.99	2.05
12	A	816	CLA	MG-ND	-2.99	1.99	2.05
12	H	819	CLA	C3D-C2D	2.99	1.47	1.39
12	a	824	CLA	CHD-C4C	2.99	1.46	1.39
12	G	819	CLA	C4D-CHA	2.99	1.48	1.38
12	H	829	CLA	C4D-CHA	2.99	1.48	1.38
12	B	838	CLA	MG-ND	-2.98	1.99	2.05
12	H	850	CLA	C3D-C2D	2.98	1.47	1.39
12	b	814	CLA	OBD-CAD	2.98	1.27	1.22
12	S	203	CLA	C3D-C2D	2.98	1.47	1.39
12	A	823	CLA	C3D-C2D	2.98	1.47	1.39
12	a	824	CLA	C4D-CHA	2.98	1.48	1.38
12	G	805	CLA	MG-NC	2.98	2.13	2.06
12	b	826	CLA	CHC-C4B	2.98	1.46	1.39
12	a	804	CLA	MG-NC	2.98	2.13	2.06
12	a	826	CLA	OBD-CAD	2.98	1.27	1.22
12	G	826	CLA	C3D-C2D	2.98	1.47	1.39
12	H	814	CLA	C3D-C2D	2.98	1.47	1.39
12	A	809	CLA	MG-NC	2.98	2.13	2.06
12	H	827	CLA	MG-NC	2.98	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	816	CLA	C4D-CHA	2.98	1.48	1.38
12	H	832	CLA	C3D-C2D	2.98	1.47	1.39
12	L	202	CLA	C3D-C2D	2.98	1.47	1.39
12	a	811	CLA	C1D-ND	-2.98	1.33	1.37
12	A	855	CLA	C4B-NB	-2.98	1.33	1.37
12	a	822	CLA	C3D-C2D	2.98	1.47	1.39
12	l	202	CLA	C3D-C2D	2.98	1.47	1.39
12	A	804	CLA	C1B-NB	-2.98	1.33	1.37
12	b	817	CLA	C4D-CHA	2.98	1.48	1.38
12	A	811	CLA	C4D-CHA	2.98	1.48	1.38
12	a	808	CLA	MG-NC	2.98	2.13	2.06
12	A	807	CLA	MG-NC	2.98	2.13	2.06
12	A	828	CLA	C3D-C2D	2.98	1.47	1.39
12	G	821	CLA	C4D-CHA	2.98	1.48	1.38
12	A	804	CLA	C1D-ND	-2.98	1.33	1.37
12	H	818	CLA	C3D-C2D	2.98	1.47	1.39
12	H	815	CLA	C3D-C2D	2.98	1.47	1.39
12	b	823	CLA	OBD-CAD	2.98	1.27	1.22
12	H	826	CLA	C1C-NC	-2.98	1.33	1.37
12	A	826	CLA	OBD-CAD	2.98	1.27	1.22
12	a	838	CLA	C1B-NB	-2.98	1.33	1.37
12	B	804	CLA	MG-ND	-2.98	1.99	2.05
12	b	821	CLA	CHB-C1B	2.98	1.46	1.39
12	b	806	CLA	C3D-C2D	2.98	1.47	1.39
12	b	807	CLA	C4D-CHA	2.98	1.48	1.38
12	G	833	CLA	MG-NC	2.98	2.13	2.06
12	b	822	CLA	MG-NC	2.98	2.13	2.06
12	a	811	CLA	C3D-C2D	2.98	1.47	1.39
12	B	812	CLA	C3D-C2D	2.97	1.47	1.39
12	b	811	CLA	MG-NC	2.97	2.13	2.06
12	b	809	CLA	C3D-C2D	2.97	1.47	1.39
12	B	816	CLA	C4D-CHA	2.97	1.48	1.38
12	H	809	CLA	C4D-CHA	2.97	1.48	1.38
12	H	815	CLA	OBD-CAD	2.97	1.27	1.22
12	A	805	CLA	C1C-NC	-2.97	1.33	1.37
12	L	205	CLA	C1B-NB	-2.97	1.34	1.37
12	b	817	CLA	MG-ND	-2.97	1.99	2.05
12	a	812	CLA	MG-NC	2.97	2.13	2.06
12	a	840	CLA	MG-NC	2.97	2.13	2.06
12	G	841	CLA	MG-ND	-2.97	1.99	2.05
12	b	815	CLA	C4D-CHA	2.97	1.48	1.38
12	f	203	CLA	C4D-CHA	2.97	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	823	CLA	C3D-C2D	2.97	1.47	1.39
12	a	820	CLA	CHB-C1B	2.97	1.46	1.39
12	G	838	CLA	MG-NC	2.97	2.13	2.06
12	b	837	CLA	C4D-CHA	2.97	1.48	1.38
12	F	203	CLA	C4D-CHA	2.97	1.48	1.38
12	G	816	CLA	C3D-C2D	2.97	1.47	1.39
12	B	812	CLA	OBD-CAD	2.97	1.27	1.22
12	B	826	CLA	CHC-C4B	2.97	1.46	1.39
12	B	827	CLA	MG-ND	-2.97	1.99	2.05
12	G	815	CLA	C1C-NC	-2.96	1.33	1.37
12	b	837	CLA	C3D-C2D	2.96	1.47	1.39
12	A	802	CLA	CHB-C1B	2.96	1.46	1.39
12	b	818	CLA	C3D-C2D	2.96	1.47	1.39
12	B	808	CLA	C4D-CHA	2.96	1.48	1.38
12	A	821	CLA	C3D-C2D	2.96	1.47	1.39
12	B	810	CLA	C3D-C2D	2.96	1.47	1.39
12	B	829	CLA	MG-NC	2.96	2.13	2.06
12	a	805	CLA	OBD-CAD	2.96	1.27	1.22
12	B	825	CLA	MG-NC	2.96	2.13	2.06
12	H	832	CLA	C1B-NB	-2.96	1.34	1.37
12	j	102	CLA	C4D-CHA	2.96	1.48	1.38
12	a	825	CLA	MG-ND	-2.96	1.99	2.05
12	B	820	CLA	C1B-NB	-2.96	1.34	1.37
12	B	824	CLA	CHC-C4B	2.96	1.46	1.39
12	j	102	CLA	MG-ND	-2.96	1.99	2.05
12	b	816	CLA	MG-NC	2.96	2.13	2.06
12	a	812	CLA	C4D-CHA	2.96	1.48	1.38
12	a	812	CLA	C3D-C2D	2.96	1.47	1.39
12	B	802	CLA	CHD-C4C	2.96	1.45	1.39
12	L	206	CLA	C1B-C2B	2.96	1.50	1.43
12	H	836	CLA	C1B-NB	-2.96	1.34	1.37
12	a	821	CLA	C4D-CHA	2.96	1.48	1.38
12	H	821	CLA	C4D-CHA	2.96	1.48	1.38
12	a	855	CLA	C3D-C2D	2.96	1.47	1.39
12	A	818	CLA	C4D-CHA	2.96	1.48	1.38
12	a	830	CLA	C1B-NB	-2.96	1.34	1.37
12	G	831	CLA	C1B-NB	-2.96	1.34	1.37
12	G	822	CLA	C4D-CHA	2.96	1.48	1.38
12	B	838	CLA	C4D-CHA	2.96	1.48	1.38
12	l	202	CLA	C4D-CHA	2.95	1.48	1.38
12	A	824	CLA	C4D-CHA	2.95	1.48	1.38
12	b	829	CLA	C3D-C2D	2.95	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	202	CLA	MG-ND	-2.95	1.99	2.05
12	a	839	CLA	C3D-C2D	2.95	1.47	1.39
12	H	808	CLA	MG-NC	2.95	2.13	2.06
12	H	830	CLA	C3D-C2D	2.95	1.47	1.39
12	a	812	CLA	MG-ND	-2.95	1.99	2.05
12	G	822	CLA	C3D-C2D	2.95	1.47	1.39
12	b	827	CLA	MG-ND	-2.95	1.99	2.05
12	G	823	CLA	C3D-C2D	2.95	1.47	1.39
12	H	824	CLA	C4D-CHA	2.95	1.48	1.38
12	A	836	CLA	C4D-CHA	2.95	1.48	1.38
12	A	827	CLA	C1B-NB	-2.95	1.34	1.37
12	a	832	CLA	C3D-C2D	2.95	1.47	1.39
12	H	817	CLA	C4D-CHA	2.95	1.48	1.38
12	a	802	CLA	C1C-NC	-2.95	1.33	1.37
12	A	833	CLA	C1C-NC	-2.95	1.33	1.37
12	b	816	CLA	C1B-NB	-2.95	1.34	1.37
12	G	815	CLA	C1B-C2B	2.95	1.50	1.43
12	a	833	CLA	C1B-NB	-2.95	1.34	1.37
12	b	806	CLA	MG-ND	-2.95	1.99	2.05
12	a	841	CLA	OBD-CAD	2.95	1.27	1.22
12	H	817	CLA	C1D-ND	-2.95	1.34	1.37
12	b	810	CLA	CHD-C4C	2.94	1.45	1.39
12	G	804	CLA	C1B-NB	-2.94	1.34	1.37
12	G	834	CLA	C1B-NB	-2.94	1.34	1.37
12	H	812	CLA	MG-NC	2.94	2.13	2.06
12	A	823	CLA	C4D-CHA	2.94	1.48	1.38
12	B	838	CLA	C3D-C2D	2.94	1.47	1.39
12	a	840	CLA	C4D-CHA	2.94	1.48	1.38
12	L	205	CLA	MG-NC	2.94	2.13	2.06
12	A	835	CLA	C1B-C2B	2.94	1.50	1.43
12	a	834	CLA	C1B-NB	-2.94	1.34	1.37
12	b	811	CLA	C1B-NB	-2.94	1.34	1.37
12	b	832	CLA	C4D-CHA	2.94	1.48	1.38
12	a	835	CLA	C1B-C2B	2.94	1.50	1.43
12	H	814	CLA	C4D-CHA	2.94	1.48	1.38
12	b	831	CLA	C4D-CHA	2.94	1.48	1.38
12	G	812	CLA	C4D-CHA	2.94	1.48	1.38
12	H	833	CLA	C4D-CHA	2.94	1.48	1.38
12	b	805	CLA	C1B-C2B	2.94	1.50	1.43
12	G	832	CLA	MG-NC	2.94	2.13	2.06
12	G	839	CLA	C3D-C2D	2.94	1.47	1.39
12	A	814	CLA	C3D-C2D	2.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	811	CLA	MG-NC	2.94	2.13	2.06
12	B	812	CLA	MG-ND	-2.94	2.00	2.05
12	G	815	CLA	C4D-CHA	2.94	1.48	1.38
12	B	807	CLA	C4D-CHA	2.94	1.48	1.38
12	b	817	CLA	C3D-C2D	2.94	1.47	1.39
12	j	102	CLA	C1B-NB	-2.94	1.34	1.37
12	A	826	CLA	C1B-NB	-2.94	1.34	1.37
12	b	813	CLA	C3D-C2D	2.94	1.47	1.39
12	B	832	CLA	C4D-CHA	2.94	1.48	1.38
12	H	837	CLA	CHB-C1B	2.94	1.46	1.39
12	a	834	CLA	MG-NC	2.94	2.13	2.06
12	B	806	CLA	C3D-C2D	2.94	1.47	1.39
12	G	842	CLA	C3D-C2D	2.94	1.47	1.39
12	B	837	CLA	C3D-C2D	2.94	1.47	1.39
12	a	840	CLA	C3D-C2D	2.94	1.47	1.39
12	B	811	CLA	C1D-ND	-2.94	1.34	1.37
12	L	202	CLA	C1B-NB	-2.94	1.34	1.37
12	A	832	CLA	MG-NC	2.94	2.13	2.06
12	a	818	CLA	C1C-NC	-2.94	1.33	1.37
12	G	808	CLA	MG-ND	-2.93	2.00	2.05
12	G	836	CLA	C4B-NB	-2.93	1.34	1.37
12	a	814	CLA	C4D-CHA	2.93	1.48	1.38
12	B	833	CLA	C4D-CHA	2.93	1.48	1.38
12	G	813	CLA	C4B-NB	-2.93	1.34	1.37
12	b	814	CLA	CHB-C1B	2.93	1.46	1.39
12	B	814	CLA	MG-ND	-2.93	2.00	2.05
12	A	815	CLA	CHB-C1B	2.93	1.46	1.39
12	a	809	CLA	C4D-CHA	2.93	1.48	1.38
12	B	811	CLA	C4D-CHA	2.93	1.48	1.38
12	H	822	CLA	C1C-NC	-2.93	1.33	1.37
12	A	830	CLA	C1B-NB	-2.93	1.34	1.37
12	H	816	CLA	C3D-C2D	2.93	1.47	1.39
12	l	205	CLA	C1B-NB	-2.93	1.34	1.37
12	P	201	CLA	C3D-C2D	2.93	1.47	1.39
12	H	830	CLA	MG-NC	2.93	2.13	2.06
12	B	823	CLA	MG-NC	2.93	2.13	2.06
12	H	822	CLA	C3D-C2D	2.93	1.47	1.39
12	a	815	CLA	C4D-CHA	2.93	1.48	1.38
12	B	813	CLA	MG-NC	2.93	2.13	2.06
12	a	813	CLA	C4D-CHA	2.93	1.48	1.38
12	b	827	CLA	C4D-CHA	2.93	1.48	1.38
12	H	839	CLA	MG-NC	2.93	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	810	CLA	MG-NC	2.93	2.13	2.06
12	l	205	CLA	C3D-C2D	2.93	1.47	1.39
12	H	829	CLA	MG-ND	-2.93	2.00	2.05
12	b	835	CLA	C1C-NC	-2.93	1.33	1.37
12	A	812	CLA	C1C-NC	-2.93	1.33	1.37
12	G	820	CLA	C3D-C2D	2.93	1.47	1.39
12	G	838	CLA	C1B-NB	-2.93	1.34	1.37
12	H	803	CLA	MG-NC	2.93	2.13	2.06
12	a	834	CLA	C4D-CHA	2.93	1.48	1.38
12	A	840	CLA	C3D-C2D	2.93	1.47	1.39
12	a	813	CLA	MG-NC	2.93	2.13	2.06
12	H	814	CLA	MG-NC	2.93	2.13	2.06
12	H	834	CLA	C4D-CHA	2.92	1.48	1.38
12	B	827	CLA	C1B-NB	-2.92	1.34	1.37
12	a	814	CLA	C1C-NC	-2.92	1.33	1.37
12	a	804	CLA	MG-ND	-2.92	2.00	2.05
12	A	840	CLA	C4D-CHA	2.92	1.48	1.38
12	b	811	CLA	C4B-NB	-2.92	1.34	1.37
12	B	813	CLA	C3D-C2D	2.92	1.47	1.39
12	a	832	CLA	MG-NC	2.92	2.13	2.06
12	B	809	CLA	C3D-C2D	2.92	1.47	1.39
12	H	810	CLA	C3D-C2D	2.92	1.47	1.39
12	a	839	CLA	MG-NC	2.92	2.13	2.06
12	G	842	CLA	MG-ND	-2.92	2.00	2.05
12	B	835	CLA	C1B-NB	-2.92	1.34	1.37
12	A	811	CLA	C3D-C2D	2.92	1.47	1.39
12	B	828	CLA	C3D-C2D	2.92	1.47	1.39
12	A	814	CLA	C4D-CHA	2.92	1.48	1.38
12	B	817	CLA	C3D-C2D	2.92	1.47	1.39
12	a	804	CLA	C1D-ND	-2.92	1.34	1.37
12	A	815	CLA	C1B-NB	-2.92	1.34	1.37
12	l	204	CLA	MG-NC	2.92	2.13	2.06
12	S	204	CLA	C1B-C2B	2.92	1.50	1.43
12	H	801	CLA	C3D-C2D	2.92	1.47	1.39
12	A	824	CLA	C3D-C2D	2.92	1.47	1.39
12	b	820	CLA	C4D-CHA	2.92	1.48	1.38
12	B	805	CLA	C1B-C2B	2.92	1.50	1.43
12	b	813	CLA	MG-NC	2.92	2.13	2.06
12	L	205	CLA	C3D-C2D	2.92	1.46	1.39
12	a	823	CLA	C4D-CHA	2.92	1.48	1.38
12	G	827	CLA	C1C-NC	-2.92	1.33	1.37
12	A	815	CLA	C4D-CHA	2.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	834	CLA	C1C-NC	-2.92	1.33	1.37
12	A	834	CLA	C1C-NC	-2.92	1.33	1.37
12	B	816	CLA	C1B-NB	-2.92	1.34	1.37
12	H	825	CLA	OBD-CAD	2.91	1.27	1.22
12	H	812	CLA	C4B-NB	-2.91	1.34	1.37
12	a	809	CLA	C1B-C2B	2.91	1.50	1.43
12	B	833	CLA	C1C-NC	-2.91	1.33	1.37
12	a	833	CLA	MG-NC	2.91	2.13	2.06
12	a	805	CLA	C1B-C2B	2.91	1.50	1.43
12	H	826	CLA	MG-NC	2.91	2.13	2.06
12	b	803	CLA	C4D-CHA	2.91	1.48	1.38
12	G	834	CLA	MG-ND	-2.91	2.00	2.05
12	H	810	CLA	C3B-C4B	2.91	1.51	1.42
12	G	806	CLA	C1B-NB	-2.91	1.34	1.37
12	G	805	CLA	C3D-C2D	2.91	1.46	1.39
12	G	808	CLA	C3D-C2D	2.91	1.46	1.39
12	b	823	CLA	C3D-C2D	2.91	1.46	1.39
12	B	820	CLA	C4D-CHA	2.91	1.48	1.38
12	H	807	CLA	C4D-CHA	2.91	1.48	1.38
12	G	824	CLA	C4D-CHA	2.91	1.48	1.38
12	A	832	CLA	C3D-C2D	2.91	1.46	1.39
12	G	842	CLA	C1B-C2B	2.91	1.50	1.43
12	a	833	CLA	C4B-NB	-2.91	1.34	1.37
12	H	808	CLA	C4D-CHA	2.91	1.48	1.38
12	H	811	CLA	OBD-CAD	2.91	1.27	1.22
12	G	809	CLA	MG-NC	2.91	2.13	2.06
12	S	204	CLA	MG-NC	2.91	2.13	2.06
12	B	811	CLA	C3D-C2D	2.91	1.46	1.39
12	G	825	CLA	C4D-CHA	2.91	1.48	1.38
12	G	816	CLA	C4D-CHA	2.91	1.48	1.38
12	G	814	CLA	CHB-C1B	2.91	1.45	1.39
12	H	820	CLA	C1B-C2B	2.91	1.49	1.43
12	H	812	CLA	C3D-C2D	2.91	1.46	1.39
12	G	819	CLA	C1B-NB	-2.91	1.34	1.37
12	G	840	CLA	C1B-NB	-2.91	1.34	1.37
12	b	817	CLA	C1B-C2B	2.90	1.49	1.43
12	B	816	CLA	MG-NC	2.90	2.13	2.06
12	H	821	CLA	C1B-NB	-2.90	1.34	1.37
12	a	803	CLA	C1B-NB	-2.90	1.34	1.37
12	A	822	CLA	MG-ND	-2.90	2.00	2.05
12	B	830	CLA	MG-ND	-2.90	2.00	2.05
12	F	201	CLA	C4D-CHA	2.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	201	CLA	C4D-CHA	2.90	1.48	1.38
12	b	802	CLA	MG-ND	-2.90	2.00	2.05
12	H	850	CLA	C1B-C2B	2.90	1.49	1.43
12	a	820	CLA	MG-ND	-2.90	2.00	2.05
12	H	813	CLA	C3D-C2D	2.90	1.46	1.39
12	P	203	CLA	C1B-C2B	2.90	1.49	1.43
12	A	818	CLA	C3D-C2D	2.90	1.46	1.39
12	a	808	CLA	C1D-ND	-2.90	1.34	1.37
12	H	837	CLA	C1C-NC	-2.90	1.33	1.37
12	G	817	CLA	MG-ND	-2.90	2.00	2.05
12	a	811	CLA	MG-ND	-2.90	2.00	2.05
12	G	836	CLA	C4D-CHA	2.90	1.48	1.38
12	B	819	CLA	C1B-C2B	2.90	1.49	1.43
12	b	820	CLA	C1B-NB	-2.90	1.34	1.37
12	B	833	CLA	MG-ND	-2.90	2.00	2.05
12	G	842	CLA	C1B-NB	-2.90	1.34	1.37
12	S	203	CLA	C1B-NB	-2.90	1.34	1.37
12	G	821	CLA	CHB-C1B	2.90	1.45	1.39
12	b	812	CLA	C3D-C2D	2.90	1.46	1.39
12	G	826	CLA	C1B-NB	-2.90	1.34	1.37
12	G	856	CLA	C3D-C2D	2.89	1.46	1.39
12	a	836	CLA	C4D-CHA	2.89	1.48	1.38
12	B	811	CLA	MG-ND	-2.89	2.00	2.05
12	A	814	CLA	MG-NC	2.89	2.13	2.06
12	A	822	CLA	C4D-CHA	2.89	1.48	1.38
12	A	814	CLA	C1B-NB	-2.89	1.34	1.37
12	A	836	CLA	C4B-NB	-2.89	1.34	1.37
12	H	839	CLA	C4D-CHA	2.89	1.48	1.38
12	A	831	CLA	C3D-C2D	2.89	1.46	1.39
12	A	831	CLA	C4D-CHA	2.89	1.48	1.38
12	A	814	CLA	MG-ND	-2.89	2.00	2.05
12	L	202	CLA	MG-NC	2.89	2.13	2.06
12	b	824	CLA	CHD-C4C	2.89	1.45	1.39
12	b	831	CLA	C1B-C2B	2.89	1.49	1.43
12	B	809	CLA	C3B-C4B	2.89	1.51	1.42
12	B	811	CLA	C4B-NB	-2.89	1.34	1.37
12	H	824	CLA	C1C-NC	-2.88	1.33	1.37
12	A	805	CLA	C1B-C2B	2.88	1.49	1.43
12	A	854	CLA	MG-NC	2.88	2.13	2.06
12	b	832	CLA	MG-ND	-2.88	2.00	2.05
12	A	855	CLA	C3D-C2D	2.88	1.46	1.39
12	G	819	CLA	C1D-ND	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	804	CLA	OBD-CAD	2.88	1.27	1.22
12	G	820	CLA	MG-NC	2.88	2.13	2.06
12	H	822	CLA	MG-NC	2.88	2.13	2.06
12	b	823	CLA	C1C-NC	-2.88	1.33	1.37
12	G	838	CLA	OBD-CAD	2.88	1.27	1.22
12	a	807	CLA	C3D-C2D	2.88	1.46	1.39
11	G	801	CL0	C1C-NC	-2.88	1.33	1.37
12	a	841	CLA	C1B-C2B	2.88	1.49	1.43
12	G	812	CLA	MG-ND	-2.88	2.00	2.05
12	H	807	CLA	MG-NC	2.88	2.13	2.06
12	G	804	CLA	C3D-C2D	2.88	1.46	1.39
12	G	821	CLA	C1D-ND	-2.88	1.34	1.37
12	G	828	CLA	C1B-NB	-2.88	1.34	1.37
12	a	811	CLA	C1B-NB	-2.88	1.34	1.37
12	L	202	CLA	C4D-CHA	2.88	1.48	1.38
12	a	818	CLA	C1B-NB	-2.88	1.34	1.37
12	A	839	CLA	C1B-NB	-2.88	1.34	1.37
12	A	810	CLA	C1C-NC	-2.88	1.33	1.37
12	H	821	CLA	MG-ND	-2.88	2.00	2.05
12	B	829	CLA	MG-ND	-2.88	2.00	2.05
12	H	811	CLA	MG-NC	2.88	2.13	2.06
12	H	812	CLA	C4D-CHA	2.88	1.48	1.38
12	a	816	CLA	C4D-CHA	2.88	1.48	1.38
12	A	816	CLA	C1D-ND	-2.88	1.34	1.37
12	l	206	CLA	C1B-C2B	2.88	1.49	1.43
12	B	811	CLA	C1C-NC	-2.88	1.33	1.37
12	a	840	CLA	C1B-NB	-2.88	1.34	1.37
12	B	818	CLA	C1B-C2B	2.88	1.49	1.43
12	G	802	CLA	CHD-C1D	2.88	1.44	1.38
12	A	812	CLA	MG-ND	-2.88	2.00	2.05
12	b	811	CLA	C3D-C2D	2.88	1.46	1.39
12	B	836	CLA	C1C-NC	-2.88	1.33	1.37
12	A	814	CLA	C1D-ND	-2.88	1.34	1.37
12	a	817	CLA	MG-NC	2.88	2.13	2.06
12	B	827	CLA	C3D-C2D	2.87	1.46	1.39
12	b	808	CLA	C4D-CHA	2.87	1.48	1.38
12	a	819	CLA	C1B-C2B	2.87	1.49	1.43
12	b	815	CLA	CHB-C1B	2.87	1.45	1.39
12	H	811	CLA	C3D-C2D	2.87	1.46	1.39
12	H	818	CLA	C1B-C2B	2.87	1.49	1.43
12	B	826	CLA	MG-NC	2.87	2.13	2.06
12	b	837	CLA	MG-NC	2.87	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	801	CL0	C1B-C2B	2.87	1.49	1.43
12	a	814	CLA	C1B-C2B	2.87	1.49	1.43
12	H	839	CLA	MG-ND	-2.87	2.00	2.05
12	G	855	CLA	MG-NC	2.87	2.13	2.06
12	a	839	CLA	C1B-C2B	2.87	1.49	1.43
12	B	822	CLA	C4D-CHA	2.87	1.48	1.38
12	A	808	CLA	MG-NC	2.87	2.13	2.06
12	A	816	CLA	C4D-CHA	2.87	1.48	1.38
11	A	801	CL0	C1B-C2B	2.87	1.49	1.43
12	A	831	CLA	C1C-NC	-2.87	1.33	1.37
12	B	822	CLA	C1C-NC	-2.87	1.33	1.37
12	G	823	CLA	C1D-ND	-2.87	1.34	1.37
12	B	817	CLA	C1B-C2B	2.87	1.49	1.43
12	L	206	CLA	MG-NC	2.87	2.13	2.06
12	A	807	CLA	C3D-C2D	2.86	1.46	1.39
12	H	816	CLA	C4D-CHA	2.86	1.48	1.38
12	a	802	CLA	OBD-CAD	2.86	1.27	1.22
12	H	815	CLA	MG-ND	-2.86	2.00	2.05
12	B	812	CLA	C1D-ND	-2.86	1.34	1.37
12	a	802	CLA	C3D-C2D	2.86	1.46	1.39
12	A	830	CLA	OBD-CAD	2.86	1.27	1.22
12	a	838	CLA	OBD-CAD	2.86	1.27	1.22
12	H	808	CLA	C1B-NB	-2.86	1.34	1.37
12	G	820	CLA	C1B-C2B	2.86	1.49	1.43
12	H	803	CLA	C3D-C2D	2.86	1.46	1.39
12	a	807	CLA	C1B-NB	-2.86	1.34	1.37
12	A	838	CLA	C1B-NB	-2.86	1.34	1.37
12	H	839	CLA	C3D-C2D	2.86	1.46	1.39
12	H	801	CLA	C4D-CHA	2.86	1.48	1.38
12	H	803	CLA	C4D-CHA	2.86	1.48	1.38
12	A	829	CLA	CHC-C4B	2.86	1.45	1.39
12	a	831	CLA	C4D-CHA	2.86	1.48	1.38
12	l	205	CLA	MG-NC	2.86	2.13	2.06
12	H	833	CLA	C1B-C2B	2.86	1.49	1.43
12	a	809	CLA	C1B-NB	-2.86	1.34	1.37
12	G	841	CLA	C4D-CHA	2.86	1.48	1.38
12	A	854	CLA	C4D-CHA	2.86	1.48	1.38
12	H	819	CLA	C1B-C2B	2.86	1.49	1.43
12	a	819	CLA	C3D-C2D	2.86	1.46	1.39
12	B	827	CLA	C4D-CHA	2.86	1.48	1.38
12	b	813	CLA	C4D-CHA	2.86	1.48	1.38
12	B	804	CLA	OBD-CAD	2.86	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	824	CLA	C1B-C2B	2.86	1.49	1.43
12	a	814	CLA	C1B-NB	-2.86	1.34	1.37
12	a	818	CLA	C1B-C2B	2.86	1.49	1.43
12	H	825	CLA	C4D-CHA	2.85	1.48	1.38
12	f	201	CLA	C3D-C2D	2.85	1.46	1.39
12	H	805	CLA	MG-NC	2.85	2.13	2.06
13	H	840	1L3	C25-C26	2.85	1.39	1.33
12	S	204	CLA	C1B-NB	-2.85	1.34	1.37
12	a	837	CLA	MG-ND	-2.85	2.00	2.05
12	a	820	CLA	C1D-ND	-2.85	1.34	1.37
12	A	818	CLA	C1D-ND	-2.85	1.34	1.37
12	B	837	CLA	C1B-NB	-2.85	1.34	1.37
12	F	203	CLA	C1B-C2B	2.85	1.49	1.43
12	a	820	CLA	MG-NC	2.85	2.13	2.06
12	G	835	CLA	C3D-C2D	2.85	1.46	1.39
12	H	824	CLA	OBD-CAD	2.85	1.27	1.22
12	b	826	CLA	MG-NC	2.85	2.13	2.06
12	L	204	CLA	MG-ND	-2.85	2.00	2.05
12	H	822	CLA	CHD-C4C	2.85	1.45	1.39
12	a	827	CLA	C1B-NB	-2.85	1.34	1.37
12	b	833	CLA	C4D-CHA	2.85	1.48	1.38
12	b	803	CLA	C3D-C2D	2.85	1.46	1.39
12	G	811	CLA	C1C-NC	-2.85	1.33	1.37
12	b	809	CLA	C1B-NB	-2.85	1.34	1.37
12	H	823	CLA	C4D-CHA	2.85	1.48	1.38
12	G	837	CLA	C3D-C2D	2.85	1.46	1.39
12	b	828	CLA	MG-ND	-2.85	2.00	2.05
12	a	836	CLA	MG-ND	-2.85	2.00	2.05
12	l	206	CLA	MG-NC	2.85	2.13	2.06
12	a	805	CLA	C1C-NC	-2.85	1.33	1.37
12	G	802	CLA	CHB-C1B	2.85	1.45	1.39
12	A	819	CLA	C1B-C2B	2.85	1.49	1.43
12	G	837	CLA	MG-NC	2.84	2.13	2.06
12	A	833	CLA	MG-NC	2.84	2.13	2.06
12	A	837	CLA	MG-NC	2.84	2.13	2.06
12	A	828	CLA	C4D-CHA	2.84	1.48	1.38
12	b	824	CLA	CHB-C1B	2.84	1.45	1.39
12	B	814	CLA	OBD-CAD	2.84	1.27	1.22
12	G	841	CLA	OBD-CAD	2.84	1.27	1.22
12	b	848	CLA	MG-NC	2.84	2.13	2.06
12	G	805	CLA	C1D-ND	-2.84	1.34	1.37
12	a	837	CLA	C4D-CHA	2.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	806	CLA	C1C-NC	-2.84	1.33	1.37
12	G	835	CLA	C1B-C2B	2.84	1.49	1.43
12	G	811	CLA	C3D-C2D	2.84	1.46	1.39
12	A	814	CLA	C1C-NC	-2.84	1.33	1.37
12	b	834	CLA	MG-NC	2.84	2.13	2.06
12	A	819	CLA	C4D-CHA	2.84	1.48	1.38
12	b	811	CLA	C4D-CHA	2.84	1.48	1.38
11	a	801	CL0	C1B-C2B	2.84	1.49	1.43
12	G	817	CLA	C4D-CHA	2.84	1.48	1.38
12	a	814	CLA	MG-NC	2.84	2.13	2.06
12	a	825	CLA	C1B-NB	-2.84	1.34	1.37
12	b	814	CLA	C4D-CHA	2.84	1.48	1.38
12	a	803	CLA	C3D-C2D	2.84	1.46	1.39
12	A	841	CLA	C1B-NB	-2.84	1.34	1.37
12	b	818	CLA	C1B-C2B	2.84	1.49	1.43
12	B	817	CLA	MG-ND	-2.84	2.00	2.05
12	B	828	CLA	MG-ND	-2.84	2.00	2.05
12	H	850	CLA	MG-ND	-2.84	2.00	2.05
12	A	815	CLA	MG-NC	2.84	2.13	2.06
12	H	837	CLA	MG-ND	-2.84	2.00	2.05
12	G	812	CLA	C3D-C2D	2.84	1.46	1.39
12	A	802	CLA	C3D-C2D	2.84	1.46	1.39
12	a	814	CLA	C1D-ND	-2.84	1.34	1.37
12	G	830	CLA	C4D-CHA	2.84	1.48	1.38
12	H	850	CLA	MG-NC	2.84	2.13	2.06
12	H	835	CLA	C1C-NC	-2.84	1.33	1.37
12	G	809	CLA	C1D-ND	-2.84	1.34	1.37
12	B	813	CLA	C4D-CHA	2.83	1.48	1.38
12	G	815	CLA	MG-NC	2.83	2.13	2.06
12	H	839	CLA	C1B-NB	-2.83	1.34	1.37
12	b	822	CLA	C4D-CHA	2.83	1.48	1.38
12	H	827	CLA	C4D-CHA	2.83	1.48	1.38
12	A	812	CLA	C3D-C2D	2.83	1.46	1.39
12	a	809	CLA	C1D-ND	-2.83	1.34	1.37
12	G	819	CLA	MG-NC	2.83	2.13	2.06
12	H	818	CLA	MG-ND	-2.83	2.00	2.05
12	b	848	CLA	MG-ND	-2.83	2.00	2.05
12	B	810	CLA	OBD-CAD	2.83	1.27	1.22
12	H	834	CLA	MG-ND	-2.83	2.00	2.05
12	G	837	CLA	C4D-CHA	2.83	1.48	1.38
12	a	821	CLA	C1B-NB	-2.83	1.34	1.37
12	B	808	CLA	C4B-NB	-2.83	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	801	CL0	C1C-NC	-2.83	1.33	1.37
12	B	821	CLA	C1C-NC	-2.83	1.33	1.37
12	B	812	CLA	C1B-C2B	2.83	1.49	1.43
12	G	824	CLA	C1D-ND	-2.83	1.34	1.37
12	a	808	CLA	C1B-NB	-2.83	1.34	1.37
12	G	803	CLA	C3D-C2D	2.83	1.46	1.39
12	L	206	CLA	C1C-NC	-2.83	1.33	1.37
12	H	811	CLA	C1D-ND	-2.83	1.34	1.37
12	a	808	CLA	C4B-NB	-2.83	1.34	1.37
12	A	841	CLA	C4D-CHA	2.83	1.48	1.38
12	G	840	CLA	C4D-CHA	2.83	1.48	1.38
12	H	809	CLA	MG-NC	2.83	2.13	2.06
12	A	803	CLA	C3D-C2D	2.83	1.46	1.39
12	G	826	CLA	C1C-NC	-2.83	1.33	1.37
12	l	202	CLA	C1B-NB	-2.83	1.34	1.37
13	G	843	1L3	C25-C26	2.83	1.39	1.33
12	b	814	CLA	MG-ND	-2.83	2.00	2.05
12	a	829	CLA	C4D-CHA	2.83	1.48	1.38
12	H	812	CLA	C1B-NB	-2.82	1.34	1.37
12	H	828	CLA	C4D-CHA	2.82	1.48	1.38
12	a	806	CLA	C1B-C2B	2.82	1.49	1.43
12	A	812	CLA	C1B-NB	-2.82	1.34	1.37
12	F	201	CLA	C3D-C2D	2.82	1.46	1.39
12	A	831	CLA	MG-NC	2.82	2.13	2.06
12	a	822	CLA	C1B-C2B	2.82	1.49	1.43
12	H	809	CLA	C4B-NB	-2.82	1.34	1.37
12	j	104	CLA	C1B-NB	-2.82	1.34	1.37
12	A	803	CLA	C1B-NB	-2.82	1.34	1.37
12	a	815	CLA	C1B-C2B	2.82	1.49	1.43
12	a	841	CLA	C4D-CHA	2.82	1.48	1.38
12	G	813	CLA	C1D-ND	-2.82	1.34	1.37
12	B	809	CLA	C1B-NB	-2.82	1.34	1.37
12	a	808	CLA	C3D-C2D	2.82	1.46	1.39
12	b	819	CLA	C1B-C2B	2.82	1.49	1.43
12	B	818	CLA	C1D-ND	-2.82	1.34	1.37
12	H	808	CLA	C1C-NC	-2.82	1.33	1.37
12	L	204	CLA	C1C-NC	-2.82	1.33	1.37
12	A	835	CLA	C3D-C2D	2.82	1.46	1.39
12	G	827	CLA	C1B-C2B	2.82	1.49	1.43
12	G	813	CLA	MG-NC	2.82	2.13	2.06
13	b	838	1L3	C25-C26	2.82	1.39	1.33
12	B	830	CLA	C1B-NB	-2.82	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	803	CLA	MG-NC	2.82	2.13	2.06
12	H	817	CLA	C1B-NB	-2.82	1.34	1.37
12	b	812	CLA	MG-ND	-2.81	2.00	2.05
12	A	837	CLA	MG-ND	-2.81	2.00	2.05
12	A	816	CLA	C1B-C2B	2.81	1.49	1.43
12	A	834	CLA	MG-ND	-2.81	2.00	2.05
12	A	835	CLA	C1B-NB	-2.81	1.34	1.37
12	G	823	CLA	C1B-C2B	2.81	1.49	1.43
12	A	825	CLA	C1B-NB	-2.81	1.34	1.37
12	G	829	CLA	C4D-CHA	2.81	1.48	1.38
12	A	813	CLA	C1B-NB	-2.81	1.34	1.37
12	b	833	CLA	MG-ND	-2.81	2.00	2.05
12	G	841	CLA	C1B-C2B	2.81	1.49	1.43
12	G	808	CLA	C1B-NB	-2.81	1.34	1.37
12	A	834	CLA	MG-NC	2.81	2.12	2.06
12	G	821	CLA	MG-ND	-2.81	2.00	2.05
12	b	837	CLA	MG-ND	-2.81	2.00	2.05
12	a	855	CLA	C4B-NB	-2.81	1.34	1.37
12	B	835	CLA	MG-NC	2.81	2.12	2.06
12	G	803	CLA	OBD-CAD	2.81	1.27	1.22
12	L	205	CLA	C1C-NC	-2.81	1.33	1.37
12	b	833	CLA	MG-NC	2.81	2.12	2.06
12	b	802	CLA	C1B-C2B	2.81	1.49	1.43
12	b	804	CLA	MG-ND	-2.81	2.00	2.05
12	A	823	CLA	C1B-C2B	2.81	1.49	1.43
12	a	819	CLA	MG-NC	2.81	2.12	2.06
12	a	813	CLA	C3D-C2D	2.81	1.46	1.39
12	a	854	CLA	MG-NC	2.81	2.12	2.06
12	a	821	CLA	C1B-C2B	2.81	1.49	1.43
12	a	809	CLA	MG-NC	2.81	2.12	2.06
12	G	822	CLA	C1B-C2B	2.81	1.49	1.43
12	H	814	CLA	C1D-ND	-2.81	1.34	1.37
12	a	810	CLA	MG-NC	2.81	2.12	2.06
12	H	838	CLA	C4D-CHA	2.80	1.48	1.38
12	a	818	CLA	MG-NC	2.80	2.12	2.06
12	b	833	CLA	C1C-NC	-2.80	1.33	1.37
12	A	829	CLA	C4D-CHA	2.80	1.48	1.38
12	b	827	CLA	C3D-C2D	2.80	1.46	1.39
12	b	836	CLA	C4D-CHA	2.80	1.48	1.38
12	b	829	CLA	MG-ND	-2.80	2.00	2.05
12	A	821	CLA	C1B-C2B	2.80	1.49	1.43
12	G	809	CLA	C4B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	j	104	CLA	C1D-ND	-2.80	1.34	1.37
12	G	831	CLA	C4D-CHA	2.80	1.48	1.38
12	a	810	CLA	C1C-NC	-2.80	1.33	1.37
12	G	815	CLA	C1B-NB	-2.80	1.34	1.37
12	A	820	CLA	MG-ND	-2.80	2.00	2.05
12	a	828	CLA	C4D-CHA	2.80	1.48	1.38
12	B	803	CLA	C1C-NC	-2.80	1.33	1.37
12	A	818	CLA	MG-NC	2.80	2.12	2.06
13	a	842	1L3	C25-C26	2.80	1.39	1.33
12	a	837	CLA	C3D-C2D	2.80	1.46	1.39
12	H	828	CLA	C1B-NB	-2.80	1.34	1.37
12	A	808	CLA	C3D-C2D	2.80	1.46	1.39
12	H	819	CLA	C1D-ND	-2.80	1.34	1.37
12	B	821	CLA	C4D-CHA	2.80	1.48	1.38
12	H	810	CLA	C1C-NC	-2.80	1.33	1.37
12	B	838	CLA	C1B-C2B	2.80	1.49	1.43
12	S	204	CLA	MG-ND	-2.80	2.00	2.05
12	A	834	CLA	C4D-CHA	2.80	1.48	1.38
12	a	823	CLA	MG-NC	2.80	2.12	2.06
12	b	812	CLA	C1B-NB	-2.79	1.34	1.37
11	a	801	CL0	CHD-C4C	2.79	1.45	1.39
12	G	815	CLA	C1D-ND	-2.79	1.34	1.37
12	j	102	CLA	MG-NC	2.79	2.12	2.06
12	b	837	CLA	C1B-C2B	2.79	1.49	1.43
12	H	833	CLA	C1B-NB	-2.79	1.34	1.37
12	a	819	CLA	C4D-CHA	2.79	1.48	1.38
12	H	830	CLA	C1B-NB	-2.79	1.34	1.37
12	B	837	CLA	C4D-CHA	2.79	1.48	1.38
12	H	815	CLA	MG-NC	2.79	2.12	2.06
12	b	826	CLA	C4D-CHA	2.79	1.48	1.38
12	G	822	CLA	C1B-NB	-2.79	1.34	1.37
12	B	801	CLA	CHB-C1B	2.79	1.45	1.39
12	a	827	CLA	C3D-C2D	2.79	1.46	1.39
12	a	826	CLA	C1C-NC	-2.79	1.33	1.37
12	H	801	CLA	C4B-NB	-2.79	1.34	1.37
12	G	820	CLA	C4D-CHA	2.79	1.48	1.38
12	A	818	CLA	C1B-C2B	2.79	1.49	1.43
12	G	811	CLA	C4D-CHA	2.79	1.48	1.38
12	H	802	CLA	CHD-C4C	2.79	1.45	1.39
12	G	811	CLA	MG-NC	2.79	2.12	2.06
12	A	810	CLA	C1B-NB	-2.79	1.34	1.37
12	B	803	CLA	MG-NC	2.79	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	807	CLA	CHC-C4B	2.79	1.45	1.39
12	H	801	CLA	C1C-NC	-2.79	1.33	1.37
12	G	838	CLA	C3D-C2D	2.79	1.46	1.39
12	B	837	CLA	MG-ND	-2.79	2.00	2.05
11	A	801	CL0	C1C-NC	-2.79	1.33	1.37
12	A	841	CLA	C1B-C2B	2.79	1.49	1.43
12	B	806	CLA	C4D-CHA	2.78	1.47	1.38
12	B	816	CLA	C1D-ND	-2.78	1.34	1.37
12	G	815	CLA	MG-ND	-2.78	2.00	2.05
12	A	806	CLA	MG-ND	-2.78	2.00	2.05
12	G	814	CLA	C4D-CHA	2.78	1.47	1.38
12	l	205	CLA	C1C-NC	-2.78	1.33	1.37
12	A	811	CLA	C1B-C2B	2.78	1.49	1.43
12	A	823	CLA	MG-NC	2.78	2.12	2.06
12	H	813	CLA	C1B-C2B	2.78	1.49	1.43
12	A	854	CLA	C4B-NB	-2.78	1.34	1.37
12	a	829	CLA	C4B-NB	-2.78	1.34	1.37
12	a	807	CLA	C1B-C2B	2.78	1.49	1.43
12	H	834	CLA	C3D-C2D	2.78	1.46	1.39
12	S	203	CLA	C1C-NC	-2.78	1.33	1.37
12	A	826	CLA	C1B-C2B	2.78	1.49	1.43
12	b	809	CLA	C3B-C4B	2.78	1.50	1.42
12	H	807	CLA	C4B-NB	-2.78	1.34	1.37
12	a	831	CLA	MG-NC	2.78	2.12	2.06
12	B	830	CLA	MG-NC	2.78	2.12	2.06
12	A	839	CLA	MG-ND	-2.78	2.00	2.05
12	B	808	CLA	MG-ND	-2.78	2.00	2.05
12	l	205	CLA	C4D-CHA	2.78	1.47	1.38
12	H	850	CLA	C1B-NB	-2.78	1.34	1.37
12	A	806	CLA	C3D-C2D	2.78	1.46	1.39
13	A	842	1L3	C25-C26	2.78	1.39	1.33
12	A	839	CLA	C1D-ND	-2.78	1.34	1.37
12	b	831	CLA	C1D-ND	-2.78	1.34	1.37
12	a	823	CLA	C1C-NC	-2.78	1.33	1.37
12	L	202	CLA	C1C-NC	-2.78	1.33	1.37
12	A	811	CLA	C1B-NB	-2.77	1.34	1.37
12	A	808	CLA	MG-ND	-2.77	2.00	2.05
12	B	826	CLA	C4D-CHA	2.77	1.47	1.38
12	G	809	CLA	MG-ND	-2.77	2.00	2.05
12	B	832	CLA	C1D-ND	-2.77	1.34	1.37
12	J	103	CLA	C1B-C2B	2.77	1.49	1.43
12	a	831	CLA	MG-ND	-2.77	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	826	CLA	C4B-NB	-2.77	1.34	1.37
12	a	839	CLA	C4B-NB	-2.77	1.34	1.37
12	G	842	CLA	MG-NC	2.77	2.12	2.06
12	b	810	CLA	C3D-C2D	2.77	1.46	1.39
12	H	833	CLA	C1D-ND	-2.77	1.34	1.37
12	b	801	CLA	C4B-NB	-2.77	1.34	1.37
12	B	823	CLA	OBD-CAD	2.77	1.27	1.22
12	B	815	CLA	C1C-NC	-2.77	1.33	1.37
12	G	835	CLA	C1D-ND	-2.77	1.34	1.37
12	H	827	CLA	CHC-C4B	2.77	1.45	1.39
12	b	825	CLA	MG-NC	2.77	2.12	2.06
12	A	839	CLA	C1B-C2B	2.77	1.49	1.43
12	H	804	CLA	MG-ND	-2.77	2.00	2.05
12	b	807	CLA	C4B-NB	-2.77	1.34	1.37
12	b	821	CLA	C4D-CHA	2.77	1.47	1.38
12	b	835	CLA	MG-ND	-2.77	2.00	2.05
12	B	807	CLA	CHC-C4B	2.77	1.45	1.39
12	B	830	CLA	C1C-NC	-2.77	1.33	1.37
12	a	805	CLA	C3D-C2D	2.77	1.46	1.39
12	a	838	CLA	C3D-C2D	2.77	1.46	1.39
12	H	802	CLA	MG-NC	2.77	2.12	2.06
12	f	203	CLA	C1B-C2B	2.77	1.49	1.43
12	b	811	CLA	MG-ND	-2.77	2.00	2.05
12	A	837	CLA	C1C-NC	-2.77	1.33	1.37
12	B	803	CLA	C4D-CHA	2.77	1.47	1.38
12	H	839	CLA	C1B-C2B	2.77	1.49	1.43
12	b	807	CLA	CHC-C4B	2.77	1.45	1.39
12	A	837	CLA	C4D-CHA	2.77	1.47	1.38
12	l	206	CLA	MG-ND	-2.77	2.00	2.05
12	a	814	CLA	MG-ND	-2.77	2.00	2.05
12	B	833	CLA	C1B-NB	-2.77	1.34	1.37
12	H	812	CLA	C1C-NC	-2.76	1.33	1.37
12	L	206	CLA	MG-ND	-2.76	2.00	2.05
12	B	831	CLA	C1C-NC	-2.76	1.33	1.37
12	A	833	CLA	MG-ND	-2.76	2.00	2.05
13	B	839	1L3	C25-C26	2.76	1.39	1.33
12	b	832	CLA	C1B-C2B	2.76	1.49	1.43
12	a	813	CLA	MG-ND	-2.76	2.00	2.05
12	H	801	CLA	MG-NC	2.76	2.12	2.06
12	A	813	CLA	MG-NC	2.76	2.12	2.06
12	B	836	CLA	MG-ND	-2.76	2.00	2.05
12	H	812	CLA	MG-ND	-2.76	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	814	CLA	C1B-C2B	2.76	1.49	1.43
12	B	834	CLA	MG-ND	-2.76	2.00	2.05
12	b	806	CLA	C4D-CHA	2.76	1.47	1.38
12	B	825	CLA	C3D-C2D	2.76	1.46	1.39
12	G	817	CLA	C1D-ND	-2.76	1.34	1.37
12	G	855	CLA	C4D-CHA	2.76	1.47	1.38
12	b	805	CLA	C3D-C2D	2.76	1.46	1.39
12	G	834	CLA	C4D-CHA	2.76	1.47	1.38
12	G	812	CLA	C1B-C2B	2.76	1.49	1.43
12	G	802	CLA	C3D-C2D	2.76	1.46	1.39
12	G	809	CLA	C1D-C2D	2.76	1.50	1.45
12	b	829	CLA	C1B-NB	-2.76	1.34	1.37
12	G	819	CLA	C4B-NB	-2.76	1.34	1.37
12	b	817	CLA	C1B-NB	-2.76	1.34	1.37
12	S	202	CLA	C1C-NC	-2.76	1.33	1.37
12	H	836	CLA	MG-NC	2.76	2.12	2.06
12	H	804	CLA	OBD-CAD	2.76	1.27	1.22
12	G	808	CLA	MG-NC	2.76	2.12	2.06
12	A	810	CLA	C3D-C2D	2.76	1.46	1.39
12	B	832	CLA	C1B-C2B	2.76	1.49	1.43
12	H	839	CLA	C1C-NC	-2.76	1.33	1.37
12	H	831	CLA	MG-ND	-2.76	2.00	2.05
12	B	808	CLA	C1D-ND	-2.76	1.34	1.37
12	A	826	CLA	C3D-C2D	2.76	1.46	1.39
12	A	837	CLA	C3D-C2D	2.76	1.46	1.39
12	a	802	CLA	MG-NC	2.75	2.12	2.06
12	B	803	CLA	C3D-C2D	2.75	1.46	1.39
12	l	206	CLA	C4D-CHA	2.75	1.47	1.38
12	a	837	CLA	MG-NC	2.75	2.12	2.06
12	H	835	CLA	MG-NC	2.75	2.12	2.06
12	a	837	CLA	C1C-NC	-2.75	1.33	1.37
12	A	813	CLA	C4D-CHA	2.75	1.47	1.38
12	B	825	CLA	C4D-CHA	2.75	1.47	1.38
12	G	837	CLA	MG-ND	-2.75	2.00	2.05
12	A	807	CLA	MG-ND	-2.75	2.00	2.05
12	a	831	CLA	C1C-NC	-2.75	1.33	1.37
12	A	855	CLA	CHD-C1D	2.75	1.43	1.38
12	B	824	CLA	C4D-CHA	2.75	1.47	1.38
12	G	856	CLA	C4B-NB	-2.75	1.34	1.37
12	A	838	CLA	OBD-CAD	2.75	1.27	1.22
12	B	838	CLA	C1B-NB	-2.75	1.34	1.37
12	G	807	CLA	C3D-C2D	2.75	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	806	CLA	C1B-C2B	2.75	1.49	1.43
12	A	822	CLA	C1B-C2B	2.75	1.49	1.43
12	a	836	CLA	C4B-NB	-2.75	1.34	1.37
12	G	817	CLA	C1B-C2B	2.75	1.49	1.43
12	L	202	CLA	MG-ND	-2.75	2.00	2.05
12	A	825	CLA	OBD-CAD	2.75	1.27	1.22
12	G	828	CLA	C3D-C2D	2.75	1.46	1.39
12	H	830	CLA	C4B-NB	-2.75	1.34	1.37
12	H	821	CLA	C1C-NC	-2.75	1.33	1.37
12	a	822	CLA	MG-ND	-2.74	2.00	2.05
12	A	824	CLA	C4B-NB	-2.74	1.34	1.37
12	H	826	CLA	C4D-CHA	2.74	1.47	1.38
12	R	103	CLA	C1D-ND	-2.74	1.34	1.37
12	B	832	CLA	C1B-NB	-2.74	1.34	1.37
12	G	840	CLA	C3D-C2D	2.74	1.46	1.39
12	A	810	CLA	MG-NC	2.74	2.12	2.06
12	S	204	CLA	C4D-CHA	2.74	1.47	1.38
12	B	808	CLA	MG-NC	2.74	2.12	2.06
12	B	816	CLA	MG-ND	-2.74	2.00	2.05
12	b	822	CLA	C1C-NC	-2.74	1.33	1.37
12	A	806	CLA	C4D-CHA	2.74	1.47	1.38
12	b	819	CLA	C1D-ND	-2.74	1.34	1.37
12	A	808	CLA	C1D-ND	-2.74	1.34	1.37
12	A	821	CLA	C1B-NB	-2.74	1.34	1.37
12	a	803	CLA	C3B-C4B	2.74	1.50	1.42
12	G	834	CLA	MG-NC	2.74	2.12	2.06
12	b	805	CLA	MG-NC	2.74	2.12	2.06
12	B	817	CLA	C1B-NB	-2.74	1.34	1.37
12	b	848	CLA	C1B-C2B	2.74	1.49	1.43
12	B	804	CLA	C4D-CHA	2.74	1.47	1.38
12	B	833	CLA	C4C-C3C	2.74	1.49	1.45
12	H	810	CLA	C1B-NB	-2.74	1.34	1.37
12	A	838	CLA	C1C-NC	-2.74	1.33	1.37
12	a	810	CLA	C1B-C2B	2.74	1.49	1.43
12	b	829	CLA	C4B-NB	-2.74	1.34	1.37
12	A	830	CLA	C4D-CHA	2.74	1.47	1.38
12	A	820	CLA	C4C-C3C	2.74	1.49	1.45
12	G	835	CLA	C1B-NB	-2.74	1.34	1.37
12	b	818	CLA	C1D-ND	-2.74	1.34	1.37
12	a	854	CLA	C4D-CHA	2.74	1.47	1.38
12	H	835	CLA	C4D-CHA	2.74	1.47	1.38
12	H	822	CLA	C4D-CHA	2.74	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	839	CLA	C1C-NC	-2.74	1.33	1.37
12	b	816	CLA	MG-ND	-2.74	2.00	2.05
12	a	806	CLA	C3D-C2D	2.73	1.46	1.39
12	H	815	CLA	C4D-CHA	2.73	1.47	1.38
12	L	206	CLA	C4D-CHA	2.73	1.47	1.38
12	j	104	CLA	MG-ND	-2.73	2.00	2.05
12	G	811	CLA	C1B-C2B	2.73	1.49	1.43
12	G	812	CLA	C1B-NB	-2.73	1.34	1.37
12	b	835	CLA	C4B-NB	-2.73	1.34	1.37
12	b	848	CLA	C1D-ND	-2.73	1.34	1.37
13	a	842	1L3	C14-C03	2.73	1.56	1.51
11	A	801	CL0	MG-NC	2.73	2.12	2.06
12	A	813	CLA	C3D-C2D	2.73	1.46	1.39
12	H	834	CLA	C1B-NB	-2.73	1.34	1.37
12	S	203	CLA	C4D-CHA	2.73	1.47	1.38
12	A	827	CLA	C4D-CHA	2.73	1.47	1.38
12	a	835	CLA	C3D-C2D	2.73	1.46	1.39
12	G	839	CLA	C1D-ND	-2.73	1.34	1.37
12	a	813	CLA	C1B-C2B	2.73	1.49	1.43
12	A	803	CLA	C3B-C4B	2.73	1.50	1.42
12	B	834	CLA	MG-NC	2.73	2.12	2.06
12	G	817	CLA	C4B-NB	-2.73	1.34	1.37
12	B	808	CLA	C1B-NB	-2.73	1.34	1.37
12	B	836	CLA	C4B-NB	-2.73	1.34	1.37
12	A	819	CLA	MG-ND	-2.73	2.00	2.05
12	G	804	CLA	C1D-ND	-2.73	1.34	1.37
12	A	826	CLA	C4B-NB	-2.73	1.34	1.37
12	B	805	CLA	C1B-NB	-2.73	1.34	1.37
12	H	834	CLA	C1C-NC	-2.73	1.33	1.37
12	a	819	CLA	C1C-NC	-2.73	1.33	1.37
12	B	819	CLA	C1D-ND	-2.73	1.34	1.37
12	G	807	CLA	C1B-C2B	2.73	1.49	1.43
12	G	816	CLA	C1B-C2B	2.73	1.49	1.43
12	A	807	CLA	C1B-C2B	2.73	1.49	1.43
12	a	815	CLA	C1D-ND	-2.73	1.34	1.37
12	A	802	CLA	C4D-CHA	2.73	1.47	1.38
12	H	828	CLA	C4B-NB	-2.73	1.34	1.37
12	b	829	CLA	C4C-C3C	2.73	1.49	1.45
12	H	813	CLA	MG-NC	2.73	2.12	2.06
12	H	805	CLA	C3D-C2D	2.73	1.46	1.39
12	B	801	CLA	C3D-C2D	2.73	1.46	1.39
12	A	838	CLA	C3B-C4B	2.72	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	205	CLA	C4D-CHA	2.72	1.47	1.38
12	B	805	CLA	C3D-C2D	2.72	1.46	1.39
12	G	839	CLA	C1B-C2B	2.72	1.49	1.43
12	A	838	CLA	C3D-C2D	2.72	1.46	1.39
12	b	801	CLA	CHB-C1B	2.72	1.45	1.39
12	B	834	CLA	C1C-NC	-2.72	1.33	1.37
12	a	811	CLA	C1B-C2B	2.72	1.49	1.43
12	A	819	CLA	C1D-ND	-2.72	1.34	1.37
13	H	840	1L3	C14-C03	2.72	1.56	1.51
12	a	806	CLA	MG-ND	-2.72	2.00	2.05
12	B	833	CLA	C1B-C2B	2.72	1.49	1.43
12	b	834	CLA	C1B-NB	-2.72	1.34	1.37
13	A	842	1L3	C14-C03	2.72	1.56	1.51
12	G	820	CLA	MG-ND	-2.72	2.00	2.05
12	G	804	CLA	C1C-NC	-2.72	1.33	1.37
12	l	205	CLA	C1B-C2B	2.72	1.49	1.43
12	A	810	CLA	C4D-CHA	2.72	1.47	1.38
12	a	838	CLA	C1C-NC	-2.72	1.33	1.37
12	A	816	CLA	C4B-NB	-2.72	1.34	1.37
13	G	843	1L3	C14-C03	2.72	1.56	1.51
12	A	808	CLA	C4B-NB	-2.72	1.34	1.37
12	j	102	CLA	C1B-C2B	2.72	1.49	1.43
12	b	808	CLA	C1B-NB	-2.72	1.34	1.37
12	b	818	CLA	C1B-NB	-2.72	1.34	1.37
12	A	812	CLA	C4B-NB	-2.72	1.34	1.37
12	A	823	CLA	C1B-NB	-2.72	1.34	1.37
12	b	825	CLA	C3D-C2D	2.72	1.46	1.39
12	b	824	CLA	C4D-CHA	2.72	1.47	1.38
12	B	807	CLA	C4B-NB	-2.72	1.34	1.37
12	B	823	CLA	C1C-NC	-2.72	1.33	1.37
12	a	824	CLA	C1B-C2B	2.72	1.49	1.43
12	B	814	CLA	C4D-CHA	2.72	1.47	1.38
12	G	820	CLA	C1C-NC	-2.72	1.33	1.37
12	a	823	CLA	C1B-C2B	2.72	1.49	1.43
12	b	832	CLA	C1C-NC	-2.72	1.33	1.37
12	A	822	CLA	C3D-C2D	2.71	1.46	1.39
12	b	835	CLA	CHB-C1B	2.71	1.45	1.39
12	H	817	CLA	MG-ND	-2.71	2.00	2.05
12	A	810	CLA	MG-ND	-2.71	2.00	2.05
12	H	823	CLA	C4B-NB	-2.71	1.34	1.37
12	B	834	CLA	C4D-CHA	2.71	1.47	1.38
12	b	805	CLA	MG-ND	-2.71	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	204	CLA	C1B-C2B	2.71	1.49	1.43
12	G	839	CLA	C1C-NC	-2.71	1.33	1.37
12	A	818	CLA	C1B-NB	-2.71	1.34	1.37
12	H	802	CLA	CHD-C1D	2.71	1.43	1.38
12	a	806	CLA	C4D-CHA	2.71	1.47	1.38
12	B	822	CLA	C4B-NB	-2.71	1.34	1.37
12	b	848	CLA	C1B-NB	-2.71	1.34	1.37
12	B	829	CLA	C1B-NB	-2.71	1.34	1.37
12	a	807	CLA	MG-ND	-2.71	2.00	2.05
12	G	837	CLA	C1C-NC	-2.71	1.33	1.37
12	l	202	CLA	MG-ND	-2.71	2.00	2.05
12	A	813	CLA	C4B-NB	-2.71	1.34	1.37
12	A	808	CLA	C1B-C2B	2.71	1.49	1.43
12	B	801	CLA	C1C-NC	-2.71	1.33	1.37
12	H	813	CLA	C1D-ND	-2.71	1.34	1.37
12	A	808	CLA	C1D-C2D	2.71	1.50	1.45
12	G	820	CLA	C1D-ND	-2.71	1.34	1.37
12	B	835	CLA	C1C-NC	-2.71	1.33	1.37
12	a	824	CLA	C4B-NB	-2.71	1.34	1.37
12	l	206	CLA	C1C-NC	-2.71	1.33	1.37
12	a	810	CLA	C3D-C2D	2.70	1.46	1.39
12	H	839	CLA	C4B-NB	-2.70	1.34	1.37
12	a	802	CLA	C4D-CHA	2.70	1.47	1.38
12	G	839	CLA	MG-ND	-2.70	2.00	2.05
12	A	802	CLA	OBD-CAD	2.70	1.27	1.22
12	a	827	CLA	C4D-CHA	2.70	1.47	1.38
12	a	803	CLA	C1C-NC	-2.70	1.33	1.37
12	B	823	CLA	C3D-C2D	2.70	1.46	1.39
12	B	827	CLA	C4B-NB	-2.70	1.34	1.37
12	G	821	CLA	C1C-NC	-2.70	1.33	1.37
12	G	805	CLA	MG-ND	-2.70	2.00	2.05
12	H	819	CLA	C1B-NB	-2.70	1.34	1.37
12	H	828	CLA	C3D-C2D	2.70	1.46	1.39
12	a	814	CLA	C4B-NB	-2.70	1.34	1.37
12	S	204	CLA	C1C-NC	-2.70	1.33	1.37
12	b	808	CLA	MG-NC	2.70	2.12	2.06
12	a	840	CLA	C1C-NC	-2.70	1.33	1.37
12	H	825	CLA	C3D-C2D	2.70	1.46	1.39
12	B	833	CLA	C3D-C2D	2.70	1.46	1.39
12	A	835	CLA	C1D-ND	-2.70	1.34	1.37
12	A	833	CLA	C4D-CHA	2.70	1.47	1.38
12	a	810	CLA	C4D-CHA	2.70	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	817	CLA	C1C-NC	-2.70	1.33	1.37
12	l	202	CLA	C1C-NC	-2.70	1.33	1.37
12	b	803	CLA	C1C-NC	-2.70	1.33	1.37
12	a	812	CLA	C1B-C2B	2.70	1.49	1.43
12	b	808	CLA	C1D-ND	-2.70	1.34	1.37
12	G	818	CLA	C4D-CHA	2.70	1.47	1.38
12	a	830	CLA	C4D-CHA	2.70	1.47	1.38
12	B	824	CLA	C3D-C2D	2.70	1.46	1.39
12	a	826	CLA	C1B-NB	-2.69	1.34	1.37
12	a	810	CLA	MG-ND	-2.69	2.00	2.05
12	b	828	CLA	C1B-C2B	2.69	1.49	1.43
12	a	839	CLA	C1D-ND	-2.69	1.34	1.37
12	G	819	CLA	MG-ND	-2.69	2.00	2.05
12	H	808	CLA	MG-ND	-2.69	2.00	2.05
12	l	204	CLA	MG-ND	-2.69	2.00	2.05
12	a	815	CLA	C1B-NB	-2.69	1.34	1.37
17	T	101	45D	C17-C15	2.69	1.53	1.47
12	R	103	CLA	C1B-C2B	2.69	1.49	1.43
12	b	811	CLA	C1B-C2B	2.69	1.49	1.43
12	b	804	CLA	C4D-CHA	2.69	1.47	1.38
12	G	807	CLA	C4D-CHA	2.69	1.47	1.38
12	b	831	CLA	MG-ND	-2.69	2.00	2.05
12	A	807	CLA	C1B-NB	-2.69	1.34	1.37
12	A	817	CLA	MG-NC	2.69	2.12	2.06
12	a	816	CLA	C4B-NB	-2.69	1.34	1.37
12	A	827	CLA	C3D-C2D	2.69	1.46	1.39
12	b	813	CLA	MG-ND	-2.69	2.00	2.05
12	G	825	CLA	C1B-C2B	2.69	1.49	1.43
12	L	204	CLA	C4B-NB	-2.69	1.34	1.37
12	a	819	CLA	MG-ND	-2.69	2.00	2.05
12	G	803	CLA	C4D-CHA	2.69	1.47	1.38
12	B	813	CLA	MG-ND	-2.69	2.00	2.05
12	b	825	CLA	C4D-CHA	2.69	1.47	1.38
12	a	835	CLA	C1D-ND	-2.69	1.34	1.37
12	G	814	CLA	C1C-NC	-2.69	1.33	1.37
12	b	801	CLA	C3D-C2D	2.69	1.46	1.39
12	A	815	CLA	C1B-C2B	2.69	1.49	1.43
12	A	828	CLA	C4B-NB	-2.69	1.34	1.37
12	a	824	CLA	OBD-CAD	2.68	1.27	1.22
12	B	820	CLA	MG-NC	2.68	2.12	2.06
12	a	827	CLA	MG-NC	2.68	2.12	2.06
12	B	838	CLA	C1C-NC	-2.68	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	808	CLA	MG-ND	-2.68	2.00	2.05
12	a	822	CLA	C1B-NB	-2.68	1.34	1.37
12	G	838	CLA	C1C-NC	-2.68	1.33	1.37
12	b	832	CLA	C1B-NB	-2.68	1.34	1.37
12	G	856	CLA	CHD-C1D	2.68	1.43	1.38
12	a	821	CLA	MG-ND	-2.68	2.00	2.05
12	a	812	CLA	C4B-NB	-2.68	1.34	1.37
12	G	818	CLA	C1C-NC	-2.68	1.33	1.37
12	a	818	CLA	C4B-NB	-2.68	1.34	1.37
12	L	205	CLA	C1B-C2B	2.68	1.49	1.43
12	A	833	CLA	C4B-NB	-2.68	1.34	1.37
12	H	836	CLA	MG-ND	-2.68	2.00	2.05
12	b	803	CLA	C1B-C2B	2.68	1.49	1.43
12	b	809	CLA	C1C-NC	-2.68	1.33	1.37
12	H	809	CLA	MG-ND	-2.68	2.00	2.05
12	S	203	CLA	C1B-C2B	2.68	1.49	1.43
12	b	802	CLA	C1C-NC	-2.68	1.33	1.37
13	b	838	1L3	C14-C03	2.68	1.56	1.51
12	G	813	CLA	C3D-C2D	2.68	1.46	1.39
12	a	810	CLA	C1B-NB	-2.68	1.34	1.37
12	G	811	CLA	C1B-NB	-2.68	1.34	1.37
12	a	841	CLA	C1B-NB	-2.68	1.34	1.37
12	b	816	CLA	C1D-ND	-2.68	1.34	1.37
12	B	835	CLA	MG-ND	-2.67	2.00	2.05
12	H	836	CLA	C1C-NC	-2.67	1.33	1.37
12	H	830	CLA	MG-ND	-2.67	2.00	2.05
12	a	826	CLA	C3D-C2D	2.67	1.46	1.39
12	a	839	CLA	C1C-NC	-2.67	1.33	1.37
12	B	832	CLA	MG-ND	-2.67	2.00	2.05
12	G	839	CLA	C4B-NB	-2.67	1.34	1.37
12	H	833	CLA	MG-ND	-2.67	2.00	2.05
12	B	805	CLA	MG-NC	2.67	2.12	2.06
12	H	810	CLA	C1D-ND	-2.67	1.34	1.37
12	H	820	CLA	C1D-ND	-2.67	1.34	1.37
12	G	815	CLA	C4B-NB	-2.67	1.34	1.37
12	H	804	CLA	MG-NC	2.67	2.12	2.06
12	B	819	CLA	MG-ND	-2.67	2.00	2.05
12	A	802	CLA	MG-NC	2.67	2.12	2.06
12	a	833	CLA	C4D-CHA	2.67	1.47	1.38
12	b	836	CLA	C1B-NB	-2.67	1.34	1.37
12	F	201	CLA	C3B-C4B	2.67	1.50	1.42
12	G	806	CLA	C3D-C2D	2.67	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	m	101	45D	C17-C15	2.67	1.53	1.47
12	G	809	CLA	C3D-C2D	2.67	1.46	1.39
12	a	835	CLA	MG-ND	-2.67	2.00	2.05
12	A	825	CLA	C1C-NC	-2.67	1.33	1.37
12	B	809	CLA	C1C-NC	-2.67	1.33	1.37
12	H	818	CLA	C1B-NB	-2.67	1.34	1.37
12	B	818	CLA	C1B-NB	-2.67	1.34	1.37
19	B	847	LMT	O3'-C3'	-2.67	1.36	1.43
12	A	809	CLA	C1C-NC	-2.67	1.33	1.37
12	G	828	CLA	C4D-CHA	2.67	1.47	1.38
12	R	103	CLA	MG-ND	-2.67	2.00	2.05
12	b	809	CLA	MG-ND	-2.67	2.00	2.05
12	G	808	CLA	C1B-C2B	2.67	1.49	1.43
12	A	812	CLA	C1B-C2B	2.67	1.49	1.43
12	B	835	CLA	C4D-CHA	2.67	1.47	1.38
12	B	814	CLA	MG-NC	2.67	2.12	2.06
12	a	828	CLA	C1C-NC	-2.67	1.33	1.37
12	A	803	CLA	C1C-NC	-2.67	1.33	1.37
17	M	101	45D	C17-C15	2.67	1.53	1.47
12	H	819	CLA	MG-ND	-2.66	2.00	2.05
12	A	839	CLA	C4B-NB	-2.66	1.34	1.37
12	b	835	CLA	C4D-CHA	2.66	1.47	1.38
12	l	204	CLA	C1C-NC	-2.66	1.33	1.37
12	a	824	CLA	C3D-C2D	2.66	1.46	1.39
12	J	103	CLA	C1D-ND	-2.66	1.34	1.37
12	H	804	CLA	C4D-CHA	2.66	1.47	1.38
12	A	854	CLA	C3B-C4B	2.66	1.50	1.42
12	B	836	CLA	CHB-C1B	2.66	1.45	1.39
12	H	850	CLA	C1D-ND	-2.66	1.34	1.37
13	B	839	1L3	C14-C03	2.66	1.56	1.51
12	H	830	CLA	C4D-CHA	2.66	1.47	1.38
12	A	822	CLA	C1B-NB	-2.66	1.34	1.37
12	H	805	CLA	C4D-CHA	2.66	1.47	1.38
12	G	816	CLA	C1B-NB	-2.66	1.34	1.37
12	A	814	CLA	C4B-NB	-2.66	1.34	1.37
12	A	818	CLA	C4B-NB	-2.66	1.34	1.37
12	B	802	CLA	C1B-C2B	2.66	1.49	1.43
12	A	815	CLA	C1D-ND	-2.66	1.34	1.37
12	b	804	CLA	C1B-C2B	2.66	1.49	1.43
12	b	802	CLA	C4B-NB	-2.66	1.34	1.37
12	A	817	CLA	C1B-NB	-2.66	1.34	1.37
12	A	805	CLA	C3A-C2A	-2.66	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	814	CLA	MG-NC	2.66	2.12	2.06
12	b	815	CLA	MG-ND	-2.66	2.00	2.05
12	B	828	CLA	C1B-C2B	2.66	1.49	1.43
12	B	807	CLA	MG-NC	2.66	2.12	2.06
12	H	806	CLA	C3D-C2D	2.66	1.46	1.39
12	H	809	CLA	C1D-ND	-2.66	1.34	1.37
12	b	822	CLA	C4B-NB	-2.66	1.34	1.37
12	B	804	CLA	C3D-C2D	2.66	1.46	1.39
12	A	810	CLA	C1B-C2B	2.65	1.49	1.43
12	G	817	CLA	C1C-NC	-2.65	1.33	1.37
12	H	813	CLA	MG-ND	-2.65	2.00	2.05
12	H	837	CLA	C4B-NB	-2.65	1.34	1.37
12	H	830	CLA	C1B-C2B	2.65	1.49	1.43
12	B	820	CLA	MG-ND	-2.65	2.00	2.05
12	G	808	CLA	C1C-NC	-2.65	1.33	1.37
12	G	821	CLA	MG-NC	2.65	2.12	2.06
12	H	809	CLA	C1B-NB	-2.65	1.34	1.37
12	b	804	CLA	C3D-C2D	2.65	1.46	1.39
12	A	823	CLA	C1C-NC	-2.65	1.33	1.37
12	G	827	CLA	C3D-C2D	2.65	1.46	1.39
12	G	810	CLA	C1C-NC	-2.65	1.33	1.37
12	b	804	CLA	MG-NC	2.65	2.12	2.06
12	a	817	CLA	C4D-CHA	2.65	1.47	1.38
12	G	823	CLA	MG-ND	-2.65	2.00	2.05
17	m	101	45D	C18-C16	2.65	1.53	1.47
12	B	805	CLA	MG-ND	-2.64	2.00	2.05
12	A	835	CLA	MG-ND	-2.64	2.00	2.05
12	G	823	CLA	C1B-NB	-2.64	1.34	1.37
12	B	818	CLA	MG-ND	-2.64	2.00	2.05
12	b	807	CLA	MG-NC	2.64	2.12	2.06
12	B	821	CLA	C3D-C2D	2.64	1.46	1.39
12	b	819	CLA	MG-ND	-2.64	2.00	2.05
12	a	854	CLA	C4B-NB	-2.64	1.34	1.37
12	H	812	CLA	C1B-C2B	2.64	1.49	1.43
12	b	837	CLA	C1C-NC	-2.64	1.33	1.37
12	G	824	CLA	MG-ND	-2.64	2.00	2.05
12	G	856	CLA	C4D-CHA	2.64	1.47	1.38
12	f	203	CLA	C1B-NB	-2.64	1.34	1.37
17	T	101	45D	C18-C16	2.64	1.53	1.47
12	a	838	CLA	C3B-C4B	2.64	1.50	1.42
12	H	814	CLA	C1B-NB	-2.64	1.34	1.37
12	B	813	CLA	C1B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	841	CLA	C1B-NB	-2.64	1.34	1.37
12	b	811	CLA	C1C-NC	-2.64	1.33	1.37
12	B	809	CLA	MG-ND	-2.64	2.00	2.05
12	G	816	CLA	C1D-ND	-2.64	1.34	1.37
12	A	817	CLA	C3B-C4B	2.64	1.50	1.42
12	a	805	CLA	MG-ND	-2.64	2.00	2.05
12	H	802	CLA	C4B-NB	-2.64	1.34	1.37
12	B	805	CLA	C4D-CHA	2.64	1.47	1.38
12	B	836	CLA	C4D-CHA	2.64	1.47	1.38
12	H	820	CLA	MG-ND	-2.63	2.00	2.05
12	G	855	CLA	C4B-NB	-2.63	1.34	1.37
12	b	827	CLA	C4B-NB	-2.63	1.34	1.37
12	A	854	CLA	C1C-C2C	2.63	1.49	1.44
12	b	829	CLA	C4D-CHA	2.63	1.47	1.38
12	H	834	CLA	C1B-C2B	2.63	1.49	1.43
12	B	829	CLA	C4D-CHA	2.63	1.47	1.38
12	R	103	CLA	C1B-NB	-2.63	1.34	1.37
12	a	835	CLA	C1B-NB	-2.63	1.34	1.37
12	B	806	CLA	C1D-ND	-2.63	1.34	1.37
12	P	203	CLA	MG-ND	-2.63	2.00	2.05
12	G	819	CLA	C1B-C2B	2.63	1.49	1.43
12	P	203	CLA	C1C-NC	-2.63	1.33	1.37
12	a	802	CLA	C4B-NB	-2.63	1.34	1.37
12	H	821	CLA	C1B-C2B	2.63	1.49	1.43
17	M	101	45D	C18-C16	2.63	1.53	1.47
12	b	832	CLA	C3D-C2D	2.63	1.46	1.39
12	a	826	CLA	C1B-C2B	2.63	1.49	1.43
12	a	828	CLA	C4B-NB	-2.63	1.34	1.37
12	H	837	CLA	MG-NC	2.63	2.12	2.06
12	B	803	CLA	C1B-C2B	2.63	1.49	1.43
12	a	841	CLA	C4B-NB	-2.63	1.34	1.37
12	A	805	CLA	C3D-C2D	2.63	1.46	1.39
12	b	805	CLA	C4D-CHA	2.63	1.47	1.38
12	P	203	CLA	C1D-ND	-2.63	1.34	1.37
12	a	819	CLA	C1D-ND	-2.63	1.34	1.37
12	a	823	CLA	C1B-NB	-2.63	1.34	1.37
12	G	802	CLA	C4B-NB	-2.62	1.34	1.37
12	b	831	CLA	C1B-NB	-2.62	1.34	1.37
12	A	807	CLA	C1C-NC	-2.62	1.33	1.37
12	H	806	CLA	C4D-CHA	2.62	1.47	1.38
12	A	818	CLA	MG-ND	-2.62	2.00	2.05
12	a	834	CLA	C4B-NB	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	834	CLA	MG-ND	-2.62	2.00	2.05
12	f	201	CLA	C3B-C4B	2.62	1.50	1.42
12	b	809	CLA	C1D-ND	-2.62	1.34	1.37
12	B	833	CLA	C4B-NB	-2.62	1.34	1.37
12	b	820	CLA	MG-ND	-2.62	2.00	2.05
12	l	204	CLA	C1B-C2B	2.62	1.49	1.43
12	G	833	CLA	C4D-CHA	2.62	1.47	1.38
12	B	838	CLA	C4B-NB	-2.62	1.34	1.37
12	H	805	CLA	MG-ND	-2.62	2.00	2.05
12	b	818	CLA	MG-ND	-2.62	2.00	2.05
12	P	203	CLA	C1B-NB	-2.62	1.34	1.37
12	G	804	CLA	C3B-C4B	2.62	1.50	1.42
12	b	819	CLA	C1B-NB	-2.62	1.34	1.37
12	G	802	CLA	C1C-NC	-2.62	1.33	1.37
12	b	820	CLA	C1C-NC	-2.62	1.33	1.37
12	B	831	CLA	C4C-C3C	2.62	1.49	1.45
12	B	821	CLA	MG-NC	2.61	2.12	2.06
12	b	834	CLA	C4D-CHA	2.61	1.47	1.38
12	A	824	CLA	C1B-C2B	2.61	1.49	1.43
12	f	203	CLA	MG-ND	-2.61	2.00	2.05
12	G	840	CLA	C1C-NC	-2.61	1.33	1.37
12	a	809	CLA	MG-ND	-2.61	2.00	2.05
12	A	829	CLA	OBD-CAD	2.61	1.27	1.22
12	A	855	CLA	C4D-CHA	2.61	1.47	1.38
12	F	203	CLA	C1D-ND	-2.61	1.34	1.37
12	A	819	CLA	C1B-NB	-2.61	1.34	1.37
12	S	203	CLA	C4B-NB	-2.61	1.34	1.37
12	A	812	CLA	C1D-ND	-2.61	1.34	1.37
12	H	832	CLA	C1C-NC	-2.61	1.33	1.37
12	H	827	CLA	C3D-C2D	2.61	1.46	1.39
12	H	804	CLA	CHD-C1D	2.61	1.43	1.38
12	a	813	CLA	C1C-NC	-2.61	1.33	1.37
12	a	835	CLA	C1C-NC	-2.61	1.33	1.37
12	H	826	CLA	C3D-C2D	2.61	1.46	1.39
12	H	836	CLA	C4D-CHA	2.60	1.47	1.38
12	b	801	CLA	C1C-NC	-2.60	1.33	1.37
12	B	829	CLA	C1C-NC	-2.60	1.33	1.37
12	B	829	CLA	C1B-C2B	2.60	1.49	1.43
12	G	810	CLA	C1D-ND	-2.60	1.34	1.37
12	G	824	CLA	C1B-NB	-2.60	1.34	1.37
12	G	855	CLA	CHB-C1B	2.60	1.45	1.39
12	H	814	CLA	MG-ND	-2.60	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	810	CLA	MG-ND	-2.60	2.00	2.05
12	b	805	CLA	C1B-NB	-2.60	1.34	1.37
13	B	839	1L3	C22-C21	2.60	1.57	1.50
12	b	837	CLA	C1B-NB	-2.60	1.34	1.37
12	a	838	CLA	C4D-CHA	2.60	1.47	1.38
12	G	838	CLA	C4D-CHA	2.60	1.47	1.38
12	H	834	CLA	C4B-NB	-2.60	1.34	1.37
12	H	802	CLA	C1B-C2B	2.60	1.49	1.43
12	G	802	CLA	C4D-CHA	2.60	1.47	1.38
12	l	202	CLA	C1B-C2B	2.60	1.49	1.43
12	J	103	CLA	MG-ND	-2.60	2.00	2.05
12	b	829	CLA	C1B-C2B	2.60	1.49	1.43
13	b	838	1L3	O05-C04	-2.60	1.17	1.23
12	H	815	CLA	C1C-NC	-2.60	1.33	1.37
12	H	801	CLA	OBD-CAD	2.59	1.27	1.22
12	G	855	CLA	C3B-C4B	2.59	1.50	1.42
13	b	838	1L3	C22-C21	2.59	1.57	1.50
12	G	818	CLA	MG-NC	2.59	2.12	2.06
12	H	814	CLA	C1B-C2B	2.59	1.49	1.43
12	H	821	CLA	MG-NC	2.59	2.12	2.06
12	A	831	CLA	C4B-NB	-2.59	1.34	1.37
12	A	816	CLA	C1C-NC	-2.59	1.33	1.37
12	b	812	CLA	C4B-NB	-2.59	1.34	1.37
12	G	838	CLA	C3B-C4B	2.59	1.50	1.42
13	H	840	1L3	C22-C21	2.59	1.57	1.50
12	A	820	CLA	CHB-C1B	2.59	1.45	1.39
12	G	830	CLA	C4B-NB	-2.59	1.34	1.37
12	P	201	CLA	C3B-C4B	2.59	1.50	1.42
12	a	855	CLA	C4D-CHA	2.59	1.47	1.38
12	S	202	CLA	C1B-C2B	2.59	1.49	1.43
12	G	835	CLA	MG-ND	-2.59	2.00	2.05
12	B	814	CLA	C1C-NC	-2.59	1.33	1.37
12	A	815	CLA	MG-ND	-2.59	2.00	2.05
12	b	820	CLA	C1B-C2B	2.59	1.49	1.43
12	a	808	CLA	C1D-C2D	2.59	1.50	1.45
12	H	808	CLA	C3B-C4B	2.59	1.50	1.42
12	F	203	CLA	C1C-NC	-2.58	1.33	1.37
12	G	830	CLA	MG-NC	2.58	2.12	2.06
12	b	821	CLA	MG-NC	2.58	2.12	2.06
12	A	840	CLA	C1C-NC	-2.58	1.33	1.37
12	b	820	CLA	MG-NC	2.58	2.12	2.06
12	S	202	CLA	C4B-NB	-2.58	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	820	CLA	C1B-NB	-2.58	1.34	1.37
12	G	829	CLA	C1C-NC	-2.58	1.33	1.37
12	a	817	CLA	C1B-NB	-2.58	1.34	1.37
12	B	802	CLA	C1C-NC	-2.58	1.33	1.37
12	B	829	CLA	C4B-NB	-2.57	1.34	1.37
12	a	854	CLA	C3B-C4B	2.57	1.50	1.42
12	A	825	CLA	C4B-NB	-2.57	1.34	1.37
12	A	808	CLA	C1C-NC	-2.57	1.33	1.37
12	B	828	CLA	C1C-NC	-2.57	1.33	1.37
12	b	806	CLA	C1B-C2B	2.57	1.49	1.43
12	B	811	CLA	C1B-C2B	2.57	1.49	1.43
12	j	102	CLA	C4B-NB	-2.57	1.34	1.37
12	G	818	CLA	C1B-C2B	2.57	1.49	1.43
12	b	833	CLA	C1B-C2B	2.57	1.49	1.43
12	G	810	CLA	MG-ND	-2.57	2.00	2.05
12	G	855	CLA	C1C-NC	-2.57	1.33	1.37
12	A	828	CLA	C1C-NC	-2.57	1.33	1.37
12	A	829	CLA	MG-NC	2.57	2.12	2.06
12	b	814	CLA	C1C-NC	-2.57	1.33	1.37
12	A	821	CLA	MG-ND	-2.57	2.00	2.05
12	a	816	CLA	C1C-NC	-2.57	1.33	1.37
12	f	203	CLA	C4C-C3C	2.57	1.49	1.45
12	b	821	CLA	C1C-NC	-2.57	1.33	1.37
11	G	801	CL0	C3D-C2D	2.57	1.46	1.39
12	G	804	CLA	MG-ND	-2.57	2.00	2.05
12	A	837	CLA	C1B-C2B	2.56	1.49	1.43
12	A	833	CLA	C1B-NB	-2.56	1.34	1.37
12	b	831	CLA	C1D-C2D	2.56	1.50	1.45
12	a	855	CLA	CHD-C1D	2.56	1.43	1.38
12	b	830	CLA	C1C-NC	-2.56	1.33	1.37
12	A	823	CLA	MG-ND	-2.56	2.00	2.05
12	H	836	CLA	C3B-C4B	2.56	1.50	1.42
12	a	815	CLA	MG-ND	-2.56	2.00	2.05
12	J	103	CLA	C1B-NB	-2.56	1.34	1.37
12	b	810	CLA	OBD-CAD	2.56	1.26	1.22
12	l	202	CLA	C3B-C4B	2.56	1.50	1.42
12	G	816	CLA	MG-ND	-2.56	2.00	2.05
12	H	802	CLA	C3D-C2D	2.56	1.46	1.39
12	A	812	CLA	C4C-C3C	2.56	1.49	1.45
12	f	203	CLA	C1C-NC	-2.56	1.33	1.37
12	b	813	CLA	C1B-NB	-2.56	1.34	1.37
12	H	802	CLA	C4D-CHA	2.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	825	CLA	C1C-NC	-2.56	1.33	1.37
12	G	814	CLA	C1B-C2B	2.56	1.49	1.43
12	a	829	CLA	OBD-CAD	2.56	1.26	1.22
12	H	808	CLA	C1B-C2B	2.56	1.49	1.43
12	H	832	CLA	C1B-C2B	2.56	1.49	1.43
12	b	826	CLA	C4C-C3C	2.56	1.49	1.45
12	F	203	CLA	MG-ND	-2.56	2.00	2.05
12	A	819	CLA	C1C-NC	-2.56	1.33	1.37
12	F	201	CLA	C1C-NC	-2.56	1.33	1.37
12	B	837	CLA	MG-NC	2.55	2.12	2.06
12	H	837	CLA	C4D-CHA	2.55	1.47	1.38
19	H	848	LMT	O3'-C3'	-2.55	1.36	1.43
12	B	809	CLA	C1D-ND	-2.55	1.34	1.37
12	G	813	CLA	C1B-C2B	2.55	1.49	1.43
12	a	804	CLA	C4B-NB	-2.55	1.34	1.37
12	G	806	CLA	C4D-CHA	2.55	1.47	1.38
12	A	803	CLA	MG-ND	-2.55	2.00	2.05
12	b	802	CLA	C4D-CHA	2.55	1.47	1.38
12	H	822	CLA	C4B-NB	-2.55	1.34	1.37
12	l	204	CLA	C4B-NB	-2.55	1.34	1.37
12	H	824	CLA	C3D-C2D	2.55	1.45	1.39
12	H	829	CLA	C1C-NC	-2.55	1.33	1.37
12	a	819	CLA	C1B-NB	-2.55	1.34	1.37
12	a	826	CLA	C4B-NB	-2.55	1.34	1.37
12	A	838	CLA	C4D-CHA	2.55	1.47	1.38
17	M	101	45D	C39-C35	2.55	1.56	1.50
12	H	804	CLA	C3D-C2D	2.55	1.45	1.39
12	A	817	CLA	C4D-CHA	2.55	1.47	1.38
17	T	101	45D	C39-C35	2.55	1.56	1.50
12	B	802	CLA	C4B-NB	-2.55	1.34	1.37
12	b	834	CLA	C1C-NC	-2.55	1.33	1.37
12	B	802	CLA	MG-NC	2.55	2.12	2.06
12	b	812	CLA	C1C-NC	-2.55	1.33	1.37
12	A	827	CLA	C1B-C2B	2.54	1.49	1.43
11	a	801	CL0	C4B-NB	-2.54	1.34	1.37
12	G	825	CLA	C4B-NB	-2.54	1.34	1.37
12	B	815	CLA	C1A-CHA	2.54	1.53	1.43
12	a	808	CLA	C1B-C2B	2.54	1.49	1.43
12	j	104	CLA	C3B-C4B	2.54	1.50	1.42
11	G	801	CL0	C4D-CHA	2.54	1.47	1.38
12	a	812	CLA	C4C-C3C	2.54	1.49	1.45
12	B	830	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	829	CLA	MG-NC	2.54	2.12	2.06
12	a	817	CLA	C3D-C2D	2.54	1.45	1.39
12	B	827	CLA	C1C-NC	-2.54	1.33	1.37
12	B	812	CLA	C4B-NB	-2.54	1.34	1.37
12	a	823	CLA	MG-ND	-2.54	2.00	2.05
12	A	804	CLA	C4B-NB	-2.54	1.34	1.37
12	a	803	CLA	MG-ND	-2.54	2.00	2.05
12	B	802	CLA	C4D-CHA	2.53	1.47	1.38
12	H	819	CLA	C4C-C3C	2.53	1.49	1.45
12	b	809	CLA	C1B-C2B	2.53	1.49	1.43
12	b	835	CLA	MG-NC	2.53	2.12	2.06
12	a	837	CLA	C1B-C2B	2.53	1.49	1.43
12	B	834	CLA	C1B-C2B	2.53	1.49	1.43
12	a	824	CLA	C1C-NC	-2.53	1.33	1.37
12	G	828	CLA	C1B-C2B	2.53	1.49	1.43
12	B	813	CLA	C1B-C2B	2.53	1.49	1.43
12	f	203	CLA	C1D-ND	-2.53	1.34	1.37
12	a	839	CLA	MG-ND	-2.53	2.00	2.05
12	B	835	CLA	C3D-C2D	2.53	1.45	1.39
12	H	831	CLA	C1D-C2D	2.53	1.50	1.45
12	b	833	CLA	C4B-NB	-2.53	1.34	1.37
12	B	801	CLA	C4B-NB	-2.53	1.34	1.37
12	b	810	CLA	C1B-C2B	2.53	1.49	1.43
12	H	838	CLA	C1B-NB	-2.52	1.34	1.37
12	H	803	CLA	C1C-NC	-2.52	1.33	1.37
12	H	816	CLA	C1B-C2B	2.52	1.49	1.43
12	B	822	CLA	C1B-C2B	2.52	1.49	1.43
12	H	833	CLA	C1C-NC	-2.52	1.33	1.37
12	b	813	CLA	C1B-C2B	2.52	1.49	1.43
12	A	819	CLA	C4C-C3C	2.52	1.49	1.45
12	G	811	CLA	MG-ND	-2.52	2.00	2.05
12	B	836	CLA	MG-NC	2.52	2.12	2.06
12	B	820	CLA	C1C-NC	-2.52	1.33	1.37
12	a	831	CLA	C4B-NB	-2.52	1.34	1.37
12	B	812	CLA	C1C-NC	-2.52	1.33	1.37
12	L	202	CLA	C3B-C4B	2.52	1.50	1.42
12	A	804	CLA	C1B-C2B	2.52	1.49	1.43
12	a	808	CLA	C1C-NC	-2.52	1.33	1.37
12	A	836	CLA	C1C-NC	-2.52	1.33	1.37
12	a	823	CLA	C4B-NB	-2.52	1.34	1.37
12	b	837	CLA	C4B-NB	-2.52	1.34	1.37
12	B	824	CLA	MG-NC	2.52	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	801	CLA	C4D-CHA	2.52	1.47	1.38
12	B	809	CLA	C4C-C3C	2.52	1.49	1.45
12	H	810	CLA	C1B-C2B	2.51	1.49	1.43
12	G	829	CLA	C4B-NB	-2.51	1.34	1.37
12	H	835	CLA	C1B-C2B	2.51	1.49	1.43
12	a	805	CLA	C3A-C2A	-2.51	1.47	1.54
12	b	809	CLA	C4C-C3C	2.51	1.49	1.45
12	B	809	CLA	C1B-C2B	2.51	1.49	1.43
12	a	804	CLA	C1B-C2B	2.51	1.49	1.43
12	B	803	CLA	C4B-NB	-2.51	1.34	1.37
12	b	821	CLA	C3D-C2D	2.51	1.45	1.39
12	B	826	CLA	C4C-C3C	2.51	1.49	1.45
12	G	822	CLA	MG-ND	-2.51	2.00	2.05
12	H	827	CLA	C4B-NB	-2.51	1.34	1.37
12	A	817	CLA	C3D-C2D	2.51	1.45	1.39
17	m	101	45D	C39-C35	2.51	1.55	1.50
12	b	801	CLA	C4D-CHA	2.50	1.47	1.38
12	B	810	CLA	C1B-C2B	2.50	1.49	1.43
12	H	820	CLA	C1B-NB	-2.50	1.34	1.37
12	l	205	CLA	C4B-NB	-2.50	1.34	1.37
12	a	817	CLA	C4B-NB	-2.50	1.34	1.37
12	a	827	CLA	C1B-C2B	2.50	1.49	1.43
12	B	829	CLA	C4C-C3C	2.50	1.49	1.45
12	G	837	CLA	C1B-C2B	2.50	1.49	1.43
12	a	840	CLA	C1B-C2B	2.50	1.49	1.43
12	A	833	CLA	C1B-C2B	2.50	1.49	1.43
12	B	831	CLA	C1B-C2B	2.50	1.49	1.43
12	H	829	CLA	C1B-C2B	2.50	1.49	1.43
12	H	810	CLA	C4C-C3C	2.50	1.49	1.45
12	H	833	CLA	C1D-C2D	2.50	1.50	1.45
12	G	828	CLA	MG-NC	2.50	2.12	2.06
12	a	806	CLA	C1C-NC	-2.50	1.34	1.37
12	b	815	CLA	C1C-NC	-2.50	1.34	1.37
12	B	819	CLA	C1B-NB	-2.49	1.34	1.37
12	B	806	CLA	C1B-C2B	2.49	1.49	1.43
12	A	834	CLA	C4B-NB	-2.49	1.34	1.37
12	G	818	CLA	C4C-C3C	2.49	1.49	1.45
12	b	831	CLA	C4C-C3C	2.49	1.49	1.45
12	A	824	CLA	OBD-CAD	2.49	1.26	1.22
12	L	206	CLA	C4B-NB	-2.49	1.34	1.37
12	G	807	CLA	MG-ND	-2.49	2.00	2.05
12	A	813	CLA	C4C-C3C	2.49	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	806	CLA	C1C-NC	-2.49	1.34	1.37
12	G	841	CLA	C4B-NB	-2.49	1.34	1.37
12	L	202	CLA	C1B-C2B	2.49	1.49	1.43
12	H	834	CLA	C4C-C3C	2.49	1.49	1.45
12	G	827	CLA	C4B-NB	-2.49	1.34	1.37
12	G	831	CLA	C3D-C2D	2.49	1.45	1.39
12	B	820	CLA	C1B-C2B	2.49	1.49	1.43
12	H	828	CLA	C1C-NC	-2.49	1.34	1.37
12	H	825	CLA	MG-NC	2.49	2.12	2.06
12	G	810	CLA	C1B-NB	-2.49	1.34	1.37
12	a	830	CLA	C4B-NB	-2.49	1.34	1.37
12	G	840	CLA	C1B-C2B	2.49	1.49	1.43
12	a	817	CLA	C1B-C2B	2.49	1.49	1.43
12	A	832	CLA	C1C-NC	-2.49	1.34	1.37
12	a	803	CLA	C1D-ND	-2.48	1.34	1.37
12	A	813	CLA	C3B-C4B	2.48	1.50	1.42
12	B	832	CLA	C1D-C2D	2.48	1.50	1.45
12	G	806	CLA	C4B-NB	-2.48	1.34	1.37
12	H	815	CLA	C4B-NB	-2.48	1.34	1.37
12	b	802	CLA	C3D-C2D	2.48	1.45	1.39
12	a	815	CLA	C1D-C2D	2.48	1.50	1.45
12	a	854	CLA	C1C-NC	-2.48	1.34	1.37
12	G	818	CLA	C3D-C2D	2.48	1.45	1.39
12	A	819	CLA	C1D-C2D	2.48	1.50	1.45
12	G	805	CLA	C1B-C2B	2.48	1.48	1.43
12	A	830	CLA	C1C-NC	-2.48	1.34	1.37
12	b	830	CLA	C1B-C2B	2.48	1.48	1.43
12	b	834	CLA	C3D-C2D	2.48	1.45	1.39
12	B	802	CLA	C3D-C2D	2.48	1.45	1.39
12	a	817	CLA	C4C-C3C	2.48	1.49	1.45
12	H	835	CLA	C4B-NB	-2.48	1.34	1.37
12	b	819	CLA	C1C-NC	-2.48	1.34	1.37
12	F	203	CLA	C1B-NB	-2.48	1.34	1.37
12	A	817	CLA	C1B-C2B	2.48	1.48	1.43
13	H	840	1L3	C03-C04	2.48	1.53	1.47
12	A	815	CLA	C1C-NC	-2.48	1.34	1.37
12	A	823	CLA	C4B-NB	-2.47	1.34	1.37
12	B	813	CLA	C1C-NC	-2.47	1.34	1.37
12	G	804	CLA	C1B-C2B	2.47	1.48	1.43
12	b	824	CLA	C3D-C2D	2.47	1.45	1.39
12	P	203	CLA	C1D-C2D	2.47	1.50	1.45
12	j	104	CLA	C1D-C2D	2.47	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	834	CLA	C3B-C4B	2.47	1.49	1.42
12	G	812	CLA	C1C-NC	-2.47	1.34	1.37
12	G	824	CLA	C1C-NC	-2.47	1.34	1.37
12	H	824	CLA	C4B-NB	-2.47	1.34	1.37
12	A	805	CLA	C4B-NB	-2.47	1.34	1.37
12	A	824	CLA	C1C-NC	-2.47	1.34	1.37
12	a	836	CLA	C3D-C2D	2.47	1.45	1.39
12	H	830	CLA	C1D-C2D	2.47	1.50	1.45
12	H	833	CLA	C4C-C3C	2.47	1.49	1.45
12	G	814	CLA	MG-NC	2.47	2.12	2.06
12	b	836	CLA	MG-NC	2.47	2.12	2.06
12	A	809	CLA	MG-ND	-2.47	2.00	2.05
13	G	843	1L3	C22-C21	2.47	1.56	1.50
12	A	816	CLA	C1B-NB	-2.47	1.34	1.37
12	A	809	CLA	C1D-C2D	2.46	1.50	1.45
12	B	826	CLA	C4B-NB	-2.46	1.34	1.37
12	G	818	CLA	C3B-C4B	2.46	1.49	1.42
12	A	822	CLA	C4C-C3C	2.46	1.49	1.45
12	A	803	CLA	C1B-C2B	2.46	1.48	1.43
12	b	848	CLA	C4B-NB	-2.46	1.34	1.37
12	b	828	CLA	C4B-NB	-2.46	1.34	1.37
12	f	203	CLA	C1D-C2D	2.46	1.50	1.45
12	A	809	CLA	C1B-NB	-2.46	1.34	1.37
12	B	808	CLA	C4C-C3C	2.46	1.49	1.45
12	a	836	CLA	C1B-C2B	2.46	1.48	1.43
11	A	801	CL0	C4D-CHA	2.46	1.46	1.38
12	A	830	CLA	C4B-NB	-2.46	1.34	1.37
12	a	806	CLA	MG-NC	2.46	2.12	2.06
12	b	848	CLA	C1A-CHA	2.46	1.53	1.43
12	F	203	CLA	C1D-C2D	2.46	1.50	1.45
12	A	805	CLA	C4D-CHA	2.46	1.46	1.38
19	b	846	LMT	O3'-C3'	-2.46	1.36	1.43
12	a	820	CLA	C1C-NC	-2.46	1.34	1.37
12	G	817	CLA	C1B-NB	-2.46	1.34	1.37
12	A	854	CLA	C1C-NC	-2.45	1.34	1.37
12	H	811	CLA	C1B-C2B	2.45	1.48	1.43
12	a	820	CLA	C1D-C2D	2.45	1.50	1.45
12	b	829	CLA	C1C-NC	-2.45	1.34	1.37
12	R	103	CLA	C1D-C2D	2.45	1.50	1.45
12	a	855	CLA	CMC-C2C	-2.45	1.45	1.50
12	G	806	CLA	MG-ND	-2.45	2.00	2.05
12	b	816	CLA	C1D-C2D	2.45	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	201	CLA	C1C-NC	-2.45	1.34	1.37
12	B	832	CLA	C4C-C3C	2.45	1.49	1.45
12	H	805	CLA	C1B-NB	-2.45	1.34	1.37
12	a	805	CLA	C4B-NB	-2.45	1.34	1.37
12	B	836	CLA	C3B-C4B	2.45	1.49	1.42
12	L	205	CLA	C4B-NB	-2.44	1.34	1.37
12	G	821	CLA	C4C-C3C	2.44	1.49	1.45
12	A	805	CLA	MG-ND	-2.44	2.00	2.05
12	B	835	CLA	C3B-C4B	2.44	1.49	1.42
12	G	809	CLA	C1B-C2B	2.44	1.48	1.43
12	G	831	CLA	C4B-NB	-2.44	1.34	1.37
12	B	804	CLA	C1B-C2B	2.44	1.48	1.43
12	G	836	CLA	C4C-C3C	2.44	1.49	1.45
12	G	816	CLA	C1D-C2D	2.44	1.50	1.45
12	b	828	CLA	C1C-NC	-2.44	1.34	1.37
17	T	101	45D	C40-C36	2.44	1.55	1.50
12	A	809	CLA	C1D-ND	-2.44	1.34	1.37
12	P	203	CLA	C4B-NB	-2.44	1.34	1.37
12	a	854	CLA	CHB-C1B	2.44	1.44	1.39
12	G	809	CLA	C1C-NC	-2.43	1.34	1.37
12	H	836	CLA	C3D-C2D	2.43	1.45	1.39
12	b	813	CLA	C1C-NC	-2.43	1.34	1.37
12	A	811	CLA	C1C-NC	-2.43	1.34	1.37
12	B	832	CLA	C1C-NC	-2.43	1.34	1.37
12	b	834	CLA	C1B-C2B	2.43	1.48	1.43
12	l	206	CLA	C4B-NB	-2.43	1.34	1.37
12	B	816	CLA	C1C-NC	-2.43	1.34	1.37
12	H	804	CLA	C1B-C2B	2.43	1.48	1.43
12	A	839	CLA	C1A-CHA	2.43	1.53	1.43
12	H	830	CLA	C1C-NC	-2.43	1.34	1.37
12	F	203	CLA	C4C-C3C	2.43	1.49	1.45
12	H	821	CLA	C4B-NB	-2.43	1.34	1.37
12	H	838	CLA	MG-NC	2.43	2.12	2.06
12	f	201	CLA	C1C-NC	-2.43	1.34	1.37
12	b	812	CLA	C1A-CHA	2.43	1.53	1.43
12	a	831	CLA	C1B-C2B	2.43	1.48	1.43
12	S	204	CLA	C4B-NB	-2.43	1.34	1.37
12	a	820	CLA	C4C-C3C	2.43	1.49	1.45
12	G	832	CLA	C1C-NC	-2.43	1.34	1.37
12	a	832	CLA	C1C-NC	-2.43	1.34	1.37
12	b	803	CLA	C4B-NB	-2.42	1.34	1.37
12	B	804	CLA	C1C-NC	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	808	CLA	C4C-C3C	2.42	1.49	1.45
13	b	838	1L3	C03-C04	2.42	1.53	1.47
12	A	815	CLA	C1D-C2D	2.42	1.50	1.45
12	A	804	CLA	C1C-NC	-2.42	1.34	1.37
12	G	856	CLA	MG-NC	2.42	2.12	2.06
12	H	813	CLA	C1A-CHA	2.42	1.53	1.43
13	B	839	1L3	C03-C04	2.42	1.53	1.47
12	H	809	CLA	C4C-C3C	2.42	1.49	1.45
13	B	839	1L3	O05-C04	-2.42	1.18	1.23
12	G	834	CLA	C4B-NB	-2.42	1.34	1.37
12	P	203	CLA	C4C-C3C	2.42	1.49	1.45
12	G	835	CLA	C1C-NC	-2.42	1.34	1.37
12	a	803	CLA	C1B-C2B	2.42	1.48	1.43
11	G	801	CL0	C4B-NB	-2.42	1.34	1.37
12	A	803	CLA	C1D-ND	-2.42	1.34	1.37
12	B	804	CLA	C4B-NB	-2.42	1.34	1.37
12	H	819	CLA	C1D-C2D	2.42	1.50	1.45
12	b	808	CLA	C1D-C2D	2.42	1.50	1.45
12	A	813	CLA	C1C-NC	-2.41	1.34	1.37
12	a	831	CLA	C1D-C2D	2.41	1.50	1.45
12	G	842	CLA	C4B-NB	-2.41	1.34	1.37
12	H	850	CLA	C4B-NB	-2.41	1.34	1.37
12	a	811	CLA	C1C-NC	-2.41	1.34	1.37
13	G	843	1L3	C18-C16	2.41	1.56	1.51
12	B	816	CLA	C4C-C3C	2.41	1.49	1.45
12	B	808	CLA	C1D-C2D	2.41	1.50	1.45
12	a	805	CLA	C4D-CHA	2.41	1.46	1.38
11	A	801	CL0	C3D-C2D	2.41	1.45	1.39
12	b	823	CLA	C1B-C2B	2.41	1.48	1.43
12	H	814	CLA	C1C-NC	-2.41	1.34	1.37
12	b	821	CLA	C4B-NB	-2.41	1.34	1.37
12	b	823	CLA	C4B-NB	-2.41	1.34	1.37
12	B	828	CLA	C4C-C3C	2.41	1.49	1.45
13	A	842	1L3	C22-C21	2.41	1.56	1.50
12	A	817	CLA	C1C-NC	-2.41	1.34	1.37
12	A	836	CLA	C3D-C2D	2.41	1.45	1.39
12	H	803	CLA	C4B-NB	-2.41	1.34	1.37
12	H	829	CLA	C4B-NB	-2.41	1.34	1.37
17	m	101	45D	C40-C36	2.40	1.55	1.50
12	b	804	CLA	C1C-NC	-2.40	1.34	1.37
13	b	838	1L3	O13-C12	-2.40	1.18	1.23
12	B	829	CLA	C1D-C2D	2.40	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	833	CLA	C1B-C2B	2.40	1.48	1.43
12	a	807	CLA	C1A-CHA	2.40	1.53	1.43
12	a	809	CLA	C1C-NC	-2.40	1.34	1.37
12	a	830	CLA	C1B-C2B	2.40	1.48	1.43
12	H	802	CLA	C1C-NC	-2.40	1.34	1.37
12	a	830	CLA	C1C-NC	-2.40	1.34	1.37
12	H	828	CLA	C1B-C2B	2.40	1.48	1.43
12	B	816	CLA	C1D-C2D	2.40	1.50	1.45
12	A	820	CLA	C1D-ND	-2.40	1.34	1.37
12	B	823	CLA	C4B-NB	-2.39	1.34	1.37
12	A	827	CLA	MG-NC	2.39	2.12	2.06
12	a	807	CLA	C1C-NC	-2.39	1.34	1.37
12	b	806	CLA	MG-NC	2.39	2.12	2.06
12	B	828	CLA	C4B-NB	-2.39	1.34	1.37
12	H	817	CLA	C1D-C2D	2.39	1.50	1.45
12	A	836	CLA	C1B-C2B	2.39	1.48	1.43
12	H	813	CLA	C4B-NB	-2.39	1.34	1.37
12	A	806	CLA	MG-NC	2.39	2.11	2.06
12	b	801	CLA	C1A-CHA	2.39	1.52	1.43
12	G	836	CLA	C1C-NC	-2.39	1.34	1.37
17	M	101	45D	C40-C36	2.39	1.55	1.50
12	B	804	CLA	MG-NC	2.38	2.11	2.06
12	G	807	CLA	C1C-NC	-2.38	1.34	1.37
12	a	831	CLA	C4C-C3C	2.38	1.49	1.45
12	G	832	CLA	C4B-NB	-2.38	1.34	1.37
12	b	827	CLA	C4C-C3C	2.38	1.49	1.45
12	G	807	CLA	MG-NC	2.38	2.11	2.06
12	b	816	CLA	C4C-C3C	2.38	1.49	1.45
12	b	835	CLA	C3D-C2D	2.38	1.45	1.39
12	G	813	CLA	C4C-C3C	2.38	1.49	1.45
12	B	836	CLA	CHB-C4A	-2.38	1.31	1.37
12	G	838	CLA	C1B-C2B	2.38	1.48	1.43
13	a	842	1L3	C22-C21	2.38	1.56	1.50
12	B	819	CLA	C1C-NC	-2.38	1.34	1.37
12	b	829	CLA	C1D-C2D	2.38	1.50	1.45
12	a	825	CLA	C4B-NB	-2.38	1.34	1.37
12	B	801	CLA	C1A-CHA	2.38	1.52	1.43
12	H	828	CLA	C4C-C3C	2.38	1.49	1.45
12	H	806	CLA	C1B-C2B	2.38	1.48	1.43
12	J	103	CLA	C1D-C2D	2.38	1.50	1.45
12	B	806	CLA	MG-NC	2.37	2.11	2.06
12	G	839	CLA	C1A-CHA	2.37	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	836	CLA	C3D-C2D	2.37	1.45	1.39
12	a	823	CLA	C1A-CHA	2.37	1.52	1.43
12	A	835	CLA	C1A-CHA	2.37	1.52	1.43
12	a	836	CLA	C1D-C2D	2.37	1.50	1.45
12	H	803	CLA	C1B-C2B	2.37	1.48	1.43
12	H	837	CLA	C3B-C4B	2.37	1.49	1.42
11	A	801	CL0	C4B-NB	-2.37	1.34	1.37
12	A	834	CLA	C3B-C4B	2.37	1.49	1.42
12	B	830	CLA	C4B-NB	-2.37	1.34	1.37
12	A	823	CLA	C1A-CHA	2.37	1.52	1.43
12	a	803	CLA	C1D-C2D	2.37	1.50	1.45
12	b	822	CLA	C1B-C2B	2.37	1.48	1.43
12	B	805	CLA	C4B-NB	-2.37	1.34	1.37
12	H	813	CLA	C1C-NC	-2.37	1.34	1.37
12	G	818	CLA	C1B-NB	-2.37	1.34	1.37
12	a	822	CLA	C1C-NC	-2.37	1.34	1.37
12	A	817	CLA	C4C-C3C	2.37	1.49	1.45
12	H	836	CLA	C1B-C2B	2.37	1.48	1.43
12	A	836	CLA	OBD-CAD	2.37	1.26	1.22
12	A	828	CLA	C1B-C2B	2.37	1.48	1.43
12	G	825	CLA	C1C-NC	-2.36	1.34	1.37
12	H	804	CLA	C4B-NB	-2.36	1.34	1.37
12	B	827	CLA	C1B-C2B	2.36	1.48	1.43
12	A	803	CLA	C1D-C2D	2.36	1.50	1.45
12	b	816	CLA	C1C-NC	-2.36	1.34	1.37
12	H	830	CLA	C4C-C3C	2.36	1.49	1.45
12	b	814	CLA	C1D-C2D	2.36	1.50	1.45
12	b	804	CLA	C4B-NB	-2.36	1.34	1.37
12	H	823	CLA	C1B-C2B	2.36	1.48	1.43
12	G	841	CLA	C4C-C3C	2.36	1.49	1.45
12	H	831	CLA	C1A-CHA	2.36	1.52	1.43
12	a	835	CLA	C1A-CHA	2.36	1.52	1.43
12	G	855	CLA	C1C-C2C	2.36	1.49	1.44
12	b	815	CLA	MG-NC	2.36	2.11	2.06
12	H	809	CLA	C1D-C2D	2.36	1.50	1.45
12	B	818	CLA	C1D-C2D	2.36	1.50	1.45
12	G	839	CLA	C4C-C3C	2.35	1.49	1.45
12	b	812	CLA	C4C-C3C	2.35	1.49	1.45
12	b	818	CLA	C4C-C3C	2.35	1.49	1.45
12	a	818	CLA	MG-ND	-2.35	2.01	2.05
12	A	855	CLA	CMC-C2C	-2.35	1.45	1.50
12	B	815	CLA	C1D-C2D	2.35	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	820	CLA	C1C-NC	-2.35	1.34	1.37
12	G	837	CLA	C1D-C2D	2.35	1.50	1.45
12	H	810	CLA	C1D-C2D	2.35	1.50	1.45
12	G	806	CLA	MG-NC	2.35	2.11	2.06
12	a	812	CLA	C1D-C2D	2.35	1.50	1.45
12	G	824	CLA	C4B-NB	-2.35	1.34	1.37
12	A	832	CLA	C4B-NB	-2.35	1.34	1.37
12	a	854	CLA	C1C-C2C	2.35	1.49	1.44
12	G	814	CLA	C1D-C2D	2.35	1.50	1.45
12	G	810	CLA	C1D-C2D	2.35	1.50	1.45
12	G	835	CLA	C1A-CHA	2.35	1.52	1.43
12	b	805	CLA	C4B-NB	-2.35	1.34	1.37
12	B	823	CLA	C1B-C2B	2.35	1.48	1.43
12	A	835	CLA	C1C-NC	-2.35	1.34	1.37
12	H	806	CLA	MG-ND	-2.35	2.01	2.05
12	b	827	CLA	C1C-NC	-2.35	1.34	1.37
12	a	826	CLA	C3B-C4B	2.35	1.49	1.42
12	A	841	CLA	C4C-C3C	2.34	1.49	1.45
12	H	820	CLA	C1D-C2D	2.34	1.50	1.45
12	A	854	CLA	CHB-C4A	-2.34	1.31	1.37
12	G	805	CLA	C4B-NB	-2.34	1.34	1.37
12	G	813	CLA	C1A-CHA	2.34	1.52	1.43
12	a	815	CLA	C1C-NC	-2.34	1.34	1.37
12	A	809	CLA	C4B-NB	-2.34	1.34	1.37
12	H	801	CLA	C1B-C2B	2.34	1.48	1.43
12	G	827	CLA	C1A-CHA	2.34	1.52	1.43
12	A	826	CLA	C1A-CHA	2.34	1.52	1.43
12	a	806	CLA	C4B-NB	-2.34	1.34	1.37
12	A	822	CLA	C1C-NC	-2.34	1.34	1.37
12	a	836	CLA	C1C-NC	-2.34	1.34	1.37
12	a	825	CLA	C1B-C2B	2.34	1.48	1.43
12	G	834	CLA	C3B-C4B	2.34	1.49	1.42
19	b	846	LMT	O2'-C2'	-2.34	1.37	1.43
12	b	831	CLA	C1C-NC	-2.34	1.34	1.37
12	b	815	CLA	C1B-C2B	2.34	1.48	1.43
12	A	822	CLA	C4B-NB	-2.33	1.34	1.37
12	j	104	CLA	C1B-C2B	2.33	1.48	1.43
12	b	835	CLA	CHB-C4A	-2.33	1.31	1.37
12	A	821	CLA	C1A-CHA	2.33	1.52	1.43
12	H	825	CLA	C1B-C2B	2.33	1.48	1.43
12	b	818	CLA	C1D-C2D	2.33	1.50	1.45
12	G	823	CLA	C4C-C3C	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	815	CLA	C4B-NB	-2.33	1.34	1.37
12	G	821	CLA	C1D-C2D	2.33	1.49	1.45
12	b	835	CLA	C3B-C4B	2.33	1.49	1.42
12	B	812	CLA	C1A-CHA	2.33	1.52	1.43
12	a	822	CLA	C4C-C3C	2.33	1.49	1.45
12	H	833	CLA	C4B-NB	-2.33	1.34	1.37
12	A	812	CLA	C1A-CHA	2.33	1.52	1.43
12	b	819	CLA	C1D-C2D	2.33	1.49	1.45
12	a	821	CLA	C1A-CHA	2.33	1.52	1.43
12	G	822	CLA	C4C-C3C	2.33	1.49	1.45
12	H	834	CLA	C1A-CHA	2.33	1.52	1.43
12	a	804	CLA	C1C-NC	-2.33	1.34	1.37
12	b	809	CLA	C1A-CHA	2.33	1.52	1.43
12	b	826	CLA	CMB-C2B	-2.33	1.46	1.50
12	A	806	CLA	C4B-NB	-2.32	1.34	1.37
12	a	837	CLA	C1D-C2D	2.32	1.49	1.45
12	G	831	CLA	C1C-NC	-2.32	1.34	1.37
12	a	832	CLA	C4B-NB	-2.32	1.34	1.37
12	b	820	CLA	C4B-NB	-2.32	1.34	1.37
12	a	826	CLA	C1A-CHA	2.32	1.52	1.43
12	H	818	CLA	C1A-CHA	2.32	1.52	1.43
12	H	802	CLA	C1C-C2C	2.32	1.49	1.44
12	a	855	CLA	C1A-CHA	2.32	1.52	1.43
12	A	807	CLA	C1A-CHA	2.32	1.52	1.43
12	H	806	CLA	MG-NC	2.32	2.11	2.06
12	G	814	CLA	C4C-C3C	2.32	1.49	1.45
12	A	820	CLA	C1A-CHA	2.32	1.52	1.43
12	A	838	CLA	C1B-C2B	2.32	1.48	1.43
12	B	820	CLA	C4B-NB	-2.32	1.34	1.37
12	B	817	CLA	C1C-NC	-2.32	1.34	1.37
12	B	832	CLA	C4B-NB	-2.32	1.34	1.37
12	a	855	CLA	C1B-C2B	2.32	1.48	1.43
12	l	204	CLA	C1A-CHA	2.32	1.52	1.43
12	f	203	CLA	C3B-C4B	2.32	1.49	1.42
12	a	812	CLA	C1A-CHA	2.32	1.52	1.43
12	H	804	CLA	C1C-NC	-2.32	1.34	1.37
12	G	820	CLA	C1D-C2D	2.32	1.49	1.45
12	G	823	CLA	C1D-C2D	2.32	1.49	1.45
12	G	810	CLA	C1A-CHA	2.32	1.52	1.43
12	b	832	CLA	C4C-C3C	2.31	1.49	1.45
12	b	828	CLA	C1A-CHA	2.31	1.52	1.43
12	B	817	CLA	C1A-CHA	2.31	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	811	CLA	C1A-CHA	2.31	1.52	1.43
12	B	809	CLA	C1A-CHA	2.31	1.52	1.43
12	H	824	CLA	C1B-C2B	2.31	1.48	1.43
12	B	819	CLA	C1D-C2D	2.31	1.49	1.45
17	T	101	45D	C28-C26	2.31	1.55	1.50
17	m	101	45D	C28-C26	2.31	1.55	1.50
12	a	818	CLA	C1A-CHA	2.31	1.52	1.43
12	G	836	CLA	OBD-CAD	2.31	1.26	1.22
12	G	832	CLA	C1D-C2D	2.31	1.49	1.45
17	M	101	45D	C28-C26	2.31	1.55	1.50
12	b	815	CLA	C1D-ND	-2.31	1.34	1.37
12	b	831	CLA	C4B-NB	-2.31	1.34	1.37
12	A	837	CLA	C4B-NB	-2.31	1.34	1.37
13	a	842	1L3	C03-C04	2.31	1.52	1.47
12	A	837	CLA	C1D-C2D	2.31	1.49	1.45
12	B	824	CLA	C1B-C2B	2.31	1.48	1.43
12	H	807	CLA	C1B-C2B	2.31	1.48	1.43
12	A	820	CLA	C1D-C2D	2.31	1.49	1.45
12	H	818	CLA	C1C-NC	-2.31	1.34	1.37
12	a	839	CLA	C1A-CHA	2.31	1.52	1.43
12	a	837	CLA	C4B-NB	-2.30	1.34	1.37
11	a	801	CL0	C4D-CHA	2.30	1.46	1.38
12	H	837	CLA	C4C-C3C	2.30	1.48	1.45
12	a	839	CLA	C4C-C3C	2.30	1.48	1.45
12	G	842	CLA	C1A-CHA	2.30	1.52	1.43
12	a	839	CLA	C1D-C2D	2.30	1.49	1.45
12	B	828	CLA	C1A-CHA	2.30	1.52	1.43
12	G	821	CLA	C4B-NB	-2.30	1.34	1.37
12	H	805	CLA	C3B-C4B	2.30	1.49	1.42
12	G	822	CLA	C1A-CHA	2.30	1.52	1.43
12	A	818	CLA	C1A-CHA	2.30	1.52	1.43
12	a	835	CLA	C4B-NB	-2.30	1.34	1.37
12	G	816	CLA	C1C-NC	-2.30	1.34	1.37
12	G	802	CLA	MG-NC	2.30	2.11	2.06
12	b	817	CLA	C1A-CHA	2.30	1.52	1.43
12	G	824	CLA	C1A-CHA	2.30	1.52	1.43
12	a	854	CLA	CHB-C4A	-2.30	1.31	1.37
12	a	803	CLA	C4C-C3C	2.30	1.48	1.45
12	B	818	CLA	C4C-C3C	2.30	1.48	1.45
12	G	824	CLA	C1D-C2D	2.30	1.49	1.45
12	A	830	CLA	C1B-C2B	2.30	1.48	1.43
12	b	832	CLA	C4B-NB	-2.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	813	CLA	C4B-NB	-2.29	1.34	1.37
12	b	836	CLA	C1A-CHA	2.29	1.52	1.43
12	a	828	CLA	C1B-C2B	2.29	1.48	1.43
12	a	833	CLA	C4C-C3C	2.29	1.48	1.45
12	H	819	CLA	C4B-NB	-2.29	1.34	1.37
12	B	807	CLA	C1A-CHA	2.29	1.52	1.43
12	G	808	CLA	C1A-CHA	2.29	1.52	1.43
13	a	842	1L3	C18-C16	2.29	1.56	1.51
12	H	815	CLA	C1B-C2B	2.29	1.48	1.43
12	B	815	CLA	C1B-NB	-2.29	1.34	1.37
12	A	804	CLA	C1A-CHA	2.29	1.52	1.43
12	H	817	CLA	C3B-C4B	2.29	1.49	1.42
12	G	823	CLA	C1C-NC	-2.29	1.34	1.37
12	H	829	CLA	C4C-C3C	2.29	1.48	1.45
12	b	827	CLA	C1B-C2B	2.29	1.48	1.43
12	G	856	CLA	C1B-C2B	2.29	1.48	1.43
12	b	802	CLA	MG-NC	2.29	2.11	2.06
12	B	814	CLA	C4B-NB	-2.29	1.34	1.37
12	l	205	CLA	C1A-CHA	2.29	1.52	1.43
12	a	813	CLA	C1D-C2D	2.29	1.49	1.45
12	H	819	CLA	C1C-NC	-2.29	1.34	1.37
12	a	855	CLA	MG-NC	2.29	2.11	2.06
12	G	816	CLA	C4C-C3C	2.29	1.48	1.45
12	a	811	CLA	C4C-C3C	2.29	1.48	1.45
12	H	826	CLA	CMD-C2D	-2.29	1.46	1.50
12	A	831	CLA	OBD-CAD	2.28	1.26	1.22
12	H	829	CLA	C1A-CHA	2.28	1.52	1.43
12	b	824	CLA	C1A-CHA	2.28	1.52	1.43
12	a	826	CLA	C1C-C2C	2.28	1.49	1.44
12	A	815	CLA	C4C-C3C	2.28	1.48	1.45
12	G	812	CLA	C1A-CHA	2.28	1.52	1.43
12	B	835	CLA	C1B-C2B	2.28	1.48	1.43
12	A	830	CLA	C1C-C2C	2.28	1.49	1.44
12	a	816	CLA	C4C-C3C	2.28	1.48	1.45
12	S	202	CLA	C1A-CHA	2.28	1.52	1.43
12	A	812	CLA	C1D-C2D	2.28	1.49	1.45
12	H	816	CLA	MG-NC	2.28	2.11	2.06
12	B	837	CLA	C1A-CHA	2.28	1.52	1.43
12	L	204	CLA	C1A-CHA	2.28	1.52	1.43
11	A	801	CL0	CMD-C2D	-2.28	1.46	1.50
12	B	831	CLA	C1A-CHA	2.28	1.52	1.43
12	H	850	CLA	C1A-CHA	2.28	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	838	CLA	C1A-CHA	2.28	1.52	1.43
12	G	807	CLA	C4B-NB	-2.28	1.34	1.37
12	b	825	CLA	C3B-C4B	2.28	1.49	1.42
12	G	829	CLA	C1B-C2B	2.28	1.48	1.43
12	A	839	CLA	C1D-C2D	2.27	1.49	1.45
12	B	821	CLA	C4B-NB	-2.27	1.34	1.37
12	A	837	CLA	C3B-C4B	2.27	1.49	1.42
12	B	833	CLA	C1A-CHA	2.27	1.52	1.43
12	b	828	CLA	C4C-C3C	2.27	1.48	1.45
12	a	804	CLA	C1D-C2D	2.27	1.49	1.45
12	a	804	CLA	C4C-C3C	2.27	1.48	1.45
12	a	821	CLA	C4C-C3C	2.27	1.48	1.45
12	G	805	CLA	C1C-NC	-2.27	1.34	1.37
12	b	819	CLA	C4B-NB	-2.27	1.34	1.37
12	G	806	CLA	C3A-C2A	-2.27	1.48	1.54
12	b	801	CLA	CHB-C4A	-2.27	1.32	1.37
12	a	822	CLA	C1D-C2D	2.27	1.49	1.45
12	H	805	CLA	C1D-C2D	2.27	1.49	1.45
12	a	830	CLA	C1C-C2C	2.27	1.49	1.44
12	a	810	CLA	C4B-NB	-2.27	1.34	1.37
12	A	828	CLA	C1A-CHA	2.27	1.52	1.43
12	a	834	CLA	C3B-C4B	2.27	1.49	1.42
12	a	819	CLA	C4B-NB	-2.27	1.34	1.37
12	A	855	CLA	C1B-C2B	2.27	1.48	1.43
12	a	804	CLA	C1A-CHA	2.27	1.52	1.43
12	b	807	CLA	C1A-CHA	2.26	1.52	1.43
12	B	809	CLA	C1D-C2D	2.26	1.49	1.45
12	H	820	CLA	C4C-C3C	2.26	1.48	1.45
12	A	855	CLA	C1A-CHA	2.26	1.52	1.43
12	a	838	CLA	C1B-C2B	2.26	1.48	1.43
12	H	839	CLA	C3B-C4B	2.26	1.49	1.42
12	a	821	CLA	C1C-NC	-2.26	1.34	1.37
12	G	837	CLA	C3B-C4B	2.26	1.49	1.42
12	A	854	CLA	CHB-C1B	2.26	1.44	1.39
12	A	841	CLA	C4B-NB	-2.26	1.34	1.37
13	A	842	1L3	C03-C04	2.26	1.52	1.47
12	G	838	CLA	C4C-C3C	2.26	1.48	1.45
12	b	817	CLA	C1C-NC	-2.26	1.34	1.37
12	B	826	CLA	C3D-C2D	2.26	1.45	1.39
12	G	831	CLA	C1C-C2C	2.26	1.49	1.44
12	H	827	CLA	CMB-C2B	-2.26	1.46	1.50
12	b	809	CLA	C1D-C2D	2.26	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	826	CLA	C3D-C2D	2.25	1.45	1.39
12	B	807	CLA	C1B-C2B	2.25	1.48	1.43
12	H	815	CLA	C1D-C2D	2.25	1.49	1.45
12	b	823	CLA	C1A-CHA	2.25	1.52	1.43
12	B	810	CLA	C1A-CHA	2.25	1.52	1.43
12	B	818	CLA	C1C-NC	-2.25	1.34	1.37
12	H	820	CLA	C4B-NB	-2.25	1.34	1.37
12	a	813	CLA	C4B-NB	-2.25	1.34	1.37
12	J	103	CLA	C1A-CHA	2.25	1.52	1.43
12	B	835	CLA	C4B-NB	-2.25	1.34	1.37
12	B	826	CLA	CMD-C2D	-2.25	1.46	1.50
12	B	801	CLA	CHB-C4A	-2.25	1.32	1.37
12	A	831	CLA	C1B-C2B	2.25	1.48	1.43
12	S	203	CLA	C1A-CHA	2.25	1.52	1.43
12	b	820	CLA	C3B-C4B	2.25	1.49	1.42
12	G	815	CLA	C1A-CHA	2.25	1.52	1.43
12	G	835	CLA	C4C-C3C	2.25	1.48	1.45
12	G	826	CLA	C1B-C2B	2.25	1.48	1.43
12	j	104	CLA	C4C-C3C	2.25	1.48	1.45
12	G	837	CLA	C4B-NB	-2.25	1.34	1.37
12	F	203	CLA	C3B-C4B	2.25	1.49	1.42
13	H	840	1L3	O05-C04	-2.25	1.18	1.23
12	b	816	CLA	C1B-C2B	2.25	1.48	1.43
12	A	810	CLA	C1D-C2D	2.25	1.49	1.45
12	b	816	CLA	C4B-NB	-2.25	1.34	1.37
12	A	811	CLA	C4B-NB	-2.25	1.34	1.37
12	a	811	CLA	C4B-NB	-2.25	1.34	1.37
12	a	819	CLA	C1D-C2D	2.25	1.49	1.45
12	a	818	CLA	C1D-C2D	2.25	1.49	1.45
12	B	835	CLA	C1D-C2D	2.25	1.49	1.45
19	B	847	LMT	O2'-C2'	-2.25	1.37	1.43
12	b	835	CLA	C4C-C3C	2.24	1.48	1.45
12	b	818	CLA	C4B-NB	-2.24	1.34	1.37
12	b	824	CLA	CHC-C4B	2.24	1.44	1.39
12	L	205	CLA	C1A-CHA	2.24	1.52	1.43
12	A	832	CLA	C1D-C2D	2.24	1.49	1.45
12	H	817	CLA	C4C-C3C	2.24	1.48	1.45
12	G	812	CLA	C4B-NB	-2.24	1.34	1.37
12	H	812	CLA	C4C-C3C	2.24	1.48	1.45
12	H	819	CLA	C1A-CHA	2.24	1.52	1.43
13	B	839	1L3	O13-C12	-2.24	1.18	1.23
12	a	837	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	811	CLA	C4C-C3C	2.24	1.48	1.45
12	H	832	CLA	C1A-CHA	2.24	1.52	1.43
12	a	840	CLA	C1A-CHA	2.24	1.52	1.43
12	b	801	CLA	MG-NC	2.24	2.11	2.06
12	b	830	CLA	C4C-C3C	2.24	1.48	1.45
12	G	833	CLA	C1B-C2B	2.24	1.48	1.43
12	G	802	CLA	C1A-CHA	2.24	1.52	1.43
12	B	805	CLA	C3B-C4B	2.24	1.49	1.42
12	a	809	CLA	C1D-C2D	2.24	1.49	1.45
12	H	807	CLA	C1A-CHA	2.24	1.52	1.43
12	b	818	CLA	C1A-CHA	2.24	1.52	1.43
12	a	813	CLA	C1A-CHA	2.24	1.52	1.43
12	A	808	CLA	C1A-CHA	2.24	1.52	1.43
12	A	839	CLA	C4C-C3C	2.24	1.48	1.45
12	G	831	CLA	C1B-C2B	2.24	1.48	1.43
12	G	805	CLA	C1A-CHA	2.24	1.52	1.43
12	G	802	CLA	CHB-C4A	-2.24	1.32	1.37
12	G	839	CLA	C1D-C2D	2.23	1.49	1.45
12	a	822	CLA	C1A-CHA	2.23	1.52	1.43
12	b	818	CLA	C1C-NC	-2.23	1.34	1.37
12	a	815	CLA	C4C-C3C	2.23	1.48	1.45
12	a	829	CLA	C1B-C2B	2.23	1.48	1.43
12	b	830	CLA	C1A-CHA	2.23	1.52	1.43
12	b	816	CLA	C1A-CHA	2.23	1.52	1.43
12	B	825	CLA	C3B-C4B	2.23	1.49	1.42
12	b	810	CLA	C1A-CHA	2.23	1.52	1.43
12	G	836	CLA	C1B-C2B	2.23	1.48	1.43
12	a	830	CLA	C3D-C2D	2.23	1.45	1.39
12	A	809	CLA	C1A-CHA	2.23	1.52	1.43
12	R	103	CLA	C4C-C3C	2.23	1.48	1.45
12	A	825	CLA	C1B-C2B	2.23	1.48	1.43
12	A	855	CLA	MG-NC	2.23	2.11	2.06
12	A	819	CLA	C4B-NB	-2.23	1.34	1.37
12	A	803	CLA	C4C-C3C	2.23	1.48	1.45
12	G	816	CLA	C1A-CHA	2.23	1.52	1.43
12	H	810	CLA	C1A-CHA	2.23	1.52	1.43
12	B	819	CLA	C4C-C3C	2.23	1.48	1.45
12	b	819	CLA	C4C-C3C	2.22	1.48	1.45
12	B	813	CLA	C1D-C2D	2.22	1.49	1.45
12	a	836	CLA	C1A-CHA	2.22	1.52	1.43
12	G	811	CLA	C4B-NB	-2.22	1.34	1.37
12	G	811	CLA	C1D-C2D	2.22	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	848	LMT	O2'-C2'	-2.22	1.37	1.43
12	H	807	CLA	C4C-C3C	2.22	1.48	1.45
12	a	809	CLA	C1A-CHA	2.22	1.52	1.43
12	B	820	CLA	C3B-C4B	2.22	1.49	1.42
12	G	856	CLA	CMC-C2C	-2.22	1.46	1.50
12	B	818	CLA	C1A-CHA	2.22	1.52	1.43
12	A	810	CLA	C4B-NB	-2.22	1.34	1.37
12	B	834	CLA	C4B-NB	-2.22	1.34	1.37
12	H	813	CLA	C1D-C2D	2.22	1.49	1.45
12	G	836	CLA	C3D-C2D	2.22	1.45	1.39
12	H	814	CLA	C3B-C4B	2.22	1.49	1.42
12	G	820	CLA	C4B-NB	-2.22	1.35	1.37
12	H	814	CLA	C1D-C2D	2.22	1.49	1.45
12	f	201	CLA	C4C-C3C	2.21	1.48	1.45
12	b	837	CLA	C3B-C4B	2.21	1.49	1.42
12	G	835	CLA	C1D-C2D	2.21	1.49	1.45
12	A	805	CLA	C3B-C4B	2.21	1.49	1.42
12	H	821	CLA	C3B-C4B	2.21	1.49	1.42
12	A	823	CLA	C1D-C2D	2.21	1.49	1.45
12	a	814	CLA	C1A-CHA	2.21	1.52	1.43
12	j	104	CLA	C1A-CHA	2.21	1.52	1.43
12	G	835	CLA	C4B-NB	-2.21	1.35	1.37
12	a	818	CLA	C4C-C3C	2.21	1.48	1.45
12	A	804	CLA	C1D-C2D	2.21	1.49	1.45
12	A	832	CLA	C1B-C2B	2.21	1.48	1.43
13	A	842	1L3	C18-C16	2.21	1.55	1.51
12	H	816	CLA	C4C-C3C	2.21	1.48	1.45
12	a	831	CLA	C1A-CHA	2.21	1.52	1.43
12	A	821	CLA	C1C-NC	-2.21	1.34	1.37
12	a	807	CLA	C4C-C3C	2.21	1.48	1.45
12	H	837	CLA	CHB-C4A	-2.21	1.32	1.37
12	H	818	CLA	C4B-NB	-2.21	1.35	1.37
12	A	814	CLA	C1A-CHA	2.21	1.52	1.43
13	H	840	1L3	O13-C12	-2.21	1.18	1.23
12	G	826	CLA	OBD-CAD	2.21	1.26	1.22
12	A	829	CLA	C1B-C2B	2.21	1.48	1.43
12	B	826	CLA	CMB-C2B	-2.21	1.46	1.50
12	b	814	CLA	C4B-NB	-2.20	1.35	1.37
12	A	802	CLA	CBD-CAD	-2.20	1.46	1.56
12	a	815	CLA	C1A-CHA	2.20	1.52	1.43
12	B	818	CLA	C4B-NB	-2.20	1.35	1.37
12	b	832	CLA	C1A-CHA	2.20	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	834	CLA	C1A-CHA	2.20	1.52	1.43
12	A	837	CLA	C1A-CHA	2.20	1.52	1.43
12	P	201	CLA	C1A-CHA	2.20	1.52	1.43
12	H	805	CLA	C4C-C3C	2.20	1.48	1.45
12	G	810	CLA	C4B-NB	-2.20	1.35	1.37
12	b	825	CLA	C4B-NB	-2.20	1.35	1.37
12	a	821	CLA	C4B-NB	-2.20	1.35	1.37
12	A	807	CLA	C3B-C4B	2.20	1.49	1.42
12	A	816	CLA	C4C-C3C	2.20	1.48	1.45
12	B	814	CLA	C1B-C2B	2.20	1.48	1.43
12	B	838	CLA	C3B-C4B	2.20	1.49	1.42
12	G	815	CLA	C4C-C3C	2.20	1.48	1.45
12	b	820	CLA	C1A-CHA	2.20	1.52	1.43
13	G	843	1L3	O13-C12	-2.20	1.18	1.23
12	J	103	CLA	C4C-C3C	2.20	1.48	1.45
12	a	825	CLA	C1A-CHA	2.20	1.52	1.43
12	b	815	CLA	C1A-CHA	2.20	1.52	1.43
12	H	803	CLA	C3B-C4B	2.20	1.49	1.42
12	B	813	CLA	C3B-C4B	2.20	1.49	1.42
12	G	814	CLA	C1A-CHA	2.19	1.52	1.43
12	a	835	CLA	C1D-C2D	2.19	1.49	1.45
12	H	820	CLA	C1A-CHA	2.19	1.52	1.43
12	G	810	CLA	C4C-C3C	2.19	1.48	1.45
12	A	822	CLA	C1D-C2D	2.19	1.49	1.45
12	B	816	CLA	C4B-NB	-2.19	1.35	1.37
12	b	805	CLA	C3B-C4B	2.19	1.49	1.42
12	G	819	CLA	C1A-CHA	2.19	1.52	1.43
12	B	824	CLA	C1A-CHA	2.19	1.52	1.43
12	B	815	CLA	C1B-C2B	2.19	1.48	1.43
12	H	801	CLA	C4C-C3C	2.19	1.48	1.45
12	a	808	CLA	C1A-CHA	2.19	1.52	1.43
12	R	103	CLA	C1C-NC	-2.19	1.34	1.37
12	B	830	CLA	C1A-CHA	2.19	1.52	1.43
12	R	103	CLA	C4B-NB	-2.19	1.35	1.37
12	A	827	CLA	C1A-CHA	2.19	1.52	1.43
13	b	838	1L3	C18-C16	2.19	1.55	1.51
12	G	830	CLA	C4C-C3C	2.19	1.48	1.45
12	B	803	CLA	C4C-C3C	2.19	1.48	1.45
13	G	843	1L3	O05-C04	-2.19	1.18	1.23
12	A	804	CLA	C4C-C3C	2.19	1.48	1.45
12	a	811	CLA	C1A-CHA	2.19	1.52	1.43
12	H	816	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	815	CLA	C3B-C4B	2.19	1.49	1.42
12	b	834	CLA	C1D-C2D	2.18	1.49	1.45
12	B	819	CLA	C4B-NB	-2.18	1.35	1.37
12	A	809	CLA	C4C-C3C	2.18	1.48	1.45
12	G	855	CLA	CHB-C4A	-2.18	1.32	1.37
12	b	811	CLA	C1D-C2D	2.18	1.49	1.45
12	G	856	CLA	C1A-CHA	2.18	1.52	1.43
12	H	814	CLA	C4B-NB	-2.18	1.35	1.37
12	G	840	CLA	C3B-C4B	2.18	1.49	1.42
12	H	809	CLA	C1A-CHA	2.18	1.52	1.43
12	A	821	CLA	C4B-NB	-2.18	1.35	1.37
12	G	817	CLA	C1D-C2D	2.18	1.49	1.45
12	H	827	CLA	C1D-C2D	2.18	1.49	1.45
12	b	837	CLA	C1A-CHA	2.18	1.52	1.43
12	G	812	CLA	C4C-C3C	2.18	1.48	1.45
12	A	840	CLA	C1A-CHA	2.18	1.52	1.43
12	A	840	CLA	C1B-C2B	2.18	1.48	1.43
12	G	823	CLA	C1A-CHA	2.18	1.52	1.43
12	B	801	CLA	MG-NC	2.18	2.11	2.06
12	H	838	CLA	C3B-C4B	2.18	1.49	1.42
12	b	824	CLA	O2D-CED	-2.18	1.40	1.45
12	H	821	CLA	C1A-CHA	2.18	1.52	1.43
12	A	840	CLA	C3B-C4B	2.18	1.49	1.42
12	A	835	CLA	C1D-C2D	2.18	1.49	1.45
12	B	815	CLA	MG-ND	-2.18	2.01	2.05
12	G	837	CLA	C1A-CHA	2.17	1.52	1.43
12	A	813	CLA	C1A-CHA	2.17	1.52	1.43
12	J	103	CLA	C1C-NC	-2.17	1.34	1.37
12	G	820	CLA	C3B-C4B	2.17	1.49	1.42
12	G	823	CLA	C4B-NB	-2.17	1.35	1.37
12	A	832	CLA	C1A-CHA	2.17	1.52	1.43
12	A	825	CLA	C1C-C2C	2.17	1.48	1.44
12	B	816	CLA	C3B-C4B	2.17	1.49	1.42
12	H	837	CLA	C3D-C2D	2.17	1.44	1.39
12	j	102	CLA	C4C-C3C	2.17	1.48	1.45
12	H	812	CLA	C1A-CHA	2.17	1.52	1.43
12	B	821	CLA	C1B-C2B	2.17	1.48	1.43
12	b	806	CLA	C1A-CHA	2.17	1.52	1.43
12	H	839	CLA	C1A-CHA	2.17	1.52	1.43
13	B	839	1L3	C18-C16	2.17	1.55	1.51
12	A	821	CLA	C4C-C3C	2.17	1.48	1.45
12	a	803	CLA	C1A-CHA	2.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	822	CLA	C4B-NB	-2.17	1.35	1.37
12	a	824	CLA	C1A-CHA	2.17	1.52	1.43
12	b	813	CLA	C1D-C2D	2.17	1.49	1.45
12	b	824	CLA	C1B-C2B	2.17	1.48	1.43
12	B	819	CLA	C1A-CHA	2.17	1.52	1.43
12	G	827	CLA	C3B-C4B	2.17	1.49	1.42
12	a	840	CLA	C3B-C4B	2.17	1.49	1.42
12	b	828	CLA	C1D-C2D	2.17	1.49	1.45
12	G	804	CLA	C1A-CHA	2.17	1.52	1.43
12	a	820	CLA	C3B-C4B	2.17	1.49	1.42
12	B	837	CLA	C4B-NB	-2.17	1.35	1.37
13	H	840	1L3	C18-C16	2.16	1.55	1.51
12	B	823	CLA	C1A-CHA	2.16	1.52	1.43
12	G	819	CLA	C3B-C4B	2.16	1.49	1.42
12	H	812	CLA	C1D-C2D	2.16	1.49	1.45
12	A	811	CLA	C1A-CHA	2.16	1.52	1.43
12	G	831	CLA	C3B-C4B	2.16	1.49	1.42
12	L	206	CLA	C1D-C2D	2.16	1.49	1.45
12	B	811	CLA	C1A-CHA	2.16	1.52	1.43
12	A	817	CLA	C1C-C2C	2.16	1.48	1.44
12	H	811	CLA	C4C-C3C	2.16	1.48	1.45
19	B	847	LMT	C3B-C2B	2.16	1.57	1.52
12	G	829	CLA	C1A-CHA	2.16	1.52	1.43
12	G	803	CLA	CBD-CAD	-2.16	1.46	1.56
12	a	809	CLA	C4B-NB	-2.16	1.35	1.37
12	a	818	CLA	C3B-C4B	2.16	1.49	1.42
12	B	827	CLA	C4C-C3C	2.16	1.48	1.45
12	a	820	CLA	C4B-NB	-2.16	1.35	1.37
12	b	807	CLA	C1B-C2B	2.16	1.48	1.43
12	A	838	CLA	C1C-C2C	2.16	1.48	1.44
12	H	829	CLA	C1D-C2D	2.16	1.49	1.45
12	B	817	CLA	C4B-NB	-2.16	1.35	1.37
12	G	821	CLA	C3B-C4B	2.16	1.49	1.42
12	F	201	CLA	C4C-C3C	2.16	1.48	1.45
12	H	822	CLA	C1A-CHA	2.15	1.52	1.43
12	a	832	CLA	C1D-C2D	2.15	1.49	1.45
12	b	825	CLA	CMD-C2D	-2.15	1.46	1.50
12	B	813	CLA	C4B-NB	-2.15	1.35	1.37
12	J	103	CLA	C4B-NB	-2.15	1.35	1.37
12	b	819	CLA	C1A-CHA	2.15	1.52	1.43
12	G	817	CLA	C4C-C3C	2.15	1.48	1.45
12	A	822	CLA	C1A-CHA	2.15	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	818	CLA	C3B-C4B	2.15	1.49	1.42
12	G	822	CLA	C1C-NC	-2.15	1.34	1.37
12	a	832	CLA	C1B-C2B	2.15	1.48	1.43
12	H	824	CLA	C1A-CHA	2.15	1.52	1.43
19	H	848	LMT	O2B-C2B	-2.15	1.37	1.43
12	a	823	CLA	C1D-C2D	2.15	1.49	1.45
12	H	825	CLA	C1A-CHA	2.15	1.51	1.43
12	b	811	CLA	C4C-C3C	2.15	1.48	1.45
12	A	835	CLA	C4C-C3C	2.15	1.48	1.45
12	G	816	CLA	C3B-C4B	2.15	1.49	1.42
12	A	821	CLA	C1D-C2D	2.15	1.49	1.45
12	A	830	CLA	C3D-C2D	2.15	1.44	1.39
12	A	829	CLA	C4C-C3C	2.15	1.48	1.45
12	a	841	CLA	C4C-C3C	2.15	1.48	1.45
12	H	814	CLA	C1A-CHA	2.15	1.51	1.43
12	G	809	CLA	C1A-CHA	2.15	1.51	1.43
12	R	103	CLA	C1A-CHA	2.15	1.51	1.43
12	H	805	CLA	C4B-NB	-2.15	1.35	1.37
12	H	817	CLA	C1A-CHA	2.14	1.51	1.43
12	G	833	CLA	C4C-C3C	2.14	1.48	1.45
12	b	822	CLA	C3B-C4B	2.14	1.49	1.42
12	A	803	CLA	C1A-CHA	2.14	1.51	1.43
12	a	819	CLA	C3B-C4B	2.14	1.49	1.42
12	G	822	CLA	C3B-C4B	2.14	1.49	1.42
12	J	103	CLA	C3B-C4B	2.14	1.49	1.42
12	B	825	CLA	CMD-C2D	-2.14	1.46	1.50
12	B	802	CLA	C3A-C2A	-2.14	1.48	1.54
12	G	805	CLA	C1D-C2D	2.14	1.49	1.45
12	b	824	CLA	MG-NC	2.14	2.11	2.06
12	G	830	CLA	C1B-C2B	2.14	1.48	1.43
12	B	828	CLA	C1D-C2D	2.14	1.49	1.45
12	R	103	CLA	C3B-C4B	2.14	1.49	1.42
12	G	832	CLA	C1A-CHA	2.13	1.51	1.43
13	A	842	1L3	C19-C20	2.13	1.56	1.50
12	a	838	CLA	C4C-C3C	2.13	1.48	1.45
12	A	838	CLA	C4C-C3C	2.13	1.48	1.45
12	G	822	CLA	C4B-NB	-2.13	1.35	1.37
12	B	810	CLA	C4C-C3C	2.13	1.48	1.45
12	a	814	CLA	C4C-C3C	2.13	1.48	1.45
12	G	819	CLA	C1D-C2D	2.13	1.49	1.45
12	F	203	CLA	C4B-NB	-2.13	1.35	1.37
12	A	805	CLA	C1D-C2D	2.13	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	820	CLA	C1A-CHA	2.13	1.51	1.43
12	a	811	CLA	C3B-C4B	2.13	1.48	1.42
12	G	838	CLA	C1C-C2C	2.13	1.48	1.44
12	j	104	CLA	C1C-C2C	2.13	1.48	1.44
12	H	832	CLA	C4B-NB	-2.13	1.35	1.37
12	b	817	CLA	C4B-NB	-2.13	1.35	1.37
12	H	826	CLA	C3B-C4B	2.13	1.48	1.42
12	B	812	CLA	C4C-C3C	2.13	1.48	1.45
12	H	818	CLA	C1C-C2C	2.13	1.48	1.44
12	B	834	CLA	C3B-C4B	2.13	1.48	1.42
12	G	804	CLA	C4C-C3C	2.13	1.48	1.45
12	H	838	CLA	C4B-NB	-2.13	1.35	1.37
12	G	811	CLA	C1A-CHA	2.13	1.51	1.43
12	G	842	CLA	C4C-C3C	2.13	1.48	1.45
12	A	811	CLA	C3B-C4B	2.13	1.48	1.42
12	A	808	CLA	C4C-C3C	2.13	1.48	1.45
12	B	838	CLA	C1C-C2C	2.12	1.48	1.44
12	G	839	CLA	C3B-C4B	2.12	1.48	1.42
12	b	818	CLA	C3B-C4B	2.12	1.48	1.42
12	b	808	CLA	C1A-CHA	2.12	1.51	1.43
12	a	828	CLA	C1A-CHA	2.12	1.51	1.43
12	H	839	CLA	C1C-C2C	2.12	1.48	1.44
12	b	827	CLA	C1D-C2D	2.12	1.49	1.45
12	a	815	CLA	C3B-C4B	2.12	1.48	1.42
12	a	835	CLA	C4C-C3C	2.12	1.48	1.45
12	b	803	CLA	C4C-C3C	2.12	1.48	1.45
12	G	816	CLA	C4B-NB	-2.12	1.35	1.37
12	b	824	CLA	CMC-C2C	-2.12	1.46	1.50
12	b	817	CLA	C1C-C2C	2.12	1.48	1.44
12	G	856	CLA	C3B-C4B	2.12	1.48	1.42
12	F	203	CLA	C1A-CHA	2.12	1.51	1.43
12	G	834	CLA	C1B-C2B	2.12	1.48	1.43
12	F	201	CLA	C1A-CHA	2.12	1.51	1.43
12	G	812	CLA	C3B-C4B	2.12	1.48	1.42
12	b	834	CLA	C4B-NB	-2.12	1.35	1.37
12	A	815	CLA	C1A-CHA	2.12	1.51	1.43
12	B	811	CLA	C1D-C2D	2.12	1.49	1.45
12	H	814	CLA	C1C-C2C	2.12	1.48	1.44
12	A	821	CLA	C3B-C4B	2.11	1.48	1.42
12	b	801	CLA	O2D-CED	-2.11	1.40	1.45
12	B	820	CLA	C1D-C2D	2.11	1.49	1.45
12	G	808	CLA	C4B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	833	CLA	C1A-CHA	2.11	1.51	1.43
12	B	825	CLA	C1A-CHA	2.11	1.51	1.43
12	H	837	CLA	C1D-C2D	2.11	1.49	1.45
12	a	805	CLA	MG-NC	2.11	2.11	2.06
12	b	825	CLA	C3A-C2A	-2.11	1.48	1.54
12	a	837	CLA	C1A-CHA	2.11	1.51	1.43
12	b	807	CLA	C4C-C3C	2.11	1.48	1.45
12	B	838	CLA	C1A-CHA	2.11	1.51	1.43
12	a	838	CLA	C1C-C2C	2.11	1.48	1.44
19	b	846	LMT	O2B-C2B	-2.11	1.37	1.43
12	B	816	CLA	C1A-CHA	2.11	1.51	1.43
12	B	821	CLA	C1A-CHA	2.11	1.51	1.43
12	G	836	CLA	CBD-CAD	-2.11	1.47	1.56
12	B	836	CLA	C1D-C2D	2.11	1.49	1.45
12	B	813	CLA	C1A-CHA	2.11	1.51	1.43
12	a	824	CLA	C1C-C2C	2.11	1.48	1.44
13	A	842	1L3	C02-C12	2.11	1.52	1.47
12	b	821	CLA	C1B-C2B	2.11	1.48	1.43
12	a	821	CLA	C3B-C4B	2.11	1.48	1.42
12	H	801	CLA	C1A-CHA	2.11	1.51	1.43
12	A	836	CLA	C1A-CHA	2.11	1.51	1.43
12	B	816	CLA	C1B-C2B	2.11	1.48	1.43
12	G	824	CLA	C4C-C3C	2.11	1.48	1.45
12	G	855	CLA	C1A-CHA	2.11	1.51	1.43
12	a	821	CLA	C1D-C2D	2.11	1.49	1.45
12	a	834	CLA	C1B-C2B	2.10	1.48	1.43
12	a	829	CLA	C4C-C3C	2.10	1.48	1.45
12	A	855	CLA	C3B-C4B	2.10	1.48	1.42
12	H	826	CLA	C4B-NB	-2.10	1.35	1.37
12	B	832	CLA	C1A-CHA	2.10	1.51	1.43
12	B	821	CLA	C3B-C4B	2.10	1.48	1.42
12	G	825	CLA	C1A-CHA	2.10	1.51	1.43
12	a	807	CLA	C3B-C4B	2.10	1.48	1.42
12	b	811	CLA	C1A-CHA	2.10	1.51	1.43
12	G	809	CLA	C4C-C3C	2.10	1.48	1.45
12	G	804	CLA	C1D-C2D	2.10	1.49	1.45
12	b	813	CLA	C3B-C4B	2.10	1.48	1.42
12	P	203	CLA	C1A-CHA	2.10	1.51	1.43
12	B	822	CLA	C1A-CHA	2.10	1.51	1.43
12	B	805	CLA	C4C-C3C	2.10	1.48	1.45
12	A	806	CLA	C1D-C2D	2.10	1.49	1.45
12	H	801	CLA	C1D-C2D	2.10	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	803	CLA	CMA-C3A	-2.10	1.48	1.53
12	H	804	CLA	C1A-CHA	2.10	1.51	1.43
12	G	830	CLA	C1A-CHA	2.10	1.51	1.43
12	a	817	CLA	C3B-C4B	2.10	1.48	1.42
12	G	838	CLA	C1D-C2D	2.10	1.49	1.45
12	G	825	CLA	C1C-C2C	2.09	1.48	1.44
12	B	805	CLA	C1D-C2D	2.09	1.49	1.45
12	a	813	CLA	C4C-C3C	2.09	1.48	1.45
12	b	814	CLA	C1A-CHA	2.09	1.51	1.43
12	F	201	CLA	C1C-C2C	2.09	1.48	1.44
12	G	808	CLA	C3B-C4B	2.09	1.48	1.42
12	A	820	CLA	C1B-C2B	2.09	1.48	1.43
12	b	830	CLA	C3B-C4B	2.09	1.48	1.42
12	G	836	CLA	C1D-C2D	2.09	1.49	1.45
12	a	832	CLA	C1A-CHA	2.09	1.51	1.43
19	H	848	LMT	O3B-C3B	-2.09	1.37	1.43
19	b	846	LMT	O3B-C3B	-2.09	1.37	1.43
12	G	821	CLA	C1A-CHA	2.09	1.51	1.43
12	G	829	CLA	C1C-C2C	2.09	1.48	1.44
12	B	817	CLA	C1C-C2C	2.09	1.48	1.44
12	H	823	CLA	C1A-CHA	2.09	1.51	1.43
12	A	816	CLA	C1A-CHA	2.09	1.51	1.43
12	B	808	CLA	C1A-CHA	2.09	1.51	1.43
12	B	806	CLA	C1A-CHA	2.09	1.51	1.43
12	a	802	CLA	CBD-CAD	-2.09	1.47	1.56
12	B	813	CLA	C1C-C2C	2.08	1.48	1.44
12	A	825	CLA	C3B-C4B	2.08	1.48	1.42
12	H	805	CLA	C1A-CHA	2.08	1.51	1.43
13	G	843	1L3	C03-C04	2.08	1.52	1.47
12	b	803	CLA	C3B-C4B	2.08	1.48	1.42
12	B	804	CLA	C1A-CHA	2.08	1.51	1.43
12	J	103	CLA	C1C-C2C	2.08	1.48	1.44
12	a	827	CLA	C1A-CHA	2.08	1.51	1.43
12	B	814	CLA	C1D-C2D	2.08	1.49	1.45
12	G	832	CLA	C1B-C2B	2.08	1.48	1.43
12	b	813	CLA	C1A-CHA	2.08	1.51	1.43
13	a	842	1L3	O13-C12	-2.08	1.18	1.23
12	A	819	CLA	C3B-C4B	2.08	1.48	1.42
12	G	827	CLA	C1C-C2C	2.08	1.48	1.44
12	H	836	CLA	C1D-C2D	2.08	1.49	1.45
13	G	843	1L3	C19-C20	2.08	1.56	1.50
13	a	842	1L3	C19-C20	2.08	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	204	CLA	C1D-C2D	2.08	1.49	1.45
12	G	820	CLA	C4C-C3C	2.08	1.48	1.45
12	B	822	CLA	C1C-C2C	2.08	1.48	1.44
12	A	824	CLA	C4C-C3C	2.08	1.48	1.45
12	b	813	CLA	C4C-C3C	2.08	1.48	1.45
12	l	206	CLA	C1D-C2D	2.08	1.49	1.45
12	A	825	CLA	C1A-CHA	2.08	1.51	1.43
12	B	822	CLA	C3B-C4B	2.08	1.48	1.42
12	B	815	CLA	CHB-C4A	-2.08	1.32	1.37
12	H	819	CLA	C3B-C4B	2.08	1.48	1.42
13	a	842	1L3	C27-C26	2.07	1.55	1.50
12	b	804	CLA	C1A-CHA	2.07	1.51	1.43
12	a	813	CLA	C1B-NB	-2.07	1.35	1.37
12	B	829	CLA	C1A-CHA	2.07	1.51	1.43
12	H	817	CLA	C1C-NC	-2.07	1.34	1.37
12	b	836	CLA	C4B-NB	-2.07	1.35	1.37
12	B	815	CLA	C4B-NB	-2.07	1.35	1.37
12	B	831	CLA	C4B-NB	-2.07	1.35	1.37
12	b	827	CLA	C3B-C4B	2.07	1.48	1.42
12	B	834	CLA	C1A-CHA	2.07	1.51	1.43
12	G	840	CLA	C1A-CHA	2.07	1.51	1.43
12	A	833	CLA	C1A-CHA	2.07	1.51	1.43
12	b	815	CLA	C1D-C2D	2.07	1.49	1.45
12	b	835	CLA	C1D-C2D	2.07	1.49	1.45
12	l	202	CLA	C4C-C3C	2.07	1.48	1.45
12	H	808	CLA	C4B-NB	-2.07	1.35	1.37
12	G	829	CLA	C3B-C4B	2.07	1.48	1.42
12	b	834	CLA	C1C-C2C	2.07	1.48	1.44
12	a	810	CLA	C3B-C4B	2.07	1.48	1.42
12	H	822	CLA	C1B-C2B	2.07	1.48	1.43
12	B	831	CLA	C3B-C4B	2.06	1.48	1.42
12	H	830	CLA	C1A-CHA	2.06	1.51	1.43
12	a	839	CLA	C3B-C4B	2.06	1.48	1.42
12	A	831	CLA	C3B-C4B	2.06	1.48	1.42
12	G	815	CLA	C1D-C2D	2.06	1.49	1.45
12	b	833	CLA	C1A-CHA	2.06	1.51	1.43
12	A	834	CLA	C1A-CHA	2.06	1.51	1.43
17	m	101	45D	C22-C16	2.06	1.55	1.50
12	A	854	CLA	C1A-CHA	2.06	1.51	1.43
12	a	838	CLA	C1D-C2D	2.06	1.49	1.45
12	A	839	CLA	C3B-C4B	2.06	1.48	1.42
12	H	823	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	833	CLA	C3B-C4B	2.06	1.48	1.42
12	b	831	CLA	C1A-CHA	2.06	1.51	1.43
12	G	819	CLA	C4C-C3C	2.06	1.48	1.45
12	B	803	CLA	C3B-C4B	2.06	1.48	1.42
12	H	831	CLA	C4C-C3C	2.06	1.48	1.45
12	a	820	CLA	C1A-CHA	2.06	1.51	1.43
12	b	821	CLA	C1A-CHA	2.06	1.51	1.43
12	B	836	CLA	C4C-C3C	2.06	1.48	1.45
12	f	203	CLA	C1A-CHA	2.06	1.51	1.43
12	F	201	CLA	C1B-C2B	2.06	1.48	1.43
12	f	201	CLA	C1A-CHA	2.06	1.51	1.43
12	j	102	CLA	C1A-CHA	2.06	1.51	1.43
12	a	825	CLA	C1C-C2C	2.05	1.48	1.44
12	B	812	CLA	C1D-C2D	2.05	1.49	1.45
12	a	817	CLA	C3B-C2B	2.05	1.48	1.41
13	A	842	1L3	O05-C04	-2.05	1.19	1.23
12	H	823	CLA	C4C-C3C	2.05	1.48	1.45
12	B	829	CLA	C3B-C4B	2.05	1.48	1.42
12	G	836	CLA	C3B-C2B	2.05	1.48	1.41
12	H	813	CLA	C3B-C4B	2.05	1.48	1.42
12	a	805	CLA	C1D-C2D	2.05	1.49	1.45
17	T	101	45D	C22-C16	2.05	1.55	1.50
12	A	810	CLA	C1A-CHA	2.05	1.51	1.43
12	B	825	CLA	C1B-C2B	2.05	1.47	1.43
12	P	201	CLA	C4C-C3C	2.05	1.48	1.45
12	a	825	CLA	C3B-C4B	2.05	1.48	1.42
12	B	829	CLA	O2D-CED	-2.05	1.40	1.45
12	A	828	CLA	C1C-C2C	2.05	1.48	1.44
12	H	803	CLA	C4C-C3C	2.05	1.48	1.45
12	G	811	CLA	C4C-C3C	2.05	1.48	1.45
12	G	817	CLA	C1A-CHA	2.05	1.51	1.43
12	f	201	CLA	C1C-C2C	2.05	1.48	1.44
12	G	805	CLA	C3B-C4B	2.05	1.48	1.42
12	b	837	CLA	C1C-C2C	2.05	1.48	1.44
13	G	843	1L3	C02-C12	2.05	1.52	1.47
12	G	802	CLA	C3A-C2A	-2.05	1.48	1.54
12	B	815	CLA	C4C-C3C	2.05	1.48	1.45
12	G	828	CLA	C1A-CHA	2.05	1.51	1.43
12	b	826	CLA	C4B-NB	-2.05	1.35	1.37
12	G	807	CLA	C1D-C2D	2.05	1.49	1.45
12	A	814	CLA	C4C-C3C	2.05	1.48	1.45
12	a	817	CLA	C1A-CHA	2.04	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	835	CLA	C1A-CHA	2.04	1.51	1.43
12	G	822	CLA	C1D-C2D	2.04	1.49	1.45
13	G	843	1L3	C27-C26	2.04	1.55	1.50
12	G	818	CLA	C1C-C2C	2.04	1.48	1.44
12	A	829	CLA	C1A-CHA	2.04	1.51	1.43
12	B	808	CLA	C3A-C2A	-2.04	1.48	1.54
12	a	810	CLA	C1D-C2D	2.04	1.49	1.45
12	A	833	CLA	C1D-C2D	2.04	1.49	1.45
12	a	819	CLA	C1A-CHA	2.04	1.51	1.43
12	b	822	CLA	C1C-C2C	2.04	1.48	1.44
12	G	805	CLA	C1C-C2C	2.04	1.48	1.44
12	b	820	CLA	C1D-C2D	2.04	1.49	1.45
12	l	202	CLA	C4B-NB	-2.04	1.35	1.37
12	G	813	CLA	C1D-C2D	2.04	1.49	1.45
12	b	813	CLA	C1C-C2C	2.04	1.48	1.44
12	H	835	CLA	C3B-C4B	2.04	1.48	1.42
13	H	840	1L3	C27-C26	2.04	1.55	1.50
12	H	832	CLA	C4C-C3C	2.04	1.48	1.45
12	B	802	CLA	C1C-C2C	2.04	1.48	1.44
12	b	821	CLA	C3B-C4B	2.04	1.48	1.42
12	b	833	CLA	C1D-C2D	2.04	1.49	1.45
12	A	831	CLA	C3B-C2B	2.04	1.48	1.41
12	G	832	CLA	C4C-C3C	2.04	1.48	1.45
12	b	805	CLA	C1A-CHA	2.04	1.51	1.43
12	G	826	CLA	C1A-CHA	2.04	1.51	1.43
12	A	830	CLA	C3B-C4B	2.04	1.48	1.42
12	B	811	CLA	C4C-C3C	2.03	1.48	1.45
12	B	812	CLA	C3B-C4B	2.03	1.48	1.42
12	A	834	CLA	C1B-C2B	2.03	1.47	1.43
12	G	834	CLA	C1A-CHA	2.03	1.51	1.43
12	A	838	CLA	C1D-C2D	2.03	1.49	1.45
12	a	835	CLA	C3B-C4B	2.03	1.48	1.42
12	B	812	CLA	C3B-C2B	2.03	1.48	1.41
12	B	830	CLA	C4C-C3C	2.03	1.48	1.45
12	B	814	CLA	C1A-CHA	2.03	1.51	1.43
12	H	836	CLA	C1C-C2C	2.03	1.48	1.44
12	B	818	CLA	C3B-C4B	2.03	1.48	1.42
13	A	842	1L3	C27-C26	2.03	1.55	1.50
12	a	854	CLA	C1A-CHA	2.03	1.51	1.43
19	B	847	LMT	O1'-C1'	-2.03	1.36	1.40
12	H	832	CLA	C3B-C4B	2.03	1.48	1.42
12	H	828	CLA	C1D-C2D	2.03	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	801	CL0	CMD-C2D	-2.03	1.46	1.50
12	a	810	CLA	C1A-CHA	2.02	1.51	1.43
12	a	830	CLA	C3B-C4B	2.02	1.48	1.42
12	A	818	CLA	C1D-C2D	2.02	1.49	1.45
12	G	835	CLA	C3B-C4B	2.02	1.48	1.42
12	a	833	CLA	C1A-CHA	2.02	1.51	1.43
12	H	836	CLA	C4B-NB	-2.02	1.35	1.37
12	G	811	CLA	C3B-C4B	2.02	1.48	1.42
12	L	202	CLA	C1A-CHA	2.02	1.51	1.43
13	a	842	1L3	O05-C04	-2.02	1.19	1.23
12	G	818	CLA	C4B-NB	-2.02	1.35	1.37
12	A	824	CLA	C1C-C2C	2.02	1.48	1.44
12	b	802	CLA	C3A-C2A	-2.02	1.49	1.54
12	A	810	CLA	C4C-C3C	2.02	1.48	1.45
12	G	832	CLA	C3B-C4B	2.02	1.48	1.42
12	G	807	CLA	C3B-C2B	2.02	1.48	1.41
12	b	829	CLA	C1A-CHA	2.02	1.51	1.43
12	G	840	CLA	C4B-NB	-2.02	1.35	1.37
12	B	803	CLA	C1D-C2D	2.02	1.49	1.45
12	A	802	CLA	CHB-C4A	-2.02	1.32	1.37
12	l	202	CLA	C1A-CHA	2.02	1.51	1.43
12	A	836	CLA	C3B-C2B	2.02	1.48	1.41
12	b	836	CLA	C3B-C4B	2.02	1.48	1.42
12	a	836	CLA	C3B-C4B	2.02	1.48	1.42
12	A	812	CLA	C3B-C4B	2.02	1.48	1.42
12	H	816	CLA	C1A-CHA	2.02	1.51	1.43
12	G	823	CLA	C3B-C4B	2.02	1.48	1.42
12	B	827	CLA	C3B-C4B	2.02	1.48	1.42
12	A	831	CLA	C1A-CHA	2.01	1.51	1.43
17	M	101	45D	C22-C16	2.01	1.54	1.50
12	a	824	CLA	C3B-C2B	2.01	1.48	1.41
12	A	805	CLA	C3B-C2B	2.01	1.48	1.41
12	a	817	CLA	C1D-C2D	2.01	1.49	1.45
12	a	854	CLA	C3A-C4A	-2.01	1.45	1.51
12	A	819	CLA	C1A-CHA	2.01	1.51	1.43
12	b	828	CLA	C3B-C2B	2.01	1.48	1.41
12	j	104	CLA	C1C-NC	-2.01	1.34	1.37
12	b	816	CLA	C3B-C4B	2.01	1.48	1.42
12	A	834	CLA	C1D-C2D	2.01	1.49	1.45
12	H	829	CLA	C3B-C4B	2.01	1.48	1.42
12	a	840	CLA	C4B-NB	-2.01	1.35	1.37
12	b	822	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	817	CLA	C1B-C2B	2.01	1.47	1.43
12	H	812	CLA	C3B-C2B	2.01	1.47	1.41
12	H	801	CLA	C3B-C4B	2.01	1.48	1.42
12	b	828	CLA	C3B-C4B	2.01	1.48	1.42
12	b	822	CLA	C4C-C3C	2.01	1.48	1.45
12	G	825	CLA	C3B-C2B	2.01	1.47	1.41
12	A	824	CLA	C3B-C2B	2.01	1.47	1.41
12	B	828	CLA	C3B-C4B	2.01	1.48	1.42
12	A	854	CLA	C3A-C4A	-2.00	1.45	1.51
12	H	826	CLA	C1A-CHA	2.00	1.51	1.43
12	H	817	CLA	C4B-NB	-2.00	1.35	1.37
12	a	813	CLA	C3B-C2B	2.00	1.47	1.41
12	A	814	CLA	C3B-C2B	2.00	1.47	1.41
12	H	802	CLA	C3B-C4B	2.00	1.48	1.42
12	H	850	CLA	C3B-C4B	2.00	1.48	1.42
12	a	805	CLA	C3B-C4B	2.00	1.48	1.42
12	a	829	CLA	C1A-CHA	2.00	1.51	1.43
12	H	806	CLA	C1A-CHA	2.00	1.51	1.43
12	H	818	CLA	C3B-C4B	2.00	1.48	1.42

All (8897) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	i	101	BCR	C16-C17-C18	24.83	162.10	127.28
15	A	846	BCR	C16-C17-C18	24.60	161.77	127.28
15	R	102	BCR	C16-C17-C18	24.51	161.65	127.28
15	j	103	BCR	C16-C17-C18	24.44	161.55	127.28
15	G	849	BCR	C20-C21-C22	24.28	161.33	127.28
15	a	848	BCR	C20-C21-C22	24.22	161.24	127.28
15	J	102	BCR	C16-C17-C18	23.93	160.84	127.28
15	B	844	BCR	C20-C21-C22	23.85	160.73	127.28
15	A	848	BCR	C20-C21-C22	23.75	160.59	127.28
15	Q	101	BCR	C16-C17-C18	23.68	160.49	127.28
15	A	846	BCR	C20-C21-C22	23.67	160.47	127.28
15	J	102	BCR	C20-C21-C22	23.52	160.26	127.28
15	b	842	BCR	C16-C17-C18	23.51	160.25	127.28
15	H	844	BCR	C16-C17-C18	23.44	160.15	127.28
15	H	845	BCR	C20-C21-C22	23.37	160.05	127.28
15	b	843	BCR	C16-C17-C18	23.25	159.88	127.28
15	I	101	BCR	C16-C17-C18	23.25	159.88	127.28
15	b	843	BCR	C20-C21-C22	23.23	159.86	127.28
15	B	843	BCR	C16-C17-C18	23.09	159.66	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	m	101	45D	C19-C23-C25	-22.88	92.39	126.23
15	Q	101	BCR	C20-C21-C22	22.79	159.24	127.28
15	R	102	BCR	C20-C21-C22	22.78	159.23	127.28
15	H	845	BCR	C16-C17-C18	22.78	159.23	127.28
15	G	846	BCR	C20-C21-C22	22.75	159.19	127.28
15	B	844	BCR	C16-C17-C18	22.69	159.10	127.28
15	i	101	BCR	C20-C21-C22	22.65	159.05	127.28
17	M	101	45D	C19-C23-C25	-22.64	92.74	126.23
15	B	845	BCR	C20-C21-C22	22.63	159.02	127.28
15	a	852	BCR	C16-C17-C18	22.53	158.87	127.28
15	G	853	BCR	C16-C17-C18	22.46	158.78	127.28
15	H	846	BCR	C20-C21-C22	22.46	158.77	127.28
15	A	852	BCR	C16-C17-C18	22.43	158.74	127.28
17	T	101	45D	C19-C23-C25	-22.42	93.07	126.23
15	b	844	BCR	C20-C21-C22	22.39	158.68	127.28
15	G	850	BCR	C20-C21-C22	22.34	158.60	127.28
15	j	103	BCR	C20-C21-C22	22.33	158.59	127.28
15	I	101	BCR	C20-C21-C22	22.19	158.40	127.28
15	A	847	BCR	C20-C21-C22	22.09	158.26	127.28
15	a	847	BCR	C20-C21-C22	22.03	158.18	127.28
15	H	842	BCR	C20-C21-C22	21.96	158.08	127.28
15	R	101	BCR	C16-C17-C18	21.89	157.97	127.28
15	a	849	BCR	C20-C21-C22	21.81	157.87	127.28
15	G	846	BCR	C15-C16-C17	21.81	168.14	123.52
15	G	848	BCR	C20-C21-C22	21.77	157.81	127.28
15	B	840	BCR	C20-C21-C22	21.74	157.77	127.28
15	A	849	BCR	C20-C21-C22	21.71	157.73	127.28
15	a	846	BCR	C16-C17-C18	21.71	157.72	127.28
15	i	102	BCR	C20-C21-C22	21.68	157.69	127.28
15	P	202	BCR	C15-C16-C17	21.67	167.86	123.52
15	b	847	BCR	C15-C16-C17	21.65	167.83	123.52
15	P	204	BCR	C15-C16-C17	21.64	167.79	123.52
15	a	845	BCR	C20-C21-C22	21.62	157.60	127.28
15	b	842	BCR	C20-C21-C22	21.61	157.58	127.28
15	A	845	BCR	C20-C21-C22	21.59	157.55	127.28
15	b	839	BCR	C20-C21-C22	21.58	157.54	127.28
15	f	202	BCR	C15-C16-C17	21.57	167.66	123.52
15	H	844	BCR	C20-C21-C22	21.57	157.52	127.28
15	Q	102	BCR	C20-C21-C22	21.57	157.52	127.28
15	J	101	BCR	C16-C17-C18	21.53	157.47	127.28
15	F	204	BCR	C15-C16-C17	21.53	167.57	123.52
15	j	101	BCR	C16-C17-C18	21.49	157.42	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	104	BCR	C15-C16-C17	21.47	167.44	123.52
15	B	843	BCR	C20-C21-C22	21.47	157.38	127.28
15	B	841	BCR	C20-C21-C22	21.41	157.30	127.28
15	J	104	BCR	C20-C21-C22	21.41	157.30	127.28
15	F	202	BCR	C15-C16-C17	21.37	167.25	123.52
15	b	840	BCR	C20-C21-C22	21.36	157.24	127.28
15	L	201	BCR	C16-C17-C18	21.35	157.22	127.28
15	G	847	BCR	C16-C17-C18	21.31	157.17	127.28
15	L	207	BCR	C20-C21-C22	21.28	157.12	127.28
15	H	841	BCR	C20-C21-C22	21.27	157.11	127.28
15	f	204	BCR	C15-C16-C17	21.25	166.99	123.52
15	a	845	BCR	C15-C16-C17	21.23	166.96	123.52
15	S	205	BCR	C16-C17-C18	21.17	156.97	127.28
15	A	845	BCR	C15-C16-C17	21.16	166.82	123.52
15	P	204	BCR	C20-C21-C22	21.14	156.92	127.28
15	P	202	BCR	C20-C21-C22	21.13	156.92	127.28
15	f	204	BCR	C20-C21-C22	21.04	156.78	127.28
15	H	849	BCR	C15-C16-C17	21.03	166.55	123.52
15	F	204	BCR	C20-C21-C22	21.02	156.76	127.28
15	G	845	BCR	C20-C21-C22	21.01	156.74	127.28
15	G	848	BCR	C16-C17-C18	21.00	156.72	127.28
15	l	201	BCR	C16-C17-C18	20.99	156.71	127.28
15	A	844	BCR	C20-C21-C22	20.93	156.64	127.28
15	L	203	BCR	C16-C17-C18	20.93	156.64	127.28
15	a	844	BCR	C20-C21-C22	20.92	156.62	127.28
15	b	847	BCR	C20-C21-C22	20.92	156.61	127.28
15	A	847	BCR	C16-C17-C18	20.86	156.54	127.28
15	b	841	BCR	C16-C17-C18	20.86	156.53	127.28
15	A	847	BCR	C15-C16-C17	20.82	166.11	123.52
15	l	203	BCR	C16-C17-C18	20.81	156.46	127.28
15	H	849	BCR	C20-C21-C22	20.80	156.44	127.28
15	A	849	BCR	C16-C17-C18	20.80	156.44	127.28
15	H	843	BCR	C16-C17-C18	20.78	156.42	127.28
15	a	847	BCR	C16-C17-C18	20.78	156.42	127.28
15	B	842	BCR	C16-C17-C18	20.75	156.38	127.28
15	S	201	BCR	C16-C17-C18	20.72	156.34	127.28
15	a	847	BCR	C15-C16-C17	20.70	165.87	123.52
15	H	846	BCR	C15-C16-C17	20.67	165.82	123.52
15	a	844	BCR	C16-C17-C18	20.62	156.19	127.28
15	G	848	BCR	C15-C16-C17	20.60	165.68	123.52
15	B	845	BCR	C15-C16-C17	20.60	165.67	123.52
15	b	844	BCR	C15-C16-C17	20.57	165.60	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	101	BCR	C20-C21-C22	20.56	156.12	127.28
15	i	102	BCR	C15-C16-C17	20.55	165.57	123.52
15	j	101	BCR	C20-C21-C22	20.54	156.08	127.28
15	F	202	BCR	C16-C17-C18	20.52	156.06	127.28
15	Q	102	BCR	C15-C16-C17	20.52	165.50	123.52
15	G	850	BCR	C16-C17-C18	20.49	156.02	127.28
15	Q	102	BCR	C16-C17-C18	20.49	156.02	127.28
15	a	849	BCR	C16-C17-C18	20.45	155.96	127.28
12	P	203	CLA	O2A-CGA-O1A	-20.44	70.77	123.33
15	L	207	BCR	C15-C16-C17	20.42	165.31	123.52
12	F	203	CLA	O2A-CGA-O1A	-20.42	70.82	123.33
15	a	849	BCR	C15-C16-C17	20.40	165.26	123.52
12	f	203	CLA	O2A-CGA-O1A	-20.40	70.87	123.33
15	b	839	BCR	C16-C17-C18	20.39	155.87	127.28
15	f	202	BCR	C20-C21-C22	20.37	155.84	127.28
15	G	850	BCR	C15-C16-C17	20.34	165.13	123.52
15	P	202	BCR	C16-C17-C18	20.32	155.78	127.28
15	G	845	BCR	C16-C17-C18	20.25	155.68	127.28
15	A	848	BCR	C16-C17-C18	20.23	155.65	127.28
15	b	840	BCR	C16-C17-C18	20.23	155.64	127.28
15	A	844	BCR	C15-C16-C17	20.22	164.90	123.52
15	F	202	BCR	C20-C21-C22	20.19	155.59	127.28
15	L	207	BCR	C16-C17-C18	20.18	155.59	127.28
15	f	202	BCR	C16-C17-C18	20.17	155.57	127.28
15	S	205	BCR	C15-C16-C17	20.15	164.74	123.52
15	H	841	BCR	C16-C17-C18	20.14	155.53	127.28
15	R	101	BCR	C20-C21-C22	20.14	155.53	127.28
15	B	841	BCR	C16-C17-C18	20.06	155.41	127.28
15	A	849	BCR	C15-C16-C17	20.06	164.56	123.52
15	B	840	BCR	C16-C17-C18	20.05	155.40	127.28
15	i	102	BCR	C16-C17-C18	20.01	155.34	127.28
15	G	845	BCR	C15-C16-C17	19.98	164.41	123.52
15	H	842	BCR	C15-C16-C17	19.97	164.37	123.52
15	l	201	BCR	C15-C16-C17	19.89	164.21	123.52
15	B	841	BCR	C15-C16-C17	19.87	164.17	123.52
15	a	848	BCR	C16-C17-C18	19.86	155.13	127.28
15	a	844	BCR	C15-C16-C17	19.83	164.10	123.52
15	B	840	BCR	C15-C16-C17	19.83	164.09	123.52
15	H	843	BCR	C15-C16-C17	19.79	164.02	123.52
15	a	848	BCR	C15-C16-C17	19.79	164.00	123.52
15	L	201	BCR	C15-C16-C17	19.77	163.98	123.52
15	A	848	BCR	C15-C16-C17	19.74	163.91	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	842	BCR	C16-C17-C18	19.73	154.94	127.28
15	b	841	BCR	C15-C16-C17	19.68	163.79	123.52
15	B	842	BCR	C15-C16-C17	19.66	163.74	123.52
15	G	849	BCR	C16-C17-C18	19.64	154.82	127.28
15	b	840	BCR	C15-C16-C17	19.63	163.69	123.52
15	S	201	BCR	C15-C16-C17	19.62	163.67	123.52
15	A	845	BCR	C16-C17-C18	19.56	154.71	127.28
15	G	849	BCR	C15-C16-C17	19.54	163.51	123.52
15	l	203	BCR	C15-C16-C17	19.53	163.49	123.52
15	b	839	BCR	C15-C16-C17	19.47	163.36	123.52
15	A	844	BCR	C16-C17-C18	19.45	154.56	127.28
15	H	841	BCR	C15-C16-C17	19.42	163.25	123.52
15	H	843	BCR	C20-C21-C22	19.41	154.50	127.28
15	L	203	BCR	C15-C16-C17	19.41	163.24	123.52
15	i	101	BCR	C15-C16-C17	19.35	163.12	123.52
15	b	841	BCR	C20-C21-C22	19.34	154.40	127.28
15	H	845	BCR	C15-C16-C17	19.33	163.07	123.52
15	Q	101	BCR	C15-C16-C17	19.32	163.06	123.52
15	l	203	BCR	C20-C21-C22	19.31	154.36	127.28
15	a	845	BCR	C16-C17-C18	19.29	154.34	127.28
15	B	842	BCR	C20-C21-C22	19.29	154.33	127.28
15	a	852	BCR	C20-C21-C22	19.28	154.32	127.28
15	I	101	BCR	C15-C16-C17	19.27	162.95	123.52
15	l	201	BCR	C20-C21-C22	19.25	154.27	127.28
15	L	201	BCR	C20-C21-C22	19.22	154.23	127.28
15	A	852	BCR	C20-C21-C22	19.21	154.21	127.28
15	B	844	BCR	C15-C16-C17	19.20	162.80	123.52
15	G	853	BCR	C20-C21-C22	19.18	154.18	127.28
15	a	846	BCR	C20-C21-C22	19.16	154.15	127.28
15	L	201	BCR	C10-C11-C12	19.15	178.68	123.20
15	S	201	BCR	C20-C21-C22	19.13	154.11	127.28
15	H	845	BCR	C10-C11-C12	19.05	178.41	123.20
15	j	103	BCR	C10-C11-C12	19.00	178.25	123.20
15	b	843	BCR	C15-C16-C17	18.99	162.38	123.52
15	l	201	BCR	C10-C11-C12	18.94	178.07	123.20
15	a	846	BCR	C10-C11-C12	18.92	178.02	123.20
15	b	843	BCR	C10-C11-C12	18.91	178.00	123.20
15	J	101	BCR	C10-C11-C12	18.91	177.99	123.20
15	f	204	BCR	C16-C17-C18	18.88	153.76	127.28
15	H	841	BCR	C10-C11-C12	18.88	177.91	123.20
15	A	847	BCR	C10-C11-C12	18.88	177.90	123.20
15	A	846	BCR	C10-C11-C12	18.87	177.87	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	845	BCR	C10-C11-C12	18.86	177.86	123.20
15	f	202	BCR	C10-C11-C12	18.79	177.65	123.20
15	R	101	BCR	C10-C11-C12	18.78	177.60	123.20
15	P	202	BCR	C10-C11-C12	18.75	177.52	123.20
15	J	101	BCR	C15-C16-C17	18.75	161.88	123.52
15	F	204	BCR	C16-C17-C18	18.71	153.52	127.28
15	R	102	BCR	C10-C11-C12	18.70	177.40	123.20
15	B	844	BCR	C10-C11-C12	18.70	177.37	123.20
15	A	844	BCR	C10-C11-C12	18.69	177.35	123.20
15	H	846	BCR	C10-C11-C12	18.67	177.31	123.20
15	B	845	BCR	C10-C11-C12	18.64	177.20	123.20
15	J	104	BCR	C10-C11-C12	18.63	177.19	123.20
15	L	207	BCR	C10-C11-C12	18.63	177.18	123.20
15	j	101	BCR	C10-C11-C12	18.62	177.16	123.20
15	b	840	BCR	C10-C11-C12	18.62	177.14	123.20
15	J	102	BCR	C10-C11-C12	18.61	177.13	123.20
15	B	841	BCR	C10-C11-C12	18.60	177.11	123.20
15	H	849	BCR	C10-C11-C12	18.60	177.09	123.20
15	H	842	BCR	C10-C11-C12	18.59	177.06	123.20
15	a	847	BCR	C10-C11-C12	18.59	177.05	123.20
15	B	840	BCR	C10-C11-C12	18.58	177.04	123.20
15	a	844	BCR	C10-C11-C12	18.55	176.94	123.20
15	G	847	BCR	C15-C16-C17	18.53	161.44	123.52
15	P	204	BCR	C16-C17-C18	18.53	153.27	127.28
15	G	848	BCR	C10-C11-C12	18.53	176.89	123.20
15	a	852	BCR	C15-C16-C17	18.50	161.37	123.52
15	i	101	BCR	C10-C11-C12	18.48	176.75	123.20
15	S	205	BCR	C20-C21-C22	18.48	153.20	127.28
15	L	203	BCR	C10-C11-C12	18.47	176.71	123.20
15	l	203	BCR	C10-C11-C12	18.44	176.64	123.20
15	P	204	BCR	C10-C11-C12	18.44	176.63	123.20
15	Q	102	BCR	C10-C11-C12	18.44	176.63	123.20
15	J	104	BCR	C16-C17-C18	18.42	153.12	127.28
15	i	102	BCR	C10-C11-C12	18.42	176.57	123.20
15	I	101	BCR	C10-C11-C12	18.42	176.56	123.20
15	G	846	BCR	C16-C17-C18	18.41	153.10	127.28
15	a	846	BCR	C15-C16-C17	18.41	161.19	123.52
15	S	205	BCR	C10-C11-C12	18.41	176.54	123.20
15	H	849	BCR	C16-C17-C18	18.40	153.08	127.28
15	A	845	BCR	C10-C11-C12	18.35	176.36	123.20
15	Q	101	BCR	C10-C11-C12	18.32	176.29	123.20
15	a	845	BCR	C10-C11-C12	18.32	176.27	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	847	BCR	C16-C17-C18	18.31	152.96	127.28
15	G	853	BCR	C15-C16-C17	18.30	160.97	123.52
15	S	201	BCR	C10-C11-C12	18.29	176.21	123.20
15	j	101	BCR	C15-C16-C17	18.28	160.93	123.52
15	a	848	BCR	C10-C11-C12	18.26	176.12	123.20
15	b	844	BCR	C10-C11-C12	18.24	176.04	123.20
15	B	843	BCR	C15-C16-C17	18.21	160.78	123.52
15	b	847	BCR	C10-C11-C12	18.20	175.95	123.20
15	H	844	BCR	C15-C16-C17	18.20	160.76	123.52
15	A	848	BCR	C10-C11-C12	18.20	175.93	123.20
15	H	846	BCR	C16-C17-C18	18.19	152.79	127.28
15	G	849	BCR	C10-C11-C12	18.17	175.86	123.20
15	A	852	BCR	C15-C16-C17	18.16	160.68	123.52
15	b	844	BCR	C16-C17-C18	18.14	152.72	127.28
15	f	204	BCR	C10-C11-C12	18.14	175.76	123.20
15	R	101	BCR	C15-C16-C17	18.14	160.63	123.52
15	F	204	BCR	C10-C11-C12	18.13	175.74	123.20
15	G	847	BCR	C20-C21-C22	18.13	152.71	127.28
15	B	845	BCR	C16-C17-C18	18.13	152.70	127.28
15	G	846	BCR	C10-C11-C12	18.12	175.71	123.20
15	G	847	BCR	C10-C11-C12	18.11	175.69	123.20
15	L	203	BCR	C20-C21-C22	18.08	152.63	127.28
15	b	842	BCR	C15-C16-C17	17.98	160.30	123.52
15	A	852	BCR	C10-C11-C12	17.89	175.04	123.20
15	J	102	BCR	C15-C16-C17	17.80	159.93	123.52
15	j	103	BCR	C15-C16-C17	17.76	159.86	123.52
15	H	843	BCR	C10-C11-C12	17.75	174.63	123.20
15	b	841	BCR	C10-C11-C12	17.75	174.63	123.20
15	B	842	BCR	C10-C11-C12	17.69	174.45	123.20
15	a	852	BCR	C10-C11-C12	17.68	174.42	123.20
15	b	839	BCR	C10-C11-C12	17.67	174.41	123.20
15	G	853	BCR	C10-C11-C12	17.54	174.02	123.20
15	R	102	BCR	C15-C16-C17	17.51	159.34	123.52
16	G	854	LHG	O8-C23-O10	-17.30	80.34	123.63
16	A	853	LHG	O8-C23-O10	-17.23	80.52	123.63
15	A	846	BCR	C15-C16-C17	17.20	158.71	123.52
15	F	202	BCR	C10-C11-C12	17.19	173.02	123.20
17	m	101	45D	C20-C24-C26	17.07	151.49	126.23
17	T	101	45D	C20-C24-C26	17.04	151.45	126.23
15	G	850	BCR	C10-C11-C12	16.99	172.44	123.20
15	a	849	BCR	C10-C11-C12	16.87	172.09	123.20
17	M	101	45D	C20-C24-C26	16.85	151.17	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	849	BCR	C10-C11-C12	16.67	171.50	123.20
17	M	101	45D	C27-C25-C23	-16.44	92.98	118.09
17	m	101	45D	C41-C42-C38	-16.20	90.37	123.52
17	T	101	45D	C41-C42-C38	-16.19	90.39	123.52
17	m	101	45D	C27-C25-C23	-16.16	93.39	118.09
17	T	101	45D	C27-C25-C23	-16.15	93.42	118.09
15	A	849	BCR	C11-C10-C9	16.02	149.74	127.28
17	m	101	45D	C39-C35-C33	-15.99	93.66	118.09
17	M	101	45D	C39-C35-C33	-15.91	93.79	118.09
16	A	853	LHG	O8-C23-C24	15.87	160.21	111.83
17	T	101	45D	C39-C35-C33	-15.81	93.93	118.09
16	G	854	LHG	O8-C23-C24	15.79	159.99	111.83
15	a	849	BCR	C11-C10-C9	15.77	149.40	127.28
17	M	101	45D	C41-C42-C38	-15.77	91.26	123.52
15	b	841	BCR	C11-C10-C9	15.63	149.19	127.28
15	A	846	BCR	C16-C15-C14	15.53	155.30	123.52
17	M	101	45D	C40-C36-C34	-15.53	94.37	118.09
15	B	842	BCR	C11-C10-C9	15.51	149.03	127.28
17	T	101	45D	C40-C36-C34	-15.49	94.43	118.09
17	m	101	45D	C40-C36-C34	-15.47	94.45	118.09
15	b	844	BCR	C21-C20-C19	15.46	168.00	123.20
15	H	846	BCR	C21-C20-C19	15.42	167.89	123.20
15	H	843	BCR	C11-C10-C9	15.39	148.86	127.28
15	B	845	BCR	C21-C20-C19	15.39	167.79	123.20
15	G	850	BCR	C11-C10-C9	15.39	148.86	127.28
15	G	847	BCR	C21-C20-C19	15.31	167.57	123.20
15	a	846	BCR	C21-C20-C19	15.27	167.43	123.20
15	L	203	BCR	C21-C20-C19	15.25	167.39	123.20
17	M	101	45D	C28-C26-C24	-15.25	94.79	118.09
15	S	201	BCR	C21-C20-C19	15.20	167.24	123.20
15	F	202	BCR	C11-C10-C9	15.18	148.56	127.28
17	m	101	45D	C28-C26-C24	-15.16	94.93	118.09
17	T	101	45D	C28-C26-C24	-15.05	95.10	118.09
15	l	203	BCR	C21-C20-C19	15.03	166.75	123.20
15	R	102	BCR	C16-C15-C14	15.01	154.24	123.52
15	G	847	BCR	C16-C15-C14	15.01	154.23	123.52
15	a	846	BCR	C16-C15-C14	14.91	154.02	123.52
15	b	844	BCR	C11-C10-C9	14.76	147.98	127.28
15	B	842	BCR	C21-C20-C19	14.73	165.88	123.20
15	B	840	BCR	C11-C10-C9	14.72	147.92	127.28
15	G	849	BCR	C21-C20-C19	14.68	165.74	123.20
15	H	843	BCR	C21-C20-C19	14.64	165.62	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	845	BCR	C11-C10-C9	14.59	147.74	127.28
15	b	841	BCR	C21-C20-C19	14.54	165.34	123.20
15	b	842	BCR	C16-C15-C14	14.54	153.26	123.52
15	l	201	BCR	C21-C20-C19	14.51	165.25	123.20
15	i	101	BCR	C21-C20-C19	14.45	165.07	123.20
15	L	201	BCR	C21-C20-C19	14.44	165.05	123.20
15	H	849	BCR	C21-C20-C19	14.38	164.86	123.20
15	F	204	BCR	C21-C20-C19	14.35	164.79	123.20
15	a	849	BCR	C21-C20-C19	14.35	164.78	123.20
15	f	202	BCR	C21-C20-C19	14.34	164.74	123.20
15	H	846	BCR	C11-C10-C9	14.33	147.38	127.28
15	F	202	BCR	C21-C20-C19	14.33	164.71	123.20
15	j	103	BCR	C16-C15-C14	14.31	152.79	123.52
15	f	204	BCR	C21-C20-C19	14.30	164.62	123.20
15	B	843	BCR	C16-C15-C14	14.29	152.75	123.52
15	H	841	BCR	C21-C20-C19	14.29	164.59	123.20
15	H	844	BCR	C16-C15-C14	14.28	152.73	123.52
15	J	102	BCR	C16-C15-C14	14.27	152.72	123.52
15	A	849	BCR	C21-C20-C19	14.27	164.55	123.20
15	A	852	BCR	C16-C15-C14	14.27	152.71	123.52
15	P	204	BCR	C21-C20-C19	14.26	164.53	123.20
15	b	839	BCR	C21-C20-C19	14.25	164.50	123.20
15	S	205	BCR	C21-C20-C19	14.24	164.46	123.20
15	G	850	BCR	C21-C20-C19	14.23	164.43	123.20
15	i	101	BCR	C11-C10-C9	14.22	147.22	127.28
15	a	848	BCR	C21-C20-C19	14.22	164.40	123.20
15	A	848	BCR	C21-C20-C19	14.21	164.38	123.20
15	J	104	BCR	C21-C20-C19	14.20	164.34	123.20
15	A	845	BCR	C21-C20-C19	14.16	164.24	123.20
15	B	840	BCR	C21-C20-C19	14.15	164.19	123.20
15	R	101	BCR	C16-C15-C14	14.11	152.40	123.52
15	P	202	BCR	C21-C20-C19	14.11	164.09	123.20
15	I	101	BCR	C21-C20-C19	14.11	164.07	123.20
15	A	844	BCR	C21-C20-C19	14.09	164.01	123.20
15	a	852	BCR	C21-C20-C19	14.05	163.90	123.20
15	Q	101	BCR	C11-C10-C9	14.04	146.97	127.28
15	a	852	BCR	C16-C15-C14	14.03	152.23	123.52
15	G	853	BCR	C16-C15-C14	14.02	152.20	123.52
15	A	852	BCR	C21-C20-C19	14.01	163.80	123.20
15	i	102	BCR	C21-C20-C19	14.01	163.80	123.20
15	Q	101	BCR	C21-C20-C19	13.99	163.74	123.20
15	I	101	BCR	C11-C10-C9	13.96	146.86	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Q	102	BCR	C21-C20-C19	13.94	163.60	123.20
15	a	845	BCR	C21-C20-C19	13.94	163.59	123.20
15	j	101	BCR	C16-C15-C14	13.93	152.03	123.52
15	G	853	BCR	C21-C20-C19	13.92	163.54	123.20
15	a	844	BCR	C21-C20-C19	13.92	163.54	123.20
15	G	845	BCR	C21-C20-C19	13.88	163.41	123.20
15	b	839	BCR	C16-C15-C14	13.85	151.86	123.52
15	b	847	BCR	C21-C20-C19	13.85	163.32	123.20
15	G	846	BCR	C21-C20-C19	13.83	163.26	123.20
15	B	841	BCR	C21-C20-C19	13.79	163.16	123.20
15	a	844	BCR	C11-C10-C9	13.69	146.48	127.28
15	H	842	BCR	C21-C20-C19	13.68	162.85	123.20
15	A	849	BCR	C11-C12-C13	13.65	163.80	126.36
15	b	840	BCR	C21-C20-C19	13.64	162.72	123.20
15	I	101	BCR	C16-C15-C14	13.61	151.38	123.52
15	J	101	BCR	C16-C15-C14	13.60	151.35	123.52
15	H	841	BCR	C16-C15-C14	13.60	151.34	123.52
15	L	207	BCR	C21-C20-C19	13.51	162.35	123.20
15	i	101	BCR	C16-C15-C14	13.50	151.13	123.52
15	B	844	BCR	C16-C15-C14	13.43	150.99	123.52
15	A	844	BCR	C11-C10-C9	13.42	146.10	127.28
12	f	203	CLA	O2A-CGA-CBA	13.40	156.35	114.00
15	b	843	BCR	C16-C15-C14	13.40	150.94	123.52
12	F	203	CLA	O2A-CGA-CBA	13.37	156.25	114.00
12	P	203	CLA	O2A-CGA-CBA	13.34	156.14	114.00
15	G	848	BCR	C21-C20-C19	13.30	161.74	123.20
15	H	845	BCR	C21-C20-C19	13.29	161.71	123.20
15	b	844	BCR	C16-C15-C14	13.29	150.71	123.52
15	Q	101	BCR	C16-C15-C14	13.28	150.70	123.52
15	a	844	BCR	C16-C15-C14	13.26	150.65	123.52
15	H	845	BCR	C16-C15-C14	13.24	150.61	123.52
15	b	843	BCR	C21-C20-C19	13.24	161.56	123.20
15	a	847	BCR	C21-C20-C19	13.20	161.44	123.20
15	B	844	BCR	C21-C20-C19	13.18	161.38	123.20
15	B	840	BCR	C16-C15-C14	13.13	150.39	123.52
15	A	847	BCR	C21-C20-C19	13.13	161.24	123.20
15	G	845	BCR	C11-C10-C9	13.09	145.64	127.28
15	B	843	BCR	C21-C20-C19	13.08	161.10	123.20
15	B	845	BCR	C16-C15-C14	13.06	150.23	123.52
15	G	846	BCR	C11-C10-C9	13.05	145.58	127.28
15	A	848	BCR	C11-C10-C9	13.01	145.53	127.28
15	H	842	BCR	C16-C15-C14	13.00	150.12	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	849	BCR	C16-C15-C14	12.98	150.08	123.52
15	b	840	BCR	C16-C15-C14	12.97	150.06	123.52
15	H	846	BCR	C16-C15-C14	12.97	150.05	123.52
15	b	839	BCR	C11-C10-C9	12.97	145.47	127.28
15	H	841	BCR	C11-C10-C9	12.96	145.46	127.28
15	B	841	BCR	C16-C15-C14	12.96	150.03	123.52
15	G	845	BCR	C16-C15-C14	12.95	150.02	123.52
15	a	848	BCR	C16-C15-C14	12.93	149.97	123.52
15	j	103	BCR	C11-C10-C9	12.90	145.37	127.28
15	b	842	BCR	C21-C20-C19	12.89	160.56	123.20
15	R	102	BCR	C21-C20-C19	12.88	160.51	123.20
15	A	848	BCR	C16-C15-C14	12.87	149.85	123.52
15	R	101	BCR	C21-C20-C19	12.86	160.47	123.20
15	A	844	BCR	C16-C15-C14	12.85	149.82	123.52
15	B	842	BCR	C16-C15-C14	12.83	149.77	123.52
15	a	845	BCR	C11-C10-C9	12.83	145.27	127.28
15	b	841	BCR	C16-C15-C14	12.82	149.76	123.52
15	H	844	BCR	C21-C20-C19	12.80	160.29	123.20
15	a	846	BCR	C11-C10-C9	12.79	145.21	127.28
15	H	843	BCR	C16-C15-C14	12.78	149.66	123.52
15	F	202	BCR	C11-C12-C13	12.75	161.32	126.36
15	A	846	BCR	C21-C20-C19	12.74	160.11	123.20
15	J	102	BCR	C11-C10-C9	12.74	145.14	127.28
15	i	102	BCR	C16-C15-C14	12.73	149.56	123.52
15	j	101	BCR	C21-C20-C19	12.71	160.03	123.20
15	A	845	BCR	C11-C10-C9	12.71	145.10	127.28
15	P	204	BCR	C11-C10-C9	12.70	145.09	127.28
15	Q	102	BCR	C11-C10-C9	12.68	145.06	127.28
15	i	102	BCR	C11-C10-C9	12.68	145.06	127.28
15	Q	102	BCR	C16-C15-C14	12.66	149.43	123.52
15	L	207	BCR	C16-C15-C14	12.66	149.42	123.52
15	G	848	BCR	C11-C10-C9	12.65	145.02	127.28
15	j	103	BCR	C21-C20-C19	12.63	159.78	123.20
15	L	207	BCR	C24-C23-C22	-12.60	107.60	126.23
15	S	205	BCR	C16-C15-C14	12.59	149.29	123.52
17	m	101	45D	C42-C38-C36	-12.59	109.62	127.28
15	a	849	BCR	C11-C12-C13	12.58	160.87	126.36
15	P	202	BCR	C11-C10-C9	12.58	144.92	127.28
15	R	102	BCR	C11-C10-C9	12.55	144.88	127.28
15	l	201	BCR	C16-C15-C14	12.55	149.20	123.52
15	H	842	BCR	C11-C10-C9	12.55	144.88	127.28
17	M	101	45D	C42-C38-C36	-12.54	109.70	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	101	BCR	C21-C20-C19	12.53	159.50	123.20
15	B	841	BCR	C11-C10-C9	12.52	144.84	127.28
15	b	847	BCR	C11-C10-C9	12.49	144.80	127.28
15	a	847	BCR	C11-C10-C9	12.47	144.76	127.28
17	T	101	45D	C42-C38-C36	-12.45	109.81	127.28
15	J	102	BCR	C21-C20-C19	12.42	159.19	123.20
15	L	203	BCR	C16-C15-C14	12.35	148.80	123.52
15	L	201	BCR	C16-C15-C14	12.34	148.76	123.52
15	l	203	BCR	C16-C15-C14	12.33	148.76	123.52
15	F	204	BCR	C11-C10-C9	12.30	144.53	127.28
15	S	201	BCR	C16-C15-C14	12.29	148.67	123.52
15	l	203	BCR	C11-C10-C9	12.29	144.51	127.28
15	L	203	BCR	C11-C10-C9	12.29	144.51	127.28
15	L	207	BCR	C11-C10-C9	12.23	144.44	127.28
15	H	849	BCR	C16-C15-C14	12.23	148.54	123.52
15	b	840	BCR	C11-C10-C9	12.22	144.42	127.28
15	S	201	BCR	C11-C10-C9	12.19	144.37	127.28
15	G	850	BCR	C11-C12-C13	12.15	159.67	126.36
15	f	202	BCR	C11-C10-C9	12.14	144.31	127.28
15	A	846	BCR	C11-C10-C9	12.14	144.31	127.28
17	T	101	45D	C32-C30-C26	-12.10	110.31	127.28
15	a	848	BCR	C11-C10-C9	12.08	144.22	127.28
15	b	843	BCR	C11-C10-C9	12.04	144.16	127.28
15	G	846	BCR	C11-C12-C13	12.02	159.32	126.36
15	b	847	BCR	C16-C15-C14	12.01	148.09	123.52
17	M	101	45D	C32-C30-C26	-12.00	110.45	127.28
15	a	848	BCR	C11-C12-C13	11.98	159.21	126.36
15	G	849	BCR	C11-C10-C9	11.95	144.03	127.28
15	H	845	BCR	C11-C10-C9	11.90	143.97	127.28
12	P	203	CLA	O1A-CGA-CBA	-11.89	85.37	123.09
15	a	845	BCR	C11-C12-C13	11.89	158.98	126.36
15	A	849	BCR	C16-C15-C14	11.89	147.85	123.52
12	F	203	CLA	O1A-CGA-CBA	-11.88	85.43	123.09
15	j	101	BCR	C11-C10-C9	11.87	143.93	127.28
15	J	104	BCR	C11-C12-C13	11.87	158.91	126.36
12	f	203	CLA	O1A-CGA-CBA	-11.86	85.48	123.09
15	A	847	BCR	C11-C10-C9	11.81	143.84	127.28
15	G	849	BCR	C11-C12-C13	11.81	158.74	126.36
15	f	204	BCR	C11-C10-C9	11.80	143.83	127.28
17	m	101	45D	C32-C30-C26	-11.79	110.75	127.28
15	A	845	BCR	C11-C12-C13	11.76	158.62	126.36
15	B	842	BCR	C11-C12-C13	11.73	158.52	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	849	BCR	C16-C15-C14	11.72	147.50	123.52
15	A	848	BCR	C11-C12-C13	11.71	158.46	126.36
15	H	843	BCR	C11-C12-C13	11.70	158.46	126.36
15	J	104	BCR	C16-C15-C14	11.69	147.43	123.52
15	G	848	BCR	C16-C15-C14	11.68	147.42	123.52
17	T	101	45D	C31-C33-C35	-11.68	94.35	126.36
15	b	841	BCR	C11-C12-C13	11.67	158.37	126.36
15	a	847	BCR	C16-C15-C14	11.65	147.36	123.52
15	G	848	BCR	C11-C12-C13	11.65	158.30	126.36
15	G	850	BCR	C16-C15-C14	11.64	147.33	123.52
17	M	101	45D	C31-C33-C35	-11.62	94.51	126.36
15	B	844	BCR	C11-C10-C9	11.61	143.56	127.28
15	G	847	BCR	C11-C10-C9	11.60	143.55	127.28
15	b	847	BCR	C11-C12-C13	11.60	158.17	126.36
15	H	849	BCR	C11-C12-C13	11.58	158.12	126.36
15	a	847	BCR	C11-C12-C13	11.58	158.11	126.36
15	R	101	BCR	C11-C10-C9	11.54	143.47	127.28
17	m	101	45D	C31-C33-C35	-11.52	94.78	126.36
15	P	202	BCR	C16-C15-C14	11.51	147.06	123.52
15	f	204	BCR	C16-C15-C14	11.40	146.84	123.52
15	A	845	BCR	C16-C15-C14	11.34	146.72	123.52
15	b	840	BCR	C11-C12-C13	11.31	157.38	126.36
15	a	845	BCR	C16-C15-C14	11.30	146.64	123.52
15	A	847	BCR	C11-C12-C13	11.29	157.32	126.36
15	l	201	BCR	C11-C10-C9	11.28	143.10	127.28
16	G	854	LHG	O10-C23-C24	-11.28	79.67	123.78
16	A	853	LHG	O10-C23-C24	-11.27	79.70	123.78
15	f	202	BCR	C11-C12-C13	11.24	157.19	126.36
15	J	101	BCR	C11-C10-C9	11.24	143.04	127.28
15	P	202	BCR	C11-C12-C13	11.22	157.14	126.36
15	A	847	BCR	C16-C15-C14	11.22	146.47	123.52
15	L	201	BCR	C11-C10-C9	11.22	143.01	127.28
15	S	201	BCR	C11-C12-C13	11.21	157.11	126.36
15	i	102	BCR	C11-C12-C13	11.20	157.07	126.36
15	H	842	BCR	C11-C12-C13	11.18	157.03	126.36
15	i	102	BCR	C24-C23-C22	-11.18	109.70	126.23
15	J	101	BCR	C11-C12-C13	11.18	157.01	126.36
15	f	202	BCR	C16-C15-C14	11.16	146.36	123.52
15	j	101	BCR	C11-C12-C13	11.15	156.94	126.36
15	b	843	BCR	C11-C12-C13	11.15	156.93	126.36
15	R	101	BCR	C11-C12-C13	11.11	156.82	126.36
15	L	207	BCR	C11-C12-C13	11.09	156.78	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	841	BCR	C11-C12-C13	11.09	156.78	126.36
15	H	845	BCR	C11-C12-C13	11.09	156.77	126.36
15	Q	102	BCR	C11-C12-C13	11.07	156.72	126.36
15	Q	102	BCR	C24-C23-C22	-11.06	109.87	126.23
15	L	201	BCR	C11-C12-C13	11.04	156.64	126.36
15	G	846	BCR	C16-C15-C14	11.02	146.06	123.52
15	F	204	BCR	C16-C15-C14	10.94	145.90	123.52
15	P	204	BCR	C16-C15-C14	10.93	145.88	123.52
15	A	844	BCR	C11-C12-C13	10.85	156.12	126.36
15	G	845	BCR	C11-C12-C13	10.85	156.12	126.36
15	L	203	BCR	C11-C12-C13	10.84	156.09	126.36
17	m	101	45D	C41-C37-C35	-10.82	112.11	127.28
15	a	844	BCR	C11-C12-C13	10.81	155.99	126.36
17	M	101	45D	C41-C37-C35	-10.79	112.14	127.28
15	B	844	BCR	C11-C12-C13	10.77	155.89	126.36
15	S	205	BCR	C11-C10-C9	10.73	142.33	127.28
15	l	203	BCR	C11-C12-C13	10.73	155.79	126.36
17	m	101	45D	C33-C35-C37	10.72	135.87	119.01
15	l	201	BCR	C11-C12-C13	10.68	155.65	126.36
15	j	103	BCR	C11-C12-C13	10.64	155.55	126.36
15	F	202	BCR	C16-C15-C14	10.64	145.28	123.52
15	S	205	BCR	C11-C12-C13	10.63	155.51	126.36
15	H	849	BCR	C11-C10-C9	10.61	142.16	127.28
17	M	101	45D	C33-C35-C37	10.60	135.69	119.01
15	J	102	BCR	C11-C12-C13	10.49	155.13	126.36
17	T	101	45D	C41-C37-C35	-10.44	112.64	127.28
15	B	840	BCR	C11-C12-C13	10.42	154.94	126.36
15	H	841	BCR	C11-C12-C13	10.40	154.88	126.36
17	T	101	45D	C33-C35-C37	10.32	135.23	119.01
15	J	104	BCR	C11-C10-C9	10.25	141.66	127.28
15	R	102	BCR	C11-C12-C13	10.20	154.33	126.36
15	A	852	BCR	C11-C10-C9	10.16	141.52	127.28
12	G	836	CLA	CMD-C2D-C1D	10.12	142.55	124.73
15	G	847	BCR	C11-C12-C13	9.97	153.69	126.36
15	G	853	BCR	C11-C10-C9	9.94	141.22	127.28
15	a	846	BCR	C11-C12-C13	9.91	153.53	126.36
15	A	846	BCR	C11-C12-C13	9.87	153.43	126.36
15	Q	101	BCR	C11-C12-C13	9.83	153.33	126.36
15	b	844	BCR	C11-C12-C13	9.82	153.29	126.36
15	B	845	BCR	C11-C12-C13	9.80	153.24	126.36
15	a	852	BCR	C11-C12-C13	9.79	153.21	126.36
15	I	101	BCR	C11-C12-C13	9.77	153.16	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	852	BCR	C11-C10-C9	9.75	140.96	127.28
12	a	836	CLA	CMD-C2D-C1D	9.75	141.90	124.73
15	H	846	BCR	C11-C12-C13	9.61	152.71	126.36
15	A	852	BCR	C11-C12-C13	9.60	152.69	126.36
12	H	837	CLA	CMD-C2D-C1D	9.59	141.62	124.73
15	b	839	BCR	C11-C12-C13	9.59	152.65	126.36
12	G	809	CLA	CMD-C2D-C1D	9.59	141.61	124.73
17	M	101	45D	C34-C36-C38	9.49	133.94	119.01
15	i	101	BCR	C11-C12-C13	9.46	152.31	126.36
17	m	101	45D	C34-C36-C38	9.45	133.88	119.01
15	F	204	BCR	C11-C12-C13	9.43	152.21	126.36
12	b	802	CLA	C4A-NA-C1A	9.40	110.97	106.68
12	A	808	CLA	CMD-C2D-C1D	9.37	141.23	124.73
12	B	826	CLA	CMD-C2D-C1D	9.31	141.13	124.73
17	T	101	45D	C34-C36-C38	9.31	133.66	119.01
12	a	808	CLA	CMD-C2D-C1D	9.18	140.90	124.73
12	a	855	CLA	C4A-NA-C1A	9.18	110.87	106.68
12	b	806	CLA	C4A-NA-C1A	9.13	110.84	106.68
12	A	836	CLA	CMD-C2D-C1D	9.10	140.75	124.73
15	P	204	BCR	C11-C12-C13	9.06	151.20	126.36
12	H	827	CLA	CMD-C2D-C1D	9.05	140.66	124.73
12	b	826	CLA	CMD-C2D-C1D	9.03	140.63	124.73
12	B	836	CLA	CMD-C2D-C1D	9.03	140.62	124.73
17	M	101	45D	C23-C25-C29	9.01	133.18	119.01
12	A	855	CLA	C4A-NA-C1A	9.00	110.78	106.68
17	T	101	45D	C23-C25-C29	8.96	133.11	119.01
15	f	204	BCR	C11-C12-C13	8.94	150.86	126.36
17	m	101	45D	C23-C25-C29	8.93	133.06	119.01
12	b	835	CLA	CMD-C2D-C1D	8.90	140.41	124.73
15	G	853	BCR	C11-C12-C13	8.89	150.73	126.36
12	A	812	CLA	CMD-C2D-C1D	8.81	140.25	124.73
17	T	101	45D	C24-C26-C30	8.78	132.81	119.01
12	H	836	CLA	CMD-C2D-C1D	8.77	140.18	124.73
17	M	101	45D	C24-C26-C30	8.77	132.80	119.01
12	b	834	CLA	CMD-C2D-C1D	8.74	140.12	124.73
17	m	101	45D	C24-C26-C30	8.71	132.70	119.01
12	a	817	CLA	CMD-C2D-C1D	8.69	140.03	124.73
12	A	803	CLA	CMD-C2D-C1D	8.68	140.02	124.73
12	G	813	CLA	CMD-C2D-C1D	8.67	139.99	124.73
12	B	835	CLA	CMD-C2D-C1D	8.66	139.99	124.73
12	H	805	CLA	CMD-C2D-C1D	8.61	139.89	124.73
12	a	803	CLA	CMD-C2D-C1D	8.60	139.88	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	m	101	45D	C32-C34-C36	8.59	149.92	126.36
12	A	813	CLA	CMD-C2D-C1D	8.59	139.85	124.73
17	T	101	45D	C32-C34-C36	8.58	149.89	126.36
17	M	101	45D	C32-C34-C36	8.58	149.88	126.36
12	a	835	CLA	CMD-C2D-C1D	8.57	139.82	124.73
12	A	810	CLA	CMD-C2D-C1D	8.55	139.79	124.73
15	A	846	BCR	C20-C19-C18	8.54	149.78	126.36
12	a	812	CLA	CMD-C2D-C1D	8.50	139.70	124.73
12	A	822	CLA	CMD-C2D-C1D	8.49	139.69	124.73
12	A	805	CLA	CMD-C2D-C1D	8.47	139.64	124.73
12	H	828	CLA	CMD-C2D-C1D	8.46	139.62	124.73
12	G	806	CLA	CMD-C2D-C1D	8.42	139.56	124.73
12	A	817	CLA	CMD-C2D-C1D	8.40	139.52	124.73
12	b	831	CLA	CMD-C2D-C1D	8.39	139.50	124.73
12	G	811	CLA	CMD-C2D-C1D	8.38	139.49	124.73
12	B	837	CLA	C4A-NA-C1A	8.37	110.50	106.68
12	A	830	CLA	CMD-C2D-C1D	8.37	139.46	124.73
12	A	832	CLA	CMD-C2D-C1D	8.36	139.46	124.73
12	H	813	CLA	CMD-C2D-C1D	8.36	139.45	124.73
12	A	838	CLA	CMD-C2D-C1D	8.35	139.43	124.73
15	R	102	BCR	C20-C19-C18	8.34	149.24	126.36
15	J	102	BCR	C20-C19-C18	8.33	149.21	126.36
12	B	802	CLA	C4A-NA-C1A	8.33	110.48	106.68
12	A	806	CLA	CMD-C2D-C1D	8.33	139.40	124.73
12	H	833	CLA	CMD-C2D-C1D	8.30	139.35	124.73
12	B	832	CLA	CMD-C2D-C1D	8.29	139.33	124.73
12	H	819	CLA	CMD-C2D-C1D	8.29	139.33	124.73
12	G	818	CLA	CMD-C2D-C1D	8.29	139.33	124.73
12	G	824	CLA	CMD-C2D-C1D	8.29	139.32	124.73
12	G	807	CLA	CMD-C2D-C1D	8.28	139.32	124.73
12	G	835	CLA	CMD-C2D-C1D	8.28	139.31	124.73
12	B	806	CLA	C4A-NA-C1A	8.28	110.46	106.68
12	a	810	CLA	CMD-C2D-C1D	8.27	139.30	124.73
12	A	837	CLA	CMD-C2D-C1D	8.27	139.29	124.73
12	B	818	CLA	CMD-C2D-C1D	8.27	139.29	124.73
12	a	838	CLA	CMD-C2D-C1D	8.27	139.29	124.73
12	A	835	CLA	CMD-C2D-C1D	8.27	139.29	124.73
12	G	838	CLA	CMD-C2D-C1D	8.26	139.28	124.73
12	a	806	CLA	CMD-C2D-C1D	8.25	139.26	124.73
12	H	814	CLA	CMD-C2D-C1D	8.25	139.25	124.73
15	H	844	BCR	C20-C19-C18	8.25	148.97	126.36
12	G	816	CLA	CMD-C2D-C1D	8.24	139.23	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	855	CLA	C2D-C1D-ND	8.24	118.28	110.13
12	b	818	CLA	CMD-C2D-C1D	8.22	139.20	124.73
12	G	814	CLA	CMD-C2D-C1D	8.22	139.20	124.73
12	b	827	CLA	CMD-C2D-C1D	8.21	139.19	124.73
15	R	101	BCR	C20-C19-C18	8.21	148.88	126.36
15	j	101	BCR	C20-C19-C18	8.20	148.86	126.36
12	a	805	CLA	CMD-C2D-C1D	8.20	139.18	124.73
12	B	805	CLA	CMD-C2D-C1D	8.20	139.17	124.73
12	a	815	CLA	CMD-C2D-C1D	8.18	139.14	124.73
12	A	815	CLA	CMD-C2D-C1D	8.17	139.11	124.73
12	B	815	CLA	CMD-C2D-C1D	8.16	139.10	124.73
12	G	820	CLA	CMD-C2D-C1D	8.16	139.09	124.73
12	A	823	CLA	CMD-C2D-C1D	8.16	139.09	124.73
15	b	842	BCR	C20-C19-C18	8.16	148.73	126.36
12	A	819	CLA	CMD-C2D-C1D	8.15	139.08	124.73
12	f	203	CLA	CMD-C2D-C1D	8.15	139.07	124.73
12	G	810	CLA	CMD-C2D-C1D	8.14	139.07	124.73
12	B	813	CLA	CMD-C2D-C1D	8.14	139.06	124.73
12	a	819	CLA	CMD-C2D-C1D	8.14	139.06	124.73
12	G	831	CLA	CMD-C2D-C1D	8.14	139.05	124.73
12	P	203	CLA	CMD-C2D-C1D	8.13	139.05	124.73
12	F	203	CLA	CMD-C2D-C1D	8.12	139.03	124.73
12	G	823	CLA	CMD-C2D-C1D	8.12	139.03	124.73
12	H	810	CLA	CMD-C2D-C1D	8.11	139.02	124.73
12	H	804	CLA	CMD-C2D-C1D	8.11	139.01	124.73
12	a	830	CLA	CMD-C2D-C1D	8.11	139.00	124.73
12	H	806	CLA	C4A-NA-C1A	8.11	110.38	106.68
12	a	813	CLA	CMD-C2D-C1D	8.10	139.00	124.73
12	J	103	CLA	CMD-C2D-C1D	8.10	138.99	124.73
12	a	837	CLA	CMD-C2D-C1D	8.09	138.98	124.73
12	B	828	CLA	CMD-C2D-C1D	8.09	138.98	124.73
15	J	101	BCR	C20-C19-C18	8.09	148.54	126.36
15	B	843	BCR	C20-C19-C18	8.09	148.53	126.36
12	b	829	CLA	CMD-C2D-C1D	8.08	138.95	124.73
12	a	822	CLA	CMD-C2D-C1D	8.08	138.95	124.73
12	B	809	CLA	CMD-C2D-C1D	8.07	138.93	124.73
12	R	103	CLA	CMD-C2D-C1D	8.07	138.93	124.73
15	A	847	BCR	C20-C19-C18	8.06	148.46	126.36
12	G	832	CLA	CMD-C2D-C1D	8.06	138.92	124.73
12	b	832	CLA	CMD-C2D-C1D	8.05	138.91	124.73
15	a	847	BCR	C20-C19-C18	8.05	148.43	126.36
12	b	809	CLA	CMD-C2D-C1D	8.05	138.90	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	823	CLA	CMD-C2D-C1D	8.04	138.89	124.73
12	H	816	CLA	CMD-C2D-C1D	8.03	138.88	124.73
12	B	829	CLA	CMD-C2D-C1D	8.03	138.87	124.73
12	j	104	CLA	CMD-C2D-C1D	8.03	138.87	124.73
12	B	821	CLA	CMD-C2D-C1D	8.03	138.87	124.73
12	b	813	CLA	CMD-C2D-C1D	8.03	138.87	124.73
12	b	804	CLA	CMD-C2D-C1D	8.03	138.87	124.73
12	H	830	CLA	CMD-C2D-C1D	8.03	138.86	124.73
12	G	839	CLA	CMD-C2D-C1D	8.02	138.85	124.73
12	a	809	CLA	CMD-C2D-C1D	8.02	138.85	124.73
15	G	848	BCR	C20-C19-C18	8.01	148.32	126.36
12	b	819	CLA	CMD-C2D-C1D	7.99	138.80	124.73
12	a	804	CLA	CMD-C2D-C1D	7.97	138.76	124.73
12	B	804	CLA	CMD-C2D-C1D	7.97	138.76	124.73
12	a	832	CLA	CMD-C2D-C1D	7.96	138.75	124.73
12	A	807	CLA	CMD-C2D-C1D	7.96	138.75	124.73
12	H	801	CLA	CMD-C2D-C1D	7.96	138.74	124.73
12	H	804	CLA	C2D-C1D-ND	7.95	118.00	110.13
12	G	804	CLA	CMD-C2D-C1D	7.95	138.73	124.73
12	A	821	CLA	CMD-C2D-C1D	7.95	138.72	124.73
12	a	820	CLA	CMD-C2D-C1D	7.94	138.71	124.73
12	b	810	CLA	CMD-C2D-C1D	7.94	138.71	124.73
12	G	805	CLA	CMD-C2D-C1D	7.94	138.71	124.73
12	b	812	CLA	CMD-C2D-C1D	7.94	138.70	124.73
12	H	820	CLA	CMD-C2D-C1D	7.93	138.69	124.73
12	b	815	CLA	CMD-C2D-C1D	7.92	138.68	124.73
12	b	828	CLA	CMD-C2D-C1D	7.92	138.68	124.73
12	H	815	CLA	CMD-C2D-C1D	7.92	138.67	124.73
12	A	804	CLA	CMD-C2D-C1D	7.90	138.64	124.73
12	b	808	CLA	CMD-C2D-C1D	7.89	138.63	124.73
12	B	808	CLA	CMD-C2D-C1D	7.89	138.63	124.73
12	B	803	CLA	CMD-C2D-C1D	7.88	138.61	124.73
12	G	819	CLA	CMD-C2D-C1D	7.88	138.60	124.73
12	H	802	CLA	C4A-NA-C1A	7.87	110.27	106.68
12	b	805	CLA	CMD-C2D-C1D	7.87	138.58	124.73
12	G	822	CLA	CMD-C2D-C1D	7.86	138.58	124.73
12	a	839	CLA	CMD-C2D-C1D	7.86	138.57	124.73
12	G	837	CLA	CMD-C2D-C1D	7.86	138.57	124.73
12	B	833	CLA	CMD-C2D-C1D	7.86	138.56	124.73
12	H	829	CLA	CMD-C2D-C1D	7.85	138.55	124.73
12	H	827	CLA	C2C-C1C-NC	7.85	118.22	109.98
15	j	103	BCR	C20-C19-C18	7.85	147.88	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	809	CLA	CMD-C2D-C1D	7.84	138.54	124.73
12	b	821	CLA	CMD-C2D-C1D	7.84	138.53	124.73
12	a	807	CLA	CMD-C2D-C1D	7.84	138.53	124.73
12	H	816	CLA	C2C-C1C-NC	7.83	118.20	109.98
12	A	836	CLA	OBD-CAD-C3D	-7.83	110.12	128.42
12	a	821	CLA	CMD-C2D-C1D	7.82	138.51	124.73
12	H	811	CLA	CMD-C2D-C1D	7.81	138.49	124.73
12	b	811	CLA	CMD-C2D-C1D	7.81	138.49	124.73
12	b	822	CLA	O2D-CGD-CBD	7.80	124.87	111.23
12	H	834	CLA	CMD-C2D-C1D	7.79	138.46	124.73
12	A	836	CLA	O2D-CGD-CBD	7.79	124.85	111.23
12	B	819	CLA	CMD-C2D-C1D	7.79	138.45	124.73
12	H	850	CLA	CMD-C2D-C1D	7.79	138.45	124.73
12	l	205	CLA	CMD-C2D-C1D	7.78	138.44	124.73
12	b	816	CLA	CMD-C2D-C1D	7.77	138.41	124.73
12	G	821	CLA	CMD-C2D-C1D	7.77	138.41	124.73
12	a	818	CLA	CMD-C2D-C1D	7.76	138.39	124.73
12	A	833	CLA	CMD-C2D-C1D	7.74	138.37	124.73
12	a	831	CLA	CMD-C2D-C1D	7.74	138.35	124.73
12	H	812	CLA	CMD-C2D-C1D	7.73	138.34	124.73
12	A	839	CLA	CMD-C2D-C1D	7.72	138.33	124.73
12	B	812	CLA	CMD-C2D-C1D	7.72	138.33	124.73
12	H	816	CLA	C1C-C2C-C3C	-7.72	98.86	106.98
12	b	836	CLA	C4A-NA-C1A	7.71	110.20	106.68
12	A	818	CLA	CMD-C2D-C1D	7.71	138.31	124.73
12	B	817	CLA	CMD-C2D-C1D	7.69	138.28	124.73
12	b	802	CLA	O2D-CGD-CBD	7.69	124.67	111.23
12	B	810	CLA	CMD-C2D-C1D	7.68	138.25	124.73
12	B	811	CLA	CMD-C2D-C1D	7.68	138.25	124.73
12	b	814	CLA	CMD-C2D-C1D	7.68	138.25	124.73
12	H	817	CLA	CMD-C2D-C1D	7.68	138.24	124.73
12	B	816	CLA	CMD-C2D-C1D	7.65	138.19	124.73
12	a	833	CLA	CMD-C2D-C1D	7.64	138.19	124.73
12	B	814	CLA	CMD-C2D-C1D	7.63	138.17	124.73
12	A	855	CLA	C2D-C1D-ND	7.62	117.67	110.13
12	A	814	CLA	CMD-C2D-C1D	7.61	138.13	124.73
12	A	831	CLA	CMD-C2D-C1D	7.61	138.12	124.73
12	G	808	CLA	CMD-C2D-C1D	7.61	138.12	124.73
12	H	824	CLA	CMD-C2D-C1D	7.60	138.12	124.73
12	G	856	CLA	C2D-C1D-ND	7.60	117.65	110.13
12	A	826	CLA	CMD-C2D-C1D	7.59	138.10	124.73
12	A	820	CLA	C4A-NA-C1A	7.58	110.14	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	827	CLA	CMD-C2D-C1D	7.58	138.08	124.73
12	A	809	CLA	CMD-C2D-C1D	7.58	138.07	124.73
12	G	817	CLA	CMD-C2D-C1D	7.57	138.06	124.73
15	G	853	BCR	C20-C19-C18	7.55	147.06	126.36
12	b	824	CLA	C4A-NA-C1A	7.53	110.11	106.68
12	B	807	CLA	C4A-NA-C1A	7.53	110.11	106.68
12	L	205	CLA	CMD-C2D-C1D	7.52	137.97	124.73
12	G	856	CLA	C4A-NA-C1A	7.52	110.11	106.68
12	B	823	CLA	CMD-C2D-C1D	7.51	137.96	124.73
12	H	816	CLA	C1D-ND-C4D	-7.51	101.04	106.31
12	A	820	CLA	CMD-C2D-C1D	7.51	137.95	124.73
12	H	822	CLA	C4A-NA-C1A	7.50	110.10	106.68
12	H	803	CLA	O2A-CGA-O1A	-7.49	104.89	123.63
12	l	202	CLA	CMD-C2D-C1D	7.48	137.89	124.73
12	H	807	CLA	C2C-C1C-NC	7.47	117.83	109.98
12	H	807	CLA	C4A-NA-C1A	7.46	110.08	106.68
12	a	814	CLA	CMD-C2D-C1D	7.46	137.86	124.73
12	b	833	CLA	CMD-C2D-C1D	7.45	137.85	124.73
15	a	852	BCR	C20-C19-C18	7.44	146.77	126.36
12	b	803	CLA	CMD-C2D-C1D	7.44	137.83	124.73
12	b	837	CLA	CMD-C2D-C1D	7.44	137.83	124.73
12	L	206	CLA	CMD-C2D-C1D	7.43	137.81	124.73
12	H	832	CLA	O2D-CGD-CBD	7.41	124.19	111.23
12	B	826	CLA	C2C-C1C-NC	7.41	117.77	109.98
12	B	803	CLA	C4A-NA-C1A	7.41	110.06	106.68
15	b	840	BCR	C20-C19-C18	7.41	146.67	126.36
12	a	826	CLA	CMD-C2D-C1D	7.41	137.77	124.73
12	A	820	CLA	C2C-C1C-NC	7.40	117.75	109.98
12	H	831	CLA	O2D-CGD-CBD	7.40	124.16	111.23
15	a	845	BCR	C20-C19-C18	7.38	146.61	126.36
12	H	802	CLA	O2D-CGD-CBD	7.38	124.13	111.23
12	A	854	CLA	C2D-C1D-ND	7.37	117.42	110.13
12	H	838	CLA	C4A-NA-C1A	7.37	110.04	106.68
12	L	202	CLA	CMD-C2D-C1D	7.37	137.71	124.73
12	G	826	CLA	CMD-C2D-C1D	7.37	137.70	124.73
15	A	852	BCR	C20-C19-C18	7.37	146.56	126.36
12	b	820	CLA	CMD-C2D-C1D	7.36	137.68	124.73
15	B	844	BCR	C20-C19-C18	7.35	146.51	126.36
12	G	842	CLA	C4A-NA-C1A	7.34	110.03	106.68
12	b	830	CLA	O2D-CGD-CBD	7.34	124.06	111.23
12	G	815	CLA	CMD-C2D-C1D	7.33	137.64	124.73
12	G	855	CLA	C2D-C1D-ND	7.33	117.38	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	848	CLA	CMD-C2D-C1D	7.32	137.62	124.73
12	b	836	CLA	CMD-C2D-C1D	7.30	137.59	124.73
12	G	827	CLA	CMD-C2D-C1D	7.30	137.59	124.73
12	a	837	CLA	O2D-CGD-CBD	7.30	123.98	111.23
12	a	807	CLA	C4A-NA-C1A	7.29	110.01	106.68
12	H	802	CLA	C2D-C1D-ND	7.29	117.34	110.13
15	G	846	BCR	C20-C19-C18	7.29	146.34	126.36
12	H	808	CLA	CMD-C2D-C1D	7.29	137.56	124.73
12	a	816	CLA	C2C-C1C-NC	7.28	117.63	109.98
12	A	829	CLA	C2C-C1C-NC	7.28	117.63	109.98
15	b	839	BCR	C7-C8-C9	-7.28	115.46	126.23
15	a	844	BCR	C20-C19-C18	7.27	146.30	126.36
12	B	834	CLA	CMD-C2D-C1D	7.27	137.53	124.73
12	b	824	CLA	CMD-C2D-C1D	7.26	137.51	124.73
12	a	854	CLA	C2D-C1D-ND	7.24	117.30	110.13
15	b	843	BCR	C20-C19-C18	7.24	146.22	126.36
15	B	841	BCR	C20-C19-C18	7.23	146.18	126.36
12	G	812	CLA	CMD-C2D-C1D	7.22	137.45	124.73
12	b	807	CLA	C2C-C1C-NC	7.22	117.57	109.98
12	H	803	CLA	CMD-C2D-C1D	7.22	137.44	124.73
12	B	820	CLA	CMD-C2D-C1D	7.22	137.43	124.73
12	l	206	CLA	CMD-C2D-C1D	7.20	137.41	124.73
15	L	207	BCR	C20-C19-C18	7.20	146.11	126.36
12	B	837	CLA	C2C-C1C-NC	7.20	117.54	109.98
12	B	831	CLA	O2D-CGD-CBD	7.19	123.80	111.23
12	b	826	CLA	C2C-C1C-NC	7.18	117.52	109.98
15	G	845	BCR	C20-C19-C18	7.17	146.03	126.36
12	A	818	CLA	C4A-NA-C1A	7.17	109.95	106.68
12	A	841	CLA	C2C-C1C-NC	7.16	117.50	109.98
12	S	204	CLA	CMD-C2D-C1D	7.15	137.33	124.73
11	A	801	CL0	C4A-NA-C1A	7.15	109.94	106.68
12	b	804	CLA	C2D-C1D-ND	7.15	117.20	110.13
12	b	836	CLA	C2C-C1C-NC	7.14	117.48	109.98
12	H	838	CLA	CMD-C2D-C1D	7.13	137.28	124.73
12	H	828	CLA	O2D-CGD-CBD	7.12	123.67	111.23
12	H	818	CLA	CMD-C2D-C1D	7.12	137.26	124.73
15	H	845	BCR	C20-C19-C18	7.12	145.88	126.36
12	a	829	CLA	C2C-C1C-NC	7.12	117.46	109.98
12	G	808	CLA	C4A-NA-C1A	7.10	109.92	106.68
12	A	810	CLA	C4A-NA-C1A	7.10	109.92	106.68
15	b	847	BCR	C20-C19-C18	7.09	145.81	126.36
12	S	203	CLA	CMD-C2D-C1D	7.09	137.22	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	830	CLA	C2C-C1C-NC	7.08	117.42	109.98
12	G	842	CLA	CMD-C2D-C1D	7.08	137.20	124.73
12	B	804	CLA	C2D-C1D-ND	7.08	117.13	110.13
12	b	807	CLA	CMD-C2D-C1D	7.07	137.18	124.73
12	B	821	CLA	C4A-NA-C1A	7.07	109.90	106.68
12	P	201	CLA	CMD-C2D-C1D	7.06	137.17	124.73
12	G	840	CLA	CMD-C2D-C1D	7.05	137.15	124.73
15	b	841	BCR	C20-C19-C18	7.05	145.70	126.36
12	B	830	CLA	CMD-C2D-C1D	7.04	137.13	124.73
12	G	841	CLA	C2C-C1C-NC	7.04	117.37	109.98
12	B	806	CLA	CMD-C2D-C1D	7.03	137.11	124.73
12	a	811	CLA	CMD-C2D-C1D	7.03	137.10	124.73
12	G	811	CLA	C4A-NA-C1A	7.02	109.88	106.68
12	A	854	CLA	C3B-C2B-C1B	-7.01	98.90	107.17
12	B	838	CLA	CMD-C2D-C1D	7.01	137.08	124.73
15	B	842	BCR	C20-C19-C18	7.01	145.59	126.36
12	b	803	CLA	O2A-CGA-O1A	-7.00	106.11	123.63
12	A	834	CLA	CMD-C2D-C1D	7.00	137.06	124.73
12	H	821	CLA	CMD-C2D-C1D	6.99	137.03	124.73
12	B	802	CLA	O2D-CGD-CBD	6.99	123.44	111.23
12	H	838	CLA	C2C-C1C-NC	6.99	117.32	109.98
12	G	815	CLA	C4A-NA-C1A	6.98	109.86	106.68
12	H	813	CLA	C4A-NA-C1A	6.98	109.86	106.68
15	H	842	BCR	C20-C19-C18	6.97	145.49	126.36
15	A	845	BCR	C20-C19-C18	6.97	145.47	126.36
12	B	837	CLA	CMD-C2D-C1D	6.95	136.97	124.73
17	M	101	45D	C42-C41-C37	-6.95	109.31	123.52
12	b	812	CLA	C4A-NA-C1A	6.94	109.84	106.68
12	b	810	CLA	O2D-CGD-CBD	6.94	123.35	111.23
12	H	804	CLA	C3D-C2D-C1D	-6.93	96.37	105.83
12	A	816	CLA	CMD-C2D-C1D	6.93	136.93	124.73
15	H	843	BCR	C20-C19-C18	6.93	145.37	126.36
15	A	844	BCR	C20-C19-C18	6.93	145.36	126.36
12	b	834	CLA	C4A-NA-C1A	6.92	109.84	106.68
15	Q	102	BCR	C20-C19-C18	6.91	145.32	126.36
12	B	838	CLA	O2D-CGD-CBD	6.91	123.31	111.23
12	H	839	CLA	CMD-C2D-C1D	6.89	136.87	124.73
12	G	803	CLA	CMD-C2D-C1D	6.89	136.87	124.73
12	b	807	CLA	C4A-NA-C1A	6.89	109.82	106.68
15	S	205	BCR	C20-C19-C18	6.89	145.26	126.36
15	J	104	BCR	C20-C19-C18	6.88	145.22	126.36
15	A	847	BCR	C3-C4-C5	-6.88	101.79	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	807	CLA	O2D-CGD-CBD	6.87	123.23	111.23
12	A	825	CLA	CMD-C2D-C1D	6.87	136.82	124.73
12	B	803	CLA	O2A-CGA-O1A	-6.86	106.47	123.63
12	a	841	CLA	C2C-C1C-NC	6.86	117.19	109.98
12	A	840	CLA	CMD-C2D-C1D	6.85	136.80	124.73
12	A	811	CLA	CMD-C2D-C1D	6.84	136.78	124.73
12	b	817	CLA	CMD-C2D-C1D	6.84	136.78	124.73
12	G	819	CLA	C4A-NA-C1A	6.84	109.80	106.68
12	a	816	CLA	CMD-C2D-C1D	6.84	136.77	124.73
12	G	814	CLA	O2D-CGD-CBD	6.83	123.17	111.23
12	G	813	CLA	C2C-C1C-NC	6.83	117.16	109.98
12	b	805	CLA	C4A-NA-C1A	6.83	109.80	106.68
12	H	834	CLA	C2C-C1C-NC	6.83	117.15	109.98
12	l	205	CLA	C4A-NA-C1A	6.82	109.79	106.68
12	H	827	CLA	CAC-C3C-C4C	6.82	133.66	124.79
12	A	816	CLA	C2C-C1C-NC	6.82	117.14	109.98
12	S	203	CLA	C4A-NA-C1A	6.81	109.79	106.68
12	A	827	CLA	CMD-C2D-C1D	6.81	136.71	124.73
12	b	821	CLA	C4A-NA-C1A	6.80	109.78	106.68
12	G	834	CLA	C4A-NA-C1A	6.80	109.78	106.68
17	m	101	45D	C42-C41-C37	-6.80	109.61	123.52
12	a	827	CLA	CMD-C2D-C1D	6.79	136.68	124.73
17	M	101	45D	C27-C25-C29	6.79	133.81	122.82
15	P	202	BCR	C20-C19-C18	6.78	144.96	126.36
12	B	825	CLA	C2C-C1C-NC	6.78	117.11	109.98
12	G	833	CLA	CMD-C2D-C1D	6.78	136.66	124.73
12	L	204	CLA	C4A-NA-C1A	6.77	109.77	106.68
12	H	806	CLA	CMD-C2D-C1D	6.77	136.64	124.73
17	T	101	45D	C42-C41-C37	-6.76	109.68	123.52
12	H	825	CLA	CMD-C2D-C1D	6.76	136.63	124.73
12	H	836	CLA	C4A-NA-C1A	6.76	109.76	106.68
15	P	204	BCR	C20-C19-C18	6.76	144.89	126.36
12	a	834	CLA	C4A-NA-C1A	6.75	109.76	106.68
15	l	201	BCR	C20-C19-C18	6.75	144.87	126.36
12	b	830	CLA	C2C-C1C-NC	6.74	117.06	109.98
12	B	833	CLA	C2C-C1C-NC	6.74	117.06	109.98
12	b	823	CLA	CMD-C2D-C1D	6.74	136.59	124.73
12	G	811	CLA	O2D-CGD-CBD	6.74	123.00	111.23
12	G	834	CLA	CMD-C2D-C1D	6.73	136.59	124.73
12	H	831	CLA	C2D-C1D-ND	6.73	116.78	110.13
12	a	840	CLA	CMD-C2D-C1D	6.72	136.57	124.73
12	H	820	CLA	C4A-NA-C1A	6.72	109.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	807	CLA	C2C-C1C-NC	6.72	117.04	109.98
12	B	835	CLA	C4A-NA-C1A	6.72	109.74	106.68
15	I	101	BCR	C20-C19-C18	6.72	144.78	126.36
12	a	855	CLA	CAC-C3C-C4C	6.71	133.53	124.79
12	A	813	CLA	O2D-CGD-CBD	6.71	122.96	111.23
12	L	205	CLA	C4A-NA-C1A	6.71	109.74	106.68
12	a	802	CLA	CMD-C2D-C1D	6.71	136.54	124.73
12	L	204	CLA	O2D-CGD-CBD	6.71	122.95	111.23
12	A	830	CLA	O2D-CGD-CBD	6.70	122.95	111.23
15	f	204	BCR	C20-C19-C18	6.69	144.72	126.36
12	a	818	CLA	C2C-C1C-NC	6.69	117.01	109.98
12	B	833	CLA	C4A-NA-C1A	6.69	109.73	106.68
12	a	825	CLA	CMD-C2D-C1D	6.68	136.50	124.73
12	a	807	CLA	O2D-CGD-CBD	6.67	122.90	111.23
11	a	801	CL0	C2C-C1C-NC	6.67	116.98	109.98
12	A	827	CLA	C4A-NA-C1A	6.66	109.72	106.68
12	B	819	CLA	C4A-NA-C1A	6.66	109.72	106.68
15	a	848	BCR	C20-C19-C18	6.66	144.62	126.36
11	G	801	CL0	C4A-NA-C1A	6.65	109.72	106.68
12	A	807	CLA	C4A-NA-C1A	6.65	109.72	106.68
12	a	855	CLA	C1D-ND-C4D	-6.65	101.64	106.31
12	L	205	CLA	C2D-C1D-ND	6.65	116.70	110.13
12	B	824	CLA	CMD-C2D-C1D	6.65	136.43	124.73
15	i	102	BCR	C20-C19-C18	6.64	144.58	126.36
15	a	847	BCR	C3-C4-C5	-6.64	102.21	114.06
12	S	203	CLA	C2D-C1D-ND	6.64	116.69	110.13
12	a	854	CLA	C3B-C2B-C1B	-6.63	99.35	107.17
12	B	801	CLA	C4A-NA-C1A	6.63	109.70	106.68
12	G	828	CLA	CMD-C2D-C1D	6.63	136.40	124.73
12	H	835	CLA	C4A-NA-C1A	6.63	109.70	106.68
12	b	821	CLA	O2D-CGD-CBD	6.62	122.81	111.23
12	S	202	CLA	C4A-NA-C1A	6.62	109.70	106.68
12	H	804	CLA	C1D-ND-C4D	-6.62	101.67	106.31
12	b	848	CLA	C4A-NA-C1A	6.61	109.69	106.68
12	B	801	CLA	C2D-C1D-ND	6.61	116.67	110.13
12	H	839	CLA	C4A-NA-C1A	6.61	109.69	106.68
12	B	805	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	Q	101	BCR	C20-C19-C18	6.61	144.47	126.36
17	m	101	45D	C27-C25-C29	6.61	133.52	122.82
15	B	840	BCR	C20-C19-C18	6.59	144.44	126.36
12	H	823	CLA	C2D-C1D-ND	6.59	116.65	110.13
12	F	201	CLA	CMD-C2D-C1D	6.59	136.34	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	829	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	b	837	CLA	O2D-CGD-CBD	6.58	122.74	111.23
12	G	817	CLA	C2C-C1C-NC	6.58	116.89	109.98
12	H	809	CLA	C2C-C1C-NC	6.58	116.89	109.98
12	l	205	CLA	C2D-C1D-ND	6.57	116.63	110.13
12	b	802	CLA	CMD-C2D-C1D	6.57	136.29	124.73
12	a	814	CLA	C4A-NA-C1A	6.56	109.67	106.68
12	b	817	CLA	C4A-NA-C1A	6.56	109.67	106.68
12	B	817	CLA	C4A-NA-C1A	6.56	109.67	106.68
17	T	101	45D	C27-C25-C29	6.56	133.44	122.82
12	B	808	CLA	C2C-C1C-NC	6.55	116.86	109.98
12	b	815	CLA	C4A-NA-C1A	6.55	109.67	106.68
12	H	816	CLA	C2D-C1D-ND	6.54	116.60	110.13
15	L	201	BCR	C20-C19-C18	6.54	144.30	126.36
15	f	202	BCR	C20-C19-C18	6.54	144.30	126.36
15	A	848	BCR	C20-C19-C18	6.54	144.30	126.36
12	G	855	CLA	C3B-C2B-C1B	-6.54	99.46	107.17
12	G	837	CLA	O2D-CGD-CBD	6.53	122.65	111.23
12	a	827	CLA	C4A-NA-C1A	6.53	109.66	106.68
12	b	803	CLA	C4A-NA-C1A	6.53	109.66	106.68
15	b	839	BCR	C20-C19-C18	6.53	144.27	126.36
12	B	804	CLA	C3D-C2D-C1D	-6.52	96.94	105.83
12	A	809	CLA	C4A-NA-C1A	6.51	109.65	106.68
12	H	850	CLA	C4A-NA-C1A	6.51	109.65	106.68
12	b	801	CLA	C4A-NA-C1A	6.51	109.65	106.68
12	A	824	CLA	C2C-C1C-NC	6.51	116.82	109.98
12	A	809	CLA	O2D-CGD-CBD	6.50	122.60	111.23
12	b	825	CLA	C2C-C1C-NC	6.50	116.81	109.98
12	a	829	CLA	C4A-NA-C1A	6.49	109.64	106.68
12	G	802	CLA	C2D-C1D-ND	6.49	116.55	110.13
12	b	833	CLA	C4A-NA-C1A	6.49	109.64	106.68
12	H	806	CLA	C1D-ND-C4D	-6.49	101.76	106.31
12	b	812	CLA	C2C-C1C-NC	6.49	116.79	109.98
12	H	802	CLA	C1D-ND-C4D	-6.48	101.76	106.31
12	a	818	CLA	C4A-NA-C1A	6.48	109.64	106.68
12	B	834	CLA	C4A-NA-C1A	6.48	109.64	106.68
12	b	822	CLA	CMD-C2D-C1D	6.48	136.14	124.73
11	a	801	CL0	C1C-C2C-C3C	-6.48	100.17	106.98
12	b	808	CLA	C2C-C1C-NC	6.47	116.78	109.98
15	F	202	BCR	C20-C19-C18	6.47	144.10	126.36
12	G	825	CLA	C2C-C1C-NC	6.47	116.78	109.98
12	a	804	CLA	O2D-CGD-CBD	6.46	122.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	839	CLA	C4A-NA-C1A	6.46	109.63	106.68
12	A	806	CLA	C1C-C2C-C3C	-6.46	100.19	106.98
12	b	802	CLA	C2D-C1D-ND	6.45	116.51	110.13
12	A	802	CLA	CMD-C2D-C1D	6.45	136.09	124.73
12	b	810	CLA	C3D-C2D-C1D	-6.45	97.03	105.83
12	G	828	CLA	C3B-C2B-C1B	-6.45	99.57	107.17
12	b	804	CLA	C3D-C2D-C1D	-6.43	97.05	105.83
12	B	810	CLA	C3D-C2D-C1D	-6.43	97.05	105.83
12	H	813	CLA	O2D-CGD-CBD	6.43	122.47	111.23
12	H	806	CLA	O2D-CGD-CBD	6.42	122.46	111.23
12	G	808	CLA	O2D-CGD-CBD	6.42	122.46	111.23
12	G	835	CLA	C2C-C1C-NC	6.42	116.73	109.98
15	F	204	BCR	C20-C19-C18	6.42	143.97	126.36
11	A	801	CL0	C1C-C2C-C3C	-6.42	100.23	106.98
12	a	827	CLA	C3B-C2B-C1B	-6.42	99.61	107.17
12	a	816	CLA	C1C-C2C-C3C	-6.42	100.23	106.98
12	l	204	CLA	C4A-NA-C1A	6.42	109.61	106.68
12	F	203	CLA	C2C-C1C-NC	6.41	116.71	109.98
12	G	830	CLA	C4A-NA-C1A	6.41	109.60	106.68
12	A	826	CLA	O2D-CGD-CBD	6.41	122.43	111.23
12	A	805	CLA	C1D-ND-C4D	-6.40	101.82	106.31
12	a	810	CLA	C4A-NA-C1A	6.40	109.60	106.68
12	B	810	CLA	O2D-CGD-CBD	6.40	122.42	111.23
12	A	827	CLA	C3B-C2B-C1B	-6.39	99.63	107.17
12	H	822	CLA	O2D-CGD-CBD	6.39	122.41	111.23
12	a	824	CLA	C2C-C1C-NC	6.39	116.69	109.98
12	b	832	CLA	C2C-C1C-NC	6.39	116.69	109.98
12	H	826	CLA	C2C-C1C-NC	6.38	116.69	109.98
12	A	824	CLA	O2D-CGD-CBD	6.38	122.38	111.23
15	H	841	BCR	C20-C19-C18	6.38	143.84	126.36
12	A	815	CLA	C4A-NA-C1A	6.37	109.58	106.68
12	G	833	CLA	O2D-CGD-CBD	6.37	122.36	111.23
12	a	809	CLA	C2C-C1C-NC	6.37	116.67	109.98
12	G	810	CLA	C4A-NA-C1A	6.37	109.58	106.68
12	b	806	CLA	CMD-C2D-C1D	6.37	135.94	124.73
11	G	801	CL0	C2C-C1C-NC	6.37	116.67	109.98
12	f	201	CLA	CMD-C2D-C1D	6.37	135.94	124.73
12	G	830	CLA	CMD-C2D-C1D	6.37	135.94	124.73
12	L	204	CLA	C2C-C1C-NC	6.36	116.67	109.98
12	G	805	CLA	O2D-CGD-CBD	6.35	122.34	111.23
12	G	807	CLA	C1C-C2C-C3C	-6.35	100.30	106.98
12	A	826	CLA	C4A-NA-C1A	6.35	109.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	825	CLA	C4A-NA-C1A	6.35	109.58	106.68
12	b	831	CLA	C2C-C1C-NC	6.34	116.64	109.98
12	a	841	CLA	C4A-NA-C1A	6.34	109.57	106.68
12	a	831	CLA	C2C-C1C-NC	6.34	116.64	109.98
12	b	801	CLA	C2D-C1D-ND	6.33	116.39	110.13
12	G	836	CLA	C2C-C1C-NC	6.33	116.63	109.98
12	b	808	CLA	C4A-NA-C1A	6.33	109.56	106.68
12	A	855	CLA	C3B-C2B-C1B	-6.32	99.72	107.17
12	a	809	CLA	C4A-NA-C1A	6.32	109.56	106.68
12	G	827	CLA	C4A-NA-C1A	6.32	109.56	106.68
12	H	809	CLA	C4A-NA-C1A	6.32	109.56	106.68
12	H	818	CLA	C4A-NA-C1A	6.32	109.56	106.68
12	H	839	CLA	O2D-CGD-CBD	6.31	122.27	111.23
12	a	807	CLA	C2C-C1C-NC	6.31	116.61	109.98
12	l	204	CLA	O2D-CGD-CBD	6.31	122.26	111.23
12	B	802	CLA	C2D-C1D-ND	6.30	116.37	110.13
12	A	835	CLA	C4A-NA-C1A	6.30	109.55	106.68
12	A	804	CLA	O2D-CGD-CBD	6.30	122.25	111.23
12	b	809	CLA	C2C-C1C-NC	6.30	116.60	109.98
12	b	823	CLA	O2D-CGD-CBD	6.30	122.24	111.23
12	S	204	CLA	O2D-CGD-CBD	6.30	122.24	111.23
12	A	854	CLA	C2B-C1B-NB	6.29	116.85	110.33
12	H	806	CLA	C2D-C1D-ND	6.29	116.35	110.13
12	A	810	CLA	O2D-CGD-CBD	6.29	122.22	111.23
12	b	802	CLA	C1C-C2C-C3C	-6.28	100.37	106.98
12	a	826	CLA	C2D-C1D-ND	6.28	116.34	110.13
12	H	811	CLA	C2C-C1C-NC	6.28	116.58	109.98
12	G	814	CLA	C4A-NA-C1A	6.28	109.54	106.68
12	H	827	CLA	C1C-C2C-C3C	-6.28	100.38	106.98
12	a	806	CLA	C2D-C1D-ND	6.28	116.34	110.13
12	A	841	CLA	CMD-C2D-C1D	6.28	135.78	124.73
12	b	815	CLA	C2D-C1D-ND	6.28	116.34	110.13
15	H	849	BCR	C20-C19-C18	6.27	143.57	126.36
12	H	812	CLA	C4A-NA-C1A	6.27	109.54	106.68
12	B	826	CLA	C1C-C2C-C3C	-6.27	100.38	106.98
12	f	203	CLA	C2C-C1C-NC	6.27	116.57	109.98
12	B	819	CLA	C2C-C1C-NC	6.26	116.56	109.98
12	S	202	CLA	O2D-CGD-CBD	6.26	122.18	111.23
12	B	824	CLA	C4A-NA-C1A	6.26	109.54	106.68
12	H	820	CLA	C2C-C1C-NC	6.26	116.56	109.98
12	G	802	CLA	C4A-NA-C1A	6.26	109.53	106.68
12	a	835	CLA	C2C-C1C-NC	6.26	116.55	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	819	CLA	C4A-NA-C1A	6.25	109.53	106.68
12	a	809	CLA	C1C-C2C-C3C	-6.25	100.41	106.98
12	G	833	CLA	C2C-C1C-NC	6.25	116.54	109.98
12	B	809	CLA	C2C-C1C-NC	6.25	116.54	109.98
12	b	806	CLA	O2D-CGD-CBD	6.24	122.15	111.23
12	H	831	CLA	C2C-C1C-NC	6.24	116.54	109.98
12	H	805	CLA	C4A-NA-C1A	6.24	109.53	106.68
12	B	823	CLA	O2D-CGD-CBD	6.24	122.14	111.23
15	B	840	BCR	C7-C8-C9	-6.24	117.01	126.23
12	H	833	CLA	C2C-C1C-NC	6.24	116.53	109.98
12	H	829	CLA	C2C-C1C-NC	6.24	116.53	109.98
12	B	812	CLA	O2D-CGD-CBD	6.23	122.13	111.23
12	a	826	CLA	O2D-CGD-CBD	6.23	122.12	111.23
12	A	834	CLA	C4A-NA-C1A	6.23	109.52	106.68
12	B	822	CLA	C2D-C1D-ND	6.23	116.29	110.13
12	a	821	CLA	C2D-C1D-ND	6.22	116.29	110.13
15	L	203	BCR	C20-C19-C18	6.22	143.43	126.36
12	b	812	CLA	O2D-CGD-CBD	6.22	122.11	111.23
12	a	804	CLA	C2C-C1C-NC	6.22	116.52	109.98
12	b	811	CLA	C4A-NA-C1A	6.22	109.52	106.68
12	A	855	CLA	C1D-ND-C4D	-6.21	101.95	106.31
12	b	828	CLA	C4A-NA-C1A	6.21	109.51	106.68
12	G	822	CLA	C2D-C1D-ND	6.20	116.27	110.13
12	H	810	CLA	C2C-C1C-NC	6.20	116.50	109.98
12	G	814	CLA	C3B-C2B-C1B	-6.20	99.86	107.17
12	b	810	CLA	C2C-C1C-NC	6.20	116.50	109.98
12	B	806	CLA	C2C-C1C-NC	6.20	116.49	109.98
12	b	815	CLA	C1C-C2C-C3C	-6.20	100.46	106.98
12	G	835	CLA	C4A-NA-C1A	6.20	109.51	106.68
12	a	838	CLA	O2D-CGD-CBD	6.20	122.07	111.23
12	a	806	CLA	C3D-C2D-C1D	-6.20	97.37	105.83
12	a	824	CLA	O2D-CGD-CBD	6.20	122.06	111.23
12	a	834	CLA	C2C-C1C-NC	6.20	116.49	109.98
12	A	835	CLA	C2C-C1C-NC	6.19	116.49	109.98
12	a	808	CLA	C3B-C2B-C1B	-6.19	99.87	107.17
12	B	828	CLA	C2C-C1C-NC	6.19	116.49	109.98
12	B	810	CLA	C2C-C1C-NC	6.19	116.48	109.98
12	H	813	CLA	C2C-C1C-NC	6.19	116.48	109.98
12	a	826	CLA	C3D-C2D-C1D	-6.19	97.38	105.83
12	a	828	CLA	C2C-C1C-NC	6.19	116.48	109.98
12	A	822	CLA	C2C-C1C-NC	6.19	116.48	109.98
12	a	833	CLA	O2D-CGD-CBD	6.18	122.04	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	826	CLA	O2D-CGD-CBD	6.18	122.04	111.23
12	b	804	CLA	C1C-C2C-C3C	-6.18	100.48	106.98
12	G	815	CLA	C2C-C1C-NC	6.18	116.47	109.98
11	A	801	CL0	C2C-C1C-NC	6.18	116.47	109.98
12	B	804	CLA	C1C-C2C-C3C	-6.17	100.49	106.98
12	H	813	CLA	C1C-C2C-C3C	-6.17	100.49	106.98
12	B	808	CLA	O2D-CGD-CBD	6.17	122.01	111.23
12	H	811	CLA	C3D-C2D-C1D	-6.17	97.42	105.83
12	a	803	CLA	C2C-C1C-NC	6.16	116.46	109.98
12	A	812	CLA	C2C-C1C-NC	6.16	116.45	109.98
12	A	809	CLA	C2C-C1C-NC	6.16	116.45	109.98
12	a	835	CLA	C4A-NA-C1A	6.16	109.49	106.68
12	H	835	CLA	CMD-C2D-C1D	6.16	135.57	124.73
12	H	832	CLA	C2C-C1C-NC	6.16	116.45	109.98
12	b	827	CLA	O2D-CGD-CBD	6.16	121.99	111.23
12	A	838	CLA	O2D-CGD-CBD	6.15	121.99	111.23
12	A	819	CLA	C2C-C1C-NC	6.15	116.44	109.98
12	H	824	CLA	O2D-CGD-CBD	6.15	121.98	111.23
12	l	206	CLA	C4A-NA-C1A	6.15	109.48	106.68
12	H	831	CLA	C3D-C2D-C1D	-6.15	97.44	105.83
12	G	825	CLA	O2D-CGD-CBD	6.15	121.98	111.23
12	b	828	CLA	C2C-C1C-NC	6.15	116.44	109.98
12	G	821	CLA	C2C-C1C-NC	6.14	116.44	109.98
12	a	814	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	A	804	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	B	832	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	a	833	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	b	819	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	A	808	CLA	C2C-C1C-NC	6.14	116.43	109.98
15	F	202	BCR	C24-C23-C22	-6.14	117.16	126.23
12	b	802	CLA	C1D-ND-C4D	-6.13	102.01	106.31
12	A	836	CLA	C2C-C1C-NC	6.13	116.42	109.98
12	B	817	CLA	O2D-CGD-CBD	6.13	121.95	111.23
12	B	837	CLA	C1C-C2C-C3C	-6.13	100.53	106.98
12	B	826	CLA	O2D-CGD-CBD	6.13	121.94	111.23
12	G	856	CLA	C3B-C2B-C1B	-6.13	99.95	107.17
12	b	837	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	B	845	BCR	C20-C19-C18	6.12	143.15	126.36
12	a	822	CLA	C2C-C1C-NC	6.12	116.41	109.98
12	P	203	CLA	C2C-C1C-NC	6.12	116.41	109.98
12	B	831	CLA	CMD-C2D-C1D	6.12	135.50	124.73
12	B	838	CLA	C4A-NA-C1A	6.12	109.47	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	804	CLA	C1D-ND-C4D	-6.12	102.02	106.31
12	H	821	CLA	C4A-NA-C1A	6.11	109.47	106.68
12	G	814	CLA	C2C-C1C-NC	6.11	116.40	109.98
12	G	819	CLA	C2C-C1C-NC	6.11	116.39	109.98
12	H	835	CLA	C2D-C1D-ND	6.10	116.17	110.13
12	a	815	CLA	C2C-C1C-NC	6.10	116.39	109.98
12	A	807	CLA	C2C-C1C-NC	6.10	116.39	109.98
12	l	206	CLA	O2D-CGD-CBD	6.10	121.90	111.23
12	G	813	CLA	C4A-NA-C1A	6.10	109.46	106.68
12	G	809	CLA	C3B-C2B-C1B	-6.10	99.98	107.17
12	B	827	CLA	O2D-CGD-CBD	6.09	121.88	111.23
12	A	836	CLA	C3D-C2D-C1D	-6.09	97.52	105.83
12	j	102	CLA	O2D-CGD-CBD	6.09	121.87	111.23
12	A	838	CLA	C2D-C1D-ND	6.09	116.15	110.13
12	B	812	CLA	C2C-C1C-NC	6.08	116.37	109.98
12	A	855	CLA	CAC-C3C-C4C	6.08	132.70	124.79
12	a	806	CLA	C1C-C2C-C3C	-6.08	100.59	106.98
12	G	828	CLA	C4A-NA-C1A	6.07	109.45	106.68
12	L	206	CLA	C4A-NA-C1A	6.07	109.45	106.68
12	A	803	CLA	C2C-C1C-NC	6.07	116.36	109.98
12	G	836	CLA	O2A-CGA-O1A	-6.07	108.45	123.63
12	l	204	CLA	C1C-C2C-C3C	-6.07	100.60	106.98
12	H	819	CLA	C2C-C1C-NC	6.07	116.36	109.98
15	H	846	BCR	C20-C19-C18	6.07	143.00	126.36
12	l	205	CLA	C3D-C2D-C1D	-6.06	97.55	105.83
12	l	204	CLA	C2C-C1C-NC	6.06	116.35	109.98
12	A	811	CLA	C2C-C1C-NC	6.06	116.35	109.98
12	A	813	CLA	C2C-C1C-NC	6.06	116.35	109.98
12	a	808	CLA	C2C-C1C-NC	6.06	116.35	109.98
12	G	804	CLA	C2C-C1C-NC	6.06	116.35	109.98
12	A	803	CLA	O2D-CGD-CBD	6.06	121.82	111.23
12	G	827	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	G	838	CLA	O2D-CGD-CBD	6.06	121.82	111.23
12	H	804	CLA	C1C-C2C-C3C	-6.05	100.61	106.98
15	S	201	BCR	C20-C19-C18	6.05	142.94	126.36
12	G	812	CLA	C4A-NA-C1A	6.05	109.44	106.68
12	B	815	CLA	C3D-C2D-C1D	-6.04	97.58	105.83
12	b	808	CLA	O2D-CGD-CBD	6.04	121.79	111.23
12	a	805	CLA	C1D-ND-C4D	-6.04	102.07	106.31
12	B	806	CLA	C2D-C1D-ND	6.04	116.11	110.13
12	G	816	CLA	C2C-C1C-NC	6.04	116.33	109.98
12	G	823	CLA	C2C-C1C-NC	6.04	116.32	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	836	CLA	O2A-CGA-O1A	-6.04	108.53	123.63
12	b	826	CLA	O2D-CGD-CBD	6.04	121.78	111.23
12	A	826	CLA	C3D-C2D-C1D	-6.04	97.59	105.83
12	G	810	CLA	C2C-C1C-NC	6.04	116.32	109.98
12	L	204	CLA	C1C-C2C-C3C	-6.04	100.63	106.98
12	H	824	CLA	C2C-C1C-NC	6.04	116.32	109.98
12	B	818	CLA	C2C-C1C-NC	6.03	116.32	109.98
12	G	807	CLA	C3D-C2D-C1D	-6.03	97.60	105.83
12	G	808	CLA	C2C-C1C-NC	6.03	116.31	109.98
12	A	816	CLA	C1C-C2C-C3C	-6.02	100.64	106.98
12	A	821	CLA	C4A-NA-C1A	6.02	109.43	106.68
12	A	812	CLA	O2D-CGD-CBD	6.02	121.76	111.23
12	a	838	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	a	836	CLA	C2C-C1C-NC	6.02	116.30	109.98
12	G	808	CLA	C3D-C2D-C1D	-6.02	97.62	105.83
12	G	807	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	A	806	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	a	811	CLA	O2D-CGD-CBD	6.01	121.74	111.23
12	a	821	CLA	C4A-NA-C1A	6.01	109.42	106.68
12	A	839	CLA	C4A-NA-C1A	6.01	109.42	106.68
12	a	839	CLA	C3B-C2B-C1B	-6.01	100.08	107.17
12	G	808	CLA	C2D-C1D-ND	6.01	116.08	110.13
12	L	205	CLA	C3D-C2D-C1D	-6.01	97.63	105.83
12	B	811	CLA	C4A-NA-C1A	6.01	109.42	106.68
15	l	203	BCR	C20-C19-C18	6.01	142.84	126.36
12	A	834	CLA	C2C-C1C-NC	6.01	116.29	109.98
12	A	833	CLA	C4A-NA-C1A	6.01	109.42	106.68
12	S	202	CLA	C2C-C1C-NC	6.01	116.29	109.98
15	G	849	BCR	C20-C19-C18	6.01	142.83	126.36
12	a	812	CLA	C2C-C1C-NC	6.00	116.29	109.98
12	B	810	CLA	O2A-CGA-O1A	-6.00	108.61	123.63
12	A	841	CLA	C4A-NA-C1A	6.00	109.42	106.68
12	a	811	CLA	C2C-C1C-NC	6.00	116.28	109.98
12	A	831	CLA	C3D-C2D-C1D	-6.00	97.65	105.83
12	B	815	CLA	C2C-C1C-NC	6.00	116.28	109.98
12	b	830	CLA	C4A-NA-C1A	5.99	109.41	106.68
12	G	839	CLA	C2C-C1C-NC	5.99	116.27	109.98
12	H	823	CLA	C4A-NA-C1A	5.99	109.41	106.68
12	A	821	CLA	C2C-C1C-NC	5.99	116.27	109.98
12	B	806	CLA	C1D-ND-C4D	-5.99	102.11	106.31
12	A	805	CLA	C4A-NA-C1A	5.99	109.41	106.68
12	a	838	CLA	C3D-C2D-C1D	-5.99	97.66	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	823	CLA	C2C-C1C-NC	5.99	116.27	109.98
12	H	838	CLA	C1C-C2C-C3C	-5.99	100.69	106.98
12	b	817	CLA	C2C-C1C-NC	5.98	116.27	109.98
12	G	838	CLA	C2D-C1D-ND	5.98	116.05	110.13
12	A	806	CLA	C3D-C2D-C1D	-5.98	97.67	105.83
12	A	806	CLA	O2A-CGA-O1A	-5.98	108.67	123.63
12	B	808	CLA	C4A-NA-C1A	5.98	109.41	106.68
12	B	815	CLA	C2D-C1D-ND	5.98	116.04	110.13
12	B	817	CLA	C2C-C1C-NC	5.98	116.26	109.98
12	G	806	CLA	C1D-ND-C4D	-5.98	102.12	106.31
12	B	829	CLA	C3B-C2B-C1B	-5.97	100.13	107.17
12	b	829	CLA	C3B-C2B-C1B	-5.97	100.13	107.17
12	b	824	CLA	C3D-C2D-C1D	-5.97	97.68	105.83
12	S	204	CLA	C4A-NA-C1A	5.97	109.40	106.68
12	G	812	CLA	C2C-C1C-NC	5.97	116.25	109.98
12	b	812	CLA	C2D-C1D-ND	5.97	116.03	110.13
12	B	806	CLA	C1C-C2C-C3C	-5.97	100.70	106.98
12	a	828	CLA	C4A-NA-C1A	5.97	109.40	106.68
12	a	855	CLA	C3D-C2D-C1D	-5.96	97.69	105.83
12	B	802	CLA	C1D-ND-C4D	-5.96	102.13	106.31
12	B	828	CLA	C4A-NA-C1A	5.96	109.40	106.68
12	A	838	CLA	C3D-C2D-C1D	-5.96	97.70	105.83
12	A	839	CLA	C3B-C2B-C1B	-5.96	100.15	107.17
12	H	801	CLA	C2C-C1C-NC	5.95	116.23	109.98
12	A	839	CLA	C2C-C1C-NC	5.95	116.23	109.98
12	a	813	CLA	C4A-NA-C1A	5.95	109.39	106.68
15	b	844	BCR	C20-C19-C18	5.95	142.67	126.36
12	a	803	CLA	O2D-CGD-CBD	5.95	121.62	111.23
11	a	801	CL0	C4A-NA-C1A	5.94	109.39	106.68
12	L	205	CLA	O2D-CGD-CBD	5.94	121.62	111.23
12	G	834	CLA	C2C-C1C-NC	5.94	116.22	109.98
12	a	839	CLA	C2C-C1C-NC	5.94	116.22	109.98
12	H	811	CLA	O2A-CGA-O1A	-5.94	108.78	123.63
12	a	806	CLA	O2A-CGA-O1A	-5.94	108.78	123.63
12	S	202	CLA	C2D-C1D-ND	5.94	116.00	110.13
12	a	823	CLA	C4A-NA-C1A	5.93	109.39	106.68
12	G	811	CLA	C2C-C1C-NC	5.93	116.21	109.98
12	a	810	CLA	O2D-CGD-CBD	5.93	121.60	111.23
12	H	830	CLA	C3B-C2B-C1B	-5.93	100.18	107.17
12	A	833	CLA	O2D-CGD-CBD	5.93	121.59	111.23
12	G	838	CLA	C3D-C2D-C1D	-5.93	97.74	105.83
12	G	855	CLA	C3D-C2D-C1D	-5.92	97.75	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	804	CLA	C4A-NA-C1A	5.92	109.38	106.68
12	A	815	CLA	C2C-C1C-NC	5.92	116.20	109.98
12	a	813	CLA	C3B-C2B-C1B	-5.92	100.19	107.17
12	a	829	CLA	CMD-C2D-C1D	5.92	135.15	124.73
12	B	821	CLA	O2D-CGD-CBD	5.92	121.57	111.23
17	M	101	45D	C28-C26-C30	5.92	132.40	122.82
12	A	811	CLA	O2D-CGD-CBD	5.91	121.57	111.23
12	b	804	CLA	C4A-NA-C1A	5.91	109.38	106.68
12	B	822	CLA	C4A-NA-C1A	5.91	109.38	106.68
12	a	841	CLA	CMD-C2D-C1D	5.91	135.13	124.73
12	G	832	CLA	C2C-C1C-NC	5.91	116.19	109.98
12	b	806	CLA	C3B-C2B-C1B	-5.90	100.21	107.17
12	b	836	CLA	C1C-C2C-C3C	-5.90	100.77	106.98
12	A	855	CLA	O2A-C1-C2	5.90	130.82	108.11
12	G	824	CLA	O2A-CGA-O1A	-5.90	108.87	123.63
12	B	806	CLA	O2D-CGD-CBD	5.90	121.55	111.23
12	b	834	CLA	C2C-C1C-NC	5.90	116.18	109.98
12	a	855	CLA	C3B-C2B-C1B	-5.90	100.22	107.17
12	b	806	CLA	C2D-C1D-ND	5.90	115.96	110.13
15	b	847	BCR	C32-C1-C6	-5.89	101.00	110.24
12	G	817	CLA	C1C-C2C-C3C	-5.89	100.78	106.98
12	b	822	CLA	C2D-C1D-ND	5.89	115.95	110.13
12	A	821	CLA	C2D-C1D-ND	5.89	115.95	110.13
12	b	818	CLA	C2C-C1C-NC	5.88	116.16	109.98
12	b	815	CLA	C1D-ND-C4D	-5.88	102.18	106.31
12	H	836	CLA	C1C-C2C-C3C	-5.88	100.79	106.98
12	b	807	CLA	C1C-C2C-C3C	-5.88	100.79	106.98
12	j	102	CLA	CMD-C2D-C1D	5.88	135.09	124.73
17	m	101	45D	C28-C26-C30	5.88	132.35	122.82
12	G	856	CLA	C1D-ND-C4D	-5.88	102.19	106.31
12	H	812	CLA	C2C-C1C-NC	5.88	116.16	109.98
12	b	823	CLA	C2D-C1D-ND	5.88	115.94	110.13
12	G	837	CLA	C2C-C1C-NC	5.88	116.15	109.98
12	b	811	CLA	C2C-C1C-NC	5.87	116.15	109.98
12	b	826	CLA	C1C-C2C-C3C	-5.87	100.80	106.98
12	H	830	CLA	C2C-C1C-NC	5.87	116.15	109.98
12	G	804	CLA	O2D-CGD-CBD	5.87	121.50	111.23
12	S	203	CLA	C2C-C1C-NC	5.87	116.15	109.98
12	B	835	CLA	C2C-C1C-NC	5.87	116.15	109.98
12	B	833	CLA	C2D-C1D-ND	5.87	115.94	110.13
12	b	815	CLA	C3D-C2D-C1D	-5.87	97.82	105.83
12	A	810	CLA	C2C-C1C-NC	5.87	116.14	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	848	CLA	C3D-C2D-C1D	-5.86	97.83	105.83
12	P	201	CLA	C2C-C1C-NC	5.86	116.14	109.98
12	H	818	CLA	O2D-CGD-CBD	5.86	121.48	111.23
12	G	855	CLA	C2B-C1B-NB	5.86	116.40	110.33
12	a	854	CLA	C2B-C1B-NB	5.86	116.40	110.33
12	A	805	CLA	C2D-C1D-ND	5.86	115.92	110.13
12	H	825	CLA	C2C-C1C-NC	5.86	116.14	109.98
12	A	841	CLA	C1C-C2C-C3C	-5.86	100.82	106.98
12	b	817	CLA	O2D-CGD-CBD	5.85	121.46	111.23
11	a	801	CL0	CMD-C2D-C1D	5.85	135.04	124.73
12	H	836	CLA	C2C-C1C-NC	5.85	116.13	109.98
12	a	840	CLA	O2D-CGD-CBD	5.85	121.46	111.23
12	G	806	CLA	C2D-C1D-ND	5.85	115.91	110.13
12	a	812	CLA	C4A-NA-C1A	5.85	109.35	106.68
12	S	203	CLA	C3D-C2D-C1D	-5.85	97.85	105.83
12	a	821	CLA	C2C-C1C-NC	5.84	116.12	109.98
12	G	856	CLA	C3D-C2D-C1D	-5.84	97.86	105.83
12	H	850	CLA	C3D-C2D-C1D	-5.84	97.86	105.83
12	G	830	CLA	C1C-C2C-C3C	-5.84	100.84	106.98
12	A	836	CLA	O2A-CGA-O1A	-5.84	109.02	123.63
12	B	831	CLA	C4A-NA-C1A	5.84	109.34	106.68
12	A	826	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	b	829	CLA	C2D-C1D-ND	5.84	115.90	110.13
12	H	829	CLA	C4A-NA-C1A	5.84	109.34	106.68
12	S	203	CLA	C1C-C2C-C3C	-5.84	100.84	106.98
12	b	816	CLA	C2C-C1C-NC	5.84	116.11	109.98
12	B	835	CLA	C1C-C2C-C3C	-5.83	100.84	106.98
12	A	818	CLA	C2C-C1C-NC	5.83	116.11	109.98
12	b	834	CLA	C1C-C2C-C3C	-5.83	100.85	106.98
12	A	808	CLA	C3B-C2B-C1B	-5.83	100.30	107.17
12	A	814	CLA	C4A-NA-C1A	5.83	109.34	106.68
12	a	821	CLA	C3D-C2D-C1D	-5.83	97.88	105.83
15	S	201	BCR	C31-C1-C6	-5.83	101.11	110.24
12	f	201	CLA	C2C-C1C-NC	5.82	116.10	109.98
12	G	830	CLA	O2D-CGD-CBD	5.82	121.41	111.23
12	A	805	CLA	O2D-CGD-CBD	5.82	121.41	111.23
12	H	818	CLA	C2C-C1C-NC	5.82	116.10	109.98
12	G	827	CLA	C3D-C2D-C1D	-5.82	97.89	105.83
12	A	838	CLA	C1D-ND-C4D	-5.82	102.23	106.31
12	B	810	CLA	OBD-CAD-C3D	-5.82	114.81	128.42
12	H	802	CLA	CMC-C2C-C1C	5.82	134.12	125.03
12	B	831	CLA	C2C-C1C-NC	5.81	116.09	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	827	CLA	O2D-CGD-CBD	5.81	121.39	111.23
12	A	837	CLA	C4A-NA-C1A	5.81	109.33	106.68
12	L	202	CLA	O2D-CGD-CBD	5.81	121.39	111.23
12	H	830	CLA	C2D-C1D-ND	5.81	115.88	110.13
12	B	810	CLA	C4A-NA-C1A	5.81	109.33	106.68
15	i	101	BCR	C20-C19-C18	5.81	142.28	126.36
12	b	823	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
12	G	839	CLA	C4A-NA-C1A	5.80	109.33	106.68
12	B	811	CLA	C2C-C1C-NC	5.80	116.08	109.98
12	H	834	CLA	C4A-NA-C1A	5.80	109.33	106.68
12	B	834	CLA	C2D-C1D-ND	5.80	115.87	110.13
12	a	820	CLA	C2C-C1C-NC	5.80	116.07	109.98
12	B	804	CLA	C1D-ND-C4D	-5.80	102.25	106.31
12	b	812	CLA	C3D-C2D-C1D	-5.80	97.92	105.83
12	B	825	CLA	C4A-NA-C1A	5.80	109.32	106.68
12	A	823	CLA	C2C-C1C-NC	5.80	116.07	109.98
12	G	806	CLA	O2D-CGD-CBD	5.79	121.36	111.23
12	a	840	CLA	C4A-NA-C1A	5.79	109.32	106.68
12	A	832	CLA	C2C-C1C-NC	5.79	116.07	109.98
12	b	824	CLA	C2D-C1D-ND	5.79	115.86	110.13
12	b	810	CLA	C4A-NA-C1A	5.79	109.32	106.68
12	H	833	CLA	C4A-NA-C1A	5.79	109.32	106.68
12	a	810	CLA	C2C-C1C-NC	5.79	116.06	109.98
12	B	824	CLA	C2C-C1C-NC	5.79	116.06	109.98
12	A	828	CLA	C2C-C1C-NC	5.78	116.05	109.98
12	G	842	CLA	C2D-C1D-ND	5.78	115.84	110.13
12	G	841	CLA	C1C-C2C-C3C	-5.78	100.90	106.98
12	a	832	CLA	C2C-C1C-NC	5.78	116.05	109.98
12	G	822	CLA	C4A-NA-C1A	5.78	109.31	106.68
12	H	832	CLA	C4A-NA-C1A	5.78	109.31	106.68
12	A	837	CLA	O2D-CGD-CBD	5.78	121.33	111.23
12	H	823	CLA	O2D-CGD-CBD	5.77	121.32	111.23
12	a	813	CLA	O2D-CGD-CBD	5.77	121.32	111.23
12	b	829	CLA	C3D-C2D-C1D	-5.77	97.95	105.83
12	G	822	CLA	C2C-C1C-NC	5.77	116.04	109.98
12	a	822	CLA	C4A-NA-C1A	5.77	109.31	106.68
12	G	839	CLA	C3B-C2B-C1B	-5.77	100.37	107.17
12	B	829	CLA	C3D-C2D-C1D	-5.77	97.96	105.83
12	b	829	CLA	C2C-C1C-NC	5.76	116.04	109.98
12	G	822	CLA	C3D-C2D-C1D	-5.76	97.97	105.83
12	G	816	CLA	C4A-NA-C1A	5.76	109.31	106.68
12	A	825	CLA	C3D-C2D-C1D	-5.76	97.97	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	840	CLA	O2D-CGD-CBD	5.76	121.30	111.23
12	B	805	CLA	O2A-CGA-O1A	-5.76	109.23	123.63
12	L	204	CLA	C2D-C1D-ND	5.75	115.82	110.13
12	A	855	CLA	C3D-C2D-C1D	-5.75	97.98	105.83
12	a	829	CLA	C1C-C2C-C3C	-5.75	100.93	106.98
12	l	206	CLA	C2C-C1C-NC	5.75	116.02	109.98
12	A	804	CLA	C3B-C2B-C1B	-5.74	100.40	107.17
12	b	813	CLA	C2D-C1D-ND	5.74	115.81	110.13
12	a	835	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
12	B	804	CLA	C4A-NA-C1A	5.74	109.30	106.68
12	b	830	CLA	C1C-C2C-C3C	-5.74	100.95	106.98
12	b	809	CLA	O2D-CGD-CBD	5.73	121.25	111.23
12	a	825	CLA	C3B-C2B-C1B	-5.73	100.41	107.17
12	H	805	CLA	C1D-ND-C4D	-5.73	102.29	106.31
15	f	202	BCR	C24-C23-C22	-5.73	117.76	126.23
12	b	832	CLA	C3D-C2D-C1D	-5.73	98.01	105.83
12	b	810	CLA	O2A-CGA-O1A	-5.73	109.30	123.63
12	A	829	CLA	CMD-C2D-C1D	5.73	134.82	124.73
12	G	824	CLA	C2C-C1C-NC	5.73	116.00	109.98
12	H	808	CLA	O2D-CGD-CBD	5.73	121.24	111.23
11	G	801	CL0	C1C-C2C-C3C	-5.73	100.96	106.98
12	A	825	CLA	C3B-C2B-C1B	-5.72	100.42	107.17
12	b	803	CLA	O2D-CGD-CBD	5.72	121.24	111.23
12	B	813	CLA	C2D-C1D-ND	5.72	115.79	110.13
12	B	818	CLA	O2D-CGD-CBD	5.72	121.23	111.23
12	b	805	CLA	C1D-ND-C4D	-5.72	102.30	106.31
12	l	204	CLA	C2D-C1D-ND	5.72	115.79	110.13
12	a	818	CLA	C1C-C2C-C3C	-5.72	100.96	106.98
12	b	825	CLA	C4A-NA-C1A	5.72	109.29	106.68
12	H	811	CLA	C3B-C2B-C1B	-5.72	100.43	107.17
12	B	803	CLA	O2D-CGD-CBD	5.72	121.22	111.23
12	B	815	CLA	O2D-CGD-CBD	5.72	121.22	111.23
12	b	810	CLA	C2D-C1D-ND	5.72	115.78	110.13
12	b	848	CLA	C2D-C1D-ND	5.72	115.78	110.13
17	T	101	45D	C28-C26-C30	5.72	132.07	122.82
12	G	841	CLA	C4A-NA-C1A	5.71	109.29	106.68
12	H	805	CLA	C2C-C1C-NC	5.71	115.98	109.98
12	H	821	CLA	C3B-C2B-C1B	-5.71	100.44	107.17
12	a	804	CLA	O2A-CGA-O1A	-5.71	109.34	123.63
15	H	841	BCR	C7-C8-C9	-5.71	117.79	126.23
12	B	803	CLA	C2C-C1C-NC	5.71	115.98	109.98
12	B	830	CLA	O2D-CGD-CBD	5.71	121.21	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	826	CLA	C3B-C2B-C1B	-5.71	100.44	107.17
12	l	202	CLA	O2D-CGD-CBD	5.71	121.20	111.23
12	S	204	CLA	O2A-CGA-O1A	-5.71	109.36	123.63
12	A	827	CLA	O2A-CGA-O1A	-5.70	109.36	123.63
12	b	804	CLA	C2C-C1C-NC	5.70	115.97	109.98
12	b	815	CLA	C3B-C2B-C1B	-5.70	100.45	107.17
12	l	205	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
12	H	801	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
12	b	803	CLA	C2C-C1C-NC	5.70	115.97	109.98
12	G	809	CLA	C2C-C1C-NC	5.70	115.97	109.98
12	l	205	CLA	C2C-C1C-NC	5.70	115.96	109.98
12	G	823	CLA	C4A-NA-C1A	5.69	109.28	106.68
12	G	805	CLA	O2A-CGA-O1A	-5.69	109.38	123.63
12	a	817	CLA	C3B-C2B-C1B	-5.69	100.46	107.17
12	A	804	CLA	O2A-CGA-O1A	-5.69	109.39	123.63
12	B	822	CLA	O2D-CGD-CBD	5.69	121.18	111.23
12	G	841	CLA	CMD-C2D-C1D	5.69	134.75	124.73
12	A	821	CLA	C3D-C2D-C1D	-5.69	98.07	105.83
12	B	833	CLA	C3D-C2D-C1D	-5.69	98.07	105.83
12	A	817	CLA	C3B-C2B-C1B	-5.69	100.47	107.17
12	G	856	CLA	CAC-C3C-C4C	5.69	132.19	124.79
12	B	816	CLA	C2C-C1C-NC	5.68	115.95	109.98
12	G	815	CLA	O2D-CGD-CBD	5.68	121.16	111.23
12	G	838	CLA	C1D-ND-C4D	-5.68	102.33	106.31
12	b	820	CLA	C2D-C1D-ND	5.67	115.74	110.13
12	B	830	CLA	C2C-C1C-NC	5.67	115.94	109.98
12	B	811	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
12	B	825	CLA	C1C-C2C-C3C	-5.67	101.02	106.98
12	b	815	CLA	C2C-C1C-NC	5.67	115.94	109.98
12	A	854	CLA	C3D-C2D-C1D	-5.67	98.09	105.83
12	a	835	CLA	C2D-C1D-ND	5.67	115.74	110.13
12	b	826	CLA	O2A-CGA-O1A	-5.67	109.45	123.63
12	b	805	CLA	O2A-CGA-O1A	-5.67	109.45	123.63
12	A	807	CLA	C3D-C2D-C1D	-5.66	98.10	105.83
12	a	808	CLA	C1C-C2C-C3C	-5.66	101.02	106.98
12	A	814	CLA	C2C-C1C-NC	5.66	115.93	109.98
15	b	847	BCR	C24-C23-C22	-5.66	117.86	126.23
12	A	837	CLA	C2C-C1C-NC	5.66	115.93	109.98
17	m	101	45D	C31-C29-C25	-5.66	119.34	127.28
12	H	816	CLA	C3D-C2D-C1D	-5.66	98.11	105.83
12	A	823	CLA	C4A-NA-C1A	5.66	109.26	106.68
12	a	827	CLA	C2D-C1D-ND	5.66	115.73	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	813	CLA	C3B-C2B-C1B	-5.66	100.50	107.17
12	a	837	CLA	C2C-C1C-NC	5.66	115.92	109.98
12	B	829	CLA	C2D-C1D-ND	5.66	115.73	110.13
12	H	814	CLA	C3B-C2B-C1B	-5.66	100.50	107.17
12	A	836	CLA	CAC-C3C-C4C	5.66	132.15	124.79
12	B	807	CLA	CMD-C2D-C1D	5.66	134.69	124.73
12	A	836	CLA	C3B-C2B-C1B	-5.66	100.50	107.17
12	G	836	CLA	C3B-C2B-C1B	-5.65	100.50	107.17
12	l	204	CLA	CMD-C2D-C1D	5.65	134.68	124.73
12	L	206	CLA	O2D-CGD-CBD	5.65	121.11	111.23
12	S	204	CLA	C2C-C1C-NC	5.65	115.92	109.98
12	a	834	CLA	CMD-C2D-C1D	5.65	134.68	124.73
12	G	840	CLA	O2A-CGA-O1A	-5.65	109.50	123.63
12	B	837	CLA	C2D-C1D-ND	5.65	115.72	110.13
12	H	839	CLA	C2D-C1D-ND	5.65	115.71	110.13
12	A	804	CLA	C1C-C2C-C3C	-5.65	101.04	106.98
12	A	823	CLA	O2A-CGA-O1A	-5.65	109.51	123.63
12	G	807	CLA	C4A-NA-C1A	5.64	109.25	106.68
12	A	826	CLA	C2C-C1C-NC	5.64	115.91	109.98
12	G	826	CLA	C3B-C2B-C1B	-5.64	100.52	107.17
12	b	817	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	H	850	CLA	C2D-C1D-ND	5.64	115.71	110.13
12	G	827	CLA	C3B-C2B-C1B	-5.64	100.52	107.17
12	G	805	CLA	C2C-C1C-NC	5.64	115.90	109.98
12	A	821	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	A	854	CLA	O2D-CGD-CBD	5.64	121.08	111.23
12	H	807	CLA	O2D-CGD-CBD	5.64	121.08	111.23
12	B	805	CLA	C2C-C1C-NC	5.64	115.90	109.98
12	a	804	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	a	836	CLA	CAC-C3C-C4C	5.63	132.12	124.79
12	B	806	CLA	O2A-CGA-O1A	-5.63	109.53	123.63
12	b	803	CLA	O2A-CGA-CBA	5.63	129.01	111.83
12	G	826	CLA	C3D-C2D-C1D	-5.63	98.14	105.83
12	a	833	CLA	C4A-NA-C1A	5.63	109.25	106.68
12	B	832	CLA	C4A-NA-C1A	5.63	109.25	106.68
12	B	838	CLA	C2D-C1D-ND	5.63	115.70	110.13
12	H	830	CLA	C3D-C2D-C1D	-5.63	98.15	105.83
12	H	806	CLA	C2C-C1C-NC	5.63	115.89	109.98
12	A	829	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
12	b	820	CLA	C4A-NA-C1A	5.63	109.25	106.68
12	B	823	CLA	C3D-C2D-C1D	-5.63	98.15	105.83
12	R	103	CLA	C2C-C1C-NC	5.62	115.89	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	825	CLA	O2A-CGA-O1A	-5.62	109.56	123.63
12	A	807	CLA	C2D-C1D-ND	5.62	115.69	110.13
12	b	822	CLA	C3B-C2B-C1B	-5.62	100.54	107.17
12	a	824	CLA	CMD-C2D-C1D	5.62	134.62	124.73
12	a	807	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
12	b	808	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
12	H	834	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
12	b	825	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
15	a	846	BCR	C20-C19-C18	5.62	141.76	126.36
12	b	806	CLA	C2C-C1C-NC	5.62	115.88	109.98
12	A	840	CLA	C2C-C1C-NC	5.62	115.88	109.98
12	G	840	CLA	O2D-CGD-CBD	5.61	121.05	111.23
17	T	101	45D	C40-C36-C38	5.61	131.91	122.82
12	H	830	CLA	C4A-NA-C1A	5.61	109.24	106.68
12	H	803	CLA	O2D-CGD-CBD	5.61	121.04	111.23
12	a	812	CLA	C3D-C2D-C1D	-5.61	98.18	105.83
12	B	804	CLA	C2C-C1C-NC	5.61	115.87	109.98
12	J	103	CLA	C2C-C1C-NC	5.61	115.87	109.98
12	l	202	CLA	C2C-C1C-NC	5.61	115.87	109.98
12	B	810	CLA	C2D-C1D-ND	5.61	115.68	110.13
12	L	206	CLA	C2C-C1C-NC	5.61	115.87	109.98
12	a	823	CLA	O2A-CGA-O1A	-5.61	109.61	123.63
12	H	808	CLA	C2C-C1C-NC	5.61	115.87	109.98
12	b	813	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
12	b	805	CLA	C2C-C1C-NC	5.60	115.87	109.98
12	j	102	CLA	C2C-C1C-NC	5.60	115.87	109.98
12	H	836	CLA	O2D-CGD-CBD	5.60	121.03	111.23
12	B	820	CLA	C3B-C2B-C1B	-5.60	100.56	107.17
12	A	840	CLA	O2A-CGA-O1A	-5.60	109.61	123.63
12	a	804	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
12	a	805	CLA	C2D-C1D-ND	5.60	115.67	110.13
12	a	824	CLA	C2D-C1D-ND	5.60	115.67	110.13
12	A	815	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
12	b	807	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
12	G	807	CLA	O2A-CGA-O1A	-5.59	109.64	123.63
12	a	827	CLA	O2A-CGA-O1A	-5.59	109.64	123.63
12	G	838	CLA	C2C-C1C-NC	5.59	115.85	109.98
12	b	806	CLA	CBA-CAA-C2A	5.59	130.42	113.79
12	a	815	CLA	C4A-NA-C1A	5.59	109.23	106.68
12	B	812	CLA	C4A-NA-C1A	5.59	109.23	106.68
12	b	818	CLA	O2D-CGD-CBD	5.58	120.99	111.23
12	A	821	CLA	O2D-CGD-CBD	5.58	120.99	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	835	CLA	C3D-C2D-C1D	-5.58	98.21	105.83
12	G	813	CLA	O2D-CGD-CBD	5.58	120.99	111.23
12	b	805	CLA	C2D-C1D-ND	5.58	115.65	110.13
12	A	814	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
12	H	811	CLA	C4A-NA-C1A	5.58	109.22	106.68
12	b	832	CLA	C2D-C1D-ND	5.58	115.65	110.13
12	B	807	CLA	C2D-C1D-ND	5.58	115.65	110.13
12	G	827	CLA	O2D-CGD-CBD	5.58	120.98	111.23
12	A	828	CLA	C4A-NA-C1A	5.58	109.22	106.68
15	G	848	BCR	C3-C4-C5	-5.58	104.11	114.06
12	a	838	CLA	C2C-C1C-NC	5.58	115.84	109.98
12	b	813	CLA	C4A-NA-C1A	5.58	109.22	106.68
12	a	840	CLA	O2A-CGA-O1A	-5.58	109.68	123.63
12	a	825	CLA	O2D-CGD-CBD	5.58	120.98	111.23
12	H	836	CLA	C1D-ND-C4D	-5.57	102.40	106.31
12	a	819	CLA	O2D-CGD-CBD	5.57	120.97	111.23
12	H	816	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
12	B	832	CLA	O2D-CGD-CBD	5.57	120.97	111.23
12	a	841	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
12	a	813	CLA	C2C-C1C-NC	5.57	115.83	109.98
12	H	812	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
12	b	820	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
12	a	854	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
12	H	823	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
12	H	810	CLA	O2D-CGD-CBD	5.57	120.96	111.23
12	H	807	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
12	S	203	CLA	O2D-CGD-CBD	5.56	120.96	111.23
12	B	806	CLA	C3B-C2B-C1B	-5.56	100.61	107.17
12	A	827	CLA	C2D-C1D-ND	5.56	115.63	110.13
12	B	805	CLA	C1D-ND-C4D	-5.56	102.41	106.31
12	B	814	CLA	C2C-C1C-NC	5.56	115.82	109.98
12	H	813	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
12	H	819	CLA	O2D-CGD-CBD	5.56	120.95	111.23
12	b	827	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
12	a	836	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
12	G	820	CLA	O2D-CGD-CBD	5.56	120.94	111.23
12	G	835	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
12	H	809	CLA	O2D-CGD-CBD	5.55	120.94	111.23
12	A	819	CLA	O2D-CGD-CBD	5.55	120.93	111.23
12	H	827	CLA	O2A-CGA-O1A	-5.55	109.75	123.63
12	G	817	CLA	C4A-NA-C1A	5.55	109.21	106.68
12	L	205	CLA	C2C-C1C-NC	5.55	115.81	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	l	203	BCR	C31-C1-C6	-5.55	101.55	110.24
12	H	830	CLA	C1D-ND-C4D	-5.54	102.42	106.31
12	B	822	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
12	G	805	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
12	L	202	CLA	C2C-C1C-NC	5.54	115.80	109.98
12	H	805	CLA	C2D-C1D-ND	5.54	115.61	110.13
12	G	806	CLA	C4A-NA-C1A	5.54	109.21	106.68
12	G	817	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
12	A	812	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
12	b	811	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
12	a	838	CLA	C1D-ND-C4D	-5.54	102.43	106.31
12	L	205	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
12	a	817	CLA	C3D-C2D-C1D	-5.54	98.27	105.83
12	H	834	CLA	C2D-C1D-ND	5.54	115.61	110.13
12	H	814	CLA	C4A-NA-C1A	5.54	109.20	106.68
12	b	822	CLA	C4A-NA-C1A	5.54	109.20	106.68
12	G	829	CLA	C2C-C1C-NC	5.54	115.80	109.98
12	b	811	CLA	O2A-CGA-O1A	-5.53	109.78	123.63
12	j	104	CLA	C2C-C1C-NC	5.53	115.79	109.98
15	G	845	BCR	C7-C8-C9	-5.53	118.05	126.23
12	a	817	CLA	C2D-C1D-ND	5.53	115.60	110.13
12	b	801	CLA	C1C-C2C-C3C	-5.53	101.16	106.98
12	A	827	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
12	H	822	CLA	C2C-C1C-NC	5.53	115.79	109.98
15	J	101	BCR	C24-C23-C22	-5.53	118.05	126.23
12	b	822	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
12	b	817	CLA	C2D-C1D-ND	5.53	115.60	110.13
12	H	834	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
12	b	837	CLA	C2D-C1D-ND	5.53	115.60	110.13
12	G	855	CLA	C1D-ND-C4D	-5.53	102.43	106.31
12	A	826	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
12	B	813	CLA	C3D-C2D-C1D	-5.53	98.29	105.83
12	F	201	CLA	C2C-C1C-NC	5.53	115.79	109.98
12	b	812	CLA	C1C-C2C-C3C	-5.53	101.17	106.98
12	B	817	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
12	H	811	CLA	O2D-CGD-CBD	5.52	120.89	111.23
12	a	829	CLA	O2D-CGD-CBD	5.52	120.88	111.23
12	A	830	CLA	C3B-C2B-C1B	-5.52	100.66	107.17
12	H	828	CLA	C2C-C1C-NC	5.52	115.78	109.98
12	H	806	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
12	B	813	CLA	C2C-C1C-NC	5.52	115.78	109.98
12	A	813	CLA	C3B-C2B-C1B	-5.52	100.67	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	819	CLA	C3B-C2B-C1B	-5.52	100.67	107.17
12	A	820	CLA	C1C-C2C-C3C	-5.52	101.18	106.98
12	A	834	CLA	C1C-C2C-C3C	-5.52	101.18	106.98
12	b	814	CLA	O2D-CGD-CBD	5.52	120.87	111.23
12	H	828	CLA	C3B-C2B-C1B	-5.52	100.67	107.17
12	B	819	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
12	G	836	CLA	O2A-CGA-CBA	5.51	128.65	111.83
12	b	837	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
12	A	806	CLA	C2C-C1C-NC	5.51	115.77	109.98
12	G	806	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
12	a	824	CLA	C4A-NA-C1A	5.51	109.19	106.68
12	B	822	CLA	C2C-C1C-NC	5.51	115.77	109.98
12	B	809	CLA	C4A-NA-C1A	5.51	109.19	106.68
12	B	815	CLA	C4A-NA-C1A	5.51	109.19	106.68
12	a	806	CLA	C1D-ND-C4D	-5.51	102.45	106.31
12	b	834	CLA	C1D-ND-C4D	-5.51	102.45	106.31
12	B	814	CLA	O2D-CGD-CBD	5.51	120.86	111.23
12	b	835	CLA	C3B-C2B-C1B	-5.51	100.68	107.17
12	a	805	CLA	O2D-CGD-CBD	5.50	120.85	111.23
12	b	831	CLA	O2D-CGD-CBD	5.50	120.85	111.23
12	S	202	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
12	H	804	CLA	C2C-C1C-NC	5.50	115.76	109.98
12	G	842	CLA	C3D-C2D-C1D	-5.50	98.32	105.83
12	P	203	CLA	C3B-C2B-C1B	-5.50	100.69	107.17
12	a	806	CLA	C4A-NA-C1A	5.50	109.19	106.68
12	a	828	CLA	CMD-C2D-C1D	5.50	134.41	124.73
12	B	815	CLA	C3B-C2B-C1B	-5.50	100.69	107.17
12	A	833	CLA	C2C-C1C-NC	5.50	115.76	109.98
12	G	814	CLA	C2B-C1B-NB	5.50	116.03	110.33
12	j	102	CLA	C4A-NA-C1A	5.50	109.19	106.68
12	a	854	CLA	C1D-ND-C4D	-5.50	102.46	106.31
12	a	833	CLA	C3B-C2B-C1B	-5.49	100.69	107.17
12	R	103	CLA	C3B-C2B-C1B	-5.49	100.70	107.17
12	A	825	CLA	C2D-C1D-ND	5.49	115.56	110.13
12	a	825	CLA	O2A-CGA-O1A	-5.49	109.89	123.63
12	S	203	CLA	C3B-C2B-C1B	-5.49	100.70	107.17
12	G	821	CLA	C4A-NA-C1A	5.49	109.18	106.68
12	B	803	CLA	C2D-C1D-ND	5.49	115.56	110.13
12	A	818	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
12	G	822	CLA	O2D-CGD-CBD	5.49	120.82	111.23
12	H	823	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
12	a	821	CLA	C1C-C2C-C3C	-5.49	101.21	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	828	CLA	O2A-CGA-O1A	-5.48	109.91	123.63
12	B	838	CLA	C3B-C2B-C1B	-5.48	100.70	107.17
12	a	814	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
12	H	839	CLA	C2C-C1C-NC	5.48	115.74	109.98
12	A	835	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
12	P	201	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
12	G	832	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
12	H	818	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
12	b	832	CLA	C4A-NA-C1A	5.48	109.18	106.68
12	G	815	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
17	M	101	45D	C40-C36-C38	5.48	131.69	122.82
12	A	812	CLA	C3D-C2D-C1D	-5.48	98.36	105.83
12	H	825	CLA	C3D-C2D-C1D	-5.48	98.36	105.83
12	a	840	CLA	C2C-C1C-NC	5.47	115.73	109.98
12	A	808	CLA	C1C-C2C-C3C	-5.47	101.22	106.98
12	G	833	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
12	B	812	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
12	G	828	CLA	O2D-CGD-CBD	5.47	120.80	111.23
12	G	836	CLA	C1C-C2C-C3C	-5.47	101.22	106.98
12	H	820	CLA	C1C-C2C-C3C	-5.47	101.22	106.98
12	b	813	CLA	C2C-C1C-NC	5.47	115.73	109.98
12	H	839	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
12	H	818	CLA	C2D-C1D-ND	5.47	115.54	110.13
12	A	818	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
12	G	802	CLA	C1-O2A-CGA	5.47	129.89	116.65
12	A	833	CLA	C3B-C2B-C1B	-5.47	100.73	107.17
17	m	101	45D	C40-C36-C38	5.47	131.67	122.82
12	F	203	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
12	b	848	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
12	H	815	CLA	O2D-CGD-CBD	5.46	120.78	111.23
12	a	828	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
12	a	823	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
12	B	810	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
12	l	205	CLA	O2D-CGD-CBD	5.46	120.78	111.23
12	A	803	CLA	O2A-CGA-O1A	-5.46	109.97	123.63
12	b	831	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
12	G	811	CLA	C2D-C1D-ND	5.46	115.53	110.13
15	G	847	BCR	C15-C14-C13	-5.46	119.63	127.28
15	R	101	BCR	C24-C23-C22	-5.46	118.16	126.23
12	b	813	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
12	b	830	CLA	CMD-C2D-C1D	5.45	134.33	124.73
12	G	814	CLA	C1C-C2C-C3C	-5.45	101.25	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	831	CLA	C4A-NA-C1A	5.45	109.17	106.68
12	a	825	CLA	C2C-C1C-NC	5.45	115.70	109.98
12	a	819	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
12	G	826	CLA	O2A-CGA-O1A	-5.45	110.00	123.63
12	a	819	CLA	C4A-NA-C1A	5.45	109.16	106.68
12	G	817	CLA	O2D-CGD-CBD	5.45	120.75	111.23
12	A	812	CLA	C4A-NA-C1A	5.44	109.16	106.68
12	B	834	CLA	C3D-C2D-C1D	-5.44	98.40	105.83
12	A	805	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
12	a	818	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
12	B	811	CLA	O2D-CGD-CBD	5.44	120.74	111.23
12	l	205	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
12	l	206	CLA	O2A-CGA-O1A	-5.44	110.02	123.63
12	B	829	CLA	C2C-C1C-NC	5.44	115.70	109.98
12	G	840	CLA	C2C-C1C-NC	5.44	115.69	109.98
12	G	811	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
12	G	828	CLA	C2D-C1D-ND	5.44	115.51	110.13
12	G	835	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
12	G	842	CLA	C2C-C1C-NC	5.44	115.69	109.98
12	J	103	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
12	b	836	CLA	O2A-CGA-O1A	-5.44	110.03	123.63
12	A	832	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
12	B	823	CLA	C2C-C1C-NC	5.43	115.69	109.98
12	a	803	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
12	b	818	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
12	G	826	CLA	C2C-C1C-NC	5.43	115.69	109.98
12	H	803	CLA	O2A-CGA-CBA	5.43	128.40	111.83
12	A	823	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
12	H	826	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
12	A	818	CLA	C2D-C1D-ND	5.43	115.50	110.13
12	G	804	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
12	a	827	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
12	H	830	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
12	B	818	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
12	B	824	CLA	C2D-C1D-ND	5.43	115.50	110.13
12	B	837	CLA	O2A-CGA-O1A	-5.43	110.05	123.63
12	b	828	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
15	a	846	BCR	C24-C23-C22	-5.43	118.21	126.23
12	A	832	CLA	O2A-CGA-O1A	-5.43	110.05	123.63
12	B	827	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
12	a	815	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
12	a	821	CLA	O2D-CGD-CBD	5.43	120.71	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	855	CLA	O2A-C1-C2	5.42	128.98	108.11
15	a	845	BCR	C3-C4-C5	-5.42	104.39	114.06
12	b	848	CLA	O2D-CGD-CBD	5.42	120.70	111.23
12	H	803	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
12	B	817	CLA	C2D-C1D-ND	5.42	115.49	110.13
12	b	807	CLA	C2D-C1D-ND	5.42	115.49	110.13
12	A	806	CLA	C1D-ND-C4D	-5.41	102.51	106.31
12	H	802	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
12	H	819	CLA	C3B-C2B-C1B	-5.41	100.79	107.17
12	H	806	CLA	C3B-C2B-C1B	-5.41	100.79	107.17
12	G	805	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
12	H	823	CLA	C2C-C1C-NC	5.41	115.66	109.98
12	B	821	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
12	G	824	CLA	C4A-NA-C1A	5.41	109.15	106.68
12	G	816	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
12	H	806	CLA	O2A-CGA-O1A	-5.41	110.10	123.63
12	b	829	CLA	O2A-CGA-O1A	-5.41	110.11	123.63
12	G	820	CLA	C2C-C1C-NC	5.41	115.66	109.98
12	B	802	CLA	CMD-C2D-C1D	5.40	134.25	124.73
12	b	836	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
12	a	832	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
12	B	836	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
12	A	815	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
12	b	812	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
12	A	835	CLA	C2D-C1D-ND	5.40	115.47	110.13
12	A	810	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
12	A	838	CLA	C2C-C1C-NC	5.40	115.65	109.98
12	G	832	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
12	B	803	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
12	A	833	CLA	C3D-C2D-C1D	-5.40	98.47	105.83
12	a	830	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
12	A	835	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
12	A	808	CLA	C4A-NA-C1A	5.40	109.14	106.68
12	B	818	CLA	C4A-NA-C1A	5.40	109.14	106.68
12	H	816	CLA	O2D-CGD-CBD	5.40	120.66	111.23
12	b	803	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
12	H	815	CLA	C2C-C1C-NC	5.40	115.65	109.98
12	b	819	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
12	a	811	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
12	G	819	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
12	A	832	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
12	G	837	CLA	C3D-C2D-C1D	-5.39	98.47	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	803	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
12	B	827	CLA	C2C-C1C-NC	5.39	115.64	109.98
15	P	202	BCR	C7-C8-C9	-5.39	118.26	126.23
12	A	816	CLA	C4A-NA-C1A	5.39	109.14	106.68
12	H	838	CLA	O2A-CGA-O1A	-5.39	110.15	123.63
12	L	206	CLA	O2A-CGA-O1A	-5.39	110.15	123.63
12	H	836	CLA	C2D-C1D-ND	5.39	115.46	110.13
12	B	821	CLA	C2D-C1D-ND	5.39	115.46	110.13
12	a	809	CLA	C2D-C1D-ND	5.39	115.46	110.13
12	G	818	CLA	C3B-C2B-C1B	-5.38	100.82	107.17
12	b	833	CLA	C2C-C1C-NC	5.38	115.64	109.98
12	A	830	CLA	O2A-CGA-O1A	-5.38	110.17	123.63
12	a	809	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
12	b	833	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
12	H	822	CLA	C2D-C1D-ND	5.38	115.45	110.13
12	H	830	CLA	O2A-CGA-O1A	-5.38	110.18	123.63
12	A	814	CLA	O2D-CGD-CBD	5.38	120.63	111.23
12	b	801	CLA	CMD-C2D-C1D	5.37	134.19	124.73
12	B	820	CLA	C2D-C1D-ND	5.37	115.44	110.13
12	b	837	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	a	822	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
12	H	839	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
12	G	813	CLA	O2A-CGA-O1A	-5.37	110.19	123.63
12	H	815	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	B	819	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	a	807	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	a	837	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
12	a	806	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
12	A	823	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	B	801	CLA	C1C-C2C-C3C	-5.37	101.34	106.98
12	B	814	CLA	C1C-C2C-C3C	-5.37	101.34	106.98
12	G	827	CLA	C2C-C1C-NC	5.37	115.62	109.98
12	B	824	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
12	b	818	CLA	C4A-NA-C1A	5.36	109.13	106.68
12	B	817	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
12	H	833	CLA	O2D-CGD-CBD	5.36	120.61	111.23
12	G	818	CLA	C1D-ND-C4D	-5.36	102.55	106.31
12	A	854	CLA	C1D-ND-C4D	-5.36	102.55	106.31
12	H	835	CLA	C2C-C1C-NC	5.36	115.61	109.98
12	j	104	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
12	a	812	CLA	C2D-C1D-ND	5.36	115.43	110.13
12	a	827	CLA	O2D-CGD-CBD	5.36	120.59	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	830	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
12	A	805	CLA	C3D-C2D-C1D	-5.35	98.52	105.83
12	a	822	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
12	G	807	CLA	C2C-C1C-NC	5.35	115.61	109.98
12	G	824	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
12	b	822	CLA	O2D-CGD-O1D	-5.35	113.43	123.85
12	B	803	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
12	H	821	CLA	C2D-C1D-ND	5.35	115.42	110.13
12	b	827	CLA	C2C-C1C-NC	5.35	115.60	109.98
12	a	814	CLA	O2D-CGD-CBD	5.35	120.58	111.23
12	B	812	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
12	a	811	CLA	C4A-NA-C1A	5.35	109.12	106.68
12	G	805	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
12	B	829	CLA	O2A-CGA-O1A	-5.35	110.25	123.63
12	G	823	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
12	H	821	CLA	C2C-C1C-NC	5.35	115.60	109.98
12	a	803	CLA	O2A-CGA-O1A	-5.35	110.25	123.63
12	H	801	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
12	B	818	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
12	B	835	CLA	C1D-ND-C4D	-5.34	102.56	106.31
12	a	831	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
12	A	837	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
12	G	822	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
12	A	816	CLA	O2D-CGD-CBD	5.34	120.56	111.23
12	G	822	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
12	G	825	CLA	C4A-NA-C1A	5.34	109.11	106.68
12	H	837	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	b	814	CLA	C3D-C2D-C1D	-5.33	98.55	105.83
12	A	813	CLA	C2D-C1D-ND	5.33	115.41	110.13
12	a	823	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	G	802	CLA	C1D-ND-C4D	-5.33	102.57	106.31
12	a	812	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
12	b	810	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
12	G	821	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	a	834	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	B	830	CLA	C4A-NA-C1A	5.33	109.11	106.68
12	H	820	CLA	C3D-C2D-C1D	-5.33	98.55	105.83
12	b	811	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	f	201	CLA	O2A-CGA-O1A	-5.33	110.29	123.63
12	H	809	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
12	G	813	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
12	b	829	CLA	C1D-ND-C4D	-5.33	102.57	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	838	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
12	H	838	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
12	H	813	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
12	H	813	CLA	C2D-C1D-ND	5.33	115.40	110.13
12	H	817	CLA	C2C-C1C-NC	5.33	115.58	109.98
12	A	831	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
15	G	847	BCR	C20-C19-C18	5.33	140.97	126.36
12	b	824	CLA	C2C-C1C-NC	5.33	115.58	109.98
12	B	817	CLA	O2A-CGA-O1A	-5.32	109.64	123.33
12	G	837	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
12	B	809	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	G	811	CLA	O2A-CGA-O1A	-5.32	110.31	123.63
12	A	803	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	A	825	CLA	C2C-C1C-NC	5.32	115.57	109.98
12	b	811	CLA	O2D-CGD-CBD	5.32	120.53	111.23
12	A	812	CLA	O2A-CGA-O1A	-5.32	110.32	123.63
12	H	832	CLA	CMD-C2D-C1D	5.32	134.10	124.73
15	G	847	BCR	C24-C23-C22	-5.32	118.37	126.23
12	G	818	CLA	C2D-C1D-ND	5.32	115.39	110.13
12	H	814	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	a	835	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
12	H	826	CLA	CMD-C2D-C1D	5.32	134.09	124.73
12	B	814	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	G	832	CLA	O2A-CGA-O1A	-5.32	110.33	123.63
12	A	822	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
12	A	837	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
12	l	206	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
12	a	812	CLA	O2A-CGA-O1A	-5.32	110.33	123.63
12	B	806	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
12	A	822	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
12	b	833	CLA	C2D-C1D-ND	5.31	115.39	110.13
12	B	818	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
12	H	824	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
12	B	838	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	H	815	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
12	a	803	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
12	B	813	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
15	G	846	BCR	C3-C4-C5	-5.31	104.58	114.06
12	a	836	CLA	O2A-CGA-CBA	5.31	128.03	111.83
12	G	812	CLA	C2D-C1D-ND	5.31	115.38	110.13
12	H	814	CLA	C2D-C1D-ND	5.31	115.38	110.13
12	G	808	CLA	C1C-C2C-C3C	-5.31	101.40	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	837	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	H	803	CLA	C4A-NA-C1A	5.31	109.10	106.68
12	B	835	CLA	O2D-CGD-CBD	5.31	120.51	111.23
12	G	804	CLA	O2A-CGA-O1A	-5.31	110.36	123.63
12	b	809	CLA	C4A-NA-C1A	5.30	109.10	106.68
12	B	833	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	b	813	CLA	C1D-ND-C4D	-5.30	102.59	106.31
12	S	202	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
12	b	822	CLA	C2C-C1C-NC	5.30	115.55	109.98
12	G	811	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
12	b	815	CLA	O2D-CGD-CBD	5.30	120.50	111.23
12	b	820	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
12	G	840	CLA	C4A-NA-C1A	5.30	109.10	106.68
12	G	820	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
12	H	818	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	G	831	CLA	O2A-CGA-O1A	-5.30	110.37	123.63
12	H	829	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
12	G	807	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	B	817	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	G	809	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
12	G	835	CLA	C2D-C1D-ND	5.30	115.37	110.13
12	G	834	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
12	B	815	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
12	a	807	CLA	C2D-C1D-ND	5.30	115.37	110.13
12	A	811	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
12	a	854	CLA	O2D-CGD-CBD	5.29	120.49	111.23
12	B	835	CLA	C2D-C1D-ND	5.29	115.37	110.13
12	A	810	CLA	O2A-CGA-O1A	-5.29	110.39	123.63
12	H	808	CLA	C2D-C1D-ND	5.29	115.36	110.13
12	a	810	CLA	O2A-CGA-O1A	-5.29	110.39	123.63
12	a	819	CLA	C2D-C1D-ND	5.29	115.36	110.13
12	A	827	CLA	O2D-CGD-CBD	5.29	120.48	111.23
12	H	832	CLA	C2D-C1D-ND	5.29	115.36	110.13
12	G	823	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
12	A	806	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
12	b	806	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
12	H	805	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
12	B	805	CLA	C2D-C1D-ND	5.29	115.36	110.13
12	B	801	CLA	C1D-ND-C4D	-5.29	102.60	106.31
12	G	831	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
12	b	837	CLA	C2C-C1C-NC	5.28	115.53	109.98
12	b	834	CLA	O2D-CGD-CBD	5.28	120.47	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	813	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
12	B	835	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
12	a	820	CLA	O2A-CGA-O1A	-5.28	110.42	123.63
12	H	803	CLA	C2C-C1C-NC	5.28	115.53	109.98
15	a	852	BCR	C24-C23-C22	-5.28	118.42	126.23
12	l	204	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
12	b	819	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
12	b	828	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
12	H	837	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
12	b	836	CLA	C2D-C1D-ND	5.28	115.35	110.13
12	b	814	CLA	C4A-NA-C1A	5.28	109.09	106.68
12	a	805	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
12	b	818	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
12	B	802	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
12	a	840	CLA	C2D-C1D-ND	5.28	115.35	110.13
12	b	823	CLA	C4A-NA-C1A	5.28	109.09	106.68
12	a	821	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
12	a	832	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
12	G	820	CLA	C4A-NA-C1A	5.27	109.08	106.68
12	a	823	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
17	M	101	45D	C23-C19-C07	-5.27	112.91	127.00
12	L	202	CLA	C2D-C1D-ND	5.27	115.34	110.13
12	G	855	CLA	O2D-CGD-CBD	5.27	120.45	111.23
12	B	814	CLA	C4A-NA-C1A	5.27	109.08	106.68
12	A	831	CLA	C2D-C1D-ND	5.27	115.34	110.13
12	B	837	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
12	B	811	CLA	O2A-CGA-O1A	-5.27	110.45	123.63
12	a	806	CLA	O2A-CGA-CBA	5.27	127.90	111.83
12	H	833	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
12	G	837	CLA	C2D-C1D-ND	5.26	115.34	110.13
12	A	823	CLA	C1C-C2C-C3C	-5.26	101.44	106.98
12	H	850	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
12	A	807	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
12	B	808	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
12	A	806	CLA	C4A-NA-C1A	5.26	109.08	106.68
12	B	828	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
12	a	839	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
15	L	203	BCR	C31-C1-C6	-5.26	102.00	110.24
12	A	804	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
12	b	832	CLA	O2D-CGD-CBD	5.26	120.42	111.23
12	B	826	CLA	O2A-CGA-O1A	-5.26	110.48	123.63
12	A	836	CLA	O2A-CGA-CBA	5.25	127.85	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	818	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
12	H	815	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
12	a	826	CLA	C4A-NA-C1A	5.25	109.08	106.68
12	L	205	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
12	H	838	CLA	C2D-C1D-ND	5.25	115.32	110.13
15	G	853	BCR	C24-C23-C22	-5.25	118.47	126.23
12	A	821	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
12	G	837	CLA	C4A-NA-C1A	5.25	109.07	106.68
12	P	203	CLA	C4A-NA-C1A	5.25	109.07	106.68
12	B	833	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
12	G	815	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
12	F	201	CLA	O2A-CGA-O1A	-5.25	110.51	123.63
12	A	816	CLA	C3B-C2B-C1B	-5.25	100.99	107.17
12	b	809	CLA	C3D-C2D-C1D	-5.24	98.67	105.83
12	f	203	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
12	G	839	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	B	832	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	a	822	CLA	O2D-CGD-CBD	5.24	120.39	111.23
12	b	819	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
12	A	813	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
12	G	823	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	H	808	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	L	204	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	G	812	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
12	b	813	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
12	B	802	CLA	CMC-C2C-C1C	5.24	133.22	125.03
12	B	820	CLA	C2C-C1C-NC	5.24	115.48	109.98
12	H	816	CLA	C4A-NA-C1A	5.24	109.07	106.68
12	B	807	CLA	O2D-CGD-CBD	5.24	120.38	111.23
12	B	813	CLA	C4A-NA-C1A	5.23	109.07	106.68
12	b	813	CLA	O2D-CGD-CBD	5.23	120.38	111.23
12	b	834	CLA	C2D-C1D-ND	5.23	115.31	110.13
12	l	204	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
12	B	836	CLA	O2D-CGD-CBD	5.23	120.38	111.23
12	G	807	CLA	C1D-ND-C4D	-5.23	102.64	106.31
12	B	832	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
12	a	832	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
12	H	836	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
12	G	828	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
12	b	801	CLA	O2A-C1-C2	5.22	128.22	108.11
12	a	811	CLA	C1C-C2C-C3C	-5.22	101.48	106.98
12	P	203	CLA	C3D-C2D-C1D	-5.22	98.70	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	816	CLA	C3B-C2B-C1B	-5.22	101.01	107.17
12	A	820	CLA	O2A-CGA-O1A	-5.22	110.56	123.63
12	H	819	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
12	H	819	CLA	C4A-NA-C1A	5.22	109.06	106.68
12	b	809	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
12	B	809	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
12	a	830	CLA	C2D-C1D-ND	5.22	115.29	110.13
12	b	832	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
15	f	204	BCR	C24-C23-C22	-5.22	118.51	126.23
12	B	819	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
12	G	805	CLA	C2D-C1D-ND	5.22	115.29	110.13
12	F	203	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
12	b	802	CLA	C2C-C1C-NC	5.22	115.46	109.98
12	B	830	CLA	C2D-C1D-ND	5.22	115.29	110.13
12	a	821	CLA	C1D-ND-C4D	-5.22	102.65	106.31
12	A	814	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
15	P	202	BCR	C24-C23-C22	-5.22	118.52	126.23
12	j	102	CLA	C2D-C1D-ND	5.22	115.29	110.13
12	A	810	CLA	C2D-C1D-ND	5.21	115.29	110.13
12	a	804	CLA	C4A-NA-C1A	5.21	109.06	106.68
12	a	824	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
12	G	802	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
12	S	202	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
12	A	811	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
12	J	103	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
12	H	810	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
12	G	829	CLA	CMD-C2D-C1D	5.21	133.90	124.73
12	B	807	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
12	G	810	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
12	H	831	CLA	CMD-C2D-C1D	5.21	133.90	124.73
12	H	802	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
12	A	839	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
12	B	819	CLA	C2D-C1D-ND	5.21	115.28	110.13
12	l	202	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
12	H	810	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
17	m	101	45D	C23-C19-C07	-5.20	113.09	127.00
12	b	829	CLA	O2D-CGD-CBD	5.20	120.33	111.23
12	G	839	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
12	H	812	CLA	O2A-CGA-O1A	-5.20	110.61	123.63
12	G	825	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
15	F	202	BCR	C3-C4-C5	-5.20	104.78	114.06
11	A	801	CL0	C1D-ND-C4D	-5.20	102.66	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	844	BCR	C7-C8-C9	-5.20	118.55	126.23
12	H	833	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
12	A	810	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
12	A	832	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
12	A	817	CLA	C2B-C1B-NB	5.20	115.71	110.33
12	b	835	CLA	O2D-CGD-CBD	5.19	120.31	111.23
12	B	836	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
12	S	203	CLA	C1D-ND-C4D	-5.19	102.67	106.31
12	H	821	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
12	A	806	CLA	O2A-CGA-CBA	5.19	127.66	111.83
12	b	832	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
12	H	814	CLA	C2C-C1C-NC	5.19	115.43	109.98
12	b	823	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
12	L	205	CLA	C1D-ND-C4D	-5.19	102.67	106.31
12	a	814	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
12	A	837	CLA	C2D-C1D-ND	5.19	115.26	110.13
12	a	825	CLA	C1C-C2C-C3C	-5.19	101.53	106.98
12	b	835	CLA	C1C-C2C-C3C	-5.19	101.53	106.98
12	S	204	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
12	H	811	CLA	C2D-C1D-ND	5.18	115.26	110.13
12	A	822	CLA	C4A-NA-C1A	5.18	109.04	106.68
12	H	834	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
12	b	837	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
12	a	819	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
12	G	824	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
12	a	814	CLA	C2D-C1D-ND	5.18	115.25	110.13
12	G	812	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
12	G	831	CLA	C2C-C1C-NC	5.18	115.42	109.98
12	G	837	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
12	B	834	CLA	C1D-ND-C4D	-5.18	102.68	106.31
12	G	807	CLA	O2A-CGA-CBA	5.17	127.61	111.83
12	G	814	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
12	H	831	CLA	C4A-NA-C1A	5.17	109.04	106.68
12	P	201	CLA	O2A-CGA-O1A	-5.17	110.70	123.63
12	H	820	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
12	H	825	CLA	C2D-C1D-ND	5.17	115.24	110.13
12	B	823	CLA	C2D-C1D-ND	5.17	115.24	110.13
12	G	818	CLA	O2D-CGD-CBD	5.17	120.26	111.23
12	H	812	CLA	C1C-C2C-C3C	-5.17	101.55	106.98
12	G	815	CLA	C2D-C1D-ND	5.17	115.24	110.13
12	L	202	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
15	f	202	BCR	C7-C8-C9	-5.16	118.59	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	822	CLA	C1D-ND-C4D	-5.16	102.69	106.31
12	H	814	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
12	H	819	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
12	a	822	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
12	G	829	CLA	O2D-CGD-CBD	5.16	120.25	111.23
12	H	812	CLA	O2D-CGD-CBD	5.16	120.25	111.23
12	b	834	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
12	A	804	CLA	C4A-NA-C1A	5.16	109.03	106.68
12	H	807	CLA	C2D-C1D-ND	5.16	115.23	110.13
12	A	828	CLA	CMD-C2D-C1D	5.16	133.81	124.73
12	H	831	CLA	O2D-CGD-O1D	-5.16	113.81	123.85
12	b	823	CLA	C2C-C1C-NC	5.16	115.40	109.98
12	l	202	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
12	G	829	CLA	C4A-NA-C1A	5.15	109.03	106.68
12	b	802	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
12	a	816	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
12	H	834	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
12	B	813	CLA	C1D-ND-C4D	-5.15	102.70	106.31
12	b	828	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
12	G	833	CLA	C4A-NA-C1A	5.15	109.03	106.68
12	H	825	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
12	b	817	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
12	G	816	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
12	H	802	CLA	CMD-C2D-C1D	5.15	133.79	124.73
12	H	806	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
12	b	805	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
12	j	104	CLA	C1C-C2C-C3C	-5.15	101.57	106.98
12	b	817	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
12	B	822	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
12	H	803	CLA	C2D-C1D-ND	5.14	115.22	110.13
12	G	810	CLA	C2D-C1D-ND	5.14	115.22	110.13
12	a	810	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
12	a	815	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
12	A	831	CLA	C2C-C1C-NC	5.14	115.38	109.98
12	a	804	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
12	G	813	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	a	806	CLA	C2C-C1C-NC	5.14	115.38	109.98
12	H	818	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
12	G	819	CLA	C2D-C1D-ND	5.14	115.21	110.13
17	T	101	45D	C23-C19-C07	-5.14	113.27	127.00
12	G	820	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	A	828	CLA	C3B-C2B-C1B	-5.14	101.11	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	842	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
12	A	814	CLA	C2D-C1D-ND	5.14	115.21	110.13
12	B	833	CLA	O2A-CGA-O1A	-5.14	110.78	123.63
12	B	833	CLA	O2D-CGD-CBD	5.14	120.21	111.23
12	b	810	CLA	OBD-CAD-C3D	-5.13	116.42	128.42
12	f	201	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
12	L	202	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
12	B	820	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
12	a	825	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
12	H	808	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
12	a	820	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
12	a	818	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
12	G	806	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	a	830	CLA	O2A-CGA-O1A	-5.13	110.80	123.63
12	a	831	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	B	820	CLA	C4A-NA-C1A	5.13	109.02	106.68
12	A	824	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
12	L	206	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
12	a	805	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
12	G	833	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
12	B	801	CLA	C2C-C1C-NC	5.13	115.36	109.98
12	A	808	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
12	H	830	CLA	O2D-CGD-CBD	5.12	120.18	111.23
15	J	102	BCR	C7-C8-C9	-5.12	118.66	126.23
12	B	812	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
12	a	819	CLA	C2C-C1C-NC	5.12	115.36	109.98
12	b	835	CLA	C2C-C1C-NC	5.12	115.36	109.98
12	L	204	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
12	l	205	CLA	C1D-ND-C4D	-5.12	102.72	106.31
12	G	818	CLA	O2A-CGA-O1A	-5.12	110.82	123.63
12	A	823	CLA	C2D-C1D-ND	5.12	115.19	110.13
12	G	821	CLA	O2A-CGA-O1A	-5.12	110.83	123.63
12	B	814	CLA	C2D-C1D-ND	5.12	115.19	110.13
12	a	837	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
12	A	830	CLA	C2C-C1C-NC	5.12	115.36	109.98
12	H	832	CLA	C1C-C2C-C3C	-5.11	101.60	106.98
12	H	822	CLA	O2A-CGA-O1A	-5.11	110.84	123.63
12	b	831	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	l	202	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	G	842	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
12	a	830	CLA	C1D-ND-C4D	-5.11	102.73	106.31
12	R	103	CLA	C3D-C2D-C1D	-5.11	98.86	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	808	CLA	C4A-NA-C1A	5.11	109.01	106.68
12	H	815	CLA	C2D-C1D-ND	5.11	115.18	110.13
12	G	802	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
12	H	817	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
12	B	812	CLA	C2D-C1D-ND	5.11	115.18	110.13
12	b	801	CLA	C1D-ND-C4D	-5.11	102.73	106.31
12	b	804	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
12	J	103	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
12	B	803	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
12	a	834	CLA	C2D-C1D-ND	5.10	115.18	110.13
12	H	829	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
12	a	837	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
12	A	819	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
12	B	803	CLA	O2A-CGA-CBA	5.10	127.39	111.83
12	B	821	CLA	C2C-C1C-NC	5.10	115.34	109.98
12	A	836	CLA	C2D-C1D-ND	5.10	115.17	110.13
12	A	819	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
12	A	820	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
12	B	836	CLA	C2B-C1B-NB	5.09	115.61	110.33
12	G	804	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
12	H	839	CLA	O2A-C1-C2	5.09	127.70	108.11
12	A	811	CLA	C4A-NA-C1A	5.09	109.00	106.68
12	H	824	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
12	f	203	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
12	a	833	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
12	R	103	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
12	B	818	CLA	C2D-C1D-ND	5.09	115.16	110.13
12	a	820	CLA	O2D-CGD-CBD	5.09	120.12	111.23
15	A	852	BCR	C24-C23-C22	-5.09	118.71	126.23
12	B	826	CLA	CMD-C2D-C3D	-5.09	116.02	127.69
12	H	809	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
12	a	816	CLA	O2D-CGD-CBD	5.09	120.12	111.23
12	a	839	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
12	H	820	CLA	C2D-C1D-ND	5.08	115.16	110.13
12	a	810	CLA	C2D-C1D-ND	5.08	115.15	110.13
12	A	831	CLA	O2D-CGD-CBD	5.08	120.11	111.23
12	b	801	CLA	C2C-C1C-NC	5.08	115.32	109.98
12	a	810	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
12	G	834	CLA	C2D-C1D-ND	5.08	115.15	110.13
12	b	821	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
12	A	839	CLA	C2B-C1B-NB	5.08	115.59	110.33
12	b	821	CLA	C2C-C1C-NC	5.08	115.32	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	809	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
12	G	838	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
12	H	839	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	a	823	CLA	C2D-C1D-ND	5.08	115.15	110.13
12	A	815	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	H	803	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	P	203	CLA	O2D-CGD-CBD	5.07	120.10	111.23
12	A	840	CLA	C4A-NA-C1A	5.07	108.99	106.68
12	a	833	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
12	H	801	CLA	C1C-C2C-C3C	-5.07	101.64	106.98
12	G	832	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
17	M	101	45D	C31-C29-C25	-5.07	120.17	127.28
12	b	831	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
12	b	833	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
12	A	855	CLA	CMD-C2D-C1D	5.07	133.65	124.73
12	G	825	CLA	C2D-C1D-ND	5.07	115.14	110.13
12	b	806	CLA	O2A-CGA-O1A	-5.06	110.96	123.63
12	H	835	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
12	b	848	CLA	O2A-CGA-O1A	-5.06	110.96	123.63
12	B	834	CLA	O2A-CGA-O1A	-5.06	110.96	123.63
12	F	203	CLA	O2D-CGD-CBD	5.06	120.08	111.23
12	b	806	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
12	b	818	CLA	C2D-C1D-ND	5.06	115.14	110.13
12	b	819	CLA	C2D-C1D-ND	5.06	115.14	110.13
12	B	838	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
12	F	203	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
12	b	827	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
15	A	848	BCR	C24-C23-C22	-5.06	118.75	126.23
12	A	837	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
12	l	202	CLA	C4A-NA-C1A	5.06	108.99	106.68
12	G	810	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
12	L	202	CLA	C4A-NA-C1A	5.06	108.99	106.68
12	H	825	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
12	L	202	CLA	O2A-CGA-O1A	-5.06	110.98	123.63
12	b	820	CLA	C1D-ND-C4D	-5.06	102.77	106.31
12	a	808	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
12	H	801	CLA	C2D-C1D-ND	5.05	115.13	110.13
12	B	820	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
12	a	830	CLA	O2D-CGD-CBD	5.05	120.06	111.23
11	A	801	CL0	O2A-CGA-O1A	-5.05	110.99	123.63
12	B	828	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
12	a	825	CLA	C2D-C1D-ND	5.05	115.12	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	840	CLA	C2D-C1D-ND	5.05	115.12	110.13
12	G	818	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
12	H	829	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
12	a	820	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
12	a	818	CLA	O2D-CGD-CBD	5.05	120.05	111.23
12	b	821	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
15	I	101	BCR	C3-C4-C5	-5.05	105.06	114.06
12	B	834	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
12	G	836	CLA	C1-O2A-CGA	5.04	128.86	116.65
12	b	833	CLA	O2D-CGD-CBD	5.04	120.05	111.23
12	a	810	CLA	C1D-ND-C4D	-5.04	102.77	106.31
12	B	809	CLA	C2D-C1D-ND	5.04	115.12	110.13
12	L	204	CLA	CMD-C2D-C1D	5.04	133.60	124.73
12	b	848	CLA	C2C-C1C-NC	5.04	115.27	109.98
12	B	808	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
12	j	104	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
12	a	831	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
12	B	821	CLA	O2A-CGA-O1A	-5.04	111.03	123.63
15	G	849	BCR	C24-C23-C22	-5.03	118.79	126.23
17	T	101	45D	C31-C29-C25	-5.03	120.22	127.28
12	G	807	CLA	O2D-CGD-CBD	5.03	120.03	111.23
12	B	823	CLA	C4A-NA-C1A	5.03	108.97	106.68
12	A	817	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
12	b	814	CLA	C2D-C1D-ND	5.03	115.10	110.13
12	B	833	CLA	C1D-ND-C4D	-5.03	102.78	106.31
12	a	815	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
12	b	821	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
12	j	102	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
12	b	829	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
12	B	801	CLA	O2A-C1-C2	5.02	127.44	108.11
12	H	808	CLA	O2A-CGA-O1A	-5.02	111.06	123.63
12	B	809	CLA	O2D-CGD-CBD	5.02	120.01	111.23
12	b	817	CLA	O2A-CGA-O1A	-5.02	110.42	123.33
12	H	821	CLA	CAA-C2A-C3A	-5.02	99.43	113.00
12	a	838	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
12	A	839	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
12	G	827	CLA	C1D-ND-C4D	-5.02	102.79	106.31
12	B	824	CLA	O2A-CGA-O1A	-5.02	111.07	123.63
12	B	823	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
12	G	811	CLA	C1D-ND-C4D	-5.02	102.79	106.31
12	H	850	CLA	O2A-CGA-O1A	-5.02	111.08	123.63
12	b	814	CLA	C2C-C1C-NC	5.02	115.25	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	835	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
12	B	801	CLA	O2A-CGA-O1A	-5.02	111.08	123.63
12	B	828	CLA	C2D-C1D-ND	5.02	115.09	110.13
12	A	819	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
12	H	833	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
12	b	803	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
12	b	816	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
12	a	837	CLA	C4A-NA-C1A	5.01	108.96	106.68
12	S	204	CLA	C2D-C1D-ND	5.01	115.08	110.13
12	A	817	CLA	O2D-CGD-CBD	5.01	119.98	111.23
12	B	816	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
12	b	806	CLA	C1D-ND-C4D	-5.00	102.80	106.31
12	a	839	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
12	G	817	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
12	G	812	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
12	b	808	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
12	A	834	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
12	B	832	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
12	a	840	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
12	a	817	CLA	C2C-C1C-NC	5.00	115.23	109.98
12	H	822	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
15	A	849	BCR	C20-C19-C18	5.00	140.06	126.36
15	P	204	BCR	C24-C23-C22	-5.00	118.84	126.23
12	b	835	CLA	C2B-C1B-NB	4.99	115.50	110.33
12	b	803	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	Q	101	BCR	C3-C4-C5	-4.99	105.16	114.06
12	G	808	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
12	l	202	CLA	C2D-C1D-ND	4.99	115.06	110.13
12	A	809	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
12	b	830	CLA	C2D-C1D-ND	4.99	115.06	110.13
12	A	854	CLA	O2A-C1-C2	4.99	127.30	108.11
12	B	805	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
12	l	206	CLA	C2D-C1D-ND	4.99	115.06	110.13
12	A	825	CLA	C1C-C2C-C3C	-4.98	101.74	106.98
12	G	831	CLA	O2D-CGD-CBD	4.98	119.94	111.23
12	G	820	CLA	C2D-C1D-ND	4.98	115.06	110.13
12	f	203	CLA	O2D-CGD-CBD	4.98	119.94	111.23
12	G	856	CLA	CMD-C2D-C1D	4.98	133.50	124.73
12	a	830	CLA	C2C-C1C-NC	4.98	115.21	109.98
11	G	801	CL0	O2A-CGA-O1A	-4.98	111.17	123.63
12	G	809	CLA	C4A-NA-C1A	4.98	108.95	106.68
12	H	850	CLA	C2C-C1C-NC	4.98	115.21	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	201	CLA	O2D-CGD-CBD	4.97	119.93	111.23
12	G	803	CLA	C2C-C1C-NC	4.97	115.21	109.98
12	J	103	CLA	C4A-NA-C1A	4.97	108.95	106.68
12	H	809	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
12	G	816	CLA	C2D-C1D-ND	4.97	115.05	110.13
12	S	204	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
12	G	805	CLA	C4A-NA-C1A	4.97	108.95	106.68
12	B	829	CLA	O2D-CGD-CBD	4.97	119.92	111.23
15	A	844	BCR	C7-C8-C9	-4.97	118.89	126.23
12	L	206	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
12	A	833	CLA	C2D-C1D-ND	4.97	115.04	110.13
12	A	824	CLA	C2D-C1D-ND	4.97	115.04	110.13
12	G	802	CLA	O2A-C1-C2	4.96	127.20	108.11
12	b	824	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
12	A	813	CLA	C1D-ND-C4D	-4.96	102.83	106.31
12	A	819	CLA	C4A-NA-C1A	4.96	108.94	106.68
12	L	206	CLA	C2D-C1D-ND	4.96	115.03	110.13
12	G	855	CLA	CMD-C2D-C1D	4.96	133.46	124.73
12	b	808	CLA	C1C-C2C-C3C	-4.96	101.77	106.98
12	H	818	CLA	O2A-CGA-O1A	-4.96	110.58	123.33
12	B	811	CLA	C1C-C2C-C3C	-4.96	101.77	106.98
12	H	828	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
12	G	823	CLA	C2D-C1D-ND	4.96	115.03	110.13
15	R	102	BCR	C7-C8-C9	-4.96	118.90	126.23
12	R	103	CLA	O2D-CGD-CBD	4.95	119.89	111.23
12	b	804	CLA	O2A-CGA-O1A	-4.95	111.24	123.63
12	a	810	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
12	A	824	CLA	O2A-CGA-O1A	-4.95	111.24	123.63
12	a	832	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
12	B	808	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
12	G	855	CLA	O2A-C1-C2	4.95	127.15	108.11
12	a	803	CLA	C2D-C1D-ND	4.95	115.02	110.13
12	a	841	CLA	C2D-C1D-ND	4.95	115.02	110.13
12	G	802	CLA	C2C-C1C-NC	4.95	115.18	109.98
12	G	856	CLA	O2A-C1-C2	4.95	127.14	108.11
12	a	837	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
12	G	824	CLA	C1C-C2C-C3C	-4.95	101.78	106.98
12	b	833	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
12	G	819	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
12	J	103	CLA	C2D-C1D-ND	4.94	115.02	110.13
12	B	820	CLA	O2A-CGA-O1A	-4.94	110.62	123.33
12	A	806	CLA	O2D-CGD-CBD	4.94	119.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	801	CL0	C2D-C1D-ND	4.94	115.02	110.13
12	H	835	CLA	O2A-CGA-O1A	-4.94	111.27	123.63
12	G	814	CLA	O2A-CGA-O1A	-4.94	110.64	123.33
12	B	828	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
12	H	821	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
12	a	812	CLA	O2D-CGD-CBD	4.93	119.86	111.23
12	a	826	CLA	C1D-ND-C4D	-4.93	102.85	106.31
12	G	831	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
12	H	802	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
12	b	830	CLA	O2A-CGA-O1A	-4.93	110.65	123.33
12	G	823	CLA	O2D-CGD-CBD	4.93	119.85	111.23
15	J	104	BCR	C24-C23-C22	-4.93	118.94	126.23
12	f	203	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
12	a	824	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
12	A	828	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
12	H	812	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	a	801	CL0	O2D-CGD-CBD	4.93	119.85	111.23
12	B	816	CLA	C1C-C2C-C3C	-4.93	101.80	106.98
12	a	830	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
12	S	202	CLA	O2A-CGA-O1A	-4.93	111.31	123.63
15	A	845	BCR	C3-C4-C5	-4.93	105.27	114.06
15	j	101	BCR	C7-C8-C9	-4.93	118.95	126.23
12	H	817	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
12	B	831	CLA	O2A-CGA-O1A	-4.92	110.67	123.33
12	B	834	CLA	C2C-C1C-NC	4.92	115.15	109.98
12	a	819	CLA	C1D-ND-C4D	-4.92	102.86	106.31
12	l	206	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
12	b	814	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
12	H	810	CLA	C4A-NA-C1A	4.92	108.92	106.68
12	H	810	CLA	O2A-CGA-O1A	-4.92	110.67	123.33
12	b	836	CLA	O2D-CGD-CBD	4.92	119.84	111.23
12	H	823	CLA	C1D-ND-C4D	-4.92	102.86	106.31
12	b	809	CLA	C2D-C1D-ND	4.92	115.00	110.13
12	b	828	CLA	C2D-C1D-ND	4.92	115.00	110.13
12	b	828	CLA	O2A-CGA-O1A	-4.92	110.68	123.33
12	A	834	CLA	C2D-C1D-ND	4.92	115.00	110.13
12	H	838	CLA	O2D-CGD-CBD	4.92	119.83	111.23
12	a	824	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
12	l	204	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
12	G	821	CLA	O2D-CGD-CBD	4.92	119.83	111.23
12	H	824	CLA	C4A-NA-C1A	4.92	108.92	106.68
12	L	204	CLA	O2A-CGA-O1A	-4.92	111.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	834	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
12	b	820	CLA	C2C-C1C-NC	4.92	115.15	109.98
12	a	806	CLA	O2D-CGD-CBD	4.92	119.82	111.23
12	H	817	CLA	C3B-C2B-C1B	-4.92	101.38	107.17
12	a	815	CLA	C2D-C1D-ND	4.92	114.99	110.13
12	G	812	CLA	O2D-CGD-CBD	4.92	119.82	111.23
12	b	813	CLA	O2A-CGA-O1A	-4.91	111.33	123.63
12	B	829	CLA	C2B-C1B-NB	4.91	115.42	110.33
12	A	818	CLA	O2D-CGD-CBD	4.91	119.82	111.23
12	G	821	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
12	b	820	CLA	O2A-CGA-O1A	-4.91	110.71	123.33
12	A	807	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	B	827	CLA	C1C-C2C-C3C	-4.91	101.82	106.98
12	A	807	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
12	H	832	CLA	O2A-CGA-O1A	-4.91	110.71	123.33
12	G	811	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
12	H	804	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
12	H	803	CLA	C1C-C2C-C3C	-4.90	101.82	106.98
12	G	837	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
12	A	816	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
12	a	822	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
12	H	801	CLA	O2D-CGD-CBD	4.90	119.80	111.23
12	G	831	CLA	C2D-C1D-ND	4.90	114.98	110.13
12	G	840	CLA	C2D-C1D-ND	4.90	114.98	110.13
12	G	834	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
12	A	809	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
12	a	840	CLA	C1C-C2C-C3C	-4.90	101.83	106.98
12	b	824	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
12	A	837	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
12	H	831	CLA	C1C-C2C-C3C	-4.90	101.83	106.98
12	A	840	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
12	H	810	CLA	C2D-C1D-ND	4.90	114.97	110.13
12	G	810	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
12	A	824	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
12	B	836	CLA	C2C-C1C-NC	4.89	115.12	109.98
12	G	825	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
12	a	822	CLA	C2D-C1D-ND	4.89	114.97	110.13
12	B	804	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
12	a	827	CLA	C2C-C1C-NC	4.89	115.12	109.98
17	T	101	45D	C39-C35-C37	4.89	130.74	122.82
12	A	813	CLA	O2A-CGA-O1A	-4.89	110.76	123.33
12	G	823	CLA	O2A-CGA-O1A	-4.89	111.40	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	206	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
12	G	824	CLA	C2D-C1D-ND	4.89	114.96	110.13
12	a	824	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
12	A	821	CLA	C1D-ND-C4D	-4.88	102.89	106.31
12	a	807	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
12	P	203	CLA	C1C-C2C-C3C	-4.88	101.84	106.98
12	H	839	CLA	C1D-ND-C4D	-4.88	102.89	106.31
12	G	810	CLA	O2A-CGA-O1A	-4.88	110.78	123.33
12	G	826	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
12	A	838	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
12	B	802	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
12	F	203	CLA	C4A-NA-C1A	4.87	108.90	106.68
12	a	836	CLA	C1-O2A-CGA	4.87	128.45	116.65
12	a	839	CLA	C2B-C1B-NB	4.87	115.38	110.33
12	H	815	CLA	OBD-CAD-C3D	-4.87	117.02	128.42
12	A	808	CLA	O2A-CGA-O1A	-4.87	111.44	123.63
12	G	841	CLA	O2A-CGA-O1A	-4.87	111.44	123.63
12	G	835	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
12	G	829	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
11	a	801	CL0	C4D-C3D-CAD	4.87	113.39	108.11
12	G	804	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
12	H	821	CLA	O2A-CGA-O1A	-4.87	110.81	123.33
12	H	829	CLA	O2A-CGA-O1A	-4.87	110.81	123.33
15	J	101	BCR	C7-C8-C9	-4.87	119.03	126.23
12	A	815	CLA	C2D-C1D-ND	4.87	114.94	110.13
12	B	804	CLA	O2A-CGA-O1A	-4.86	111.46	123.63
12	a	835	CLA	C1D-ND-C4D	-4.86	102.90	106.31
12	b	815	CLA	CHD-C1D-ND	-4.86	117.96	124.80
12	a	813	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
12	H	807	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
12	b	807	CLA	O2D-CGD-CBD	4.86	119.73	111.23
12	b	811	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
12	b	827	CLA	C1C-C2C-C3C	-4.86	101.87	106.98
12	b	807	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
12	H	824	CLA	C2D-C1D-ND	4.86	114.94	110.13
12	b	820	CLA	CAA-C2A-C3A	-4.86	99.87	113.00
12	a	817	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
12	H	821	CLA	C2B-C1B-NB	4.86	115.36	110.33
12	A	855	CLA	C2B-C1B-NB	4.86	115.36	110.33
12	b	827	CLA	C2D-C1D-ND	4.86	114.93	110.13
12	a	819	CLA	O2A-CGA-O1A	-4.86	110.84	123.33
12	H	823	CLA	O2A-CGA-O1A	-4.86	111.48	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	203	CLA	C2D-C1D-ND	4.86	114.93	110.13
12	b	816	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
12	A	822	CLA	O2A-CGA-O1A	-4.86	111.48	123.63
12	a	839	CLA	C2D-C1D-ND	4.85	114.93	110.13
12	b	826	CLA	CMD-C2D-C3D	-4.85	116.56	127.69
12	b	805	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
12	B	801	CLA	O2A-CGA-CBA	4.85	126.63	111.83
12	B	831	CLA	C2D-C1D-ND	4.85	114.93	110.13
12	a	817	CLA	C1D-ND-C4D	-4.85	102.91	106.31
12	b	816	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
11	a	801	CL0	O2A-CGA-O1A	-4.85	111.50	123.63
12	H	835	CLA	C1D-ND-C4D	-4.85	102.91	106.31
12	G	825	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
12	A	819	CLA	O2A-CGA-O1A	-4.85	110.87	123.33
12	G	814	CLA	C2D-C1D-ND	4.84	114.92	110.13
12	A	817	CLA	C2D-C1D-ND	4.84	114.92	110.13
12	b	822	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
12	B	837	CLA	C1D-ND-C4D	-4.84	102.91	106.31
12	B	820	CLA	CAA-C2A-C3A	-4.84	99.91	113.00
12	A	841	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
15	j	101	BCR	C24-C23-C22	-4.84	119.07	126.23
12	a	826	CLA	C2C-C1C-NC	4.84	115.07	109.98
12	B	837	CLA	O2D-CGD-CBD	4.84	119.69	111.23
12	b	837	CLA	O2A-C1-C2	4.84	126.73	108.11
12	a	841	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
12	B	822	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
15	i	101	BCR	C3-C4-C5	-4.84	105.43	114.06
12	a	817	CLA	O2D-CGD-CBD	4.84	119.68	111.23
12	G	826	CLA	C2D-C1D-ND	4.84	114.91	110.13
12	a	813	CLA	O2A-CGA-O1A	-4.83	110.90	123.33
12	G	820	CLA	O2A-CGA-O1A	-4.83	110.90	123.33
12	l	206	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
12	b	834	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
12	S	203	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
12	H	814	CLA	C1D-ND-C4D	-4.83	102.92	106.31
12	B	807	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
12	S	204	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
12	a	828	CLA	O2D-CGD-CBD	4.83	119.67	111.23
12	a	834	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
12	a	841	CLA	CMB-C2B-C1B	4.83	132.77	125.42
12	G	813	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
12	b	801	CLA	C3D-C2D-C1D	-4.83	99.24	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	829	CLA	C4A-NA-C1A	4.83	108.88	106.68
12	G	839	CLA	C2B-C1B-NB	4.83	115.33	110.33
12	G	834	CLA	O2D-CGD-CBD	4.82	119.66	111.23
12	F	201	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
12	B	829	CLA	C1D-ND-C4D	-4.82	102.93	106.31
12	H	805	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
12	a	835	CLA	O2A-CGA-O1A	-4.82	110.94	123.33
12	L	205	CLA	O2A-CGA-O1A	-4.82	111.58	123.63
12	a	809	CLA	O2A-CGA-O1A	-4.82	110.94	123.33
12	H	837	CLA	O2D-CGD-CBD	4.82	119.65	111.23
12	B	820	CLA	C1D-ND-C4D	-4.82	102.93	106.31
12	G	816	CLA	O2D-CGD-CBD	4.82	119.65	111.23
12	H	823	CLA	CMD-C2D-C1D	4.81	133.21	124.73
12	b	822	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
12	a	826	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
12	B	807	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
12	H	829	CLA	C2D-C1D-ND	4.81	114.89	110.13
12	a	813	CLA	C2B-C1B-NB	4.81	115.31	110.33
12	A	830	CLA	C2D-C1D-ND	4.81	114.89	110.13
12	B	816	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
12	A	818	CLA	C1D-ND-C4D	-4.81	102.94	106.31
12	H	808	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
12	B	805	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
12	B	822	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
12	H	828	CLA	C2D-C1D-ND	4.81	114.88	110.13
12	G	809	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
11	A	801	CL0	CMD-C2D-C1D	4.80	133.19	124.73
12	H	833	CLA	O2A-CGA-O1A	-4.80	110.98	123.33
12	A	834	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
15	A	844	BCR	C24-C23-C22	-4.80	119.14	126.23
12	H	814	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
12	H	809	CLA	O2A-CGA-O1A	-4.80	111.00	123.33
12	b	803	CLA	C2D-C1D-ND	4.80	114.87	110.13
12	A	830	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
12	A	803	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
12	B	835	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
12	A	838	CLA	O2A-CGA-O1A	-4.79	111.01	123.33
12	b	834	CLA	O2A-CGA-O1A	-4.79	111.01	123.33
12	b	825	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
12	B	831	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
12	G	810	CLA	C1D-ND-C4D	-4.79	102.95	106.31
12	G	855	CLA	C4A-NA-C1A	4.78	108.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	832	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
15	j	103	BCR	C7-C8-C9	-4.78	119.16	126.23
12	R	103	CLA	C2D-C1D-ND	4.78	114.86	110.13
12	j	104	CLA	O2D-CGD-CBD	4.78	119.59	111.23
12	A	835	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
12	B	801	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	G	804	CLA	C2D-C1D-ND	4.78	114.85	110.13
12	B	811	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	b	831	CLA	O2A-CGA-O1A	-4.77	111.05	123.33
12	J	103	CLA	O2A-CGA-O1A	-4.77	111.05	123.33
12	a	834	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
12	A	816	CLA	C2D-C1D-ND	4.77	114.85	110.13
12	a	854	CLA	C4A-NA-C1A	4.77	108.86	106.68
12	A	809	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
12	G	831	CLA	C1C-C2C-C3C	-4.77	101.96	106.98
12	B	802	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
12	G	809	CLA	O2D-CGD-CBD	4.77	119.57	111.23
12	G	842	CLA	C1D-ND-C4D	-4.77	102.97	106.31
12	H	819	CLA	C2D-C1D-ND	4.77	114.84	110.13
12	H	832	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
12	A	826	CLA	O2A-CGA-O1A	-4.77	111.71	123.63
12	A	803	CLA	C2D-C1D-ND	4.77	114.84	110.13
12	a	854	CLA	O2A-C1-C2	4.77	126.45	108.11
12	A	811	CLA	O2A-CGA-O1A	-4.77	111.08	123.33
12	A	836	CLA	C1-O2A-CGA	4.77	128.19	116.65
12	B	828	CLA	O2A-CGA-O1A	-4.77	111.08	123.33
12	A	840	CLA	C1C-C2C-C3C	-4.77	101.97	106.98
12	B	813	CLA	O2A-CGA-O1A	-4.76	111.71	123.63
12	B	832	CLA	C2D-C1D-ND	4.76	114.84	110.13
12	G	840	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
12	B	829	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
12	A	821	CLA	O2A-CGA-O1A	-4.76	111.09	123.33
15	G	845	BCR	C24-C23-C22	-4.76	119.20	126.23
17	m	101	45D	C24-C20-C08	-4.76	114.29	127.00
12	H	830	CLA	O2A-CGA-CBA	4.76	126.34	111.83
12	l	202	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
12	G	810	CLA	O2D-CGD-CBD	4.76	119.55	111.23
12	J	103	CLA	O2D-CGD-CBD	4.76	119.55	111.23
15	I	101	BCR	C24-C23-C22	-4.76	119.20	126.23
12	a	831	CLA	O2A-CGA-O1A	-4.76	111.73	123.63
12	A	824	CLA	CMD-C2D-C1D	4.76	133.10	124.73
12	l	205	CLA	O2A-CGA-O1A	-4.75	111.73	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	812	CLA	C2D-C1D-ND	4.75	114.83	110.13
12	G	835	CLA	O2A-CGA-O1A	-4.75	111.11	123.33
12	P	203	CLA	C2D-C1D-ND	4.75	114.83	110.13
12	A	824	CLA	CMA-C3A-C4A	4.75	124.55	111.77
12	a	829	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
12	b	806	CLA	CAA-C2A-C3A	-4.75	100.16	113.00
12	b	835	CLA	O2A-CGA-O1A	-4.75	111.74	123.63
12	G	838	CLA	O2A-CGA-O1A	-4.75	111.11	123.33
12	b	809	CLA	O2A-CGA-O1A	-4.75	111.11	123.33
12	A	814	CLA	O2A-CGA-O1A	-4.75	111.12	123.33
12	a	808	CLA	O2A-CGA-O1A	-4.75	111.75	123.63
12	L	206	CLA	C1D-ND-C4D	-4.75	102.98	106.31
12	G	829	CLA	C1C-C2C-C3C	-4.75	101.99	106.98
12	A	802	CLA	CAC-C3C-C4C	4.75	130.97	124.79
12	a	814	CLA	O2A-CGA-O1A	-4.75	111.12	123.33
12	b	812	CLA	O2A-CGA-O1A	-4.75	111.13	123.33
12	B	827	CLA	C2D-C1D-ND	4.75	114.82	110.13
12	G	839	CLA	C2D-C1D-ND	4.74	114.82	110.13
12	H	820	CLA	O2A-CGA-O1A	-4.74	111.13	123.33
12	a	811	CLA	O2A-CGA-O1A	-4.74	111.13	123.33
12	A	833	CLA	C1C-C2C-C3C	-4.74	101.99	106.98
12	b	822	CLA	C1D-ND-C4D	-4.74	102.98	106.31
12	B	822	CLA	C1D-ND-C4D	-4.74	102.98	106.31
12	A	815	CLA	O2D-CGD-CBD	4.74	119.52	111.23
12	H	828	CLA	C1C-C2C-C3C	-4.74	102.00	106.98
12	B	812	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
12	B	827	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
12	b	811	CLA	C2D-C1D-ND	4.74	114.81	110.13
12	B	832	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
12	a	813	CLA	C1C-C2C-C3C	-4.74	102.00	106.98
12	a	841	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
12	b	829	CLA	O2A-CGA-CBA	4.73	126.27	111.83
12	a	817	CLA	C4A-NA-C1A	4.73	108.84	106.68
12	G	815	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
12	H	819	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
12	a	838	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
12	H	806	CLA	CBA-CAA-C2A	4.73	127.87	113.79
12	B	838	CLA	O2A-C1-C2	4.73	126.32	108.11
12	H	805	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
12	H	837	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
12	A	839	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
12	G	809	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	A	835	CLA	O2A-CGA-O1A	-4.73	111.17	123.33
12	B	813	CLA	O2D-CGD-CBD	4.73	119.50	111.23
12	a	821	CLA	O2A-CGA-O1A	-4.73	111.17	123.33
12	G	822	CLA	O2A-CGA-O1A	-4.73	111.18	123.33
12	b	801	CLA	O2A-CGA-O1A	-4.73	111.81	123.63
12	a	831	CLA	C2D-C1D-ND	4.73	114.80	110.13
12	G	808	CLA	O2A-CGA-O1A	-4.73	111.81	123.63
12	A	825	CLA	O2D-CGD-CBD	4.72	119.49	111.23
12	A	810	CLA	C1D-ND-C4D	-4.72	103.00	106.31
12	G	818	CLA	O2A-CGA-CBA	4.72	126.23	111.83
12	A	834	CLA	O2A-CGA-O1A	-4.72	111.82	123.63
12	H	836	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
12	H	835	CLA	O2D-CGD-CBD	4.72	119.48	111.23
12	B	821	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
12	G	841	CLA	CMB-C2B-C1B	4.72	132.60	125.42
12	a	811	CLA	C2D-C1D-ND	4.72	114.80	110.13
12	H	820	CLA	O2D-CGD-CBD	4.72	119.48	111.23
12	G	834	CLA	O2A-CGA-O1A	-4.72	111.83	123.63
12	a	809	CLA	C1D-ND-C4D	-4.72	103.00	106.31
12	a	855	CLA	C1-O2A-CGA	4.72	128.07	116.65
12	G	803	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
12	B	815	CLA	O2A-CGA-CBA	4.72	126.21	111.83
12	R	103	CLA	O2A-CGA-O1A	-4.71	111.21	123.33
12	b	818	CLA	O2A-CGA-O1A	-4.71	111.21	123.33
12	a	814	CLA	C1C-C2C-C3C	-4.71	102.02	106.98
12	a	831	CLA	O2D-CGD-CBD	4.71	119.47	111.23
12	F	201	CLA	O2D-CGD-CBD	4.71	119.47	111.23
12	S	202	CLA	CMD-C2D-C1D	4.71	133.03	124.73
12	G	816	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
12	A	830	CLA	C1D-ND-C4D	-4.71	103.01	106.31
12	B	834	CLA	O2D-CGD-CBD	4.71	119.46	111.23
12	B	830	CLA	C1C-C2C-C3C	-4.71	102.03	106.98
12	f	203	CLA	C2D-C1D-ND	4.71	114.78	110.13
12	A	841	CLA	C2D-C1D-ND	4.71	114.78	110.13
12	b	802	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
12	b	812	CLA	C1D-ND-C4D	-4.70	103.01	106.31
12	B	818	CLA	O2A-CGA-O1A	-4.70	111.23	123.33
12	A	828	CLA	C2D-C1D-ND	4.70	114.78	110.13
12	H	804	CLA	O2A-CGA-O1A	-4.70	111.86	123.63
17	M	101	45D	C39-C35-C37	4.70	130.44	122.82
12	a	815	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
12	a	807	CLA	O2A-CGA-O1A	-4.70	111.86	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	819	CLA	O2D-CGD-CBD	4.70	119.45	111.23
12	b	820	CLA	C1C-C2C-C3C	-4.70	102.03	106.98
12	B	816	CLA	O2A-CGA-O1A	-4.70	111.87	123.63
12	G	840	CLA	O2A-CGA-CBA	4.70	126.17	111.83
12	A	820	CLA	C2B-C1B-NB	4.70	115.20	110.33
12	G	829	CLA	C2D-C1D-ND	4.70	114.78	110.13
12	b	802	CLA	O2A-CGA-O1A	-4.70	111.88	123.63
12	G	833	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
12	A	829	CLA	O2D-CGD-CBD	4.70	119.44	111.23
12	H	817	CLA	C2D-C1D-ND	4.70	114.77	110.13
12	b	801	CLA	C3B-C2B-C1B	-4.70	101.64	107.17
12	H	813	CLA	O2A-CGA-O1A	-4.69	111.26	123.33
12	b	819	CLA	O2A-CGA-O1A	-4.69	111.26	123.33
12	a	815	CLA	O2D-CGD-CBD	4.69	119.44	111.23
12	b	819	CLA	O2D-CGD-CBD	4.69	119.44	111.23
12	G	806	CLA	C2C-C1C-NC	4.69	114.91	109.98
12	f	203	CLA	C4A-NA-C1A	4.69	108.82	106.68
12	A	804	CLA	C2D-C1D-ND	4.69	114.77	110.13
12	G	840	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
12	a	802	CLA	O2D-CGD-CBD	4.69	119.43	111.23
12	B	803	CLA	C1D-ND-C4D	-4.69	103.02	106.31
12	H	803	CLA	C2B-C1B-NB	4.69	115.19	110.33
12	H	833	CLA	C2D-C1D-ND	4.69	114.77	110.13
12	a	811	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
12	H	826	CLA	C4A-NA-C1A	4.69	108.82	106.68
12	G	812	CLA	C1D-ND-C4D	-4.69	103.02	106.31
15	a	848	BCR	C24-C23-C22	-4.69	119.30	126.23
15	G	850	BCR	C36-C18-C19	-4.69	110.93	118.09
12	a	802	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
12	A	802	CLA	O2A-CGA-O1A	-4.68	111.91	123.63
12	H	805	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
12	G	839	CLA	O2A-CGA-O1A	-4.68	111.92	123.63
12	H	828	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
12	B	827	CLA	O2A-CGA-O1A	-4.68	111.30	123.33
12	G	827	CLA	O2A-CGA-O1A	-4.68	111.92	123.63
17	M	101	45D	C24-C20-C08	-4.68	114.50	127.00
12	B	809	CLA	O2A-CGA-O1A	-4.68	111.30	123.33
12	B	836	CLA	O2A-CGA-O1A	-4.68	111.92	123.63
12	B	819	CLA	O2A-CGA-O1A	-4.68	111.30	123.33
12	B	837	CLA	CMB-C2B-C1B	4.68	132.54	125.42
12	A	808	CLA	O2D-CGD-CBD	4.68	119.41	111.23
12	B	829	CLA	C4A-NA-C1A	4.68	108.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	816	CLA	O2A-CGA-CBA	4.68	126.10	111.83
12	a	829	CLA	C2D-C1D-ND	4.68	114.75	110.13
12	a	837	CLA	C2D-C1D-ND	4.68	114.75	110.13
12	A	818	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
12	B	808	CLA	O2A-CGA-O1A	-4.68	111.31	123.33
12	b	816	CLA	C4A-NA-C1A	4.68	108.81	106.68
15	b	844	BCR	C19-C18-C17	4.68	126.36	119.01
12	B	820	CLA	C2B-C1B-NB	4.67	115.17	110.33
12	a	834	CLA	O2A-CGA-O1A	-4.67	111.94	123.63
12	a	803	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
12	a	855	CLA	CMD-C2D-C1D	4.67	132.96	124.73
12	B	806	CLA	O2A-CGA-CBA	4.67	126.08	111.83
12	B	829	CLA	O2A-CGA-CBA	4.67	126.08	111.83
17	m	101	45D	C39-C35-C37	4.67	130.39	122.82
12	A	817	CLA	O2A-CGA-O1A	-4.67	111.94	123.63
12	A	802	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	A	810	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
12	G	816	CLA	C1D-ND-C4D	-4.67	103.04	106.31
12	G	804	CLA	C4A-NA-C1A	4.67	108.81	106.68
12	R	103	CLA	C4A-NA-C1A	4.67	108.81	106.68
12	B	816	CLA	C2D-C1D-ND	4.67	114.75	110.13
12	A	815	CLA	O2A-CGA-O1A	-4.67	111.33	123.33
15	a	846	BCR	C15-C14-C13	-4.66	120.74	127.28
12	B	801	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
12	a	802	CLA	O2A-CGA-O1A	-4.66	111.97	123.63
12	A	829	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
12	B	823	CLA	OBD-CAD-C3D	-4.66	117.52	128.42
12	A	827	CLA	C2B-C1B-NB	4.66	115.16	110.33
12	l	206	CLA	C1D-ND-C4D	-4.66	103.04	106.31
12	B	802	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
12	j	104	CLA	O2A-CGA-O1A	-4.66	111.36	123.33
12	H	827	CLA	C4A-NA-C1A	4.66	108.80	106.68
12	H	801	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
11	G	801	CL0	C1D-ND-C4D	-4.65	103.05	106.31
12	L	202	CLA	C1D-ND-C4D	-4.65	103.05	106.31
12	G	837	CLA	C1D-ND-C4D	-4.65	103.05	106.31
12	b	808	CLA	O2A-CGA-O1A	-4.65	111.38	123.33
12	B	824	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
12	b	830	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
12	G	815	CLA	C1C-C2C-C3C	-4.65	102.09	106.98
12	B	828	CLA	O2D-CGD-CBD	4.65	119.35	111.23
15	i	101	BCR	C24-C23-C22	-4.65	119.36	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	830	CLA	O2A-CGA-O1A	-4.65	112.01	123.63
12	G	809	CLA	O2A-CGA-O1A	-4.64	112.01	123.63
12	G	806	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
12	a	809	CLA	O2D-CGD-CBD	4.64	119.34	111.23
12	H	815	CLA	C4A-NA-C1A	4.64	108.80	106.68
12	a	805	CLA	C4A-NA-C1A	4.64	108.80	106.68
12	A	819	CLA	C2D-C1D-ND	4.64	114.72	110.13
12	B	835	CLA	O2A-CGA-O1A	-4.64	111.40	123.33
12	a	825	CLA	C4A-NA-C1A	4.64	108.80	106.68
12	A	811	CLA	C2D-C1D-ND	4.64	114.72	110.13
12	a	829	CLA	O2A-CGA-O1A	-4.64	112.03	123.63
12	G	817	CLA	C2D-C1D-ND	4.64	114.71	110.13
12	A	815	CLA	C2B-C1B-NB	4.63	115.13	110.33
12	A	812	CLA	C2D-C1D-ND	4.63	114.71	110.13
12	S	204	CLA	C1D-ND-C4D	-4.63	103.06	106.31
12	j	104	CLA	C2D-C1D-ND	4.63	114.71	110.13
12	L	202	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	B	805	CLA	O2D-CGD-CBD	4.63	119.32	111.23
12	H	828	CLA	C4A-NA-C1A	4.63	108.79	106.68
15	Q	101	BCR	C24-C23-C22	-4.63	119.39	126.23
12	b	826	CLA	O2A-CGA-CBA	4.63	125.94	111.83
12	a	812	CLA	O2A-CGA-CBA	4.62	125.94	111.83
12	b	827	CLA	O2A-CGA-O1A	-4.62	111.44	123.33
15	a	844	BCR	C24-C23-C22	-4.62	119.39	126.23
12	B	814	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
12	G	828	CLA	C2C-C1C-NC	4.62	114.84	109.98
15	A	846	BCR	C15-C14-C13	-4.62	120.80	127.28
12	b	829	CLA	CHD-C1D-ND	-4.62	118.30	124.80
12	B	803	CLA	C2B-C1B-NB	4.62	115.12	110.33
15	F	204	BCR	C24-C23-C22	-4.62	119.40	126.23
12	a	816	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	G	841	CLA	C2D-C1D-ND	4.62	114.70	110.13
12	A	835	CLA	C1D-ND-C4D	-4.62	103.07	106.31
12	j	104	CLA	C2B-C1B-NB	4.62	115.11	110.33
12	a	839	CLA	O2A-CGA-CBA	4.62	125.91	111.83
12	a	824	CLA	CMA-C3A-C4A	4.61	124.18	111.77
12	G	813	CLA	O2A-CGA-CBA	4.61	125.90	111.83
12	A	854	CLA	O2A-CGA-O1A	-4.61	112.09	123.63
12	a	816	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
12	b	829	CLA	C2B-C1B-NB	4.61	115.11	110.33
12	A	804	CLA	O2A-CGA-CBA	4.61	125.89	111.83
12	H	824	CLA	O2A-CGA-O1A	-4.61	112.10	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	825	CLA	O2A-CGA-CBA	4.61	125.89	111.83
12	A	841	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	a	836	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
12	B	816	CLA	O2D-CGD-CBD	4.60	119.28	111.23
12	B	829	CLA	CHD-C1D-ND	-4.60	118.32	124.80
12	H	808	CLA	C1D-ND-C4D	-4.60	103.08	106.31
12	A	837	CLA	C1D-ND-C4D	-4.60	103.08	106.31
12	a	818	CLA	C2D-C1D-ND	4.60	114.68	110.13
12	H	815	CLA	C1D-ND-C4D	-4.60	103.09	106.31
17	T	101	45D	C24-C20-C08	-4.60	114.72	127.00
12	H	834	CLA	C1D-ND-C4D	-4.60	103.09	106.31
12	A	815	CLA	C1D-ND-C4D	-4.60	103.09	106.31
12	A	820	CLA	O2D-CGD-CBD	4.60	119.26	111.23
12	b	833	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
12	G	856	CLA	C1-O2A-CGA	4.59	127.77	116.65
12	G	832	CLA	C2B-C1B-NB	4.59	115.09	110.33
15	G	848	BCR	C24-C23-C22	-4.59	119.44	126.23
12	G	812	CLA	O2A-CGA-O1A	-4.59	111.53	123.33
12	H	817	CLA	O2A-CGA-O1A	-4.59	112.15	123.63
12	B	810	CLA	O2A-CGA-CBA	4.59	125.83	111.83
12	H	811	CLA	O2A-CGA-CBA	4.59	125.82	111.83
12	a	840	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
12	A	811	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
12	b	820	CLA	C2B-C1B-NB	4.59	115.08	110.33
12	G	840	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
12	b	805	CLA	O2D-CGD-CBD	4.58	119.25	111.23
12	a	815	CLA	C1D-ND-C4D	-4.58	103.10	106.31
12	b	837	CLA	CMC-C2C-C1C	4.58	132.19	125.03
12	A	812	CLA	O2A-CGA-CBA	4.58	125.80	111.83
12	H	830	CLA	CHD-C1D-ND	-4.58	118.36	124.80
12	G	828	CLA	CAA-C2A-C3A	-4.57	100.64	113.00
12	b	823	CLA	O2A-CGA-O1A	-4.57	112.19	123.63
12	b	832	CLA	C1D-ND-C4D	-4.57	103.11	106.31
12	B	819	CLA	O2D-CGD-CBD	4.57	119.22	111.23
12	H	837	CLA	CMD-C2D-C3D	-4.57	117.22	127.69
12	b	805	CLA	C1C-C2C-C3C	-4.57	102.18	106.98
12	b	837	CLA	C1D-ND-C4D	-4.57	103.11	106.31
12	a	831	CLA	C4A-NA-C1A	4.57	108.76	106.68
12	B	836	CLA	C4A-NA-C1A	4.57	108.76	106.68
12	B	821	CLA	C1D-ND-C4D	-4.57	103.11	106.31
12	H	822	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
12	G	803	CLA	O2A-CGA-O1A	-4.56	112.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	826	CLA	C4D-C3D-CAD	4.56	113.06	108.11
12	H	837	CLA	C2B-C1B-NB	4.56	115.06	110.33
12	a	854	CLA	C4-C3-C5	4.56	123.14	115.23
12	B	823	CLA	O2A-CGA-O1A	-4.56	112.22	123.63
12	G	831	CLA	C1D-ND-C4D	-4.56	103.11	106.31
12	b	833	CLA	C1D-ND-C4D	-4.56	103.11	106.31
12	H	826	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
12	b	831	CLA	C2D-C1D-ND	4.55	114.63	110.13
15	G	850	BCR	C20-C19-C18	4.55	138.85	126.36
12	A	822	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
12	B	838	CLA	CMC-C2C-C1C	4.55	132.15	125.03
12	H	802	CLA	O2A-CGA-O1A	-4.55	112.24	123.63
12	a	825	CLA	O2A-CGA-CBA	4.55	125.71	111.83
12	H	811	CLA	C1C-C2C-C3C	-4.55	102.19	106.98
12	A	827	CLA	O2A-CGA-CBA	4.55	125.71	111.83
12	G	836	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
12	a	833	CLA	C2D-C1D-ND	4.55	114.63	110.13
12	b	811	CLA	O2A-CGA-CBA	4.55	125.70	111.83
15	a	847	BCR	C24-C23-C22	-4.55	119.51	126.23
12	H	825	CLA	O2D-CGD-CBD	4.55	119.18	111.23
12	b	815	CLA	C2B-C1B-NB	4.54	115.04	110.33
12	G	802	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
12	j	102	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
12	H	818	CLA	C1D-ND-C4D	-4.54	103.12	106.31
12	H	807	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
12	A	802	CLA	C2D-C1D-ND	4.54	114.62	110.13
12	A	836	CLA	C1C-C2C-C3C	-4.54	102.20	106.98
15	J	104	BCR	C34-C9-C10	-4.54	115.46	122.82
12	a	818	CLA	C2B-C1B-NB	4.54	115.03	110.33
12	G	820	CLA	C1D-ND-C4D	-4.54	103.13	106.31
12	A	816	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
12	H	835	CLA	C1C-C2C-C3C	-4.54	102.21	106.98
12	A	829	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
12	a	817	CLA	C2B-C1B-NB	4.53	115.03	110.33
12	A	824	CLA	C4A-NA-C1A	4.53	108.75	106.68
12	a	804	CLA	O2A-CGA-CBA	4.53	125.65	111.83
15	G	849	BCR	C28-C27-C26	-4.53	105.97	114.06
12	G	819	CLA	C2B-C1B-NB	4.53	115.03	110.33
12	H	813	CLA	C2B-C1B-NB	4.53	115.03	110.33
12	A	820	CLA	CMC-C2C-C3C	4.53	138.40	126.15
12	A	855	CLA	C1-O2A-CGA	4.53	127.62	116.65
12	b	810	CLA	C1C-C2C-C3C	-4.53	102.22	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	849	BCR	C20-C19-C18	4.53	138.78	126.36
12	B	811	CLA	C2D-C1D-ND	4.53	114.61	110.13
12	H	836	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
12	A	817	CLA	O2A-CGA-CBA	4.52	125.63	111.83
12	b	816	CLA	O2A-CGA-O1A	-4.52	112.32	123.63
12	H	805	CLA	O2D-CGD-CBD	4.52	119.13	111.23
12	a	830	CLA	C4A-NA-C1A	4.52	108.74	106.68
12	A	807	CLA	C1D-ND-C4D	-4.52	103.14	106.31
12	B	804	CLA	O2D-CGD-CBD	4.52	119.13	111.23
15	P	204	BCR	C28-C27-C26	-4.52	106.00	114.06
12	A	824	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
12	A	827	CLA	C2C-C1C-NC	4.51	114.72	109.98
12	G	802	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
12	H	824	CLA	C1C-C2C-C3C	-4.51	102.23	106.98
15	A	848	BCR	C28-C27-C26	-4.51	106.01	114.06
12	A	808	CLA	C2B-C1B-NB	4.51	115.01	110.33
12	b	821	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
12	G	828	CLA	C2B-C1B-NB	4.51	115.00	110.33
12	G	841	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
12	A	831	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
12	G	835	CLA	C1D-ND-C4D	-4.51	103.15	106.31
12	A	839	CLA	C2D-C1D-ND	4.51	114.59	110.13
12	G	839	CLA	O2A-CGA-CBA	4.50	125.57	111.83
11	G	801	CL0	C2D-C1D-ND	4.50	114.58	110.13
12	b	811	CLA	C1D-ND-C4D	-4.50	103.16	106.31
15	B	845	BCR	C19-C18-C17	4.50	126.08	119.01
12	a	854	CLA	O2A-CGA-O1A	-4.50	112.38	123.63
12	a	804	CLA	C2D-C1D-ND	4.50	114.58	110.13
12	G	805	CLA	O2A-CGA-CBA	4.50	125.54	111.83
12	A	830	CLA	C4A-NA-C1A	4.50	108.73	106.68
12	A	834	CLA	O2D-CGD-CBD	4.49	119.08	111.23
15	a	849	BCR	C36-C18-C19	-4.49	111.22	118.09
12	A	831	CLA	O2A-CGA-O1A	-4.49	112.39	123.63
12	a	828	CLA	C2D-C1D-ND	4.49	114.57	110.13
12	G	817	CLA	O2A-CGA-O1A	-4.49	112.39	123.63
12	a	840	CLA	O2A-CGA-CBA	4.49	125.53	111.83
12	B	819	CLA	C1D-ND-C4D	-4.49	103.16	106.31
12	b	810	CLA	O2A-CGA-CBA	4.49	125.52	111.83
12	a	802	CLA	CAA-C2A-C3A	-4.49	100.88	113.00
12	G	828	CLA	C1D-ND-C4D	-4.49	103.17	106.31
12	a	837	CLA	C2B-C1B-NB	4.48	114.98	110.33
12	B	817	CLA	C1D-ND-C4D	-4.48	103.17	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	817	CLA	C1D-ND-C4D	-4.48	103.17	106.31
12	b	808	CLA	C2D-C1D-ND	4.48	114.56	110.13
12	a	836	CLA	C2B-C1B-NB	4.48	114.97	110.33
12	A	826	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
12	A	832	CLA	C2D-C1D-ND	4.48	114.56	110.13
12	A	828	CLA	O2D-CGD-CBD	4.48	119.06	111.23
12	b	828	CLA	C2B-C1B-NB	4.48	114.97	110.33
12	A	804	CLA	C2B-C1B-NB	4.48	114.97	110.33
12	B	821	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
12	A	832	CLA	C2B-C1B-NB	4.47	114.96	110.33
12	H	809	CLA	C2D-C1D-ND	4.47	114.55	110.13
12	A	829	CLA	C2D-C1D-ND	4.47	114.55	110.13
12	H	839	CLA	C1-O2A-CGA	4.47	127.47	116.65
12	b	821	CLA	C2B-C1B-NB	4.47	114.96	110.33
12	a	814	CLA	C1D-ND-C4D	-4.47	103.18	106.31
12	b	818	CLA	C1D-ND-C4D	-4.47	103.18	106.31
12	H	807	CLA	CMD-C2D-C1D	4.47	132.60	124.73
15	b	847	BCR	C7-C8-C9	-4.46	119.63	126.23
12	a	804	CLA	C2B-C1B-NB	4.46	114.96	110.33
15	a	849	BCR	C3-C4-C5	-4.46	106.09	114.06
12	G	834	CLA	C1D-ND-C4D	-4.46	103.18	106.31
12	H	830	CLA	C2B-C1B-NB	4.46	114.95	110.33
12	a	841	CLA	O2D-CGD-CBD	4.46	119.03	111.23
12	B	805	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
12	b	821	CLA	C2D-C1D-ND	4.46	114.54	110.13
12	f	201	CLA	O2A-CGA-CBA	4.46	125.42	111.83
12	H	821	CLA	C1D-ND-C4D	-4.46	103.19	106.31
12	G	819	CLA	CBA-CAA-C2A	4.45	127.05	113.79
12	B	838	CLA	C1D-ND-C4D	-4.45	103.19	106.31
12	A	830	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
12	b	803	CLA	C2B-C1B-NB	4.45	114.94	110.33
12	a	836	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
12	a	808	CLA	C2B-C1B-NB	4.45	114.94	110.33
12	B	801	CLA	CMD-C2D-C1D	4.45	132.57	124.73
12	B	825	CLA	O2A-CGA-O1A	-4.45	112.50	123.63
12	a	830	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
12	G	819	CLA	C1D-ND-C4D	-4.45	103.19	106.31
15	J	102	BCR	C24-C23-C22	-4.45	119.65	126.23
15	A	849	BCR	C3-C4-C5	-4.45	106.12	114.06
12	G	855	CLA	O2A-CGA-O1A	-4.45	112.50	123.63
12	f	201	CLA	O2D-CGD-CBD	4.45	119.01	111.23
12	B	802	CLA	C2C-C1C-NC	4.45	114.65	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	832	CLA	O2D-CGD-CBD	4.45	119.00	111.23
12	a	802	CLA	C2D-C1D-ND	4.45	114.53	110.13
15	A	847	BCR	C24-C23-C22	-4.45	119.66	126.23
12	G	808	CLA	C1D-ND-C4D	-4.45	103.19	106.31
12	a	832	CLA	C2D-C1D-ND	4.44	114.53	110.13
12	b	819	CLA	C1D-ND-C4D	-4.44	103.19	106.31
15	H	846	BCR	C19-C18-C17	4.44	126.00	119.01
12	b	804	CLA	O2D-CGD-CBD	4.44	118.99	111.23
12	B	814	CLA	C1D-ND-C4D	-4.44	103.20	106.31
12	G	802	CLA	CMB-C2B-C3B	4.44	136.99	126.55
12	P	201	CLA	O2A-CGA-CBA	4.44	125.36	111.83
12	G	821	CLA	C2B-C1B-NB	4.44	114.93	110.33
12	B	822	CLA	CMD-C2D-C1D	4.43	132.53	124.73
12	P	201	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
12	a	823	CLA	O2A-CGA-CBA	4.43	125.34	111.83
12	a	808	CLA	O2D-CGD-CBD	4.43	118.97	111.23
12	B	815	CLA	O2A-CGA-O1A	-4.43	112.56	123.63
15	F	202	BCR	C7-C8-C9	-4.43	119.69	126.23
12	b	814	CLA	O2A-CGA-O1A	-4.42	112.56	123.63
12	B	805	CLA	O2A-CGA-CBA	4.42	125.32	111.83
12	b	815	CLA	O2A-CGA-CBA	4.42	125.32	111.83
12	G	826	CLA	O2A-CGA-CBA	4.42	125.32	111.83
12	a	834	CLA	O2D-CGD-CBD	4.42	118.96	111.23
12	a	827	CLA	C1D-ND-C4D	-4.42	103.21	106.31
12	a	803	CLA	C1D-ND-C4D	-4.42	103.21	106.31
12	a	839	CLA	C1D-ND-C4D	-4.42	103.21	106.31
12	H	804	CLA	CHD-C1D-ND	-4.42	118.58	124.80
12	A	809	CLA	C2D-C1D-ND	4.42	114.50	110.13
12	H	807	CLA	O2A-CGA-CBA	4.42	125.30	111.83
12	a	809	CLA	C3B-C2B-C1B	-4.42	101.97	107.17
12	B	826	CLA	C4D-C3D-CAD	4.41	112.90	108.11
12	b	825	CLA	CMD-C2D-C1D	4.41	132.50	124.73
12	a	827	CLA	C2B-C1B-NB	4.41	114.90	110.33
12	G	830	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
12	b	805	CLA	O2A-CGA-CBA	4.41	125.28	111.83
12	G	856	CLA	C2B-C1B-NB	4.41	114.89	110.33
12	G	824	CLA	O2A-CGA-CBA	4.41	125.27	111.83
12	G	855	CLA	C4-C3-C5	4.41	122.88	115.23
12	A	840	CLA	O2A-CGA-CBA	4.40	125.27	111.83
12	G	805	CLA	C1D-ND-C4D	-4.40	103.22	106.31
12	A	828	CLA	O2A-CGA-O1A	-4.40	112.61	123.63
12	a	807	CLA	C1D-ND-C4D	-4.40	103.22	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	818	CLA	C1D-ND-C4D	-4.40	103.22	106.31
12	A	818	CLA	CBA-CAA-C2A	4.40	126.89	113.79
12	G	828	CLA	O2A-CGA-CBA	4.40	125.25	111.83
12	G	829	CLA	O2A-CGA-O1A	-4.40	112.62	123.63
15	a	848	BCR	C28-C27-C26	-4.40	106.21	114.06
12	A	823	CLA	O2A-CGA-CBA	4.40	125.24	111.83
12	H	823	CLA	C1C-C2C-C3C	-4.40	102.36	106.98
12	b	801	CLA	C2B-C1B-NB	4.40	114.89	110.33
12	A	854	CLA	C4A-NA-C1A	4.39	108.68	106.68
12	l	205	CLA	CHD-C1D-ND	-4.39	118.62	124.80
12	F	201	CLA	C2D-C1D-ND	4.39	114.47	110.13
12	G	821	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
12	H	817	CLA	O2D-CGD-CBD	4.39	118.90	111.23
12	B	834	CLA	C1C-C2C-C3C	-4.39	102.37	106.98
12	A	835	CLA	O2D-CGD-CBD	4.39	118.90	111.23
12	A	837	CLA	C2B-C1B-NB	4.39	114.88	110.33
15	l	201	BCR	C40-C30-C25	4.39	117.12	110.24
12	G	815	CLA	C1D-ND-C4D	-4.39	103.23	106.31
12	b	836	CLA	CMB-C2B-C1B	4.39	132.10	125.42
12	G	825	CLA	CMA-C3A-C4A	4.38	123.55	111.77
12	a	820	CLA	C4A-NA-C1A	4.38	108.68	106.68
12	A	813	CLA	C4A-NA-C1A	4.38	108.68	106.68
12	A	841	CLA	O2D-CGD-CBD	4.38	118.88	111.23
12	b	822	CLA	C2B-C1B-NB	4.38	114.86	110.33
12	H	812	CLA	C1D-ND-C4D	-4.38	103.24	106.31
12	B	808	CLA	C2D-C1D-ND	4.37	114.45	110.13
12	A	820	CLA	C3B-C4B-NB	4.37	114.43	110.53
12	G	833	CLA	C2D-C1D-ND	4.37	114.45	110.13
12	A	814	CLA	C1D-ND-C4D	-4.37	103.24	106.31
12	H	810	CLA	C1D-ND-C4D	-4.37	103.25	106.31
12	a	825	CLA	C2B-C1B-NB	4.37	114.86	110.33
12	G	833	CLA	O2A-CGA-O1A	-4.37	112.70	123.63
12	A	854	CLA	O2D-CGD-O1D	-4.37	115.35	123.85
12	a	833	CLA	O2A-CGA-O1A	-4.37	112.70	123.63
12	G	841	CLA	O2D-CGD-CBD	4.37	118.86	111.23
12	H	837	CLA	C4D-C3D-CAD	4.37	112.85	108.11
12	B	810	CLA	C1C-C2C-C3C	-4.37	102.39	106.98
12	b	816	CLA	C2D-C1D-ND	4.37	114.45	110.13
12	F	203	CLA	C1D-ND-C4D	-4.37	103.25	106.31
12	B	811	CLA	C2B-C1B-NB	4.36	114.85	110.33
12	H	820	CLA	C1D-ND-C4D	-4.36	103.25	106.31
12	G	803	CLA	C2D-C1D-ND	4.36	114.44	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	816	CLA	CHD-C1D-ND	-4.36	118.66	124.80
12	G	842	CLA	O2D-CGD-CBD	4.36	118.86	111.23
12	A	820	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
12	G	813	CLA	C2D-C1D-ND	4.36	114.44	110.13
12	A	812	CLA	C1C-C2C-C3C	-4.36	102.40	106.98
11	G	801	CL0	O2D-CGD-CBD	4.36	118.85	111.23
12	A	825	CLA	CAA-C2A-C3A	-4.36	101.22	113.00
12	H	827	CLA	O2A-CGA-CBA	4.36	125.12	111.83
12	A	833	CLA	O2A-CGA-O1A	-4.36	112.73	123.63
12	B	809	CLA	C1D-ND-C4D	-4.36	103.26	106.31
12	a	808	CLA	C4A-NA-C1A	4.36	108.67	106.68
12	B	831	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
12	B	824	CLA	O2D-CGD-CBD	4.35	118.84	111.23
12	a	816	CLA	O2A-CGA-CBA	4.35	125.11	111.83
12	B	831	CLA	C1C-C2C-C3C	-4.35	102.40	106.98
12	B	833	CLA	CAC-C3C-C4C	4.35	130.45	124.79
12	B	826	CLA	C4A-NA-C1A	4.35	108.66	106.68
12	G	802	CLA	O2A-CGA-CBA	4.35	125.10	111.83
12	B	815	CLA	C2B-C1B-NB	4.35	114.84	110.33
15	H	849	BCR	C24-C23-C22	-4.35	119.80	126.23
12	G	810	CLA	CMB-C2B-C1B	4.35	132.04	125.42
12	G	840	CLA	C1D-ND-C4D	-4.35	103.26	106.31
12	A	818	CLA	O2A-C1-C2	4.35	124.84	108.11
12	H	831	CLA	O2A-CGA-O1A	-4.35	112.75	123.63
12	b	809	CLA	C3B-C2B-C1B	-4.35	102.05	107.17
12	a	820	CLA	C2B-C1B-NB	4.35	114.83	110.33
12	a	828	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
12	B	813	CLA	C2B-C1B-NB	4.34	114.83	110.33
12	H	813	CLA	C1D-ND-C4D	-4.34	103.26	106.31
12	f	203	CLA	C1D-ND-C4D	-4.34	103.27	106.31
12	A	822	CLA	O2D-CGD-CBD	4.34	118.82	111.23
12	H	814	CLA	C2B-C1B-NB	4.34	114.83	110.33
12	a	820	CLA	C3B-C2B-C1B	-4.34	102.06	107.17
12	a	805	CLA	CAA-C2A-C3A	-4.34	101.28	113.00
12	a	855	CLA	C2B-C1B-NB	4.34	114.82	110.33
12	B	809	CLA	C3B-C2B-C1B	-4.34	102.06	107.17
12	a	827	CLA	O2A-CGA-CBA	4.34	125.06	111.83
12	H	828	CLA	C1D-ND-C4D	-4.34	103.27	106.31
12	G	803	CLA	CAA-C2A-C3A	-4.33	101.29	113.00
12	F	201	CLA	O2A-CGA-CBA	4.33	125.05	111.83
12	H	810	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
12	G	827	CLA	C1C-C2C-C3C	-4.33	102.42	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	821	CLA	C2D-C1D-ND	4.33	114.41	110.13
12	H	838	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
12	b	814	CLA	C1D-ND-C4D	-4.33	103.28	106.31
12	b	848	CLA	O2A-CGA-CBA	4.32	125.02	111.83
12	G	804	CLA	C1D-ND-C4D	-4.32	103.28	106.31
15	b	841	BCR	C34-C9-C10	-4.32	115.81	122.82
12	G	832	CLA	C2D-C1D-ND	4.32	114.40	110.13
12	J	103	CLA	C1D-ND-C4D	-4.32	103.28	106.31
12	B	830	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
12	A	830	CLA	O2A-CGA-CBA	4.32	125.00	111.83
12	H	804	CLA	O2D-CGD-CBD	4.32	118.78	111.23
12	a	840	CLA	O2A-C1-C2	4.31	124.70	108.11
12	P	201	CLA	C4A-NA-C1A	4.31	108.65	106.68
12	A	839	CLA	O2A-CGA-CBA	4.31	124.98	111.83
12	A	814	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
12	A	854	CLA	O2A-CGA-CBA	4.31	124.97	111.83
12	H	829	CLA	O2D-CGD-CBD	4.31	118.76	111.23
12	G	837	CLA	C2B-C1B-NB	4.30	114.79	110.33
12	A	808	CLA	C2D-C1D-ND	4.30	114.39	110.13
12	G	836	CLA	CMD-C2D-C3D	-4.30	117.82	127.69
12	R	103	CLA	C1D-ND-C4D	-4.30	103.29	106.31
12	A	809	CLA	CMB-C2B-C1B	4.30	131.97	125.42
12	A	802	CLA	CAA-C2A-C3A	-4.30	101.38	113.00
12	b	807	CLA	CAA-C2A-C3A	-4.30	101.38	113.00
12	H	850	CLA	C1D-ND-C4D	-4.30	103.30	106.31
12	H	829	CLA	C2B-C1B-NB	4.30	114.78	110.33
12	B	821	CLA	C2B-C1B-NB	4.30	114.78	110.33
12	G	835	CLA	O2D-CGD-CBD	4.30	118.75	111.23
12	H	824	CLA	OBD-CAD-C3D	-4.30	118.37	128.42
12	H	802	CLA	C2C-C1C-NC	4.30	114.50	109.98
12	b	827	CLA	C4A-NA-C1A	4.30	108.64	106.68
15	F	202	BCR	C12-C13-C14	-4.30	112.25	119.01
12	a	854	CLA	O2D-CGD-O1D	-4.29	115.49	123.85
12	a	840	CLA	C1D-ND-C4D	-4.29	103.30	106.31
12	G	820	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
16	G	854	LHG	O7-C7-C8	4.29	120.76	111.48
12	B	801	CLA	CMB-C2B-C3B	4.29	136.64	126.55
12	a	828	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
12	l	202	CLA	C1D-ND-C4D	-4.29	103.30	106.31
12	A	817	CLA	C1D-ND-C4D	-4.29	103.30	106.31
12	G	823	CLA	C1D-ND-C4D	-4.28	103.31	106.31
12	b	827	CLA	C1D-ND-C4D	-4.28	103.31	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	815	CLA	O2A-CGA-O1A	-4.28	112.92	123.63
12	G	809	CLA	CHD-C1D-ND	-4.28	118.78	124.80
12	b	835	CLA	C4A-NA-C1A	4.28	108.63	106.68
12	f	201	CLA	C2D-C1D-ND	4.28	114.36	110.13
12	B	827	CLA	C1D-ND-C4D	-4.28	103.31	106.31
12	A	806	CLA	CAA-C2A-C3A	-4.28	101.44	113.00
15	H	843	BCR	C34-C9-C10	-4.28	115.89	122.82
12	A	802	CLA	CMC-C2C-C1C	4.28	131.72	125.03
12	B	814	CLA	O2A-CGA-O1A	-4.28	112.93	123.63
12	A	805	CLA	C1C-C2C-C3C	-4.27	102.48	106.98
12	l	204	CLA	C1D-ND-C4D	-4.27	103.31	106.31
12	H	832	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
12	H	825	CLA	O2A-C1-C2	4.27	124.56	108.11
12	a	832	CLA	C2B-C1B-NB	4.27	114.76	110.33
12	G	814	CLA	C1D-ND-C4D	-4.27	103.32	106.31
12	P	201	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
12	G	832	CLA	O2D-CGD-CBD	4.27	118.69	111.23
12	G	803	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
12	B	804	CLA	O2A-CGA-CBA	4.27	124.84	111.83
12	f	201	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
15	R	101	BCR	C7-C8-C9	-4.26	119.93	126.23
12	H	812	CLA	C2B-C1B-NB	4.26	114.75	110.33
12	A	805	CLA	C2B-C1B-NB	4.26	114.75	110.33
12	G	824	CLA	C1D-ND-C4D	-4.26	103.32	106.31
12	A	818	CLA	C2B-C1B-NB	4.26	114.75	110.33
12	b	801	CLA	CMB-C2B-C3B	4.26	136.57	126.55
12	a	809	CLA	CMB-C2B-C1B	4.26	131.91	125.42
12	A	802	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
12	a	805	CLA	C2C-C1C-NC	4.26	114.45	109.98
12	B	811	CLA	O2A-CGA-CBA	4.26	124.81	111.83
12	a	813	CLA	C2D-C1D-ND	4.26	114.34	110.13
12	a	854	CLA	O2A-CGA-CBA	4.26	124.81	111.83
12	H	834	CLA	O2A-CGA-CBA	4.25	124.81	111.83
12	a	805	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
12	G	829	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
12	G	838	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
15	P	202	BCR	C3-C4-C5	-4.25	106.48	114.06
12	b	828	CLA	O2D-CGD-CBD	4.25	118.66	111.23
12	a	820	CLA	C2D-C1D-ND	4.25	114.33	110.13
12	G	842	CLA	O2A-CGA-CBA	4.25	124.78	111.83
12	b	814	CLA	OBD-CAD-C3D	-4.24	118.49	128.42
12	L	205	CLA	CHD-C1D-ND	-4.24	118.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	831	CLA	C2B-C1B-NB	4.24	114.73	110.33
12	H	807	CLA	CAA-C2A-C3A	-4.24	101.54	113.00
12	A	803	CLA	C1D-ND-C4D	-4.24	103.34	106.31
12	H	838	CLA	CMB-C2B-C1B	4.24	131.88	125.42
12	G	805	CLA	C2B-C1B-NB	4.24	114.72	110.33
11	A	801	CL0	O2D-CGD-CBD	4.23	118.63	111.23
12	G	802	CLA	C2B-C1B-NB	4.23	114.71	110.33
12	G	831	CLA	O2A-CGA-CBA	4.23	124.73	111.83
12	A	805	CLA	C2C-C1C-NC	4.23	114.42	109.98
15	G	850	BCR	C3-C4-C5	-4.23	106.51	114.06
12	B	807	CLA	O2A-CGA-CBA	4.23	124.73	111.83
12	B	801	CLA	C2B-C1B-NB	4.23	114.71	110.33
12	a	823	CLA	C1D-ND-C4D	-4.23	103.35	106.31
12	b	807	CLA	O2A-CGA-CBA	4.23	124.72	111.83
15	B	842	BCR	C34-C9-C10	-4.23	115.97	122.82
11	G	801	CL0	CMD-C2D-C1D	4.22	132.16	124.73
12	H	814	CLA	O2D-CGD-CBD	4.22	118.60	111.23
12	a	826	CLA	C2B-C1B-NB	4.22	114.70	110.33
12	b	836	CLA	O2A-CGA-CBA	4.21	124.69	111.83
12	B	811	CLA	C1D-ND-C4D	-4.21	103.36	106.31
15	S	205	BCR	C40-C30-C25	4.21	116.85	110.24
12	l	202	CLA	O2A-CGA-CBA	4.21	124.68	111.83
12	H	812	CLA	O2A-CGA-CBA	4.21	124.68	111.83
12	a	817	CLA	C1C-C2C-C3C	-4.21	102.55	106.98
12	B	832	CLA	C1D-ND-C4D	-4.21	103.36	106.31
12	G	818	CLA	C2B-C1B-NB	4.21	114.69	110.33
12	B	821	CLA	O2A-CGA-CBA	4.21	124.66	111.83
12	H	817	CLA	C1D-ND-C4D	-4.21	103.36	106.31
12	G	804	CLA	O2A-CGA-CBA	4.21	124.66	111.83
12	b	832	CLA	O2A-CGA-CBA	4.21	124.66	111.83
12	a	817	CLA	O2A-CGA-CBA	4.20	124.66	111.83
12	G	855	CLA	O2A-CGA-CBA	4.20	124.65	111.83
12	G	807	CLA	CAA-C2A-C3A	-4.20	101.64	113.00
12	G	818	CLA	C4D-C3D-CAD	4.20	112.67	108.11
12	j	102	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
12	G	838	CLA	CHD-C1D-ND	-4.20	118.89	124.80
12	a	841	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
12	j	102	CLA	O2A-CGA-O1A	-4.20	113.13	123.63
12	A	832	CLA	O2A-CGA-CBA	4.20	124.63	111.83
12	A	831	CLA	OBD-CAD-C3D	-4.20	118.61	128.42
12	B	824	CLA	O2A-C1-C2	4.20	124.26	108.11
12	B	830	CLA	O2A-CGA-O1A	-4.20	113.13	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	819	CLA	C1D-ND-C4D	-4.20	103.37	106.31
12	G	813	CLA	OBD-CAD-C3D	-4.19	118.61	128.42
12	H	838	CLA	O2A-CGA-CBA	4.19	124.62	111.83
12	A	807	CLA	O2A-CGA-CBA	4.19	124.62	111.83
12	b	823	CLA	C1D-ND-C4D	-4.19	103.37	106.31
12	a	816	CLA	C4A-NA-C1A	4.19	108.59	106.68
12	A	803	CLA	O2A-CGA-CBA	4.19	124.60	111.83
12	H	822	CLA	O2A-CGA-CBA	4.19	124.60	111.83
12	b	809	CLA	C1D-ND-C4D	-4.19	103.38	106.31
12	a	803	CLA	O2A-CGA-CBA	4.19	124.60	111.83
12	H	816	CLA	C2B-C1B-NB	4.18	114.67	110.33
12	b	811	CLA	C2B-C1B-NB	4.18	114.67	110.33
12	a	818	CLA	O2A-CGA-O1A	-4.18	113.16	123.63
12	B	812	CLA	C2B-C1B-NB	4.18	114.66	110.33
12	a	830	CLA	O2A-CGA-CBA	4.18	124.58	111.83
12	G	818	CLA	C2C-C1C-NC	4.18	114.37	109.98
12	a	828	CLA	O2A-CGA-O1A	-4.18	113.17	123.63
13	b	838	1L3	C22-C21-C23	4.18	122.48	115.23
15	B	844	BCR	C24-C23-C22	-4.18	120.06	126.23
12	B	826	CLA	O2A-CGA-CBA	4.18	124.57	111.83
12	a	831	CLA	C1D-ND-C4D	-4.18	103.38	106.31
12	b	813	CLA	C2B-C1B-NB	4.17	114.66	110.33
12	A	805	CLA	CAA-C2A-C3A	-4.17	101.72	113.00
12	b	821	CLA	O2A-CGA-CBA	4.17	124.56	111.83
12	A	812	CLA	C2B-C1B-NB	4.17	114.65	110.33
12	H	827	CLA	CMD-C2D-C3D	-4.17	118.12	127.69
12	B	836	CLA	C4D-C3D-CAD	4.17	112.64	108.11
12	A	828	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
12	P	203	CLA	C1D-ND-C4D	-4.17	103.39	106.31
12	A	823	CLA	C1D-ND-C4D	-4.17	103.39	106.31
12	H	811	CLA	C2B-C1B-NB	4.17	114.65	110.33
12	S	202	CLA	C1D-ND-C4D	-4.17	103.39	106.31
12	H	822	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
12	P	201	CLA	C2D-C1D-ND	4.17	114.25	110.13
12	A	840	CLA	O2A-C1-C2	4.17	124.15	108.11
12	a	833	CLA	C2B-C1B-NB	4.17	114.65	110.33
12	A	840	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
12	b	837	CLA	C2B-C1B-NB	4.17	114.65	110.33
12	H	811	CLA	OBD-CAD-C3D	-4.16	118.68	128.42
12	B	837	CLA	O2A-CGA-CBA	4.16	124.53	111.83
12	A	826	CLA	C1D-ND-C4D	-4.16	103.39	106.31
12	F	201	CLA	C3D-C2D-C1D	-4.16	100.16	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	801	CLA	C2B-C1B-NB	4.16	114.64	110.33
12	a	811	CLA	C1D-ND-C4D	-4.16	103.39	106.31
12	A	838	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
12	A	825	CLA	C4A-NA-C1A	4.15	108.57	106.68
12	A	806	CLA	CHD-C1D-ND	-4.15	118.96	124.80
12	A	825	CLA	C2B-C1B-NB	4.15	114.63	110.33
11	a	801	CL0	C1D-ND-C4D	-4.15	103.40	106.31
12	H	823	CLA	C2B-C1B-NB	4.15	114.63	110.33
12	a	812	CLA	C1D-ND-C4D	-4.15	103.40	106.31
12	B	833	CLA	O2A-CGA-CBA	4.15	124.49	111.83
12	A	841	CLA	CMB-C2B-C1B	4.14	131.73	125.42
12	A	838	CLA	CHD-C1D-ND	-4.14	118.97	124.80
12	B	838	CLA	O2A-CGA-O1A	-4.14	113.26	123.63
12	b	824	CLA	O2A-CGA-CBA	4.14	124.47	111.83
12	a	812	CLA	CHD-C1D-ND	-4.14	118.97	124.80
12	a	805	CLA	CHD-C1D-ND	-4.14	118.97	124.80
12	A	822	CLA	C2D-C1D-ND	4.14	114.22	110.13
12	b	823	CLA	O2A-CGA-CBA	4.14	124.45	111.83
12	B	827	CLA	C4A-NA-C1A	4.14	108.57	106.68
12	a	824	CLA	C3C-C4C-NC	4.14	115.73	110.43
12	B	816	CLA	C4A-NA-C1A	4.14	108.57	106.68
12	b	816	CLA	O2D-CGD-CBD	4.13	118.46	111.23
12	B	836	CLA	C1D-ND-C4D	-4.13	103.41	106.31
12	F	201	CLA	C1D-ND-C4D	-4.13	103.41	106.31
12	H	831	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
12	a	837	CLA	C1D-ND-C4D	-4.13	103.41	106.31
12	A	803	CLA	C2B-C1B-NB	4.13	114.61	110.33
12	a	812	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
12	A	811	CLA	C1D-ND-C4D	-4.13	103.42	106.31
12	a	806	CLA	CAA-C2A-C3A	-4.13	101.85	113.00
12	A	827	CLA	C1D-ND-C4D	-4.13	103.42	106.31
12	B	828	CLA	C1D-ND-C4D	-4.12	103.42	106.31
12	L	204	CLA	C1D-ND-C4D	-4.12	103.42	106.31
12	b	804	CLA	O2A-CGA-CBA	4.12	124.40	111.83
12	a	818	CLA	CBA-CAA-C2A	4.12	126.05	113.79
12	H	850	CLA	O2A-CGA-CBA	4.12	124.40	111.83
16	A	853	LHG	O7-C7-C8	4.12	120.39	111.48
12	H	808	CLA	O2A-CGA-CBA	4.12	124.39	111.83
12	B	816	CLA	C1D-ND-C4D	-4.12	103.42	106.31
12	H	837	CLA	C1D-ND-C4D	-4.12	103.42	106.31
12	b	801	CLA	O2A-CGA-CBA	4.12	124.39	111.83
12	A	829	CLA	O2A-C1-C2	4.12	123.95	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	822	CLA	C2B-C1B-NB	4.11	114.59	110.33
12	H	838	CLA	CAC-C3C-C2C	4.11	135.12	127.56
12	A	841	CLA	O2A-CGA-CBA	4.11	124.38	111.83
12	j	102	CLA	C1D-ND-C4D	-4.11	103.43	106.31
12	A	831	CLA	C4A-NA-C1A	4.11	108.56	106.68
12	F	201	CLA	C4A-NA-C1A	4.11	108.56	106.68
12	a	838	CLA	CHD-C1D-ND	-4.11	119.02	124.80
12	b	823	CLA	C3C-C4C-NC	4.11	115.69	110.43
12	A	834	CLA	C1D-ND-C4D	-4.11	103.43	106.31
16	A	850	LHG	O7-C7-C8	4.10	120.36	111.48
12	b	802	CLA	CMC-C2C-C1C	4.10	131.44	125.03
12	H	833	CLA	C1D-ND-C4D	-4.10	103.43	106.31
12	S	204	CLA	O2A-CGA-CBA	4.10	124.34	111.83
12	b	827	CLA	C2B-C1B-NB	4.10	114.58	110.33
12	a	802	CLA	C2C-C1C-NC	4.10	114.29	109.98
15	H	849	BCR	C34-C9-C10	-4.10	116.18	122.82
12	A	854	CLA	CMC-C2C-C1C	4.10	131.44	125.03
12	b	806	CLA	C2B-C1B-NB	4.10	114.58	110.33
12	H	823	CLA	O2A-CGA-CBA	4.10	124.33	111.83
12	H	839	CLA	O2A-CGA-O1A	-4.10	113.38	123.63
12	b	818	CLA	C2B-C1B-NB	4.10	114.57	110.33
12	G	830	CLA	C2D-C1D-ND	4.10	114.18	110.13
12	H	803	CLA	C1D-ND-C4D	-4.09	103.44	106.31
12	G	814	CLA	CHD-C1D-ND	-4.09	119.04	124.80
12	b	808	CLA	C1D-ND-C4D	-4.09	103.44	106.31
12	G	855	CLA	O2D-CGD-O1D	-4.09	115.89	123.85
12	S	203	CLA	CHD-C1D-ND	-4.09	119.05	124.80
12	a	806	CLA	CHD-C1D-ND	-4.09	119.05	124.80
12	b	831	CLA	C1D-ND-C4D	-4.08	103.45	106.31
12	P	201	CLA	O2A-C1-C2	4.08	123.83	108.11
12	G	840	CLA	O2A-C1-C2	4.08	123.83	108.11
12	a	826	CLA	C3C-C4C-NC	4.08	115.66	110.43
12	R	103	CLA	C2B-C1B-NB	4.08	114.56	110.33
12	A	837	CLA	O2A-CGA-CBA	4.08	124.28	111.83
12	a	819	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
12	A	805	CLA	O2A-CGA-O1A	-4.08	113.42	123.63
12	b	848	CLA	C1D-ND-C4D	-4.08	103.45	106.31
12	b	815	CLA	O2A-CGA-O1A	-4.08	113.43	123.63
12	a	836	CLA	CMD-C2D-C3D	-4.08	118.34	127.69
12	H	819	CLA	C1D-ND-C4D	-4.08	103.45	106.31
15	L	201	BCR	C40-C30-C25	4.08	116.64	110.24
12	A	855	CLA	O2A-CGA-O1A	-4.07	113.44	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	826	CLA	CAA-C2A-C3A	-4.07	101.99	113.00
12	H	831	CLA	C1D-ND-C4D	-4.07	103.45	106.31
12	G	838	CLA	C4A-NA-C1A	4.07	108.54	106.68
12	A	802	CLA	C2C-C1C-NC	4.07	114.26	109.98
12	B	834	CLA	O2A-CGA-CBA	4.07	124.25	111.83
15	A	849	BCR	C7-C8-C9	-4.07	120.21	126.23
12	B	815	CLA	C1D-ND-C4D	-4.07	103.46	106.31
12	H	806	CLA	O2A-CGA-CBA	4.07	124.25	111.83
12	b	836	CLA	CAC-C3C-C2C	4.07	135.03	127.56
12	G	803	CLA	O2A-CGA-CBA	4.07	124.24	111.83
12	A	816	CLA	C1D-ND-C4D	-4.07	103.46	106.31
12	f	201	CLA	C3B-C2B-C1B	-4.07	102.38	107.17
12	a	803	CLA	C2B-C1B-NB	4.07	114.54	110.33
12	A	814	CLA	C2B-C1B-NB	4.06	114.54	110.33
12	a	831	CLA	C2B-C1B-NB	4.06	114.54	110.33
12	b	833	CLA	C2B-C1B-NB	4.06	114.54	110.33
12	A	840	CLA	C1D-ND-C4D	-4.06	103.46	106.31
12	L	202	CLA	O2A-CGA-CBA	4.06	124.22	111.83
12	G	825	CLA	O2A-CGA-CBA	4.06	124.21	111.83
12	B	823	CLA	O2A-CGA-CBA	4.06	124.21	111.83
12	G	804	CLA	C2B-C1B-NB	4.06	114.53	110.33
12	H	850	CLA	O2D-CGD-CBD	4.06	118.33	111.23
12	G	807	CLA	CHD-C1D-ND	-4.06	119.09	124.80
12	B	838	CLA	C1-O2A-CGA	4.06	126.47	116.65
13	B	839	1L3	C22-C21-C23	4.05	122.27	115.23
12	a	816	CLA	C2D-C1D-ND	4.05	114.14	110.13
12	G	818	CLA	O2A-C1-C2	4.05	123.70	108.11
15	R	101	BCR	C15-C14-C13	-4.05	121.60	127.28
12	A	820	CLA	C2D-C1D-ND	4.05	114.13	110.13
12	A	833	CLA	C2B-C1B-NB	4.05	114.52	110.33
12	G	806	CLA	CAA-C2A-C3A	-4.05	102.06	113.00
12	a	802	CLA	O2A-C1-C2	4.05	123.68	108.11
15	b	840	BCR	C24-C23-C22	-4.05	120.25	126.23
12	B	822	CLA	O2A-C1-C2	4.05	123.68	108.11
12	G	817	CLA	C1D-ND-C4D	-4.05	103.47	106.31
12	B	814	CLA	OBD-CAD-C3D	-4.05	118.96	128.42
15	b	843	BCR	C24-C23-C22	-4.04	120.25	126.23
12	a	841	CLA	O2A-CGA-CBA	4.04	124.17	111.83
12	b	837	CLA	O2A-CGA-O1A	-4.04	113.51	123.63
12	A	821	CLA	C2B-C1B-NB	4.04	114.52	110.33
15	G	849	BCR	C27-C26-C25	-4.04	117.24	122.70
12	A	833	CLA	C1D-ND-C4D	-4.04	103.48	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	814	CLA	O2A-CGA-CBA	4.04	124.15	111.83
12	a	805	CLA	O2A-CGA-O1A	-4.04	113.52	123.63
12	a	821	CLA	C2B-C1B-NB	4.04	114.52	110.33
15	b	839	BCR	C15-C14-C13	-4.04	121.61	127.28
12	G	841	CLA	O2A-CGA-CBA	4.04	124.15	111.83
12	A	834	CLA	C2B-C1B-NB	4.04	114.51	110.33
12	b	822	CLA	O2A-CGA-CBA	4.04	124.14	111.83
12	P	201	CLA	C2B-C1B-NB	4.03	114.51	110.33
12	a	810	CLA	O2A-CGA-CBA	4.03	124.14	111.83
12	a	802	CLA	CMC-C2C-C1C	4.03	131.34	125.03
12	a	827	CLA	CAA-C2A-C3A	-4.03	102.10	113.00
12	G	815	CLA	C2B-C1B-NB	4.03	114.51	110.33
12	H	819	CLA	C2B-C1B-NB	4.03	114.51	110.33
12	B	838	CLA	C2B-C1B-NB	4.03	114.51	110.33
12	a	822	CLA	C1D-ND-C4D	-4.03	103.48	106.31
12	a	854	CLA	CMD-C2D-C1D	4.03	131.83	124.73
16	G	851	LHG	O7-C7-C8	4.03	120.20	111.48
12	G	811	CLA	O2A-CGA-CBA	4.03	124.13	111.83
12	G	827	CLA	C2B-C1B-NB	4.03	114.51	110.33
12	H	805	CLA	CHD-C1D-ND	-4.03	119.13	124.80
12	A	817	CLA	CHD-C1D-ND	-4.03	119.13	124.80
12	a	808	CLA	C2D-C1D-ND	4.03	114.11	110.13
13	H	840	1L3	C22-C21-C23	4.03	122.22	115.23
12	H	822	CLA	C1D-ND-C4D	-4.03	103.48	106.31
12	G	841	CLA	C3B-C2B-C1B	-4.03	102.42	107.17
12	A	813	CLA	C2B-C1B-NB	4.02	114.50	110.33
12	B	834	CLA	C2B-C1B-NB	4.02	114.50	110.33
12	G	841	CLA	CAC-C3C-C4C	4.02	130.03	124.79
12	A	804	CLA	CMC-C2C-C1C	4.02	131.32	125.03
12	a	834	CLA	C1D-ND-C4D	-4.02	103.49	106.31
15	a	849	BCR	C28-C27-C26	-4.02	106.89	114.06
12	G	811	CLA	CHD-C1D-ND	-4.02	119.15	124.80
12	a	803	CLA	C4A-NA-C1A	4.02	108.51	106.68
12	G	836	CLA	C2B-C1B-NB	4.02	114.49	110.33
12	H	801	CLA	C1D-ND-C4D	-4.02	103.49	106.31
12	G	825	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
12	b	848	CLA	C2B-C1B-NB	4.02	114.49	110.33
12	a	823	CLA	O2D-CGD-CBD	4.02	118.25	111.23
12	b	825	CLA	O2A-CGA-CBA	4.01	124.08	111.83
12	H	816	CLA	CBA-CAA-C2A	4.01	125.73	113.79
15	G	850	BCR	C7-C8-C9	-4.01	120.30	126.23
12	H	831	CLA	O2A-CGA-CBA	4.01	124.07	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	805	CLA	CHD-C1D-ND	-4.01	119.16	124.80
12	H	835	CLA	O2A-CGA-CBA	4.01	124.06	111.83
12	G	802	CLA	CAA-C2A-C3A	-4.01	102.16	113.00
15	a	852	BCR	C15-C14-C13	-4.01	121.66	127.28
12	A	802	CLA	O2A-CGA-CBA	4.01	124.06	111.83
12	a	837	CLA	O2A-CGA-CBA	4.01	124.06	111.83
12	a	819	CLA	CAC-C3C-C4C	4.01	130.01	124.79
12	H	839	CLA	CMC-C2C-C1C	4.01	131.30	125.03
12	G	802	CLA	CMD-C2D-C1D	4.01	131.79	124.73
12	B	830	CLA	C1D-ND-C4D	-4.01	103.50	106.31
12	l	202	CLA	C2B-C1B-NB	4.01	114.48	110.33
12	B	828	CLA	C2B-C1B-NB	4.01	114.48	110.33
15	a	848	BCR	C34-C9-C8	4.01	124.21	118.09
12	H	805	CLA	CMB-C2B-C1B	4.01	131.52	125.42
12	A	810	CLA	O2A-CGA-CBA	4.01	124.05	111.83
12	B	836	CLA	CMD-C2D-C3D	-4.00	118.51	127.69
12	H	815	CLA	O2A-CGA-CBA	4.00	124.04	111.83
15	G	850	BCR	C28-C27-C26	-4.00	106.92	114.06
12	G	834	CLA	C2B-C1B-NB	4.00	114.48	110.33
12	a	821	CLA	CHD-C1D-ND	-4.00	119.17	124.80
12	a	822	CLA	C2B-C1B-NB	4.00	114.48	110.33
12	G	803	CLA	O2D-CGD-CBD	4.00	118.22	111.23
12	b	826	CLA	C4A-NA-C1A	4.00	108.50	106.68
12	B	822	CLA	C2B-C1B-NB	4.00	114.47	110.33
12	A	808	CLA	CHD-C1D-ND	-4.00	119.17	124.80
12	a	818	CLA	O2A-CGA-CBA	4.00	124.03	111.83
12	b	837	CLA	C1-O2A-CGA	4.00	126.33	116.65
12	G	807	CLA	C2B-C1B-NB	4.00	114.47	110.33
12	G	809	CLA	C2D-C1D-ND	4.00	114.08	110.13
12	G	816	CLA	C2B-C1B-NB	4.00	114.47	110.33
12	G	805	CLA	CMC-C2C-C1C	4.00	131.28	125.03
12	a	827	CLA	C1C-C2C-C3C	-4.00	102.78	106.98
12	A	836	CLA	C2B-C1B-NB	4.00	114.47	110.33
12	G	806	CLA	CAC-C3C-C4C	3.99	129.99	124.79
12	G	822	CLA	CHD-C1D-ND	-3.99	119.18	124.80
12	H	832	CLA	C1D-ND-C4D	-3.99	103.51	106.31
12	b	836	CLA	C1D-ND-C4D	-3.99	103.51	106.31
15	a	848	BCR	C27-C26-C25	-3.99	117.31	122.70
12	H	837	CLA	CMA-C3A-C4A	3.99	122.50	111.77
12	H	815	CLA	C2B-C1B-NB	3.98	114.46	110.33
12	G	819	CLA	O2A-CGA-O1A	-3.98	113.67	123.63
12	a	811	CLA	C2B-C1B-NB	3.98	114.45	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	825	CLA	CMD-C2D-C1D	3.98	131.74	124.73
12	j	104	CLA	C1D-ND-C4D	-3.98	103.52	106.31
12	G	819	CLA	O2A-C1-C2	3.98	123.42	108.11
12	B	806	CLA	O2A-C1-C2	3.98	123.42	108.11
12	B	823	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
12	H	824	CLA	O2A-CGA-CBA	3.97	123.95	111.83
12	B	822	CLA	O2A-CGA-CBA	3.97	123.95	111.83
12	A	802	CLA	C1D-ND-C4D	-3.97	103.53	106.31
12	L	206	CLA	O2A-CGA-CBA	3.97	123.94	111.83
15	F	202	BCR	C35-C13-C12	3.97	124.16	118.09
12	b	828	CLA	C1D-ND-C4D	-3.97	103.53	106.31
12	A	806	CLA	C2B-C1B-NB	3.97	114.44	110.33
12	l	206	CLA	O2A-CGA-CBA	3.97	123.94	111.83
12	J	103	CLA	C2B-C1B-NB	3.97	114.44	110.33
12	H	825	CLA	O2A-CGA-CBA	3.96	123.92	111.83
12	a	814	CLA	C2B-C1B-NB	3.96	114.44	110.33
12	H	817	CLA	C2B-C1B-NB	3.96	114.43	110.33
12	A	810	CLA	CHD-C1D-ND	-3.96	119.23	124.80
12	a	829	CLA	O2A-C1-C2	3.96	123.34	108.11
12	H	821	CLA	O2D-CGD-CBD	3.96	118.15	111.23
12	a	832	CLA	O2A-CGA-CBA	3.96	123.90	111.83
12	a	816	CLA	CMA-C3A-C4A	3.96	122.41	111.77
12	A	803	CLA	C4A-NA-C1A	3.96	108.48	106.68
12	a	818	CLA	O2A-C1-C2	3.96	123.33	108.11
15	B	842	BCR	C33-C5-C6	-3.95	120.17	124.48
12	H	839	CLA	C2B-C1B-NB	3.95	114.42	110.33
12	A	833	CLA	O2A-C1-C2	3.95	123.31	108.11
12	a	823	CLA	O2A-C1-C2	3.95	123.31	108.11
12	b	833	CLA	O2A-CGA-CBA	3.95	123.88	111.83
12	G	806	CLA	O2A-CGA-O1A	-3.95	113.75	123.63
12	B	807	CLA	CAA-C2A-C3A	-3.95	102.34	113.00
15	f	202	BCR	C3-C4-C5	-3.95	107.02	114.06
12	A	818	CLA	O2A-CGA-CBA	3.94	123.86	111.83
12	j	104	CLA	C4A-NA-C1A	3.94	108.48	106.68
12	b	821	CLA	C1D-ND-C4D	-3.94	103.55	106.31
12	b	835	CLA	C4D-C3D-CAD	3.94	112.39	108.11
12	H	837	CLA	C4A-NA-C1A	3.94	108.48	106.68
12	G	833	CLA	CAA-C2A-C3A	-3.94	102.36	113.00
12	B	818	CLA	C2B-C1B-NB	3.94	114.41	110.33
12	b	803	CLA	C1D-ND-C4D	-3.94	103.55	106.31
12	a	820	CLA	O2A-C1-C2	3.94	123.26	108.11
12	H	827	CLA	C4B-C3B-C2B	-3.94	102.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	830	CLA	O2A-C1-C2	3.94	123.26	108.11
15	a	845	BCR	C24-C23-C22	-3.94	120.41	126.23
12	H	808	CLA	C2B-C1B-NB	3.94	114.41	110.33
11	a	801	CL0	O2A-CGA-CBA	3.94	123.84	111.83
12	G	808	CLA	O2A-CGA-CBA	3.94	123.83	111.83
12	A	820	CLA	O2A-CGA-CBA	3.93	123.83	111.83
15	G	853	BCR	C15-C14-C13	-3.93	121.76	127.28
12	A	826	CLA	C2B-C1B-NB	3.93	114.40	110.33
12	A	820	CLA	O2A-C1-C2	3.93	123.23	108.11
12	L	202	CLA	C2B-C1B-NB	3.93	114.40	110.33
12	b	824	CLA	O2A-C1-C2	3.93	123.22	108.11
12	a	805	CLA	O2A-CGA-CBA	3.93	123.80	111.83
12	H	806	CLA	CAA-C2A-C3A	-3.92	102.39	113.00
12	A	823	CLA	C2B-C1B-NB	3.92	114.40	110.33
12	A	837	CLA	C4D-C3D-CAD	3.92	112.37	108.11
12	G	836	CLA	O2D-CGD-CBD	3.92	118.09	111.23
15	F	202	BCR	C28-C27-C26	-3.92	107.06	114.06
12	G	821	CLA	O2A-C1-C2	3.92	123.20	108.11
12	b	836	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
12	a	817	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	B	825	CLA	O2D-CGD-CBD	3.92	118.08	111.23
12	H	816	CLA	O2A-CGA-O1A	-3.92	113.83	123.63
12	A	823	CLA	O2A-C1-C2	3.92	123.19	108.11
12	A	809	CLA	C1D-ND-C4D	-3.92	103.56	106.31
12	G	823	CLA	C2B-C1B-NB	3.92	114.39	110.33
12	a	833	CLA	CAA-C2A-C3A	-3.91	102.42	113.00
12	b	814	CLA	C3B-C2B-C1B	-3.91	102.56	107.17
15	B	840	BCR	C24-C23-C22	-3.91	120.44	126.23
12	H	809	CLA	C1D-ND-C4D	-3.91	103.57	106.31
12	B	830	CLA	O2A-CGA-CBA	3.91	123.77	111.83
12	A	808	CLA	O2A-C1-C2	3.91	123.16	108.11
12	G	803	CLA	C3B-C2B-C1B	-3.91	102.56	107.17
17	m	101	45D	C29-C31-C33	-3.91	111.87	123.20
12	G	837	CLA	O2A-CGA-CBA	3.91	123.75	111.83
15	J	102	BCR	C28-C27-C26	-3.91	107.09	114.06
12	A	808	CLA	O2A-CGA-CBA	3.91	123.75	111.83
12	A	833	CLA	CAA-C2A-C3A	-3.90	102.45	113.00
12	G	806	CLA	CMC-C2C-C1C	3.90	131.13	125.03
12	a	812	CLA	C2B-C1B-NB	3.90	114.37	110.33
12	a	826	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
12	G	832	CLA	O2A-CGA-CBA	3.90	123.73	111.83
12	a	855	CLA	O2A-CGA-O1A	-3.90	113.87	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	841	CLA	O2A-C1-C2	3.90	123.11	108.11
12	a	808	CLA	CHD-C1D-ND	-3.90	119.31	124.80
15	A	847	BCR	C34-C9-C8	3.90	124.04	118.09
11	A	801	CL0	O2A-CGA-CBA	3.90	123.71	111.83
12	b	824	CLA	C2B-C1B-NB	3.90	114.37	110.33
12	b	802	CLA	CAA-C2A-C3A	-3.89	102.48	113.00
12	B	831	CLA	CAC-C3C-C4C	3.89	129.85	124.79
12	G	833	CLA	C2B-C1B-NB	3.89	114.36	110.33
12	A	805	CLA	O2A-CGA-CBA	3.89	123.70	111.83
12	G	802	CLA	CAA-C2A-C1A	-3.89	99.23	111.97
12	G	841	CLA	O2A-C1-C2	3.89	123.08	108.11
12	b	835	CLA	CMD-C2D-C3D	-3.89	118.77	127.69
12	A	820	CLA	CHB-C4A-NA	3.89	130.01	124.40
12	H	835	CLA	C2B-C1B-NB	3.89	114.36	110.33
12	B	824	CLA	O2A-CGA-CBA	3.89	123.69	111.83
12	B	816	CLA	CMB-C2B-C1B	3.89	131.34	125.42
12	a	806	CLA	C2B-C1B-NB	3.88	114.35	110.33
12	a	833	CLA	O2A-C1-C2	3.88	123.06	108.11
12	a	836	CLA	C4A-NA-C1A	3.88	108.45	106.68
12	a	802	CLA	C1D-ND-C4D	-3.88	103.59	106.31
12	a	824	CLA	O2A-CGA-CBA	3.88	123.67	111.83
12	G	821	CLA	O2A-CGA-CBA	3.88	123.67	111.83
12	H	823	CLA	O2A-C1-C2	3.88	123.03	108.11
15	a	849	BCR	C7-C8-C9	-3.88	120.50	126.23
12	a	825	CLA	CAA-C2A-C3A	-3.87	102.53	113.00
12	b	835	CLA	C1D-ND-C4D	-3.87	103.59	106.31
12	G	806	CLA	O2A-CGA-CBA	3.87	123.64	111.83
12	B	836	CLA	CMB-C2B-C3B	3.87	135.65	126.55
12	B	804	CLA	CHD-C1D-ND	-3.87	119.36	124.80
12	A	821	CLA	CHD-C1D-ND	-3.87	119.36	124.80
12	B	808	CLA	C1D-ND-C4D	-3.87	103.60	106.31
15	A	845	BCR	C24-C23-C22	-3.87	120.52	126.23
12	G	836	CLA	CMB-C2B-C3B	3.87	135.64	126.55
12	b	816	CLA	C1D-ND-C4D	-3.87	103.60	106.31
12	B	824	CLA	C1D-ND-C4D	-3.87	103.60	106.31
15	b	841	BCR	C33-C5-C6	-3.86	120.27	124.48
12	a	841	CLA	C1D-ND-C4D	-3.86	103.60	106.31
12	A	824	CLA	O2A-CGA-CBA	3.86	123.61	111.83
12	H	829	CLA	C1D-ND-C4D	-3.86	103.60	106.31
12	a	838	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
12	P	203	CLA	C2B-C1B-NB	3.86	114.33	110.33
12	S	202	CLA	O2A-CGA-CBA	3.86	123.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	802	CLA	O2D-CGD-CBD	3.86	117.97	111.23
12	j	102	CLA	O2A-CGA-CBA	3.86	123.59	111.83
12	b	822	CLA	O2A-C1-C2	3.86	122.95	108.11
12	G	831	CLA	C4A-NA-C1A	3.86	108.44	106.68
12	G	829	CLA	O2A-C1-C2	3.86	122.94	108.11
12	G	855	CLA	C2C-C1C-NC	3.86	114.03	109.98
12	G	827	CLA	O2A-CGA-CBA	3.85	123.59	111.83
12	H	810	CLA	C2B-C1B-NB	3.85	114.32	110.33
12	a	823	CLA	C2B-C1B-NB	3.85	114.32	110.33
12	G	809	CLA	C1D-ND-C4D	-3.85	103.61	106.31
12	a	829	CLA	C1D-ND-C4D	-3.85	103.61	106.31
15	H	843	BCR	C33-C5-C6	-3.85	120.28	124.48
12	B	811	CLA	O2A-C1-C2	3.85	122.92	108.11
12	A	826	CLA	O2A-CGA-CBA	3.85	123.57	111.83
17	M	101	45D	C29-C31-C33	-3.85	112.05	123.20
12	B	807	CLA	C1D-ND-C4D	-3.85	103.61	106.31
12	a	826	CLA	O2A-CGA-CBA	3.85	123.57	111.83
12	G	832	CLA	CHD-C1D-ND	-3.85	119.39	124.80
12	l	205	CLA	C2B-C1B-NB	3.85	114.31	110.33
12	H	802	CLA	C11-C12-C13	-3.84	103.19	115.97
12	A	817	CLA	C4D-C3D-CAD	3.84	112.28	108.11
12	G	830	CLA	O2A-CGA-CBA	3.84	123.55	111.83
12	a	841	CLA	O2A-C1-C2	3.84	122.89	108.11
12	B	816	CLA	C2B-C1B-NB	3.84	114.31	110.33
12	b	821	CLA	C4-C3-C5	3.84	121.89	115.23
15	H	842	BCR	C27-C26-C25	-3.84	117.52	122.70
12	A	832	CLA	O2D-CGD-CBD	3.84	117.94	111.23
12	A	822	CLA	C1D-ND-C4D	-3.84	103.62	106.31
12	A	832	CLA	C4A-NA-C1A	3.84	108.43	106.68
12	A	807	CLA	O2A-C1-C2	3.83	122.86	108.11
12	H	838	CLA	C1D-ND-C4D	-3.83	103.62	106.31
12	B	806	CLA	CBA-CAA-C2A	3.83	125.19	113.79
12	b	813	CLA	O2A-CGA-CBA	3.83	123.52	111.83
12	b	813	CLA	O2A-C1-C2	3.83	122.85	108.11
12	B	809	CLA	C2B-C1B-NB	3.83	114.30	110.33
12	H	802	CLA	C4-C3-C5	3.83	121.87	115.23
15	A	849	BCR	C28-C27-C26	-3.83	107.23	114.06
16	a	853	LHG	O7-C7-C8	3.83	119.76	111.48
12	B	806	CLA	CAA-C2A-C3A	-3.82	102.66	113.00
12	b	816	CLA	C2B-C1B-NB	3.82	114.29	110.33
12	b	802	CLA	C4-C3-C5	3.82	121.87	115.23
12	A	818	CLA	O2A-CGA-O1A	-3.82	114.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	834	CLA	C2B-C1B-NB	3.82	114.29	110.33
12	f	203	CLA	C2B-C1B-NB	3.82	114.29	110.33
12	G	855	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
15	j	101	BCR	C15-C14-C13	-3.82	121.92	127.28
12	G	824	CLA	O2D-CGD-CBD	3.82	117.91	111.23
12	A	822	CLA	C2B-C1B-NB	3.82	114.29	110.33
15	H	841	BCR	C24-C23-C22	-3.82	120.58	126.23
12	H	826	CLA	O2A-CGA-CBA	3.82	123.48	111.83
12	B	837	CLA	CAC-C3C-C2C	3.82	134.58	127.56
12	G	805	CLA	O2A-C1-C2	3.82	122.81	108.11
12	G	808	CLA	C2B-C1B-NB	3.82	114.29	110.33
12	b	806	CLA	O2A-CGA-CBA	3.82	123.48	111.83
12	B	835	CLA	C2B-C1B-NB	3.82	114.29	110.33
12	A	825	CLA	C1D-ND-C4D	-3.82	103.63	106.31
12	G	825	CLA	C3C-C4C-NC	3.82	115.32	110.43
15	A	849	BCR	C33-C5-C6	-3.82	120.32	124.48
12	G	813	CLA	C2B-C1B-NB	3.82	114.28	110.33
12	A	826	CLA	C3C-C4C-NC	3.82	115.32	110.43
12	a	804	CLA	O2A-C1-C2	3.81	122.79	108.11
12	A	808	CLA	C1D-ND-C4D	-3.81	103.64	106.31
12	B	824	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
15	b	844	BCR	C34-C9-C10	-3.81	116.64	122.82
12	B	810	CLA	C2B-C1B-NB	3.81	114.28	110.33
15	i	102	BCR	C15-C14-C13	-3.80	121.94	127.28
12	G	827	CLA	C3C-C4C-NC	3.80	115.30	110.43
12	b	824	CLA	C4C-C3C-C2C	-3.80	101.35	106.89
12	a	812	CLA	O2A-C1-C2	3.80	122.75	108.11
15	G	850	BCR	C34-C9-C10	-3.80	116.65	122.82
18	H	847	LMG	O7-C10-C11	3.80	119.71	111.48
12	a	854	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
11	G	801	CL0	O2A-CGA-CBA	3.80	123.43	111.83
12	A	823	CLA	CHD-C1D-ND	-3.80	119.45	124.80
12	G	833	CLA	O2A-C1-C2	3.80	122.74	108.11
12	B	807	CLA	CAC-C3C-C4C	3.80	129.74	124.79
12	A	804	CLA	O2A-C1-C2	3.80	122.73	108.11
12	b	809	CLA	C2B-C1B-NB	3.80	114.27	110.33
12	b	824	CLA	C1D-ND-C4D	-3.80	103.65	106.31
12	G	834	CLA	C4-C3-C5	3.80	121.82	115.23
12	B	812	CLA	C1D-ND-C4D	-3.79	103.65	106.31
12	b	808	CLA	C2B-C1B-NB	3.79	114.26	110.33
12	l	204	CLA	C4-C3-C5	3.79	121.81	115.23
12	a	820	CLA	O2A-CGA-CBA	3.79	123.39	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	806	CLA	O2A-C1-C2	3.79	122.69	108.11
12	a	825	CLA	C1D-ND-C4D	-3.79	103.66	106.31
12	H	804	CLA	O2A-CGA-CBA	3.79	123.38	111.83
12	L	204	CLA	O2A-CGA-CBA	3.79	123.38	111.83
12	B	825	CLA	C2D-C1D-ND	3.79	113.87	110.13
12	G	829	CLA	C2B-C1B-NB	3.79	114.25	110.33
12	H	801	CLA	C4A-NA-C1A	3.79	108.41	106.68
15	a	852	BCR	C38-C26-C25	-3.78	120.35	124.48
12	G	826	CLA	C2B-C1B-NB	3.78	114.25	110.33
12	a	822	CLA	O2A-CGA-CBA	3.78	123.37	111.83
12	G	803	CLA	C1D-ND-C4D	-3.78	103.66	106.31
12	G	808	CLA	O2A-C1-C2	3.78	122.66	108.11
12	G	834	CLA	O2A-C1-C2	3.78	122.66	108.11
12	A	831	CLA	C1D-ND-C4D	-3.78	103.66	106.31
12	A	812	CLA	O2A-C1-C2	3.78	122.64	108.11
12	a	819	CLA	CAA-C2A-C3A	-3.78	102.80	113.00
12	b	810	CLA	C3C-C4C-NC	3.78	115.27	110.43
12	A	828	CLA	O2A-C1-C2	3.77	122.64	108.11
12	L	205	CLA	O2A-CGA-CBA	3.77	123.34	111.83
12	A	823	CLA	O2D-CGD-CBD	3.77	117.83	111.23
12	a	836	CLA	C1D-ND-C4D	-3.77	103.67	106.31
12	A	817	CLA	C4-C3-C5	3.77	121.78	115.23
12	a	802	CLA	O2A-CGA-CBA	3.77	123.33	111.83
12	G	820	CLA	C2B-C1B-NB	3.77	114.23	110.33
12	A	828	CLA	C2B-C1B-NB	3.77	114.23	110.33
15	S	201	BCR	C32-C1-C6	3.77	116.15	110.24
12	A	836	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
12	a	832	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	b	836	CLA	O2A-C1-C2	3.77	122.60	108.11
12	l	202	CLA	O2A-C1-C2	3.77	122.60	108.11
15	A	848	BCR	C27-C26-C25	-3.76	117.62	122.70
12	A	817	CLA	C4-C3-C2	-3.76	113.96	123.63
12	A	819	CLA	C2B-C1B-NB	3.76	114.23	110.33
12	G	823	CLA	O2A-CGA-CBA	3.76	123.31	111.83
12	l	204	CLA	O2A-CGA-CBA	3.76	123.31	111.83
12	a	805	CLA	C2B-C1B-NB	3.76	114.23	110.33
12	A	839	CLA	O2D-CGD-CBD	3.76	117.80	111.23
12	B	802	CLA	C4-C3-C5	3.76	121.75	115.23
12	A	841	CLA	C1D-ND-C4D	-3.76	103.67	106.31
12	G	812	CLA	C2B-C1B-NB	3.76	114.22	110.33
12	l	204	CLA	C2B-C1B-NB	3.76	114.22	110.33
15	H	844	BCR	C28-C27-C26	-3.76	107.36	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	844	BCR	C28-C27-C26	-3.76	107.36	114.06
12	b	807	CLA	C1D-ND-C4D	-3.75	103.68	106.31
12	a	824	CLA	C1D-ND-C4D	-3.75	103.68	106.31
12	G	842	CLA	C2B-C1B-NB	3.75	114.22	110.33
12	B	827	CLA	C2B-C1B-NB	3.75	114.22	110.33
12	A	822	CLA	O2A-CGA-CBA	3.75	123.27	111.83
12	H	850	CLA	C2B-C1B-NB	3.75	114.21	110.33
12	A	811	CLA	C2B-C1B-NB	3.75	114.21	110.33
12	G	839	CLA	C1D-ND-C4D	-3.75	103.68	106.31
12	F	201	CLA	O2A-C1-C2	3.75	122.53	108.11
12	H	833	CLA	C2B-C1B-NB	3.75	114.21	110.33
12	H	812	CLA	O2A-C1-C2	3.74	122.51	108.11
12	G	856	CLA	CAA-C2A-C3A	-3.74	102.88	113.00
12	b	804	CLA	CHD-C1D-ND	-3.74	119.53	124.80
12	A	819	CLA	CAA-C2A-C3A	-3.74	102.89	113.00
12	a	808	CLA	O2A-CGA-CBA	3.74	123.24	111.83
12	A	827	CLA	CAA-C2A-C3A	-3.74	102.89	113.00
12	a	819	CLA	C2B-C1B-NB	3.74	114.21	110.33
12	G	809	CLA	CMD-C2D-C3D	-3.74	119.11	127.69
15	B	841	BCR	C24-C23-C22	-3.74	120.71	126.23
12	S	202	CLA	C2B-C1B-NB	3.74	114.20	110.33
12	B	813	CLA	CHD-C1D-ND	-3.73	119.55	124.80
12	a	831	CLA	C4-C3-C5	3.73	121.70	115.23
12	b	812	CLA	C2B-C1B-NB	3.73	114.19	110.33
17	T	101	45D	C29-C31-C33	-3.73	112.39	123.20
12	H	814	CLA	O2A-CGA-CBA	3.73	123.20	111.83
15	G	845	BCR	C28-C27-C26	-3.73	107.41	114.06
12	a	804	CLA	CMC-C2C-C1C	3.73	130.86	125.03
12	G	825	CLA	C1D-ND-C4D	-3.73	103.70	106.31
12	a	807	CLA	C2B-C1B-NB	3.72	114.19	110.33
12	G	804	CLA	O2A-C1-C2	3.72	122.44	108.11
12	H	807	CLA	CAC-C3C-C4C	3.72	129.63	124.79
12	a	836	CLA	C2D-C1D-ND	3.72	113.81	110.13
12	G	809	CLA	CAA-C2A-C3A	-3.72	102.94	113.00
12	L	204	CLA	C4-C3-C5	3.72	121.69	115.23
12	F	201	CLA	CAA-C2A-C3A	-3.72	102.94	113.00
15	H	842	BCR	C24-C23-C22	-3.72	120.73	126.23
12	B	837	CLA	O2A-C1-C2	3.72	122.42	108.11
12	b	822	CLA	CMA-C3A-C4A	3.72	121.77	111.77
12	b	823	CLA	OBD-CAD-C3D	-3.72	119.72	128.42
12	G	825	CLA	O2A-C1-C2	3.72	122.41	108.11
12	H	817	CLA	C4A-NA-C1A	3.72	108.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	830	CLA	CMC-C2C-C1C	3.72	130.84	125.03
12	a	834	CLA	O2A-CGA-CBA	3.71	123.16	111.83
12	b	810	CLA	O1D-CGD-CBD	-3.71	117.19	124.52
12	F	203	CLA	C2B-C1B-NB	3.71	114.18	110.33
12	a	817	CLA	C4-C3-C5	3.71	121.67	115.23
12	G	842	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
15	l	203	BCR	C37-C22-C23	3.71	123.76	118.09
15	G	848	BCR	C34-C9-C8	3.71	123.76	118.09
12	B	810	CLA	C3C-C4C-NC	3.71	115.18	110.43
12	A	817	CLA	O2A-C1-C2	3.71	122.39	108.11
11	A	801	CL0	CAA-C2A-C3A	-3.71	102.97	113.00
12	H	827	CLA	CMB-C2B-C3B	3.71	135.27	126.55
12	b	825	CLA	C2D-C1D-ND	3.71	113.80	110.13
12	G	820	CLA	CAA-C2A-C3A	-3.71	102.98	113.00
15	a	844	BCR	C28-C27-C26	-3.71	107.45	114.06
12	A	832	CLA	CHD-C1D-ND	-3.71	119.59	124.80
12	G	841	CLA	C1D-ND-C4D	-3.71	103.71	106.31
12	a	833	CLA	C1D-ND-C4D	-3.71	103.71	106.31
12	b	831	CLA	CHD-C1D-ND	-3.70	119.59	124.80
12	B	832	CLA	C2B-C1B-NB	3.70	114.17	110.33
15	b	839	BCR	C24-C23-C22	-3.70	120.76	126.23
12	a	807	CLA	O2A-CGA-CBA	3.70	123.12	111.83
12	H	835	CLA	CMA-C3A-C4A	3.70	121.72	111.77
12	H	837	CLA	CHD-C1D-ND	-3.70	119.59	124.80
12	F	203	CLA	CAA-C2A-C3A	-3.70	103.00	113.00
12	a	807	CLA	O2A-C1-C2	3.70	122.34	108.11
12	a	837	CLA	O2A-C1-C2	3.70	122.34	108.11
12	A	824	CLA	C3C-C4C-NC	3.70	115.17	110.43
12	G	811	CLA	O2A-C1-C2	3.70	122.34	108.11
12	a	828	CLA	O2A-C1-C2	3.70	122.34	108.11
12	B	817	CLA	O2A-CGA-CBA	3.70	125.68	114.00
15	P	202	BCR	C28-C27-C26	-3.70	107.46	114.06
12	A	831	CLA	C4-C3-C5	3.70	121.64	115.23
12	G	813	CLA	O2A-C1-C2	3.69	122.33	108.11
12	b	805	CLA	CMB-C2B-C1B	3.69	131.04	125.42
12	B	821	CLA	C4-C3-C5	3.69	121.64	115.23
12	a	808	CLA	O2A-C1-C2	3.69	122.31	108.11
12	A	813	CLA	CHD-C1D-ND	-3.69	119.61	124.80
15	G	853	BCR	C38-C26-C25	-3.69	120.46	124.48
12	G	837	CLA	CHD-C1D-ND	-3.69	119.61	124.80
12	A	802	CLA	C4-C3-C5	3.69	121.63	115.23
12	b	810	CLA	C2B-C1B-NB	3.68	114.15	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	829	CLA	C1D-ND-C4D	-3.68	103.73	106.31
12	H	822	CLA	C4-C3-C5	3.68	121.62	115.23
12	H	809	CLA	C2B-C1B-NB	3.68	114.14	110.33
12	B	817	CLA	C2B-C1B-NB	3.68	114.14	110.33
12	H	814	CLA	O2A-C1-C2	3.68	122.28	108.11
12	A	854	CLA	CMD-C2D-C1D	3.68	131.21	124.73
12	B	822	CLA	CBA-CAA-C2A	3.68	124.74	113.79
12	f	201	CLA	CAA-C2A-C3A	-3.68	103.06	113.00
12	a	837	CLA	C4D-C3D-CAD	3.68	112.10	108.11
18	B	846	LMG	O7-C10-C11	3.68	119.44	111.48
12	L	204	CLA	C2B-C1B-NB	3.68	114.14	110.33
12	b	835	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
12	A	810	CLA	O2A-C1-C2	3.68	122.26	108.11
12	b	835	CLA	CHD-C1D-ND	-3.68	119.63	124.80
12	a	829	CLA	O2A-CGA-CBA	3.68	123.05	111.83
12	a	805	CLA	O2A-C1-C2	3.68	122.26	108.11
12	b	820	CLA	O2D-CGD-CBD	3.68	117.66	111.23
12	A	834	CLA	O2A-C1-C2	3.67	122.25	108.11
12	a	803	CLA	O2A-C1-C2	3.67	122.25	108.11
12	G	818	CLA	C1-O2A-CGA	3.67	125.54	116.65
12	a	855	CLA	CAA-C2A-C3A	-3.67	103.07	113.00
12	b	834	CLA	C2B-C1B-NB	3.67	114.14	110.33
15	a	848	BCR	C30-C25-C26	-3.67	117.62	122.64
12	B	801	CLA	CAA-C2A-C1A	-3.67	99.94	111.97
12	B	836	CLA	CHD-C1D-ND	-3.67	119.64	124.80
12	A	828	CLA	C1D-ND-C4D	-3.67	103.74	106.31
12	H	831	CLA	O2A-C1-C2	3.67	122.23	108.11
12	B	818	CLA	CHD-C1D-ND	-3.67	119.64	124.80
12	a	810	CLA	C2B-C1B-NB	3.67	114.13	110.33
12	b	848	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
15	H	845	BCR	C24-C23-C22	-3.67	120.81	126.23
12	B	816	CLA	C4-C3-C5	3.67	121.59	115.23
12	b	816	CLA	C4-C3-C5	3.67	121.59	115.23
12	b	826	CLA	C4B-C3B-C2B	-3.67	102.74	107.30
12	H	818	CLA	C2B-C1B-NB	3.67	114.13	110.33
12	b	804	CLA	CMC-C2C-C1C	3.67	130.76	125.03
12	A	855	CLA	CAA-C2A-C3A	-3.67	103.09	113.00
12	a	811	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
12	H	838	CLA	O2A-C1-C2	3.66	122.21	108.11
12	B	835	CLA	CHD-C1D-ND	-3.66	119.65	124.80
12	H	817	CLA	CMB-C2B-C1B	3.66	131.00	125.42
12	a	815	CLA	C2B-C1B-NB	3.66	114.12	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	829	CLA	O2A-CGA-CBA	3.66	123.00	111.83
12	S	202	CLA	C4-C3-C5	3.66	121.58	115.23
12	G	856	CLA	C2C-C1C-NC	3.66	113.83	109.98
12	S	203	CLA	O2A-CGA-CBA	3.66	123.00	111.83
12	b	830	CLA	C3B-C2B-C1B	-3.66	102.86	107.17
12	B	826	CLA	C4B-C3B-C2B	-3.66	102.75	107.30
12	b	835	CLA	O2A-CGA-CBA	3.66	122.99	111.83
12	A	830	CLA	CMC-C2C-C1C	3.66	130.75	125.03
12	B	813	CLA	O2A-CGA-CBA	3.65	122.98	111.83
12	H	824	CLA	C1D-ND-C4D	-3.65	103.75	106.31
12	a	831	CLA	CHD-C1D-ND	-3.65	119.66	124.80
12	b	816	CLA	CMB-C2B-C1B	3.65	130.98	125.42
12	A	836	CLA	C1D-ND-C4D	-3.65	103.75	106.31
12	H	828	CLA	C2B-C1B-NB	3.65	114.11	110.33
12	B	837	CLA	C3B-C2B-C1B	-3.65	102.87	107.17
12	a	834	CLA	O2A-C1-C2	3.65	122.14	108.11
15	B	841	BCR	C34-C9-C10	-3.65	116.91	122.82
12	G	806	CLA	CHD-C1D-ND	-3.65	119.67	124.80
12	A	813	CLA	O1D-CGD-CBD	-3.65	117.33	124.52
12	f	201	CLA	C4A-NA-C1A	3.65	108.34	106.68
12	G	819	CLA	O2A-CGA-CBA	3.64	122.95	111.83
12	L	205	CLA	C2B-C1B-NB	3.64	114.11	110.33
12	b	823	CLA	O2A-C1-C2	3.64	122.13	108.11
12	a	855	CLA	CMA-C3A-C4A	3.64	121.56	111.77
12	b	833	CLA	CMA-C3A-C4A	3.64	121.56	111.77
12	G	831	CLA	C2B-C1B-NB	3.64	114.10	110.33
12	B	805	CLA	CHD-C1D-ND	-3.64	119.68	124.80
12	B	836	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
12	A	816	CLA	O2A-CGA-CBA	3.64	122.94	111.83
12	G	818	CLA	C4-C3-C2	-3.64	114.28	123.63
12	S	203	CLA	C2B-C1B-NB	3.64	114.10	110.33
12	A	841	CLA	C3B-C2B-C1B	-3.64	102.88	107.17
12	B	805	CLA	CMB-C2B-C1B	3.64	130.96	125.42
12	b	827	CLA	CHD-C1D-ND	-3.64	119.68	124.80
12	f	203	CLA	CAA-C2A-C3A	-3.64	103.17	113.00
11	G	801	CL0	C3B-C2B-C1B	-3.64	102.88	107.17
12	H	825	CLA	C1C-C2C-C3C	-3.64	103.16	106.98
12	G	817	CLA	O2A-CGA-CBA	3.64	122.92	111.83
15	B	843	BCR	C28-C27-C26	-3.64	107.57	114.06
11	A	801	CL0	C4D-C3D-CAD	3.64	112.05	108.11
15	a	849	BCR	C34-C9-C10	-3.63	116.93	122.82
12	A	803	CLA	O2A-C1-C2	3.63	122.09	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	824	CLA	C3C-C4C-NC	3.63	115.08	110.43
15	b	842	BCR	C15-C14-C13	-3.63	121.93	127.48
12	a	837	CLA	CHD-C1D-ND	-3.63	119.69	124.80
12	A	837	CLA	CHD-C1D-ND	-3.63	119.69	124.80
12	H	823	CLA	CBA-CAA-C2A	3.63	124.60	113.79
15	H	849	BCR	C19-C18-C17	3.63	124.72	119.01
12	B	823	CLA	C1D-ND-C4D	-3.63	103.77	106.31
12	B	819	CLA	C2B-C1B-NB	3.63	114.09	110.33
12	H	802	CLA	C3C-C4C-NC	3.63	115.08	110.43
12	G	828	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
12	G	811	CLA	C2B-C1B-NB	3.63	114.09	110.33
12	B	829	CLA	CAA-C2A-C3A	-3.63	103.20	113.00
12	B	830	CLA	O2A-C1-C2	3.63	122.06	108.11
12	A	809	CLA	O2A-CGA-CBA	3.63	125.46	114.00
12	G	803	CLA	O2A-C1-C2	3.63	122.06	108.11
12	b	830	CLA	C1D-ND-C4D	-3.62	103.77	106.31
12	b	813	CLA	CHD-C1D-ND	-3.62	119.70	124.80
15	b	842	BCR	C38-C26-C25	-3.62	120.53	124.48
12	H	813	CLA	CHD-C1D-ND	-3.62	119.70	124.80
12	b	819	CLA	C2B-C1B-NB	3.62	114.08	110.33
12	H	801	CLA	C4-C3-C5	3.62	121.51	115.23
12	A	812	CLA	OBD-CAD-C3D	-3.62	119.96	128.42
12	b	810	CLA	O2A-C1-C2	3.62	122.03	108.11
12	B	813	CLA	O2A-C1-C2	3.62	122.03	108.11
12	A	834	CLA	C4-C3-C5	3.62	121.50	115.23
12	G	820	CLA	CAC-C3C-C4C	3.62	129.50	124.79
12	G	837	CLA	C4D-C3D-CAD	3.62	112.03	108.11
12	a	833	CLA	O2A-CGA-CBA	3.61	122.86	111.83
12	A	816	CLA	CMA-C3A-C4A	3.61	121.49	111.77
12	B	836	CLA	O2A-CGA-CBA	3.61	122.85	111.83
12	b	831	CLA	C2B-C1B-NB	3.61	114.07	110.33
12	b	836	CLA	CMC-C2C-C3C	3.61	135.92	126.15
12	a	834	CLA	C4-C3-C5	3.61	121.50	115.23
12	a	818	CLA	C1D-ND-C4D	-3.61	103.78	106.31
12	G	809	CLA	O2A-CGA-CBA	3.61	122.84	111.83
12	l	205	CLA	O2A-CGA-CBA	3.61	122.84	111.83
12	b	802	CLA	C4D-C3D-CAD	3.61	112.03	108.11
15	P	204	BCR	C35-C13-C14	-3.61	116.97	122.82
15	a	848	BCR	C34-C9-C10	-3.61	116.97	122.82
12	H	815	CLA	CHD-C1D-ND	-3.61	119.73	124.80
12	a	822	CLA	CHD-C1D-ND	-3.61	119.73	124.80
12	B	832	CLA	CHD-C1D-ND	-3.61	119.73	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	809	CLA	CHD-C1D-ND	-3.61	119.73	124.80
12	b	834	CLA	CHD-C1D-ND	-3.60	119.73	124.80
12	B	810	CLA	O2A-C1-C2	3.60	121.98	108.11
12	A	838	CLA	C4A-NA-C1A	3.60	108.32	106.68
15	H	842	BCR	C34-C9-C10	-3.60	116.98	122.82
12	A	831	CLA	CMB-C2B-C3B	3.60	135.02	126.55
15	B	843	BCR	C30-C25-C26	-3.60	117.72	122.64
12	A	855	CLA	O2A-CGA-CBA	3.60	122.81	111.83
12	A	841	CLA	CAC-C3C-C4C	3.60	129.47	124.79
12	G	839	CLA	O2D-CGD-CBD	3.60	117.52	111.23
12	B	815	CLA	O2A-C1-C2	3.60	121.95	108.11
12	b	814	CLA	CHD-C1D-ND	-3.60	119.74	124.80
12	A	819	CLA	CAC-C3C-C4C	3.60	129.47	124.79
12	a	827	CLA	O2A-C1-C2	3.59	121.94	108.11
12	H	827	CLA	CHD-C4C-NC	-3.59	118.66	124.23
15	G	849	BCR	C34-C9-C8	3.59	123.58	118.09
15	b	844	BCR	C7-C8-C9	-3.59	120.92	126.23
15	l	201	BCR	C7-C8-C9	-3.59	120.92	126.23
12	G	831	CLA	CMC-C2C-C1C	3.59	130.65	125.03
12	B	834	CLA	CMA-C3A-C4A	3.59	121.42	111.77
12	H	814	CLA	CHD-C1D-ND	-3.59	119.75	124.80
12	B	815	CLA	CBA-CAA-C2A	3.59	124.47	113.79
12	A	807	CLA	C2B-C1B-NB	3.59	114.05	110.33
12	H	815	CLA	O2A-C1-C2	3.59	121.91	108.11
12	A	833	CLA	CHD-C1D-ND	-3.59	119.76	124.80
15	B	843	BCR	C23-C24-C25	-3.59	117.42	127.00
12	b	835	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
12	a	823	CLA	CHD-C1D-ND	-3.59	119.76	124.80
12	b	805	CLA	CHD-C1D-ND	-3.59	119.76	124.80
12	B	816	CLA	O2A-CGA-CBA	3.58	122.76	111.83
12	a	810	CLA	CHD-C1D-ND	-3.58	119.76	124.80
12	H	836	CLA	CHD-C1D-ND	-3.58	119.76	124.80
11	a	801	CL0	C2D-C1D-ND	3.58	113.67	110.13
15	A	852	BCR	C15-C14-C13	-3.58	122.26	127.28
15	H	846	BCR	C34-C9-C10	-3.58	117.02	122.82
12	G	826	CLA	C4A-NA-C1A	3.58	108.31	106.68
12	H	826	CLA	O2A-C1-C2	3.58	121.88	108.11
15	S	205	BCR	C3-C4-C5	-3.58	107.68	114.06
12	B	804	CLA	O2A-C1-C2	3.58	121.87	108.11
12	a	836	CLA	CHD-C1D-ND	-3.57	119.77	124.80
12	A	855	CLA	C2C-C1C-NC	3.57	113.74	109.98
12	G	806	CLA	O2A-C1-C2	3.57	121.86	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	809	CLA	O2A-CGA-CBA	3.57	125.29	114.00
12	a	838	CLA	C4A-NA-C1A	3.57	108.31	106.68
12	G	824	CLA	C2B-C1B-NB	3.57	114.03	110.33
12	b	825	CLA	O2D-CGD-CBD	3.57	117.47	111.23
12	B	826	CLA	CMB-C2B-C3B	3.57	134.95	126.55
12	A	824	CLA	C1D-ND-C4D	-3.57	103.81	106.31
15	A	852	BCR	C38-C26-C25	-3.57	120.59	124.48
12	A	837	CLA	O2A-C1-C2	3.57	121.84	108.11
12	H	824	CLA	C2B-C1B-NB	3.57	114.03	110.33
12	a	810	CLA	O2A-C1-C2	3.57	121.84	108.11
12	G	835	CLA	C2B-C1B-NB	3.57	114.03	110.33
12	a	802	CLA	CAC-C3C-C4C	3.57	129.43	124.79
12	H	817	CLA	C4-C3-C5	3.57	121.42	115.23
15	H	849	BCR	C2-C1-C6	3.57	115.62	110.44
15	G	849	BCR	C19-C18-C17	3.57	124.62	119.01
12	b	826	CLA	CMB-C2B-C3B	3.56	134.93	126.55
15	J	104	BCR	C19-C18-C17	3.56	124.61	119.01
12	a	813	CLA	CHD-C1D-ND	-3.56	119.79	124.80
12	f	201	CLA	C2B-C1B-NB	3.56	114.02	110.33
12	b	825	CLA	O2A-C1-C2	3.56	121.81	108.11
12	H	837	CLA	O2A-CGA-CBA	3.56	122.69	111.83
12	H	817	CLA	CHD-C1D-ND	-3.56	119.79	124.80
12	L	205	CLA	O2A-C1-C2	3.56	121.81	108.11
12	H	816	CLA	O2A-C1-C2	3.56	121.80	108.11
12	H	824	CLA	O2A-C1-C2	3.56	121.80	108.11
12	A	824	CLA	O2A-C1-C2	3.56	121.80	108.11
12	A	838	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
12	H	802	CLA	C11-C10-C8	-3.56	104.14	115.97
12	b	809	CLA	O2A-CGA-CBA	3.55	125.23	114.00
15	G	853	BCR	C37-C22-C21	-3.55	117.06	122.82
12	a	816	CLA	O2A-C1-C2	3.55	121.78	108.11
12	G	818	CLA	C4-C3-C5	3.55	121.39	115.23
15	l	201	BCR	C33-C5-C6	-3.55	120.61	124.48
15	a	847	BCR	C34-C9-C8	3.55	123.51	118.09
12	B	825	CLA	O2A-CGA-CBA	3.55	122.66	111.83
12	H	826	CLA	O2D-CGD-CBD	3.55	117.44	111.23
12	G	834	CLA	O2A-CGA-CBA	3.55	122.66	111.83
12	B	831	CLA	C1D-ND-C4D	-3.55	103.82	106.31
12	B	823	CLA	C2B-C1B-NB	3.55	114.00	110.33
12	G	814	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
12	a	855	CLA	O2A-CGA-CBA	3.55	122.65	111.83
12	A	812	CLA	C1D-ND-C4D	-3.55	103.82	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	827	CLA	CHD-C1D-ND	-3.54	119.81	124.80
12	a	824	CLA	O2A-C1-C2	3.54	121.74	108.11
12	a	854	CLA	C2C-C1C-NC	3.54	113.70	109.98
12	A	805	CLA	O2A-C1-C2	3.54	121.73	108.11
12	L	206	CLA	O2A-C1-C2	3.54	121.73	108.11
12	A	829	CLA	C3B-C2B-C1B	-3.54	103.00	107.17
12	L	204	CLA	O2A-C1-C2	3.54	121.73	108.11
12	H	833	CLA	CHD-C1D-ND	-3.54	119.82	124.80
15	a	852	BCR	C37-C22-C21	-3.54	117.08	122.82
12	A	830	CLA	C3C-C4C-NC	3.54	114.96	110.43
12	B	814	CLA	O2A-CGA-CBA	3.54	122.62	111.83
12	G	837	CLA	CMA-C3A-C4A	3.54	121.28	111.77
12	A	827	CLA	O2A-C1-C2	3.54	121.72	108.11
12	G	832	CLA	C4A-NA-C1A	3.54	108.29	106.68
12	B	808	CLA	C2B-C1B-NB	3.54	113.99	110.33
12	A	834	CLA	O2A-CGA-CBA	3.53	122.61	111.83
12	S	203	CLA	CMA-C3A-C4A	3.53	121.27	111.77
12	G	837	CLA	O2A-C1-C2	3.53	121.71	108.11
12	a	809	CLA	CED-O2D-CGD	3.53	123.93	115.92
12	j	104	CLA	CHD-C1D-ND	-3.53	119.83	124.80
12	A	854	CLA	C3C-C4C-NC	3.53	114.96	110.43
12	G	824	CLA	O2A-C1-C2	3.53	121.70	108.11
12	A	838	CLA	CMC-C2C-C1C	3.53	130.55	125.03
12	b	836	CLA	CHD-C1D-ND	-3.53	119.83	124.80
12	f	201	CLA	C1D-ND-C4D	-3.53	103.83	106.31
12	H	836	CLA	C2B-C1B-NB	3.53	113.99	110.33
12	H	827	CLA	C4D-C3D-CAD	3.53	111.94	108.11
15	H	849	BCR	C38-C26-C25	-3.53	120.63	124.48
12	G	821	CLA	C1D-ND-C4D	-3.53	103.84	106.31
15	H	846	BCR	C36-C18-C17	-3.53	117.10	122.82
12	H	802	CLA	CAA-C2A-C3A	-3.53	103.46	113.00
12	A	830	CLA	C2B-C1B-NB	3.53	113.98	110.33
15	l	203	BCR	C32-C1-C6	3.53	115.78	110.24
15	L	203	BCR	C32-C1-C6	3.53	115.78	110.24
12	H	805	CLA	C1-O2A-CGA	3.53	125.19	116.65
15	Q	102	BCR	C15-C14-C13	-3.53	122.33	127.28
12	b	823	CLA	C2B-C1B-NB	3.53	113.98	110.33
15	S	205	BCR	C33-C5-C6	-3.53	120.64	124.48
12	j	102	CLA	O2A-C1-C2	3.52	121.67	108.11
12	a	835	CLA	C2B-C1B-NB	3.52	113.98	110.33
12	B	804	CLA	C2B-C1B-NB	3.52	113.98	110.33
12	H	830	CLA	CAA-C2A-C3A	-3.52	103.48	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	807	CLA	C1D-ND-C4D	-3.52	103.84	106.31
12	P	201	CLA	C1D-ND-C4D	-3.52	103.84	106.31
15	G	846	BCR	C24-C23-C22	-3.52	121.02	126.23
12	H	802	CLA	O1D-CGD-CBD	-3.52	117.57	124.52
15	b	847	BCR	C2-C1-C6	3.52	115.56	110.44
15	H	842	BCR	C19-C18-C17	3.52	124.55	119.01
12	B	806	CLA	CHD-C1D-ND	-3.52	119.85	124.80
12	H	810	CLA	O2A-CGA-CBA	3.52	125.12	114.00
12	A	820	CLA	CHC-C1C-C2C	-3.52	116.95	126.95
12	F	201	CLA	C3B-C2B-C1B	-3.52	103.02	107.17
12	b	820	CLA	CHD-C1D-ND	-3.52	119.85	124.80
11	G	801	CL0	C3C-C4C-NC	3.52	114.94	110.43
15	H	841	BCR	C33-C5-C6	-3.52	120.65	124.48
12	B	823	CLA	O2A-C1-C2	3.52	121.64	108.11
12	a	802	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
12	j	102	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
15	B	845	BCR	C36-C18-C17	-3.51	117.12	122.82
12	a	832	CLA	C4A-NA-C1A	3.51	108.28	106.68
12	G	824	CLA	CHD-C1D-ND	-3.51	119.86	124.80
12	b	804	CLA	O2A-C1-C2	3.51	121.63	108.11
12	G	833	CLA	O2A-CGA-CBA	3.51	122.55	111.83
15	A	849	BCR	C36-C18-C19	-3.51	112.72	118.09
15	J	104	BCR	C2-C1-C6	3.51	115.54	110.44
16	a	851	LHG	O7-C7-C8	3.51	119.08	111.48
12	A	819	CLA	CHD-C1D-ND	-3.51	119.86	124.80
12	B	814	CLA	CHD-C1D-ND	-3.51	119.86	124.80
12	a	817	CLA	C4D-C3D-CAD	3.51	111.92	108.11
12	a	838	CLA	CMC-C2C-C1C	3.51	130.52	125.03
12	H	827	CLA	CAC-C3C-C2C	-3.51	121.11	127.56
15	A	848	BCR	C30-C25-C26	-3.51	117.84	122.64
12	H	822	CLA	CMC-C2C-C1C	3.51	130.52	125.03
12	H	823	CLA	CMA-C3A-C4A	3.51	121.20	111.77
12	b	809	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
12	a	839	CLA	O2D-CGD-CBD	3.51	117.36	111.23
11	G	801	CL0	CAA-C2A-C3A	-3.51	103.53	113.00
12	H	825	CLA	C2B-C1B-NB	3.51	113.96	110.33
15	b	840	BCR	C34-C9-C10	-3.50	117.14	122.82
12	H	850	CLA	C1C-C2C-C3C	-3.50	103.29	106.98
12	a	838	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
12	H	838	CLA	CMC-C2C-C3C	3.50	135.62	126.15
12	b	833	CLA	O2A-C1-C2	3.50	121.59	108.11
12	G	817	CLA	C2B-C1B-NB	3.50	113.96	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	820	CLA	C2B-C1B-NB	3.50	113.96	110.33
12	B	822	CLA	CMA-C3A-C4A	3.50	121.18	111.77
15	L	201	BCR	C7-C8-C9	-3.50	121.06	126.23
16	A	851	LHG	O7-C7-C8	3.50	119.06	111.48
12	b	829	CLA	CAA-C2A-C3A	-3.50	103.54	113.00
12	B	801	CLA	C1-O2A-CGA	3.50	125.12	116.65
12	a	820	CLA	CHD-C1D-ND	-3.50	119.88	124.80
12	S	202	CLA	O2A-C1-C2	3.50	121.57	108.11
11	G	801	CL0	C4D-C3D-CAD	3.50	111.90	108.11
12	b	802	CLA	O1D-CGD-CBD	-3.49	117.63	124.52
12	H	823	CLA	C3C-C4C-NC	3.49	114.91	110.43
12	B	803	CLA	CHD-C1D-ND	-3.49	119.89	124.80
12	P	203	CLA	CAA-C2A-C3A	-3.49	103.56	113.00
11	A	801	CL0	C3D-C2D-C1D	-3.49	101.07	105.83
12	B	824	CLA	C2B-C1B-NB	3.49	113.95	110.33
15	L	201	BCR	C3-C4-C5	-3.49	107.83	114.06
15	B	844	BCR	C3-C4-C5	-3.49	107.83	114.06
12	B	837	CLA	CMC-C2C-C3C	3.49	135.58	126.15
12	b	814	CLA	C2B-C1B-NB	3.49	113.94	110.33
12	b	802	CLA	O2A-CGA-CBA	3.49	122.46	111.83
12	B	823	CLA	C3C-C4C-NC	3.48	114.89	110.43
12	A	817	CLA	C2C-C1C-NC	3.48	113.64	109.98
16	a	850	LHG	O7-C7-C8	3.48	119.02	111.48
12	A	807	CLA	C1-O2A-CGA	3.48	125.08	116.65
12	A	804	CLA	CHD-C1D-ND	-3.48	119.90	124.80
12	a	836	CLA	C4D-C3D-CAD	3.48	111.89	108.11
12	a	806	CLA	CMC-C2C-C1C	3.48	130.47	125.03
11	a	801	CL0	C4D-CHA-C1A	-3.48	117.09	121.24
12	L	205	CLA	CMA-C3A-C4A	3.48	121.12	111.77
12	B	820	CLA	CHD-C1D-ND	-3.48	119.91	124.80
15	H	846	BCR	C7-C8-C9	-3.48	121.09	126.23
12	G	833	CLA	C1D-ND-C4D	-3.48	103.87	106.31
15	F	204	BCR	C12-C13-C14	3.48	124.48	119.01
12	H	837	CLA	CMB-C2B-C3B	3.48	134.73	126.55
12	B	802	CLA	O2A-CGA-CBA	3.48	122.44	111.83
15	A	846	BCR	C24-C23-C22	-3.48	121.09	126.23
15	L	201	BCR	C33-C5-C6	-3.47	120.69	124.48
12	A	810	CLA	C2B-C1B-NB	3.47	113.93	110.33
15	J	104	BCR	C38-C26-C25	-3.47	120.69	124.48
12	A	822	CLA	C4D-C3D-CAD	3.47	111.88	108.11
12	b	821	CLA	CMC-C2C-C1C	3.47	130.46	125.03
12	H	806	CLA	C2B-C1B-NB	3.47	113.92	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	813	CLA	C4D-C3D-CAD	3.47	111.87	108.11
12	H	838	CLA	CHD-C1D-ND	-3.47	119.92	124.80
12	B	802	CLA	C11-C12-C13	-3.47	104.44	115.97
12	G	839	CLA	O2A-C1-C2	3.47	121.45	108.11
12	B	836	CLA	O2A-C1-C2	3.47	121.44	108.11
15	l	201	BCR	C3-C4-C5	-3.47	107.88	114.06
12	a	812	CLA	C3C-C4C-NC	3.46	114.87	110.43
12	G	838	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
12	a	829	CLA	CAA-C2A-C3A	-3.46	103.64	113.00
12	b	810	CLA	C1D-ND-C4D	-3.46	103.88	106.31
12	B	802	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
15	G	849	BCR	C30-C25-C26	-3.46	117.91	122.64
12	G	810	CLA	O2A-CGA-CBA	3.46	124.94	114.00
11	a	801	CL0	CMA-C3A-C2A	-3.46	100.61	113.98
12	B	802	CLA	CAA-C2A-C3A	-3.46	103.65	113.00
12	H	801	CLA	CMB-C2B-C3B	3.46	134.69	126.55
12	G	818	CLA	C4A-NA-C1A	3.46	108.26	106.68
12	f	201	CLA	O2A-C1-C2	3.46	121.41	108.11
12	a	808	CLA	CAA-C2A-C3A	-3.46	103.66	113.00
12	A	809	CLA	CED-O2D-CGD	3.46	123.75	115.92
12	G	818	CLA	C1C-C2C-C3C	-3.46	103.35	106.98
12	B	802	CLA	C4D-C3D-CAD	3.45	111.86	108.11
12	A	833	CLA	O2A-CGA-CBA	3.45	122.37	111.83
12	b	814	CLA	O2A-C1-C2	3.45	121.40	108.11
12	a	830	CLA	C3C-C4C-NC	3.45	114.85	110.43
12	A	810	CLA	CMA-C3A-C4A	3.45	121.05	111.77
12	H	819	CLA	CHD-C1D-ND	-3.45	119.94	124.80
12	G	816	CLA	CHD-C1D-ND	-3.45	119.95	124.80
12	G	823	CLA	CHD-C1D-ND	-3.45	119.95	124.80
12	A	815	CLA	CHD-C1D-ND	-3.45	119.95	124.80
12	H	801	CLA	CHD-C1D-ND	-3.45	119.95	124.80
12	B	809	CLA	O2A-CGA-CBA	3.45	124.90	114.00
12	a	854	CLA	CMC-C2C-C1C	3.45	130.42	125.03
12	H	827	CLA	CMB-C2B-C1B	-3.45	120.17	125.42
12	H	818	CLA	O2A-CGA-CBA	3.44	124.88	114.00
12	a	802	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
11	a	801	CL0	C3C-C4C-NC	3.44	114.84	110.43
12	G	830	CLA	CAA-C2A-C3A	-3.44	103.69	113.00
12	A	836	CLA	CMB-C2B-C3B	3.44	134.65	126.55
12	G	823	CLA	O2A-C1-C2	3.44	121.34	108.11
12	a	837	CLA	CMA-C3A-C4A	3.44	121.02	111.77
12	a	818	CLA	CHD-C1D-ND	-3.44	119.96	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	822	CLA	O2A-C1-C2	3.44	121.33	108.11
15	b	842	BCR	C28-C27-C26	-3.44	107.93	114.06
15	b	844	BCR	C36-C18-C17	-3.44	117.25	122.82
12	a	836	CLA	CMB-C2B-C3B	3.44	134.63	126.55
12	a	803	CLA	CHD-C1D-ND	-3.44	119.97	124.80
18	b	845	LMG	O7-C10-C11	3.44	118.92	111.48
12	A	804	CLA	C1D-ND-C4D	-3.44	103.90	106.31
12	A	839	CLA	C1D-ND-C4D	-3.44	103.90	106.31
12	G	825	CLA	CMD-C2D-C1D	3.44	130.78	124.73
12	l	205	CLA	CMA-C3A-C4A	3.44	121.01	111.77
12	a	832	CLA	C1D-ND-C4D	-3.43	103.90	106.31
12	B	820	CLA	O2A-CGA-CBA	3.43	124.85	114.00
15	H	842	BCR	C33-C5-C6	-3.43	120.74	124.48
12	H	837	CLA	C3D-C2D-C1D	-3.43	101.15	105.83
12	H	811	CLA	O2A-C1-C2	3.43	121.32	108.11
12	A	822	CLA	O2A-C1-C2	3.43	121.32	108.11
12	l	206	CLA	C2B-C1B-NB	3.43	113.89	110.33
12	a	802	CLA	C4-C3-C5	3.43	121.18	115.23
12	A	831	CLA	CAA-C2A-C3A	-3.43	103.73	113.00
12	B	816	CLA	CHD-C1D-ND	-3.43	119.98	124.80
12	a	805	CLA	C3D-C4D-ND	3.43	115.56	109.99
12	G	824	CLA	CMA-C3A-C4A	3.43	120.98	111.77
12	H	834	CLA	O2D-CGD-CBD	3.43	117.22	111.23
15	B	841	BCR	C27-C26-C25	-3.43	118.07	122.70
12	B	808	CLA	CHD-C1D-ND	-3.43	119.98	124.80
12	b	823	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
12	A	828	CLA	O2A-CGA-CBA	3.42	122.27	111.83
12	P	201	CLA	CAA-C2A-C3A	-3.42	103.75	113.00
12	R	103	CLA	CHD-C1D-ND	-3.42	119.99	124.80
12	l	204	CLA	O2A-C1-C2	3.42	121.28	108.11
12	G	811	CLA	CMA-C3A-C4A	3.42	120.97	111.77
12	H	822	CLA	C3C-C4C-NC	3.42	114.81	110.43
12	b	817	CLA	O2A-CGA-CBA	3.42	124.81	114.00
15	A	846	BCR	C28-C27-C26	-3.42	107.95	114.06
12	H	837	CLA	CAA-C2A-C3A	-3.42	103.76	113.00
15	A	852	BCR	C37-C22-C21	-3.42	117.28	122.82
12	H	837	CLA	O2A-C1-C2	3.42	121.26	108.11
12	H	820	CLA	CHD-C1D-ND	-3.42	119.99	124.80
12	H	825	CLA	C1D-ND-C4D	-3.41	103.92	106.31
12	b	804	CLA	C2B-C1B-NB	3.41	113.87	110.33
12	a	817	CLA	C4-C3-C2	-3.41	114.86	123.63
12	S	203	CLA	O2A-C1-C2	3.41	121.25	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	821	CLA	CHD-C1D-ND	-3.41	120.00	124.80
12	a	819	CLA	CHD-C1D-ND	-3.41	120.00	124.80
12	a	805	CLA	CAC-C3C-C4C	3.41	129.23	124.79
12	H	829	CLA	O2A-CGA-CBA	3.41	124.78	114.00
12	a	808	CLA	C4D-C3D-CAD	3.41	111.81	108.11
15	H	841	BCR	C15-C14-C13	-3.41	122.50	127.28
15	G	847	BCR	C28-C27-C26	-3.41	107.98	114.06
12	b	818	CLA	CHD-C1D-ND	-3.41	120.00	124.80
12	G	807	CLA	CMC-C2C-C1C	3.41	130.36	125.03
12	H	804	CLA	C2B-C1B-NB	3.41	113.86	110.33
12	b	816	CLA	CHD-C1D-ND	-3.41	120.01	124.80
12	H	820	CLA	CMB-C2B-C1B	3.41	130.61	125.42
12	H	806	CLA	O2A-C1-C2	3.41	121.22	108.11
12	B	802	CLA	CMA-C3A-C2A	-3.41	100.81	113.98
12	a	817	CLA	CMB-C2B-C3B	3.41	134.56	126.55
15	R	101	BCR	C37-C22-C21	-3.41	117.30	122.82
12	l	205	CLA	O2A-C1-C2	3.40	121.21	108.11
12	G	803	CLA	CMC-C2C-C1C	3.40	130.35	125.03
15	H	844	BCR	C15-C14-C13	-3.40	122.28	127.48
15	F	204	BCR	C35-C13-C14	-3.40	117.30	122.82
15	B	845	BCR	C34-C9-C10	-3.40	117.30	122.82
12	H	805	CLA	O2A-C1-C2	3.40	121.20	108.11
15	A	852	BCR	C7-C8-C9	-3.40	121.20	126.23
12	a	841	CLA	CAC-C3C-C4C	3.40	129.22	124.79
12	G	856	CLA	CMA-C3A-C4A	3.40	120.92	111.77
12	G	820	CLA	CHD-C1D-ND	-3.40	120.02	124.80
12	G	856	CLA	O2A-CGA-CBA	3.40	122.20	111.83
15	F	204	BCR	C28-C27-C26	-3.40	108.00	114.06
15	I	101	BCR	C34-C9-C10	-3.40	117.31	122.82
12	a	804	CLA	CHD-C1D-ND	-3.40	120.02	124.80
12	H	834	CLA	C2B-C1B-NB	3.40	113.85	110.33
12	l	205	CLA	CMC-C2C-C1C	3.40	130.34	125.03
12	a	831	CLA	O2A-CGA-CBA	3.40	122.19	111.83
12	B	819	CLA	CHD-C1D-ND	-3.40	120.02	124.80
12	f	201	CLA	C4-C3-C5	3.39	121.12	115.23
12	a	828	CLA	C1D-ND-C4D	-3.39	103.93	106.31
12	A	811	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
12	B	819	CLA	CMB-C2B-C1B	3.39	130.59	125.42
12	A	839	CLA	CHD-C1D-ND	-3.39	120.03	124.80
12	B	814	CLA	C2B-C1B-NB	3.39	113.84	110.33
15	B	843	BCR	C27-C26-C25	-3.39	118.12	122.70
12	H	807	CLA	C3B-C2B-C1B	-3.39	103.17	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	806	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
12	a	855	CLA	C2C-C1C-NC	3.39	113.54	109.98
12	H	827	CLA	C3D-C2D-C1D	-3.39	101.21	105.83
12	A	803	CLA	CHD-C1D-ND	-3.39	120.04	124.80
12	b	817	CLA	C2B-C1B-NB	3.39	113.84	110.33
12	B	833	CLA	C2B-C1B-NB	3.39	113.84	110.33
12	A	805	CLA	CAC-C3C-C4C	3.39	129.19	124.79
15	a	848	BCR	C19-C18-C17	3.39	124.33	119.01
12	H	832	CLA	O1D-CGD-CBD	-3.39	117.84	124.52
12	A	808	CLA	CMD-C2D-C3D	-3.39	119.93	127.69
15	f	202	BCR	C28-C27-C26	-3.38	108.02	114.06
12	L	206	CLA	CHD-C1D-ND	-3.38	120.04	124.80
12	H	832	CLA	O2A-CGA-CBA	3.38	124.69	114.00
15	A	849	BCR	C35-C13-C12	3.38	123.25	118.09
12	B	836	CLA	C2D-C1D-ND	3.38	113.47	110.13
15	b	842	BCR	C30-C25-C26	-3.38	118.02	122.64
12	B	825	CLA	O2A-C1-C2	3.38	121.11	108.11
12	b	815	CLA	CMC-C2C-C1C	3.38	130.31	125.03
12	f	203	CLA	CHD-C1D-ND	-3.38	120.05	124.80
12	A	808	CLA	CAA-C2A-C3A	-3.38	103.87	113.00
12	A	825	CLA	CMC-C2C-C1C	3.38	130.31	125.03
12	A	805	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
12	B	834	CLA	CHD-C1D-ND	-3.38	120.05	124.80
12	G	835	CLA	O2A-CGA-CBA	3.38	124.66	114.00
15	a	845	BCR	C4-C5-C6	-3.37	118.14	122.70
12	b	835	CLA	O2A-C1-C2	3.37	121.09	108.11
12	b	823	CLA	C1C-C2C-C3C	-3.37	103.43	106.98
12	b	822	CLA	CBA-CAA-C2A	3.37	123.83	113.79
12	b	815	CLA	CBA-CAA-C2A	3.37	123.83	113.79
15	G	848	BCR	C38-C26-C25	-3.37	120.81	124.48
15	b	840	BCR	C33-C5-C6	-3.37	120.81	124.48
12	G	809	CLA	O2A-C1-C2	3.37	121.08	108.11
12	l	206	CLA	CHD-C1D-ND	-3.37	120.06	124.80
12	H	804	CLA	O2A-C1-C2	3.37	121.07	108.11
12	B	834	CLA	O2A-C1-C2	3.37	121.07	108.11
12	H	828	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
15	A	849	BCR	C34-C9-C10	-3.37	117.36	122.82
12	a	804	CLA	C1D-ND-C4D	-3.37	103.95	106.31
12	B	806	CLA	C2B-C1B-NB	3.37	113.82	110.33
12	B	806	CLA	CBC-CAC-C3C	-3.37	103.30	112.42
15	f	204	BCR	C19-C18-C17	3.37	124.30	119.01
12	b	812	CLA	CHD-C1D-ND	-3.36	120.07	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	805	CLA	O2A-C1-C2	3.36	121.05	108.11
12	A	817	CLA	C1-O2A-CGA	3.36	124.79	116.65
12	H	835	CLA	O2A-C1-C2	3.36	121.05	108.11
12	a	805	CLA	CMC-C2C-C1C	3.36	130.29	125.03
12	a	839	CLA	CHD-C1D-ND	-3.36	120.07	124.80
12	b	835	CLA	CMB-C2B-C3B	3.36	134.46	126.55
12	b	819	CLA	CHD-C1D-ND	-3.36	120.07	124.80
15	S	205	BCR	C7-C8-C9	-3.36	121.26	126.23
12	H	806	CLA	C4D-C3D-CAD	3.36	111.76	108.11
12	a	836	CLA	O2D-CGD-CBD	3.36	117.11	111.23
12	G	802	CLA	CMC-C2C-C1C	3.36	130.28	125.03
12	G	817	CLA	CHD-C1D-ND	-3.36	120.07	124.80
12	G	809	CLA	C4D-C3D-CAD	3.36	111.75	108.11
15	H	844	BCR	C30-C25-C26	-3.36	118.05	122.64
15	b	844	BCR	C33-C5-C6	-3.36	120.82	124.48
12	a	810	CLA	CMA-C3A-C4A	3.36	120.79	111.77
15	B	843	BCR	C15-C14-C13	-3.36	122.35	127.48
12	G	856	CLA	O2A-CGA-O1A	-3.35	115.24	123.63
15	b	847	BCR	C38-C26-C25	-3.35	120.82	124.48
12	B	827	CLA	O2A-CGA-CBA	3.35	124.60	114.00
11	a	801	CL0	C3B-C2B-C1B	-3.35	103.22	107.17
15	G	846	BCR	C19-C18-C17	3.35	124.28	119.01
12	b	820	CLA	O2A-CGA-CBA	3.35	124.59	114.00
12	H	821	CLA	O2A-CGA-CBA	3.35	124.59	114.00
12	P	203	CLA	CHD-C1D-ND	-3.35	120.09	124.80
12	a	817	CLA	O2A-C1-C2	3.35	121.00	108.11
12	a	829	CLA	C3B-C2B-C1B	-3.35	103.22	107.17
12	b	830	CLA	O2A-CGA-CBA	3.35	124.58	114.00
12	G	810	CLA	CHD-C1D-ND	-3.35	120.09	124.80
12	b	807	CLA	CHD-C1D-ND	-3.35	120.09	124.80
12	G	818	CLA	CHD-C1D-ND	-3.35	120.09	124.80
12	A	822	CLA	CHD-C1D-ND	-3.35	120.09	124.80
12	L	206	CLA	C2B-C1B-NB	3.35	113.80	110.33
12	b	811	CLA	O2A-C1-C2	3.35	120.98	108.11
11	A	801	CL0	CMC-C2C-C1C	3.35	130.26	125.03
12	A	807	CLA	CMB-C2B-C1B	3.34	130.51	125.42
12	a	825	CLA	O2A-C1-C2	3.34	120.98	108.11
12	G	823	CLA	CMA-C3A-C4A	3.34	120.76	111.77
12	a	830	CLA	O2A-C1-C2	3.34	120.98	108.11
12	A	813	CLA	C4D-C3D-CAD	3.34	111.74	108.11
12	J	103	CLA	CHD-C1D-ND	-3.34	120.10	124.80
12	G	829	CLA	CMB-C2B-C3B	3.34	134.41	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	206	CLA	C4-C3-C5	3.34	121.03	115.23
12	b	823	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
12	S	204	CLA	C2B-C1B-NB	3.34	113.79	110.33
12	F	203	CLA	CHD-C1D-ND	-3.34	120.10	124.80
15	A	848	BCR	C34-C9-C8	3.34	123.19	118.09
12	A	854	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
11	A	801	CL0	C3B-C2B-C1B	-3.34	103.23	107.17
12	G	806	CLA	C2B-C1B-NB	3.34	113.79	110.33
12	A	839	CLA	O2A-C1-C2	3.34	120.95	108.11
12	a	830	CLA	C2B-C1B-NB	3.34	113.78	110.33
12	a	837	CLA	CBA-CAA-C2A	3.33	123.72	113.79
12	B	828	CLA	O2A-CGA-CBA	3.33	124.54	114.00
12	B	805	CLA	C2B-C1B-NB	3.33	113.78	110.33
12	A	855	CLA	CMA-C3A-C4A	3.33	120.73	111.77
12	G	821	CLA	CHD-C1D-ND	-3.33	120.11	124.80
15	Q	101	BCR	C34-C9-C10	-3.33	117.42	122.82
12	H	828	CLA	O2A-CGA-CBA	3.33	124.52	114.00
12	b	835	CLA	C2D-C1D-ND	3.33	113.42	110.13
12	b	831	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
12	a	825	CLA	CMC-C2C-C1C	3.33	130.23	125.03
15	G	849	BCR	C34-C9-C10	-3.33	117.43	122.82
15	A	847	BCR	C38-C26-C25	-3.33	120.86	124.48
12	a	815	CLA	CMA-C3A-C4A	3.32	120.71	111.77
12	b	830	CLA	O1D-CGD-CBD	-3.32	117.96	124.52
12	A	828	CLA	C3C-C4C-NC	3.32	114.69	110.43
12	A	835	CLA	C2B-C1B-NB	3.32	113.77	110.33
12	H	812	CLA	CHD-C1D-ND	-3.32	120.13	124.80
12	B	804	CLA	OBD-CAD-C3D	-3.32	120.66	128.42
12	b	801	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
12	a	840	CLA	C2B-C1B-NB	3.32	113.77	110.33
12	B	803	CLA	C6-C5-C3	-3.32	105.38	113.47
12	G	829	CLA	C3C-C4C-NC	3.32	114.68	110.43
12	G	826	CLA	O2A-C1-C2	3.32	120.88	108.11
12	a	804	CLA	CAC-C3C-C4C	3.32	129.11	124.79
15	i	101	BCR	C34-C9-C10	-3.32	117.44	122.82
12	b	825	CLA	C3B-C2B-C1B	-3.32	103.26	107.17
12	B	814	CLA	CBA-CAA-C2A	3.32	123.66	113.79
12	G	820	CLA	O2A-CGA-CBA	3.31	124.47	114.00
15	b	840	BCR	C34-C9-C8	3.31	123.15	118.09
12	G	825	CLA	CMC-C2C-C1C	3.31	130.21	125.03
15	F	204	BCR	C19-C18-C17	3.31	124.22	119.01
12	b	821	CLA	C4D-C3D-CAD	3.31	111.70	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	830	CLA	C4D-C3D-CAD	3.31	111.70	108.11
12	b	811	CLA	CHD-C1D-ND	-3.31	120.14	124.80
12	B	815	CLA	CMA-C3A-C4A	3.31	120.67	111.77
12	b	828	CLA	CHD-C1D-ND	-3.31	120.15	124.80
15	b	842	BCR	C37-C22-C21	-3.31	117.46	122.82
12	A	835	CLA	CMB-C2B-C1B	3.31	130.46	125.42
12	H	822	CLA	CMD-C2D-C1D	3.31	130.55	124.73
12	A	825	CLA	O2A-C1-C2	3.31	120.84	108.11
12	H	808	CLA	O2A-C1-C2	3.31	120.84	108.11
12	b	801	CLA	C4D-C3D-CAD	3.31	111.70	108.11
11	a	801	CL0	CAA-C2A-C3A	-3.31	104.06	113.00
12	A	829	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
12	G	838	CLA	CMC-C2C-C1C	3.31	130.20	125.03
12	H	817	CLA	O2A-CGA-CBA	3.31	121.92	111.83
15	B	840	BCR	C27-C26-C25	-3.31	118.24	122.70
12	H	804	CLA	CMC-C2C-C1C	3.30	130.20	125.03
12	A	835	CLA	CMA-C3A-C4A	3.30	120.65	111.77
12	G	819	CLA	CHD-C1D-ND	-3.30	120.15	124.80
12	G	816	CLA	O2A-CGA-CBA	3.30	124.44	114.00
15	L	201	BCR	C40-C30-C39	-3.30	99.18	108.63
12	B	828	CLA	CHD-C1D-ND	-3.30	120.16	124.80
12	G	837	CLA	CBA-CAA-C2A	3.30	123.62	113.79
12	a	823	CLA	CMA-C3A-C4A	3.30	120.64	111.77
12	G	824	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
12	G	836	CLA	C4D-C3D-CAD	3.30	111.69	108.11
12	H	829	CLA	CHD-C1D-ND	-3.30	120.16	124.80
12	a	835	CLA	CHD-C1D-ND	-3.30	120.16	124.80
15	J	104	BCR	C32-C1-C6	-3.30	105.07	110.24
12	G	805	CLA	CHD-C1D-ND	-3.30	120.16	124.80
12	b	828	CLA	O2A-CGA-CBA	3.30	124.42	114.00
12	a	807	CLA	C1-O2A-CGA	3.30	124.63	116.65
12	B	822	CLA	C3C-C4C-NC	3.30	114.65	110.43
15	a	846	BCR	C28-C27-C26	-3.30	108.18	114.06
12	H	836	CLA	CMC-C2C-C1C	3.29	130.18	125.03
12	A	805	CLA	C3D-C4D-ND	3.29	115.34	109.99
15	B	843	BCR	C37-C22-C21	-3.29	117.48	122.82
12	H	813	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
12	G	818	CLA	CAC-C3C-C4C	3.29	129.07	124.79
15	P	204	BCR	C19-C18-C17	3.29	124.19	119.01
12	H	838	CLA	C2B-C1B-NB	3.29	113.74	110.33
15	J	101	BCR	C15-C14-C13	-3.29	122.66	127.28
15	B	841	BCR	C33-C5-C6	-3.29	120.89	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	830	CLA	C3B-C2B-C1B	-3.29	103.29	107.17
12	A	835	CLA	O2A-CGA-CBA	3.29	124.39	114.00
12	A	834	CLA	CHD-C1D-ND	-3.29	120.17	124.80
12	a	823	CLA	CAC-C3C-C4C	3.29	129.07	124.79
12	a	820	CLA	C1D-ND-C4D	-3.29	104.00	106.31
12	a	807	CLA	CMB-C2B-C1B	3.29	130.43	125.42
12	A	823	CLA	CMA-C3A-C4A	3.29	120.61	111.77
12	H	821	CLA	CHD-C1D-ND	-3.29	120.18	124.80
12	H	828	CLA	CHD-C1D-ND	-3.29	120.18	124.80
12	A	824	CLA	CAC-C3C-C4C	3.29	129.06	124.79
12	B	831	CLA	O2A-CGA-CBA	3.28	124.38	114.00
12	B	814	CLA	O2A-C1-C2	3.28	120.74	108.11
15	f	204	BCR	C28-C27-C26	-3.28	108.20	114.06
12	a	808	CLA	CMD-C2D-C3D	-3.28	120.16	127.69
12	b	816	CLA	O2A-CGA-CBA	3.28	121.84	111.83
12	A	824	CLA	CMC-C2C-C1C	3.28	130.16	125.03
12	a	835	CLA	CMB-C2B-C1B	3.28	130.41	125.42
12	a	810	CLA	C4D-C3D-CAD	3.28	111.67	108.11
12	A	811	CLA	O2A-CGA-CBA	3.28	124.36	114.00
15	b	841	BCR	C1-C6-C5	-3.28	118.16	122.64
15	a	847	BCR	C38-C26-C25	-3.28	120.91	124.48
12	a	837	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
12	b	821	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
12	b	801	CLA	CBC-CAC-C3C	-3.28	103.54	112.42
12	H	811	CLA	CAC-C3C-C4C	3.27	129.05	124.79
12	G	830	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
12	H	850	CLA	O2A-C1-C2	3.27	120.70	108.11
12	a	815	CLA	CHD-C1D-ND	-3.27	120.20	124.80
15	a	845	BCR	C34-C9-C8	3.27	123.08	118.09
12	L	202	CLA	O2A-C1-C2	3.27	120.69	108.11
16	G	852	LHG	O7-C7-C8	3.27	118.55	111.48
12	b	825	CLA	C3D-C2D-C1D	-3.27	101.37	105.83
15	B	841	BCR	C34-C9-C8	3.27	123.08	118.09
12	S	204	CLA	CHD-C1D-ND	-3.27	120.21	124.80
11	A	801	CL0	CMA-C3A-C2A	-3.27	101.36	113.98
12	H	802	CLA	O2A-CGA-CBA	3.26	121.79	111.83
11	a	801	CL0	CMC-C2C-C1C	3.26	130.13	125.03
12	A	827	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
12	a	811	CLA	O2A-CGA-CBA	3.26	124.31	114.00
12	G	839	CLA	CED-O2D-CGD	3.26	123.31	115.92
12	H	822	CLA	C2B-C1B-NB	3.26	113.71	110.33
12	b	807	CLA	C3B-C2B-C1B	-3.26	103.33	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	808	CLA	C1D-ND-C4D	-3.26	104.02	106.31
12	b	831	CLA	O2A-CGA-CBA	3.26	124.30	114.00
12	A	813	CLA	O2A-CGA-CBA	3.26	124.30	114.00
12	G	855	CLA	C3C-C4C-NC	3.26	114.61	110.43
12	l	202	CLA	CHD-C1D-ND	-3.26	120.22	124.80
15	G	847	BCR	C37-C22-C21	-3.26	117.54	122.82
15	S	201	BCR	C7-C8-C9	-3.26	121.42	126.23
12	A	818	CLA	CMA-C3A-C4A	3.26	120.53	111.77
12	H	805	CLA	C4D-C3D-CAD	3.26	111.64	108.11
12	B	836	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
12	H	802	CLA	CHD-C4C-C3C	-3.25	120.03	124.77
12	a	819	CLA	O2A-CGA-CBA	3.25	124.27	114.00
15	A	845	BCR	C19-C18-C17	3.25	124.12	119.01
12	H	824	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
12	A	819	CLA	O2A-CGA-CBA	3.25	124.27	114.00
12	G	829	CLA	O2A-CGA-CBA	3.25	121.74	111.83
12	H	801	CLA	OBD-CAD-C3D	-3.25	120.82	128.42
12	b	834	CLA	CMC-C2C-C1C	3.25	130.11	125.03
12	b	832	CLA	O2A-C1-C2	3.25	120.61	108.11
12	a	826	CLA	OBD-CAD-C3D	-3.25	120.83	128.42
12	H	833	CLA	CAA-C2A-C3A	-3.25	104.23	113.00
12	S	203	CLA	CMC-C2C-C1C	3.25	130.11	125.03
15	P	204	BCR	C12-C13-C14	3.24	124.11	119.01
12	B	802	CLA	CHD-C4C-C3C	-3.24	120.04	124.77
12	A	816	CLA	C1-O2A-CGA	3.24	124.50	116.65
12	A	836	CLA	CED-O2D-CGD	3.24	123.27	115.92
12	B	825	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
12	H	819	CLA	O2A-CGA-CBA	3.24	124.24	114.00
12	b	827	CLA	O2A-CGA-CBA	3.24	124.24	114.00
12	H	833	CLA	O2A-CGA-CBA	3.24	124.24	114.00
12	b	808	CLA	CHD-C1D-ND	-3.24	120.24	124.80
12	a	815	CLA	O2A-CGA-CBA	3.24	124.23	114.00
12	a	835	CLA	O2A-CGA-CBA	3.24	124.23	114.00
12	b	828	CLA	CED-O2D-CGD	3.24	123.26	115.92
12	B	831	CLA	O1D-CGD-CBD	-3.24	118.13	124.52
12	a	807	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
12	G	806	CLA	CMA-C3A-C2A	-3.24	101.47	113.98
12	H	826	CLA	C4D-C3D-CAD	3.24	111.62	108.11
12	L	202	CLA	CHD-C1D-ND	-3.24	120.25	124.80
12	G	831	CLA	C4D-C3D-CAD	3.24	111.62	108.11
12	G	839	CLA	CHD-C1D-ND	-3.23	120.25	124.80
12	b	833	CLA	CHD-C1D-ND	-3.23	120.25	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	838	CLA	O2A-CGA-CBA	3.23	124.21	114.00
12	B	832	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
12	A	835	CLA	CHD-C1D-ND	-3.23	120.26	124.80
12	L	205	CLA	CMC-C2C-C1C	3.23	130.08	125.03
12	b	834	CLA	O2A-CGA-CBA	3.23	124.20	114.00
15	F	202	BCR	C39-C30-C25	-3.23	105.18	110.24
12	b	818	CLA	O2A-CGA-CBA	3.23	124.19	114.00
12	R	103	CLA	O2A-CGA-CBA	3.22	124.19	114.00
12	A	815	CLA	O2A-CGA-CBA	3.22	124.19	114.00
12	B	830	CLA	CMB-C2B-C1B	3.22	130.33	125.42
15	b	843	BCR	C3-C4-C5	-3.22	108.31	114.06
15	a	845	BCR	C7-C8-C9	-3.22	121.47	126.23
15	B	845	BCR	C33-C5-C6	-3.22	120.97	124.48
12	G	835	CLA	CHD-C1D-ND	-3.22	120.27	124.80
12	G	856	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
12	H	810	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
15	H	846	BCR	C38-C26-C25	-3.22	120.97	124.48
15	f	204	BCR	C12-C13-C14	3.22	124.07	119.01
11	G	801	CL0	C3D-C2D-C1D	-3.22	101.44	105.83
15	G	846	BCR	C34-C9-C8	3.22	123.00	118.09
12	G	826	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
15	H	844	BCR	C23-C24-C25	-3.21	118.41	127.00
12	b	826	CLA	CMB-C2B-C1B	-3.21	120.53	125.42
12	G	831	CLA	O2A-C1-C2	3.21	120.47	108.11
12	A	837	CLA	CMA-C3A-C4A	3.21	120.41	111.77
12	b	814	CLA	CBA-CAA-C2A	3.21	123.35	113.79
12	A	821	CLA	O2A-CGA-CBA	3.21	124.15	114.00
15	H	842	BCR	C34-C9-C8	3.21	123.00	118.09
15	H	849	BCR	C32-C1-C6	-3.21	105.21	110.24
12	a	839	CLA	O2A-C1-C2	3.21	120.47	108.11
12	A	812	CLA	C3C-C4C-NC	3.21	114.54	110.43
12	A	855	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	B	818	CLA	O2A-CGA-CBA	3.21	124.14	114.00
12	H	825	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	A	812	CLA	CHD-C1D-ND	-3.21	120.29	124.80
12	B	833	CLA	CHD-C1D-ND	-3.21	120.29	124.80
12	b	802	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
12	G	826	CLA	C1D-ND-C4D	-3.21	104.06	106.31
15	b	843	BCR	C7-C8-C9	-3.21	121.49	126.23
12	b	812	CLA	O2A-CGA-CBA	3.21	124.13	114.00
16	a	853	LHG	C5-O7-C7	-3.21	110.12	117.80
12	a	821	CLA	O2A-CGA-CBA	3.21	124.13	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	828	CLA	O2A-C1-C2	3.21	120.44	108.11
12	B	812	CLA	O2A-CGA-CBA	3.20	124.13	114.00
12	J	103	CLA	O2A-CGA-CBA	3.20	124.12	114.00
12	a	805	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
12	b	804	CLA	OBD-CAD-C3D	-3.20	120.93	128.42
12	A	830	CLA	C4D-C3D-CAD	3.20	111.58	108.11
15	j	101	BCR	C37-C22-C21	-3.20	117.63	122.82
12	S	204	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
15	a	846	BCR	C34-C9-C8	3.20	122.98	118.09
15	B	842	BCR	C1-C6-C5	-3.20	118.26	122.64
11	G	801	CL0	CMC-C2C-C1C	3.20	130.04	125.03
12	G	822	CLA	O2A-CGA-CBA	3.20	124.11	114.00
12	A	807	CLA	CMA-C3A-C4A	3.20	120.38	111.77
12	H	813	CLA	O2A-CGA-CBA	3.20	124.11	114.00
12	H	809	CLA	CHD-C1D-ND	-3.20	120.30	124.80
12	A	829	CLA	C1D-ND-C4D	-3.20	104.07	106.31
12	a	838	CLA	O2A-CGA-CBA	3.20	124.11	114.00
15	H	846	BCR	C33-C5-C6	-3.20	120.99	124.48
12	H	805	CLA	O2A-CGA-CBA	3.20	121.59	111.83
12	a	827	CLA	C3C-C4C-NC	3.20	114.53	110.43
12	a	813	CLA	O2A-CGA-CBA	3.20	124.10	114.00
12	G	809	CLA	CMB-C2B-C3B	3.20	134.07	126.55
12	a	835	CLA	C4D-C3D-CAD	3.20	111.58	108.11
12	G	840	CLA	C2B-C1B-NB	3.20	113.64	110.33
12	G	802	CLA	O2D-CGD-CBD	3.20	116.82	111.23
12	G	855	CLA	CHD-C1D-ND	-3.20	120.30	124.80
12	F	201	CLA	CMA-C3A-C4A	3.20	120.36	111.77
12	H	822	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
12	G	803	CLA	C4-C3-C5	3.20	120.78	115.23
12	S	204	CLA	O2A-C1-C2	3.19	120.40	108.11
12	G	814	CLA	O2A-CGA-CBA	3.19	124.09	114.00
12	a	825	CLA	CHD-C1D-ND	-3.19	120.31	124.80
12	a	833	CLA	CHD-C1D-ND	-3.19	120.31	124.80
12	a	839	CLA	CED-O2D-CGD	3.19	123.16	115.92
12	b	812	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
12	A	820	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
12	B	817	CLA	CHD-C1D-ND	-3.19	120.31	124.80
12	B	838	CLA	O2A-CGA-CBA	3.19	121.56	111.83
12	b	820	CLA	CBC-CAC-C3C	-3.19	103.77	112.42
15	A	849	BCR	C33-C5-C4	3.19	120.40	113.60
15	l	203	BCR	C34-C9-C8	3.19	122.96	118.09
12	A	831	CLA	O2A-C1-C2	3.19	120.38	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	834	CLA	O2A-C1-C2	3.19	120.37	108.11
15	L	207	BCR	C23-C24-C25	3.19	135.51	127.00
15	b	840	BCR	C27-C26-C25	-3.19	118.40	122.70
15	G	847	BCR	C3-C4-C5	-3.19	108.38	114.06
12	a	812	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
12	b	802	CLA	CMA-C3A-C2A	-3.18	101.67	113.98
15	L	203	BCR	C34-C9-C8	3.18	122.95	118.09
12	G	812	CLA	O2A-CGA-CBA	3.18	124.06	114.00
12	G	808	CLA	C1-O2A-CGA	3.18	124.36	116.65
12	H	836	CLA	O2A-CGA-CBA	3.18	124.06	114.00
12	b	810	CLA	CAA-C2A-C3A	-3.18	104.40	113.00
12	A	827	CLA	O1D-CGD-CBD	-3.18	118.24	124.52
12	B	803	CLA	CAC-C3C-C4C	3.18	128.93	124.79
15	L	207	BCR	C15-C14-C13	-3.18	122.82	127.28
12	G	838	CLA	O2A-CGA-CBA	3.18	124.05	114.00
12	G	808	CLA	CMB-C2B-C1B	3.18	130.26	125.42
12	G	855	CLA	CMC-C2C-C1C	3.18	130.00	125.03
12	B	833	CLA	O2A-C1-C2	3.18	120.35	108.11
12	B	801	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
12	B	816	CLA	O2A-C1-C2	3.18	120.34	108.11
12	H	810	CLA	CAC-C3C-C4C	3.18	128.93	124.79
19	B	847	LMT	C3'-C4'-C5'	-3.18	103.89	110.93
12	H	832	CLA	C3C-C4C-NC	3.18	114.50	110.43
15	B	843	BCR	C30-C25-C24	3.18	124.27	115.65
12	A	828	CLA	CMB-C2B-C3B	3.18	134.02	126.55
12	G	804	CLA	CHD-C1D-ND	-3.18	120.33	124.80
12	B	829	CLA	O2A-C1-C2	3.18	120.33	108.11
12	B	820	CLA	O2D-CGD-CBD	3.18	116.78	111.23
15	F	204	BCR	C34-C9-C8	3.17	122.94	118.09
12	B	832	CLA	O2A-CGA-CBA	3.17	124.03	114.00
15	H	844	BCR	C37-C22-C21	-3.17	117.67	122.82
12	H	826	CLA	CBA-CAA-C2A	3.17	123.24	113.79
12	a	815	CLA	C4D-C3D-CAD	3.17	111.55	108.11
12	L	204	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
12	a	833	CLA	CAC-C3C-C4C	3.17	128.92	124.79
12	a	820	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
12	H	830	CLA	C3D-C4D-ND	3.17	115.14	109.99
12	a	833	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
12	B	802	CLA	C3C-C4C-NC	3.17	114.49	110.43
12	a	823	CLA	CAA-C2A-C3A	-3.17	104.44	113.00
12	A	808	CLA	C4D-C3D-CAD	3.17	111.55	108.11
12	A	841	CLA	CMA-C3A-C4A	3.16	120.28	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	850	BCR	C33-C5-C6	-3.16	121.03	124.48
12	B	815	CLA	CHD-C1D-ND	-3.16	120.35	124.80
12	a	854	CLA	C3C-C4C-NC	3.16	114.48	110.43
12	A	803	CLA	CAA-C2A-C3A	-3.16	104.45	113.00
12	l	202	CLA	CMC-C2C-C1C	3.16	129.97	125.03
11	G	801	CL0	CMA-C3A-C2A	-3.16	101.76	113.98
12	a	805	CLA	C4D-C3D-CAD	3.16	111.54	108.11
12	B	803	CLA	CHB-C4A-NA	3.16	128.96	124.40
12	B	811	CLA	CHD-C1D-ND	-3.16	120.36	124.80
12	a	855	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
12	l	206	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
13	B	839	1L3	C14-C03-C02	-3.16	119.47	124.89
12	b	817	CLA	C3C-C4C-NC	3.16	114.48	110.43
12	j	104	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
15	H	845	BCR	C3-C4-C5	-3.16	108.43	114.06
12	H	801	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
12	B	810	CLA	CHD-C1D-ND	-3.16	120.36	124.80
12	B	836	CLA	CHB-C1B-C2B	-3.15	118.27	127.43
12	b	825	CLA	C1D-ND-C4D	-3.15	104.10	106.31
12	B	810	CLA	C1D-ND-C4D	-3.15	104.10	106.31
12	G	813	CLA	C1D-ND-C4D	-3.15	104.10	106.31
12	G	829	CLA	CMA-C3A-C4A	3.15	120.25	111.77
12	A	830	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
12	B	823	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
15	G	847	BCR	C19-C18-C17	3.15	123.97	119.01
15	B	840	BCR	C15-C14-C13	-3.15	122.86	127.28
12	H	826	CLA	C2D-C1D-ND	3.15	113.24	110.13
12	a	828	CLA	O2A-CGA-CBA	3.15	121.44	111.83
12	A	802	CLA	C4A-NA-C1A	3.15	108.12	106.68
12	B	801	CLA	CBC-CAC-C3C	-3.15	103.88	112.42
12	A	832	CLA	C1D-ND-C4D	-3.15	104.10	106.31
12	A	818	CLA	CHD-C1D-ND	-3.15	120.37	124.80
12	B	835	CLA	CMC-C2C-C1C	3.15	129.95	125.03
12	H	826	CLA	C3B-C2B-C1B	-3.15	103.46	107.17
12	B	835	CLA	O2A-CGA-CBA	3.14	123.94	114.00
12	A	804	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
12	H	830	CLA	O2A-C1-C2	3.14	120.21	108.11
12	a	828	CLA	C2B-C1B-NB	3.14	113.58	110.33
12	H	837	CLA	C3D-C4D-ND	3.14	115.09	109.99
12	B	807	CLA	C3B-C2B-C1B	-3.14	103.47	107.17
12	a	807	CLA	CMA-C3A-C4A	3.14	120.22	111.77
12	A	805	CLA	CHB-C4A-NA	3.14	128.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	802	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
12	G	836	CLA	C2D-C1D-ND	3.14	113.23	110.13
13	A	842	1L3	C24-C25-C26	-3.14	120.43	127.62
12	B	805	CLA	O2A-C1-C2	3.14	120.19	108.11
12	A	814	CLA	O2A-CGA-CBA	3.14	123.92	114.00
12	H	809	CLA	O2A-CGA-CBA	3.14	123.92	114.00
12	G	830	CLA	C1D-ND-C4D	-3.14	104.11	106.31
15	L	207	BCR	C34-C9-C8	3.14	122.88	118.09
12	H	803	CLA	CHB-C4A-NA	3.14	128.93	124.40
12	A	836	CLA	C4D-C3D-CAD	3.14	111.51	108.11
12	b	848	CLA	O2A-C1-C2	3.13	120.17	108.11
12	G	802	CLA	C4-C3-C5	3.13	120.67	115.23
12	A	840	CLA	CMA-C3A-C4A	3.13	120.19	111.77
12	B	827	CLA	CHD-C1D-ND	-3.13	120.39	124.80
15	R	102	BCR	C40-C30-C25	3.13	115.15	110.24
12	A	836	CLA	CHD-C1D-ND	-3.13	120.40	124.80
16	G	852	LHG	O8-C23-C24	3.13	120.65	111.15
12	G	833	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
12	H	817	CLA	CAA-C2A-C3A	-3.13	104.54	113.00
12	b	826	CLA	C1-O2A-CGA	3.13	124.23	116.65
12	H	805	CLA	C2B-C1B-NB	3.13	113.57	110.33
15	b	842	BCR	C23-C24-C25	-3.13	118.64	127.00
15	B	844	BCR	C33-C5-C6	-3.13	121.07	124.48
15	f	202	BCR	C35-C13-C12	3.13	122.86	118.09
12	B	812	CLA	O2D-CGD-O1D	-3.13	117.77	123.85
12	A	806	CLA	CMC-C2C-C1C	3.12	129.92	125.03
12	A	825	CLA	CAA-C2A-C1A	-3.12	101.74	111.97
12	A	815	CLA	CHB-C4A-NA	3.12	128.91	124.40
12	a	828	CLA	CMA-C3A-C4A	3.12	120.17	111.77
12	H	801	CLA	O2A-CGA-CBA	3.12	121.36	111.83
12	H	808	CLA	CHD-C1D-ND	-3.12	120.41	124.80
12	G	813	CLA	C3C-C4C-NC	3.12	114.43	110.43
12	A	826	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
19	b	846	LMT	C3'-C4'-C5'	-3.12	104.01	110.93
12	j	104	CLA	O2A-CGA-CBA	3.12	123.86	114.00
12	H	808	CLA	CMC-C2C-C1C	3.12	129.91	125.03
12	H	831	CLA	CMB-C2B-C1B	3.12	130.17	125.42
12	B	826	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
12	b	848	CLA	C3C-C4C-NC	3.12	114.43	110.43
15	A	847	BCR	C4-C5-C6	-3.12	118.49	122.70
12	H	834	CLA	CHD-C1D-ND	-3.12	120.41	124.80
12	A	840	CLA	C3C-C4C-NC	3.12	114.42	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	831	CLA	C3C-C4C-NC	3.12	114.42	110.43
12	G	808	CLA	CHD-C1D-ND	-3.12	120.42	124.80
15	G	846	BCR	C36-C18-C17	-3.12	117.77	122.82
15	a	846	BCR	C3-C4-C5	-3.12	108.50	114.06
12	G	842	CLA	O2A-C1-C2	3.12	120.10	108.11
15	f	204	BCR	C35-C13-C14	-3.12	117.77	122.82
12	H	820	CLA	O2A-CGA-CBA	3.11	123.84	114.00
12	H	831	CLA	CMA-C3A-C4A	3.11	120.14	111.77
12	H	813	CLA	CMC-C2C-C1C	3.11	129.90	125.03
12	A	838	CLA	OBD-CAD-C3D	-3.11	121.14	128.42
12	P	203	CLA	CMA-C3A-C4A	3.11	120.14	111.77
12	H	824	CLA	C4D-C3D-CAD	3.11	111.49	108.11
12	A	809	CLA	O1D-CGD-CBD	-3.11	118.38	124.52
12	G	830	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
12	G	819	CLA	C1-C2-C3	-3.11	121.10	126.20
12	A	815	CLA	CMA-C3A-C2A	3.11	126.00	113.98
12	a	838	CLA	OBD-CAD-C3D	-3.11	121.15	128.42
12	b	824	CLA	CMC-C2C-C3C	3.11	134.56	126.15
15	a	849	BCR	C33-C5-C6	-3.11	121.09	124.48
12	a	831	CLA	O2A-C1-C2	3.11	120.07	108.11
12	G	816	CLA	C4D-C3D-CAD	3.11	111.48	108.11
12	a	814	CLA	O2A-CGA-CBA	3.11	123.82	114.00
12	H	827	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
12	l	204	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	B	845	BCR	C7-C8-C9	-3.11	121.64	126.23
12	j	102	CLA	CAA-CBA-CGA	-3.11	104.39	113.21
12	b	826	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
12	H	829	CLA	CMB-C2B-C3B	3.10	133.85	126.55
15	A	848	BCR	C19-C18-C17	3.10	123.89	119.01
12	H	811	CLA	CAA-C2A-C3A	-3.10	104.61	113.00
12	B	830	CLA	CHD-C1D-ND	-3.10	120.44	124.80
12	G	810	CLA	C2B-C1B-NB	3.10	113.54	110.33
12	G	814	CLA	CMB-C2B-C3B	3.10	133.85	126.55
13	G	843	1L3	C17-C16-C18	3.10	120.61	115.23
15	B	844	BCR	C7-C8-C9	-3.10	121.64	126.23
15	A	846	BCR	C3-C4-C5	-3.10	108.53	114.06
12	H	805	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
17	T	101	45D	C22-C16-C08	-3.10	119.13	124.11
12	A	807	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
11	a	801	CL0	C1-C2-C3	-3.10	121.12	126.20
12	b	805	CLA	C2B-C1B-NB	3.10	113.54	110.33
12	b	805	CLA	C3C-C4C-NC	3.10	114.40	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	203	CLA	CMA-C3A-C4A	3.10	120.10	111.77
12	a	804	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
12	A	802	CLA	O2A-C1-C2	3.10	120.02	108.11
15	B	843	BCR	C38-C26-C27	3.10	120.19	113.60
12	A	818	CLA	C1-C2-C3	-3.09	121.13	126.20
12	B	817	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
11	A	801	CL0	O2A-C1-C2	3.09	120.01	108.11
15	i	101	BCR	C34-C9-C8	3.09	122.81	118.09
12	A	825	CLA	CHD-C1D-ND	-3.09	120.45	124.80
12	B	805	CLA	C3D-C4D-ND	3.09	115.01	109.99
12	H	819	CLA	CMA-C3A-C4A	3.09	120.08	111.77
12	B	836	CLA	C3D-C4D-ND	3.09	115.01	109.99
12	a	803	CLA	C4D-C3D-CAD	3.09	111.46	108.11
12	a	808	CLA	CMA-C3A-C4A	3.09	120.08	111.77
12	B	808	CLA	O2A-CGA-CBA	3.09	123.76	114.00
12	A	807	CLA	CHD-C1D-ND	-3.09	120.45	124.80
12	b	837	CLA	CHD-C1D-ND	-3.09	120.46	124.80
12	H	806	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
12	G	815	CLA	O2A-CGA-CBA	3.09	123.75	114.00
15	S	201	BCR	C34-C9-C8	3.09	122.80	118.09
13	a	842	1L3	C24-C25-C26	-3.09	120.56	127.62
12	G	832	CLA	C1D-ND-C4D	-3.09	104.15	106.31
12	H	826	CLA	C3D-C2D-C1D	-3.08	101.62	105.83
12	H	839	CLA	C1-C2-C3	-3.08	121.14	126.20
12	a	854	CLA	CHB-C4A-NA	3.08	128.85	124.40
12	A	840	CLA	C2B-C1B-NB	3.08	113.52	110.33
12	H	815	CLA	CMC-C2C-C1C	3.08	129.85	125.03
12	B	810	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
12	A	827	CLA	C3C-C4C-NC	3.08	114.38	110.43
12	A	823	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
12	B	828	CLA	C4D-C3D-CAD	3.08	111.45	108.11
12	A	831	CLA	O2A-CGA-CBA	3.08	121.23	111.83
12	A	854	CLA	CHB-C1B-C2B	-3.08	118.48	127.43
12	G	805	CLA	C4D-C3D-CAD	3.08	111.45	108.11
12	a	825	CLA	CMA-C3A-C4A	3.08	120.05	111.77
15	L	203	BCR	C37-C22-C23	3.08	122.79	118.09
12	H	802	CLA	C4D-C3D-CAD	3.08	111.45	108.11
15	G	848	BCR	C34-C9-C10	-3.08	117.83	122.82
12	G	807	CLA	O2A-C1-C2	3.08	119.96	108.11
12	H	829	CLA	C4D-C3D-CAD	3.08	111.45	108.11
12	A	809	CLA	CHD-C1D-ND	-3.08	120.47	124.80
15	A	849	BCR	C31-C1-C6	-3.08	105.42	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	848	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
12	H	850	CLA	C3C-C4C-NC	3.08	114.37	110.43
12	B	826	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
12	b	828	CLA	C4D-C3D-CAD	3.07	111.44	108.11
15	a	846	BCR	C34-C9-C10	-3.07	117.84	122.82
12	G	841	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
12	G	840	CLA	CMA-C3A-C4A	3.07	120.03	111.77
12	G	836	CLA	CHD-C1D-ND	-3.07	120.48	124.80
12	B	825	CLA	C1D-ND-C4D	-3.07	104.16	106.31
12	f	203	CLA	CMA-C3A-C4A	3.07	120.03	111.77
12	B	804	CLA	CMC-C2C-C1C	3.07	129.83	125.03
12	H	813	CLA	C4D-C3D-CAD	3.07	111.44	108.11
12	H	814	CLA	CMC-C2C-C1C	3.07	129.83	125.03
12	H	825	CLA	C3C-C4C-NC	3.07	114.36	110.43
12	G	832	CLA	O2A-C1-C2	3.07	119.92	108.11
12	G	840	CLA	C3C-C4C-NC	3.07	114.36	110.43
12	P	201	CLA	CMC-C2C-C1C	3.07	129.83	125.03
12	j	102	CLA	CAC-C3C-C4C	3.07	128.78	124.79
12	H	802	CLA	CMA-C3A-C2A	-3.07	102.13	113.98
15	b	841	BCR	C29-C30-C25	3.07	114.89	110.44
12	G	827	CLA	O2A-C1-C2	3.06	119.90	108.11
12	f	201	CLA	CMC-C2C-C1C	3.06	129.82	125.03
12	A	816	CLA	CHD-C1D-ND	-3.06	120.49	124.80
11	A	801	CL0	C3C-C4C-NC	3.06	114.35	110.43
12	A	815	CLA	C4D-C3D-CAD	3.06	111.43	108.11
12	b	807	CLA	CAC-C3C-C4C	3.06	128.77	124.79
12	b	811	CLA	C4D-C3D-CAD	3.06	111.43	108.11
12	b	829	CLA	C3D-C4D-ND	3.06	114.96	109.99
12	A	854	CLA	C2C-C1C-NC	3.06	113.20	109.98
12	A	814	CLA	CMA-C3A-C4A	3.06	120.00	111.77
15	H	845	BCR	C33-C5-C4	3.06	120.12	113.60
12	H	810	CLA	CHD-C1D-ND	-3.06	120.50	124.80
12	A	831	CLA	CHD-C1D-ND	-3.06	120.50	124.80
12	A	854	CLA	CHB-C4A-NA	3.06	128.81	124.40
12	B	837	CLA	C3C-C4C-NC	3.06	114.35	110.43
12	A	816	CLA	CMB-C2B-C1B	3.06	130.07	125.42
15	f	202	BCR	C39-C30-C25	-3.06	105.45	110.24
12	A	824	CLA	C2B-C1B-NB	3.06	113.50	110.33
12	A	824	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
15	b	839	BCR	C19-C18-C17	3.06	123.82	119.01
12	b	805	CLA	C3D-C4D-ND	3.06	114.95	109.99
15	L	203	BCR	C7-C8-C9	-3.06	121.71	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	831	CLA	CHD-C1D-ND	-3.06	120.50	124.80
12	A	815	CLA	CMB-C2B-C1B	3.06	130.07	125.42
12	B	809	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
11	a	801	CL0	CMB-C2B-C1B	3.05	130.07	125.42
12	G	834	CLA	CHD-C1D-ND	-3.05	120.50	124.80
12	H	837	CLA	CHB-C1B-C2B	-3.05	118.56	127.43
12	B	814	CLA	CMC-C2C-C1C	3.05	129.80	125.03
12	a	828	CLA	CMB-C2B-C3B	3.05	133.73	126.55
12	A	835	CLA	C4D-C3D-CAD	3.05	111.42	108.11
12	a	840	CLA	C3C-C4C-NC	3.05	114.34	110.43
15	a	847	BCR	C34-C9-C10	-3.05	117.87	122.82
15	A	845	BCR	C36-C18-C17	-3.05	117.87	122.82
12	G	807	CLA	C6-C5-C3	-3.05	106.04	113.47
12	G	840	CLA	C1-O2A-CGA	3.05	124.03	116.65
12	A	855	CLA	CED-O2D-CGD	3.05	122.83	115.92
12	A	822	CLA	CMD-C2D-C3D	-3.05	120.70	127.69
12	A	809	CLA	C2B-C1B-NB	3.05	113.49	110.33
12	b	818	CLA	CMA-C3A-C4A	3.05	119.97	111.77
12	a	819	CLA	CMA-C3A-C4A	3.05	119.97	111.77
15	S	201	BCR	C35-C13-C12	3.05	122.74	118.09
15	j	101	BCR	C29-C28-C27	3.05	117.98	111.28
12	b	812	CLA	C4D-C3D-CAD	3.05	111.41	108.11
12	B	826	CLA	CAA-C2A-C3A	-3.05	104.77	113.00
12	b	829	CLA	O2A-C1-C2	3.05	119.83	108.11
12	A	802	CLA	C2B-C1B-NB	3.05	113.48	110.33
12	F	201	CLA	C2B-C1B-NB	3.05	113.48	110.33
12	A	813	CLA	CAC-C3C-C4C	3.05	128.75	124.79
12	G	855	CLA	C4-C3-C2	-3.04	115.81	123.63
12	G	820	CLA	CMA-C3A-C4A	3.04	119.95	111.77
12	b	837	CLA	O2A-CGA-CBA	3.04	121.11	111.83
12	B	819	CLA	O2A-CGA-CBA	3.04	123.61	114.00
12	B	838	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
12	b	824	CLA	CAC-C3C-C4C	3.04	128.75	124.79
12	B	831	CLA	CHD-C4C-NC	-3.04	119.52	124.23
11	A	801	CL0	C3D-C4D-ND	3.04	114.93	109.99
12	a	807	CLA	C4D-C3D-CAD	3.04	111.41	108.11
12	F	201	CLA	C4-C3-C5	3.04	120.50	115.23
12	A	817	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
19	H	848	LMT	C3'-C4'-C5'	-3.04	104.19	110.93
12	a	826	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
12	b	835	CLA	CHB-C1B-C2B	-3.04	118.61	127.43
12	H	811	CLA	C3C-C4C-NC	3.04	114.32	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	810	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
13	G	843	1L3	C24-C25-C26	-3.04	120.67	127.62
15	I	101	BCR	C15-C14-C13	-3.04	123.02	127.28
12	H	825	CLA	C1-C2-C3	-3.04	121.22	126.20
12	b	808	CLA	O2A-CGA-CBA	3.04	123.59	114.00
12	a	825	CLA	CAA-C2A-C1A	-3.04	102.03	111.97
12	H	805	CLA	C3D-C4D-ND	3.04	114.92	109.99
12	G	809	CLA	CMA-C3A-C4A	3.04	119.93	111.77
12	b	809	CLA	CAC-C3C-C4C	3.03	128.74	124.79
12	B	818	CLA	CMA-C3A-C4A	3.03	119.93	111.77
12	b	815	CLA	O2A-C1-C2	3.03	119.78	108.11
12	A	830	CLA	CMA-C3A-C4A	3.03	119.92	111.77
12	b	834	CLA	C4D-C3D-CAD	3.03	111.40	108.11
12	B	809	CLA	CAC-C3C-C4C	3.03	128.74	124.79
16	a	851	LHG	O8-C23-C24	3.03	120.36	111.15
12	H	803	CLA	CHD-C1D-ND	-3.03	120.53	124.80
12	B	837	CLA	CHD-C1D-ND	-3.03	120.53	124.80
15	H	845	BCR	C4-C5-C6	-3.03	118.61	122.70
12	G	838	CLA	C2B-C1B-NB	3.03	113.47	110.33
12	B	805	CLA	C4D-C3D-CAD	3.03	111.40	108.11
12	a	837	CLA	C6-C5-C3	-3.03	106.09	113.47
12	G	813	CLA	CMC-C2C-C3C	3.03	134.34	126.15
15	L	201	BCR	C34-C9-C10	-3.03	117.91	122.82
12	a	837	CLA	O1D-CGD-CBD	-3.03	118.55	124.52
12	a	831	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
15	B	844	BCR	C33-C5-C4	3.03	120.05	113.60
12	A	837	CLA	CBA-CAA-C2A	3.03	122.80	113.79
12	G	804	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
12	j	102	CLA	CMB-C2B-C1B	3.03	130.03	125.42
12	R	103	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
12	A	823	CLA	CAC-C3C-C4C	3.03	128.73	124.79
12	H	839	CLA	C4D-C3D-CAD	3.02	111.39	108.11
12	H	825	CLA	O1D-CGD-CBD	-3.02	118.55	124.52
12	A	819	CLA	CMA-C3A-C4A	3.02	119.90	111.77
12	G	825	CLA	C2B-C1B-NB	3.02	113.46	110.33
15	G	846	BCR	C4-C5-C6	-3.02	118.62	122.70
12	A	826	CLA	OBD-CAD-C3D	-3.02	121.35	128.42
12	A	816	CLA	CMC-C2C-C1C	3.02	129.76	125.03
12	H	832	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
12	G	856	CLA	CED-O2D-CGD	3.02	122.77	115.92
12	A	836	CLA	C4A-NA-C1A	3.02	108.06	106.68
15	b	843	BCR	C4-C5-C6	-3.02	118.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	843	BCR	C1-C6-C5	-3.02	118.51	122.64
12	H	834	CLA	CMB-C2B-C1B	3.02	130.02	125.42
12	H	836	CLA	C4D-C3D-CAD	3.02	111.39	108.11
12	b	832	CLA	CHD-C1D-ND	-3.02	120.55	124.80
12	a	814	CLA	CMA-C3A-C4A	3.02	119.89	111.77
12	B	816	CLA	CAA-C2A-C3A	-3.02	104.84	113.00
12	H	817	CLA	O2A-C1-C2	3.02	119.72	108.11
12	A	808	CLA	C1-C2-C3	-3.02	121.88	126.76
12	a	824	CLA	CAC-C3C-C4C	3.02	128.72	124.79
12	A	822	CLA	CMA-C3A-C4A	3.02	119.88	111.77
12	b	812	CLA	CMA-C3A-C4A	3.02	119.88	111.77
15	H	845	BCR	C7-C8-C9	-3.02	121.77	126.23
12	B	812	CLA	CMA-C3A-C4A	3.02	119.88	111.77
12	A	807	CLA	C4D-C3D-CAD	3.02	111.38	108.11
12	B	817	CLA	C4D-C3D-CAD	3.02	111.38	108.11
12	H	837	CLA	C2D-C1D-ND	3.02	113.11	110.13
15	a	845	BCR	C19-C18-C17	3.01	123.75	119.01
12	b	830	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
15	G	853	BCR	C7-C8-C9	-3.01	121.78	126.23
12	b	822	CLA	OBD-CAD-C3D	-3.01	121.37	128.42
12	G	826	CLA	CMA-C3A-C4A	3.01	119.87	111.77
17	m	101	45D	C30-C32-C34	-3.01	114.47	123.20
12	G	806	CLA	C4D-C3D-CAD	3.01	111.38	108.11
12	G	810	CLA	C4D-C3D-CAD	3.01	111.38	108.11
12	H	809	CLA	CAA-C2A-C3A	-3.01	104.87	113.00
12	j	102	CLA	C2B-C1B-NB	3.01	113.45	110.33
11	G	801	CL0	C3D-C4D-ND	3.01	114.88	109.99
15	A	845	BCR	C34-C9-C8	3.01	122.68	118.09
12	B	820	CLA	CMC-C2C-C1C	3.01	129.74	125.03
12	A	803	CLA	CMB-C2B-C1B	3.01	130.00	125.42
15	l	203	BCR	C7-C8-C9	-3.01	121.79	126.23
15	A	844	BCR	C36-C18-C17	-3.01	117.95	122.82
12	S	203	CLA	C4-C3-C5	3.01	120.44	115.23
12	B	830	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
12	G	806	CLA	C3D-C4D-ND	3.01	114.87	109.99
12	A	825	CLA	CMA-C3A-C4A	3.01	119.85	111.77
12	H	801	CLA	O2A-C1-C2	3.00	119.67	108.11
12	G	810	CLA	CMA-C3A-C4A	3.00	119.85	111.77
12	L	205	CLA	C4-C3-C5	3.00	120.44	115.23
15	H	844	BCR	C38-C26-C27	3.00	120.00	113.60
12	F	201	CLA	CMC-C2C-C1C	3.00	129.72	125.03
12	G	834	CLA	CBA-CAA-C2A	3.00	122.72	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	828	CLA	C3C-C4C-NC	3.00	114.27	110.43
12	b	820	CLA	CMC-C2C-C1C	3.00	129.72	125.03
15	b	839	BCR	C33-C5-C6	-3.00	121.21	124.48
16	A	851	LHG	O8-C23-C24	3.00	120.26	111.15
12	G	830	CLA	C2B-C1B-NB	3.00	113.44	110.33
12	a	824	CLA	CMC-C2C-C1C	3.00	129.72	125.03
12	l	202	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
12	b	835	CLA	C3D-C4D-ND	3.00	114.86	109.99
12	H	807	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
12	H	818	CLA	C3C-C4C-NC	3.00	114.27	110.43
12	B	817	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	G	846	BCR	C28-C27-C26	-3.00	108.71	114.06
12	H	806	CLA	C3D-C4D-ND	3.00	114.86	109.99
12	b	807	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
15	J	104	BCR	C7-C8-C9	-2.99	121.81	126.23
12	b	803	CLA	CHB-C4A-NA	2.99	128.72	124.40
12	B	820	CLA	CED-O2D-CGD	2.99	122.70	115.92
12	H	839	CLA	O2A-CGA-CBA	2.99	120.96	111.83
12	b	816	CLA	O2A-C1-C2	2.99	119.62	108.11
12	b	837	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
12	b	826	CLA	O2A-C1-C2	2.99	119.62	108.11
12	A	820	CLA	CAC-C3C-C4C	2.99	128.68	124.79
12	B	807	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
12	a	827	CLA	O1D-CGD-CBD	-2.99	118.62	124.52
12	b	803	CLA	CHD-C1D-ND	-2.99	120.59	124.80
12	B	803	CLA	C4D-C3D-CAD	2.99	111.35	108.11
12	b	835	CLA	CAA-C2A-C3A	-2.99	104.92	113.00
12	J	103	CLA	CAA-C2A-C3A	-2.99	104.92	113.00
12	H	828	CLA	C4D-C3D-CAD	2.99	111.35	108.11
12	b	801	CLA	CAA-CBA-CGA	-2.99	104.72	113.21
12	A	837	CLA	C6-C5-C3	-2.99	106.19	113.47
12	B	807	CLA	O2A-C1-C2	2.99	119.61	108.11
12	H	804	CLA	OBD-CAD-C3D	-2.99	121.43	128.42
12	H	828	CLA	CMB-C2B-C1B	2.99	129.97	125.42
12	b	821	CLA	CHD-C1D-ND	-2.99	120.60	124.80
12	B	809	CLA	CHD-C1D-ND	-2.99	120.60	124.80
12	G	835	CLA	C4D-C3D-CAD	2.99	111.35	108.11
12	B	825	CLA	C3C-C4C-NC	2.99	114.26	110.43
15	Q	101	BCR	C34-C9-C8	2.99	122.65	118.09
15	b	842	BCR	C38-C26-C27	2.99	119.96	113.60
12	G	811	CLA	CED-O2D-CGD	2.99	122.69	115.92
12	H	828	CLA	CAC-C3C-C4C	2.99	128.68	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	805	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
15	b	843	BCR	C33-C5-C4	2.99	119.96	113.60
12	G	838	CLA	C3D-C4D-ND	2.99	114.84	109.99
15	a	845	BCR	C36-C18-C17	-2.99	117.98	122.82
17	m	101	45D	C21-C15-C07	-2.99	119.31	124.11
12	a	829	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
15	R	102	BCR	C24-C23-C22	-2.99	121.82	126.23
12	A	836	CLA	O1D-CGD-CBD	-2.98	118.63	124.52
15	H	844	BCR	C38-C26-C25	-2.98	121.23	124.48
15	B	842	BCR	C34-C9-C8	2.98	122.65	118.09
12	B	813	CLA	C4D-C3D-CAD	2.98	111.34	108.11
12	B	831	CLA	C2B-C1B-NB	2.98	113.42	110.33
12	a	802	CLA	CMB-C2B-C1B	2.98	129.96	125.42
15	b	841	BCR	C34-C9-C8	2.98	122.64	118.09
12	b	822	CLA	CHD-C1D-ND	-2.98	120.61	124.80
12	b	803	CLA	C6-C5-C3	-2.98	106.21	113.47
15	A	847	BCR	C12-C13-C14	-2.98	114.32	119.01
12	H	811	CLA	C1D-ND-C4D	-2.98	104.22	106.31
12	H	810	CLA	C4D-C3D-CAD	2.98	111.34	108.11
12	B	817	CLA	C3C-C4C-NC	2.98	114.25	110.43
15	H	849	BCR	C36-C18-C17	-2.98	117.99	122.82
12	A	817	CLA	CAC-C3C-C4C	2.98	128.66	124.79
12	l	205	CLA	C4-C3-C5	2.98	120.40	115.23
12	G	835	CLA	CMB-C2B-C1B	2.98	129.95	125.42
12	A	838	CLA	C2B-C1B-NB	2.98	113.41	110.33
12	G	817	CLA	O2A-C1-C2	2.98	119.56	108.11
12	B	802	CLA	C2B-C1B-NB	2.98	113.41	110.33
12	A	830	CLA	O2A-C1-C2	2.98	119.56	108.11
12	b	817	CLA	CMA-C3A-C4A	2.98	119.77	111.77
12	A	827	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
12	a	837	CLA	OBD-CAD-C3D	-2.97	121.46	128.42
12	H	827	CLA	CED-O2D-CGD	2.97	122.66	115.92
12	a	824	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
12	b	805	CLA	C4D-C3D-CAD	2.97	111.34	108.11
12	L	202	CLA	CMC-C2C-C1C	2.97	129.68	125.03
12	b	828	CLA	CMB-C2B-C3B	2.97	133.54	126.55
12	A	838	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
15	H	842	BCR	C38-C26-C27	2.97	119.93	113.60
12	F	201	CLA	C3C-C4C-NC	2.97	114.24	110.43
12	a	830	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
12	b	802	CLA	C11-C10-C8	-2.97	106.08	115.97
15	I	101	BCR	C34-C9-C8	2.97	122.63	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	852	BCR	C34-C9-C10	-2.97	118.00	122.82
12	A	812	CLA	C4D-C3D-CAD	2.97	111.33	108.11
12	b	809	CLA	CHD-C1D-ND	-2.97	120.62	124.80
12	B	827	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
12	B	831	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
12	B	821	CLA	CAC-C3C-C4C	2.97	128.65	124.79
12	a	829	CLA	CMC-C2C-C3C	2.97	134.18	126.15
12	b	819	CLA	CMA-C3A-C4A	2.97	119.75	111.77
12	b	825	CLA	CBA-CAA-C2A	2.97	122.63	113.79
12	a	816	CLA	CHD-C1D-ND	-2.97	120.62	124.80
12	b	810	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
12	H	805	CLA	C3C-C4C-NC	2.97	114.23	110.43
12	b	835	CLA	CMA-C3A-C4A	2.97	119.74	111.77
12	G	836	CLA	C4A-NA-C1A	2.97	108.03	106.68
15	l	201	BCR	C33-C5-C4	2.97	119.92	113.60
12	j	104	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
15	a	849	BCR	C24-C23-C22	-2.96	121.85	126.23
12	b	836	CLA	C3C-C4C-NC	2.96	114.23	110.43
12	l	204	CLA	CHD-C1D-ND	-2.96	120.63	124.80
12	H	807	CLA	O2A-C1-C2	2.96	119.51	108.11
12	a	829	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	a	806	CLA	O2A-C1-C2	2.96	119.51	108.11
15	A	844	BCR	C19-C18-C17	2.96	123.67	119.01
15	H	841	BCR	C27-C26-C25	-2.96	118.70	122.70
12	B	820	CLA	CBC-CAC-C3C	-2.96	104.39	112.42
12	L	206	CLA	C3D-C4D-ND	2.96	114.80	109.99
12	b	832	CLA	C3C-C4C-NC	2.96	114.22	110.43
12	A	804	CLA	C4-C3-C5	2.96	120.37	115.23
12	A	838	CLA	C3D-C4D-ND	2.96	114.80	109.99
12	j	104	CLA	CMC-C2C-C1C	2.96	129.66	125.03
15	A	846	BCR	C34-C9-C8	2.96	122.61	118.09
15	H	844	BCR	C30-C25-C24	2.96	123.68	115.65
12	H	831	CLA	CAA-CBA-CGA	-2.96	104.80	113.21
12	l	204	CLA	CMC-C2C-C1C	2.96	129.66	125.03
15	S	205	BCR	C23-C22-C21	2.96	123.66	119.01
12	b	814	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	a	842	1L3	C17-C16-C18	2.96	120.36	115.23
12	b	819	CLA	O2A-CGA-CBA	2.96	123.34	114.00
11	a	801	CL0	O2A-C1-C2	2.96	119.49	108.11
12	B	803	CLA	CMA-C3A-C2A	-2.96	102.55	113.98
12	H	802	CLA	C2B-C1B-NB	2.96	113.39	110.33
12	b	804	CLA	C4D-C3D-CAD	2.96	111.32	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	813	CLA	CMA-C3A-C4A	2.96	119.72	111.77
12	a	813	CLA	C1D-ND-C4D	-2.96	104.24	106.31
12	G	833	CLA	C3C-C4C-NC	2.96	114.22	110.43
12	b	834	CLA	C3D-C4D-ND	2.95	114.79	109.99
15	a	847	BCR	C4-C5-C6	-2.95	118.71	122.70
12	a	822	CLA	CMA-C3A-C4A	2.95	119.71	111.77
12	a	802	CLA	CHD-C1D-ND	-2.95	120.64	124.80
12	B	829	CLA	C3D-C4D-ND	2.95	114.79	109.99
12	A	826	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
13	b	838	1L3	C14-C15-C16	-2.95	121.74	126.83
13	A	842	1L3	C14-C03-C02	-2.95	119.83	124.89
13	b	838	1L3	C14-C03-C02	-2.95	119.83	124.89
12	A	820	CLA	CMC-C2C-C1C	-2.95	120.42	125.03
15	G	848	BCR	C2-C1-C6	2.95	114.73	110.44
12	A	809	CLA	CBA-CAA-C2A	2.95	122.57	113.79
12	G	831	CLA	C3C-C4C-NC	2.95	114.21	110.43
12	a	816	CLA	C1D-ND-C4D	-2.95	104.24	106.31
12	B	823	CLA	CMA-C3A-C4A	2.95	119.70	111.77
12	b	824	CLA	C3C-C4C-NC	2.95	114.21	110.43
17	T	101	45D	C30-C32-C34	-2.95	114.66	123.20
15	H	843	BCR	C34-C9-C8	2.95	122.59	118.09
15	S	201	BCR	C37-C22-C23	2.95	122.59	118.09
15	H	845	BCR	C33-C5-C6	-2.95	121.27	124.48
12	a	854	CLA	CHB-C1B-C2B	-2.95	118.88	127.43
15	S	205	BCR	C34-C9-C10	-2.95	118.04	122.82
12	B	825	CLA	C4D-C3D-CAD	2.95	111.31	108.11
12	H	825	CLA	CAC-C3C-C4C	2.95	128.62	124.79
13	H	840	1L3	C14-C03-C02	-2.95	119.84	124.89
15	H	849	BCR	C7-C8-C9	-2.94	121.88	126.23
15	I	101	BCR	C7-C8-C9	-2.94	121.88	126.23
12	B	801	CLA	C4D-C3D-CAD	2.94	111.30	108.11
12	G	803	CLA	CHD-C1D-ND	-2.94	120.66	124.80
12	b	837	CLA	C1-C2-C3	-2.94	121.38	126.20
12	G	856	CLA	CMC-C2C-C1C	2.94	129.63	125.03
12	H	816	CLA	CMC-C2C-C1C	2.94	129.63	125.03
12	J	103	CLA	CMC-C2C-C1C	2.94	129.63	125.03
15	S	201	BCR	C34-C9-C10	-2.94	118.05	122.82
12	H	818	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
12	f	201	CLA	C3C-C4C-NC	2.94	114.20	110.43
15	b	842	BCR	C30-C25-C24	2.94	123.63	115.65
12	H	818	CLA	CMA-C3A-C4A	2.94	119.68	111.77
12	a	807	CLA	CHD-C1D-ND	-2.94	120.66	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	815	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	i	102	BCR	C34-C9-C8	2.94	122.58	118.09
15	L	203	BCR	C35-C13-C12	2.94	122.58	118.09
12	H	835	CLA	CAA-C2A-C3A	-2.94	105.06	113.00
12	L	202	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
12	G	840	CLA	C4D-C3D-CAD	2.94	111.30	108.11
15	A	847	BCR	C34-C9-C10	-2.94	118.06	122.82
15	B	841	BCR	C19-C18-C17	2.94	123.63	119.01
12	H	816	CLA	CMB-C2B-C3B	2.94	133.46	126.55
12	H	828	CLA	CMA-C3A-C4A	2.94	119.67	111.77
12	H	850	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
12	a	823	CLA	CMC-C2C-C1C	2.94	129.62	125.03
12	H	818	CLA	CHD-C1D-ND	-2.94	120.67	124.80
12	B	805	CLA	C3C-C4C-NC	2.94	114.19	110.43
12	B	829	CLA	CMB-C2B-C3B	2.94	133.45	126.55
12	B	809	CLA	C4D-C3D-CAD	2.94	111.29	108.11
12	B	812	CLA	CHD-C1D-ND	-2.93	120.67	124.80
12	B	809	CLA	CMA-C3A-C4A	2.93	119.66	111.77
12	a	826	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
12	a	802	CLA	C3C-C4C-NC	2.93	114.19	110.43
12	G	838	CLA	OBD-CAD-C3D	-2.93	121.56	128.42
12	G	837	CLA	C6-C5-C3	-2.93	106.33	113.47
12	a	812	CLA	C4D-C3D-CAD	2.93	111.29	108.11
12	A	854	CLA	CMB-C2B-C3B	2.93	133.44	126.55
12	B	830	CLA	CMA-C3A-C4A	2.93	119.65	111.77
12	b	813	CLA	C4D-C3D-CAD	2.93	111.29	108.11
12	A	818	CLA	CAC-C3C-C4C	2.93	128.60	124.79
11	A	801	CL0	C1-C2-C3	-2.93	121.40	126.20
12	H	839	CLA	C3C-C4C-NC	2.93	114.18	110.43
12	b	825	CLA	C4D-C3D-CAD	2.93	111.29	108.11
12	G	841	CLA	CHD-C1D-ND	-2.93	120.68	124.80
12	G	842	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
12	G	815	CLA	CMA-C3A-C4A	2.93	119.64	111.77
12	H	832	CLA	CMC-C2C-C1C	2.93	129.61	125.03
12	A	805	CLA	C4D-C3D-CAD	2.93	111.28	108.11
15	J	101	BCR	C37-C22-C21	-2.93	118.07	122.82
12	A	816	CLA	C2B-C1B-NB	2.93	113.36	110.33
12	B	817	CLA	OBD-CAD-C3D	-2.92	121.58	128.42
12	b	827	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
12	b	827	CLA	C4D-C3D-CAD	2.92	111.28	108.11
12	G	839	CLA	CAC-C3C-C4C	2.92	128.59	124.79
12	b	836	CLA	C1-O2A-CGA	2.92	123.73	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	821	CLA	CMC-C2C-C1C	2.92	129.60	125.03
12	G	829	CLA	C1-C2-C3	-2.92	121.41	126.20
12	b	807	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
12	H	850	CLA	CMA-C3A-C4A	2.92	119.63	111.77
13	a	842	1L3	C14-C03-C02	-2.92	119.88	124.89
12	G	856	CLA	C3C-C4C-NC	2.92	114.17	110.43
12	a	839	CLA	C4D-C3D-CAD	2.92	111.28	108.11
13	B	839	1L3	C14-C03-C04	2.92	121.66	118.58
12	H	815	CLA	CBA-CAA-C2A	2.92	122.48	113.79
12	b	809	CLA	C4D-C3D-CAD	2.92	111.28	108.11
12	b	809	CLA	CMA-C3A-C4A	2.92	119.62	111.77
12	b	832	CLA	CMB-C2B-C1B	2.92	129.86	125.42
12	B	833	CLA	CMB-C2B-C1B	2.92	129.86	125.42
12	B	838	CLA	O1D-CGD-CBD	-2.92	118.76	124.52
12	A	841	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
15	H	844	BCR	C27-C26-C25	-2.92	118.76	122.70
12	H	816	CLA	C3D-C4D-ND	2.92	114.73	109.99
12	G	825	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
12	H	824	CLA	CMA-C3A-C4A	2.92	119.61	111.77
12	a	841	CLA	CAA-C2A-C3A	-2.92	105.12	113.00
12	b	816	CLA	CAA-C2A-C3A	-2.92	105.12	113.00
12	a	831	CLA	CMB-C2B-C3B	2.92	133.41	126.55
12	B	814	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
12	L	206	CLA	CAA-C2A-C3A	-2.91	105.12	113.00
12	H	816	CLA	C4D-C3D-CAD	2.91	111.27	108.11
17	M	101	45D	C30-C32-C34	-2.91	114.76	123.20
12	G	842	CLA	CMA-C3A-C4A	2.91	119.60	111.77
15	Q	101	BCR	C7-C8-C9	-2.91	121.93	126.23
12	A	808	CLA	CMA-C3A-C4A	2.91	119.60	111.77
12	G	834	CLA	C4D-C3D-CAD	2.91	111.27	108.11
12	R	103	CLA	C4D-C3D-CAD	2.91	111.27	108.11
12	A	829	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
12	B	808	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
12	G	815	CLA	CHD-C1D-ND	-2.91	120.70	124.80
12	G	811	CLA	O1D-CGD-CBD	-2.91	118.78	124.52
11	G	801	CL0	CMB-C2B-C1B	2.91	129.85	125.42
12	A	829	CLA	CMC-C2C-C3C	2.91	134.02	126.15
12	b	802	CLA	C2B-C1B-NB	2.91	113.34	110.33
15	B	841	BCR	C38-C26-C27	2.91	119.80	113.60
11	G	801	CL0	C1-C2-C3	-2.91	121.43	126.20
12	A	823	CLA	CMC-C2C-C1C	2.91	129.58	125.03
15	H	843	BCR	C7-C8-C9	-2.91	121.93	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	811	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
12	b	806	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
12	G	808	CLA	CBA-CAA-C2A	2.91	122.45	113.79
12	H	819	CLA	CAC-C3C-C4C	2.91	128.57	124.79
12	B	826	CLA	O2A-C1-C2	2.91	119.30	108.11
12	G	814	CLA	CHB-C4A-NA	2.91	128.60	124.40
12	b	829	CLA	CMB-C2B-C3B	2.91	133.39	126.55
12	H	827	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
12	b	833	CLA	CAA-C2A-C3A	-2.91	105.15	113.00
12	B	828	CLA	CMB-C2B-C3B	2.91	133.38	126.55
12	B	818	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
12	a	816	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
12	H	850	CLA	CHD-C1D-ND	-2.90	120.72	124.80
15	L	201	BCR	C37-C22-C21	-2.90	118.11	122.82
12	B	824	CLA	C4D-C3D-CAD	2.90	111.26	108.11
12	H	835	CLA	CHD-C1D-ND	-2.90	120.72	124.80
15	b	847	BCR	C19-C18-C17	2.90	123.57	119.01
12	A	807	CLA	CBA-CAA-C2A	2.90	122.43	113.79
12	A	854	CLA	C4-C3-C5	2.90	120.26	115.23
12	A	824	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
12	a	828	CLA	CMC-C2C-C1C	2.90	129.57	125.03
12	A	802	CLA	C3C-C4C-NC	2.90	114.15	110.43
12	a	818	CLA	CMA-C3A-C4A	2.90	119.57	111.77
12	b	832	CLA	CMA-C3A-C4A	2.90	119.57	111.77
12	l	206	CLA	C3D-C4D-ND	2.90	114.70	109.99
12	G	808	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
12	l	206	CLA	O2A-C1-C2	2.90	119.27	108.11
15	S	205	BCR	C33-C5-C4	2.90	119.78	113.60
12	G	819	CLA	CMA-C3A-C4A	2.90	119.57	111.77
12	B	834	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
12	G	804	CLA	C4D-C3D-CAD	2.90	111.25	108.11
12	B	805	CLA	CAA-C2A-C3A	-2.90	105.17	113.00
12	H	814	CLA	C4D-C3D-CAD	2.90	111.25	108.11
12	b	825	CLA	C3C-C4C-NC	2.90	114.14	110.43
15	a	844	BCR	C15-C14-C13	-2.90	123.21	127.28
12	A	810	CLA	C4D-C3D-CAD	2.90	111.25	108.11
12	H	838	CLA	CHD-C4C-C3C	-2.90	120.55	124.77
12	a	806	CLA	C6-C5-C3	-2.90	106.41	113.47
12	B	836	CLA	CAA-C2A-C3A	-2.90	105.17	113.00
12	S	204	CLA	C3D-C4D-ND	2.90	114.69	109.99
12	A	812	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
12	a	803	CLA	CAA-C2A-C3A	-2.89	105.18	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	804	CLA	CAC-C3C-C4C	2.89	128.56	124.79
12	a	816	CLA	C1-O2A-CGA	2.89	123.66	116.65
12	b	824	CLA	C4D-CHA-C1A	2.89	124.70	121.24
12	a	804	CLA	C4-C3-C5	2.89	120.25	115.23
12	b	848	CLA	CMA-C3A-C4A	2.89	119.55	111.77
12	b	811	CLA	CAA-C2A-C3A	-2.89	105.18	113.00
12	b	810	CLA	CHD-C1D-ND	-2.89	120.73	124.80
12	a	838	CLA	CAA-C2A-C3A	-2.89	105.19	113.00
12	B	811	CLA	C4D-C3D-CAD	2.89	111.24	108.11
15	B	845	BCR	C38-C26-C25	-2.89	121.33	124.48
12	A	817	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
12	b	823	CLA	CMA-C3A-C4A	2.89	119.53	111.77
12	H	823	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
12	b	808	CLA	CMA-C3A-C2A	-2.89	102.82	113.98
12	S	202	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
12	b	814	CLA	C6-C5-C3	-2.89	106.44	113.47
12	A	825	CLA	C3C-C4C-NC	2.89	114.13	110.43
12	a	818	CLA	C1-C2-C3	-2.89	121.47	126.20
12	G	803	CLA	CAC-C3C-C4C	2.89	128.54	124.79
12	G	808	CLA	C3C-C4C-NC	2.89	114.13	110.43
15	A	847	BCR	C38-C26-C27	2.88	119.75	113.60
12	a	831	CLA	CMA-C3A-C4A	2.88	119.53	111.77
12	b	848	CLA	C4C-C3C-C2C	-2.88	102.69	106.89
11	a	801	CL0	CBC-CAC-C3C	-2.88	104.60	112.42
12	a	819	CLA	CMC-C2C-C1C	2.88	129.54	125.03
12	J	103	CLA	CMA-C3A-C4A	2.88	119.52	111.77
12	B	838	CLA	C3C-C4C-NC	2.88	114.12	110.43
15	P	204	BCR	C27-C26-C25	-2.88	118.81	122.70
12	b	834	CLA	CMD-C2D-C3D	-2.88	121.08	127.69
12	G	824	CLA	CAC-C3C-C4C	2.88	128.54	124.79
12	b	822	CLA	C3C-C4C-NC	2.88	114.12	110.43
12	A	833	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	G	828	CLA	C4D-C3D-CAD	2.88	111.23	108.11
15	l	203	BCR	C34-C9-C10	-2.88	118.15	122.82
12	G	827	CLA	OBD-CAD-C3D	-2.88	121.68	128.42
12	H	819	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
12	F	201	CLA	C4D-C3D-CAD	2.88	111.23	108.11
12	b	818	CLA	C4D-C3D-CAD	2.88	111.23	108.11
12	G	826	CLA	CHD-C1D-ND	-2.88	120.75	124.80
12	b	808	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
12	B	835	CLA	C3D-C4D-ND	2.88	114.67	109.99
12	a	820	CLA	CMB-C2B-C3B	2.88	133.32	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	852	BCR	C7-C8-C9	-2.88	121.98	126.23
12	a	817	CLA	CAC-C3C-C4C	2.88	128.53	124.79
12	a	840	CLA	CMC-C2C-C1C	2.88	129.53	125.03
12	a	826	CLA	O2A-C1-C2	2.87	119.17	108.11
13	B	839	1L3	C14-C15-C16	-2.87	121.88	126.83
12	H	802	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
12	H	839	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	H	821	CLA	CBC-CAC-C3C	-2.87	104.63	112.42
17	M	101	45D	C21-C15-C07	-2.87	119.49	124.11
12	a	816	CLA	C2B-C1B-NB	2.87	113.31	110.33
12	b	824	CLA	C3B-C4B-NB	2.87	113.09	110.53
12	H	836	CLA	C3D-C4D-ND	2.87	114.65	109.99
15	H	842	BCR	C36-C18-C17	-2.87	118.17	122.82
12	P	201	CLA	CHD-C1D-ND	-2.87	120.76	124.80
12	B	824	CLA	C1-C2-C3	-2.87	121.50	126.20
12	b	818	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
15	S	201	BCR	C12-C13-C14	-2.87	114.50	119.01
12	H	838	CLA	C3C-C4C-NC	2.87	114.11	110.43
12	B	823	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
12	a	854	CLA	CHD-C1D-ND	-2.87	120.77	124.80
12	A	818	CLA	CAA-C2A-C1A	-2.87	102.57	111.97
12	a	810	CLA	CED-O2D-CGD	2.87	122.42	115.92
12	G	817	CLA	CMA-C3A-C4A	2.87	119.48	111.77
12	H	820	CLA	CMA-C3A-C4A	2.87	119.48	111.77
12	A	836	CLA	C3C-C4C-NC	2.87	114.10	110.43
12	l	205	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
12	a	838	CLA	C3D-C4D-ND	2.87	114.65	109.99
12	b	829	CLA	CAC-C3C-C4C	2.87	128.52	124.79
12	a	829	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
12	b	826	CLA	CAC-C3C-C4C	2.87	128.52	124.79
12	A	833	CLA	C1-C2-C3	-2.86	121.50	126.20
12	b	817	CLA	C4D-C3D-CAD	2.86	111.22	108.11
12	b	830	CLA	CMC-C2C-C1C	2.86	129.51	125.03
12	H	836	CLA	CMD-C2D-C3D	-2.86	121.12	127.69
12	A	826	CLA	O2A-C1-C2	2.86	119.12	108.11
12	B	825	CLA	C3B-C2B-C1B	-2.86	103.80	107.17
12	B	807	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
12	a	830	CLA	CMB-C2B-C1B	2.86	129.78	125.42
12	H	837	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
12	H	835	CLA	C3C-C4C-NC	2.86	114.10	110.43
12	L	204	CLA	CMC-C2C-C1C	2.86	129.50	125.03
12	B	821	CLA	C4D-C3D-CAD	2.86	111.21	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	808	CLA	CMA-C3A-C2A	-2.86	102.93	113.98
15	H	849	BCR	C34-C9-C8	2.86	122.46	118.09
12	G	836	CLA	C1D-ND-C4D	-2.86	104.31	106.31
12	a	821	CLA	CMC-C2C-C1C	2.86	129.50	125.03
12	G	818	CLA	C3D-C4D-ND	2.86	114.63	109.99
15	a	847	BCR	C38-C26-C27	2.86	119.69	113.60
12	A	814	CLA	C4D-C3D-CAD	2.86	111.21	108.11
15	L	203	BCR	C34-C9-C10	-2.86	118.19	122.82
12	A	814	CLA	C3C-C4C-NC	2.86	114.09	110.43
12	a	832	CLA	O2A-C1-C2	2.86	119.11	108.11
12	H	807	CLA	C6-C5-C3	-2.86	106.51	113.47
15	H	844	BCR	C37-C22-C23	2.86	122.45	118.09
15	G	847	BCR	C34-C9-C10	-2.86	118.19	122.82
12	a	830	CLA	CGD-CBD-CAD	-2.86	101.60	110.85
12	G	830	CLA	CMC-C2C-C3C	2.86	133.88	126.15
12	a	840	CLA	C1-O2A-CGA	2.86	123.56	116.65
16	G	854	LHG	C5-O7-C7	-2.86	110.96	117.80
12	G	819	CLA	CAC-C3C-C4C	2.86	128.51	124.79
15	A	845	BCR	C4-C5-C6	-2.86	118.85	122.70
15	A	846	BCR	C27-C26-C25	-2.86	118.85	122.70
12	b	808	CLA	CMC-C2C-C3C	2.85	133.87	126.15
16	a	853	LHG	O8-C23-C24	2.85	120.54	111.83
12	a	828	CLA	C1-C2-C3	-2.85	121.52	126.20
12	A	833	CLA	CAC-C3C-C4C	2.85	128.50	124.79
12	b	817	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
12	A	814	CLA	CHD-C1D-ND	-2.85	120.79	124.80
15	a	852	BCR	C34-C9-C8	2.85	122.45	118.09
12	B	822	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	j	101	BCR	C38-C26-C25	-2.85	121.37	124.48
12	B	811	CLA	CAA-C2A-C3A	-2.85	105.29	113.00
12	a	814	CLA	CHD-C1D-ND	-2.85	120.79	124.80
12	a	855	CLA	CMC-C2C-C1C	2.85	129.49	125.03
15	F	202	BCR	C29-C30-C25	2.85	114.58	110.44
12	G	812	CLA	C3C-C4C-NC	2.85	114.08	110.43
12	A	834	CLA	C4D-C3D-CAD	2.85	111.20	108.11
12	a	825	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
12	a	840	CLA	CMA-C3A-C4A	2.85	119.43	111.77
12	A	826	CLA	CMA-C3A-C4A	2.85	119.43	111.77
12	B	821	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	b	840	BCR	C19-C18-C17	2.85	123.49	119.01
12	B	802	CLA	C3D-C4D-ND	2.85	114.61	109.99
12	a	838	CLA	C3C-C4C-NC	2.85	114.08	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	841	CLA	CMC-C2C-C1C	2.85	129.48	125.03
15	A	845	BCR	C28-C27-C26	-2.85	108.98	114.06
12	A	806	CLA	O2A-C1-C2	2.85	119.06	108.11
12	G	830	CLA	CHD-C1D-ND	-2.84	120.80	124.80
12	B	824	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
12	b	822	CLA	CMC-C2C-C1C	2.84	129.48	125.03
12	a	804	CLA	CBA-CAA-C2A	2.84	122.26	113.79
12	b	826	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
15	L	201	BCR	C33-C5-C4	2.84	119.66	113.60
11	G	801	CL0	O2A-C1-C2	2.84	119.04	108.11
12	a	810	CLA	C3D-C4D-ND	2.84	114.60	109.99
12	B	806	CLA	CMB-C2B-C1B	2.84	129.74	125.42
12	B	801	CLA	CHD-C1D-ND	-2.84	120.81	124.80
12	G	837	CLA	O1D-CGD-CBD	-2.84	118.92	124.52
12	A	839	CLA	C4D-C3D-CAD	2.84	111.19	108.11
12	b	807	CLA	C6-C7-C8	-2.84	106.53	115.97
12	H	808	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
15	j	103	BCR	C24-C23-C22	-2.84	122.04	126.23
15	G	848	BCR	C38-C26-C27	2.84	119.64	113.60
13	A	842	1L3	C17-C16-C18	2.84	120.15	115.23
15	B	844	BCR	C4-C5-C6	-2.84	118.87	122.70
12	G	817	CLA	C1-O2A-CGA	2.84	123.52	116.65
15	R	101	BCR	C38-C26-C25	-2.84	121.39	124.48
12	A	804	CLA	CBA-CAA-C2A	2.84	122.23	113.79
12	b	821	CLA	CMB-C2B-C3B	2.84	133.22	126.55
12	a	826	CLA	CMC-C2C-C1C	2.84	129.47	125.03
12	A	813	CLA	CMB-C2B-C3B	2.84	133.22	126.55
12	a	813	CLA	CAC-C3C-C4C	2.84	128.48	124.79
12	G	842	CLA	C3C-C4C-NC	2.83	114.06	110.43
12	b	814	CLA	CMC-C2C-C1C	2.83	129.46	125.03
15	b	843	BCR	C1-C6-C5	-2.83	118.76	122.64
12	G	806	CLA	C1-C2-C3	-2.83	121.55	126.20
12	H	834	CLA	CMA-C3A-C4A	2.83	119.39	111.77
12	H	824	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
15	a	845	BCR	C28-C27-C26	-2.83	109.01	114.06
12	G	841	CLA	CMC-C2C-C1C	2.83	129.46	125.03
15	A	852	BCR	C34-C9-C10	-2.83	118.23	122.82
12	G	803	CLA	C3C-C4C-NC	2.83	114.06	110.43
12	G	816	CLA	CMA-C3A-C4A	2.83	119.38	111.77
15	A	846	BCR	C34-C9-C10	-2.83	118.23	122.82
12	B	819	CLA	CMA-C3A-C4A	2.83	119.38	111.77
12	a	824	CLA	C2B-C1B-NB	2.83	113.26	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	808	CLA	CMB-C2B-C3B	2.83	133.21	126.55
12	G	802	CLA	C3D-C4D-ND	2.83	114.59	109.99
15	H	843	BCR	C29-C30-C25	2.83	114.55	110.44
12	G	830	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
18	H	847	LMG	O8-C28-C29	2.83	120.46	111.83
12	H	828	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
12	G	827	CLA	C4D-C3D-CAD	2.83	111.18	108.11
12	H	812	CLA	C4D-C3D-CAD	2.83	111.18	108.11
15	Q	102	BCR	C34-C9-C8	2.83	122.41	118.09
12	G	817	CLA	CMC-C2C-C1C	2.83	129.45	125.03
12	A	807	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
15	L	207	BCR	C37-C22-C21	-2.83	118.24	122.82
12	B	804	CLA	C4D-C3D-CAD	2.83	111.17	108.11
13	a	842	1L3	C19-C20-C21	-2.83	121.16	127.62
12	H	823	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
12	B	811	CLA	CMB-C2B-C3B	2.82	133.19	126.55
12	A	838	CLA	C3C-C4C-NC	2.82	114.05	110.43
17	M	101	45D	C22-C16-C08	-2.82	119.57	124.11
12	b	848	CLA	CHD-C1D-ND	-2.82	120.83	124.80
12	A	829	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
12	a	840	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
15	B	844	BCR	C1-C6-C5	-2.82	118.78	122.64
17	T	101	45D	C21-C15-C07	-2.82	119.57	124.11
12	B	810	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	B	847	LMT	O2B-C2B-C1B	-2.82	103.35	110.08
12	A	829	CLA	C2B-C1B-NB	2.82	113.25	110.33
12	H	826	CLA	C3C-C4C-NC	2.82	114.04	110.43
12	A	839	CLA	CED-O2D-CGD	2.82	122.31	115.92
12	G	826	CLA	CAA-C2A-C1A	-2.82	102.73	111.97
12	b	814	CLA	CHB-C4A-NA	2.82	128.47	124.40
12	B	813	CLA	CMC-C2C-C1C	2.82	129.44	125.03
12	B	830	CLA	CAA-CBA-CGA	-2.82	105.20	113.21
12	b	826	CLA	CED-O2D-CGD	2.82	122.31	115.92
12	L	205	CLA	O1D-CGD-CBD	-2.82	118.96	124.52
12	A	830	CLA	CMD-C2D-C3D	-2.82	121.23	127.69
12	B	823	CLA	C4D-C3D-CAD	2.82	111.17	108.11
13	H	840	1L3	C14-C15-C16	-2.82	121.98	126.83
12	a	805	CLA	CMA-C3A-C2A	-2.82	103.09	113.98
12	a	854	CLA	C4-C3-C2	-2.82	116.40	123.63
15	b	843	BCR	C33-C5-C6	-2.82	121.41	124.48
12	G	835	CLA	CMC-C2C-C1C	2.82	129.43	125.03
12	H	821	CLA	CMC-C2C-C1C	2.82	129.43	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	835	CLA	C4D-C3D-CAD	2.81	111.16	108.11
15	H	845	BCR	C1-C6-C5	-2.81	118.79	122.64
12	A	840	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
12	a	815	CLA	CMB-C2B-C1B	2.81	129.70	125.42
12	G	825	CLA	CAC-C3C-C4C	2.81	128.45	124.79
12	H	814	CLA	CMA-C3A-C4A	2.81	119.33	111.77
12	b	832	CLA	C2B-C1B-NB	2.81	113.24	110.33
12	A	805	CLA	C1-C2-C3	-2.81	121.59	126.20
12	H	806	CLA	CBC-CAC-C3C	-2.81	104.80	112.42
12	a	827	CLA	C4D-C3D-CAD	2.81	111.16	108.11
12	B	818	CLA	C4D-C3D-CAD	2.81	111.16	108.11
12	b	802	CLA	CHD-C4C-C3C	-2.81	120.68	124.77
12	B	817	CLA	CMC-C2C-C1C	2.81	129.42	125.03
12	B	838	CLA	CHD-C1D-ND	-2.81	120.85	124.80
12	a	814	CLA	C4D-C3D-CAD	2.81	111.15	108.11
12	b	818	CLA	CMC-C2C-C1C	2.81	129.42	125.03
12	b	805	CLA	CAA-C2A-C3A	-2.81	105.42	113.00
12	A	803	CLA	C4D-C3D-CAD	2.80	111.15	108.11
12	b	830	CLA	C3C-C4C-NC	2.80	114.02	110.43
12	H	805	CLA	CAC-C3C-C4C	2.80	128.44	124.79
12	a	816	CLA	C1-C2-C3	-2.80	122.23	126.76
12	B	808	CLA	CAA-C2A-C3A	-2.80	105.42	113.00
12	G	855	CLA	CHB-C1B-C2B	-2.80	119.29	127.43
15	P	202	BCR	C29-C30-C25	2.80	114.51	110.44
12	H	850	CLA	CAA-C2A-C3A	-2.80	105.43	113.00
12	a	835	CLA	CMA-C3A-C4A	2.80	119.31	111.77
12	A	802	CLA	C1-O2A-CGA	2.80	123.43	116.65
12	B	808	CLA	CMC-C2C-C3C	2.80	133.73	126.15
12	A	816	CLA	O2A-C1-C2	2.80	118.89	108.11
12	A	854	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
12	H	827	CLA	O2A-C1-C2	2.80	118.89	108.11
12	H	838	CLA	CAC-C3C-C4C	-2.80	121.14	124.79
12	H	827	CLA	CAA-C2A-C3A	-2.80	105.43	113.00
12	a	823	CLA	C4D-C3D-CAD	2.80	111.15	108.11
15	B	842	BCR	C7-C8-C9	-2.80	122.09	126.23
12	A	811	CLA	CMA-C3A-C4A	2.80	119.30	111.77
12	A	814	CLA	CMB-C2B-C3B	2.80	133.13	126.55
18	b	845	LMG	O8-C28-C29	2.80	120.37	111.83
15	G	847	BCR	C34-C9-C8	2.80	122.36	118.09
15	f	204	BCR	C36-C18-C17	-2.80	118.28	122.82
12	b	824	CLA	C4D-C3D-CAD	2.80	111.14	108.11
12	B	824	CLA	C3C-C4C-NC	2.80	114.01	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	803	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
15	b	840	BCR	C36-C18-C17	-2.80	118.28	122.82
12	B	820	CLA	CMB-C2B-C3B	2.80	133.13	126.55
12	G	826	CLA	C3C-C4C-NC	2.80	114.01	110.43
12	b	819	CLA	CMB-C2B-C1B	2.80	129.68	125.42
15	b	841	BCR	C7-C8-C9	-2.80	122.10	126.23
12	a	829	CLA	CHD-C1D-ND	-2.80	120.87	124.80
12	H	825	CLA	CED-O2D-CGD	2.79	122.25	115.92
12	H	816	CLA	CHB-C4A-NA	2.79	128.43	124.40
12	G	813	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
12	H	808	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
12	b	832	CLA	C4D-C3D-CAD	2.79	111.14	108.11
12	b	833	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
12	H	807	CLA	C6-C7-C8	-2.79	106.68	115.97
12	B	806	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
11	a	801	CL0	C2A-C3A-C4A	2.79	106.38	101.87
12	A	828	CLA	CMC-C2C-C1C	2.79	129.40	125.03
15	A	844	BCR	C15-C14-C13	-2.79	123.36	127.28
12	B	834	CLA	C3D-C4D-ND	2.79	114.52	109.99
15	l	201	BCR	C34-C9-C10	-2.79	118.29	122.82
12	A	816	CLA	C4D-C3D-CAD	2.79	111.14	108.11
12	A	828	CLA	CMA-C3A-C4A	2.79	119.27	111.77
12	j	104	CLA	C4D-C3D-CAD	2.79	111.14	108.11
12	B	806	CLA	C3D-C4D-ND	2.79	114.52	109.99
12	B	805	CLA	CAC-C3C-C4C	2.79	128.42	124.79
12	G	840	CLA	CMC-C2C-C1C	2.79	129.39	125.03
12	S	202	CLA	CMC-C2C-C1C	2.79	129.39	125.03
12	b	801	CLA	CMC-C2C-C1C	2.79	129.39	125.03
12	G	837	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
12	b	802	CLA	C3D-C4D-ND	2.79	114.52	109.99
12	b	836	CLA	C2B-C1B-NB	2.79	113.22	110.33
12	B	830	CLA	C2B-C1B-NB	2.79	113.22	110.33
15	a	846	BCR	C37-C22-C21	-2.79	118.30	122.82
12	B	827	CLA	C4D-C3D-CAD	2.79	111.13	108.11
12	H	810	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
12	G	802	CLA	CHB-C1B-C2B	-2.78	119.34	127.43
12	G	802	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
12	B	814	CLA	C4D-C3D-CAD	2.78	111.13	108.11
12	b	808	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
12	G	836	CLA	CAC-C3C-C4C	2.78	128.41	124.79
12	G	828	CLA	CHD-C1D-ND	-2.78	120.89	124.80
12	G	828	CLA	C4C-C3C-C2C	-2.78	102.84	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	205	BCR	C40-C30-C39	-2.78	100.66	108.63
12	b	817	CLA	CMC-C2C-C1C	2.78	129.38	125.03
12	H	803	CLA	CMB-C2B-C3B	2.78	133.09	126.55
12	b	824	CLA	CHC-C1C-C2C	-2.78	119.04	126.95
12	H	828	CLA	CMD-C2D-C3D	-2.78	121.31	127.69
15	H	841	BCR	C19-C18-C17	2.78	123.38	119.01
15	B	844	BCR	C36-C18-C17	-2.78	118.31	122.82
12	H	815	CLA	C4D-C3D-CAD	2.78	111.13	108.11
12	a	816	CLA	CMC-C2C-C1C	2.78	129.38	125.03
12	B	818	CLA	CMC-C2C-C1C	2.78	129.38	125.03
15	G	848	BCR	C30-C25-C24	2.78	123.19	115.65
12	G	840	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	b	813	CLA	CMC-C2C-C1C	2.78	129.38	125.03
15	J	101	BCR	C36-C18-C17	-2.78	118.31	122.82
12	G	826	CLA	CMC-C2C-C1C	2.78	129.38	125.03
12	b	825	CLA	C2B-C1B-NB	2.78	113.21	110.33
12	A	807	CLA	C3C-C4C-NC	2.78	113.99	110.43
12	A	803	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	b	813	CLA	C4-C3-C5	2.78	120.05	115.23
12	G	827	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
12	G	855	CLA	CHB-C4A-NA	2.78	128.41	124.40
15	b	842	BCR	C37-C22-C23	2.78	122.33	118.09
15	H	846	BCR	C34-C9-C8	2.78	122.33	118.09
12	B	825	CLA	CBA-CAA-C2A	2.78	122.05	113.79
12	A	818	CLA	CMC-C2C-C1C	2.77	129.37	125.03
12	A	835	CLA	CMC-C2C-C1C	2.77	129.37	125.03
15	l	201	BCR	C36-C18-C17	-2.77	118.32	122.82
12	a	810	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
12	R	103	CLA	CMA-C3A-C4A	2.77	119.22	111.77
12	H	816	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
12	A	812	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
12	A	833	CLA	CMA-C3A-C4A	2.77	119.22	111.77
12	H	821	CLA	CMB-C2B-C3B	2.77	133.07	126.55
12	A	820	CLA	C1D-ND-C4D	-2.77	104.37	106.31
12	A	828	CLA	CED-O2D-CGD	2.77	122.20	115.92
15	G	850	BCR	C24-C23-C22	-2.77	122.14	126.23
12	A	855	CLA	CHB-C4A-NA	2.77	128.40	124.40
12	a	855	CLA	CED-O2D-CGD	2.77	122.20	115.92
12	L	206	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
12	H	806	CLA	CAA-CBA-CGA	2.77	121.07	113.21
12	b	801	CLA	C4-C3-C5	2.77	120.03	115.23
12	G	812	CLA	CHD-C1D-ND	-2.77	120.91	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	832	CLA	CMC-C2C-C1C	2.77	129.36	125.03
12	a	834	CLA	C3C-C4C-NC	2.77	113.97	110.43
15	b	844	BCR	C15-C14-C13	-2.77	123.40	127.28
12	H	820	CLA	CMC-C2C-C1C	2.76	129.35	125.03
12	b	831	CLA	CAC-C3C-C4C	2.76	128.39	124.79
12	a	805	CLA	C4-C3-C5	2.76	120.03	115.23
12	B	824	CLA	OBD-CAD-C3D	-2.76	121.96	128.42
15	P	204	BCR	C36-C18-C17	-2.76	118.34	122.82
12	S	202	CLA	C3C-C4C-NC	2.76	113.97	110.43
12	B	812	CLA	CMB-C2B-C3B	2.76	133.05	126.55
15	B	840	BCR	C19-C18-C17	2.76	123.35	119.01
12	G	804	CLA	CMB-C2B-C1B	2.76	129.62	125.42
15	B	845	BCR	C34-C9-C8	2.76	122.31	118.09
12	a	855	CLA	CHD-C1D-ND	-2.76	120.92	124.80
12	H	818	CLA	C4D-C3D-CAD	2.76	111.11	108.11
12	a	835	CLA	C3C-C4C-NC	2.76	113.97	110.43
12	a	826	CLA	CMB-C2B-C3B	2.76	133.04	126.55
12	B	808	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
12	G	805	CLA	C4-C3-C5	2.76	120.02	115.23
12	B	810	CLA	C1-C2-C3	-2.76	121.68	126.20
12	H	810	CLA	CMA-C3A-C4A	2.76	119.19	111.77
12	G	812	CLA	CMC-C2C-C1C	2.76	129.34	125.03
12	G	817	CLA	C4D-C3D-CAD	2.76	111.10	108.11
12	B	819	CLA	CMC-C2C-C1C	2.76	129.34	125.03
12	f	201	CLA	C4D-C3D-CAD	2.76	111.10	108.11
12	H	817	CLA	CMC-C2C-C1C	2.76	129.34	125.03
12	A	820	CLA	CHD-C1D-ND	-2.76	120.92	124.80
12	L	206	CLA	C4-C3-C5	2.75	120.01	115.23
12	B	821	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
12	G	838	CLA	C3C-C4C-NC	2.75	113.96	110.43
15	A	845	BCR	C7-C8-C9	-2.75	122.16	126.23
12	G	819	CLA	CAA-C2A-C1A	-2.75	102.95	111.97
12	b	802	CLA	CHD-C1D-ND	-2.75	120.93	124.80
12	H	832	CLA	C2B-C1B-NB	2.75	113.18	110.33
12	a	838	CLA	C2B-C1B-NB	2.75	113.18	110.33
12	A	834	CLA	CBA-CAA-C2A	2.75	121.98	113.79
12	L	202	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
17	m	101	45D	C22-C16-C08	-2.75	119.69	124.11
12	G	803	CLA	C1-O2A-CGA	2.75	123.31	116.65
15	b	847	BCR	C37-C22-C21	-2.75	118.36	122.82
15	i	101	BCR	C7-C8-C9	-2.75	122.17	126.23
15	a	847	BCR	C35-C13-C12	2.75	122.29	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	844	BCR	C37-C22-C21	-2.75	118.36	122.82
12	A	823	CLA	C4D-C3D-CAD	2.75	111.09	108.11
12	B	829	CLA	CMA-C3A-C4A	2.75	119.16	111.77
12	A	827	CLA	CAC-C3C-C4C	2.75	128.37	124.79
12	b	806	CLA	C4D-C3D-CAD	2.75	111.09	108.11
12	B	835	CLA	CMD-C2D-C3D	-2.75	121.39	127.69
12	b	812	CLA	C3C-C4C-NC	2.75	113.95	110.43
12	a	804	CLA	C4D-C3D-CAD	2.75	111.09	108.11
12	G	827	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
12	A	854	CLA	C3B-C4B-NB	-2.75	108.08	110.53
12	b	837	CLA	C4D-C3D-CAD	2.75	111.09	108.11
12	b	820	CLA	CMB-C2B-C3B	2.75	133.01	126.55
12	B	830	CLA	CAC-C3C-C4C	2.74	128.36	124.79
12	a	826	CLA	CHD-C4C-C3C	-2.74	120.77	124.77
12	G	841	CLA	C3D-C4D-ND	2.74	114.45	109.99
12	H	804	CLA	C4D-C3D-CAD	2.74	111.09	108.11
12	A	812	CLA	CMD-C2D-C3D	-2.74	121.40	127.69
12	G	855	CLA	OBD-CAD-C3D	-2.74	122.00	128.42
12	H	825	CLA	OBD-CAD-C3D	-2.74	122.00	128.42
15	G	853	BCR	C34-C9-C8	2.74	122.28	118.09
12	H	834	CLA	C3C-C4C-NC	2.74	113.94	110.43
15	G	847	BCR	C27-C26-C25	-2.74	119.00	122.70
12	b	805	CLA	CAC-C3C-C4C	2.74	128.36	124.79
12	B	831	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
15	L	201	BCR	C23-C22-C21	2.74	123.32	119.01
12	B	820	CLA	C3D-C4D-ND	2.74	114.44	109.99
12	A	810	CLA	CMB-C2B-C1B	2.74	129.59	125.42
12	H	833	CLA	CMA-C3A-C4A	2.74	119.14	111.77
12	G	828	CLA	O1D-CGD-CBD	-2.74	119.12	124.52
15	G	845	BCR	C37-C22-C21	-2.74	118.38	122.82
12	G	825	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
12	b	826	CLA	CHA-C4D-ND	2.74	138.20	132.55
12	A	803	CLA	CMD-C2D-C3D	-2.74	121.41	127.69
12	B	838	CLA	C1-C2-C3	-2.74	121.71	126.20
12	a	854	CLA	OBD-CAD-C3D	-2.74	122.02	128.42
15	J	104	BCR	C36-C18-C17	-2.74	118.38	122.82
12	H	829	CLA	CED-O2D-CGD	2.73	122.12	115.92
12	B	803	CLA	CMB-C2B-C3B	2.73	132.98	126.55
12	H	819	CLA	C4D-C3D-CAD	2.73	111.08	108.11
12	A	855	CLA	CMB-C2B-C3B	2.73	132.98	126.55
12	H	804	CLA	CAA-C2A-C3A	-2.73	105.61	113.00
12	b	801	CLA	C1-O2A-CGA	2.73	123.27	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	822	CLA	C3C-C4C-NC	2.73	113.93	110.43
12	A	817	CLA	C3C-C4C-NC	2.73	113.93	110.43
12	B	811	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	H	818	CLA	CMC-C2C-C1C	2.73	129.30	125.03
12	P	201	CLA	C4D-C3D-CAD	2.73	111.07	108.11
12	A	811	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
12	a	803	CLA	CMC-C2C-C1C	2.73	129.30	125.03
12	H	809	CLA	CMC-C2C-C3C	2.73	133.53	126.15
15	P	202	BCR	C35-C13-C12	2.73	122.26	118.09
12	H	804	CLA	CED-O2D-CGD	2.73	122.11	115.92
12	G	813	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	a	832	CLA	CMC-C2C-C1C	2.73	129.30	125.03
12	B	823	CLA	CAA-CBA-CGA	-2.73	105.46	113.21
15	F	204	BCR	C34-C9-C10	-2.73	118.40	122.82
15	A	848	BCR	C34-C9-C10	-2.73	118.40	122.82
12	b	823	CLA	C4-C3-C5	2.73	119.96	115.23
15	b	841	BCR	C23-C22-C21	-2.73	114.72	119.01
12	G	822	CLA	CMC-C2C-C1C	2.73	129.29	125.03
12	b	801	CLA	CHD-C1D-ND	-2.73	120.97	124.80
12	J	103	CLA	C4D-C3D-CAD	2.73	111.07	108.11
12	G	839	CLA	CMB-C2B-C3B	2.73	132.96	126.55
15	B	842	BCR	C40-C30-C25	2.72	114.52	110.24
12	G	822	CLA	C4D-C3D-CAD	2.72	111.06	108.11
12	B	812	CLA	C3C-C4C-NC	2.72	113.92	110.43
15	B	841	BCR	C36-C18-C17	-2.72	118.41	122.82
12	H	813	CLA	CMB-C2B-C3B	2.72	132.95	126.55
12	G	813	CLA	CMD-C2D-C3D	-2.72	121.45	127.69
12	G	838	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
12	b	807	CLA	O2A-C1-C2	2.72	118.58	108.11
15	b	844	BCR	C34-C9-C8	2.72	122.24	118.09
12	a	815	CLA	CMC-C2C-C1C	2.72	129.28	125.03
12	G	821	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
12	A	804	CLA	C4D-C3D-CAD	2.72	111.06	108.11
12	B	811	CLA	C3C-C4C-NC	2.72	113.91	110.43
15	l	203	BCR	C35-C13-C12	2.72	122.24	118.09
12	b	811	CLA	C3D-C4D-ND	2.72	114.41	109.99
12	A	834	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
12	A	821	CLA	C4D-C3D-CAD	2.72	111.06	108.11
12	B	807	CLA	C6-C7-C8	-2.72	106.93	115.97
12	b	824	CLA	C1D-CHD-C4C	-2.72	120.24	126.02
12	A	829	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
12	G	803	CLA	C2B-C1B-NB	2.72	113.14	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Q	101	BCR	C38-C26-C25	-2.72	121.52	124.48
12	a	831	CLA	C3D-C4D-ND	2.72	114.40	109.99
12	b	801	CLA	C3D-C4D-ND	2.72	114.40	109.99
12	b	824	CLA	C1-C2-C3	-2.71	121.75	126.20
12	A	820	CLA	C4B-CHC-C1C	2.71	132.63	126.25
12	b	803	CLA	CBA-CAA-C2A	2.71	121.87	113.79
12	A	837	CLA	OBD-CAD-C3D	-2.71	122.07	128.42
12	b	808	CLA	CMB-C2B-C1B	2.71	129.55	125.42
12	j	104	CLA	CMA-C3A-C4A	2.71	119.07	111.77
13	A	842	1L3	C01-C02-C03	-2.71	119.99	124.45
12	B	828	CLA	CAC-C3C-C4C	2.71	128.32	124.79
12	R	103	CLA	CMC-C2C-C1C	2.71	129.27	125.03
12	A	841	CLA	CHD-C1D-ND	-2.71	120.99	124.80
12	A	824	CLA	CMB-C2B-C3B	2.71	132.93	126.55
12	G	824	CLA	C4D-C3D-CAD	2.71	111.05	108.11
15	a	847	BCR	C30-C25-C24	2.71	123.00	115.65
12	B	836	CLA	CMA-C3A-C4A	2.71	119.06	111.77
12	G	805	CLA	CBA-CAA-C2A	2.71	121.86	113.79
12	B	818	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
15	R	102	BCR	C15-C14-C13	-2.71	123.48	127.28
12	b	801	CLA	CHB-C1B-C2B	-2.71	119.56	127.43
12	B	838	CLA	C4-C3-C5	2.71	119.93	115.23
12	A	836	CLA	CBC-CAC-C3C	2.71	119.77	112.42
12	B	826	CLA	CHD-C1D-ND	-2.71	120.99	124.80
12	b	809	CLA	C3C-C4C-NC	2.71	113.90	110.43
12	A	810	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
12	a	805	CLA	C1-C2-C3	-2.71	121.76	126.20
12	A	827	CLA	CED-O2D-CGD	2.71	122.06	115.92
15	S	205	BCR	C37-C22-C21	-2.71	118.43	122.82
12	b	848	CLA	CAA-C2A-C3A	-2.71	105.68	113.00
12	B	806	CLA	CMA-C3A-C4A	2.71	119.05	111.77
12	b	806	CLA	CMA-C3A-C4A	2.71	119.05	111.77
12	S	204	CLA	C4-C3-C5	2.71	119.93	115.23
12	G	812	CLA	CMB-C2B-C1B	2.71	129.54	125.42
15	A	847	BCR	C30-C25-C24	2.71	122.99	115.65
12	A	855	CLA	CAA-C2A-C1A	-2.71	103.11	111.97
12	a	811	CLA	C3C-C4C-NC	2.71	113.90	110.43
12	a	828	CLA	C3C-C4C-NC	2.71	113.90	110.43
12	A	840	CLA	C1-O2A-CGA	2.71	123.20	116.65
12	l	206	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
12	G	804	CLA	CMC-C2C-C1C	2.70	129.26	125.03
12	F	203	CLA	CMB-C2B-C1B	2.70	129.54	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	842	CLA	CHD-C1D-ND	-2.70	121.00	124.80
12	B	810	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
12	H	809	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
12	G	807	CLA	CMB-C2B-C3B	2.70	132.91	126.55
12	A	854	CLA	OBD-CAD-C3D	-2.70	122.10	128.42
15	b	844	BCR	C38-C26-C25	-2.70	121.53	124.48
12	A	811	CLA	C3C-C4C-NC	2.70	113.89	110.43
12	H	805	CLA	CMD-C2D-C3D	-2.70	121.49	127.69
12	G	842	CLA	C4-C3-C5	2.70	119.92	115.23
12	b	808	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
15	P	204	BCR	C34-C9-C8	2.70	122.22	118.09
12	b	802	CLA	C11-C12-C13	-2.70	106.99	115.97
15	b	839	BCR	C27-C26-C25	-2.70	119.05	122.70
15	Q	101	BCR	C15-C14-C13	-2.70	123.49	127.28
12	A	831	CLA	C3C-C4C-NC	2.70	113.89	110.43
12	H	827	CLA	C1-O2A-CGA	2.70	123.19	116.65
12	G	836	CLA	CHA-C4D-ND	2.70	138.12	132.55
12	A	854	CLA	CHD-C1D-ND	-2.70	121.00	124.80
12	G	826	CLA	OBD-CAD-C3D	-2.70	122.11	128.42
12	H	836	CLA	CBC-CAC-C3C	-2.70	105.10	112.42
12	a	817	CLA	C3C-C4C-NC	2.70	113.89	110.43
12	B	801	CLA	C3D-C4D-ND	2.70	114.37	109.99
12	b	820	CLA	C3D-C4D-ND	2.70	114.37	109.99
12	B	809	CLA	C3C-C4C-NC	2.70	113.88	110.43
12	a	841	CLA	CMC-C2C-C1C	2.70	129.25	125.03
12	G	855	CLA	CMB-C2B-C3B	2.70	132.89	126.55
12	G	811	CLA	C3D-C4D-ND	2.70	114.37	109.99
12	G	804	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
12	b	817	CLA	CHD-C1D-ND	-2.70	121.01	124.80
15	f	202	BCR	C29-C30-C25	2.70	114.35	110.44
12	G	804	CLA	C3C-C4C-NC	2.69	113.88	110.43
12	b	831	CLA	CMA-C3A-C4A	2.69	119.02	111.77
15	l	201	BCR	C37-C22-C21	-2.69	118.45	122.82
12	G	813	CLA	CHD-C1D-ND	-2.69	121.01	124.80
12	B	814	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
12	H	807	CLA	C3C-C4C-NC	2.69	113.88	110.43
12	b	813	CLA	C3D-C4D-ND	2.69	114.36	109.99
12	A	810	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
12	A	817	CLA	CMD-C2D-C3D	-2.69	121.52	127.69
12	G	823	CLA	C3C-C4C-NC	2.69	113.88	110.43
12	A	840	CLA	CMC-C2C-C1C	2.69	129.24	125.03
12	a	855	CLA	C3D-C4D-ND	2.69	114.36	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	811	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
12	a	824	CLA	OBD-CAD-C3D	-2.69	122.13	128.42
12	H	809	CLA	C4D-C3D-CAD	2.69	111.03	108.11
12	b	806	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
12	B	826	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
12	a	811	CLA	CHD-C1D-ND	-2.69	121.02	124.80
12	B	838	CLA	C4D-C3D-CAD	2.69	111.03	108.11
12	G	817	CLA	OBD-CAD-C3D	-2.69	122.14	128.42
12	A	828	CLA	C4D-C3D-CAD	2.69	111.02	108.11
12	A	813	CLA	CMD-C2D-C3D	-2.69	121.53	127.69
15	S	205	BCR	C36-C18-C17	-2.69	118.46	122.82
12	a	813	CLA	C3C-C4C-NC	2.69	113.87	110.43
15	b	840	BCR	C38-C26-C27	2.69	119.32	113.60
12	b	804	CLA	CED-O2D-CGD	2.69	122.01	115.92
12	G	829	CLA	C4D-C3D-CAD	2.69	111.02	108.11
12	G	816	CLA	CMB-C2B-C1B	2.69	129.51	125.42
12	B	834	CLA	C3C-C4C-NC	2.69	113.87	110.43
12	H	815	CLA	C6-C5-C3	-2.69	106.93	113.47
12	A	811	CLA	CMC-C2C-C1C	2.69	129.23	125.03
12	H	831	CLA	CHC-C1C-C2C	-2.69	119.32	126.95
12	J	103	CLA	CMB-C2B-C1B	2.68	129.51	125.42
12	G	833	CLA	CAC-C3C-C4C	2.68	128.28	124.79
15	G	848	BCR	C35-C13-C12	2.68	122.19	118.09
12	H	830	CLA	CMC-C2C-C1C	2.68	129.23	125.03
12	a	855	CLA	CHB-C4A-NA	2.68	128.27	124.40
15	A	844	BCR	C37-C22-C21	-2.68	118.47	122.82
12	a	811	CLA	CMC-C2C-C1C	2.68	129.23	125.03
15	B	842	BCR	C36-C18-C17	-2.68	118.47	122.82
12	A	803	CLA	C3C-C4C-NC	2.68	113.87	110.43
12	A	817	CLA	CMB-C2B-C3B	2.68	132.86	126.55
15	F	202	BCR	C31-C1-C6	-2.68	106.03	110.24
12	b	814	CLA	C4D-C3D-CAD	2.68	111.02	108.11
12	G	818	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
12	a	803	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
12	a	827	CLA	CHD-C1D-ND	-2.68	121.03	124.80
12	a	833	CLA	C1-C2-C3	-2.68	121.80	126.20
12	G	815	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
13	G	843	1L3	C15-C14-C03	-2.68	105.48	112.08
12	G	811	CLA	C4D-C3D-CAD	2.68	111.02	108.11
15	a	844	BCR	C36-C18-C17	-2.68	118.47	122.82
12	B	801	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	b	823	CLA	CHD-C4C-C3C	-2.68	120.87	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	806	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
12	A	805	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	B	815	CLA	CMB-C2B-C3B	2.68	132.85	126.55
12	a	819	CLA	CMB-C2B-C1B	2.68	129.50	125.42
12	A	811	CLA	CHD-C1D-ND	-2.68	121.03	124.80
12	b	834	CLA	CBC-CAC-C3C	-2.68	105.16	112.42
12	A	836	CLA	O2A-C1-C2	2.68	118.41	108.11
12	b	837	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
12	H	809	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
12	A	802	CLA	C3D-C4D-ND	2.67	114.33	109.99
12	B	822	CLA	CMC-C2C-C1C	2.67	129.21	125.03
12	G	810	CLA	CED-O2D-CGD	2.67	121.98	115.92
12	a	808	CLA	C1-C2-C3	-2.67	122.44	126.76
15	B	842	BCR	C39-C30-C25	-2.67	106.05	110.24
12	f	203	CLA	CAC-C3C-C4C	2.67	128.27	124.79
12	S	204	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
12	B	834	CLA	C4D-C3D-CAD	2.67	111.01	108.11
12	R	103	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
12	b	848	CLA	C4-C3-C5	2.67	119.86	115.23
12	A	810	CLA	C3D-C4D-ND	2.67	114.33	109.99
12	H	819	CLA	CMC-C2C-C1C	2.67	129.21	125.03
12	G	839	CLA	C4D-C3D-CAD	2.67	111.01	108.11
12	b	808	CLA	C4D-C3D-CAD	2.67	111.01	108.11
12	B	806	CLA	C4D-C3D-CAD	2.67	111.01	108.11
12	l	202	CLA	C1-O2A-CGA	2.67	123.11	116.65
12	H	815	CLA	C3D-C4D-ND	2.67	114.33	109.99
12	G	839	CLA	CMC-C2C-C1C	2.67	129.20	125.03
12	B	826	CLA	C1-C2-C3	-2.67	121.83	126.20
12	G	821	CLA	C4D-C3D-CAD	2.67	111.00	108.11
15	j	101	BCR	C36-C18-C17	-2.67	118.50	122.82
12	a	816	CLA	OBD-CAD-C3D	-2.67	122.19	128.42
12	a	814	CLA	C3C-C4C-NC	2.67	113.84	110.43
16	G	852	LHG	C5-O7-C7	-2.66	111.42	117.80
12	H	817	CLA	C3D-C4D-ND	2.66	114.32	109.99
12	b	807	CLA	C6-C5-C3	-2.66	106.98	113.47
12	G	827	CLA	CMC-C2C-C1C	2.66	129.20	125.03
15	a	847	BCR	C12-C13-C14	-2.66	114.82	119.01
12	B	823	CLA	C4-C3-C5	2.66	119.85	115.23
18	B	846	LMG	O8-C28-C29	2.66	119.95	111.83
15	P	204	BCR	C38-C26-C27	2.66	119.27	113.60
12	b	814	CLA	C3D-C4D-ND	2.66	114.31	109.99
12	A	816	CLA	OBD-CAD-C3D	-2.66	122.19	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	804	CLA	CMB-C2B-C1B	2.66	129.47	125.42
12	A	819	CLA	CMB-C2B-C1B	2.66	129.47	125.42
12	G	807	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
12	f	201	CLA	CAC-C3C-C4C	2.66	128.25	124.79
11	a	801	CL0	C3D-C4D-ND	2.66	114.31	109.99
12	H	807	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
12	G	812	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
15	i	101	BCR	C38-C26-C25	-2.66	121.58	124.48
15	H	849	BCR	C37-C22-C21	-2.66	118.51	122.82
12	a	822	CLA	C4D-C3D-CAD	2.66	110.99	108.11
12	A	819	CLA	C4D-C3D-CAD	2.66	110.99	108.11
12	G	818	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
12	l	205	CLA	C1-C2-C3	-2.66	121.84	126.20
12	G	813	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
12	B	838	CLA	CAC-C3C-C4C	2.66	128.25	124.79
15	A	847	BCR	C35-C13-C12	2.66	122.15	118.09
12	b	824	CLA	OBD-CAD-C3D	-2.66	122.20	128.42
12	H	812	CLA	CMB-C2B-C3B	2.66	132.80	126.55
12	A	839	CLA	CAC-C3C-C4C	2.66	128.25	124.79
12	G	835	CLA	CMA-C3A-C4A	2.66	118.91	111.77
11	A	801	CL0	CMB-C2B-C1B	2.66	129.46	125.42
15	B	843	BCR	C37-C22-C23	2.66	122.15	118.09
12	G	816	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	G	815	CLA	C4D-C3D-CAD	2.66	110.99	108.11
15	L	203	BCR	C12-C13-C14	-2.66	114.83	119.01
12	G	856	CLA	CMB-C2B-C3B	2.66	132.80	126.55
12	G	834	CLA	C3D-C4D-ND	2.66	114.30	109.99
12	a	811	CLA	CMB-C2B-C1B	2.66	129.46	125.42
12	a	803	CLA	CMB-C2B-C1B	2.66	129.46	125.42
12	G	855	CLA	C4C-C3C-C2C	-2.65	103.03	106.89
15	G	845	BCR	C36-C18-C17	-2.65	118.52	122.82
12	a	802	CLA	C3D-C4D-ND	2.65	114.30	109.99
15	F	204	BCR	C36-C18-C17	-2.65	118.52	122.82
15	I	101	BCR	C32-C1-C6	-2.65	106.08	110.24
12	b	818	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
12	G	806	CLA	C4-C3-C5	2.65	119.83	115.23
12	b	811	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	a	837	CLA	C1-C2-C3	-2.65	121.85	126.20
12	B	815	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	A	817	CLA	C4A-NA-C1A	2.65	107.89	106.68
12	b	819	CLA	C3C-C4C-NC	2.65	113.82	110.43
15	Q	101	BCR	C32-C1-C6	-2.65	106.09	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	841	CLA	CMA-C3A-C4A	2.65	118.89	111.77
15	b	839	BCR	C36-C18-C17	-2.65	118.53	122.82
12	A	815	CLA	C3D-C4D-ND	2.65	114.29	109.99
12	b	832	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
12	A	813	CLA	CMC-C2C-C1C	2.65	129.17	125.03
12	B	815	CLA	C4D-C3D-CAD	2.65	110.98	108.11
12	a	840	CLA	CHD-C1D-ND	-2.65	121.08	124.80
12	b	803	CLA	CMB-C2B-C3B	2.65	132.77	126.55
15	G	846	BCR	C35-C13-C12	2.65	122.13	118.09
12	G	828	CLA	CBA-CAA-C2A	2.65	121.66	113.79
15	J	101	BCR	C31-C1-C6	-2.64	106.10	110.24
12	a	802	CLA	C4A-NA-C1A	2.64	107.89	106.68
12	A	822	CLA	C3C-C4C-NC	2.64	113.82	110.43
15	L	203	BCR	C38-C26-C25	-2.64	121.60	124.48
12	a	810	CLA	CMD-C2D-C3D	-2.64	121.63	127.69
12	j	102	CLA	CMA-C3A-C4A	2.64	118.87	111.77
15	H	846	BCR	C15-C14-C13	-2.64	123.57	127.28
12	A	809	CLA	C4D-C3D-CAD	2.64	110.97	108.11
15	l	201	BCR	C19-C18-C17	2.64	123.16	119.01
11	a	801	CL0	C3D-C2D-C1D	-2.64	102.23	105.83
12	G	812	CLA	CMA-C3A-C4A	2.64	118.87	111.77
12	A	817	CLA	CHB-C1B-C2B	-2.64	119.76	127.43
13	b	838	1L3	C14-C03-C04	2.64	121.36	118.58
12	b	811	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
12	G	827	CLA	CMA-C3A-C4A	2.64	118.87	111.77
12	H	802	CLA	C3D-C4D-ND	2.64	114.28	109.99
12	H	808	CLA	CMB-C2B-C1B	2.64	129.44	125.42
15	j	103	BCR	C30-C25-C26	-2.64	119.03	122.64
15	i	102	BCR	C38-C26-C25	-2.64	121.61	124.48
12	b	831	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
12	A	802	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
12	G	821	CLA	CHB-C4A-NA	2.64	128.21	124.40
12	A	832	CLA	O2A-C1-C2	2.64	118.26	108.11
12	A	826	CLA	C4D-C3D-CAD	2.64	110.97	108.11
12	A	830	CLA	O1D-CGD-CBD	-2.64	119.32	124.52
12	a	839	CLA	CHB-C4A-NA	2.64	128.20	124.40
12	B	831	CLA	CHD-C1D-ND	-2.64	121.09	124.80
12	L	205	CLA	CBC-CAC-C3C	-2.63	105.28	112.42
12	b	804	CLA	CAA-C2A-C3A	-2.63	105.88	113.00
12	G	820	CLA	C4D-C3D-CAD	2.63	110.97	108.11
12	b	837	CLA	CAC-C3C-C4C	2.63	128.22	124.79
12	H	826	CLA	C1D-ND-C4D	-2.63	104.46	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	820	CLA	CMB-C2B-C1B	2.63	129.43	125.42
12	G	842	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
12	H	832	CLA	CAC-C3C-C4C	2.63	128.22	124.79
12	G	803	CLA	C4A-NA-C1A	2.63	107.88	106.68
15	B	842	BCR	C33-C5-C4	2.63	119.21	113.60
12	H	823	CLA	CAC-C3C-C4C	2.63	128.21	124.79
12	a	840	CLA	C4D-C3D-CAD	2.63	110.96	108.11
12	F	201	CLA	C3D-C4D-ND	2.63	114.26	109.99
15	I	101	BCR	C38-C26-C25	-2.63	121.61	124.48
12	G	812	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
12	a	839	CLA	CAC-C3C-C4C	2.63	128.21	124.79
12	B	813	CLA	C3D-C4D-ND	2.63	114.26	109.99
12	G	821	CLA	CMB-C2B-C3B	2.63	132.74	126.55
12	a	817	CLA	CBA-CAA-C2A	2.63	121.62	113.79
12	H	838	CLA	C1-O2A-CGA	2.63	123.02	116.65
12	H	803	CLA	CMC-C2C-C1C	2.63	129.14	125.03
12	H	812	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
12	b	833	CLA	C3C-C4C-NC	2.63	113.80	110.43
12	b	836	CLA	C4-C3-C5	2.63	119.79	115.23
12	G	803	CLA	C3D-C4D-ND	2.63	114.26	109.99
12	b	820	CLA	CED-O2D-CGD	2.63	121.87	115.92
12	B	824	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
15	L	201	BCR	C35-C13-C12	2.63	122.10	118.09
12	S	203	CLA	CBC-CAC-C3C	-2.63	105.30	112.42
12	B	819	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
12	b	807	CLA	C4-C3-C5	2.63	119.79	115.23
12	a	827	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
12	b	816	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
12	L	204	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
15	a	849	BCR	C33-C5-C4	2.62	119.19	113.60
12	A	806	CLA	CMB-C2B-C3B	2.62	132.72	126.55
15	H	843	BCR	C36-C18-C17	-2.62	118.56	122.82
12	G	840	CLA	CHD-C1D-ND	-2.62	121.11	124.80
12	G	817	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
12	H	803	CLA	C4D-C3D-CAD	2.62	110.96	108.11
12	G	804	CLA	OBD-CAD-C3D	-2.62	122.28	128.42
12	a	815	CLA	C3D-C4D-ND	2.62	114.25	109.99
12	B	814	CLA	C3D-C4D-ND	2.62	114.25	109.99
12	G	808	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
12	G	838	CLA	CMB-C2B-C1B	2.62	129.41	125.42
15	G	850	BCR	C37-C22-C23	2.62	122.09	118.09
12	A	855	CLA	C3D-C4D-ND	2.62	114.25	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	834	CLA	CMC-C2C-C1C	2.62	129.13	125.03
12	a	813	CLA	C4D-C3D-CAD	2.62	110.95	108.11
12	b	803	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
12	P	203	CLA	CAC-C3C-C4C	2.62	128.20	124.79
15	I	101	BCR	C33-C5-C6	-2.62	121.63	124.48
12	G	814	CLA	C4D-C3D-CAD	2.62	110.95	108.11
12	B	833	CLA	C3C-C4C-NC	2.62	113.78	110.43
12	H	835	CLA	CBA-CAA-C2A	2.62	121.58	113.79
12	b	821	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
12	a	817	CLA	CMD-C2D-C3D	-2.62	121.69	127.69
12	A	836	CLA	CHA-C4D-ND	2.62	137.95	132.55
12	b	831	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
12	A	809	CLA	C3C-C4C-NC	2.62	113.78	110.43
12	b	803	CLA	C4D-C3D-CAD	2.62	110.95	108.11
12	b	819	CLA	C4D-C3D-CAD	2.62	110.95	108.11
12	H	812	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
12	A	808	CLA	CMB-C2B-C3B	2.62	132.70	126.55
12	a	819	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
12	a	826	CLA	C4D-C3D-CAD	2.61	110.95	108.11
12	G	816	CLA	C3D-C4D-ND	2.61	114.24	109.99
12	a	818	CLA	CAA-C2A-C1A	-2.61	103.41	111.97
15	G	850	BCR	C19-C18-C17	2.61	123.12	119.01
12	a	820	CLA	CAC-C3C-C4C	2.61	128.19	124.79
12	J	103	CLA	C3C-C4C-NC	2.61	113.78	110.43
12	B	804	CLA	CED-O2D-CGD	2.61	121.84	115.92
12	G	824	CLA	CMC-C2C-C1C	2.61	129.12	125.03
12	G	837	CLA	C3D-C4D-ND	2.61	114.23	109.99
12	b	826	CLA	CMC-C2C-C3C	2.61	133.21	126.15
12	B	827	CLA	C3C-C4C-NC	2.61	113.77	110.43
12	H	808	CLA	C3C-C4C-NC	2.61	113.77	110.43
12	a	825	CLA	C3C-C4C-NC	2.61	113.77	110.43
12	A	840	CLA	C4D-C3D-CAD	2.61	110.94	108.11
12	H	835	CLA	C3D-C4D-ND	2.61	114.22	109.99
12	A	819	CLA	C3D-C4D-ND	2.61	114.22	109.99
12	G	811	CLA	CMB-C2B-C1B	2.61	129.39	125.42
12	a	809	CLA	CMC-C2C-C1C	2.61	129.11	125.03
12	b	824	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
12	B	805	CLA	C4C-C3C-C2C	-2.61	103.10	106.89
12	b	833	CLA	C3D-C4D-ND	2.61	114.22	109.99
12	b	831	CLA	C3D-C4D-ND	2.61	114.22	109.99
12	a	841	CLA	CHD-C1D-ND	-2.61	121.14	124.80
12	b	807	CLA	C3B-C4B-NB	2.60	112.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	822	CLA	O2A-C1-C2	2.60	118.13	108.11
12	a	824	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
12	b	836	CLA	CAC-C3C-C4C	-2.60	121.40	124.79
12	B	809	CLA	CMC-C2C-C1C	2.60	129.10	125.03
12	f	203	CLA	C3D-C4D-ND	2.60	114.22	109.99
15	P	202	BCR	C39-C30-C25	-2.60	106.16	110.24
12	H	803	CLA	CAC-C3C-C4C	2.60	128.18	124.79
12	H	812	CLA	C3D-C4D-ND	2.60	114.22	109.99
12	G	806	CLA	CAA-CBA-CGA	-2.60	105.82	113.21
12	A	836	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
12	a	809	CLA	CMA-C3A-C4A	2.60	118.77	111.77
12	B	802	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
12	A	811	CLA	CMB-C2B-C1B	2.60	129.38	125.42
12	B	816	CLA	CED-O2D-CGD	2.60	121.81	115.92
12	B	819	CLA	C3C-C4C-NC	2.60	113.76	110.43
12	G	814	CLA	C3D-C4D-ND	2.60	114.21	109.99
12	l	202	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
12	A	841	CLA	C1-C2-C3	-2.60	121.94	126.20
12	P	201	CLA	CMB-C2B-C3B	2.60	132.66	126.55
12	A	834	CLA	C3D-C4D-ND	2.60	114.21	109.99
12	a	821	CLA	CBA-CAA-C2A	2.60	121.53	113.79
12	G	818	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
12	A	825	CLA	CMB-C2B-C3B	2.60	132.66	126.55
12	B	832	CLA	CMA-C3A-C4A	2.60	118.76	111.77
12	A	855	CLA	C4D-C3D-CAD	2.60	110.93	108.11
12	f	203	CLA	C4D-C3D-CAD	2.60	110.93	108.11
12	b	824	CLA	O2D-CGD-CBD	2.60	115.77	111.23
15	B	840	BCR	C30-C25-C26	-2.60	119.09	122.64
12	G	810	CLA	C3D-C4D-ND	2.60	114.21	109.99
12	A	833	CLA	CMC-C2C-C1C	2.60	129.09	125.03
15	j	101	BCR	C31-C1-C6	-2.60	106.17	110.24
12	A	819	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
15	A	845	BCR	C34-C9-C10	-2.59	118.61	122.82
12	B	804	CLA	CAA-C2A-C3A	-2.59	105.99	113.00
12	B	807	CLA	C3C-C4C-NC	2.59	113.75	110.43
12	B	837	CLA	C4D-C3D-CAD	2.59	110.92	108.11
15	a	849	BCR	C35-C13-C12	2.59	122.05	118.09
12	B	827	CLA	CMB-C2B-C1B	2.59	129.37	125.42
12	G	833	CLA	C1-C2-C3	-2.59	121.95	126.20
12	a	855	CLA	C3C-C4C-NC	2.59	113.75	110.43
12	A	818	CLA	C3C-C4C-NC	2.59	113.75	110.43
12	a	829	CLA	C3D-C4D-ND	2.59	114.20	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	837	CLA	C1-O2A-CGA	2.59	122.93	116.65
12	B	826	CLA	CMC-C2C-C3C	2.59	133.16	126.15
12	b	815	CLA	C4-C3-C5	2.59	119.73	115.23
12	B	811	CLA	C3D-C4D-ND	2.59	114.20	109.99
12	A	805	CLA	C4-C3-C5	2.59	119.73	115.23
12	S	204	CLA	C3C-C4C-NC	2.59	113.75	110.43
12	G	829	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	b	812	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	H	805	CLA	CMA-C3A-C4A	2.59	118.74	111.77
12	b	826	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
15	H	841	BCR	C30-C25-C26	-2.59	119.10	122.64
12	H	820	CLA	C3C-C4C-NC	2.59	113.75	110.43
12	H	838	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
12	H	820	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
12	A	810	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
15	a	845	BCR	C35-C13-C12	2.59	122.04	118.09
12	A	816	CLA	C3D-C4D-ND	2.59	114.20	109.99
12	b	805	CLA	C1-O2A-CGA	2.59	122.92	116.65
12	B	810	CLA	CHD-C4C-C3C	-2.59	121.00	124.77
12	G	815	CLA	C3C-C4C-NC	2.59	113.75	110.43
12	G	829	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
15	b	843	BCR	C1-C6-C7	2.59	122.67	115.65
12	G	820	CLA	C3D-C4D-ND	2.59	114.19	109.99
12	b	808	CLA	C3D-C4D-ND	2.59	114.19	109.99
12	H	827	CLA	CHD-C4C-C3C	2.59	128.55	124.77
12	H	814	CLA	C3D-C4D-ND	2.59	114.19	109.99
12	a	809	CLA	C4D-C3D-CAD	2.59	110.92	108.11
12	b	815	CLA	CHB-C4A-NA	2.59	128.13	124.40
12	B	835	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
12	B	837	CLA	CMA-C3A-C4A	2.59	118.73	111.77
12	A	804	CLA	CMB-C2B-C1B	2.59	129.36	125.42
12	H	838	CLA	C4-C3-C5	2.59	119.72	115.23
12	H	819	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
15	l	201	BCR	C23-C22-C21	2.59	123.08	119.01
12	a	821	CLA	CMA-C3A-C4A	2.59	118.72	111.77
12	j	102	CLA	C3C-C4C-NC	2.59	113.74	110.43
12	a	810	CLA	CMB-C2B-C1B	2.58	129.35	125.42
12	b	817	CLA	CMB-C2B-C1B	2.58	129.35	125.42
12	j	102	CLA	C4C-C3C-C2C	-2.58	103.13	106.89
12	B	816	CLA	C3D-C4D-ND	2.58	114.19	109.99
15	a	844	BCR	C33-C5-C6	-2.58	121.66	124.48
12	a	811	CLA	CAA-C2A-C3A	-2.58	106.02	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	823	CLA	C4D-C3D-CAD	2.58	110.91	108.11
12	B	810	CLA	C4D-C3D-CAD	2.58	110.91	108.11
12	b	819	CLA	CMC-C2C-C1C	2.58	129.07	125.03
12	b	837	CLA	C3C-C4C-NC	2.58	113.74	110.43
12	b	834	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
12	a	807	CLA	C3C-C4C-NC	2.58	113.74	110.43
12	A	835	CLA	C3C-C4C-NC	2.58	113.74	110.43
12	A	830	CLA	CHD-C1D-ND	-2.58	121.17	124.80
15	A	845	BCR	C38-C26-C25	-2.58	121.67	124.48
15	l	201	BCR	C40-C30-C39	-2.58	101.24	108.63
11	a	801	CL0	CHA-C4D-ND	2.58	137.87	132.55
12	A	828	CLA	C1-C2-C3	-2.58	121.97	126.20
15	I	101	BCR	C38-C26-C27	2.58	119.10	113.60
12	L	204	CLA	C3C-C4C-NC	2.58	113.73	110.43
12	B	821	CLA	C1-O2A-CGA	2.58	122.89	116.65
12	a	829	CLA	C2B-C1B-NB	2.58	113.00	110.33
12	A	802	CLA	CHD-C1D-ND	-2.58	121.17	124.80
12	G	817	CLA	C3D-C4D-ND	2.58	114.18	109.99
12	a	835	CLA	CMC-C2C-C1C	2.58	129.06	125.03
12	a	830	CLA	CAC-C3C-C4C	2.58	128.14	124.79
12	G	812	CLA	C4D-C3D-CAD	2.58	110.91	108.11
12	b	809	CLA	CMC-C2C-C1C	2.58	129.06	125.03
12	G	834	CLA	C3C-C4C-NC	2.58	113.73	110.43
12	B	802	CLA	C11-C10-C8	-2.58	107.40	115.97
12	B	833	CLA	C4D-C3D-CAD	2.58	110.90	108.11
12	b	805	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
12	a	805	CLA	CAA-CBA-CGA	-2.58	105.90	113.21
12	A	815	CLA	CMC-C2C-C1C	2.58	129.06	125.03
12	b	816	CLA	C3D-C4D-ND	2.57	114.17	109.99
15	G	853	BCR	C34-C9-C10	-2.57	118.64	122.82
12	B	821	CLA	O2A-C1-C2	2.57	118.02	108.11
12	H	812	CLA	CMC-C2C-C1C	2.57	129.06	125.03
12	L	202	CLA	C3C-C4C-NC	2.57	113.73	110.43
12	a	802	CLA	CAA-CBA-CGA	-2.57	105.90	113.21
15	B	843	BCR	C38-C26-C25	-2.57	121.68	124.48
12	A	833	CLA	C3D-C4D-ND	2.57	114.17	109.99
12	A	829	CLA	CED-O2D-CGD	2.57	121.75	115.92
12	b	806	CLA	C3C-C4C-NC	2.57	113.72	110.43
12	A	830	CLA	CMB-C2B-C1B	2.57	129.34	125.42
12	a	819	CLA	C4D-C3D-CAD	2.57	110.90	108.11
12	b	815	CLA	CMB-C2B-C3B	2.57	132.60	126.55
12	H	810	CLA	C3C-C4C-NC	2.57	113.72	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	811	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
12	b	821	CLA	CMD-C2D-C3D	-2.57	121.79	127.69
12	b	806	CLA	C3D-C4D-ND	2.57	114.17	109.99
12	A	814	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
12	a	815	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
15	l	201	BCR	C1-C6-C5	-2.57	119.12	122.64
15	b	847	BCR	C36-C18-C17	-2.57	118.65	122.82
12	B	827	CLA	C3D-C4D-ND	2.57	114.16	109.99
12	A	809	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
12	b	831	CLA	CMB-C2B-C1B	2.57	129.33	125.42
12	A	831	CLA	CMA-C3A-C4A	2.57	118.67	111.77
11	a	801	CL0	CGD-CBD-CAD	-2.57	102.53	110.85
12	a	819	CLA	C3D-C4D-ND	2.57	114.16	109.99
12	B	826	CLA	C2B-C1B-NB	2.57	112.99	110.33
15	i	101	BCR	C38-C26-C27	2.57	119.07	113.60
12	b	825	CLA	C3D-C4D-ND	2.57	114.16	109.99
12	A	832	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
12	A	818	CLA	C4D-C3D-CAD	2.57	110.89	108.11
12	B	837	CLA	CHC-C1C-C2C	-2.57	119.66	126.95
12	B	805	CLA	CMD-C2D-C3D	-2.57	121.81	127.69
12	G	822	CLA	CBA-CAA-C2A	2.57	121.42	113.79
12	a	809	CLA	C2B-C1B-NB	2.57	112.99	110.33
12	a	807	CLA	CBA-CAA-C2A	2.56	121.42	113.79
12	a	803	CLA	C3C-C4C-NC	2.56	113.72	110.43
11	G	801	CL0	O2D-CGD-O1D	-2.56	118.86	123.85
12	F	201	CLA	CHD-C1D-ND	-2.56	121.19	124.80
12	H	827	CLA	C1-C2-C3	-2.56	122.00	126.20
12	a	813	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
12	B	808	CLA	CMB-C2B-C1B	2.56	129.32	125.42
12	H	828	CLA	C3C-C4C-NC	2.56	113.71	110.43
15	l	203	BCR	C38-C26-C25	-2.56	121.69	124.48
12	l	202	CLA	CMB-C2B-C1B	2.56	129.32	125.42
12	A	806	CLA	C3D-C4D-ND	2.56	114.15	109.99
15	a	852	BCR	C23-C22-C21	2.56	123.04	119.01
12	A	840	CLA	CHD-C1D-ND	-2.56	121.20	124.80
12	H	836	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
12	B	801	CLA	CHB-C1B-C2B	-2.56	119.99	127.43
12	J	103	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	G	825	CLA	CMB-C2B-C3B	2.56	132.57	126.55
12	a	822	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	B	808	CLA	C3D-C4D-ND	2.56	114.15	109.99
12	B	837	CLA	C3D-C4D-ND	2.56	114.15	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	816	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	G	830	CLA	C4-C3-C5	2.56	119.67	115.23
12	A	803	CLA	CMC-C2C-C1C	2.56	129.03	125.03
15	b	839	BCR	C30-C25-C26	-2.56	119.14	122.64
12	B	835	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
12	G	856	CLA	C4D-C3D-CAD	2.56	110.89	108.11
12	a	824	CLA	CMB-C2B-C3B	2.56	132.57	126.55
12	A	817	CLA	C3D-C4D-ND	2.56	114.14	109.99
12	G	802	CLA	C4D-C3D-CAD	2.56	110.88	108.11
12	a	821	CLA	C4D-C3D-CAD	2.56	110.88	108.11
12	b	836	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
12	A	831	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
12	A	837	CLA	C1-C2-C3	-2.56	122.01	126.20
12	a	826	CLA	C4-C3-C5	2.56	119.67	115.23
12	H	839	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
12	B	805	CLA	C1-O2A-CGA	2.56	122.84	116.65
12	A	830	CLA	CAC-C3C-C4C	2.56	128.12	124.79
12	R	103	CLA	CMB-C2B-C1B	2.56	129.31	125.42
12	l	206	CLA	C3C-C4C-NC	2.56	113.70	110.43
15	G	850	BCR	C33-C5-C4	2.56	119.05	113.60
12	G	802	CLA	CHD-C1D-ND	-2.56	121.21	124.80
12	G	832	CLA	CMC-C2C-C1C	2.56	129.03	125.03
15	Q	101	BCR	C38-C26-C27	2.56	119.04	113.60
12	a	834	CLA	C4D-C3D-CAD	2.56	110.88	108.11
12	A	826	CLA	CHD-C1D-ND	-2.55	121.21	124.80
12	H	827	CLA	CMC-C2C-C1C	2.55	129.03	125.03
15	S	205	BCR	C1-C6-C5	-2.55	119.14	122.64
15	I	101	BCR	C37-C22-C21	-2.55	118.68	122.82
12	b	810	CLA	C4D-C3D-CAD	2.55	110.88	108.11
12	A	821	CLA	CBA-CAA-C2A	2.55	121.39	113.79
15	B	845	BCR	C15-C14-C13	-2.55	123.70	127.28
15	B	844	BCR	C1-C6-C7	2.55	122.58	115.65
12	j	104	CLA	C3C-C4C-NC	2.55	113.70	110.43
12	A	821	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
12	H	830	CLA	CMB-C2B-C3B	2.55	132.56	126.55
12	G	815	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
12	F	201	CLA	CAC-C3C-C4C	2.55	128.11	124.79
12	A	805	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
12	H	824	CLA	C4-C3-C5	2.55	119.66	115.23
12	H	821	CLA	C3D-C4D-ND	2.55	114.14	109.99
12	G	815	CLA	CMC-C2C-C3C	2.55	133.05	126.15
12	A	837	CLA	C3D-C4D-ND	2.55	114.13	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	104	BCR	C34-C9-C8	2.55	121.98	118.09
12	A	809	CLA	CMA-C3A-C4A	2.55	118.63	111.77
12	b	829	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
15	f	202	BCR	C2-C1-C6	2.55	114.14	110.44
12	A	829	CLA	CHD-C1D-ND	-2.55	121.22	124.80
12	b	827	CLA	CAC-C3C-C4C	2.55	128.10	124.79
12	b	830	CLA	CAC-C3C-C4C	2.55	128.10	124.79
12	G	831	CLA	CMD-C2D-C3D	-2.55	121.85	127.69
15	b	841	BCR	C33-C5-C4	2.55	119.03	113.60
15	A	849	BCR	C4-C5-C6	-2.55	119.26	122.70
15	Q	101	BCR	C33-C5-C6	-2.55	121.70	124.48
12	b	832	CLA	CAC-C3C-C4C	2.55	128.10	124.79
12	f	203	CLA	CMB-C2B-C1B	2.55	129.30	125.42
12	G	822	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
12	a	814	CLA	CMC-C2C-C3C	2.55	133.03	126.15
12	L	205	CLA	C3C-C4C-NC	2.55	113.69	110.43
12	B	815	CLA	C1-C2-C3	-2.55	122.03	126.20
12	F	203	CLA	C4D-C3D-CAD	2.54	110.87	108.11
12	A	839	CLA	CMB-C2B-C3B	2.54	132.53	126.55
12	B	806	CLA	CAA-CBA-CGA	2.54	120.43	113.21
15	I	101	BCR	C27-C26-C25	-2.54	119.27	122.70
12	b	806	CLA	CHD-C1D-ND	-2.54	121.22	124.80
12	a	816	CLA	C4D-C3D-CAD	2.54	110.87	108.11
12	a	828	CLA	C4D-C3D-CAD	2.54	110.87	108.11
12	a	834	CLA	C3D-C4D-ND	2.54	114.12	109.99
12	F	203	CLA	C3D-C4D-ND	2.54	114.12	109.99
12	H	808	CLA	C4-C3-C5	2.54	119.64	115.23
12	F	203	CLA	CAC-C3C-C4C	2.54	128.10	124.79
12	G	820	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
12	H	827	CLA	C2B-C1B-NB	2.54	112.96	110.33
12	A	854	CLA	C4-C3-C2	-2.54	117.10	123.63
12	H	828	CLA	C3D-C4D-ND	2.54	114.12	109.99
12	L	202	CLA	C3D-C4D-ND	2.54	114.12	109.99
12	A	855	CLA	C3C-C4C-NC	2.54	113.68	110.43
12	H	837	CLA	CED-O2D-CGD	2.54	121.68	115.92
12	H	850	CLA	C4-C3-C5	2.54	119.64	115.23
12	B	828	CLA	C3C-C4C-NC	2.54	113.68	110.43
12	a	830	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
12	A	829	CLA	C4-C3-C5	2.54	119.64	115.23
12	B	803	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
12	G	831	CLA	CMA-C3A-C4A	2.54	118.59	111.77
12	S	203	CLA	C3C-C4C-NC	2.54	113.68	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	804	CLA	CBC-CAC-C3C	-2.54	105.54	112.42
12	a	802	CLA	C2B-C1B-NB	2.54	112.96	110.33
12	H	812	CLA	C3C-C4C-NC	2.54	113.68	110.43
17	T	101	45D	C06-C04-C08	2.54	114.12	110.44
15	G	850	BCR	C40-C30-C25	2.54	114.22	110.24
15	A	845	BCR	C35-C13-C12	2.54	121.96	118.09
15	A	847	BCR	C2-C1-C6	2.54	114.12	110.44
12	A	822	CLA	C1-C2-C3	-2.54	122.66	126.76
12	G	822	CLA	CMA-C3A-C4A	2.54	118.59	111.77
12	G	818	CLA	C3C-C4C-NC	2.54	113.68	110.43
12	R	103	CLA	C3C-C4C-NC	2.54	113.68	110.43
12	a	833	CLA	C3D-C4D-ND	2.54	114.11	109.99
12	l	205	CLA	O1D-CGD-CBD	-2.54	119.52	124.52
15	a	848	BCR	C36-C18-C17	-2.53	118.71	122.82
12	H	819	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
12	B	810	CLA	C4-C3-C5	2.53	119.63	115.23
15	L	201	BCR	C1-C6-C5	-2.53	119.17	122.64
12	b	827	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
12	a	813	CLA	CAA-C2A-C3A	-2.53	106.15	113.00
12	A	838	CLA	CMB-C2B-C1B	2.53	129.28	125.42
12	B	803	CLA	C3D-C4D-ND	2.53	114.11	109.99
12	a	830	CLA	CHD-C1D-ND	-2.53	121.24	124.80
12	A	834	CLA	C3C-C4C-NC	2.53	113.67	110.43
12	H	802	CLA	CHC-C1C-NC	-2.53	120.50	124.31
16	a	851	LHG	C5-O7-C7	-2.53	111.73	117.80
12	L	205	CLA	C1-C2-C3	-2.53	122.05	126.20
12	G	810	CLA	C3C-C4C-NC	2.53	113.67	110.43
12	G	835	CLA	C3C-C4C-NC	2.53	113.67	110.43
12	A	821	CLA	CMA-C3A-C4A	2.53	118.58	111.77
12	B	819	CLA	C4D-C3D-CAD	2.53	110.86	108.11
12	L	206	CLA	C4D-C3D-CAD	2.53	110.86	108.11
12	G	808	CLA	CMA-C3A-C4A	2.53	118.58	111.77
12	H	805	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
12	a	806	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
12	A	833	CLA	C3C-C4C-NC	2.53	113.67	110.43
12	B	833	CLA	CMC-C2C-C1C	2.53	128.99	125.03
12	b	824	CLA	C6-C5-C3	-2.53	107.31	113.47
12	A	825	CLA	C1-C2-C3	-2.53	122.05	126.20
12	a	834	CLA	CHD-C1D-ND	-2.53	121.24	124.80
12	b	811	CLA	CMB-C2B-C3B	2.53	132.50	126.55
12	H	820	CLA	C4D-C3D-CAD	2.53	110.85	108.11
12	a	825	CLA	C1-C2-C3	-2.53	122.06	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	829	CLA	C3C-C4C-NC	2.53	113.67	110.43
12	A	836	CLA	CHA-C1A-NA	-2.53	120.67	126.39
12	B	837	CLA	CHD-C4C-C3C	-2.53	121.09	124.77
12	a	820	CLA	CHB-C1B-C2B	-2.53	120.09	127.43
12	A	817	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
15	G	845	BCR	C33-C5-C6	-2.53	121.73	124.48
12	A	855	CLA	CHD-C1D-ND	-2.53	121.25	124.80
12	A	812	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
11	a	801	CL0	CHC-C1C-NC	-2.52	120.51	124.31
12	S	203	CLA	C3D-C4D-ND	2.52	114.09	109.99
12	H	833	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
12	G	836	CLA	CHA-C1A-NA	-2.52	120.67	126.39
15	F	202	BCR	C37-C22-C21	-2.52	118.73	122.82
12	a	826	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
12	B	827	CLA	CMC-C2C-C1C	2.52	128.98	125.03
15	R	101	BCR	C29-C28-C27	2.52	116.83	111.28
12	b	819	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
12	G	836	CLA	C3C-C4C-NC	2.52	113.66	110.43
12	H	806	CLA	CHD-C1D-ND	-2.52	121.25	124.80
12	G	820	CLA	CMC-C2C-C1C	2.52	128.98	125.03
12	A	823	CLA	C1-C2-C3	-2.52	122.06	126.20
12	H	833	CLA	C4D-C3D-CAD	2.52	110.85	108.11
12	f	201	CLA	CMB-C2B-C3B	2.52	132.48	126.55
12	H	822	CLA	CGD-CBD-CAD	-2.52	102.68	110.85
15	f	202	BCR	C37-C22-C21	-2.52	118.73	122.82
12	H	825	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
12	l	204	CLA	C3C-C4C-NC	2.52	113.66	110.43
12	B	815	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
12	a	854	CLA	C4C-C3C-C2C	-2.52	103.22	106.89
12	G	825	CLA	C4D-C3D-CAD	2.52	110.84	108.11
12	G	833	CLA	CHD-C1D-ND	-2.52	121.25	124.80
15	H	843	BCR	C33-C5-C4	2.52	118.97	113.60
12	a	821	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
12	a	817	CLA	C4C-C3C-C2C	-2.52	103.22	106.89
12	B	806	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	a	854	CLA	C3D-C4D-ND	2.52	114.08	109.99
12	G	826	CLA	C1-C2-C3	-2.52	122.07	126.20
12	A	855	CLA	C4-C3-C5	2.52	119.60	115.23
12	H	807	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
12	H	811	CLA	C6-C5-C3	-2.52	107.33	113.47
12	a	841	CLA	C1-C2-C3	-2.52	122.07	126.20
12	a	837	CLA	C3D-C4D-ND	2.52	114.08	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	839	CLA	CHD-C1D-ND	-2.52	121.26	124.80
12	a	817	CLA	C3D-C4D-ND	2.52	114.08	109.99
12	A	803	CLA	CMA-C3A-C4A	2.52	118.54	111.77
12	G	819	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
12	b	826	CLA	C1-C2-C3	-2.52	122.07	126.20
12	G	824	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
12	P	203	CLA	C3D-C4D-ND	2.52	114.08	109.99
12	P	201	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
12	a	832	CLA	C3C-C4C-NC	2.52	113.65	110.43
15	S	205	BCR	C19-C18-C17	2.52	122.97	119.01
15	b	841	BCR	C36-C18-C17	-2.52	118.74	122.82
12	H	816	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
12	B	832	CLA	C3D-C4D-ND	2.52	114.08	109.99
12	a	807	CLA	O1D-CGD-CBD	-2.52	119.56	124.52
15	H	845	BCR	C1-C6-C7	2.52	122.47	115.65
12	b	822	CLA	CMB-C2B-C3B	2.51	132.47	126.55
15	A	849	BCR	C24-C23-C22	-2.51	122.52	126.23
12	G	830	CLA	C3D-C4D-ND	2.51	114.07	109.99
12	a	825	CLA	CMB-C2B-C3B	2.51	132.46	126.55
12	A	802	CLA	CHA-C1A-NA	-2.51	120.70	126.39
12	B	836	CLA	CBA-CAA-C2A	2.51	121.27	113.79
12	B	807	CLA	CHD-C1D-ND	-2.51	121.27	124.80
15	a	848	BCR	C35-C13-C12	2.51	121.92	118.09
15	A	847	BCR	C30-C25-C26	-2.51	119.20	122.64
15	G	846	BCR	C38-C26-C25	-2.51	121.74	124.48
12	b	807	CLA	C2B-C1B-NB	2.51	112.93	110.33
12	B	837	CLA	C4-C3-C5	2.51	119.58	115.23
12	b	831	CLA	CMC-C2C-C1C	2.51	128.96	125.03
15	a	848	BCR	C38-C26-C27	2.51	118.95	113.60
12	S	202	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
12	G	819	CLA	C3C-C4C-NC	2.51	113.64	110.43
12	a	841	CLA	CMA-C3A-C4A	2.51	118.52	111.77
12	A	805	CLA	CMA-C3A-C2A	-2.51	104.28	113.98
12	A	825	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
12	G	805	CLA	CAC-C3C-C4C	2.51	128.05	124.79
12	A	836	CLA	C4C-C3C-C2C	-2.51	103.24	106.89
12	B	801	CLA	C4-C3-C5	2.51	119.58	115.23
12	H	801	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
12	A	841	CLA	C3D-C4D-ND	2.51	114.06	109.99
12	H	817	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
12	G	827	CLA	CMB-C2B-C3B	2.51	132.44	126.55
12	B	807	CLA	C6-C5-C3	-2.51	107.36	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	831	CLA	C3D-C4D-ND	2.50	114.06	109.99
12	G	842	CLA	C4D-C3D-CAD	2.50	110.83	108.11
12	A	826	CLA	CMB-C2B-C3B	2.50	132.44	126.55
13	B	839	1L3	C17-C16-C18	2.50	119.57	115.23
12	a	836	CLA	C3D-C4D-ND	2.50	114.06	109.99
12	H	810	CLA	CMC-C2C-C1C	2.50	128.95	125.03
12	G	823	CLA	C1-C2-C3	-2.50	122.71	126.76
12	a	823	CLA	C1-C2-C3	-2.50	122.10	126.20
15	a	845	BCR	C34-C9-C10	-2.50	118.76	122.82
15	R	101	BCR	C31-C1-C6	-2.50	106.32	110.24
12	H	839	CLA	C3D-C4D-ND	2.50	114.06	109.99
12	H	826	CLA	C2B-C1B-NB	2.50	112.92	110.33
12	b	824	CLA	CHA-C1A-NA	-2.50	120.72	126.39
12	A	837	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
12	b	803	CLA	C3C-C4C-NC	2.50	113.64	110.43
12	L	202	CLA	C4D-C3D-CAD	2.50	110.82	108.11
13	A	842	1L3	C14-C15-C16	-2.50	122.52	126.83
12	B	829	CLA	C3C-C4C-NC	2.50	113.63	110.43
15	F	204	BCR	C38-C26-C25	-2.50	121.75	124.48
12	G	817	CLA	CMB-C2B-C1B	2.50	129.23	125.42
15	i	101	BCR	C27-C26-C25	-2.50	119.33	122.70
12	G	807	CLA	C3D-C4D-ND	2.50	114.05	109.99
12	A	818	CLA	C3D-C4D-ND	2.50	114.05	109.99
12	R	103	CLA	C3D-C4D-ND	2.50	114.05	109.99
15	B	840	BCR	C36-C18-C17	-2.50	118.77	122.82
12	B	807	CLA	C3B-C4B-NB	2.50	112.76	110.53
12	a	836	CLA	O2A-C1-C2	2.50	117.72	108.11
12	b	805	CLA	CMC-C2C-C1C	2.50	128.94	125.03
12	a	815	CLA	C3C-C4C-NC	2.50	113.63	110.43
12	b	834	CLA	C3C-C4C-NC	2.50	113.63	110.43
12	B	803	CLA	C11-C10-C8	-2.50	107.66	115.97
12	H	814	CLA	C4-C3-C5	2.50	119.56	115.23
12	B	825	CLA	C3D-C4D-ND	2.50	114.05	109.99
12	G	816	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
12	b	815	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
15	A	849	BCR	C34-C9-C8	2.50	121.90	118.09
12	a	830	CLA	C3D-C4D-ND	2.50	114.05	109.99
12	a	813	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
12	b	811	CLA	C3C-C4C-NC	2.50	113.63	110.43
12	G	833	CLA	C3D-C4D-ND	2.50	114.04	109.99
12	G	841	CLA	C1-C2-C3	-2.50	122.11	126.20
12	G	855	CLA	CAA-C2A-C3A	-2.50	106.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	827	CLA	C3D-C4D-ND	2.50	114.04	109.99
12	b	801	CLA	CAA-C2A-C3A	-2.50	106.26	113.00
12	b	821	CLA	C1-O2A-CGA	2.49	122.69	116.65
12	A	822	CLA	C3D-C4D-ND	2.49	114.04	109.99
12	B	833	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
12	G	819	CLA	C3D-C4D-ND	2.49	114.04	109.99
15	f	204	BCR	C34-C9-C8	2.49	121.90	118.09
12	H	801	CLA	C3C-C4C-NC	2.49	113.62	110.43
12	b	836	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
12	G	837	CLA	C1-C2-C3	-2.49	122.11	126.20
12	a	854	CLA	C3B-C4B-NB	-2.49	108.30	110.53
12	G	833	CLA	CMC-C2C-C1C	2.49	128.93	125.03
12	H	831	CLA	C3D-C4D-ND	2.49	114.04	109.99
12	A	832	CLA	C4D-C3D-CAD	2.49	110.81	108.11
12	a	814	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
12	B	832	CLA	CAC-C3C-C4C	2.49	128.03	124.79
15	a	847	BCR	C30-C25-C26	-2.49	119.23	122.64
12	A	839	CLA	CMC-C2C-C1C	2.49	128.93	125.03
12	B	837	CLA	CAC-C3C-C4C	-2.49	121.55	124.79
12	a	808	CLA	CMC-C2C-C1C	2.49	128.93	125.03
12	B	802	CLA	C1-C2-C3	-2.49	122.12	126.20
12	H	808	CLA	C3D-C4D-ND	2.49	114.03	109.99
15	a	852	BCR	C38-C26-C27	2.49	118.90	113.60
12	B	823	CLA	CHA-C1A-NA	-2.49	120.75	126.39
12	a	820	CLA	C4D-C3D-CAD	2.49	110.81	108.11
12	b	819	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
12	A	834	CLA	CMC-C2C-C1C	2.49	128.92	125.03
12	B	801	CLA	CAA-CBA-CGA	-2.49	106.14	113.21
12	B	826	CLA	CHA-C4D-ND	2.49	137.68	132.55
12	B	832	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
12	B	825	CLA	CMC-C2C-C3C	2.49	132.88	126.15
12	B	836	CLA	C4-C3-C5	2.49	119.54	115.23
12	A	815	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
12	H	833	CLA	C3D-C4D-ND	2.49	114.03	109.99
15	G	849	BCR	C15-C14-C13	-2.49	123.79	127.28
12	G	809	CLA	C3D-C4D-ND	2.49	114.03	109.99
12	a	805	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
12	H	822	CLA	CMB-C2B-C3B	2.48	132.39	126.55
15	G	849	BCR	C36-C18-C17	-2.48	118.79	122.82
12	H	829	CLA	CBA-CAA-C2A	2.48	121.18	113.79
12	b	835	CLA	C4-C3-C5	2.48	119.54	115.23
12	B	829	CLA	O2D-CGD-O1D	-2.48	119.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	837	CLA	CBA-CAA-C2A	2.48	121.18	113.79
12	S	203	CLA	CBA-CAA-C2A	2.48	121.18	113.79
12	H	820	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
12	A	810	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
12	H	811	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
12	a	809	CLA	C3D-C4D-ND	2.48	114.02	109.99
12	B	825	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
12	B	828	CLA	CBA-CAA-C2A	2.48	121.18	113.79
12	a	835	CLA	CBA-CAA-C2A	2.48	121.18	113.79
12	l	205	CLA	CBA-CAA-C2A	2.48	121.18	113.79
12	a	841	CLA	C3D-C4D-ND	2.48	114.02	109.99
12	a	802	CLA	C4C-C3C-C2C	-2.48	103.28	106.89
12	G	805	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
12	b	833	CLA	C4D-C3D-CAD	2.48	110.80	108.11
12	a	822	CLA	C1-C2-C3	-2.48	122.75	126.76
12	F	203	CLA	CMC-C2C-C1C	2.48	128.91	125.03
12	b	831	CLA	C4D-C3D-CAD	2.48	110.80	108.11
12	H	838	CLA	CMA-C3A-C4A	2.48	118.43	111.77
12	G	821	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
15	a	846	BCR	C27-C26-C25	-2.48	119.36	122.70
12	G	824	CLA	C3D-C4D-ND	2.48	114.01	109.99
12	b	802	CLA	OBD-CAD-C3D	-2.48	122.63	128.42
12	a	834	CLA	CMC-C2C-C1C	2.48	128.90	125.03
12	b	805	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
12	a	824	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
12	H	803	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
12	l	205	CLA	C3D-C4D-ND	2.47	114.01	109.99
15	a	845	BCR	C38-C26-C25	-2.47	121.78	124.48
12	A	816	CLA	CBC-CAC-C3C	-2.47	105.71	112.42
12	a	813	CLA	CMB-C2B-C3B	2.47	132.37	126.55
12	H	803	CLA	C6-C5-C3	-2.47	107.44	113.47
12	A	836	CLA	CMC-C2C-C1C	2.47	128.90	125.03
15	A	849	BCR	C12-C13-C14	-2.47	115.12	119.01
12	P	203	CLA	CMB-C2B-C1B	2.47	129.18	125.42
12	H	824	CLA	CAA-CBA-CGA	-2.47	106.19	113.21
12	G	837	CLA	OBD-CAD-C3D	-2.47	122.64	128.42
12	a	855	CLA	O2D-CGD-CBD	2.47	115.55	111.23
12	G	805	CLA	C1-O2A-CGA	2.47	122.63	116.65
12	B	804	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
12	H	810	CLA	CMB-C2B-C1B	2.47	129.18	125.42
12	H	833	CLA	CAC-C3C-C4C	2.47	128.00	124.79
12	a	839	CLA	C3D-C4D-ND	2.47	114.00	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	822	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	b	828	CLA	C3C-C4C-NC	2.47	113.59	110.43
12	b	825	CLA	CHB-C4A-NA	2.47	127.96	124.40
12	b	827	CLA	CMB-C2B-C1B	2.47	129.18	125.42
12	a	806	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	L	205	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	G	842	CLA	CAC-C3C-C4C	2.47	128.00	124.79
12	a	832	CLA	C4D-C3D-CAD	2.47	110.79	108.11
12	a	804	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
12	G	814	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
12	a	807	CLA	CMC-C2C-C1C	2.47	128.89	125.03
12	H	837	CLA	C4-C3-C5	2.47	119.51	115.23
12	H	819	CLA	C3C-C4C-NC	2.47	113.59	110.43
12	A	841	CLA	C3C-C4C-NC	2.47	113.59	110.43
15	R	101	BCR	C23-C22-C21	2.47	122.89	119.01
12	B	826	CLA	CHD-C4C-NC	-2.47	120.41	124.23
15	a	846	BCR	C19-C18-C17	2.47	122.89	119.01
12	G	804	CLA	CMA-C3A-C4A	2.47	118.40	111.77
12	a	841	CLA	C3C-C4C-NC	2.47	113.59	110.43
12	H	826	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	G	829	CLA	C3D-C4D-ND	2.46	113.99	109.99
12	H	809	CLA	C3D-C4D-ND	2.46	113.99	109.99
12	A	816	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
12	B	804	CLA	C4-C3-C5	2.46	119.50	115.23
12	B	819	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
12	B	820	CLA	C4D-C3D-CAD	2.46	110.78	108.11
12	l	202	CLA	C3D-C4D-ND	2.46	113.99	109.99
12	G	828	CLA	CAC-C3C-C4C	2.46	127.99	124.79
12	a	815	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
12	f	203	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
12	f	201	CLA	CMA-C3A-C4A	2.46	118.39	111.77
12	b	824	CLA	CMC-C2C-C1C	-2.46	121.19	125.03
15	L	207	BCR	C38-C26-C25	-2.46	121.80	124.48
12	H	814	CLA	C3C-C4C-NC	2.46	113.58	110.43
12	H	815	CLA	CAA-CBA-CGA	-2.46	106.22	113.21
12	B	816	CLA	CMA-C3A-C4A	2.46	118.39	111.77
12	A	818	CLA	CMB-C2B-C1B	2.46	129.17	125.42
12	P	201	CLA	C4-C3-C5	2.46	119.50	115.23
15	l	201	BCR	C24-C23-C22	-2.46	122.59	126.23
12	b	823	CLA	C7-C6-C5	-2.46	106.70	113.26
12	H	835	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
12	A	819	CLA	CMD-C2D-C3D	-2.46	122.05	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	821	CLA	CED-O2D-CGD	2.46	121.50	115.92
15	j	103	BCR	C34-C9-C10	-2.46	118.83	122.82
12	G	836	CLA	CMC-C2C-C1C	2.46	128.88	125.03
15	b	847	BCR	C31-C1-C6	2.46	114.10	110.24
15	H	841	BCR	C36-C18-C17	-2.46	118.83	122.82
12	b	812	CLA	OBD-CAD-C3D	-2.46	122.67	128.42
12	H	834	CLA	C4D-C3D-CAD	2.46	110.77	108.11
12	G	831	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
12	b	806	CLA	CMB-C2B-C1B	2.46	129.16	125.42
12	G	855	CLA	C3D-C4D-ND	2.46	113.98	109.99
12	B	826	CLA	CAC-C3C-C4C	2.46	127.98	124.79
12	A	806	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
12	B	801	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
12	A	813	CLA	C3D-C4D-ND	2.46	113.98	109.99
12	A	837	CLA	C3C-C4C-NC	2.46	113.58	110.43
13	b	838	1L3	C22-C21-C20	-2.45	117.32	123.63
15	P	202	BCR	C34-C9-C10	-2.45	118.84	122.82
12	a	831	CLA	C4D-C3D-CAD	2.45	110.77	108.11
12	B	821	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	A	826	CLA	CHD-C4C-C3C	-2.45	121.19	124.77
12	A	830	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
12	H	836	CLA	C3C-C4C-NC	2.45	113.57	110.43
12	A	816	CLA	C3C-C4C-NC	2.45	113.57	110.43
12	A	805	CLA	CMB-C2B-C3B	2.45	132.32	126.55
12	H	828	CLA	CMC-C2C-C1C	2.45	128.87	125.03
13	A	842	1L3	C19-C20-C21	-2.45	122.01	127.62
12	H	806	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
12	b	807	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
15	H	843	BCR	C29-C28-C27	2.45	116.67	111.28
12	a	811	CLA	CAC-C3C-C4C	2.45	127.98	124.79
15	R	101	BCR	C36-C18-C17	-2.45	118.84	122.82
12	j	104	CLA	CHB-C1B-C2B	-2.45	120.31	127.43
12	B	809	CLA	C4B-CHC-C1C	2.45	132.01	126.25
12	A	820	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
12	G	838	CLA	CAC-C3C-C4C	2.45	127.98	124.79
12	A	829	CLA	C3B-C4B-NB	2.45	112.72	110.53
12	H	807	CLA	C4-C3-C5	2.45	119.48	115.23
12	a	855	CLA	C4D-C3D-CAD	2.45	110.77	108.11
12	F	203	CLA	C3C-C4C-NC	2.45	113.57	110.43
12	A	806	CLA	C6-C5-C3	-2.45	107.50	113.47
12	G	841	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
12	a	813	CLA	O2D-CGD-O1D	-2.45	119.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	826	CLA	CMA-C3A-C4A	2.45	118.35	111.77
12	A	818	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
15	G	845	BCR	C19-C18-C17	2.45	122.86	119.01
12	G	856	CLA	C3D-C4D-ND	2.45	113.97	109.99
16	A	851	LHG	C5-O7-C7	-2.45	111.94	117.80
15	A	847	BCR	C27-C26-C25	-2.45	119.40	122.70
12	a	827	CLA	CMC-C2C-C1C	2.45	128.86	125.03
12	G	822	CLA	C3C-C4C-NC	2.45	113.56	110.43
12	b	833	CLA	CBA-CAA-C2A	2.45	121.07	113.79
13	a	842	1L3	C14-C03-C04	2.45	121.16	118.58
12	b	821	CLA	O2A-C1-C2	2.45	117.52	108.11
12	A	813	CLA	CMA-C3A-C4A	2.45	118.35	111.77
12	H	825	CLA	CMC-C2C-C3C	2.45	132.76	126.15
12	H	810	CLA	C4B-CHC-C1C	2.45	132.00	126.25
12	b	819	CLA	C3D-C4D-ND	2.45	113.96	109.99
12	H	824	CLA	CMB-C2B-C3B	2.45	132.30	126.55
12	G	840	CLA	C3D-C4D-ND	2.44	113.96	109.99
12	a	814	CLA	C3D-C4D-ND	2.44	113.96	109.99
15	R	101	BCR	C34-C9-C10	-2.44	118.86	122.82
12	b	821	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
12	a	811	CLA	C4D-C3D-CAD	2.44	110.76	108.11
15	a	847	BCR	C27-C26-C25	-2.44	119.40	122.70
12	G	827	CLA	CHD-C1D-ND	-2.44	121.36	124.80
12	A	837	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
12	H	817	CLA	C4D-C3D-CAD	2.44	110.76	108.11
12	G	832	CLA	CHB-C1B-C2B	-2.44	120.33	127.43
12	a	802	CLA	C1-O2A-CGA	2.44	122.56	116.65
12	H	831	CLA	C2B-C1B-NB	2.44	112.86	110.33
12	a	812	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
12	a	839	CLA	C4-C3-C5	2.44	119.47	115.23
12	H	812	CLA	CMA-C3A-C4A	2.44	118.33	111.77
12	a	809	CLA	C3C-C4C-NC	2.44	113.56	110.43
12	a	833	CLA	C3C-C4C-NC	2.44	113.56	110.43
12	A	827	CLA	CBA-CAA-C2A	2.44	121.06	113.79
15	Q	102	BCR	C38-C26-C25	-2.44	121.82	124.48
15	J	102	BCR	C37-C22-C21	-2.44	118.86	122.82
12	H	806	CLA	C4-C3-C5	2.44	119.46	115.23
11	a	801	CL0	O2D-CGD-O1D	-2.44	119.10	123.85
12	H	825	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
12	A	837	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
12	a	826	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
12	B	818	CLA	C3C-C4C-NC	2.44	113.56	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	822	CLA	CAC-C3C-C4C	2.44	127.96	124.79
15	f	202	BCR	C1-C6-C5	-2.44	119.30	122.64
12	B	825	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
15	G	853	BCR	C23-C22-C21	2.44	122.84	119.01
15	Q	101	BCR	C27-C26-C25	-2.44	119.41	122.70
15	G	848	BCR	C30-C25-C26	-2.44	119.30	122.64
15	L	207	BCR	C34-C9-C10	-2.44	118.87	122.82
12	L	202	CLA	CAC-C3C-C4C	2.44	127.96	124.79
12	G	809	CLA	C1-C2-C3	-2.44	122.82	126.76
12	a	855	CLA	CAA-C2A-C1A	-2.44	103.99	111.97
12	b	827	CLA	CMC-C2C-C1C	2.44	128.84	125.03
12	G	830	CLA	C3B-C4B-NB	2.44	112.70	110.53
12	G	811	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
12	a	836	CLA	CMC-C2C-C1C	2.44	128.84	125.03
12	a	826	CLA	C1-C2-C3	-2.44	122.21	126.20
12	a	813	CLA	CMA-C3A-C4A	2.44	118.32	111.77
12	b	815	CLA	C3D-C4D-ND	2.44	113.95	109.99
12	A	828	CLA	C3D-C4D-ND	2.44	113.95	109.99
12	b	835	CLA	CED-O2D-CGD	2.44	121.44	115.92
12	a	837	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
12	j	104	CLA	C3D-C4D-ND	2.44	113.94	109.99
12	B	822	CLA	C4C-C3C-C2C	-2.44	103.35	106.89
12	j	102	CLA	C4-C3-C5	2.43	119.45	115.23
12	a	834	CLA	CAA-C2A-C3A	-2.43	106.42	113.00
12	a	823	CLA	CMB-C2B-C1B	2.43	129.13	125.42
15	a	847	BCR	C2-C1-C6	2.43	113.97	110.44
12	H	802	CLA	C1-C2-C3	-2.43	122.21	126.20
12	B	810	CLA	CMB-C2B-C3B	2.43	132.28	126.55
12	B	815	CLA	C3C-C4C-NC	2.43	113.55	110.43
12	b	830	CLA	C2B-C1B-NB	2.43	112.85	110.33
12	H	811	CLA	CHD-C1D-ND	-2.43	121.38	124.80
12	A	854	CLA	C1-O2A-CGA	2.43	122.54	116.65
15	B	844	BCR	C15-C14-C13	-2.43	123.87	127.28
15	G	850	BCR	C35-C13-C12	2.43	121.80	118.09
12	A	824	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
12	a	818	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
12	A	803	CLA	C1-C2-C3	-2.43	122.21	126.20
12	H	825	CLA	C4D-C3D-CAD	2.43	110.75	108.11
12	a	828	CLA	C4-C3-C5	2.43	119.45	115.23
12	b	803	CLA	CMC-C2C-C1C	2.43	128.83	125.03
12	G	814	CLA	CAC-C3C-C4C	2.43	127.95	124.79
12	b	810	CLA	C1-C2-C3	-2.43	122.22	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	815	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
13	H	840	1L3	C14-C03-C04	2.43	121.14	118.58
12	a	836	CLA	CHA-C1A-NA	-2.43	120.89	126.39
12	B	832	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
12	H	836	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
12	P	201	CLA	C3C-C4C-NC	2.43	113.54	110.43
12	b	834	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
12	a	821	CLA	C3D-C4D-ND	2.43	113.93	109.99
12	G	810	CLA	CBA-CAA-C2A	2.43	121.02	113.79
12	a	814	CLA	CMB-C2B-C3B	2.43	132.26	126.55
12	H	816	CLA	C1-C2-C3	-2.43	122.22	126.20
12	H	829	CLA	C3C-C4C-NC	2.43	113.54	110.43
15	G	845	BCR	C15-C14-C13	-2.43	123.88	127.28
15	i	101	BCR	C32-C1-C6	-2.43	106.44	110.24
12	b	836	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
12	a	812	CLA	CMD-C2D-C3D	-2.43	122.13	127.69
12	A	854	CLA	CHD-C4C-C3C	-2.43	121.24	124.77
12	A	825	CLA	C1-O2A-CGA	2.43	122.52	116.65
15	B	841	BCR	C23-C24-C25	-2.43	120.52	127.00
12	B	808	CLA	O1D-CGD-CBD	-2.42	119.73	124.52
12	j	102	CLA	C3D-C4D-ND	2.42	113.93	109.99
12	A	854	CLA	C3D-C4D-ND	2.42	113.93	109.99
12	b	836	CLA	CHD-C4C-C3C	-2.42	121.24	124.77
12	B	818	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
12	a	854	CLA	CMB-C2B-C3B	2.42	132.25	126.55
12	b	828	CLA	OBD-CAD-C3D	-2.42	122.75	128.42
12	B	824	CLA	CAC-C3C-C4C	2.42	127.94	124.79
12	a	824	CLA	C4D-C3D-CAD	2.42	110.74	108.11
12	H	850	CLA	C1-C2-C3	-2.42	122.23	126.20
12	b	818	CLA	C3C-C4C-NC	2.42	113.53	110.43
12	A	803	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
12	b	818	CLA	CAC-C3C-C4C	2.42	127.94	124.79
12	G	806	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
12	l	202	CLA	C3C-C4C-NC	2.42	113.53	110.43
12	G	822	CLA	C3D-C4D-ND	2.42	113.92	109.99
12	H	839	CLA	C6-C5-C3	-2.42	107.57	113.47
12	b	818	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
12	G	828	CLA	C3D-C4D-ND	2.42	113.92	109.99
12	b	827	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
12	H	811	CLA	C4-C3-C5	2.42	119.43	115.23
12	b	809	CLA	CMB-C2B-C1B	2.42	129.10	125.42
12	b	802	CLA	C3C-C4C-NC	2.42	113.53	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	820	CLA	C1-C2-C3	-2.42	122.23	126.20
12	B	832	CLA	C4D-C3D-CAD	2.42	110.73	108.11
12	G	836	CLA	CGD-CBD-CAD	-2.42	103.01	110.85
12	A	830	CLA	C3D-C4D-ND	2.42	113.92	109.99
15	a	849	BCR	C12-C13-C14	-2.42	115.20	119.01
12	B	819	CLA	C3D-C4D-ND	2.42	113.92	109.99
12	B	808	CLA	C4D-C3D-CAD	2.42	110.73	108.11
12	G	815	CLA	C3D-C4D-ND	2.42	113.92	109.99
13	a	842	1L3	C14-C15-C16	-2.42	122.66	126.83
12	A	826	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
15	H	843	BCR	C19-C18-C17	2.42	122.81	119.01
12	A	832	CLA	C3C-C4C-NC	2.42	113.53	110.43
12	b	818	CLA	C3D-C4D-ND	2.42	113.92	109.99
12	A	838	CLA	CAC-C3C-C4C	2.42	127.93	124.79
15	H	842	BCR	C7-C8-C9	-2.42	122.66	126.23
12	H	830	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
12	f	203	CLA	C3C-C4C-NC	2.42	113.52	110.43
12	a	828	CLA	C3D-C4D-ND	2.41	113.91	109.99
12	b	804	CLA	C4-C3-C5	2.41	119.42	115.23
12	H	811	CLA	C1-C2-C3	-2.41	122.24	126.20
13	H	840	1L3	C22-C21-C20	-2.41	117.43	123.63
12	H	833	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
15	b	840	BCR	C33-C5-C4	2.41	118.74	113.60
15	B	841	BCR	C7-C8-C9	-2.41	122.67	126.23
12	H	822	CLA	C4D-C3D-CAD	2.41	110.73	108.11
12	b	822	CLA	C4D-C3D-CAD	2.41	110.73	108.11
12	G	827	CLA	C6-C5-C3	-2.41	107.59	113.47
15	A	844	BCR	C33-C5-C6	-2.41	121.85	124.48
12	G	816	CLA	C3C-C4C-NC	2.41	113.52	110.43
12	G	856	CLA	CHD-C1D-ND	-2.41	121.41	124.80
12	a	814	CLA	C4C-C3C-C2C	-2.41	103.38	106.89
15	a	849	BCR	C37-C22-C23	2.41	121.77	118.09
12	H	831	CLA	CHD-C1D-C2D	-2.41	120.47	125.49
12	B	818	CLA	C3D-C4D-ND	2.41	113.91	109.99
12	G	823	CLA	C3D-C4D-ND	2.41	113.91	109.99
12	H	838	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
12	A	811	CLA	C3D-C4D-ND	2.41	113.90	109.99
12	a	806	CLA	CMB-C2B-C3B	2.41	132.22	126.55
12	A	822	CLA	CED-O2D-CGD	2.41	121.38	115.92
12	S	203	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
15	i	102	BCR	C36-C18-C17	-2.41	118.91	122.82
12	H	831	CLA	CAC-C3C-C4C	2.41	127.92	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	201	CLA	CHB-C1B-C2B	-2.41	120.43	127.43
12	a	818	CLA	CHC-C1C-C2C	-2.41	120.10	126.95
15	G	849	BCR	C38-C26-C27	2.41	118.73	113.60
12	H	818	CLA	CMB-C2B-C1B	2.41	129.09	125.42
12	a	832	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
15	G	848	BCR	C12-C13-C14	-2.41	115.22	119.01
13	B	839	1L3	C22-C21-C20	-2.41	117.45	123.63
12	G	832	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
12	j	104	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
12	H	814	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
15	H	842	BCR	C23-C24-C25	-2.41	120.57	127.00
12	a	826	CLA	CHD-C1D-ND	-2.41	121.42	124.80
13	G	843	1L3	C01-C02-C03	-2.41	120.50	124.45
12	G	832	CLA	CMB-C2B-C3B	2.41	132.21	126.55
12	b	807	CLA	CMC-C2C-C3C	2.40	132.65	126.15
12	B	823	CLA	CMB-C2B-C3B	2.40	132.21	126.55
12	H	802	CLA	C5-C3-C2	-2.40	115.77	121.17
12	B	837	CLA	CAA-C2A-C3A	-2.40	106.50	113.00
15	A	849	BCR	C19-C18-C17	2.40	122.79	119.01
12	A	826	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
12	A	824	CLA	C1-C2-C3	-2.40	122.26	126.20
12	a	835	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
12	a	829	CLA	C4-C3-C5	2.40	119.40	115.23
12	G	814	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
12	A	834	CLA	C1-O2A-CGA	2.40	122.47	116.65
12	A	812	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
12	b	837	CLA	C3D-C4D-ND	2.40	113.89	109.99
12	B	813	CLA	CMA-C3A-C4A	2.40	118.23	111.77
12	B	835	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
12	b	805	CLA	CMA-C3A-C4A	2.40	118.23	111.77
12	H	803	CLA	C4-C3-C5	2.40	119.40	115.23
15	H	843	BCR	C37-C22-C23	2.40	121.76	118.09
12	B	813	CLA	C3C-C4C-NC	2.40	113.51	110.43
13	H	840	1L3	C17-C16-C18	2.40	119.39	115.23
15	B	844	BCR	C19-C18-C17	2.40	122.78	119.01
12	A	810	CLA	C1-C2-C3	-2.40	122.88	126.76
12	f	201	CLA	CHD-C1D-ND	-2.40	121.42	124.80
12	H	811	CLA	C4D-C3D-CAD	2.40	110.71	108.11
12	l	202	CLA	C4D-C3D-CAD	2.40	110.71	108.11
12	S	203	CLA	C1-C2-C3	-2.40	122.27	126.20
12	B	833	CLA	CMA-C3A-C4A	2.40	118.22	111.77
12	b	811	CLA	CED-O2D-CGD	2.40	121.36	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	203	BCR	C23-C22-C21	-2.40	115.24	119.01
15	L	203	BCR	C36-C18-C17	-2.40	118.93	122.82
12	G	813	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
12	l	205	CLA	C4D-C3D-CAD	2.40	110.71	108.11
12	G	824	CLA	CMB-C2B-C1B	2.40	129.07	125.42
12	G	835	CLA	CAC-C3C-C4C	2.40	127.91	124.79
15	B	842	BCR	C35-C13-C12	2.40	121.75	118.09
12	a	817	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
12	a	804	CLA	CHA-C1A-NA	-2.40	120.97	126.39
15	f	204	BCR	C39-C30-C25	-2.40	106.49	110.24
15	S	201	BCR	C2-C3-C4	-2.40	106.01	111.28
12	G	805	CLA	C3C-C4C-NC	2.39	113.50	110.43
12	B	835	CLA	C3C-C4C-NC	2.39	113.50	110.43
12	H	803	CLA	C3C-C4C-NC	2.39	113.50	110.43
15	b	847	BCR	C29-C28-C27	2.39	116.54	111.28
13	B	839	1L3	C19-C20-C21	-2.39	122.14	127.62
12	a	838	CLA	CAC-C3C-C4C	2.39	127.90	124.79
17	M	101	45D	C22-C16-C18	2.39	119.11	115.49
15	l	201	BCR	C4-C5-C6	-2.39	119.47	122.70
12	G	817	CLA	CAC-C3C-C4C	2.39	127.90	124.79
12	G	812	CLA	C3D-C4D-ND	2.39	113.88	109.99
12	a	820	CLA	C1-C2-C3	-2.39	122.28	126.20
12	a	828	CLA	CHD-C1D-ND	-2.39	121.44	124.80
12	B	811	CLA	C1-C2-C3	-2.39	122.28	126.20
12	G	824	CLA	C4-C3-C5	2.39	119.38	115.23
12	B	824	CLA	CBA-CAA-C2A	2.39	120.91	113.79
12	H	808	CLA	CAC-C3C-C4C	2.39	127.90	124.79
12	b	815	CLA	CHB-C1B-C2B	-2.39	120.48	127.43
12	G	830	CLA	C4D-C3D-CAD	2.39	110.70	108.11
12	A	811	CLA	C4D-C3D-CAD	2.39	110.70	108.11
12	b	814	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
12	B	822	CLA	C3D-C4D-ND	2.39	113.87	109.99
12	b	802	CLA	C1-C2-C3	-2.39	122.28	126.20
12	B	834	CLA	CBA-CAA-C2A	2.39	120.91	113.79
12	G	810	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
12	a	811	CLA	C3D-C4D-ND	2.39	113.87	109.99
12	R	103	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
15	A	848	BCR	C15-C14-C13	-2.39	123.93	127.28
15	J	101	BCR	C34-C9-C10	-2.39	118.94	122.82
12	G	841	CLA	C4-C3-C5	2.39	119.38	115.23
12	a	835	CLA	CHA-C1A-NA	-2.39	120.98	126.39
12	b	801	CLA	CMB-C2B-C1B	-2.39	121.78	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	202	CLA	C1-O2A-CGA	2.39	122.43	116.65
12	B	837	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
12	a	836	CLA	CBC-CAC-C3C	2.39	118.89	112.42
12	H	807	CLA	CMC-C2C-C3C	2.39	132.61	126.15
12	b	802	CLA	C5-C3-C2	-2.39	115.81	121.17
15	L	201	BCR	C36-C18-C17	-2.39	118.95	122.82
12	a	828	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
15	H	845	BCR	C29-C30-C25	2.39	113.91	110.44
12	G	856	CLA	CHB-C4A-NA	2.39	127.84	124.40
15	l	203	BCR	C23-C22-C21	-2.39	115.26	119.01
12	a	809	CLA	CBA-CAA-C2A	2.38	120.89	113.79
12	a	838	CLA	CAA-CBA-CGA	-2.38	106.13	112.49
12	b	813	CLA	C3C-C4C-NC	2.38	113.48	110.43
12	A	832	CLA	C4-C3-C5	2.38	119.37	115.23
12	A	825	CLA	CHB-C1B-C2B	-2.38	120.51	127.43
12	B	834	CLA	OBD-CAD-C3D	-2.38	122.85	128.42
12	L	204	CLA	CHD-C1D-ND	-2.38	121.45	124.80
12	b	812	CLA	CBA-CAA-C2A	2.38	120.88	113.79
15	a	848	BCR	C12-C13-C14	-2.38	115.26	119.01
12	H	835	CLA	CMC-C2C-C1C	2.38	128.76	125.03
12	B	813	CLA	C4-C3-C5	2.38	119.36	115.23
12	b	808	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
12	H	805	CLA	CMC-C2C-C1C	2.38	128.75	125.03
12	a	823	CLA	C3D-C4D-ND	2.38	113.86	109.99
11	G	801	CL0	C1-O2A-CGA	2.38	122.41	116.65
12	a	834	CLA	CBA-CAA-C2A	2.38	120.88	113.79
12	A	814	CLA	C3D-C4D-ND	2.38	113.86	109.99
12	a	830	CLA	CHC-C1C-NC	-2.38	120.73	124.31
12	H	839	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
12	H	838	CLA	C4D-C3D-CAD	2.38	110.69	108.11
12	b	820	CLA	C4D-C3D-CAD	2.38	110.69	108.11
12	l	206	CLA	C4D-C3D-CAD	2.38	110.69	108.11
15	b	843	BCR	C15-C14-C13	-2.38	123.94	127.28
12	G	806	CLA	C11-C10-C8	-2.38	108.06	115.97
13	a	842	1L3	C22-C21-C23	2.38	119.36	115.23
12	A	855	CLA	CMC-C2C-C1C	2.38	128.75	125.03
12	a	810	CLA	C1-C2-C3	-2.38	122.92	126.76
12	B	802	CLA	O2A-C1-C2	2.38	117.25	108.11
12	H	832	CLA	CMB-C2B-C1B	2.38	129.04	125.42
12	B	805	CLA	CMA-C3A-C4A	2.38	118.16	111.77
12	G	838	CLA	CAA-CBA-CGA	-2.38	106.15	112.49
12	B	815	CLA	O2D-CGD-O1D	-2.38	119.22	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	809	CLA	C3D-C4D-ND	2.38	113.85	109.99
12	B	826	CLA	CHB-C1B-C2B	-2.38	120.53	127.43
13	a	842	1L3	C01-C02-C03	-2.38	120.55	124.45
12	a	836	CLA	CHD-C4C-NC	-2.38	120.55	124.23
12	b	803	CLA	C3D-C4D-ND	2.37	113.85	109.99
12	A	826	CLA	CAC-C3C-C2C	2.37	131.92	127.56
12	B	809	CLA	CMB-C2B-C1B	2.37	129.03	125.42
12	B	836	CLA	CED-O2D-CGD	2.37	121.30	115.92
15	a	846	BCR	C7-C8-C9	-2.37	122.72	126.23
12	a	808	CLA	OBD-CAD-C3D	-2.37	122.87	128.42
12	A	816	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
12	A	812	CLA	CHA-C1A-NA	-2.37	121.02	126.39
12	G	832	CLA	C3C-C4C-NC	2.37	113.47	110.43
12	L	206	CLA	C3C-C4C-NC	2.37	113.47	110.43
12	G	821	CLA	C3D-C4D-ND	2.37	113.84	109.99
12	G	813	CLA	CHA-C1A-NA	-2.37	121.02	126.39
15	b	841	BCR	C38-C26-C25	2.37	127.07	124.48
12	B	825	CLA	CHC-C1C-C2C	-2.37	120.20	126.95
15	Q	102	BCR	C37-C22-C21	-2.37	118.97	122.82
12	B	821	CLA	CMB-C2B-C3B	2.37	132.13	126.55
12	P	203	CLA	C3C-C4C-NC	2.37	113.47	110.43
12	a	855	CLA	C4-C3-C5	2.37	119.35	115.23
15	A	848	BCR	C38-C26-C27	2.37	118.65	113.60
12	b	837	CLA	C6-C5-C3	-2.37	107.69	113.47
12	H	824	CLA	CHA-C1A-NA	-2.37	121.02	126.39
12	P	203	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
12	H	827	CLA	CHB-C1B-C2B	-2.37	120.55	127.43
12	a	835	CLA	CAC-C3C-C4C	2.37	127.87	124.79
15	b	842	BCR	C27-C26-C25	-2.37	119.50	122.70
12	a	834	CLA	CED-O2D-CGD	2.37	121.29	115.92
15	a	849	BCR	C1-C6-C7	2.37	122.08	115.65
12	b	835	CLA	CBA-CAA-C2A	2.37	120.84	113.79
12	H	815	CLA	CMB-C2B-C3B	2.37	132.12	126.55
12	H	803	CLA	C3D-C4D-ND	2.37	113.84	109.99
12	H	807	CLA	C3D-C4D-ND	2.37	113.84	109.99
12	P	201	CLA	C3D-C4D-ND	2.37	113.84	109.99
12	G	825	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
11	G	801	CL0	C6-C5-C3	-2.37	107.70	113.47
12	B	826	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
12	G	828	CLA	CMA-C3A-C4A	2.37	118.14	111.77
12	a	822	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
12	G	812	CLA	CAC-C3C-C4C	2.37	127.87	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	203	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
15	S	205	BCR	C35-C13-C12	2.37	121.70	118.09
12	H	813	CLA	OBD-CAD-C3D	-2.37	122.88	128.42
12	b	836	CLA	CMA-C3A-C4A	2.37	118.14	111.77
12	a	834	CLA	CAC-C3C-C4C	2.37	127.87	124.79
12	H	810	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
12	H	810	CLA	C3D-C4D-ND	2.37	113.83	109.99
12	B	805	CLA	CED-O2D-CGD	2.37	121.28	115.92
12	G	811	CLA	C1-C2-C3	-2.37	122.93	126.76
12	H	836	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
12	S	203	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
12	P	203	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
12	a	831	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
12	B	806	CLA	CMC-C2C-C1C	2.37	128.73	125.03
12	a	832	CLA	CAA-C2A-C3A	-2.37	106.61	113.00
12	b	816	CLA	C4D-C3D-CAD	2.37	110.67	108.11
12	S	202	CLA	CHD-C1D-ND	-2.37	121.47	124.80
12	G	826	CLA	CMB-C2B-C3B	2.37	132.11	126.55
15	H	841	BCR	C34-C9-C10	-2.36	118.98	122.82
12	G	834	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
12	H	812	CLA	C1-C2-C3	-2.36	122.32	126.20
12	A	821	CLA	C3D-C4D-ND	2.36	113.83	109.99
12	A	854	CLA	CAA-C2A-C1A	2.36	119.72	111.97
12	G	816	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
15	a	847	BCR	C36-C18-C17	-2.36	118.99	122.82
12	A	832	CLA	CHA-C1A-NA	-2.36	121.04	126.39
12	H	827	CLA	CHA-C4D-ND	2.36	137.43	132.55
11	A	801	CL0	CBC-CAC-C3C	-2.36	106.01	112.42
12	B	830	CLA	C4-C3-C5	2.36	119.33	115.23
12	B	816	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
12	B	828	CLA	CMA-C3A-C4A	2.36	118.12	111.77
12	B	817	CLA	CMB-C2B-C1B	2.36	129.02	125.42
12	a	831	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
12	G	828	CLA	CMB-C2B-C3B	2.36	132.11	126.55
15	a	849	BCR	C19-C18-C17	2.36	122.72	119.01
12	A	804	CLA	C1-O2A-CGA	2.36	122.37	116.65
12	a	830	CLA	C4C-C3C-C2C	-2.36	103.45	106.89
12	B	803	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
12	G	814	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
12	G	807	CLA	CHB-C4A-NA	2.36	127.81	124.40
12	H	824	CLA	C7-C6-C5	-2.36	106.97	113.26
12	A	835	CLA	O2D-CGD-O1D	-2.36	119.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	846	BCR	C7-C8-C9	-2.36	122.74	126.23
12	A	841	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
12	G	808	CLA	CHB-C4A-NA	2.36	127.81	124.40
12	B	826	CLA	C3D-C4D-ND	2.36	113.82	109.99
12	G	823	CLA	CMC-C2C-C1C	2.36	128.72	125.03
12	G	835	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
15	l	203	BCR	C12-C13-C14	-2.36	115.30	119.01
12	a	854	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
15	J	104	BCR	C3-C4-C5	-2.36	109.85	114.06
12	G	841	CLA	CED-O2D-CGD	2.36	121.27	115.92
12	G	837	CLA	C3C-C4C-NC	2.36	113.45	110.43
12	l	205	CLA	C3C-C4C-NC	2.36	113.45	110.43
12	a	818	CLA	CAC-C3C-C4C	2.36	127.86	124.79
12	b	823	CLA	CHA-C1A-NA	-2.36	121.05	126.39
12	A	823	CLA	C3D-C4D-ND	2.36	113.82	109.99
12	a	816	CLA	C3C-C4C-NC	2.36	113.45	110.43
15	B	844	BCR	C40-C30-C25	2.36	113.94	110.24
15	i	101	BCR	C33-C5-C6	-2.36	121.91	124.48
15	A	844	BCR	C34-C9-C10	-2.36	119.00	122.82
12	b	804	CLA	C3D-C4D-ND	2.36	113.82	109.99
12	b	823	CLA	CMB-C2B-C3B	2.36	132.09	126.55
12	F	201	CLA	C1-C2-C3	-2.36	122.34	126.20
12	H	823	CLA	C3D-C4D-ND	2.36	113.82	109.99
12	J	103	CLA	C3D-C4D-ND	2.36	113.82	109.99
15	B	840	BCR	C38-C26-C27	2.36	118.62	113.60
15	P	204	BCR	C38-C26-C25	-2.36	121.91	124.48
12	B	807	CLA	C4C-C3C-C2C	-2.36	103.46	106.89
12	H	809	CLA	CMA-C3A-C2A	-2.36	104.87	113.98
12	G	804	CLA	C1-C2-C3	-2.36	122.34	126.20
12	A	808	CLA	CAC-C3C-C4C	2.36	127.86	124.79
12	G	833	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
12	l	204	CLA	C4-C3-C2	-2.36	117.58	123.63
12	A	827	CLA	CHD-C1D-ND	-2.36	121.49	124.80
12	b	836	CLA	C3D-C4D-ND	2.36	113.81	109.99
12	G	839	CLA	C4-C3-C5	2.35	119.31	115.23
12	J	103	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
12	a	816	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
12	H	822	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
12	G	821	CLA	C1-C2-C3	-2.35	122.34	126.20
12	G	823	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
12	B	808	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
12	A	835	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	G	837	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
12	B	829	CLA	CHB-C1B-C2B	-2.35	120.60	127.43
12	a	824	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
12	b	826	CLA	CHD-C4C-NC	-2.35	120.58	124.23
12	H	811	CLA	CMB-C2B-C3B	2.35	132.08	126.55
12	j	102	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
12	H	829	CLA	C3D-C4D-ND	2.35	113.81	109.99
12	B	815	CLA	CAC-C3C-C4C	2.35	127.85	124.79
12	G	834	CLA	CMC-C2C-C1C	2.35	128.71	125.03
12	a	822	CLA	CMC-C2C-C1C	2.35	128.71	125.03
12	b	809	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
12	H	805	CLA	CBA-CAA-C2A	2.35	120.79	113.79
15	P	202	BCR	C2-C1-C6	2.35	113.85	110.44
12	b	811	CLA	CMA-C3A-C4A	2.35	118.09	111.77
12	A	810	CLA	CAC-C3C-C4C	2.35	127.85	124.79
12	H	804	CLA	C3D-C4D-ND	2.35	113.81	109.99
12	a	825	CLA	CHB-C1B-C2B	-2.35	120.61	127.43
12	G	820	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
12	a	816	CLA	C3D-C4D-ND	2.35	113.80	109.99
12	H	813	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
12	L	204	CLA	CBC-CAC-C3C	-2.35	106.06	112.42
12	A	808	CLA	C3D-C4D-ND	2.35	113.80	109.99
12	a	836	CLA	CGD-CBD-CAD	-2.35	103.25	110.85
12	b	810	CLA	CHA-C1A-NA	-2.35	121.08	126.39
12	H	802	CLA	CHD-C1D-C2D	-2.35	120.61	125.49
12	B	826	CLA	C1-O2A-CGA	2.34	122.33	116.65
12	G	802	CLA	C3C-C4C-NC	2.34	113.43	110.43
12	b	810	CLA	CMB-C2B-C3B	2.34	132.06	126.55
12	A	839	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
12	A	821	CLA	C3C-C4C-NC	2.34	113.43	110.43
12	A	841	CLA	C4D-C3D-CAD	2.34	110.65	108.11
12	B	833	CLA	C3D-C4D-ND	2.34	113.80	109.99
12	a	803	CLA	OBD-CAD-C3D	-2.34	122.94	128.42
12	b	813	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
12	H	850	CLA	CED-O2D-CGD	2.34	121.23	115.92
12	b	836	CLA	C4D-C3D-CAD	2.34	110.65	108.11
12	A	827	CLA	C4D-C3D-CAD	2.34	110.65	108.11
12	A	830	CLA	CHC-C1C-NC	-2.34	120.78	124.31
12	b	811	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
12	G	842	CLA	CHC-C1C-C2C	-2.34	120.29	126.95
12	G	832	CLA	CHA-C1A-NA	-2.34	121.09	126.39
12	A	812	CLA	CMC-C2C-C3C	2.34	132.48	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	824	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
12	b	829	CLA	C3C-C4C-NC	2.34	113.43	110.43
12	b	837	CLA	CMA-C3A-C4A	2.34	118.07	111.77
12	H	819	CLA	C3D-C4D-ND	2.34	113.79	109.99
12	S	204	CLA	C1-C2-C3	-2.34	122.36	126.20
12	a	838	CLA	CMB-C2B-C1B	2.34	128.98	125.42
12	A	829	CLA	C3D-C4D-ND	2.34	113.79	109.99
12	A	813	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
12	G	804	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
12	a	841	CLA	CHC-C1C-C2C	-2.34	120.30	126.95
12	B	802	CLA	C5-C3-C2	-2.34	115.92	121.17
12	H	839	CLA	CHC-C1C-NC	-2.34	120.79	124.31
12	H	826	CLA	CHC-C1C-C2C	-2.34	120.30	126.95
12	a	804	CLA	C1-O2A-CGA	2.34	122.31	116.65
12	S	203	CLA	CMB-C2B-C3B	2.34	132.05	126.55
12	a	821	CLA	C3C-C4C-NC	2.34	113.43	110.43
12	A	834	CLA	C4-C3-C2	-2.34	117.62	123.63
12	H	820	CLA	C3D-C4D-ND	2.34	113.79	109.99
12	f	201	CLA	CHB-C1B-C2B	-2.34	120.64	127.43
12	B	832	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
12	A	811	CLA	CAC-C3C-C4C	2.34	127.83	124.79
12	a	825	CLA	C3D-C4D-ND	2.34	113.79	109.99
12	H	829	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
15	A	852	BCR	C23-C22-C21	2.34	122.69	119.01
12	B	824	CLA	CHA-C1A-NA	-2.34	121.10	126.39
12	B	825	CLA	C4-C3-C5	2.34	119.28	115.23
12	G	825	CLA	C3D-C4D-ND	2.34	113.78	109.99
12	b	821	CLA	CHB-C4A-NA	2.34	127.77	124.40
12	A	816	CLA	CAC-C3C-C4C	2.34	127.83	124.79
12	b	810	CLA	C4-C3-C5	2.33	119.28	115.23
15	a	852	BCR	C29-C28-C27	2.33	116.41	111.28
15	G	848	BCR	C27-C26-C25	-2.33	119.55	122.70
12	P	203	CLA	C4D-C3D-CAD	2.33	110.64	108.11
12	a	830	CLA	CMA-C3A-C4A	2.33	118.05	111.77
12	b	807	CLA	CMA-C3A-C4A	2.33	118.05	111.77
15	a	846	BCR	C39-C30-C25	-2.33	106.58	110.24
12	A	806	CLA	CHB-C4A-NA	2.33	127.77	124.40
12	H	801	CLA	CMA-C3A-C4A	2.33	118.04	111.77
12	b	821	CLA	CGD-CBD-CAD	-2.33	103.29	110.85
15	J	102	BCR	C29-C28-C27	-2.33	106.15	111.28
12	b	827	CLA	CMA-C3A-C4A	2.33	118.04	111.77
12	A	808	CLA	CHC-C1C-C2C	-2.33	120.32	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	806	CLA	CED-O2D-CGD	2.33	121.20	115.92
12	a	825	CLA	C1-O2A-CGA	2.33	122.29	116.65
12	a	820	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
12	a	821	CLA	CMB-C2B-C3B	2.33	132.03	126.55
12	a	812	CLA	CHB-C4A-NA	2.33	127.76	124.40
12	B	832	CLA	C3C-C4C-NC	2.33	113.42	110.43
12	G	816	CLA	CMA-C3A-C2A	2.33	122.99	113.98
12	A	826	CLA	C4-C3-C5	2.33	119.27	115.23
12	f	203	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
12	B	805	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
12	B	824	CLA	CHD-C4C-C3C	-2.33	121.38	124.77
12	b	823	CLA	C4D-C3D-CAD	2.33	110.64	108.11
12	a	827	CLA	CMB-C2B-C3B	2.33	132.03	126.55
12	A	813	CLA	C3C-C4C-NC	2.33	113.41	110.43
12	B	830	CLA	C3C-C4C-NC	2.33	113.41	110.43
12	b	829	CLA	CMC-C2C-C1C	2.33	128.67	125.03
18	B	846	LMG	O7-C10-O9	-2.33	118.26	123.70
12	S	202	CLA	C4-C3-C2	-2.33	117.65	123.63
12	a	804	CLA	CHB-C4A-NA	2.33	127.76	124.40
12	B	823	CLA	C7-C6-C5	-2.33	107.06	113.26
12	H	803	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
15	b	840	BCR	C37-C22-C21	-2.33	119.05	122.82
15	G	850	BCR	C12-C13-C14	-2.33	115.35	119.01
12	H	827	CLA	C4-C3-C5	2.33	119.27	115.23
15	b	840	BCR	C7-C8-C9	-2.33	122.79	126.23
12	a	815	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
12	H	838	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
13	b	838	1L3	C19-C20-C21	-2.33	122.30	127.62
12	H	818	CLA	C3D-C4D-ND	2.33	113.77	109.99
12	l	204	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
12	H	803	CLA	CHA-C1A-NA	-2.33	121.12	126.39
15	B	840	BCR	C33-C5-C6	-2.33	121.95	124.48
12	a	812	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
15	H	845	BCR	C15-C14-C13	-2.33	124.02	127.28
12	H	822	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
12	A	832	CLA	CHB-C1B-C2B	-2.32	120.68	127.43
15	j	101	BCR	C34-C9-C8	2.32	121.64	118.09
15	a	845	BCR	C33-C5-C4	2.32	118.55	113.60
12	a	810	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
12	a	822	CLA	C3D-C4D-ND	2.32	113.76	109.99
12	L	206	CLA	C1-C2-C3	-2.32	122.39	126.20
12	A	814	CLA	O1D-CGD-CBD	-2.32	119.94	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	828	CLA	C3D-C4D-ND	2.32	113.76	109.99
12	G	820	CLA	C3C-C4C-NC	2.32	113.41	110.43
12	L	204	CLA	C4-C3-C2	-2.32	117.66	123.63
12	A	835	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
12	H	838	CLA	C3D-C4D-ND	2.32	113.76	109.99
12	a	812	CLA	CHA-C1A-NA	-2.32	121.13	126.39
12	a	833	CLA	CMC-C2C-C1C	2.32	128.66	125.03
12	b	808	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
12	b	832	CLA	OBD-CAD-C3D	-2.32	122.99	128.42
12	L	205	CLA	CBA-CAA-C2A	2.32	120.70	113.79
12	B	828	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
12	B	825	CLA	C2B-C1B-NB	2.32	112.73	110.33
12	a	837	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
12	a	814	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
12	H	839	CLA	CMB-C2B-C3B	2.32	132.01	126.55
12	G	840	CLA	C1-C2-C3	-2.32	123.01	126.76
15	H	849	BCR	C29-C28-C27	2.32	116.38	111.28
12	H	802	CLA	O2A-C1-C2	2.32	117.04	108.11
12	a	832	CLA	CHB-C1B-C2B	-2.32	120.69	127.43
12	a	831	CLA	CED-O2D-CGD	2.32	121.18	115.92
12	a	811	CLA	CMA-C3A-C4A	2.32	118.01	111.77
12	B	807	CLA	C4D-C3D-CAD	2.32	110.62	108.11
12	B	813	CLA	CED-O2D-CGD	2.32	121.18	115.92
16	G	851	LHG	C6-C5-C4	-2.32	106.38	111.78
15	G	848	BCR	C37-C22-C21	-2.32	119.06	122.82
12	G	834	CLA	CHB-C4A-NA	2.32	127.75	124.40
12	H	806	CLA	CHB-C4A-NA	2.32	127.75	124.40
15	G	853	BCR	C38-C26-C27	2.32	118.54	113.60
12	a	806	CLA	C4-C3-C5	2.32	119.25	115.23
12	S	202	CLA	CHB-C4A-NA	2.32	127.75	124.40
12	S	204	CLA	CMC-C2C-C1C	2.32	128.66	125.03
12	G	829	CLA	C4C-C3C-C2C	-2.32	103.52	106.89
12	b	827	CLA	C3C-C4C-NC	2.32	113.40	110.43
12	G	809	CLA	CMC-C2C-C1C	2.32	128.66	125.03
12	a	841	CLA	C4-C3-C5	2.32	119.25	115.23
12	H	829	CLA	CAC-C3C-C4C	2.32	127.80	124.79
15	H	842	BCR	C33-C5-C4	2.32	118.53	113.60
12	a	832	CLA	CHA-C1A-NA	-2.32	121.15	126.39
12	B	809	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
15	G	848	BCR	C4-C5-C6	-2.31	119.58	122.70
12	G	826	CLA	CHB-C1B-C2B	-2.31	120.71	127.43
12	a	803	CLA	C1-C2-C3	-2.31	122.41	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	823	CLA	CHD-C1D-ND	-2.31	121.55	124.80
12	G	805	CLA	CHA-C1A-NA	-2.31	121.15	126.39
12	a	832	CLA	CMB-C2B-C3B	2.31	131.99	126.55
13	A	842	1L3	C22-C21-C23	2.31	119.24	115.23
12	A	816	CLA	C1-C2-C3	-2.31	123.02	126.76
12	B	822	CLA	C1-O2A-CGA	2.31	122.25	116.65
12	B	838	CLA	C3D-C4D-ND	2.31	113.75	109.99
12	G	804	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
15	S	205	BCR	C4-C5-C6	-2.31	119.58	122.70
12	G	807	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
12	a	805	CLA	CMB-C2B-C3B	2.31	131.99	126.55
12	b	816	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
12	G	805	CLA	C3D-C4D-ND	2.31	113.74	109.99
12	G	832	CLA	C4D-C3D-CAD	2.31	110.62	108.11
12	B	812	CLA	C4D-C3D-CAD	2.31	110.62	108.11
15	G	848	BCR	C36-C18-C17	-2.31	119.07	122.82
12	H	826	CLA	CMC-C2C-C3C	2.31	132.40	126.15
12	b	803	CLA	CAC-C3C-C4C	2.31	127.80	124.79
12	f	201	CLA	C3D-C4D-ND	2.31	113.74	109.99
12	a	806	CLA	CHB-C4A-NA	2.31	127.73	124.40
12	A	812	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
15	B	841	BCR	C37-C22-C21	-2.31	119.08	122.82
12	a	831	CLA	CMC-C2C-C3C	2.31	132.39	126.15
12	A	839	CLA	CMA-C3A-C4A	2.31	117.98	111.77
12	a	832	CLA	C3D-C4D-ND	2.31	113.74	109.99
12	G	818	CLA	CBA-CAA-C2A	2.31	120.66	113.79
12	G	804	CLA	C3D-C4D-ND	2.31	113.74	109.99
12	G	817	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
12	B	824	CLA	CED-O2D-CGD	2.31	121.15	115.92
12	L	202	CLA	CMB-C2B-C1B	2.31	128.93	125.42
12	l	205	CLA	CMB-C2B-C3B	2.31	131.98	126.55
12	B	815	CLA	C4-C3-C5	2.31	119.23	115.23
12	A	817	CLA	CMA-C3A-C4A	2.31	117.97	111.77
12	A	819	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
12	H	834	CLA	CAC-C3C-C4C	2.31	127.79	124.79
11	A	801	CL0	C6-C5-C3	-2.31	107.85	113.47
12	A	823	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
12	A	838	CLA	CAA-CBA-CGA	-2.31	106.34	112.49
12	B	807	CLA	CMA-C3A-C4A	2.31	117.97	111.77
12	H	823	CLA	CMB-C2B-C3B	2.31	131.97	126.55
12	B	807	CLA	C4-C3-C5	2.31	119.23	115.23
12	A	807	CLA	CHB-C4A-NA	2.31	127.73	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	204	CLA	CHB-C4A-NA	2.31	127.73	124.40
12	a	803	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
12	A	820	CLA	CMB-C2B-C3B	2.31	131.97	126.55
12	H	807	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
12	A	806	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
12	B	816	CLA	C4D-C3D-CAD	2.30	110.61	108.11
12	H	817	CLA	CHB-C1B-C2B	-2.30	120.74	127.43
12	H	834	CLA	C3D-C4D-ND	2.30	113.73	109.99
12	b	826	CLA	C3D-C4D-ND	2.30	113.73	109.99
12	a	835	CLA	O2D-CGD-CBD	2.30	115.26	111.23
12	a	827	CLA	CED-O2D-CGD	2.30	121.14	115.92
12	a	817	CLA	CMA-C3A-C4A	2.30	117.96	111.77
15	J	101	BCR	C34-C9-C8	2.30	121.61	118.09
12	a	810	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
17	T	101	45D	C22-C16-C18	2.30	118.98	115.49
12	H	822	CLA	C3D-C4D-ND	2.30	113.73	109.99
12	L	205	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
12	a	831	CLA	C3C-C4C-NC	2.30	113.38	110.43
12	G	824	CLA	C3C-C4C-NC	2.30	113.38	110.43
12	b	836	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
12	a	816	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
12	A	815	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
12	a	840	CLA	C3D-C4D-ND	2.30	113.73	109.99
12	S	204	CLA	C4D-C3D-CAD	2.30	110.61	108.11
12	H	809	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
12	a	807	CLA	CHB-C4A-NA	2.30	127.72	124.40
12	G	835	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
15	G	846	BCR	C33-C5-C4	2.30	118.50	113.60
12	l	202	CLA	CAC-C3C-C4C	2.30	127.78	124.79
17	M	101	45D	C21-C15-C17	2.30	118.97	115.49
12	G	803	CLA	CHA-C1A-NA	-2.30	121.18	126.39
12	a	839	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
12	A	817	CLA	CBA-CAA-C2A	2.30	120.63	113.79
12	a	830	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
12	G	835	CLA	CBA-CAA-C2A	2.30	120.63	113.79
12	G	827	CLA	C4-C3-C5	2.30	119.22	115.23
15	H	845	BCR	C36-C18-C17	-2.30	119.09	122.82
12	a	804	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
12	B	828	CLA	C3D-C4D-ND	2.30	113.72	109.99
12	a	841	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
12	A	834	CLA	CHB-C1B-C2B	-2.30	120.76	127.43
12	b	817	CLA	C3D-C4D-ND	2.30	113.72	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	841	BCR	C15-C14-C13	-2.30	124.06	127.28
11	G	801	CL0	C4D-CHA-C1A	-2.30	118.50	121.24
12	b	809	CLA	C4B-CHC-C1C	2.30	131.65	126.25
12	b	821	CLA	C3D-C4D-ND	2.30	113.72	109.99
12	S	202	CLA	C3D-C4D-ND	2.29	113.72	109.99
12	a	818	CLA	C3D-C4D-ND	2.29	113.72	109.99
12	b	806	CLA	C1-C2-C3	-2.29	122.44	126.20
12	L	204	CLA	C3D-C4D-ND	2.29	113.72	109.99
12	l	204	CLA	C3D-C4D-ND	2.29	113.72	109.99
12	B	803	CLA	C1-C2-C3	-2.29	122.44	126.20
12	G	827	CLA	CAA-C2A-C3A	-2.29	106.80	113.00
12	b	809	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
12	G	834	CLA	C4-C3-C2	-2.29	117.74	123.63
15	b	841	BCR	C19-C18-C17	2.29	122.61	119.01
12	A	824	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
12	B	812	CLA	CMC-C2C-C1C	2.29	128.62	125.03
12	b	815	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
12	B	838	CLA	CHC-C1C-NC	-2.29	120.86	124.31
12	a	841	CLA	CED-O2D-CGD	2.29	121.11	115.92
12	A	817	CLA	CED-O2D-CGD	2.29	121.11	115.92
12	L	205	CLA	C4D-C3D-CAD	2.29	110.59	108.11
12	G	831	CLA	C1-C2-C3	-2.29	123.06	126.76
12	B	811	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
12	A	840	CLA	C3D-C4D-ND	2.29	113.71	109.99
12	a	828	CLA	C1-O2A-CGA	2.29	122.19	116.65
15	B	841	BCR	C30-C25-C26	-2.29	119.51	122.64
12	B	812	CLA	CHA-C1A-NA	-2.29	121.21	126.39
12	P	203	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
12	B	827	CLA	CAC-C3C-C4C	2.29	127.77	124.79
12	B	806	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
12	B	828	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
12	A	830	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
12	H	813	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
12	a	818	CLA	C4D-C3D-CAD	2.29	110.59	108.11
12	B	830	CLA	C3D-C4D-ND	2.29	113.70	109.99
12	H	803	CLA	CBA-CAA-C2A	2.29	120.59	113.79
12	L	205	CLA	CMB-C2B-C3B	2.29	131.93	126.55
13	G	843	1L3	C22-C21-C23	2.29	119.20	115.23
12	H	821	CLA	CAC-C3C-C4C	2.29	127.76	124.79
12	H	811	CLA	C4B-CHC-C1C	2.29	131.62	126.25
12	H	817	CLA	C3C-C4C-NC	2.29	113.36	110.43
12	G	817	CLA	CAA-C2A-C3A	-2.29	106.82	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	837	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
12	b	832	CLA	C4-C3-C5	2.29	119.19	115.23
12	A	804	CLA	CHA-C1A-NA	-2.29	121.22	126.39
12	H	833	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
15	A	849	BCR	C37-C22-C23	2.28	121.58	118.09
12	b	803	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
12	b	824	CLA	C6-C7-C8	-2.28	108.37	115.97
12	A	815	CLA	C3C-C4C-NC	2.28	113.36	110.43
12	G	805	CLA	C1-C2-C3	-2.28	122.45	126.20
12	B	812	CLA	CAC-C3C-C4C	2.28	127.76	124.79
12	G	830	CLA	CMB-C2B-C3B	2.28	131.92	126.55
15	P	202	BCR	C31-C1-C6	-2.28	106.66	110.24
12	H	835	CLA	CAC-C3C-C4C	2.28	127.76	124.79
11	A	801	CL0	O2D-CGD-O1D	-2.28	119.41	123.85
12	H	802	CLA	CMB-C2B-C3B	2.28	131.92	126.55
12	a	812	CLA	CHD-C4C-NC	-2.28	120.69	124.23
12	B	806	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
12	b	833	CLA	CAC-C3C-C4C	2.28	127.76	124.79
12	F	201	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
12	a	828	CLA	CAA-CBA-CGA	-2.28	106.73	113.21
12	G	833	CLA	C4D-C3D-CAD	2.28	110.58	108.11
12	B	807	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
15	a	845	BCR	C12-C13-C14	-2.28	115.42	119.01
12	G	805	CLA	CMB-C2B-C1B	2.28	128.89	125.42
12	G	821	CLA	CAC-C3C-C4C	2.28	127.76	124.79
12	B	829	CLA	C1-C2-C3	-2.28	122.46	126.20
13	H	840	1L3	C19-C20-C21	-2.28	122.41	127.62
15	f	204	BCR	C38-C26-C25	-2.28	122.00	124.48
12	b	821	CLA	CAC-C3C-C4C	2.28	127.75	124.79
12	G	821	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
16	a	850	LHG	O8-C23-C24	2.28	118.78	111.83
12	b	825	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
12	a	855	CLA	CMB-C2B-C3B	2.28	131.91	126.55
12	H	808	CLA	C4D-C3D-CAD	2.28	110.58	108.11
12	A	804	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	B	827	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	H	809	CLA	CMB-C2B-C1B	2.28	128.89	125.42
12	A	804	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
12	b	826	CLA	C2B-C1B-NB	2.28	112.69	110.33
12	G	802	CLA	C3A-C2A-C1A	2.28	104.75	101.34
12	G	839	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
12	l	206	CLA	CMC-C2C-C1C	2.28	128.59	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	j	101	BCR	C3-C4-C5	-2.28	110.00	114.06
12	a	825	CLA	CBA-CAA-C2A	2.28	120.56	113.79
12	G	818	CLA	OBD-CAD-C3D	-2.28	123.10	128.42
15	H	843	BCR	C40-C30-C25	2.28	113.81	110.24
12	S	203	CLA	C4D-C3D-CAD	2.28	110.58	108.11
12	B	803	CLA	CMC-C2C-C1C	2.27	128.59	125.03
12	B	830	CLA	CHC-C1C-C2C	-2.27	120.48	126.95
12	G	833	CLA	C4C-C3C-C2C	-2.27	103.58	106.89
12	b	810	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
12	H	807	CLA	C4D-C3D-CAD	2.27	110.58	108.11
15	G	846	BCR	C34-C9-C10	-2.27	119.13	122.82
12	G	822	CLA	CMB-C2B-C3B	2.27	131.90	126.55
12	H	826	CLA	CED-O2D-CGD	2.27	121.07	115.92
12	a	823	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
12	b	802	CLA	O2A-C1-C2	2.27	116.86	108.11
12	a	809	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
12	A	806	CLA	C4D-C3D-CAD	2.27	110.57	108.11
12	G	803	CLA	C4C-C3C-C2C	-2.27	103.58	106.89
12	A	828	CLA	C1-O2A-CGA	2.27	122.15	116.65
12	G	835	CLA	C3D-C4D-ND	2.27	113.68	109.99
12	B	817	CLA	C3D-C4D-ND	2.27	113.68	109.99
15	J	104	BCR	C37-C22-C21	-2.27	119.14	122.82
12	H	839	CLA	CHB-C4A-NA	2.27	127.68	124.40
12	B	804	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
15	S	201	BCR	C36-C18-C17	-2.27	119.14	122.82
12	B	827	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
15	J	102	BCR	C34-C9-C10	-2.27	119.14	122.82
12	G	818	CLA	CMA-C3A-C4A	2.27	117.87	111.77
12	a	828	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
12	b	824	CLA	CBA-CAA-C2A	2.27	120.55	113.79
12	B	828	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
12	G	826	CLA	C1-O2A-CGA	2.27	122.14	116.65
12	A	829	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
12	A	820	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
12	G	816	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
12	b	848	CLA	C1-C2-C3	-2.27	122.48	126.20
12	A	817	CLA	CMC-C2C-C1C	2.27	128.58	125.03
12	H	805	CLA	C6-C7-C8	-2.27	108.43	115.97
12	H	805	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
15	L	201	BCR	C4-C5-C6	-2.27	119.64	122.70
12	A	814	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
12	F	203	CLA	O2D-CGD-O1D	-2.27	119.44	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	842	BCR	C19-C18-C17	2.27	122.57	119.01
12	A	834	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
15	a	844	BCR	C19-C18-C17	2.27	122.57	119.01
12	A	831	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
12	G	819	CLA	CMC-C2C-C1C	2.27	128.57	125.03
12	A	816	CLA	CED-O2D-CGD	2.27	121.05	115.92
12	G	810	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
12	b	816	CLA	CAC-C3C-C4C	2.27	127.74	124.79
12	A	835	CLA	CAC-C3C-C4C	2.27	127.74	124.79
12	f	201	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
15	G	850	BCR	C34-C9-C8	2.26	121.55	118.09
12	B	838	CLA	CMB-C2B-C3B	2.26	131.88	126.55
12	G	856	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
15	S	201	BCR	C15-C14-C13	-2.26	124.10	127.28
12	A	817	CLA	CHA-C1A-NA	-2.26	121.26	126.39
12	A	802	CLA	CMB-C2B-C1B	2.26	128.87	125.42
12	a	839	CLA	CMB-C2B-C3B	2.26	131.88	126.55
12	H	822	CLA	CHB-C4A-NA	2.26	127.67	124.40
12	b	802	CLA	C7-C6-C5	-2.26	107.23	113.26
12	G	833	CLA	C1-O2A-CGA	2.26	122.13	116.65
12	a	820	CLA	C3D-C4D-ND	2.26	113.67	109.99
12	a	827	CLA	C3D-C4D-ND	2.26	113.67	109.99
12	B	821	CLA	C3D-C4D-ND	2.26	113.67	109.99
15	b	843	BCR	C29-C30-C25	2.26	113.73	110.44
12	G	827	CLA	C1-C2-C3	-2.26	122.49	126.20
15	J	102	BCR	C40-C30-C25	2.26	113.79	110.24
12	b	831	CLA	C3C-C4C-NC	2.26	113.33	110.43
11	A	801	CL0	C2A-C3A-C4A	2.26	105.52	101.87
12	A	841	CLA	CED-O2D-CGD	2.26	121.05	115.92
12	H	812	CLA	CHB-C4A-NA	2.26	127.66	124.40
12	a	812	CLA	C3D-C4D-ND	2.26	113.66	109.99
12	a	830	CLA	C1-C2-C3	-2.26	123.10	126.76
12	H	833	CLA	C3C-C4C-NC	2.26	113.33	110.43
12	B	809	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
15	a	849	BCR	C40-C30-C25	2.26	113.79	110.24
12	H	827	CLA	C3B-C4B-NB	2.26	112.55	110.53
15	A	848	BCR	C36-C18-C17	-2.26	119.15	122.82
12	B	825	CLA	C1-C2-C3	-2.26	122.49	126.20
12	B	812	CLA	CBA-CAA-C2A	2.26	120.52	113.79
12	A	827	CLA	CMB-C2B-C3B	2.26	131.87	126.55
15	H	842	BCR	C30-C25-C26	-2.26	119.55	122.64
12	B	822	CLA	C1-C2-C3	-2.26	122.50	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	801	CL0	C1-O2A-CGA	2.26	122.12	116.65
12	b	834	CLA	CMB-C2B-C1B	2.26	128.86	125.42
12	A	805	CLA	C2A-C3A-C4A	2.26	105.52	101.87
11	A	801	CL0	C16-C17-C18	-2.26	105.86	115.94
12	B	837	CLA	C6-C5-C3	-2.26	107.97	113.47
12	b	808	CLA	C3B-C4B-NB	2.26	112.55	110.53
12	H	824	CLA	CHA-C4D-ND	2.26	137.21	132.55
15	G	846	BCR	C12-C13-C14	-2.26	115.46	119.01
12	A	803	CLA	C4B-CHC-C1C	2.26	131.56	126.25
12	A	840	CLA	C4C-C3C-C2C	-2.26	103.61	106.89
15	P	202	BCR	C36-C18-C17	-2.26	119.16	122.82
12	H	829	CLA	OBD-CAD-C3D	-2.26	123.14	128.42
12	G	802	CLA	CAA-CBA-CGA	-2.26	106.80	113.21
12	G	842	CLA	C1-C2-C3	-2.26	122.50	126.20
15	J	102	BCR	C39-C30-C25	-2.26	106.70	110.24
12	H	811	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
12	A	841	CLA	C4-C3-C5	2.26	119.14	115.23
12	H	831	CLA	C4C-C3C-C2C	-2.26	103.61	106.89
15	R	102	BCR	C34-C9-C10	-2.26	119.16	122.82
12	a	835	CLA	C3D-C4D-ND	2.26	113.65	109.99
12	b	848	CLA	CHD-C4C-C3C	-2.26	121.48	124.77
15	G	845	BCR	C34-C9-C10	-2.26	119.16	122.82
12	a	855	CLA	CHD-C1D-C2D	-2.26	120.80	125.49
12	A	815	CLA	CAA-C2A-C3A	-2.26	106.91	113.00
12	b	828	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
12	G	834	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
15	b	843	BCR	C34-C9-C10	-2.25	119.16	122.82
12	a	817	CLA	CHB-C1B-C2B	-2.25	120.88	127.43
12	b	825	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
12	B	818	CLA	CAC-C3C-C4C	2.25	127.72	124.79
12	a	829	CLA	CMB-C2B-C3B	2.25	131.85	126.55
15	J	104	BCR	C8-C9-C10	2.25	122.55	119.01
12	b	822	CLA	C1-C2-C3	-2.25	122.51	126.20
12	G	819	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
12	a	834	CLA	C4-C3-C2	-2.25	117.84	123.63
12	G	842	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
12	G	825	CLA	C1-C2-C3	-2.25	122.51	126.20
12	B	810	CLA	CHA-C1A-NA	-2.25	121.29	126.39
12	B	820	CLA	C3C-C4C-NC	2.25	113.31	110.43
15	b	841	BCR	C29-C28-C27	2.25	116.23	111.28
15	J	101	BCR	C38-C26-C25	-2.25	122.03	124.48
12	B	834	CLA	CMB-C2B-C3B	2.25	131.85	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	837	CLA	C4-C3-C5	2.25	119.14	115.23
12	b	824	CLA	CMB-C2B-C3B	2.25	131.84	126.55
12	A	839	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	a	839	CLA	CMC-C2C-C1C	2.25	128.55	125.03
12	L	204	CLA	C1-C2-C3	-2.25	122.51	126.20
12	A	854	CLA	CHA-C1A-NA	-2.25	121.30	126.39
12	a	816	CLA	CAC-C3C-C4C	2.25	127.72	124.79
12	a	814	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
13	A	842	1L3	C14-C03-C04	2.25	120.95	118.58
12	A	824	CLA	CHA-C1A-NA	-2.25	121.30	126.39
15	G	847	BCR	C38-C26-C27	2.25	118.39	113.60
12	a	804	CLA	CBC-CAC-C3C	-2.25	106.33	112.42
12	G	831	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
12	H	813	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
12	b	806	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
12	b	825	CLA	C4B-C3B-C2B	-2.25	104.51	107.30
15	H	843	BCR	C23-C22-C21	-2.25	115.47	119.01
15	l	201	BCR	C1-C6-C7	2.25	121.74	115.65
15	b	841	BCR	C35-C13-C12	2.25	121.52	118.09
12	a	819	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
15	G	850	BCR	C1-C6-C7	2.25	121.74	115.65
15	L	201	BCR	C19-C18-C17	2.25	122.54	119.01
17	T	101	45D	C21-C15-C17	2.25	118.89	115.49
15	j	103	BCR	C15-C14-C13	-2.24	124.13	127.28
15	H	842	BCR	C31-C1-C6	-2.24	106.72	110.24
12	b	802	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
12	A	807	CLA	C1-C2-C3	-2.24	122.52	126.20
12	A	829	CLA	CMB-C2B-C3B	2.24	131.83	126.55
12	B	829	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
12	a	803	CLA	C3D-C4D-ND	2.24	113.63	109.99
12	H	820	CLA	CAC-C3C-C4C	2.24	127.71	124.79
12	A	803	CLA	C4-C3-C5	2.24	119.12	115.23
12	H	835	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
15	H	841	BCR	C37-C22-C21	-2.24	119.18	122.82
12	G	825	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
12	A	810	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
12	b	837	CLA	CMB-C2B-C3B	2.24	131.82	126.55
15	H	845	BCR	C34-C9-C10	-2.24	119.19	122.82
12	a	820	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
12	S	202	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
12	G	821	CLA	CHB-C1B-C2B	-2.24	120.92	127.43
15	A	849	BCR	C1-C6-C5	-2.24	119.57	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	812	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
12	A	828	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
12	B	827	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
12	A	832	CLA	CMB-C2B-C3B	2.24	131.82	126.55
12	H	831	CLA	C3C-C4C-NC	2.24	113.30	110.43
17	m	101	45D	C22-C16-C18	2.24	118.88	115.49
12	H	801	CLA	CED-O2D-CGD	2.24	120.99	115.92
12	B	812	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
12	b	826	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
12	b	828	CLA	CBA-CAA-C2A	2.24	120.45	113.79
12	G	828	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
12	B	824	CLA	CHB-C4A-NA	2.24	127.63	124.40
12	a	827	CLA	CAC-C3C-C4C	2.24	127.70	124.79
12	G	837	CLA	CMC-C2C-C1C	2.24	128.53	125.03
15	Q	101	BCR	C37-C22-C21	-2.24	119.19	122.82
12	H	808	CLA	C1-O2A-CGA	2.24	122.06	116.65
15	a	852	BCR	C3-C4-C5	-2.24	110.07	114.06
12	a	803	CLA	C4-C3-C5	2.24	119.11	115.23
15	b	840	BCR	C15-C14-C13	-2.24	124.14	127.28
12	A	805	CLA	CAA-CBA-CGA	-2.24	106.86	113.21
12	b	806	CLA	CHB-C4A-NA	2.24	127.63	124.40
12	A	813	CLA	CHA-C1A-NA	-2.24	121.33	126.39
12	S	202	CLA	C1-C2-C3	-2.24	122.53	126.20
12	b	813	CLA	CMA-C3A-C4A	2.23	117.78	111.77
12	B	821	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
12	H	812	CLA	CAC-C3C-C4C	2.23	127.70	124.79
15	H	843	BCR	C35-C13-C12	2.23	121.50	118.09
17	m	101	45D	C21-C15-C17	2.23	118.87	115.49
12	a	834	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
17	m	101	45D	C06-C04-C08	2.23	113.68	110.44
12	H	804	CLA	C1-O2A-CGA	2.23	122.05	116.65
12	B	822	CLA	CAC-C3C-C4C	2.23	127.69	124.79
12	B	807	CLA	C3D-C4D-ND	2.23	113.61	109.99
12	H	808	CLA	CHB-C4A-NA	2.23	127.62	124.40
12	A	831	CLA	CHA-C1A-NA	-2.23	121.34	126.39
15	G	847	BCR	C7-C8-C9	-2.23	122.93	126.23
12	b	819	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
12	H	831	CLA	C4-C3-C5	2.23	119.10	115.23
12	A	809	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
12	H	804	CLA	C3C-C4C-NC	2.23	113.29	110.43
12	B	821	CLA	CMC-C2C-C1C	2.23	128.52	125.03
12	H	811	CLA	CHA-C1A-NA	-2.23	121.34	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	841	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
12	b	821	CLA	CMA-C3A-C2A	2.23	122.60	113.98
12	H	832	CLA	C4D-C3D-CAD	2.23	110.53	108.11
12	B	838	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
12	H	809	CLA	C3B-C4B-NB	2.23	112.52	110.53
12	b	816	CLA	C3C-C4C-NC	2.23	113.28	110.43
12	a	824	CLA	C1-C2-C3	-2.23	122.55	126.20
15	f	204	BCR	C37-C22-C21	-2.23	119.21	122.82
12	B	814	CLA	C6-C5-C3	-2.23	108.04	113.47
15	A	852	BCR	C34-C9-C8	2.23	121.49	118.09
12	H	829	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
12	b	826	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
12	A	804	CLA	C1-C2-C3	-2.23	122.55	126.20
12	A	825	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
12	G	823	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
15	L	207	BCR	C19-C18-C17	2.23	122.51	119.01
12	A	821	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
15	H	845	BCR	C35-C13-C12	2.23	121.49	118.09
12	A	827	CLA	C4-C3-C5	2.23	119.09	115.23
15	f	202	BCR	C33-C5-C6	-2.23	122.06	124.48
12	a	822	CLA	CMB-C2B-C1B	2.23	128.81	125.42
12	a	829	CLA	C3B-C4B-NB	2.22	112.52	110.53
12	B	807	CLA	C2B-C1B-NB	2.22	112.63	110.33
12	G	813	CLA	CHB-C4A-NA	2.22	127.61	124.40
12	G	842	CLA	C3D-C4D-ND	2.22	113.60	109.99
12	a	840	CLA	CHD-C4C-C3C	-2.22	121.53	124.77
12	B	833	CLA	CHB-C4A-NA	2.22	127.61	124.40
15	F	204	BCR	C38-C26-C27	2.22	118.34	113.60
12	H	822	CLA	CHD-C4C-C3C	-2.22	121.53	124.77
12	b	828	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
12	a	808	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
12	b	826	CLA	CHD-C1D-ND	-2.22	121.67	124.80
15	P	202	BCR	C37-C22-C21	-2.22	119.22	122.82
15	R	102	BCR	C29-C28-C27	2.22	116.16	111.28
12	j	102	CLA	CHD-C1D-ND	-2.22	121.68	124.80
15	a	849	BCR	C4-C5-C6	-2.22	119.70	122.70
12	a	803	CLA	CAC-C3C-C4C	2.22	127.68	124.79
12	B	819	CLA	CAC-C3C-C4C	2.22	127.68	124.79
12	L	206	CLA	CMC-C2C-C1C	2.22	128.50	125.03
12	H	815	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
12	a	812	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
12	H	827	CLA	C3B-C2B-C1B	-2.22	104.55	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	l	203	BCR	C36-C18-C17	-2.22	119.22	122.82
12	H	834	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
12	G	815	CLA	CMB-C2B-C3B	2.22	131.77	126.55
12	b	815	CLA	C1-C2-C3	-2.22	122.56	126.20
12	b	829	CLA	C1-C2-C3	-2.22	122.56	126.20
12	H	850	CLA	CHD-C4C-C3C	-2.22	121.54	124.77
12	B	802	CLA	C7-C6-C5	-2.22	107.35	113.26
12	B	834	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
15	a	844	BCR	C38-C26-C25	-2.22	122.06	124.48
12	A	835	CLA	CHA-C1A-NA	-2.22	121.37	126.39
12	G	821	CLA	CED-O2D-CGD	2.22	120.95	115.92
12	a	832	CLA	C4-C3-C5	2.22	119.08	115.23
15	R	101	BCR	C34-C9-C8	2.22	121.48	118.09
12	B	804	CLA	CHB-C4A-NA	2.22	127.60	124.40
12	a	812	CLA	CMC-C2C-C3C	2.22	132.15	126.15
12	f	203	CLA	CMC-C2C-C1C	2.22	128.50	125.03
12	b	805	CLA	C6-C7-C8	-2.22	108.59	115.97
12	G	836	CLA	O2A-C1-C2	2.22	116.64	108.11
12	G	802	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
12	a	836	CLA	C3C-C4C-NC	2.22	113.27	110.43
12	B	823	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
13	G	843	1L3	C14-C03-C02	-2.22	121.09	124.89
12	a	808	CLA	C3D-C4D-ND	2.22	113.59	109.99
15	H	845	BCR	C34-C9-C8	2.22	121.47	118.09
12	A	812	CLA	CMB-C2B-C1B	2.22	128.79	125.42
12	S	204	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
15	J	102	BCR	C15-C14-C13	-2.22	124.17	127.28
12	A	833	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
12	a	837	CLA	C4-C3-C5	2.22	119.08	115.23
12	A	828	CLA	C4-C3-C5	2.22	119.08	115.23
13	B	839	1L3	C24-C25-C26	-2.22	122.55	127.62
12	A	824	CLA	CAA-C2A-C1A	2.22	119.24	111.97
15	H	844	BCR	C39-C30-C25	2.22	113.72	110.24
11	a	801	CL0	C3A-C2A-C1A	-2.22	98.02	101.34
12	B	826	CLA	C4-C3-C5	2.22	119.07	115.23
12	H	822	CLA	C1-O2A-CGA	2.22	122.01	116.65
12	l	204	CLA	C1-C2-C3	-2.21	122.57	126.20
12	B	817	CLA	CBA-CAA-C2A	2.21	120.38	113.79
12	b	805	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
15	a	844	BCR	C34-C9-C10	-2.21	119.23	122.82
12	A	806	CLA	C4-C3-C5	2.21	119.07	115.23
12	G	820	CLA	O1D-CGD-CBD	-2.21	120.15	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	837	CLA	CMC-C2C-C1C	2.21	128.49	125.03
12	b	802	CLA	CHB-C4A-NA	2.21	127.59	124.40
15	J	102	BCR	C33-C5-C6	-2.21	122.07	124.48
12	G	832	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
15	A	852	BCR	C29-C28-C27	2.21	116.14	111.28
12	B	809	CLA	C3D-C4D-ND	2.21	113.58	109.99
12	B	831	CLA	CMA-C3A-C4A	2.21	117.72	111.77
12	b	830	CLA	CMA-C3A-C4A	2.21	117.72	111.77
12	b	837	CLA	CHB-C4A-NA	2.21	127.59	124.40
12	H	806	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
12	B	804	CLA	C3D-C4D-ND	2.21	113.58	109.99
12	a	819	CLA	C3C-C4C-NC	2.21	113.26	110.43
12	b	822	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
15	H	845	BCR	C19-C18-C17	2.21	122.49	119.01
12	b	816	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
15	A	844	BCR	C27-C26-C25	-2.21	119.72	122.70
12	B	816	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
12	b	811	CLA	C1-C2-C3	-2.21	122.58	126.20
15	a	847	BCR	C37-C22-C21	-2.21	119.24	122.82
12	a	802	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
12	G	832	CLA	C1-C2-C3	-2.21	122.58	126.20
12	A	833	CLA	CMB-C2B-C1B	2.21	128.78	125.42
12	G	818	CLA	CHB-C4A-NA	2.21	127.59	124.40
12	b	837	CLA	CHC-C1C-NC	-2.21	120.98	124.31
12	G	818	CLA	CED-O2D-CGD	2.21	120.92	115.92
12	G	818	CLA	CMC-C2C-C1C	2.21	128.48	125.03
12	a	824	CLA	CHA-C4D-ND	2.21	137.10	132.55
12	a	810	CLA	C3C-C4C-NC	2.21	113.26	110.43
12	H	802	CLA	OBD-CAD-C3D	-2.21	123.26	128.42
12	b	833	CLA	OBD-CAD-C3D	-2.21	123.26	128.42
12	G	840	CLA	C4C-C3C-C2C	-2.21	103.68	106.89
12	H	827	CLA	C3D-C4D-ND	2.21	113.57	109.99
12	H	811	CLA	CMC-C2C-C1C	2.20	128.48	125.03
15	A	847	BCR	C33-C5-C4	2.20	118.30	113.60
11	G	801	CL0	CBC-CAC-C3C	-2.20	106.45	112.42
12	b	820	CLA	C3C-C4C-NC	2.20	113.25	110.43
12	H	839	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
15	i	102	BCR	C31-C1-C6	2.20	113.70	110.24
12	A	826	CLA	C6-C5-C3	-2.20	108.10	113.47
12	a	817	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
12	a	809	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
12	H	811	CLA	CHA-C4D-ND	2.20	137.09	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	804	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
12	B	803	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
12	A	831	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
12	H	801	CLA	C3D-C4D-ND	2.20	113.56	109.99
12	H	836	CLA	CMB-C2B-C1B	2.20	128.77	125.42
15	A	845	BCR	C37-C22-C21	-2.20	119.25	122.82
12	B	826	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
15	b	844	BCR	C2-C3-C4	2.20	116.11	111.28
12	H	817	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
12	H	825	CLA	CHB-C4A-NA	2.20	127.57	124.40
12	A	803	CLA	C3D-C4D-ND	2.20	113.56	109.99
12	A	835	CLA	C3D-C4D-ND	2.20	113.56	109.99
15	L	201	BCR	C1-C6-C7	2.20	121.61	115.65
15	B	841	BCR	C33-C5-C4	2.20	118.28	113.60
12	B	813	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
12	a	813	CLA	CMC-C2C-C1C	2.20	128.47	125.03
12	a	803	CLA	C4B-CHC-C1C	2.20	131.42	126.25
12	A	812	CLA	C1-C2-C3	-2.20	123.21	126.76
12	a	827	CLA	CHD-C4C-C3C	-2.20	121.57	124.77
12	A	818	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
12	H	807	CLA	C2B-C1B-NB	2.20	112.61	110.33
12	G	831	CLA	CMB-C2B-C1B	2.20	128.76	125.42
12	a	829	CLA	C3C-C4C-NC	2.20	113.25	110.43
12	G	839	CLA	CHB-C4A-NA	2.20	127.57	124.40
15	F	202	BCR	C1-C6-C7	2.20	121.61	115.65
12	G	808	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
15	S	201	BCR	C38-C26-C25	-2.20	122.09	124.48
12	a	840	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
12	b	810	CLA	C6-C5-C3	-2.20	108.12	113.47
12	b	820	CLA	CAC-C3C-C4C	2.20	127.65	124.79
12	H	804	CLA	C1-C2-C3	-2.20	122.60	126.20
12	G	807	CLA	C4D-C3D-CAD	2.20	110.49	108.11
12	G	825	CLA	CAA-C2A-C1A	2.20	119.17	111.97
12	B	821	CLA	CMA-C3A-C2A	2.20	122.47	113.98
15	A	852	BCR	C38-C26-C27	2.19	118.28	113.60
12	G	828	CLA	C4-C3-C5	2.19	119.04	115.23
12	A	839	CLA	C3D-C4D-ND	2.19	113.55	109.99
12	a	828	CLA	CED-O2D-CGD	2.19	120.89	115.92
12	H	825	CLA	CHA-C1A-NA	-2.19	121.42	126.39
12	B	826	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
12	b	809	CLA	C3D-C4D-ND	2.19	113.55	109.99
12	a	809	CLA	CMD-C2D-C3D	-2.19	122.66	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	832	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
15	i	102	BCR	C34-C9-C10	-2.19	119.26	122.82
12	G	821	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
12	a	803	CLA	CMA-C3A-C4A	2.19	117.67	111.77
12	B	807	CLA	CMC-C2C-C3C	2.19	132.08	126.15
15	S	205	BCR	C1-C6-C7	2.19	121.60	115.65
15	J	101	BCR	C3-C4-C5	-2.19	110.15	114.06
12	G	856	CLA	CHD-C1D-C2D	-2.19	120.93	125.49
12	a	812	CLA	OBD-CAD-C3D	-2.19	123.29	128.42
12	B	818	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
15	a	845	BCR	C37-C22-C21	-2.19	119.27	122.82
12	b	804	CLA	C3C-C4C-NC	2.19	113.24	110.43
12	B	807	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
12	A	812	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	G	804	CLA	C4-C3-C5	2.19	119.03	115.23
12	A	832	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
12	H	829	CLA	CHA-C1A-NA	-2.19	121.43	126.39
12	G	810	CLA	CAC-C3C-C4C	2.19	127.64	124.79
15	P	204	BCR	C39-C30-C25	-2.19	106.81	110.24
15	b	839	BCR	C34-C9-C10	-2.19	119.27	122.82
15	J	104	BCR	C35-C13-C12	2.19	121.43	118.09
12	l	204	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
15	B	840	BCR	C34-C9-C10	-2.19	119.27	122.82
12	B	832	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
15	b	844	BCR	C29-C28-C27	2.19	116.09	111.28
16	A	850	LHG	O8-C23-C24	2.19	118.51	111.83
12	A	814	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
15	b	841	BCR	C31-C1-C6	-2.19	106.81	110.24
15	Q	102	BCR	C36-C18-C17	-2.19	119.27	122.82
12	A	822	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
12	b	804	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	B	833	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
15	b	839	BCR	C37-C22-C21	-2.19	119.28	122.82
12	a	812	CLA	C1-C2-C3	-2.19	123.23	126.76
12	B	823	CLA	CHD-C1D-ND	-2.19	121.73	124.80
15	b	847	BCR	C4-C5-C6	-2.19	119.75	122.70
12	G	821	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
12	B	825	CLA	CMA-C3A-C4A	2.19	117.65	111.77
12	G	814	CLA	CHB-C1B-C2B	-2.18	121.08	127.43
12	B	834	CLA	CAC-C3C-C4C	2.18	127.63	124.79
12	A	836	CLA	C5-C3-C4	2.18	119.62	114.59
12	B	823	CLA	CHD-C4C-C3C	-2.18	121.59	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	807	CLA	CMC-C2C-C1C	2.18	128.45	125.03
12	B	821	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
12	L	202	CLA	CHB-C4A-NA	2.18	127.55	124.40
12	G	841	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
12	G	810	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
12	H	801	CLA	CHA-C1A-NA	-2.18	121.45	126.39
12	G	808	CLA	C4D-C3D-CAD	2.18	110.47	108.11
12	G	856	CLA	O2D-CGD-CBD	2.18	115.04	111.23
12	b	808	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
12	A	839	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
15	R	102	BCR	C33-C5-C6	-2.18	122.11	124.48
12	B	823	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
15	a	844	BCR	C27-C26-C25	-2.18	119.76	122.70
12	A	822	CLA	CMC-C2C-C1C	2.18	128.44	125.03
12	H	830	CLA	C1-C2-C3	-2.18	122.63	126.20
12	a	831	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
12	A	804	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
12	A	819	CLA	CMC-C2C-C1C	2.18	128.44	125.03
12	B	811	CLA	CMC-C2C-C1C	2.18	128.44	125.03
12	G	818	CLA	CHA-C1A-NA	-2.18	121.46	126.39
12	G	815	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
12	A	822	CLA	CAC-C3C-C4C	2.18	127.62	124.79
12	H	838	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
12	A	814	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
12	a	806	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
15	A	852	BCR	C3-C4-C5	-2.18	110.17	114.06
12	H	807	CLA	C3B-C4B-NB	2.18	112.47	110.53
13	G	843	1L3	C27-C26-C28	2.18	119.01	115.23
15	f	204	BCR	C34-C9-C10	-2.18	119.29	122.82
12	B	806	CLA	C3C-C4C-NC	2.18	113.22	110.43
12	B	817	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
12	H	824	CLA	CHD-C4C-C3C	-2.18	121.60	124.77
15	b	844	BCR	C31-C1-C6	-2.18	106.83	110.24
12	a	837	CLA	CMC-C2C-C1C	2.18	128.43	125.03
12	G	804	CLA	C4B-CHC-C1C	2.18	131.36	126.25
12	a	854	CLA	C6-C7-C8	-2.18	108.73	115.97
12	G	819	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
12	B	837	CLA	C2B-C1B-NB	2.17	112.58	110.33
12	a	833	CLA	CMA-C3A-C4A	2.17	117.62	111.77
12	a	837	CLA	C3C-C4C-NC	2.17	113.22	110.43
12	b	828	CLA	CAC-C3C-C4C	2.17	127.62	124.79
12	a	825	CLA	CAA-CBA-CGA	-2.17	107.04	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	842	1L3	C27-C26-C28	2.17	119.00	115.23
11	a	801	CL0	CMD-C2D-C3D	-2.17	122.71	127.69
12	B	814	CLA	C1-O2A-CGA	2.17	121.91	116.65
12	G	808	CLA	C4-C3-C5	2.17	119.00	115.23
12	a	813	CLA	C3D-C4D-ND	2.17	113.52	109.99
12	H	826	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
12	H	822	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
12	F	201	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
12	a	816	CLA	CHA-C1A-NA	-2.17	121.47	126.39
15	H	844	BCR	C35-C13-C12	2.17	119.58	114.59
12	a	827	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
16	A	850	LHG	O7-C7-O9	-2.17	118.63	123.70
12	H	806	CLA	CMA-C3A-C4A	2.17	117.61	111.77
12	H	839	CLA	C4B-CHC-C1C	2.17	131.35	126.25
12	H	833	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
12	a	805	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	a	820	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	B	836	CLA	CMC-C2C-C1C	2.17	128.43	125.03
12	B	808	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
12	A	839	CLA	C4-C3-C5	2.17	118.99	115.23
12	H	824	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
12	A	838	CLA	C4B-CHC-C1C	2.17	131.35	126.25
12	b	806	CLA	C3A-C2A-C1A	2.17	104.59	101.34
12	b	803	CLA	C4-C3-C5	2.17	118.99	115.23
12	H	802	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	H	819	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
12	H	824	CLA	CMC-C2C-C3C	2.17	132.01	126.15
12	a	824	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
12	G	834	CLA	C1-O2A-CGA	2.17	121.90	116.65
12	B	822	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
15	H	845	BCR	C30-C25-C24	2.17	121.53	115.65
12	A	808	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
15	B	844	BCR	C34-C9-C10	-2.17	119.30	122.82
12	a	807	CLA	C3D-C4D-ND	2.17	113.51	109.99
12	b	817	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
15	B	841	BCR	C38-C26-C25	-2.17	122.12	124.48
12	G	834	CLA	CHB-C1B-C2B	-2.17	121.14	127.43
12	G	826	CLA	CBA-CAA-C2A	2.17	120.24	113.79
12	b	826	CLA	CBC-CAC-C3C	-2.17	106.55	112.42
12	H	823	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
12	b	803	CLA	CHA-C1A-NA	-2.17	121.49	126.39
13	b	838	1L3	C24-C25-C26	-2.17	122.67	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	830	CLA	CHA-C4D-ND	2.17	137.02	132.55
15	J	101	BCR	C32-C1-C6	2.17	113.64	110.24
12	b	805	CLA	C1-C2-C3	-2.17	122.65	126.20
12	H	815	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	H	834	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	G	814	CLA	CAA-C2A-C3A	-2.16	107.15	113.00
12	H	839	CLA	CMA-C3A-C4A	2.16	117.59	111.77
12	B	819	CLA	CHB-C4A-NA	2.16	127.52	124.40
13	a	842	1L3	C33-C31-C32	2.16	119.57	114.59
12	B	837	CLA	C1-C2-C3	-2.16	122.65	126.20
13	A	842	1L3	C33-C31-C32	2.16	119.57	114.59
12	b	812	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
12	a	841	CLA	C4D-C3D-CAD	2.16	110.45	108.11
12	b	829	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
12	G	832	CLA	C3D-C4D-ND	2.16	113.50	109.99
12	B	824	CLA	C6-C7-C8	-2.16	108.78	115.97
12	b	824	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	B	822	CLA	CHD-C1D-ND	-2.16	121.76	124.80
15	L	203	BCR	C15-C14-C13	-2.16	124.25	127.28
12	b	823	CLA	C1-O2A-CGA	2.16	121.88	116.65
15	G	849	BCR	C35-C13-C12	2.16	121.39	118.09
12	a	814	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
15	H	846	BCR	C37-C22-C21	-2.16	119.32	122.82
15	F	202	BCR	C2-C1-C6	2.16	113.58	110.44
12	b	804	CLA	C1-C2-C3	-2.16	122.66	126.20
12	b	830	CLA	CHD-C1D-ND	-2.16	121.76	124.80
15	R	101	BCR	C39-C30-C25	2.16	113.63	110.24
12	H	811	CLA	CBC-CAC-C3C	2.16	118.27	112.42
15	G	845	BCR	C27-C26-C25	-2.16	119.79	122.70
12	a	811	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	H	823	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
12	b	813	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
12	H	829	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
12	A	802	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
12	a	804	CLA	C1-C2-C3	-2.16	122.66	126.20
12	A	822	CLA	CMB-C2B-C1B	2.16	128.71	125.42
12	l	206	CLA	CMB-C2B-C3B	2.16	131.62	126.55
12	A	826	CLA	C1-C2-C3	-2.16	122.66	126.20
12	a	833	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
12	H	821	CLA	C3C-C4C-NC	2.16	113.19	110.43
12	A	807	CLA	C3D-C4D-ND	2.16	113.49	109.99
12	b	833	CLA	C4C-C3C-C2C	-2.16	103.75	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	831	CLA	CAC-C3C-C4C	2.16	127.59	124.79
12	b	812	CLA	CAC-C3C-C4C	2.16	127.59	124.79
12	H	830	CLA	C3C-C4C-NC	2.16	113.19	110.43
12	B	821	CLA	C3C-C4C-NC	2.16	113.19	110.43
12	B	810	CLA	C6-C5-C3	-2.16	108.22	113.47
12	a	819	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
12	j	102	CLA	CMC-C2C-C3C	2.16	131.98	126.15
12	b	801	CLA	C3A-C2A-C1A	2.16	104.57	101.34
15	P	204	BCR	C30-C25-C26	-2.15	119.69	122.64
12	G	823	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
12	j	102	CLA	C4D-C3D-CAD	2.15	110.45	108.11
12	G	811	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
12	A	819	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
12	A	837	CLA	C4-C3-C5	2.15	118.97	115.23
12	G	815	CLA	CAC-C3C-C4C	2.15	127.59	124.79
12	G	833	CLA	CBB-CAB-C3B	-2.15	116.76	127.53
12	H	811	CLA	CHB-C4A-NA	2.15	127.51	124.40
12	a	841	CLA	C2B-C1B-NB	2.15	112.56	110.33
15	G	853	BCR	C29-C28-C27	2.15	116.01	111.28
12	b	831	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
15	J	101	BCR	C35-C13-C12	2.15	121.38	118.09
12	G	809	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
12	b	830	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
12	G	808	CLA	C1-C2-C3	-2.15	122.67	126.20
12	H	821	CLA	C4D-C3D-CAD	2.15	110.44	108.11
12	G	816	CLA	CHB-C4A-NA	2.15	127.51	124.40
12	G	815	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
12	B	823	CLA	CHA-C4D-ND	2.15	136.99	132.55
12	H	820	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
15	j	103	BCR	C33-C5-C6	-2.15	122.14	124.48
12	a	836	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
12	H	801	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
12	B	829	CLA	C4D-CHA-C1A	2.15	123.81	121.24
12	b	823	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
15	G	849	BCR	C12-C13-C14	-2.15	115.63	119.01
12	B	814	CLA	C3C-C4C-NC	2.15	113.19	110.43
12	b	810	CLA	CHD-C4C-C3C	-2.15	121.64	124.77
12	a	818	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
12	a	816	CLA	CED-O2D-CGD	2.15	120.79	115.92
12	B	825	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
12	A	838	CLA	CHC-C1C-NC	-2.15	121.07	124.31
15	L	201	BCR	C34-C9-C8	2.15	121.37	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	822	CLA	C11-C10-C8	-2.15	108.82	115.97
12	a	808	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
15	a	844	BCR	C38-C26-C27	2.15	118.18	113.60
12	B	831	CLA	C3D-C4D-ND	2.15	113.48	109.99
12	H	830	CLA	CAC-C3C-C4C	2.15	127.58	124.79
12	a	824	CLA	CHA-C1A-NA	-2.15	121.53	126.39
12	H	804	CLA	CHB-C4A-NA	2.15	127.50	124.40
11	A	801	CL0	CHC-C1C-NC	-2.15	121.08	124.31
15	S	201	BCR	C23-C22-C21	-2.15	115.63	119.01
12	H	824	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
12	A	820	CLA	C1-O2A-CGA	2.15	121.85	116.65
12	A	815	CLA	CHA-C1A-NA	-2.15	121.53	126.39
12	b	810	CLA	CMA-C3A-C4A	2.15	117.54	111.77
12	B	816	CLA	C3C-C4C-NC	2.15	113.18	110.43
12	G	822	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
12	B	824	CLA	CMC-C2C-C3C	2.15	131.95	126.15
15	i	102	BCR	C19-C18-C17	2.15	122.39	119.01
12	B	811	CLA	CHB-C4A-NA	2.15	127.50	124.40
12	a	804	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
12	a	828	CLA	CAC-C3C-C4C	2.15	127.58	124.79
12	G	855	CLA	CHA-C1A-NA	-2.15	121.53	126.39
12	G	819	CLA	CMB-C2B-C3B	2.15	131.60	126.55
12	b	827	CLA	CHB-C1B-C2B	-2.15	121.20	127.43
15	B	841	BCR	C31-C1-C6	-2.15	106.88	110.24
12	G	805	CLA	CBC-CAC-C3C	-2.15	106.61	112.42
12	l	205	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
12	a	824	CLA	CHD-C1D-C2D	-2.14	121.03	125.49
12	A	825	CLA	C4-C3-C5	2.14	118.95	115.23
12	H	825	CLA	CBA-CAA-C2A	2.14	120.17	113.79
12	H	838	CLA	C6-C5-C3	-2.14	108.25	113.47
12	a	818	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
12	H	802	CLA	C7-C6-C5	-2.14	107.55	113.26
12	a	806	CLA	C4D-C3D-CAD	2.14	110.43	108.11
12	H	808	CLA	C4B-CHC-C1C	2.14	131.28	126.25
12	b	807	CLA	C3D-C4D-ND	2.14	113.47	109.99
12	B	832	CLA	CMB-C2B-C1B	2.14	128.68	125.42
13	G	843	1L3	C19-C20-C21	-2.14	122.72	127.62
12	a	807	CLA	C4-C3-C5	2.14	118.94	115.23
12	B	821	CLA	C11-C10-C8	-2.14	108.85	115.97
12	B	820	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
12	G	817	CLA	C3C-C4C-NC	2.14	113.17	110.43
12	G	830	CLA	C3C-C4C-NC	2.14	113.17	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	832	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
11	G	801	CL0	C2A-C3A-C4A	2.14	105.33	101.87
12	H	839	CLA	CAC-C3C-C4C	2.14	127.57	124.79
12	B	811	CLA	CAC-C3C-C4C	2.14	127.57	124.79
15	S	205	BCR	C34-C9-C8	2.14	121.36	118.09
12	H	801	CLA	C4D-C3D-CAD	2.14	110.43	108.11
12	H	828	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
12	G	835	CLA	CHA-C1A-NA	-2.14	121.55	126.39
12	a	816	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
12	H	821	CLA	CAA-CBA-CGA	-2.14	106.78	112.49
15	G	845	BCR	C38-C26-C25	-2.14	122.15	124.48
12	A	815	CLA	CAC-C3C-C4C	2.14	127.57	124.79
12	a	836	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
15	B	840	BCR	C37-C22-C21	-2.14	119.35	122.82
12	b	813	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
12	B	831	CLA	CMC-C2C-C1C	2.14	128.37	125.03
12	G	835	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
12	A	854	CLA	CHC-C1C-NC	-2.14	121.09	124.31
15	l	203	BCR	C23-C24-C25	-2.14	121.29	127.00
12	b	848	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
12	B	834	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
12	a	807	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
15	Q	102	BCR	C34-C9-C10	-2.14	119.35	122.82
12	A	813	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
12	A	831	CLA	C1-O2A-CGA	2.14	121.82	116.65
12	G	842	CLA	CMC-C2C-C3C	2.14	131.93	126.15
12	a	824	CLA	CAA-C2A-C1A	2.14	118.97	111.97
12	B	836	CLA	CHB-C4A-NA	2.14	127.48	124.40
12	a	840	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
12	H	823	CLA	C1-O2A-CGA	2.14	121.82	116.65
12	H	832	CLA	CMA-C3A-C4A	2.13	117.51	111.77
12	G	834	CLA	CAC-C3C-C4C	2.13	127.57	124.79
12	H	821	CLA	CHB-C4A-NA	2.13	127.48	124.40
12	b	836	CLA	C6-C5-C3	-2.13	108.27	113.47
12	G	836	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
12	B	816	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
12	H	838	CLA	C1-C2-C3	-2.13	122.70	126.20
12	A	837	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
12	B	811	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
12	A	804	CLA	C3C-C4C-NC	2.13	113.16	110.43
12	a	836	CLA	C5-C3-C4	2.13	119.50	114.59
12	a	813	CLA	CHB-C4A-NA	2.13	127.48	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	828	CLA	CED-O2D-CGD	2.13	120.75	115.92
12	G	828	CLA	CHD-C4C-C3C	-2.13	121.67	124.77
12	H	824	CLA	C1-C2-C3	-2.13	122.70	126.20
12	G	805	CLA	CHB-C4A-NA	2.13	127.48	124.40
12	B	835	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
12	G	823	CLA	CMB-C2B-C1B	2.13	128.66	125.42
12	G	802	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
12	B	808	CLA	C3B-C4B-NB	2.13	112.43	110.53
12	H	834	CLA	C4-C3-C5	2.13	118.93	115.23
12	H	834	CLA	CHA-C1A-NA	-2.13	121.57	126.39
12	G	839	CLA	C3D-C4D-ND	2.13	113.45	109.99
12	B	816	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
12	H	835	CLA	CMB-C2B-C3B	2.13	131.56	126.55
12	b	811	CLA	CHB-C4A-NA	2.13	127.47	124.40
15	b	841	BCR	C37-C22-C23	2.13	121.34	118.09
15	F	202	BCR	C27-C26-C25	-2.13	119.83	122.70
12	b	833	CLA	CMB-C2B-C3B	2.13	131.56	126.55
12	H	807	CLA	CMA-C3A-C4A	2.13	117.49	111.77
13	A	842	1L3	C27-C26-C28	2.13	118.92	115.23
12	A	839	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
15	L	201	BCR	C24-C23-C22	-2.13	123.09	126.23
12	H	823	CLA	C1-C2-C3	-2.13	122.71	126.20
15	i	102	BCR	C37-C22-C21	-2.13	119.37	122.82
12	G	817	CLA	C1-C2-C3	-2.13	123.32	126.76
12	H	807	CLA	C4C-C3C-C2C	-2.13	103.80	106.89
12	G	841	CLA	C3C-C4C-NC	2.13	113.16	110.43
12	B	835	CLA	CMB-C2B-C1B	2.13	128.66	125.42
12	H	816	CLA	C4-C3-C5	2.13	118.92	115.23
15	P	204	BCR	C34-C9-C10	-2.13	119.37	122.82
12	B	815	CLA	C3D-C4D-ND	2.13	113.44	109.99
12	b	818	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
15	f	202	BCR	C36-C18-C17	-2.13	119.37	122.82
12	A	819	CLA	C3C-C4C-NC	2.13	113.15	110.43
12	a	823	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
12	H	823	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
12	a	825	CLA	C4-C3-C5	2.13	118.92	115.23
12	G	821	CLA	CMC-C2C-C3C	2.13	131.90	126.15
12	b	821	CLA	C11-C10-C8	-2.12	108.90	115.97
12	A	855	CLA	CHD-C1D-C2D	-2.12	121.07	125.49
12	a	834	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
15	B	844	BCR	C29-C30-C25	2.12	113.53	110.44
12	A	840	CLA	O1D-CGD-CBD	-2.12	120.33	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	813	CLA	CHA-C1A-NA	-2.12	121.58	126.39
12	S	204	CLA	CMB-C2B-C3B	2.12	131.54	126.55
12	G	813	CLA	C1-C2-C3	-2.12	123.33	126.76
12	G	825	CLA	CHA-C1A-NA	-2.12	121.58	126.39
12	B	831	CLA	CHA-C1A-NA	-2.12	121.58	126.39
15	b	841	BCR	C1-C6-C7	2.12	121.41	115.65
12	B	816	CLA	CAC-C3C-C4C	2.12	127.55	124.79
12	G	813	CLA	CHA-C4D-ND	2.12	136.93	132.55
15	R	101	BCR	C3-C4-C5	-2.12	110.27	114.06
12	F	201	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
12	b	830	CLA	C3D-C4D-ND	2.12	113.44	109.99
12	G	808	CLA	CHA-C1A-NA	-2.12	121.58	126.39
11	G	801	CL0	CHC-C1C-NC	-2.12	121.11	124.31
12	A	833	CLA	C1-O2A-CGA	2.12	121.79	116.65
15	a	846	BCR	C38-C26-C27	2.12	118.12	113.60
12	a	803	CLA	CHA-C4D-ND	2.12	136.93	132.55
16	A	853	LHG	O7-C7-O9	-2.12	118.75	123.70
12	H	815	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
12	A	838	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
12	G	819	CLA	C4D-C3D-CAD	2.12	110.41	108.11
12	a	806	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
12	A	816	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
12	b	848	CLA	CMB-C2B-C3B	2.12	131.54	126.55
12	A	831	CLA	CMC-C2C-C1C	2.12	128.35	125.03
15	f	202	BCR	C12-C13-C14	-2.12	115.67	119.01
12	b	830	CLA	C4D-C3D-CAD	2.12	110.41	108.11
12	B	801	CLA	C3C-C4C-NC	2.12	113.14	110.43
12	G	836	CLA	C5-C3-C4	2.12	119.47	114.59
15	b	844	BCR	C24-C23-C22	-2.12	123.10	126.23
16	A	850	LHG	C5-O7-C7	-2.12	112.72	117.80
12	H	824	CLA	CHD-C1D-ND	-2.12	121.82	124.80
15	b	840	BCR	C23-C24-C25	-2.12	121.34	127.00
16	A	853	LHG	C5-O7-C7	-2.12	112.73	117.80
12	b	820	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
15	A	846	BCR	C7-C8-C9	-2.12	123.10	126.23
12	a	821	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
15	i	102	BCR	C32-C1-C6	-2.12	106.92	110.24
12	B	833	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
12	G	855	CLA	CAC-C3C-C4C	2.12	127.54	124.79
12	B	808	CLA	CAC-C3C-C4C	2.12	127.54	124.79
12	G	824	CLA	C1-C2-C3	-2.12	122.73	126.20
12	A	804	CLA	C3D-C4D-ND	2.12	113.43	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	805	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
12	B	810	CLA	CHA-C4D-ND	2.12	136.91	132.55
12	b	829	CLA	CMA-C3A-C4A	2.12	117.46	111.77
12	a	804	CLA	C3D-C4D-ND	2.12	113.42	109.99
12	b	808	CLA	CHB-C4A-NA	2.11	127.45	124.40
12	B	822	CLA	C4D-C3D-CAD	2.11	110.40	108.11
15	b	842	BCR	C39-C30-C25	2.11	113.56	110.24
12	G	818	CLA	CMB-C2B-C3B	2.11	131.52	126.55
12	a	815	CLA	CAC-C3C-C4C	2.11	127.54	124.79
12	J	103	CLA	CAC-C3C-C4C	2.11	127.54	124.79
11	A	801	CL0	CHD-C4C-C3C	-2.11	121.69	124.77
15	i	101	BCR	C15-C14-C13	-2.11	124.32	127.28
12	H	826	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
15	H	842	BCR	C15-C14-C13	-2.11	124.32	127.28
12	a	802	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
11	A	801	CL0	C4D-CHA-C1A	-2.11	118.73	121.24
17	M	101	45D	C06-C04-C08	2.11	113.50	110.44
12	B	808	CLA	C3C-C4C-NC	2.11	113.13	110.43
12	B	835	CLA	CMA-C3A-C4A	2.11	117.44	111.77
12	a	802	CLA	CHA-C4D-ND	2.11	136.90	132.55
12	b	810	CLA	CHA-C4D-ND	2.11	136.90	132.55
12	A	834	CLA	CMB-C2B-C3B	2.11	131.51	126.55
12	G	817	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
12	B	801	CLA	O2D-CGD-CBD	2.11	114.92	111.23
12	a	839	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
12	b	822	CLA	C1-O2A-CGA	2.11	121.75	116.65
12	H	813	CLA	C3D-C4D-ND	2.11	113.41	109.99
12	G	829	CLA	C1-O2A-CGA	2.11	121.75	116.65
15	H	841	BCR	C38-C26-C27	2.11	118.09	113.60
12	H	809	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
12	a	806	CLA	CHD-C4C-C3C	-2.11	121.70	124.77
12	a	837	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
12	b	832	CLA	CMC-C2C-C1C	2.11	128.33	125.03
12	H	806	CLA	C3C-C4C-NC	2.11	113.13	110.43
12	H	809	CLA	C3C-C4C-NC	2.11	113.13	110.43
12	A	840	CLA	C5-C3-C4	2.11	119.44	114.59
12	a	834	CLA	CHB-C4A-NA	2.11	127.44	124.40
12	B	824	CLA	CHD-C1D-ND	-2.11	121.84	124.80
15	F	202	BCR	C33-C5-C6	-2.11	122.19	124.48
12	G	819	CLA	C7-C6-C5	-2.11	107.65	113.26
12	B	803	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
12	b	814	CLA	C3C-C4C-NC	2.11	113.13	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	833	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
12	b	828	CLA	CHB-C4A-NA	2.10	127.44	124.40
12	H	815	CLA	C3C-C4C-NC	2.10	113.13	110.43
15	F	204	BCR	C30-C25-C26	-2.10	119.76	122.64
15	f	204	BCR	C32-C1-C6	-2.10	106.94	110.24
12	S	204	CLA	C6-C5-C3	-2.10	108.34	113.47
12	G	831	CLA	CHC-C1C-NC	-2.10	121.14	124.31
12	A	838	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
12	H	830	CLA	C4D-C3D-CAD	2.10	110.39	108.11
12	H	818	CLA	CBA-CAA-C2A	2.10	120.05	113.79
15	b	843	BCR	C36-C18-C17	-2.10	119.41	122.82
12	A	823	CLA	CMB-C2B-C1B	2.10	128.62	125.42
19	B	847	LMT	O2B-C2B-C3B	2.10	115.33	110.38
15	l	203	BCR	C15-C14-C13	-2.10	124.33	127.28
12	a	810	CLA	CAC-C3C-C4C	2.10	127.53	124.79
12	a	828	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
12	G	809	CLA	CAC-C3C-C4C	2.10	127.52	124.79
12	B	833	CLA	C4C-C3C-C2C	-2.10	103.83	106.89
12	G	826	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
12	a	808	CLA	C3C-C4C-NC	2.10	113.12	110.43
12	B	838	CLA	C4-C3-C2	-2.10	118.23	123.63
12	j	102	CLA	C1-C2-C3	-2.10	122.76	126.20
12	G	826	CLA	C4C-C3C-C2C	-2.10	103.83	106.89
15	i	101	BCR	C37-C22-C21	-2.10	119.41	122.82
12	b	813	CLA	CHB-C4A-NA	2.10	127.43	124.40
12	A	808	CLA	CED-O2D-CGD	2.10	120.68	115.92
12	A	828	CLA	CHD-C1D-ND	-2.10	121.85	124.80
12	a	838	CLA	CHC-C1C-NC	-2.10	121.15	124.31
12	A	835	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
15	A	846	BCR	C39-C30-C25	-2.10	106.95	110.24
12	l	202	CLA	CHB-C4A-NA	2.10	127.43	124.40
12	a	820	CLA	CHA-C1A-NA	-2.10	121.64	126.39
12	H	838	CLA	C11-C12-C13	-2.10	108.99	115.97
12	H	807	CLA	CHD-C1D-ND	-2.10	121.85	124.80
12	G	825	CLA	CAA-CBA-CGA	-2.10	107.25	113.21
12	S	202	CLA	CAC-C3C-C4C	2.10	127.52	124.79
12	H	832	CLA	C3D-C4D-ND	2.10	113.40	109.99
12	b	821	CLA	CHA-C4D-ND	2.10	136.88	132.55
12	H	833	CLA	CMB-C2B-C1B	2.10	128.61	125.42
12	A	807	CLA	C4-C3-C5	2.10	118.87	115.23
15	b	847	BCR	C35-C13-C12	2.10	121.29	118.09
16	G	851	LHG	O8-C6-C5	-2.10	102.35	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	807	CLA	C1-C2-C3	-2.10	122.76	126.20
12	G	837	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
12	B	823	CLA	C16-C15-C13	-2.10	109.00	115.97
12	A	838	CLA	C4D-C3D-CAD	2.10	110.38	108.11
12	B	830	CLA	C4D-C3D-CAD	2.10	110.38	108.11
12	l	206	CLA	C1-C2-C3	-2.10	122.76	126.20
12	H	821	CLA	CAA-C2A-C1A	-2.10	105.11	111.97
12	a	823	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
12	L	206	CLA	CMB-C2B-C3B	2.10	131.48	126.55
15	A	847	BCR	C37-C22-C21	-2.10	119.42	122.82
12	a	840	CLA	C5-C3-C4	2.10	119.41	114.59
12	R	103	CLA	CAC-C3C-C4C	2.10	127.52	124.79
15	J	101	BCR	C23-C22-C21	2.09	122.30	119.01
12	G	826	CLA	C4-C3-C5	2.09	118.86	115.23
12	b	828	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
12	b	828	CLA	CHA-C1A-NA	-2.09	121.65	126.39
12	a	823	CLA	C3C-C4C-NC	2.09	113.11	110.43
12	B	829	CLA	CHA-C1A-NA	-2.09	121.65	126.39
12	G	828	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
12	G	838	CLA	C4D-C3D-CAD	2.09	110.38	108.11
15	P	204	BCR	C37-C22-C21	-2.09	119.42	122.82
15	G	845	BCR	C38-C26-C27	2.09	118.06	113.60
15	b	843	BCR	C30-C25-C24	2.09	121.33	115.65
15	B	843	BCR	C35-C13-C12	2.09	119.41	114.59
12	H	850	CLA	CHA-C1A-NA	-2.09	121.65	126.39
12	j	104	CLA	CHA-C1A-NA	-2.09	121.65	126.39
12	B	810	CLA	CHD-C4C-NC	-2.09	120.99	124.23
12	L	202	CLA	C4-C3-C5	2.09	118.86	115.23
12	H	809	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
12	A	814	CLA	CMC-C2C-C3C	2.09	131.81	126.15
12	a	836	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
12	H	817	CLA	CHA-C1A-NA	-2.09	121.66	126.39
12	a	822	CLA	CAC-C3C-C4C	2.09	127.51	124.79
15	B	844	BCR	C8-C7-C6	-2.09	121.41	127.00
12	A	831	CLA	CHA-C4D-ND	2.09	136.86	132.55
12	a	813	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
12	H	814	CLA	CED-O2D-CGD	2.09	120.66	115.92
12	B	831	CLA	CMB-C2B-C1B	2.09	128.60	125.42
12	A	820	CLA	C3D-C4D-ND	2.09	113.38	109.99
12	B	837	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
12	G	827	CLA	CHD-C4C-C3C	-2.09	121.73	124.77
12	f	203	CLA	CHC-C1C-C2C	-2.09	121.01	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	836	CLA	C1-C2-C3	-2.09	122.78	126.20
12	H	818	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
15	J	104	BCR	C29-C28-C27	2.09	115.87	111.28
15	G	847	BCR	C39-C30-C25	-2.09	106.97	110.24
15	A	847	BCR	C36-C18-C17	-2.09	119.43	122.82
12	b	830	CLA	CHA-C1A-NA	-2.09	121.66	126.39
12	A	809	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
12	b	815	CLA	C4D-C3D-CAD	2.09	110.37	108.11
12	G	856	CLA	C4-C3-C5	2.09	118.85	115.23
12	G	826	CLA	CHA-C4D-ND	2.09	136.85	132.55
12	H	837	CLA	CHA-C4D-ND	2.09	136.85	132.55
12	a	833	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
12	A	802	CLA	C1D-CHD-C4C	-2.09	121.58	126.02
12	b	821	CLA	C3C-C4C-NC	2.09	113.10	110.43
12	a	820	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
12	A	830	CLA	C1-C2-C3	-2.09	123.39	126.76
15	R	102	BCR	C30-C25-C26	-2.09	119.78	122.64
12	A	816	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
12	b	831	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
12	l	206	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
12	G	826	CLA	CHA-C1A-NA	-2.09	121.67	126.39
12	G	805	CLA	CMA-C3A-C4A	2.09	117.38	111.77
12	A	821	CLA	CHA-C1A-NA	-2.08	121.67	126.39
12	l	205	CLA	C4-C3-C2	-2.08	118.27	123.63
15	A	847	BCR	C31-C1-C6	-2.08	106.97	110.24
15	B	845	BCR	C29-C28-C27	2.08	115.86	111.28
12	A	803	CLA	CHA-C1A-NA	-2.08	121.67	126.39
12	b	823	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
15	S	201	BCR	C23-C24-C25	-2.08	121.43	127.00
12	A	810	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
12	G	829	CLA	CED-O2D-CGD	2.08	120.64	115.92
12	b	826	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
12	b	834	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
12	G	832	CLA	CBB-CAB-C3B	-2.08	117.12	127.53
12	H	820	CLA	CHB-C4A-NA	2.08	127.41	124.40
18	b	845	LMG	O7-C10-O9	-2.08	118.84	123.70
12	b	801	CLA	O2D-CGD-CBD	2.08	114.87	111.23
12	A	833	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
12	B	828	CLA	CHA-C1A-NA	-2.08	121.68	126.39
12	B	805	CLA	C4B-CHC-C1C	2.08	131.14	126.25
13	G	843	1L3	C33-C31-C32	2.08	119.38	114.59
12	b	818	CLA	CMB-C2B-C3B	2.08	131.44	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	843	BCR	C34-C9-C8	2.08	121.27	118.09
12	A	830	CLA	CHA-C4D-ND	2.08	136.84	132.55
12	H	850	CLA	C4D-C3D-CAD	2.08	110.36	108.11
12	a	812	CLA	CMB-C2B-C1B	2.08	128.59	125.42
12	H	819	CLA	CMB-C2B-C3B	2.08	131.44	126.55
12	H	827	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
12	G	819	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
12	H	815	CLA	C1-C2-C3	-2.08	122.79	126.20
12	b	836	CLA	C1-C2-C3	-2.08	122.79	126.20
12	a	821	CLA	CHA-C1A-NA	-2.08	121.68	126.39
12	a	824	CLA	CHC-C1C-NC	-2.08	121.18	124.31
12	a	838	CLA	C4C-C3C-C2C	-2.08	103.87	106.89
12	a	824	CLA	CHD-C4C-C3C	-2.08	121.74	124.77
12	G	822	CLA	CAC-C3C-C4C	2.08	127.49	124.79
12	B	830	CLA	C6-C5-C3	-2.08	108.41	113.47
12	B	830	CLA	C4C-C3C-C2C	-2.08	103.87	106.89
12	b	817	CLA	CHD-C4C-C3C	-2.08	121.75	124.77
12	a	836	CLA	CHA-C4D-ND	2.08	136.83	132.55
12	H	850	CLA	CAC-C3C-C4C	2.08	127.49	124.79
12	G	829	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
16	G	854	LHG	O7-C7-O9	-2.08	118.85	123.70
11	a	801	CL0	C11-C12-C13	-2.08	109.06	115.97
12	L	206	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
12	G	825	CLA	CHC-C1C-NC	-2.08	121.18	124.31
12	a	803	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
12	A	829	CLA	C1-C2-C3	-2.08	122.80	126.20
12	G	832	CLA	C4-C3-C5	2.08	118.83	115.23
12	A	824	CLA	C3D-C4D-ND	2.08	113.36	109.99
12	G	841	CLA	C2B-C1B-NB	2.08	112.48	110.33
12	S	203	CLA	CHC-C1C-NC	-2.07	121.19	124.31
12	G	816	CLA	CAC-C3C-C4C	2.07	127.49	124.79
12	b	810	CLA	CAC-C3C-C4C	2.07	127.49	124.79
12	a	840	CLA	C1-C2-C3	-2.07	123.41	126.76
12	G	822	CLA	CHA-C1A-NA	-2.07	121.69	126.39
12	b	833	CLA	C1-O2A-CGA	2.07	121.67	116.65
12	H	809	CLA	CAC-C3C-C4C	2.07	127.49	124.79
12	A	828	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
12	G	817	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
15	b	844	BCR	C37-C22-C21	-2.07	119.46	122.82
12	H	822	CLA	CMA-C3A-C2A	2.07	122.00	113.98
12	H	808	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
12	A	806	CLA	CMD-C2D-C3D	-2.07	122.94	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	814	CLA	C4-C3-C5	2.07	118.83	115.23
12	j	102	CLA	C1-O2A-CGA	2.07	121.67	116.65
12	b	821	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
12	B	813	CLA	CMB-C2B-C3B	2.07	131.42	126.55
12	H	821	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
12	H	805	CLA	C4B-CHC-C1C	2.07	131.12	126.25
12	G	832	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
15	b	840	BCR	C30-C25-C26	-2.07	119.81	122.64
12	A	804	CLA	CMA-C3A-C4A	2.07	117.34	111.77
12	H	835	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
12	H	801	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
12	a	834	CLA	C1-O2A-CGA	2.07	121.66	116.65
12	H	832	CLA	CHA-C1A-NA	-2.07	121.70	126.39
12	b	825	CLA	CHA-C4D-ND	2.07	136.82	132.55
12	b	825	CLA	C4C-C3C-C2C	-2.07	103.88	106.89
15	P	202	BCR	C29-C28-C27	-2.07	106.73	111.28
15	G	850	BCR	C4-C5-C6	-2.07	119.91	122.70
15	F	204	BCR	C27-C26-C25	-2.07	119.91	122.70
15	B	842	BCR	C1-C6-C7	2.07	121.26	115.65
12	B	830	CLA	C1-C2-C3	-2.07	122.81	126.20
12	b	829	CLA	CHA-C1A-NA	-2.07	121.71	126.39
12	A	830	CLA	CHD-C4C-C3C	-2.07	121.76	124.77
12	G	803	CLA	C6-C5-C3	-2.07	108.43	113.47
12	A	827	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
12	b	811	CLA	CAC-C3C-C4C	2.07	127.48	124.79
12	a	818	CLA	C3C-C4C-NC	2.07	113.08	110.43
12	A	803	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
12	a	818	CLA	CMC-C2C-C1C	2.07	128.26	125.03
15	G	848	BCR	C31-C1-C6	-2.07	107.00	110.24
15	j	103	BCR	C37-C22-C23	2.07	121.25	118.09
13	b	838	1L3	C27-C26-C28	2.07	118.81	115.23
12	B	832	CLA	CMC-C2C-C1C	2.07	128.26	125.03
12	H	814	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
12	G	837	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
12	b	812	CLA	C3D-C4D-ND	2.06	113.34	109.99
12	b	808	CLA	CAC-C3C-C4C	2.06	127.48	124.79
12	A	840	CLA	C1-C2-C3	-2.06	123.42	126.76
13	G	843	1L3	O05-C04-C03	-2.06	117.36	120.67
12	G	825	CLA	CHD-C4C-C3C	-2.06	121.76	124.77
12	b	830	CLA	CMB-C2B-C1B	2.06	128.56	125.42
15	A	846	BCR	C38-C26-C27	2.06	118.00	113.60
12	B	823	CLA	C1-O2A-CGA	2.06	121.65	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	f	202	BCR	C29-C28-C27	-2.06	106.74	111.28
12	a	810	CLA	CMC-C2C-C1C	2.06	128.26	125.03
12	a	828	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
12	G	820	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
12	A	818	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
15	G	853	BCR	C3-C4-C5	-2.06	110.38	114.06
15	a	849	BCR	C34-C9-C8	2.06	121.24	118.09
12	G	833	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
12	A	834	CLA	CMA-C3A-C4A	2.06	117.32	111.77
12	a	854	CLA	CHA-C1A-NA	-2.06	121.72	126.39
15	b	842	BCR	C35-C13-C12	2.06	119.33	114.59
12	a	841	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
12	A	841	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
12	G	802	CLA	CED-O2D-CGD	2.06	120.59	115.92
12	A	828	CLA	CAC-C3C-C4C	2.06	127.47	124.79
12	H	831	CLA	CHA-C1A-NA	-2.06	121.72	126.39
12	b	816	CLA	CHA-C1A-NA	-2.06	121.72	126.39
12	H	831	CLA	CMC-C2C-C3C	2.06	131.72	126.15
12	A	837	CLA	C1-O2A-CGA	2.06	121.64	116.65
12	b	821	CLA	C5-C3-C2	-2.06	116.54	121.17
12	A	821	CLA	CMB-C2B-C3B	2.06	131.40	126.55
12	b	803	CLA	CMA-C3A-C2A	-2.06	106.01	113.98
12	A	820	CLA	C4D-C3D-CAD	2.06	110.34	108.11
12	A	807	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
12	H	801	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
15	A	844	BCR	C38-C26-C27	2.06	117.99	113.60
12	b	825	CLA	CED-O2D-CGD	2.06	120.59	115.92
12	G	839	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
12	B	826	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
12	b	805	CLA	C4B-CHC-C1C	2.06	131.09	126.25
12	H	830	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
12	a	807	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
13	A	842	1L3	C15-C14-C03	-2.06	107.01	112.08
12	a	838	CLA	C4D-C3D-CAD	2.06	110.34	108.11
12	B	804	CLA	C6-C5-C3	-2.06	108.46	113.47
12	G	820	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
12	A	827	CLA	CHD-C4C-C3C	-2.06	121.77	124.77
12	F	201	CLA	CED-O2D-CGD	2.06	120.58	115.92
19	b	846	LMT	C4B-C3B-C2B	2.06	114.44	110.83
12	A	839	CLA	C3C-C4C-NC	2.06	113.06	110.43
12	b	829	CLA	C4D-C3D-CAD	2.06	110.34	108.11
12	a	831	CLA	CHB-C1B-C2B	-2.06	121.46	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	813	CLA	CBA-CAA-C2A	2.06	119.91	113.79
12	G	838	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
12	H	816	CLA	CHA-C1A-NA	-2.06	121.73	126.39
15	f	202	BCR	C34-C9-C10	-2.06	119.48	122.82
12	B	813	CLA	CHB-C1B-C2B	-2.06	121.46	127.43
12	b	817	CLA	CBA-CAA-C2A	2.06	119.91	113.79
12	l	204	CLA	C1-O2A-CGA	2.06	121.62	116.65
12	G	813	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
12	H	816	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
12	G	811	CLA	CAC-C3C-C4C	2.05	127.46	124.79
12	A	836	CLA	CHB-C1B-C2B	-2.05	121.46	127.43
12	b	832	CLA	C3D-C4D-ND	2.05	113.33	109.99
12	b	836	CLA	C11-C12-C13	-2.05	109.14	115.97
12	a	834	CLA	C4C-C3C-C2C	-2.05	103.90	106.89
12	G	837	CLA	C1-O2A-CGA	2.05	121.62	116.65
13	H	840	1L3	C24-C25-C26	-2.05	122.92	127.62
12	A	855	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
12	b	807	CLA	CMB-C2B-C3B	2.05	131.38	126.55
15	A	848	BCR	C35-C13-C12	2.05	121.22	118.09
12	A	827	CLA	C3D-C4D-ND	2.05	113.32	109.99
12	G	838	CLA	CHC-C1C-NC	-2.05	121.22	124.31
12	G	810	CLA	CMC-C2C-C1C	2.05	128.24	125.03
12	H	830	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
12	G	817	CLA	CED-O2D-CGD	2.05	120.57	115.92
12	G	839	CLA	CMA-C3A-C4A	2.05	117.29	111.77
12	b	813	CLA	CMB-C2B-C1B	2.05	128.54	125.42
12	a	816	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
12	A	833	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
13	a	842	1L3	C15-C14-C03	-2.05	107.03	112.08
15	A	845	BCR	C12-C13-C14	-2.05	115.78	119.01
12	B	827	CLA	C4C-C3C-C2C	-2.05	103.91	106.89
12	G	811	CLA	C3C-C4C-NC	2.05	113.06	110.43
12	A	820	CLA	CHA-C1A-NA	-2.05	121.75	126.39
15	a	848	BCR	C15-C14-C13	-2.05	124.41	127.28
12	b	812	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	b	835	CLA	C1-C2-C3	-2.05	122.84	126.20
12	b	816	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
12	B	820	CLA	CAC-C3C-C4C	2.05	127.45	124.79
12	S	202	CLA	CHA-C1A-NA	-2.05	121.75	126.39
12	b	812	CLA	CHA-C1A-NA	-2.05	121.75	126.39
12	a	818	CLA	CMB-C2B-C1B	2.05	128.54	125.42
12	A	837	CLA	CHB-C1B-C2B	-2.05	121.48	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	827	CLA	CAC-C3C-C4C	2.05	127.45	124.79
12	G	821	CLA	C1-O2A-CGA	2.05	121.60	116.65
15	f	204	BCR	C30-C25-C26	-2.05	119.84	122.64
12	F	203	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
12	l	204	CLA	CHB-C4A-NA	2.04	127.35	124.40
12	b	835	CLA	CHA-C4D-ND	2.04	136.77	132.55
11	G	801	CL0	C4C-C3C-C2C	-2.04	103.92	106.89
12	a	854	CLA	C1-O2A-CGA	2.04	121.60	116.65
12	G	836	CLA	C3D-C4D-ND	2.04	113.31	109.99
12	A	831	CLA	CED-O2D-CGD	2.04	120.55	115.92
15	H	842	BCR	C1-C6-C5	-2.04	119.84	122.64
11	a	801	CL0	C11-C10-C8	-2.04	109.17	115.97
12	L	202	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
12	B	836	CLA	CHA-C4D-ND	2.04	136.77	132.55
12	A	854	CLA	CAC-C3C-C4C	2.04	127.45	124.79
12	A	826	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
15	b	847	BCR	C34-C9-C8	2.04	121.21	118.09
18	H	847	LMG	O8-C28-O10	-2.04	118.52	123.63
12	a	840	CLA	CMB-C2B-C1B	2.04	128.53	125.42
12	H	826	CLA	C1-C2-C3	-2.04	122.85	126.20
12	G	827	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
12	b	810	CLA	C4B-CHC-C1C	2.04	131.05	126.25
12	H	824	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
15	H	842	BCR	C37-C22-C21	-2.04	119.51	122.82
12	a	808	CLA	CHA-C4D-ND	2.04	136.76	132.55
12	P	203	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
12	b	823	CLA	CHD-C1D-ND	-2.04	121.93	124.80
13	B	839	1L3	C27-C26-C28	2.04	118.77	115.23
12	a	829	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
12	H	817	CLA	CAC-C3C-C4C	2.04	127.44	124.79
12	b	833	CLA	CMC-C2C-C1C	2.04	128.22	125.03
15	j	101	BCR	C32-C1-C6	2.04	113.44	110.24
12	G	804	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
12	A	840	CLA	CAC-C3C-C4C	2.04	127.44	124.79
12	H	814	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
12	A	836	CLA	CHD-C4C-NC	-2.04	121.07	124.23
12	H	802	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
12	A	855	CLA	C1C-C2C-C3C	-2.04	104.83	106.98
12	B	825	CLA	CED-O2D-CGD	2.04	120.54	115.92
12	G	817	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
12	B	802	CLA	CHB-C4A-NA	2.04	127.34	124.40
12	b	824	CLA	C4B-C3B-C2B	-2.04	104.77	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	816	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
12	H	820	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
12	G	839	CLA	C3C-C4C-NC	2.04	113.04	110.43
12	G	838	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
12	a	835	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
12	B	838	CLA	C6-C7-C8	-2.04	109.19	115.97
12	B	835	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
12	H	831	CLA	C1-O2A-CGA	2.04	121.58	116.65
12	B	829	CLA	CAC-C3C-C4C	2.04	127.44	124.79
15	P	202	BCR	C8-C9-C10	2.04	122.21	119.01
12	A	803	CLA	CHA-C4D-ND	2.04	136.75	132.55
12	G	831	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
12	G	811	CLA	CMC-C2C-C1C	2.04	128.22	125.03
12	B	819	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
12	B	820	CLA	CAA-CBA-CGA	-2.04	107.06	112.49
15	a	847	BCR	C31-C1-C6	-2.03	107.05	110.24
12	b	835	CLA	CHB-C4A-NA	2.03	127.34	124.40
12	B	816	CLA	CHA-C1A-NA	-2.03	121.78	126.39
12	B	806	CLA	C1-C2-C3	-2.03	122.86	126.20
12	b	825	CLA	CMA-C3A-C2A	-2.03	106.12	113.98
12	a	810	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
15	A	847	BCR	C1-C6-C5	-2.03	119.86	122.64
12	a	833	CLA	C1-O2A-CGA	2.03	121.57	116.65
12	B	812	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
12	b	837	CLA	C4B-CHC-C1C	2.03	131.03	126.25
12	b	815	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
12	A	854	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
15	a	849	BCR	C1-C6-C5	-2.03	119.86	122.64
12	A	825	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
15	H	843	BCR	C31-C1-C6	-2.03	107.06	110.24
12	L	202	CLA	C4B-CHC-C1C	2.03	131.03	126.25
12	a	837	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
12	a	819	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
12	H	804	CLA	C4-C3-C5	2.03	118.75	115.23
12	a	809	CLA	CHD-C4C-C3C	-2.03	121.81	124.77
12	b	822	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
12	A	810	CLA	CED-O2D-CGD	2.03	120.52	115.92
12	b	817	CLA	OBD-CAD-C3D	-2.03	123.67	128.42
12	b	815	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
15	Q	101	BCR	C35-C13-C12	2.03	121.19	118.09
12	B	804	CLA	CMB-C2B-C3B	2.03	131.32	126.55
12	b	832	CLA	CHA-C1A-NA	-2.03	121.80	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	816	CLA	CHB-C4A-NA	2.03	127.33	124.40
12	G	809	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	G	840	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	H	832	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
12	A	823	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
12	G	826	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
12	G	827	CLA	C3D-C4D-ND	2.03	113.28	109.99
12	b	802	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
15	b	843	BCR	C35-C13-C12	2.03	121.18	118.09
12	A	817	CLA	OBD-CAD-C3D	-2.03	123.68	128.42
12	b	814	CLA	CAC-C3C-C4C	2.03	127.43	124.79
12	B	813	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
12	B	822	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	A	822	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
12	b	809	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
12	B	819	CLA	CED-O2D-CGD	2.03	120.51	115.92
12	A	823	CLA	O2D-CGD-O1D	-2.03	119.91	123.85
12	G	803	CLA	CMB-C2B-C1B	2.02	128.50	125.42
12	a	819	CLA	CHC-C1C-C2C	-2.02	121.19	126.95
12	H	835	CLA	C1-O2A-CGA	2.02	121.55	116.65
12	a	855	CLA	C1C-C2C-C3C	-2.02	104.85	106.98
12	B	838	CLA	C4B-CHC-C1C	2.02	131.01	126.25
15	b	841	BCR	C40-C30-C25	2.02	113.42	110.24
12	b	813	CLA	C1-C2-C3	-2.02	122.88	126.20
12	a	838	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
12	B	819	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
15	b	840	BCR	C38-C26-C25	-2.02	122.28	124.48
12	P	201	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
12	B	828	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
12	A	833	CLA	C4D-C3D-CAD	2.02	110.30	108.11
15	b	840	BCR	C31-C1-C6	-2.02	107.07	110.24
12	b	829	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
12	G	840	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
12	b	835	CLA	CAC-C3C-C4C	2.02	127.42	124.79
12	a	826	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
12	G	809	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
15	a	847	BCR	C33-C5-C4	2.02	117.90	113.60
11	a	801	CL0	CHC-C4B-NB	2.02	127.08	124.05
12	G	840	CLA	C5-C3-C4	2.02	119.24	114.59
12	b	833	CLA	C6-C7-C8	-2.02	109.25	115.97
12	G	831	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
12	B	838	CLA	CHB-C4A-NA	2.02	127.31	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	809	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
12	A	827	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
12	B	834	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
12	B	821	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
12	P	201	CLA	CMA-C3A-C4A	2.02	117.20	111.77
12	G	829	CLA	CHD-C1D-ND	-2.02	121.96	124.80
12	H	826	CLA	CMA-C3A-C2A	-2.02	106.18	113.98
12	S	202	CLA	C1-O2A-CGA	2.02	121.54	116.65
12	A	839	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
12	H	850	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
12	a	838	CLA	C4B-CHC-C1C	2.02	130.99	126.25
12	a	827	CLA	CMA-C3A-C4A	2.02	117.19	111.77
12	a	833	CLA	C4C-C3C-C2C	-2.02	103.96	106.89
12	B	820	CLA	CHB-C4A-NA	2.02	127.31	124.40
12	G	803	CLA	CHA-C4D-ND	2.02	136.71	132.55
12	A	832	CLA	C3D-C4D-ND	2.02	113.26	109.99
12	F	203	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
12	H	831	CLA	C1-C2-C3	-2.02	122.89	126.20
12	B	823	CLA	C1-C2-C3	-2.02	122.89	126.20
12	H	850	CLA	C1D-CHD-C4C	-2.01	121.74	126.02
12	H	817	CLA	CHB-C4A-NA	2.01	127.31	124.40
12	L	205	CLA	C4-C3-C2	-2.01	118.45	123.63
12	B	803	CLA	CBA-CAA-C2A	2.01	119.79	113.79
12	B	821	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
12	b	808	CLA	C3C-C4C-NC	2.01	113.01	110.43
12	b	832	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
12	A	827	CLA	CMB-C2B-C1B	2.01	128.49	125.42
15	L	207	BCR	C33-C5-C6	-2.01	122.29	124.48
12	A	839	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
12	G	827	CLA	CHA-C1A-NA	-2.01	121.83	126.39
12	b	848	CLA	C4D-C3D-CAD	2.01	110.29	108.11
12	j	104	CLA	CAC-C3C-C4C	2.01	127.41	124.79
12	G	837	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
12	j	102	CLA	C6-C5-C3	-2.01	108.57	113.47
15	H	846	BCR	C31-C1-C6	-2.01	107.09	110.24
12	B	816	CLA	CHB-C4A-NA	2.01	127.30	124.40
12	H	806	CLA	C1-O2A-CGA	2.01	121.52	116.65
12	G	819	CLA	C4C-C3C-C2C	-2.01	103.96	106.89
12	a	829	CLA	C4C-C3C-C2C	-2.01	103.96	106.89
12	a	816	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
12	G	831	CLA	CHA-C4D-ND	2.01	136.70	132.55
12	G	807	CLA	CMD-C2D-C3D	-2.01	123.08	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	101	BCR	C32-C1-C6	2.01	113.40	110.24
12	H	813	CLA	CHB-C4A-NA	2.01	127.30	124.40
12	G	817	CLA	C5-C3-C4	2.01	119.22	114.59
12	A	831	CLA	C1-C2-C3	-2.01	122.90	126.20
12	A	832	CLA	CBB-CAB-C3B	-2.01	117.48	127.53
15	B	844	BCR	C34-C9-C8	2.01	121.16	118.09
12	A	814	CLA	CHA-C1A-NA	-2.01	121.84	126.39
12	B	802	CLA	C4D-CHA-C1A	-2.01	118.85	121.24
15	b	839	BCR	C38-C26-C27	2.01	117.88	113.60
12	G	831	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
12	l	202	CLA	C4B-CHC-C1C	2.01	130.97	126.25
12	A	855	CLA	O2D-CGD-CBD	2.01	114.74	111.23
12	H	829	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
12	A	809	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
15	F	204	BCR	C23-C24-C25	-2.01	121.64	127.00
12	a	832	CLA	C1-C2-C3	-2.01	122.91	126.20
18	H	847	LMG	O7-C10-O9	-2.01	119.01	123.70
12	b	816	CLA	CMA-C3A-C4A	2.01	117.17	111.77
12	a	833	CLA	C4D-C3D-CAD	2.01	110.29	108.11
12	A	822	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
15	Q	102	BCR	C35-C13-C12	2.01	121.15	118.09
15	A	844	BCR	C38-C26-C25	-2.01	122.29	124.48
12	b	810	CLA	CMC-C2C-C1C	2.01	128.17	125.03
12	a	832	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
12	H	826	CLA	C4B-C3B-C2B	-2.01	104.81	107.30
12	B	805	CLA	C6-C7-C8	-2.01	109.30	115.97
12	a	803	CLA	CHA-C1A-NA	-2.01	121.85	126.39
12	b	833	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
12	b	832	CLA	CHC-C1C-C2C	-2.01	121.25	126.95
12	b	819	CLA	CHB-C4A-NA	2.01	127.29	124.40
15	j	101	BCR	C34-C9-C10	-2.01	119.57	122.82
12	a	806	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
12	H	818	CLA	CHD-C4C-C3C	-2.00	121.85	124.77
12	G	821	CLA	CHA-C1A-NA	-2.00	121.85	126.39
12	b	814	CLA	CHA-C1A-NA	-2.00	121.85	126.39
12	a	822	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
12	b	823	CLA	C16-C15-C13	-2.00	109.30	115.97
12	A	813	CLA	C4B-CHC-C1C	2.00	130.96	126.25
12	H	834	CLA	C1-O2A-CGA	2.00	121.50	116.65
12	A	825	CLA	CBA-CAA-C2A	2.00	119.75	113.79
12	b	833	CLA	C6-C5-C3	-2.00	108.59	113.47
12	H	826	CLA	CHA-C4D-ND	2.00	136.68	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	821	CLA	CAC-C3C-C4C	2.00	127.40	124.79
12	H	825	CLA	CHD-C1D-ND	-2.00	121.98	124.80
11	a	801	CL0	C1-O2A-CGA	2.00	121.50	116.65
12	b	823	CLA	CAC-C3C-C4C	2.00	127.39	124.79
12	A	829	CLA	CAC-C3C-C4C	2.00	127.39	124.79
12	B	809	CLA	C4C-C3C-C2C	-2.00	103.98	106.89
12	a	827	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
12	H	850	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
15	a	846	BCR	C37-C22-C23	2.00	121.15	118.09
12	G	834	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
16	G	852	LHG	O8-C23-O10	-2.00	118.62	123.63
12	H	822	CLA	CHA-C1A-NA	-2.00	121.86	126.39
12	f	201	CLA	CHA-C4D-ND	2.00	136.68	132.55
12	B	834	CLA	C6-C7-C8	-2.00	109.31	115.97
12	G	818	CLA	CHA-C4D-ND	2.00	136.68	132.55
12	B	802	CLA	OBD-CAD-C3D	-2.00	123.74	128.42

There are no chirality outliers.

All (4013) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	805	CLA	C1A-C2A-CAA-CBA
12	G	805	CLA	C3A-C2A-CAA-CBA
12	G	806	CLA	CAD-CBD-CGD-O1D
12	G	806	CLA	CAD-CBD-CGD-O2D
12	G	807	CLA	C1A-C2A-CAA-CBA
12	G	807	CLA	CBD-CGD-O2D-CED
12	G	808	CLA	C1A-C2A-CAA-CBA
12	G	808	CLA	C3A-C2A-CAA-CBA
12	G	808	CLA	C4B-C3B-CAB-CBB
12	G	808	CLA	CHA-CBD-CGD-O1D
12	G	808	CLA	CHA-CBD-CGD-O2D
12	G	810	CLA	C1A-C2A-CAA-CBA
12	G	810	CLA	C3A-C2A-CAA-CBA
12	G	810	CLA	C2B-C3B-CAB-CBB
12	G	810	CLA	C4B-C3B-CAB-CBB
12	G	811	CLA	C2B-C3B-CAB-CBB
12	G	811	CLA	C4B-C3B-CAB-CBB
12	G	812	CLA	C2B-C3B-CAB-CBB
12	G	812	CLA	C4B-C3B-CAB-CBB
12	G	816	CLA	C2B-C3B-CAB-CBB
12	G	816	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	G	817	CLA	CBD-CGD-O2D-CED
12	G	818	CLA	C1A-C2A-CAA-CBA
12	G	818	CLA	C3A-C2A-CAA-CBA
12	G	818	CLA	C2-C1-O2A-CGA
12	G	818	CLA	CBD-CGD-O2D-CED
12	G	819	CLA	C1A-C2A-CAA-CBA
12	G	819	CLA	C3A-C2A-CAA-CBA
12	G	820	CLA	C1A-C2A-CAA-CBA
12	G	820	CLA	C3A-C2A-CAA-CBA
12	G	820	CLA	C2B-C3B-CAB-CBB
12	G	820	CLA	C4B-C3B-CAB-CBB
12	G	820	CLA	CHA-CBD-CGD-O2D
12	G	822	CLA	C3A-C2A-CAA-CBA
12	G	822	CLA	CHA-CBD-CGD-O1D
12	G	822	CLA	CHA-CBD-CGD-O2D
12	G	823	CLA	CBD-CGD-O2D-CED
12	G	825	CLA	C2-C1-O2A-CGA
12	G	826	CLA	CBA-CGA-O2A-C1
12	G	826	CLA	O1A-CGA-O2A-C1
12	G	829	CLA	CBD-CGD-O2D-CED
12	G	830	CLA	CHA-CBD-CGD-O1D
12	G	830	CLA	CHA-CBD-CGD-O2D
12	G	832	CLA	CBD-CGD-O2D-CED
12	G	833	CLA	C1A-C2A-CAA-CBA
12	G	833	CLA	CHA-CBD-CGD-O1D
12	G	833	CLA	CHA-CBD-CGD-O2D
12	G	834	CLA	C2-C1-O2A-CGA
12	G	835	CLA	C1A-C2A-CAA-CBA
12	G	835	CLA	C3A-C2A-CAA-CBA
12	G	835	CLA	C2B-C3B-CAB-CBB
12	G	835	CLA	C4B-C3B-CAB-CBB
12	G	840	CLA	CBA-CGA-O2A-C1
12	G	840	CLA	O1A-CGA-O2A-C1
12	G	840	CLA	C4B-C3B-CAB-CBB
12	G	840	CLA	CBD-CGD-O2D-CED
12	G	841	CLA	C2B-C3B-CAB-CBB
12	G	841	CLA	C4B-C3B-CAB-CBB
12	G	842	CLA	CAD-CBD-CGD-O2D
12	G	842	CLA	CBD-CGD-O2D-CED
12	G	856	CLA	C2-C1-O2A-CGA
12	H	801	CLA	C1A-C2A-CAA-CBA
12	H	803	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	H	803	CLA	C3A-C2A-CAA-CBA
12	H	804	CLA	C2B-C3B-CAB-CBB
12	H	804	CLA	C4B-C3B-CAB-CBB
12	H	805	CLA	CBD-CGD-O2D-CED
12	H	806	CLA	C2B-C3B-CAB-CBB
12	H	806	CLA	C4B-C3B-CAB-CBB
12	H	806	CLA	CHA-CBD-CGD-O1D
12	H	806	CLA	CHA-CBD-CGD-O2D
12	H	807	CLA	C1A-C2A-CAA-CBA
12	H	807	CLA	C3A-C2A-CAA-CBA
12	H	811	CLA	C1A-C2A-CAA-CBA
12	H	811	CLA	C3A-C2A-CAA-CBA
12	H	812	CLA	CBD-CGD-O2D-CED
12	H	813	CLA	C1A-C2A-CAA-CBA
12	H	813	CLA	C3A-C2A-CAA-CBA
12	H	813	CLA	CHA-CBD-CGD-O1D
12	H	813	CLA	CHA-CBD-CGD-O2D
12	H	814	CLA	C2B-C3B-CAB-CBB
12	H	814	CLA	C4B-C3B-CAB-CBB
12	H	815	CLA	C3A-C2A-CAA-CBA
12	H	816	CLA	C1A-C2A-CAA-CBA
12	H	816	CLA	C3A-C2A-CAA-CBA
12	H	817	CLA	C2B-C3B-CAB-CBB
12	H	817	CLA	C4B-C3B-CAB-CBB
12	H	817	CLA	CBD-CGD-O2D-CED
12	H	818	CLA	C1A-C2A-CAA-CBA
12	H	818	CLA	C3A-C2A-CAA-CBA
12	H	818	CLA	CHA-CBD-CGD-O1D
12	H	818	CLA	CHA-CBD-CGD-O2D
12	H	820	CLA	C2B-C3B-CAB-CBB
12	H	820	CLA	C4B-C3B-CAB-CBB
12	H	822	CLA	CHA-CBD-CGD-O1D
12	H	822	CLA	CHA-CBD-CGD-O2D
12	H	823	CLA	C1A-C2A-CAA-CBA
12	H	823	CLA	C3A-C2A-CAA-CBA
12	H	823	CLA	CHA-CBD-CGD-O1D
12	H	823	CLA	CHA-CBD-CGD-O2D
12	H	824	CLA	CHA-CBD-CGD-O1D
12	H	824	CLA	CHA-CBD-CGD-O2D
12	H	825	CLA	C1A-C2A-CAA-CBA
12	H	826	CLA	C1A-C2A-CAA-CBA
12	H	826	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	H	827	CLA	CHA-CBD-CGD-O1D
12	H	827	CLA	CHA-CBD-CGD-O2D
12	H	828	CLA	C4B-C3B-CAB-CBB
12	H	829	CLA	C1A-C2A-CAA-CBA
12	H	829	CLA	C3A-C2A-CAA-CBA
12	H	831	CLA	CHA-CBD-CGD-O1D
12	H	831	CLA	CHA-CBD-CGD-O2D
12	H	832	CLA	C4B-C3B-CAB-CBB
12	H	832	CLA	CHA-CBD-CGD-O2D
12	H	833	CLA	CBD-CGD-O2D-CED
12	H	834	CLA	C1A-C2A-CAA-CBA
12	H	834	CLA	C2B-C3B-CAB-CBB
12	H	834	CLA	C4B-C3B-CAB-CBB
12	H	835	CLA	CBD-CGD-O2D-CED
12	H	838	CLA	C2-C1-O2A-CGA
12	H	838	CLA	CBD-CGD-O2D-CED
12	H	839	CLA	C2-C1-O2A-CGA
12	H	850	CLA	CBD-CGD-O2D-CED
12	P	201	CLA	CBD-CGD-O2D-CED
12	P	201	CLA	C4-C3-C5-C6
12	R	103	CLA	C2B-C3B-CAB-CBB
12	R	103	CLA	C4B-C3B-CAB-CBB
12	S	203	CLA	C1A-C2A-CAA-CBA
12	S	203	CLA	C3A-C2A-CAA-CBA
12	a	804	CLA	C3A-C2A-CAA-CBA
12	a	804	CLA	C2B-C3B-CAB-CBB
12	a	804	CLA	C4B-C3B-CAB-CBB
12	a	805	CLA	CAD-CBD-CGD-O2D
12	a	806	CLA	CBD-CGD-O2D-CED
12	a	807	CLA	C1A-C2A-CAA-CBA
12	a	807	CLA	C3A-C2A-CAA-CBA
12	a	807	CLA	C4B-C3B-CAB-CBB
12	a	807	CLA	CHA-CBD-CGD-O1D
12	a	807	CLA	CHA-CBD-CGD-O2D
12	a	809	CLA	C1A-C2A-CAA-CBA
12	a	809	CLA	C3A-C2A-CAA-CBA
12	a	809	CLA	C2B-C3B-CAB-CBB
12	a	809	CLA	C4B-C3B-CAB-CBB
12	a	809	CLA	CBD-CGD-O2D-CED
12	a	810	CLA	C1A-C2A-CAA-CBA
12	a	810	CLA	C3A-C2A-CAA-CBA
12	a	810	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	a	810	CLA	C4B-C3B-CAB-CBB
12	a	810	CLA	CBD-CGD-O2D-CED
12	a	811	CLA	C2B-C3B-CAB-CBB
12	a	811	CLA	C4B-C3B-CAB-CBB
12	a	815	CLA	C2B-C3B-CAB-CBB
12	a	815	CLA	C4B-C3B-CAB-CBB
12	a	816	CLA	C2B-C3B-CAB-CBB
12	a	816	CLA	C4B-C3B-CAB-CBB
12	a	817	CLA	C1A-C2A-CAA-CBA
12	a	818	CLA	C1A-C2A-CAA-CBA
12	a	818	CLA	C3A-C2A-CAA-CBA
12	a	819	CLA	C1A-C2A-CAA-CBA
12	a	819	CLA	C3A-C2A-CAA-CBA
12	a	819	CLA	C2B-C3B-CAB-CBB
12	a	819	CLA	C4B-C3B-CAB-CBB
12	a	819	CLA	CHA-CBD-CGD-O1D
12	a	819	CLA	CHA-CBD-CGD-O2D
12	a	821	CLA	C3A-C2A-CAA-CBA
12	a	821	CLA	CHA-CBD-CGD-O1D
12	a	821	CLA	CHA-CBD-CGD-O2D
12	a	824	CLA	C2-C1-O2A-CGA
12	a	824	CLA	CHA-CBD-CGD-O2D
12	a	825	CLA	CBA-CGA-O2A-C1
12	a	825	CLA	O1A-CGA-O2A-C1
12	a	828	CLA	CBD-CGD-O2D-CED
12	a	829	CLA	CHA-CBD-CGD-O1D
12	a	829	CLA	CHA-CBD-CGD-O2D
12	a	830	CLA	C2B-C3B-CAB-CBB
12	a	830	CLA	C4B-C3B-CAB-CBB
12	a	832	CLA	CBD-CGD-O2D-CED
12	a	833	CLA	C1A-C2A-CAA-CBA
12	a	833	CLA	CHA-CBD-CGD-O1D
12	a	833	CLA	CHA-CBD-CGD-O2D
12	a	834	CLA	C2-C1-O2A-CGA
12	a	834	CLA	CBD-CGD-O2D-CED
12	a	835	CLA	C1A-C2A-CAA-CBA
12	a	835	CLA	C3A-C2A-CAA-CBA
12	a	835	CLA	C2B-C3B-CAB-CBB
12	a	835	CLA	C4B-C3B-CAB-CBB
12	a	840	CLA	C2-C1-O2A-CGA
12	a	840	CLA	C4B-C3B-CAB-CBB
12	a	841	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	a	841	CLA	C4B-C3B-CAB-CBB
12	a	855	CLA	C2-C1-O2A-CGA
12	b	801	CLA	C2-C1-O2A-CGA
12	b	803	CLA	C1A-C2A-CAA-CBA
12	b	803	CLA	C3A-C2A-CAA-CBA
12	b	804	CLA	C2B-C3B-CAB-CBB
12	b	804	CLA	C4B-C3B-CAB-CBB
12	b	804	CLA	CBD-CGD-O2D-CED
12	b	805	CLA	CBD-CGD-O2D-CED
12	b	806	CLA	C2B-C3B-CAB-CBB
12	b	806	CLA	C4B-C3B-CAB-CBB
12	b	806	CLA	CHA-CBD-CGD-O1D
12	b	806	CLA	CHA-CBD-CGD-O2D
12	b	810	CLA	C1A-C2A-CAA-CBA
12	b	811	CLA	CBD-CGD-O2D-CED
12	b	812	CLA	C1A-C2A-CAA-CBA
12	b	812	CLA	C3A-C2A-CAA-CBA
12	b	812	CLA	CHA-CBD-CGD-O1D
12	b	812	CLA	CHA-CBD-CGD-O2D
12	b	813	CLA	C2B-C3B-CAB-CBB
12	b	813	CLA	C4B-C3B-CAB-CBB
12	b	814	CLA	C3A-C2A-CAA-CBA
12	b	815	CLA	C1A-C2A-CAA-CBA
12	b	815	CLA	C3A-C2A-CAA-CBA
12	b	816	CLA	C2B-C3B-CAB-CBB
12	b	816	CLA	C4B-C3B-CAB-CBB
12	b	816	CLA	C4-C3-C5-C6
12	b	817	CLA	C1A-C2A-CAA-CBA
12	b	817	CLA	C3A-C2A-CAA-CBA
12	b	817	CLA	CHA-CBD-CGD-O1D
12	b	817	CLA	CHA-CBD-CGD-O2D
12	b	819	CLA	C2B-C3B-CAB-CBB
12	b	819	CLA	C4B-C3B-CAB-CBB
12	b	821	CLA	CHA-CBD-CGD-O1D
12	b	821	CLA	CHA-CBD-CGD-O2D
12	b	822	CLA	C1A-C2A-CAA-CBA
12	b	822	CLA	C3A-C2A-CAA-CBA
12	b	822	CLA	CHA-CBD-CGD-O1D
12	b	822	CLA	CHA-CBD-CGD-O2D
12	b	823	CLA	C1A-C2A-CAA-CBA
12	b	823	CLA	C3A-C2A-CAA-CBA
12	b	823	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	b	823	CLA	CHA-CBD-CGD-O2D
12	b	824	CLA	C1A-C2A-CAA-CBA
12	b	824	CLA	C3A-C2A-CAA-CBA
12	b	825	CLA	C1A-C2A-CAA-CBA
12	b	825	CLA	C3A-C2A-CAA-CBA
12	b	826	CLA	CHA-CBD-CGD-O1D
12	b	826	CLA	CHA-CBD-CGD-O2D
12	b	827	CLA	C4B-C3B-CAB-CBB
12	b	828	CLA	C1A-C2A-CAA-CBA
12	b	828	CLA	C3A-C2A-CAA-CBA
12	b	829	CLA	CBD-CGD-O2D-CED
12	b	832	CLA	C1A-C2A-CAA-CBA
12	b	832	CLA	C2B-C3B-CAB-CBB
12	b	832	CLA	C4B-C3B-CAB-CBB
12	b	832	CLA	CBD-CGD-O2D-CED
12	b	835	CLA	C4B-C3B-CAB-CBB
12	b	836	CLA	C2-C1-O2A-CGA
12	b	836	CLA	CBD-CGD-O2D-CED
12	b	837	CLA	C2-C1-O2A-CGA
12	b	837	CLA	CHA-CBD-CGD-O1D
12	b	837	CLA	CHA-CBD-CGD-O2D
12	b	848	CLA	CAD-CBD-CGD-O1D
12	b	848	CLA	CAD-CBD-CGD-O2D
12	f	201	CLA	CBD-CGD-O2D-CED
12	j	102	CLA	CHA-CBD-CGD-O1D
12	j	102	CLA	CHA-CBD-CGD-O2D
12	j	104	CLA	C4B-C3B-CAB-CBB
12	j	104	CLA	CBD-CGD-O2D-CED
12	l	202	CLA	CBD-CGD-O2D-CED
12	l	205	CLA	C1A-C2A-CAA-CBA
12	l	205	CLA	C3A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA
12	A	804	CLA	C4B-C3B-CAB-CBB
12	A	805	CLA	CAD-CBD-CGD-O1D
12	A	805	CLA	CAD-CBD-CGD-O2D
12	A	806	CLA	C1A-C2A-CAA-CBA
12	A	806	CLA	CBD-CGD-O2D-CED
12	A	807	CLA	C1A-C2A-CAA-CBA
12	A	807	CLA	C3A-C2A-CAA-CBA
12	A	807	CLA	CHA-CBD-CGD-O1D
12	A	807	CLA	CHA-CBD-CGD-O2D
12	A	809	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	809	CLA	C3A-C2A-CAA-CBA
12	A	809	CLA	C2B-C3B-CAB-CBB
12	A	809	CLA	C4B-C3B-CAB-CBB
12	A	809	CLA	CBD-CGD-O2D-CED
12	A	809	CLA	O1D-CGD-O2D-CED
12	A	810	CLA	C2B-C3B-CAB-CBB
12	A	810	CLA	C4B-C3B-CAB-CBB
12	A	811	CLA	C4B-C3B-CAB-CBB
12	A	813	CLA	CBD-CGD-O2D-CED
12	A	815	CLA	C4B-C3B-CAB-CBB
12	A	816	CLA	CBD-CGD-O2D-CED
12	A	817	CLA	C1A-C2A-CAA-CBA
12	A	817	CLA	C3A-C2A-CAA-CBA
12	A	817	CLA	C2-C1-O2A-CGA
12	A	817	CLA	CBD-CGD-O2D-CED
12	A	818	CLA	C1A-C2A-CAA-CBA
12	A	818	CLA	C3A-C2A-CAA-CBA
12	A	818	CLA	CBD-CGD-O2D-CED
12	A	819	CLA	C1A-C2A-CAA-CBA
12	A	819	CLA	C2B-C3B-CAB-CBB
12	A	819	CLA	C4B-C3B-CAB-CBB
12	A	819	CLA	CHA-CBD-CGD-O1D
12	A	819	CLA	CHA-CBD-CGD-O2D
12	A	821	CLA	C3A-C2A-CAA-CBA
12	A	821	CLA	CHA-CBD-CGD-O1D
12	A	821	CLA	CHA-CBD-CGD-O2D
12	A	822	CLA	CBD-CGD-O2D-CED
12	A	824	CLA	C2-C1-O2A-CGA
12	A	824	CLA	CHA-CBD-CGD-O1D
12	A	824	CLA	CHA-CBD-CGD-O2D
12	A	825	CLA	CBA-CGA-O2A-C1
12	A	825	CLA	O1A-CGA-O2A-C1
12	A	827	CLA	CBD-CGD-O2D-CED
12	A	828	CLA	CBD-CGD-O2D-CED
12	A	829	CLA	CHA-CBD-CGD-O1D
12	A	829	CLA	CHA-CBD-CGD-O2D
12	A	830	CLA	C4B-C3B-CAB-CBB
12	A	833	CLA	C1A-C2A-CAA-CBA
12	A	833	CLA	CHA-CBD-CGD-O1D
12	A	833	CLA	CHA-CBD-CGD-O2D
12	A	834	CLA	C2-C1-O2A-CGA
12	A	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	835	CLA	C3A-C2A-CAA-CBA
12	A	835	CLA	C2B-C3B-CAB-CBB
12	A	835	CLA	C4B-C3B-CAB-CBB
12	A	836	CLA	CBD-CGD-O2D-CED
12	A	840	CLA	C2-C1-O2A-CGA
12	A	840	CLA	C4B-C3B-CAB-CBB
12	A	855	CLA	C2-C1-O2A-CGA
12	B	801	CLA	C2-C1-O2A-CGA
12	B	803	CLA	C1A-C2A-CAA-CBA
12	B	803	CLA	C3A-C2A-CAA-CBA
12	B	804	CLA	C2B-C3B-CAB-CBB
12	B	804	CLA	C4B-C3B-CAB-CBB
12	B	806	CLA	C2B-C3B-CAB-CBB
12	B	806	CLA	C4B-C3B-CAB-CBB
12	B	806	CLA	CHA-CBD-CGD-O1D
12	B	806	CLA	CHA-CBD-CGD-O2D
12	B	807	CLA	C1A-C2A-CAA-CBA
12	B	807	CLA	C3A-C2A-CAA-CBA
12	B	810	CLA	C1A-C2A-CAA-CBA
12	B	810	CLA	C3A-C2A-CAA-CBA
12	B	811	CLA	CBD-CGD-O2D-CED
12	B	812	CLA	C1A-C2A-CAA-CBA
12	B	812	CLA	C3A-C2A-CAA-CBA
12	B	812	CLA	CHA-CBD-CGD-O1D
12	B	812	CLA	CHA-CBD-CGD-O2D
12	B	813	CLA	C2B-C3B-CAB-CBB
12	B	813	CLA	C4B-C3B-CAB-CBB
12	B	814	CLA	C3A-C2A-CAA-CBA
12	B	815	CLA	C1A-C2A-CAA-CBA
12	B	815	CLA	C3A-C2A-CAA-CBA
12	B	816	CLA	C2B-C3B-CAB-CBB
12	B	816	CLA	C4B-C3B-CAB-CBB
12	B	817	CLA	C1A-C2A-CAA-CBA
12	B	817	CLA	C3A-C2A-CAA-CBA
12	B	817	CLA	CHA-CBD-CGD-O1D
12	B	817	CLA	CHA-CBD-CGD-O2D
12	B	819	CLA	C2B-C3B-CAB-CBB
12	B	819	CLA	C4B-C3B-CAB-CBB
12	B	821	CLA	CHA-CBD-CGD-O1D
12	B	821	CLA	CHA-CBD-CGD-O2D
12	B	822	CLA	C1A-C2A-CAA-CBA
12	B	822	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	822	CLA	CHA-CBD-CGD-O1D
12	B	822	CLA	CHA-CBD-CGD-O2D
12	B	823	CLA	CHA-CBD-CGD-O1D
12	B	823	CLA	CHA-CBD-CGD-O2D
12	B	824	CLA	C1A-C2A-CAA-CBA
12	B	824	CLA	C3A-C2A-CAA-CBA
12	B	824	CLA	CBD-CGD-O2D-CED
12	B	825	CLA	C1A-C2A-CAA-CBA
12	B	825	CLA	C3A-C2A-CAA-CBA
12	B	826	CLA	CHA-CBD-CGD-O1D
12	B	826	CLA	CHA-CBD-CGD-O2D
12	B	827	CLA	C4B-C3B-CAB-CBB
12	B	828	CLA	C1A-C2A-CAA-CBA
12	B	828	CLA	C3A-C2A-CAA-CBA
12	B	829	CLA	CBD-CGD-O2D-CED
12	B	830	CLA	CHA-CBD-CGD-O1D
12	B	830	CLA	CHA-CBD-CGD-O2D
12	B	831	CLA	C4B-C3B-CAB-CBB
12	B	833	CLA	C1A-C2A-CAA-CBA
12	B	833	CLA	C3A-C2A-CAA-CBA
12	B	833	CLA	C2B-C3B-CAB-CBB
12	B	833	CLA	C4B-C3B-CAB-CBB
12	B	833	CLA	CBD-CGD-O2D-CED
12	B	834	CLA	CBD-CGD-O2D-CED
12	B	837	CLA	C2-C1-O2A-CGA
12	B	837	CLA	CBD-CGD-O2D-CED
12	B	837	CLA	C6-C7-C8-C9
12	B	838	CLA	C2-C1-O2A-CGA
12	B	838	CLA	CHA-CBD-CGD-O1D
12	B	838	CLA	CHA-CBD-CGD-O2D
12	F	201	CLA	CBD-CGD-O2D-CED
12	J	103	CLA	C2B-C3B-CAB-CBB
12	J	103	CLA	C4B-C3B-CAB-CBB
12	L	205	CLA	C1A-C2A-CAA-CBA
12	L	205	CLA	C3A-C2A-CAA-CBA
13	H	840	1L3	C16-C18-C19-C20
13	b	838	1L3	C16-C18-C19-C20
15	G	845	BCR	C11-C10-C9-C8
15	G	845	BCR	C11-C10-C9-C34
15	G	845	BCR	C19-C20-C21-C22
15	G	845	BCR	C23-C24-C25-C26
15	G	846	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	G	847	BCR	C11-C10-C9-C8
15	G	847	BCR	C11-C10-C9-C34
15	G	847	BCR	C10-C11-C12-C13
15	G	848	BCR	C11-C10-C9-C8
15	G	848	BCR	C11-C10-C9-C34
15	G	848	BCR	C23-C24-C25-C26
15	G	849	BCR	C7-C8-C9-C10
15	G	849	BCR	C11-C10-C9-C8
15	G	849	BCR	C11-C10-C9-C34
15	G	849	BCR	C21-C22-C23-C24
15	G	849	BCR	C37-C22-C23-C24
15	G	850	BCR	C7-C8-C9-C10
15	G	850	BCR	C11-C10-C9-C8
15	G	850	BCR	C11-C10-C9-C34
15	G	850	BCR	C10-C11-C12-C13
15	G	850	BCR	C21-C22-C23-C24
15	G	850	BCR	C37-C22-C23-C24
15	G	853	BCR	C7-C8-C9-C10
15	G	853	BCR	C7-C8-C9-C34
15	G	853	BCR	C11-C10-C9-C8
15	G	853	BCR	C11-C10-C9-C34
15	G	853	BCR	C17-C18-C19-C20
15	H	841	BCR	C11-C10-C9-C8
15	H	841	BCR	C11-C10-C9-C34
15	H	841	BCR	C10-C11-C12-C13
15	H	841	BCR	C19-C20-C21-C22
15	H	842	BCR	C11-C10-C9-C8
15	H	842	BCR	C11-C10-C9-C34
15	H	842	BCR	C21-C22-C23-C24
15	H	843	BCR	C21-C22-C23-C24
15	H	845	BCR	C7-C8-C9-C10
15	H	845	BCR	C7-C8-C9-C34
15	H	845	BCR	C17-C18-C19-C20
15	H	845	BCR	C36-C18-C19-C20
15	H	846	BCR	C11-C10-C9-C8
15	H	846	BCR	C11-C10-C9-C34
15	H	846	BCR	C9-C10-C11-C12
15	H	846	BCR	C10-C11-C12-C13
15	P	202	BCR	C11-C10-C9-C8
15	P	202	BCR	C11-C10-C9-C34
15	P	202	BCR	C10-C11-C12-C13
15	P	202	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
15	P	202	BCR	C36-C18-C19-C20
15	Q	101	BCR	C11-C10-C9-C8
15	Q	101	BCR	C11-C10-C9-C34
15	Q	101	BCR	C9-C10-C11-C12
15	Q	101	BCR	C10-C11-C12-C13
15	Q	101	BCR	C11-C12-C13-C14
15	Q	101	BCR	C11-C12-C13-C35
15	Q	102	BCR	C23-C24-C25-C26
15	R	101	BCR	C7-C8-C9-C10
15	R	101	BCR	C7-C8-C9-C34
15	R	101	BCR	C19-C20-C21-C22
15	R	101	BCR	C21-C22-C23-C24
15	R	101	BCR	C37-C22-C23-C24
15	R	102	BCR	C11-C10-C9-C8
15	R	102	BCR	C11-C10-C9-C34
15	R	102	BCR	C10-C11-C12-C13
15	R	102	BCR	C17-C18-C19-C20
15	S	201	BCR	C7-C8-C9-C10
15	S	201	BCR	C11-C10-C9-C8
15	S	201	BCR	C11-C10-C9-C34
15	S	201	BCR	C10-C11-C12-C13
15	S	201	BCR	C11-C12-C13-C14
15	S	201	BCR	C11-C12-C13-C35
15	S	205	BCR	C7-C8-C9-C10
15	S	205	BCR	C7-C8-C9-C34
15	S	205	BCR	C11-C10-C9-C8
15	S	205	BCR	C11-C10-C9-C34
15	a	844	BCR	C7-C8-C9-C34
15	a	844	BCR	C11-C10-C9-C8
15	a	844	BCR	C11-C10-C9-C34
15	a	844	BCR	C19-C20-C21-C22
15	a	844	BCR	C23-C24-C25-C26
15	a	845	BCR	C7-C8-C9-C10
15	a	845	BCR	C11-C10-C9-C34
15	a	845	BCR	C23-C24-C25-C26
15	a	846	BCR	C11-C10-C9-C8
15	a	846	BCR	C11-C10-C9-C34
15	a	846	BCR	C10-C11-C12-C13
15	a	847	BCR	C11-C10-C9-C34
15	a	847	BCR	C23-C24-C25-C26
15	a	848	BCR	C7-C8-C9-C10
15	a	848	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	a	848	BCR	C11-C10-C9-C34
15	a	848	BCR	C17-C18-C19-C20
15	a	848	BCR	C21-C22-C23-C24
15	a	848	BCR	C37-C22-C23-C24
15	a	849	BCR	C7-C8-C9-C10
15	a	849	BCR	C11-C10-C9-C8
15	a	849	BCR	C11-C10-C9-C34
15	a	849	BCR	C21-C22-C23-C24
15	a	849	BCR	C37-C22-C23-C24
15	a	852	BCR	C7-C8-C9-C10
15	a	852	BCR	C7-C8-C9-C34
15	a	852	BCR	C11-C10-C9-C8
15	a	852	BCR	C11-C10-C9-C34
15	a	852	BCR	C17-C18-C19-C20
15	a	852	BCR	C36-C18-C19-C20
15	b	839	BCR	C11-C10-C9-C8
15	b	839	BCR	C11-C10-C9-C34
15	b	839	BCR	C19-C20-C21-C22
15	b	840	BCR	C11-C10-C9-C8
15	b	840	BCR	C11-C10-C9-C34
15	b	840	BCR	C17-C18-C19-C20
15	b	840	BCR	C21-C22-C23-C24
15	b	841	BCR	C21-C22-C23-C24
15	b	843	BCR	C7-C8-C9-C10
15	b	843	BCR	C7-C8-C9-C34
15	b	843	BCR	C11-C10-C9-C8
15	b	843	BCR	C11-C10-C9-C34
15	b	843	BCR	C17-C18-C19-C20
15	b	843	BCR	C36-C18-C19-C20
15	b	844	BCR	C11-C10-C9-C8
15	b	844	BCR	C11-C10-C9-C34
15	b	844	BCR	C9-C10-C11-C12
15	b	844	BCR	C10-C11-C12-C13
15	b	847	BCR	C7-C8-C9-C10
15	b	847	BCR	C7-C8-C9-C34
15	f	202	BCR	C11-C10-C9-C8
15	f	202	BCR	C11-C10-C9-C34
15	f	202	BCR	C10-C11-C12-C13
15	f	202	BCR	C17-C18-C19-C20
15	f	202	BCR	C36-C18-C19-C20
15	i	101	BCR	C11-C10-C9-C8
15	i	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
15	i	101	BCR	C10-C11-C12-C13
15	i	101	BCR	C11-C12-C13-C14
15	i	101	BCR	C11-C12-C13-C35
15	i	102	BCR	C23-C24-C25-C26
15	j	101	BCR	C7-C8-C9-C10
15	j	101	BCR	C7-C8-C9-C34
15	j	101	BCR	C19-C20-C21-C22
15	j	101	BCR	C21-C22-C23-C24
15	j	101	BCR	C37-C22-C23-C24
15	j	103	BCR	C7-C8-C9-C34
15	j	103	BCR	C11-C10-C9-C8
15	j	103	BCR	C11-C10-C9-C34
15	j	103	BCR	C10-C11-C12-C13
15	l	201	BCR	C7-C8-C9-C10
15	l	201	BCR	C7-C8-C9-C34
15	l	201	BCR	C11-C10-C9-C8
15	l	201	BCR	C11-C10-C9-C34
15	l	203	BCR	C7-C8-C9-C10
15	l	203	BCR	C11-C10-C9-C8
15	l	203	BCR	C11-C10-C9-C34
15	l	203	BCR	C10-C11-C12-C13
15	l	203	BCR	C11-C12-C13-C14
15	l	203	BCR	C11-C12-C13-C35
15	A	844	BCR	C7-C8-C9-C34
15	A	844	BCR	C11-C10-C9-C8
15	A	844	BCR	C11-C10-C9-C34
15	A	844	BCR	C23-C24-C25-C26
15	A	845	BCR	C7-C8-C9-C10
15	A	845	BCR	C11-C10-C9-C8
15	A	845	BCR	C11-C10-C9-C34
15	A	845	BCR	C23-C24-C25-C26
15	A	846	BCR	C11-C10-C9-C8
15	A	846	BCR	C11-C10-C9-C34
15	A	846	BCR	C10-C11-C12-C13
15	A	847	BCR	C11-C10-C9-C34
15	A	847	BCR	C23-C24-C25-C26
15	A	848	BCR	C7-C8-C9-C10
15	A	848	BCR	C11-C10-C9-C8
15	A	848	BCR	C11-C10-C9-C34
15	A	848	BCR	C21-C22-C23-C24
15	A	848	BCR	C37-C22-C23-C24
15	A	849	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	A	849	BCR	C11-C10-C9-C8
15	A	849	BCR	C11-C10-C9-C34
15	A	849	BCR	C21-C22-C23-C24
15	A	849	BCR	C37-C22-C23-C24
15	A	849	BCR	C23-C24-C25-C26
15	A	852	BCR	C7-C8-C9-C10
15	A	852	BCR	C7-C8-C9-C34
15	A	852	BCR	C11-C10-C9-C8
15	A	852	BCR	C11-C10-C9-C34
15	A	852	BCR	C10-C11-C12-C13
15	A	852	BCR	C17-C18-C19-C20
15	B	840	BCR	C11-C10-C9-C8
15	B	840	BCR	C11-C10-C9-C34
15	B	840	BCR	C19-C20-C21-C22
15	B	841	BCR	C11-C10-C9-C8
15	B	841	BCR	C11-C10-C9-C34
15	B	841	BCR	C17-C18-C19-C20
15	B	841	BCR	C21-C22-C23-C24
15	B	842	BCR	C21-C22-C23-C24
15	B	843	BCR	C21-C22-C23-C24
15	B	844	BCR	C7-C8-C9-C10
15	B	844	BCR	C7-C8-C9-C34
15	B	844	BCR	C11-C10-C9-C8
15	B	844	BCR	C11-C10-C9-C34
15	B	844	BCR	C17-C18-C19-C20
15	B	844	BCR	C36-C18-C19-C20
15	B	845	BCR	C11-C10-C9-C8
15	B	845	BCR	C11-C10-C9-C34
15	B	845	BCR	C9-C10-C11-C12
15	B	845	BCR	C10-C11-C12-C13
15	F	202	BCR	C7-C8-C9-C34
15	F	202	BCR	C11-C10-C9-C8
15	F	202	BCR	C11-C10-C9-C34
15	F	202	BCR	C17-C18-C19-C20
15	F	202	BCR	C36-C18-C19-C20
15	F	204	BCR	C11-C10-C9-C8
15	F	204	BCR	C11-C10-C9-C34
15	F	204	BCR	C10-C11-C12-C13
15	I	101	BCR	C11-C10-C9-C8
15	I	101	BCR	C11-C10-C9-C34
15	I	101	BCR	C10-C11-C12-C13
15	I	101	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	I	101	BCR	C11-C12-C13-C35
15	J	101	BCR	C7-C8-C9-C10
15	J	101	BCR	C7-C8-C9-C34
15	J	101	BCR	C19-C20-C21-C22
15	J	101	BCR	C21-C22-C23-C24
15	J	101	BCR	C37-C22-C23-C24
15	J	102	BCR	C11-C10-C9-C8
15	J	102	BCR	C11-C10-C9-C34
15	J	102	BCR	C15-C16-C17-C18
15	L	201	BCR	C7-C8-C9-C10
15	L	201	BCR	C7-C8-C9-C34
15	L	201	BCR	C11-C10-C9-C8
15	L	201	BCR	C11-C10-C9-C34
15	L	201	BCR	C11-C12-C13-C14
15	L	203	BCR	C7-C8-C9-C10
15	L	203	BCR	C11-C10-C9-C8
15	L	203	BCR	C11-C10-C9-C34
15	L	203	BCR	C10-C11-C12-C13
15	L	203	BCR	C11-C12-C13-C14
15	L	203	BCR	C11-C12-C13-C35
16	G	851	LHG	O1-C1-C2-C3
16	G	851	LHG	C1-C2-C3-O3
16	G	851	LHG	C4-O6-P-O3
16	G	851	LHG	C4-O6-P-O4
16	G	851	LHG	O6-C4-C5-O7
16	G	852	LHG	C4-O6-P-O3
16	G	852	LHG	C4-O6-P-O4
16	G	854	LHG	O1-C1-C2-O2
16	G	854	LHG	C3-O3-P-O6
16	G	854	LHG	C4-O6-P-O3
16	G	854	LHG	C4-O6-P-O4
16	G	854	LHG	C4-O6-P-O5
16	G	854	LHG	O9-C7-O7-C5
16	G	854	LHG	C8-C7-O7-C5
16	a	850	LHG	O1-C1-C2-C3
16	a	850	LHG	C1-C2-C3-O3
16	a	850	LHG	C4-O6-P-O5
16	a	851	LHG	C4-O6-P-O4
16	a	853	LHG	C3-O3-P-O6
16	a	853	LHG	C4-O6-P-O3
16	a	853	LHG	C4-O6-P-O4
16	a	853	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
16	a	853	LHG	C8-C7-O7-C5
16	A	850	LHG	O1-C1-C2-C3
16	A	850	LHG	C1-C2-C3-O3
16	A	850	LHG	C4-O6-P-O3
16	A	851	LHG	C4-O6-P-O4
16	A	853	LHG	C3-O3-P-O6
16	A	853	LHG	C4-O6-P-O3
16	A	853	LHG	C4-O6-P-O4
16	A	853	LHG	C4-O6-P-O5
16	A	853	LHG	O9-C7-O7-C5
16	A	853	LHG	C8-C7-O7-C5
17	T	101	45D	C16-C08-C20-C24
17	T	101	45D	C20-C24-C26-C28
17	T	101	45D	C20-C24-C26-C30
17	T	101	45D	C31-C33-C35-C37
17	m	101	45D	C16-C08-C20-C24
17	m	101	45D	C20-C24-C26-C28
17	m	101	45D	C20-C24-C26-C30
17	m	101	45D	C35-C37-C41-C42
17	M	101	45D	C16-C08-C20-C24
17	M	101	45D	C20-C24-C26-C28
17	M	101	45D	C20-C24-C26-C30
19	H	848	LMT	C2-C1-O1'-C1'
19	b	846	LMT	C2-C1-O1'-C1'
19	B	847	LMT	C2-C1-O1'-C1'
12	a	822	CLA	O1D-CGD-O2D-CED
12	a	828	CLA	O1D-CGD-O2D-CED
12	G	816	CLA	O1D-CGD-O2D-CED
12	G	829	CLA	O1D-CGD-O2D-CED
12	G	835	CLA	O1D-CGD-O2D-CED
12	G	836	CLA	O1D-CGD-O2D-CED
12	P	201	CLA	O1D-CGD-O2D-CED
12	a	815	CLA	O1D-CGD-O2D-CED
12	a	820	CLA	O1D-CGD-O2D-CED
12	a	835	CLA	O1D-CGD-O2D-CED
12	f	203	CLA	O1D-CGD-O2D-CED
12	A	810	CLA	O1D-CGD-O2D-CED
12	A	815	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	O1D-CGD-O2D-CED
12	A	822	CLA	O1D-CGD-O2D-CED
12	A	828	CLA	O1D-CGD-O2D-CED
12	A	836	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	816	CLA	O1D-CGD-O2D-CED
12	F	201	CLA	O1D-CGD-O2D-CED
12	J	103	CLA	O1D-CGD-O2D-CED
12	G	803	CLA	CBD-CGD-O2D-CED
12	G	804	CLA	CBD-CGD-O2D-CED
12	G	809	CLA	CBD-CGD-O2D-CED
12	G	811	CLA	CBD-CGD-O2D-CED
12	G	813	CLA	CBD-CGD-O2D-CED
12	G	814	CLA	CBD-CGD-O2D-CED
12	G	815	CLA	CBD-CGD-O2D-CED
12	G	816	CLA	CBD-CGD-O2D-CED
12	G	819	CLA	CBD-CGD-O2D-CED
12	G	821	CLA	CBD-CGD-O2D-CED
12	G	822	CLA	CBD-CGD-O2D-CED
12	G	824	CLA	CBD-CGD-O2D-CED
12	G	828	CLA	CBD-CGD-O2D-CED
12	G	831	CLA	CBD-CGD-O2D-CED
12	G	833	CLA	CBD-CGD-O2D-CED
12	G	834	CLA	CBD-CGD-O2D-CED
12	G	835	CLA	CBD-CGD-O2D-CED
12	G	836	CLA	CBD-CGD-O2D-CED
12	H	802	CLA	CBD-CGD-O2D-CED
12	H	804	CLA	CBD-CGD-O2D-CED
12	H	808	CLA	CBD-CGD-O2D-CED
12	H	809	CLA	CBD-CGD-O2D-CED
12	H	811	CLA	CBD-CGD-O2D-CED
12	H	819	CLA	CBD-CGD-O2D-CED
12	H	820	CLA	CBD-CGD-O2D-CED
12	H	829	CLA	CBD-CGD-O2D-CED
12	H	830	CLA	CBD-CGD-O2D-CED
12	H	837	CLA	CBD-CGD-O2D-CED
12	P	203	CLA	CBD-CGD-O2D-CED
12	R	103	CLA	CBD-CGD-O2D-CED
12	a	808	CLA	CBD-CGD-O2D-CED
12	a	812	CLA	CBD-CGD-O2D-CED
12	a	813	CLA	CBD-CGD-O2D-CED
12	a	814	CLA	CBD-CGD-O2D-CED
12	a	815	CLA	CBD-CGD-O2D-CED
12	a	816	CLA	CBD-CGD-O2D-CED
12	a	817	CLA	CBD-CGD-O2D-CED
12	a	818	CLA	CBD-CGD-O2D-CED
12	a	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	a	820	CLA	CBD-CGD-O2D-CED
12	a	821	CLA	CBD-CGD-O2D-CED
12	a	822	CLA	CBD-CGD-O2D-CED
12	a	827	CLA	CBD-CGD-O2D-CED
12	a	833	CLA	CBD-CGD-O2D-CED
12	a	835	CLA	CBD-CGD-O2D-CED
12	a	836	CLA	CBD-CGD-O2D-CED
12	a	840	CLA	CBD-CGD-O2D-CED
12	b	802	CLA	CBD-CGD-O2D-CED
12	b	816	CLA	CBD-CGD-O2D-CED
12	b	817	CLA	CBD-CGD-O2D-CED
12	b	818	CLA	CBD-CGD-O2D-CED
12	b	819	CLA	CBD-CGD-O2D-CED
12	b	828	CLA	CBD-CGD-O2D-CED
12	b	831	CLA	CBD-CGD-O2D-CED
12	b	833	CLA	CBD-CGD-O2D-CED
12	b	834	CLA	CBD-CGD-O2D-CED
12	b	835	CLA	CBD-CGD-O2D-CED
12	b	848	CLA	CBD-CGD-O2D-CED
12	f	203	CLA	CBD-CGD-O2D-CED
12	A	802	CLA	CBD-CGD-O2D-CED
12	A	808	CLA	CBD-CGD-O2D-CED
12	A	810	CLA	CBD-CGD-O2D-CED
12	A	812	CLA	CBD-CGD-O2D-CED
12	A	814	CLA	CBD-CGD-O2D-CED
12	A	815	CLA	CBD-CGD-O2D-CED
12	A	820	CLA	CBD-CGD-O2D-CED
12	A	821	CLA	CBD-CGD-O2D-CED
12	A	832	CLA	CBD-CGD-O2D-CED
12	A	833	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	CBD-CGD-O2D-CED
12	A	835	CLA	CBD-CGD-O2D-CED
12	A	840	CLA	CBD-CGD-O2D-CED
12	B	802	CLA	CBD-CGD-O2D-CED
12	B	810	CLA	CBD-CGD-O2D-CED
12	B	816	CLA	CBD-CGD-O2D-CED
12	B	817	CLA	CBD-CGD-O2D-CED
12	B	819	CLA	CBD-CGD-O2D-CED
12	B	826	CLA	CBD-CGD-O2D-CED
12	B	832	CLA	CBD-CGD-O2D-CED
12	B	835	CLA	CBD-CGD-O2D-CED
12	B	836	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	F	203	CLA	CBD-CGD-O2D-CED
12	J	103	CLA	CBD-CGD-O2D-CED
12	L	202	CLA	CBD-CGD-O2D-CED
12	G	836	CLA	O1A-CGA-O2A-C1
12	G	841	CLA	O1A-CGA-O2A-C1
12	H	827	CLA	O1A-CGA-O2A-C1
12	H	838	CLA	O1A-CGA-O2A-C1
12	a	841	CLA	O1A-CGA-O2A-C1
12	l	204	CLA	O1A-CGA-O2A-C1
12	A	841	CLA	O1A-CGA-O2A-C1
16	G	854	LHG	O10-C23-O8-C6
12	H	838	CLA	C4C-C3C-CAC-CBC
12	b	836	CLA	C4C-C3C-CAC-CBC
12	G	807	CLA	O1D-CGD-O2D-CED
12	G	823	CLA	O1D-CGD-O2D-CED
12	a	806	CLA	O1D-CGD-O2D-CED
12	a	809	CLA	O1D-CGD-O2D-CED
12	f	201	CLA	O1D-CGD-O2D-CED
12	A	806	CLA	O1D-CGD-O2D-CED
12	G	809	CLA	O1D-CGD-O2D-CED
12	G	811	CLA	O1D-CGD-O2D-CED
12	G	821	CLA	O1D-CGD-O2D-CED
12	H	802	CLA	O1D-CGD-O2D-CED
12	H	804	CLA	O1D-CGD-O2D-CED
12	a	812	CLA	O1D-CGD-O2D-CED
12	a	813	CLA	O1D-CGD-O2D-CED
12	a	816	CLA	O1D-CGD-O2D-CED
12	b	819	CLA	O1D-CGD-O2D-CED
12	A	808	CLA	O1D-CGD-O2D-CED
12	A	834	CLA	O1D-CGD-O2D-CED
12	A	835	CLA	O1D-CGD-O2D-CED
12	B	819	CLA	O1D-CGD-O2D-CED
12	B	832	CLA	O1D-CGD-O2D-CED
12	F	203	CLA	O1D-CGD-O2D-CED
12	G	836	CLA	CBA-CGA-O2A-C1
12	H	822	CLA	CBA-CGA-O2A-C1
12	G	808	CLA	CBD-CGD-O2D-CED
12	G	856	CLA	CBD-CGD-O2D-CED
12	b	810	CLA	CBD-CGD-O2D-CED
12	G	802	CLA	O1A-CGA-O2A-C1
12	G	811	CLA	O1A-CGA-O2A-C1
12	G	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	H	814	CLA	O1A-CGA-O2A-C1
12	H	822	CLA	O1A-CGA-O2A-C1
12	S	202	CLA	O1A-CGA-O2A-C1
12	a	810	CLA	O1A-CGA-O2A-C1
12	a	822	CLA	O1A-CGA-O2A-C1
12	a	831	CLA	O1A-CGA-O2A-C1
12	a	836	CLA	O1A-CGA-O2A-C1
12	a	840	CLA	O1A-CGA-O2A-C1
12	b	801	CLA	O1A-CGA-O2A-C1
12	b	813	CLA	O1A-CGA-O2A-C1
12	b	821	CLA	O1A-CGA-O2A-C1
12	b	826	CLA	O1A-CGA-O2A-C1
12	b	836	CLA	O1A-CGA-O2A-C1
12	A	810	CLA	O1A-CGA-O2A-C1
12	A	822	CLA	O1A-CGA-O2A-C1
12	A	836	CLA	O1A-CGA-O2A-C1
12	A	840	CLA	O1A-CGA-O2A-C1
12	B	801	CLA	O1A-CGA-O2A-C1
12	B	813	CLA	O1A-CGA-O2A-C1
12	B	826	CLA	O1A-CGA-O2A-C1
12	B	837	CLA	O1A-CGA-O2A-C1
12	L	204	CLA	O1A-CGA-O2A-C1
16	A	853	LHG	O10-C23-O8-C6
12	G	815	CLA	O1D-CGD-O2D-CED
12	G	817	CLA	O1D-CGD-O2D-CED
12	G	818	CLA	O1D-CGD-O2D-CED
12	H	812	CLA	O1D-CGD-O2D-CED
12	H	820	CLA	O1D-CGD-O2D-CED
12	H	835	CLA	O1D-CGD-O2D-CED
12	P	203	CLA	O1D-CGD-O2D-CED
12	R	103	CLA	O1D-CGD-O2D-CED
12	a	808	CLA	O1D-CGD-O2D-CED
12	a	814	CLA	O1D-CGD-O2D-CED
12	a	832	CLA	O1D-CGD-O2D-CED
12	a	836	CLA	O1D-CGD-O2D-CED
12	b	802	CLA	O1D-CGD-O2D-CED
12	b	804	CLA	O1D-CGD-O2D-CED
12	b	831	CLA	O1D-CGD-O2D-CED
12	A	814	CLA	O1D-CGD-O2D-CED
12	A	816	CLA	O1D-CGD-O2D-CED
12	B	802	CLA	O1D-CGD-O2D-CED
12	b	836	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
12	G	840	CLA	O1D-CGD-O2D-CED
12	H	805	CLA	O1D-CGD-O2D-CED
12	H	817	CLA	O1D-CGD-O2D-CED
12	H	833	CLA	O1D-CGD-O2D-CED
12	H	850	CLA	O1D-CGD-O2D-CED
12	a	810	CLA	O1D-CGD-O2D-CED
12	a	834	CLA	O1D-CGD-O2D-CED
12	b	811	CLA	O1D-CGD-O2D-CED
12	b	829	CLA	O1D-CGD-O2D-CED
12	j	104	CLA	O1D-CGD-O2D-CED
12	A	813	CLA	O1D-CGD-O2D-CED
12	B	829	CLA	O1D-CGD-O2D-CED
12	B	837	CLA	O1D-CGD-O2D-CED
12	b	808	CLA	CBD-CGD-O2D-CED
12	B	818	CLA	CBD-CGD-O2D-CED
12	H	838	CLA	C2C-C3C-CAC-CBC
16	a	853	LHG	O9-C7-O7-C5
12	A	827	CLA	O1D-CGD-O2D-CED
12	G	805	CLA	C3-C5-C6-C7
12	G	807	CLA	C3-C5-C6-C7
12	G	808	CLA	C3-C5-C6-C7
12	G	818	CLA	C3-C5-C6-C7
12	G	824	CLA	C3-C5-C6-C7
12	G	825	CLA	C3-C5-C6-C7
12	G	826	CLA	C3-C5-C6-C7
12	G	827	CLA	C3-C5-C6-C7
12	G	832	CLA	C3-C5-C6-C7
12	G	839	CLA	C3-C5-C6-C7
12	H	806	CLA	C3-C5-C6-C7
12	H	808	CLA	C3-C5-C6-C7
12	a	804	CLA	C3-C5-C6-C7
12	a	806	CLA	C3-C5-C6-C7
12	a	807	CLA	C3-C5-C6-C7
12	a	817	CLA	C3-C5-C6-C7
12	a	824	CLA	C3-C5-C6-C7
12	a	825	CLA	C3-C5-C6-C7
12	a	826	CLA	C3-C5-C6-C7
12	a	832	CLA	C3-C5-C6-C7
12	a	834	CLA	C3-C5-C6-C7
12	a	839	CLA	C3-C5-C6-C7
12	b	802	CLA	C3-C5-C6-C7
12	b	806	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	b	836	CLA	C3-C5-C6-C7
12	A	804	CLA	C3-C5-C6-C7
12	A	806	CLA	C3-C5-C6-C7
12	A	807	CLA	C3-C5-C6-C7
12	A	824	CLA	C3-C5-C6-C7
12	A	825	CLA	C3-C5-C6-C7
12	A	826	CLA	C3-C5-C6-C7
12	A	834	CLA	C3-C5-C6-C7
12	A	839	CLA	C3-C5-C6-C7
12	B	802	CLA	C3-C5-C6-C7
12	B	806	CLA	C3-C5-C6-C7
12	B	816	CLA	C3-C5-C6-C7
12	L	202	CLA	C3-C5-C6-C7
12	H	838	CLA	O1D-CGD-O2D-CED
12	A	817	CLA	O1D-CGD-O2D-CED
12	A	818	CLA	O1D-CGD-O2D-CED
12	B	824	CLA	O1D-CGD-O2D-CED
12	G	819	CLA	CBA-CGA-O2A-C1
12	G	823	CLA	CBA-CGA-O2A-C1
12	G	825	CLA	CBA-CGA-O2A-C1
12	G	841	CLA	CBA-CGA-O2A-C1
12	H	814	CLA	CBA-CGA-O2A-C1
12	H	816	CLA	CBA-CGA-O2A-C1
12	H	827	CLA	CBA-CGA-O2A-C1
12	H	838	CLA	CBA-CGA-O2A-C1
12	P	201	CLA	CBA-CGA-O2A-C1
12	a	817	CLA	CBA-CGA-O2A-C1
12	a	818	CLA	CBA-CGA-O2A-C1
12	a	822	CLA	CBA-CGA-O2A-C1
12	a	824	CLA	CBA-CGA-O2A-C1
12	a	836	CLA	CBA-CGA-O2A-C1
12	a	840	CLA	CBA-CGA-O2A-C1
12	a	841	CLA	CBA-CGA-O2A-C1
12	b	801	CLA	CBA-CGA-O2A-C1
12	b	826	CLA	CBA-CGA-O2A-C1
12	f	201	CLA	CBA-CGA-O2A-C1
12	l	204	CLA	CBA-CGA-O2A-C1
12	A	804	CLA	CBA-CGA-O2A-C1
12	A	822	CLA	CBA-CGA-O2A-C1
12	A	824	CLA	CBA-CGA-O2A-C1
12	A	836	CLA	CBA-CGA-O2A-C1
12	A	841	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	801	CLA	CBA-CGA-O2A-C1
12	B	813	CLA	CBA-CGA-O2A-C1
12	B	815	CLA	CBA-CGA-O2A-C1
12	G	820	CLA	CBD-CGD-O2D-CED
12	G	827	CLA	CBD-CGD-O2D-CED
12	G	830	CLA	CBD-CGD-O2D-CED
12	G	841	CLA	CBD-CGD-O2D-CED
12	H	806	CLA	CBD-CGD-O2D-CED
12	H	813	CLA	CBD-CGD-O2D-CED
12	H	818	CLA	CBD-CGD-O2D-CED
12	H	824	CLA	CBD-CGD-O2D-CED
12	H	825	CLA	CBD-CGD-O2D-CED
12	H	827	CLA	CBD-CGD-O2D-CED
12	H	831	CLA	CBD-CGD-O2D-CED
12	H	834	CLA	CBD-CGD-O2D-CED
12	H	836	CLA	CBD-CGD-O2D-CED
12	a	802	CLA	CBD-CGD-O2D-CED
12	a	807	CLA	CBD-CGD-O2D-CED
12	a	823	CLA	CBD-CGD-O2D-CED
12	a	826	CLA	CBD-CGD-O2D-CED
12	a	829	CLA	CBD-CGD-O2D-CED
12	a	830	CLA	CBD-CGD-O2D-CED
12	a	841	CLA	CBD-CGD-O2D-CED
12	b	806	CLA	CBD-CGD-O2D-CED
12	b	812	CLA	CBD-CGD-O2D-CED
12	b	823	CLA	CBD-CGD-O2D-CED
12	b	826	CLA	CBD-CGD-O2D-CED
12	b	827	CLA	CBD-CGD-O2D-CED
12	j	102	CLA	CBD-CGD-O2D-CED
12	A	807	CLA	CBD-CGD-O2D-CED
12	A	819	CLA	CBD-CGD-O2D-CED
12	A	823	CLA	CBD-CGD-O2D-CED
12	A	841	CLA	CBD-CGD-O2D-CED
12	B	804	CLA	CBD-CGD-O2D-CED
12	B	806	CLA	CBD-CGD-O2D-CED
12	B	812	CLA	CBD-CGD-O2D-CED
12	B	823	CLA	CBD-CGD-O2D-CED
12	B	828	CLA	CBD-CGD-O2D-CED
12	B	830	CLA	CBD-CGD-O2D-CED
12	G	832	CLA	O1D-CGD-O2D-CED
12	G	842	CLA	O1D-CGD-O2D-CED
12	H	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	H	830	CLA	O1D-CGD-O2D-CED
12	b	805	CLA	O1D-CGD-O2D-CED
12	b	832	CLA	O1D-CGD-O2D-CED
12	b	835	CLA	O1D-CGD-O2D-CED
12	b	836	CLA	O1D-CGD-O2D-CED
12	l	202	CLA	O1D-CGD-O2D-CED
12	B	811	CLA	O1D-CGD-O2D-CED
12	B	833	CLA	O1D-CGD-O2D-CED
12	B	834	CLA	O1D-CGD-O2D-CED
12	L	202	CLA	O1D-CGD-O2D-CED
12	B	837	CLA	C2C-C3C-CAC-CBC
12	A	840	CLA	O1D-CGD-O2D-CED
12	G	818	CLA	C4-C3-C5-C6
12	G	834	CLA	C4-C3-C5-C6
12	G	855	CLA	C4-C3-C5-C6
12	H	801	CLA	C4-C3-C5-C6
12	H	802	CLA	C4-C3-C5-C6
12	H	817	CLA	C4-C3-C5-C6
12	a	817	CLA	C4-C3-C5-C6
12	a	831	CLA	C4-C3-C5-C6
12	a	834	CLA	C4-C3-C5-C6
12	a	854	CLA	C4-C3-C5-C6
12	b	802	CLA	C4-C3-C5-C6
12	f	201	CLA	C4-C3-C5-C6
12	A	804	CLA	C4-C3-C5-C6
12	A	817	CLA	C4-C3-C5-C6
12	A	831	CLA	C4-C3-C5-C6
12	A	834	CLA	C4-C3-C5-C6
12	B	802	CLA	C4-C3-C5-C6
12	B	816	CLA	C4-C3-C5-C6
12	F	201	CLA	C4-C3-C5-C6
12	G	818	CLA	C2-C3-C5-C6
12	H	801	CLA	C2-C3-C5-C6
12	H	802	CLA	C2-C3-C5-C6
12	H	817	CLA	C2-C3-C5-C6
12	P	201	CLA	C2-C3-C5-C6
12	a	817	CLA	C2-C3-C5-C6
12	a	831	CLA	C2-C3-C5-C6
12	a	834	CLA	C2-C3-C5-C6
12	b	802	CLA	C2-C3-C5-C6
12	b	816	CLA	C2-C3-C5-C6
12	f	201	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	804	CLA	C2-C3-C5-C6
12	A	817	CLA	C2-C3-C5-C6
12	A	834	CLA	C2-C3-C5-C6
12	B	802	CLA	C2-C3-C5-C6
12	B	816	CLA	C2-C3-C5-C6
12	B	837	CLA	C4C-C3C-CAC-CBC
12	A	829	CLA	CBD-CGD-O2D-CED
12	G	834	CLA	O1D-CGD-O2D-CED
12	H	837	CLA	O1D-CGD-O2D-CED
12	a	818	CLA	O1D-CGD-O2D-CED
12	b	816	CLA	O1D-CGD-O2D-CED
12	b	848	CLA	O1D-CGD-O2D-CED
12	B	836	CLA	O1D-CGD-O2D-CED
19	H	848	LMT	O5B-C5B-C6B-O6B
12	H	815	CLA	C2A-CAA-CBA-CGA
12	a	830	CLA	C2A-CAA-CBA-CGA
12	b	835	CLA	C2A-CAA-CBA-CGA
12	B	836	CLA	C2A-CAA-CBA-CGA
12	G	834	CLA	C3-C5-C6-C7
12	H	802	CLA	C3-C5-C6-C7
12	H	804	CLA	C3-C5-C6-C7
12	H	817	CLA	C3-C5-C6-C7
12	H	830	CLA	C3-C5-C6-C7
12	H	838	CLA	C3-C5-C6-C7
12	a	828	CLA	C3-C5-C6-C7
12	b	816	CLA	C3-C5-C6-C7
12	l	202	CLA	C3-C5-C6-C7
12	A	817	CLA	C3-C5-C6-C7
12	A	832	CLA	C3-C5-C6-C7
12	B	837	CLA	C3-C5-C6-C7
12	G	802	CLA	CBA-CGA-O2A-C1
12	G	805	CLA	CBA-CGA-O2A-C1
12	G	809	CLA	CBA-CGA-O2A-C1
12	G	811	CLA	CBA-CGA-O2A-C1
12	G	813	CLA	CBA-CGA-O2A-C1
12	G	830	CLA	CBA-CGA-O2A-C1
12	H	808	CLA	CBA-CGA-O2A-C1
12	S	202	CLA	CBA-CGA-O2A-C1
12	a	804	CLA	CBA-CGA-O2A-C1
12	a	810	CLA	CBA-CGA-O2A-C1
12	a	812	CLA	CBA-CGA-O2A-C1
12	a	831	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	834	CLA	CBA-CGA-O2A-C1
12	b	813	CLA	CBA-CGA-O2A-C1
12	b	815	CLA	CBA-CGA-O2A-C1
12	b	821	CLA	CBA-CGA-O2A-C1
12	b	836	CLA	CBA-CGA-O2A-C1
12	l	202	CLA	CBA-CGA-O2A-C1
12	A	810	CLA	CBA-CGA-O2A-C1
12	A	812	CLA	CBA-CGA-O2A-C1
12	A	818	CLA	CBA-CGA-O2A-C1
12	A	829	CLA	CBA-CGA-O2A-C1
12	A	840	CLA	CBA-CGA-O2A-C1
12	B	826	CLA	CBA-CGA-O2A-C1
12	B	837	CLA	CBA-CGA-O2A-C1
12	F	201	CLA	CBA-CGA-O2A-C1
12	L	204	CLA	CBA-CGA-O2A-C1
18	B	846	LMG	C41-C42-C43-C44
18	B	846	LMG	C23-C24-C25-C26
15	R	102	BCR	C15-C16-C17-C18
15	i	101	BCR	C9-C10-C11-C12
15	j	103	BCR	C15-C16-C17-C18
15	A	844	BCR	C19-C20-C21-C22
15	I	101	BCR	C9-C10-C11-C12
17	T	101	45D	C25-C29-C31-C33
17	T	101	45D	C35-C37-C41-C42
17	M	101	45D	C25-C29-C31-C33
12	G	804	CLA	O1A-CGA-O2A-C1
12	G	825	CLA	O1A-CGA-O2A-C1
12	H	808	CLA	O1A-CGA-O2A-C1
12	a	803	CLA	O1A-CGA-O2A-C1
12	a	804	CLA	O1A-CGA-O2A-C1
12	a	817	CLA	O1A-CGA-O2A-C1
12	a	824	CLA	O1A-CGA-O2A-C1
12	f	201	CLA	O1A-CGA-O2A-C1
12	l	202	CLA	O1A-CGA-O2A-C1
12	A	803	CLA	O1A-CGA-O2A-C1
12	A	804	CLA	O1A-CGA-O2A-C1
12	A	818	CLA	O1A-CGA-O2A-C1
12	A	831	CLA	O1A-CGA-O2A-C1
12	B	821	CLA	O1A-CGA-O2A-C1
12	F	201	CLA	O1A-CGA-O2A-C1
12	L	202	CLA	O1A-CGA-O2A-C1
12	B	835	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	b	845	LMG	C23-C24-C25-C26
18	b	845	LMG	C41-C42-C43-C44
18	H	847	LMG	C23-C24-C25-C26
18	H	847	LMG	C35-C36-C37-C38
18	H	847	LMG	C41-C42-C43-C44
18	b	845	LMG	C35-C36-C37-C38
18	B	846	LMG	C35-C36-C37-C38
19	b	846	LMT	O5B-C5B-C6B-O6B
12	G	814	CLA	O1D-CGD-O2D-CED
12	G	828	CLA	O1D-CGD-O2D-CED
12	a	827	CLA	O1D-CGD-O2D-CED
12	a	840	CLA	O1D-CGD-O2D-CED
12	B	817	CLA	O1D-CGD-O2D-CED
12	H	837	CLA	C3-C5-C6-C7
12	b	804	CLA	C3-C5-C6-C7
12	b	829	CLA	C3-C5-C6-C7
12	b	835	CLA	C3-C5-C6-C7
12	B	801	CLA	C3-C5-C6-C7
12	B	804	CLA	C3-C5-C6-C7
12	F	201	CLA	C3-C5-C6-C7
12	a	803	CLA	CBD-CGD-O2D-CED
12	A	826	CLA	CBD-CGD-O2D-CED
12	B	805	CLA	CBD-CGD-O2D-CED
12	B	813	CLA	CBD-CGD-O2D-CED
16	G	851	LHG	O2-C2-C3-O3
16	a	850	LHG	O2-C2-C3-O3
16	A	850	LHG	O2-C2-C3-O3
12	G	819	CLA	O1D-CGD-O2D-CED
12	G	833	CLA	O1D-CGD-O2D-CED
12	H	808	CLA	O1D-CGD-O2D-CED
12	H	829	CLA	O1D-CGD-O2D-CED
12	a	817	CLA	O1D-CGD-O2D-CED
12	a	821	CLA	O1D-CGD-O2D-CED
12	b	818	CLA	O1D-CGD-O2D-CED
12	b	828	CLA	O1D-CGD-O2D-CED
12	G	804	CLA	CBA-CGA-O2A-C1
12	G	821	CLA	CBA-CGA-O2A-C1
12	G	828	CLA	CBA-CGA-O2A-C1
12	G	831	CLA	CBA-CGA-O2A-C1
12	G	834	CLA	CBA-CGA-O2A-C1
12	G	856	CLA	CBA-CGA-O2A-C1
12	H	812	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	808	CLA	CBA-CGA-O2A-C1
12	a	827	CLA	CBA-CGA-O2A-C1
12	a	829	CLA	CBA-CGA-O2A-C1
12	a	830	CLA	CBA-CGA-O2A-C1
12	b	811	CLA	CBA-CGA-O2A-C1
12	A	820	CLA	CBA-CGA-O2A-C1
12	A	830	CLA	CBA-CGA-O2A-C1
12	A	831	CLA	CBA-CGA-O2A-C1
12	A	834	CLA	CBA-CGA-O2A-C1
12	B	811	CLA	CBA-CGA-O2A-C1
12	B	821	CLA	CBA-CGA-O2A-C1
12	L	202	CLA	CBA-CGA-O2A-C1
12	G	805	CLA	O1A-CGA-O2A-C1
12	G	830	CLA	O1A-CGA-O2A-C1
12	H	801	CLA	O1A-CGA-O2A-C1
12	P	201	CLA	O1A-CGA-O2A-C1
12	A	812	CLA	O1A-CGA-O2A-C1
12	A	824	CLA	O1A-CGA-O2A-C1
12	H	811	CLA	O1D-CGD-O2D-CED
12	A	812	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	O1D-CGD-O2D-CED
12	a	855	CLA	CBD-CGD-O2D-CED
12	B	825	CLA	CBD-CGD-O2D-CED
12	b	834	CLA	O1D-CGD-O2D-CED
12	A	802	CLA	O1D-CGD-O2D-CED
12	A	821	CLA	O1D-CGD-O2D-CED
12	G	821	CLA	O1A-CGA-O2A-C1
12	a	830	CLA	O1A-CGA-O2A-C1
12	G	813	CLA	O1D-CGD-O2D-CED
12	G	831	CLA	O1D-CGD-O2D-CED
12	B	826	CLA	O1D-CGD-O2D-CED
12	G	855	CLA	C3-C5-C6-C7
12	a	854	CLA	C3-C5-C6-C7
12	b	801	CLA	C3-C5-C6-C7
12	B	829	CLA	C3-C5-C6-C7
12	a	831	CLA	CBD-CGD-O2D-CED
12	A	804	CLA	CBD-CGD-O2D-CED
12	B	831	CLA	CBD-CGD-O2D-CED
12	G	822	CLA	O1D-CGD-O2D-CED
12	G	824	CLA	O1D-CGD-O2D-CED
12	a	819	CLA	O1D-CGD-O2D-CED
12	a	833	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	817	CLA	O1D-CGD-O2D-CED
12	b	833	CLA	O1D-CGD-O2D-CED
12	A	833	CLA	O1D-CGD-O2D-CED
12	H	801	CLA	CBA-CGA-O2A-C1
12	a	803	CLA	CBA-CGA-O2A-C1
12	a	820	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	CBA-CGA-O2A-C1
12	A	817	CLA	CBA-CGA-O2A-C1
12	S	202	CLA	C4-C3-C5-C6
12	a	804	CLA	C4-C3-C5-C6
12	l	204	CLA	C4-C3-C5-C6
12	L	204	CLA	C4-C3-C5-C6
13	H	840	1L3	C22-C21-C23-C24
13	b	838	1L3	C22-C21-C23-C24
13	B	839	1L3	C22-C21-C23-C24
12	G	834	CLA	C2-C3-C5-C6
12	G	855	CLA	C2-C3-C5-C6
12	S	202	CLA	C2-C3-C5-C6
12	l	204	CLA	C2-C3-C5-C6
12	F	201	CLA	C2-C3-C5-C6
12	L	204	CLA	C2-C3-C5-C6
13	H	840	1L3	C20-C21-C23-C24
13	b	838	1L3	C20-C21-C23-C24
13	B	839	1L3	C20-C21-C23-C24
12	G	813	CLA	O1A-CGA-O2A-C1
12	G	819	CLA	O1A-CGA-O2A-C1
12	H	812	CLA	O1A-CGA-O2A-C1
12	H	816	CLA	O1A-CGA-O2A-C1
12	a	808	CLA	O1A-CGA-O2A-C1
12	a	812	CLA	O1A-CGA-O2A-C1
12	a	834	CLA	O1A-CGA-O2A-C1
12	b	815	CLA	O1A-CGA-O2A-C1
12	A	820	CLA	O1A-CGA-O2A-C1
12	B	815	CLA	O1A-CGA-O2A-C1
12	G	804	CLA	O1D-CGD-O2D-CED
13	G	843	1L3	C21-C23-C24-C25
13	G	843	1L3	C26-C28-C29-C30
13	a	842	1L3	C21-C23-C24-C25
13	a	842	1L3	C26-C28-C29-C30
13	A	842	1L3	C21-C23-C24-C25
13	A	842	1L3	C26-C28-C29-C30
13	B	839	1L3	C26-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
13	B	839	1L3	C16-C18-C19-C20
19	H	848	LMT	C4B-C5B-C6B-O6B
12	H	801	CLA	CBD-CGD-O2D-CED
12	H	815	CLA	CBD-CGD-O2D-CED
12	G	831	CLA	C2A-CAA-CBA-CGA
12	A	830	CLA	C2A-CAA-CBA-CGA
12	G	803	CLA	O1D-CGD-O2D-CED
12	B	804	CLA	O1D-CGD-O2D-CED
12	G	809	CLA	O1A-CGA-O2A-C1
12	G	828	CLA	O1A-CGA-O2A-C1
12	G	834	CLA	O1A-CGA-O2A-C1
12	G	856	CLA	O1A-CGA-O2A-C1
12	a	818	CLA	O1A-CGA-O2A-C1
12	a	827	CLA	O1A-CGA-O2A-C1
12	a	829	CLA	O1A-CGA-O2A-C1
12	A	829	CLA	O1A-CGA-O2A-C1
12	A	830	CLA	O1A-CGA-O2A-C1
12	A	834	CLA	O1A-CGA-O2A-C1
12	B	811	CLA	O1A-CGA-O2A-C1
12	G	808	CLA	CBA-CGA-O2A-C1
12	G	818	CLA	CBA-CGA-O2A-C1
12	b	832	CLA	CBA-CGA-O2A-C1
12	A	827	CLA	CBA-CGA-O2A-C1
12	B	833	CLA	CBA-CGA-O2A-C1
12	G	805	CLA	CBD-CGD-O2D-CED
12	H	816	CLA	CBD-CGD-O2D-CED
12	H	832	CLA	CBD-CGD-O2D-CED
12	S	204	CLA	CBD-CGD-O2D-CED
12	a	804	CLA	CBD-CGD-O2D-CED
12	b	814	CLA	CBD-CGD-O2D-CED
12	b	822	CLA	CBD-CGD-O2D-CED
12	b	830	CLA	CBD-CGD-O2D-CED
12	A	803	CLA	CBD-CGD-O2D-CED
12	A	831	CLA	CBD-CGD-O2D-CED
12	A	855	CLA	CBD-CGD-O2D-CED
12	B	809	CLA	CBD-CGD-O2D-CED
12	B	814	CLA	CBD-CGD-O2D-CED
12	B	827	CLA	CBD-CGD-O2D-CED
12	G	856	CLA	O1D-CGD-O2D-CED
12	b	811	CLA	O1A-CGA-O2A-C1
12	A	817	CLA	O1A-CGA-O2A-C1
12	B	818	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	G	825	CLA	C15-C16-C17-C18
17	m	101	45D	C25-C29-C31-C33
12	G	818	CLA	O1A-CGA-O2A-C1
12	G	831	CLA	O1A-CGA-O2A-C1
12	a	820	CLA	O1A-CGA-O2A-C1
12	A	827	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	C1-C2-C3-O3
16	A	853	LHG	C1-C2-C3-O3
12	G	808	CLA	O1D-CGD-O2D-CED
12	H	803	CLA	CBA-CGA-O2A-C1
12	H	825	CLA	CBA-CGA-O2A-C1
12	H	834	CLA	CBA-CGA-O2A-C1
12	H	837	CLA	CBA-CGA-O2A-C1
12	S	204	CLA	CBA-CGA-O2A-C1
12	a	807	CLA	CBA-CGA-O2A-C1
12	a	816	CLA	CBA-CGA-O2A-C1
12	a	855	CLA	CBA-CGA-O2A-C1
12	b	803	CLA	CBA-CGA-O2A-C1
12	b	835	CLA	CBA-CGA-O2A-C1
12	b	848	CLA	CBA-CGA-O2A-C1
12	l	206	CLA	CBA-CGA-O2A-C1
12	A	807	CLA	CBA-CGA-O2A-C1
12	A	808	CLA	CBA-CGA-O2A-C1
12	A	823	CLA	CBA-CGA-O2A-C1
12	A	855	CLA	CBA-CGA-O2A-C1
12	B	803	CLA	CBA-CGA-O2A-C1
12	B	805	CLA	CBA-CGA-O2A-C1
12	B	836	CLA	CBA-CGA-O2A-C1
12	B	838	CLA	CBA-CGA-O2A-C1
12	L	206	CLA	CBA-CGA-O2A-C1
12	B	808	CLA	CBD-CGD-O2D-CED
12	H	809	CLA	O1D-CGD-O2D-CED
12	H	825	CLA	O1D-CGD-O2D-CED
12	H	827	CLA	O1D-CGD-O2D-CED
12	H	836	CLA	O1D-CGD-O2D-CED
12	A	819	CLA	O1D-CGD-O2D-CED
12	A	841	CLA	O1D-CGD-O2D-CED
12	B	810	CLA	O1D-CGD-O2D-CED
12	A	854	CLA	C4-C3-C5-C6
12	a	804	CLA	C2-C3-C5-C6
12	a	854	CLA	C2-C3-C5-C6
12	A	831	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	854	CLA	C2-C3-C5-C6
12	H	811	CLA	C11-C12-C13-C14
12	H	817	CLA	C6-C7-C8-C9
12	a	805	CLA	C14-C13-C15-C16
12	b	810	CLA	C11-C12-C13-C14
12	b	816	CLA	C6-C7-C8-C9
12	A	805	CLA	C14-C13-C15-C16
12	B	810	CLA	C11-C12-C13-C14
12	B	824	CLA	C14-C13-C15-C16
19	b	846	LMT	C4B-C5B-C6B-O6B
12	G	820	CLA	O1D-CGD-O2D-CED
12	H	813	CLA	O1D-CGD-O2D-CED
12	H	818	CLA	O1D-CGD-O2D-CED
12	a	802	CLA	O1D-CGD-O2D-CED
12	a	841	CLA	O1D-CGD-O2D-CED
12	b	810	CLA	O1D-CGD-O2D-CED
12	b	826	CLA	O1D-CGD-O2D-CED
12	A	807	CLA	O1D-CGD-O2D-CED
12	B	828	CLA	O1D-CGD-O2D-CED
16	G	854	LHG	C7-C8-C9-C10
16	A	853	LHG	C7-C8-C9-C10
12	A	808	CLA	O1A-CGA-O2A-C1
12	H	806	CLA	O1D-CGD-O2D-CED
12	a	807	CLA	O1D-CGD-O2D-CED
12	j	102	CLA	O1D-CGD-O2D-CED
15	G	845	BCR	C7-C8-C9-C34
15	G	849	BCR	C7-C8-C9-C34
15	G	849	BCR	C36-C18-C19-C20
15	G	850	BCR	C7-C8-C9-C34
15	G	853	BCR	C36-C18-C19-C20
15	H	841	BCR	C7-C8-C9-C34
15	H	842	BCR	C36-C18-C19-C20
15	H	842	BCR	C37-C22-C23-C24
15	H	843	BCR	C37-C22-C23-C24
15	P	202	BCR	C7-C8-C9-C34
15	Q	102	BCR	C7-C8-C9-C34
15	Q	102	BCR	C37-C22-C23-C24
15	R	102	BCR	C7-C8-C9-C34
15	R	102	BCR	C36-C18-C19-C20
15	S	201	BCR	C7-C8-C9-C34
15	S	205	BCR	C11-C12-C13-C35
15	a	845	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	a	848	BCR	C7-C8-C9-C34
15	a	848	BCR	C36-C18-C19-C20
15	a	849	BCR	C7-C8-C9-C34
15	b	840	BCR	C11-C12-C13-C35
15	b	840	BCR	C36-C18-C19-C20
15	b	840	BCR	C37-C22-C23-C24
15	b	841	BCR	C37-C22-C23-C24
15	b	842	BCR	C37-C22-C23-C24
15	i	102	BCR	C7-C8-C9-C34
15	i	102	BCR	C37-C22-C23-C24
15	j	103	BCR	C36-C18-C19-C20
15	l	203	BCR	C7-C8-C9-C34
15	A	845	BCR	C7-C8-C9-C34
15	A	848	BCR	C7-C8-C9-C34
15	A	848	BCR	C36-C18-C19-C20
15	A	849	BCR	C7-C8-C9-C34
15	A	849	BCR	C11-C12-C13-C35
15	A	852	BCR	C36-C18-C19-C20
15	B	840	BCR	C7-C8-C9-C34
15	B	841	BCR	C36-C18-C19-C20
15	B	841	BCR	C37-C22-C23-C24
15	B	842	BCR	C37-C22-C23-C24
15	B	843	BCR	C37-C22-C23-C24
15	F	202	BCR	C11-C12-C13-C35
15	J	102	BCR	C7-C8-C9-C34
15	J	102	BCR	C36-C18-C19-C20
15	J	104	BCR	C7-C8-C9-C34
15	L	201	BCR	C11-C12-C13-C35
15	L	203	BCR	C7-C8-C9-C34
15	L	207	BCR	C37-C22-C23-C24
17	T	101	45D	C31-C33-C35-C39
17	m	101	45D	C31-C33-C35-C39
17	M	101	45D	C31-C33-C35-C39
15	G	845	BCR	C7-C8-C9-C10
15	H	841	BCR	C7-C8-C9-C10
15	P	202	BCR	C7-C8-C9-C10
15	Q	102	BCR	C21-C22-C23-C24
15	R	102	BCR	C7-C8-C9-C10
15	a	844	BCR	C7-C8-C9-C10
15	i	102	BCR	C21-C22-C23-C24
15	j	103	BCR	C7-C8-C9-C10
15	A	844	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	B	840	BCR	C7-C8-C9-C10
15	F	202	BCR	C7-C8-C9-C10
15	J	102	BCR	C7-C8-C9-C10
15	L	207	BCR	C21-C22-C23-C24
17	m	101	45D	C31-C33-C35-C37
17	M	101	45D	C31-C33-C35-C37
12	G	824	CLA	C2A-CAA-CBA-CGA
12	b	814	CLA	C2A-CAA-CBA-CGA
18	B	846	LMG	C28-C29-C30-C31
12	b	823	CLA	O1D-CGD-O2D-CED
12	H	803	CLA	O1A-CGA-O2A-C1
12	H	837	CLA	O1A-CGA-O2A-C1
12	a	807	CLA	O1A-CGA-O2A-C1
12	a	855	CLA	O1A-CGA-O2A-C1
12	l	206	CLA	O1A-CGA-O2A-C1
12	A	807	CLA	O1A-CGA-O2A-C1
12	A	855	CLA	O1A-CGA-O2A-C1
12	B	836	CLA	O1A-CGA-O2A-C1
12	H	824	CLA	O1D-CGD-O2D-CED
12	a	823	CLA	CBA-CGA-O2A-C1
12	b	805	CLA	CBA-CGA-O2A-C1
12	b	829	CLA	CBA-CGA-O2A-C1
12	B	816	CLA	CBA-CGA-O2A-C1
12	B	824	CLA	CBA-CGA-O2A-C1
16	A	853	LHG	C24-C23-O8-C6
12	H	804	CLA	C13-C15-C16-C17
12	b	804	CLA	C10-C11-C12-C13
12	A	824	CLA	C15-C16-C17-C18
12	B	837	CLA	C5-C6-C7-C8
12	G	802	CLA	C2-C1-O2A-CGA
12	G	804	CLA	C2-C1-O2A-CGA
12	H	804	CLA	C2-C1-O2A-CGA
12	H	830	CLA	C2-C1-O2A-CGA
12	H	850	CLA	C2-C1-O2A-CGA
12	a	803	CLA	C2-C1-O2A-CGA
12	a	817	CLA	C2-C1-O2A-CGA
12	b	804	CLA	C2-C1-O2A-CGA
12	b	821	CLA	C2-C1-O2A-CGA
12	b	829	CLA	C2-C1-O2A-CGA
12	b	848	CLA	C2-C1-O2A-CGA
12	A	803	CLA	C2-C1-O2A-CGA
12	B	803	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	B	804	CLA	C2-C1-O2A-CGA
12	B	821	CLA	C2-C1-O2A-CGA
12	B	829	CLA	C2-C1-O2A-CGA
12	a	830	CLA	O1D-CGD-O2D-CED
12	b	812	CLA	O1D-CGD-O2D-CED
12	B	806	CLA	O1D-CGD-O2D-CED
12	B	812	CLA	O1D-CGD-O2D-CED
12	B	823	CLA	O1D-CGD-O2D-CED
12	H	823	CLA	CBD-CGD-O2D-CED
12	H	802	CLA	C8-C10-C11-C12
12	H	803	CLA	C13-C15-C16-C17
12	H	804	CLA	C5-C6-C7-C8
12	H	804	CLA	C10-C11-C12-C13
12	H	817	CLA	C10-C11-C12-C13
12	H	827	CLA	C8-C10-C11-C12
12	H	831	CLA	C13-C15-C16-C17
12	a	803	CLA	C5-C6-C7-C8
12	b	804	CLA	C13-C15-C16-C17
12	j	102	CLA	C13-C15-C16-C17
12	A	803	CLA	C5-C6-C7-C8
12	B	802	CLA	C13-C15-C16-C17
12	B	816	CLA	C10-C11-C12-C13
12	B	829	CLA	C13-C15-C16-C17
12	B	830	CLA	C13-C15-C16-C17
12	b	808	CLA	O1D-CGD-O2D-CED
16	G	851	LHG	O1-C1-C2-O2
16	A	853	LHG	O1-C1-C2-O2
18	b	845	LMG	C28-C29-C30-C31
12	G	830	CLA	O1D-CGD-O2D-CED
12	G	841	CLA	O1D-CGD-O2D-CED
12	a	823	CLA	O1D-CGD-O2D-CED
12	b	835	CLA	O1A-CGA-O2A-C1
12	B	804	CLA	C13-C15-C16-C17
12	B	822	CLA	CBD-CGD-O2D-CED
19	H	848	LMT	O5'-C5'-C6'-O6'
12	G	813	CLA	C2C-C3C-CAC-CBC
12	H	823	CLA	C11-C10-C8-C7
12	b	822	CLA	C11-C10-C8-C7
12	A	820	CLA	C11-C12-C13-C15
12	G	824	CLA	CBA-CGA-O2A-C1
12	G	842	CLA	CBA-CGA-O2A-C1
12	b	813	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	b	846	LMT	O5'-C5'-C6'-O6'
12	b	832	CLA	C5-C6-C7-C8
12	A	841	CLA	C10-C11-C12-C13
12	B	804	CLA	C10-C11-C12-C13
16	a	853	LHG	C7-C8-C9-C10
15	G	853	BCR	C9-C10-C11-C12
15	A	846	BCR	C9-C10-C11-C12
17	M	101	45D	C35-C37-C41-C42
19	B	847	LMT	O5'-C5'-C6'-O6'
12	G	827	CLA	O1D-CGD-O2D-CED
12	H	834	CLA	O1D-CGD-O2D-CED
12	a	826	CLA	O1D-CGD-O2D-CED
12	a	829	CLA	O1D-CGD-O2D-CED
13	G	843	1L3	C16-C18-C19-C20
13	H	840	1L3	C26-C28-C29-C30
13	a	842	1L3	C16-C18-C19-C20
13	A	842	1L3	C16-C18-C19-C20
12	A	854	CLA	C3-C5-C6-C7
12	G	804	CLA	C5-C6-C7-C8
12	G	819	CLA	C15-C16-C17-C18
12	a	823	CLA	C5-C6-C7-C8
12	a	841	CLA	C10-C11-C12-C13
12	b	816	CLA	C10-C11-C12-C13
12	b	829	CLA	C13-C15-C16-C17
12	B	830	CLA	C8-C10-C11-C12
12	b	803	CLA	O1A-CGA-O2A-C1
12	B	805	CLA	O1A-CGA-O2A-C1
12	A	823	CLA	O1D-CGD-O2D-CED
12	G	804	CLA	C15-C16-C17-C18
12	G	825	CLA	C8-C10-C11-C12
12	G	837	CLA	C8-C10-C11-C12
12	G	841	CLA	C10-C11-C12-C13
12	H	817	CLA	C15-C16-C17-C18
12	H	831	CLA	C10-C11-C12-C13
12	H	839	CLA	C15-C16-C17-C18
12	P	201	CLA	C15-C16-C17-C18
12	a	803	CLA	C15-C16-C17-C18
12	a	805	CLA	C10-C11-C12-C13
12	a	818	CLA	C13-C15-C16-C17
12	a	818	CLA	C15-C16-C17-C18
12	a	826	CLA	C8-C10-C11-C12
12	a	826	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	a	837	CLA	C5-C6-C7-C8
12	b	836	CLA	C5-C6-C7-C8
12	A	803	CLA	C15-C16-C17-C18
12	A	818	CLA	C13-C15-C16-C17
12	A	818	CLA	C15-C16-C17-C18
12	B	806	CLA	C10-C11-C12-C13
12	B	816	CLA	C15-C16-C17-C18
12	B	821	CLA	C5-C6-C7-C8
12	B	833	CLA	C8-C10-C11-C12
12	F	201	CLA	C15-C16-C17-C18
16	a	853	LHG	C5-C4-O6-P
12	G	802	CLA	C2A-CAA-CBA-CGA
12	G	804	CLA	C2A-CAA-CBA-CGA
12	G	821	CLA	C2A-CAA-CBA-CGA
12	G	829	CLA	C2A-CAA-CBA-CGA
12	H	813	CLA	C2A-CAA-CBA-CGA
12	H	825	CLA	C2A-CAA-CBA-CGA
12	H	837	CLA	C2A-CAA-CBA-CGA
12	H	839	CLA	C2A-CAA-CBA-CGA
12	a	803	CLA	C2A-CAA-CBA-CGA
12	a	817	CLA	C2A-CAA-CBA-CGA
12	a	820	CLA	C2A-CAA-CBA-CGA
12	a	823	CLA	C2A-CAA-CBA-CGA
12	a	841	CLA	C2A-CAA-CBA-CGA
12	b	801	CLA	C2A-CAA-CBA-CGA
12	b	812	CLA	C2A-CAA-CBA-CGA
12	A	803	CLA	C2A-CAA-CBA-CGA
12	A	808	CLA	C2A-CAA-CBA-CGA
12	A	820	CLA	C2A-CAA-CBA-CGA
12	A	823	CLA	C2A-CAA-CBA-CGA
12	A	828	CLA	C2A-CAA-CBA-CGA
12	B	801	CLA	C2A-CAA-CBA-CGA
12	B	812	CLA	C2A-CAA-CBA-CGA
15	H	846	BCR	C18-C19-C20-C21
15	a	849	BCR	C10-C11-C12-C13
15	a	852	BCR	C10-C11-C12-C13
15	b	844	BCR	C18-C19-C20-C21
15	B	845	BCR	C18-C19-C20-C21
12	G	807	CLA	C15-C16-C17-C18
12	G	819	CLA	C13-C15-C16-C17
12	G	827	CLA	C10-C11-C12-C13
12	G	837	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	H	802	CLA	C13-C15-C16-C17
12	H	822	CLA	C5-C6-C7-C8
12	H	824	CLA	C10-C11-C12-C13
12	H	834	CLA	C10-C11-C12-C13
12	H	850	CLA	C8-C10-C11-C12
12	P	201	CLA	C10-C11-C12-C13
12	a	805	CLA	C5-C6-C7-C8
12	a	820	CLA	C10-C11-C12-C13
12	b	821	CLA	C5-C6-C7-C8
12	b	821	CLA	C15-C16-C17-C18
12	j	102	CLA	C8-C10-C11-C12
12	A	805	CLA	C5-C6-C7-C8
12	A	806	CLA	C15-C16-C17-C18
12	A	807	CLA	C10-C11-C12-C13
12	A	818	CLA	C8-C10-C11-C12
12	A	823	CLA	C5-C6-C7-C8
12	A	834	CLA	C15-C16-C17-C18
12	B	803	CLA	C13-C15-C16-C17
12	B	829	CLA	C10-C11-C12-C13
12	B	830	CLA	C10-C11-C12-C13
12	B	838	CLA	C15-C16-C17-C18
16	A	850	LHG	C23-C24-C25-C26
18	H	847	LMG	C28-C29-C30-C31
12	B	813	CLA	O1D-CGD-O2D-CED
12	B	830	CLA	O1D-CGD-O2D-CED
12	H	834	CLA	O1A-CGA-O2A-C1
12	a	816	CLA	O1A-CGA-O2A-C1
12	B	803	CLA	O1A-CGA-O2A-C1
12	B	838	CLA	O1A-CGA-O2A-C1
12	H	839	CLA	C3-C5-C6-C7
12	j	102	CLA	C3-C5-C6-C7
16	a	850	LHG	C11-C12-C13-C14
12	H	831	CLA	O1D-CGD-O2D-CED
12	G	806	CLA	C5-C6-C7-C8
12	G	827	CLA	C8-C10-C11-C12
12	G	834	CLA	C15-C16-C17-C18
12	H	803	CLA	C5-C6-C7-C8
12	H	806	CLA	C13-C15-C16-C17
12	H	808	CLA	C10-C11-C12-C13
12	H	834	CLA	C8-C10-C11-C12
12	H	838	CLA	C5-C6-C7-C8
12	a	834	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	a	837	CLA	C8-C10-C11-C12
12	a	841	CLA	C13-C15-C16-C17
12	b	802	CLA	C15-C16-C17-C18
12	b	804	CLA	C5-C6-C7-C8
12	b	816	CLA	C15-C16-C17-C18
12	b	823	CLA	C10-C11-C12-C13
12	b	826	CLA	C13-C15-C16-C17
12	b	829	CLA	C10-C11-C12-C13
12	b	829	CLA	C15-C16-C17-C18
12	b	832	CLA	C10-C11-C12-C13
12	b	848	CLA	C8-C10-C11-C12
12	f	201	CLA	C10-C11-C12-C13
12	f	201	CLA	C15-C16-C17-C18
12	j	102	CLA	C10-C11-C12-C13
12	l	202	CLA	C10-C11-C12-C13
12	A	837	CLA	C8-C10-C11-C12
12	A	837	CLA	C13-C15-C16-C17
12	A	855	CLA	C10-C11-C12-C13
12	B	804	CLA	C5-C6-C7-C8
12	B	829	CLA	C15-C16-C17-C18
12	F	201	CLA	C10-C11-C12-C13
12	L	202	CLA	C10-C11-C12-C13
16	G	854	LHG	O2-C2-C3-O3
16	a	853	LHG	O2-C2-C3-O3
16	A	853	LHG	O2-C2-C3-O3
12	H	839	CLA	CBA-CGA-O2A-C1
12	H	850	CLA	CBA-CGA-O2A-C1
12	G	808	CLA	O1A-CGA-O2A-C1
12	H	825	CLA	O1A-CGA-O2A-C1
12	S	204	CLA	O1A-CGA-O2A-C1
12	b	832	CLA	O1A-CGA-O2A-C1
12	B	833	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	C23-C24-C25-C26
12	G	841	CLA	C13-C15-C16-C17
12	H	831	CLA	C8-C10-C11-C12
12	b	806	CLA	C10-C11-C12-C13
12	b	832	CLA	C8-C10-C11-C12
12	A	841	CLA	C13-C15-C16-C17
19	H	848	LMT	O1'-C1-C2-C3
19	B	847	LMT	O1'-C1-C2-C3
11	G	801	CL0	C3-C5-C6-C7
12	H	816	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	a	831	CLA	O1D-CGD-O2D-CED
12	b	806	CLA	O1D-CGD-O2D-CED
12	A	829	CLA	O1D-CGD-O2D-CED
12	B	805	CLA	O1D-CGD-O2D-CED
12	B	825	CLA	O1D-CGD-O2D-CED
12	G	808	CLA	C10-C11-C12-C13
12	G	819	CLA	C8-C10-C11-C12
12	H	822	CLA	C15-C16-C17-C18
12	H	830	CLA	C10-C11-C12-C13
12	a	806	CLA	C15-C16-C17-C18
12	A	805	CLA	C10-C11-C12-C13
12	B	826	CLA	C8-C10-C11-C12
12	A	823	CLA	O1A-CGA-O2A-C1
16	G	851	LHG	C11-C12-C13-C14
12	a	803	CLA	O1D-CGD-O2D-CED
19	B	847	LMT	O5B-C5B-C6B-O6B
12	G	806	CLA	C10-C11-C12-C13
12	G	837	CLA	C13-C15-C16-C17
12	G	856	CLA	C10-C11-C12-C13
12	H	830	CLA	C8-C10-C11-C12
12	H	830	CLA	C13-C15-C16-C17
12	H	837	CLA	C13-C15-C16-C17
12	H	839	CLA	C13-C15-C16-C17
12	H	850	CLA	C5-C6-C7-C8
12	a	818	CLA	C8-C10-C11-C12
12	a	839	CLA	C8-C10-C11-C12
12	b	806	CLA	C13-C15-C16-C17
12	b	835	CLA	C13-C15-C16-C17
12	b	848	CLA	C5-C6-C7-C8
12	A	826	CLA	C8-C10-C11-C12
12	A	837	CLA	C5-C6-C7-C8
12	B	821	CLA	C15-C16-C17-C18
12	B	826	CLA	C5-C6-C7-C8
12	B	833	CLA	C10-C11-C12-C13
12	B	836	CLA	C13-C15-C16-C17
12	b	816	CLA	CBA-CGA-O2A-C1
12	b	824	CLA	CBA-CGA-O2A-C1
12	B	829	CLA	CBA-CGA-O2A-C1
12	a	805	CLA	CBD-CGD-O2D-CED
12	b	813	CLA	CBD-CGD-O2D-CED
12	a	823	CLA	O1A-CGA-O2A-C1
12	b	848	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	L	206	CLA	O1A-CGA-O2A-C1
12	G	839	CLA	C8-C10-C11-C12
12	H	806	CLA	C10-C11-C12-C13
12	B	824	CLA	C10-C11-C12-C13
12	A	828	CLA	C3-C5-C6-C7
15	a	844	BCR	C13-C14-C15-C16
12	H	827	CLA	C13-C15-C16-C17
12	l	202	CLA	C5-C6-C7-C8
12	A	826	CLA	C10-C11-C12-C13
12	B	806	CLA	C13-C15-C16-C17
16	a	850	LHG	C23-C24-C25-C26
16	G	854	LHG	C1-C2-C3-O3
12	G	809	CLA	C2A-CAA-CBA-CGA
12	G	812	CLA	C2A-CAA-CBA-CGA
12	G	813	CLA	C2A-CAA-CBA-CGA
12	G	815	CLA	C2A-CAA-CBA-CGA
12	G	841	CLA	C2A-CAA-CBA-CGA
12	H	823	CLA	C2A-CAA-CBA-CGA
12	H	826	CLA	C2A-CAA-CBA-CGA
12	S	203	CLA	C2A-CAA-CBA-CGA
12	a	808	CLA	C2A-CAA-CBA-CGA
12	a	812	CLA	C2A-CAA-CBA-CGA
12	a	814	CLA	C2A-CAA-CBA-CGA
12	b	809	CLA	C2A-CAA-CBA-CGA
12	b	822	CLA	C2A-CAA-CBA-CGA
12	b	837	CLA	C2A-CAA-CBA-CGA
12	A	812	CLA	C2A-CAA-CBA-CGA
12	A	814	CLA	C2A-CAA-CBA-CGA
12	A	841	CLA	C2A-CAA-CBA-CGA
12	B	838	CLA	C2A-CAA-CBA-CGA
12	L	205	CLA	C2A-CAA-CBA-CGA
12	H	817	CLA	CBA-CGA-O2A-C1
12	H	830	CLA	CBA-CGA-O2A-C1
12	l	205	CLA	CBA-CGA-O2A-C1
12	B	810	CLA	CBA-CGA-O2A-C1
16	G	854	LHG	C24-C23-O8-C6
12	H	808	CLA	C5-C6-C7-C8
12	H	830	CLA	C15-C16-C17-C18
12	a	854	CLA	C10-C11-C12-C13
12	b	803	CLA	C13-C15-C16-C17
12	b	829	CLA	C8-C10-C11-C12
12	b	835	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	b	837	CLA	C15-C16-C17-C18
12	A	832	CLA	C5-C6-C7-C8
12	A	837	CLA	C15-C16-C17-C18
12	A	839	CLA	C8-C10-C11-C12
12	A	841	CLA	C5-C6-C7-C8
12	B	802	CLA	C8-C10-C11-C12
12	B	823	CLA	C10-C11-C12-C13
12	B	836	CLA	C10-C11-C12-C13
12	B	838	CLA	C8-C10-C11-C12
12	H	803	CLA	CBD-CGD-O2D-CED
12	l	206	CLA	CBD-CGD-O2D-CED
19	b	846	LMT	O1'-C1-C2-C3
12	B	816	CLA	O1A-CGA-O2A-C1
12	H	801	CLA	O1D-CGD-O2D-CED
12	G	807	CLA	C10-C11-C12-C13
12	H	811	CLA	C8-C10-C11-C12
12	H	825	CLA	C13-C15-C16-C17
12	a	824	CLA	C8-C10-C11-C12
12	b	802	CLA	C8-C10-C11-C12
12	b	802	CLA	C13-C15-C16-C17
12	b	803	CLA	C5-C6-C7-C8
12	A	806	CLA	C10-C11-C12-C13
12	A	824	CLA	C8-C10-C11-C12
12	B	824	CLA	C13-C15-C16-C17
12	H	811	CLA	C10-C11-C12-C13
12	H	827	CLA	C5-C6-C7-C8
12	S	203	CLA	C13-C15-C16-C17
12	a	806	CLA	C10-C11-C12-C13
12	a	807	CLA	C10-C11-C12-C13
12	a	837	CLA	C13-C15-C16-C17
12	b	810	CLA	C10-C11-C12-C13
12	b	824	CLA	C10-C11-C12-C13
12	b	826	CLA	C8-C10-C11-C12
12	l	205	CLA	C13-C15-C16-C17
12	B	826	CLA	C13-C15-C16-C17
12	F	201	CLA	C5-C6-C7-C8
12	L	202	CLA	C5-C6-C7-C8
12	H	811	CLA	CBA-CGA-O2A-C1
12	A	826	CLA	O1D-CGD-O2D-CED
12	G	832	CLA	C5-C6-C7-C8
12	H	825	CLA	C10-C11-C12-C13
12	a	805	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	G	804	CLA	C3-C5-C6-C7
12	f	201	CLA	C3-C5-C6-C7
12	A	831	CLA	C3-C5-C6-C7
12	B	836	CLA	C3-C5-C6-C7
16	A	850	LHG	C8-C7-O7-C5
12	a	841	CLA	C5-C6-C7-C8
12	b	824	CLA	C13-C15-C16-C17
12	B	833	CLA	C5-C6-C7-C8
12	B	838	CLA	C13-C15-C16-C17
12	b	810	CLA	CBA-CGA-O2A-C1
12	H	802	CLA	C16-C17-C18-C19
12	b	804	CLA	C16-C17-C18-C20
12	A	831	CLA	C6-C7-C8-C9
12	B	805	CLA	C16-C17-C18-C20
12	G	842	CLA	O1A-CGA-O2A-C1
15	H	845	BCR	C11-C10-C9-C34
15	P	204	BCR	C11-C10-C9-C34
15	Q	102	BCR	C11-C10-C9-C34
15	f	204	BCR	C11-C10-C9-C34
15	L	207	BCR	C11-C10-C9-C34
12	b	827	CLA	O1D-CGD-O2D-CED
12	B	802	CLA	C15-C16-C17-C18
12	B	803	CLA	C5-C6-C7-C8
12	B	804	CLA	C15-C16-C17-C18
15	H	841	BCR	C37-C22-C23-C24
15	H	844	BCR	C37-C22-C23-C24
15	S	201	BCR	C36-C18-C19-C20
15	b	839	BCR	C7-C8-C9-C34
15	f	202	BCR	C7-C8-C9-C34
15	l	201	BCR	C11-C12-C13-C35
15	B	841	BCR	C11-C12-C13-C35
15	F	202	BCR	C37-C22-C23-C24
15	L	207	BCR	C7-C8-C9-C34
15	S	205	BCR	C11-C12-C13-C14
15	b	839	BCR	C7-C8-C9-C10
15	f	202	BCR	C7-C8-C9-C10
15	j	103	BCR	C17-C18-C19-C20
15	A	848	BCR	C17-C18-C19-C20
15	F	202	BCR	C11-C12-C13-C14
12	G	824	CLA	O1A-CGA-O2A-C1
12	H	850	CLA	O1A-CGA-O2A-C1
12	b	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	G	803	CLA	C2A-CAA-CBA-CGA
12	G	856	CLA	C2A-CAA-CBA-CGA
12	a	828	CLA	C2A-CAA-CBA-CGA
12	a	855	CLA	C2A-CAA-CBA-CGA
12	b	825	CLA	C2A-CAA-CBA-CGA
12	l	205	CLA	C2A-CAA-CBA-CGA
12	A	802	CLA	C2A-CAA-CBA-CGA
12	A	817	CLA	C2A-CAA-CBA-CGA
12	A	835	CLA	C2A-CAA-CBA-CGA
12	B	809	CLA	C2A-CAA-CBA-CGA
12	H	802	CLA	C15-C16-C17-C18
12	H	812	CLA	C5-C6-C7-C8
16	G	852	LHG	O1-C1-C2-C3
16	G	854	LHG	O1-C1-C2-C3
16	a	851	LHG	O1-C1-C2-C3
16	a	853	LHG	O1-C1-C2-C3
16	A	851	LHG	O1-C1-C2-C3
16	A	853	LHG	O1-C1-C2-C3
12	G	806	CLA	C16-C17-C18-C20
12	G	818	CLA	C6-C7-C8-C10
12	G	855	CLA	C16-C17-C18-C20
12	H	805	CLA	C16-C17-C18-C20
12	H	830	CLA	C16-C17-C18-C19
12	a	817	CLA	C6-C7-C8-C10
12	a	831	CLA	C6-C7-C8-C9
12	a	854	CLA	C16-C17-C18-C20
12	b	829	CLA	C16-C17-C18-C19
12	A	805	CLA	C16-C17-C18-C19
12	A	817	CLA	C6-C7-C8-C10
12	H	815	CLA	O1D-CGD-O2D-CED
12	B	831	CLA	O1D-CGD-O2D-CED
12	H	839	CLA	O1A-CGA-O2A-C1
12	b	829	CLA	O1A-CGA-O2A-C1
12	B	824	CLA	O1A-CGA-O2A-C1
12	G	802	CLA	C3-C5-C6-C7
12	H	831	CLA	C3-C5-C6-C7
12	L	205	CLA	C13-C15-C16-C17
15	H	845	BCR	C11-C10-C9-C8
15	P	204	BCR	C11-C10-C9-C8
15	Q	102	BCR	C11-C10-C9-C8
15	a	845	BCR	C11-C10-C9-C8
15	a	847	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	f	204	BCR	C11-C10-C9-C8
15	A	847	BCR	C11-C10-C9-C8
15	L	207	BCR	C11-C10-C9-C8
12	b	804	CLA	C8-C10-C11-C12
12	b	813	CLA	C2-C3-C5-C6
12	a	855	CLA	O1D-CGD-O2D-CED
12	A	804	CLA	O1D-CGD-O2D-CED
12	B	814	CLA	O1D-CGD-O2D-CED
12	A	831	CLA	O1D-CGD-O2D-CED
12	S	203	CLA	CBA-CGA-O2A-C1
12	G	855	CLA	C10-C11-C12-C13
12	H	837	CLA	C10-C11-C12-C13
12	b	825	CLA	C13-C15-C16-C17
16	A	851	LHG	C7-C8-C9-C10
12	B	830	CLA	C3-C5-C6-C7
12	G	803	CLA	C2-C1-O2A-CGA
12	G	813	CLA	C2-C1-O2A-CGA
12	G	831	CLA	C2-C1-O2A-CGA
12	G	842	CLA	C2-C1-O2A-CGA
12	H	803	CLA	C2-C1-O2A-CGA
12	H	822	CLA	C2-C1-O2A-CGA
12	a	812	CLA	C2-C1-O2A-CGA
12	a	830	CLA	C2-C1-O2A-CGA
12	A	812	CLA	C2-C1-O2A-CGA
12	A	830	CLA	C2-C1-O2A-CGA
12	H	801	CLA	C6-C7-C8-C9
12	H	804	CLA	C16-C17-C18-C20
12	a	805	CLA	C16-C17-C18-C19
12	a	831	CLA	C6-C7-C8-C10
12	a	854	CLA	C16-C17-C18-C19
12	b	829	CLA	C16-C17-C18-C20
12	A	827	CLA	C11-C12-C13-C15
12	A	831	CLA	C6-C7-C8-C10
12	A	854	CLA	C16-C17-C18-C20
12	B	804	CLA	C16-C17-C18-C20
12	B	829	CLA	C16-C17-C18-C20
12	b	816	CLA	O1A-CGA-O2A-C1
12	b	824	CLA	O1A-CGA-O2A-C1
12	B	810	CLA	O1A-CGA-O2A-C1
12	H	804	CLA	C8-C10-C11-C12
18	H	847	LMG	C34-C35-C36-C37
12	b	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	a	850	LHG	C13-C14-C15-C16
16	a	853	LHG	C11-C12-C13-C14
12	H	816	CLA	O1D-CGD-O2D-CED
12	b	814	CLA	O1D-CGD-O2D-CED
12	H	826	CLA	C8-C10-C11-C12
12	B	811	CLA	C5-C6-C7-C8
16	G	851	LHG	C12-C13-C14-C15
16	a	853	LHG	C34-C35-C36-C37
16	A	853	LHG	C9-C10-C11-C12
16	A	853	LHG	C28-C29-C30-C31
18	b	845	LMG	C34-C35-C36-C37
12	H	830	CLA	O1A-CGA-O2A-C1
12	A	803	CLA	O1D-CGD-O2D-CED
16	G	854	LHG	C9-C10-C11-C12
16	G	854	LHG	C30-C31-C32-C33
18	B	846	LMG	C34-C35-C36-C37
16	A	850	LHG	O9-C7-O7-C5
16	a	853	LHG	O1-C1-C2-O2
18	B	846	LMG	C33-C34-C35-C36
12	S	204	CLA	O1D-CGD-O2D-CED
12	H	805	CLA	C13-C15-C16-C17
11	a	801	CL0	C4B-C3B-CAB-CBB
12	G	805	CLA	C4B-C3B-CAB-CBB
12	G	813	CLA	C4B-C3B-CAB-CBB
12	G	824	CLA	C4B-C3B-CAB-CBB
12	G	831	CLA	C4B-C3B-CAB-CBB
12	G	832	CLA	C4B-C3B-CAB-CBB
12	G	833	CLA	C4B-C3B-CAB-CBB
12	G	834	CLA	C4B-C3B-CAB-CBB
12	G	837	CLA	C4B-C3B-CAB-CBB
12	H	805	CLA	C4B-C3B-CAB-CBB
12	H	818	CLA	C4B-C3B-CAB-CBB
12	H	825	CLA	C4B-C3B-CAB-CBB
12	H	831	CLA	C4B-C3B-CAB-CBB
12	H	837	CLA	C4B-C3B-CAB-CBB
12	a	812	CLA	C4B-C3B-CAB-CBB
12	a	823	CLA	C4B-C3B-CAB-CBB
12	a	832	CLA	C4B-C3B-CAB-CBB
12	a	833	CLA	C4B-C3B-CAB-CBB
12	a	834	CLA	C4B-C3B-CAB-CBB
12	a	837	CLA	C4B-C3B-CAB-CBB
12	a	854	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	b	805	CLA	C4B-C3B-CAB-CBB
12	b	817	CLA	C4B-C3B-CAB-CBB
12	b	824	CLA	C4B-C3B-CAB-CBB
12	b	830	CLA	C4B-C3B-CAB-CBB
12	f	203	CLA	C4B-C3B-CAB-CBB
12	j	102	CLA	C4B-C3B-CAB-CBB
12	A	812	CLA	C4B-C3B-CAB-CBB
12	A	816	CLA	C4B-C3B-CAB-CBB
12	A	832	CLA	C4B-C3B-CAB-CBB
12	A	833	CLA	C4B-C3B-CAB-CBB
12	A	837	CLA	C4B-C3B-CAB-CBB
12	A	841	CLA	C4B-C3B-CAB-CBB
12	A	854	CLA	C4B-C3B-CAB-CBB
12	B	805	CLA	C4B-C3B-CAB-CBB
12	B	814	CLA	C4B-C3B-CAB-CBB
12	B	817	CLA	C4B-C3B-CAB-CBB
12	B	824	CLA	C4B-C3B-CAB-CBB
12	B	830	CLA	C4B-C3B-CAB-CBB
12	B	836	CLA	C4B-C3B-CAB-CBB
12	F	203	CLA	C4B-C3B-CAB-CBB
19	b	846	LMT	C11-C10-C9-C8
12	G	806	CLA	C16-C17-C18-C19
12	H	805	CLA	C16-C17-C18-C19
12	B	805	CLA	C16-C17-C18-C19
12	b	830	CLA	O1D-CGD-O2D-CED
12	G	818	CLA	C2A-CAA-CBA-CGA
12	G	822	CLA	C2A-CAA-CBA-CGA
12	G	828	CLA	C2A-CAA-CBA-CGA
12	A	827	CLA	C2A-CAA-CBA-CGA
12	A	855	CLA	C2A-CAA-CBA-CGA
12	G	829	CLA	C5-C6-C7-C8
12	H	826	CLA	C13-C15-C16-C17
12	b	825	CLA	C8-C10-C11-C12
12	B	810	CLA	C10-C11-C12-C13
16	G	852	LHG	C8-C7-O7-C5
16	a	851	LHG	C8-C7-O7-C5
16	G	854	LHG	C34-C35-C36-C37
12	b	822	CLA	O1D-CGD-O2D-CED
12	a	803	CLA	C6-C7-C8-C10
12	A	803	CLA	C6-C7-C8-C10
12	A	826	CLA	C11-C12-C13-C15
12	B	803	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	B	822	CLA	C11-C10-C8-C7
12	B	805	CLA	C13-C15-C16-C17
12	B	829	CLA	C8-C10-C11-C12
12	H	817	CLA	O1A-CGA-O2A-C1
12	G	803	CLA	C3A-C2A-CAA-CBA
12	G	806	CLA	C3A-C2A-CAA-CBA
12	G	807	CLA	C3A-C2A-CAA-CBA
12	G	809	CLA	C3A-C2A-CAA-CBA
12	G	825	CLA	C3A-C2A-CAA-CBA
12	G	855	CLA	C3A-C2A-CAA-CBA
12	H	808	CLA	C3A-C2A-CAA-CBA
12	H	821	CLA	C3A-C2A-CAA-CBA
12	H	822	CLA	C3A-C2A-CAA-CBA
12	H	824	CLA	C3A-C2A-CAA-CBA
12	H	834	CLA	C3A-C2A-CAA-CBA
12	P	203	CLA	C3A-C2A-CAA-CBA
12	a	802	CLA	C3A-C2A-CAA-CBA
12	a	805	CLA	C3A-C2A-CAA-CBA
12	a	806	CLA	C3A-C2A-CAA-CBA
12	a	808	CLA	C3A-C2A-CAA-CBA
12	a	824	CLA	C3A-C2A-CAA-CBA
12	a	854	CLA	C3A-C2A-CAA-CBA
12	b	807	CLA	C3A-C2A-CAA-CBA
12	b	810	CLA	C3A-C2A-CAA-CBA
12	b	820	CLA	C3A-C2A-CAA-CBA
12	b	821	CLA	C3A-C2A-CAA-CBA
12	b	832	CLA	C3A-C2A-CAA-CBA
12	f	203	CLA	C3A-C2A-CAA-CBA
12	l	202	CLA	C3A-C2A-CAA-CBA
12	A	802	CLA	C3A-C2A-CAA-CBA
12	A	805	CLA	C3A-C2A-CAA-CBA
12	A	808	CLA	C3A-C2A-CAA-CBA
12	A	819	CLA	C3A-C2A-CAA-CBA
12	A	824	CLA	C3A-C2A-CAA-CBA
12	B	820	CLA	C3A-C2A-CAA-CBA
12	B	821	CLA	C3A-C2A-CAA-CBA
12	B	823	CLA	C3A-C2A-CAA-CBA
12	F	203	CLA	C3A-C2A-CAA-CBA
12	L	202	CLA	C3A-C2A-CAA-CBA
12	H	832	CLA	O1D-CGD-O2D-CED
18	H	847	LMG	C16-C17-C18-C19
18	b	845	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	G	813	CLA	C4C-C3C-CAC-CBC
16	a	853	LHG	C26-C27-C28-C29
12	a	824	CLA	C15-C16-C17-C18
12	A	832	CLA	C10-C11-C12-C13
15	R	101	BCR	C13-C14-C15-C16
15	a	846	BCR	C9-C10-C11-C12
12	G	855	CLA	C16-C17-C18-C19
12	H	830	CLA	C16-C17-C18-C20
12	b	807	CLA	C16-C17-C18-C20
12	A	854	CLA	C16-C17-C18-C19
12	B	829	CLA	C16-C17-C18-C19
12	H	811	CLA	O1A-CGA-O2A-C1
12	B	829	CLA	O1A-CGA-O2A-C1
16	G	854	LHG	C33-C34-C35-C36
16	A	853	LHG	C34-C35-C36-C37
12	B	825	CLA	C8-C10-C11-C12
16	G	854	LHG	C10-C11-C12-C13
16	G	854	LHG	C24-C25-C26-C27
16	a	853	LHG	C10-C11-C12-C13
12	B	827	CLA	O1D-CGD-O2D-CED
12	H	804	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	CBA-CGA-O2A-C1
18	B	846	LMG	C16-C17-C18-C19
12	G	833	CLA	C3-C5-C6-C7
12	G	842	CLA	C3-C5-C6-C7
12	H	801	CLA	C3-C5-C6-C7
12	a	831	CLA	C3-C5-C6-C7
12	b	815	CLA	C3-C5-C6-C7
16	A	853	LHG	C23-C24-C25-C26
12	G	825	CLA	C13-C15-C16-C17
12	a	832	CLA	C5-C6-C7-C8
12	b	804	CLA	C15-C16-C17-C18
16	G	854	LHG	C28-C29-C30-C31
16	a	850	LHG	C11-C10-C9-C8
12	l	205	CLA	O1A-CGA-O2A-C1
16	A	853	LHG	C25-C26-C27-C28
12	G	805	CLA	O1D-CGD-O2D-CED
16	a	853	LHG	C24-C25-C26-C27
16	a	853	LHG	C28-C29-C30-C31
12	H	801	CLA	C6-C7-C8-C10
12	A	827	CLA	C11-C12-C13-C14
16	G	851	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	G	852	LHG	C7-C8-C9-C10
12	b	810	CLA	O1A-CGA-O2A-C1
12	G	808	CLA	C2B-C3B-CAB-CBB
12	G	834	CLA	C2B-C3B-CAB-CBB
12	G	837	CLA	C2B-C3B-CAB-CBB
12	G	840	CLA	C2B-C3B-CAB-CBB
12	H	805	CLA	C2B-C3B-CAB-CBB
12	H	828	CLA	C2B-C3B-CAB-CBB
12	H	831	CLA	C2B-C3B-CAB-CBB
12	H	832	CLA	C2B-C3B-CAB-CBB
12	H	837	CLA	C2B-C3B-CAB-CBB
12	a	807	CLA	C2B-C3B-CAB-CBB
12	a	834	CLA	C2B-C3B-CAB-CBB
12	a	837	CLA	C2B-C3B-CAB-CBB
12	a	840	CLA	C2B-C3B-CAB-CBB
12	b	805	CLA	C2B-C3B-CAB-CBB
12	b	827	CLA	C2B-C3B-CAB-CBB
12	b	830	CLA	C2B-C3B-CAB-CBB
12	b	835	CLA	C2B-C3B-CAB-CBB
12	f	203	CLA	C2B-C3B-CAB-CBB
12	j	104	CLA	C2B-C3B-CAB-CBB
12	A	804	CLA	C2B-C3B-CAB-CBB
12	A	811	CLA	C2B-C3B-CAB-CBB
12	A	815	CLA	C2B-C3B-CAB-CBB
12	A	830	CLA	C2B-C3B-CAB-CBB
12	A	837	CLA	C2B-C3B-CAB-CBB
12	A	840	CLA	C2B-C3B-CAB-CBB
12	A	841	CLA	C2B-C3B-CAB-CBB
12	B	805	CLA	C2B-C3B-CAB-CBB
12	B	827	CLA	C2B-C3B-CAB-CBB
12	B	831	CLA	C2B-C3B-CAB-CBB
12	B	836	CLA	C2B-C3B-CAB-CBB
12	F	203	CLA	C2B-C3B-CAB-CBB
15	G	845	BCR	C1-C6-C7-C8
15	G	845	BCR	C5-C6-C7-C8
15	G	845	BCR	C23-C24-C25-C30
15	G	846	BCR	C23-C24-C25-C30
15	G	847	BCR	C1-C6-C7-C8
15	G	847	BCR	C5-C6-C7-C8
15	G	848	BCR	C23-C24-C25-C30
15	G	849	BCR	C23-C24-C25-C30
15	G	850	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	G	850	BCR	C23-C24-C25-C30
15	G	853	BCR	C1-C6-C7-C8
15	G	853	BCR	C5-C6-C7-C8
15	H	841	BCR	C23-C24-C25-C26
15	H	841	BCR	C23-C24-C25-C30
15	Q	101	BCR	C1-C6-C7-C8
15	Q	101	BCR	C5-C6-C7-C8
15	Q	102	BCR	C23-C24-C25-C30
15	R	101	BCR	C23-C24-C25-C26
15	R	101	BCR	C23-C24-C25-C30
15	R	102	BCR	C1-C6-C7-C8
15	R	102	BCR	C5-C6-C7-C8
15	S	201	BCR	C23-C24-C25-C26
15	S	201	BCR	C23-C24-C25-C30
15	a	844	BCR	C1-C6-C7-C8
15	a	844	BCR	C5-C6-C7-C8
15	a	844	BCR	C23-C24-C25-C30
15	a	845	BCR	C23-C24-C25-C30
15	a	846	BCR	C1-C6-C7-C8
15	a	846	BCR	C5-C6-C7-C8
15	a	847	BCR	C23-C24-C25-C30
15	a	848	BCR	C23-C24-C25-C30
15	a	849	BCR	C23-C24-C25-C26
15	a	849	BCR	C23-C24-C25-C30
15	a	852	BCR	C1-C6-C7-C8
15	a	852	BCR	C5-C6-C7-C8
15	b	839	BCR	C23-C24-C25-C26
15	b	839	BCR	C23-C24-C25-C30
15	i	101	BCR	C1-C6-C7-C8
15	i	101	BCR	C5-C6-C7-C8
15	i	102	BCR	C23-C24-C25-C30
15	j	101	BCR	C23-C24-C25-C26
15	j	101	BCR	C23-C24-C25-C30
15	j	103	BCR	C1-C6-C7-C8
15	j	103	BCR	C5-C6-C7-C8
15	l	203	BCR	C23-C24-C25-C26
15	l	203	BCR	C23-C24-C25-C30
15	A	844	BCR	C23-C24-C25-C30
15	A	845	BCR	C23-C24-C25-C30
15	A	846	BCR	C1-C6-C7-C8
15	A	846	BCR	C5-C6-C7-C8
15	A	847	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
15	A	848	BCR	C23-C24-C25-C30
15	A	849	BCR	C23-C24-C25-C30
15	A	852	BCR	C1-C6-C7-C8
15	A	852	BCR	C5-C6-C7-C8
15	B	840	BCR	C23-C24-C25-C26
15	B	840	BCR	C23-C24-C25-C30
15	F	202	BCR	C1-C6-C7-C8
15	I	101	BCR	C1-C6-C7-C8
15	I	101	BCR	C5-C6-C7-C8
15	J	101	BCR	C23-C24-C25-C26
15	J	101	BCR	C23-C24-C25-C30
15	J	102	BCR	C1-C6-C7-C8
15	J	102	BCR	C5-C6-C7-C8
15	J	104	BCR	C23-C24-C25-C30
15	L	203	BCR	C23-C24-C25-C26
15	L	203	BCR	C23-C24-C25-C30
15	L	207	BCR	C23-C24-C25-C26
15	L	207	BCR	C23-C24-C25-C30
17	T	101	45D	C15-C07-C19-C23
17	m	101	45D	C15-C07-C19-C23
17	M	101	45D	C15-C07-C19-C23
12	H	839	CLA	CBD-CGD-O2D-CED
12	G	807	CLA	CBA-CGA-O2A-C1
12	B	816	CLA	C8-C10-C11-C12
16	G	854	LHG	C26-C27-C28-C29
16	A	850	LHG	C34-C35-C36-C37
16	A	853	LHG	C26-C27-C28-C29
16	a	850	LHG	C34-C35-C36-C37
12	G	840	CLA	C2A-CAA-CBA-CGA
12	H	810	CLA	C2A-CAA-CBA-CGA
12	H	822	CLA	C2A-CAA-CBA-CGA
12	a	802	CLA	C2A-CAA-CBA-CGA
12	a	811	CLA	C2A-CAA-CBA-CGA
12	a	821	CLA	C2A-CAA-CBA-CGA
12	a	827	CLA	C2A-CAA-CBA-CGA
12	a	835	CLA	C2A-CAA-CBA-CGA
12	b	813	CLA	C2A-CAA-CBA-CGA
12	b	824	CLA	C2A-CAA-CBA-CGA
12	A	811	CLA	C2A-CAA-CBA-CGA
12	A	821	CLA	C2A-CAA-CBA-CGA
12	B	822	CLA	C2A-CAA-CBA-CGA
12	B	824	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	H	804	CLA	C15-C16-C17-C18
12	H	837	CLA	C8-C10-C11-C12
12	H	804	CLA	O1A-CGA-O2A-C1
12	S	203	CLA	O1A-CGA-O2A-C1
16	G	851	LHG	C34-C35-C36-C37
16	a	850	LHG	C29-C30-C31-C32
16	A	853	LHG	C12-C13-C14-C15
16	G	852	LHG	O9-C7-O7-C5
16	a	851	LHG	O9-C7-O7-C5
12	G	805	CLA	C4-C3-C5-C6
12	l	205	CLA	C4-C3-C5-C6
12	L	205	CLA	C4-C3-C5-C6
16	a	850	LHG	C28-C29-C30-C31
15	H	849	BCR	C10-C11-C12-C13
15	b	839	BCR	C10-C11-C12-C13
15	f	204	BCR	C10-C11-C12-C13
15	A	846	BCR	C18-C19-C20-C21
15	B	840	BCR	C10-C11-C12-C13
15	J	102	BCR	C10-C11-C12-C13
12	b	811	CLA	C5-C6-C7-C8
12	G	805	CLA	C2-C3-C5-C6
12	l	205	CLA	C2-C3-C5-C6
12	L	205	CLA	C2-C3-C5-C6
16	G	851	LHG	C28-C29-C30-C31
16	A	850	LHG	C11-C12-C13-C14
12	b	837	CLA	CBA-CGA-O2A-C1
12	G	825	CLA	C6-C7-C8-C9
12	H	831	CLA	C11-C12-C13-C14
12	B	816	CLA	C6-C7-C8-C9
12	H	812	CLA	C10-C11-C12-C13
12	a	855	CLA	C10-C11-C12-C13
12	B	815	CLA	C8-C10-C11-C12
16	a	853	LHG	C16-C17-C18-C19
12	A	812	CLA	C2C-C3C-CAC-CBC
12	G	810	CLA	O1D-CGD-O2D-CED
12	B	820	CLA	CBD-CGD-O2D-CED
12	G	837	CLA	C15-C16-C17-C18
16	A	850	LHG	C28-C29-C30-C31
12	a	804	CLA	O1D-CGD-O2D-CED
12	H	817	CLA	C8-C10-C11-C12
15	P	202	BCR	C9-C10-C11-C12
15	P	204	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	F	202	BCR	C19-C20-C21-C22
12	H	804	CLA	C16-C17-C18-C19
16	a	853	LHG	C30-C31-C32-C33
16	A	851	LHG	C8-C7-O7-C5
16	A	853	LHG	C24-C25-C26-C27
12	G	829	CLA	C15-C16-C17-C18
12	H	806	CLA	C8-C10-C11-C12
16	a	853	LHG	C25-C26-C27-C28
18	b	845	LMG	C33-C34-C35-C36
12	H	816	CLA	C10-C11-C12-C13
12	A	828	CLA	C8-C10-C11-C12
12	B	811	CLA	C10-C11-C12-C13
15	P	202	BCR	C37-C22-C23-C24
15	a	846	BCR	C36-C18-C19-C20
15	f	202	BCR	C37-C22-C23-C24
16	a	851	LHG	C7-C8-C9-C10
11	a	801	CL0	C3-C5-C6-C7
12	b	814	CLA	C3-C5-C6-C7
12	b	848	CLA	C3-C5-C6-C7
12	L	205	CLA	C3-C5-C6-C7
15	G	849	BCR	C17-C18-C19-C20
15	H	842	BCR	C17-C18-C19-C20
15	S	201	BCR	C17-C18-C19-C20
15	b	840	BCR	C11-C12-C13-C14
15	i	102	BCR	C7-C8-C9-C10
15	l	201	BCR	C11-C12-C13-C14
15	A	849	BCR	C11-C12-C13-C14
15	J	102	BCR	C17-C18-C19-C20
15	J	104	BCR	C7-C8-C9-C10
16	G	854	LHG	C16-C17-C18-C19
12	B	814	CLA	C2A-CAA-CBA-CGA
12	b	804	CLA	C16-C17-C18-C19
12	b	805	CLA	C16-C17-C18-C19
12	b	805	CLA	C16-C17-C18-C20
16	A	853	LHG	C30-C31-C32-C33
12	A	820	CLA	C4-C3-C5-C6
12	G	807	CLA	O1A-CGA-O2A-C1
12	B	805	CLA	C8-C10-C11-C12
12	A	855	CLA	O1D-CGD-O2D-CED
12	A	806	CLA	O1A-CGA-O2A-C1
12	a	803	CLA	C3-C5-C6-C7
12	B	814	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	a	832	CLA	C10-C11-C12-C13
12	a	837	CLA	C15-C16-C17-C18
19	b	846	LMT	C4-C5-C6-C7
16	a	853	LHG	C33-C34-C35-C36
16	A	850	LHG	C13-C14-C15-C16
16	A	851	LHG	O9-C7-O7-C5
12	G	841	CLA	C5-C6-C7-C8
12	a	807	CLA	C15-C16-C17-C18
12	a	805	CLA	C16-C17-C18-C20
12	a	817	CLA	C6-C7-C8-C9
12	b	807	CLA	C16-C17-C18-C19
16	G	851	LHG	C13-C14-C15-C16
16	G	854	LHG	C11-C12-C13-C14
16	G	854	LHG	C29-C30-C31-C32
12	a	812	CLA	C2C-C3C-CAC-CBC
12	G	829	CLA	C8-C10-C11-C12
12	b	806	CLA	C8-C10-C11-C12
12	b	815	CLA	C10-C11-C12-C13
12	b	835	CLA	C8-C10-C11-C12
12	A	805	CLA	C13-C15-C16-C17
12	A	807	CLA	C15-C16-C17-C18
12	B	804	CLA	C8-C10-C11-C12
16	G	851	LHG	C24-C25-C26-C27
16	A	853	LHG	C10-C11-C12-C13
12	H	815	CLA	C3-C5-C6-C7
16	a	850	LHG	O7-C5-C6-O8
16	a	853	LHG	C32-C33-C34-C35
12	L	205	CLA	CBA-CGA-O2A-C1
12	H	834	CLA	C5-C6-C7-C8
12	a	828	CLA	C8-C10-C11-C12
12	A	807	CLA	C5-C6-C7-C8
18	H	847	LMG	C29-C30-C31-C32
12	a	802	CLA	C2-C1-O2A-CGA
12	A	802	CLA	C2-C1-O2A-CGA
12	H	802	CLA	C16-C17-C18-C20
12	A	805	CLA	C16-C17-C18-C20
12	B	804	CLA	C16-C17-C18-C19
12	P	201	CLA	C5-C6-C7-C8
12	a	824	CLA	C13-C15-C16-C17
16	A	850	LHG	C16-C17-C18-C19
12	b	829	CLA	C4-C3-C5-C6
12	H	850	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	A	803	CLA	C3-C5-C6-C7
12	A	820	CLA	C2-C3-C5-C6
12	a	805	CLA	C8-C10-C11-C12
16	a	853	LHG	C9-C10-C11-C12
12	G	835	CLA	C2A-CAA-CBA-CGA
12	G	855	CLA	C2A-CAA-CBA-CGA
12	H	814	CLA	C2A-CAA-CBA-CGA
12	a	840	CLA	C2A-CAA-CBA-CGA
12	A	840	CLA	C2A-CAA-CBA-CGA
12	B	813	CLA	C2A-CAA-CBA-CGA
12	B	825	CLA	C2A-CAA-CBA-CGA
12	G	810	CLA	CBD-CGD-O2D-CED
12	b	813	CLA	O1D-CGD-O2D-CED
16	G	851	LHG	C9-C10-C11-C12
11	G	801	CL0	C8-C10-C11-C12
12	G	832	CLA	C10-C11-C12-C13
16	G	854	LHG	C12-C13-C14-C15
16	A	853	LHG	C33-C34-C35-C36
16	a	850	LHG	O1-C1-C2-O2
16	A	850	LHG	O1-C1-C2-O2
12	H	805	CLA	O1A-CGA-O2A-C1
11	A	801	CL0	C3-C5-C6-C7
12	G	806	CLA	C1A-C2A-CAA-CBA
12	G	809	CLA	C1A-C2A-CAA-CBA
12	G	812	CLA	C1A-C2A-CAA-CBA
12	G	814	CLA	C1A-C2A-CAA-CBA
12	G	816	CLA	C1A-C2A-CAA-CBA
12	G	822	CLA	C1A-C2A-CAA-CBA
12	G	824	CLA	C1A-C2A-CAA-CBA
12	G	825	CLA	C1A-C2A-CAA-CBA
12	G	828	CLA	C1A-C2A-CAA-CBA
12	G	830	CLA	C1A-C2A-CAA-CBA
12	G	838	CLA	C1A-C2A-CAA-CBA
12	G	842	CLA	C1A-C2A-CAA-CBA
12	G	855	CLA	C1A-C2A-CAA-CBA
12	H	808	CLA	C1A-C2A-CAA-CBA
12	H	809	CLA	C1A-C2A-CAA-CBA
12	H	810	CLA	C1A-C2A-CAA-CBA
12	H	812	CLA	C1A-C2A-CAA-CBA
12	H	815	CLA	C1A-C2A-CAA-CBA
12	H	817	CLA	C1A-C2A-CAA-CBA
12	H	819	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	H	821	CLA	C1A-C2A-CAA-CBA
12	H	822	CLA	C1A-C2A-CAA-CBA
12	H	824	CLA	C1A-C2A-CAA-CBA
12	H	827	CLA	C1A-C2A-CAA-CBA
12	H	828	CLA	C1A-C2A-CAA-CBA
12	H	830	CLA	C1A-C2A-CAA-CBA
12	H	833	CLA	C1A-C2A-CAA-CBA
12	H	836	CLA	C1A-C2A-CAA-CBA
12	H	838	CLA	C1A-C2A-CAA-CBA
12	H	850	CLA	C1A-C2A-CAA-CBA
12	P	203	CLA	C1A-C2A-CAA-CBA
12	R	103	CLA	C1A-C2A-CAA-CBA
12	a	804	CLA	C1A-C2A-CAA-CBA
12	a	805	CLA	C1A-C2A-CAA-CBA
12	a	806	CLA	C1A-C2A-CAA-CBA
12	a	811	CLA	C1A-C2A-CAA-CBA
12	a	815	CLA	C1A-C2A-CAA-CBA
12	a	821	CLA	C1A-C2A-CAA-CBA
12	a	823	CLA	C1A-C2A-CAA-CBA
12	a	824	CLA	C1A-C2A-CAA-CBA
12	a	827	CLA	C1A-C2A-CAA-CBA
12	a	829	CLA	C1A-C2A-CAA-CBA
12	a	831	CLA	C1A-C2A-CAA-CBA
12	a	838	CLA	C1A-C2A-CAA-CBA
12	a	839	CLA	C1A-C2A-CAA-CBA
12	b	807	CLA	C1A-C2A-CAA-CBA
12	b	808	CLA	C1A-C2A-CAA-CBA
12	b	811	CLA	C1A-C2A-CAA-CBA
12	b	814	CLA	C1A-C2A-CAA-CBA
12	b	816	CLA	C1A-C2A-CAA-CBA
12	b	818	CLA	C1A-C2A-CAA-CBA
12	b	820	CLA	C1A-C2A-CAA-CBA
12	b	821	CLA	C1A-C2A-CAA-CBA
12	b	826	CLA	C1A-C2A-CAA-CBA
12	b	829	CLA	C1A-C2A-CAA-CBA
12	b	831	CLA	C1A-C2A-CAA-CBA
12	b	834	CLA	C1A-C2A-CAA-CBA
12	b	836	CLA	C1A-C2A-CAA-CBA
12	b	848	CLA	C1A-C2A-CAA-CBA
12	f	203	CLA	C1A-C2A-CAA-CBA
12	j	104	CLA	C1A-C2A-CAA-CBA
12	l	202	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	804	CLA	C1A-C2A-CAA-CBA
12	A	805	CLA	C1A-C2A-CAA-CBA
12	A	811	CLA	C1A-C2A-CAA-CBA
12	A	815	CLA	C1A-C2A-CAA-CBA
12	A	821	CLA	C1A-C2A-CAA-CBA
12	A	823	CLA	C1A-C2A-CAA-CBA
12	A	824	CLA	C1A-C2A-CAA-CBA
12	A	827	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C1A-C2A-CAA-CBA
12	A	831	CLA	C1A-C2A-CAA-CBA
12	A	838	CLA	C1A-C2A-CAA-CBA
12	B	808	CLA	C1A-C2A-CAA-CBA
12	B	811	CLA	C1A-C2A-CAA-CBA
12	B	814	CLA	C1A-C2A-CAA-CBA
12	B	816	CLA	C1A-C2A-CAA-CBA
12	B	818	CLA	C1A-C2A-CAA-CBA
12	B	820	CLA	C1A-C2A-CAA-CBA
12	B	821	CLA	C1A-C2A-CAA-CBA
12	B	823	CLA	C1A-C2A-CAA-CBA
12	B	826	CLA	C1A-C2A-CAA-CBA
12	B	829	CLA	C1A-C2A-CAA-CBA
12	B	832	CLA	C1A-C2A-CAA-CBA
12	B	837	CLA	C1A-C2A-CAA-CBA
12	F	203	CLA	C1A-C2A-CAA-CBA
12	J	103	CLA	C1A-C2A-CAA-CBA
12	L	202	CLA	C1A-C2A-CAA-CBA
12	b	825	CLA	CBD-CGD-O2D-CED
18	H	847	LMG	C36-C37-C38-C39
12	B	806	CLA	C8-C10-C11-C12
12	B	822	CLA	C8-C10-C11-C12
16	G	851	LHG	O6-C4-C5-C6
12	G	804	CLA	C6-C7-C8-C10
12	G	808	CLA	C11-C10-C8-C7
12	G	808	CLA	C11-C12-C13-C15
12	G	837	CLA	C11-C12-C13-C15
12	G	837	CLA	C12-C13-C15-C16
12	G	841	CLA	C6-C7-C8-C10
12	H	803	CLA	C11-C10-C8-C7
12	H	804	CLA	C6-C7-C8-C10
12	H	804	CLA	C11-C10-C8-C7
12	H	811	CLA	C11-C10-C8-C7
12	H	811	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
12	H	823	CLA	C11-C12-C13-C15
12	H	824	CLA	C6-C7-C8-C10
12	a	807	CLA	C11-C10-C8-C7
12	a	807	CLA	C11-C12-C13-C15
12	a	820	CLA	C11-C12-C13-C15
12	a	828	CLA	C12-C13-C15-C16
12	a	834	CLA	C6-C7-C8-C10
12	a	837	CLA	C11-C12-C13-C15
12	a	837	CLA	C12-C13-C15-C16
12	a	841	CLA	C6-C7-C8-C10
12	a	854	CLA	C11-C12-C13-C15
12	b	804	CLA	C11-C10-C8-C7
12	b	810	CLA	C11-C10-C8-C7
12	b	822	CLA	C11-C12-C13-C15
12	b	823	CLA	C6-C7-C8-C10
12	b	825	CLA	C12-C13-C15-C16
12	A	807	CLA	C11-C10-C8-C7
12	A	827	CLA	C6-C7-C8-C10
12	A	828	CLA	C12-C13-C15-C16
12	A	834	CLA	C6-C7-C8-C10
12	A	837	CLA	C11-C12-C13-C15
12	B	804	CLA	C6-C7-C8-C10
12	B	810	CLA	C11-C10-C8-C7
12	B	823	CLA	C6-C7-C8-C10
12	L	205	CLA	C12-C13-C15-C16
12	b	837	CLA	C16-C17-C18-C19
12	A	807	CLA	C16-C17-C18-C19
12	B	807	CLA	C16-C17-C18-C20
12	B	838	CLA	C16-C17-C18-C19
12	b	805	CLA	C8-C10-C11-C12
12	b	837	CLA	O1A-CGA-O2A-C1
12	H	805	CLA	C8-C10-C11-C12
12	a	807	CLA	C5-C6-C7-C8
12	G	832	CLA	C4-C3-C5-C6
12	S	203	CLA	C4-C3-C5-C6
12	a	820	CLA	C4-C3-C5-C6
12	A	827	CLA	C4-C3-C5-C6
12	G	832	CLA	C2-C3-C5-C6
12	H	812	CLA	C2-C3-C5-C6
12	H	830	CLA	C2-C3-C5-C6
12	a	827	CLA	C2-C3-C5-C6
12	b	811	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	824	CLA	C2-C3-C5-C6
12	A	854	CLA	C5-C6-C7-C8
12	B	826	CLA	C10-C11-C12-C13
12	a	854	CLA	C2A-CAA-CBA-CGA
12	A	854	CLA	C2A-CAA-CBA-CGA
12	G	808	CLA	C11-C10-C8-C9
12	G	827	CLA	C11-C12-C13-C14
12	G	828	CLA	C6-C7-C8-C9
12	G	834	CLA	C6-C7-C8-C9
12	G	837	CLA	C14-C13-C15-C16
12	G	841	CLA	C6-C7-C8-C9
12	G	855	CLA	C11-C12-C13-C14
12	G	856	CLA	C11-C10-C8-C9
12	H	803	CLA	C11-C10-C8-C9
12	H	803	CLA	C14-C13-C15-C16
12	H	804	CLA	C6-C7-C8-C9
12	H	811	CLA	C11-C10-C8-C9
12	H	838	CLA	C6-C7-C8-C9
12	a	826	CLA	C11-C12-C13-C14
12	a	828	CLA	C14-C13-C15-C16
12	a	837	CLA	C14-C13-C15-C16
12	b	804	CLA	C6-C7-C8-C9
12	b	823	CLA	C6-C7-C8-C9
12	b	824	CLA	C14-C13-C15-C16
12	b	825	CLA	C14-C13-C15-C16
12	l	206	CLA	C14-C13-C15-C16
12	A	828	CLA	C14-C13-C15-C16
12	A	834	CLA	C6-C7-C8-C9
12	A	854	CLA	C11-C12-C13-C14
12	B	803	CLA	C14-C13-C15-C16
12	B	804	CLA	C6-C7-C8-C9
12	L	205	CLA	C14-C13-C15-C16
18	B	846	LMG	C36-C37-C38-C39
15	L	203	BCR	C9-C10-C11-C12
12	H	805	CLA	CBA-CGA-O2A-C1
12	a	806	CLA	CBA-CGA-O2A-C1
12	b	804	CLA	CBA-CGA-O2A-C1
12	B	804	CLA	CBA-CGA-O2A-C1
12	B	834	CLA	CBA-CGA-O2A-C1
12	b	816	CLA	C8-C10-C11-C12
12	b	837	CLA	C8-C10-C11-C12
12	A	824	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	A	854	CLA	C15-C16-C17-C18
12	B	825	CLA	C13-C15-C16-C17
16	G	854	LHG	C25-C26-C27-C28
12	B	809	CLA	O1D-CGD-O2D-CED
12	A	828	CLA	C15-C16-C17-C18
13	b	838	1L3	C26-C28-C29-C30
16	A	853	LHG	C16-C17-C18-C19
12	G	808	CLA	C15-C16-C17-C18
12	a	828	CLA	C15-C16-C17-C18
16	A	853	LHG	C29-C30-C31-C32
12	a	807	CLA	C16-C17-C18-C19
12	B	837	CLA	C16-C17-C18-C20
12	H	823	CLA	O1D-CGD-O2D-CED
15	i	102	BCR	C11-C10-C9-C34
12	B	822	CLA	C10-C11-C12-C13
12	H	812	CLA	C4-C3-C5-C6
12	b	811	CLA	C4-C3-C5-C6
12	A	832	CLA	C4-C3-C5-C6
12	a	820	CLA	C2-C3-C5-C6
12	a	832	CLA	C2-C3-C5-C6
12	b	829	CLA	C2-C3-C5-C6
12	A	827	CLA	C2-C3-C5-C6
12	A	832	CLA	C2-C3-C5-C6
12	B	811	CLA	C2-C3-C5-C6
12	G	808	CLA	C5-C6-C7-C8
12	G	855	CLA	C15-C16-C17-C18
12	b	810	CLA	C8-C10-C11-C12
12	A	803	CLA	C10-C11-C12-C13
12	B	825	CLA	C15-C16-C17-C18
16	G	851	LHG	C29-C30-C31-C32
12	a	827	CLA	C11-C12-C13-C15
15	Q	102	BCR	C7-C8-C9-C10
15	b	842	BCR	C21-C22-C23-C24
17	T	101	45D	C19-C23-C25-C29
12	L	205	CLA	O1A-CGA-O2A-C1
12	b	822	CLA	C15-C16-C17-C18
16	A	853	LHG	C11-C12-C13-C14
12	S	203	CLA	C3-C5-C6-C7
16	G	854	LHG	C23-C24-C25-C26
19	H	848	LMT	C4-C5-C6-C7
12	A	854	CLA	O2A-C1-C2-C3
15	A	848	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	H	848	LMT	C1-C2-C3-C4
12	A	826	CLA	C15-C16-C17-C18
12	B	810	CLA	C8-C10-C11-C12
16	a	853	LHG	C29-C30-C31-C32
15	j	101	BCR	C13-C14-C15-C16
15	j	103	BCR	C13-C14-C15-C16
15	A	852	BCR	C19-C20-C21-C22
18	b	845	LMG	C36-C37-C38-C39
12	a	806	CLA	O1A-CGA-O2A-C1
12	b	825	CLA	O1D-CGD-O2D-CED
12	B	822	CLA	O1D-CGD-O2D-CED
16	a	850	LHG	C24-C25-C26-C27
12	H	830	CLA	C4-C3-C5-C6
12	a	827	CLA	C4-C3-C5-C6
12	a	832	CLA	C4-C3-C5-C6
12	b	821	CLA	C4-C3-C5-C6
13	a	842	1L3	C22-C21-C23-C24
12	a	818	CLA	C2-C3-C5-C6
16	A	850	LHG	C35-C36-C37-C38
16	G	854	LHG	C27-C28-C29-C30
18	B	846	LMG	C22-C23-C24-C25
12	G	818	CLA	C6-C7-C8-C9
12	b	837	CLA	C16-C17-C18-C20
18	H	847	LMG	C22-C23-C24-C25
16	G	851	LHG	O7-C5-C6-O8
12	A	832	CLA	CBA-CGA-O2A-C1
12	A	812	CLA	C4C-C3C-CAC-CBC
18	b	845	LMG	C24-C25-C26-C27
19	B	847	LMT	C11-C10-C9-C8
12	B	824	CLA	CAA-CBA-CGA-O2A
12	l	205	CLA	C3-C5-C6-C7
12	B	815	CLA	C3-C5-C6-C7
12	B	816	CLA	C5-C6-C7-C8
12	H	828	CLA	CBD-CGD-O2D-CED
12	b	804	CLA	O1A-CGA-O2A-C1
18	H	847	LMG	C24-C25-C26-C27
12	b	816	CLA	C5-C6-C7-C8
12	G	832	CLA	CBA-CGA-O2A-C1
12	a	832	CLA	CBA-CGA-O2A-C1
18	B	846	LMG	C24-C25-C26-C27
12	b	824	CLA	CAA-CBA-CGA-O2A
19	b	846	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
18	b	845	LMG	C22-C23-C24-C25
12	b	823	CLA	C5-C6-C7-C8
12	a	805	CLA	O1D-CGD-O2D-CED
12	B	823	CLA	C5-C6-C7-C8
15	A	846	BCR	C19-C20-C21-C22
12	G	821	CLA	C4-C3-C5-C6
12	H	834	CLA	C4-C3-C5-C6
12	a	802	CLA	C4-C3-C5-C6
12	b	805	CLA	C4-C3-C5-C6
12	A	802	CLA	C4-C3-C5-C6
12	B	804	CLA	O1A-CGA-O2A-C1
12	G	821	CLA	C2-C3-C5-C6
12	G	833	CLA	C2-C3-C5-C6
12	B	829	CLA	C2-C3-C5-C6
12	A	836	CLA	C2C-C3C-CAC-CBC
16	G	852	LHG	O1-C1-C2-O2
12	G	837	CLA	C11-C12-C13-C14
12	H	823	CLA	C11-C12-C13-C14
12	H	825	CLA	C14-C13-C15-C16
12	H	826	CLA	C14-C13-C15-C16
12	S	204	CLA	C14-C13-C15-C16
12	a	807	CLA	C11-C10-C8-C9
12	a	824	CLA	C6-C7-C8-C9
12	a	826	CLA	C11-C10-C8-C9
12	a	834	CLA	C6-C7-C8-C9
12	a	837	CLA	C11-C12-C13-C14
12	a	841	CLA	C6-C7-C8-C9
12	a	854	CLA	C11-C12-C13-C14
12	a	855	CLA	C11-C10-C8-C9
12	b	803	CLA	C11-C10-C8-C9
12	b	810	CLA	C11-C10-C8-C9
12	b	822	CLA	C11-C12-C13-C14
12	A	807	CLA	C11-C10-C8-C9
12	A	820	CLA	C11-C12-C13-C14
12	A	826	CLA	C11-C12-C13-C14
12	A	827	CLA	C6-C7-C8-C9
12	A	837	CLA	C11-C12-C13-C14
12	B	810	CLA	C11-C10-C8-C9
12	B	822	CLA	C11-C12-C13-C14
12	B	825	CLA	C14-C13-C15-C16
12	L	206	CLA	C14-C13-C15-C16
12	l	206	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	811	CLA	C10-C11-C12-C13
12	f	201	CLA	C5-C6-C7-C8
12	L	206	CLA	C10-C11-C12-C13
16	G	854	LHG	C5-C4-O6-P
11	G	801	CL0	C4B-C3B-CAB-CBB
11	A	801	CL0	C4B-C3B-CAB-CBB
12	G	817	CLA	C4B-C3B-CAB-CBB
12	G	823	CLA	C4B-C3B-CAB-CBB
12	G	826	CLA	C4B-C3B-CAB-CBB
12	G	855	CLA	C4B-C3B-CAB-CBB
12	G	856	CLA	C4B-C3B-CAB-CBB
12	H	815	CLA	C4B-C3B-CAB-CBB
12	H	833	CLA	C4B-C3B-CAB-CBB
12	P	203	CLA	C4B-C3B-CAB-CBB
12	a	822	CLA	C4B-C3B-CAB-CBB
12	a	855	CLA	C4B-C3B-CAB-CBB
12	b	814	CLA	C4B-C3B-CAB-CBB
12	b	823	CLA	C4B-C3B-CAB-CBB
12	b	831	CLA	C4B-C3B-CAB-CBB
12	b	836	CLA	C4B-C3B-CAB-CBB
12	A	807	CLA	C4B-C3B-CAB-CBB
12	A	822	CLA	C4B-C3B-CAB-CBB
12	A	823	CLA	C4B-C3B-CAB-CBB
12	A	834	CLA	C4B-C3B-CAB-CBB
12	B	822	CLA	C4B-C3B-CAB-CBB
12	B	832	CLA	C4B-C3B-CAB-CBB
12	B	837	CLA	C4B-C3B-CAB-CBB
16	A	850	LHG	C29-C30-C31-C32
16	G	851	LHG	C35-C36-C37-C38
12	a	812	CLA	C4C-C3C-CAC-CBC
12	H	811	CLA	C5-C6-C7-C8
12	B	815	CLA	C10-C11-C12-C13
12	B	807	CLA	C16-C17-C18-C19
12	b	833	CLA	CBA-CGA-O2A-C1
16	a	850	LHG	C35-C36-C37-C38
12	b	821	CLA	C2A-CAA-CBA-CGA
18	b	845	LMG	C11-C12-C13-C14
12	G	804	CLA	C11-C10-C8-C7
12	G	819	CLA	C12-C13-C15-C16
12	G	825	CLA	C12-C13-C15-C16
12	G	827	CLA	C11-C12-C13-C15
12	G	828	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
12	G	834	CLA	C6-C7-C8-C10
12	G	855	CLA	C11-C12-C13-C15
12	G	856	CLA	C11-C10-C8-C7
12	H	803	CLA	C12-C13-C15-C16
12	H	811	CLA	C12-C13-C15-C16
12	H	826	CLA	C12-C13-C15-C16
12	S	204	CLA	C12-C13-C15-C16
12	a	803	CLA	C11-C10-C8-C7
12	a	805	CLA	C12-C13-C15-C16
12	a	826	CLA	C11-C12-C13-C15
12	a	827	CLA	C6-C7-C8-C10
12	a	855	CLA	C11-C10-C8-C7
12	b	803	CLA	C12-C13-C15-C16
12	b	804	CLA	C6-C7-C8-C10
12	b	805	CLA	C12-C13-C15-C16
12	b	810	CLA	C12-C13-C15-C16
12	l	206	CLA	C12-C13-C15-C16
12	A	837	CLA	C12-C13-C15-C16
12	A	854	CLA	C11-C12-C13-C15
12	B	822	CLA	C11-C12-C13-C15
12	B	825	CLA	C12-C13-C15-C16
12	L	206	CLA	C12-C13-C15-C16
12	H	803	CLA	C10-C11-C12-C13
12	H	811	CLA	C15-C16-C17-C18
12	H	823	CLA	C8-C10-C11-C12
12	H	823	CLA	C15-C16-C17-C18
12	H	826	CLA	C15-C16-C17-C18
12	H	807	CLA	C8-C10-C11-C12
12	a	827	CLA	C11-C12-C13-C14
12	B	838	CLA	C16-C17-C18-C20
12	G	811	CLA	C3A-C2A-CAA-CBA
12	G	829	CLA	C3A-C2A-CAA-CBA
12	G	834	CLA	C3A-C2A-CAA-CBA
12	H	805	CLA	C4-C3-C5-C6
12	H	825	CLA	C3A-C2A-CAA-CBA
12	H	828	CLA	C3A-C2A-CAA-CBA
12	a	817	CLA	C3A-C2A-CAA-CBA
12	a	839	CLA	C3A-C2A-CAA-CBA
12	A	806	CLA	C3A-C2A-CAA-CBA
12	B	805	CLA	C4-C3-C5-C6
12	B	811	CLA	C4-C3-C5-C6
12	B	827	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	829	CLA	C4-C3-C5-C6
16	A	853	LHG	C32-C33-C34-C35
12	G	828	CLA	C2-C3-C5-C6
12	H	834	CLA	C2-C3-C5-C6
12	b	837	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	O1A-CGA-O2A-C1
12	B	834	CLA	O1A-CGA-O2A-C1
15	G	847	BCR	C9-C10-C11-C12
15	G	850	BCR	C9-C10-C11-C12
15	G	853	BCR	C19-C20-C21-C22
15	H	843	BCR	C19-C20-C21-C22
15	R	102	BCR	C9-C10-C11-C12
15	R	102	BCR	C13-C14-C15-C16
15	S	201	BCR	C9-C10-C11-C12
15	b	839	BCR	C9-C10-C11-C12
15	b	841	BCR	C19-C20-C21-C22
15	f	202	BCR	C9-C10-C11-C12
15	f	202	BCR	C19-C20-C21-C22
15	l	203	BCR	C9-C10-C11-C12
15	A	844	BCR	C13-C14-C15-C16
15	B	842	BCR	C19-C20-C21-C22
15	J	102	BCR	C9-C10-C11-C12
15	J	102	BCR	C13-C14-C15-C16
17	m	101	45D	C36-C38-C42-C41
12	A	807	CLA	C16-C17-C18-C20
15	b	839	BCR	C37-C22-C23-C24
17	T	101	45D	C19-C23-C25-C27
16	a	850	LHG	C9-C10-C11-C12
18	B	846	LMG	C29-C30-C31-C32
16	G	851	LHG	C25-C26-C27-C28
11	a	801	CL0	CBA-CGA-O2A-C1
16	G	851	LHG	C4-C5-C6-O8
16	G	852	LHG	C4-C5-C6-O8
16	G	854	LHG	C4-C5-C6-O8
16	a	850	LHG	C4-C5-C6-O8
16	a	851	LHG	C4-C5-C6-O8
16	A	853	LHG	C4-C5-C6-O8
16	G	851	LHG	C11-C10-C9-C8
12	B	807	CLA	C3-C5-C6-C7
12	G	855	CLA	C5-C6-C7-C8
12	l	206	CLA	C10-C11-C12-C13
12	B	806	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	B	846	LMG	C11-C12-C13-C14
12	G	828	CLA	C4-C3-C5-C6
12	G	833	CLA	C4-C3-C5-C6
12	H	822	CLA	C4-C3-C5-C6
12	H	823	CLA	C4-C3-C5-C6
12	a	818	CLA	C4-C3-C5-C6
12	a	833	CLA	C4-C3-C5-C6
12	A	824	CLA	C4-C3-C5-C6
12	A	833	CLA	C4-C3-C5-C6
12	H	805	CLA	C2-C3-C5-C6
12	B	805	CLA	C2-C3-C5-C6
12	G	821	CLA	C3-C5-C6-C7
12	b	848	CLA	C10-C11-C12-C13
16	a	853	LHG	C27-C28-C29-C30
12	G	828	CLA	C11-C12-C13-C15
12	H	807	CLA	C16-C17-C18-C20
12	B	802	CLA	C16-C17-C18-C20
12	a	826	CLA	C15-C16-C17-C18
12	G	831	CLA	C2B-C3B-CAB-CBB
12	A	834	CLA	C2B-C3B-CAB-CBB
15	G	849	BCR	C1-C6-C7-C8
15	G	849	BCR	C23-C24-C25-C26
15	G	853	BCR	C23-C24-C25-C30
15	H	843	BCR	C23-C24-C25-C30
15	P	202	BCR	C1-C6-C7-C8
15	P	204	BCR	C1-C6-C7-C8
15	R	102	BCR	C23-C24-C25-C30
15	S	201	BCR	C1-C6-C7-C8
15	S	205	BCR	C23-C24-C25-C30
15	a	848	BCR	C1-C6-C7-C8
15	a	852	BCR	C23-C24-C25-C30
15	b	839	BCR	C1-C6-C7-C8
15	b	847	BCR	C23-C24-C25-C30
15	f	202	BCR	C1-C6-C7-C8
15	l	203	BCR	C1-C6-C7-C8
15	A	844	BCR	C1-C6-C7-C8
15	A	848	BCR	C1-C6-C7-C8
15	A	848	BCR	C23-C24-C25-C26
15	B	842	BCR	C23-C24-C25-C30
15	L	203	BCR	C1-C6-C7-C8
17	T	101	45D	C04-C08-C20-C24
17	m	101	45D	C04-C08-C20-C24

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Mol	Chain	Res	Type	Atoms
17	M	101	45D	C04-C08-C20-C24
12	S	204	CLA	C10-C11-C12-C13
16	A	853	LHG	C5-C4-O6-P
12	a	803	CLA	C10-C11-C12-C13
12	G	827	CLA	C16-C17-C18-C19
12	a	832	CLA	C8-C10-C11-C12
12	a	832	CLA	C15-C16-C17-C18
12	A	832	CLA	C15-C16-C17-C18
16	G	852	LHG	O7-C5-C6-O8
16	G	854	LHG	O7-C5-C6-O8
16	a	851	LHG	O7-C5-C6-O8
16	A	850	LHG	O7-C5-C6-O8
12	H	839	CLA	O1D-CGD-O2D-CED
12	b	824	CLA	O1D-CGD-O2D-CED
12	G	804	CLA	C10-C11-C12-C13
12	G	842	CLA	C10-C11-C12-C13
12	H	823	CLA	C10-C11-C12-C13
12	b	822	CLA	C8-C10-C11-C12
12	S	203	CLA	C2-C3-C5-C6
12	a	833	CLA	C2-C3-C5-C6
12	A	802	CLA	C2-C3-C5-C6
12	A	833	CLA	C2-C3-C5-C6
12	H	803	CLA	O1D-CGD-O2D-CED
12	a	833	CLA	C3-C5-C6-C7
12	G	808	CLA	C11-C12-C13-C14
12	G	819	CLA	C14-C13-C15-C16
12	H	824	CLA	C6-C7-C8-C9
12	a	827	CLA	C6-C7-C8-C9
12	b	803	CLA	C14-C13-C15-C16
12	j	102	CLA	C11-C12-C13-C14
12	A	837	CLA	C14-C13-C15-C16
12	A	855	CLA	C11-C10-C8-C9
12	A	817	CLA	C6-C7-C8-C9
12	B	808	CLA	O1D-CGD-O2D-CED
12	b	824	CLA	C3-C5-C6-C7
13	H	840	1L3	C21-C23-C24-C25
13	B	839	1L3	C21-C23-C24-C25
12	a	833	CLA	C2A-CAA-CBA-CGA
12	A	833	CLA	C2A-CAA-CBA-CGA
12	G	832	CLA	C8-C10-C11-C12
16	G	854	LHG	C31-C32-C33-C34
12	B	810	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	A	851	LHG	O1-C1-C2-O2
12	A	839	CLA	CBA-CGA-O2A-C1
12	G	803	CLA	C4-C3-C5-C6
17	T	101	45D	C36-C38-C42-C41
17	M	101	45D	C36-C38-C42-C41
12	a	802	CLA	C2-C3-C5-C6
12	b	805	CLA	C2-C3-C5-C6
12	a	807	CLA	C16-C17-C18-C20
12	G	832	CLA	C15-C16-C17-C18
12	B	820	CLA	O1D-CGD-O2D-CED
16	A	853	LHG	C31-C32-C33-C34
12	H	807	CLA	C3-C5-C6-C7
12	A	833	CLA	C3-C5-C6-C7
12	B	836	CLA	C8-C10-C11-C12
16	a	851	LHG	O6-C4-C5-C6
16	A	850	LHG	O6-C4-C5-C6
12	B	815	CLA	C11-C12-C13-C14
12	G	841	CLA	C15-C16-C17-C18
17	m	101	45D	C19-C23-C25-C27
17	M	101	45D	C19-C23-C25-C27
12	G	821	CLA	C12-C13-C15-C16
12	a	818	CLA	C12-C13-C15-C16
12	a	824	CLA	C12-C13-C15-C16
12	b	803	CLA	C11-C10-C8-C7
12	l	202	CLA	C6-C7-C8-C10
12	A	803	CLA	C11-C10-C8-C7
12	A	807	CLA	C11-C12-C13-C15
12	A	818	CLA	C12-C13-C15-C16
12	A	820	CLA	C11-C10-C8-C7
12	A	824	CLA	C12-C13-C15-C16
12	A	839	CLA	C11-C12-C13-C15
12	A	855	CLA	C11-C10-C8-C7
12	B	810	CLA	C12-C13-C15-C16
15	H	841	BCR	C21-C22-C23-C24
15	H	844	BCR	C21-C22-C23-C24
15	a	846	BCR	C17-C18-C19-C20
15	B	841	BCR	C11-C12-C13-C14
15	F	202	BCR	C21-C22-C23-C24
17	m	101	45D	C19-C23-C25-C29
17	M	101	45D	C19-C23-C25-C29
12	H	835	CLA	CBA-CGA-O2A-C1
11	a	801	CL0	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	G	832	CLA	O1A-CGA-O2A-C1
12	a	832	CLA	O1A-CGA-O2A-C1
12	G	806	CLA	C13-C15-C16-C17
12	l	206	CLA	C2A-CAA-CBA-CGA
12	b	822	CLA	C4-C3-C5-C6
12	B	833	CLA	C4-C3-C5-C6
13	G	843	1L3	C22-C21-C23-C24
12	b	833	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	C31-C32-C33-C34
12	B	815	CLA	CBD-CGD-O2D-CED
12	b	815	CLA	C8-C10-C11-C12
11	A	801	CL0	O1A-CGA-O2A-C1
12	G	828	CLA	C11-C12-C13-C14
12	B	802	CLA	C16-C17-C18-C19
11	G	801	CL0	O1A-CGA-O2A-C1
12	H	817	CLA	C5-C6-C7-C8
12	H	850	CLA	C10-C11-C12-C13
12	H	825	CLA	CAA-CBA-CGA-O2A
16	G	852	LHG	O6-C4-C5-O7
16	a	851	LHG	O6-C4-C5-O7
16	A	851	LHG	O6-C4-C5-O7
16	A	851	LHG	C4-C5-C6-O8
12	b	806	CLA	C5-C6-C7-C8
12	b	822	CLA	C10-C11-C12-C13
12	A	806	CLA	C5-C6-C7-C8
12	B	837	CLA	C16-C17-C18-C19
12	B	826	CLA	C3-C5-C6-C7
12	B	815	CLA	O1D-CGD-O2D-CED
12	L	206	CLA	C13-C15-C16-C17
18	H	847	LMG	C33-C34-C35-C36
12	H	811	CLA	C4-C3-C5-C6
12	B	807	CLA	C4-C3-C5-C6
12	H	823	CLA	C2-C3-C5-C6
18	b	845	LMG	C29-C30-C31-C32
12	b	825	CLA	C15-C16-C17-C18
12	l	206	CLA	C13-C15-C16-C17
12	B	822	CLA	C15-C16-C17-C18
16	A	851	LHG	O7-C5-C6-O8
16	A	853	LHG	O7-C5-C6-O8
12	a	828	CLA	C5-C6-C7-C8
12	G	821	CLA	C14-C13-C15-C16
12	G	827	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
12	G	829	CLA	C14-C13-C15-C16
12	H	808	CLA	C11-C12-C13-C14
12	H	825	CLA	C11-C12-C13-C14
12	a	818	CLA	C14-C13-C15-C16
12	l	202	CLA	C11-C12-C13-C14
12	A	818	CLA	C14-C13-C15-C16
12	A	826	CLA	C6-C7-C8-C9
12	B	810	CLA	C6-C7-C8-C9
12	B	823	CLA	C6-C7-C8-C9
12	B	830	CLA	C11-C12-C13-C14
12	B	830	CLA	C14-C13-C15-C16
12	B	803	CLA	C10-C11-C12-C13
12	a	831	CLA	C5-C6-C7-C8
16	A	851	LHG	O8-C23-C24-C25
12	H	808	CLA	C2-C1-O2A-CGA
12	l	202	CLA	C2-C1-O2A-CGA
11	A	801	CL0	CBA-CGA-O2A-C1
12	G	842	CLA	C11-C12-C13-C15
12	B	815	CLA	C11-C12-C13-C15
12	a	828	CLA	C13-C15-C16-C17
12	b	807	CLA	C8-C10-C11-C12
12	H	807	CLA	C4-C3-C5-C6
12	b	807	CLA	C4-C3-C5-C6
12	P	201	CLA	C3-C5-C6-C7
12	G	803	CLA	C2-C3-C5-C6
12	B	807	CLA	C2-C3-C5-C6
12	H	839	CLA	C8-C10-C11-C12
12	f	201	CLA	C13-C15-C16-C17
16	A	850	LHG	C32-C33-C34-C35
16	a	850	LHG	C32-C33-C34-C35
12	H	825	CLA	C16-C17-C18-C20
12	b	836	CLA	C16-C17-C18-C20
15	H	842	BCR	C11-C12-C13-C35
12	H	826	CLA	C4B-C3B-CAB-CBB
12	H	838	CLA	C4B-C3B-CAB-CBB
12	P	201	CLA	C4B-C3B-CAB-CBB
12	a	808	CLA	C1A-C2A-CAA-CBA
12	a	854	CLA	C1A-C2A-CAA-CBA
12	b	834	CLA	C4B-C3B-CAB-CBB
12	A	854	CLA	C1A-C2A-CAA-CBA
12	B	835	CLA	C1A-C2A-CAA-CBA
12	B	835	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	G	801	CL0	CBA-CGA-O2A-C1
12	a	839	CLA	CBA-CGA-O2A-C1
12	b	810	CLA	C4-C3-C5-C6
12	B	810	CLA	C4-C3-C5-C6
12	B	822	CLA	C4-C3-C5-C6
15	b	839	BCR	C21-C22-C23-C24
15	L	207	BCR	C7-C8-C9-C10
12	G	827	CLA	C16-C17-C18-C20
12	a	818	CLA	C16-C17-C18-C20
12	B	824	CLA	C16-C17-C18-C20
16	G	851	LHG	C10-C11-C12-C13
16	G	852	LHG	O6-C4-C5-C6
16	A	851	LHG	O6-C4-C5-C6
16	G	851	LHG	C32-C33-C34-C35
12	G	829	CLA	C12-C13-C15-C16
12	G	830	CLA	C11-C10-C8-C7
12	G	834	CLA	C11-C12-C13-C15
12	G	839	CLA	C11-C12-C13-C15
12	H	822	CLA	C11-C12-C13-C15
12	H	850	CLA	C11-C10-C8-C7
12	S	203	CLA	C12-C13-C15-C16
12	a	839	CLA	C11-C12-C13-C15
12	b	802	CLA	C12-C13-C15-C16
12	b	821	CLA	C11-C12-C13-C15
12	b	829	CLA	C6-C7-C8-C10
12	b	848	CLA	C11-C10-C8-C7
12	A	805	CLA	C12-C13-C15-C16
12	A	834	CLA	C11-C12-C13-C15
12	B	805	CLA	C12-C13-C15-C16
12	B	821	CLA	C11-C12-C13-C15
12	B	829	CLA	C6-C7-C8-C10
12	B	810	CLA	C4C-C3C-CAC-CBC
12	H	807	CLA	C16-C17-C18-C19
12	H	838	CLA	C16-C17-C18-C20
12	a	834	CLA	C16-C17-C18-C19
12	b	810	CLA	C16-C17-C18-C19
12	A	826	CLA	O1A-CGA-O2A-C1
12	a	826	CLA	O1A-CGA-O2A-C1
12	S	204	CLA	C13-C15-C16-C17
16	G	854	LHG	C2-C3-O3-P
16	A	853	LHG	C2-C3-O3-P
12	a	824	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	G	819	CLA	C16-C17-C18-C20
18	H	847	LMG	C11-C12-C13-C14
12	B	810	CLA	C2C-C3C-CAC-CBC
12	a	806	CLA	C5-C6-C7-C8
12	H	835	CLA	O1A-CGA-O2A-C1
16	A	850	LHG	O6-C4-C5-O7
16	A	853	LHG	C13-C14-C15-C16
12	H	823	CLA	C11-C10-C8-C9
12	a	824	CLA	C14-C13-C15-C16
12	b	822	CLA	C11-C10-C8-C9
12	b	824	CLA	C11-C12-C13-C14
12	b	836	CLA	C6-C7-C8-C9
12	A	820	CLA	C11-C10-C8-C9
12	A	824	CLA	C14-C13-C15-C16
12	A	833	CLA	C14-C13-C15-C16
16	A	851	LHG	C9-C10-C11-C12
16	a	853	LHG	O8-C23-C24-C25
12	a	854	CLA	C5-C6-C7-C8
15	G	845	BCR	C13-C14-C15-C16
15	H	849	BCR	C19-C20-C21-C22
15	P	202	BCR	C19-C20-C21-C22
15	a	852	BCR	C19-C20-C21-C22
15	j	103	BCR	C9-C10-C11-C12
19	H	848	LMT	C11-C10-C9-C8
12	B	802	CLA	O1A-CGA-O2A-C1
12	L	205	CLA	C10-C11-C12-C13
12	H	807	CLA	C2-C3-C5-C6
12	b	807	CLA	C2-C3-C5-C6
12	b	822	CLA	C2-C3-C5-C6
12	G	815	CLA	CAD-CBD-CGD-O2D
12	G	855	CLA	CAD-CBD-CGD-O2D
12	H	803	CLA	CAD-CBD-CGD-O2D
12	H	811	CLA	CAD-CBD-CGD-O2D
12	H	850	CLA	CAD-CBD-CGD-O2D
12	a	826	CLA	CAD-CBD-CGD-O2D
12	a	830	CLA	CAD-CBD-CGD-O2D
12	a	854	CLA	CAD-CBD-CGD-O2D
12	b	810	CLA	CAD-CBD-CGD-O2D
12	b	832	CLA	CAD-CBD-CGD-O2D
12	A	814	CLA	CAD-CBD-CGD-O2D
12	A	837	CLA	CAD-CBD-CGD-O2D
12	A	854	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	B	803	CLA	CAD-CBD-CGD-O2D
12	B	810	CLA	CAD-CBD-CGD-O2D
12	B	833	CLA	CAD-CBD-CGD-O2D
12	A	825	CLA	C5-C6-C7-C8
12	A	832	CLA	C8-C10-C11-C12
12	H	838	CLA	C16-C17-C18-C19
12	a	834	CLA	C16-C17-C18-C20
12	b	836	CLA	C16-C17-C18-C19
12	G	833	CLA	C2A-CAA-CBA-CGA
12	b	810	CLA	C2A-CAA-CBA-CGA
12	G	827	CLA	C15-C16-C17-C18
12	G	814	CLA	CHA-CBD-CGD-O2D
12	G	815	CLA	CAD-CBD-CGD-O1D
12	G	820	CLA	CHA-CBD-CGD-O1D
12	G	825	CLA	CHA-CBD-CGD-O1D
12	G	825	CLA	CHA-CBD-CGD-O2D
12	G	827	CLA	CAD-CBD-CGD-O1D
12	G	842	CLA	CAD-CBD-CGD-O1D
12	G	855	CLA	CAD-CBD-CGD-O1D
12	H	803	CLA	CAD-CBD-CGD-O1D
12	H	811	CLA	CAD-CBD-CGD-O1D
12	H	812	CLA	CHA-CBD-CGD-O1D
12	H	812	CLA	CHA-CBD-CGD-O2D
12	H	832	CLA	CHA-CBD-CGD-O1D
12	H	834	CLA	CAD-CBD-CGD-O1D
12	H	839	CLA	CHA-CBD-CGD-O1D
12	H	839	CLA	CHA-CBD-CGD-O2D
12	H	850	CLA	CAD-CBD-CGD-O1D
12	a	805	CLA	CAD-CBD-CGD-O1D
12	a	814	CLA	CAD-CBD-CGD-O1D
12	a	824	CLA	CHA-CBD-CGD-O1D
12	a	826	CLA	CAD-CBD-CGD-O1D
12	a	830	CLA	CAD-CBD-CGD-O1D
12	a	854	CLA	CAD-CBD-CGD-O1D
12	b	803	CLA	CAD-CBD-CGD-O1D
12	b	810	CLA	CAD-CBD-CGD-O1D
12	b	830	CLA	CHA-CBD-CGD-O1D
12	b	830	CLA	CHA-CBD-CGD-O2D
12	b	832	CLA	CAD-CBD-CGD-O1D
12	A	814	CLA	CAD-CBD-CGD-O1D
12	A	826	CLA	CAD-CBD-CGD-O1D
12	A	837	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	A	854	CLA	CAD-CBD-CGD-O1D
12	B	803	CLA	CAD-CBD-CGD-O1D
12	B	810	CLA	CAD-CBD-CGD-O1D
12	B	811	CLA	CHA-CBD-CGD-O2D
12	B	831	CLA	CHA-CBD-CGD-O1D
12	B	831	CLA	CHA-CBD-CGD-O2D
12	B	833	CLA	CAD-CBD-CGD-O1D
15	a	844	BCR	C15-C16-C17-C18
15	a	849	BCR	C9-C10-C11-C12
15	b	847	BCR	C19-C20-C21-C22
15	i	102	BCR	C13-C14-C15-C16
16	G	851	LHG	C3-O3-P-O5
16	G	852	LHG	C3-O3-P-O5
16	G	852	LHG	C4-O6-P-O5
16	G	854	LHG	C3-O3-P-O5
16	a	850	LHG	C3-O3-P-O5
16	a	851	LHG	C3-O3-P-O5
16	a	851	LHG	C4-O6-P-O3
16	a	853	LHG	C3-O3-P-O5
16	A	850	LHG	C3-O3-P-O5
16	A	850	LHG	C4-O6-P-O4
16	A	850	LHG	C4-O6-P-O5
16	A	853	LHG	C3-O3-P-O5
12	A	823	CLA	C3-C5-C6-C7
11	a	801	CL0	C2B-C3B-CAB-CBB
12	G	805	CLA	C2B-C3B-CAB-CBB
12	G	813	CLA	C2B-C3B-CAB-CBB
12	G	817	CLA	C2B-C3B-CAB-CBB
12	G	824	CLA	C2B-C3B-CAB-CBB
12	G	832	CLA	C2B-C3B-CAB-CBB
12	G	833	CLA	C2B-C3B-CAB-CBB
12	H	818	CLA	C2B-C3B-CAB-CBB
12	H	825	CLA	C2B-C3B-CAB-CBB
12	a	812	CLA	C2B-C3B-CAB-CBB
12	a	823	CLA	C2B-C3B-CAB-CBB
12	a	832	CLA	C2B-C3B-CAB-CBB
12	a	833	CLA	C2B-C3B-CAB-CBB
12	a	854	CLA	C2B-C3B-CAB-CBB
12	b	817	CLA	C2B-C3B-CAB-CBB
12	b	824	CLA	C2B-C3B-CAB-CBB
12	b	836	CLA	C2B-C3B-CAB-CBB
12	j	102	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	807	CLA	C2B-C3B-CAB-CBB
12	A	812	CLA	C2B-C3B-CAB-CBB
12	A	816	CLA	C2B-C3B-CAB-CBB
12	A	832	CLA	C2B-C3B-CAB-CBB
12	A	833	CLA	C2B-C3B-CAB-CBB
12	A	854	CLA	C2B-C3B-CAB-CBB
12	B	814	CLA	C2B-C3B-CAB-CBB
12	B	817	CLA	C2B-C3B-CAB-CBB
12	B	824	CLA	C2B-C3B-CAB-CBB
12	B	830	CLA	C2B-C3B-CAB-CBB
12	B	837	CLA	C2B-C3B-CAB-CBB
15	R	102	BCR	C23-C24-C25-C26
15	a	848	BCR	C23-C24-C25-C26
15	b	841	BCR	C23-C24-C25-C30
15	f	204	BCR	C1-C6-C7-C8
15	A	844	BCR	C5-C6-C7-C8
15	A	852	BCR	C23-C24-C25-C30
15	B	840	BCR	C1-C6-C7-C8
15	F	204	BCR	C1-C6-C7-C8
16	G	854	LHG	C32-C33-C34-C35
12	H	811	CLA	C2-C3-C5-C6
12	a	824	CLA	C2-C3-C5-C6
12	b	821	CLA	C2-C3-C5-C6
12	H	824	CLA	C5-C6-C7-C8
12	b	823	CLA	C8-C10-C11-C12
12	F	201	CLA	C13-C15-C16-C17
16	a	853	LHG	C2-C3-O3-P
12	B	821	CLA	C13-C15-C16-C17
12	G	842	CLA	C11-C12-C13-C14
12	H	839	CLA	C16-C17-C18-C19
12	b	815	CLA	C11-C12-C13-C14
12	B	810	CLA	C16-C17-C18-C19
19	H	848	LMT	C4'-C5'-C6'-O6'
12	b	803	CLA	CBD-CGD-O2D-CED
19	B	847	LMT	C2-C3-C4-C5
12	a	823	CLA	C3-C5-C6-C7
12	B	836	CLA	C15-C16-C17-C18
15	R	101	BCR	C18-C19-C20-C21
15	R	102	BCR	C18-C19-C20-C21
15	j	101	BCR	C18-C19-C20-C21
15	j	103	BCR	C18-C19-C20-C21
15	J	101	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
15	J	102	BCR	C18-C19-C20-C21
12	G	807	CLA	CAA-CBA-CGA-O2A
13	b	838	1L3	C21-C23-C24-C25
12	H	806	CLA	C5-C6-C7-C8
12	A	820	CLA	C13-C15-C16-C17
12	H	822	CLA	C2-C3-C5-C6
12	B	833	CLA	C2-C3-C5-C6
16	a	853	LHG	C12-C13-C14-C15
12	A	826	CLA	C5-C6-C7-C8
11	G	801	CL0	C11-C12-C13-C14
12	G	806	CLA	C14-C13-C15-C16
12	G	825	CLA	C14-C13-C15-C16
12	G	833	CLA	C14-C13-C15-C16
12	S	203	CLA	C14-C13-C15-C16
12	a	803	CLA	C11-C10-C8-C9
12	a	807	CLA	C11-C12-C13-C14
12	b	802	CLA	C11-C10-C8-C9
12	b	802	CLA	C14-C13-C15-C16
12	b	805	CLA	C14-C13-C15-C16
12	b	810	CLA	C14-C13-C15-C16
12	b	829	CLA	C6-C7-C8-C9
12	l	205	CLA	C14-C13-C15-C16
12	A	803	CLA	C11-C10-C8-C9
12	A	807	CLA	C11-C12-C13-C14
12	B	802	CLA	C11-C10-C8-C9
12	B	803	CLA	C11-C10-C8-C9
12	B	810	CLA	C14-C13-C15-C16
12	L	202	CLA	C11-C12-C13-C14
12	G	833	CLA	C12-C13-C15-C16
12	a	820	CLA	C11-C10-C8-C7
12	l	205	CLA	C12-C13-C15-C16
12	A	833	CLA	C12-C13-C15-C16
12	A	841	CLA	C6-C7-C8-C10
12	B	803	CLA	C11-C10-C8-C7
15	i	102	BCR	C11-C10-C9-C8
12	P	201	CLA	C13-C15-C16-C17
16	A	850	LHG	C24-C25-C26-C27
12	A	837	CLA	C4-C3-C5-C6
18	b	845	LMG	O7-C8-C9-O8
12	A	826	CLA	CBA-CGA-O2A-C1
15	H	845	BCR	C19-C20-C21-C22
12	A	806	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	a	855	CLA	C2C-C3C-CAC-CBC
12	a	826	CLA	CBA-CGA-O2A-C1
12	A	828	CLA	C2-C1-O2A-CGA
12	L	202	CLA	C2-C1-O2A-CGA
12	b	832	CLA	C4-C3-C5-C6
12	A	841	CLA	C16-C17-C18-C20
12	a	806	CLA	CAA-CBA-CGA-O2A
12	A	828	CLA	CAA-CBA-CGA-O2A
15	a	845	BCR	C36-C18-C19-C20
15	l	203	BCR	C36-C18-C19-C20
12	H	825	CLA	C16-C17-C18-C19
18	B	846	LMG	C12-C13-C14-C15
16	A	851	LHG	O10-C23-C24-C25
16	G	852	LHG	C9-C10-C11-C12
12	b	802	CLA	O1A-CGA-O2A-C1
12	A	841	CLA	C15-C16-C17-C18
12	A	832	CLA	C2A-CAA-CBA-CGA
12	B	810	CLA	C2A-CAA-CBA-CGA
12	G	837	CLA	C4-C3-C5-C6
12	H	825	CLA	C4-C3-C5-C6
19	B	847	LMT	C4-C5-C6-C7
18	b	845	LMG	C12-C13-C14-C15
16	a	851	LHG	O8-C23-C24-C25
12	A	820	CLA	C3-C5-C6-C7
12	A	818	CLA	C16-C17-C18-C20
12	G	804	CLA	C11-C10-C8-C9
12	G	839	CLA	C11-C12-C13-C14
12	H	811	CLA	C14-C13-C15-C16
12	a	820	CLA	C11-C10-C8-C9
12	a	833	CLA	C14-C13-C15-C16
12	b	848	CLA	C11-C10-C8-C9
12	B	824	CLA	C11-C12-C13-C14
12	B	829	CLA	C6-C7-C8-C9
12	G	839	CLA	CBA-CGA-O2A-C1
12	H	823	CLA	C4B-C3B-CAB-CBB
12	H	824	CLA	C4B-C3B-CAB-CBB
12	a	802	CLA	C4B-C3B-CAB-CBB
12	G	826	CLA	C5-C6-C7-C8
12	a	837	CLA	C10-C11-C12-C13
12	A	830	CLA	CBD-CGD-O2D-CED
12	a	816	CLA	C2A-CAA-CBA-CGA
12	a	834	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	A	809	CLA	C2A-CAA-CBA-CGA
12	a	837	CLA	C4-C3-C5-C6
12	B	824	CLA	C4-C3-C5-C6
19	b	846	LMT	C4'-C5'-C6'-O6'
12	G	837	CLA	C2-C3-C5-C6
12	b	832	CLA	C2-C3-C5-C6
12	A	837	CLA	C2-C3-C5-C6
13	a	842	1L3	C20-C21-C23-C24
15	b	843	BCR	C19-C20-C21-C22
12	a	854	CLA	C15-C16-C17-C18
12	L	204	CLA	C5-C6-C7-C8
16	a	850	LHG	C24-C23-O8-C6
12	B	824	CLA	C16-C17-C18-C19
12	H	825	CLA	C11-C12-C13-C15
12	b	810	CLA	C11-C12-C13-C15
12	b	824	CLA	C11-C12-C13-C15
12	A	828	CLA	C11-C12-C13-C15
12	B	802	CLA	C11-C10-C8-C7
12	B	804	CLA	C11-C10-C8-C7
12	L	202	CLA	C6-C7-C8-C10
12	a	828	CLA	CAA-CBA-CGA-O2A
12	a	818	CLA	C16-C17-C18-C19
12	A	834	CLA	C16-C17-C18-C19
12	H	802	CLA	O1A-CGA-O2A-C1
12	A	839	CLA	O1A-CGA-O2A-C1
18	B	846	LMG	O7-C8-C9-O8
12	H	806	CLA	C4-C3-C5-C6
12	A	810	CLA	C3A-C2A-CAA-CBA
12	A	854	CLA	C3A-C2A-CAA-CBA
12	B	834	CLA	C4-C3-C5-C6
13	A	842	1L3	C22-C21-C23-C24
12	B	810	CLA	C2-C3-C5-C6
12	B	822	CLA	C2-C3-C5-C6
12	G	819	CLA	C16-C17-C18-C19
15	G	846	BCR	C11-C10-C9-C34
15	G	850	BCR	C16-C17-C18-C36
15	H	843	BCR	C11-C10-C9-C34
15	H	843	BCR	C20-C21-C22-C37
15	P	204	BCR	C35-C13-C14-C15
15	R	102	BCR	C16-C17-C18-C36
15	R	102	BCR	C20-C21-C22-C37
15	S	201	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
15	a	849	BCR	C16-C17-C18-C36
15	b	841	BCR	C11-C10-C9-C34
15	b	841	BCR	C20-C21-C22-C37
15	f	204	BCR	C35-C13-C14-C15
15	j	103	BCR	C16-C17-C18-C36
15	j	103	BCR	C20-C21-C22-C37
15	l	203	BCR	C20-C21-C22-C37
15	A	849	BCR	C16-C17-C18-C36
15	B	842	BCR	C11-C10-C9-C34
15	B	842	BCR	C20-C21-C22-C37
15	F	204	BCR	C35-C13-C14-C15
15	J	102	BCR	C16-C17-C18-C36
15	J	102	BCR	C20-C21-C22-C37
15	L	203	BCR	C20-C21-C22-C37
12	H	835	CLA	C13-C15-C16-C17
12	P	201	CLA	C2-C1-O2A-CGA
12	a	829	CLA	C2-C1-O2A-CGA
12	b	803	CLA	C2-C1-O2A-CGA
12	l	204	CLA	C2-C1-O2A-CGA
12	A	829	CLA	C2-C1-O2A-CGA
12	B	823	CLA	C2-C1-O2A-CGA
15	H	841	BCR	C9-C10-C11-C12
15	Q	102	BCR	C13-C14-C15-C16
12	A	837	CLA	C3-C5-C6-C7
12	f	201	CLA	C8-C10-C11-C12
12	A	821	CLA	CAA-CBA-CGA-O1A
12	B	812	CLA	CAA-CBA-CGA-O2A
12	B	812	CLA	CAA-CBA-CGA-O1A
12	A	837	CLA	C10-C11-C12-C13
12	B	802	CLA	C10-C11-C12-C13
15	H	842	BCR	C11-C12-C13-C14
12	b	810	CLA	C2-C3-C5-C6
12	B	824	CLA	C2-C3-C5-C6
11	a	801	CL0	C16-C17-C18-C19
12	b	824	CLA	C16-C17-C18-C20
16	a	851	LHG	C9-C10-C11-C12
12	H	811	CLA	C2A-CAA-CBA-CGA
12	G	822	CLA	CAA-CBA-CGA-O1A
12	H	818	CLA	CAA-CBA-CGA-O2A
12	b	812	CLA	CAA-CBA-CGA-O1A
12	b	817	CLA	CAA-CBA-CGA-O1A
12	G	807	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	G	829	CLA	C11-C12-C13-C14
12	H	822	CLA	C11-C12-C13-C14
12	H	831	CLA	C14-C13-C15-C16
12	H	837	CLA	C11-C12-C13-C14
12	a	806	CLA	C11-C12-C13-C14
12	j	102	CLA	C14-C13-C15-C16
12	A	805	CLA	C11-C12-C13-C14
12	A	828	CLA	C11-C12-C13-C14
12	A	841	CLA	C6-C7-C8-C9
12	B	821	CLA	C11-C12-C13-C14
12	B	836	CLA	C6-C7-C8-C9
11	G	801	CL0	C16-C17-C18-C19
16	A	850	LHG	C19-C20-C21-C22
12	a	821	CLA	CAA-CBA-CGA-O1A
12	A	821	CLA	CAA-CBA-CGA-O2A
12	A	838	CLA	CAA-CBA-CGA-O1A
12	b	812	CLA	CAA-CBA-CGA-O2A
12	B	821	CLA	C4-C3-C5-C6
12	l	202	CLA	C15-C16-C17-C18
12	H	825	CLA	C2-C3-C5-C6
12	a	837	CLA	C2-C3-C5-C6
16	a	851	LHG	O1-C1-C2-O2
12	P	201	CLA	C8-C10-C11-C12
12	G	822	CLA	CAA-CBA-CGA-O2A
12	H	813	CLA	CAA-CBA-CGA-O2A
12	a	821	CLA	CAA-CBA-CGA-O2A
12	a	838	CLA	CAA-CBA-CGA-O1A
12	S	204	CLA	C2A-CAA-CBA-CGA
12	l	204	CLA	C2A-CAA-CBA-CGA
12	G	803	CLA	C1A-C2A-CAA-CBA
12	G	811	CLA	C1A-C2A-CAA-CBA
12	G	829	CLA	C1A-C2A-CAA-CBA
12	a	802	CLA	C1A-C2A-CAA-CBA
12	A	802	CLA	C1A-C2A-CAA-CBA
12	A	808	CLA	C1A-C2A-CAA-CBA
12	B	827	CLA	C1A-C2A-CAA-CBA
15	G	850	BCR	C16-C17-C18-C19
15	H	843	BCR	C11-C10-C9-C8
15	H	843	BCR	C20-C21-C22-C23
15	P	204	BCR	C12-C13-C14-C15
15	R	102	BCR	C16-C17-C18-C19
15	R	102	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
15	S	201	BCR	C20-C21-C22-C23
15	a	849	BCR	C16-C17-C18-C19
15	b	841	BCR	C11-C10-C9-C8
15	b	841	BCR	C20-C21-C22-C23
15	f	204	BCR	C12-C13-C14-C15
15	j	103	BCR	C16-C17-C18-C19
15	j	103	BCR	C20-C21-C22-C23
15	l	203	BCR	C20-C21-C22-C23
15	A	849	BCR	C16-C17-C18-C19
15	B	842	BCR	C11-C10-C9-C8
15	B	842	BCR	C20-C21-C22-C23
15	F	204	BCR	C12-C13-C14-C15
15	J	102	BCR	C16-C17-C18-C19
15	J	102	BCR	C20-C21-C22-C23
15	L	203	BCR	C20-C21-C22-C23
12	F	201	CLA	C16-C17-C18-C19
12	A	838	CLA	CAA-CBA-CGA-O2A
12	b	833	CLA	C13-C15-C16-C17
16	a	851	LHG	O10-C23-C24-C25
12	G	823	CLA	C2B-C3B-CAB-CBB
12	G	826	CLA	C2B-C3B-CAB-CBB
12	G	856	CLA	C2B-C3B-CAB-CBB
12	H	815	CLA	C2B-C3B-CAB-CBB
12	H	823	CLA	C2B-C3B-CAB-CBB
12	H	824	CLA	C2B-C3B-CAB-CBB
12	H	838	CLA	C2B-C3B-CAB-CBB
12	P	201	CLA	C2B-C3B-CAB-CBB
12	P	203	CLA	C2B-C3B-CAB-CBB
12	a	822	CLA	C2B-C3B-CAB-CBB
12	b	823	CLA	C2B-C3B-CAB-CBB
12	b	833	CLA	C2B-C3B-CAB-CBB
12	b	834	CLA	C2B-C3B-CAB-CBB
12	A	822	CLA	C2B-C3B-CAB-CBB
12	A	823	CLA	C2B-C3B-CAB-CBB
12	B	821	CLA	C2B-C3B-CAB-CBB
12	B	835	CLA	C2B-C3B-CAB-CBB
15	G	849	BCR	C5-C6-C7-C8
15	G	853	BCR	C23-C24-C25-C26
15	H	841	BCR	C1-C6-C7-C8
15	H	843	BCR	C23-C24-C25-C26
15	H	845	BCR	C23-C24-C25-C26
15	H	845	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
15	H	849	BCR	C23-C24-C25-C30
15	P	202	BCR	C5-C6-C7-C8
15	P	204	BCR	C5-C6-C7-C8
15	Q	102	BCR	C1-C6-C7-C8
15	S	201	BCR	C5-C6-C7-C8
15	S	205	BCR	C23-C24-C25-C26
15	a	848	BCR	C5-C6-C7-C8
15	a	852	BCR	C23-C24-C25-C26
15	b	839	BCR	C5-C6-C7-C8
15	b	841	BCR	C23-C24-C25-C26
15	b	843	BCR	C23-C24-C25-C26
15	b	843	BCR	C23-C24-C25-C30
15	b	847	BCR	C23-C24-C25-C26
15	f	202	BCR	C5-C6-C7-C8
15	f	204	BCR	C5-C6-C7-C8
15	i	102	BCR	C1-C6-C7-C8
15	l	203	BCR	C5-C6-C7-C8
15	A	848	BCR	C5-C6-C7-C8
15	A	852	BCR	C23-C24-C25-C26
15	B	840	BCR	C5-C6-C7-C8
15	B	842	BCR	C23-C24-C25-C26
15	F	202	BCR	C5-C6-C7-C8
15	F	204	BCR	C5-C6-C7-C8
15	J	101	BCR	C1-C6-C7-C8
15	J	104	BCR	C23-C24-C25-C26
15	L	203	BCR	C5-C6-C7-C8
16	G	852	LHG	O8-C23-C24-C25
17	T	101	45D	C03-C07-C19-C23
17	m	101	45D	C03-C07-C19-C23
12	b	819	CLA	CAA-CBA-CGA-O1A
12	a	839	CLA	O1A-CGA-O2A-C1
16	G	851	LHG	C30-C31-C32-C33
12	H	818	CLA	CAA-CBA-CGA-O1A
12	G	826	CLA	C4-C3-C5-C6
12	b	836	CLA	C4-C3-C5-C6
12	B	838	CLA	C4-C3-C5-C6
12	a	838	CLA	CAA-CBA-CGA-O2A
12	B	817	CLA	CAA-CBA-CGA-O2A
12	S	203	CLA	C10-C11-C12-C13
11	G	801	CL0	C11-C12-C13-C15
12	G	807	CLA	C11-C12-C13-C15
12	H	805	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	H	825	CLA	C6-C7-C8-C10
12	H	830	CLA	C6-C7-C8-C10
12	a	829	CLA	C11-C10-C8-C7
12	a	833	CLA	C12-C13-C15-C16
12	a	834	CLA	C11-C12-C13-C15
12	b	802	CLA	C11-C10-C8-C7
12	A	820	CLA	C12-C13-C15-C16
12	A	829	CLA	C11-C10-C8-C7
12	B	824	CLA	C6-C7-C8-C10
12	B	837	CLA	C6-C7-C8-C10
12	B	838	CLA	C6-C7-C8-C10
16	A	850	LHG	C14-C15-C16-C17
12	H	839	CLA	C16-C17-C18-C20
12	A	834	CLA	C16-C17-C18-C20
12	a	832	CLA	C2A-CAA-CBA-CGA
12	b	819	CLA	C2A-CAA-CBA-CGA
12	B	821	CLA	C2A-CAA-CBA-CGA
12	L	206	CLA	C2A-CAA-CBA-CGA
12	H	813	CLA	CAA-CBA-CGA-O1A
12	H	822	CLA	C13-C15-C16-C17
12	A	833	CLA	C13-C15-C16-C17
12	b	817	CLA	CAA-CBA-CGA-O2A
12	B	817	CLA	CAA-CBA-CGA-O1A
12	B	823	CLA	C8-C10-C11-C12
15	a	852	BCR	C37-C22-C23-C24
12	b	819	CLA	CAA-CBA-CGA-O2A
12	a	823	CLA	C4-C3-C5-C6
12	l	206	CLA	C4-C3-C5-C6
12	A	823	CLA	C4-C3-C5-C6
12	H	806	CLA	C2-C3-C5-C6
12	A	823	CLA	C2-C3-C5-C6
12	B	834	CLA	C2-C3-C5-C6
12	B	838	CLA	O1D-CGD-O2D-CED
15	l	203	BCR	C17-C18-C19-C20
12	l	205	CLA	C10-C11-C12-C13
12	A	828	CLA	C5-C6-C7-C8
12	B	819	CLA	CAA-CBA-CGA-O1A
12	B	819	CLA	CAA-CBA-CGA-O2A
12	H	802	CLA	C11-C10-C8-C9
12	a	839	CLA	C11-C12-C13-C14
12	b	810	CLA	C6-C7-C8-C9
12	b	823	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	A	807	CLA	C14-C13-C15-C16
12	B	822	CLA	C11-C10-C8-C9
12	B	838	CLA	C11-C12-C13-C14
12	H	801	CLA	C5-C6-C7-C8
12	A	831	CLA	C5-C6-C7-C8
18	b	845	LMG	C31-C32-C33-C34
11	a	801	CL0	C8-C10-C11-C12
12	G	808	CLA	C13-C15-C16-C17
12	G	825	CLA	C5-C6-C7-C8
12	H	838	CLA	C8-C10-C11-C12
12	a	833	CLA	C13-C15-C16-C17
12	G	839	CLA	C4-C3-C5-C6
12	H	835	CLA	C4-C3-C5-C6
12	b	806	CLA	C4-C3-C5-C6
12	b	833	CLA	C4-C3-C5-C6
12	B	806	CLA	C4-C3-C5-C6
12	B	837	CLA	C4-C3-C5-C6
12	b	806	CLA	C2-C3-C5-C6
13	G	843	1L3	C20-C21-C23-C24
12	b	803	CLA	O1D-CGD-O2D-CED
12	a	820	CLA	C13-C15-C16-C17
12	G	834	CLA	C16-C17-C18-C19
12	A	837	CLA	C16-C17-C18-C20
12	A	811	CLA	CAA-CBA-CGA-O2A
12	G	833	CLA	C13-C15-C16-C17
16	a	850	LHG	O10-C23-O8-C6
12	S	202	CLA	C2A-CAA-CBA-CGA
12	G	825	CLA	C16-C17-C18-C19
12	G	827	CLA	O1A-CGA-O2A-C1
12	a	841	CLA	C15-C16-C17-C18
12	H	838	CLA	C4-C3-C5-C6
12	a	839	CLA	C4-C3-C5-C6
15	H	844	BCR	C19-C20-C21-C22
12	G	812	CLA	CAA-CBA-CGA-O2A
12	F	203	CLA	CAA-CBA-CGA-O2A
12	B	806	CLA	C2-C3-C5-C6
12	A	824	CLA	C16-C17-C18-C19
19	B	847	LMT	C4B-C5B-C6B-O6B
12	G	821	CLA	C4B-C3B-CAB-CBB
12	H	835	CLA	C4B-C3B-CAB-CBB
12	a	818	CLA	C4B-C3B-CAB-CBB
12	b	818	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	b	833	CLA	C4B-C3B-CAB-CBB
12	b	848	CLA	C4B-C3B-CAB-CBB
12	A	818	CLA	C4B-C3B-CAB-CBB
12	A	827	CLA	C4B-C3B-CAB-CBB
12	A	855	CLA	C4B-C3B-CAB-CBB
12	B	821	CLA	C4B-C3B-CAB-CBB
12	B	823	CLA	C4B-C3B-CAB-CBB
12	B	834	CLA	C4B-C3B-CAB-CBB
12	G	856	CLA	C15-C16-C17-C18
12	G	838	CLA	CAA-CBA-CGA-O2A
12	f	203	CLA	CAA-CBA-CGA-O2A
12	B	807	CLA	C8-C10-C11-C12
18	B	846	LMG	C31-C32-C33-C34
12	G	835	CLA	CAA-CBA-CGA-O2A
12	H	820	CLA	CAA-CBA-CGA-O2A
12	H	836	CLA	CAA-CBA-CGA-O2A
12	P	203	CLA	CAA-CBA-CGA-O1A
12	P	203	CLA	CAA-CBA-CGA-O2A
12	G	834	CLA	C16-C17-C18-C20
12	H	811	CLA	C16-C17-C18-C19
12	A	841	CLA	C16-C17-C18-C19
12	G	829	CLA	CAA-CBA-CGA-O2A
12	G	838	CLA	CAA-CBA-CGA-O1A
12	F	203	CLA	CAA-CBA-CGA-O1A
12	G	819	CLA	C4-C3-C5-C6
12	b	824	CLA	C4-C3-C5-C6
12	A	839	CLA	C4-C3-C5-C6
12	H	835	CLA	C2-C3-C5-C6
12	a	820	CLA	C12-C13-C15-C16
12	A	807	CLA	C12-C13-C15-C16
12	B	810	CLA	C11-C12-C13-C15
12	H	820	CLA	CAA-CBA-CGA-O1A
12	a	811	CLA	CAA-CBA-CGA-O2A
12	A	835	CLA	CAA-CBA-CGA-O2A
12	a	834	CLA	C5-C6-C7-C8
12	B	810	CLA	C15-C16-C17-C18
12	H	816	CLA	C11-C12-C13-C14
12	H	824	CLA	C11-C12-C13-C14
12	H	850	CLA	C11-C10-C8-C9
12	b	805	CLA	C6-C7-C8-C9
12	A	803	CLA	C6-C7-C8-C9
12	A	806	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	B	823	CLA	C11-C12-C13-C14
16	G	852	LHG	O10-C23-C24-C25
16	A	850	LHG	C9-C10-C11-C12
12	G	812	CLA	CAA-CBA-CGA-O1A
12	H	836	CLA	CAA-CBA-CGA-O1A
12	b	834	CLA	CAA-CBA-CGA-O1A
12	f	203	CLA	CAA-CBA-CGA-O1A
12	H	820	CLA	C2A-CAA-CBA-CGA
12	G	836	CLA	C2-C1-O2A-CGA
12	H	825	CLA	C2-C1-O2A-CGA
12	H	835	CLA	C2-C1-O2A-CGA
12	S	202	CLA	C2-C1-O2A-CGA
12	b	823	CLA	C2-C1-O2A-CGA
12	b	824	CLA	C2-C1-O2A-CGA
12	b	826	CLA	C2-C1-O2A-CGA
12	l	206	CLA	C2-C1-O2A-CGA
12	A	832	CLA	C2-C1-O2A-CGA
19	H	848	LMT	C2-C3-C4-C5
12	a	834	CLA	C3A-C2A-CAA-CBA
12	a	840	CLA	C3A-C2A-CAA-CBA
12	b	827	CLA	C3A-C2A-CAA-CBA
12	f	201	CLA	C3A-C2A-CAA-CBA
12	A	826	CLA	C3A-C2A-CAA-CBA
12	A	840	CLA	C3A-C2A-CAA-CBA
12	b	824	CLA	CAA-CBA-CGA-O1A
12	b	834	CLA	CAA-CBA-CGA-O2A
12	A	814	CLA	CAA-CBA-CGA-O2A
16	a	851	LHG	O10-C23-O8-C6
12	G	819	CLA	C2-C3-C5-C6
12	b	805	CLA	C3-C5-C6-C7
12	a	833	CLA	C5-C6-C7-C8
12	B	835	CLA	CAA-CBA-CGA-O2A
12	a	854	CLA	O2A-C1-C2-C3
15	b	847	BCR	C10-C11-C12-C13
15	A	845	BCR	C10-C11-C12-C13
12	G	815	CLA	CAA-CBA-CGA-O2A
12	j	104	CLA	CAA-CBA-CGA-O2A
12	A	811	CLA	CAA-CBA-CGA-O1A
12	A	835	CLA	CAA-CBA-CGA-O1A
12	G	837	CLA	C10-C11-C12-C13
12	a	811	CLA	CAA-CBA-CGA-O1A
12	a	814	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	B	835	CLA	CAA-CBA-CGA-O1A
12	G	829	CLA	C13-C15-C16-C17
12	G	834	CLA	C13-C15-C16-C17
12	B	834	CLA	C13-C15-C16-C17
12	H	826	CLA	CBA-CGA-O2A-C1
12	b	825	CLA	CBA-CGA-O2A-C1
16	A	850	LHG	C4-C5-C6-O8
12	b	824	CLA	CBD-CGD-O2D-CED
12	B	838	CLA	CBD-CGD-O2D-CED
12	G	807	CLA	C5-C6-C7-C8
12	a	855	CLA	C15-C16-C17-C18
12	b	810	CLA	C15-C16-C17-C18
12	A	818	CLA	C16-C17-C18-C19
12	b	807	CLA	C3-C5-C6-C7
12	B	824	CLA	CAA-CBA-CGA-O1A
12	A	834	CLA	C2A-CAA-CBA-CGA
12	H	830	CLA	CAA-CBA-CGA-O2A
12	A	814	CLA	CAA-CBA-CGA-O1A
12	G	842	CLA	C5-C6-C7-C8
12	A	824	CLA	C5-C6-C7-C8
12	J	103	CLA	CAA-CBA-CGA-O2A
16	a	851	LHG	C24-C23-O8-C6
12	a	839	CLA	CAA-CBA-CGA-O2A
12	b	805	CLA	CAA-CBA-CGA-O2A
12	A	841	CLA	CAA-CBA-CGA-O2A
18	b	845	LMG	O7-C10-C11-C12
16	a	850	LHG	C25-C26-C27-C28
12	a	814	CLA	CAA-CBA-CGA-O1A
12	A	833	CLA	C5-C6-C7-C8
12	G	804	CLA	C6-C7-C8-C9
12	a	803	CLA	C6-C7-C8-C9
12	b	821	CLA	C11-C12-C13-C14
12	b	835	CLA	C11-C12-C13-C14
12	l	202	CLA	C11-C10-C8-C9
12	A	834	CLA	C11-C12-C13-C14
12	A	839	CLA	C11-C12-C13-C14
12	B	805	CLA	C14-C13-C15-C16
12	A	824	CLA	C16-C17-C18-C20
12	G	818	CLA	CAA-CBA-CGA-O2A
12	G	841	CLA	CAA-CBA-CGA-O2A
12	G	815	CLA	CAA-CBA-CGA-O1A
12	G	835	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	j	104	CLA	CAA-CBA-CGA-O1A
16	A	850	LHG	C30-C31-C32-C33
15	f	202	BCR	C21-C22-C23-C24
12	G	817	CLA	CAA-CBA-CGA-O2A
12	A	817	CLA	CAA-CBA-CGA-O2A
16	G	851	LHG	O8-C23-C24-C25
12	L	204	CLA	C2A-CAA-CBA-CGA
12	G	829	CLA	C11-C12-C13-C15
12	H	802	CLA	C11-C10-C8-C7
12	H	808	CLA	C6-C7-C8-C10
12	H	824	CLA	C11-C12-C13-C15
12	H	827	CLA	C11-C10-C8-C7
12	H	831	CLA	C11-C12-C13-C15
12	H	837	CLA	C11-C12-C13-C15
12	H	838	CLA	C6-C7-C8-C10
12	a	806	CLA	C11-C12-C13-C15
12	a	807	CLA	C12-C13-C15-C16
12	b	805	CLA	C6-C7-C8-C10
12	b	823	CLA	C11-C12-C13-C15
12	j	102	CLA	C11-C12-C13-C15
12	A	806	CLA	C11-C12-C13-C15
12	B	823	CLA	C11-C12-C13-C15
12	B	824	CLA	C11-C12-C13-C15
12	B	824	CLA	C12-C13-C15-C16
12	B	838	CLA	C11-C12-C13-C15
11	G	801	CL0	C2B-C3B-CAB-CBB
11	A	801	CL0	C2B-C3B-CAB-CBB
12	G	855	CLA	C2B-C3B-CAB-CBB
12	H	833	CLA	C2B-C3B-CAB-CBB
12	H	835	CLA	C2B-C3B-CAB-CBB
12	S	202	CLA	C2B-C3B-CAB-CBB
12	a	802	CLA	C2B-C3B-CAB-CBB
12	a	818	CLA	C2B-C3B-CAB-CBB
12	a	855	CLA	C2B-C3B-CAB-CBB
12	b	814	CLA	C2B-C3B-CAB-CBB
12	b	831	CLA	C2B-C3B-CAB-CBB
12	A	818	CLA	C2B-C3B-CAB-CBB
12	A	820	CLA	C2B-C3B-CAB-CBB
12	A	855	CLA	C2B-C3B-CAB-CBB
12	B	822	CLA	C2B-C3B-CAB-CBB
12	B	823	CLA	C2B-C3B-CAB-CBB
12	B	832	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	H	841	BCR	C5-C6-C7-C8
15	H	846	BCR	C1-C6-C7-C8
15	H	846	BCR	C5-C6-C7-C8
15	H	846	BCR	C23-C24-C25-C26
15	H	846	BCR	C23-C24-C25-C30
15	H	849	BCR	C1-C6-C7-C8
15	H	849	BCR	C5-C6-C7-C8
15	H	849	BCR	C23-C24-C25-C26
15	Q	102	BCR	C5-C6-C7-C8
15	R	101	BCR	C5-C6-C7-C8
15	b	844	BCR	C5-C6-C7-C8
15	b	847	BCR	C5-C6-C7-C8
15	i	102	BCR	C5-C6-C7-C8
15	j	101	BCR	C1-C6-C7-C8
15	j	101	BCR	C5-C6-C7-C8
15	l	201	BCR	C23-C24-C25-C26
15	l	201	BCR	C23-C24-C25-C30
15	B	844	BCR	C23-C24-C25-C26
15	B	844	BCR	C23-C24-C25-C30
15	B	845	BCR	C5-C6-C7-C8
15	J	101	BCR	C5-C6-C7-C8
15	J	102	BCR	C23-C24-C25-C26
15	J	104	BCR	C5-C6-C7-C8
15	L	201	BCR	C23-C24-C25-C26
15	L	201	BCR	C23-C24-C25-C30
15	L	207	BCR	C5-C6-C7-C8
17	M	101	45D	C03-C07-C19-C23
16	G	851	LHG	C8-C7-O7-C5
12	B	805	CLA	CAA-CBA-CGA-O2A
12	G	830	CLA	C2-C1-O2A-CGA
12	G	837	CLA	C2-C1-O2A-CGA
12	H	824	CLA	C2-C1-O2A-CGA
12	H	827	CLA	C2-C1-O2A-CGA
12	a	810	CLA	C2-C1-O2A-CGA
12	a	837	CLA	C2-C1-O2A-CGA
12	f	201	CLA	C2-C1-O2A-CGA
18	H	847	LMG	C13-C14-C15-C16
18	B	846	LMG	C13-C14-C15-C16
12	B	803	CLA	C16-C17-C18-C19
12	b	836	CLA	C8-C10-C11-C12
12	B	837	CLA	C8-C10-C11-C12
12	F	201	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	a	807	CLA	C8-C10-C11-C12
12	G	805	CLA	CAA-CBA-CGA-O2A
18	H	847	LMG	O7-C10-C11-C12
12	P	201	CLA	C16-C17-C18-C19
12	b	824	CLA	C16-C17-C18-C19
16	a	853	LHG	O7-C7-C8-C9
18	B	846	LMG	O7-C10-C11-C12
19	B	847	LMT	C1-C2-C3-C4
12	b	805	CLA	C2A-CAA-CBA-CGA
12	B	819	CLA	C2A-CAA-CBA-CGA
12	H	805	CLA	CAA-CBA-CGA-O2A
12	A	807	CLA	C8-C10-C11-C12
12	H	824	CLA	C8-C10-C11-C12
12	a	820	CLA	C5-C6-C7-C8
19	H	848	LMT	C9-C10-C11-C12
16	G	854	LHG	O7-C7-C8-C9
16	a	850	LHG	O8-C23-C24-C25
12	B	821	CLA	C2-C3-C5-C6
12	B	838	CLA	C2-C3-C5-C6
12	G	833	CLA	C5-C6-C7-C8
16	a	850	LHG	C30-C31-C32-C33
12	G	810	CLA	C2A-CAA-CBA-CGA
12	R	103	CLA	CAA-CBA-CGA-O2A
12	H	824	CLA	CAA-CBA-CGA-O2A
12	a	817	CLA	CAA-CBA-CGA-O2A
12	a	841	CLA	CAA-CBA-CGA-O2A
12	A	804	CLA	CAA-CBA-CGA-O2A
12	b	833	CLA	C5-C6-C7-C8
19	b	846	LMT	C2-C3-C4-C5
12	H	805	CLA	C14-C13-C15-C16
12	H	830	CLA	C6-C7-C8-C9
12	H	838	CLA	C11-C10-C8-C9
12	a	834	CLA	C11-C12-C13-C14
12	b	801	CLA	C11-C10-C8-C9
12	l	202	CLA	C6-C7-C8-C9
12	A	829	CLA	C11-C10-C8-C9
12	B	824	CLA	C6-C7-C8-C9
15	H	849	BCR	C7-C8-C9-C34
15	f	202	BCR	C11-C12-C13-C35
12	B	829	CLA	CAA-CBA-CGA-O2A
16	A	850	LHG	O8-C23-C24-C25
16	A	853	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	H	826	CLA	O1A-CGA-O2A-C1
12	G	804	CLA	C4B-C3B-CAB-CBB
12	G	827	CLA	C1A-C2A-CAA-CBA
12	G	834	CLA	C1A-C2A-CAA-CBA
12	H	822	CLA	C4B-C3B-CAB-CBB
12	S	202	CLA	C4B-C3B-CAB-CBB
12	a	825	CLA	C4B-C3B-CAB-CBB
12	a	826	CLA	C1A-C2A-CAA-CBA
12	f	201	CLA	C4B-C3B-CAB-CBB
12	l	202	CLA	C4B-C3B-CAB-CBB
12	A	820	CLA	C4B-C3B-CAB-CBB
12	A	825	CLA	C4B-C3B-CAB-CBB
12	A	826	CLA	C1A-C2A-CAA-CBA
12	A	836	CLA	C1A-C2A-CAA-CBA
12	L	202	CLA	C4B-C3B-CAB-CBB
16	A	853	LHG	C27-C28-C29-C30
12	S	203	CLA	CAA-CBA-CGA-O2A
12	a	804	CLA	CAA-CBA-CGA-O2A
12	B	810	CLA	CAA-CBA-CGA-O2A
12	B	823	CLA	CAA-CBA-CGA-O2A
12	L	205	CLA	CAA-CBA-CGA-O2A
15	H	849	BCR	C7-C8-C9-C10
15	P	202	BCR	C21-C22-C23-C24
15	a	845	BCR	C17-C18-C19-C20
15	H	841	BCR	C13-C14-C15-C16
15	R	101	BCR	C15-C16-C17-C18
15	S	205	BCR	C19-C20-C21-C22
15	j	101	BCR	C15-C16-C17-C18
15	B	843	BCR	C19-C20-C21-C22
15	L	207	BCR	C13-C14-C15-C16
12	H	833	CLA	CAA-CBA-CGA-O2A
12	J	103	CLA	CAA-CBA-CGA-O1A
12	G	808	CLA	C2A-CAA-CBA-CGA
12	G	832	CLA	C2A-CAA-CBA-CGA
12	b	805	CLA	C13-C15-C16-C17
12	b	835	CLA	C15-C16-C17-C18
12	G	827	CLA	C4-C3-C5-C6
11	G	801	CL0	C2-C1-O2A-CGA
12	b	833	CLA	C2-C1-O2A-CGA
12	A	827	CLA	C2-C1-O2A-CGA
12	A	836	CLA	C2-C1-O2A-CGA
12	B	824	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	B	834	CLA	C2-C1-O2A-CGA
12	L	204	CLA	C2-C1-O2A-CGA
12	b	803	CLA	CAA-CBA-CGA-O2A
12	G	802	CLA	C6-C7-C8-C10
12	b	801	CLA	C11-C10-C8-C7
12	b	837	CLA	C11-C12-C13-C15
12	B	801	CLA	C11-C10-C8-C7
12	B	830	CLA	C11-C12-C13-C15
12	b	833	CLA	C2-C3-C5-C6
12	b	836	CLA	C2-C3-C5-C6
12	b	810	CLA	C5-C6-C7-C8
12	b	837	CLA	C13-C15-C16-C17
12	f	201	CLA	C16-C17-C18-C19
12	G	855	CLA	O2A-C1-C2-C3
12	H	837	CLA	C15-C16-C17-C18
12	A	816	CLA	CAA-CBA-CGA-O2A
12	L	206	CLA	O1D-CGD-O2D-CED
12	B	802	CLA	CBA-CGA-O2A-C1
16	G	851	LHG	O10-C23-C24-C25
12	B	805	CLA	C2A-CAA-CBA-CGA
12	A	823	CLA	C6-C7-C8-C9
12	G	827	CLA	C3A-C2A-CAA-CBA
12	a	826	CLA	C3A-C2A-CAA-CBA
18	B	846	LMG	O9-C10-C11-C12
12	a	854	CLA	C8-C10-C11-C12
12	b	824	CLA	C2-C3-C5-C6
13	A	842	1L3	C20-C21-C23-C24
12	b	810	CLA	C13-C15-C16-C17
12	a	839	CLA	CAA-CBA-CGA-O1A
12	L	205	CLA	CAA-CBA-CGA-O1A
16	G	854	LHG	O9-C7-C8-C9
16	a	853	LHG	O9-C7-C8-C9
19	B	847	LMT	C4'-C5'-C6'-O6'
12	b	825	CLA	O1A-CGA-O2A-C1
12	A	817	CLA	CAA-CBA-CGA-O1A
12	B	805	CLA	CAA-CBA-CGA-O1A
12	B	814	CLA	C6-C7-C8-C9
18	H	847	LMG	C15-C16-C17-C18
16	A	853	LHG	C35-C36-C37-C38
12	a	809	CLA	C2A-CAA-CBA-CGA
12	B	825	CLA	CBA-CGA-O2A-C1
12	G	802	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	G	830	CLA	C11-C10-C8-C9
12	G	834	CLA	C11-C12-C13-C14
12	H	825	CLA	C6-C7-C8-C9
12	a	820	CLA	C14-C13-C15-C16
12	a	829	CLA	C11-C10-C8-C9
12	A	820	CLA	C14-C13-C15-C16
12	B	838	CLA	C6-C7-C8-C9
16	a	853	LHG	O10-C23-C24-C25
18	b	845	LMG	O9-C10-C11-C12
12	B	809	CLA	CAA-CBA-CGA-O2A
12	S	202	CLA	C5-C6-C7-C8
12	H	805	CLA	CAA-CBA-CGA-O1A
12	H	835	CLA	C8-C10-C11-C12
12	H	826	CLA	O1D-CGD-O2D-CED
12	G	818	CLA	CAA-CBA-CGA-O1A
12	G	841	CLA	CAA-CBA-CGA-O1A
12	a	817	CLA	CAA-CBA-CGA-O1A
12	A	804	CLA	CAA-CBA-CGA-O1A
12	A	816	CLA	CAA-CBA-CGA-O1A
12	H	823	CLA	C5-C6-C7-C8
12	a	825	CLA	C5-C6-C7-C8
12	b	821	CLA	C13-C15-C16-C17
12	a	816	CLA	CAA-CBA-CGA-O2A
15	i	101	BCR	C17-C18-C19-C20
12	b	805	CLA	CAA-CBA-CGA-O1A
16	A	850	LHG	O10-C23-C24-C25
12	H	807	CLA	C10-C11-C12-C13
12	G	839	CLA	O1A-CGA-O2A-C1
12	H	824	CLA	CAA-CBA-CGA-O1A
12	a	841	CLA	CAA-CBA-CGA-O1A
18	H	847	LMG	O9-C10-C11-C12
12	L	206	CLA	CAA-CBA-CGA-O2A
12	l	202	CLA	C8-C10-C11-C12
12	G	823	CLA	C2A-CAA-CBA-CGA
18	b	845	LMG	C21-C22-C23-C24
12	H	833	CLA	CAA-CBA-CGA-O1A
12	R	103	CLA	CAA-CBA-CGA-O1A
12	b	809	CLA	CAA-CBA-CGA-O2A
12	G	817	CLA	CAA-CBA-CGA-O1A
12	a	804	CLA	CAA-CBA-CGA-O1A
12	A	841	CLA	CAA-CBA-CGA-O1A
16	A	853	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	H	814	CLA	C4-C3-C5-C6
16	G	851	LHG	C18-C19-C20-C21
12	G	834	CLA	C5-C6-C7-C8
12	H	835	CLA	C5-C6-C7-C8
12	S	204	CLA	CAA-CBA-CGA-O2A
12	b	829	CLA	CAA-CBA-CGA-O2A
12	b	807	CLA	C10-C11-C12-C13
15	b	842	BCR	C19-C20-C21-C22
12	G	805	CLA	CAA-CBA-CGA-O1A
12	B	810	CLA	CAA-CBA-CGA-O1A
16	a	850	LHG	O10-C23-C24-C25
16	G	851	LHG	O9-C7-O7-C5
12	H	808	CLA	CAD-CBD-CGD-O2D
12	H	816	CLA	CAD-CBD-CGD-O2D
12	H	834	CLA	CAD-CBD-CGD-O2D
12	a	814	CLA	CAD-CBD-CGD-O2D
12	A	804	CLA	CAD-CBD-CGD-O2D
12	J	103	CLA	CAD-CBD-CGD-O2D
12	H	811	CLA	CAA-CBA-CGA-O2A
12	b	803	CLA	CAA-CBA-CGA-O1A
11	A	801	CL0	C15-C16-C17-C18
12	B	803	CLA	C15-C16-C17-C18
12	A	854	CLA	C10-C11-C12-C13
12	G	828	CLA	C2-C1-O2A-CGA
12	a	832	CLA	C2-C1-O2A-CGA
12	a	836	CLA	C2-C1-O2A-CGA
12	b	810	CLA	CAA-CBA-CGA-O2A
12	G	808	CLA	C8-C10-C11-C12
12	b	811	CLA	CAA-CBA-CGA-O2A
12	l	205	CLA	CAA-CBA-CGA-O2A
12	B	811	CLA	CAA-CBA-CGA-O2A
16	a	851	LHG	O7-C7-C8-C9
16	A	851	LHG	O7-C7-C8-C9
16	a	850	LHG	C8-C7-O7-C5
12	L	206	CLA	CAA-CBA-CGA-O1A
11	a	801	CL0	CAA-CBA-CGA-O2A
12	H	803	CLA	CAA-CBA-CGA-O2A
12	H	838	CLA	CAA-CBA-CGA-O2A
12	b	807	CLA	CAA-CBA-CGA-O2A
12	B	803	CLA	CAA-CBA-CGA-O2A
12	A	819	CLA	CAA-CBA-CGA-O2A
12	B	809	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	S	203	CLA	CAA-CBA-CGA-O1A
12	a	816	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

278 monomers are involved in 560 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	803	CLA	3	0
12	G	802	CLA	5	0
12	B	810	CLA	1	0
15	b	847	BCR	4	0
12	G	842	CLA	2	0
12	A	841	CLA	1	0
12	B	814	CLA	2	0
12	A	812	CLA	1	0
12	A	826	CLA	2	0
12	b	802	CLA	3	0
12	H	816	CLA	3	0
12	S	204	CLA	3	0
12	G	827	CLA	3	0
12	A	825	CLA	2	0
12	B	835	CLA	2	0
12	b	824	CLA	2	0
12	a	855	CLA	6	0
12	B	825	CLA	4	0
15	b	840	BCR	4	0
12	L	206	CLA	4	0
16	a	850	LHG	2	0
12	H	806	CLA	2	0
12	B	833	CLA	7	0
12	B	828	CLA	2	0
12	H	829	CLA	1	0
12	J	103	CLA	1	0
15	H	849	BCR	3	0
12	B	805	CLA	6	0
12	B	836	CLA	1	0
15	L	207	BCR	1	0
12	b	806	CLA	3	0
12	b	813	CLA	1	0
12	A	832	CLA	3	0
15	G	849	BCR	3	0
12	A	818	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	803	CLA	1	0
16	A	851	LHG	3	0
12	H	831	CLA	3	0
15	L	203	BCR	2	0
18	H	847	LMG	5	0
12	G	839	CLA	2	0
12	A	831	CLA	2	0
19	b	846	LMT	1	0
12	A	823	CLA	2	0
12	a	823	CLA	1	0
12	G	819	CLA	4	0
15	G	848	BCR	2	0
12	a	807	CLA	5	0
12	A	835	CLA	1	0
12	H	817	CLA	2	0
12	F	201	CLA	3	0
15	B	842	BCR	1	0
12	a	822	CLA	1	0
12	b	821	CLA	3	0
12	H	838	CLA	4	0
15	H	845	BCR	6	0
19	B	847	LMT	2	0
12	A	816	CLA	1	0
12	b	817	CLA	1	0
17	M	101	45D	3	0
17	m	101	45D	4	0
12	B	812	CLA	1	0
12	a	831	CLA	2	0
15	j	101	BCR	2	0
15	B	843	BCR	3	0
15	G	847	BCR	3	0
15	a	848	BCR	2	0
15	b	844	BCR	3	0
12	G	841	CLA	1	0
15	G	850	BCR	3	0
15	L	201	BCR	2	0
12	H	801	CLA	1	0
12	A	824	CLA	7	0
14	K	102	SF4	1	0
12	b	804	CLA	3	0
12	H	802	CLA	3	0
12	b	830	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	852	LHG	1	0
12	H	822	CLA	2	0
12	A	839	CLA	1	0
12	A	829	CLA	4	0
12	G	803	CLA	2	0
12	S	202	CLA	1	0
12	f	203	CLA	2	0
12	a	839	CLA	2	0
12	a	827	CLA	2	0
12	H	807	CLA	3	0
12	a	834	CLA	2	0
12	b	810	CLA	3	0
15	S	205	BCR	3	0
12	G	828	CLA	1	0
12	G	856	CLA	4	0
12	G	818	CLA	4	0
12	b	822	CLA	8	0
12	B	802	CLA	2	0
12	b	803	CLA	1	0
12	a	841	CLA	2	0
15	P	204	BCR	1	0
12	S	203	CLA	3	0
12	H	837	CLA	2	0
15	J	101	BCR	2	0
12	a	840	CLA	1	0
15	f	204	BCR	2	0
12	b	805	CLA	7	0
12	A	820	CLA	2	0
12	b	815	CLA	2	0
15	J	104	BCR	2	0
15	H	841	BCR	1	0
12	B	831	CLA	2	0
12	G	806	CLA	3	0
12	a	820	CLA	1	0
15	B	841	BCR	3	0
17	T	101	45D	3	0
15	H	844	BCR	4	0
12	G	813	CLA	1	0
15	A	849	BCR	5	0
16	G	854	LHG	1	0
12	H	825	CLA	5	0
12	H	808	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	804	CLA	3	0
12	G	804	CLA	2	0
15	J	102	BCR	2	0
12	l	204	CLA	2	0
12	B	803	CLA	1	0
12	A	837	CLA	1	0
15	a	845	BCR	2	0
12	G	826	CLA	2	0
12	b	832	CLA	5	0
15	b	841	BCR	1	0
12	G	810	CLA	1	0
15	A	847	BCR	1	0
12	G	833	CLA	2	0
15	I	101	BCR	4	0
12	b	826	CLA	2	0
12	A	828	CLA	2	0
12	G	855	CLA	3	0
12	H	805	CLA	5	0
12	A	802	CLA	3	0
12	A	827	CLA	3	0
15	G	846	BCR	1	0
12	A	833	CLA	3	0
12	b	834	CLA	2	0
12	A	855	CLA	3	0
12	b	825	CLA	4	0
12	H	834	CLA	4	0
15	H	846	BCR	2	0
12	A	806	CLA	2	0
12	A	821	CLA	1	0
12	a	821	CLA	1	0
12	H	832	CLA	2	0
15	a	847	BCR	3	0
16	G	851	LHG	3	0
12	L	205	CLA	3	0
12	B	806	CLA	3	0
12	G	840	CLA	1	0
12	b	807	CLA	2	0
15	a	852	BCR	1	0
12	a	854	CLA	5	0
15	b	839	BCR	1	0
15	b	843	BCR	6	0
12	G	817	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	b	848	CLA	2	0
12	L	202	CLA	2	0
15	B	845	BCR	3	0
12	G	835	CLA	2	0
12	G	823	CLA	1	0
15	A	852	BCR	2	0
12	a	814	CLA	1	0
15	F	202	BCR	3	0
12	B	823	CLA	2	0
15	l	201	BCR	2	0
12	H	835	CLA	4	0
12	H	824	CLA	3	0
12	H	827	CLA	1	0
12	l	205	CLA	4	0
12	G	824	CLA	4	0
12	a	824	CLA	5	0
12	B	827	CLA	2	0
12	a	812	CLA	2	0
12	B	830	CLA	4	0
12	B	834	CLA	2	0
12	a	826	CLA	3	0
12	b	823	CLA	2	0
12	R	103	CLA	1	0
12	H	828	CLA	3	0
12	H	811	CLA	2	0
12	G	807	CLA	2	0
12	G	825	CLA	7	0
12	a	825	CLA	1	0
12	A	808	CLA	1	0
12	B	824	CLA	1	0
12	l	206	CLA	3	0
15	R	101	BCR	2	0
12	a	832	CLA	3	0
12	a	828	CLA	6	0
15	j	103	BCR	3	0
12	a	818	CLA	5	0
12	A	834	CLA	2	0
12	b	835	CLA	2	0
12	B	822	CLA	6	0
12	a	802	CLA	3	0
12	A	817	CLA	1	0
12	A	805	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	822	CLA	1	0
15	A	848	BCR	2	0
12	a	805	CLA	4	0
18	B	846	LMG	4	0
15	G	853	BCR	1	0
12	b	829	CLA	1	0
12	b	833	CLA	2	0
15	i	101	BCR	3	0
15	H	843	BCR	4	0
12	H	804	CLA	3	0
12	b	828	CLA	2	0
15	A	846	BCR	3	0
12	G	808	CLA	3	0
12	a	809	CLA	2	0
12	H	826	CLA	3	0
12	b	836	CLA	5	0
12	b	816	CLA	2	0
16	a	851	LHG	1	0
12	a	833	CLA	4	0
12	G	829	CLA	5	0
15	a	849	BCR	3	0
12	a	829	CLA	3	0
15	Q	102	BCR	1	0
12	H	836	CLA	3	0
12	H	815	CLA	2	0
12	a	836	CLA	1	0
15	P	202	BCR	4	0
12	B	837	CLA	3	0
15	A	845	BCR	3	0
12	B	829	CLA	1	0
12	H	823	CLA	6	0
12	A	840	CLA	4	0
12	b	812	CLA	2	0
11	G	801	CL0	1	0
12	H	812	CLA	1	0
12	P	201	CLA	5	0
18	b	845	LMG	3	0
15	R	102	BCR	3	0
12	b	837	CLA	1	0
12	G	834	CLA	3	0
12	a	835	CLA	2	0
15	Q	101	BCR	4	0

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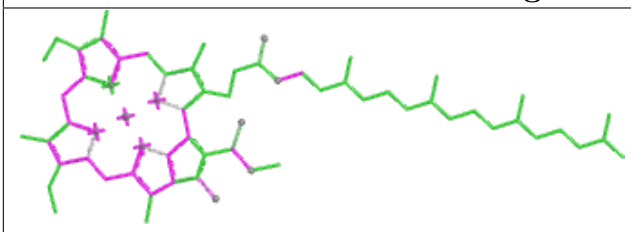
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	842	BCR	2	0
12	B	815	CLA	1	0
12	B	807	CLA	4	0
12	f	201	CLA	3	0
15	a	846	BCR	4	0
12	j	102	CLA	2	0
12	b	827	CLA	3	0
12	F	203	CLA	1	0
12	a	817	CLA	3	0
12	G	832	CLA	2	0
15	b	842	BCR	4	0
19	H	848	LMT	1	0
12	A	854	CLA	4	0
12	A	807	CLA	3	0
12	H	850	CLA	3	0
12	a	816	CLA	1	0
16	a	853	LHG	1	0
15	G	845	BCR	1	0
11	A	801	CL0	4	0
12	l	202	CLA	5	0
12	L	204	CLA	2	0
12	a	806	CLA	3	0
12	G	830	CLA	3	0
15	f	202	BCR	2	0
15	B	844	BCR	4	0
15	S	201	BCR	2	0
12	A	804	CLA	2	0
12	G	821	CLA	3	0
15	l	203	BCR	2	0
12	G	837	CLA	1	0
12	B	801	CLA	5	0
15	F	204	BCR	2	0
12	b	801	CLA	1	0

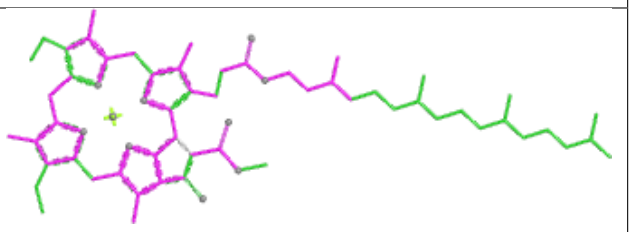
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

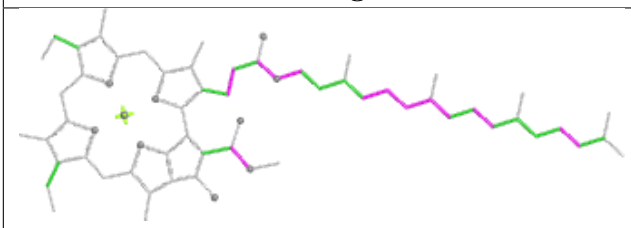
Ligand CLA A 803



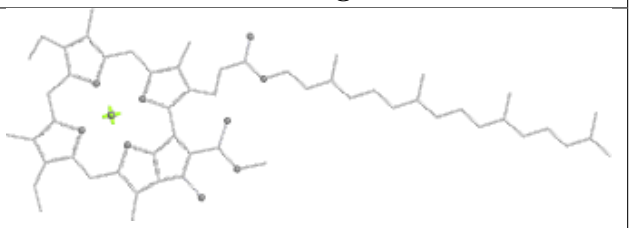
Bond lengths



Bond angles

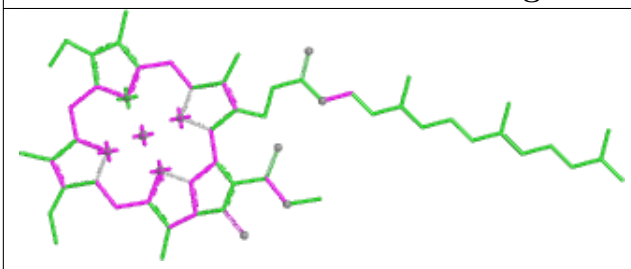


Torsions

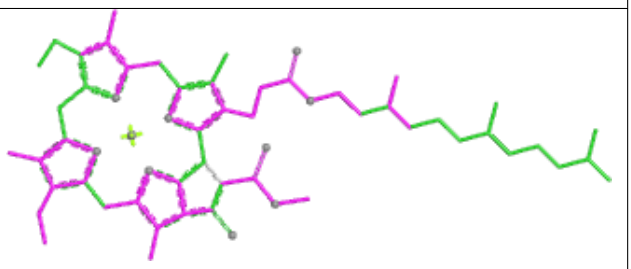


Rings

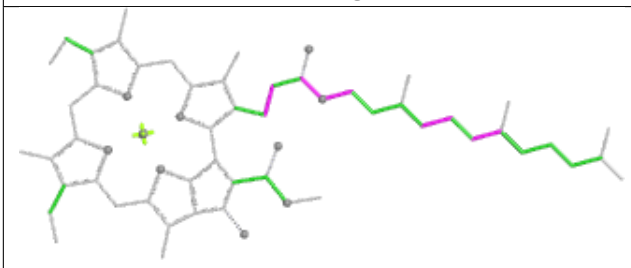
Ligand CLA G 802



Bond lengths



Bond angles



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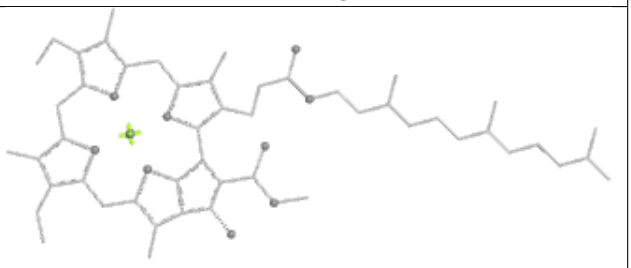
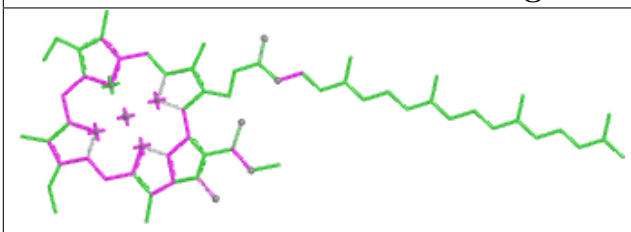
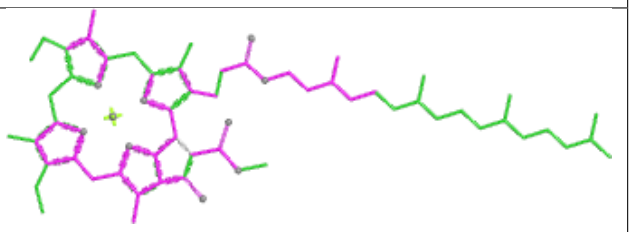


Rings

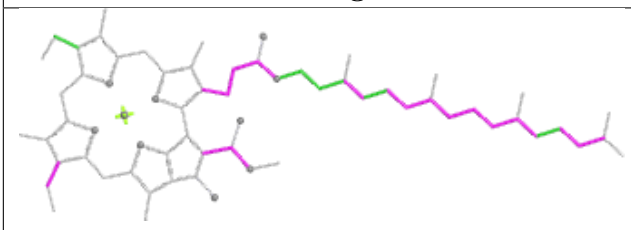
Ligand CLA B 810



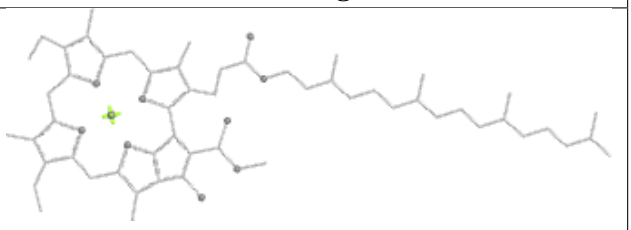
Bond lengths



Bond angles

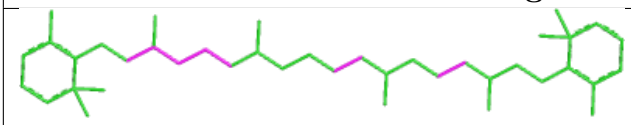


Torsions

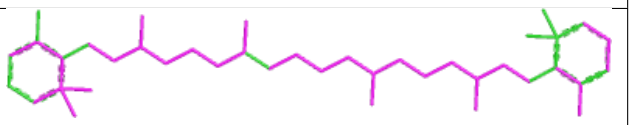


Rings

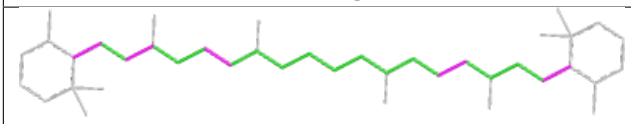
Ligand BCR b 847



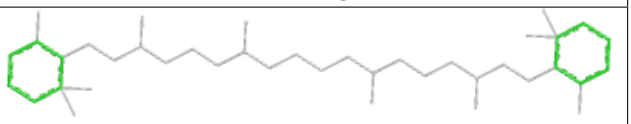
Bond lengths



Bond angles

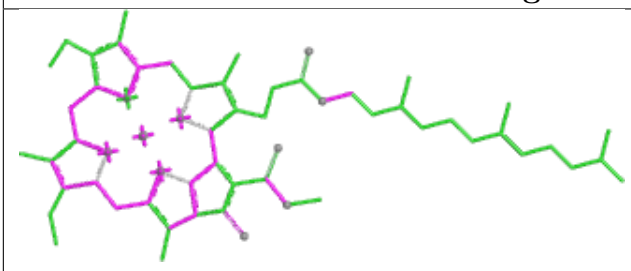


Torsions

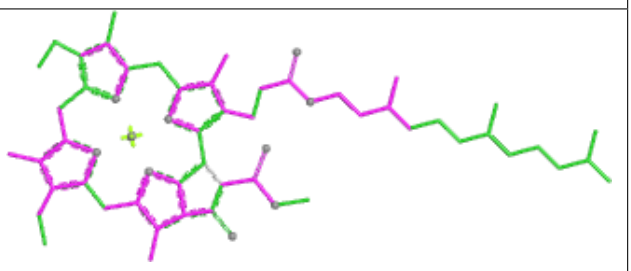


Rings

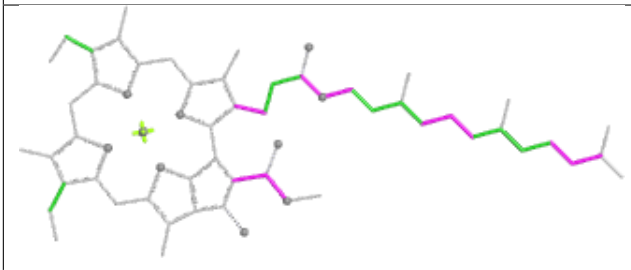
Ligand CLA G 842



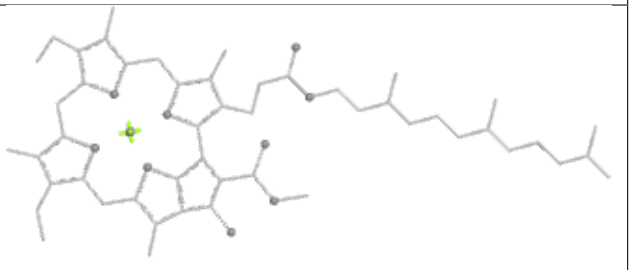
Bond lengths



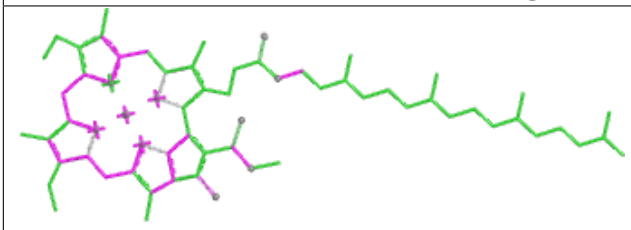
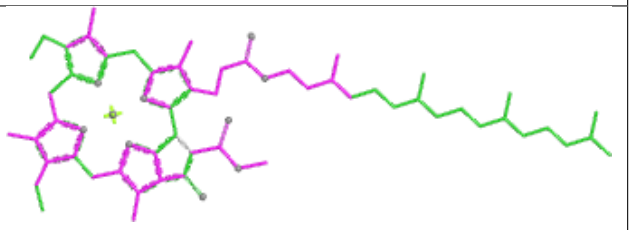
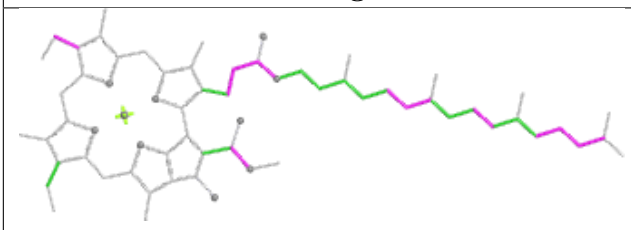
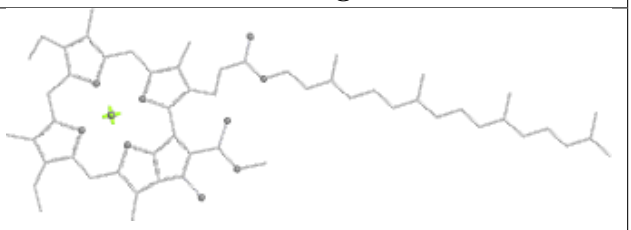
Bond angles

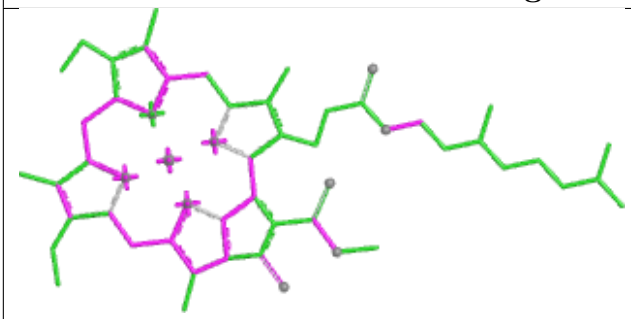
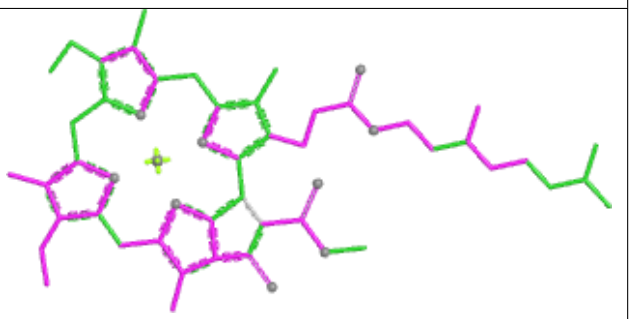
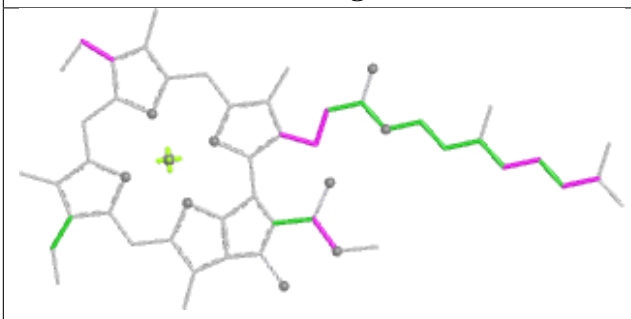
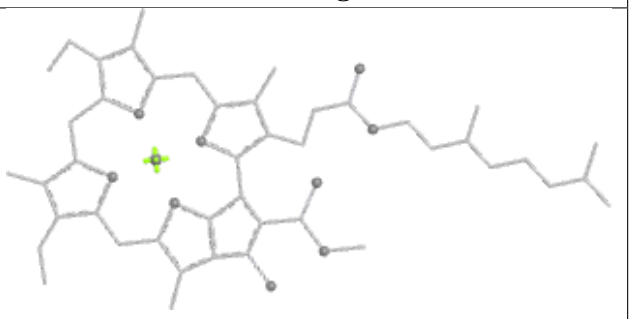


Torsions



Rings

Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

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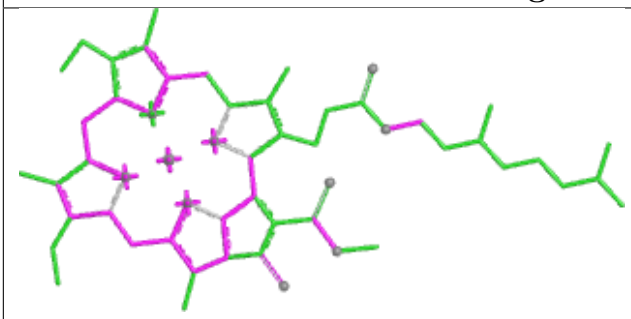
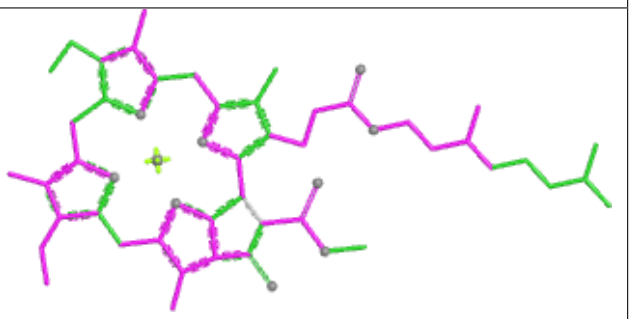
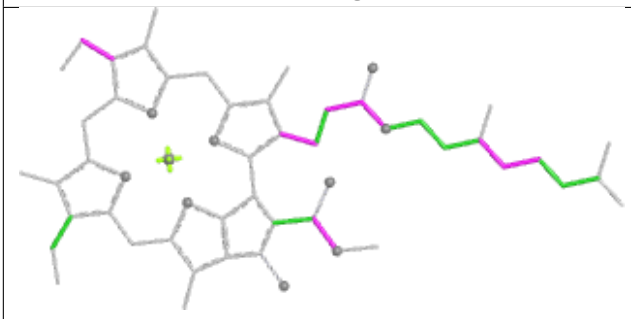
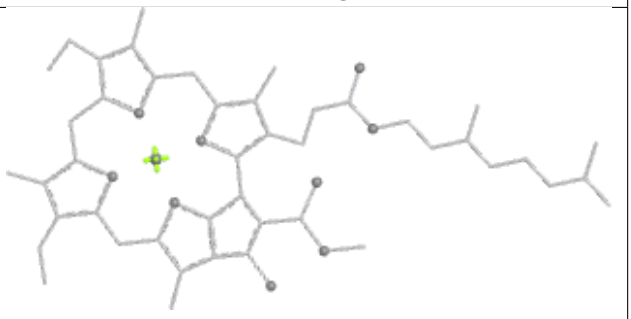
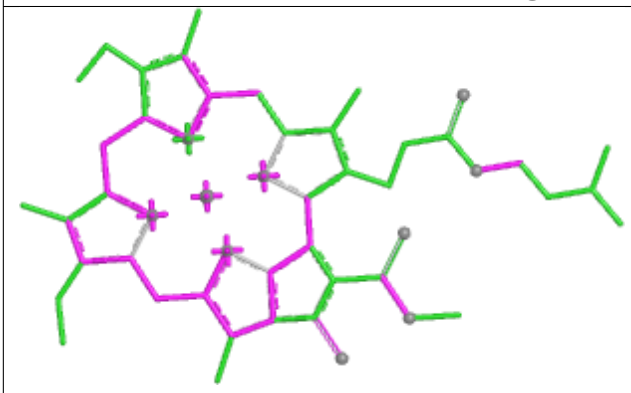
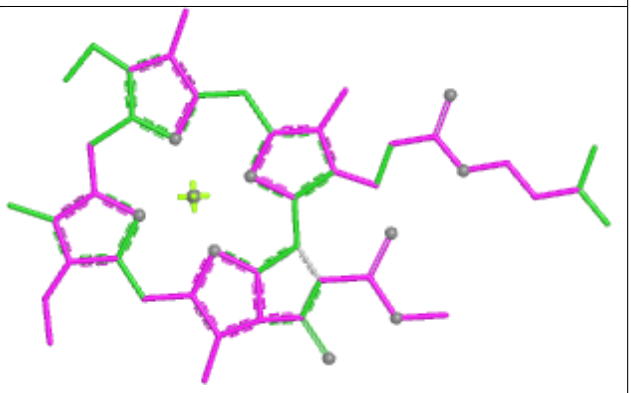
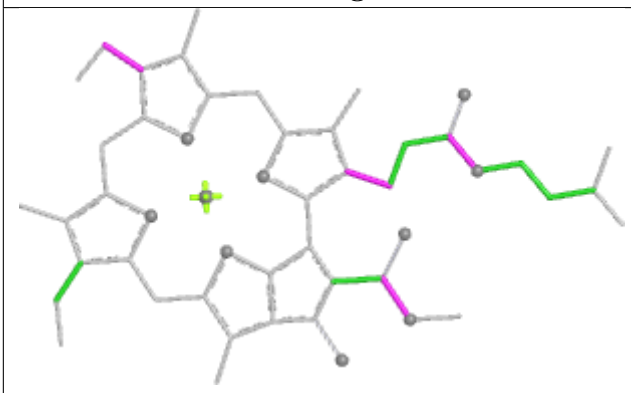
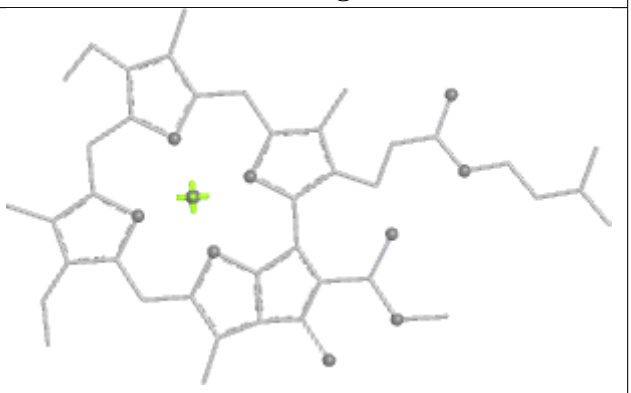
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

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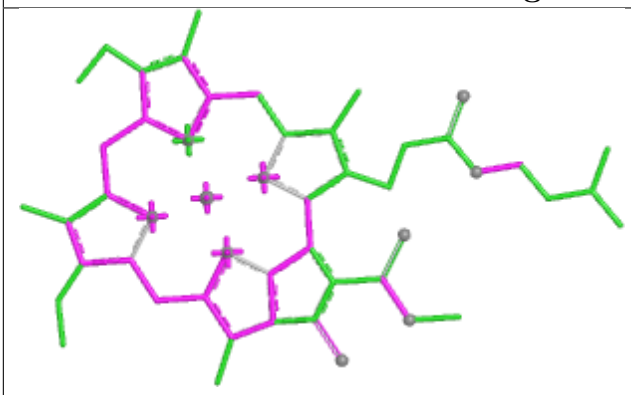
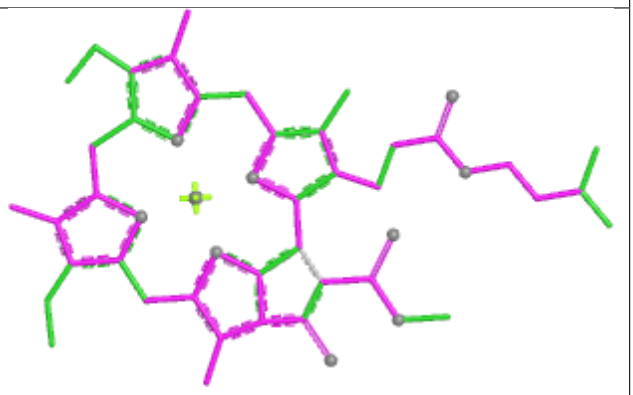
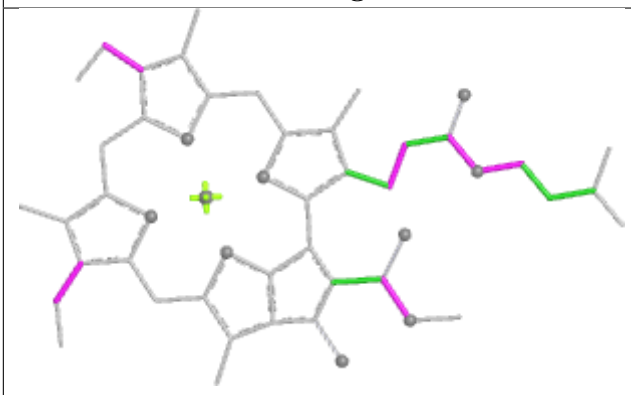


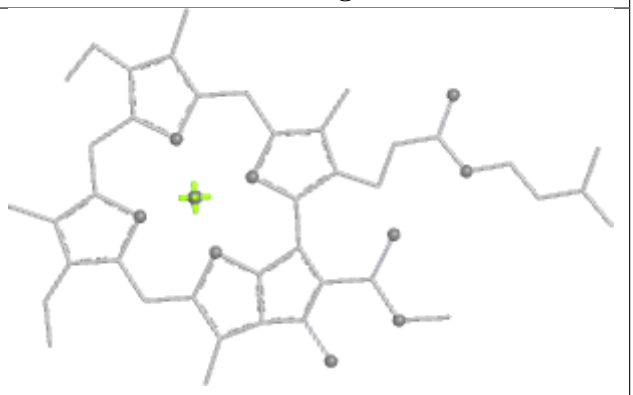
Bond lengths



Bond angles

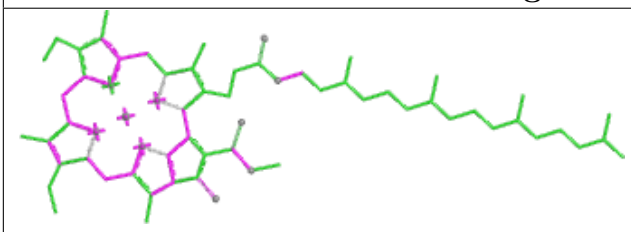


Torsions



Rings

Ligand CLA A 826



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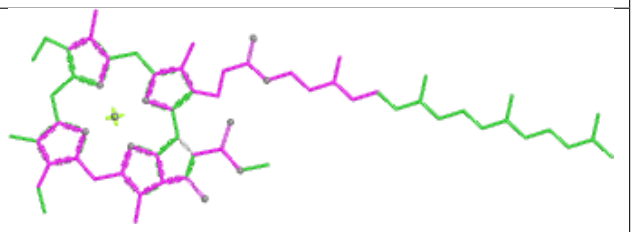
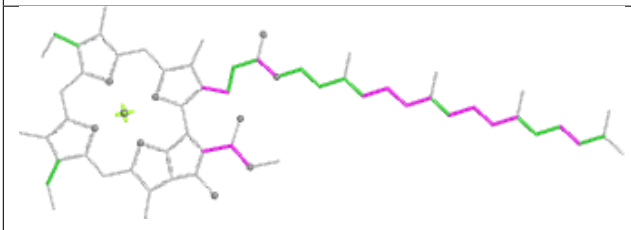


Bond angles



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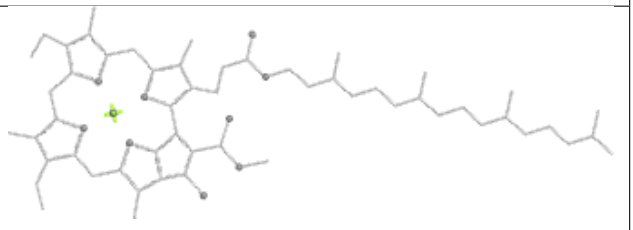
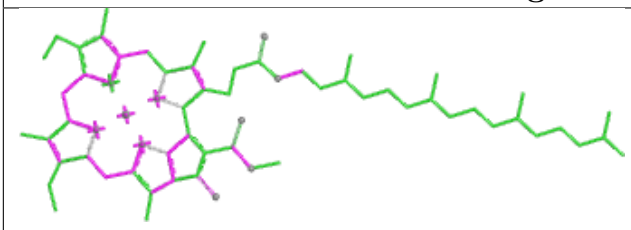


Rings

Ligand CLA b 802



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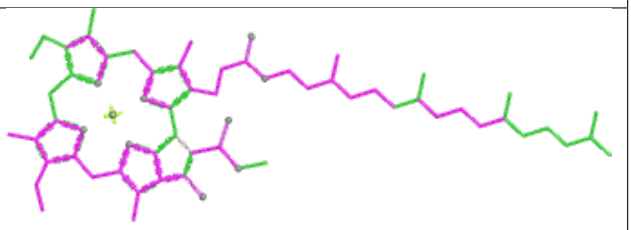

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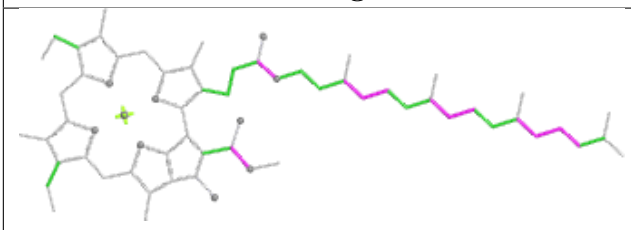

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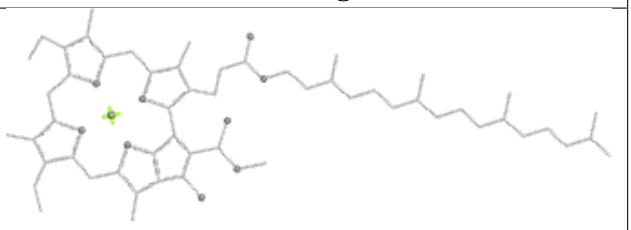
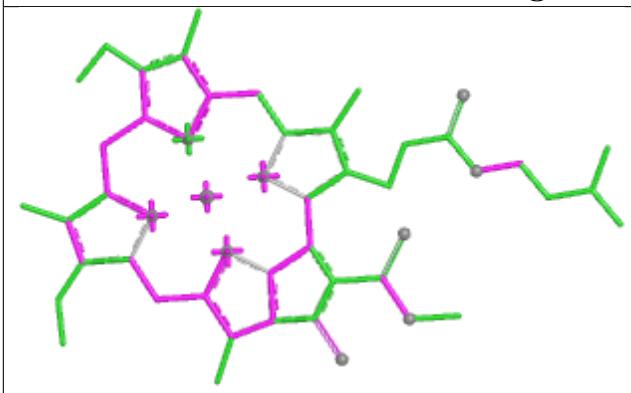


Rings

Ligand CLA a 810



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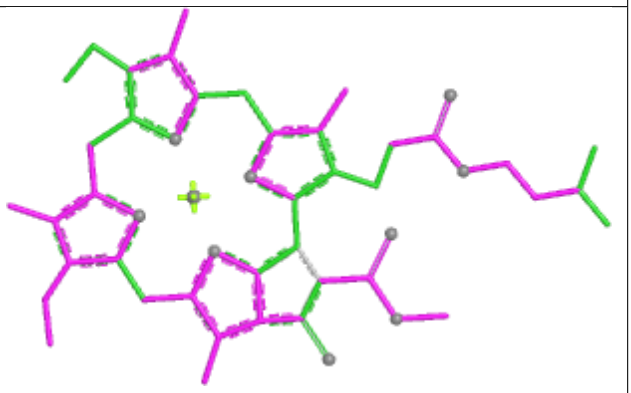

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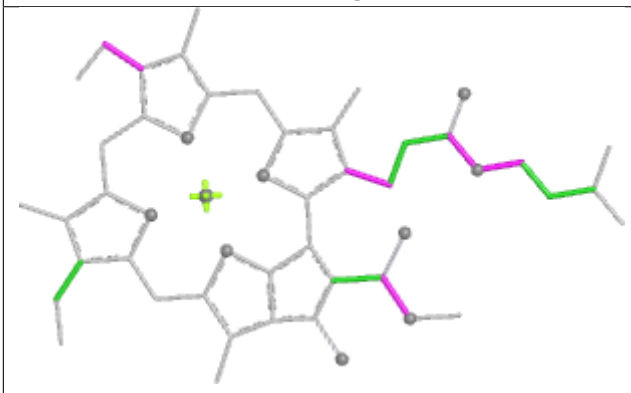

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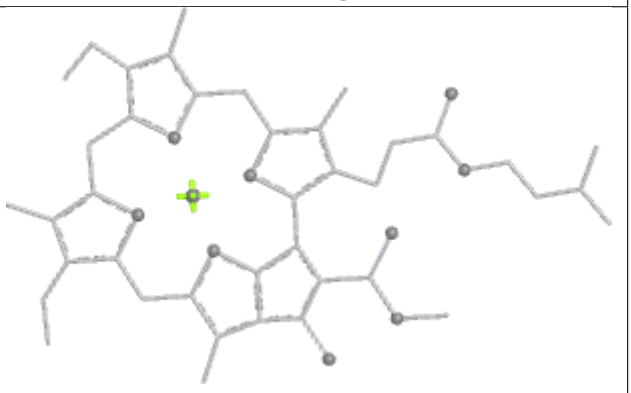
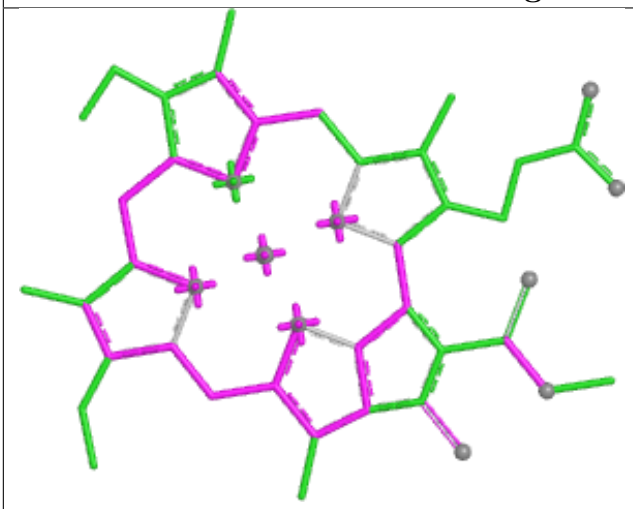


Rings

Ligand CLA B 819



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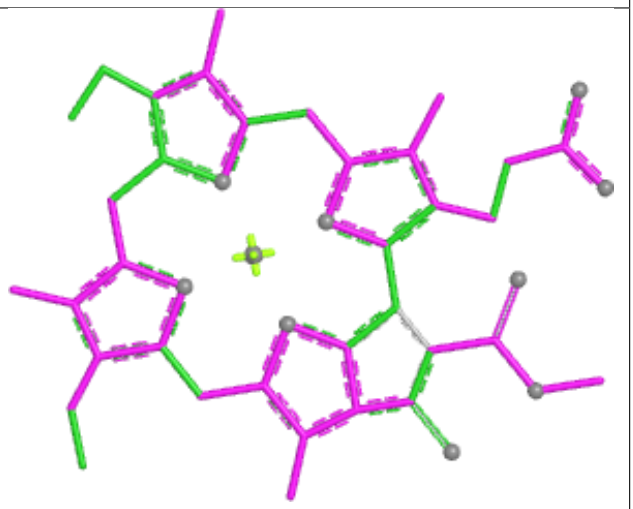
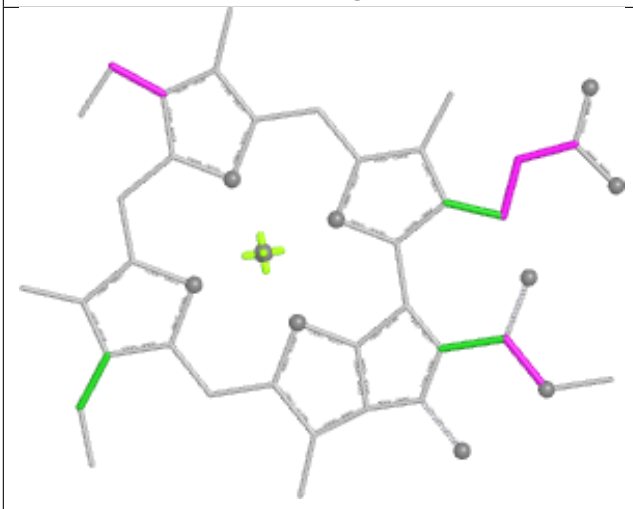


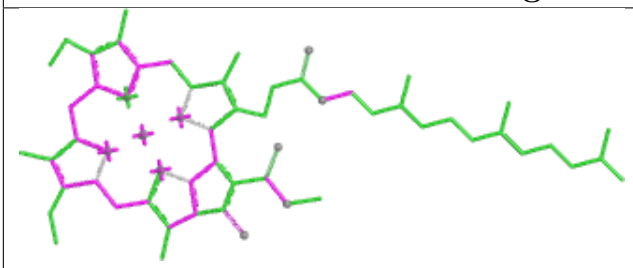
Bond angles



Torsions

Rings

Ligand CLA H 816



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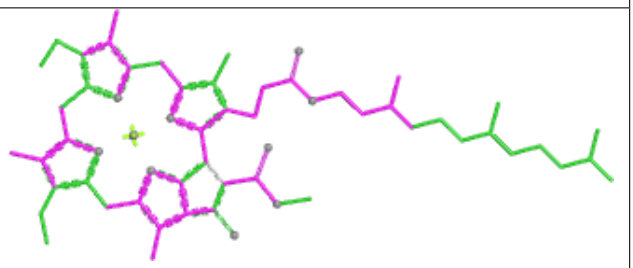

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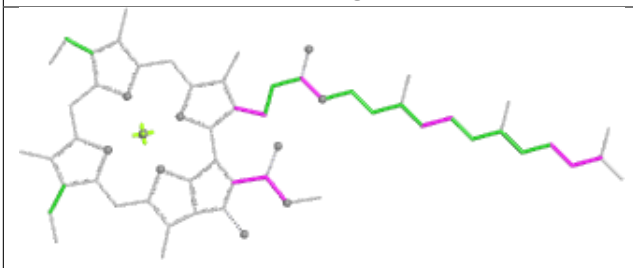
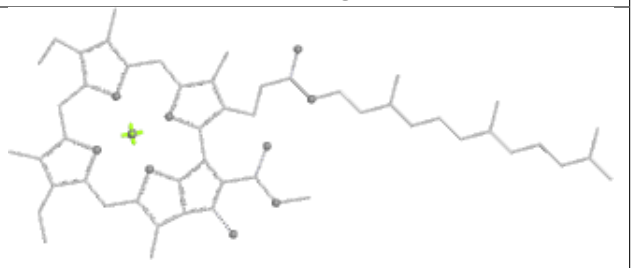
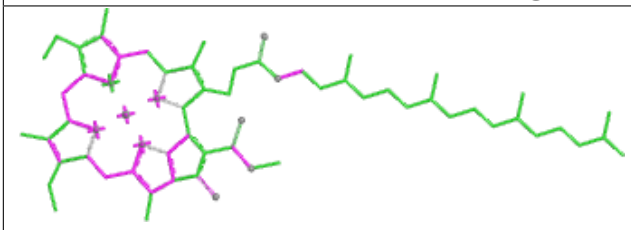
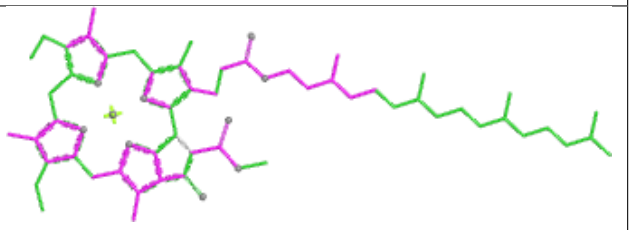
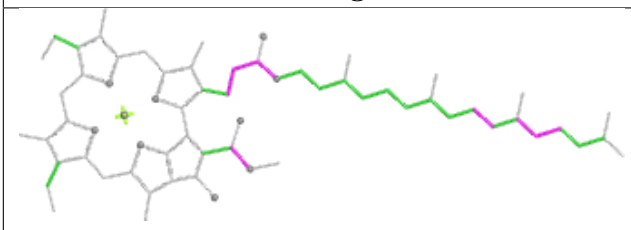
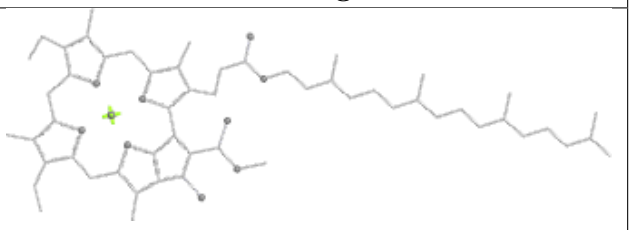


Torsions



Rings

Ligand CLA S 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

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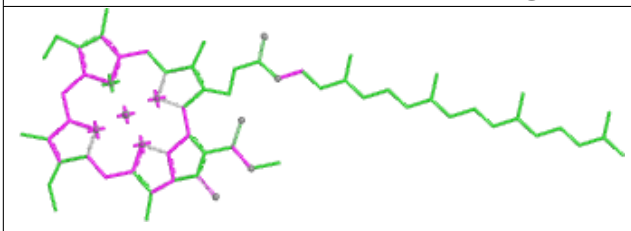
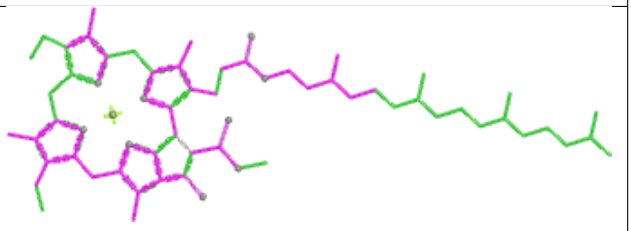
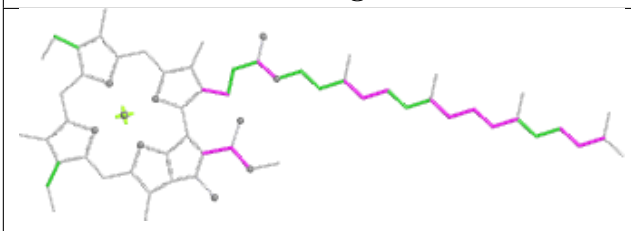
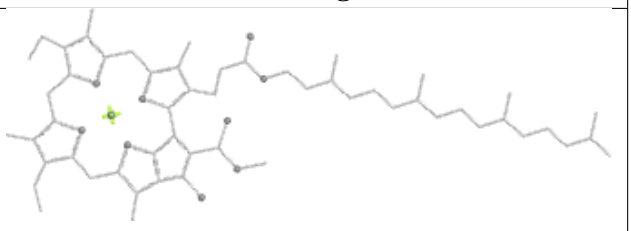
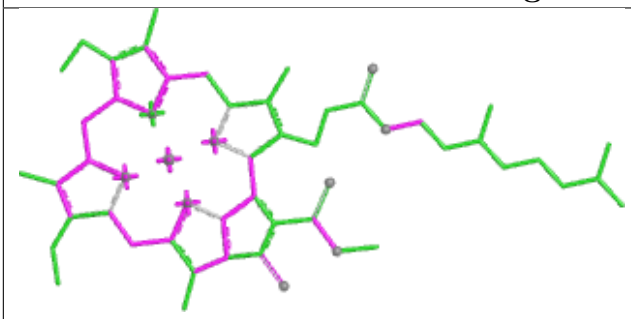
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 825



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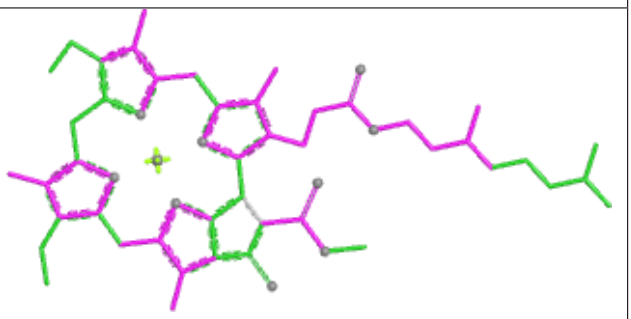
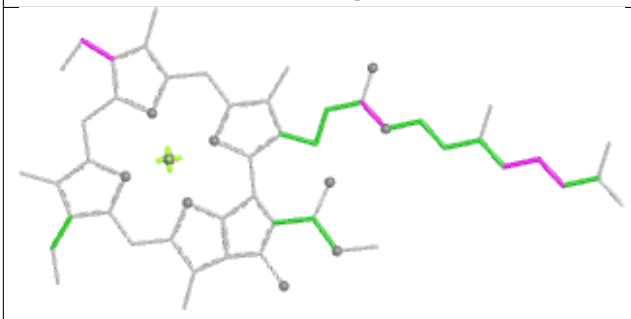
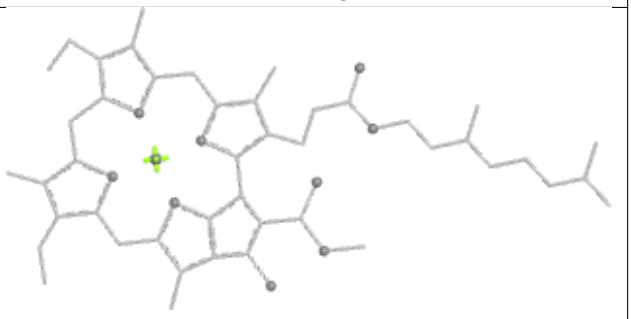


Bond angles

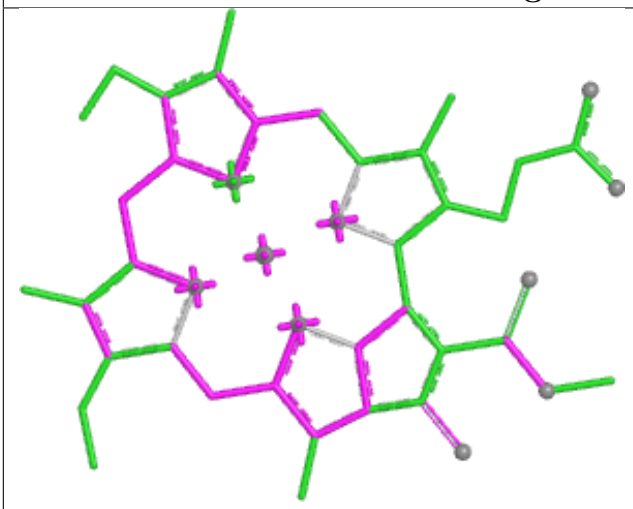


Torsions



Rings

Ligand CLA B 835



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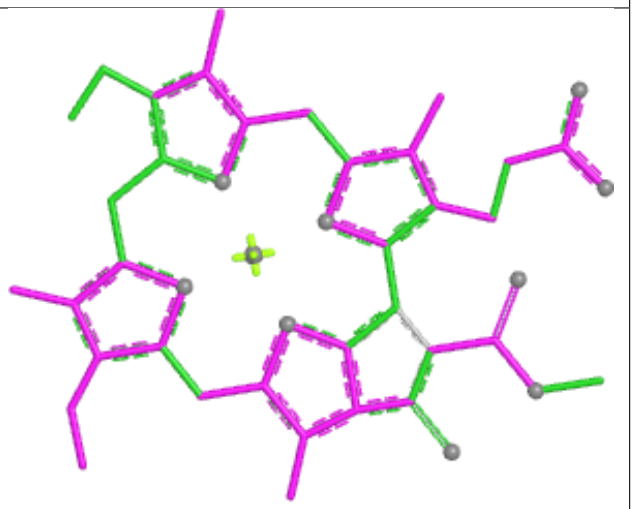
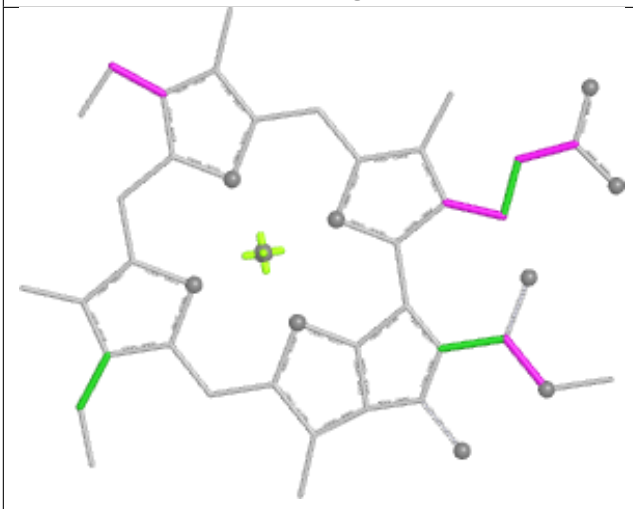


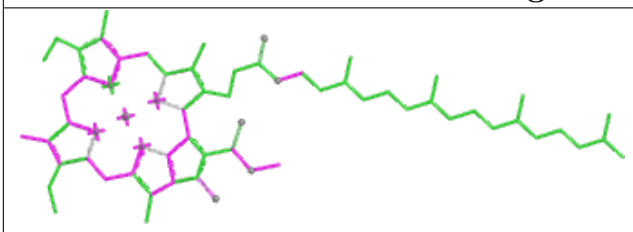
Bond angles



Torsions

Rings

Ligand CLA b 824



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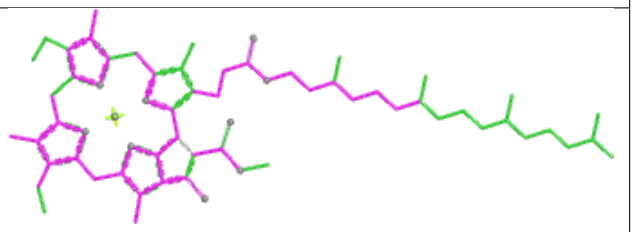
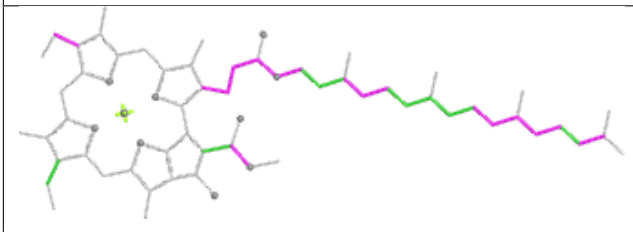


Bond angles



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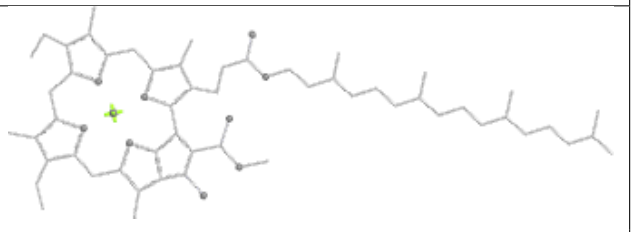
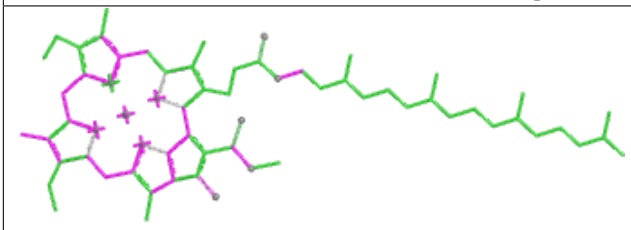
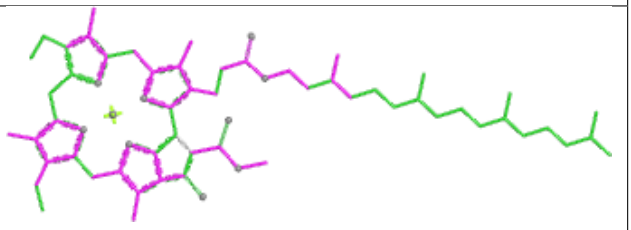


Rings

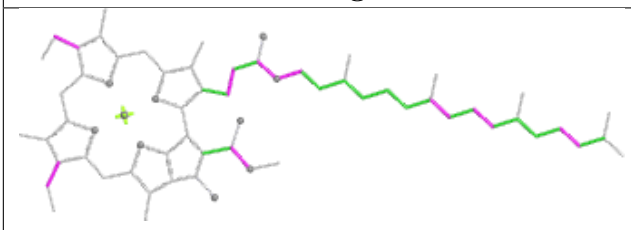
Ligand CLA a 855



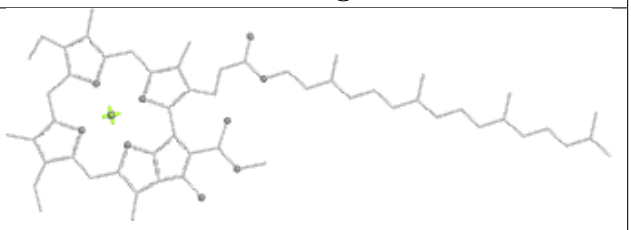
Bond lengths



Bond angles

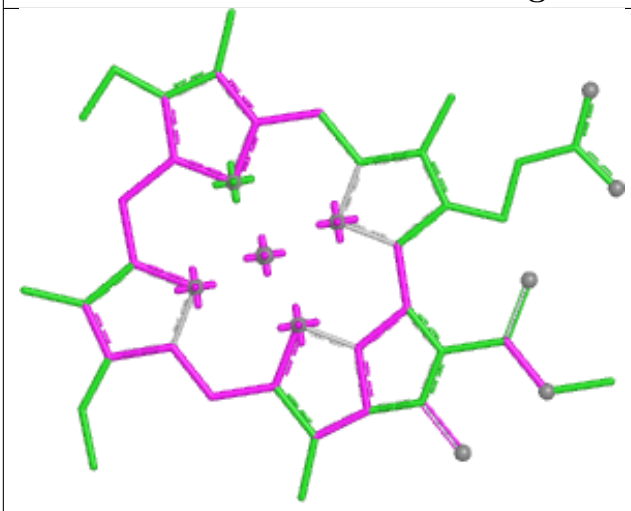


Torsions

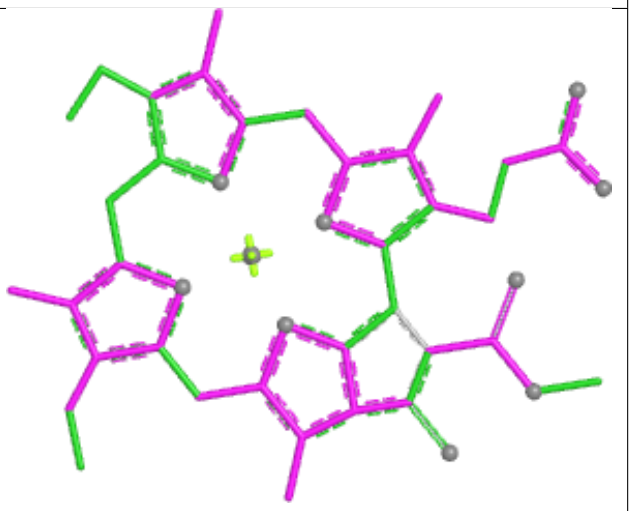


Rings

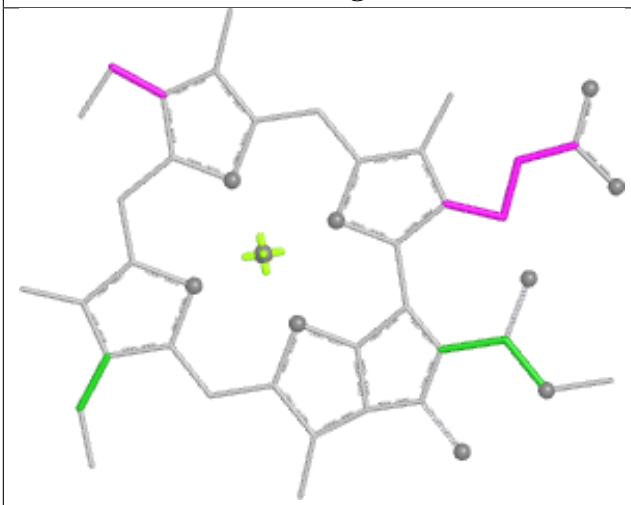
Ligand CLA a 811



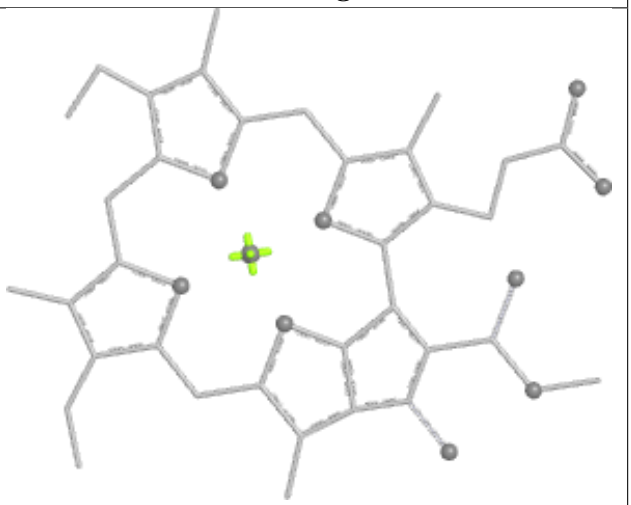
Bond lengths



Bond angles

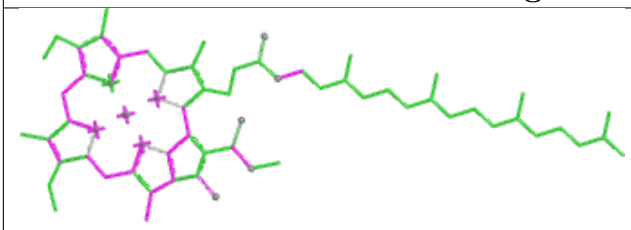


Torsions



Rings

Ligand CLA B 825



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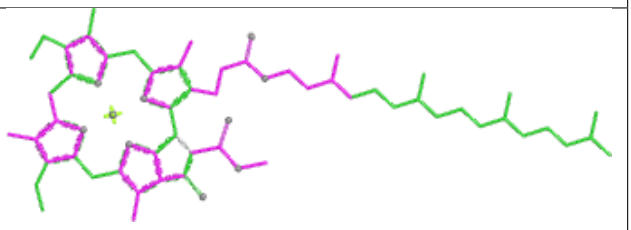
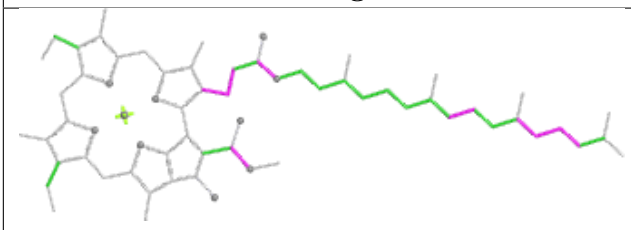
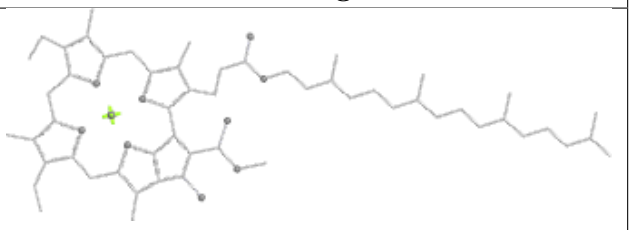


Bond angles

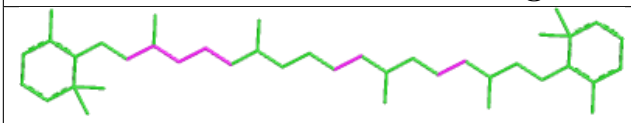


Torsions



Rings

Ligand BCR b 840



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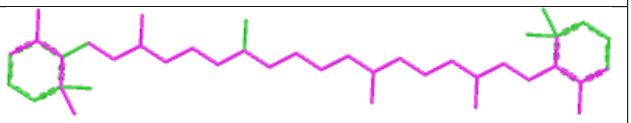
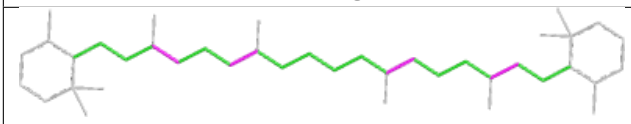
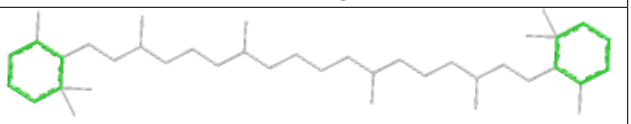


Bond angles

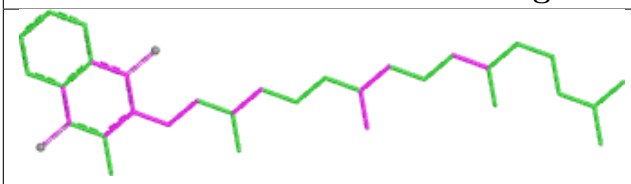


Torsions

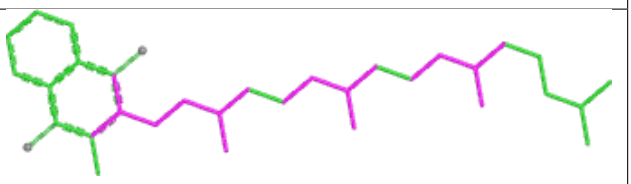


Rings

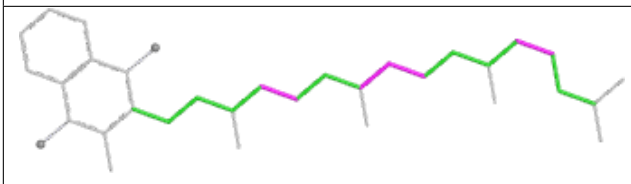
Ligand 1L3 B 839



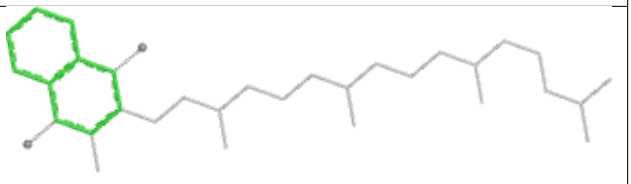
Bond lengths



Bond angles

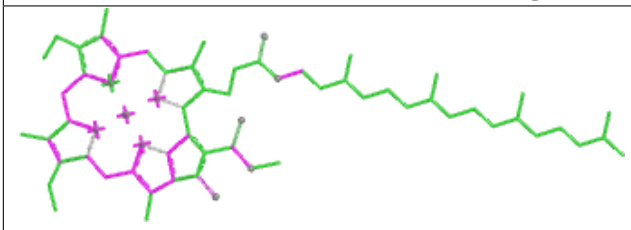


Torsions



Rings

Ligand CLA L 206



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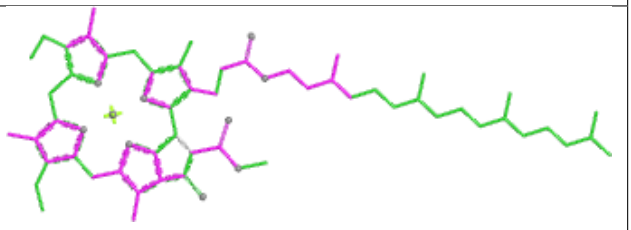
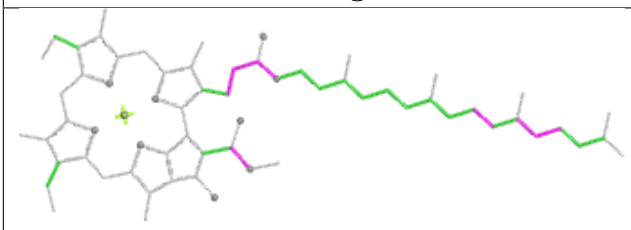
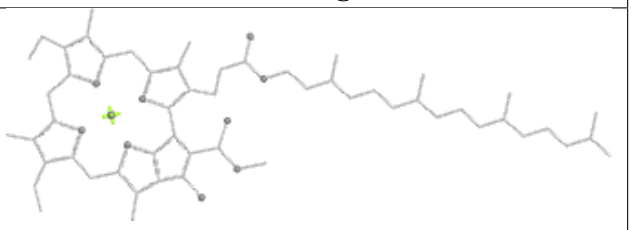


Bond angles

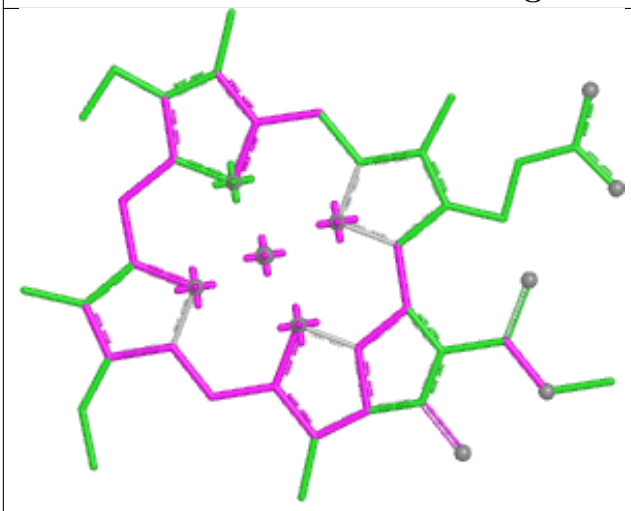


Torsions



Rings

Ligand CLA B 809



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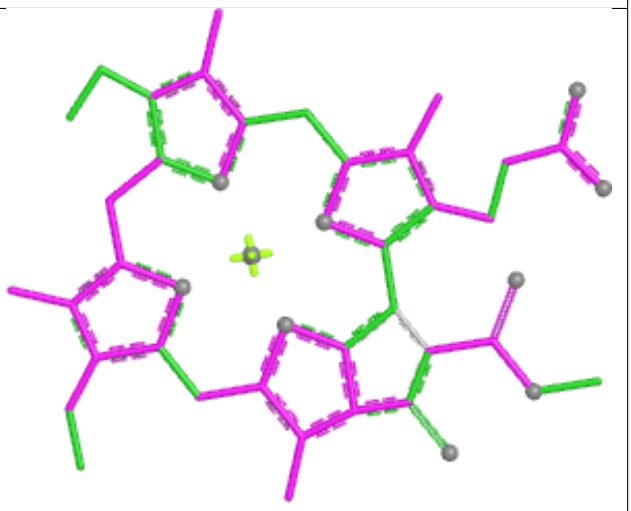
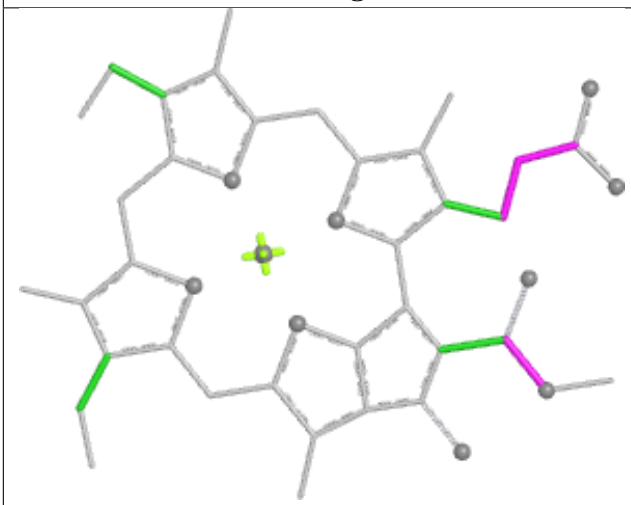
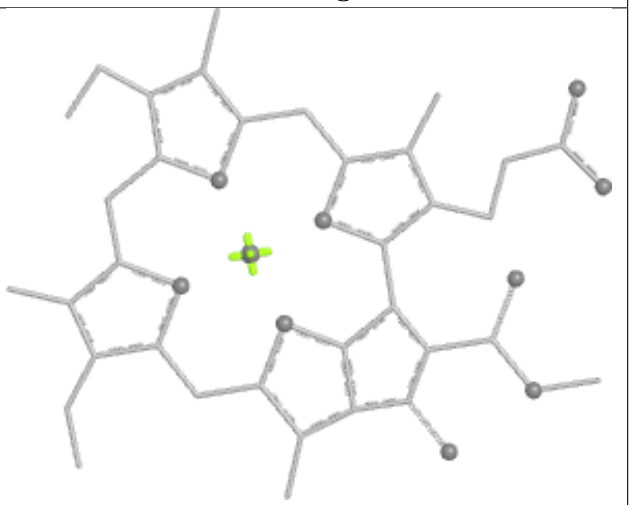


Bond angles

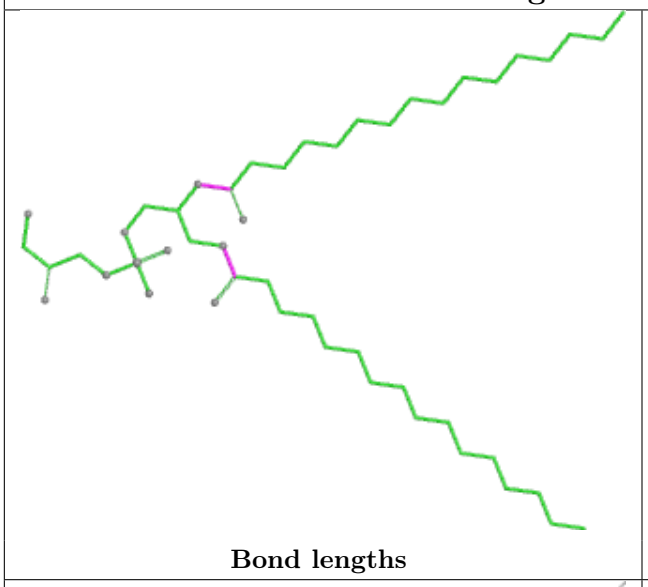


Torsions



Rings

Ligand LHG a 850



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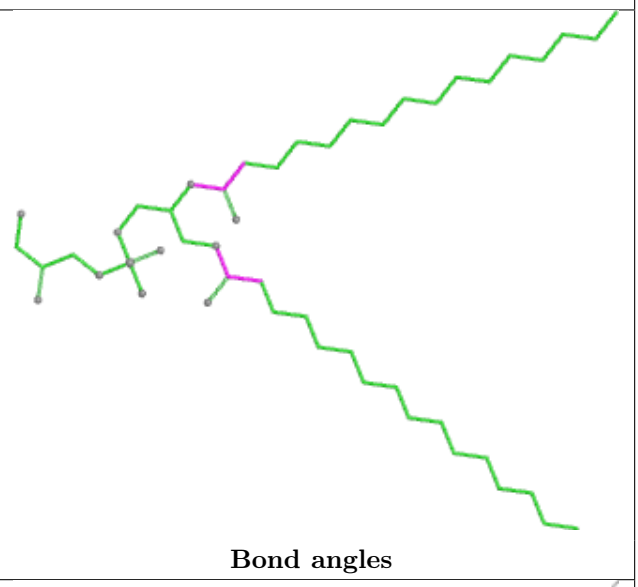
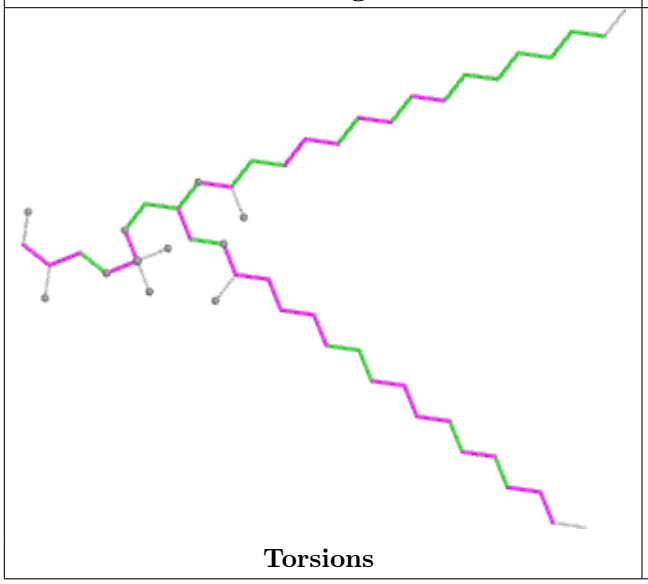


Bond angles



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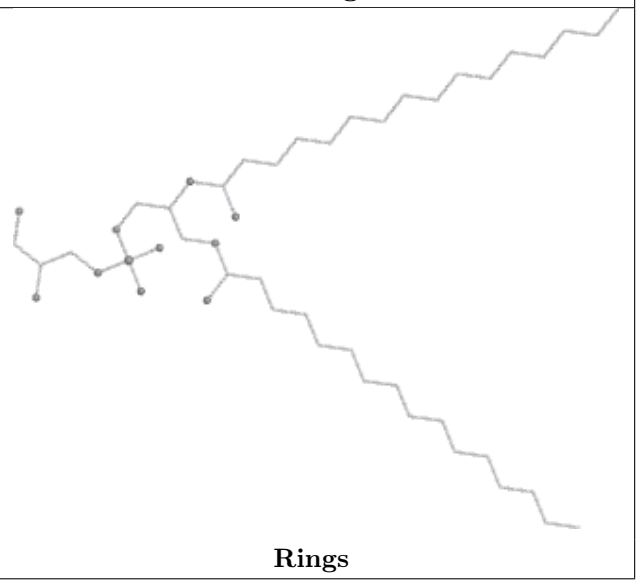
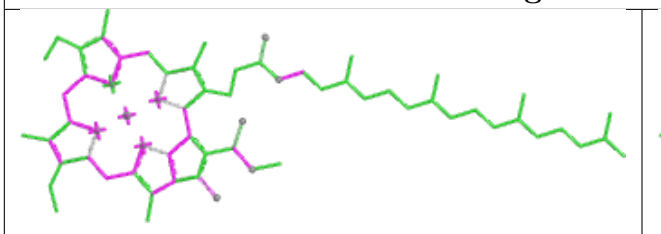
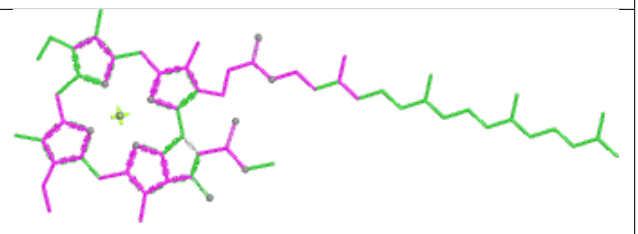


Rings

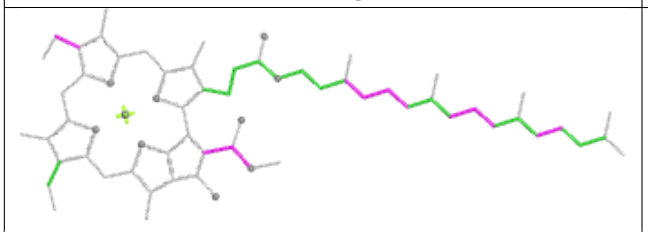
Ligand CLA H 806



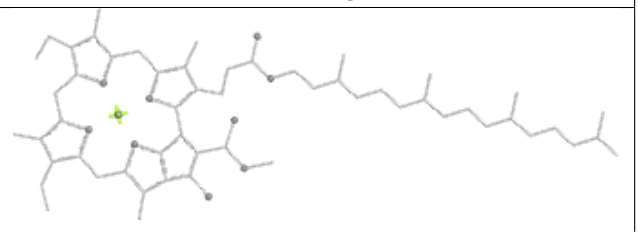
Bond lengths



Bond angles

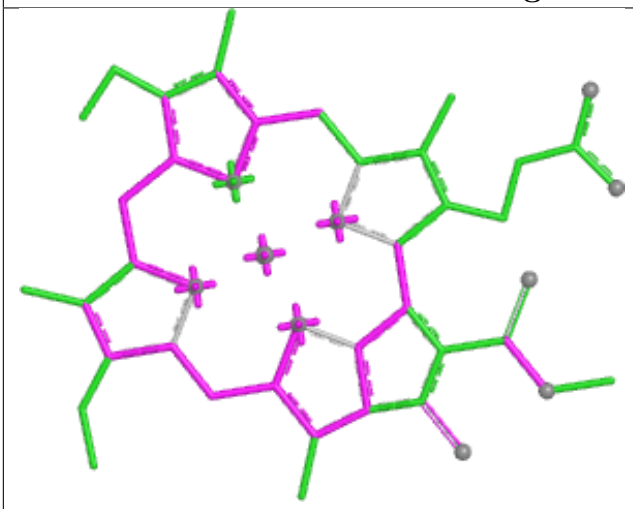


Torsions



Rings

Ligand CLA A 819



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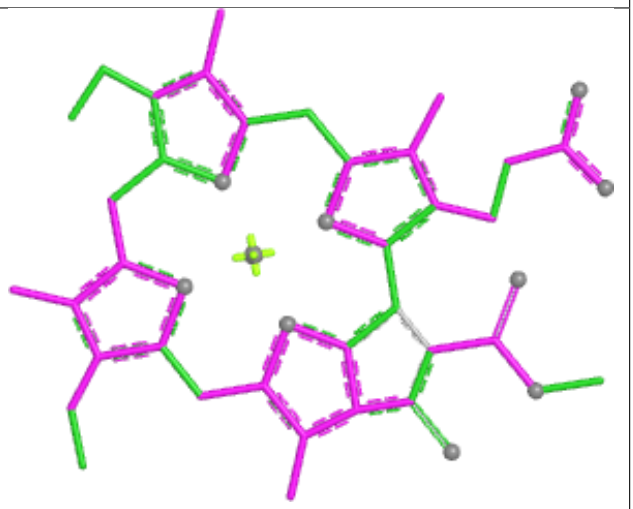
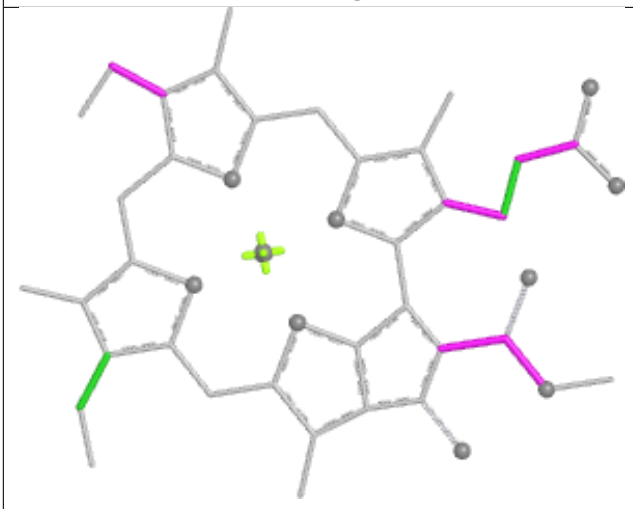


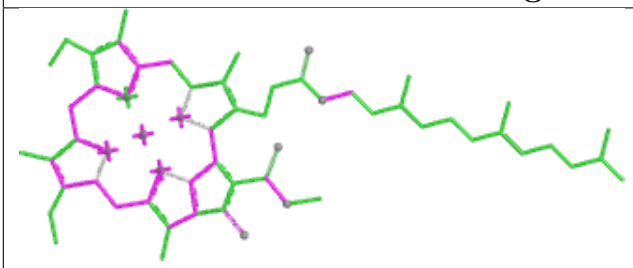
Bond angles



Torsions

Rings

Ligand CLA B 833



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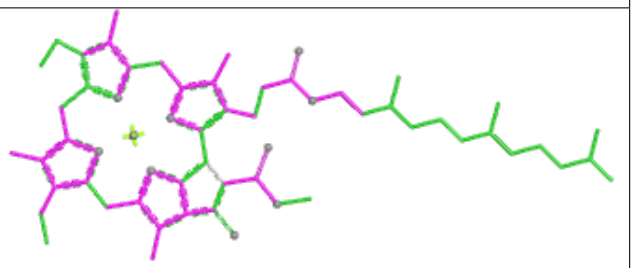
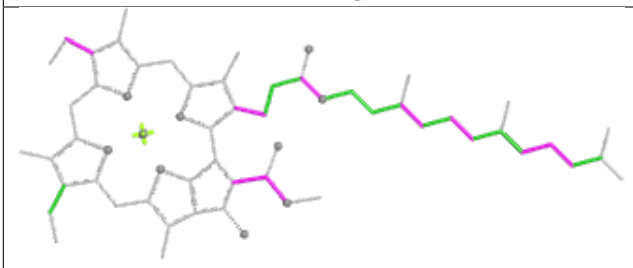


Bond angles



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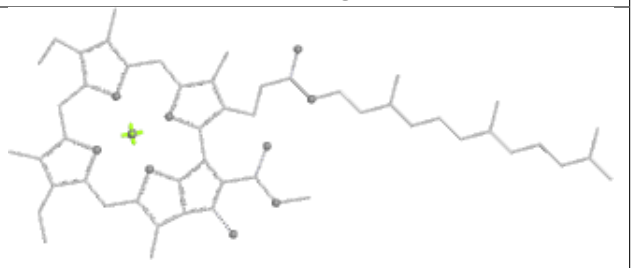
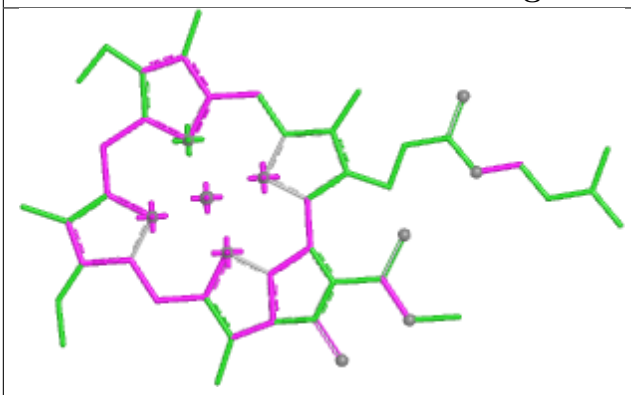


Rings

Ligand CLA A 836



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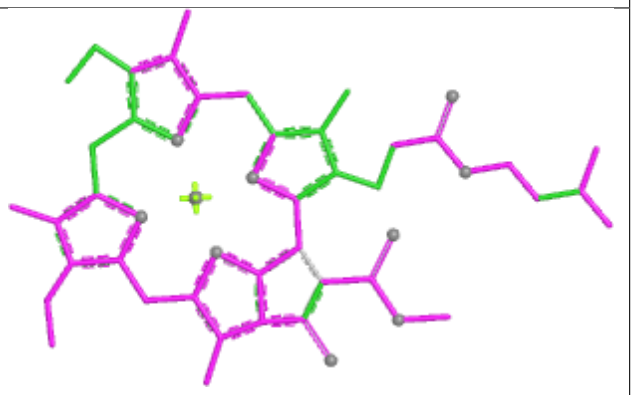
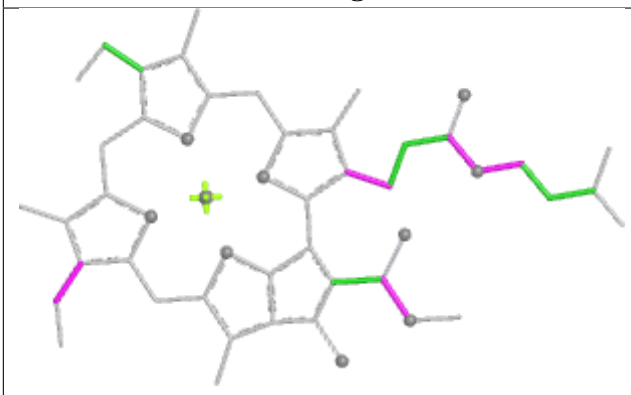


Bond angles



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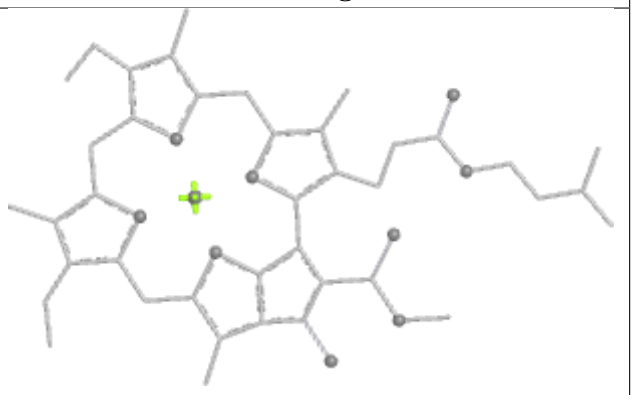
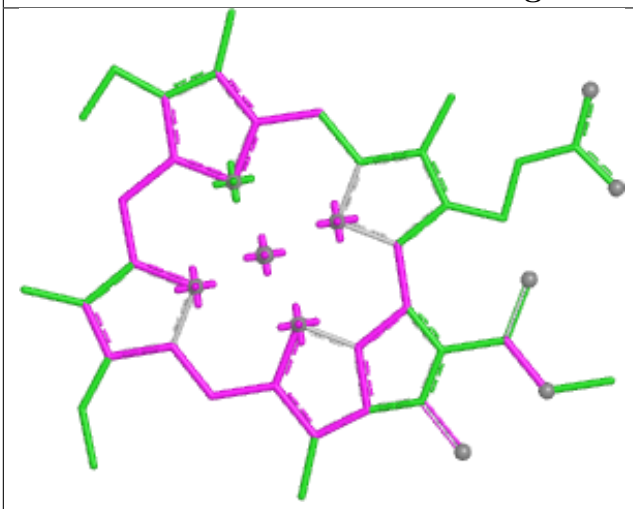


Rings

Ligand CLA B 828



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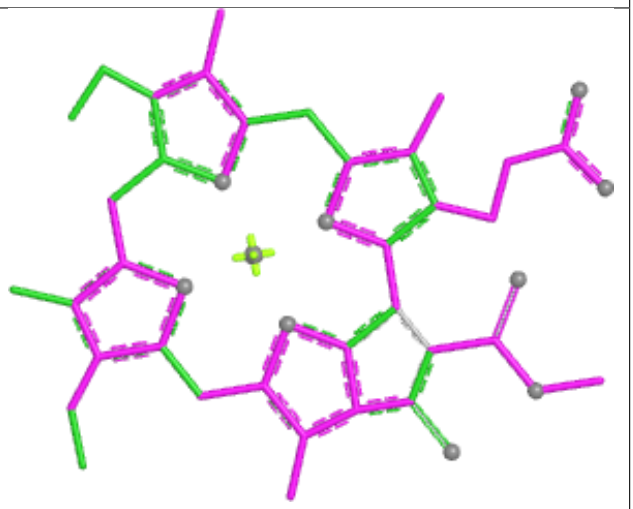
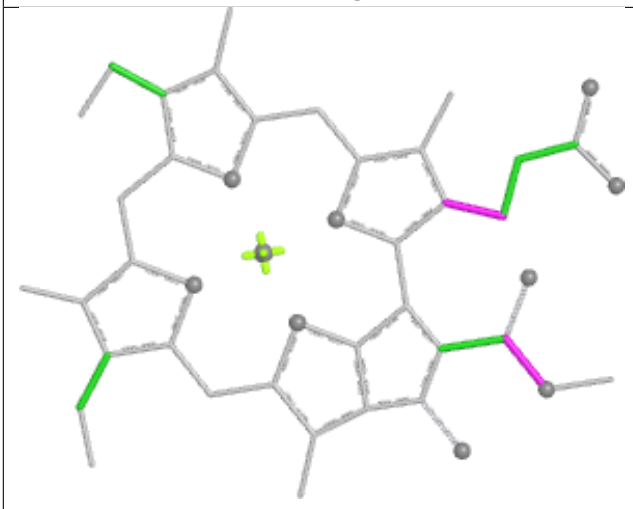


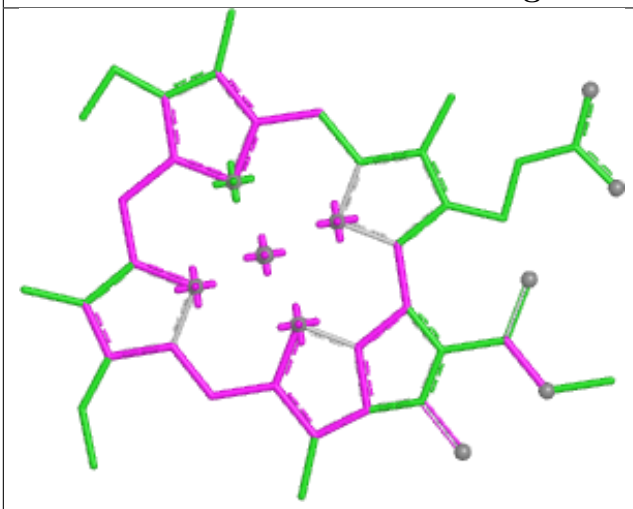
Bond angles



Torsions

Rings

Ligand CLA H 829



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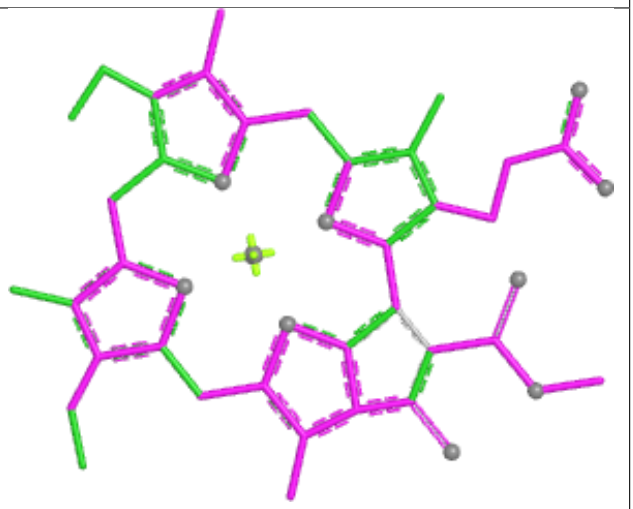
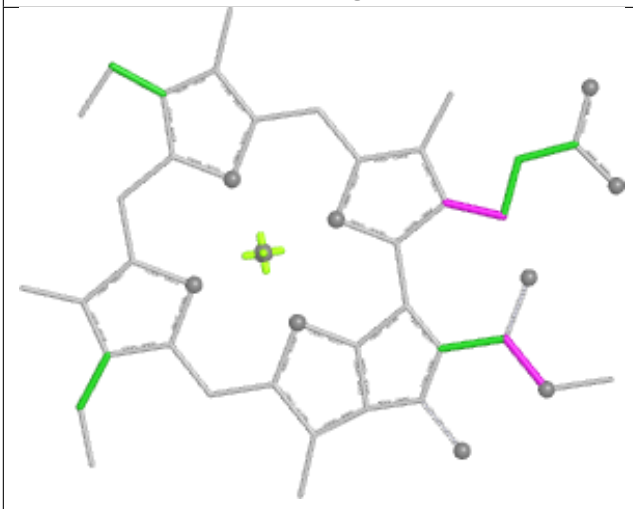


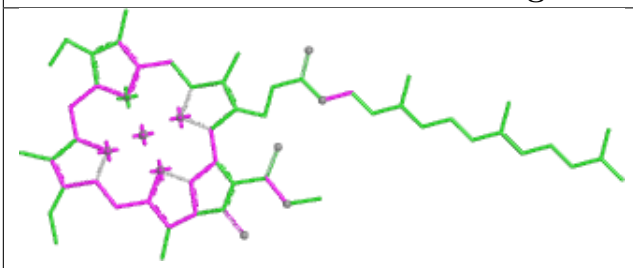
Bond angles



Torsions

Rings

Ligand CLA b 811



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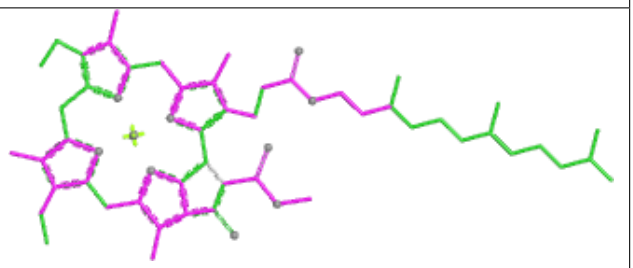
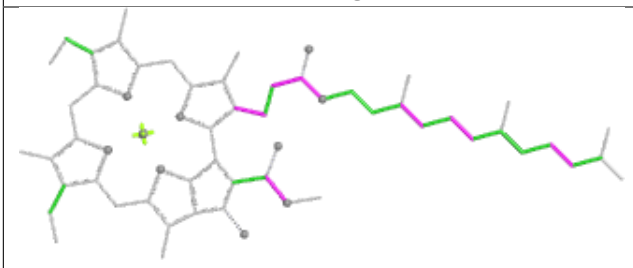
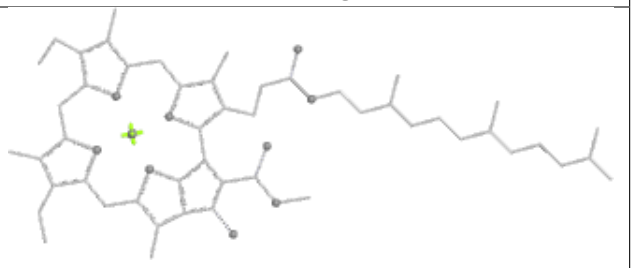


Bond angles

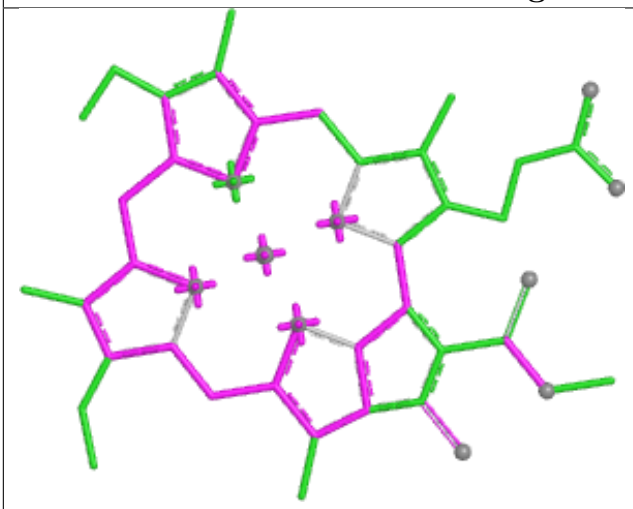


Torsions

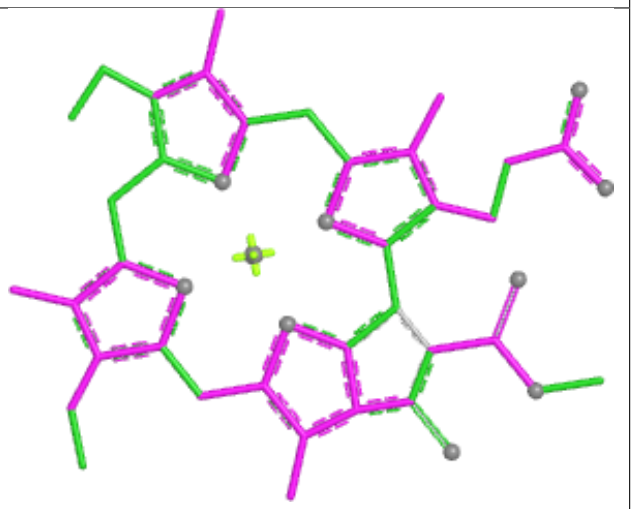


Rings

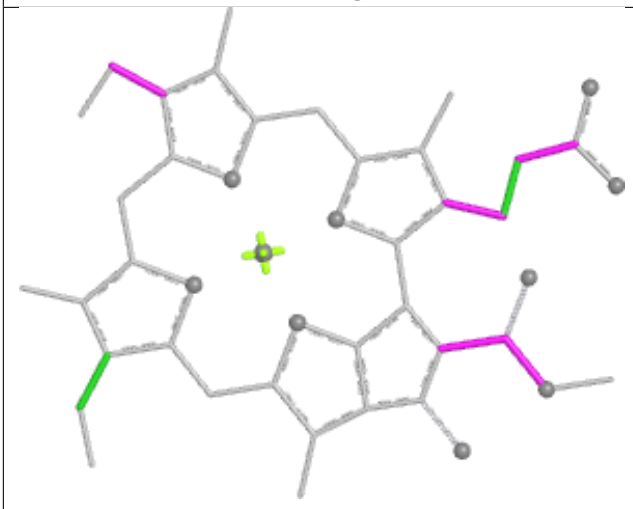
Ligand CLA J 103



Bond lengths



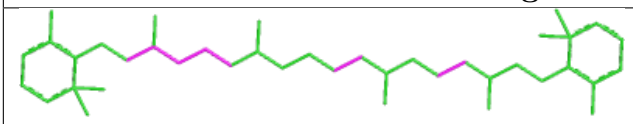
Bond angles



Torsions

Rings

Ligand BCR H 849



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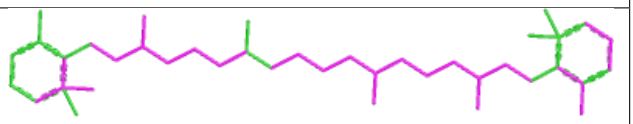
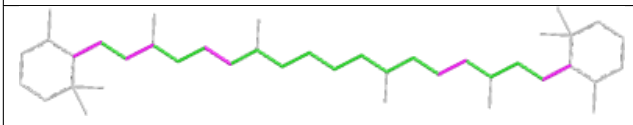
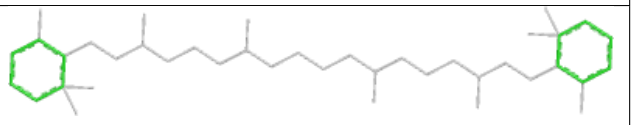


Bond angles

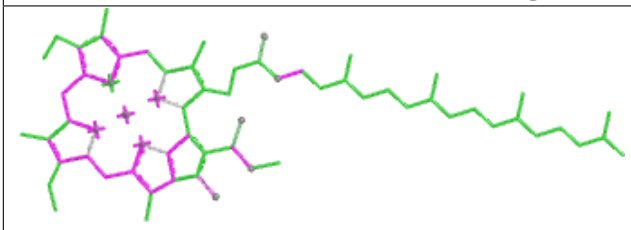


Torsions



Rings

Ligand CLA B 805



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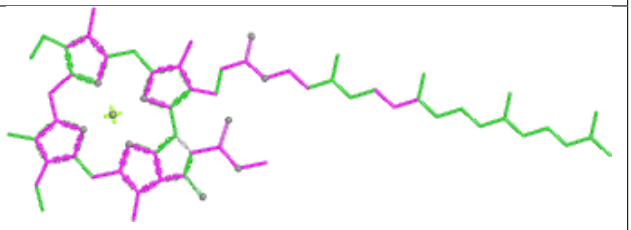
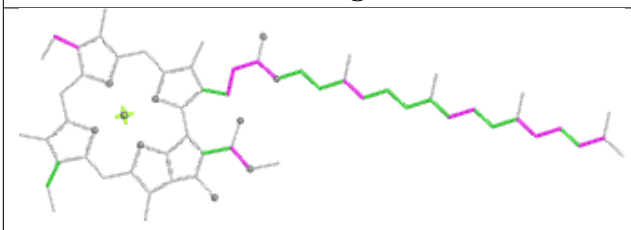
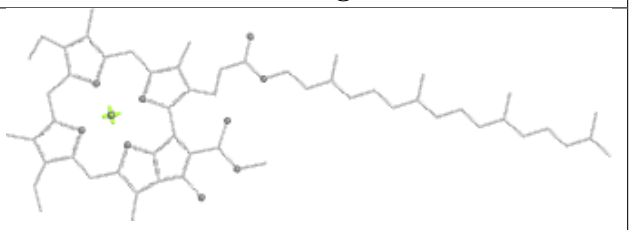


Bond angles

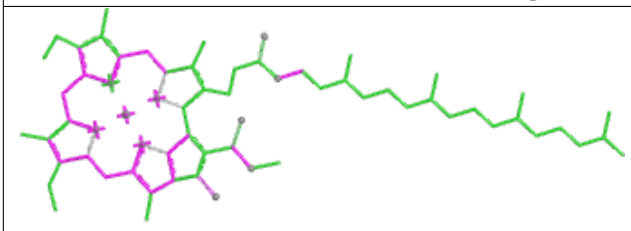


Torsions



Rings

Ligand CLA B 836



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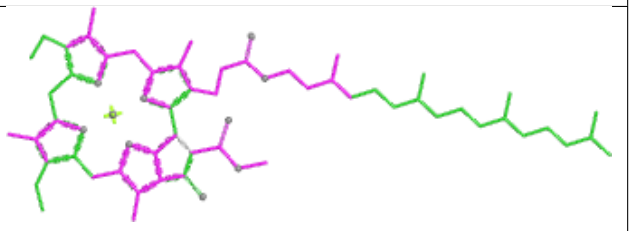
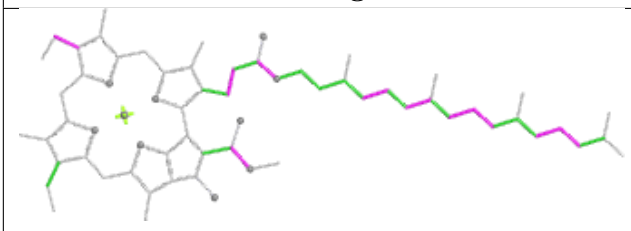
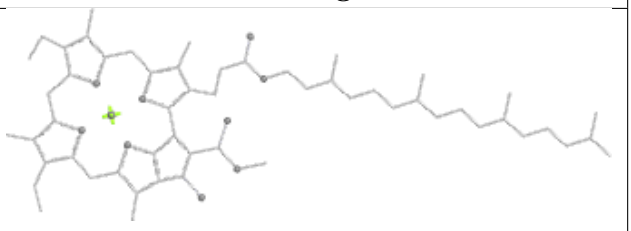


Bond angles

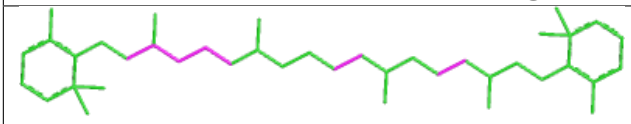


Torsions

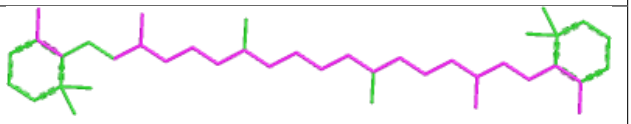


Rings

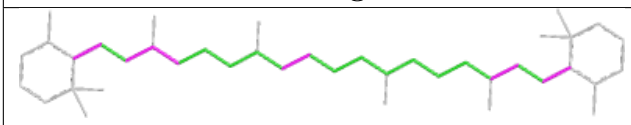
Ligand BCR L 207



Bond lengths



Bond angles



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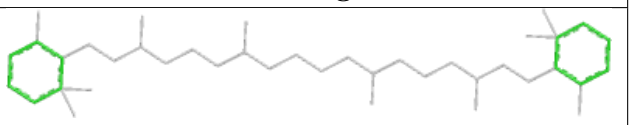
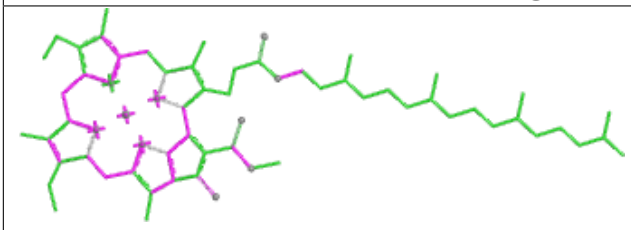
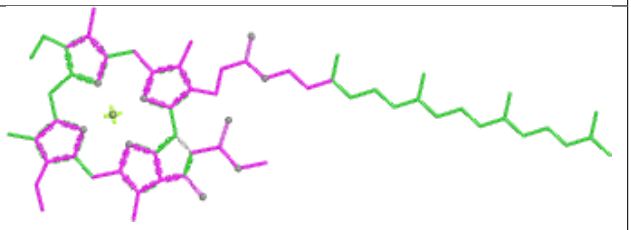
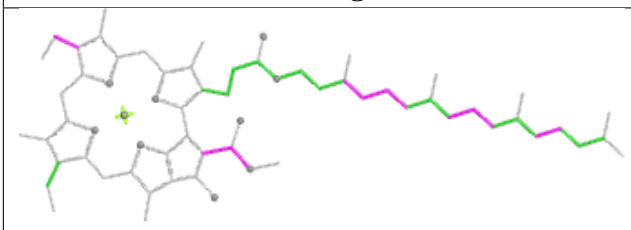
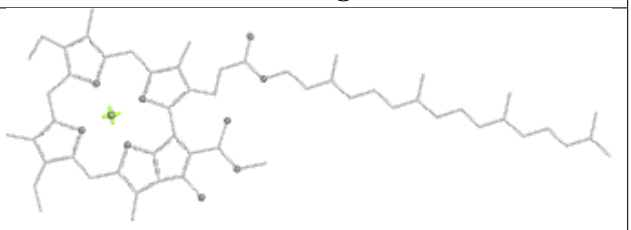
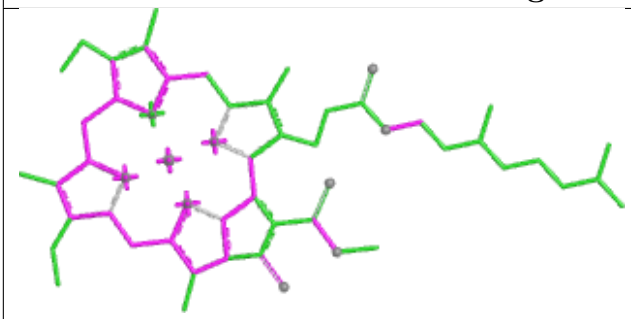
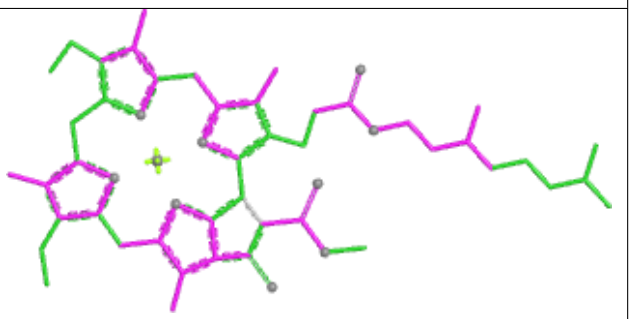
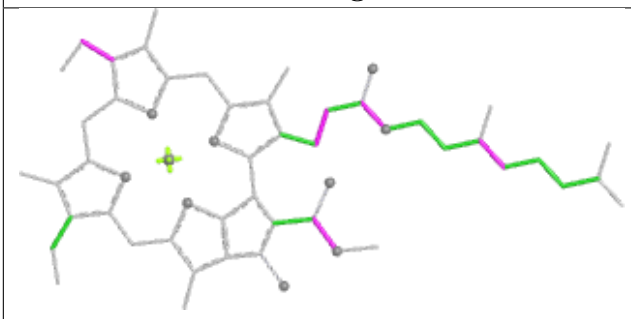
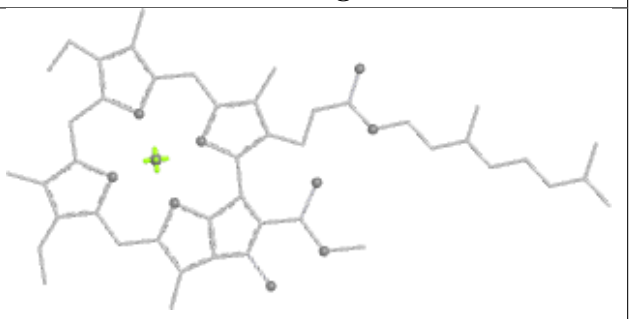
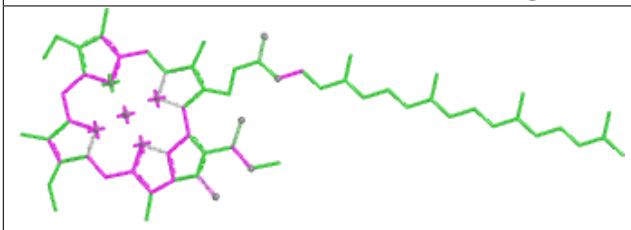


Rings

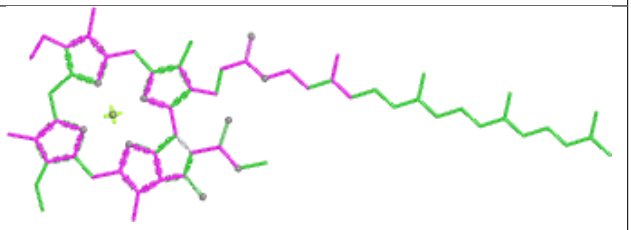
Ligand CLA b 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

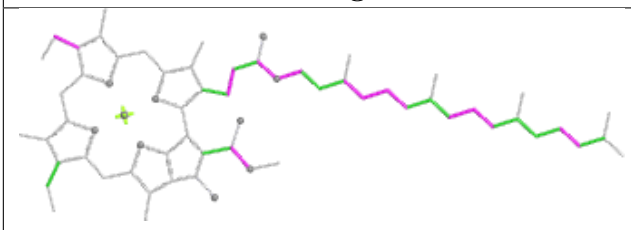
Ligand CLA A 832



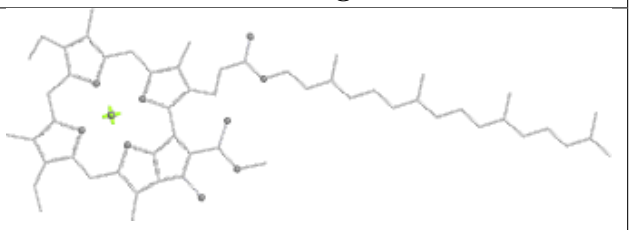
Bond lengths



Bond angles

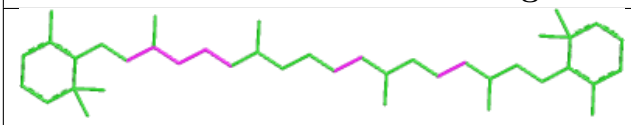


Torsions



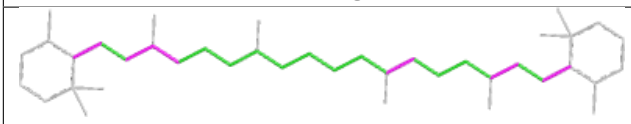
Rings

Ligand BCR G 849

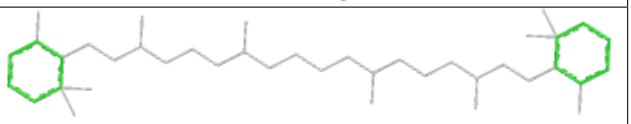


Bond lengths

Bond angles

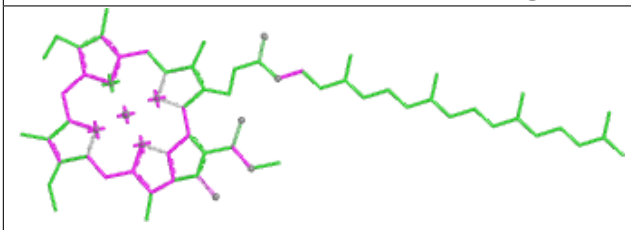


Torsions

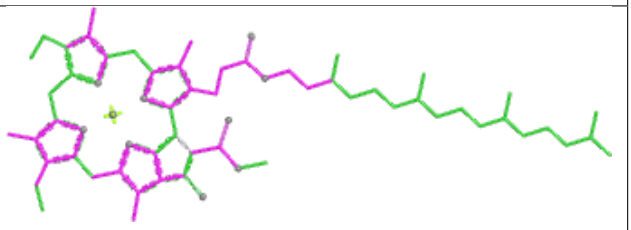


Rings

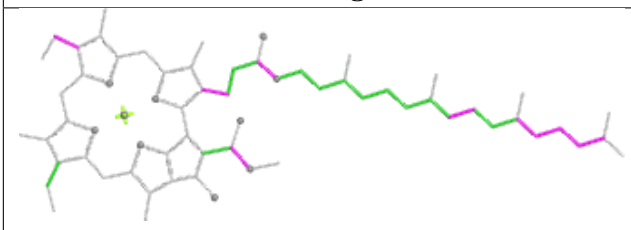
Ligand CLA A 818



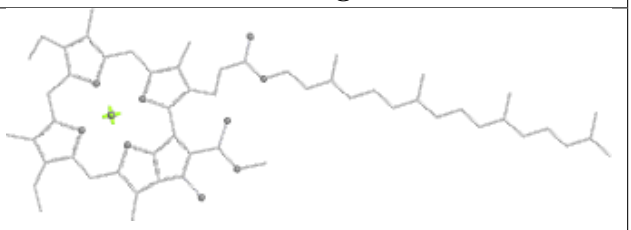
Bond lengths



Bond angles

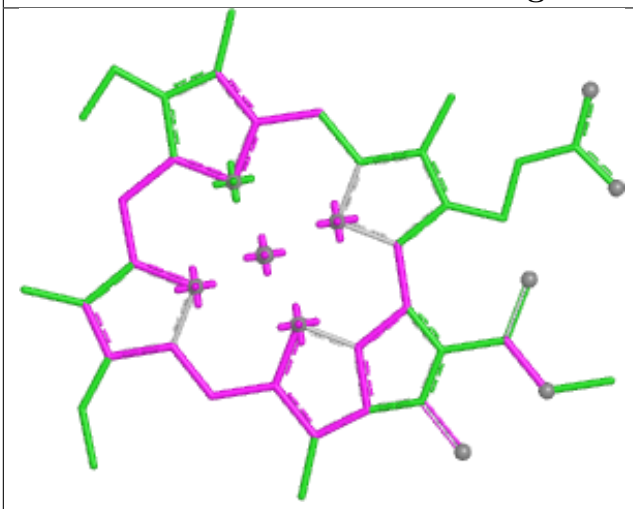


Torsions



Rings

Ligand CLA b 831



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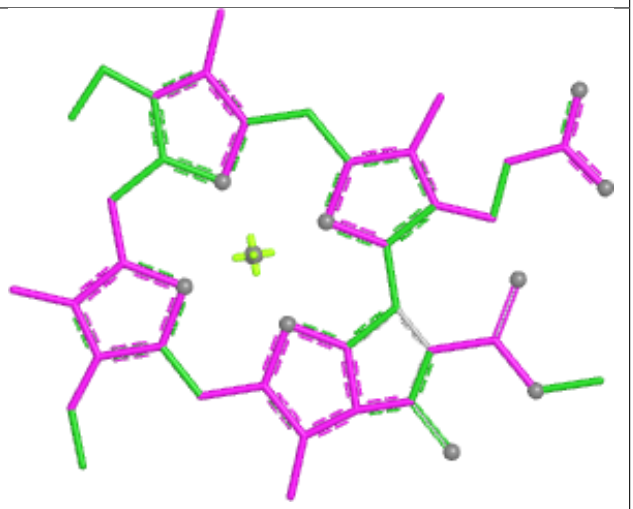
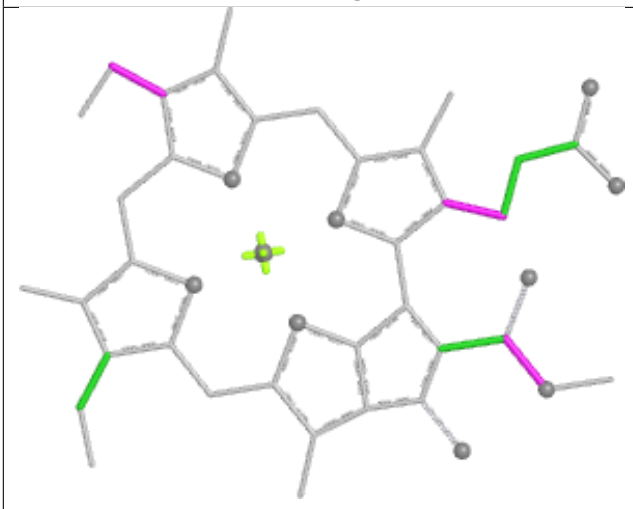


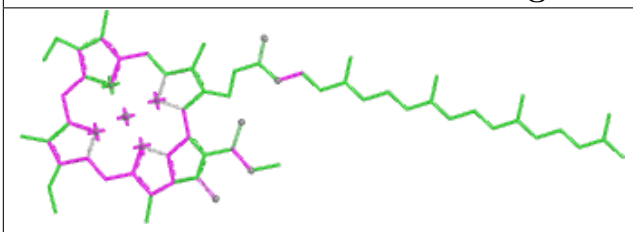
Bond angles



Torsions

Rings

Ligand CLA a 803



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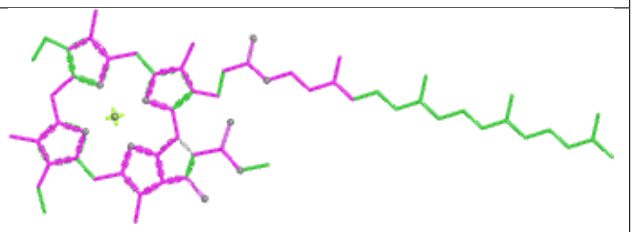
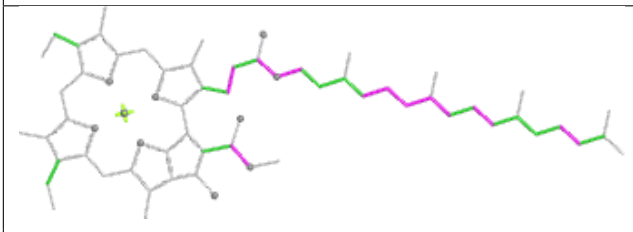
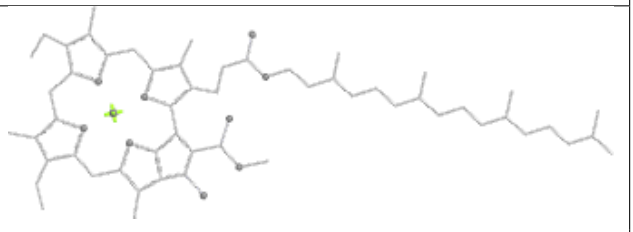


Bond angles

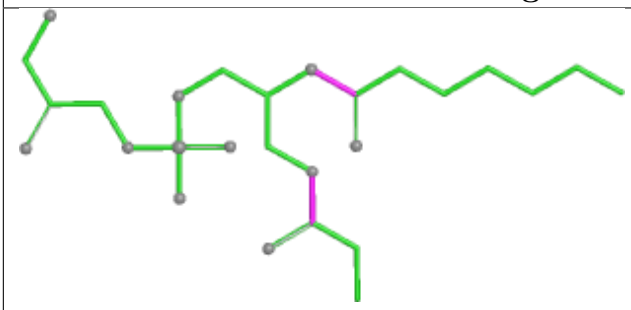


Torsions



Rings

Ligand LHG A 851



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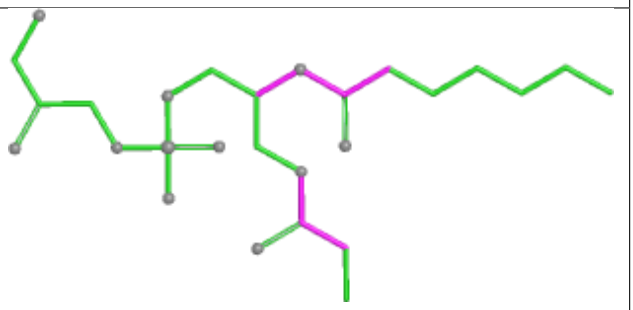
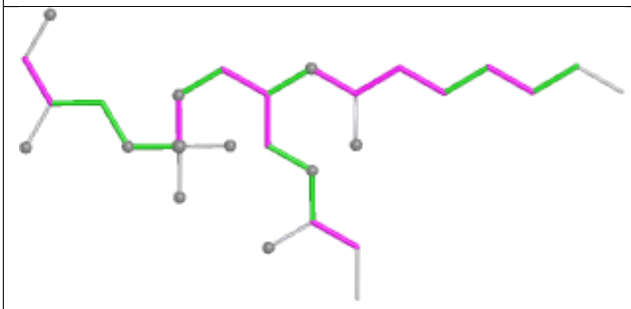
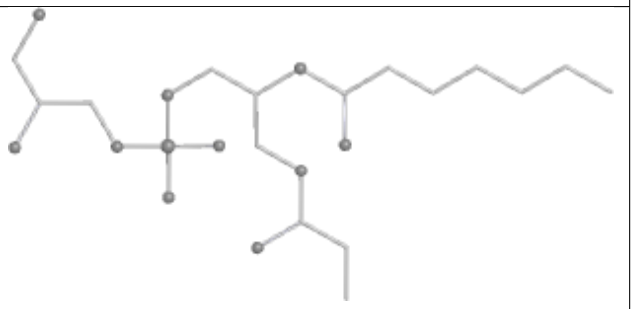


Bond angles

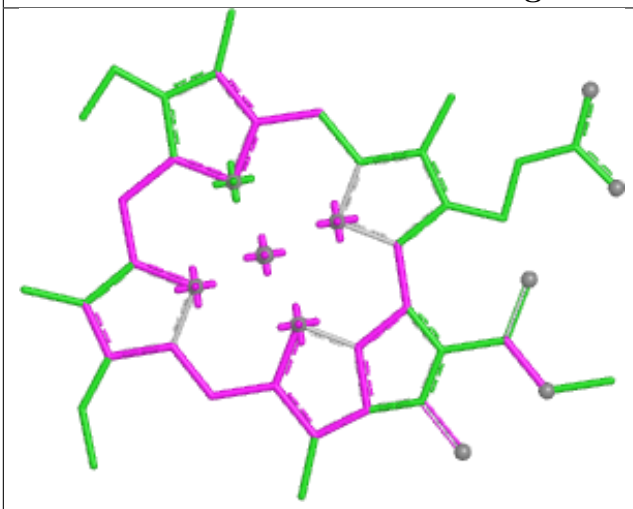


Torsions

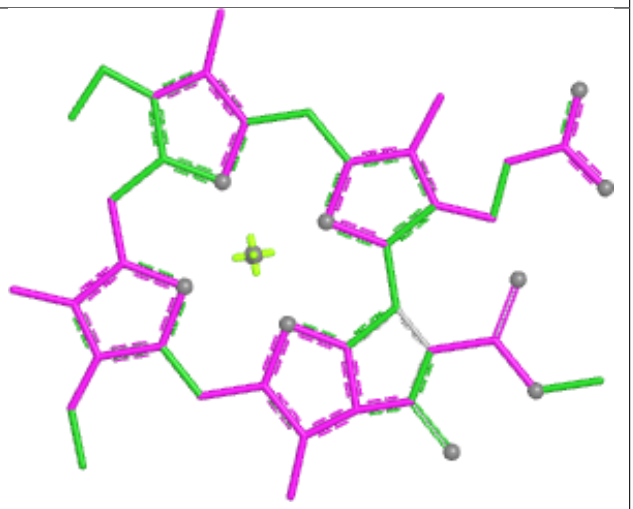


Rings

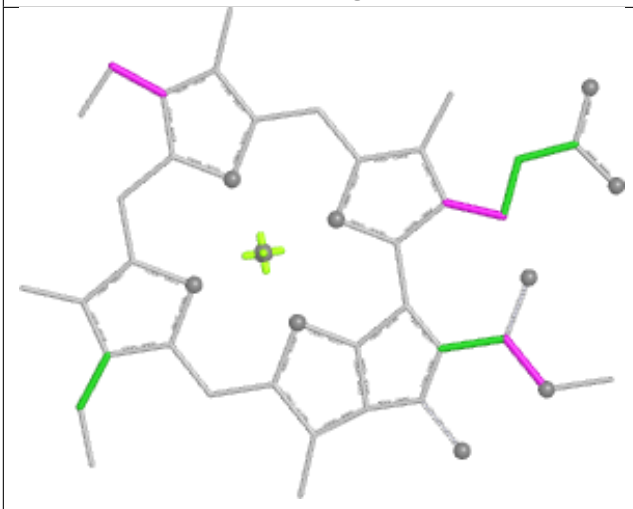
Ligand CLA B 832



Bond lengths



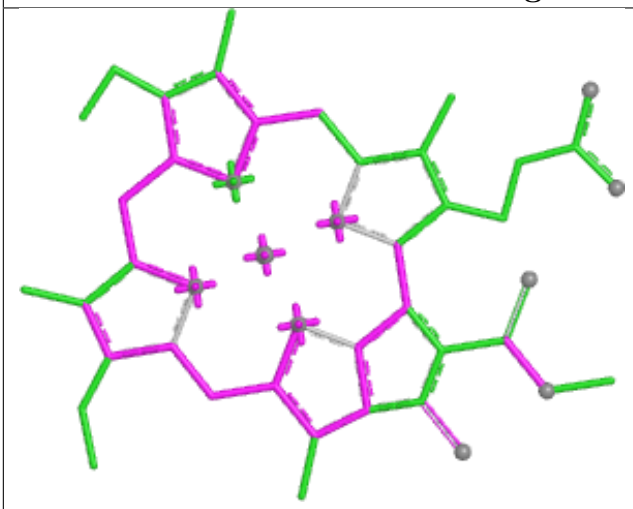
Bond angles



Torsions

Rings

Ligand CLA B 818



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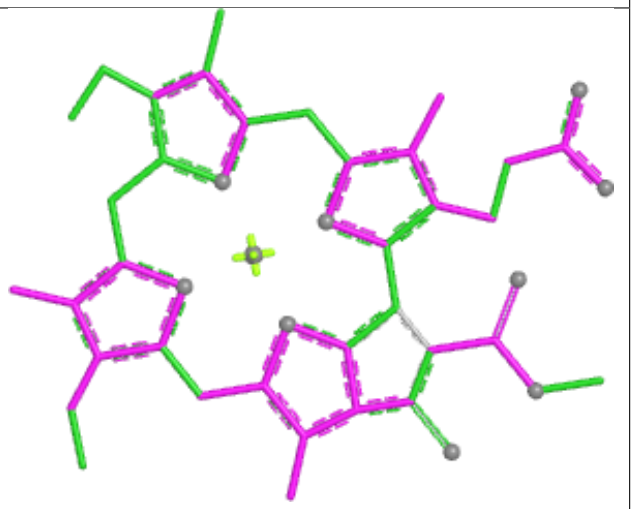
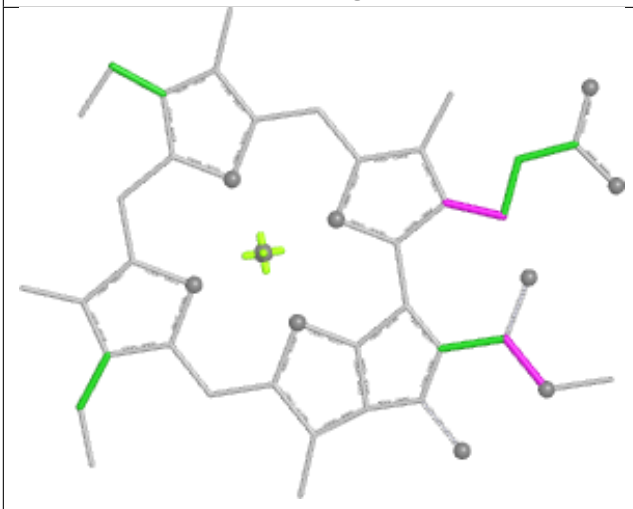


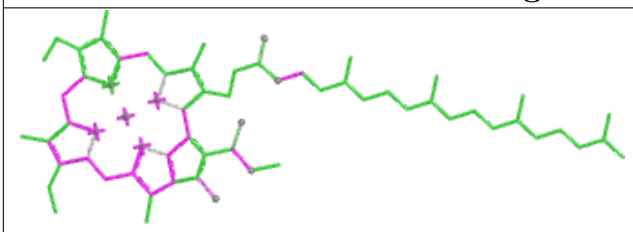
Bond angles



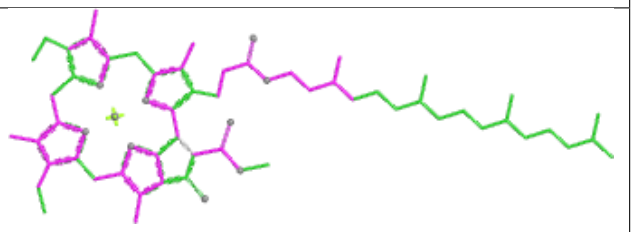
Torsions

Rings

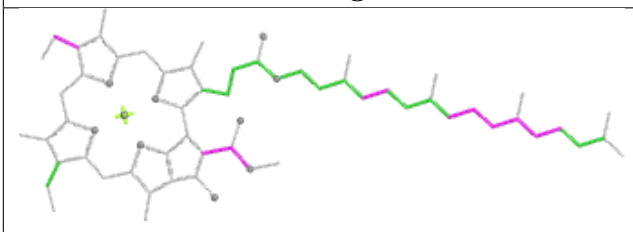
Ligand CLA H 831



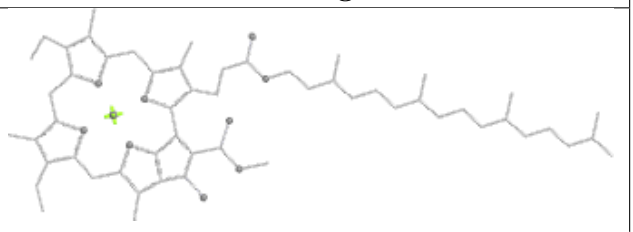
Bond lengths



Bond angles

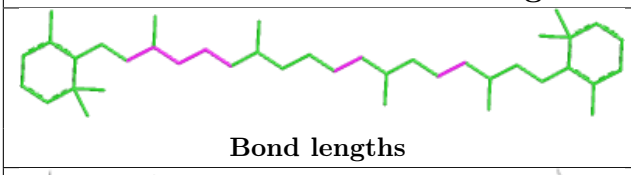


Torsions



Rings

Ligand BCR L 203



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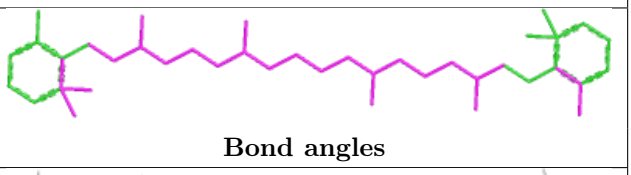
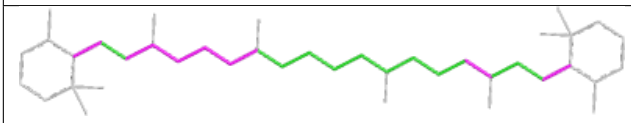
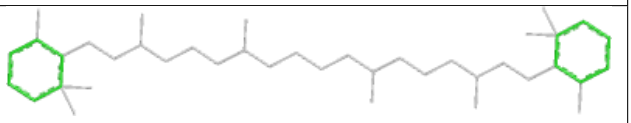


Bond angles



Torsions

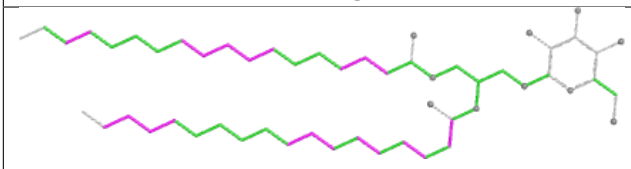


Rings

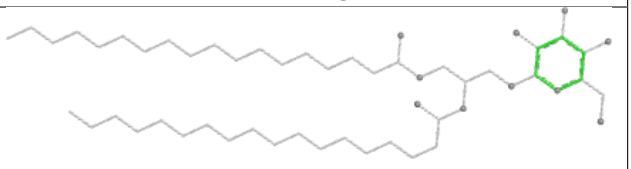
Ligand LMG H 847

Bond lengths

Bond angles

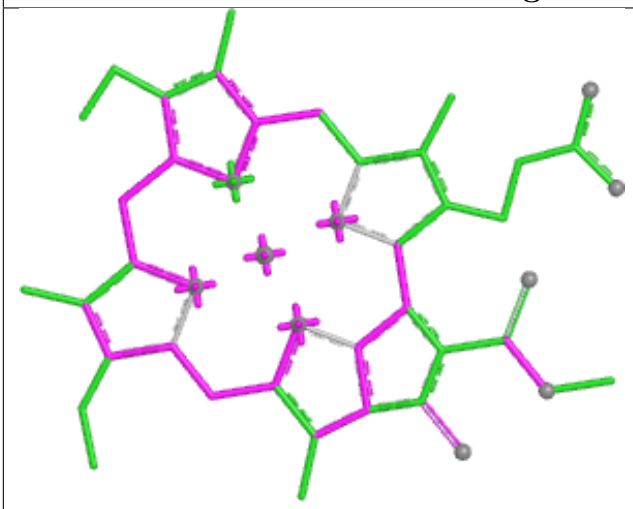


Torsions

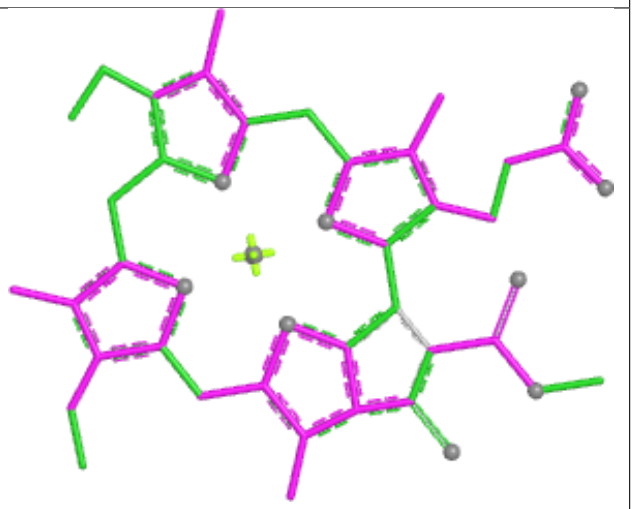


Rings

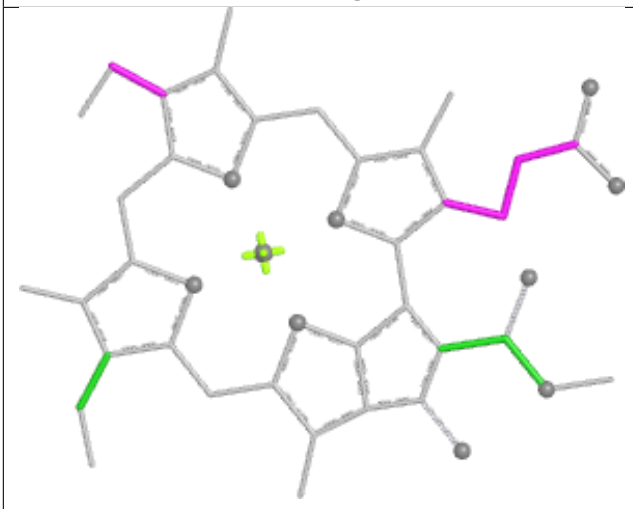
Ligand CLA G 812



Bond lengths



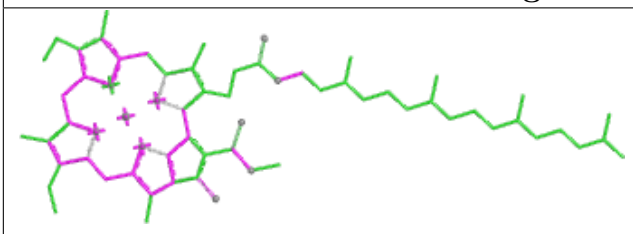
Bond angles



Torsions

Rings

Ligand CLA G 839



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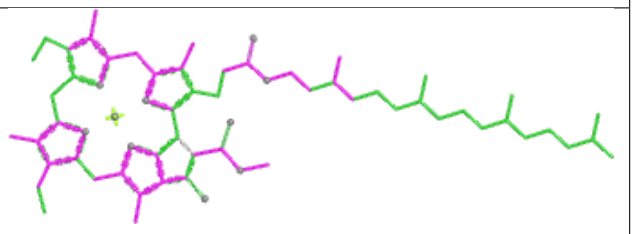
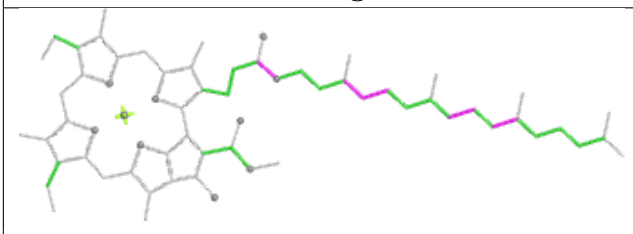
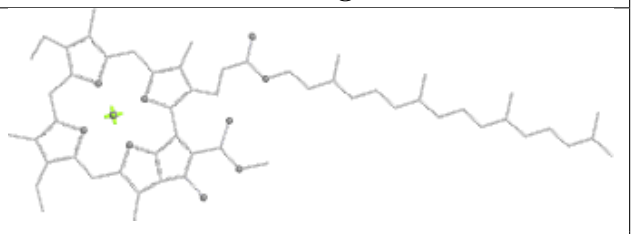


Bond angles

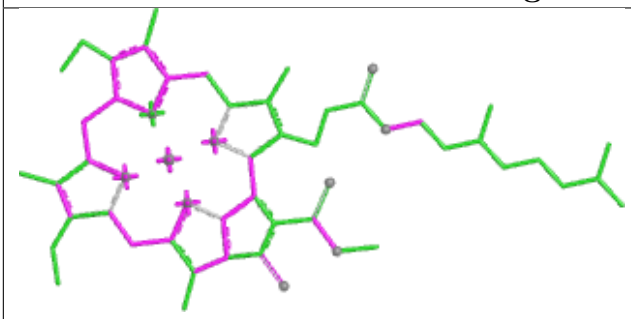


Torsions

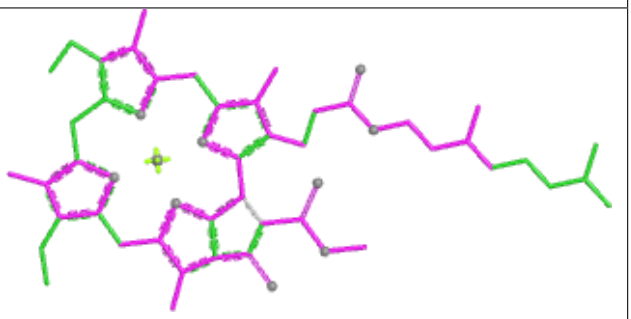


Rings

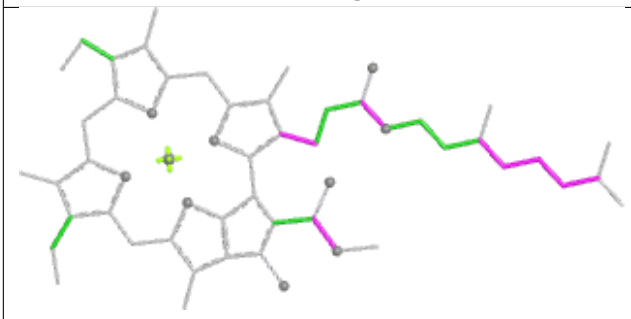
Ligand CLA A 831



Bond lengths



Bond angles



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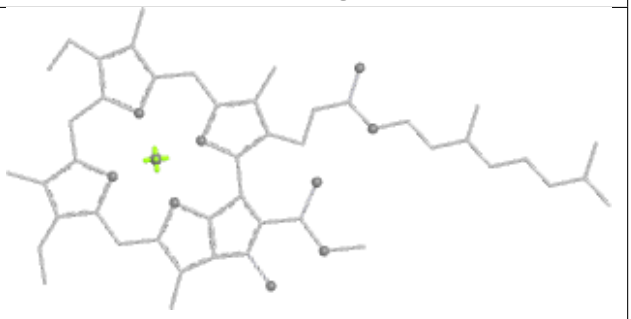
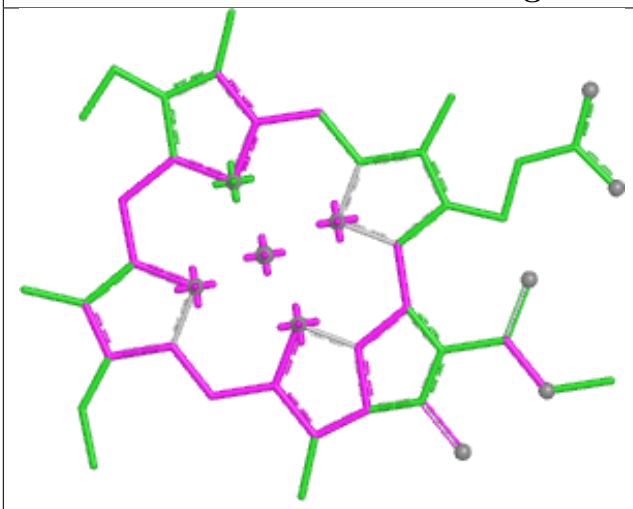


Rings

Ligand CLA A 809



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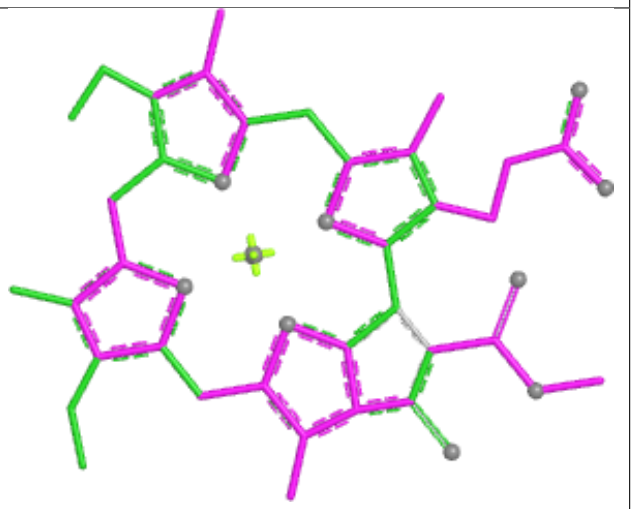
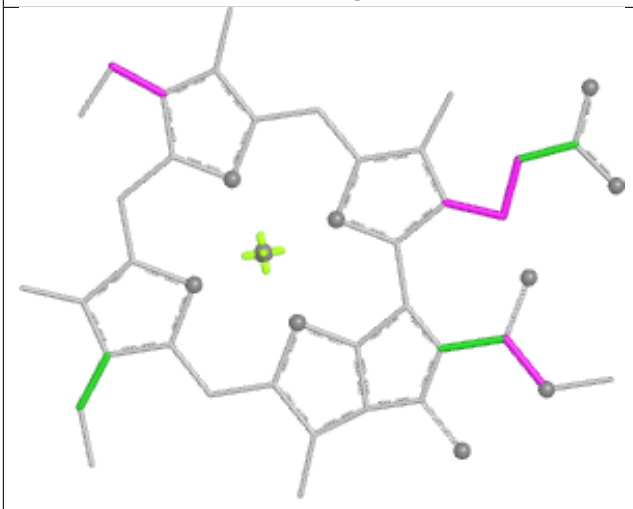


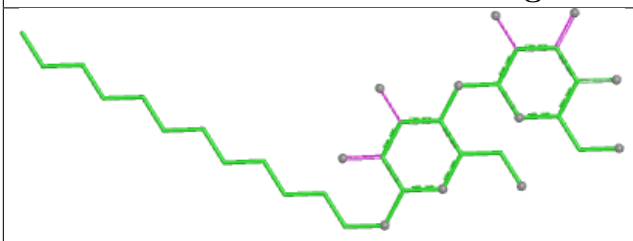
Bond angles



Torsions

Rings

Ligand LMT b 846



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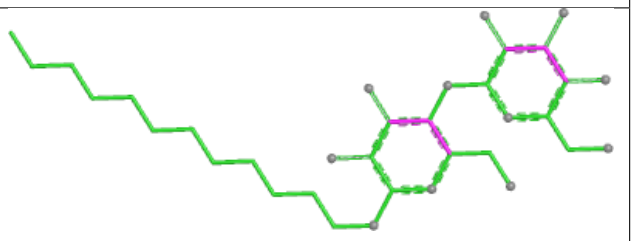
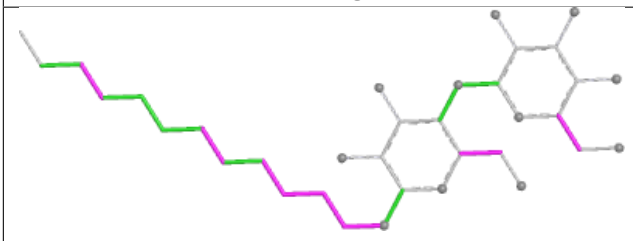
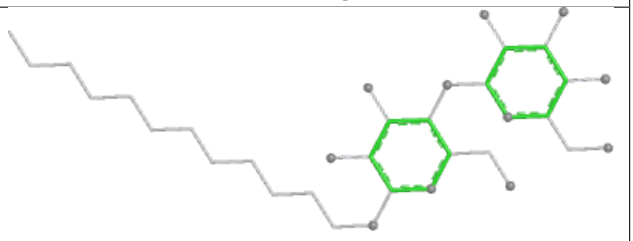


Bond angles

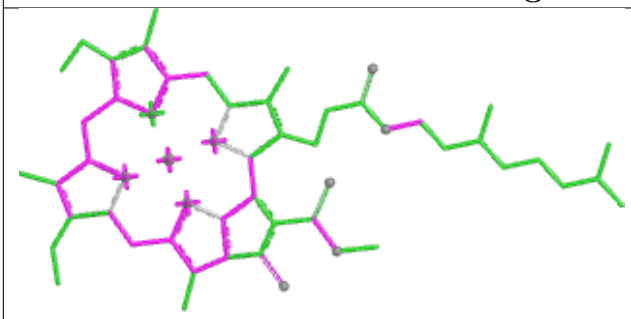


Torsions



Rings

Ligand CLA B 813



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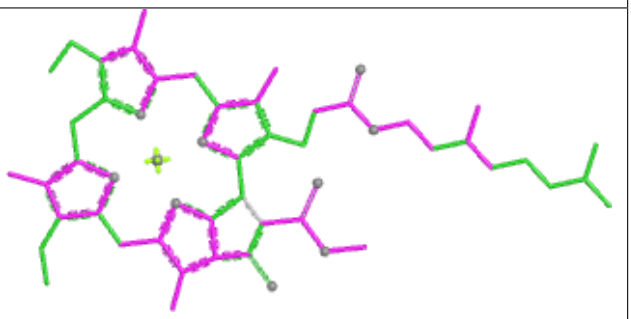
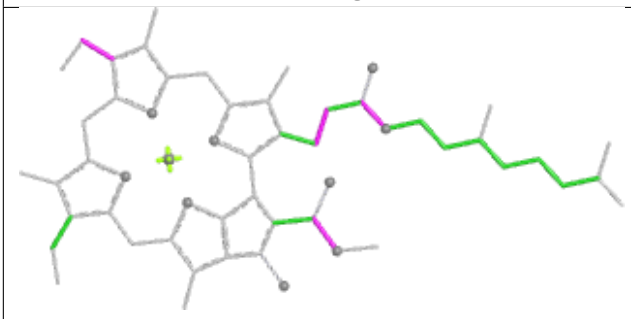
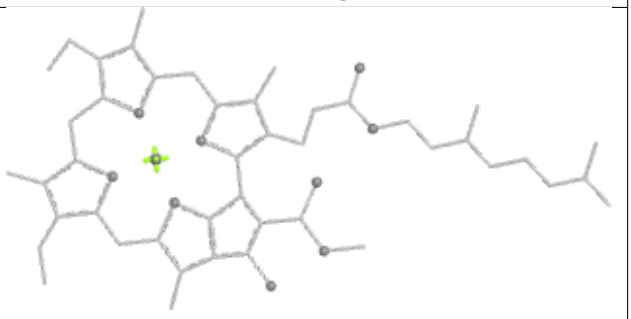


Bond angles

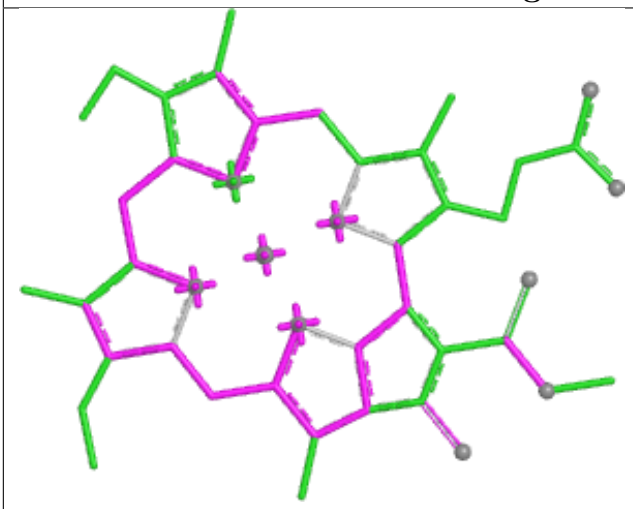


Torsions



Rings

Ligand CLA H 809



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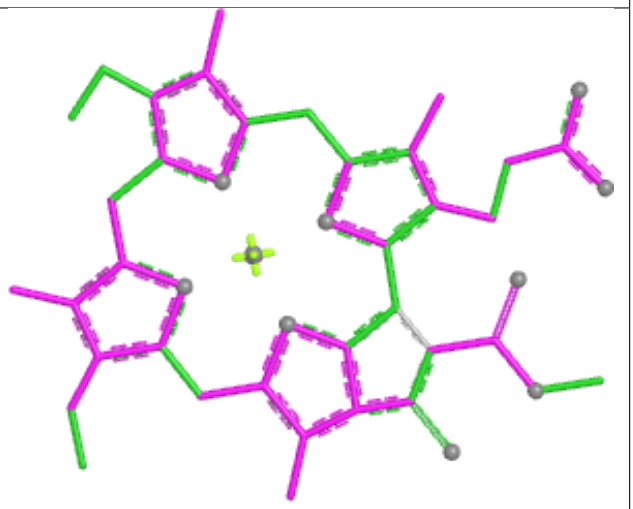
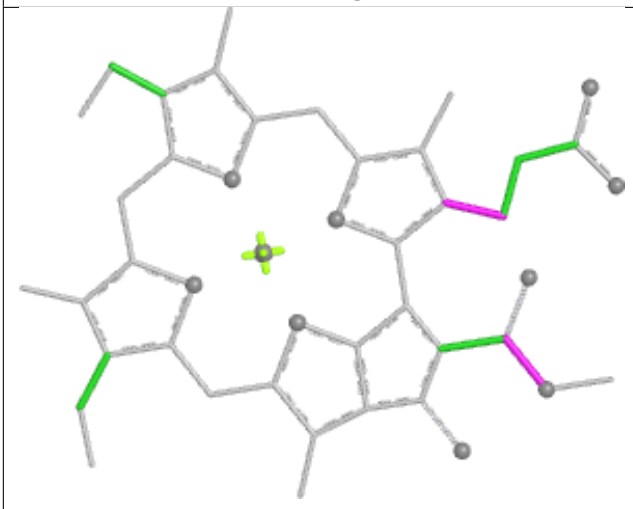


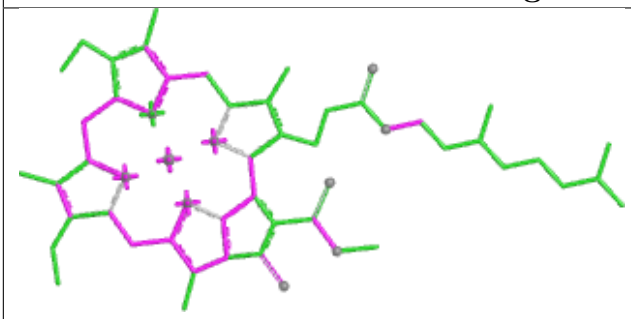
Bond angles



Torsions

Rings

Ligand CLA A 823



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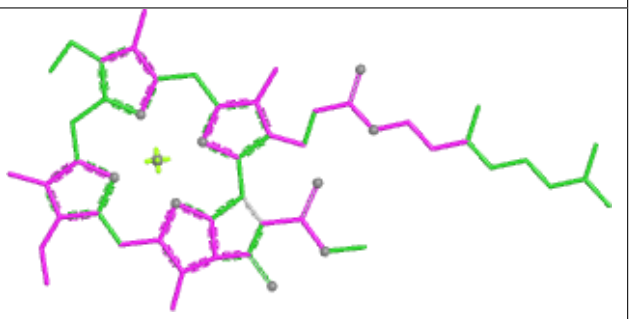
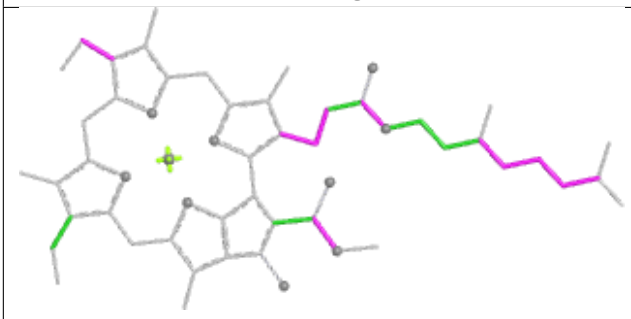
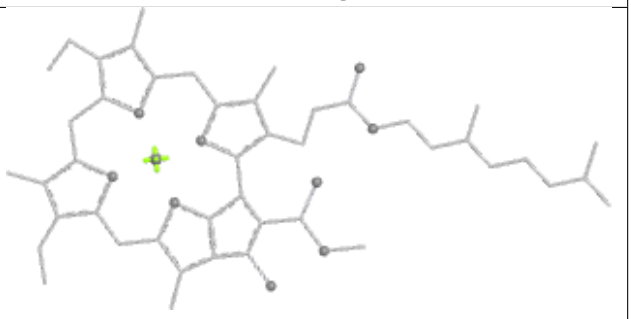


Bond angles

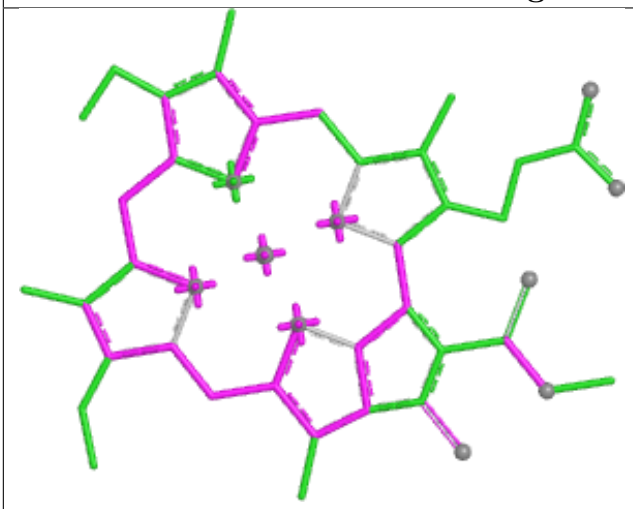


Torsions



Rings

Ligand CLA b 809



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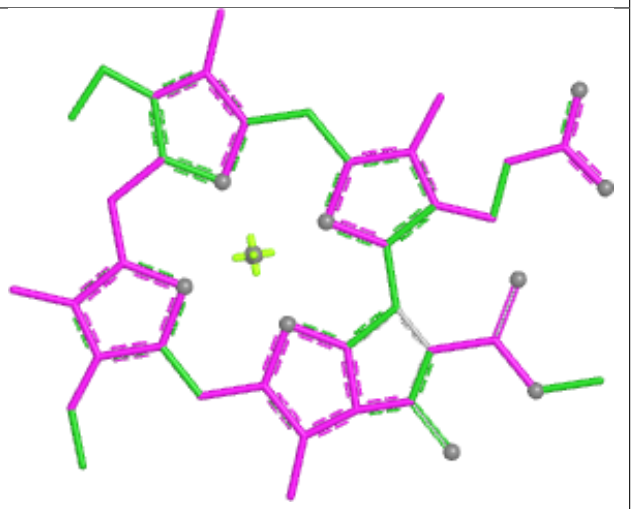
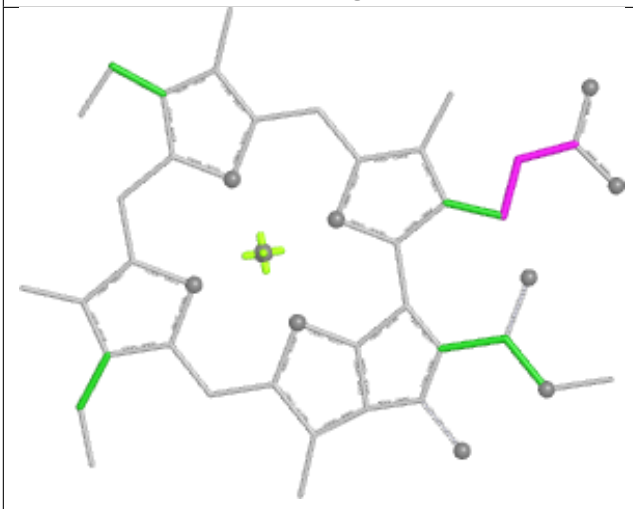


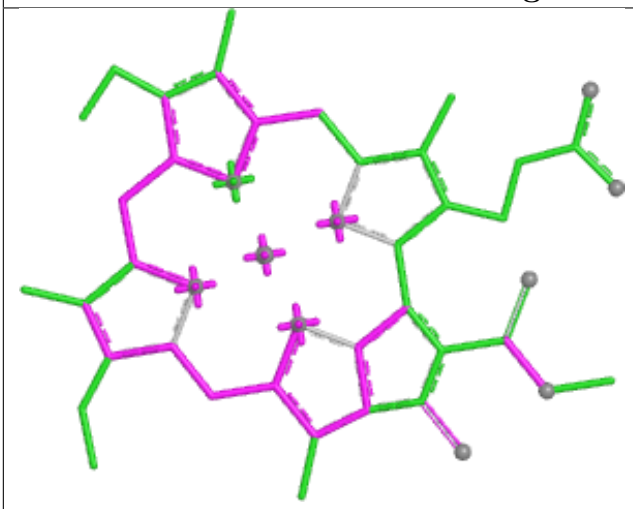
Bond angles



Torsions

Rings

Ligand CLA G 820



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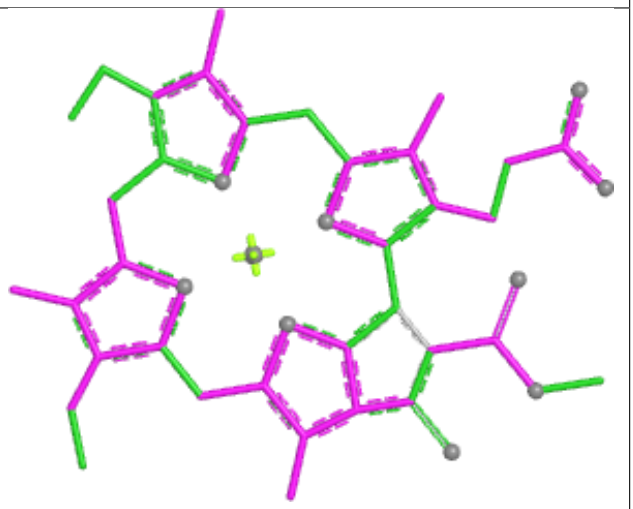
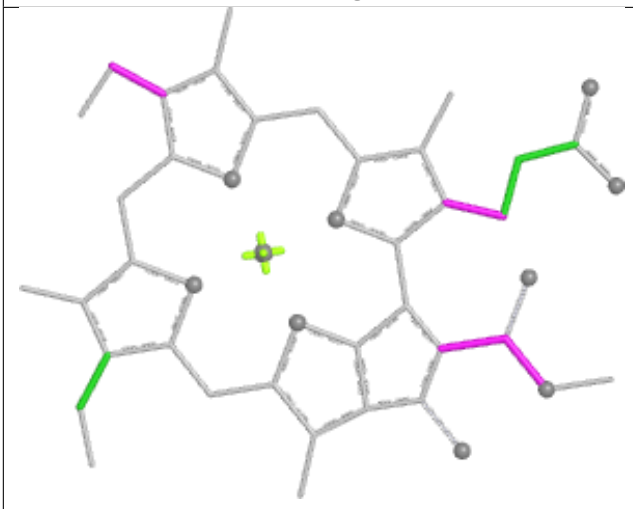


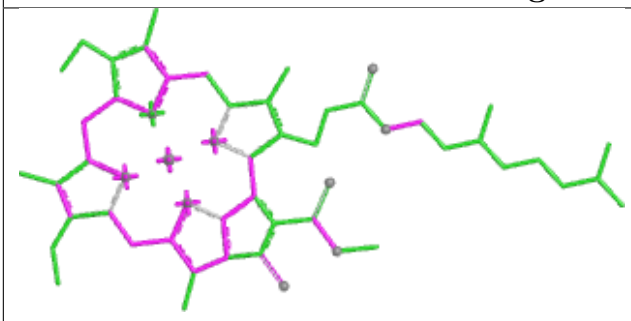
Bond angles



Torsions

Rings

Ligand CLA a 823



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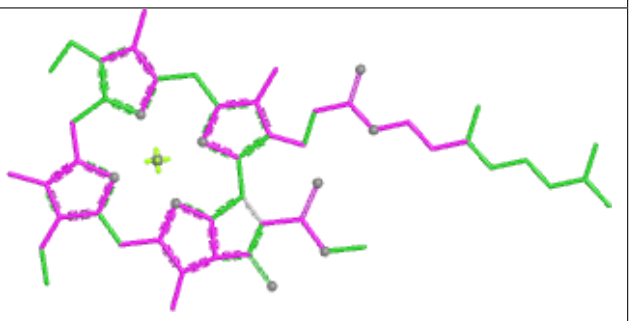
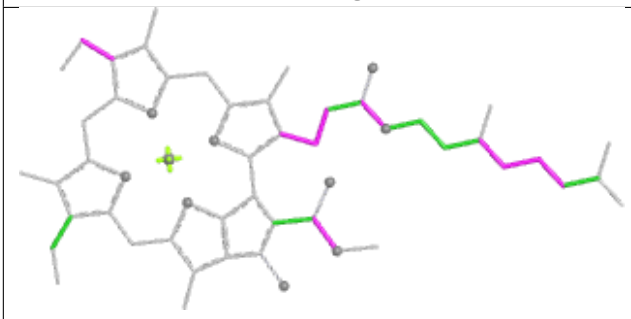
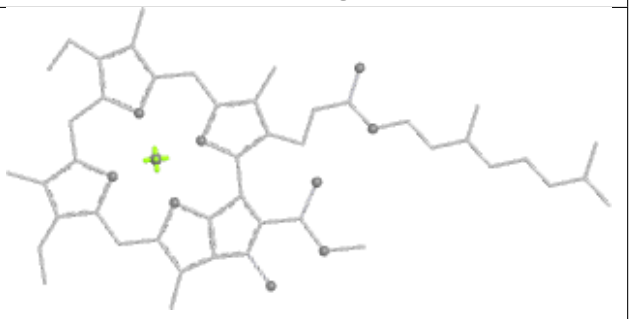


Bond angles

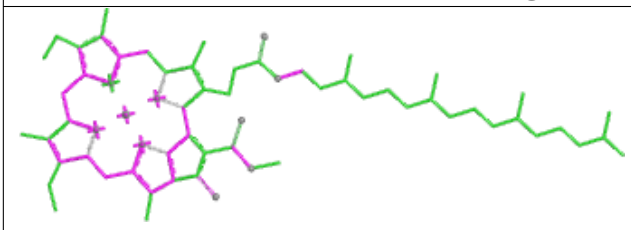


Torsions

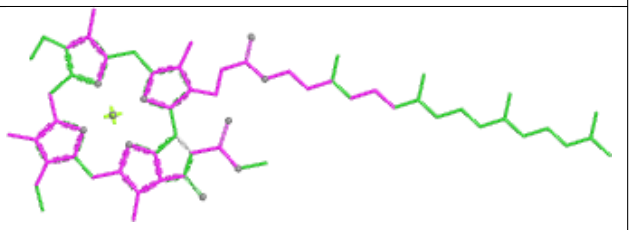


Rings

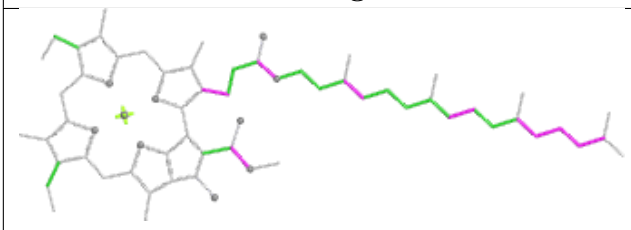
Ligand CLA G 819



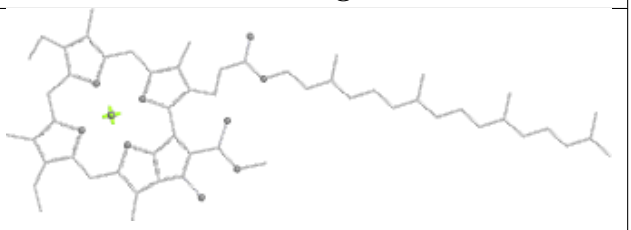
Bond lengths



Bond angles

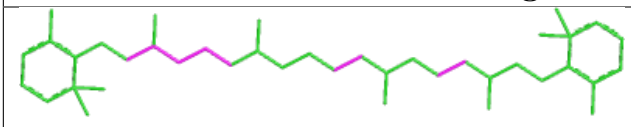


Torsions

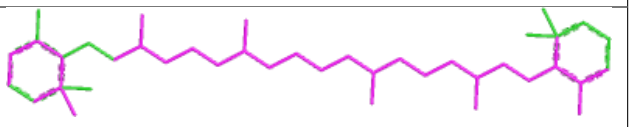


Rings

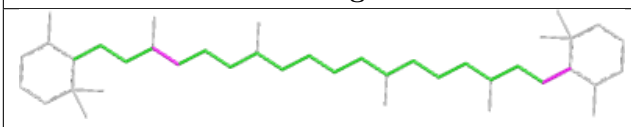
Ligand BCR G 848



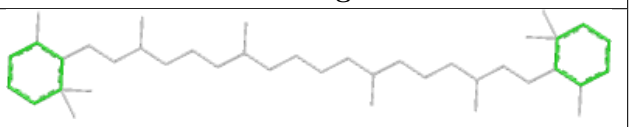
Bond lengths



Bond angles

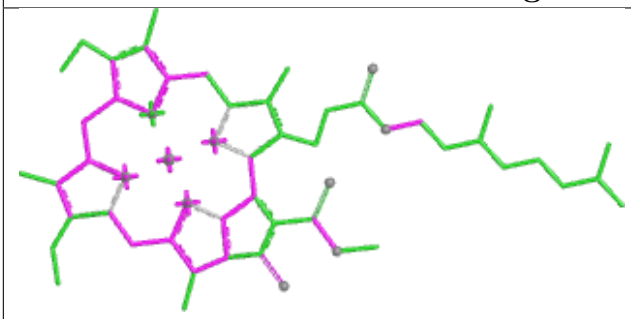


Torsions

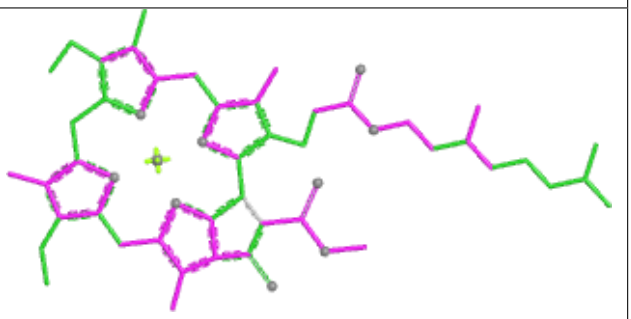


Rings

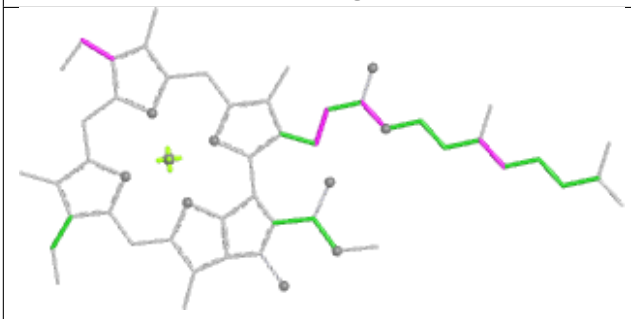
Ligand CLA H 814



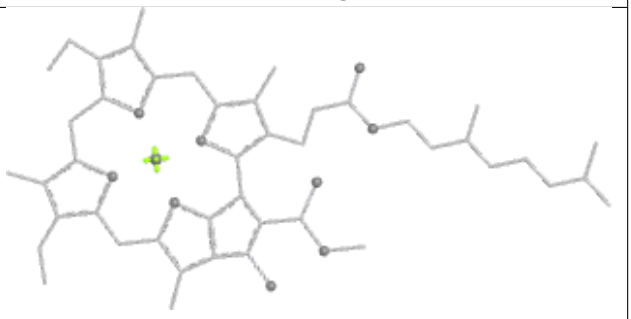
Bond lengths



Bond angles

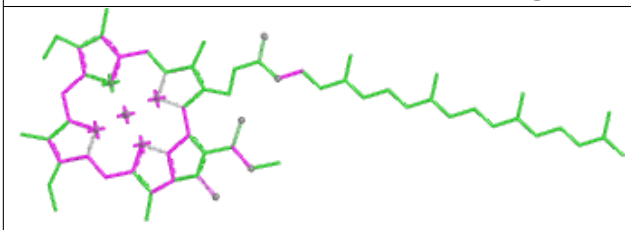


Torsions



Rings

Ligand CLA a 807



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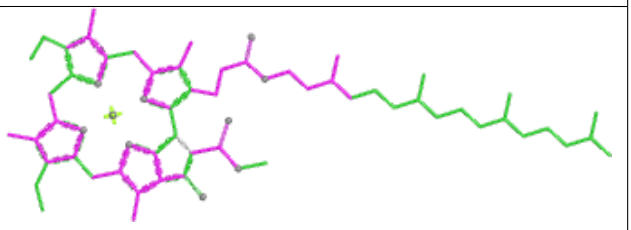
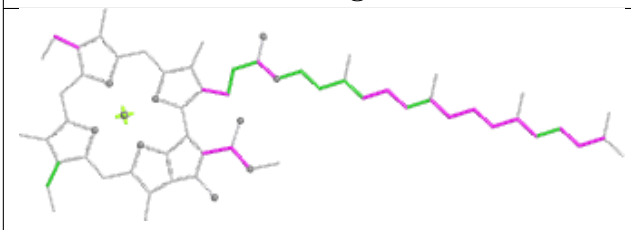
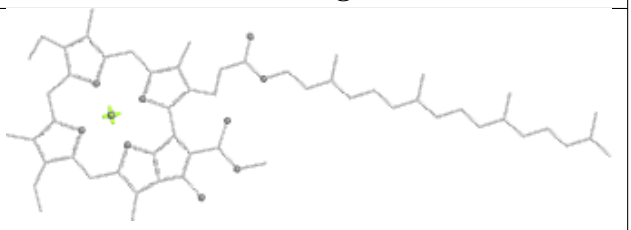


Bond angles

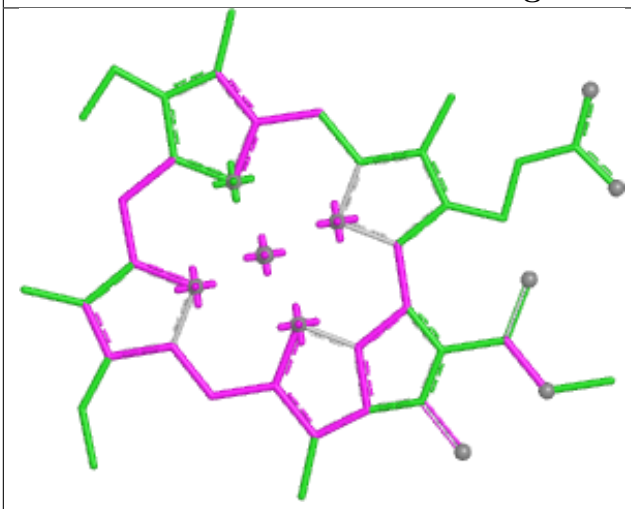


Torsions



Rings

Ligand CLA A 835



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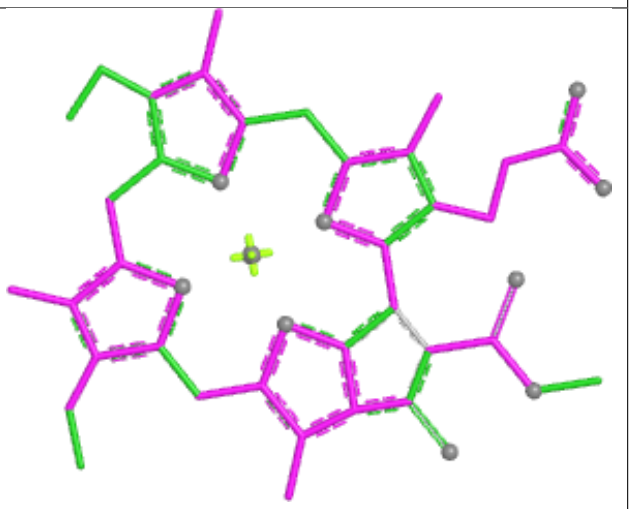
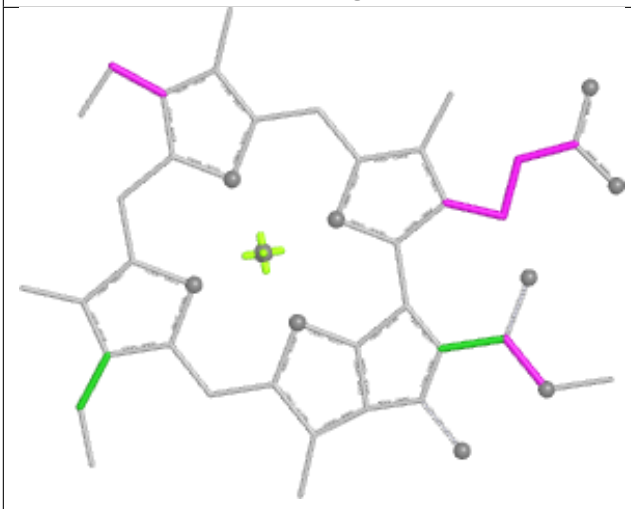


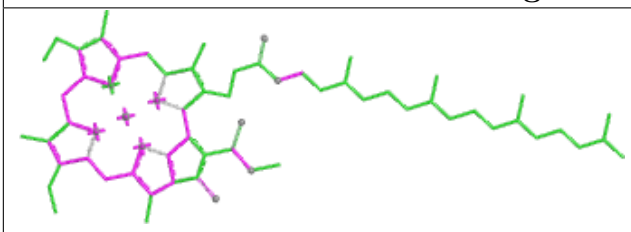
Bond angles



Torsions

Rings

Ligand CLA H 817



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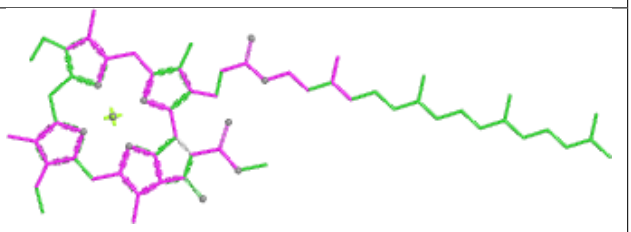
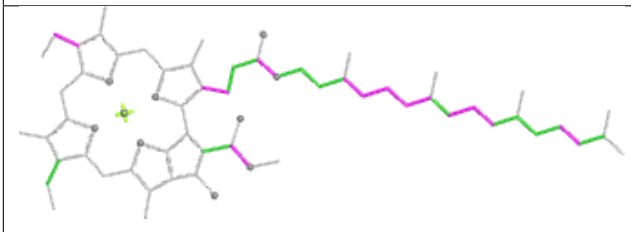
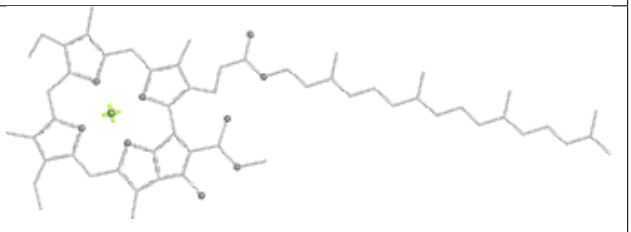


Bond angles

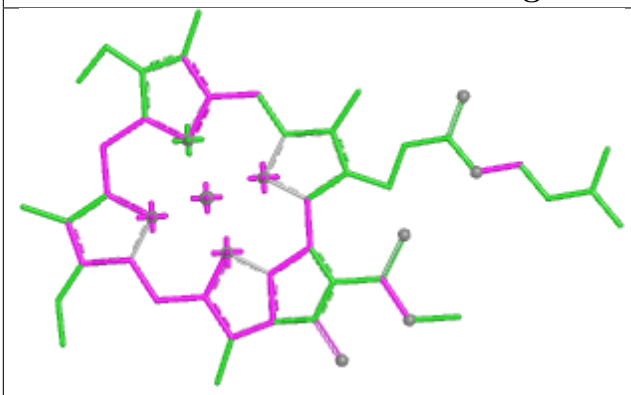


Torsions



Rings

Ligand CLA G 809



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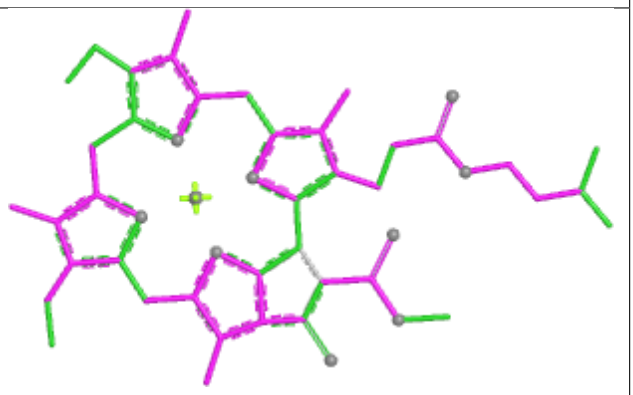
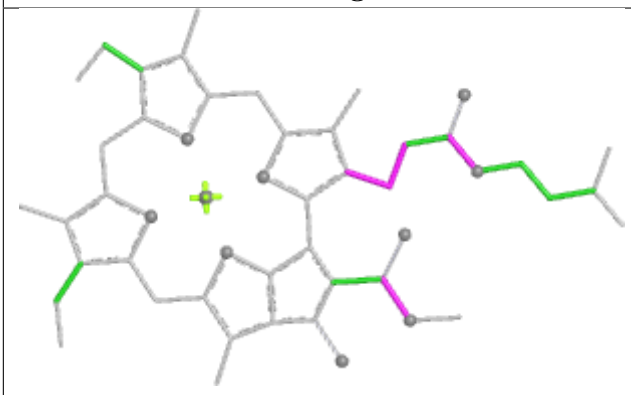
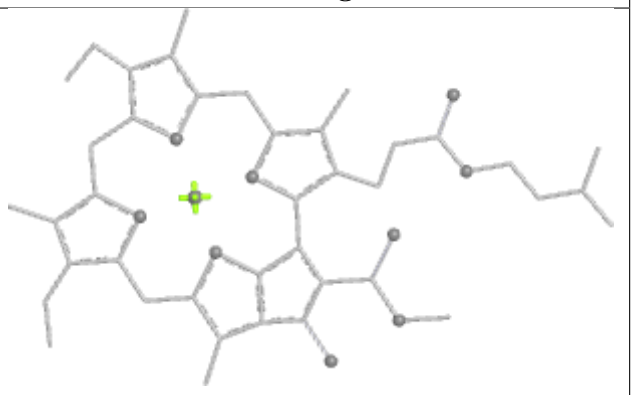


Bond angles

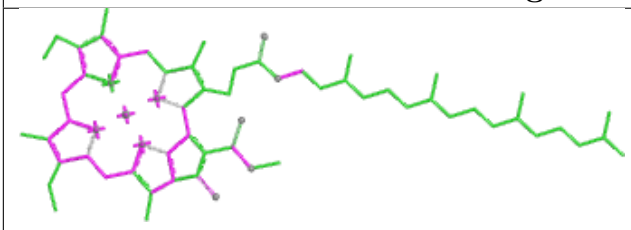


Torsions



Rings

Ligand CLA F 201



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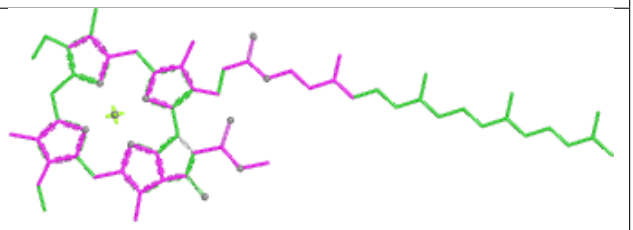
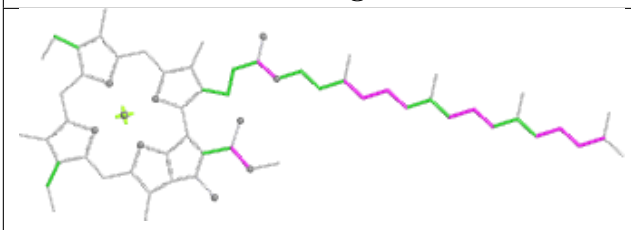


Bond angles



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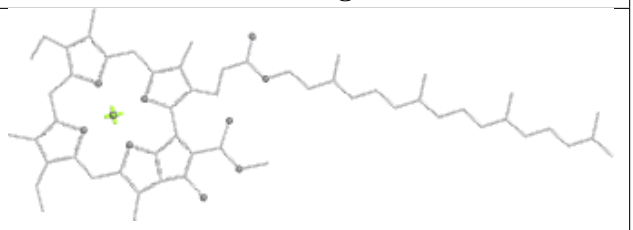
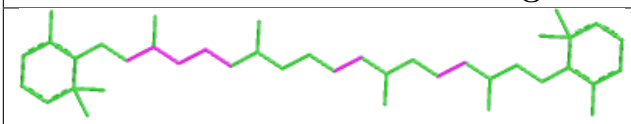


Rings

Ligand BCR B 842



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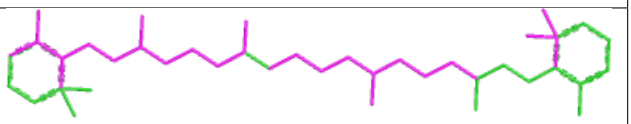
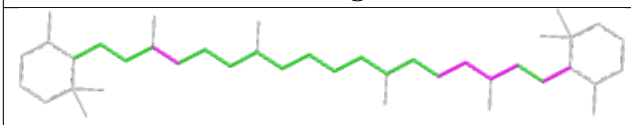
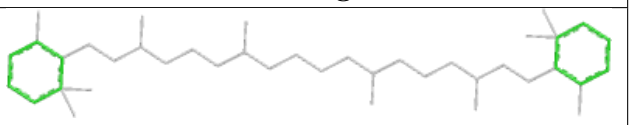


Bond angles

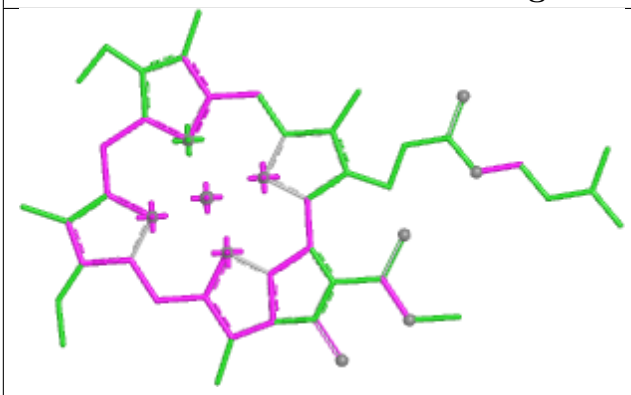


Torsions



Rings

Ligand CLA a 822



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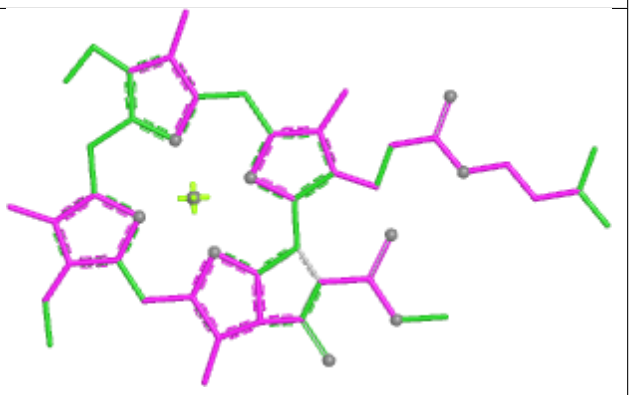
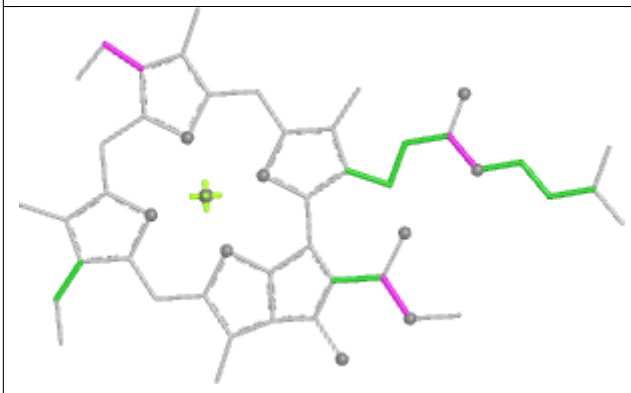


Bond angles



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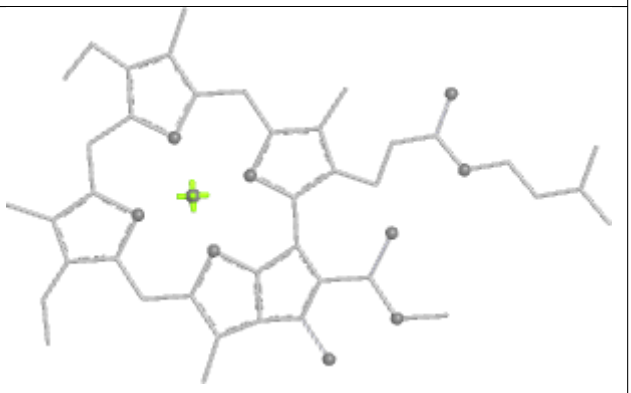
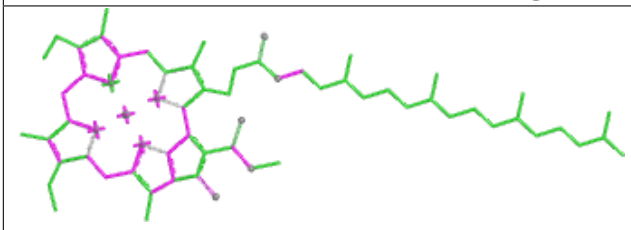


Rings

Ligand CLA b 821



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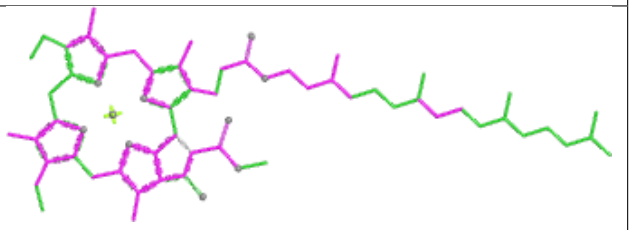
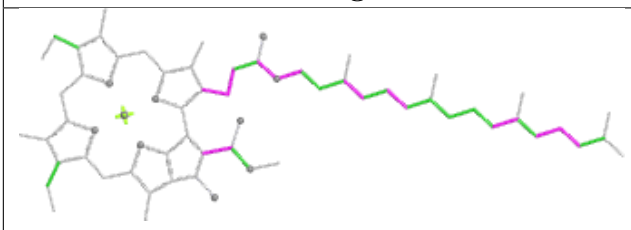


Bond angles



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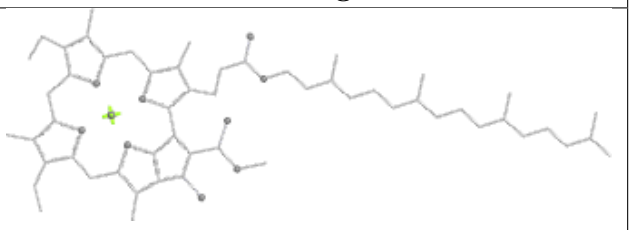
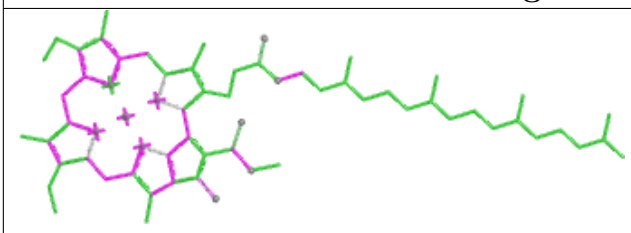


Rings

Ligand CLA H 838



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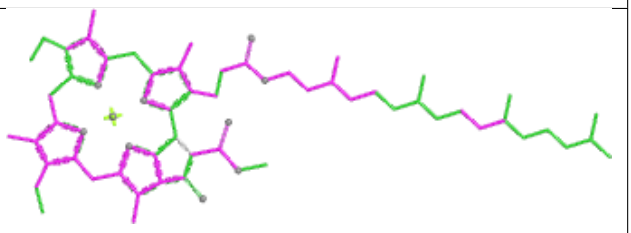
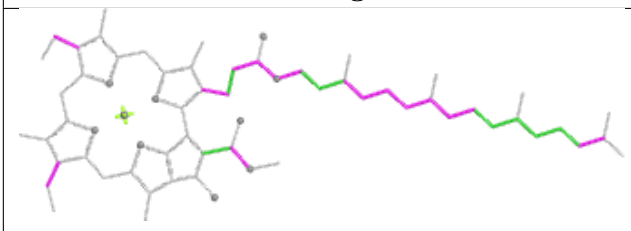
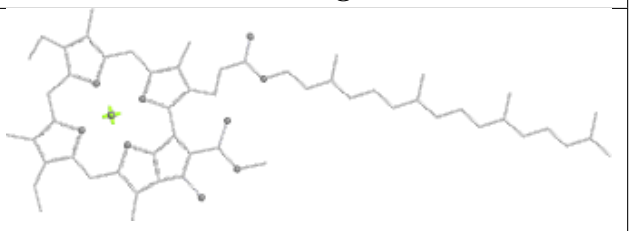


Bond angles

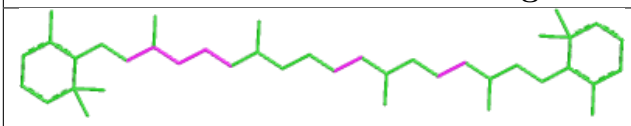


Torsions

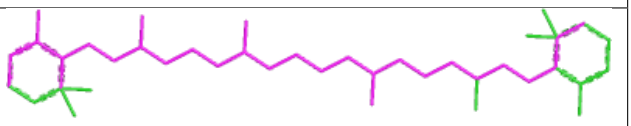


Rings

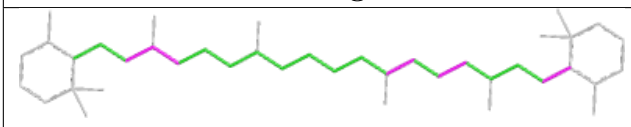
Ligand BCR H 845



Bond lengths



Bond angles



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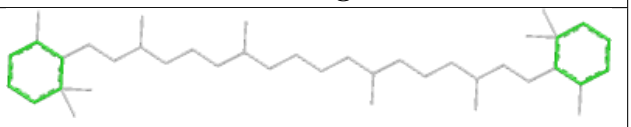
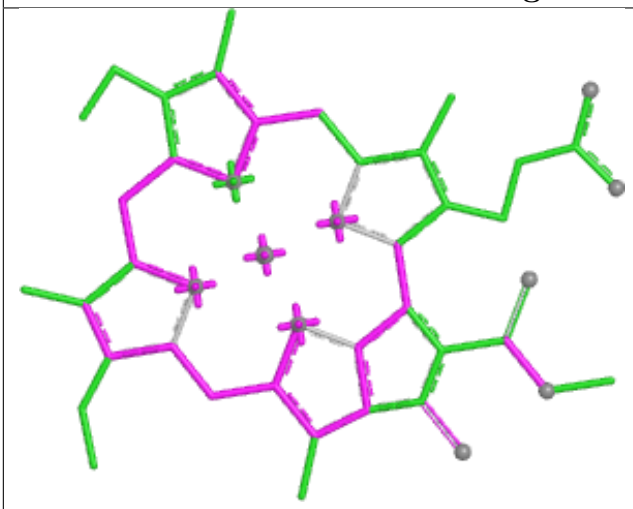


Rings

Ligand CLA G 814



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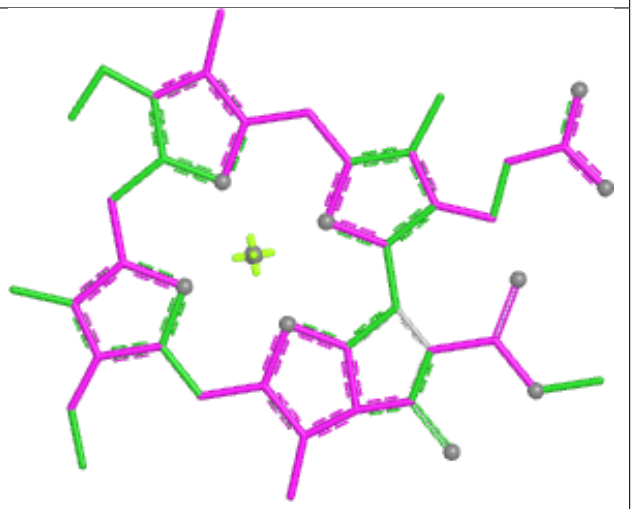
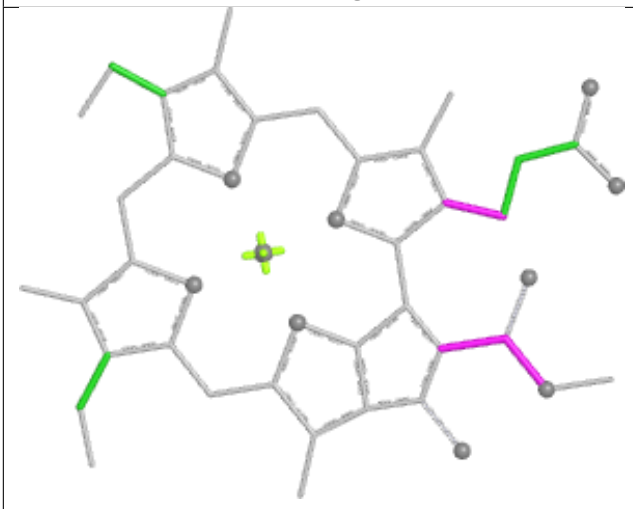


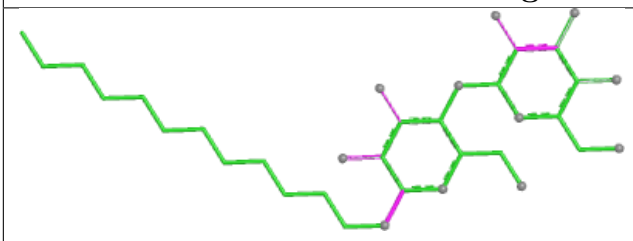
Bond angles



Torsions

Rings

Ligand LMT B 847



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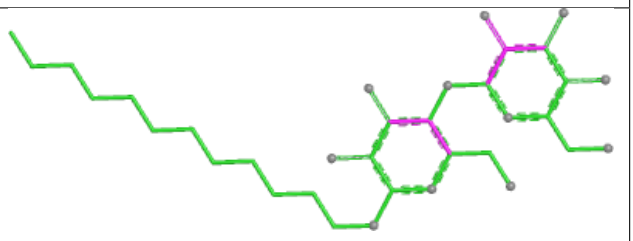
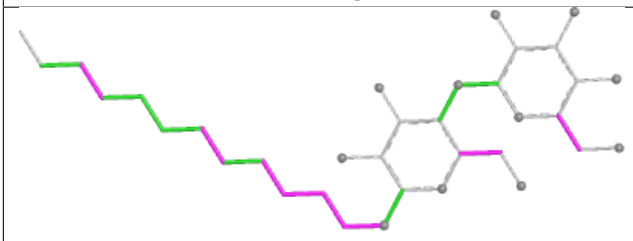
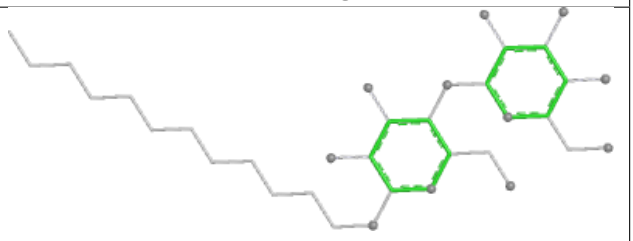


Bond angles

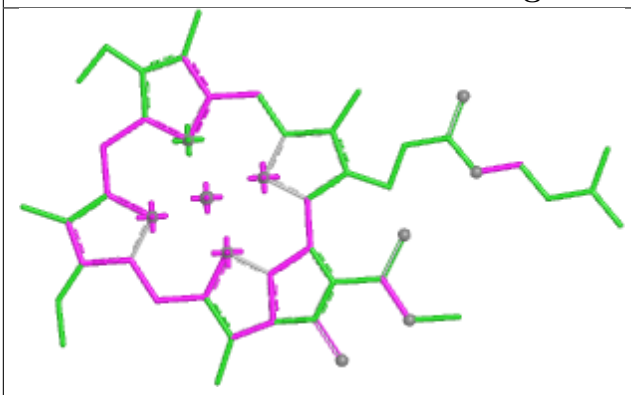


Torsions

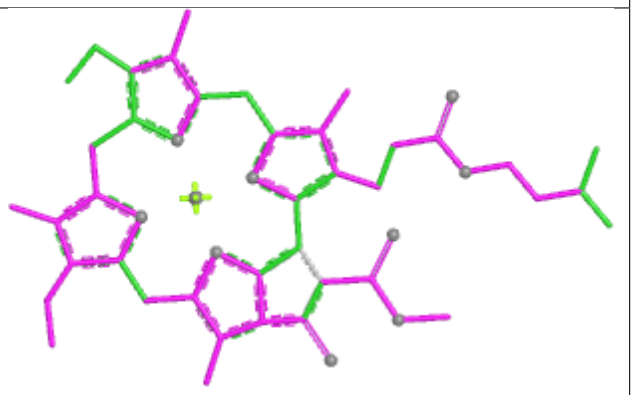


Rings

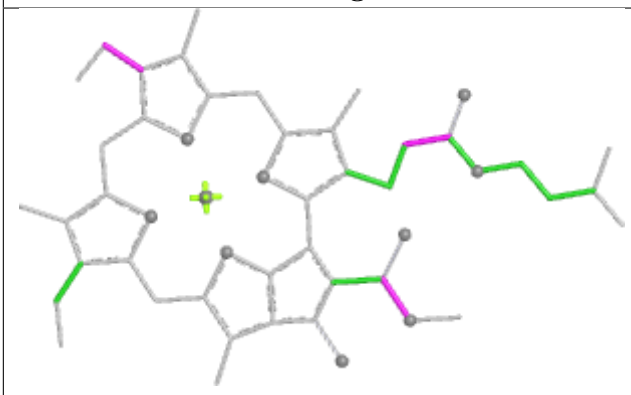
Ligand CLA A 816



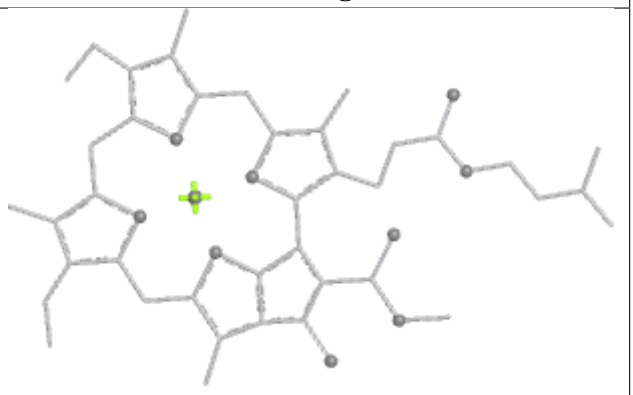
Bond lengths



Bond angles

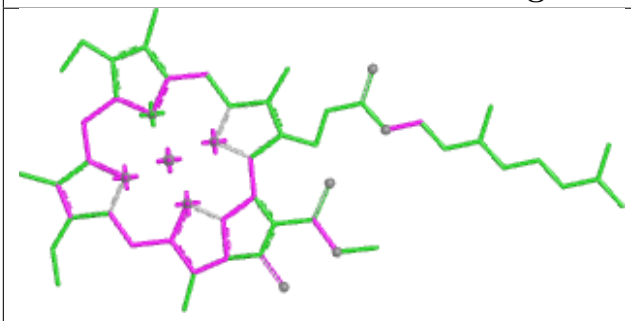


Torsions

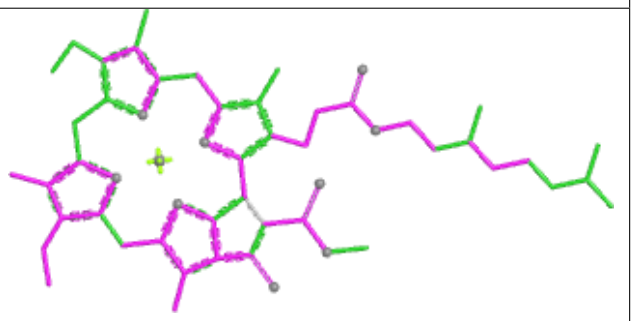


Rings

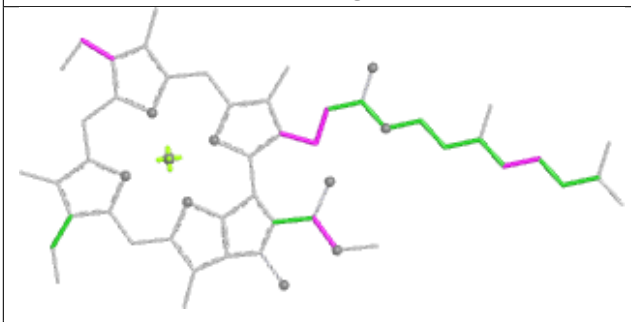
Ligand CLA b 814



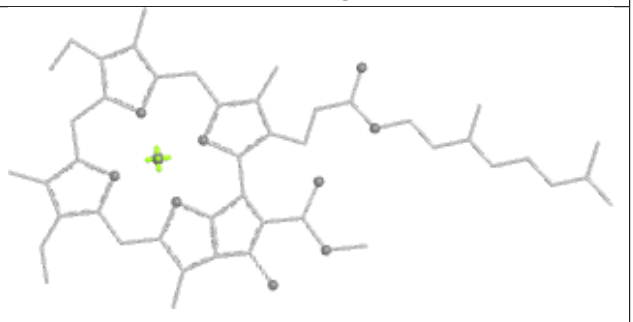
Bond lengths



Bond angles

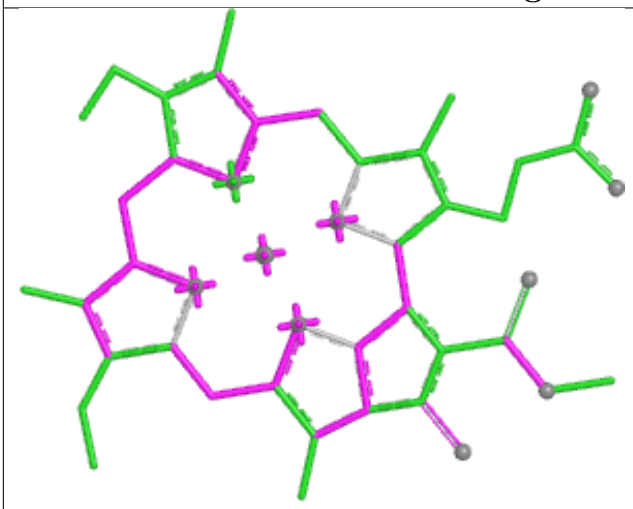


Torsions



Rings

Ligand CLA B 817



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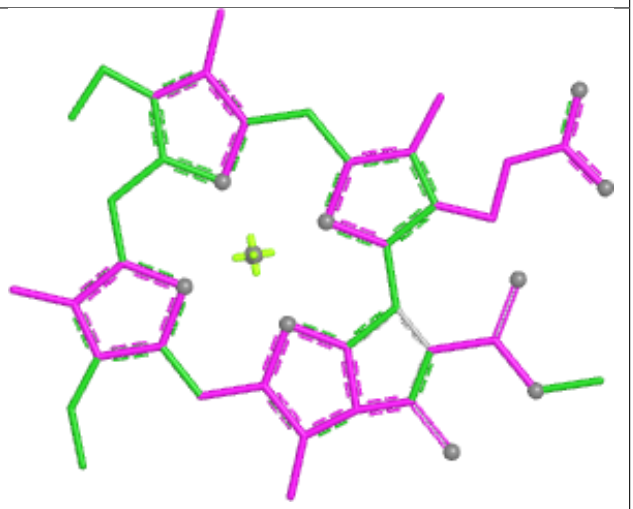
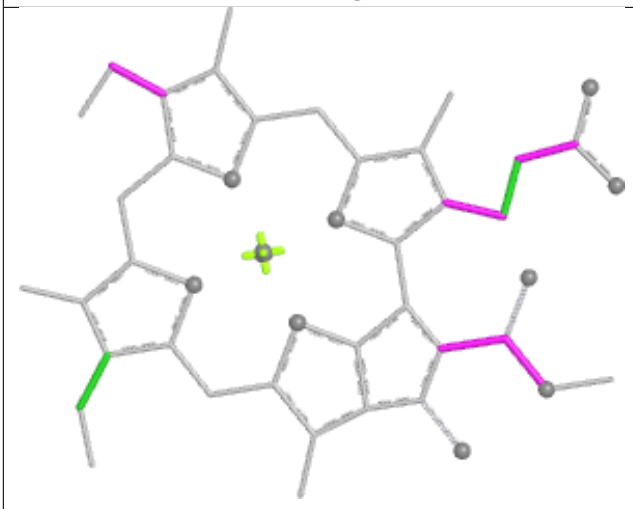


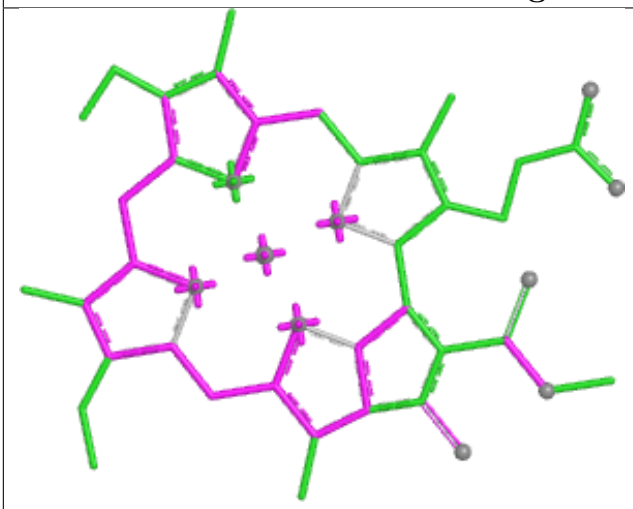
Bond angles



Torsions

Rings

Ligand CLA a 838



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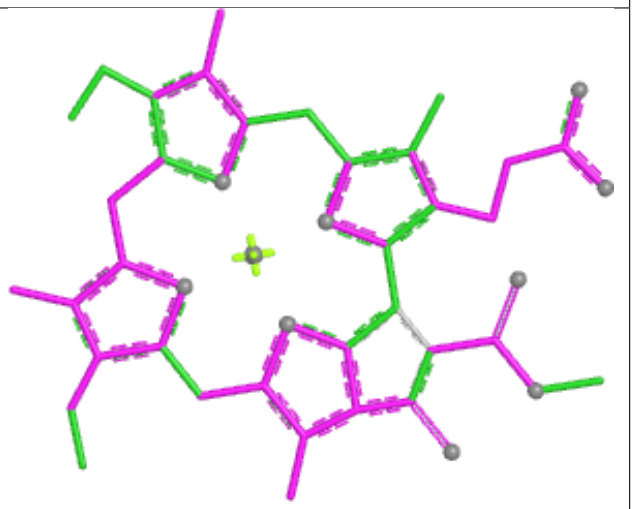
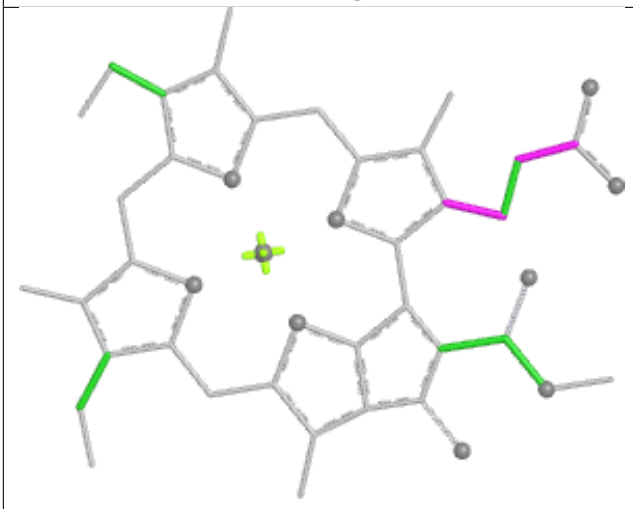


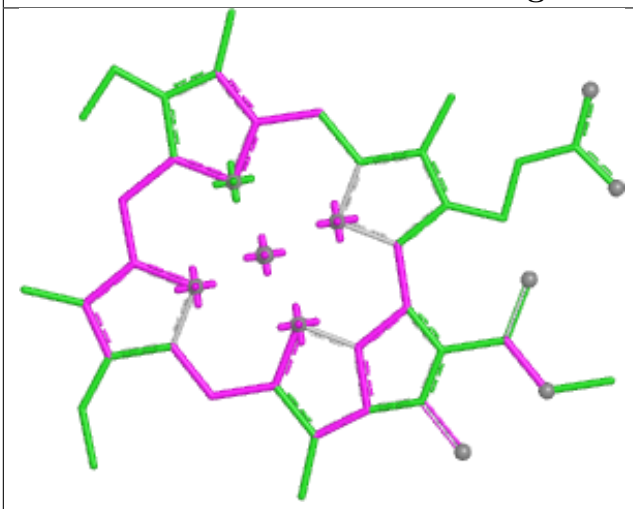
Bond angles



Torsions

Rings

Ligand CLA b 817



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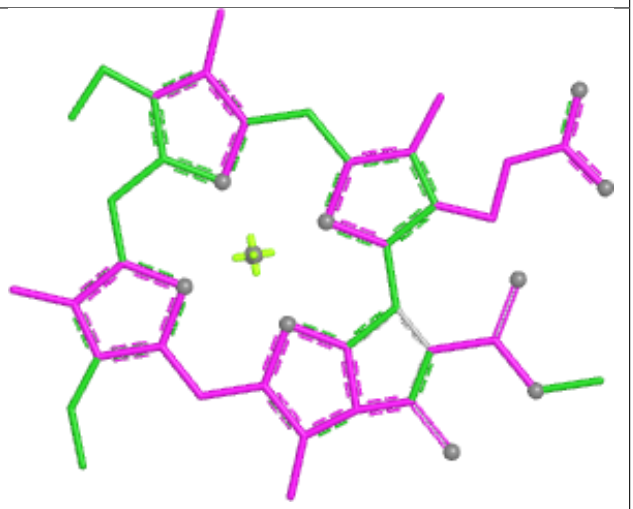
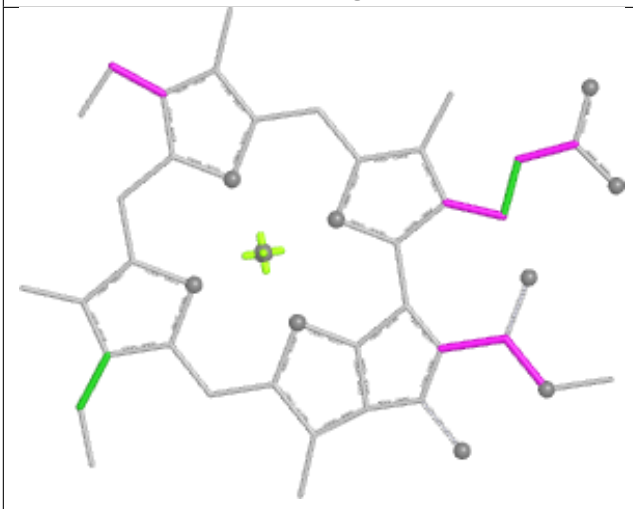


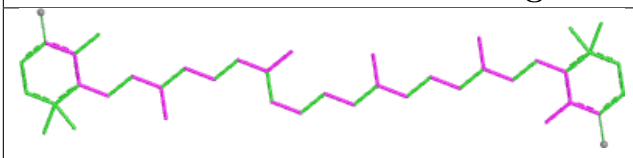
Bond angles



Torsions

Rings

Ligand 45D M 101



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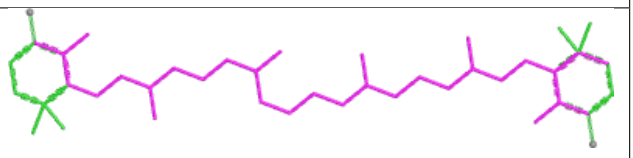
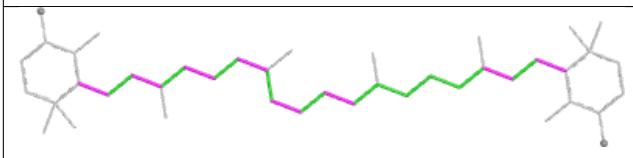
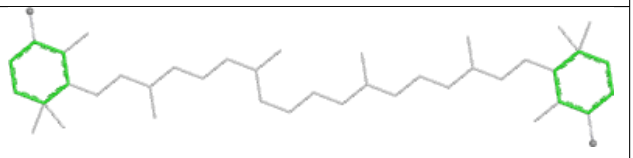


Bond angles

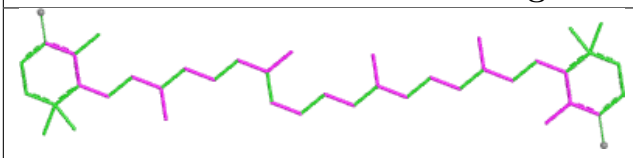


Torsions



Rings

Ligand 45D m 101



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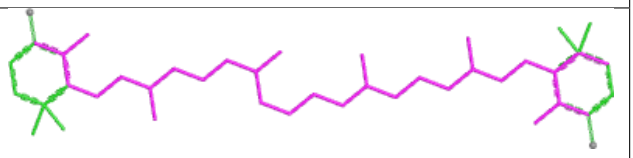
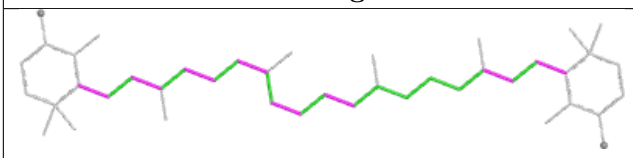


Bond angles



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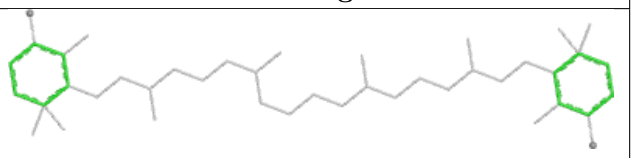
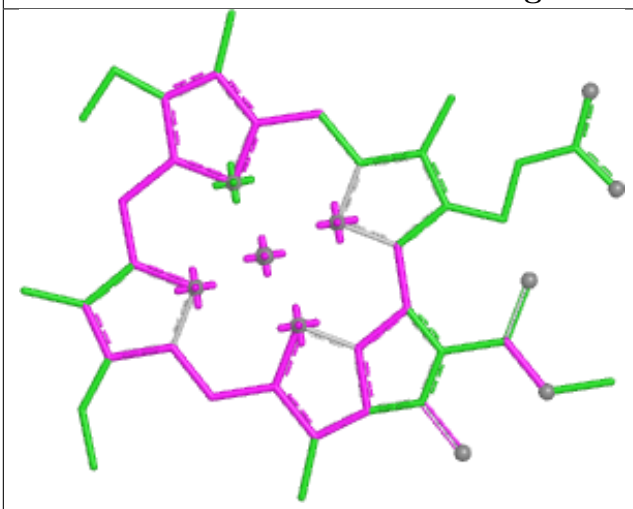


Rings

Ligand CLA B 812



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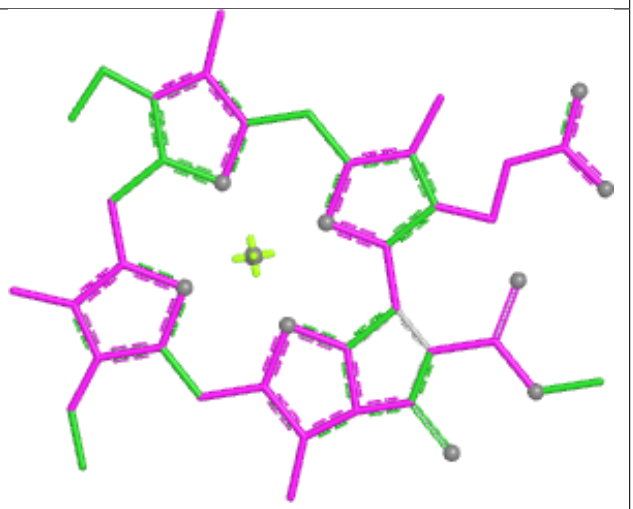
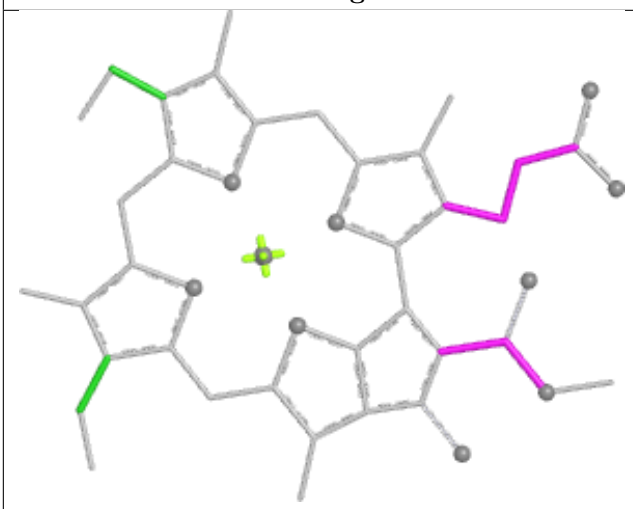


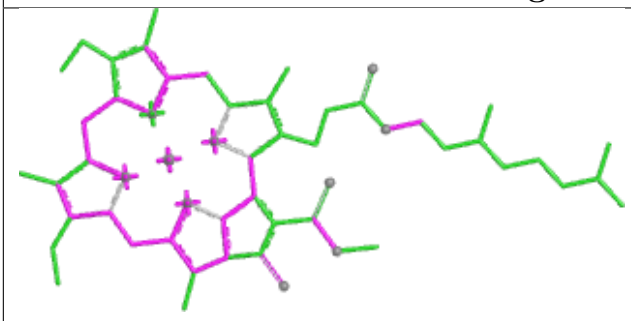
Bond angles



Torsions

Rings

Ligand CLA a 831



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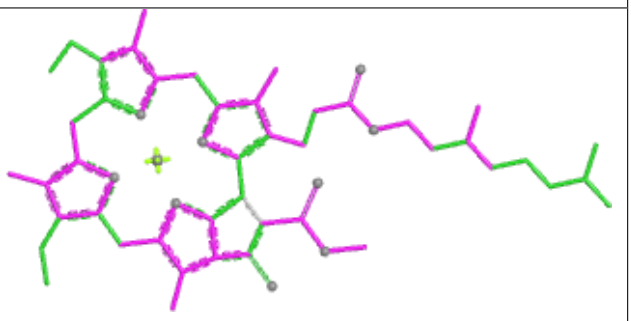
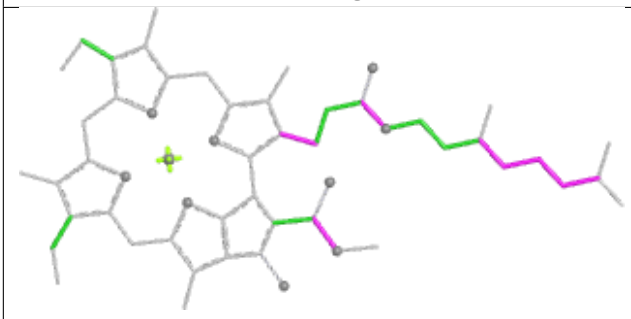


Bond angles



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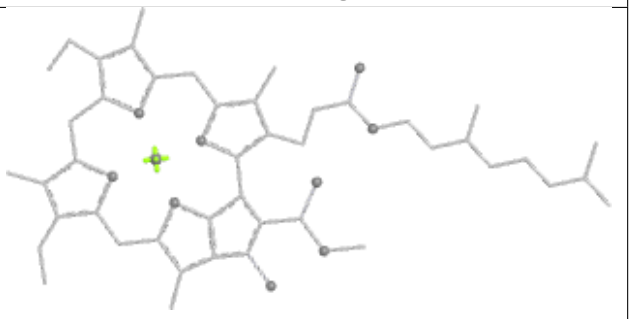
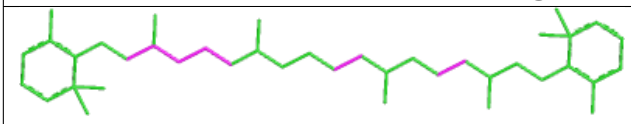


Rings

Ligand BCR j 101



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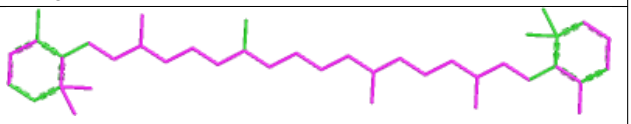
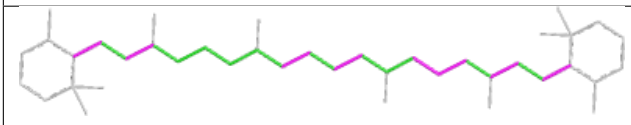
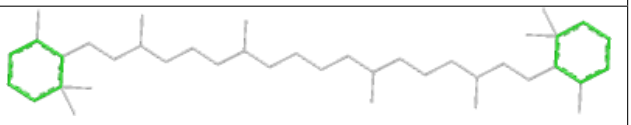


Bond angles

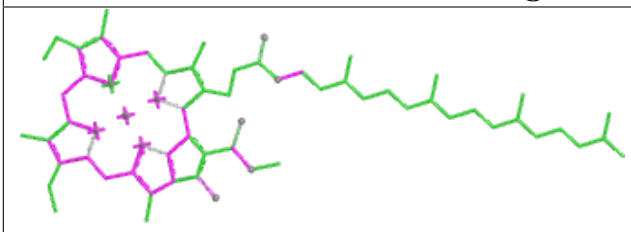


Torsions

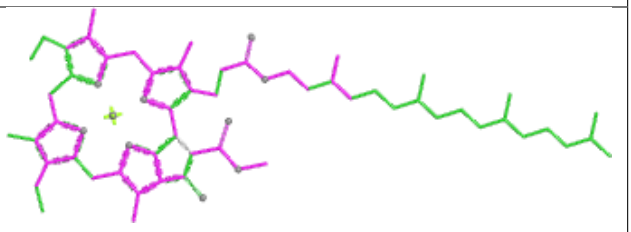


Rings

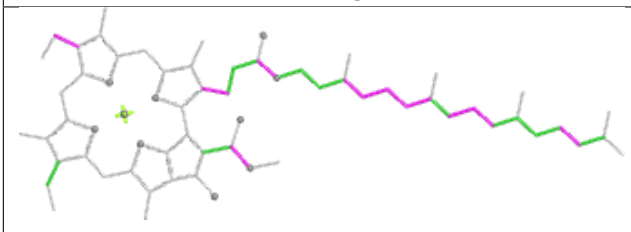
Ligand CLA B 816



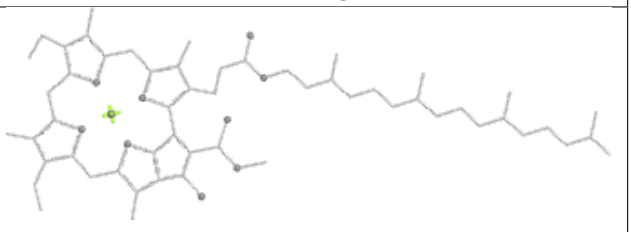
Bond lengths



Bond angles

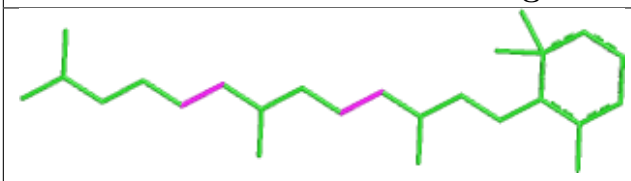


Torsions



Rings

Ligand BCR B 843



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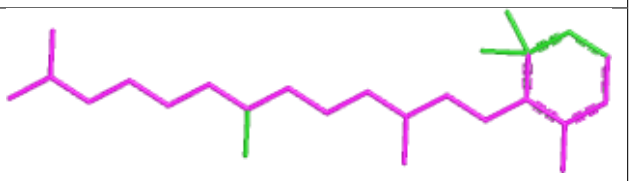
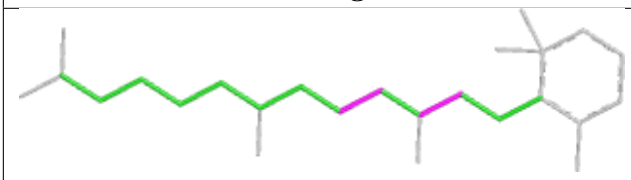
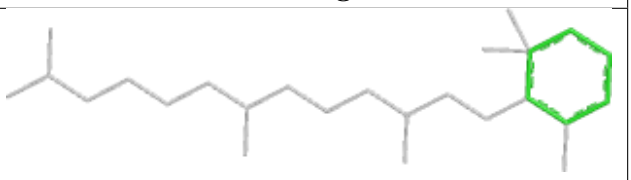


Bond angles

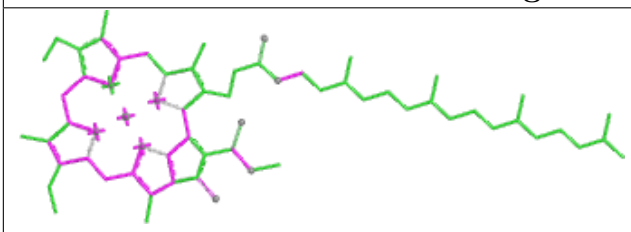


Torsions



Rings

Ligand CLA H 830



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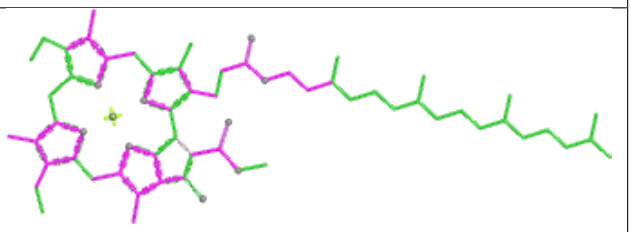
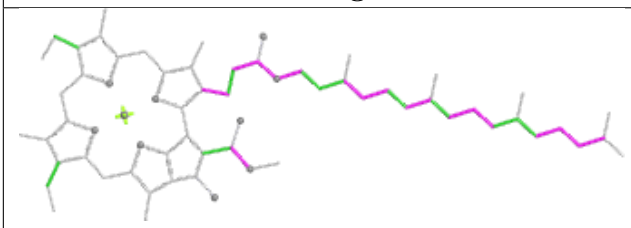
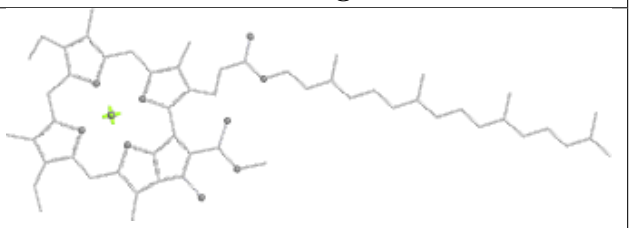


Bond angles

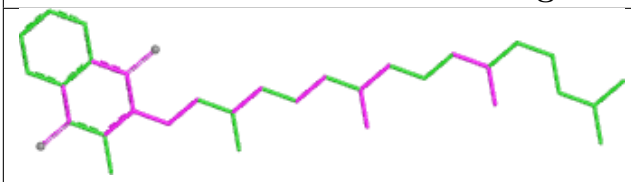


Torsions

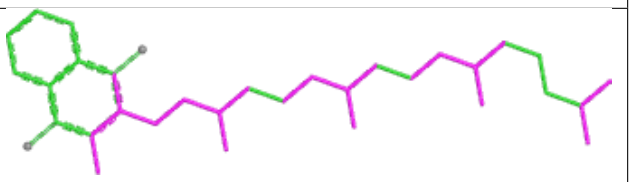


Rings

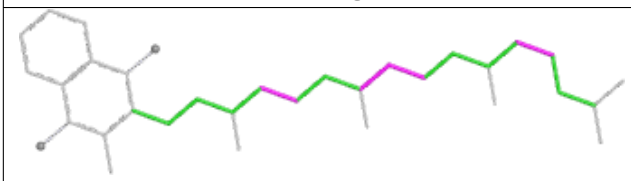
Ligand 1L3 a 842



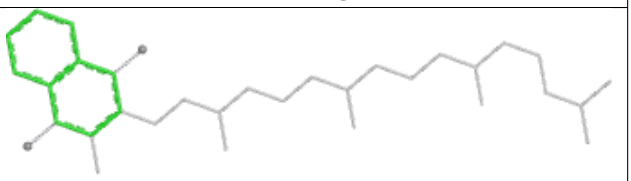
Bond lengths



Bond angles

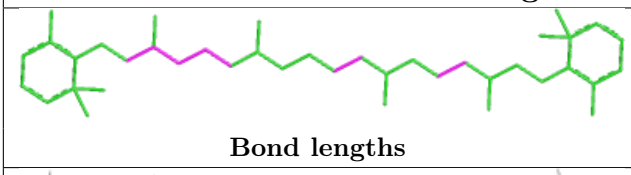


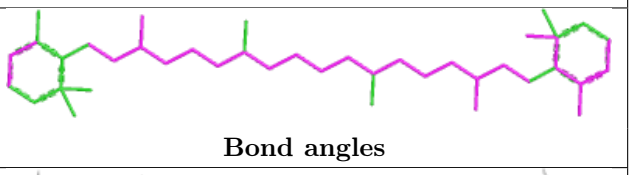
Torsions

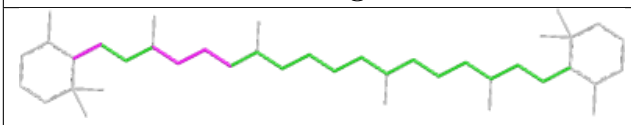


Rings

Ligand BCR G 847


Bond lengths


Bond angles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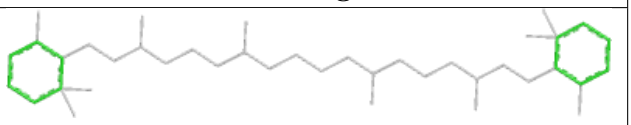
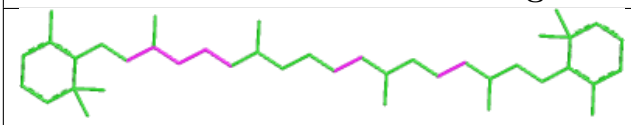
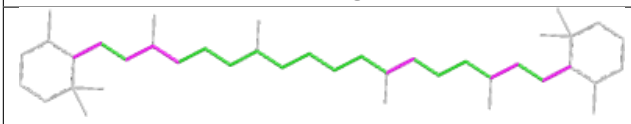
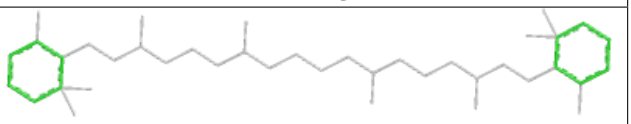

Rings

Ligand BCR a 848

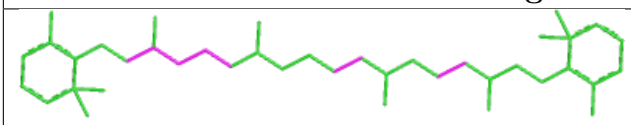

Bond lengths

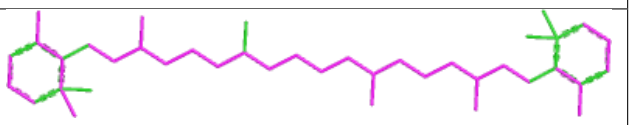
Bond angles

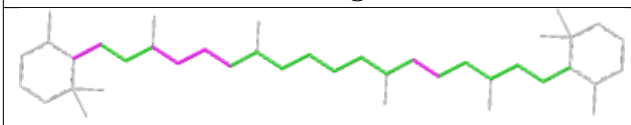

Torsions

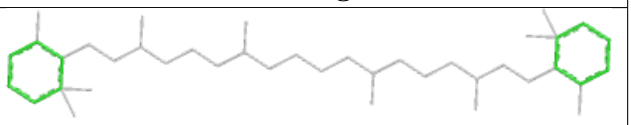

Rings

Ligand BCR b 844

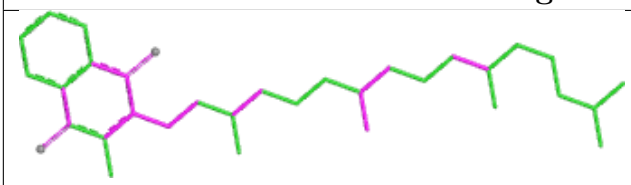

Bond lengths


Bond angles


Torsions


Rings

Ligand 1L3 b 838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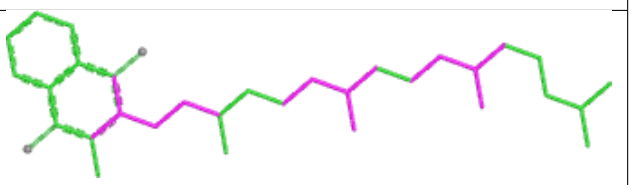
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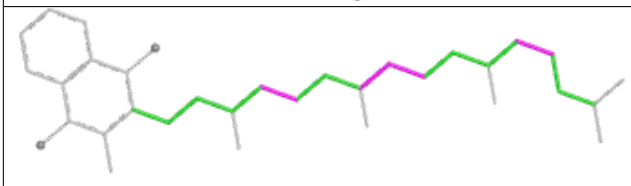
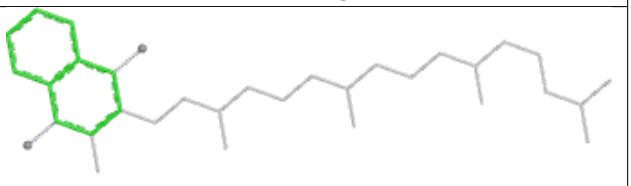
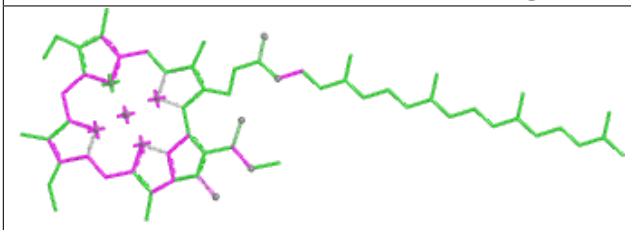
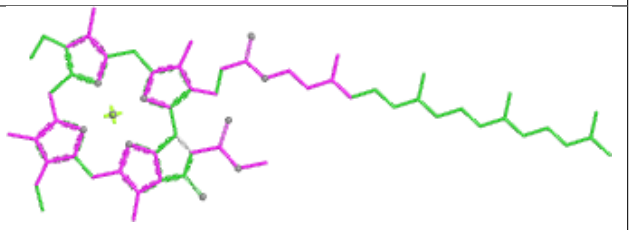

Torsions


Rings

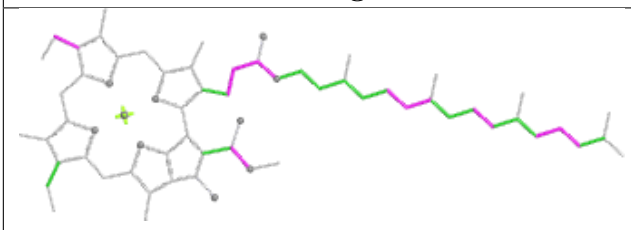
Ligand CLA G 841



Bond lengths



Bond angles



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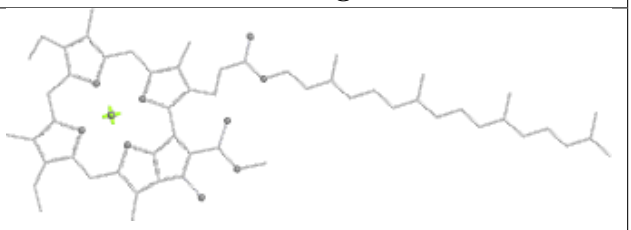
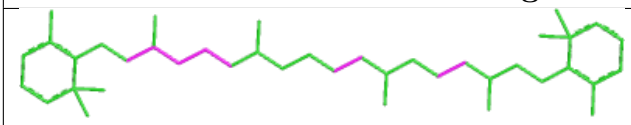


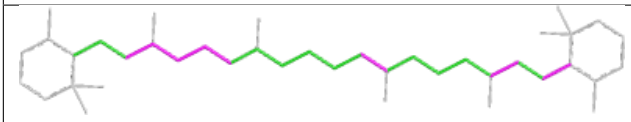
Rings

Ligand BCR G 850



Bond lengths

Bond angles



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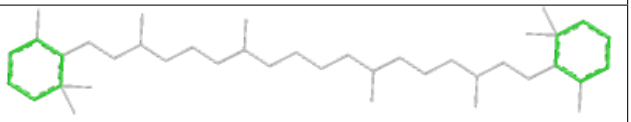
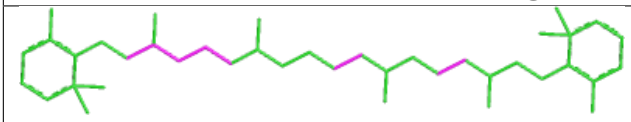
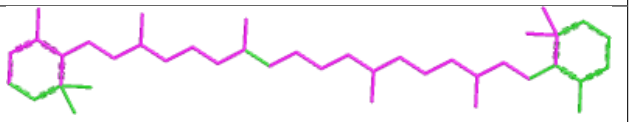


Rings

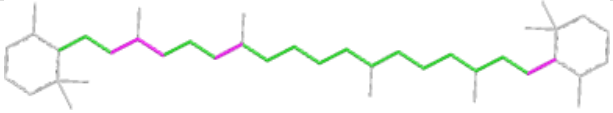
Ligand BCR L 201



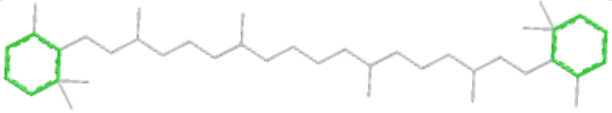
Bond lengths



Bond angles

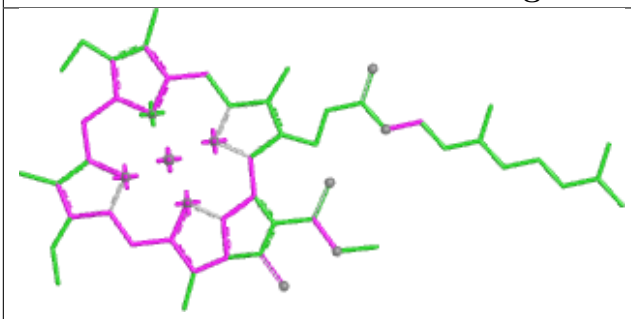


Torsions

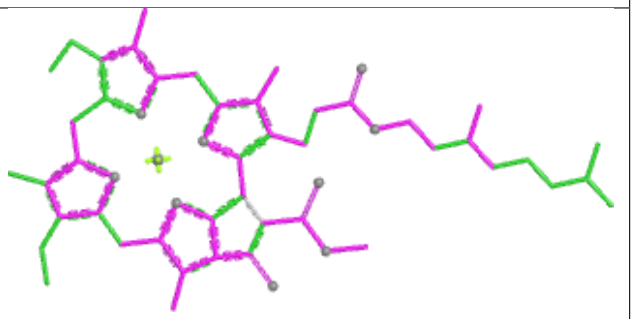


Rings

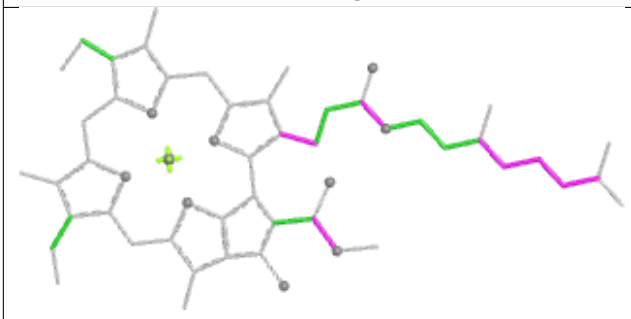
Ligand CLA H 801



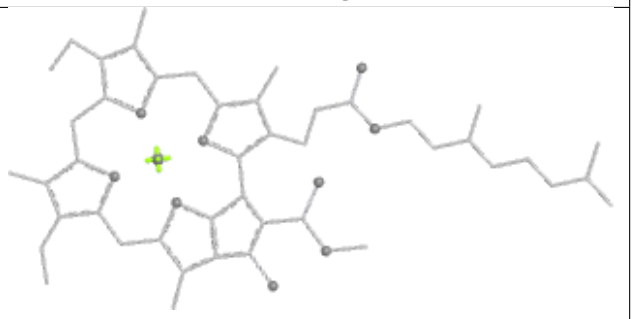
Bond lengths



Bond angles

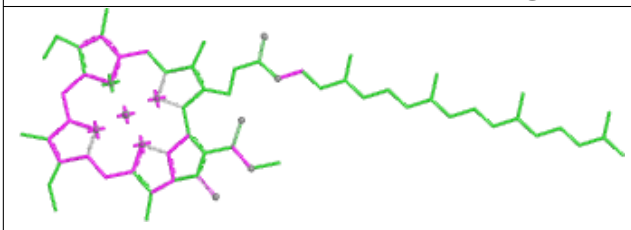


Torsions

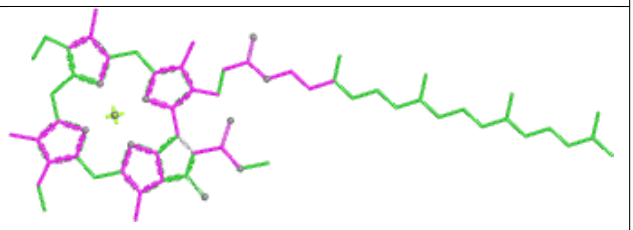


Rings

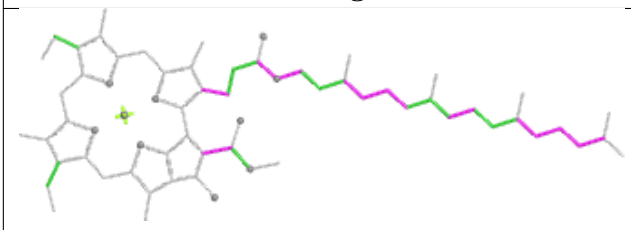
Ligand CLA A 824



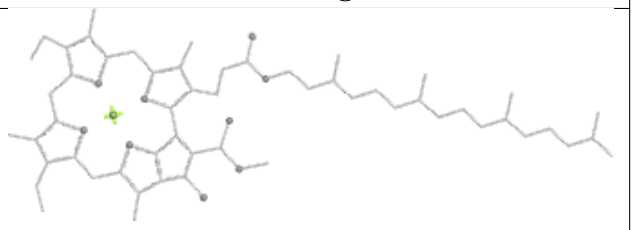
Bond lengths



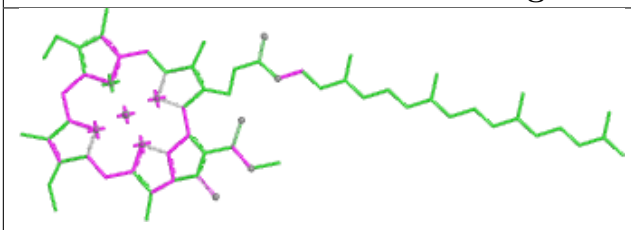
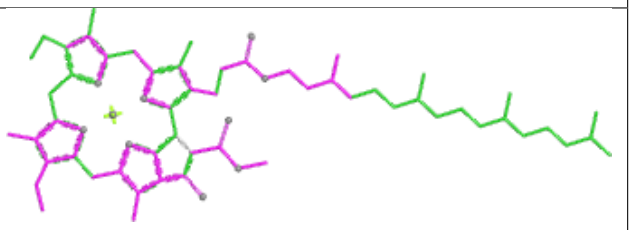
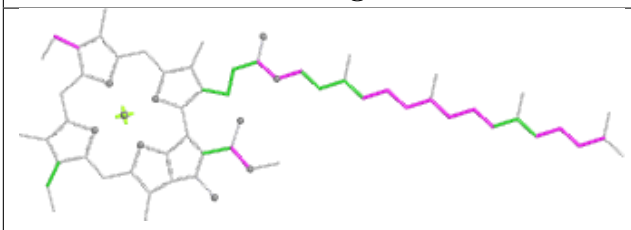
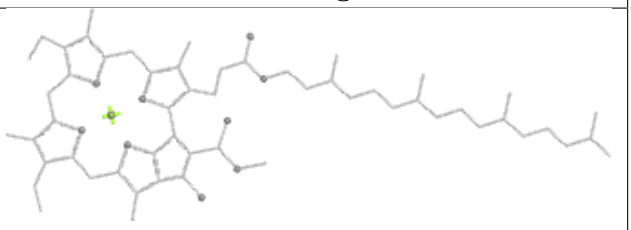
Bond angles

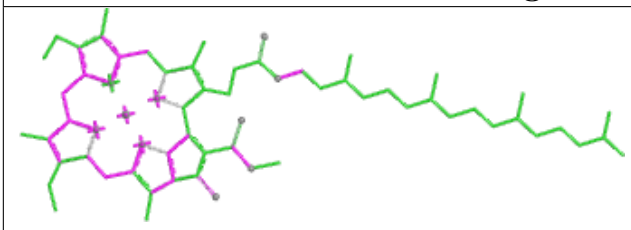
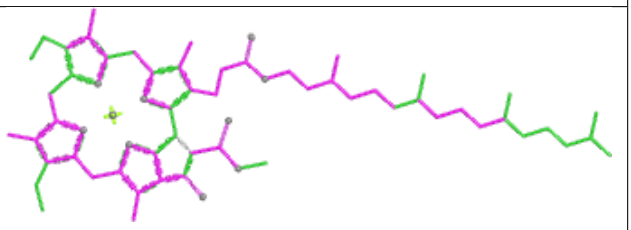
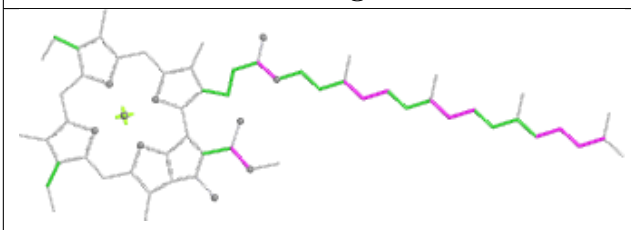
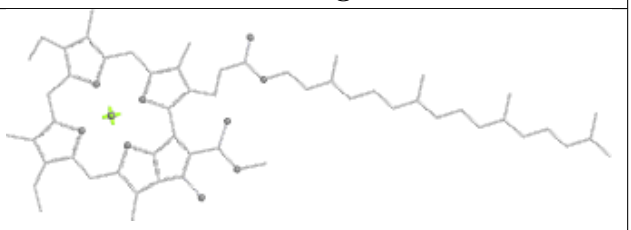


Torsions

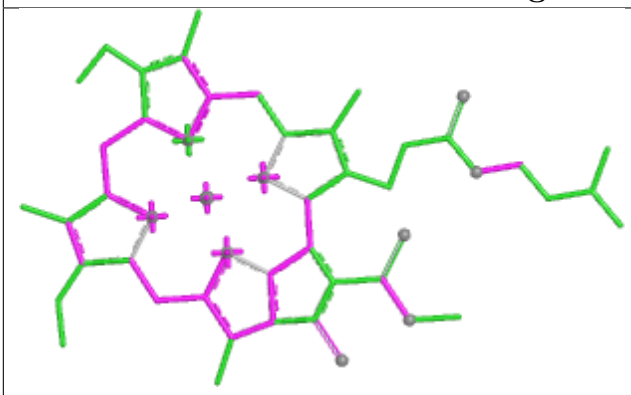


Rings

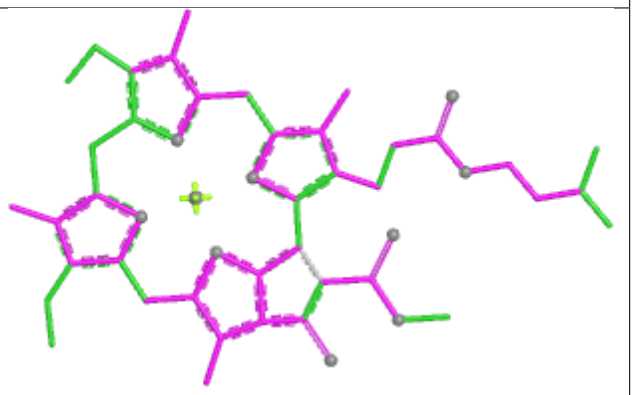
Ligand CLA b 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

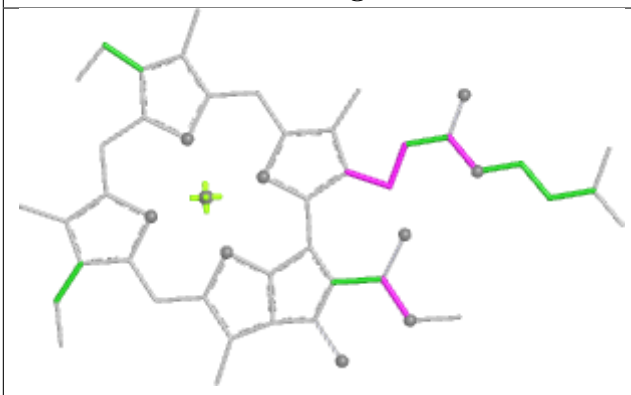
Ligand CLA a 808



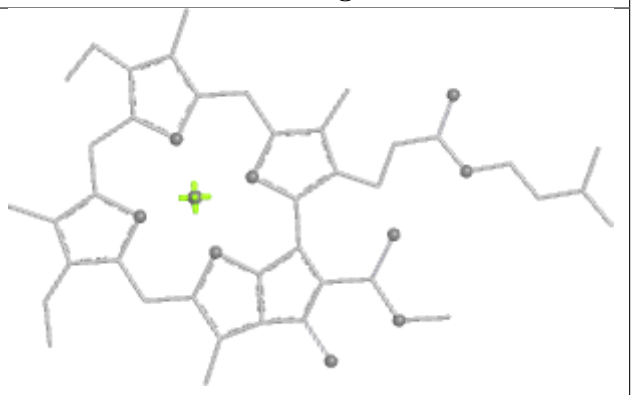
Bond lengths



Bond angles

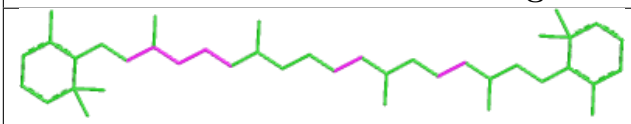


Torsions

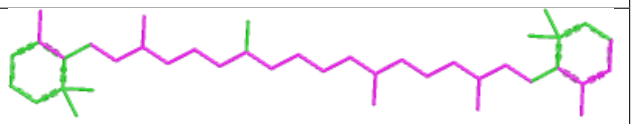


Rings

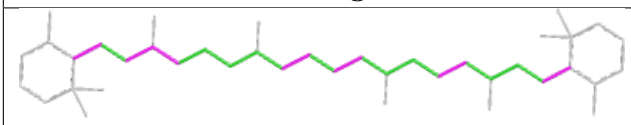
Ligand BCR a 844



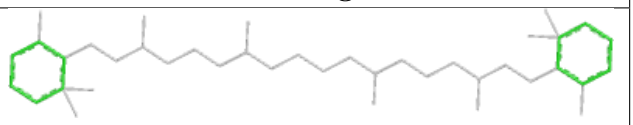
Bond lengths



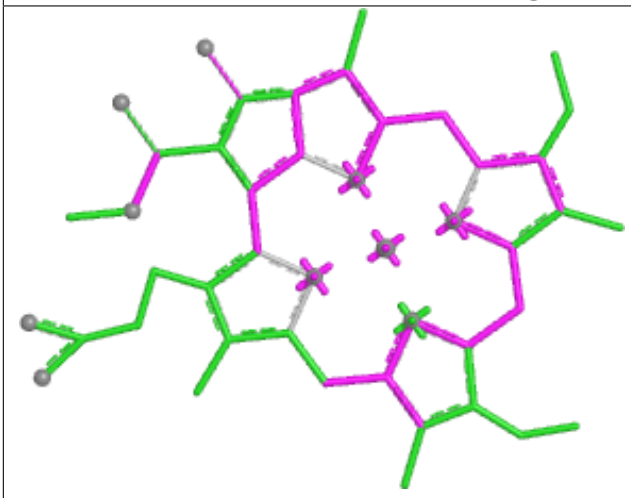
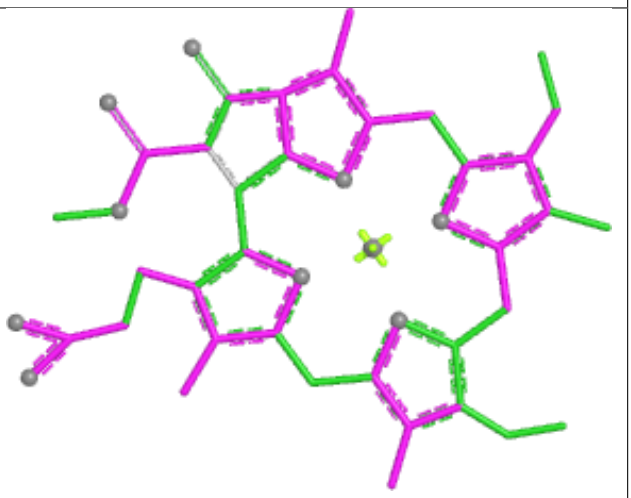
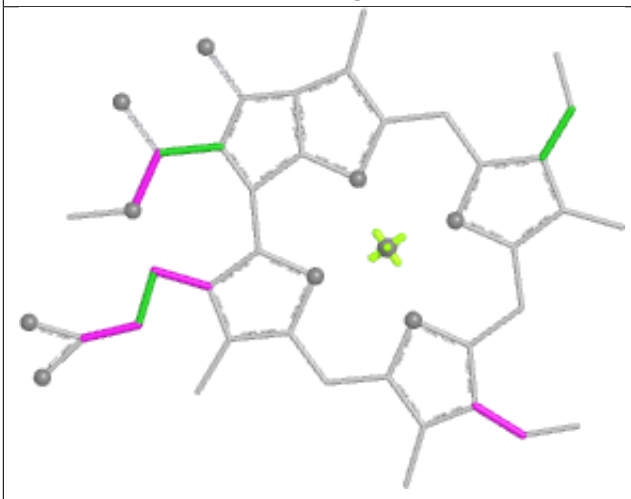
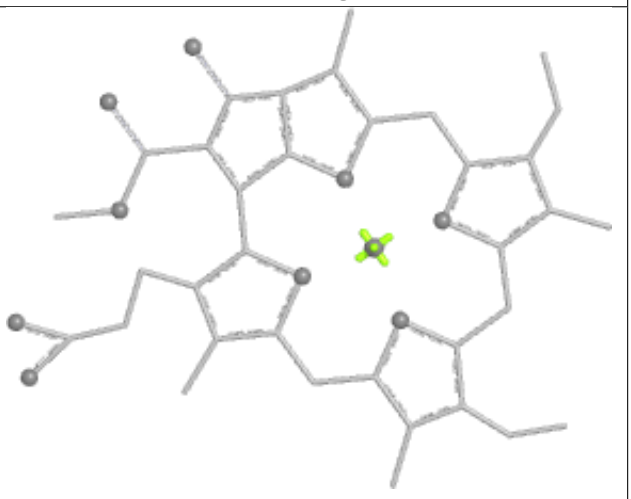
Bond angles



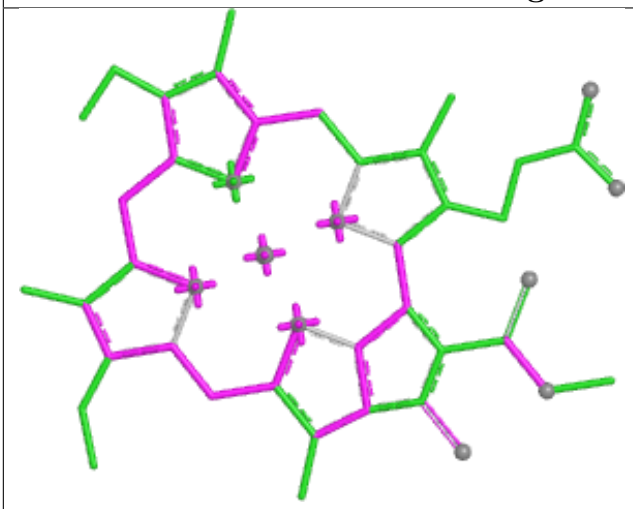
Torsions



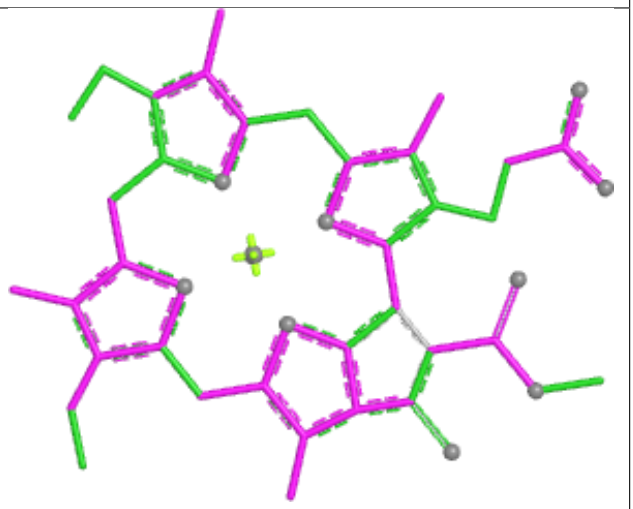
Rings

Ligand CLA P 203	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

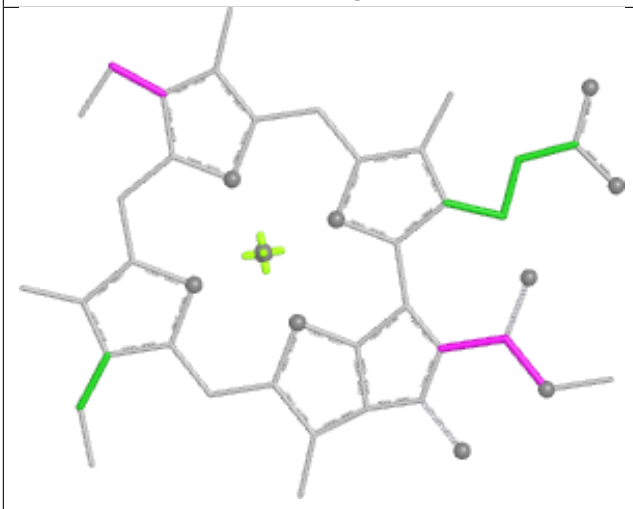
Ligand CLA b 830



Bond lengths

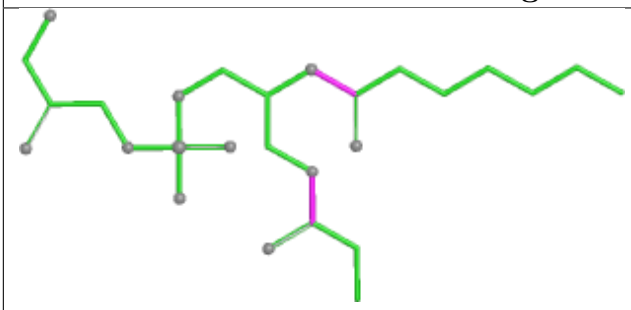
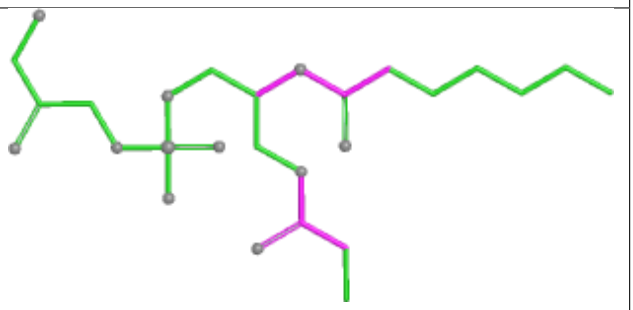
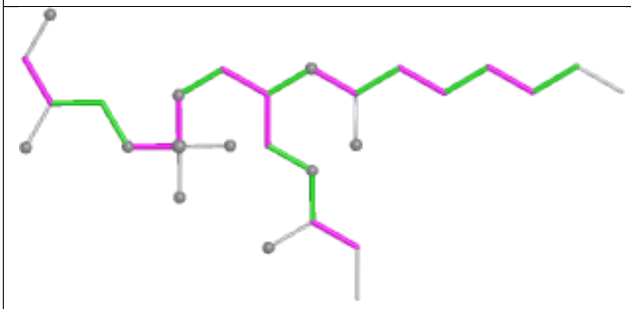
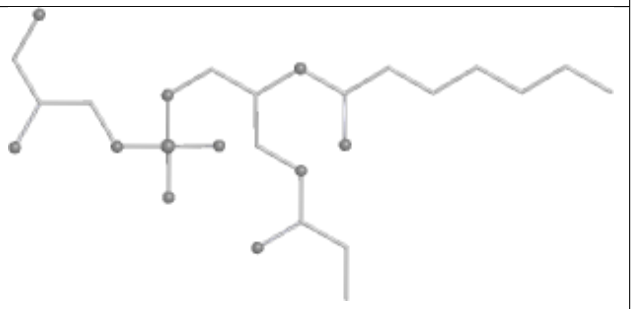


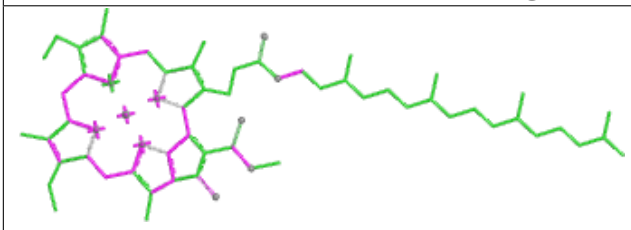
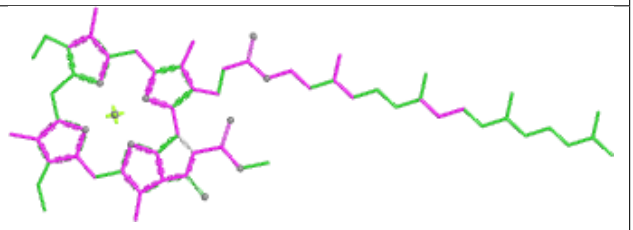
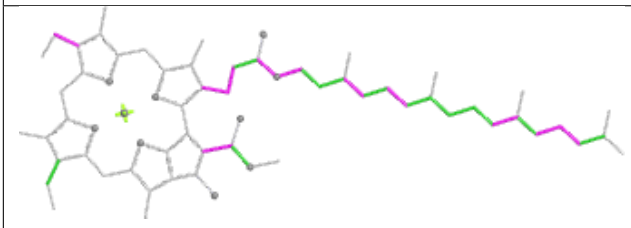
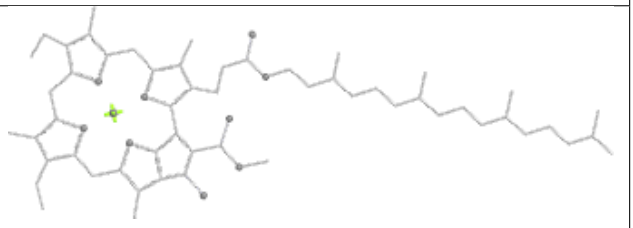
Bond angles



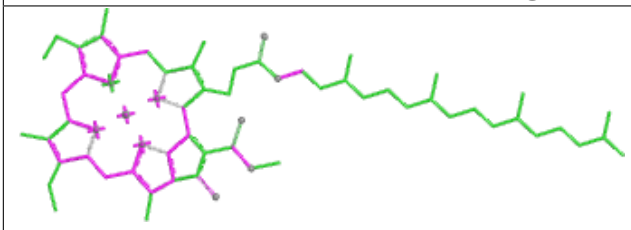
Torsions

Rings

Ligand LHG G 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 839



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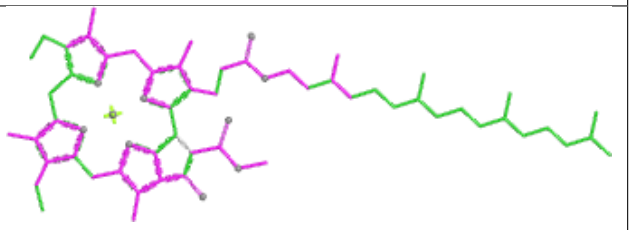

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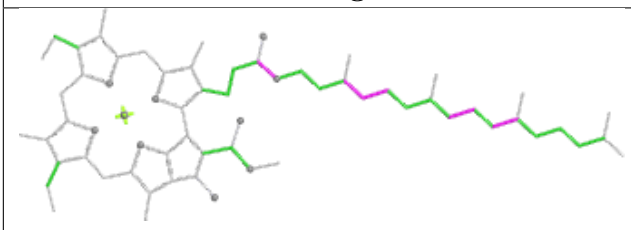
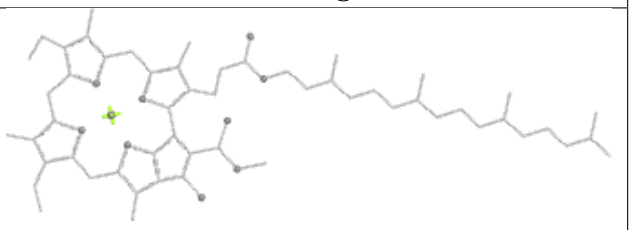
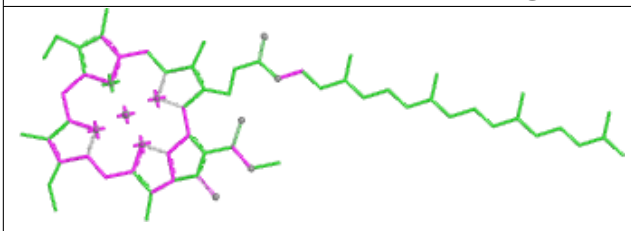


Torsions



Rings

Ligand CLA A 829



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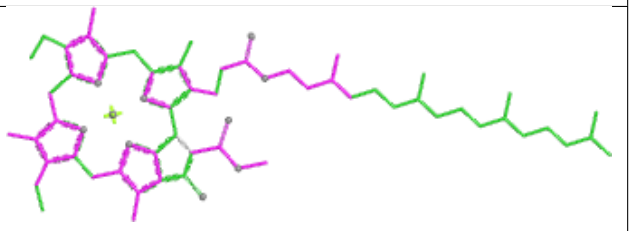

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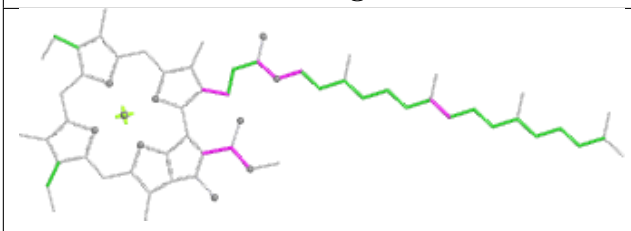

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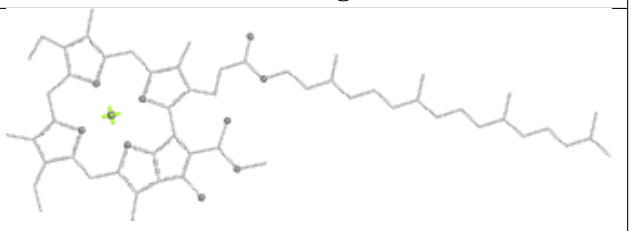

Rings

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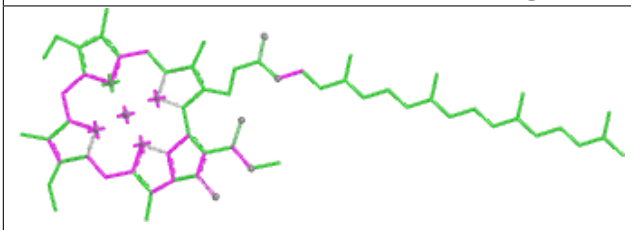

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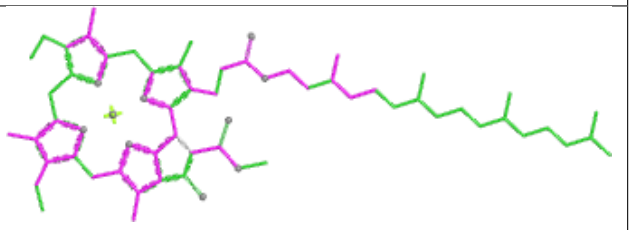
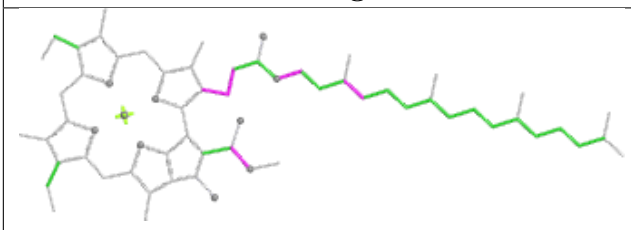


Bond angles



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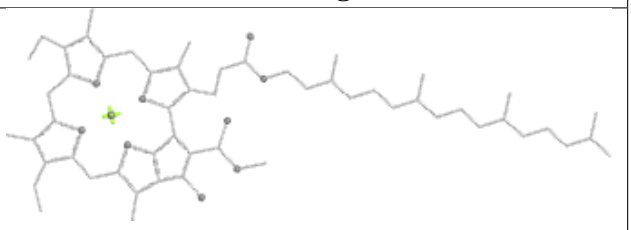
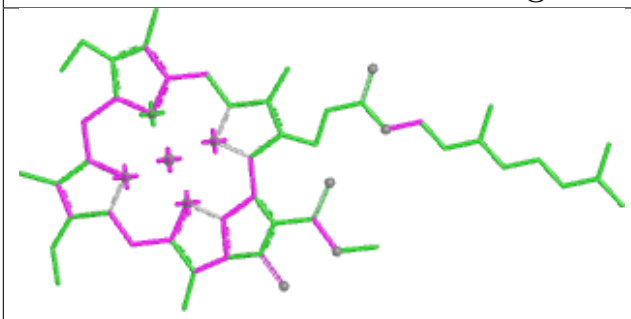


Rings

Ligand CLA S 202



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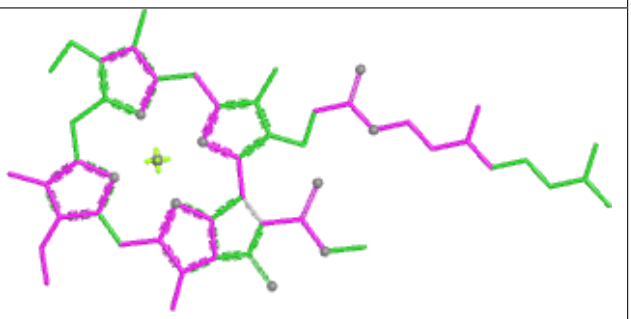
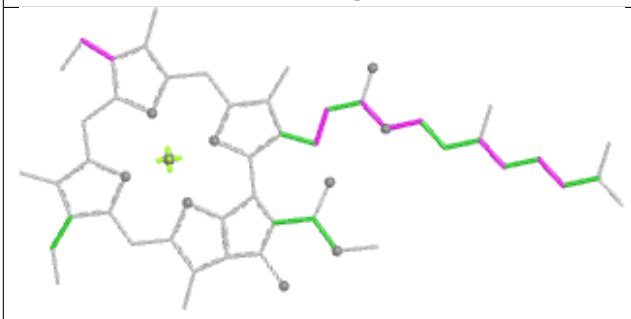


Bond angles



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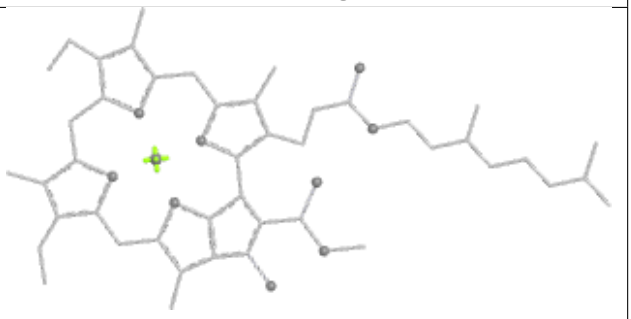
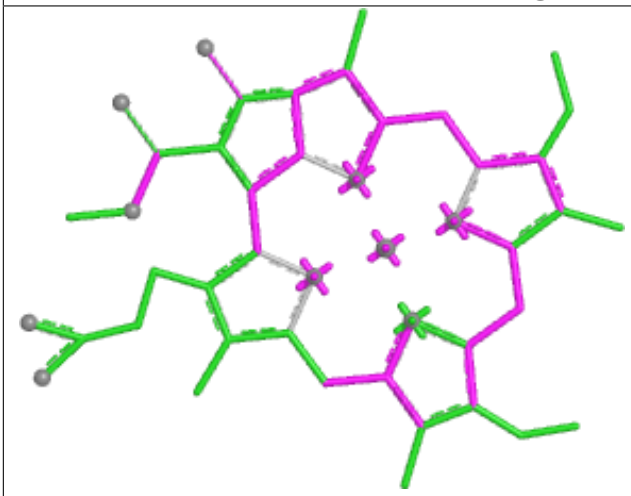
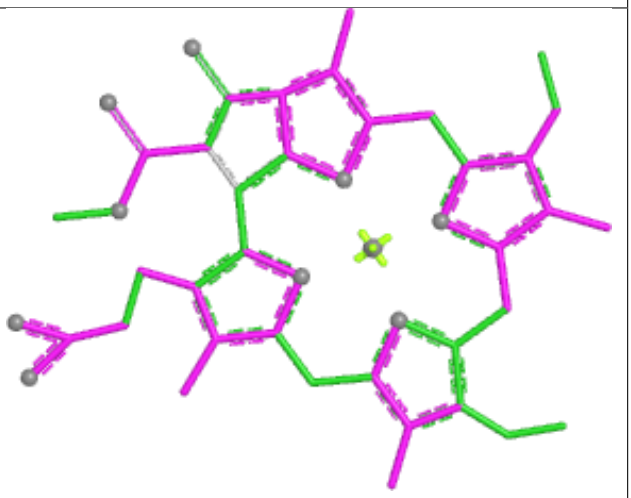
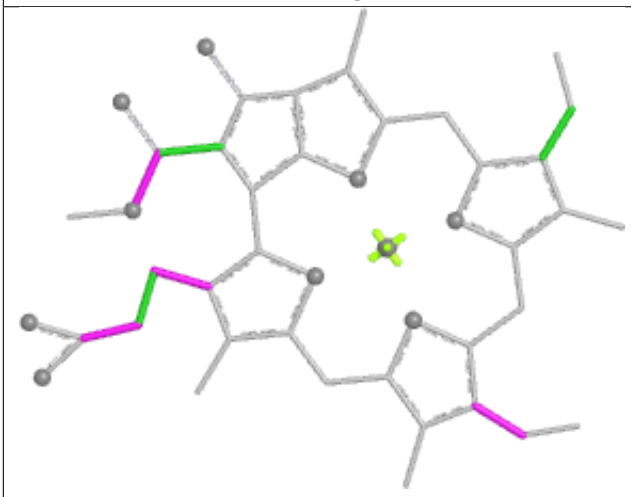
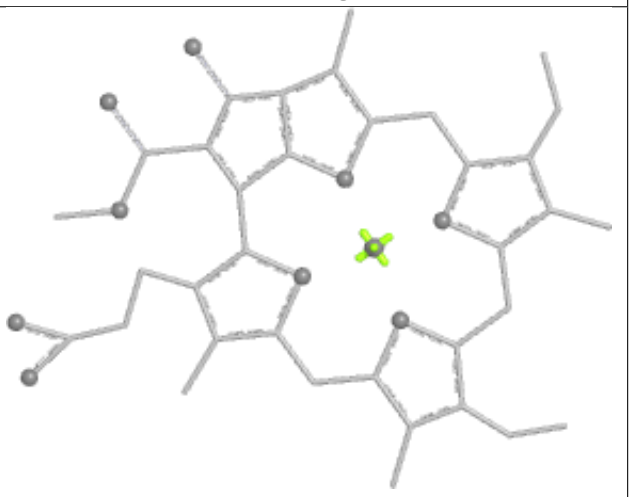
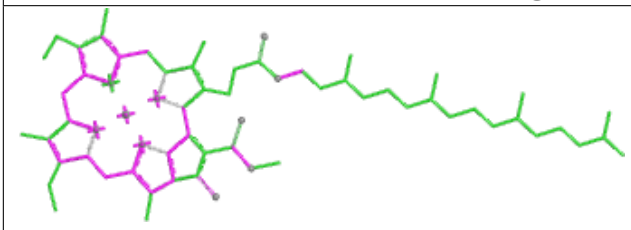
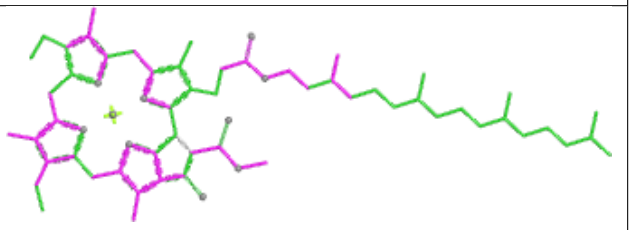
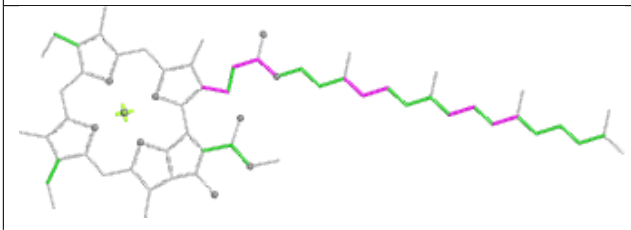
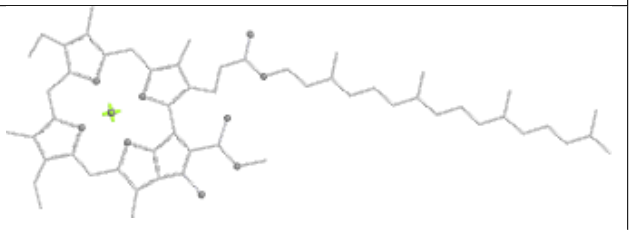
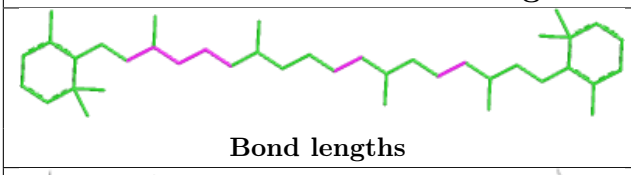


Rings

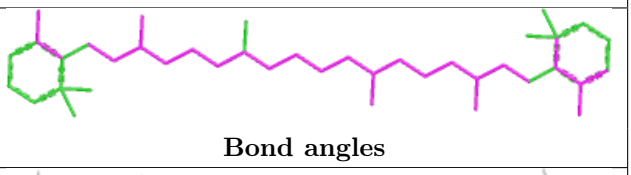
Ligand CLA f 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

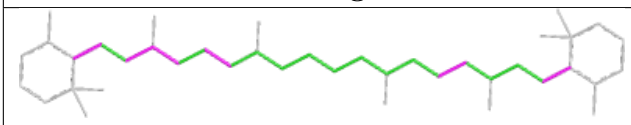
Ligand BCR B 840



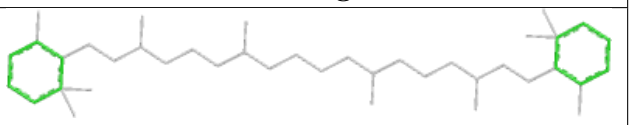
Bond lengths



Bond angles

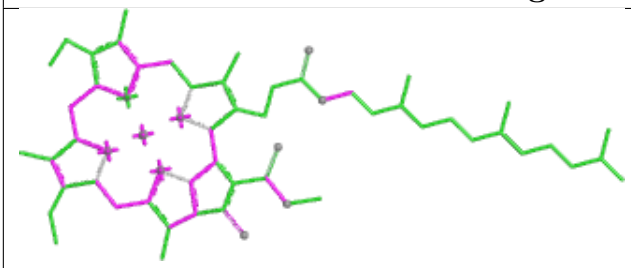


Torsions



Rings

Ligand CLA a 827



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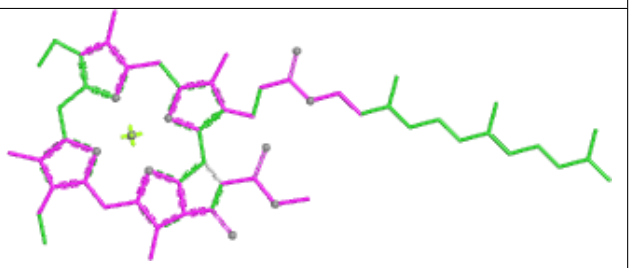
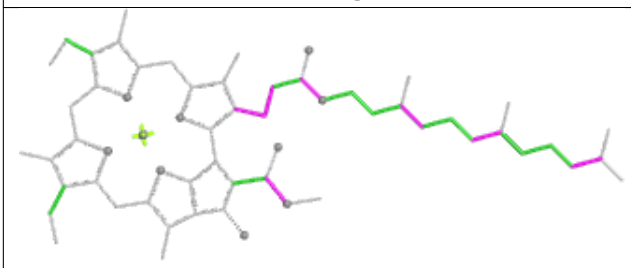
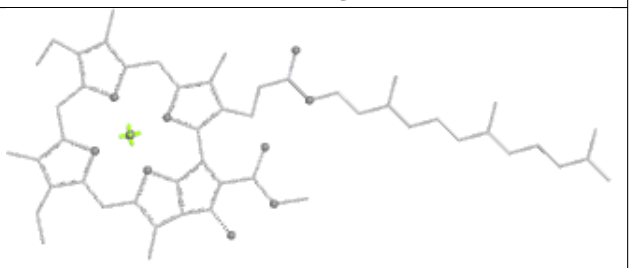


Bond angles

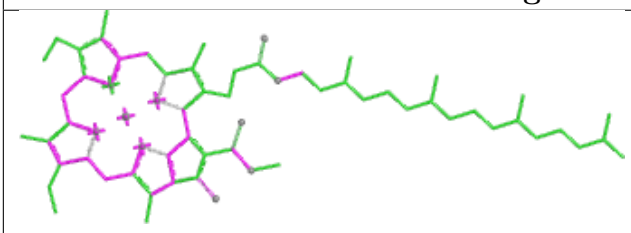


Torsions



Rings

Ligand CLA H 807



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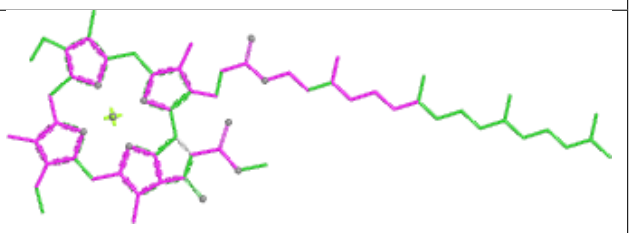
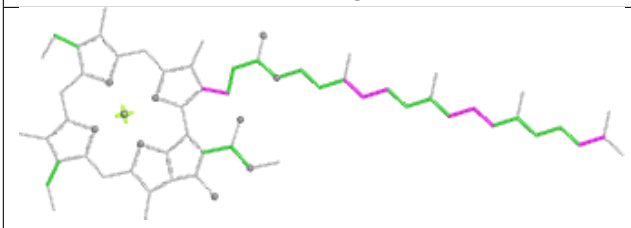


Bond angles



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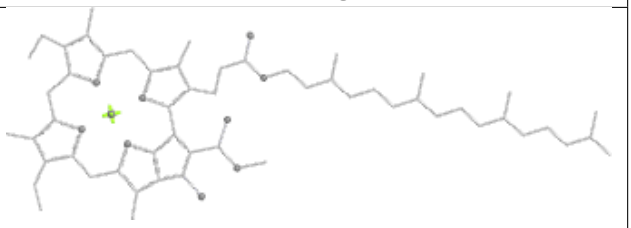
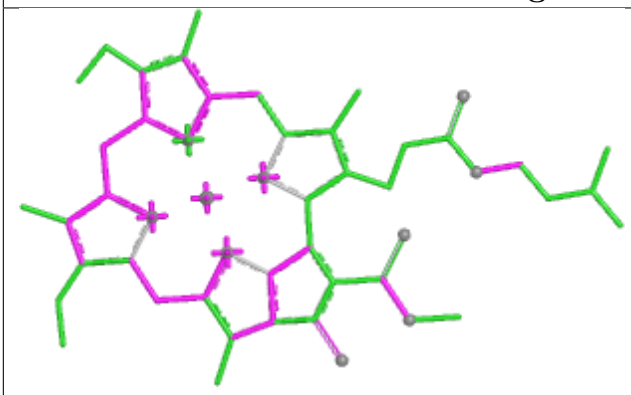
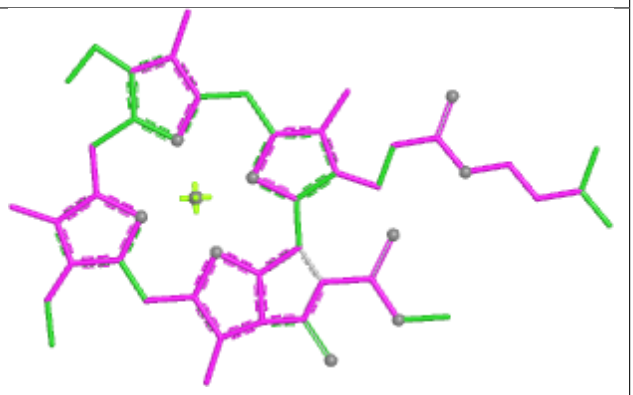


Rings

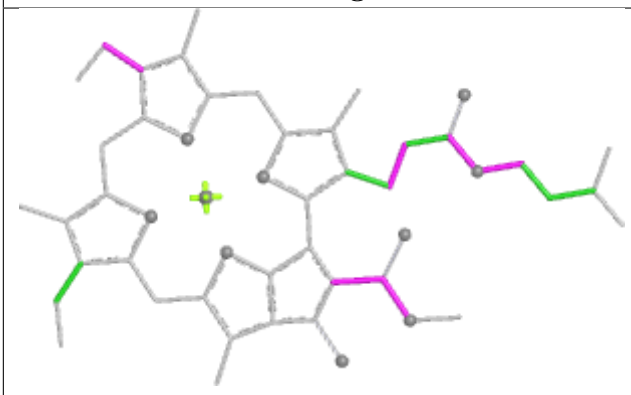
Ligand CLA a 830



Bond lengths



Bond angles



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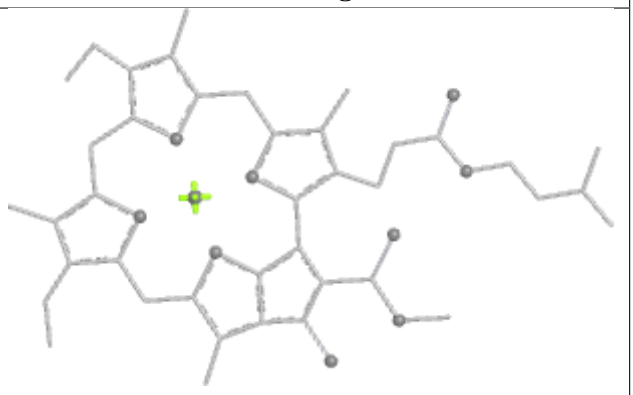
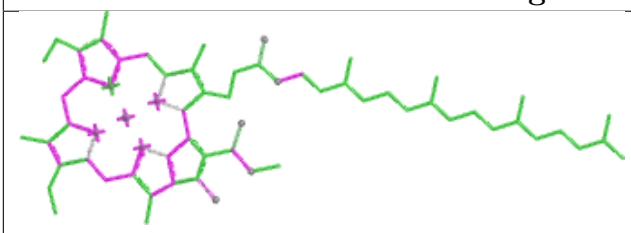


Rings

Ligand CLA a 834



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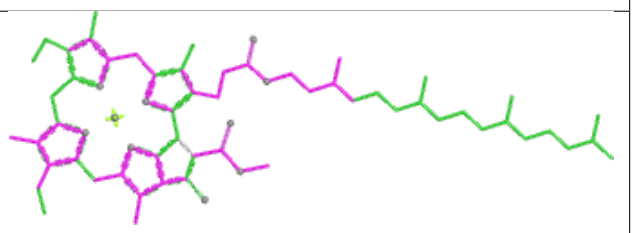
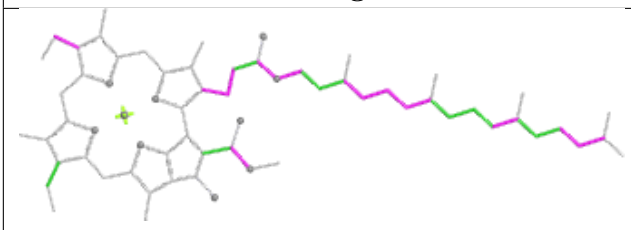


Bond angles



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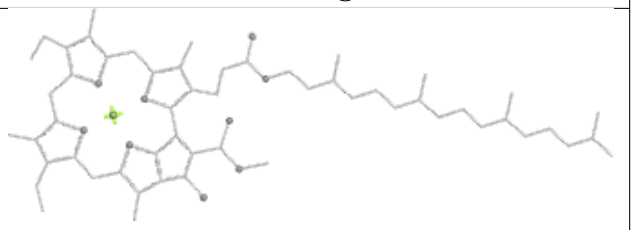
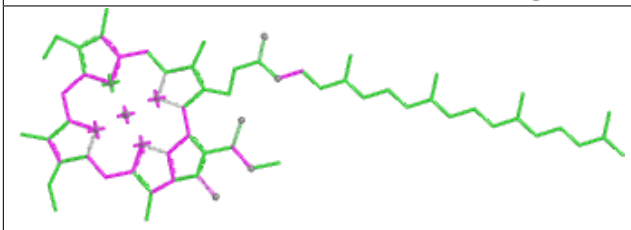


Rings

Ligand CLA b 810



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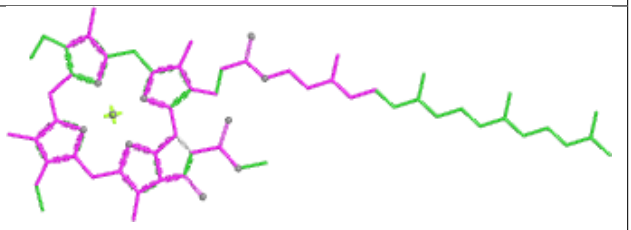
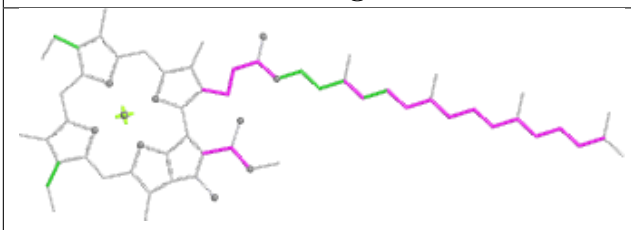
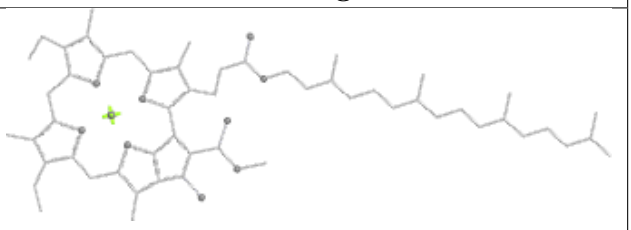


Bond angles

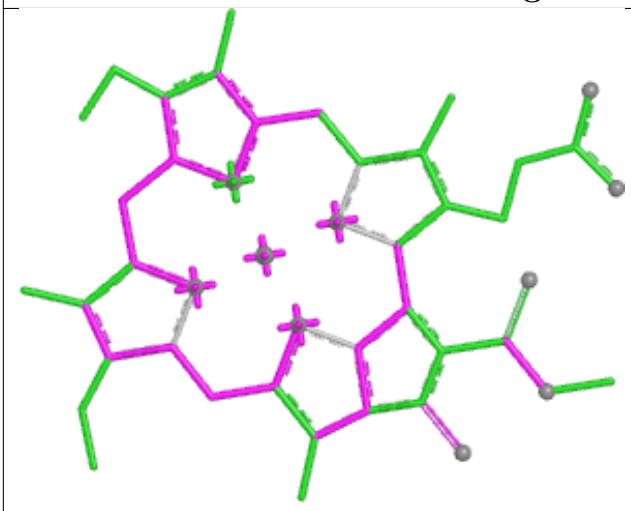


Torsions

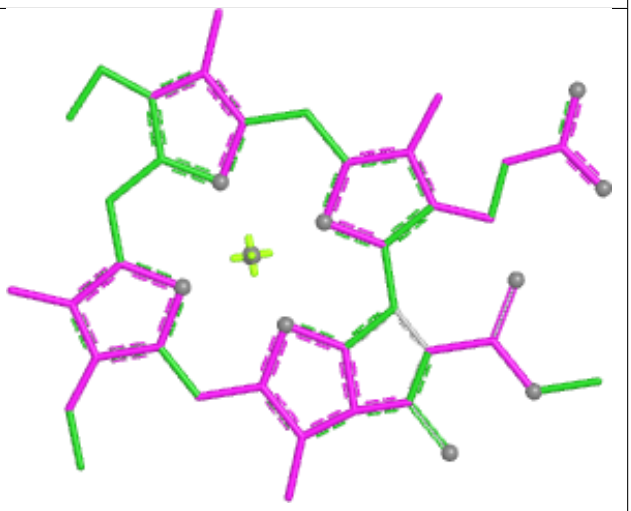


Rings

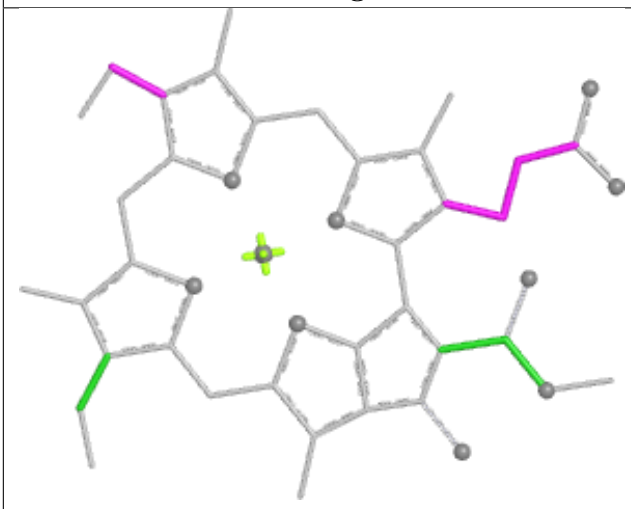
Ligand CLA A 811



Bond lengths



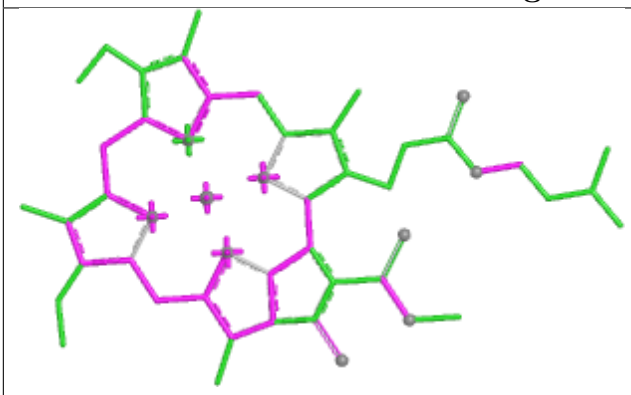
Bond angles



Torsions

Rings

Ligand CLA A 822



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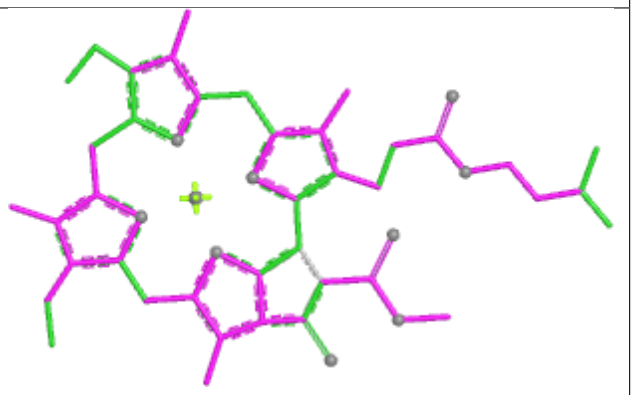
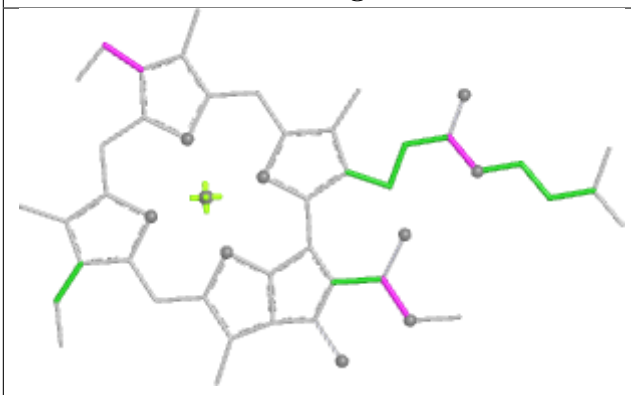
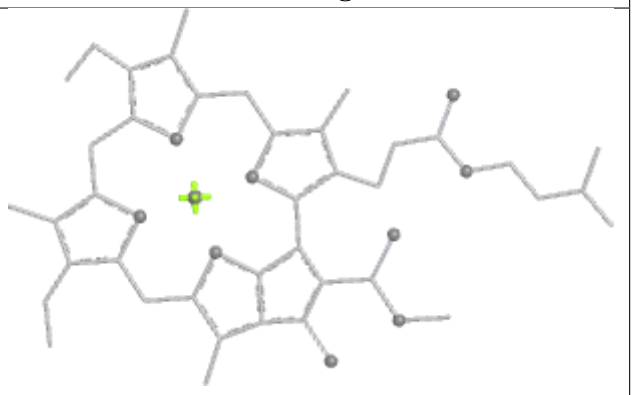


Bond angles

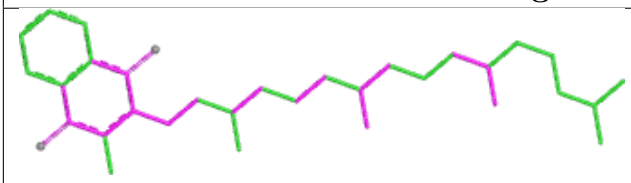


Torsions



Rings

Ligand 1L3 G 843



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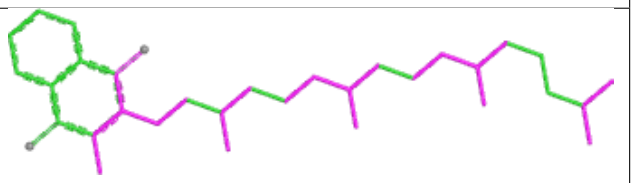
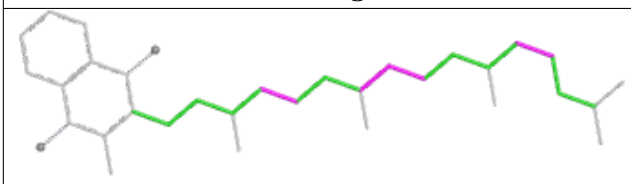
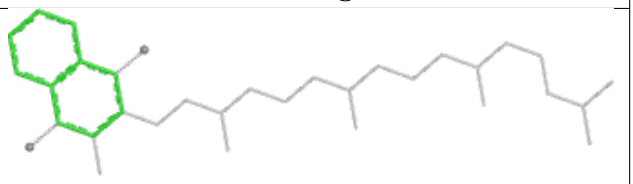


Bond angles

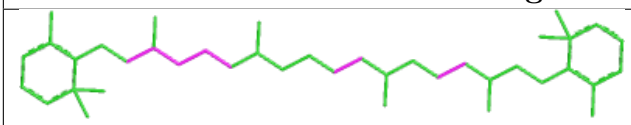


Torsions

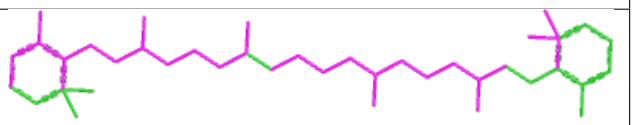


Rings

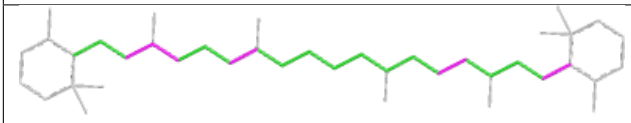
Ligand BCR S 205



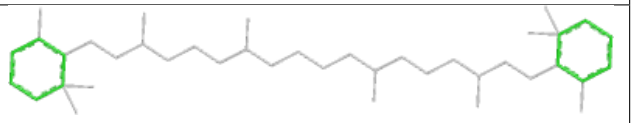
Bond lengths



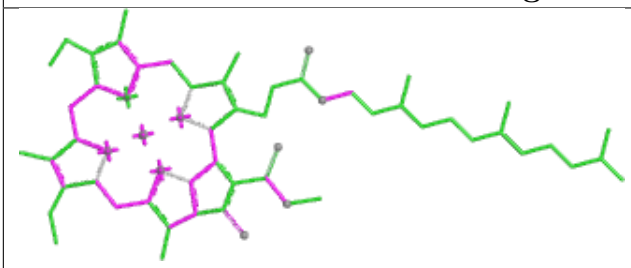
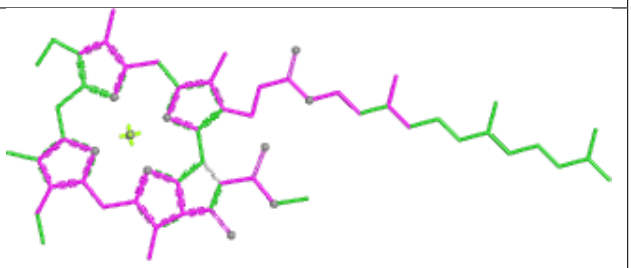
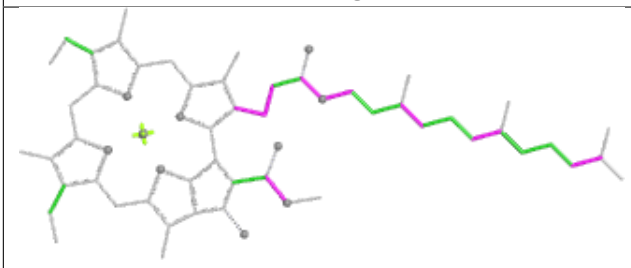
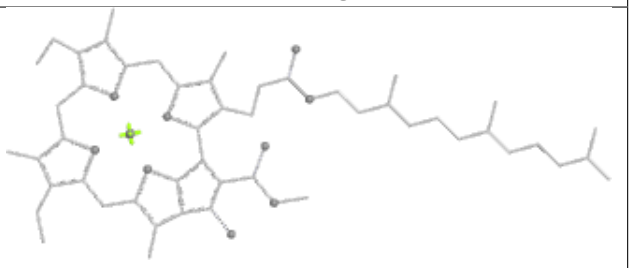
Bond angles

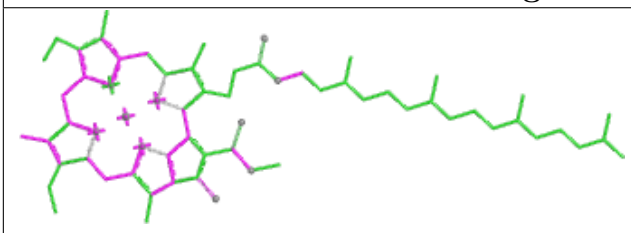
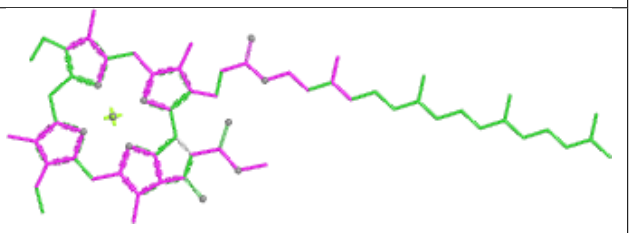
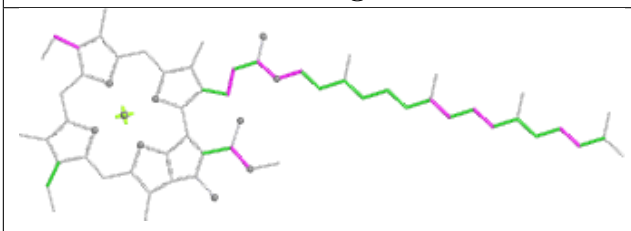
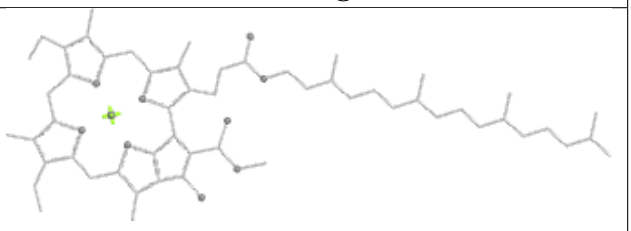


Torsions

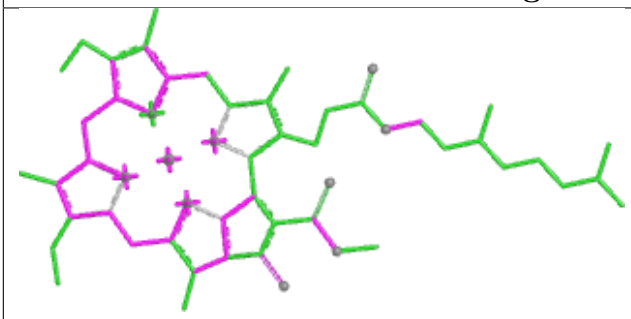


Rings

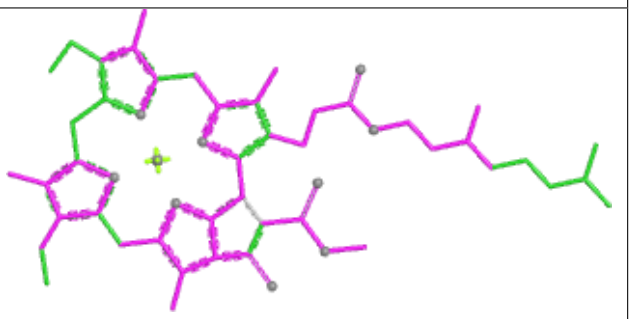
Ligand CLA G 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

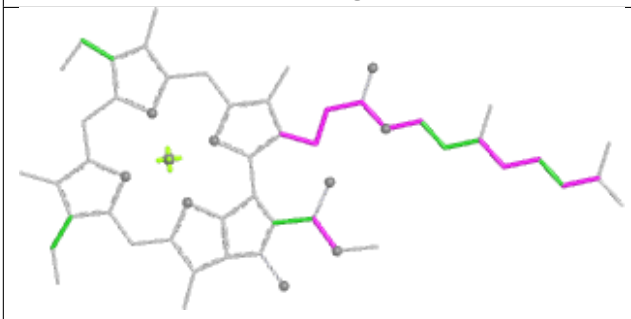
Ligand CLA G 818



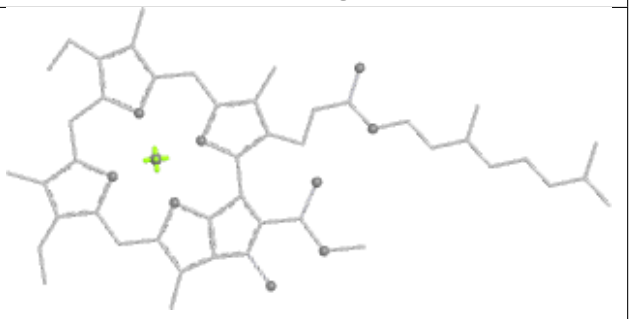
Bond lengths



Bond angles

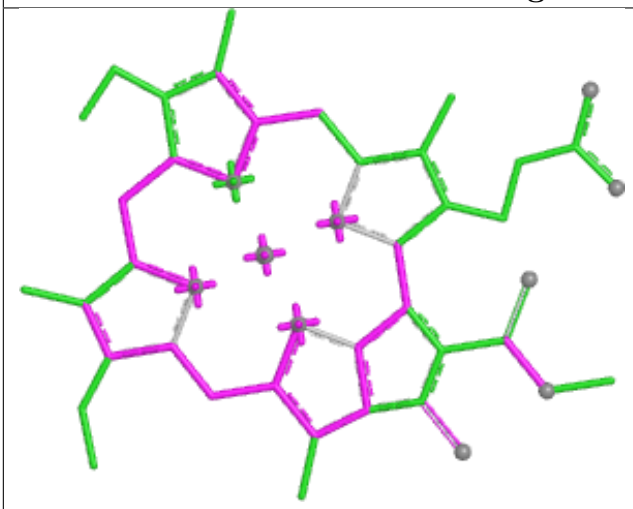


Torsions

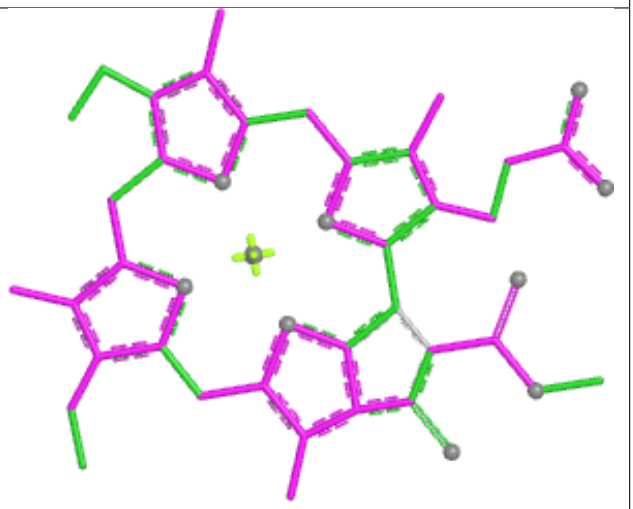


Rings

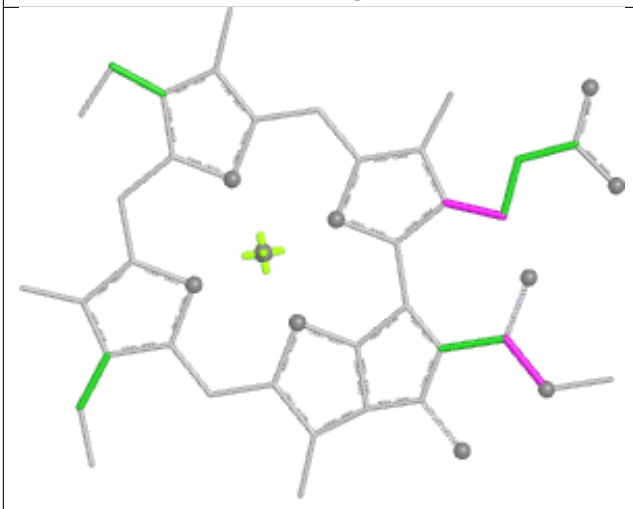
Ligand CLA b 808



Bond lengths



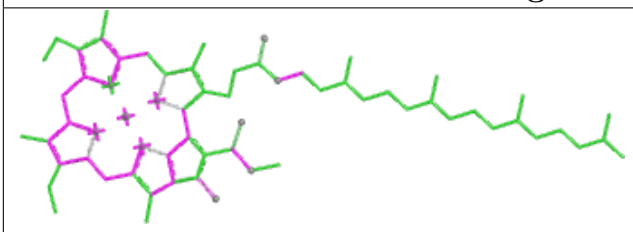
Bond angles



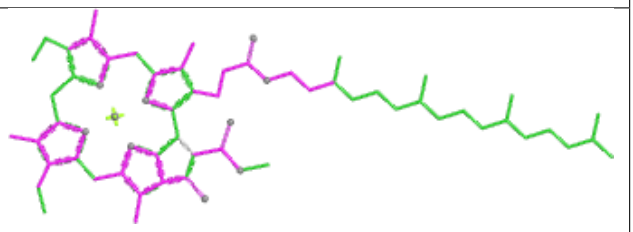
Torsions

Rings

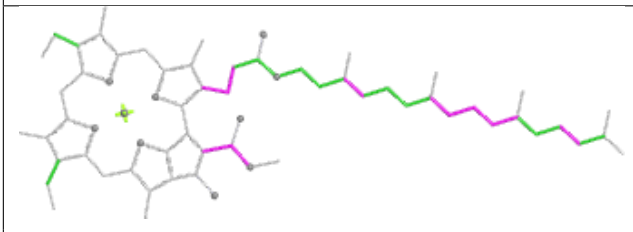
Ligand CLA b 822



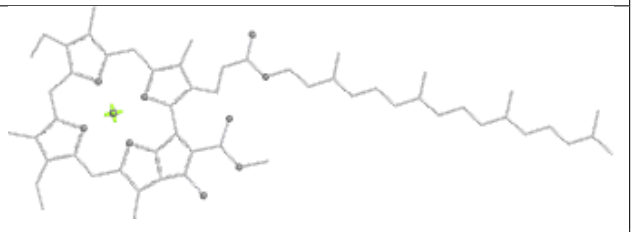
Bond lengths



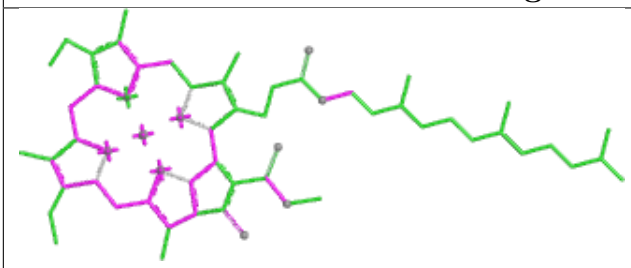
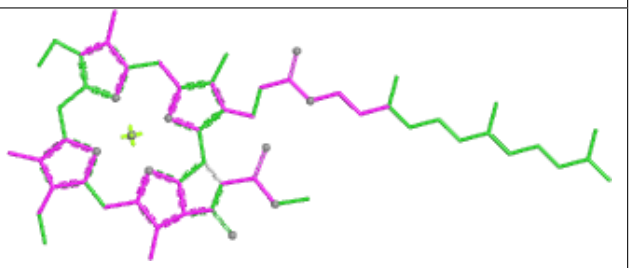
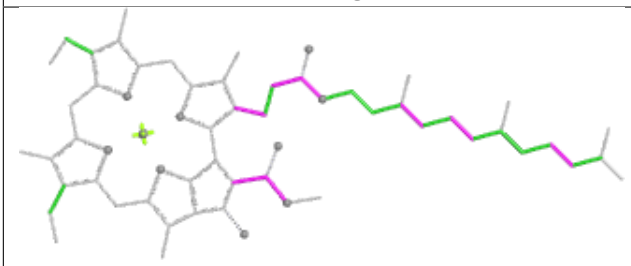
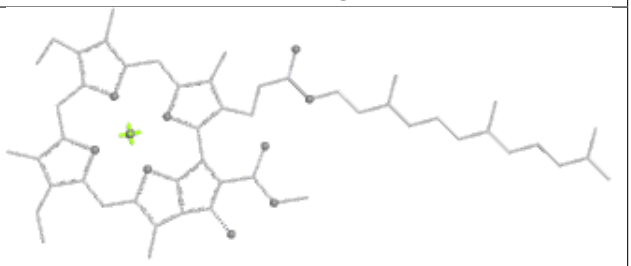
Bond angles



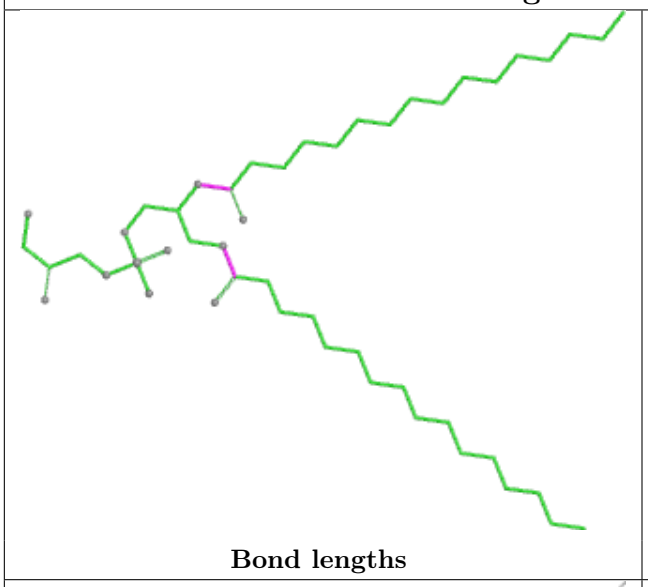
Torsions



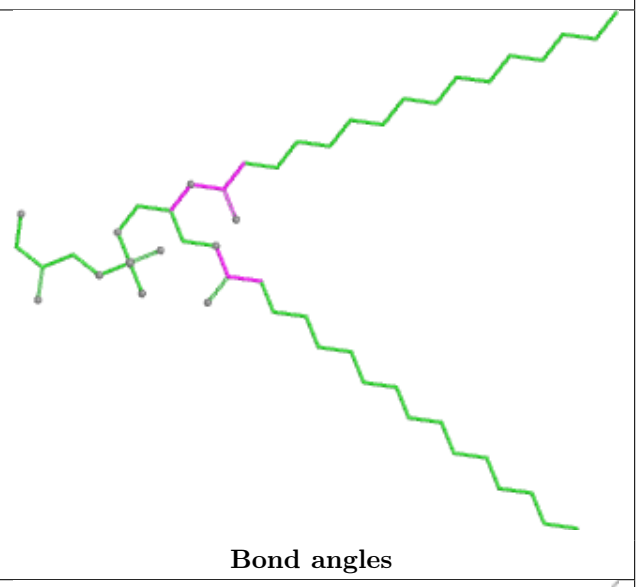
Rings

Ligand CLA B 811	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

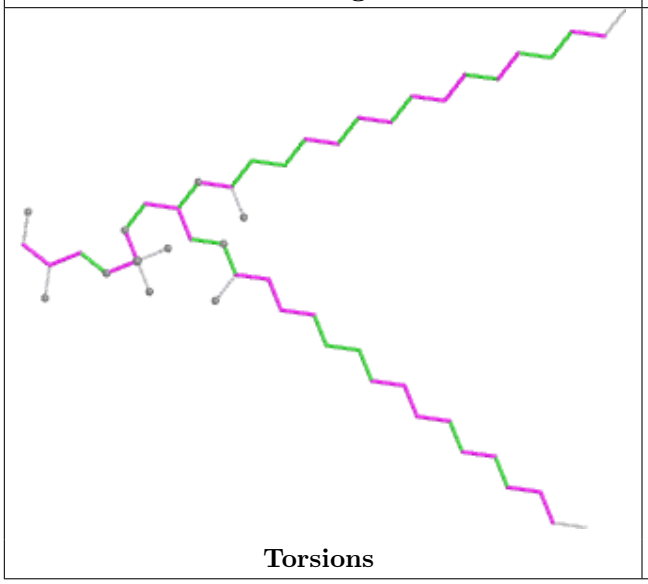
Ligand LHG A 850



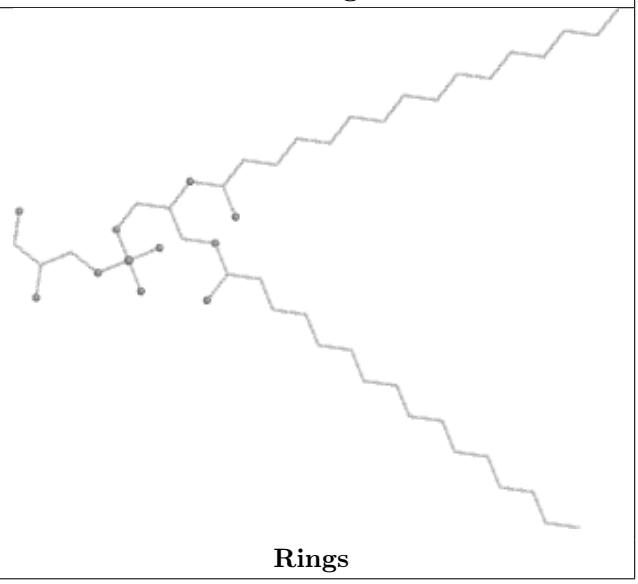
Bond lengths



Bond angles

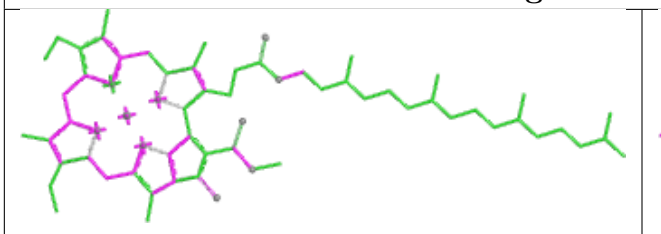


Torsions



Rings

Ligand CLA B 802



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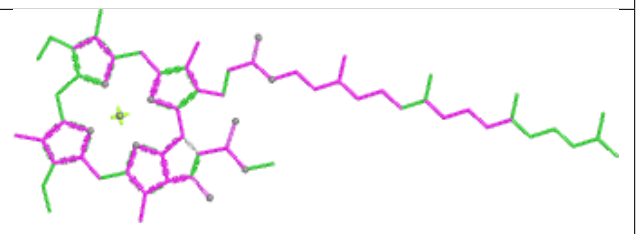
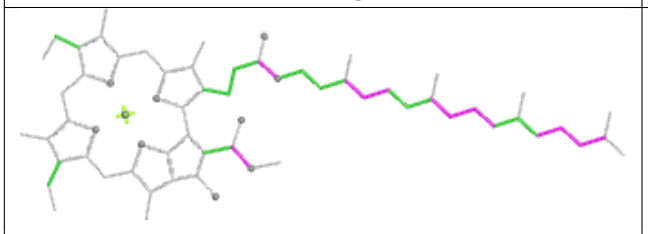


Bond angles



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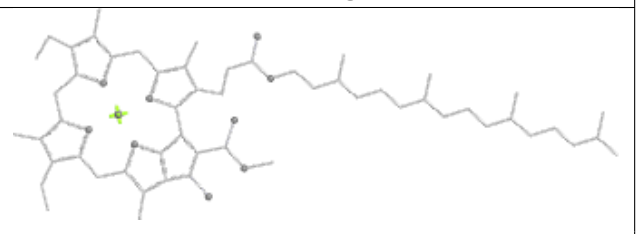
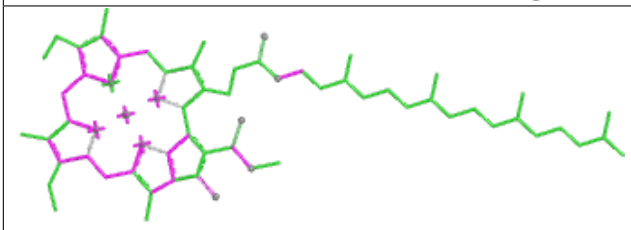
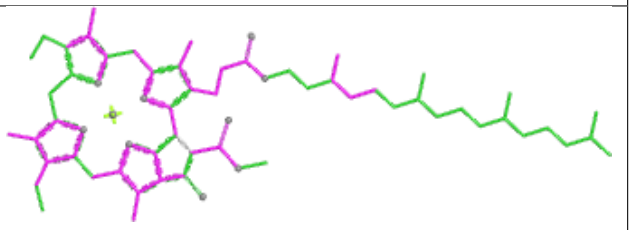


Rings

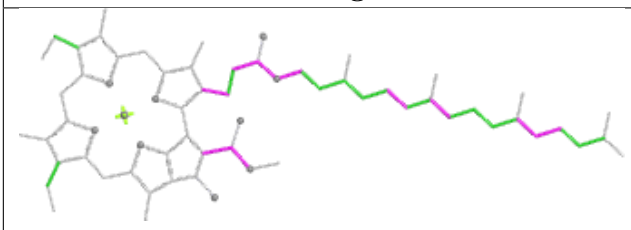
Ligand CLA b 803



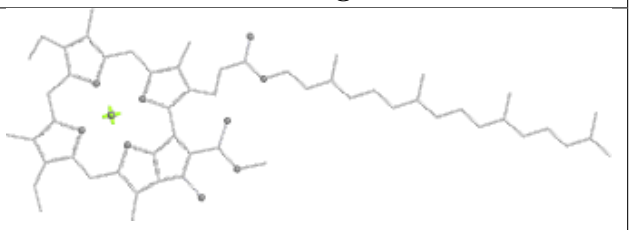
Bond lengths



Bond angles

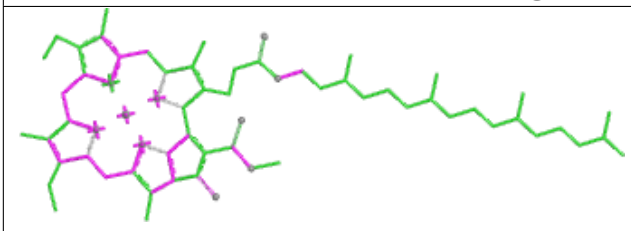


Torsions

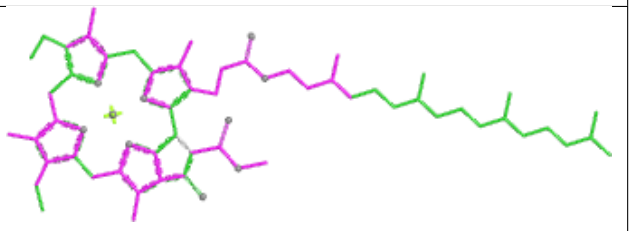


Rings

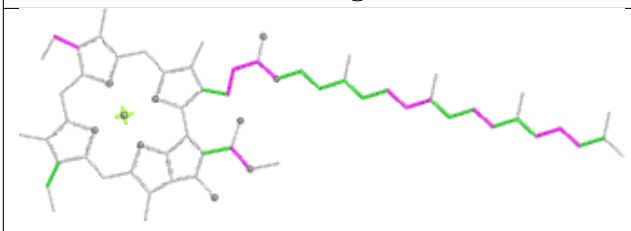
Ligand CLA a 841



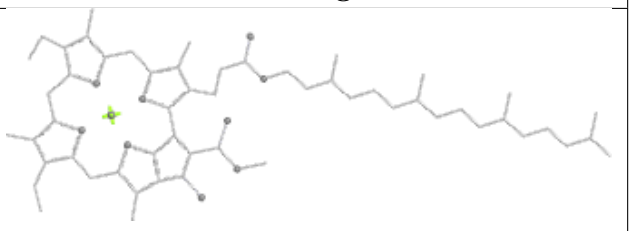
Bond lengths



Bond angles

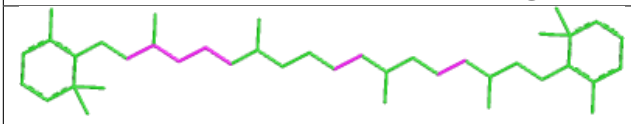


Torsions



Rings

Ligand BCR P 204



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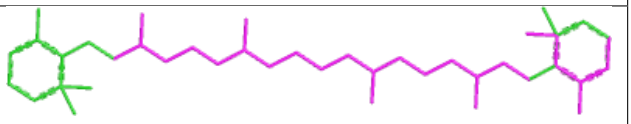
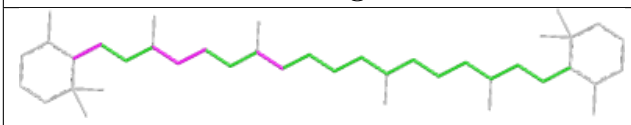
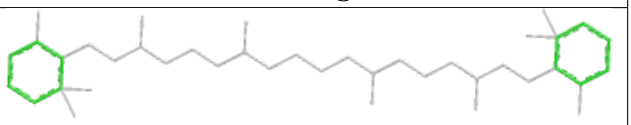


Bond angles

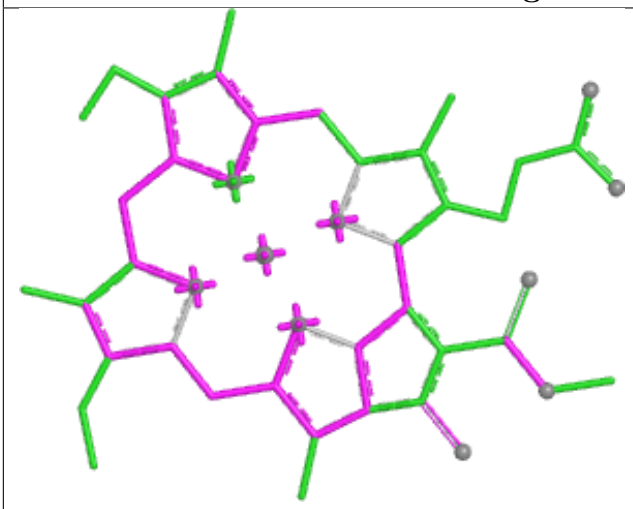


Torsions



Rings

Ligand CLA G 816



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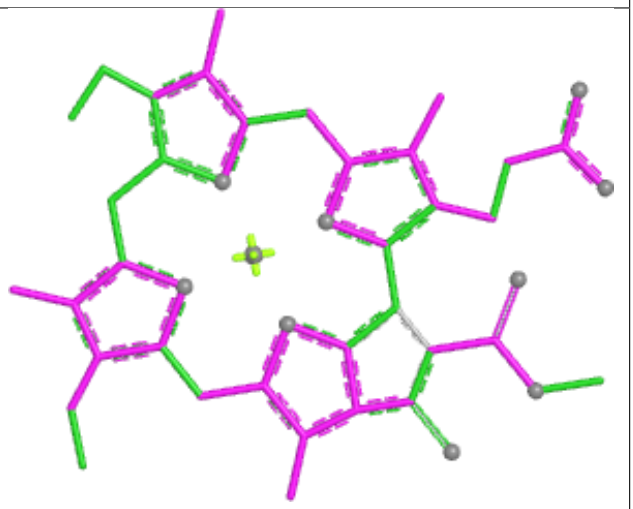
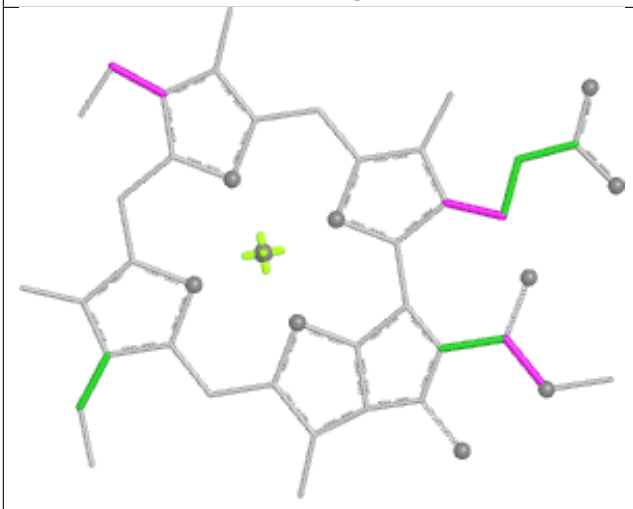


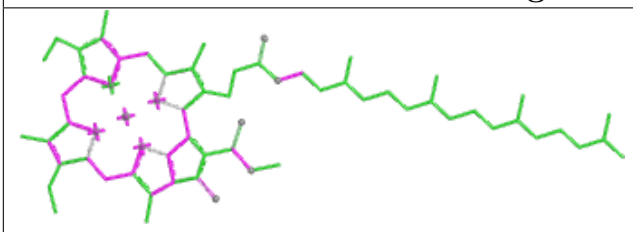
Bond angles



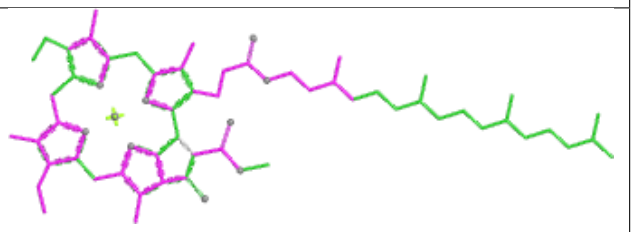
Torsions

Rings

Ligand CLA S 203



Bond lengths



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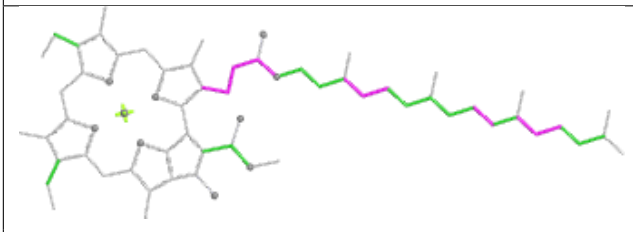
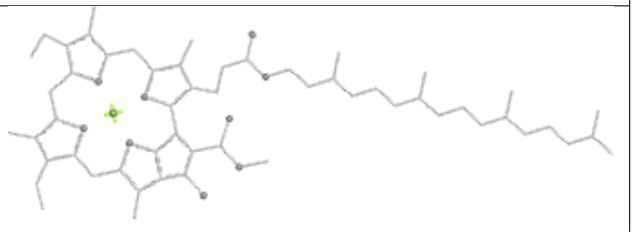
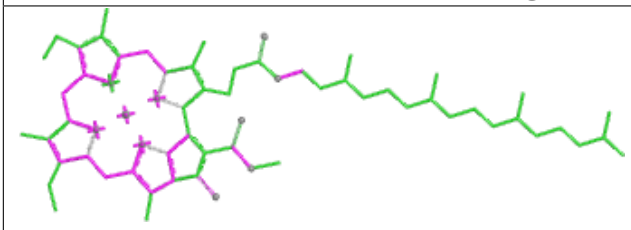


Torsions



Rings

Ligand CLA H 837



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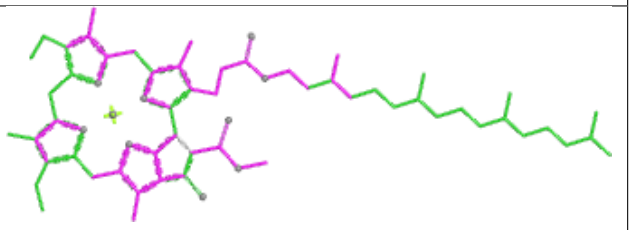
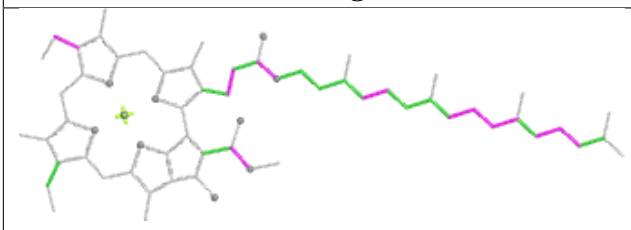


Bond angles



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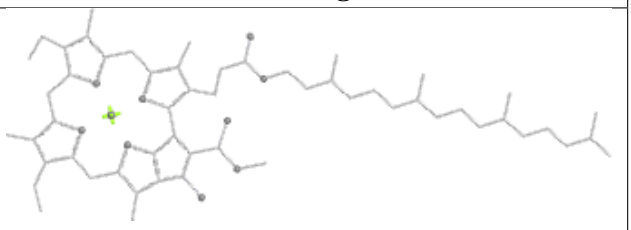
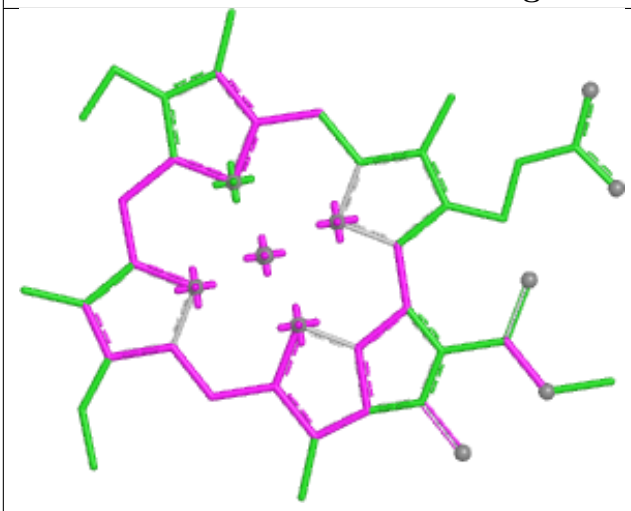


Rings

Ligand CLA G 815



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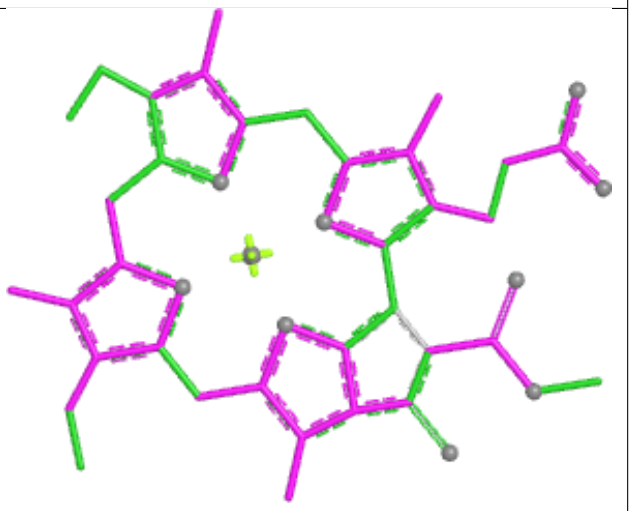
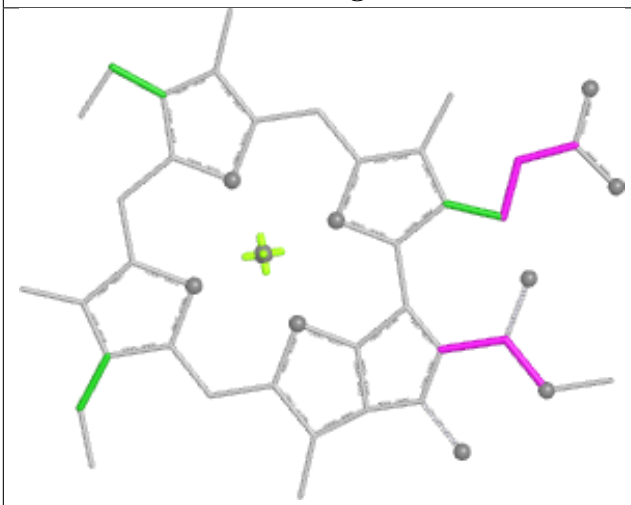


Bond angles



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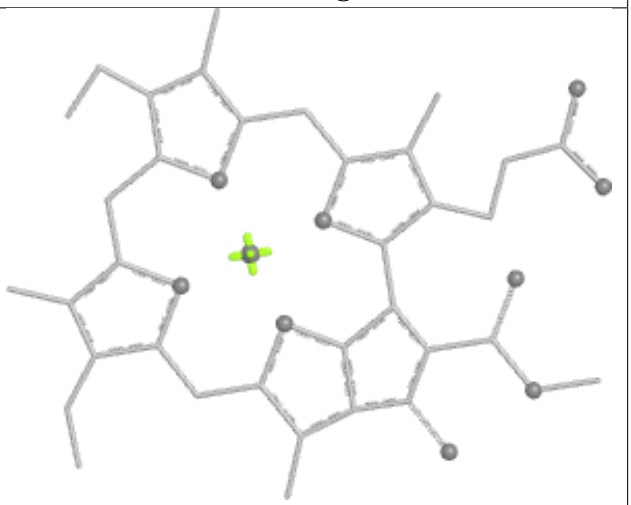
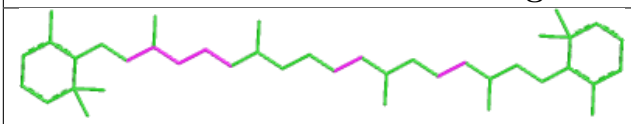


Rings

Ligand BCR J 101



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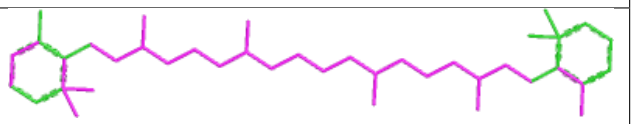
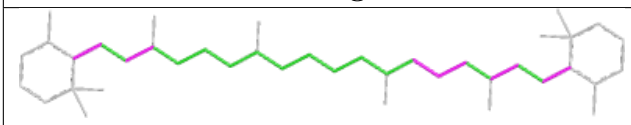


Bond angles



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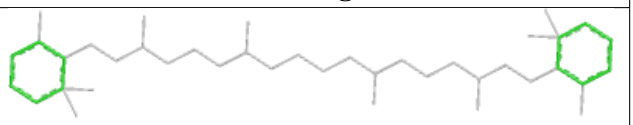
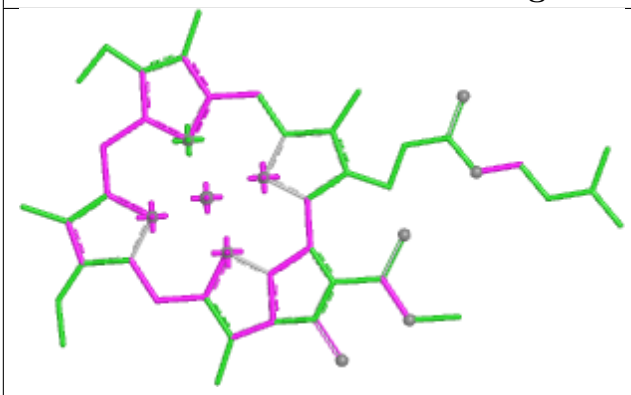


Rings

Ligand CLA a 840



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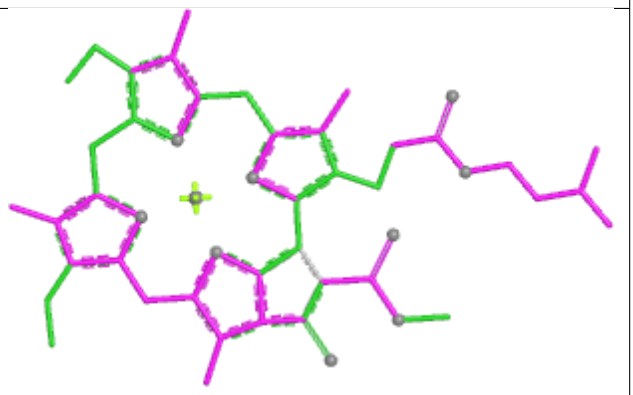
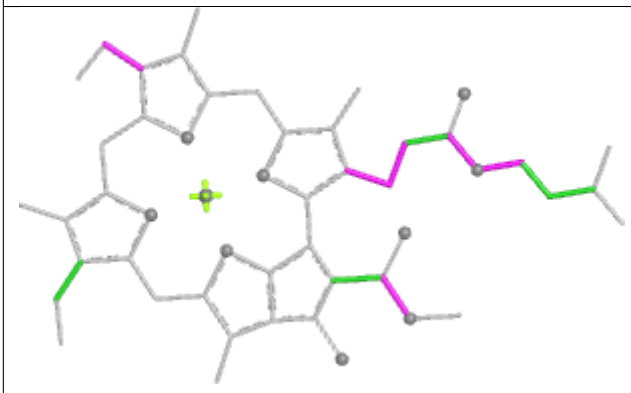


Bond angles



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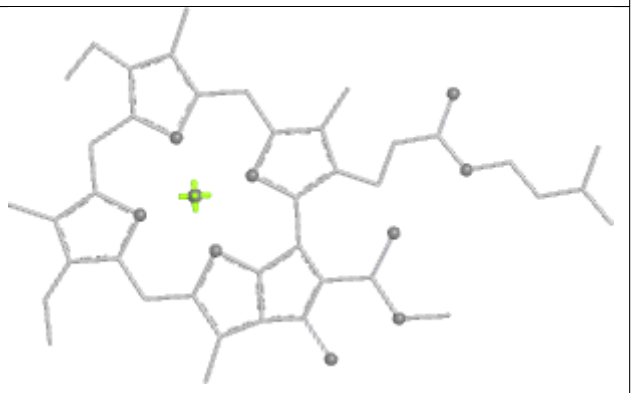
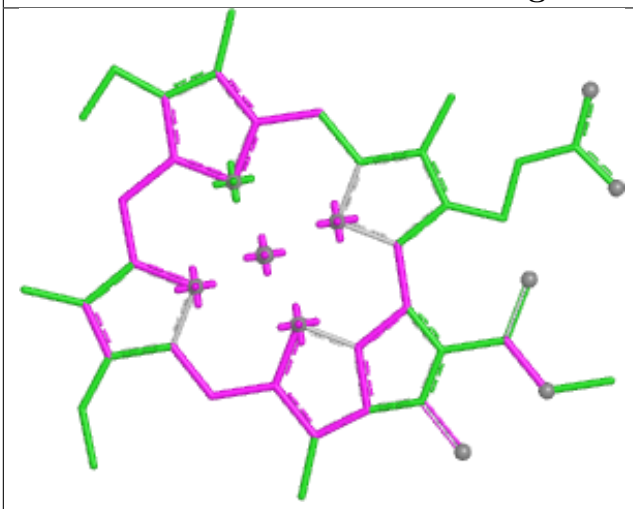


Rings

Ligand CLA a 819



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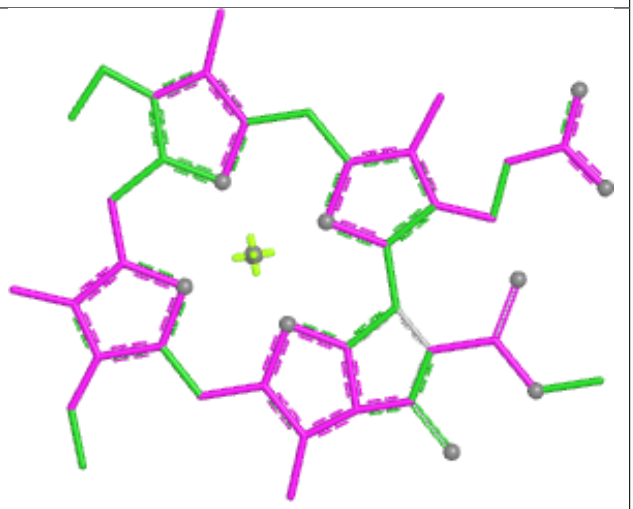
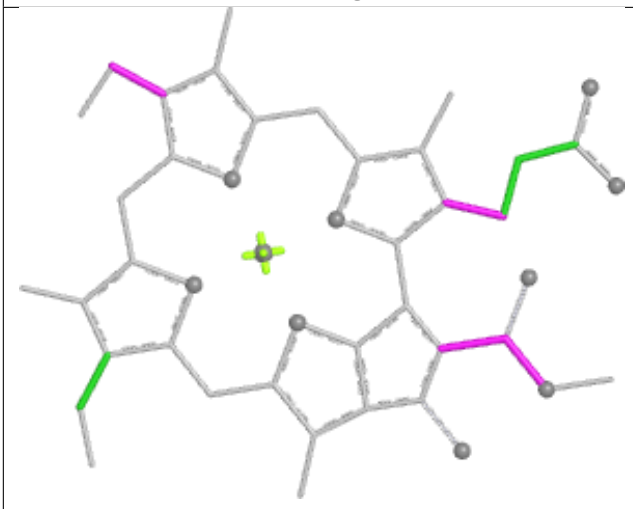


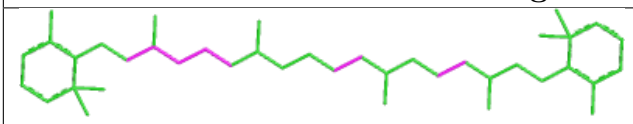
Bond angles



Torsions

Rings

Ligand BCR f 204



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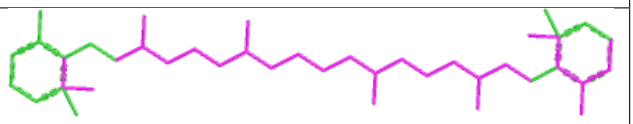
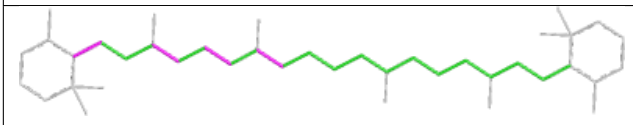


Bond angles



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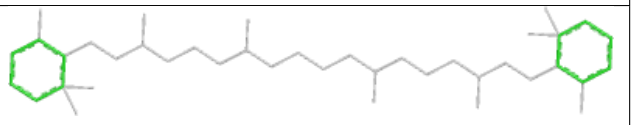
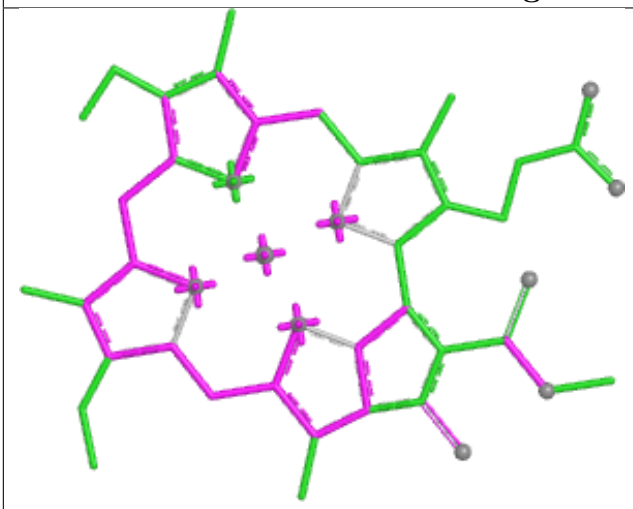


Rings

Ligand CLA G 838



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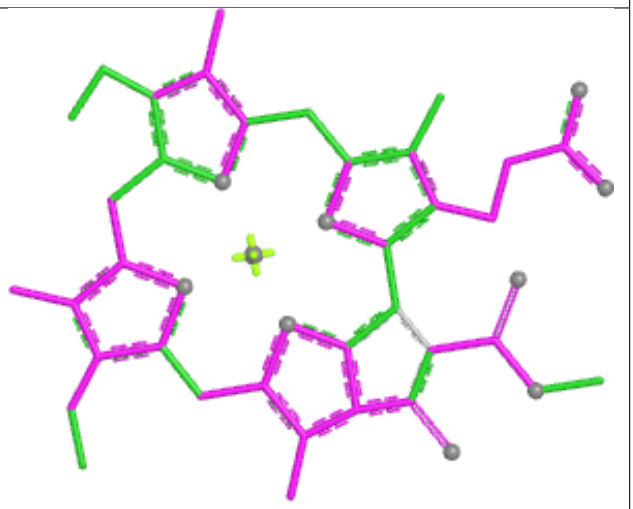
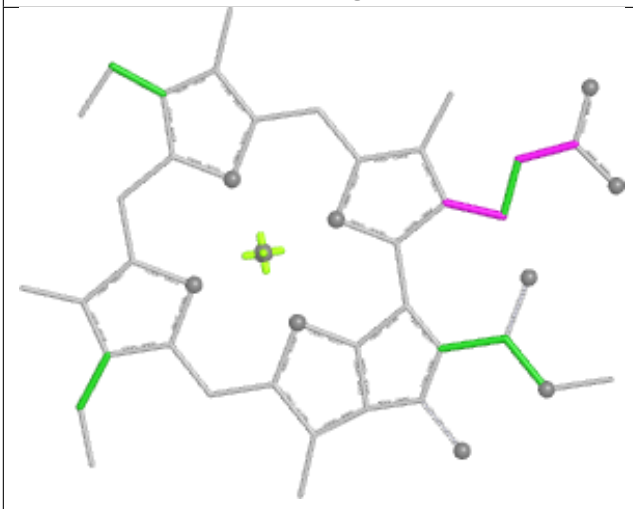


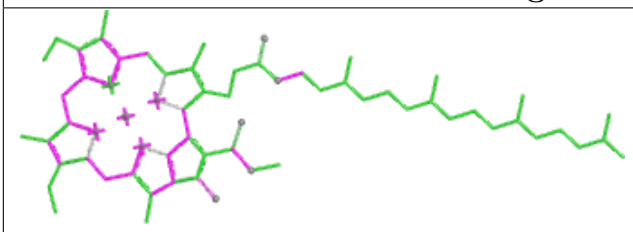
Bond angles



Torsions

Rings

Ligand CLA b 805



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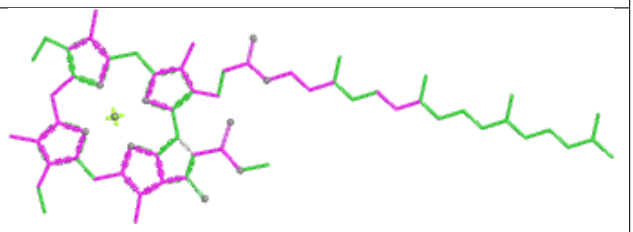
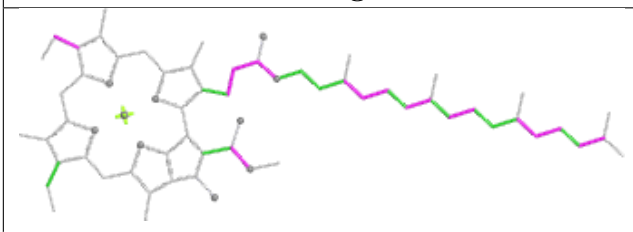


Bond angles



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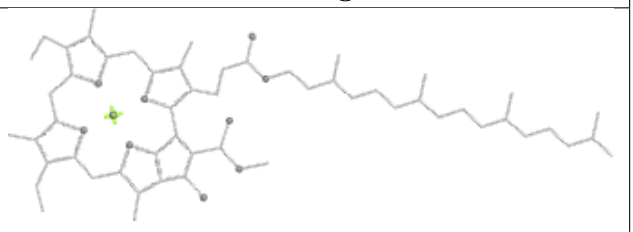
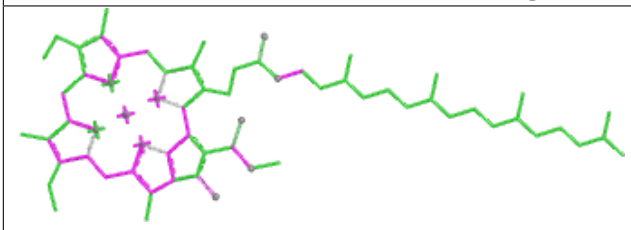


Rings

Ligand CLA A 820



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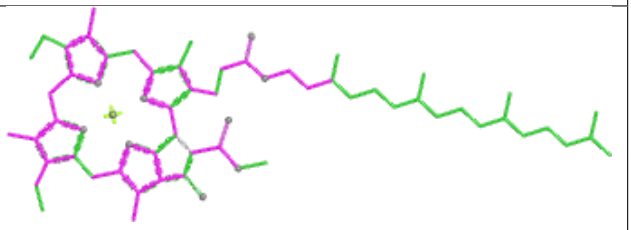
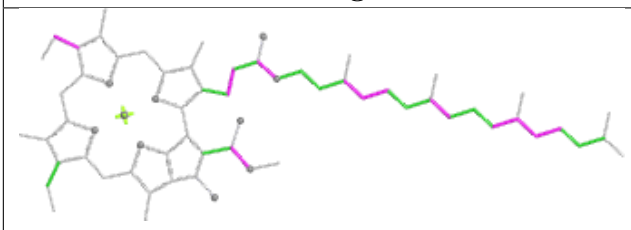


Bond angles



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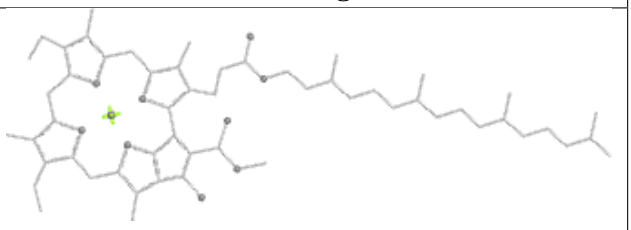
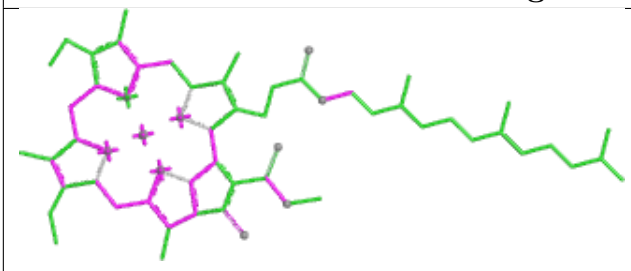


Rings

Ligand CLA b 815



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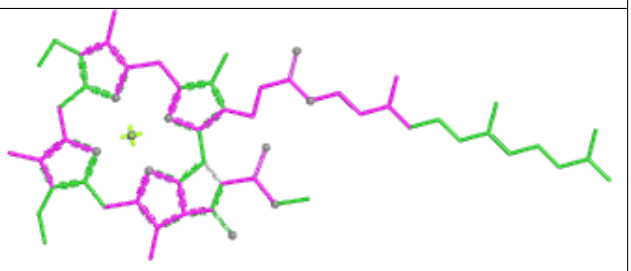
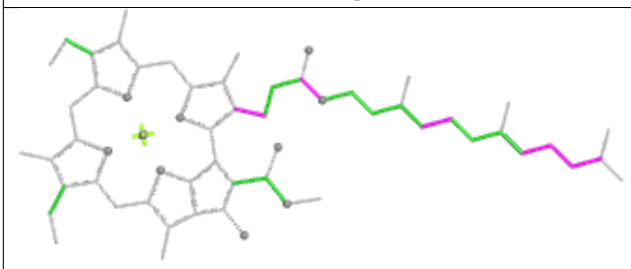


Bond angles



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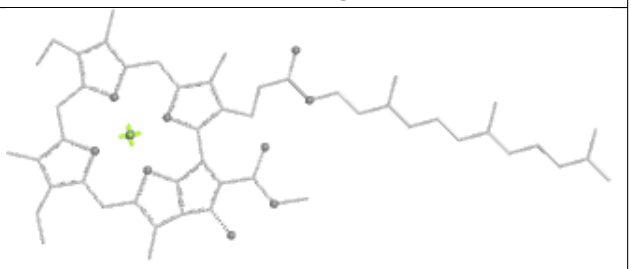
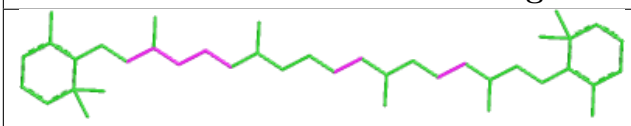


Rings

Ligand BCR J 104



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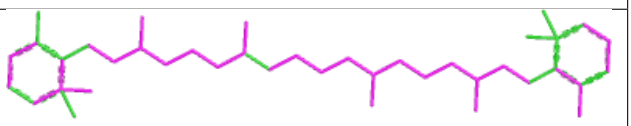
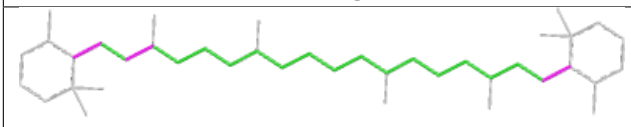


Bond angles



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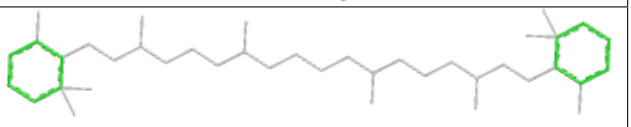
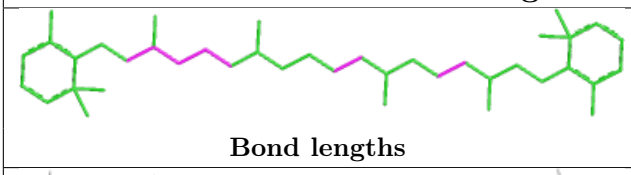


Rings

Ligand BCR H 841



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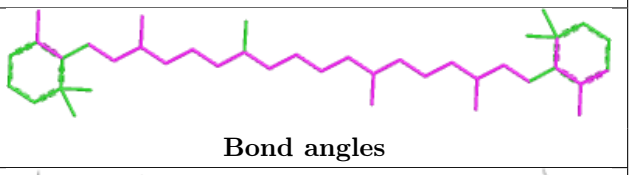
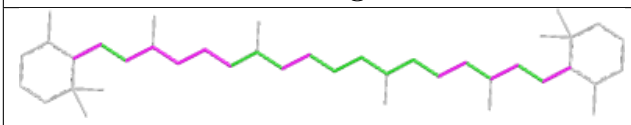


Bond angles



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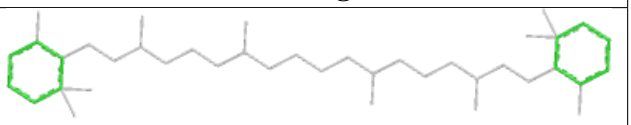
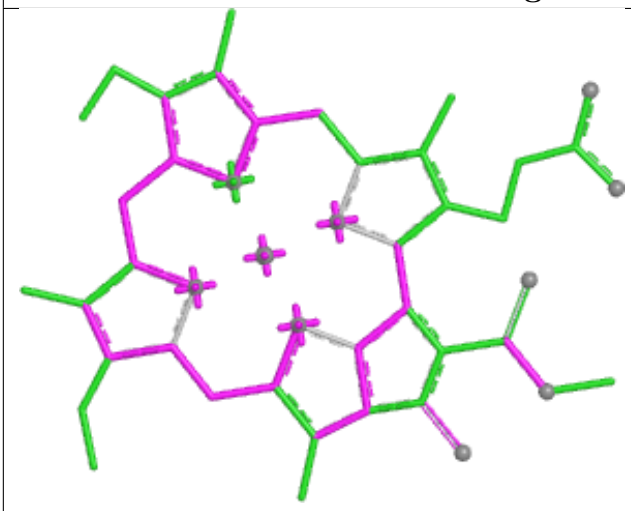


Rings

Ligand CLA B 831



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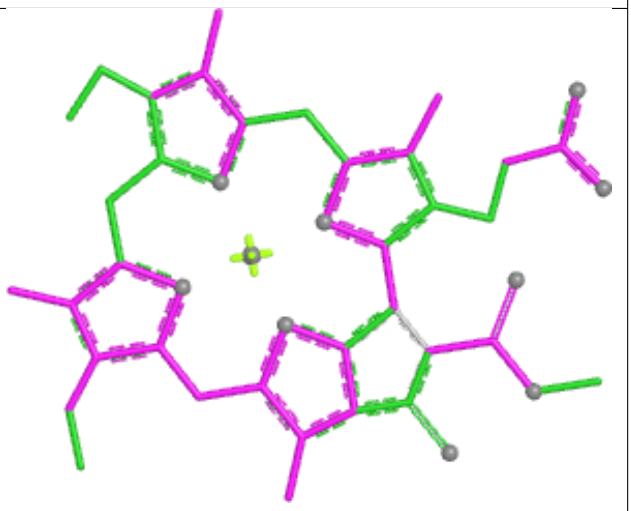
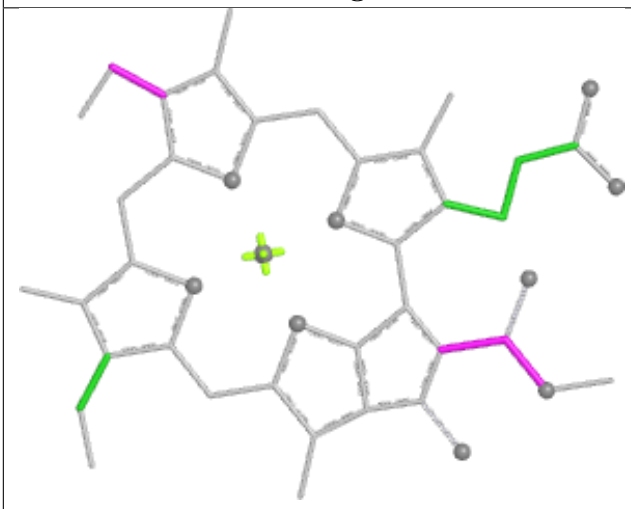


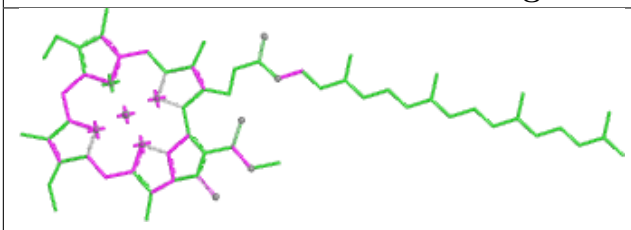
Bond angles



Torsions

Rings

Ligand CLA G 806



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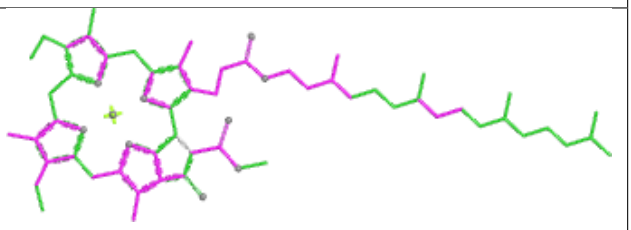
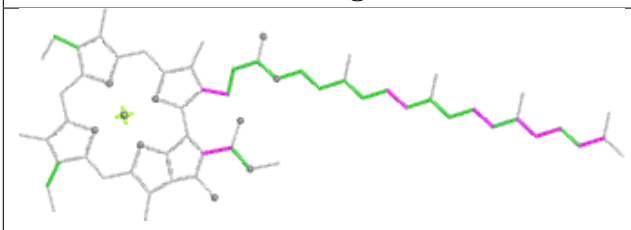
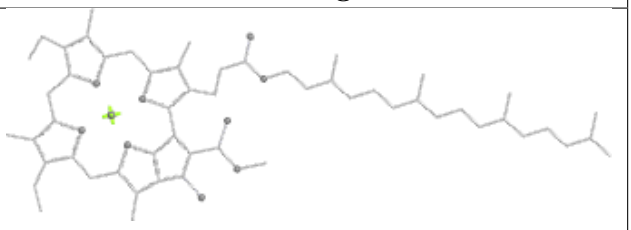


Bond angles

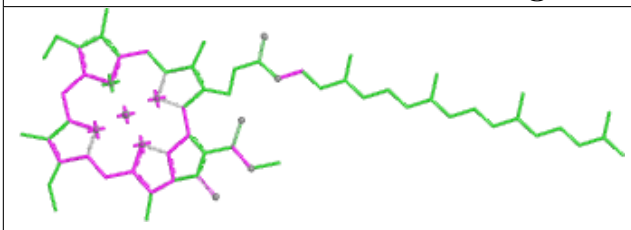


Torsions

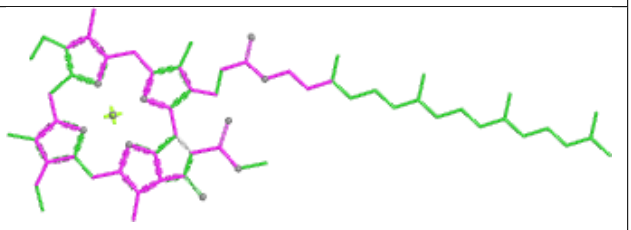


Rings

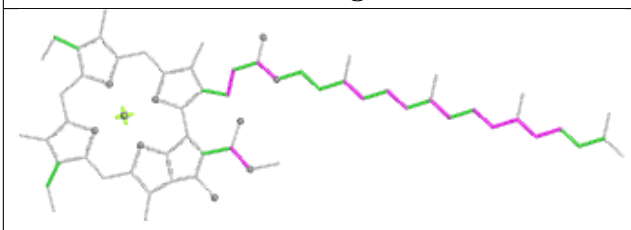
Ligand CLA a 820



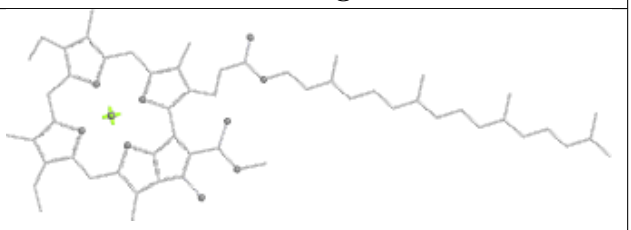
Bond lengths



Bond angles

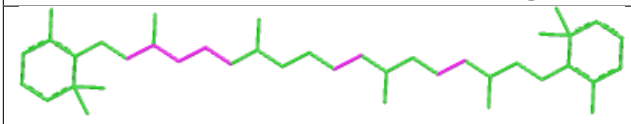


Torsions



Rings

Ligand BCR B 841



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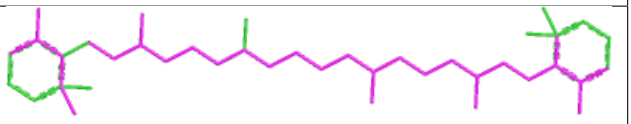
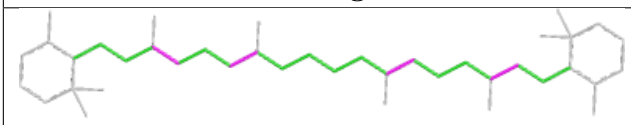
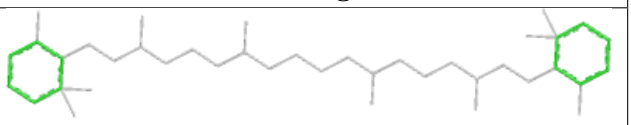


Bond angles

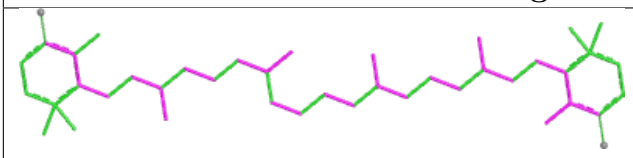


Torsions



Rings

Ligand 45D T 101



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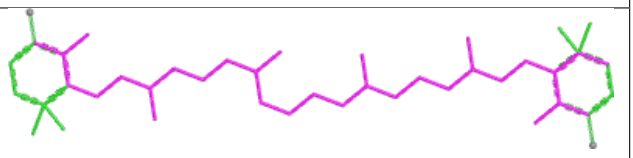
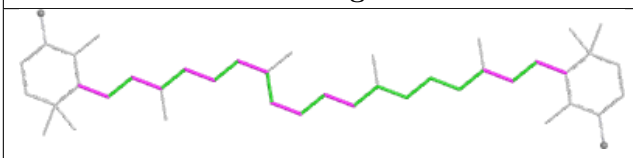


Bond angles



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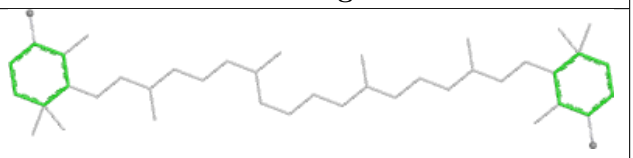
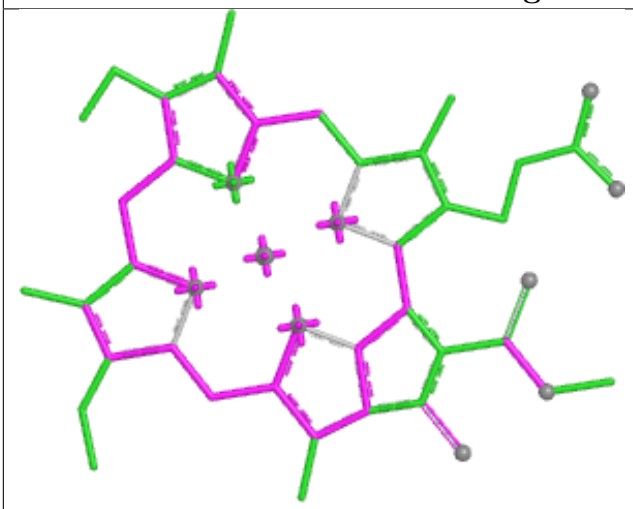


Rings

Ligand CLA H 810



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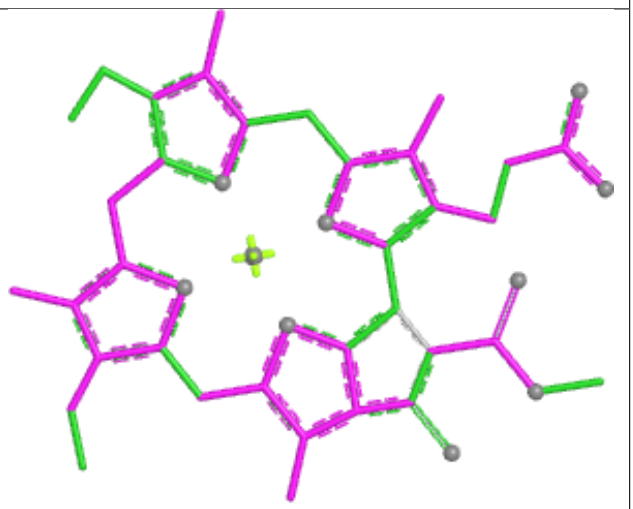
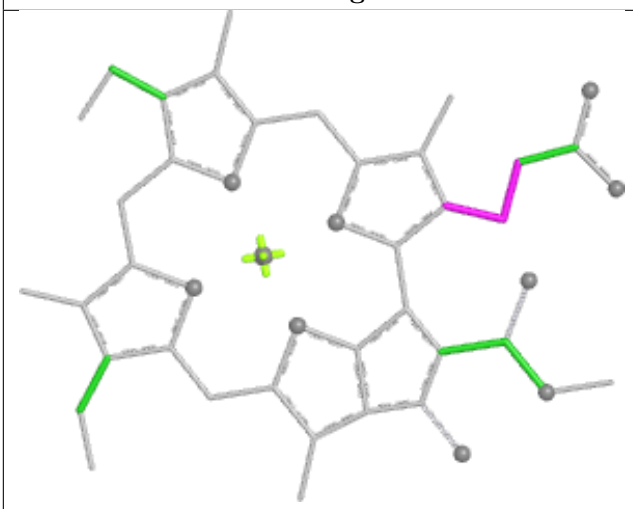


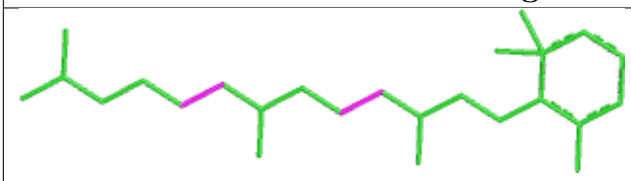
Bond angles



Torsions

Rings

Ligand BCR H 844



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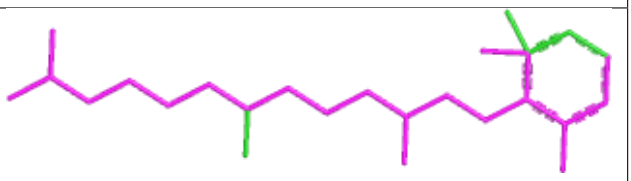
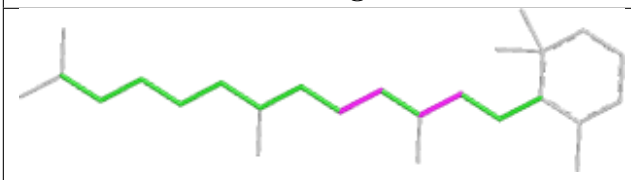
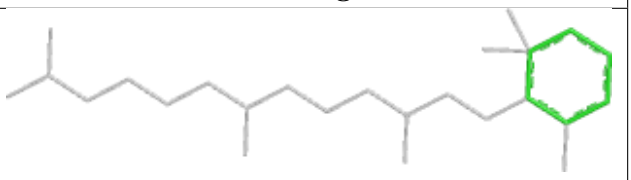


Bond angles

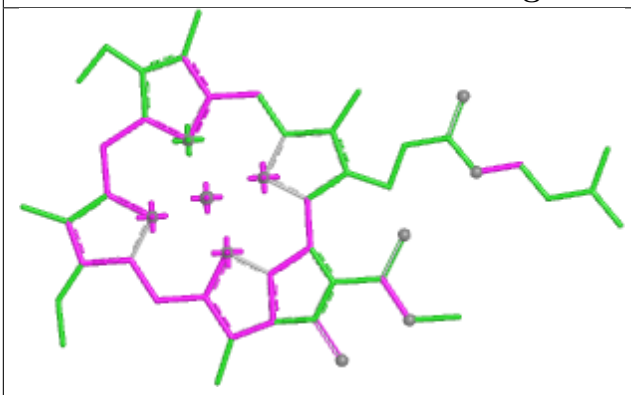


Torsions

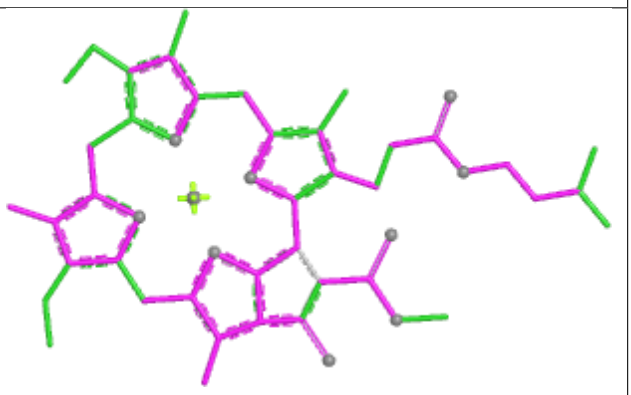


Rings

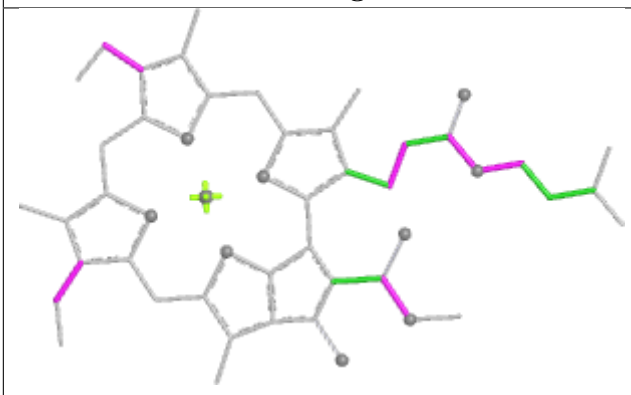
Ligand CLA G 813



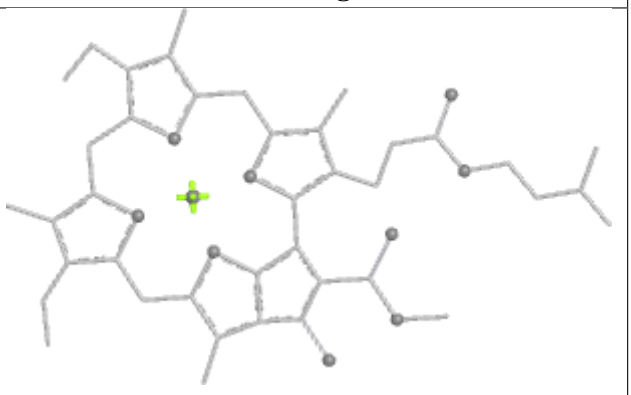
Bond lengths



Bond angles

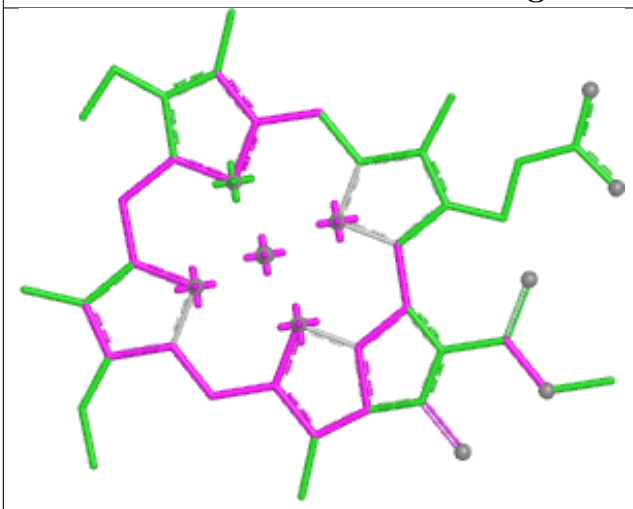


Torsions

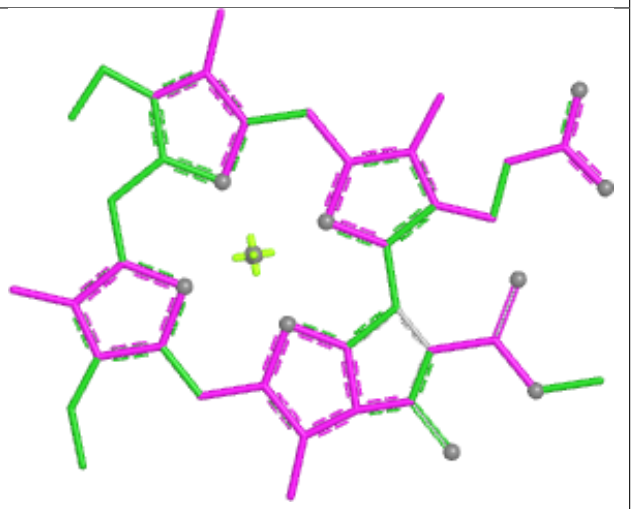


Rings

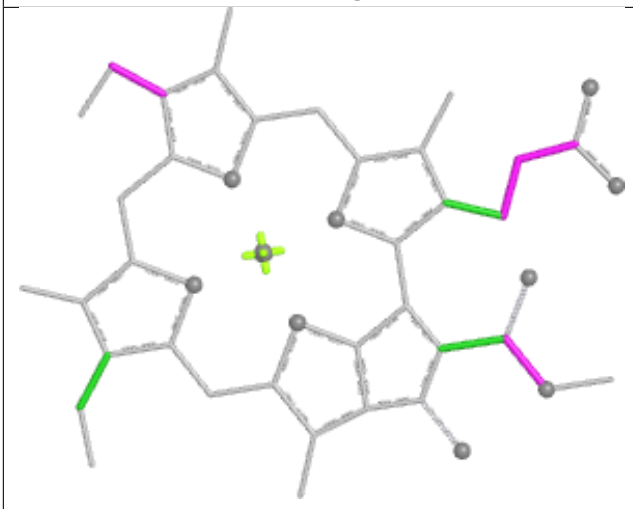
Ligand CLA b 819



Bond lengths



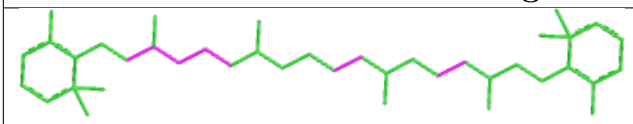
Bond angles



Torsions

Rings

Ligand BCR A 849



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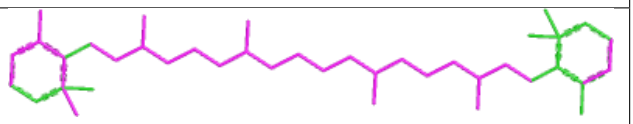
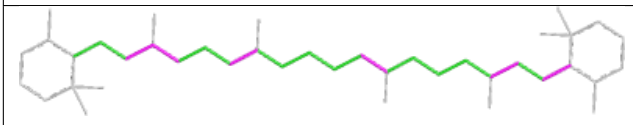
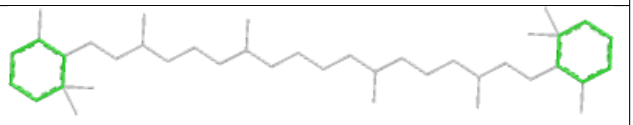


Bond angles

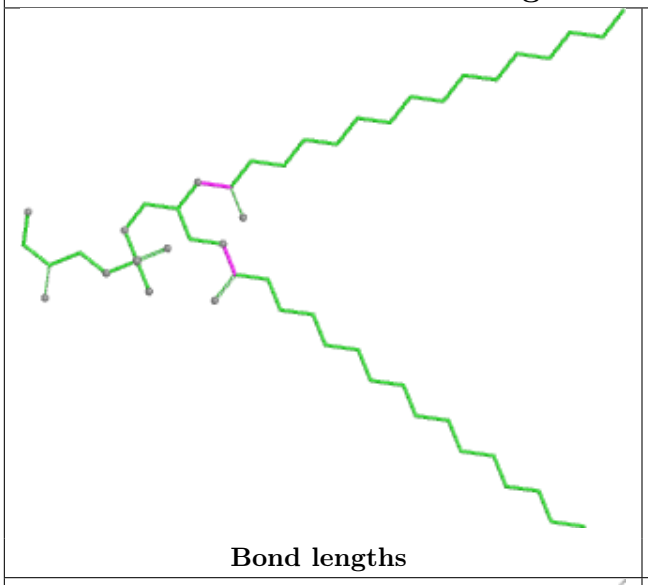


Torsions

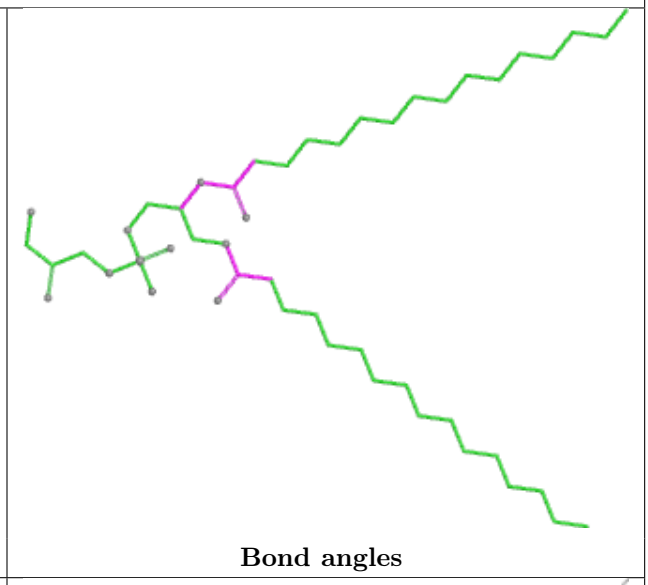


Rings

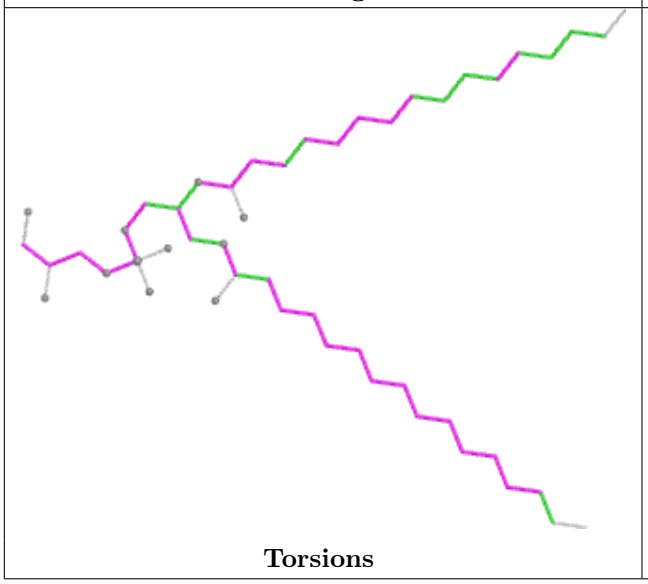
Ligand LHG G 854



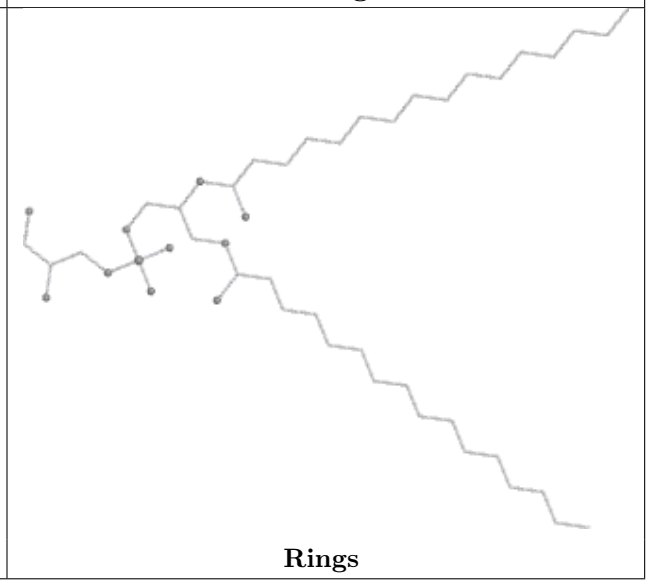
Bond lengths



Bond angles

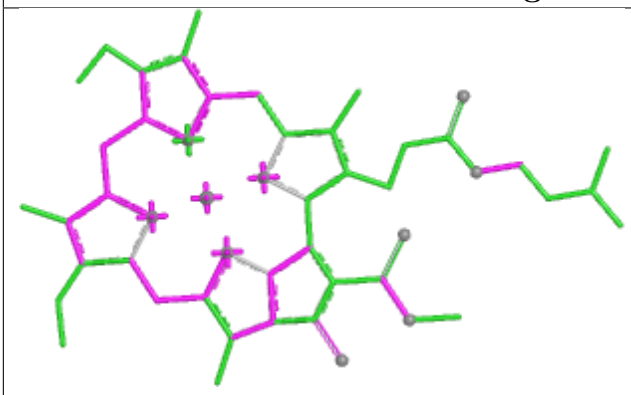


Torsions



Rings

Ligand CLA A 830



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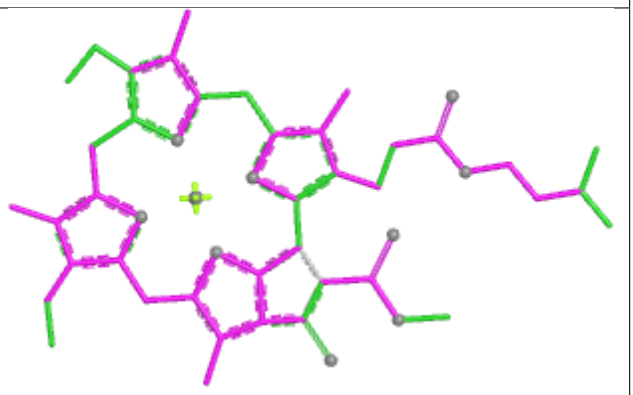
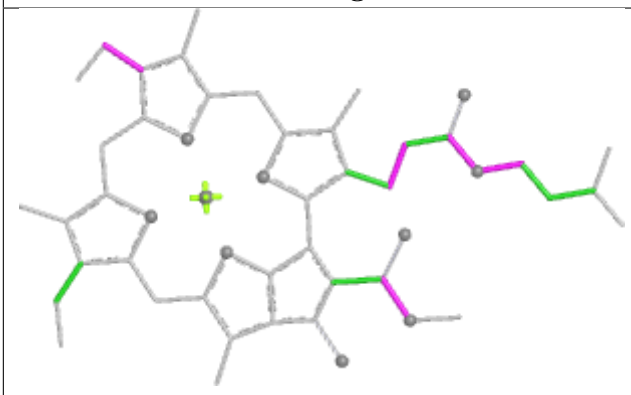


Bond angles



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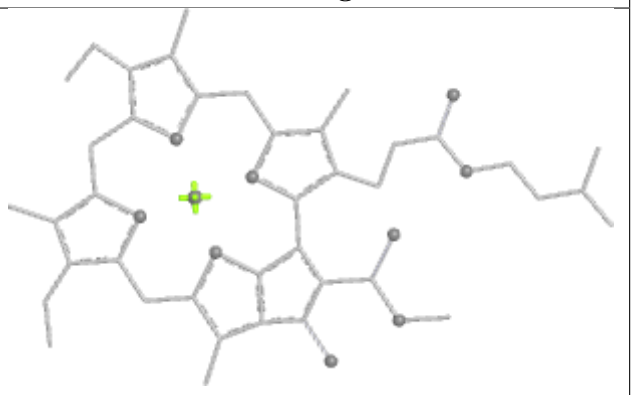
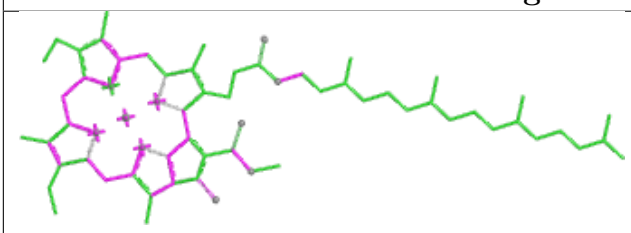


Rings

Ligand CLA H 825



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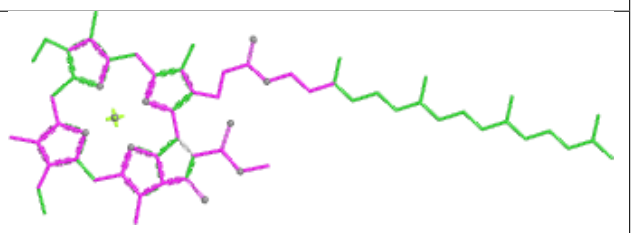
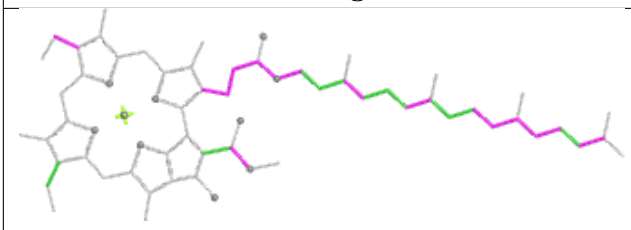


Bond angles



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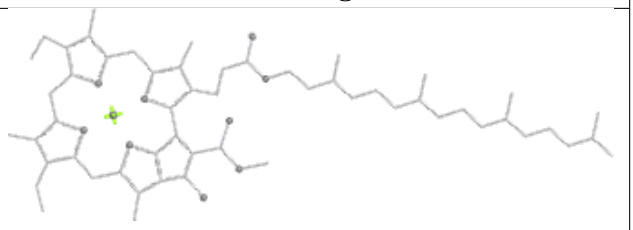
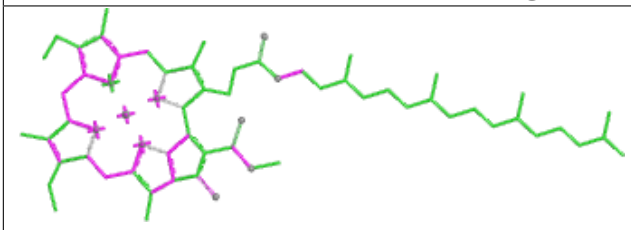


Rings

Ligand CLA H 808



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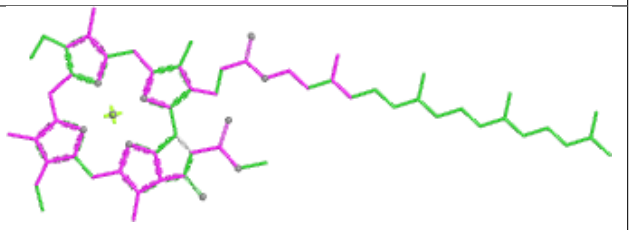
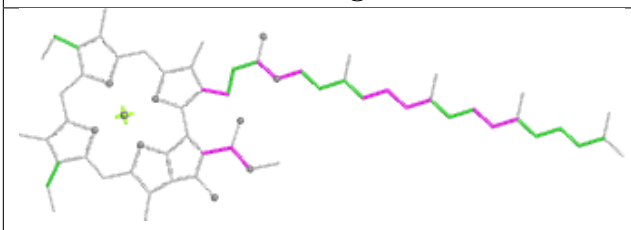
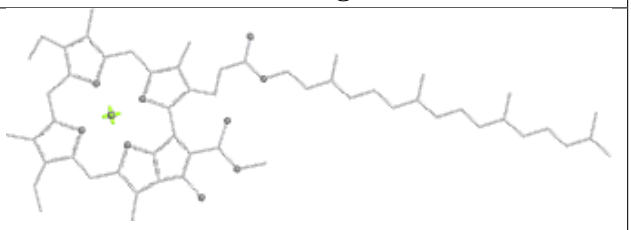


Bond angles

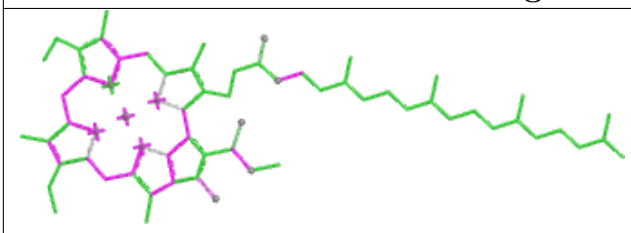


Torsions

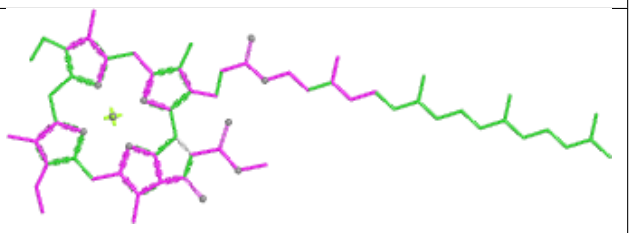


Rings

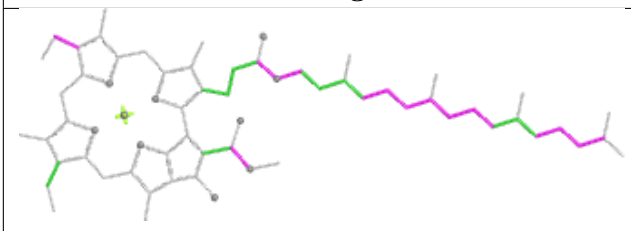
Ligand CLA B 804



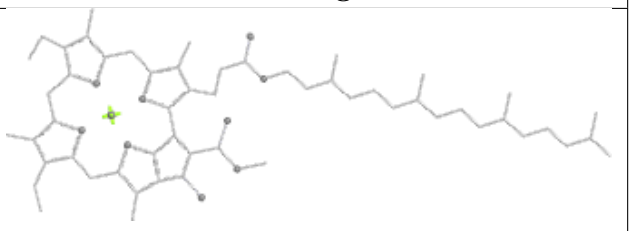
Bond lengths



Bond angles

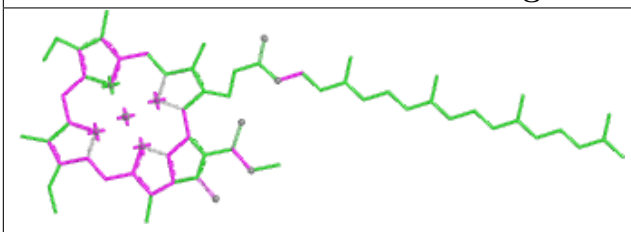


Torsions

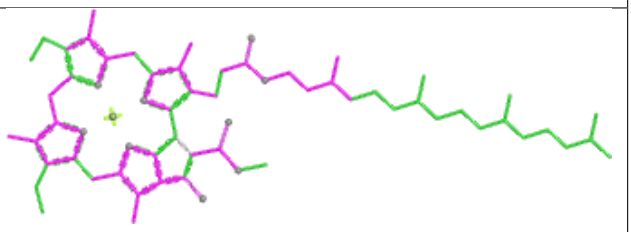


Rings

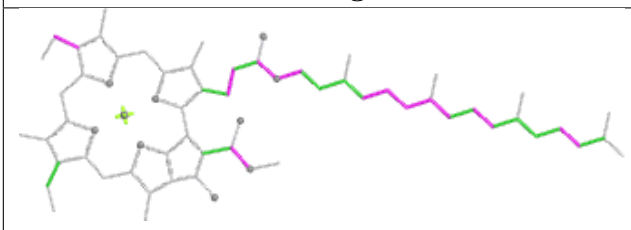
Ligand CLA G 804



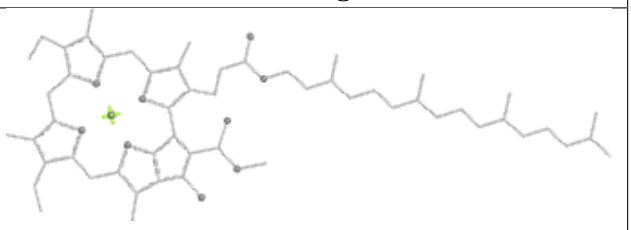
Bond lengths



Bond angles

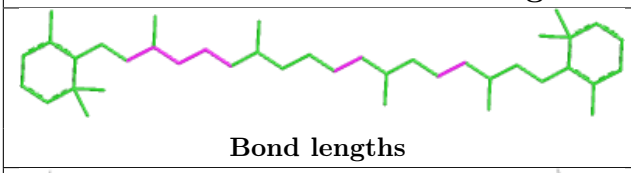


Torsions

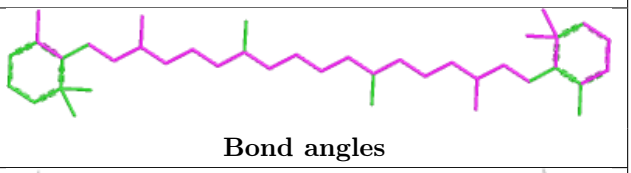


Rings

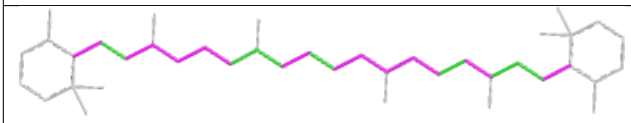
Ligand BCR J 102



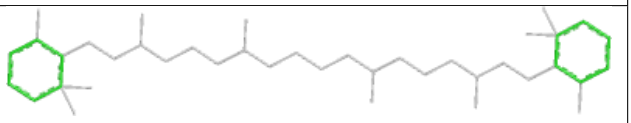
Bond lengths



Bond angles

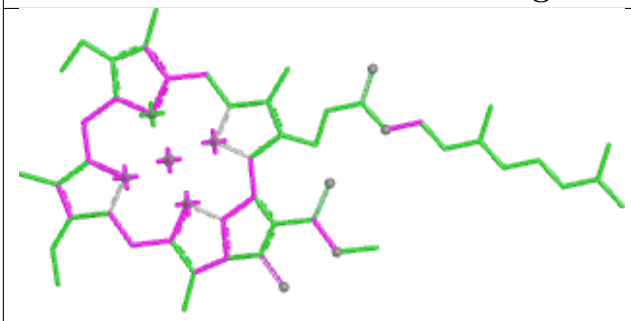


Torsions



Rings

Ligand CLA l 204



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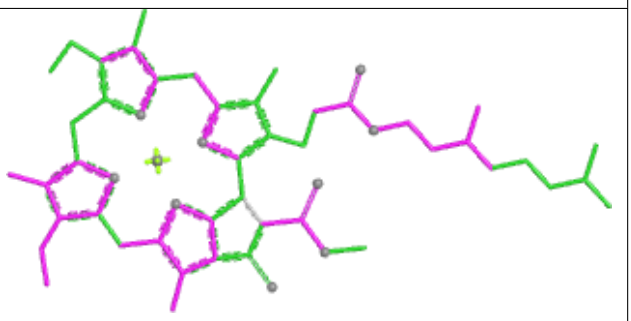
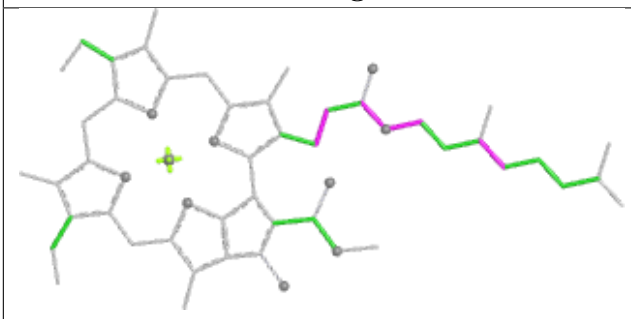
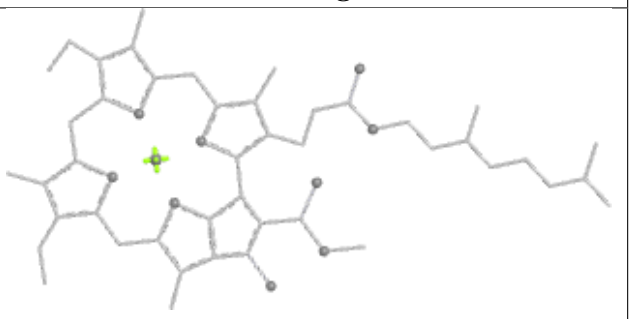


Bond angles

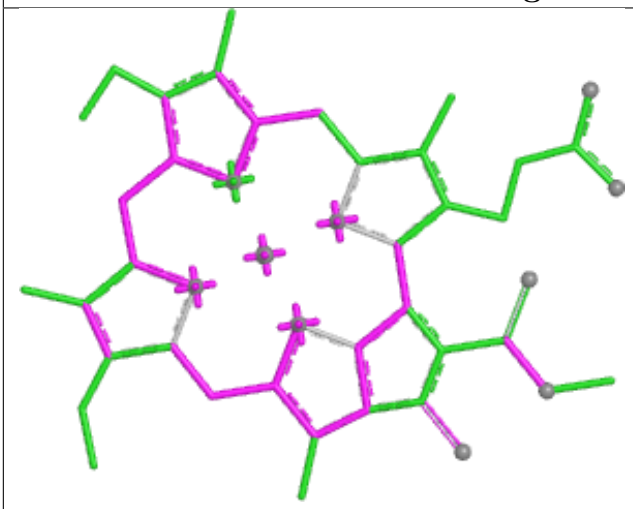


Torsions



Rings

Ligand CLA H 813



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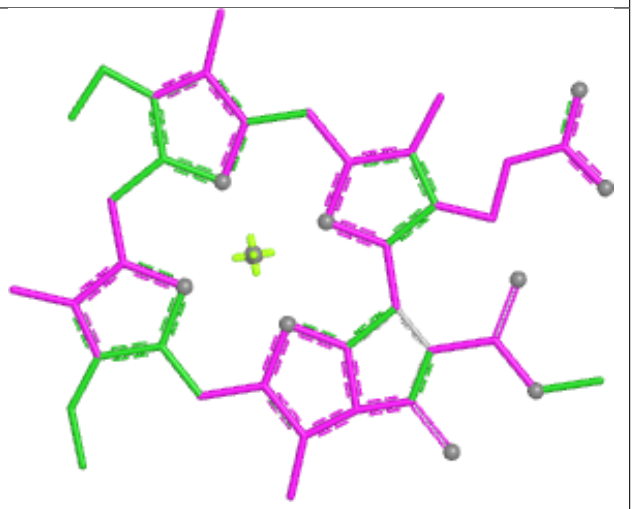
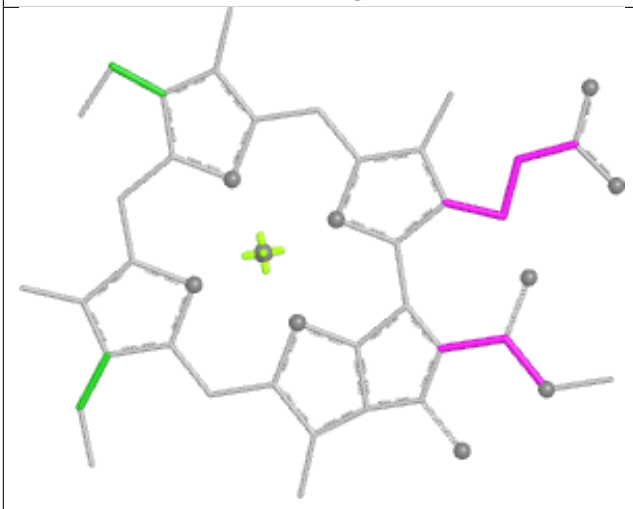


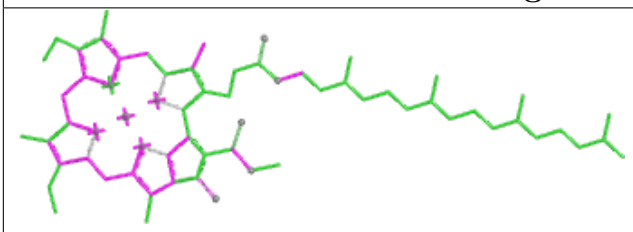
Bond angles



Torsions

Rings

Ligand CLA B 803



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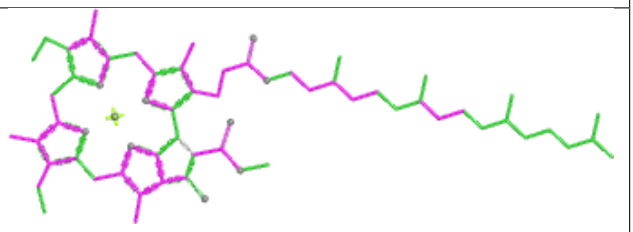
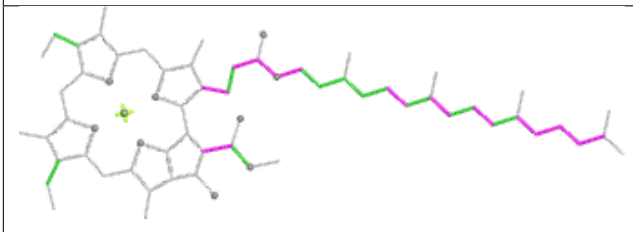
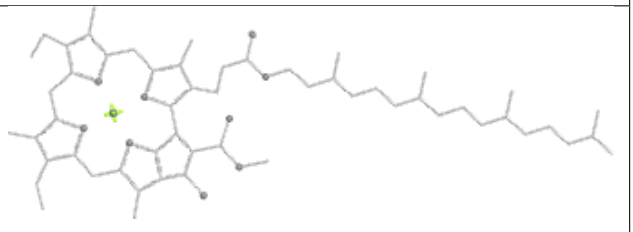


Bond angles

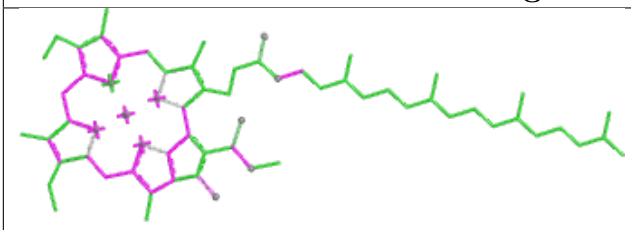


Torsions



Rings

Ligand CLA A 837



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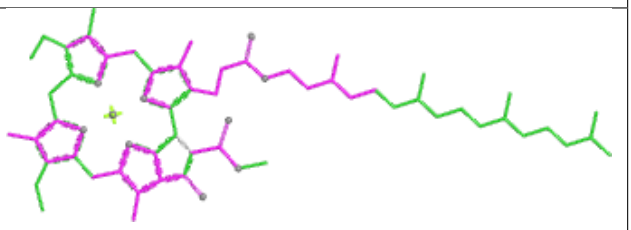
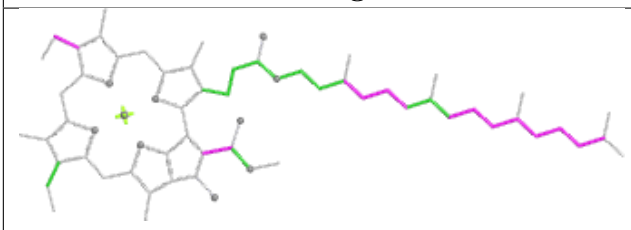


Bond angles



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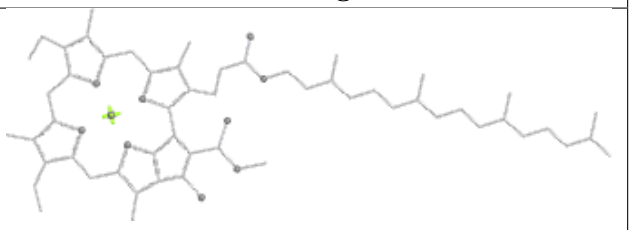
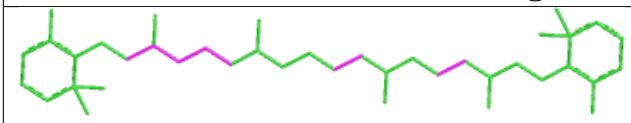


Rings

Ligand BCR a 845



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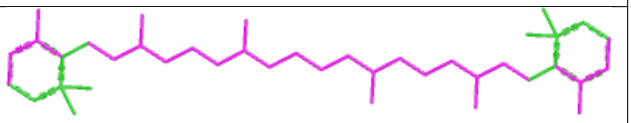
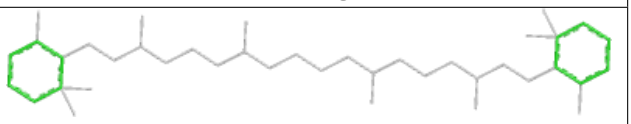


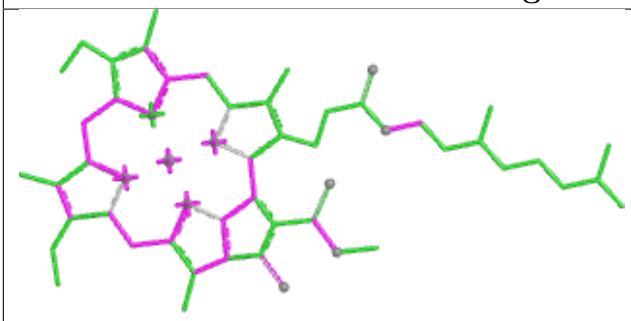
Bond angles

Torsions



Rings

Ligand CLA G 826



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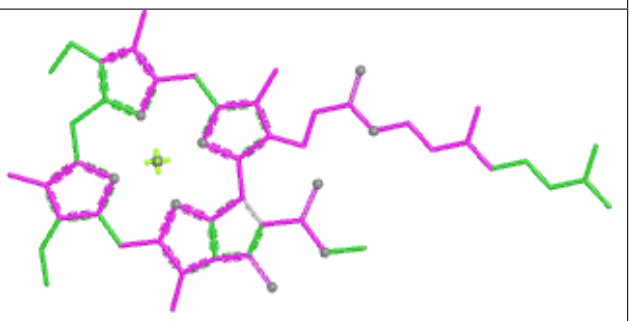
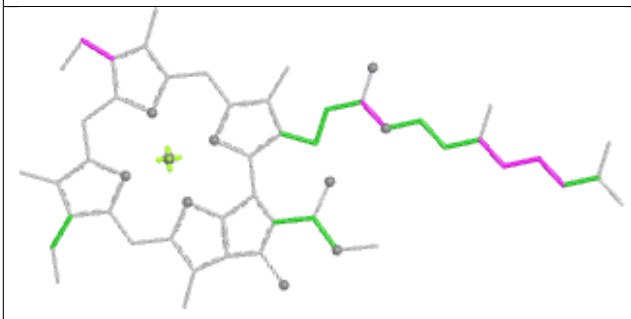


Bond angles



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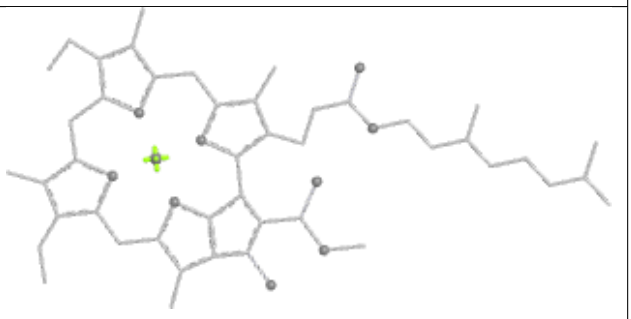
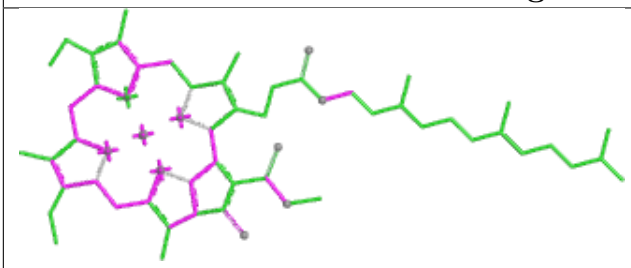
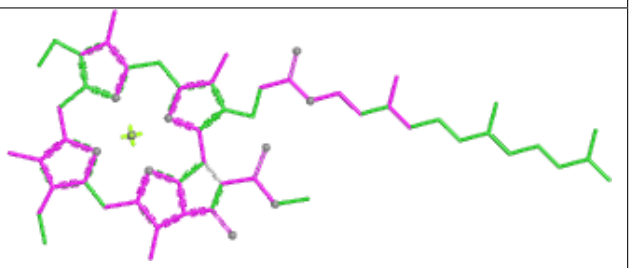
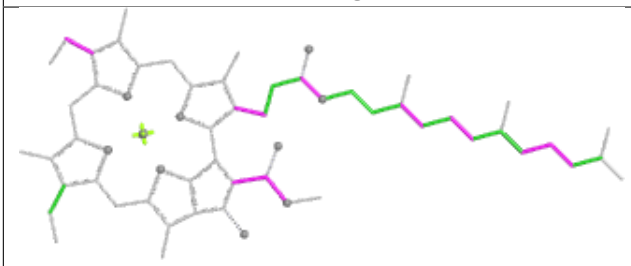
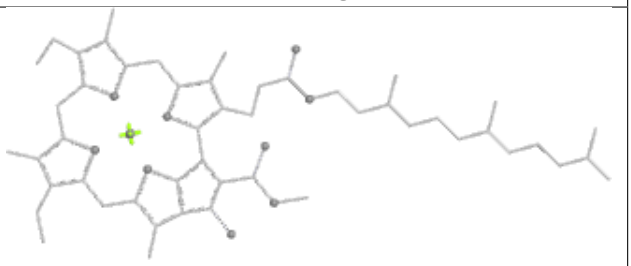
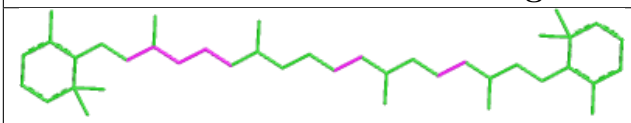
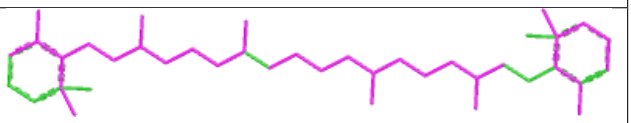
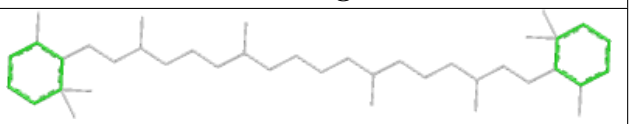
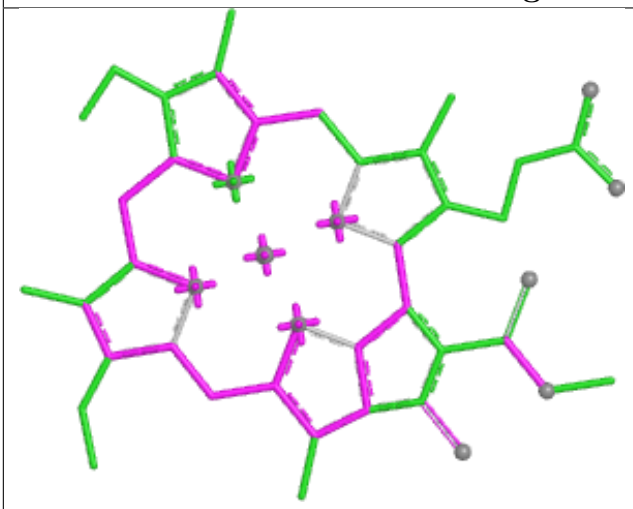


Rings

Ligand CLA b 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 810



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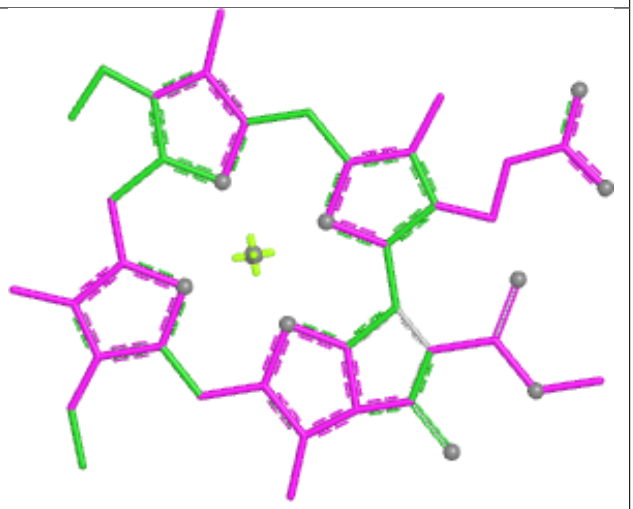
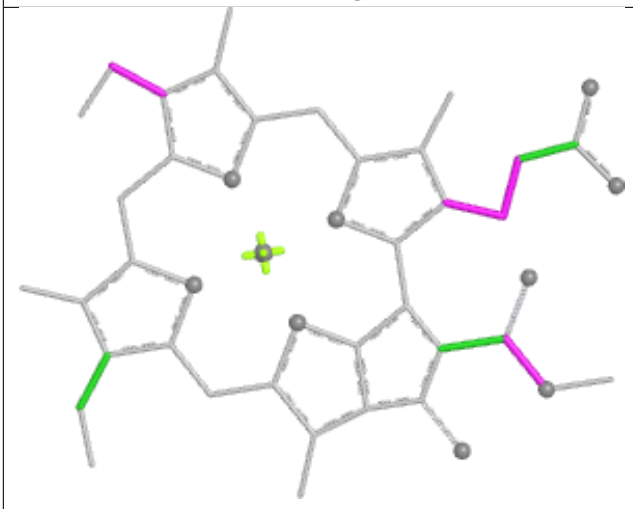


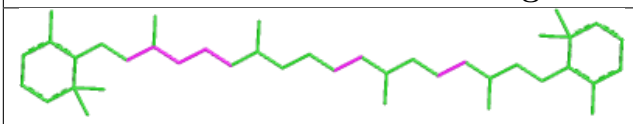
Bond angles



Torsions

Rings

Ligand BCR A 847



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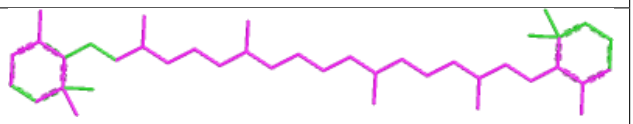
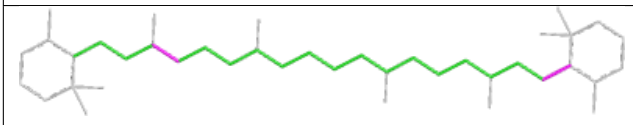


Bond angles



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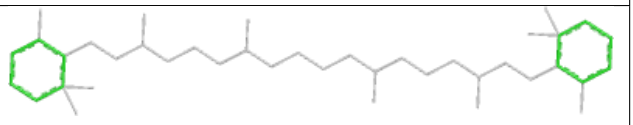
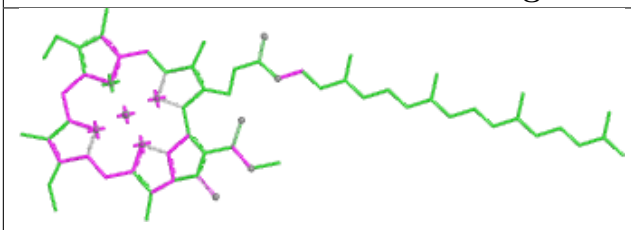


Rings

Ligand CLA G 833



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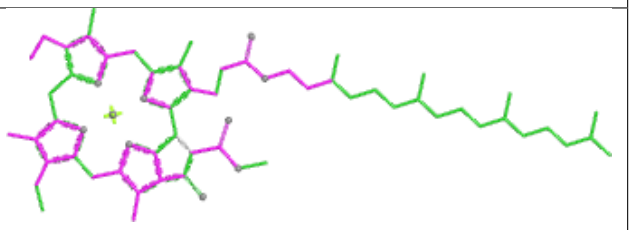
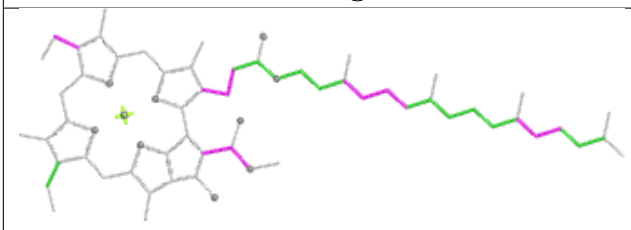


Bond angles



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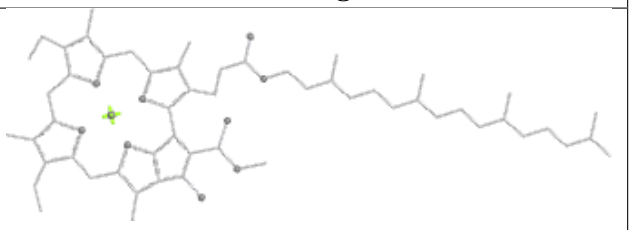
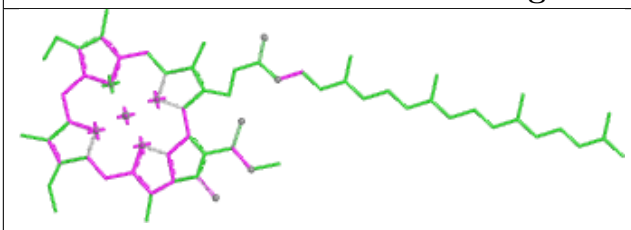
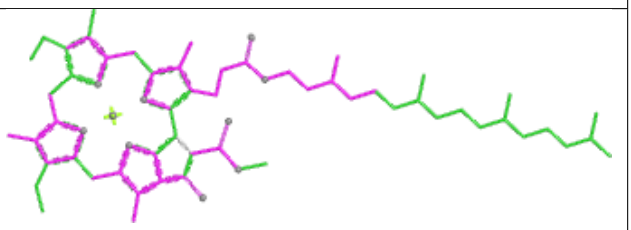


Rings

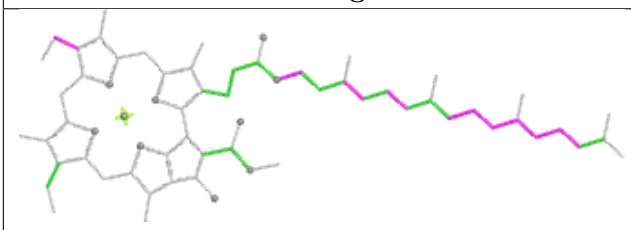
Ligand CLA a 837



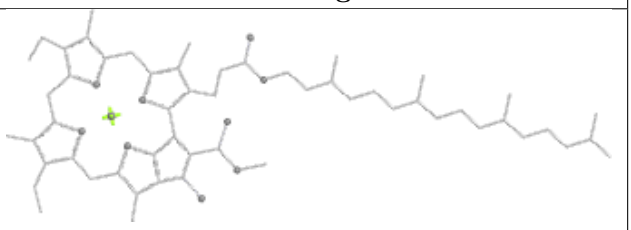
Bond lengths



Bond angles

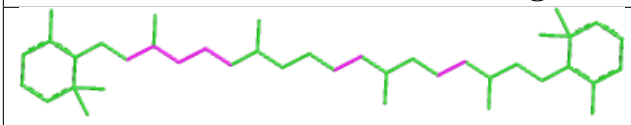


Torsions

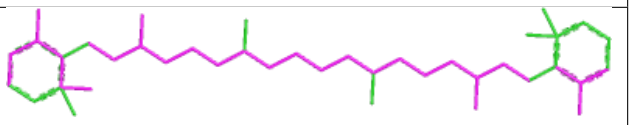


Rings

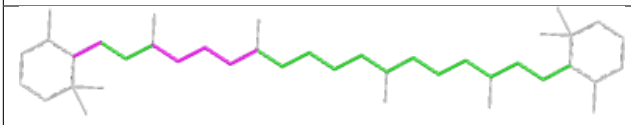
Ligand BCR I 101



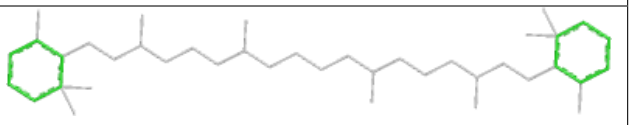
Bond lengths



Bond angles

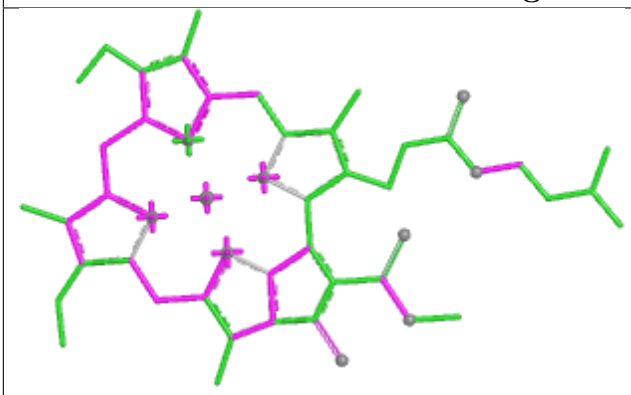


Torsions

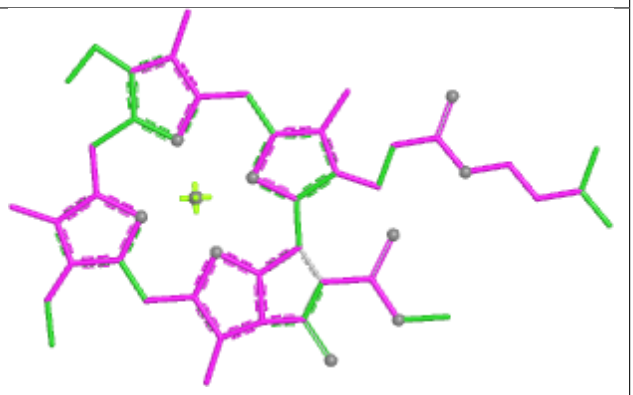


Rings

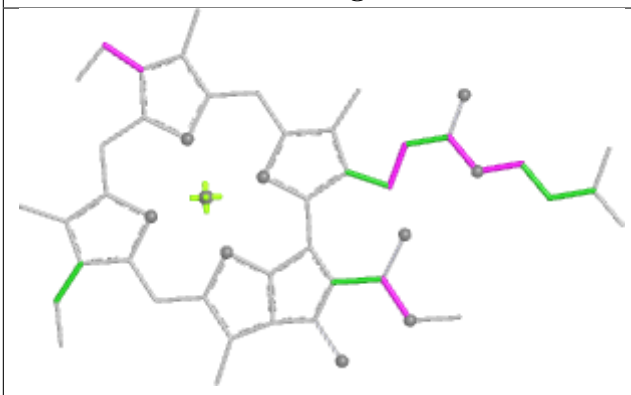
Ligand CLA G 831



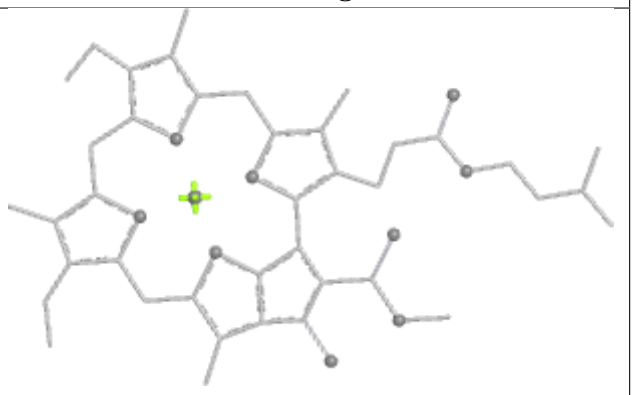
Bond lengths



Bond angles

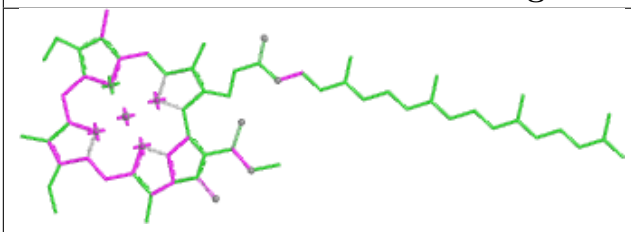


Torsions

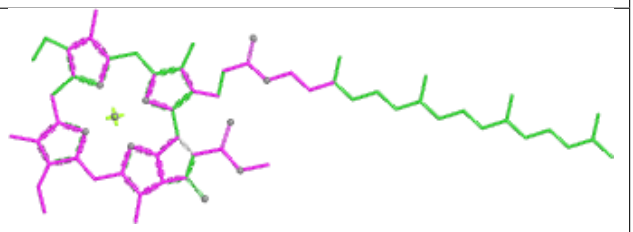


Rings

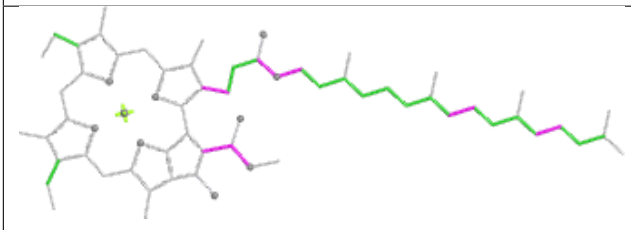
Ligand CLA b 826



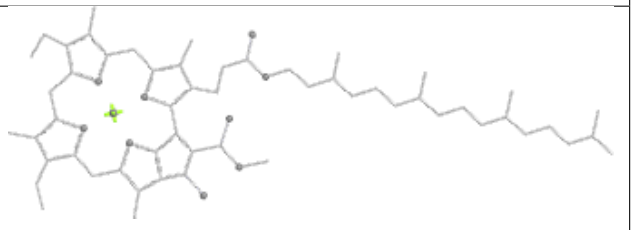
Bond lengths



Bond angles

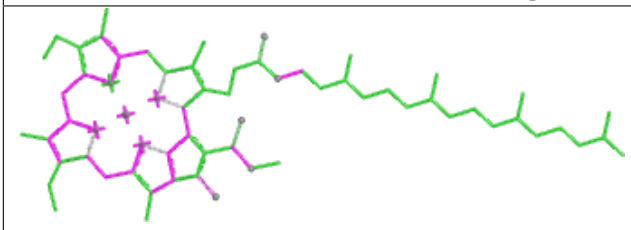


Torsions



Rings

Ligand CLA A 828



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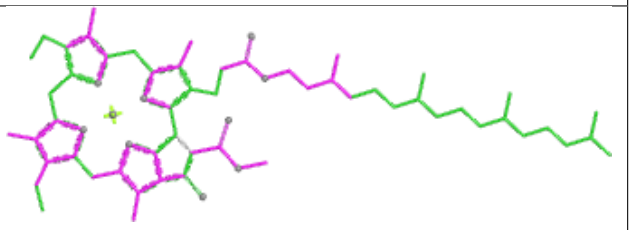
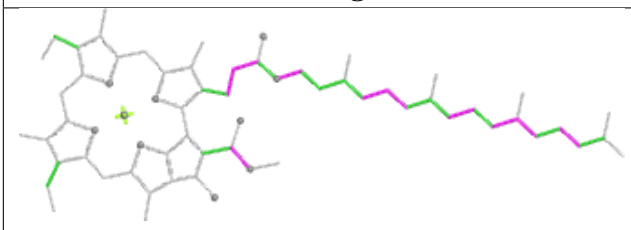
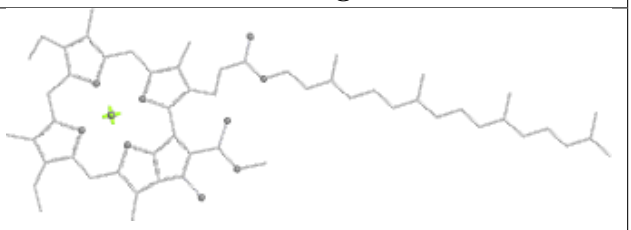


Bond angles

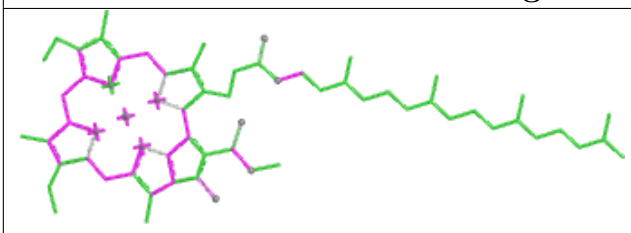


Torsions



Rings

Ligand CLA G 855



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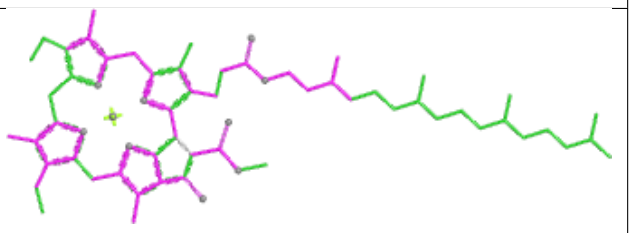
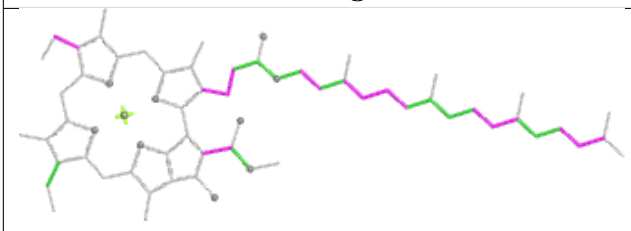
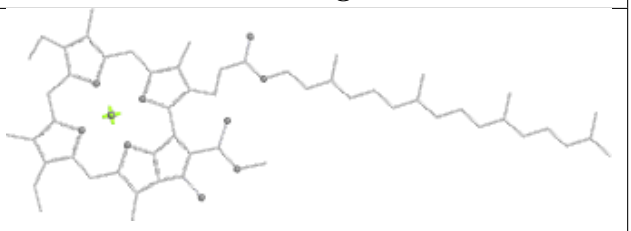


Bond angles

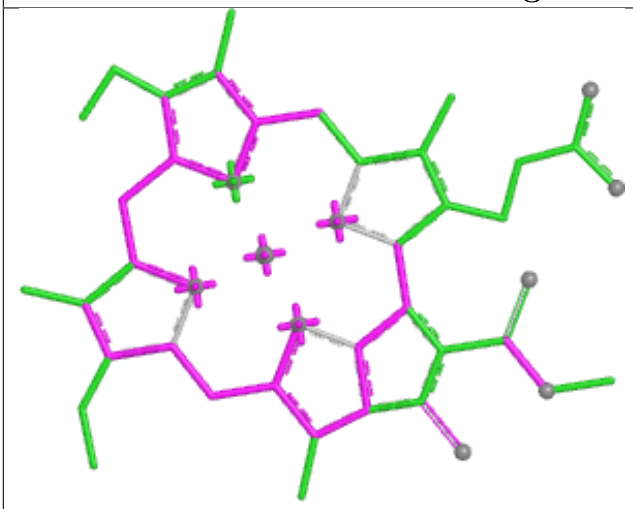


Torsions



Rings

Ligand CLA H 819



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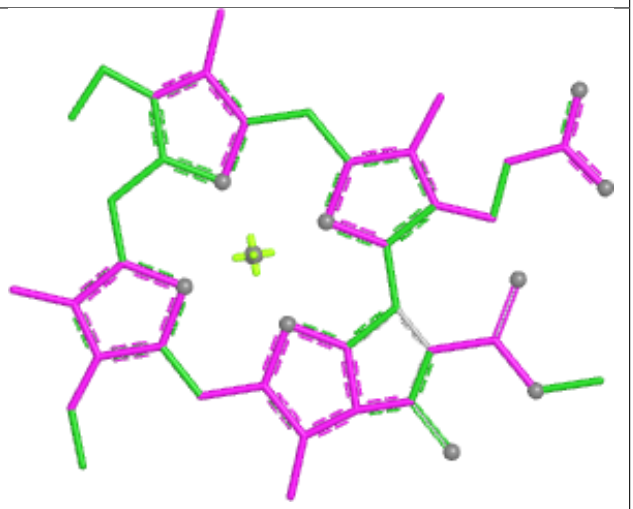
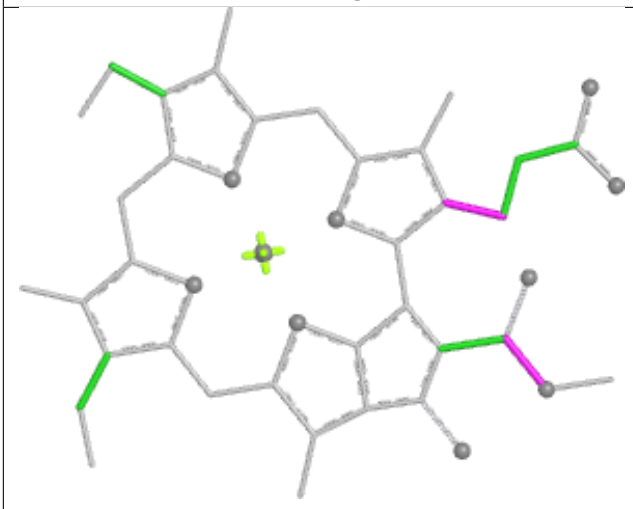


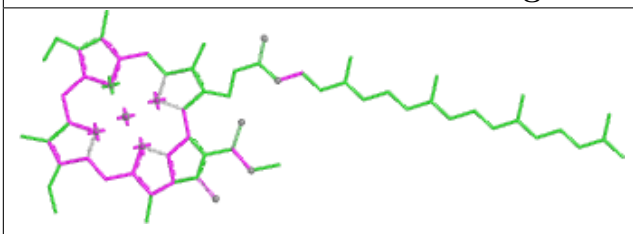
Bond angles



Torsions

Rings

Ligand CLA H 805



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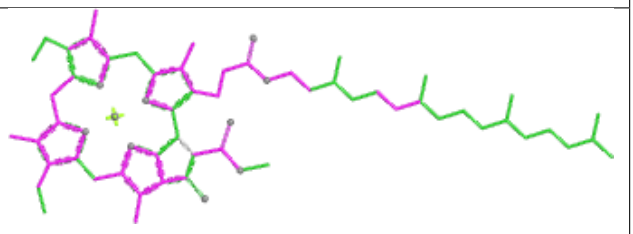
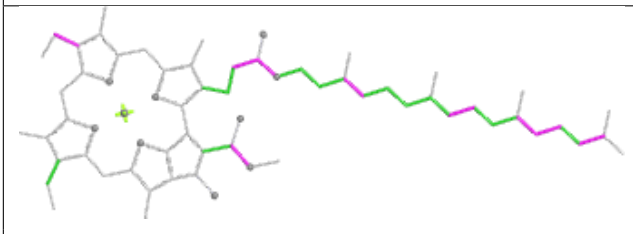
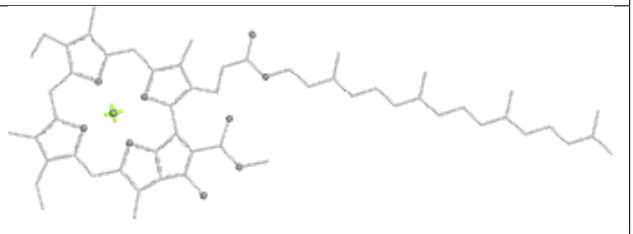


Bond angles

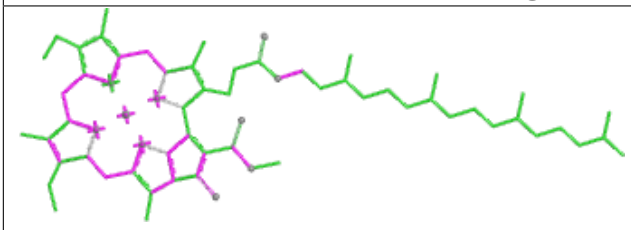


Torsions



Rings

Ligand CLA A 802



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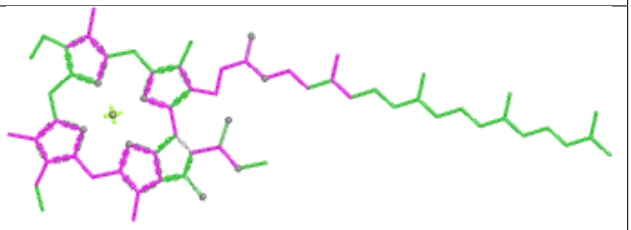
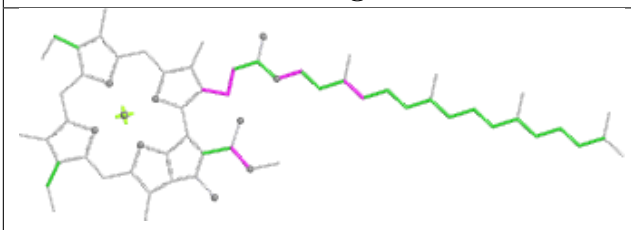


Bond angles



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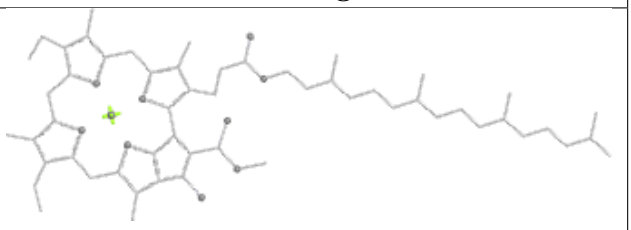
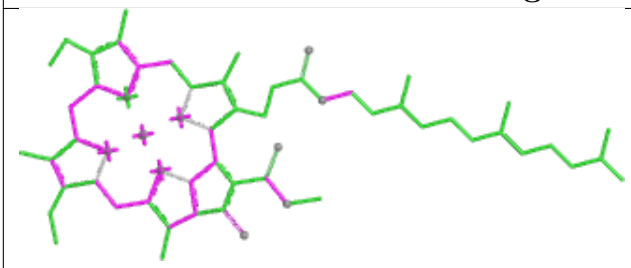


Rings

Ligand CLA A 827



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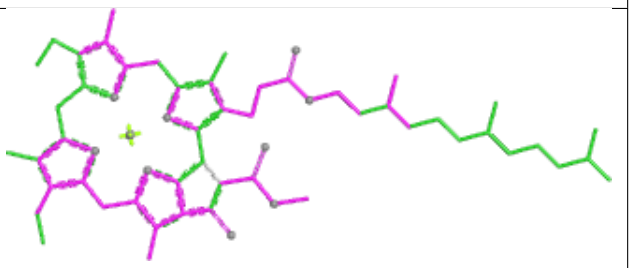
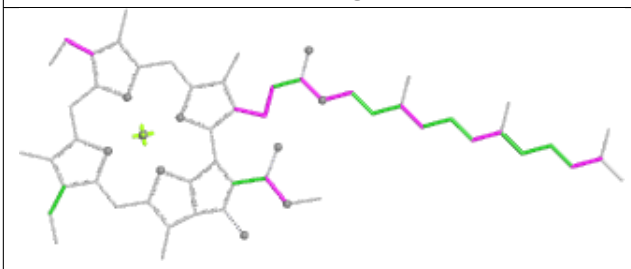


Bond angles



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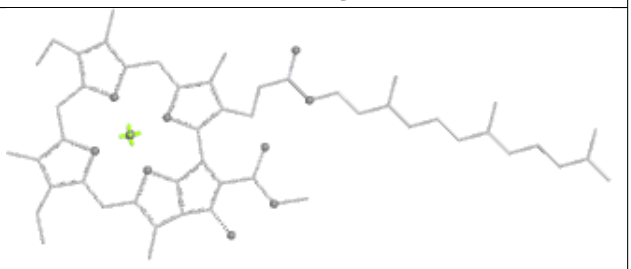
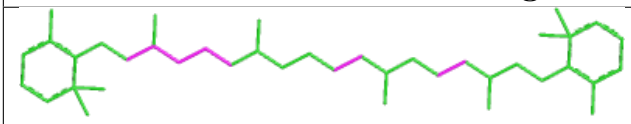


Rings

Ligand BCR G 846



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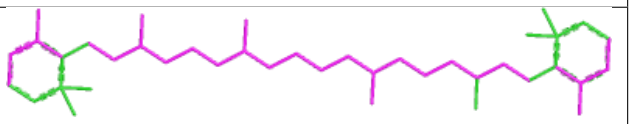
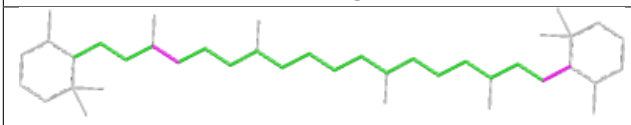
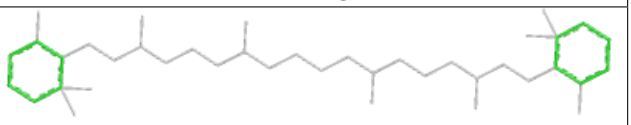


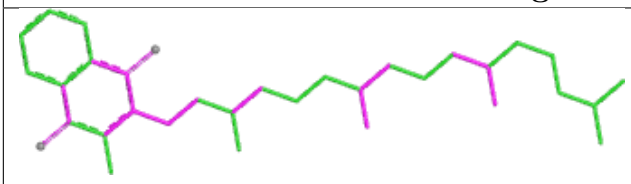
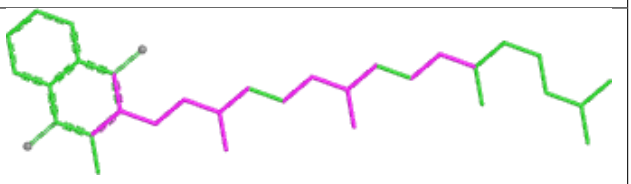
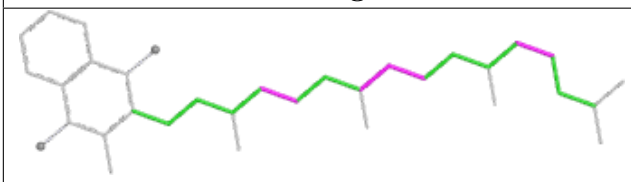
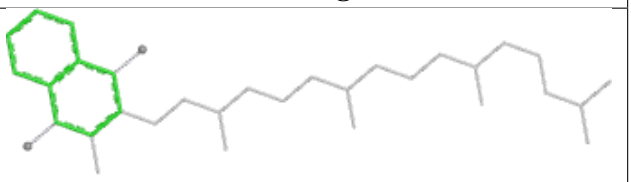
Bond angles

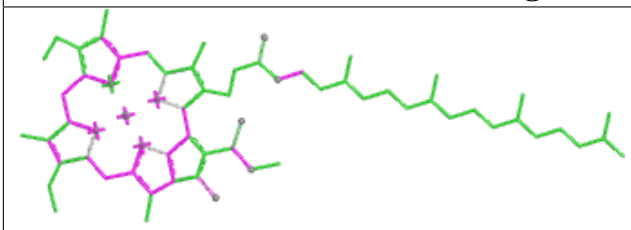
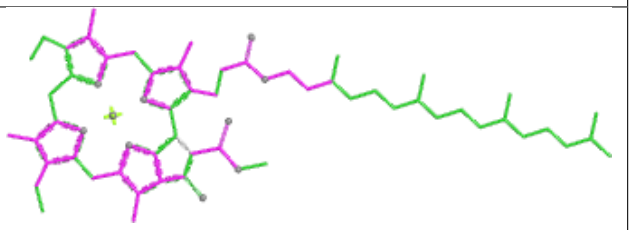
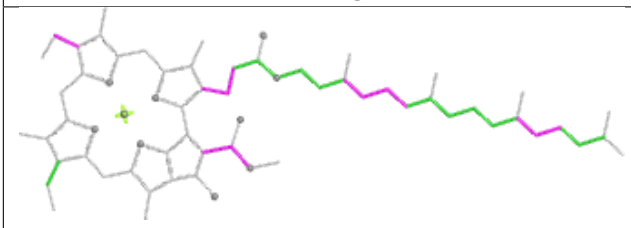
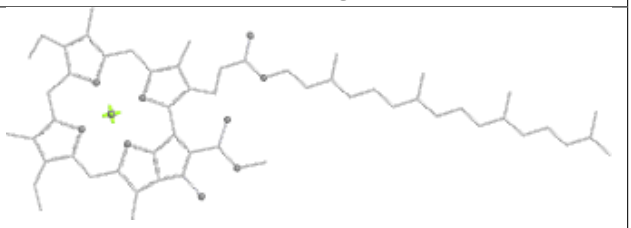


Torsions

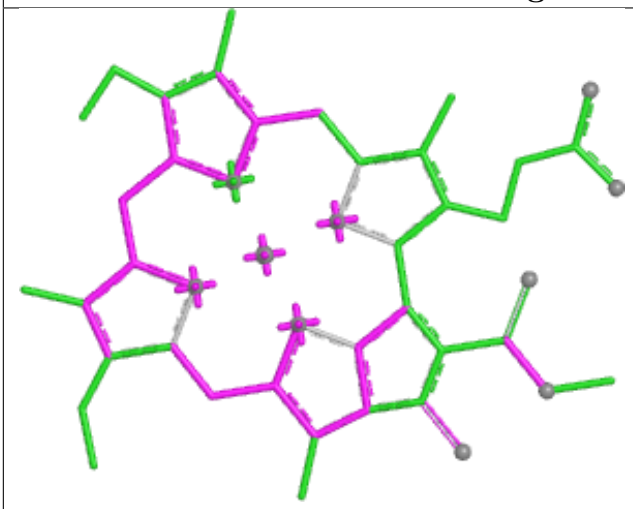


Rings

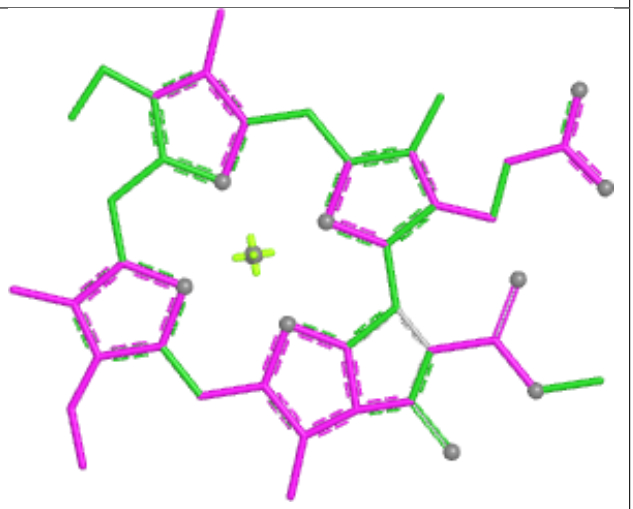
Ligand 1L3 H 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

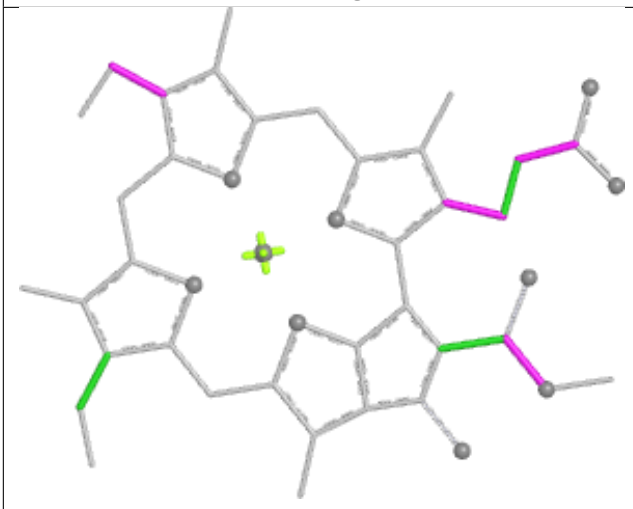
Ligand CLA b 834



Bond lengths



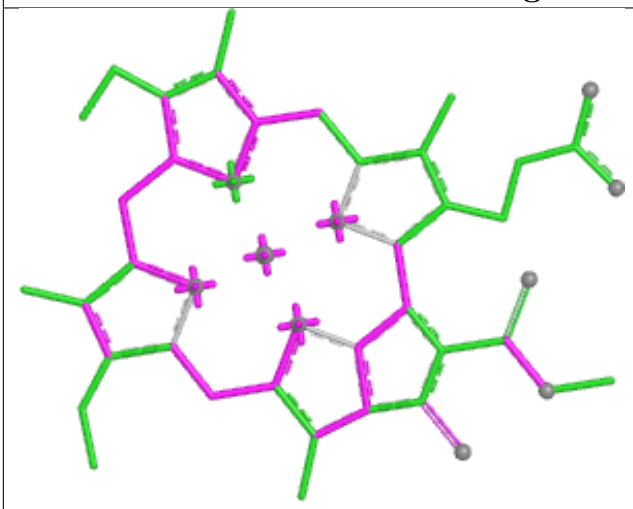
Bond angles



Torsions

Rings

Ligand CLA H 821



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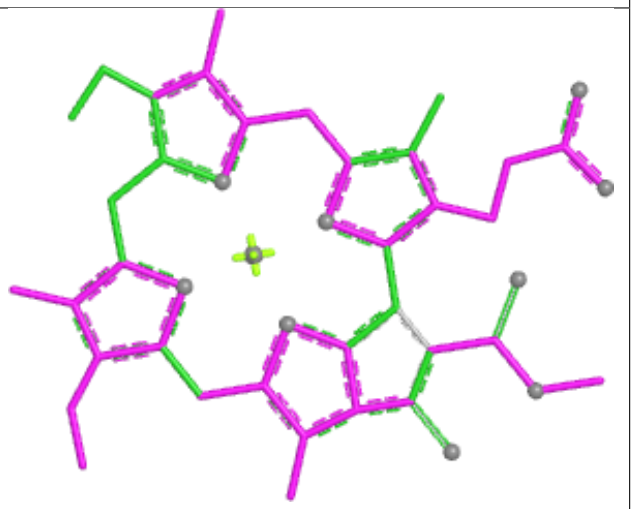
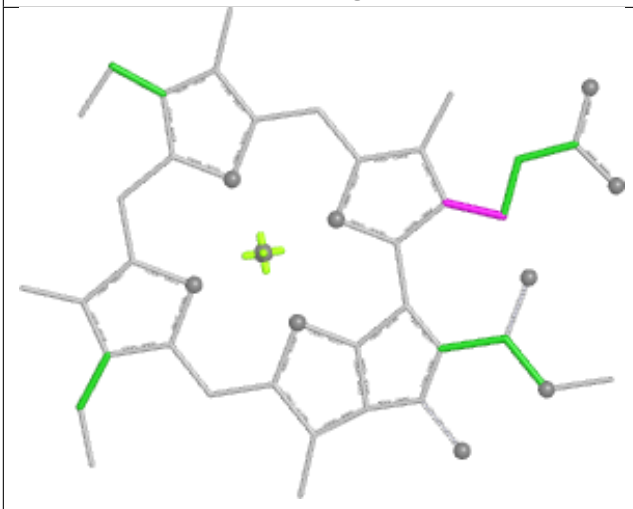


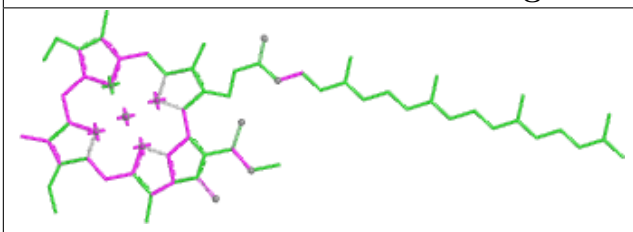
Bond angles



Torsions

Rings

Ligand CLA A 855



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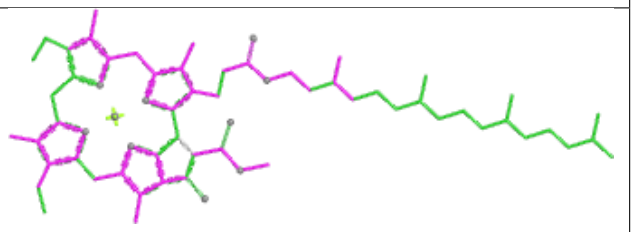
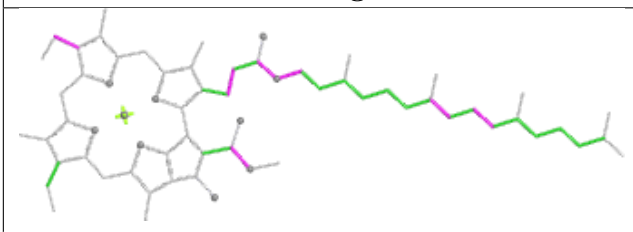
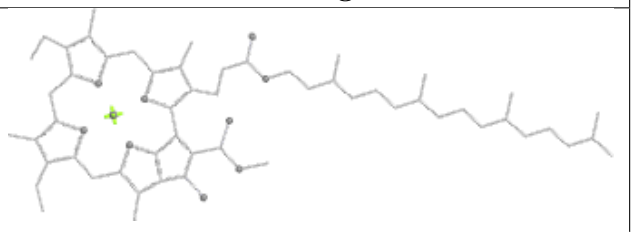


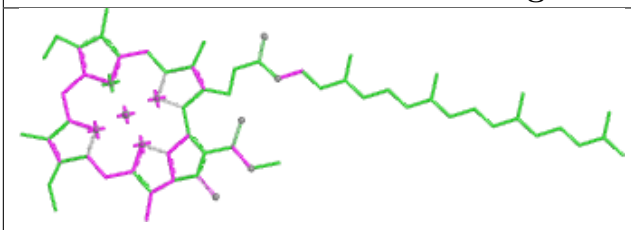
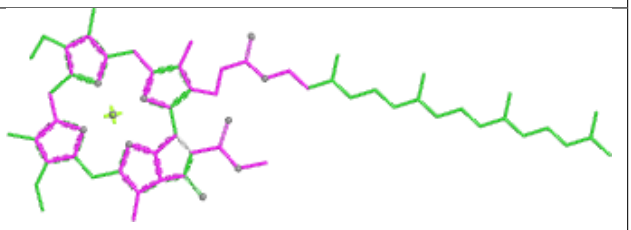
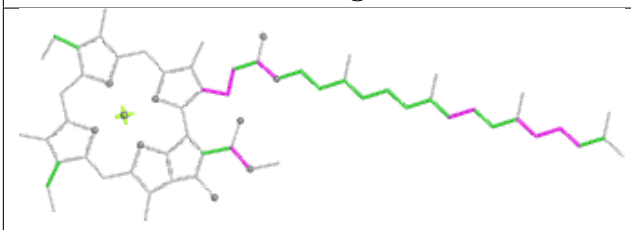
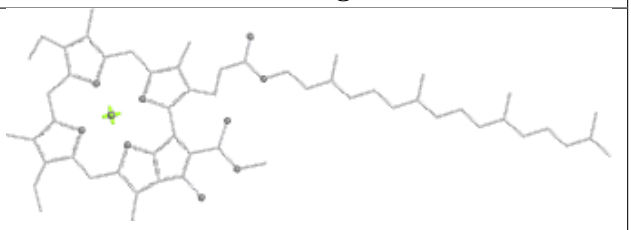
Bond angles

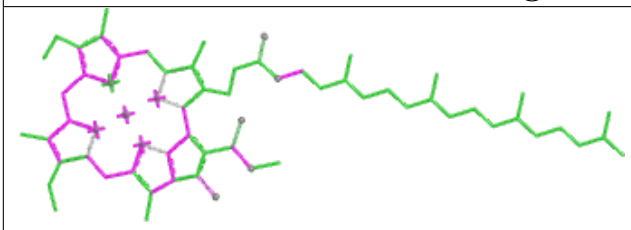
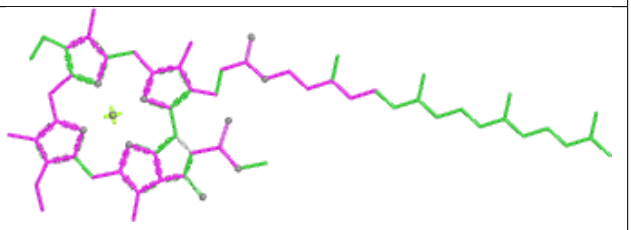
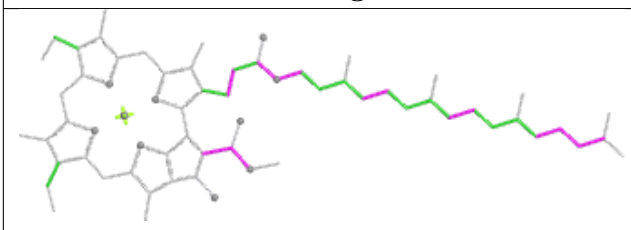
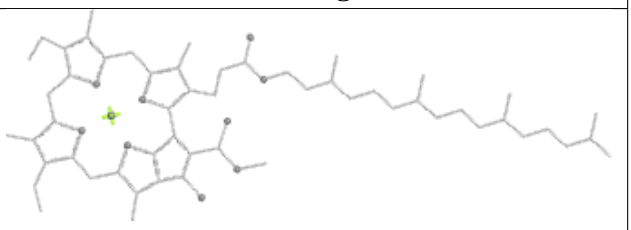


Torsions

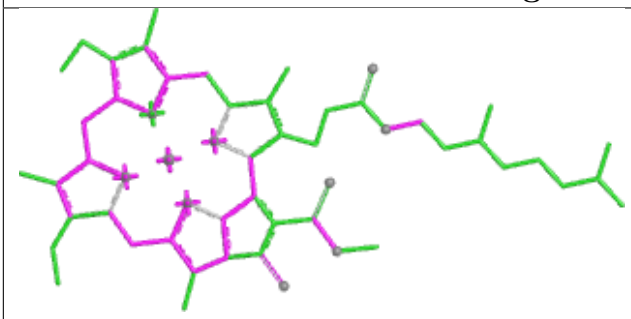


Rings

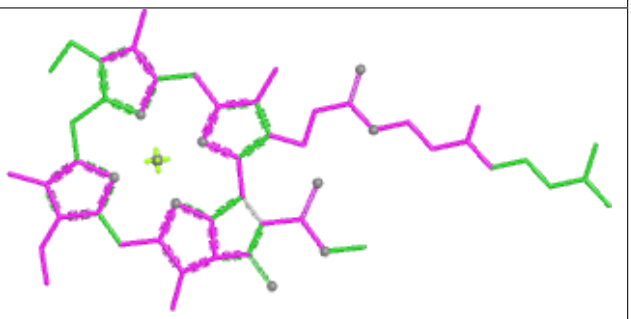
Ligand CLA b 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

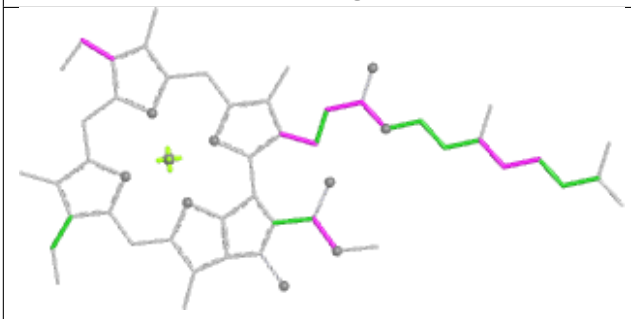
Ligand CLA G 805



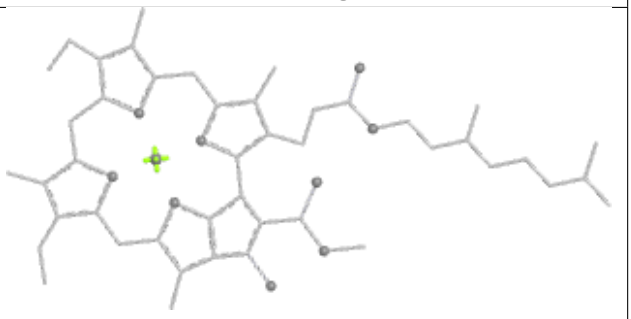
Bond lengths



Bond angles

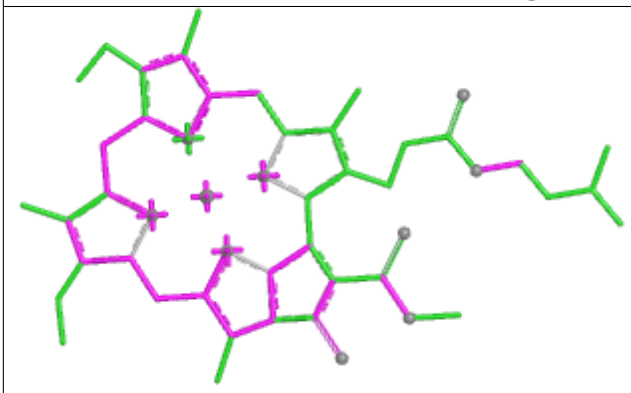


Torsions



Rings

Ligand CLA G 836



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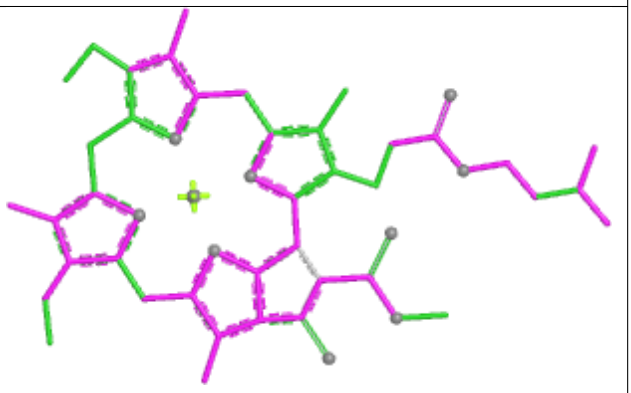
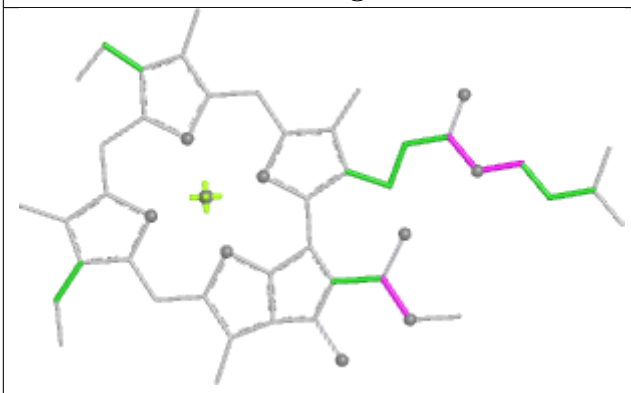
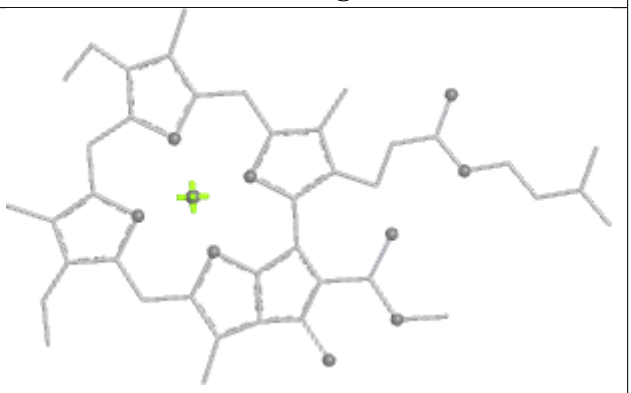


Bond angles

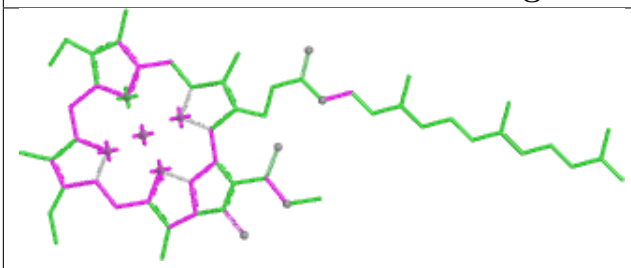


Torsions



Rings

Ligand CLA H 834



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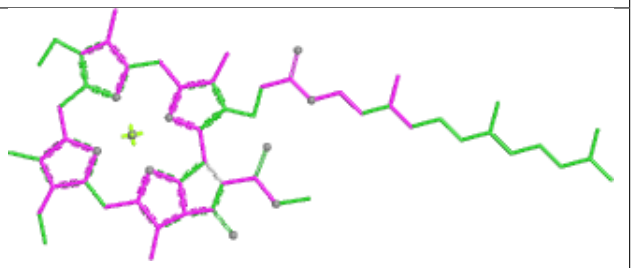
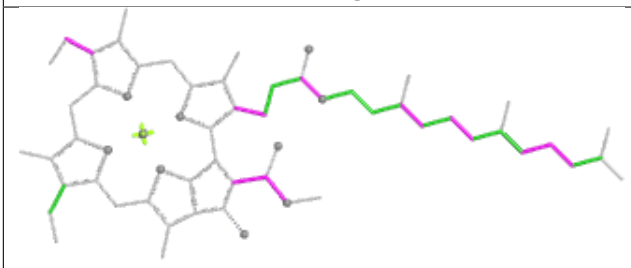
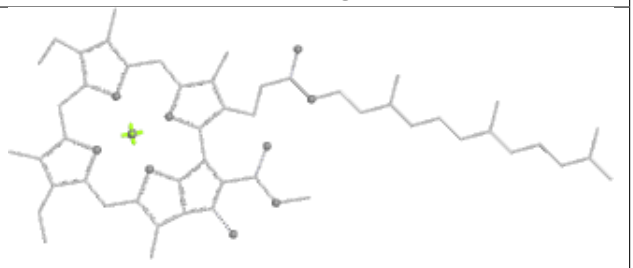


Bond angles

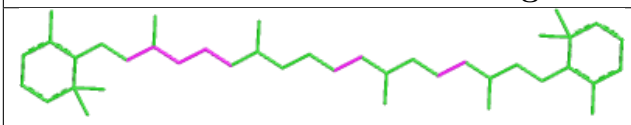


Torsions



Rings

Ligand BCR H 846



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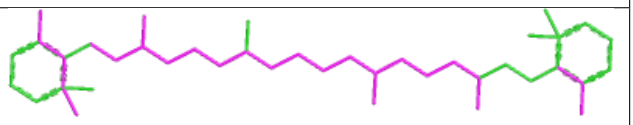
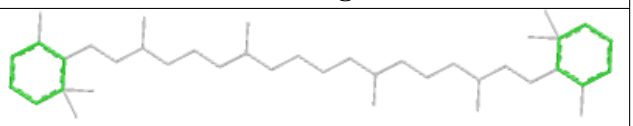


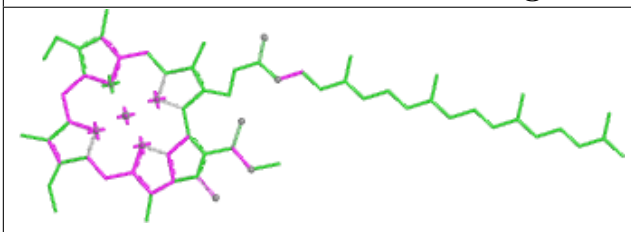
Bond angles

Torsions



Rings

Ligand CLA A 806



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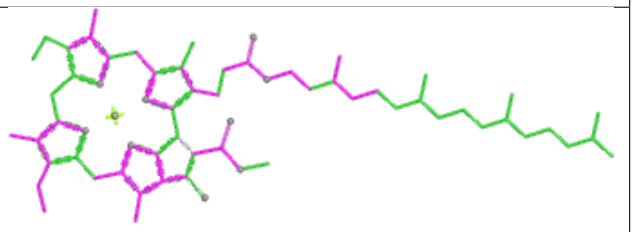
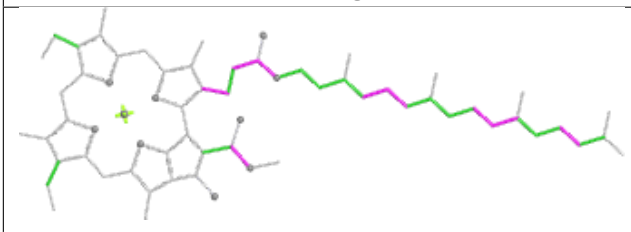
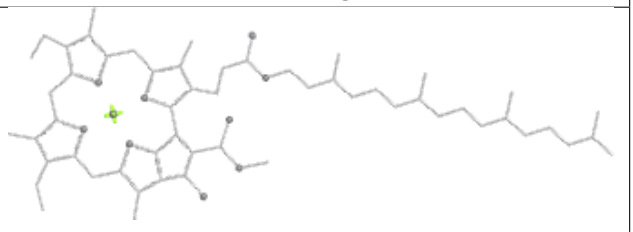


Bond angles

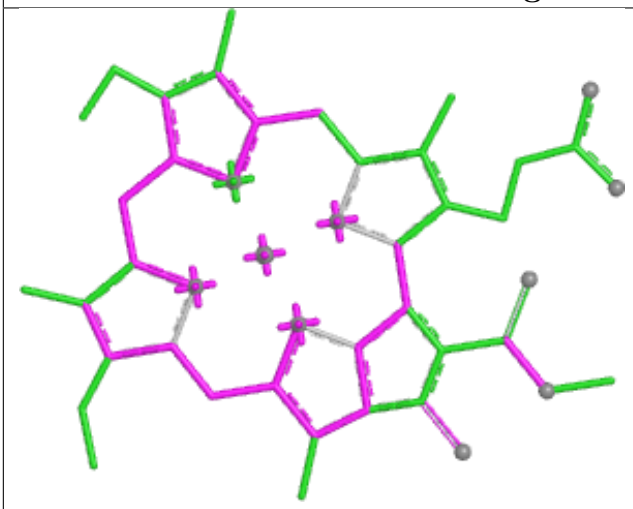


Torsions



Rings

Ligand CLA A 821



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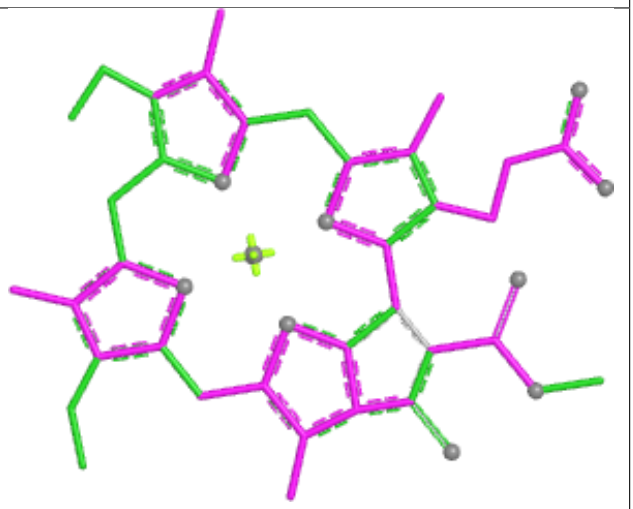

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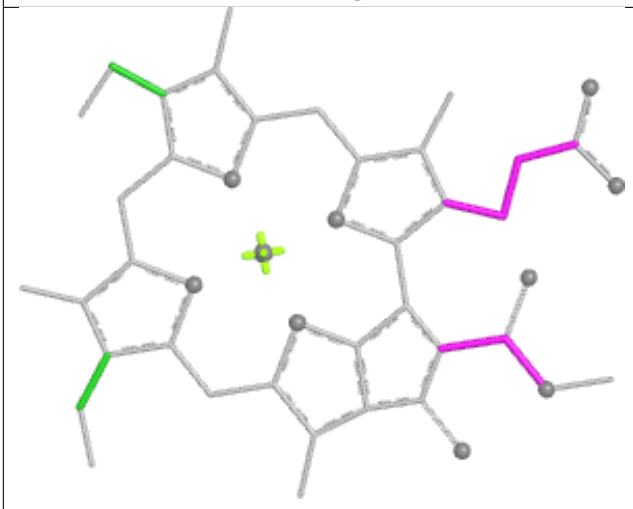
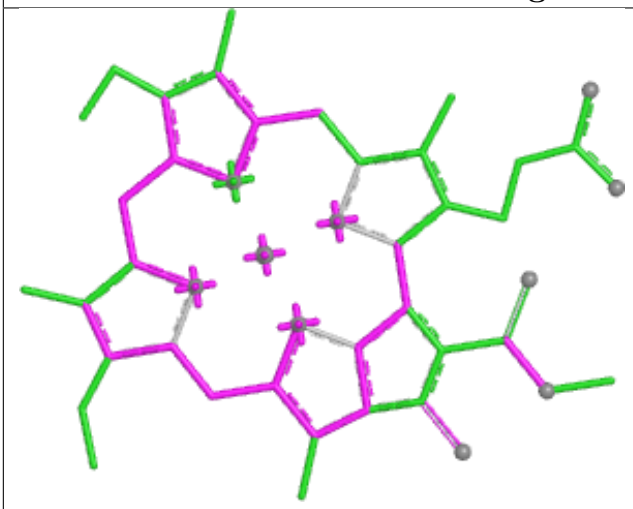


Torsions

Rings

Ligand CLA a 821



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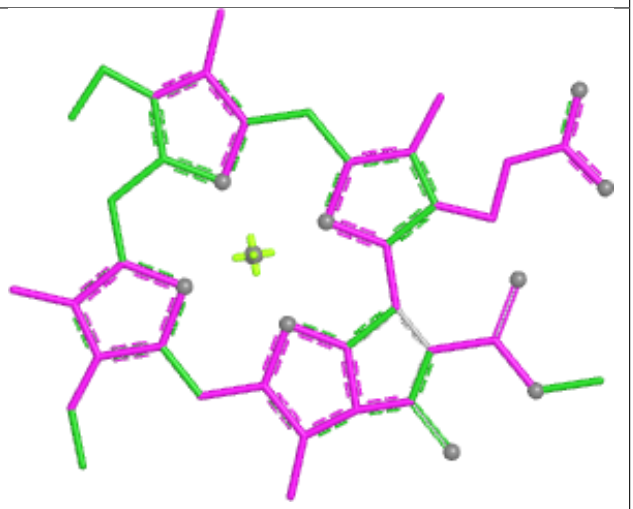

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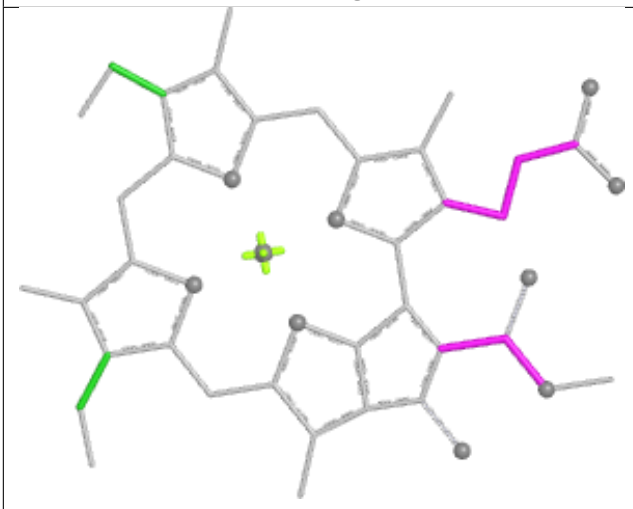
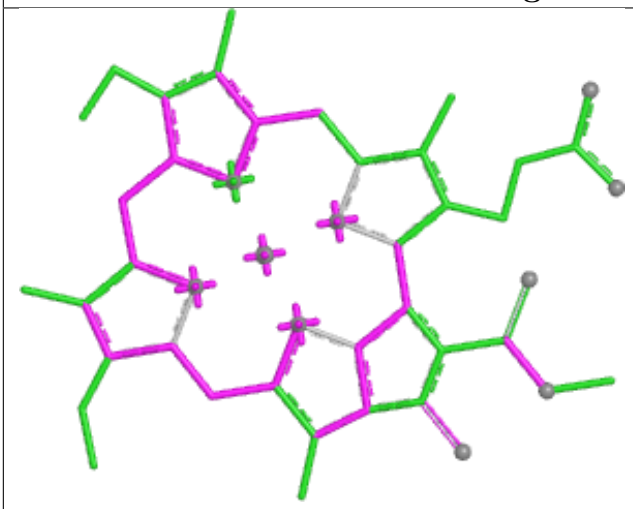


Torsions

Rings

Ligand CLA H 832



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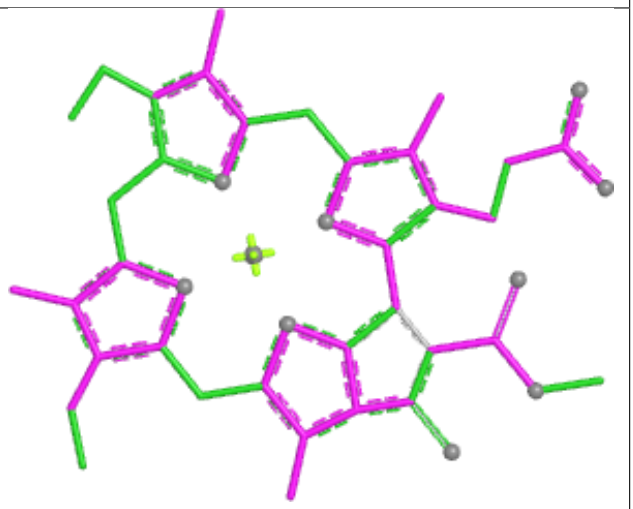
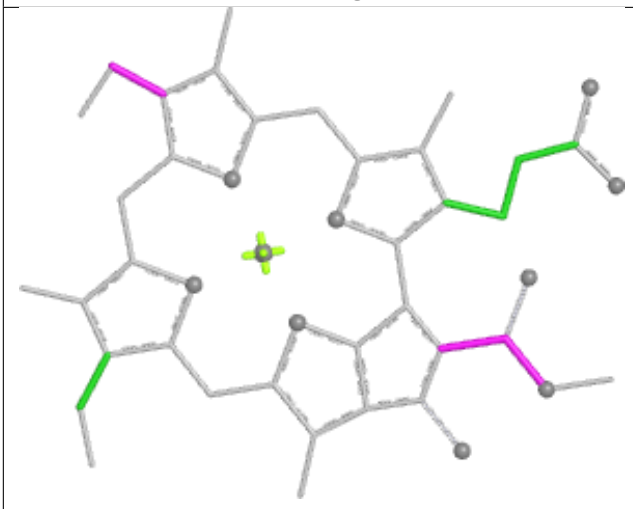


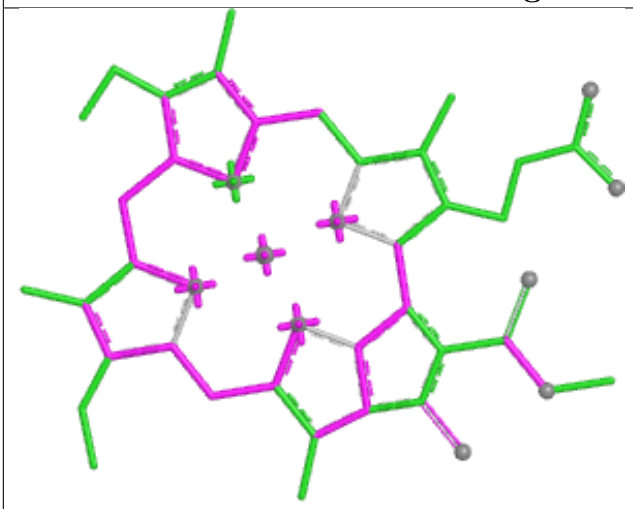
Bond angles



Torsions

Rings

Ligand CLA A 813



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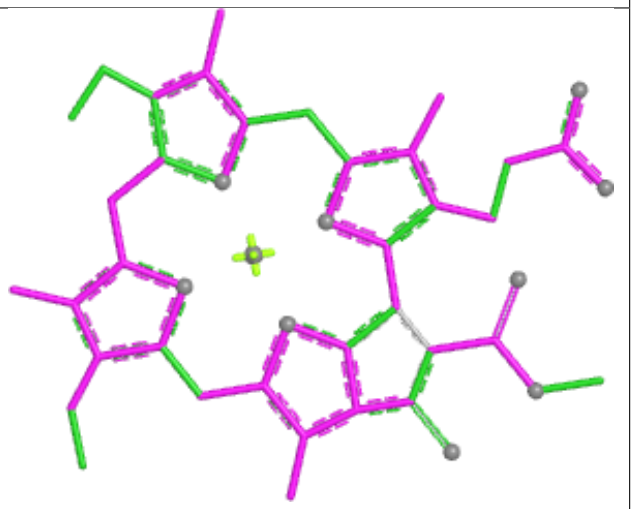
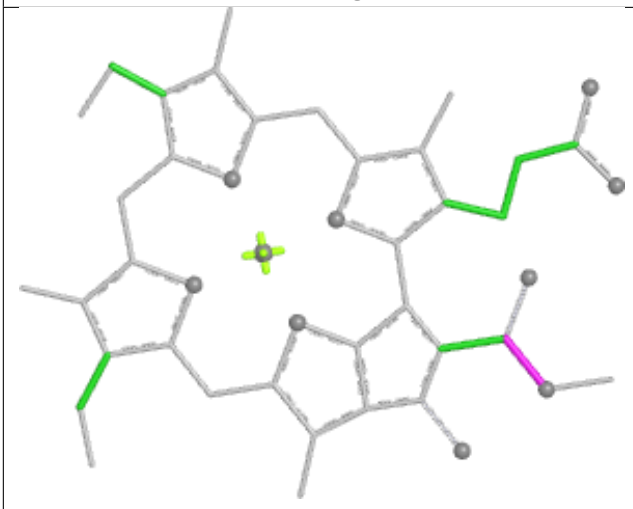


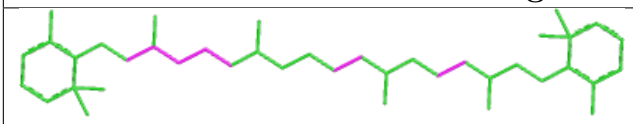
Bond angles



Torsions

Rings

Ligand BCR a 847



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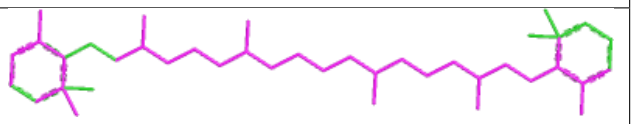
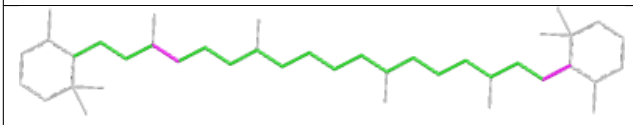
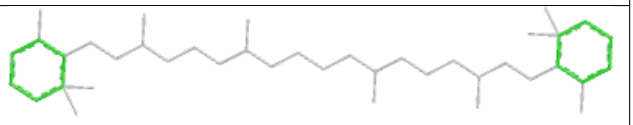


Bond angles

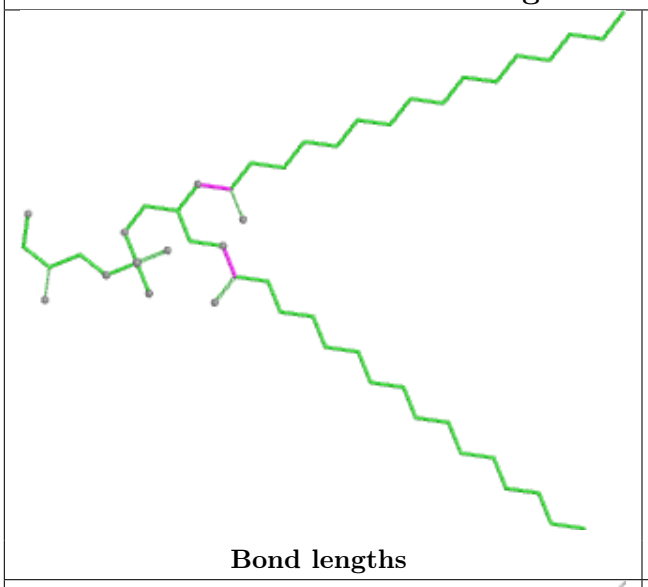


Torsions



Rings

Ligand LHG G 851



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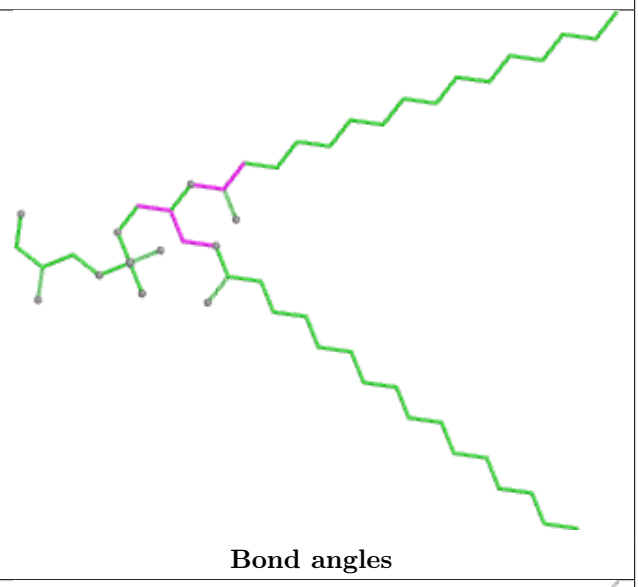
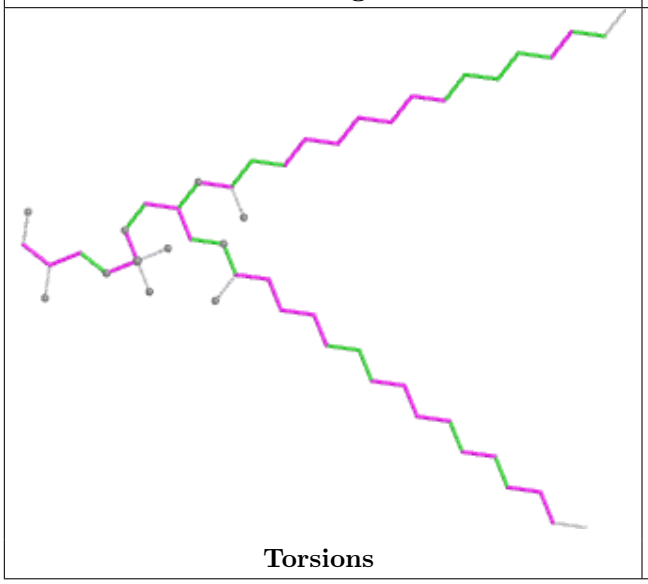


Bond angles



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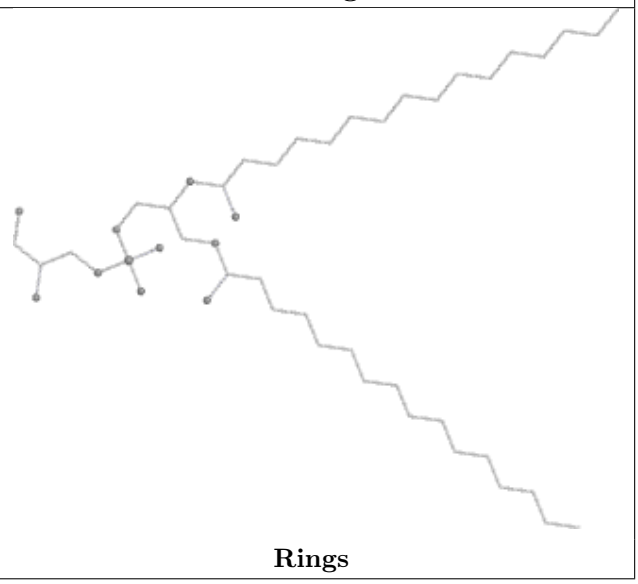
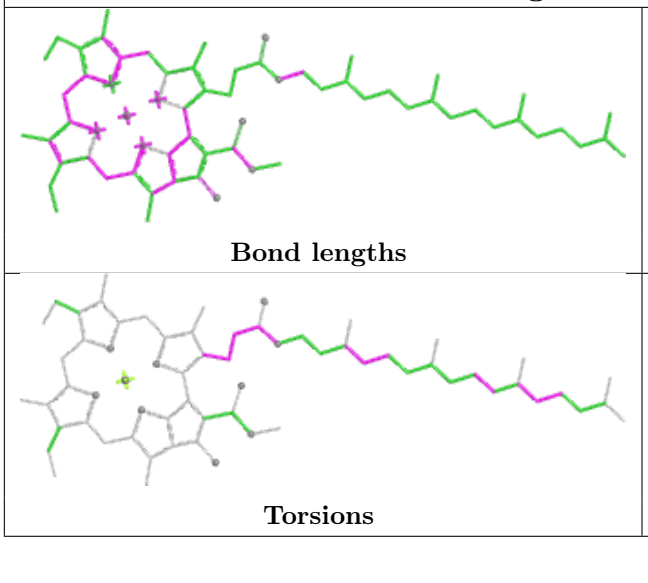


Rings

Ligand CLA L 205



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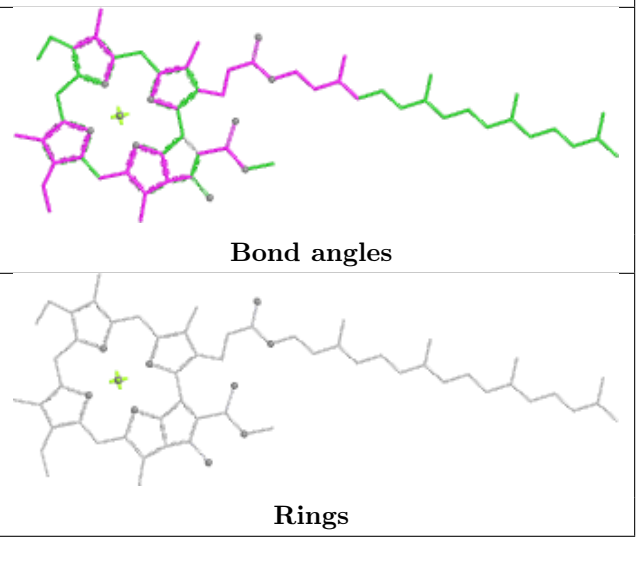
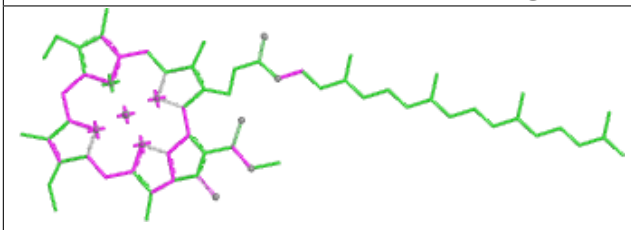
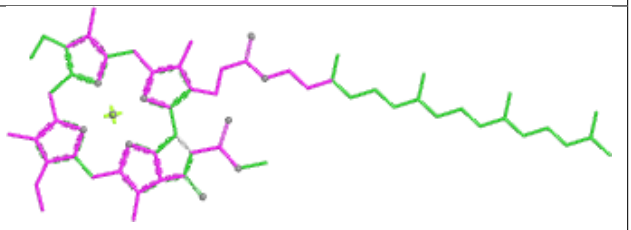
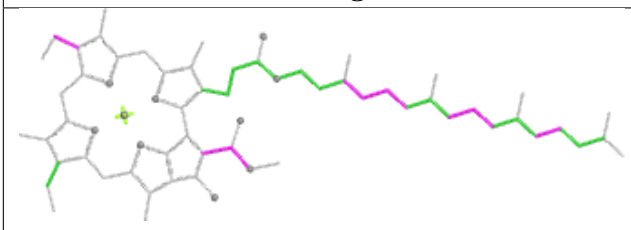
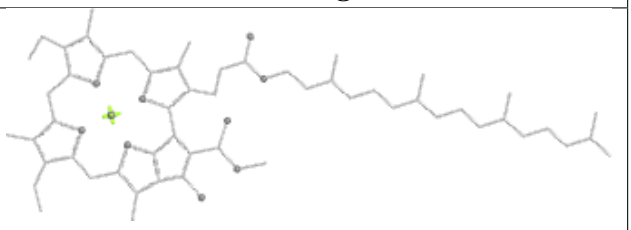
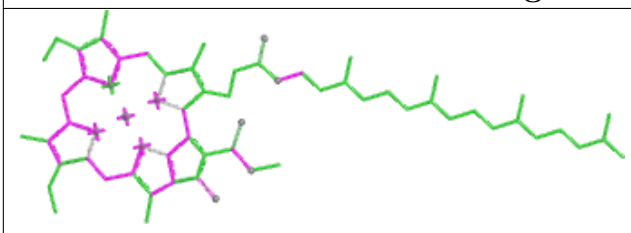
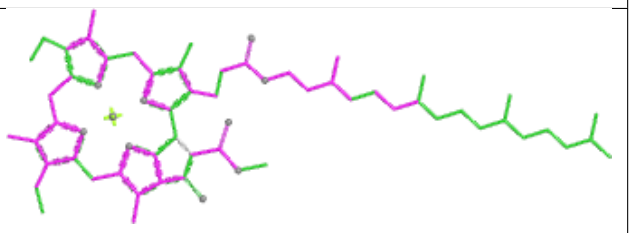
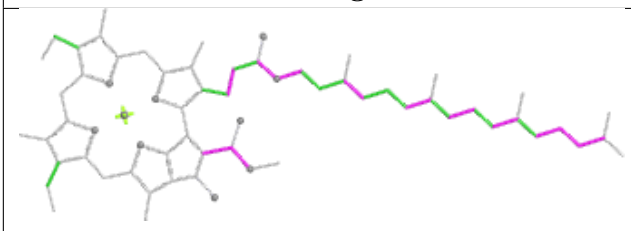
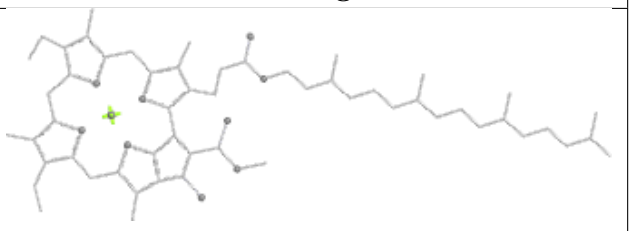


Bond angles

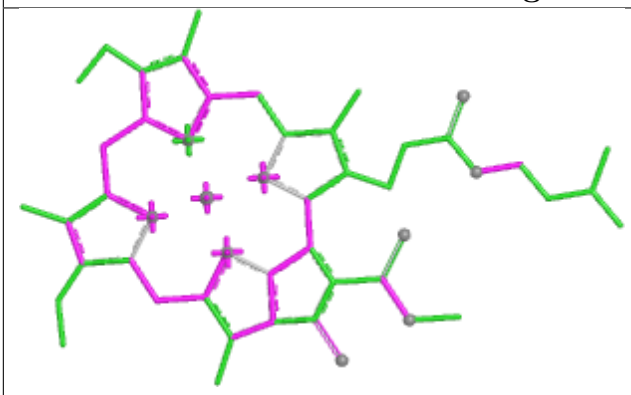
Torsions

Rings

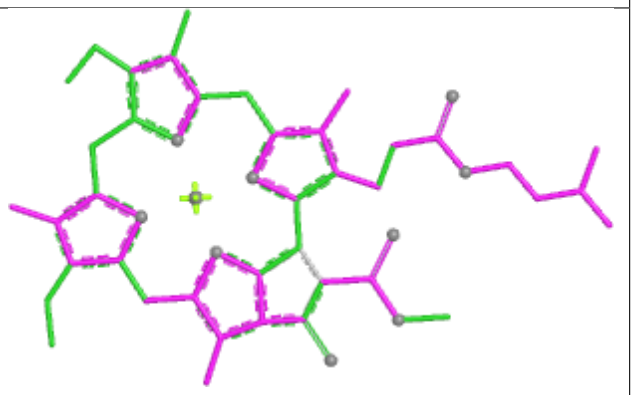
Ligand CLA B 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

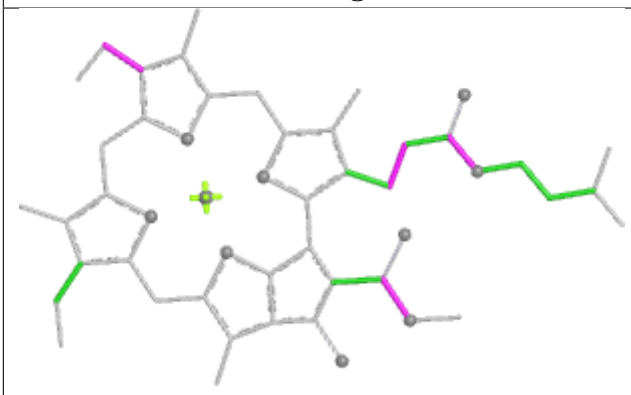
Ligand CLA G 840



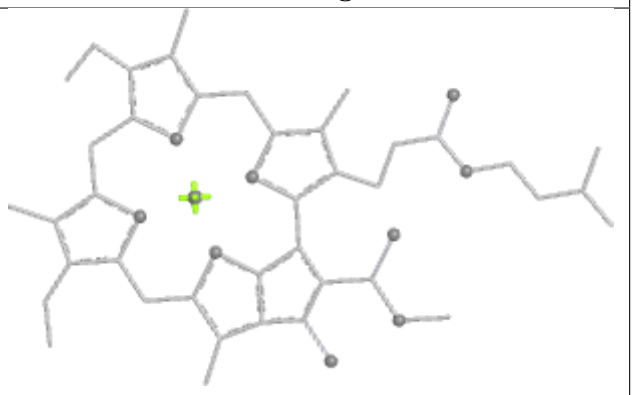
Bond lengths



Bond angles

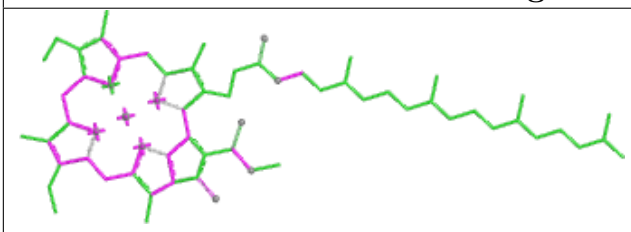


Torsions

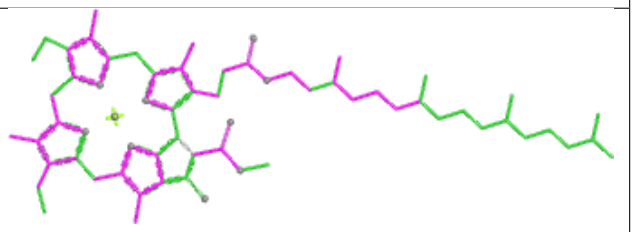


Rings

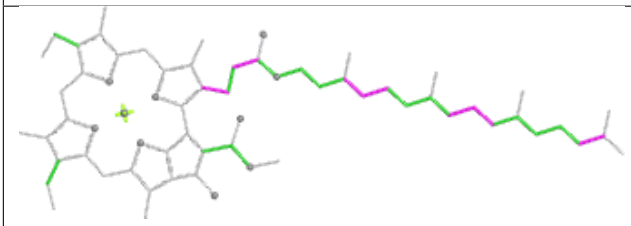
Ligand CLA b 807



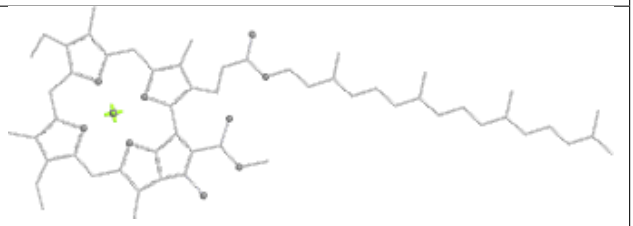
Bond lengths



Bond angles

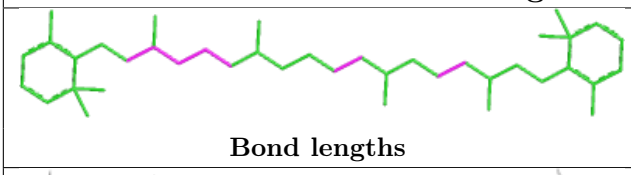


Torsions

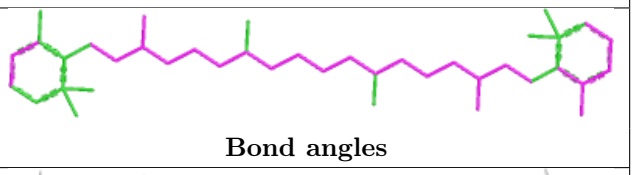


Rings

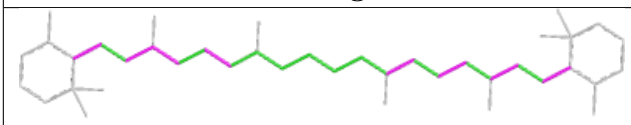
Ligand BCR a 852



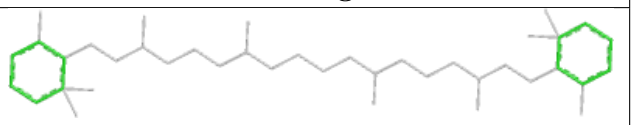
Bond lengths



Bond angles

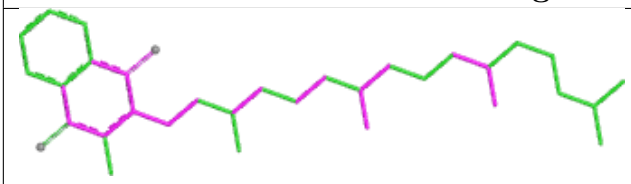


Torsions



Rings

Ligand 1L3 A 842



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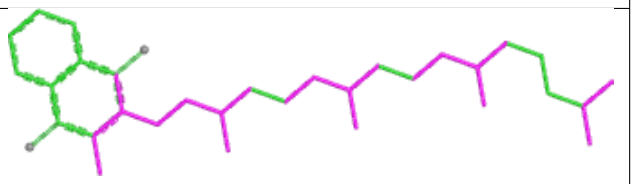
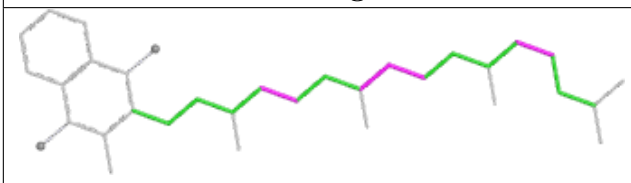
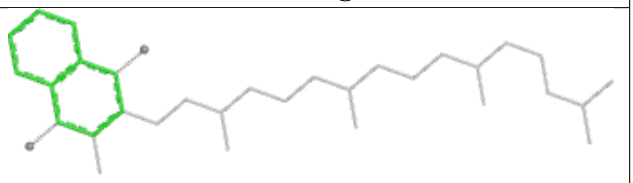


Bond angles

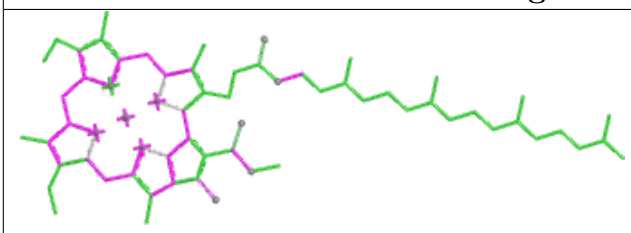


Torsions

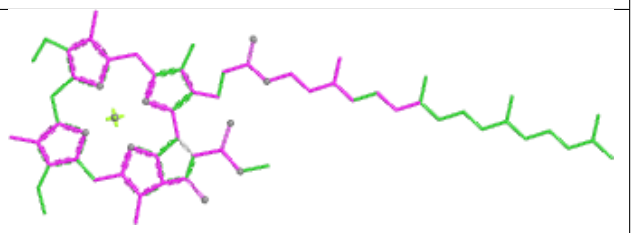


Rings

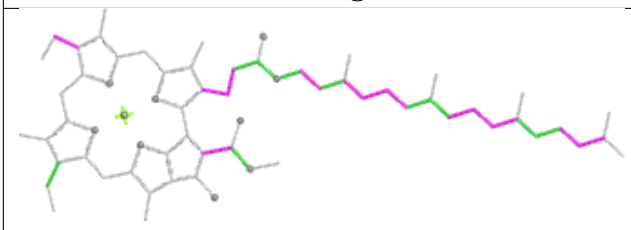
Ligand CLA a 854



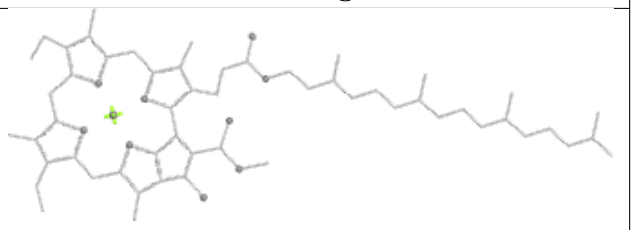
Bond lengths



Bond angles

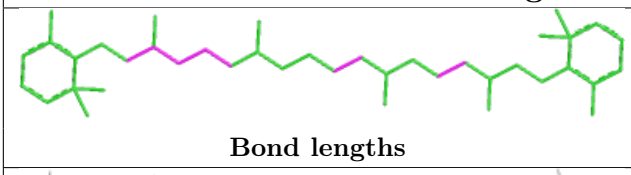


Torsions

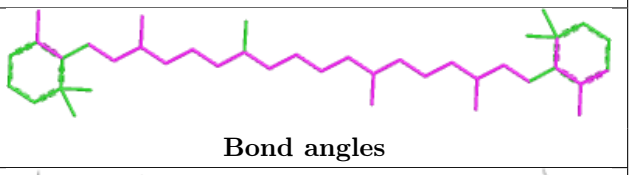


Rings

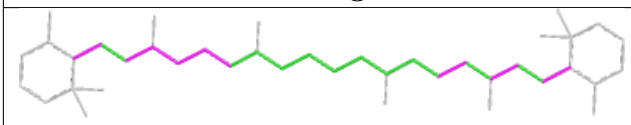
Ligand BCR b 839



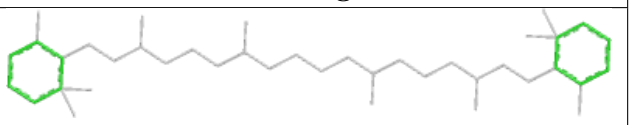
Bond lengths



Bond angles

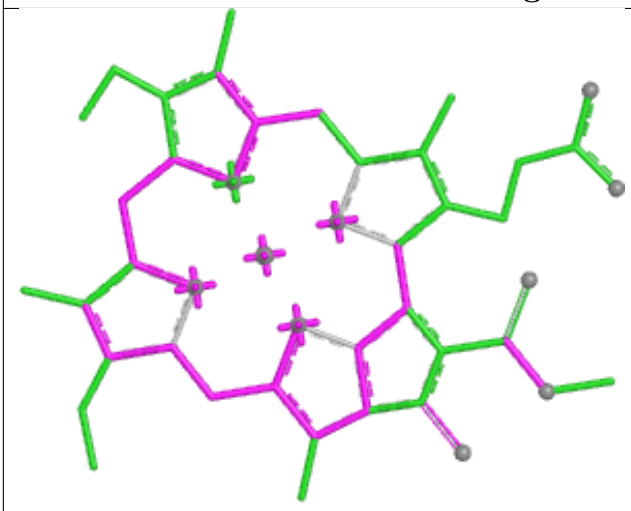


Torsions

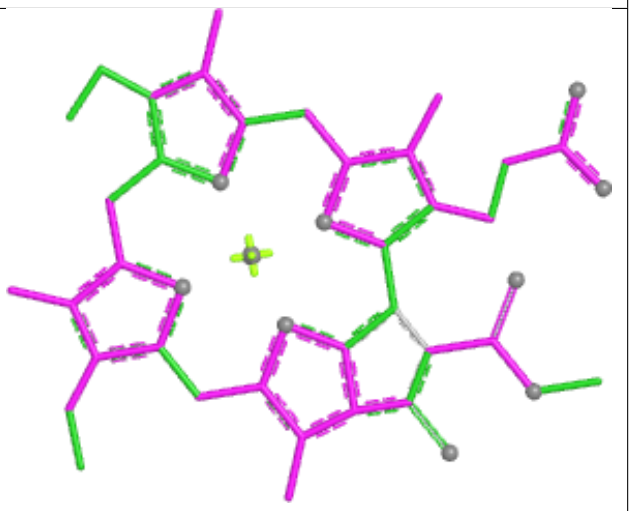


Rings

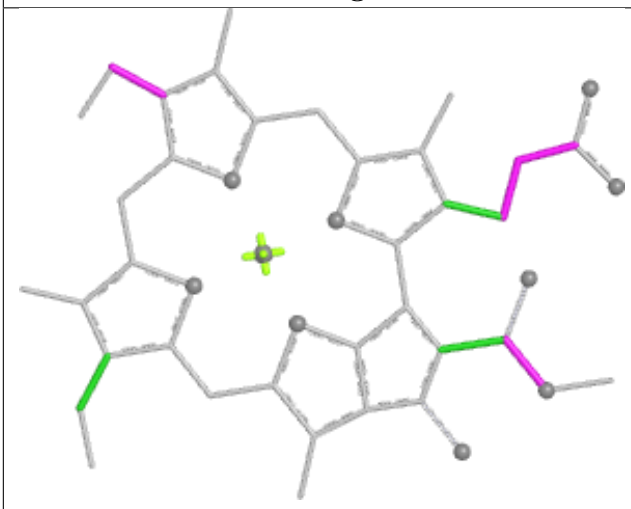
Ligand CLA H 820



Bond lengths



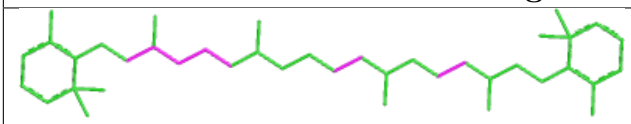
Bond angles



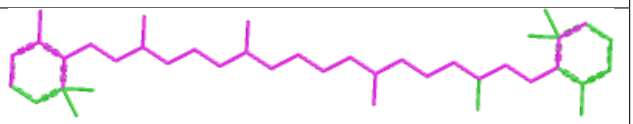
Torsions

Rings

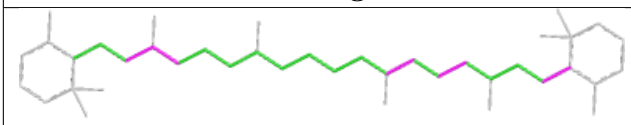
Ligand BCR b 843



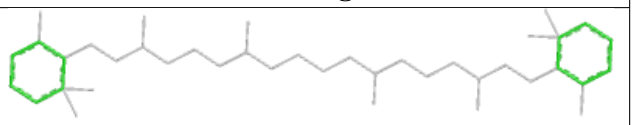
Bond lengths



Bond angles

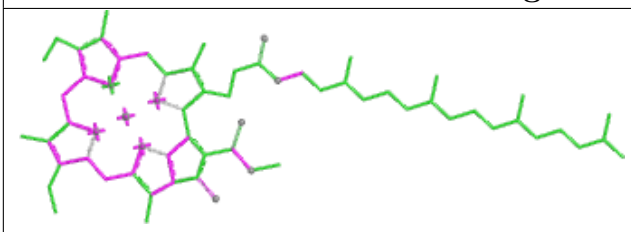


Torsions

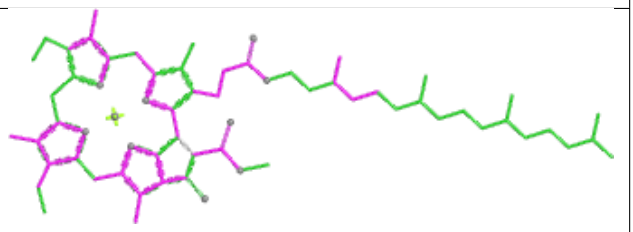


Rings

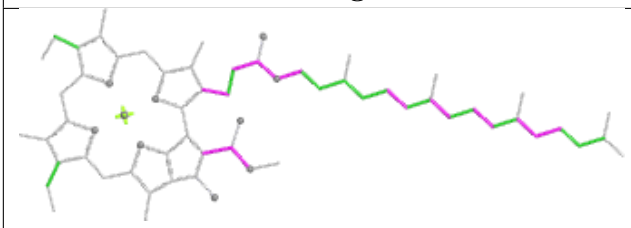
Ligand CLA H 803



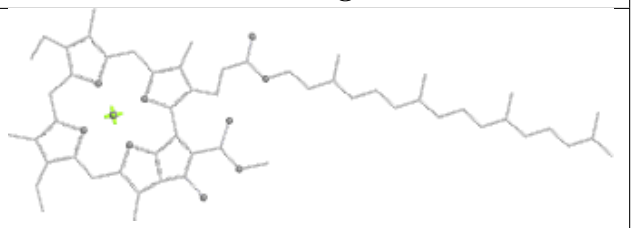
Bond lengths



Bond angles

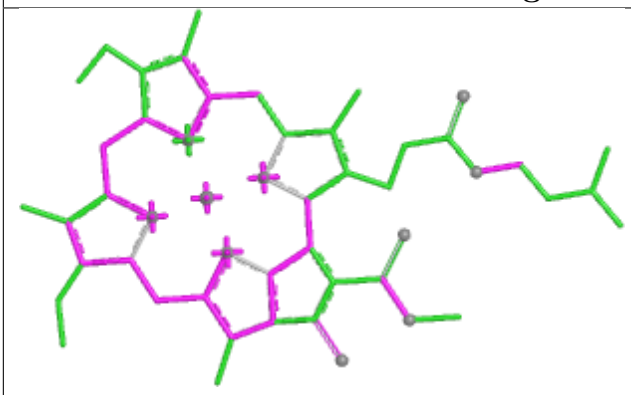


Torsions

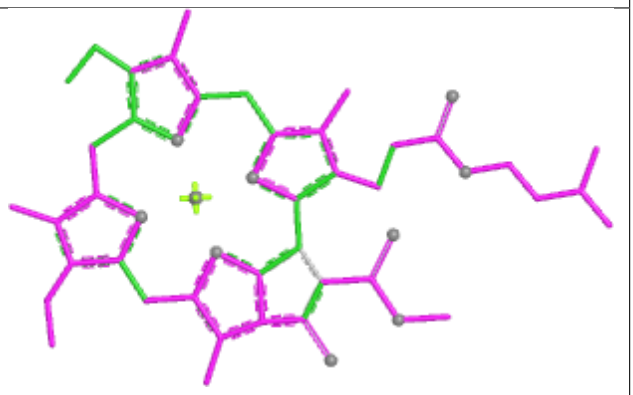


Rings

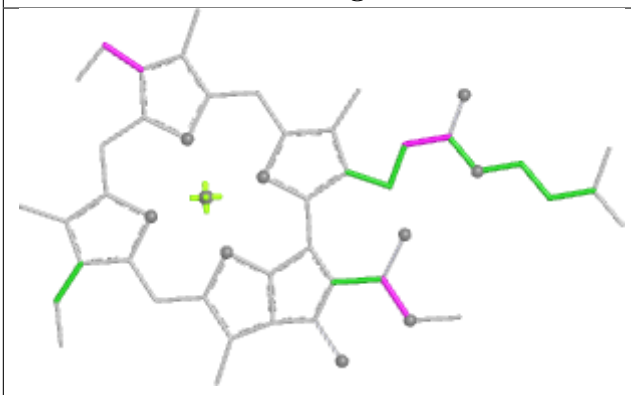
Ligand CLA G 817



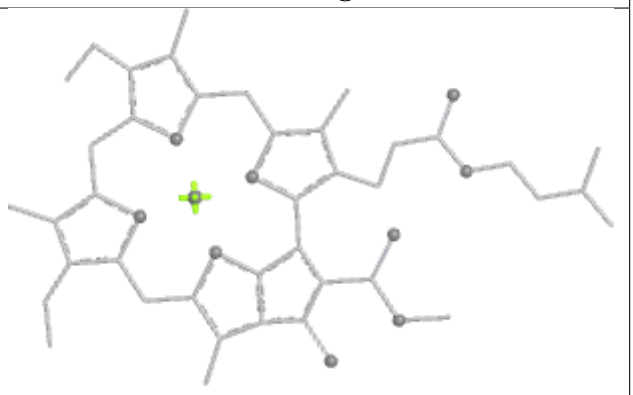
Bond lengths



Bond angles

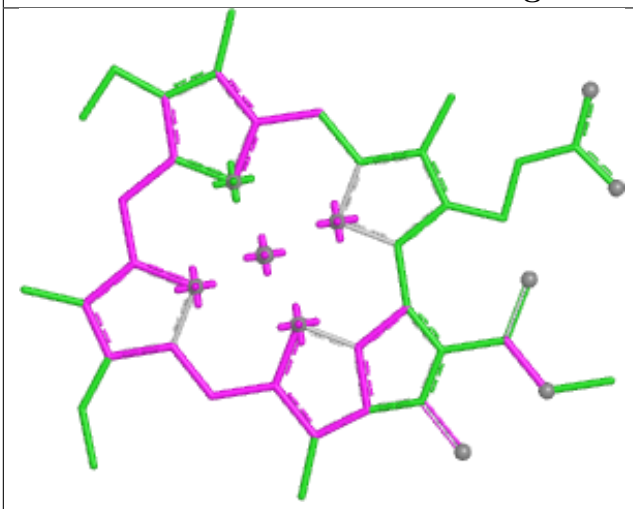


Torsions

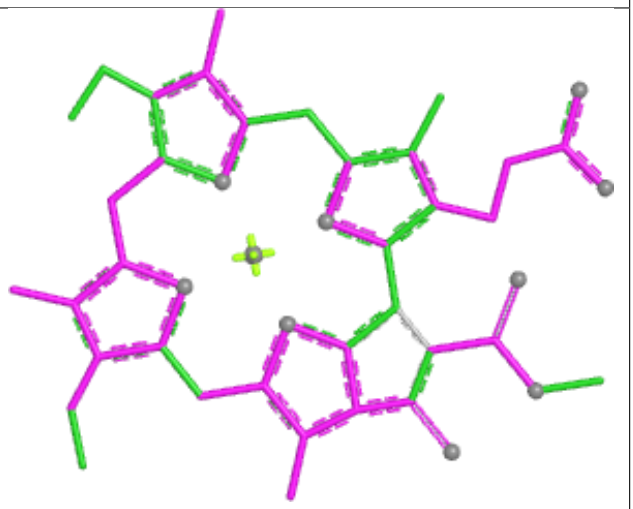


Rings

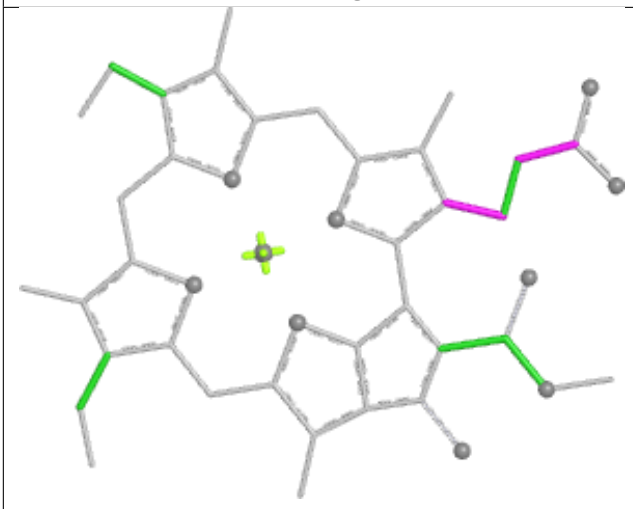
Ligand CLA A 838



Bond lengths



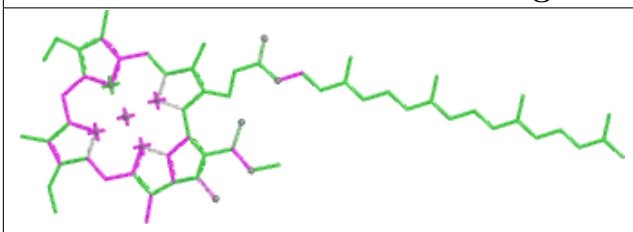
Bond angles



Torsions

Rings

Ligand CL0 a 801



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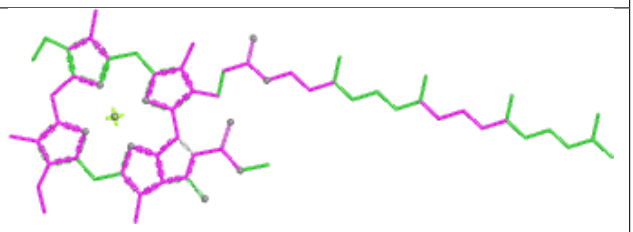
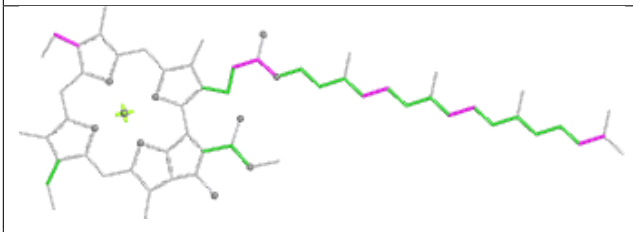
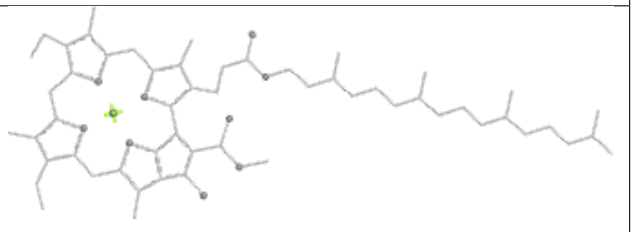


Bond angles

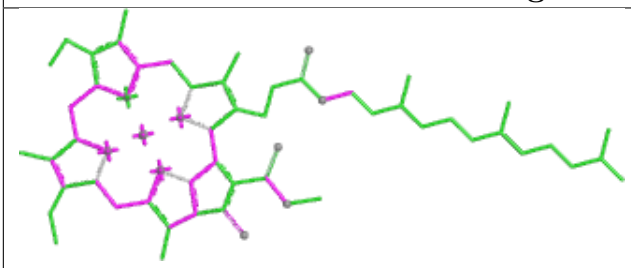


Torsions

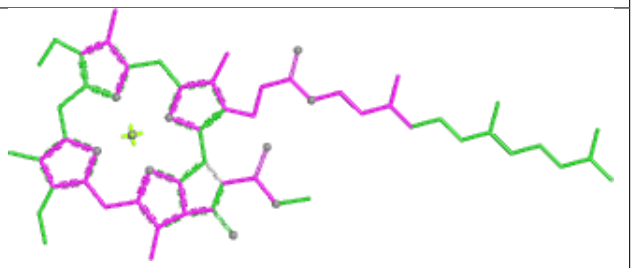


Rings

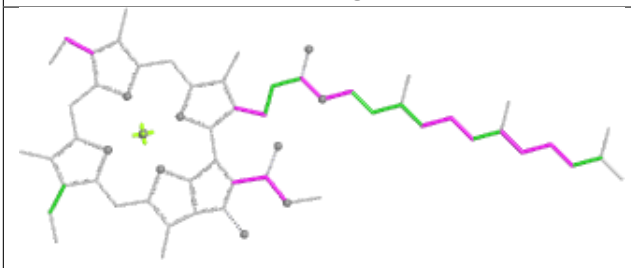
Ligand CLA b 848



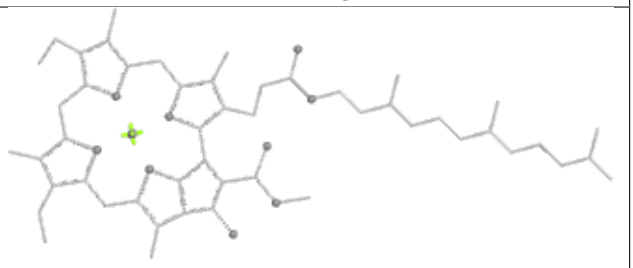
Bond lengths



Bond angles

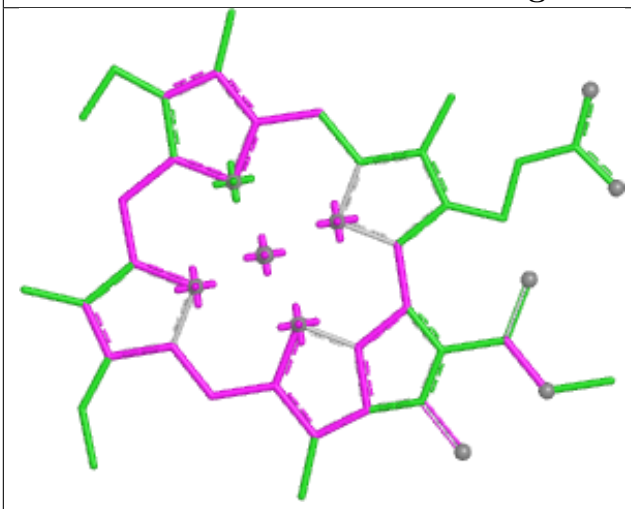


Torsions

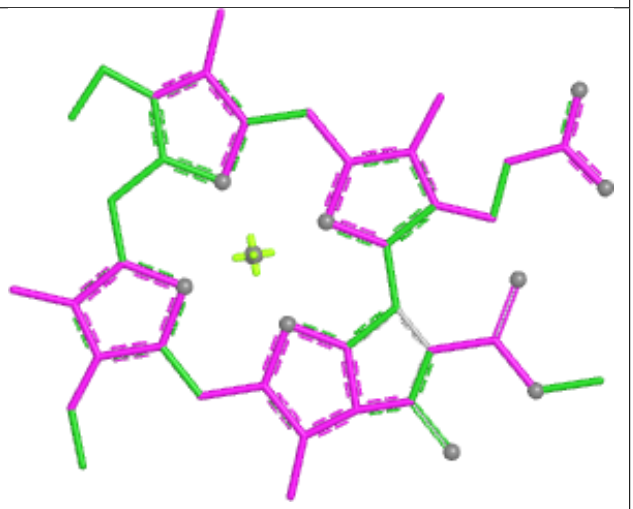


Rings

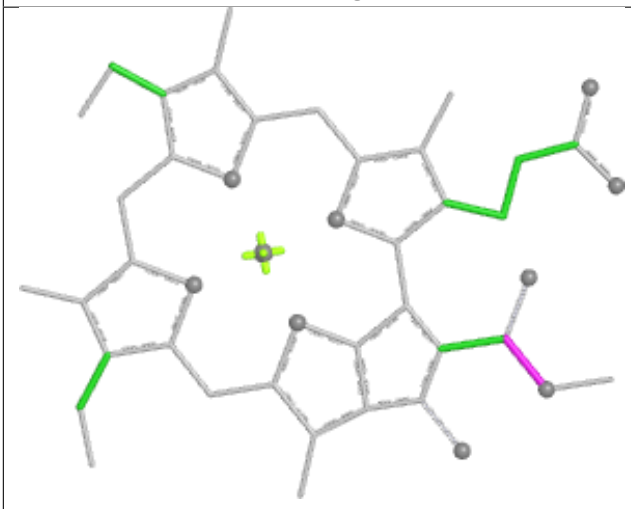
Ligand CLA a 813



Bond lengths



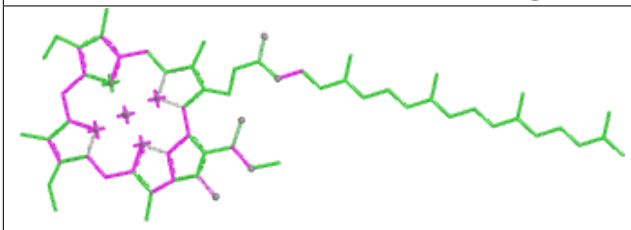
Bond angles



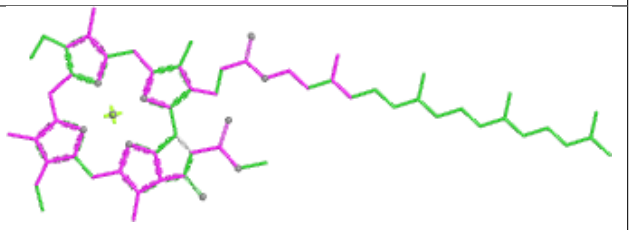
Torsions

Rings

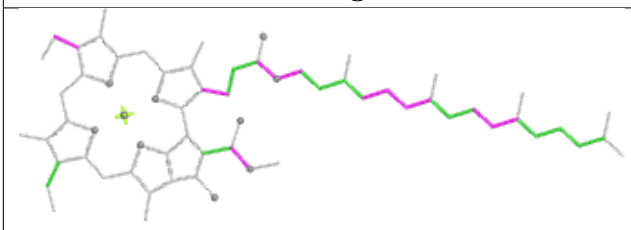
Ligand CLA L 202



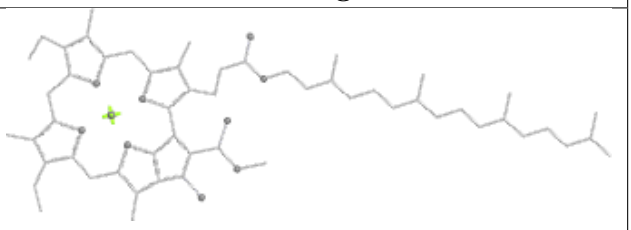
Bond lengths



Bond angles

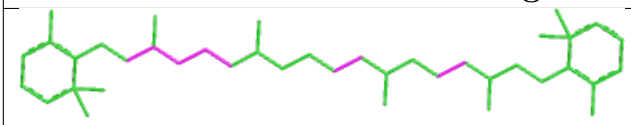


Torsions



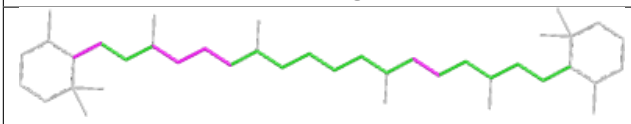
Rings

Ligand BCR B 845

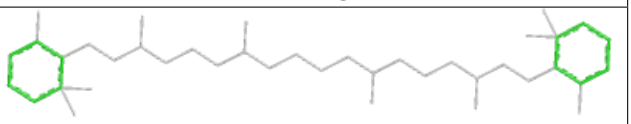


Bond lengths

Bond angles

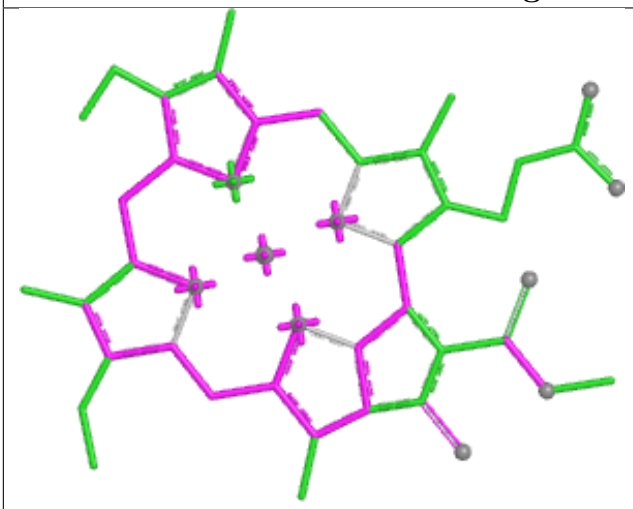


Torsions

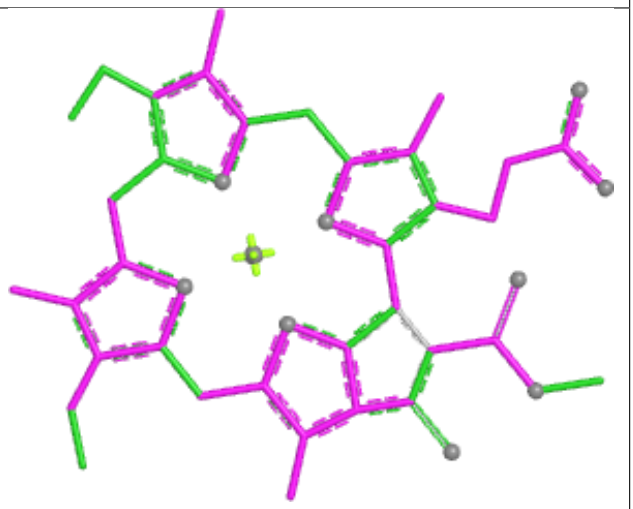


Rings

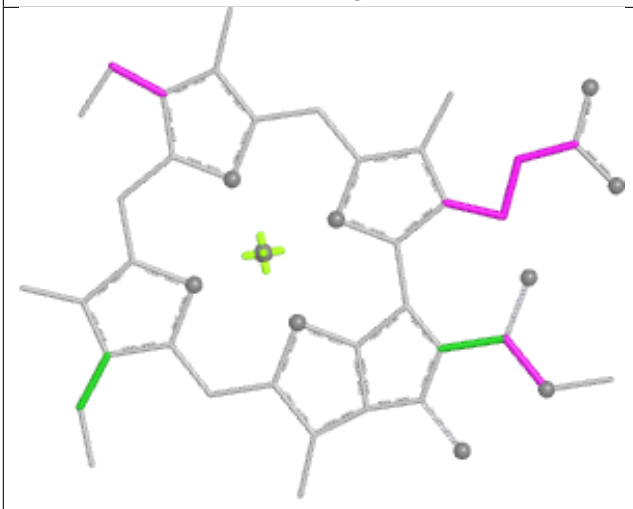
Ligand CLA G 835



Bond lengths



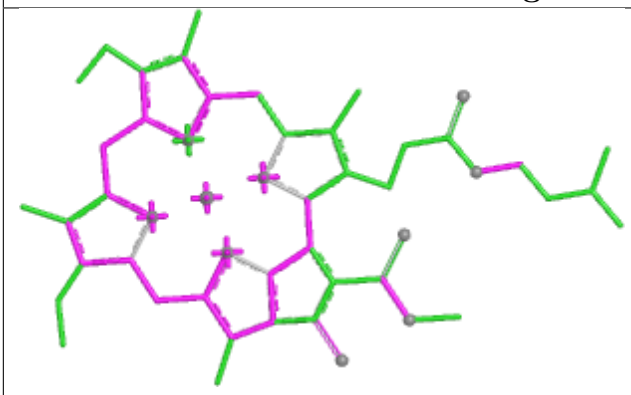
Bond angles



Torsions

Rings

Ligand CLA G 823



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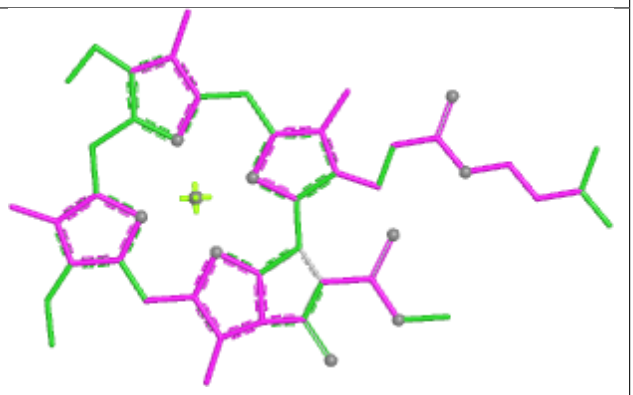
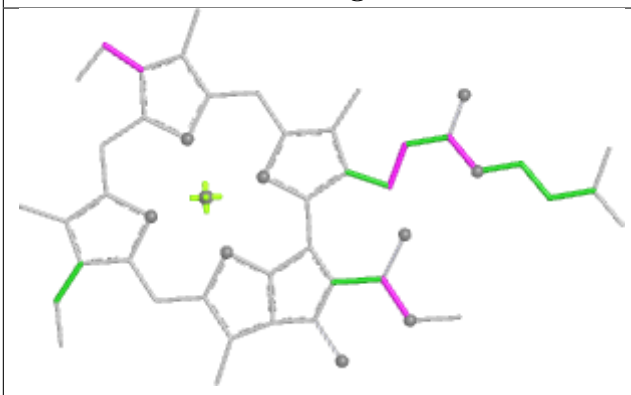
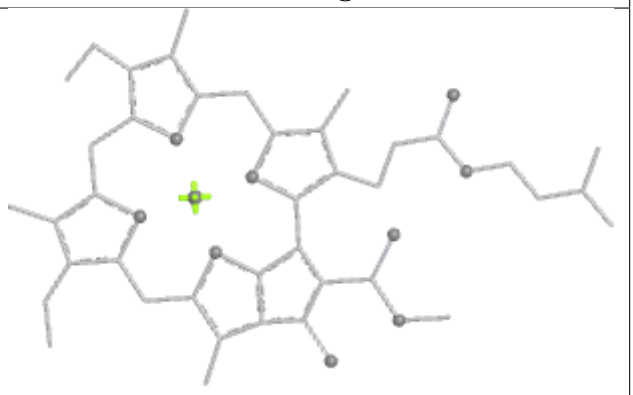


Bond angles

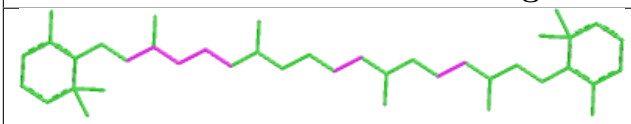


Torsions



Rings

Ligand BCR A 852



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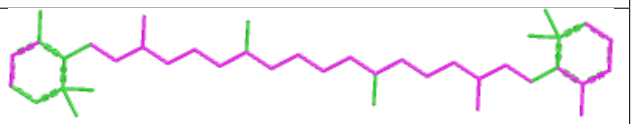

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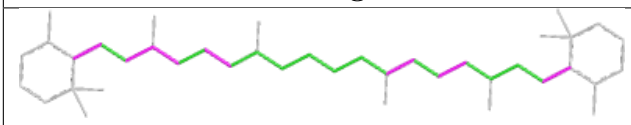

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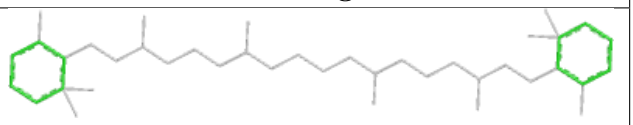
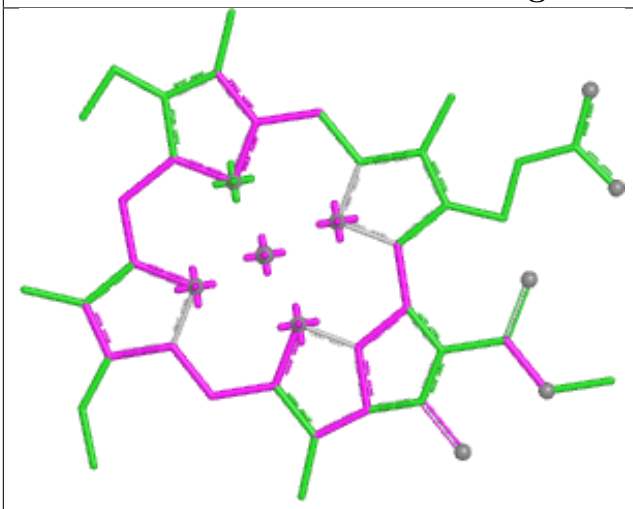
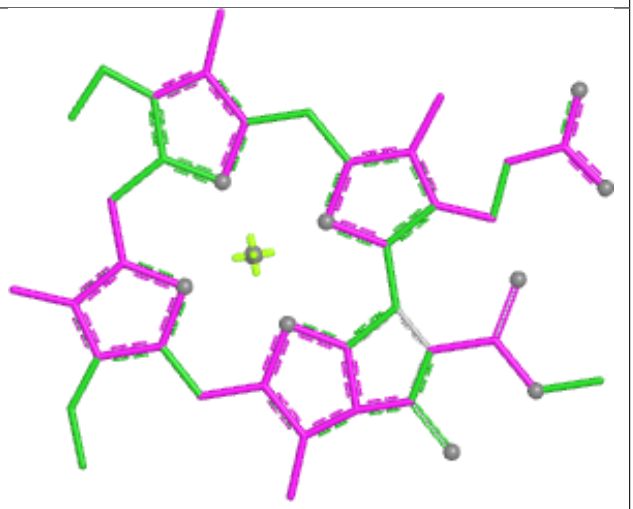


Rings

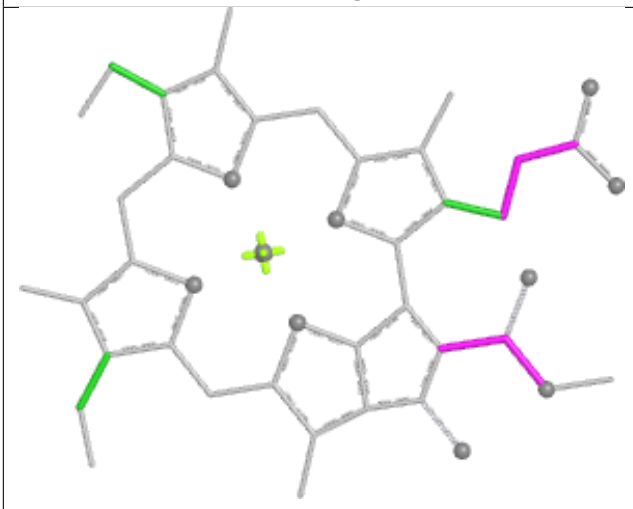
Ligand CLA a 814



Bond lengths



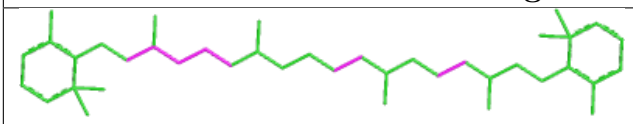
Bond angles



Torsions

Rings

Ligand BCR F 202



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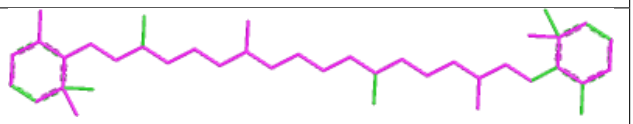
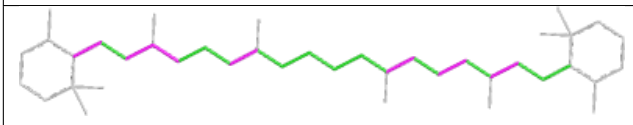


Bond angles



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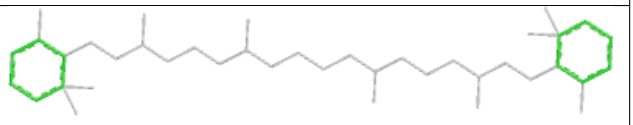
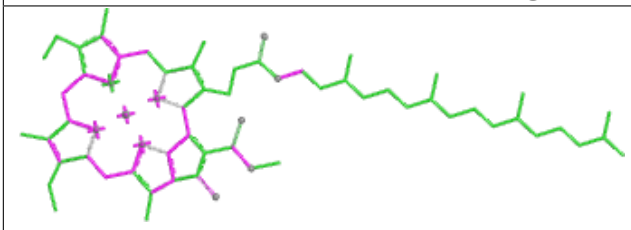


Rings

Ligand CLA B 823



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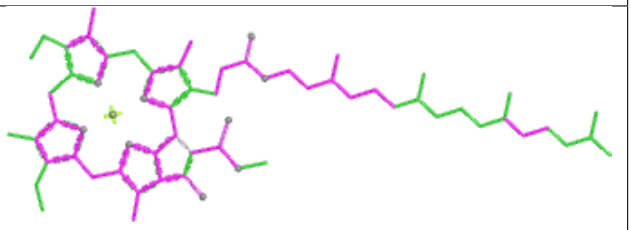
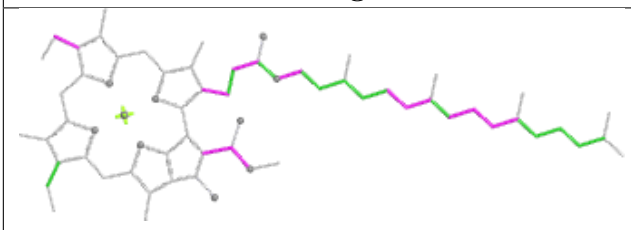


Bond angles



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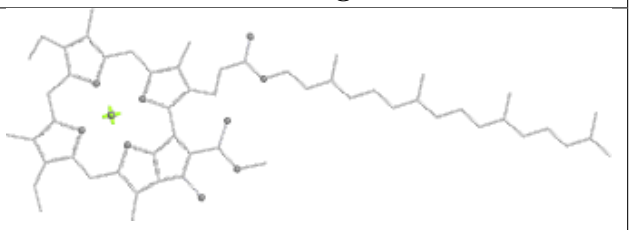
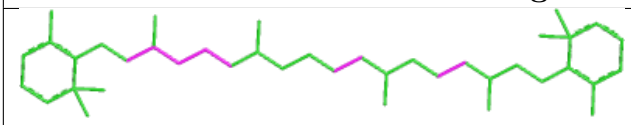


Rings

Ligand BCR l 201



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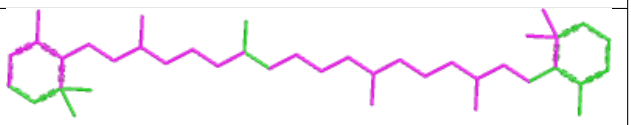
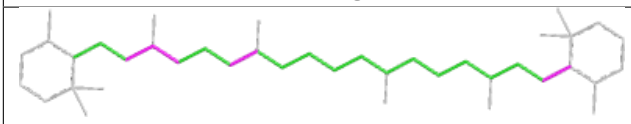


Bond angles



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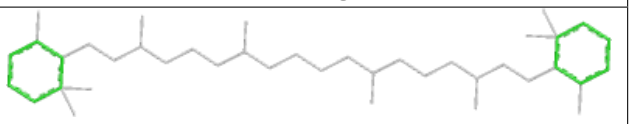
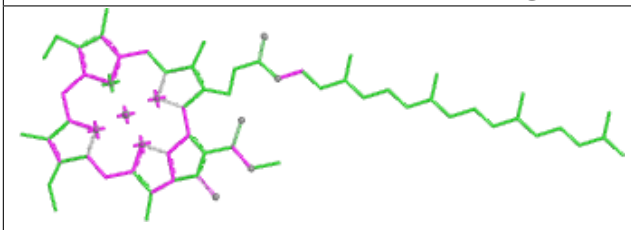


Rings

Ligand CLA H 835



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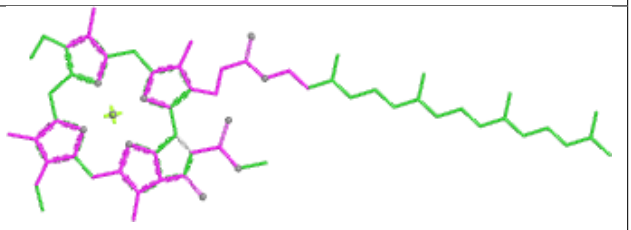
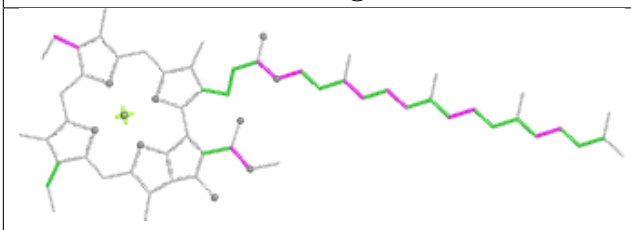


Bond angles



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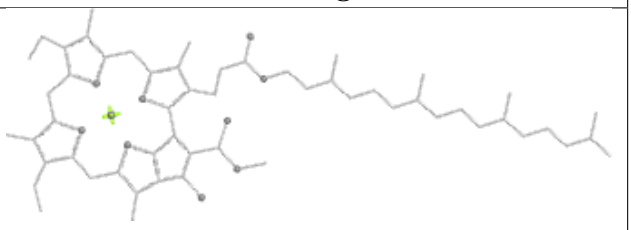
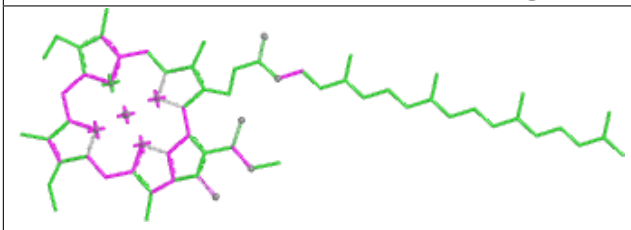


Rings

Ligand CLA H 824



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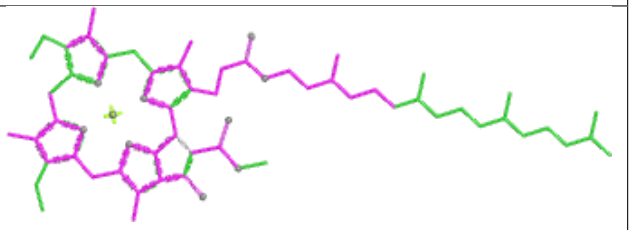
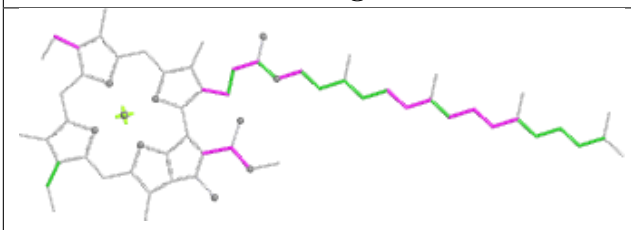


Bond angles



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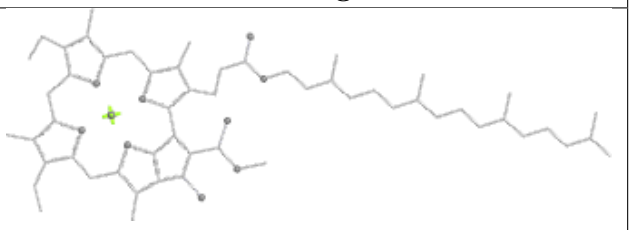
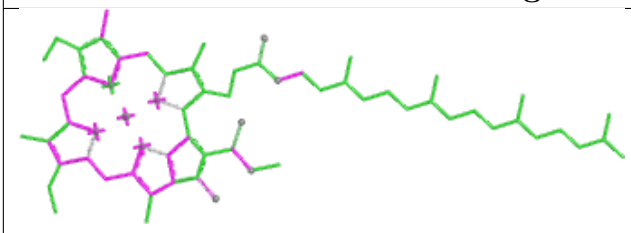


Rings

Ligand CLA H 827



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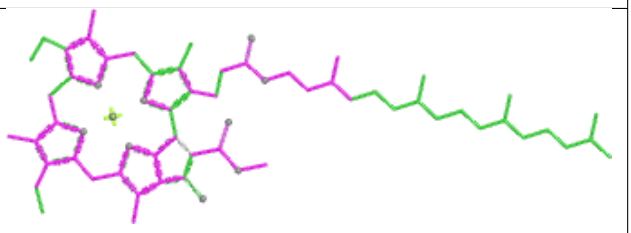
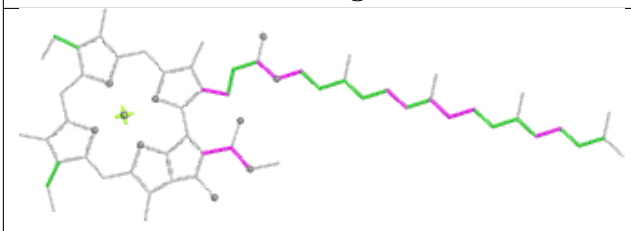


Bond angles



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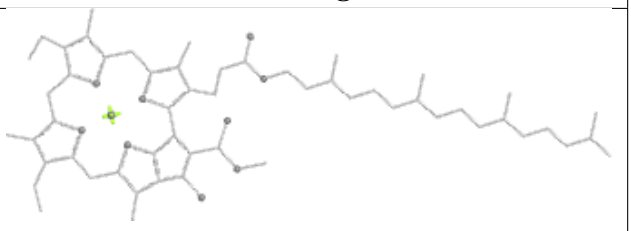
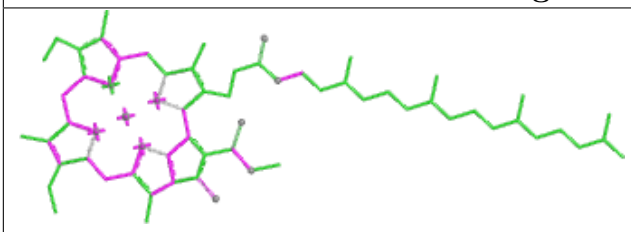


Rings

Ligand CLA l 205



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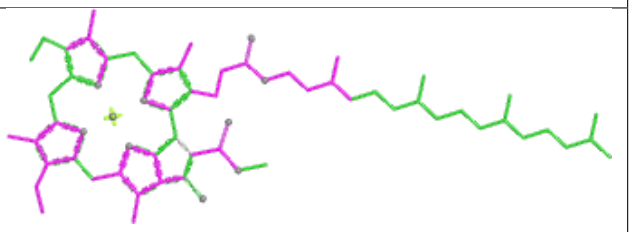
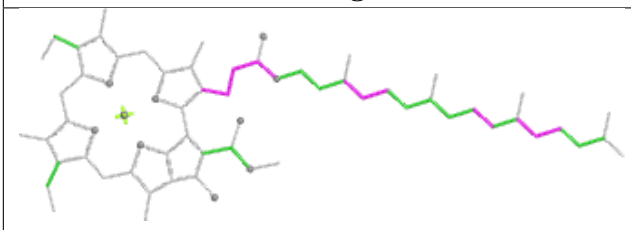
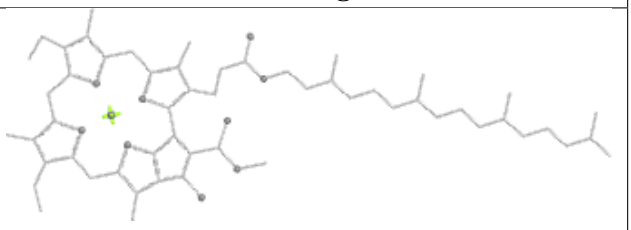


Bond angles

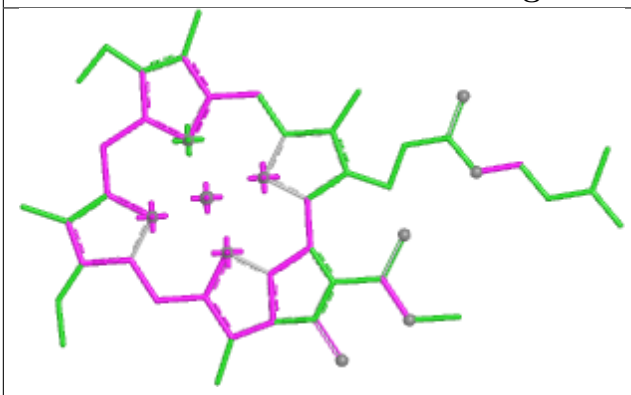


Torsions



Rings

Ligand CLA G 811



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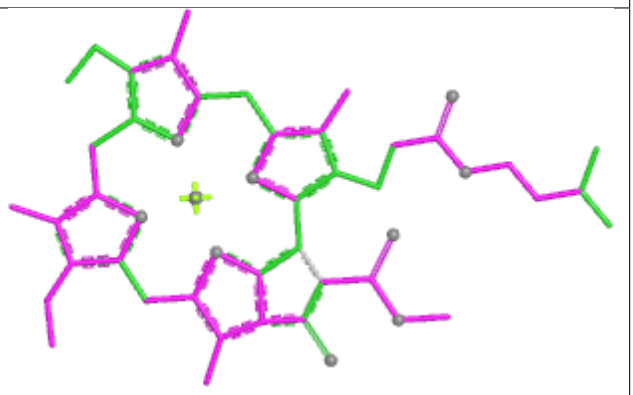
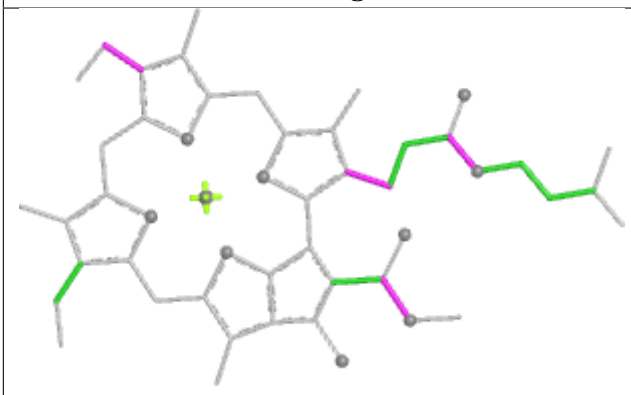
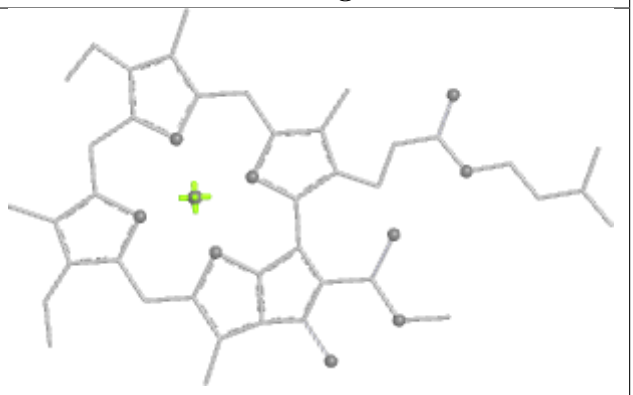


Bond angles

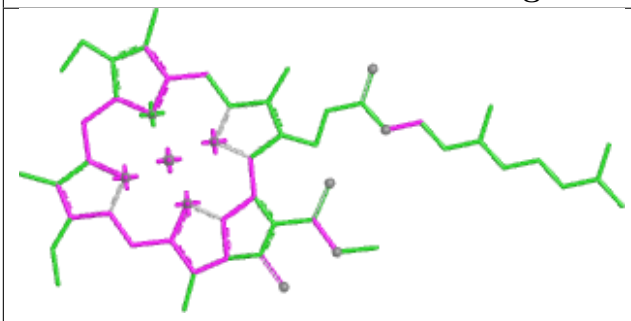


Torsions



Rings

Ligand CLA G 824



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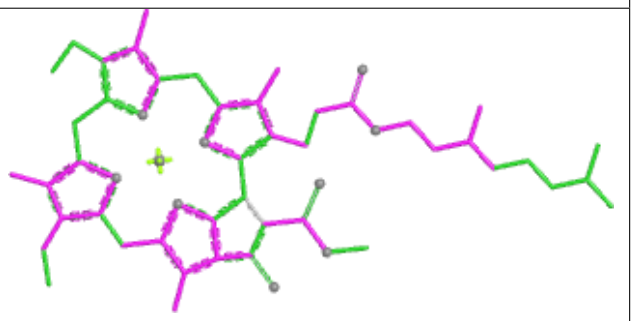
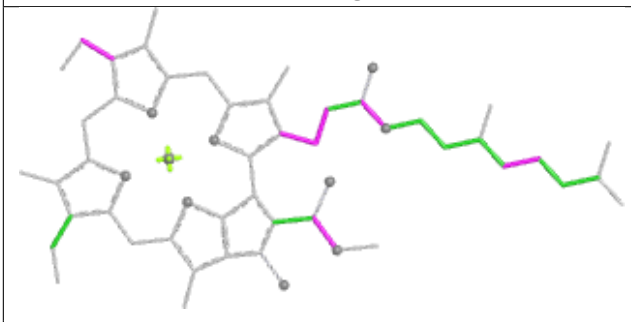
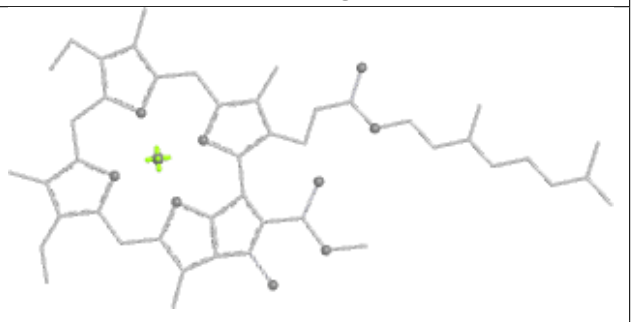


Bond angles

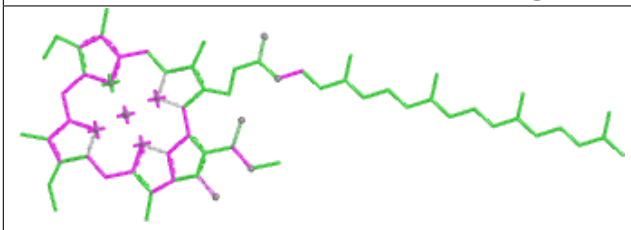


Torsions



Rings

Ligand CLA a 824



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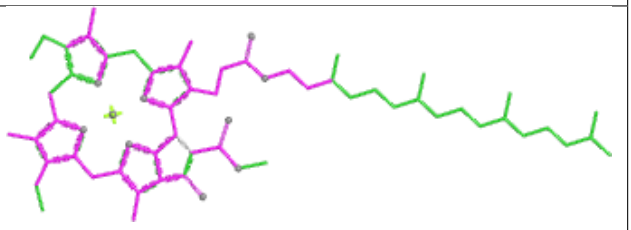
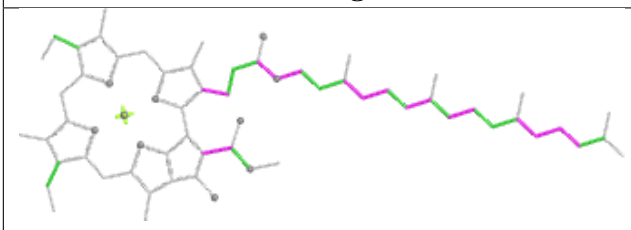
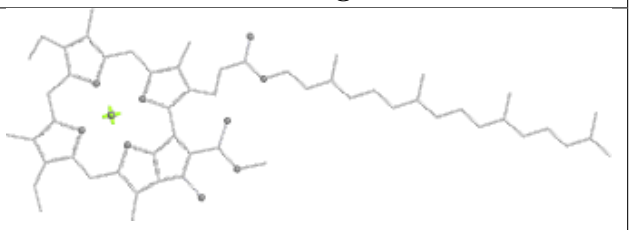


Bond angles

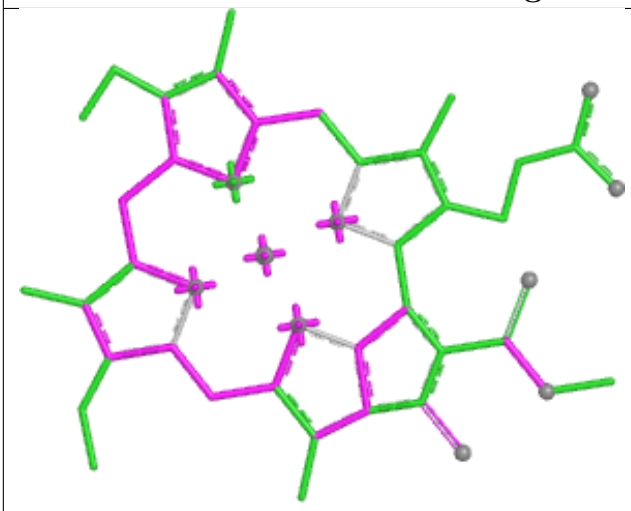


Torsions

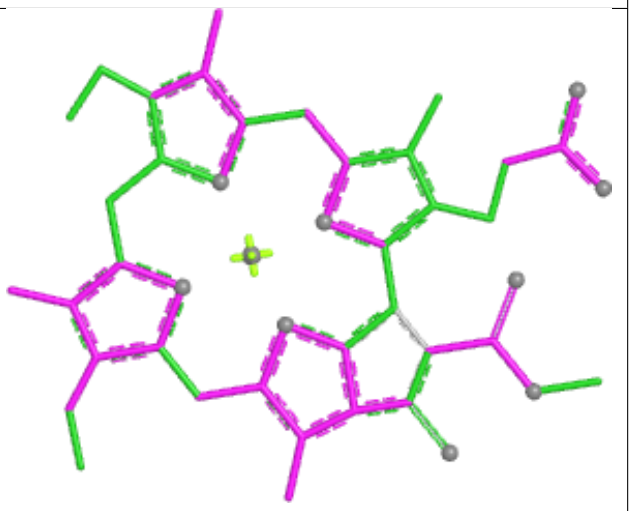


Rings

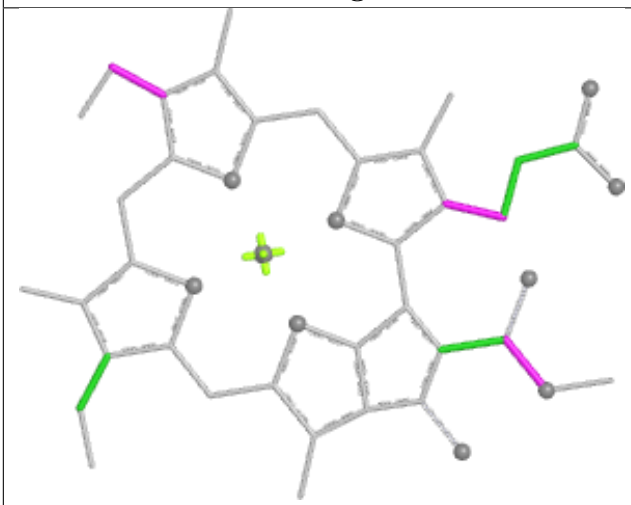
Ligand CLA B 827



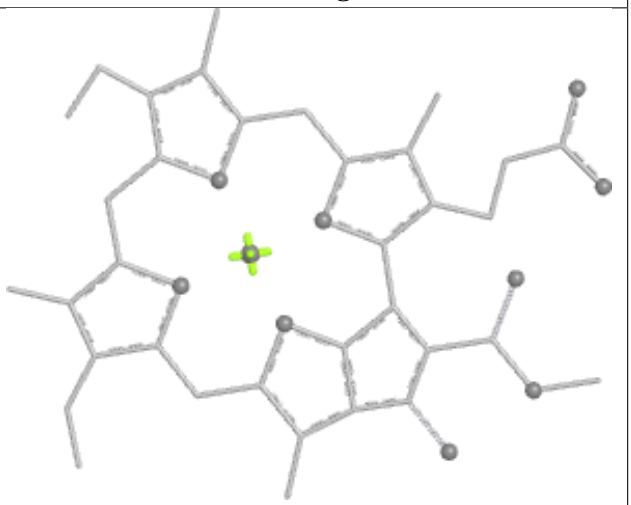
Bond lengths



Bond angles

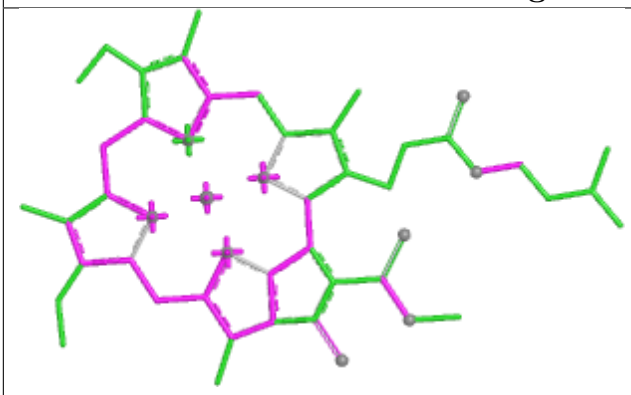


Torsions

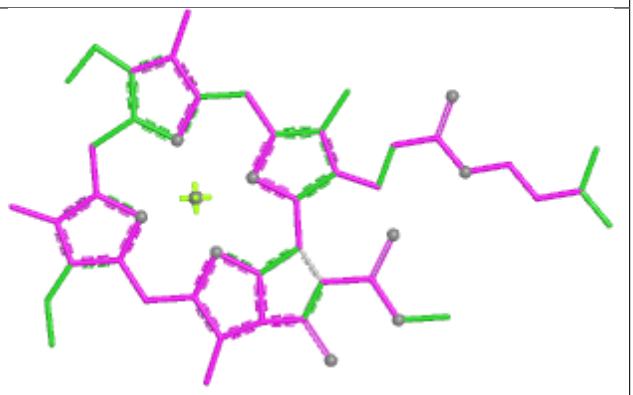


Rings

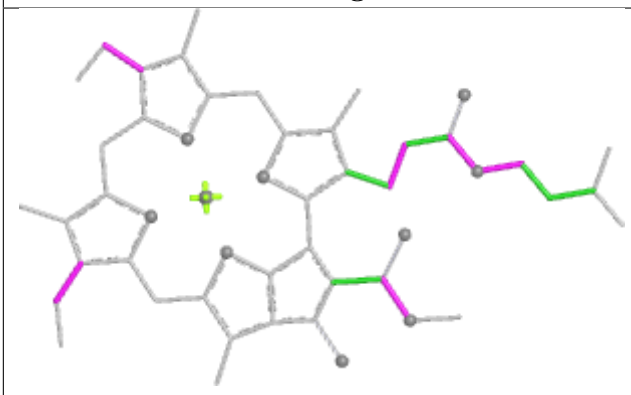
Ligand CLA a 812



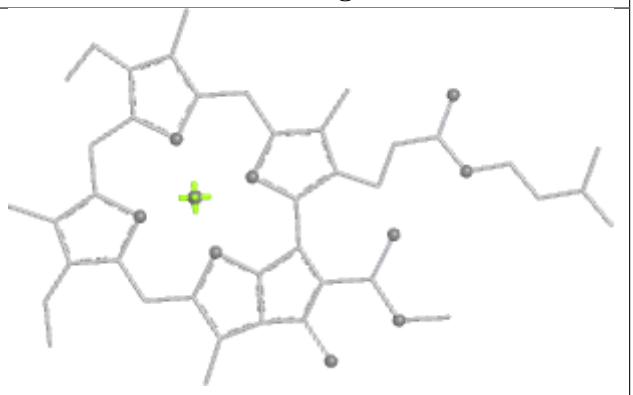
Bond lengths



Bond angles

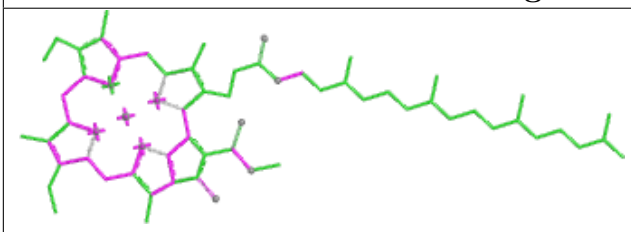


Torsions



Rings

Ligand CLA B 830



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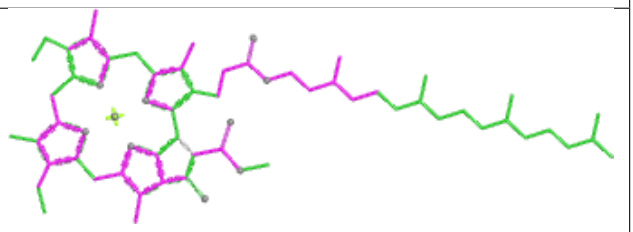
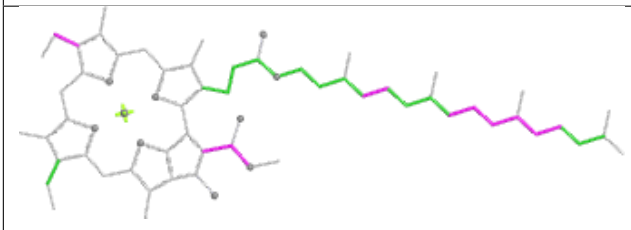


Bond angles



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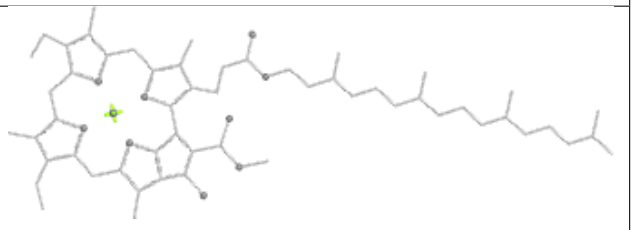
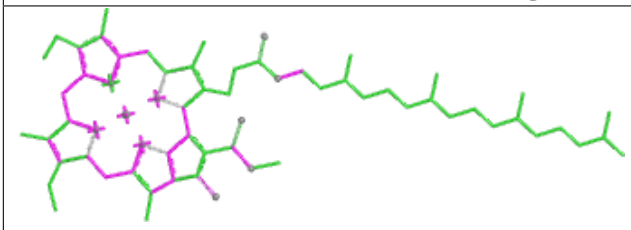


Rings

Ligand CLA B 834



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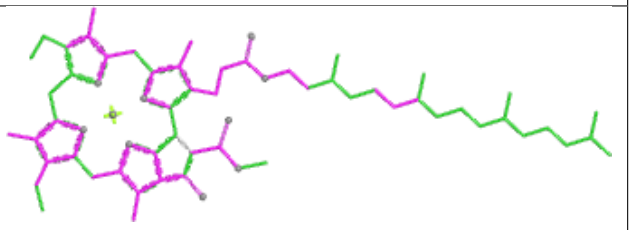
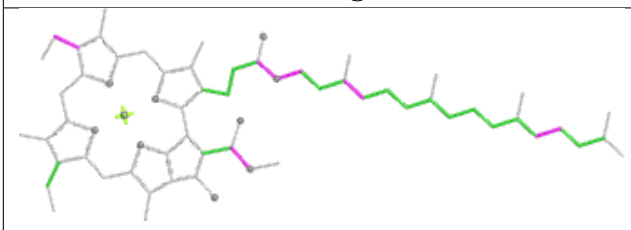


Bond angles



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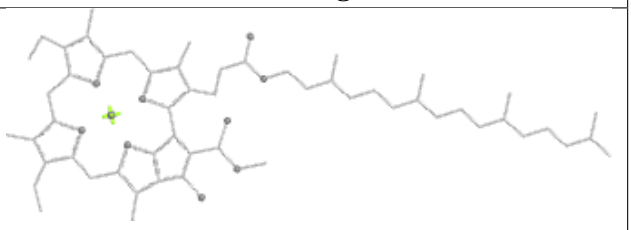
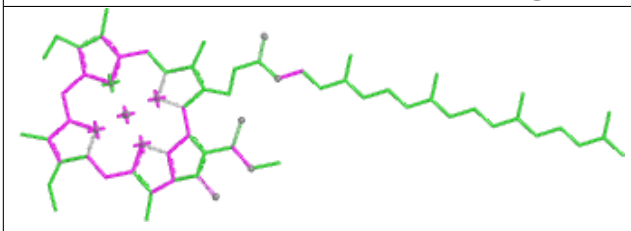
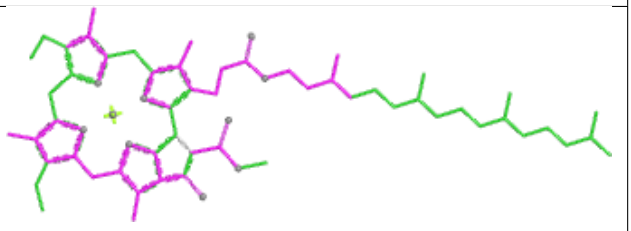


Rings

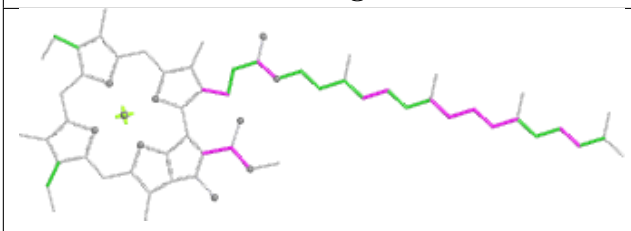
Ligand CLA a 826



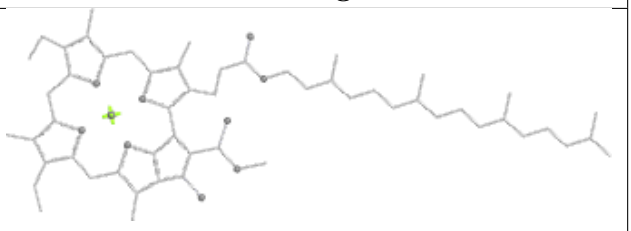
Bond lengths



Bond angles

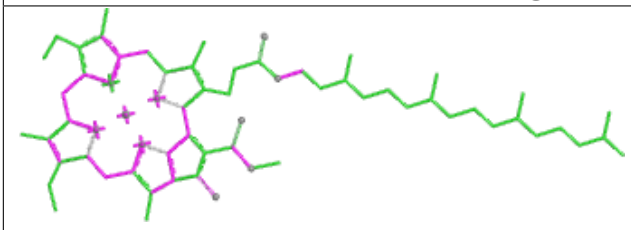


Torsions

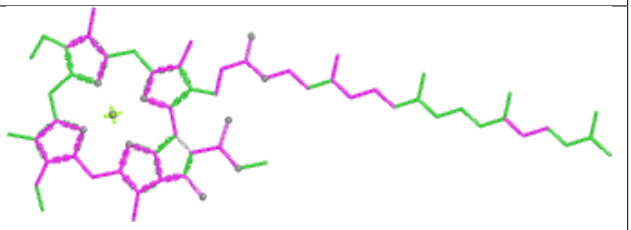


Rings

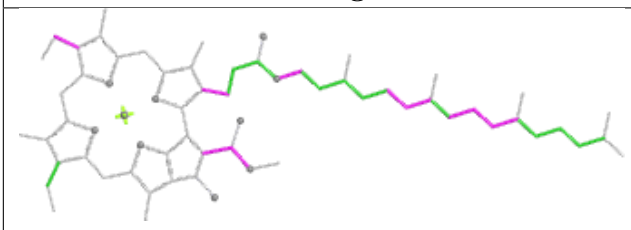
Ligand CLA b 823



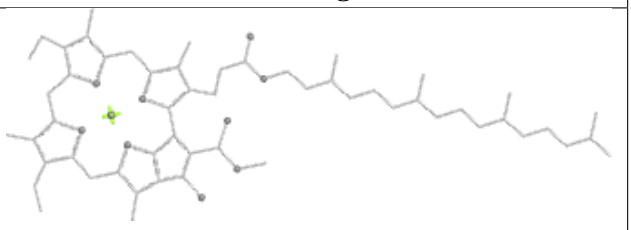
Bond lengths



Bond angles

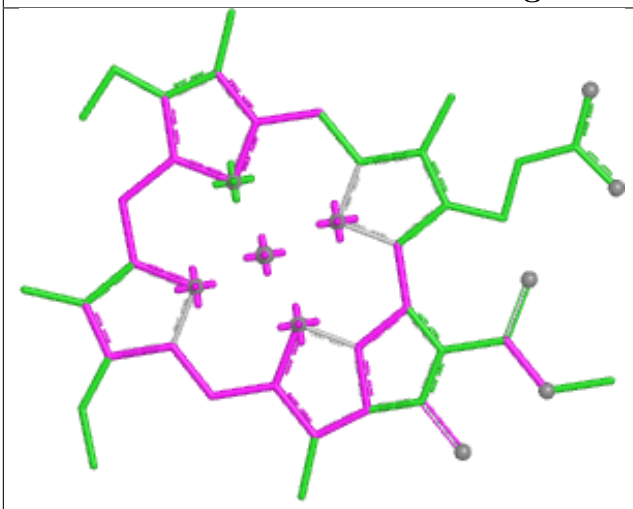


Torsions

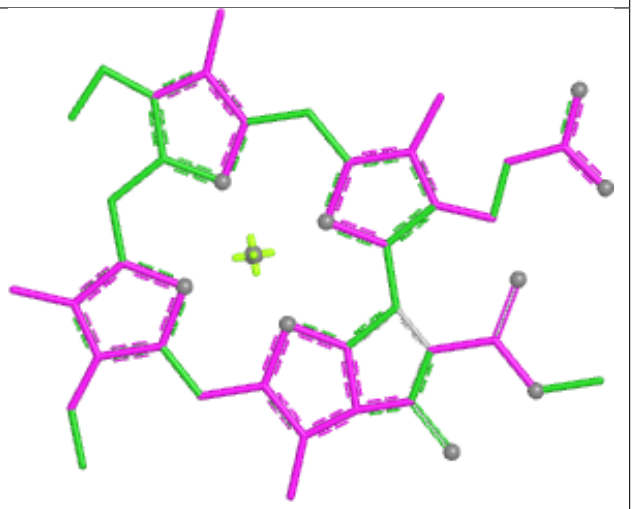


Rings

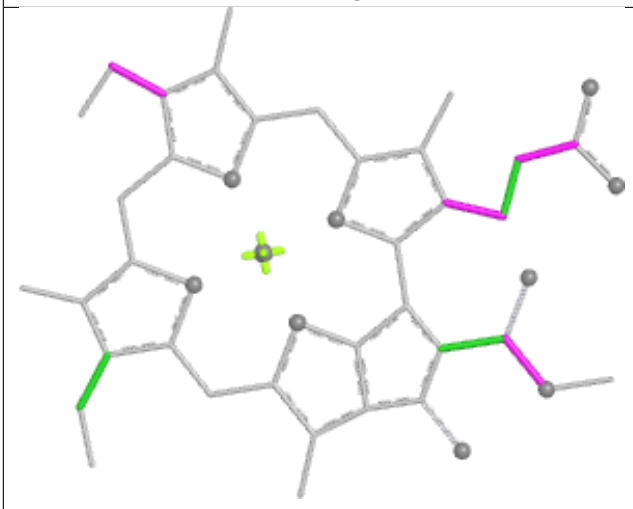
Ligand CLA R 103



Bond lengths



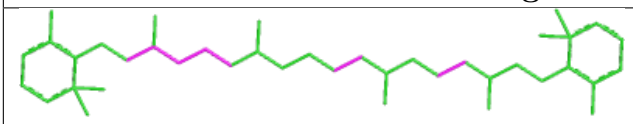
Bond angles



Torsions

Rings

Ligand BCR A 844



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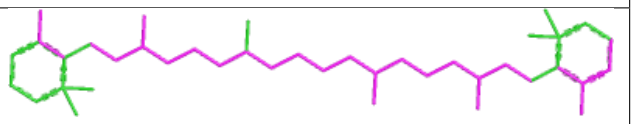
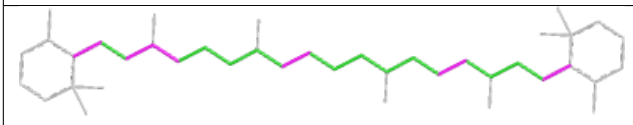
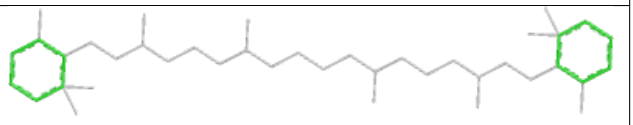


Bond angles

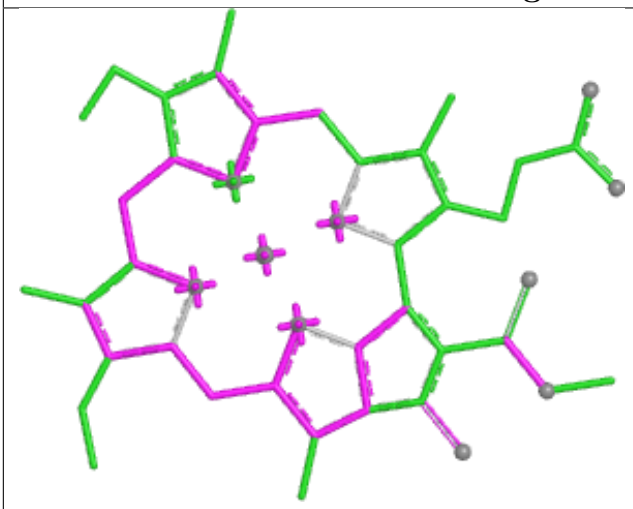


Torsions

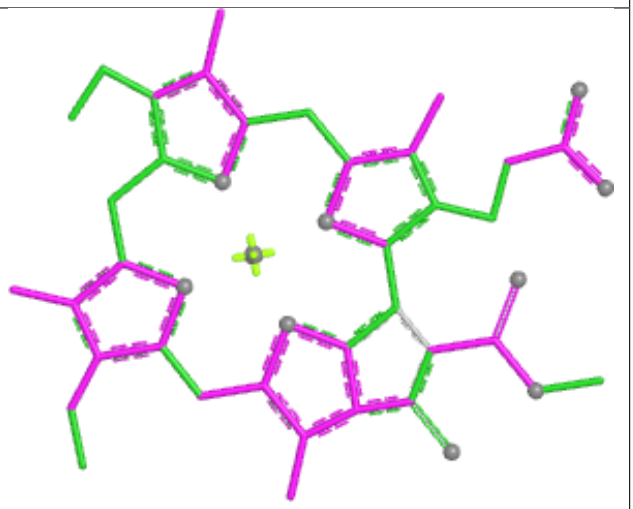


Rings

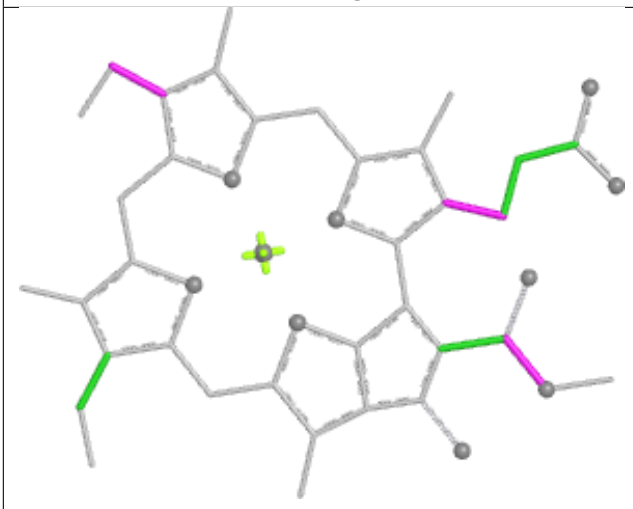
Ligand CLA H 828



Bond lengths



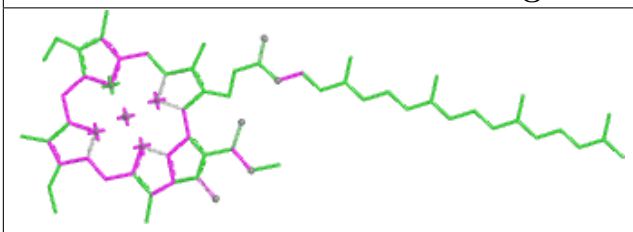
Bond angles



Torsions

Rings

Ligand CLA H 811



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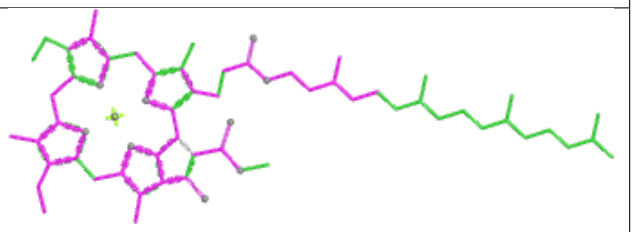
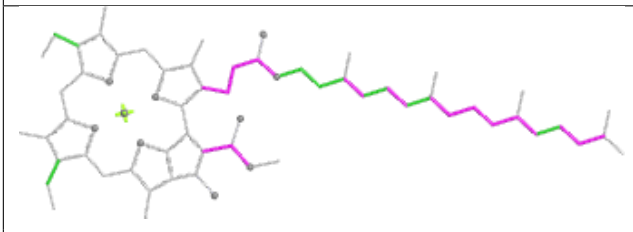
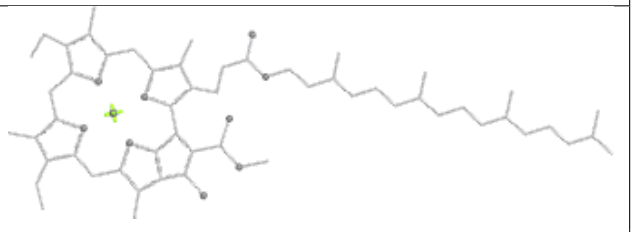


Bond angles

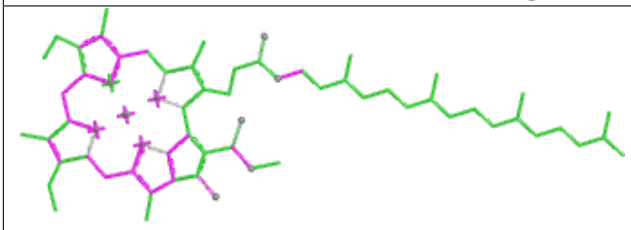


Torsions

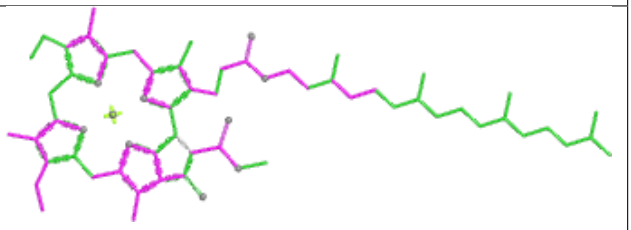


Rings

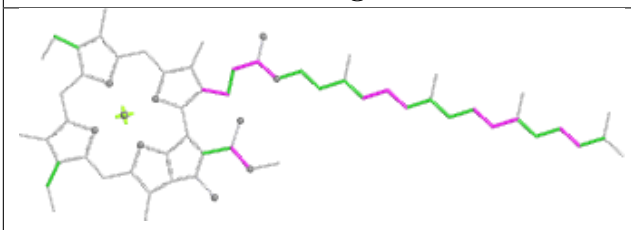
Ligand CLA G 807



Bond lengths



Bond angles



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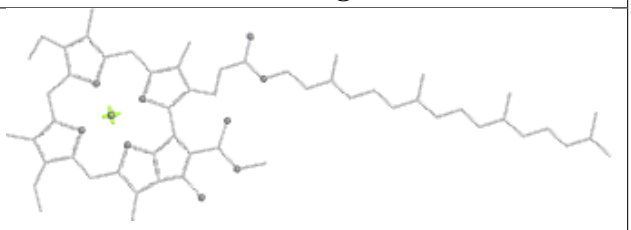
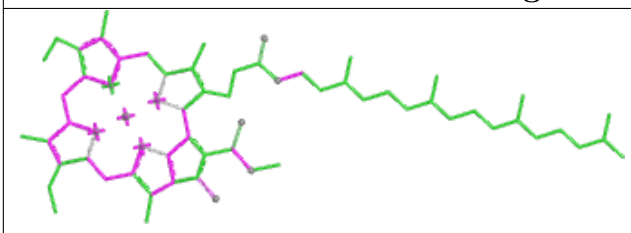


Rings

Ligand CLA G 825



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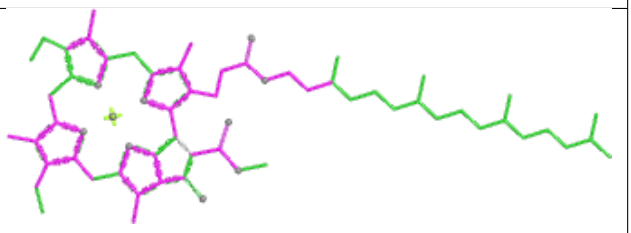
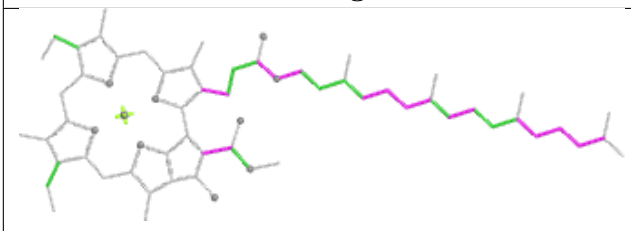
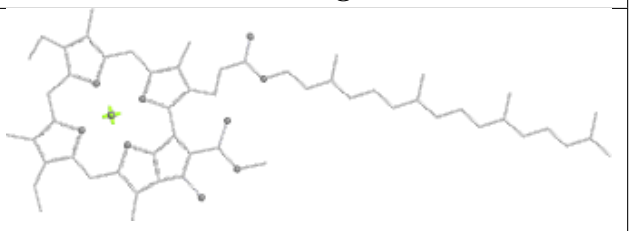


Bond angles

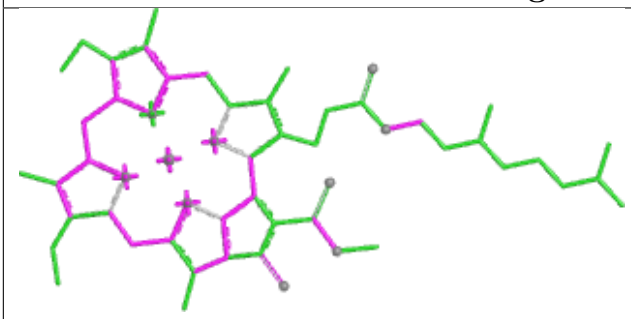


Torsions

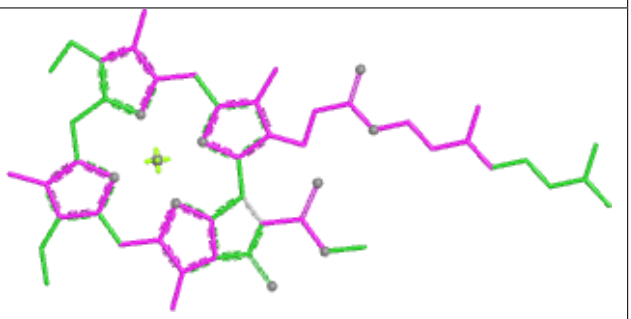


Rings

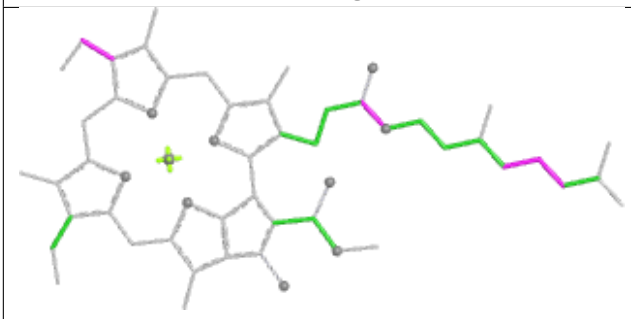
Ligand CLA a 825



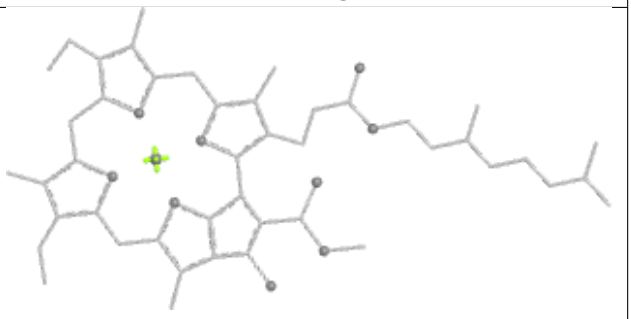
Bond lengths



Bond angles

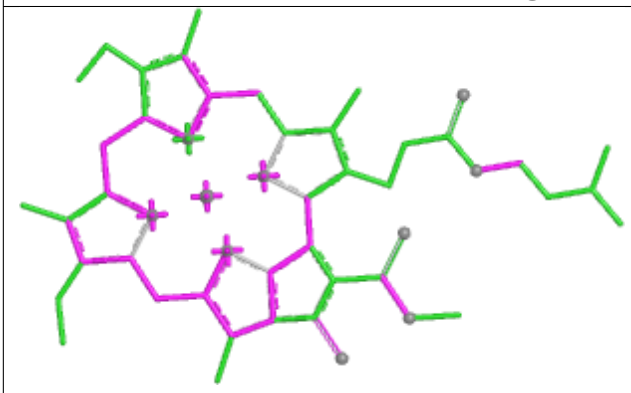


Torsions

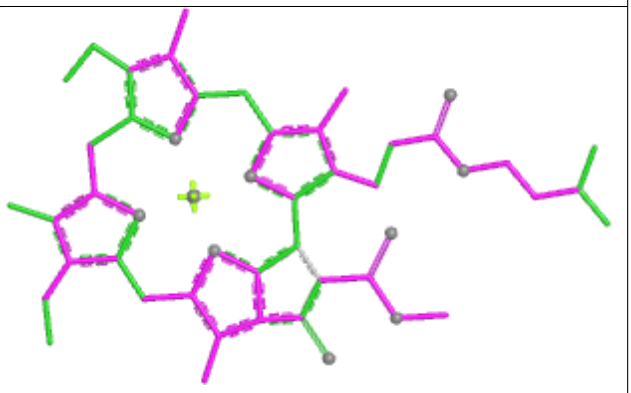


Rings

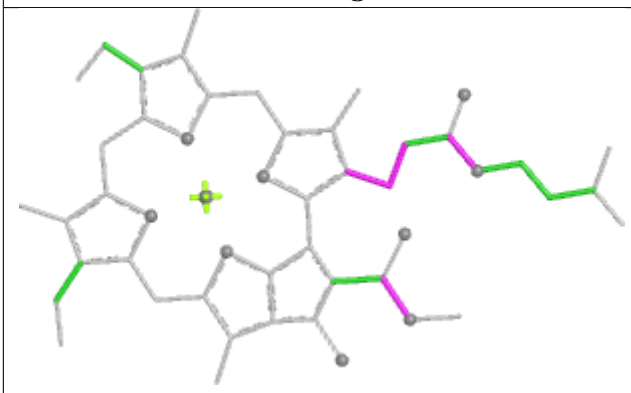
Ligand CLA A 808



Bond lengths



Bond angles



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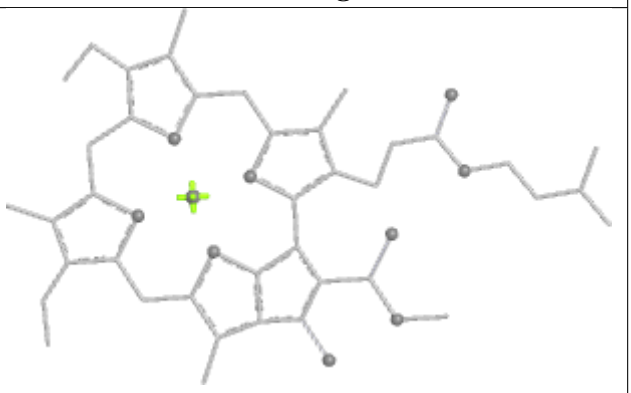
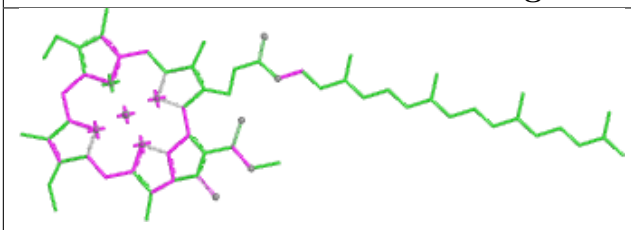
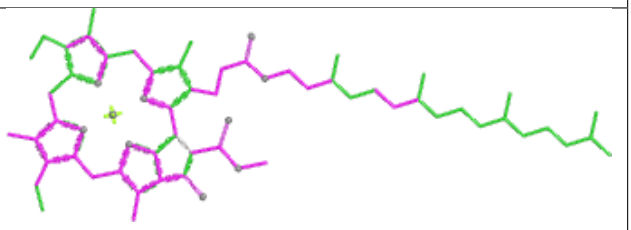


Rings

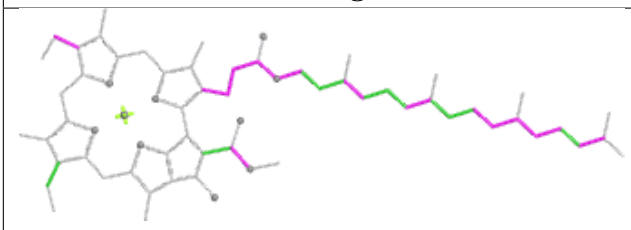
Ligand CLA B 824



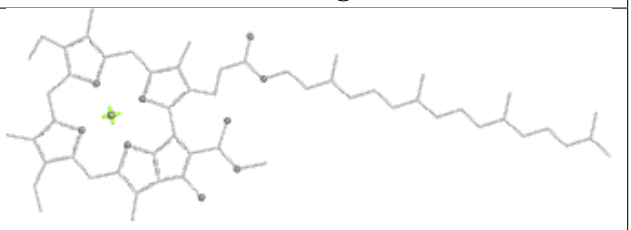
Bond lengths



Bond angles

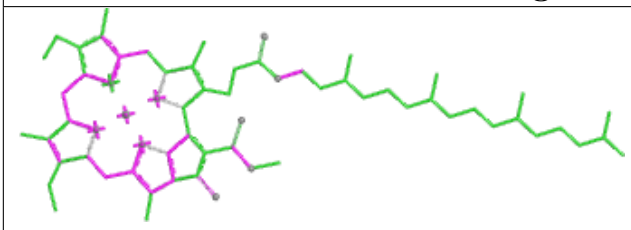


Torsions



Rings

Ligand CLA l 206



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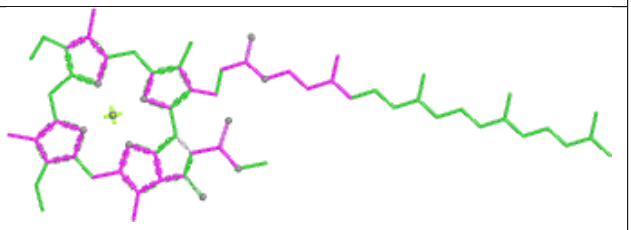
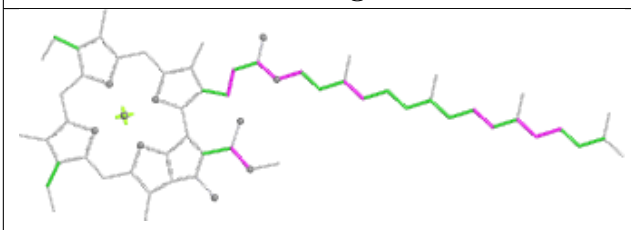
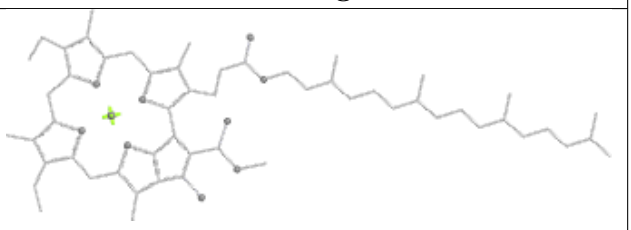


Bond angles

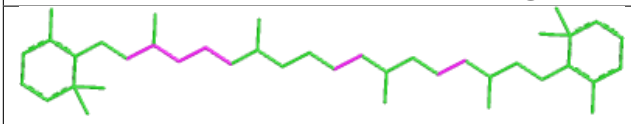


Torsions



Rings

Ligand BCR R 101



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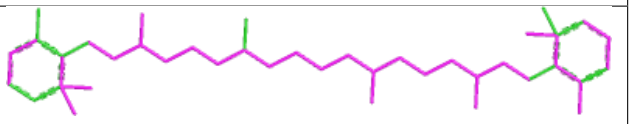
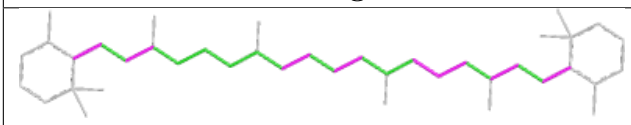
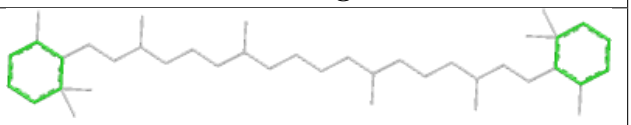


Bond angles

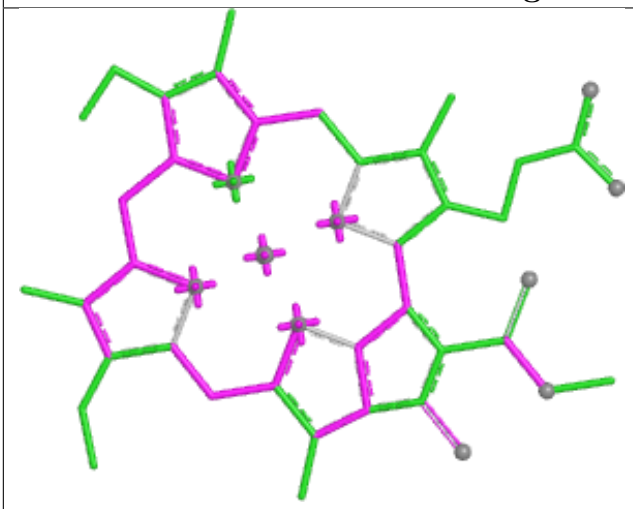


Torsions



Rings

Ligand CLA H 818



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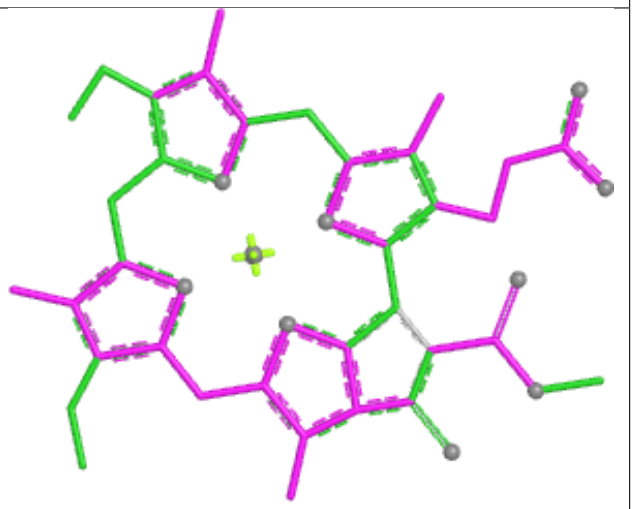
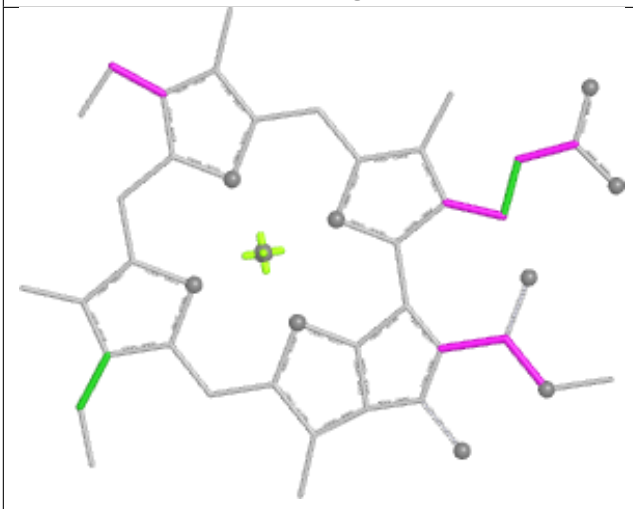


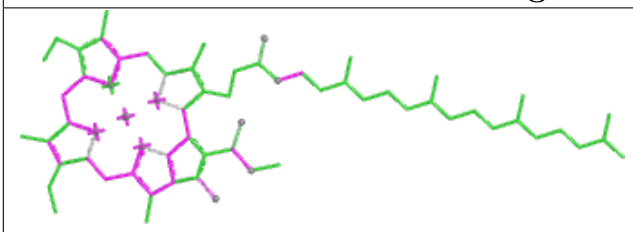
Bond angles



Torsions

Rings

Ligand CLA a 832



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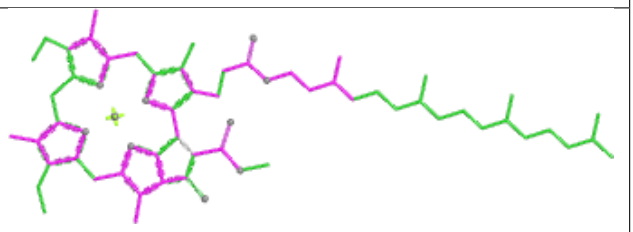
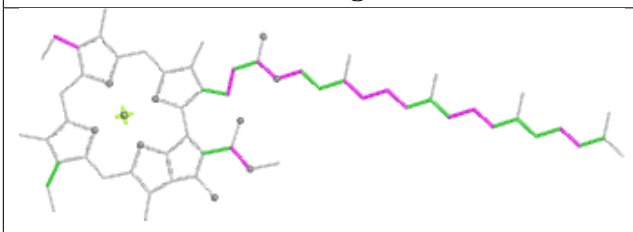
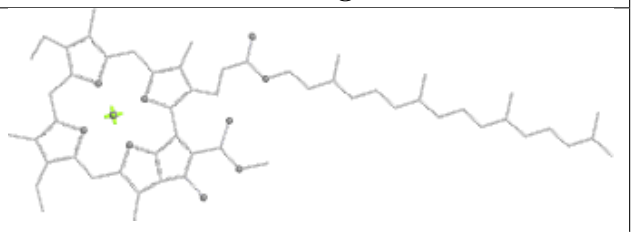


Bond angles

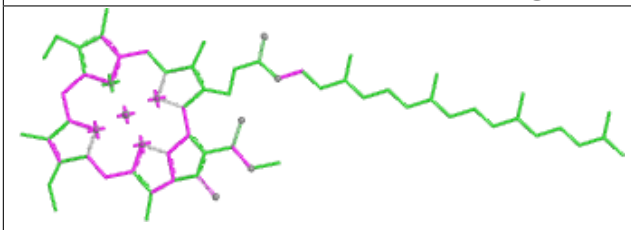


Torsions



Rings

Ligand CLA a 828



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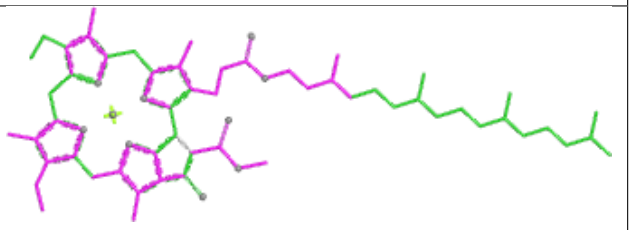
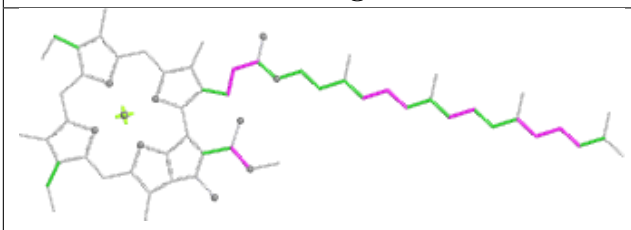
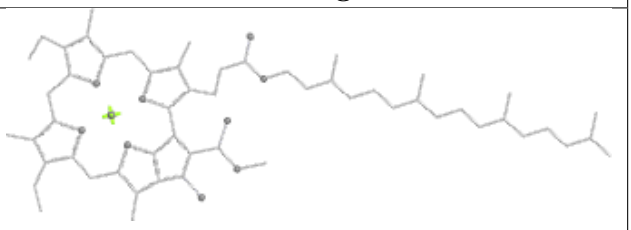


Bond angles

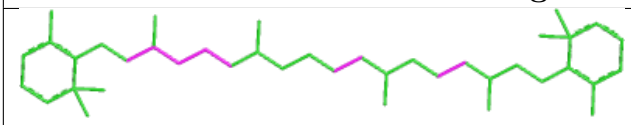


Torsions



Rings

Ligand BCR j 103



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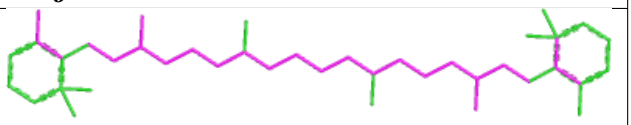
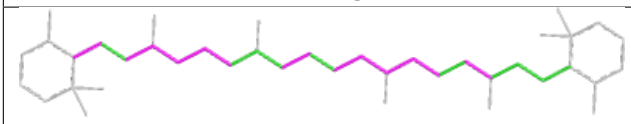


Bond angles



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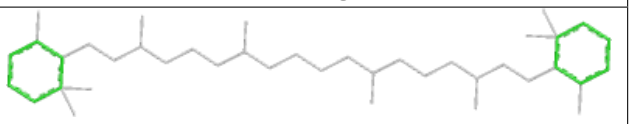
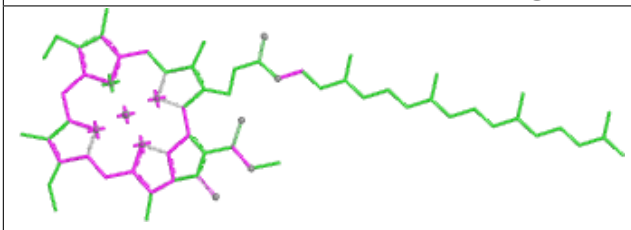


Rings

Ligand CLA a 818



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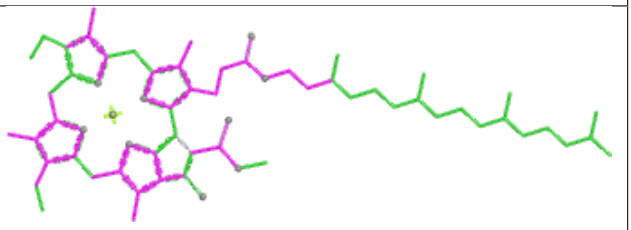
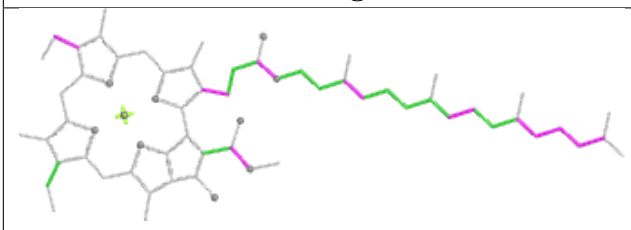
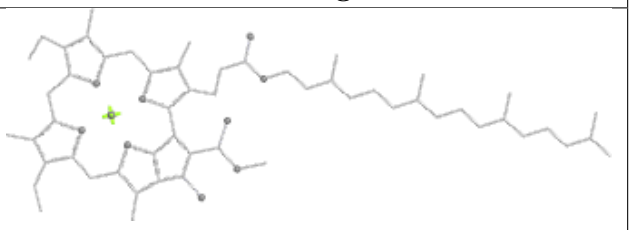


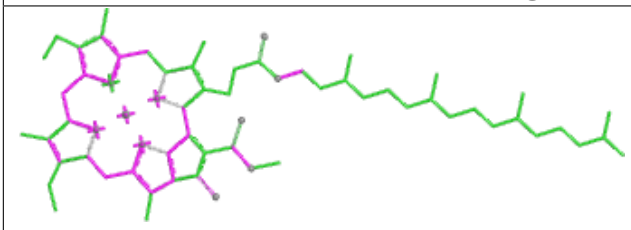
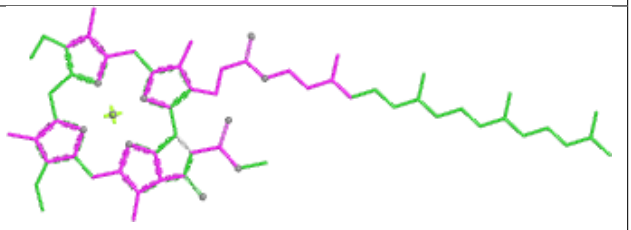
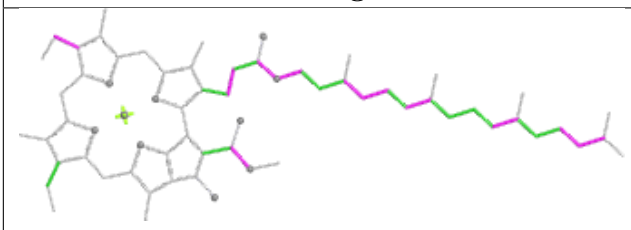
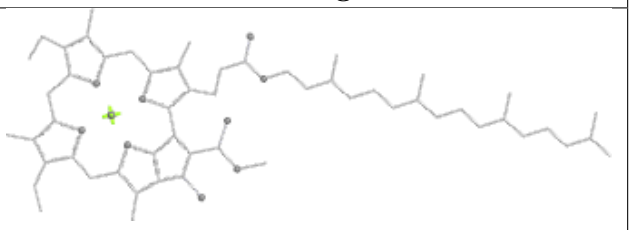
Bond angles

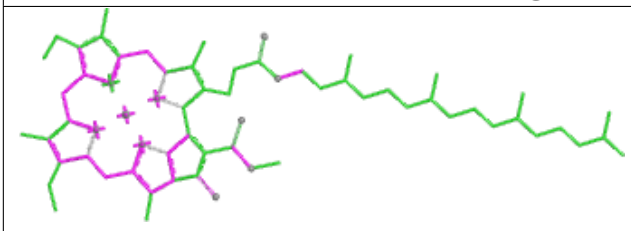
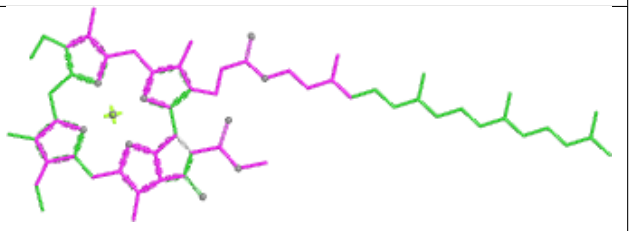
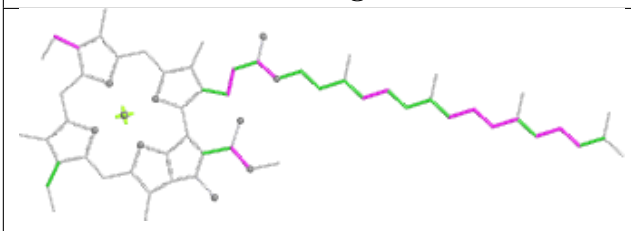
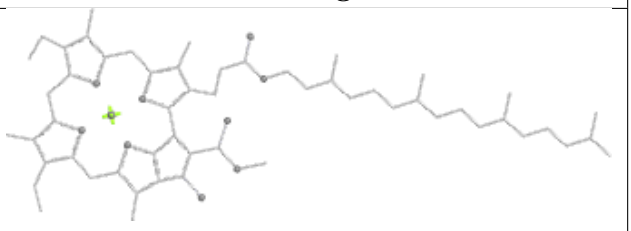


Torsions

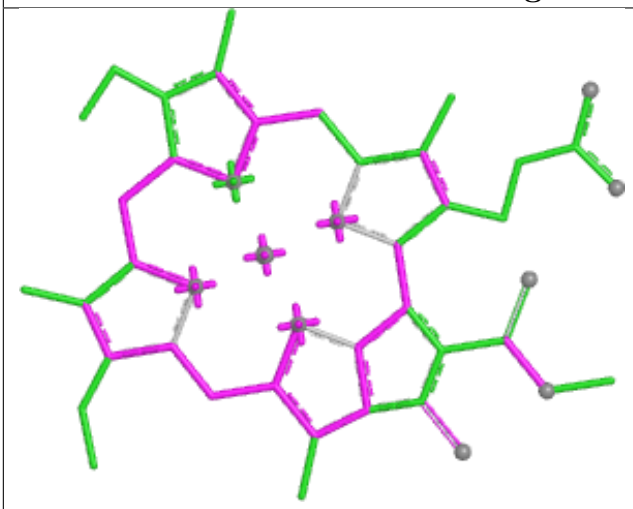


Rings

Ligand CLA A 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 808



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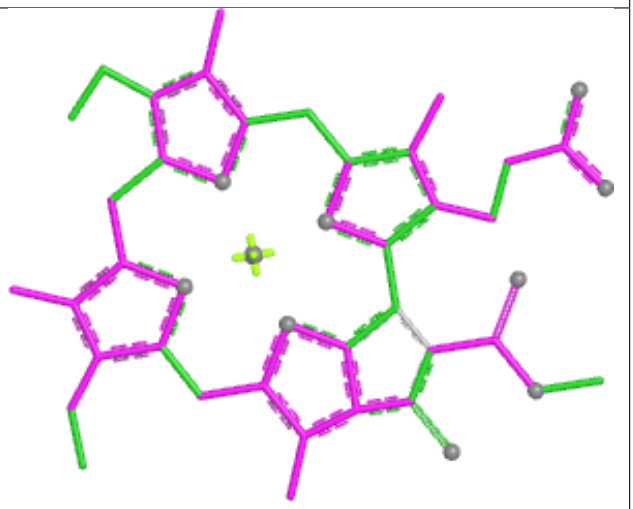
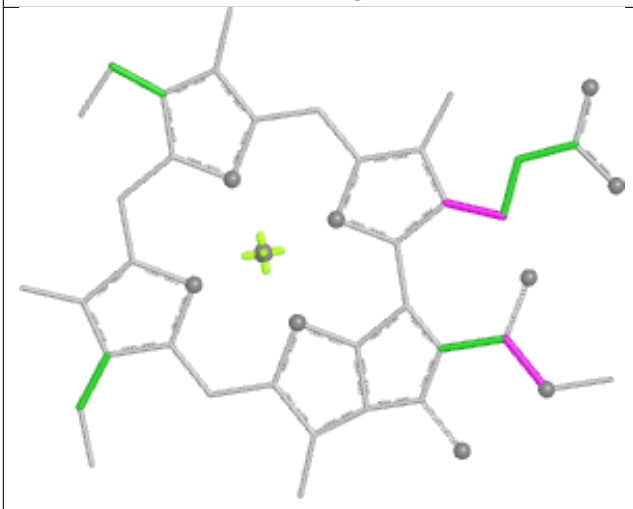


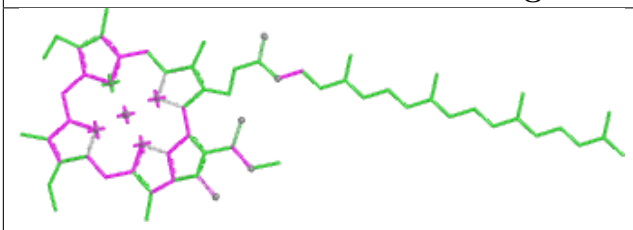
Bond angles



Torsions

Rings

Ligand CLA B 822



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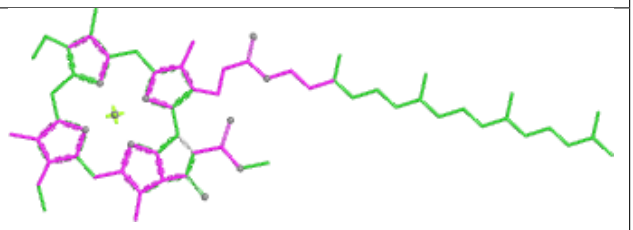
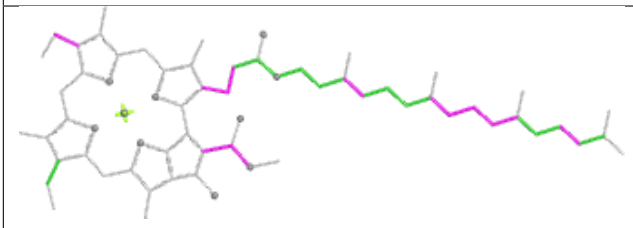
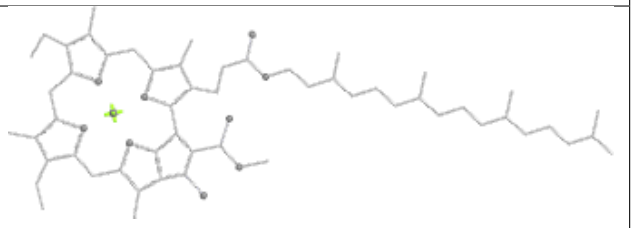


Bond angles

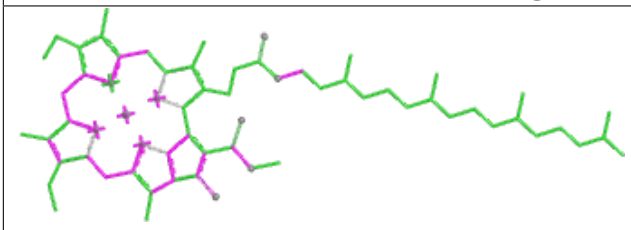


Torsions



Rings

Ligand CLA a 802



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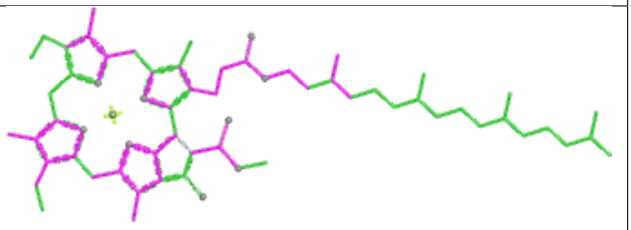
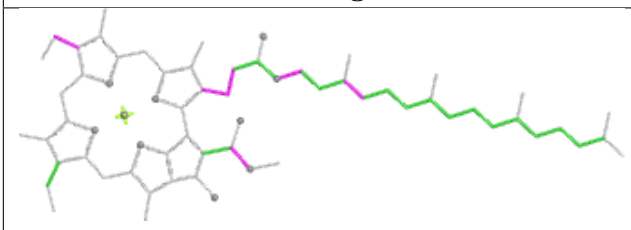
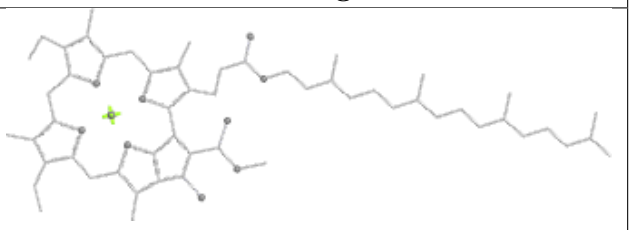


Bond angles

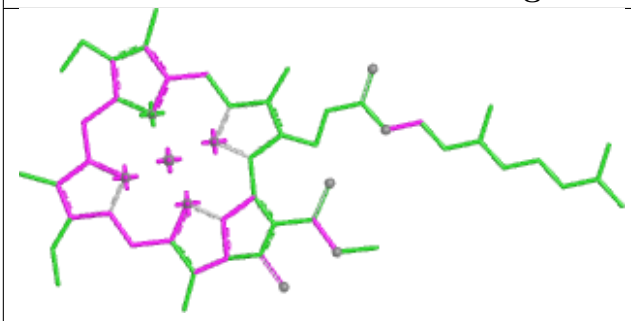


Torsions

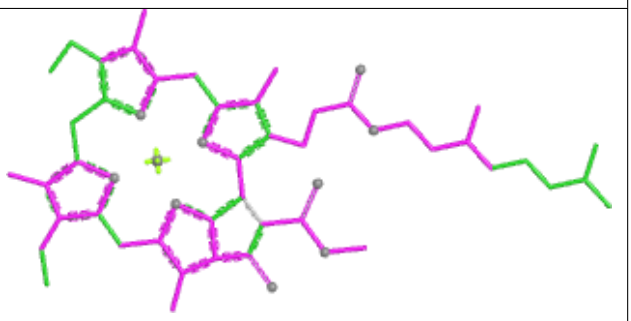


Rings

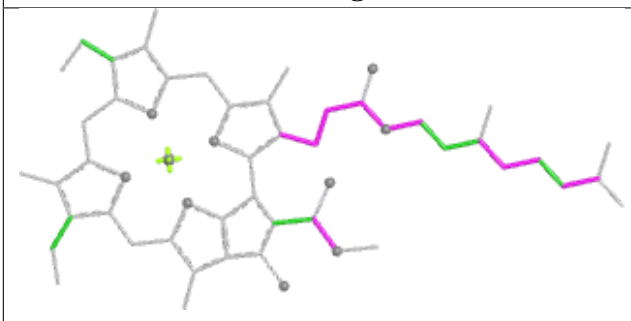
Ligand CLA A 817



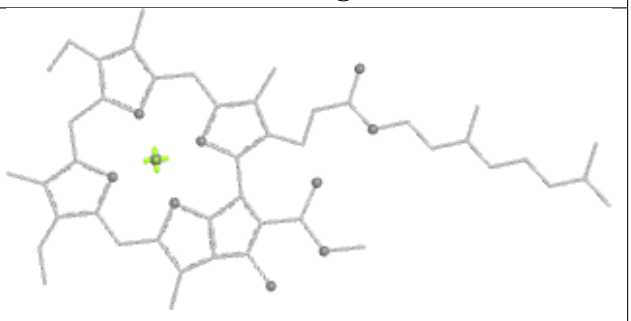
Bond lengths



Bond angles

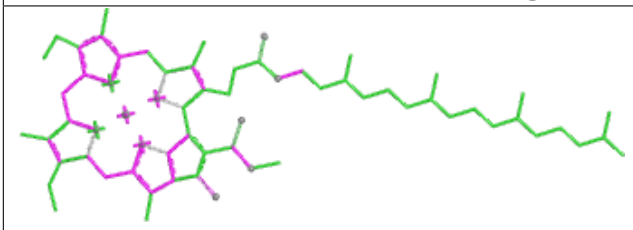


Torsions

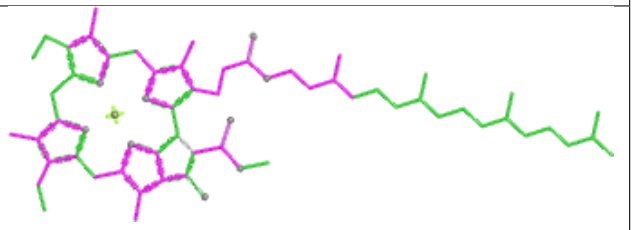


Rings

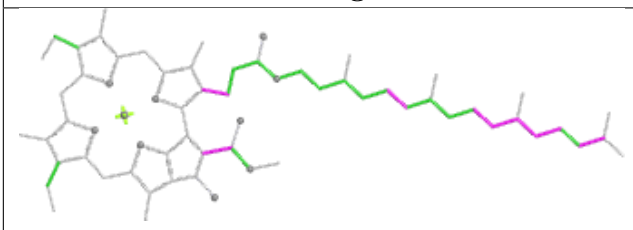
Ligand CLA A 805



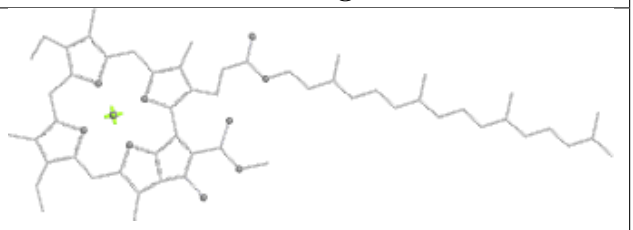
Bond lengths



Bond angles

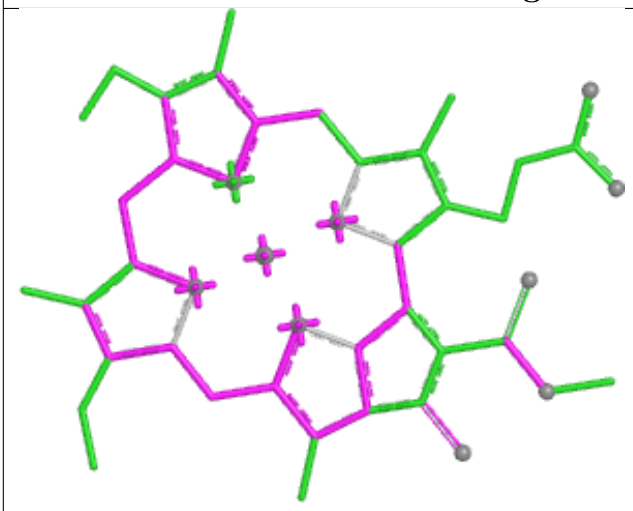


Torsions

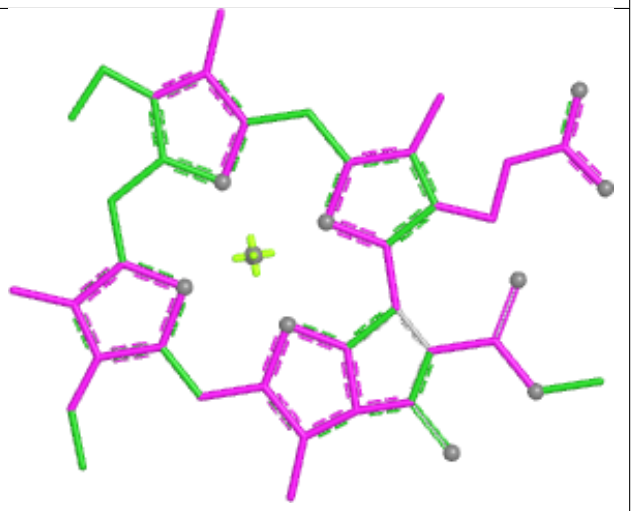


Rings

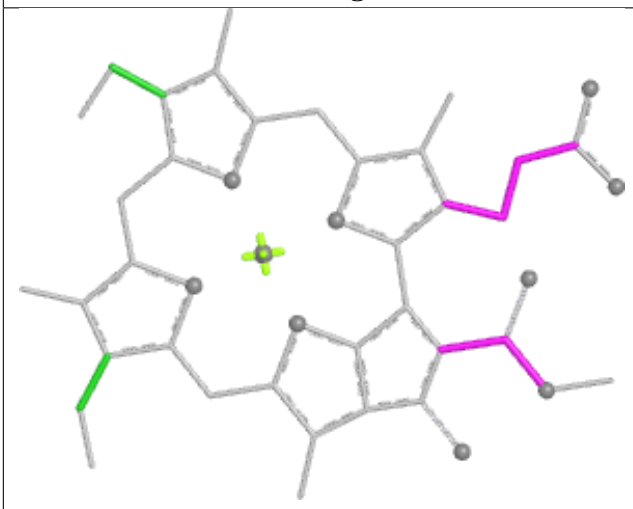
Ligand CLA G 822



Bond lengths



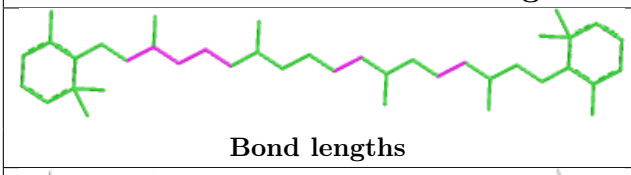
Bond angles



Torsions

Rings

Ligand BCR A 848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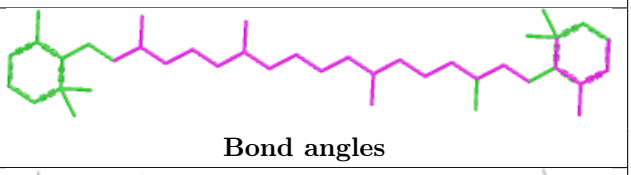
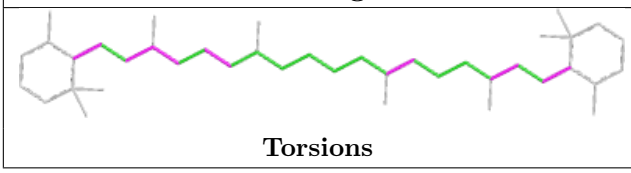
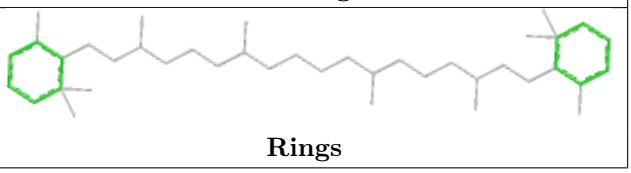
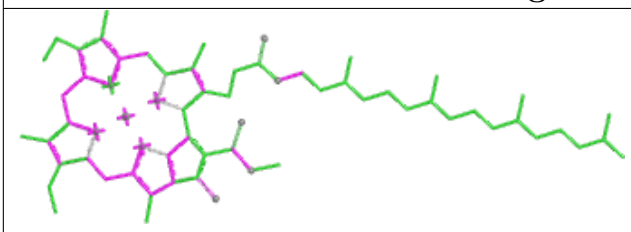

Bond angles


Torsions


Rings

Ligand CLA a 805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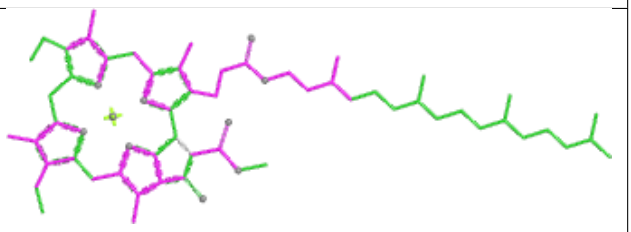
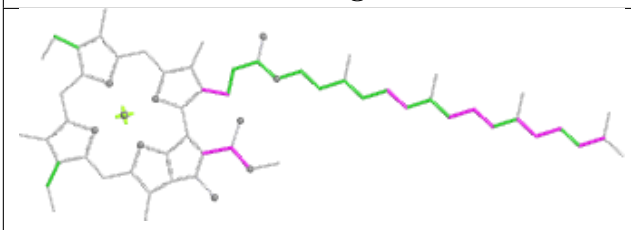
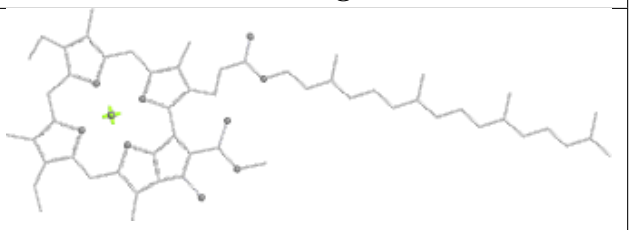
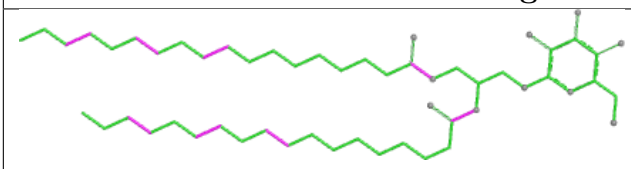
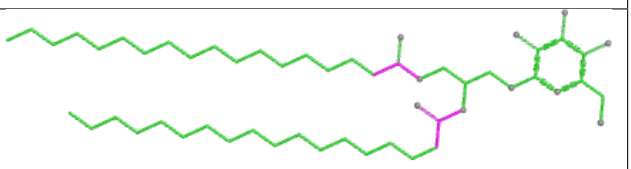

Bond angles

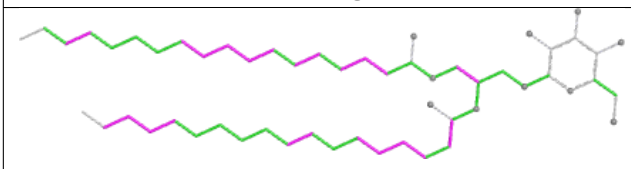

Torsions

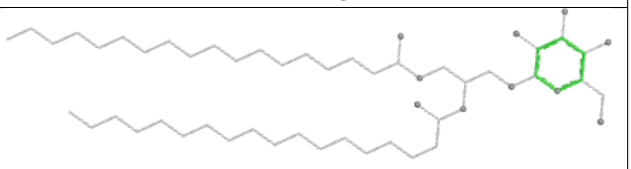

Rings

Ligand LMG B 846

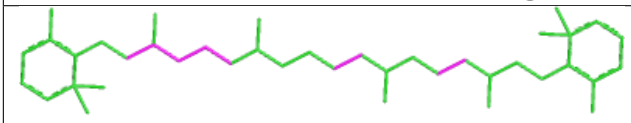

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR G 853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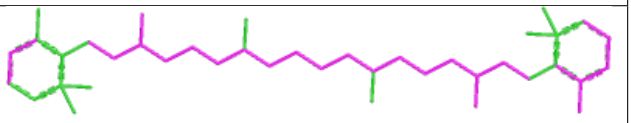
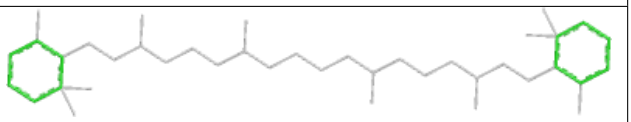
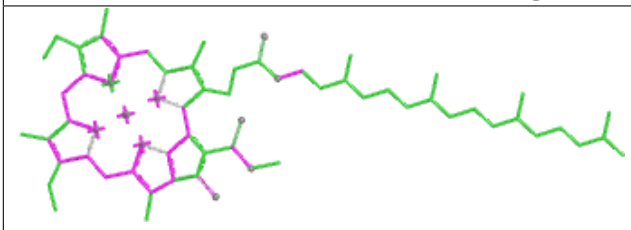

Bond angles

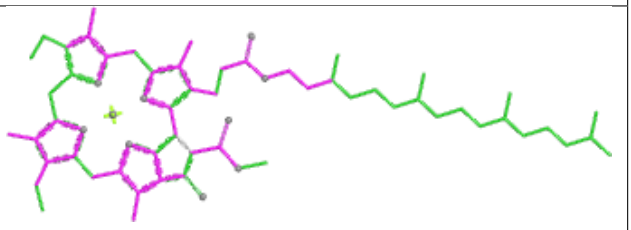
Torsions


Rings

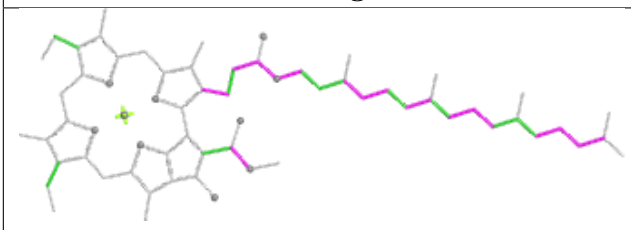
Ligand CLA b 829



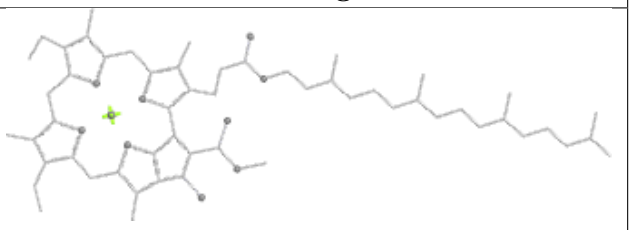
Bond lengths



Bond angles

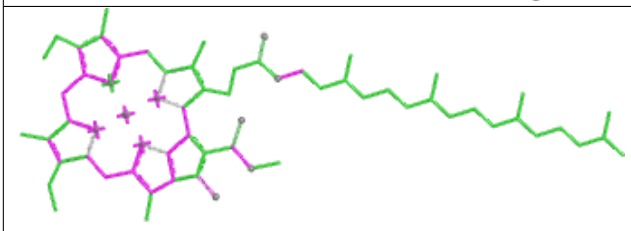


Torsions



Rings

Ligand CLA b 833



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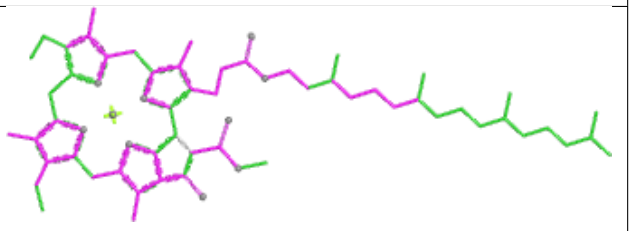
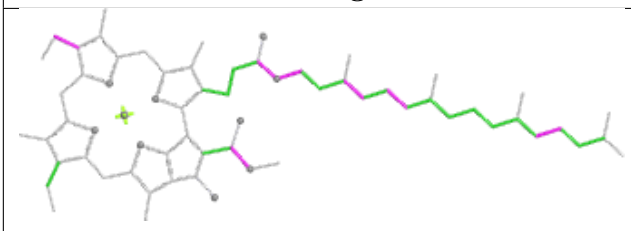
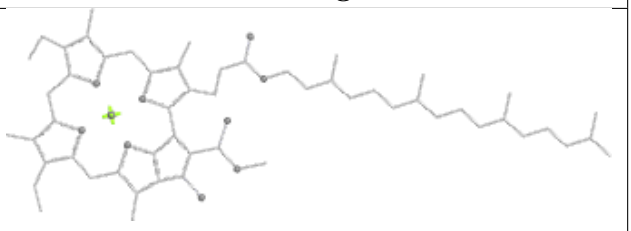


Bond angles

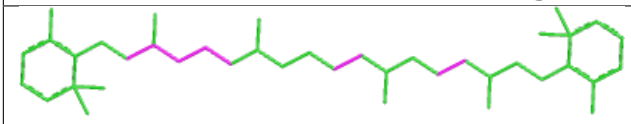


Torsions

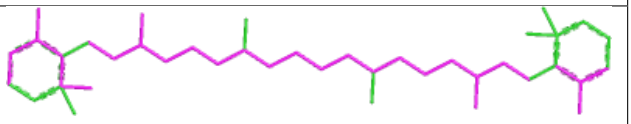


Rings

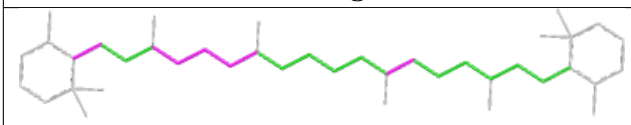
Ligand BCR i 101



Bond lengths



Bond angles



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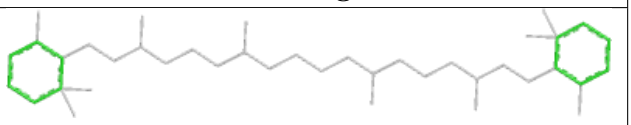
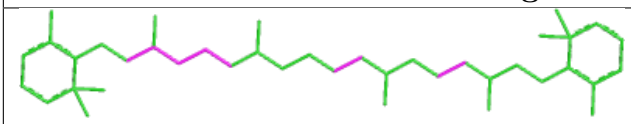
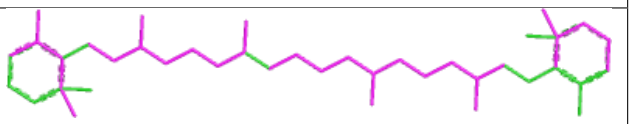


Rings

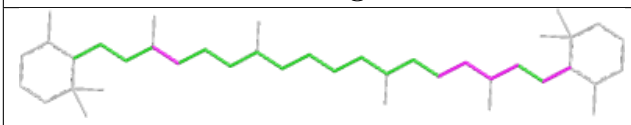
Ligand BCR H 843



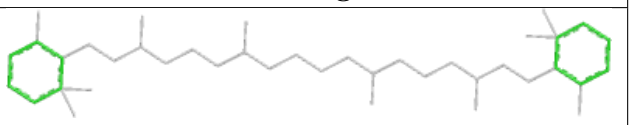
Bond lengths



Bond angles

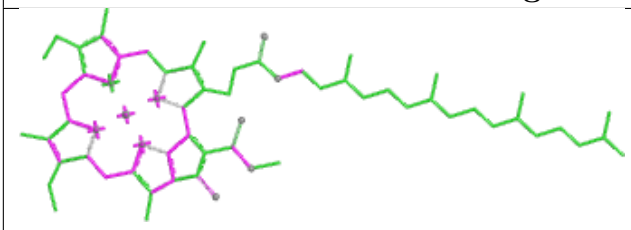


Torsions



Rings

Ligand CLA H 804



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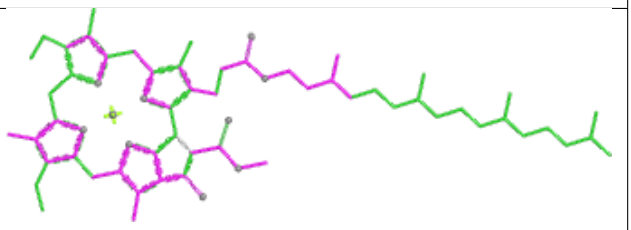
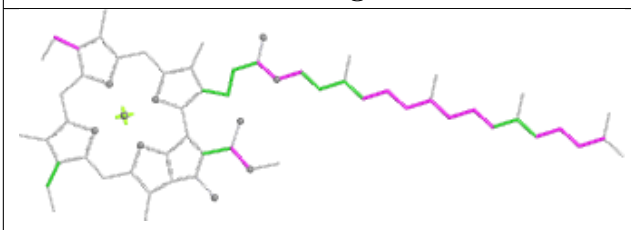
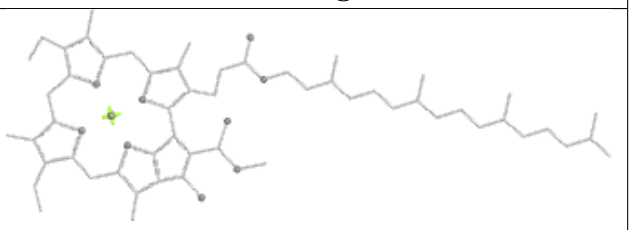


Bond angles

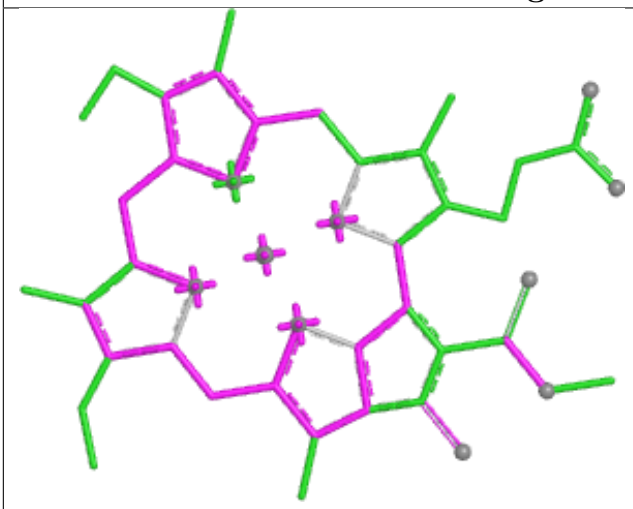


Torsions



Rings

Ligand CLA b 828



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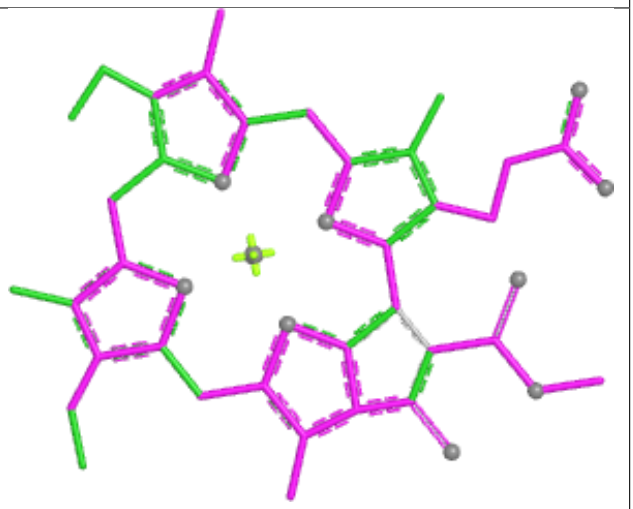
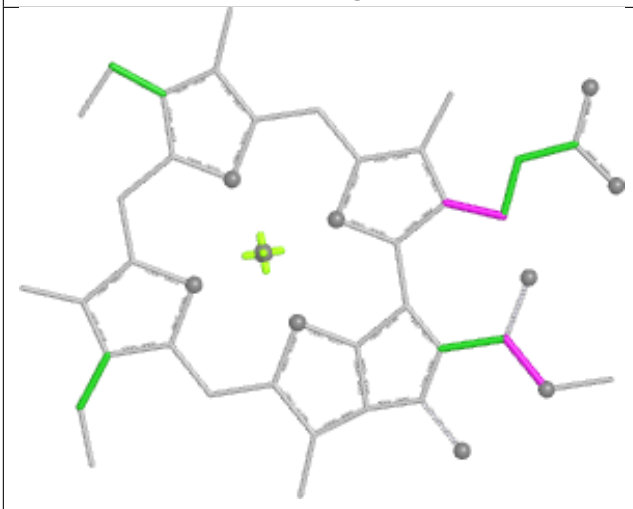


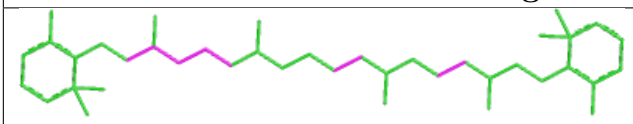
Bond angles



Torsions

Rings

Ligand BCR A 846



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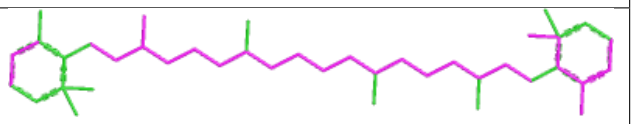
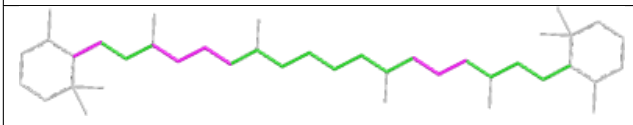
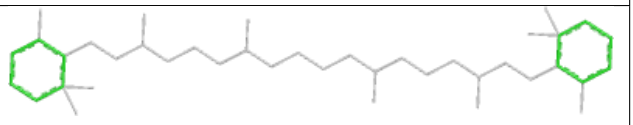


Bond angles

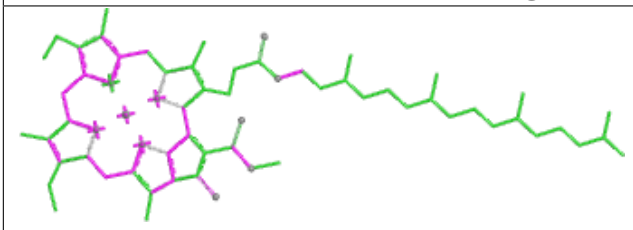


Torsions

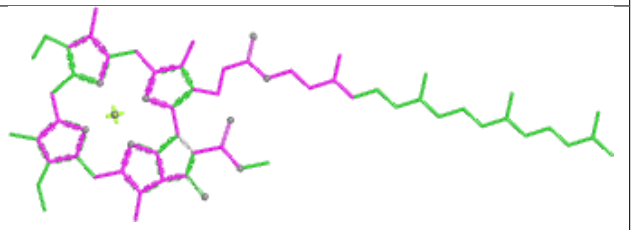


Rings

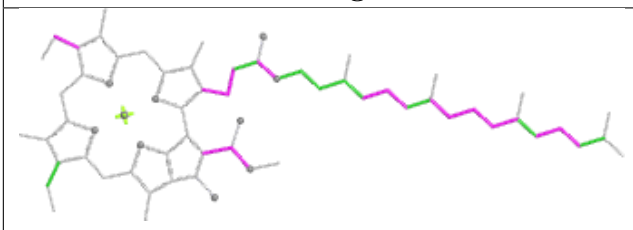
Ligand CLA G 808



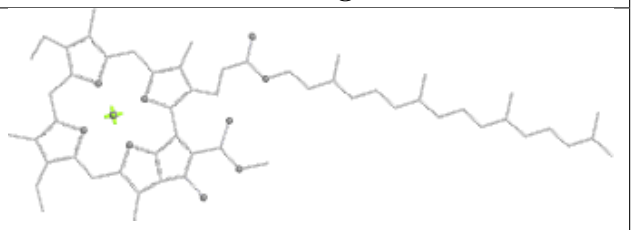
Bond lengths



Bond angles

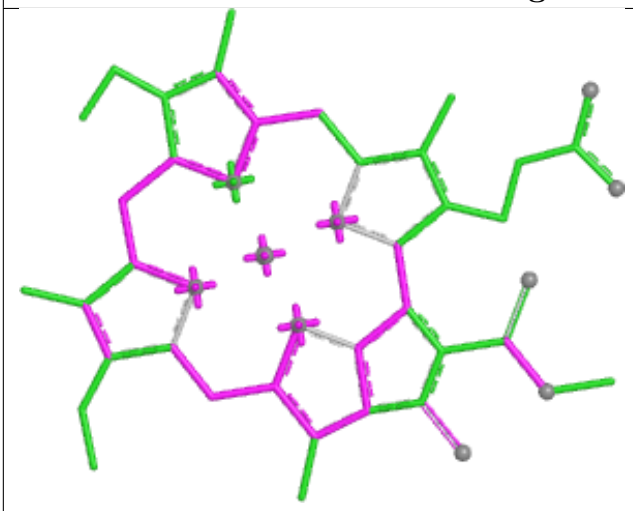


Torsions

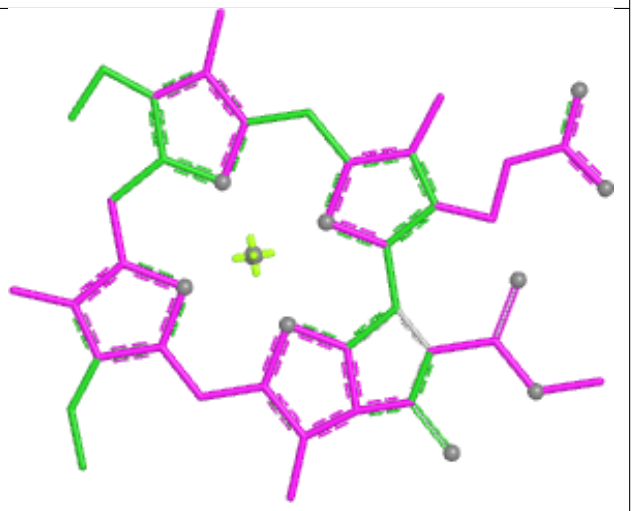


Rings

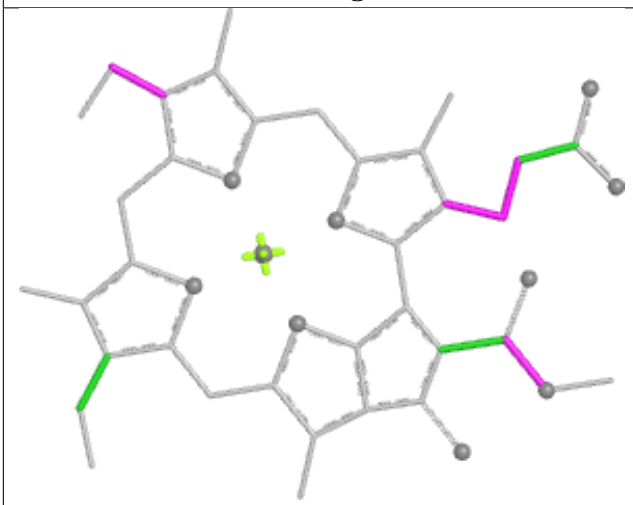
Ligand CLA a 809



Bond lengths



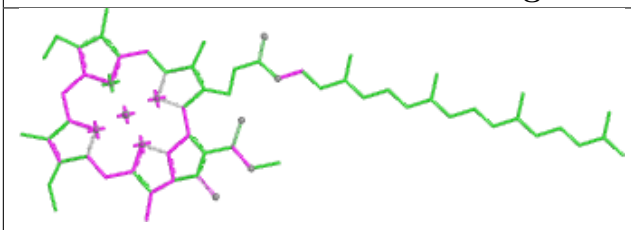
Bond angles



Torsions

Rings

Ligand CLA H 826



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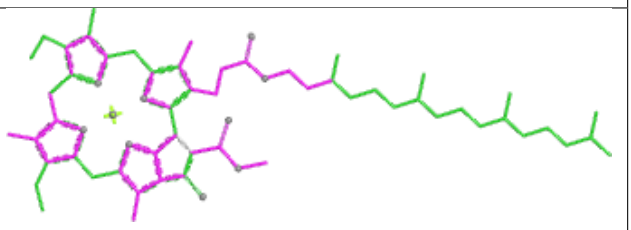
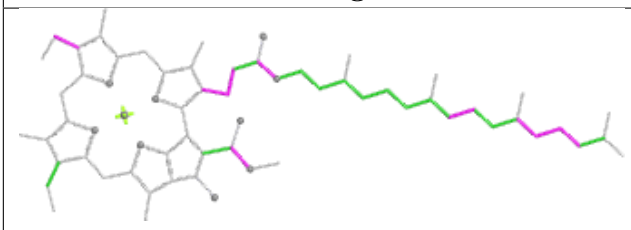
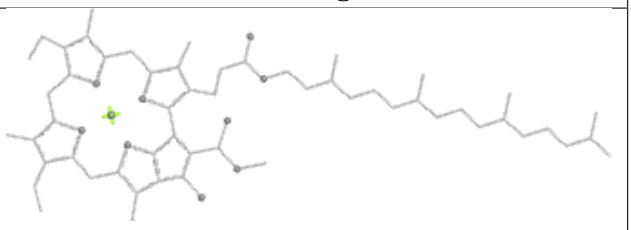


Bond angles

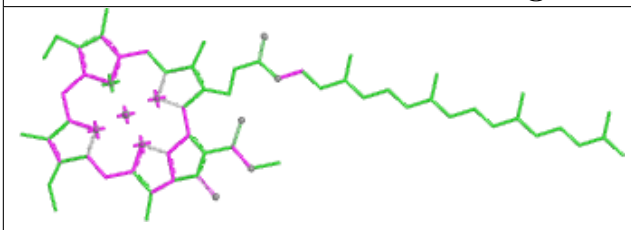


Torsions



Rings

Ligand CLA b 836



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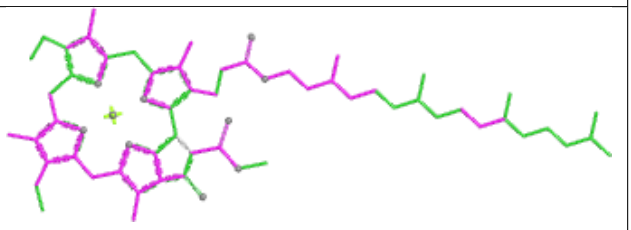
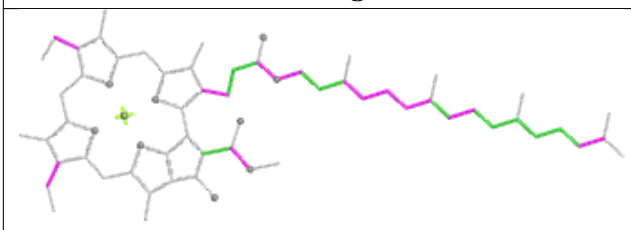
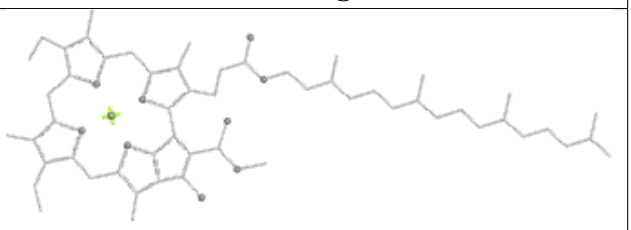


Bond angles

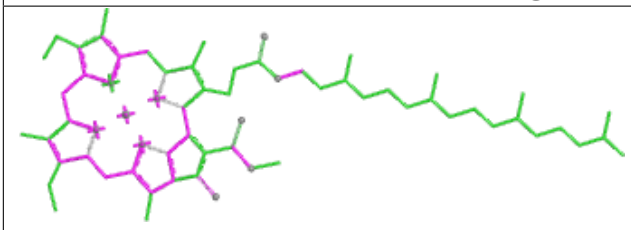


Torsions



Rings

Ligand CLA b 816



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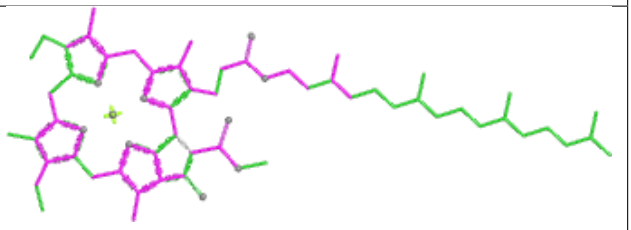
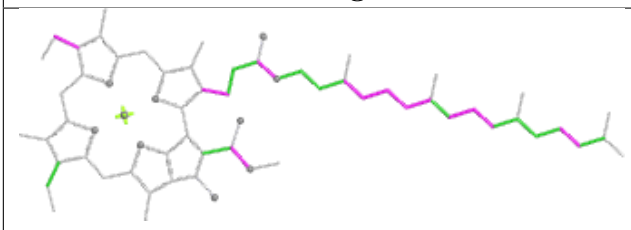
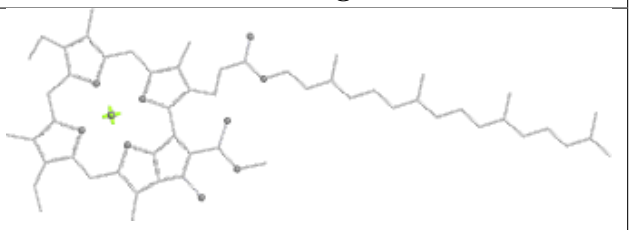


Bond angles

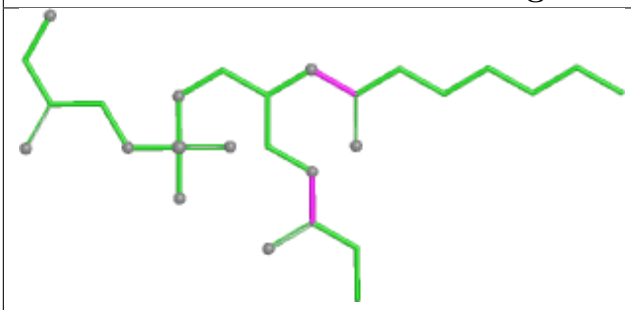


Torsions



Rings

Ligand LHG a 851



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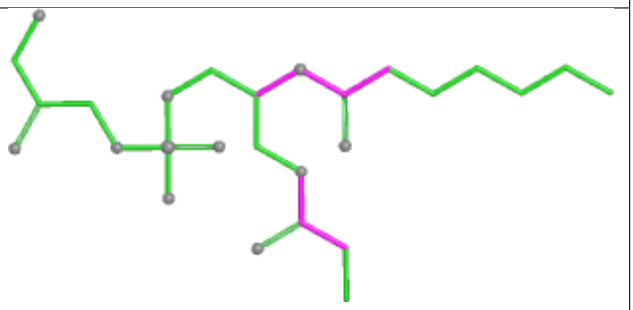
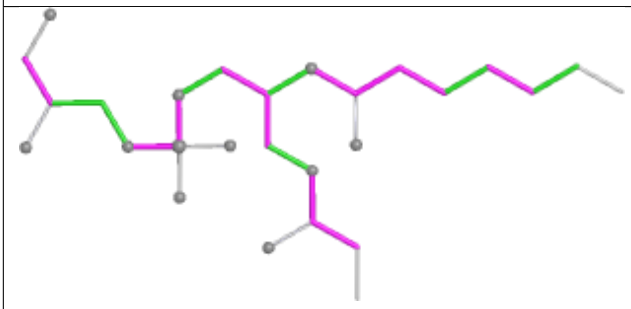
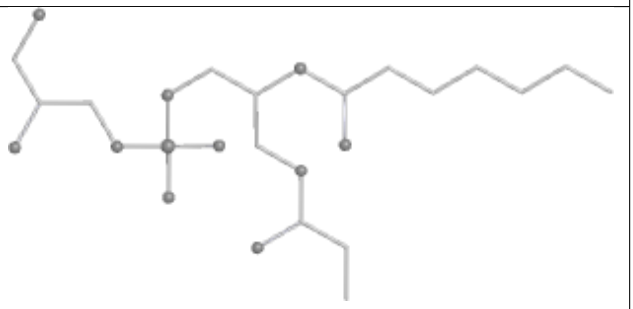


Bond angles

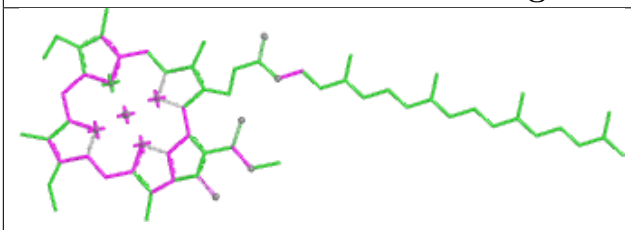


Torsions



Rings

Ligand CLA a 833



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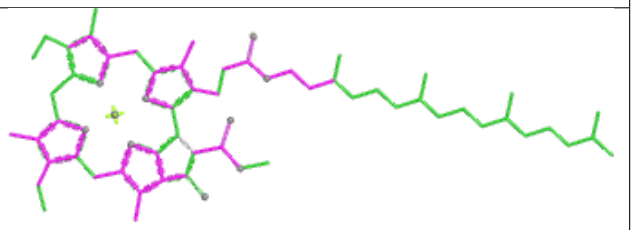
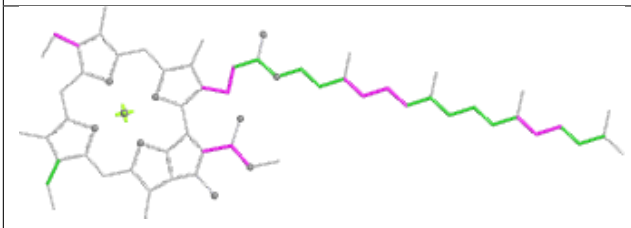


Bond angles



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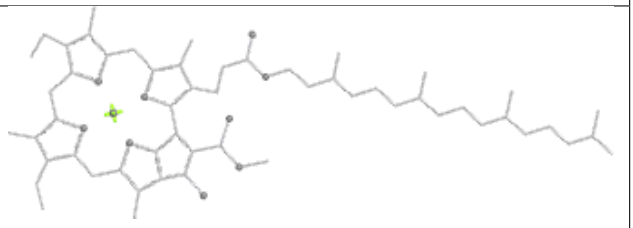
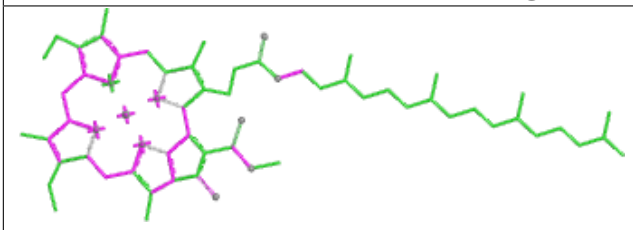


Rings

Ligand CLA G 829



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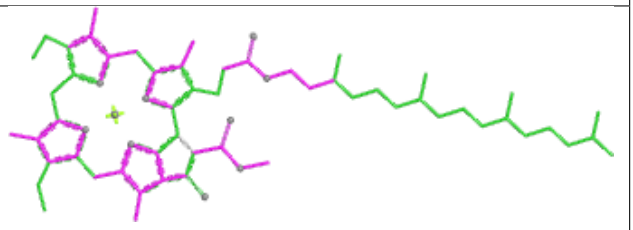
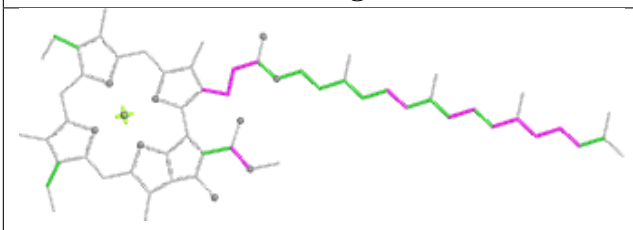


Bond angles



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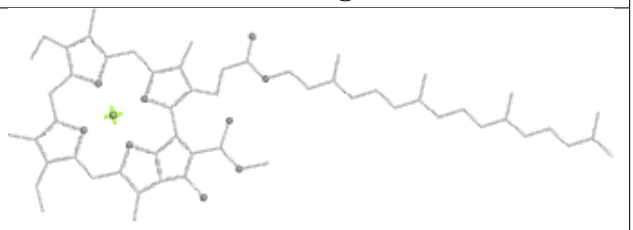
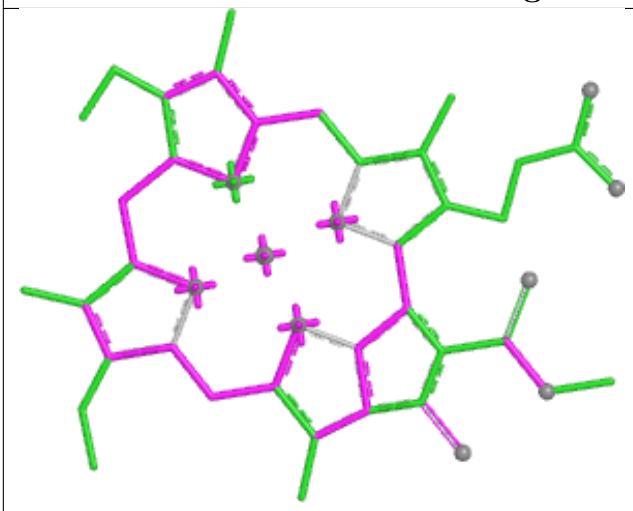


Rings

Ligand CLA A 814



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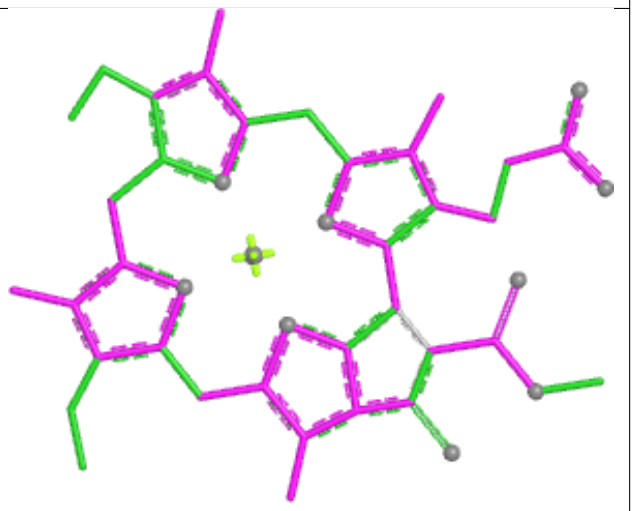

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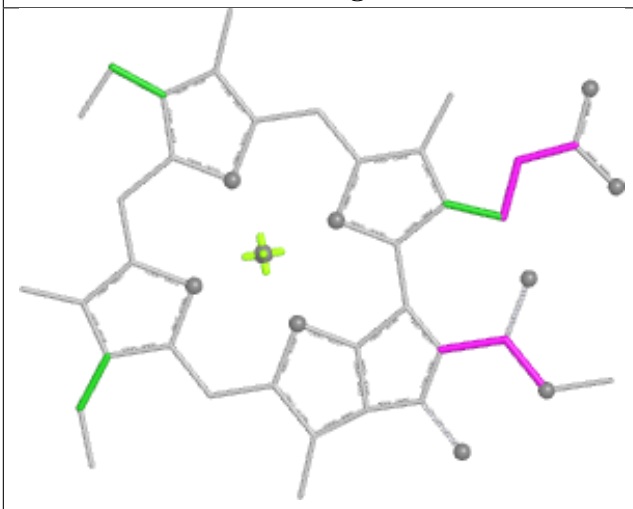
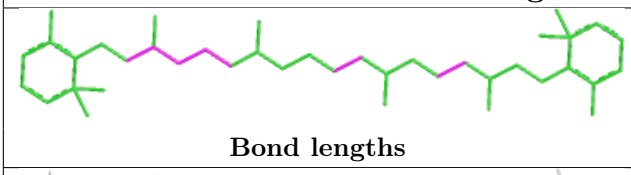


Torsions

Rings

Ligand BCR a 849



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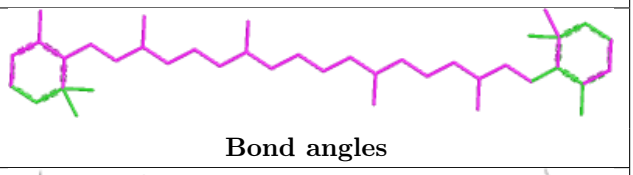
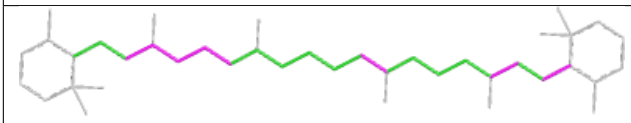
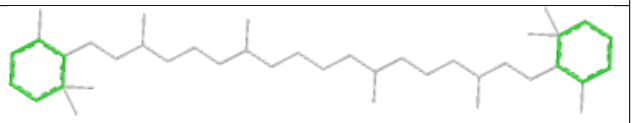


Bond angles

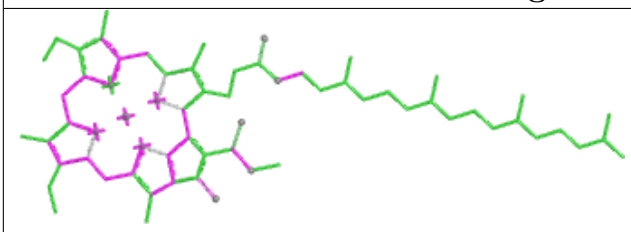


Torsions



Rings

Ligand CLA a 829



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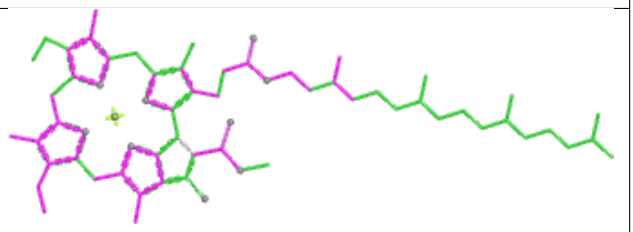
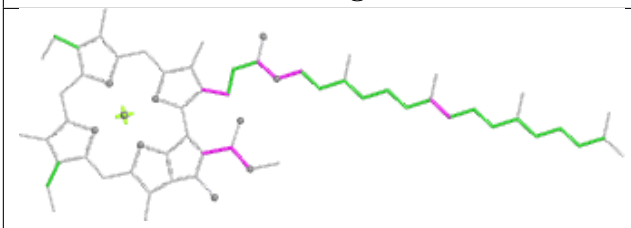


Bond angles



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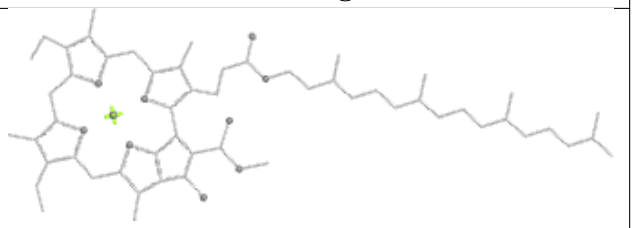
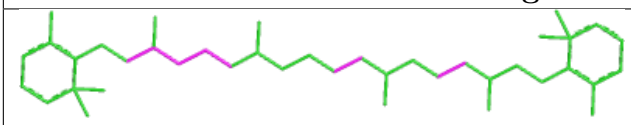


Rings

Ligand BCR Q 102



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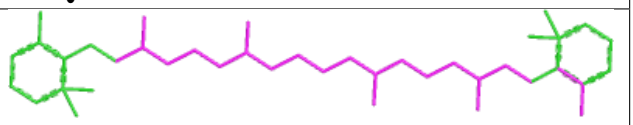
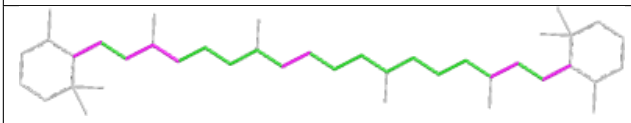


Bond angles



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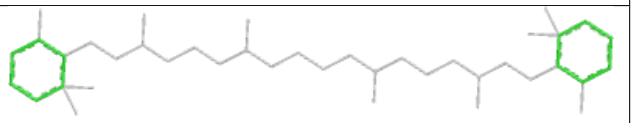
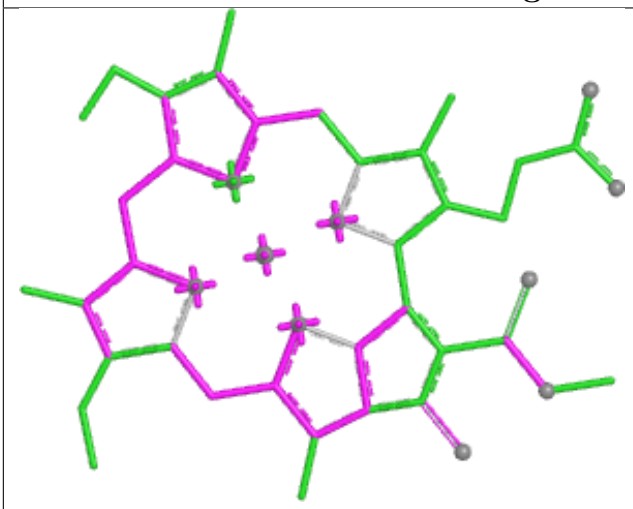


Rings

Ligand CLA H 836



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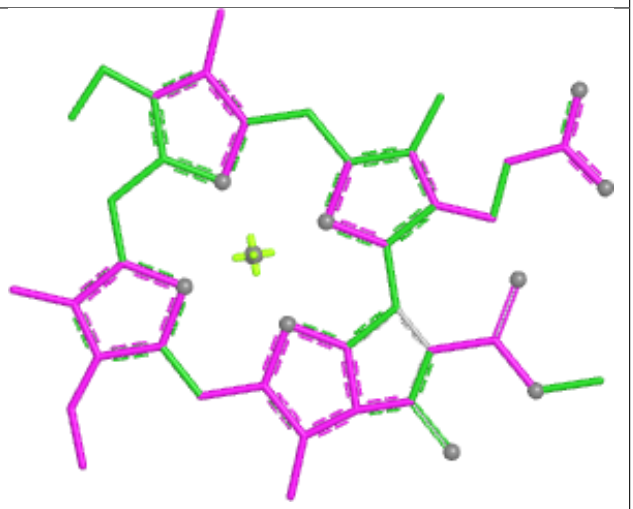
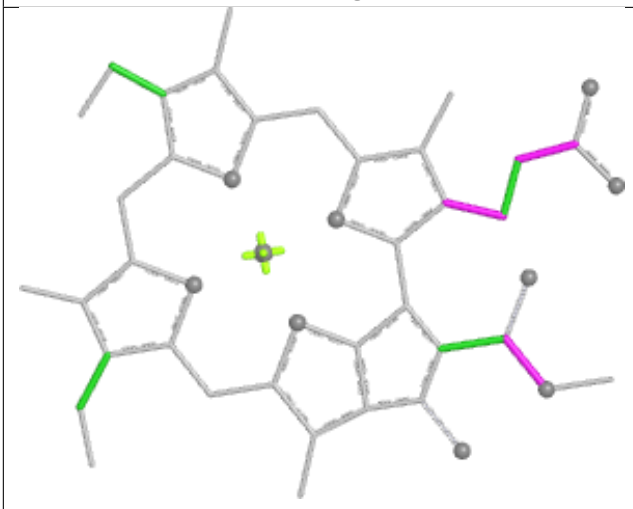


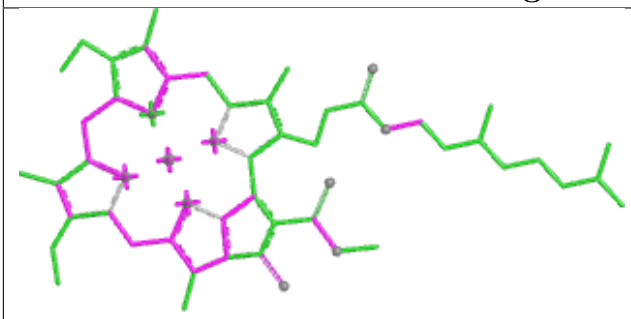
Bond angles



Torsions

Rings

Ligand CLA H 815



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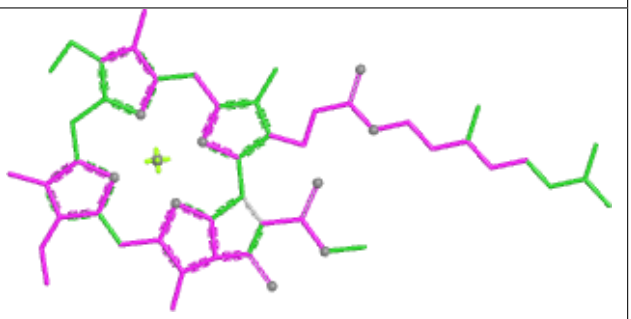
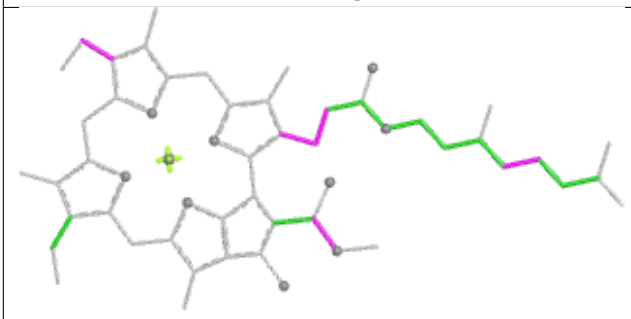
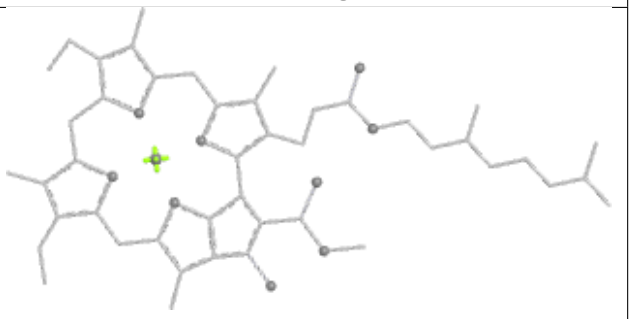


Bond angles

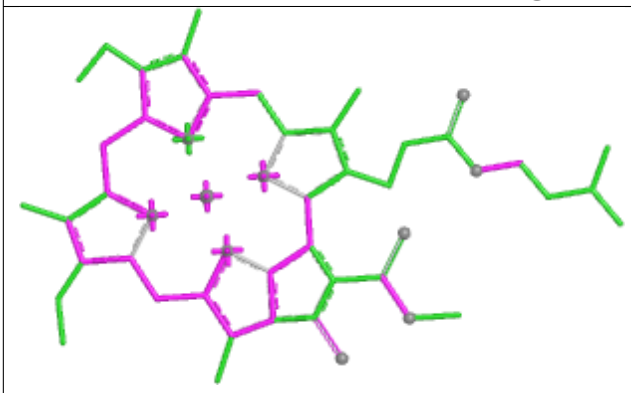


Torsions



Rings

Ligand CLA a 836



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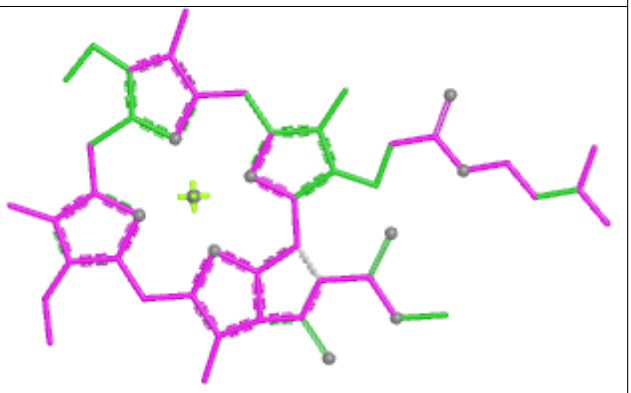
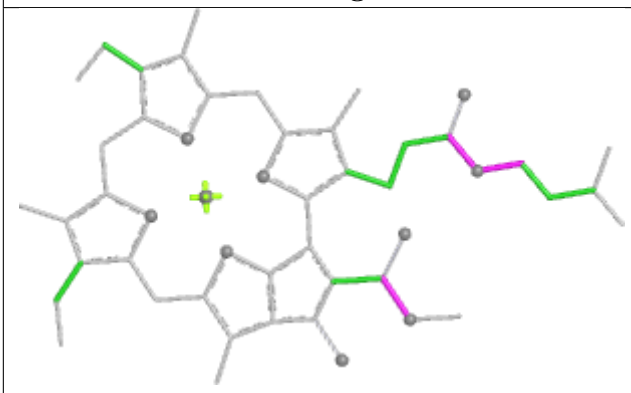


Bond angles



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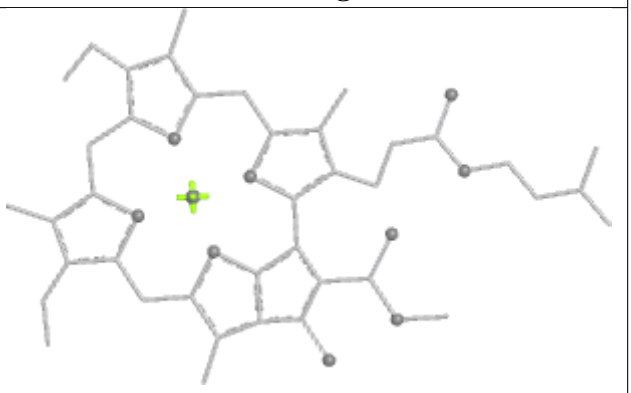
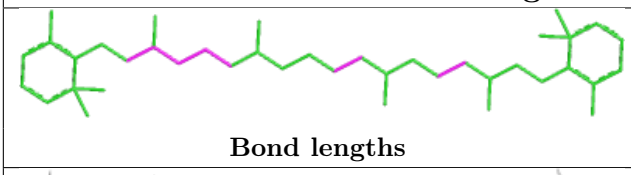
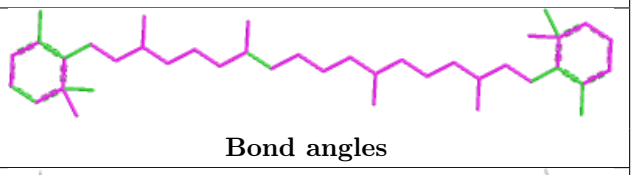
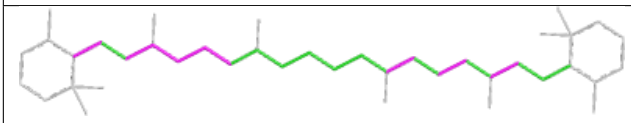


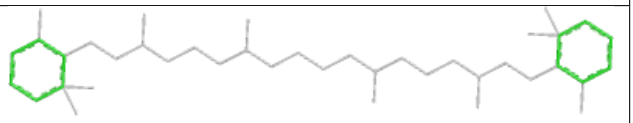
Rings

Ligand BCR P 202

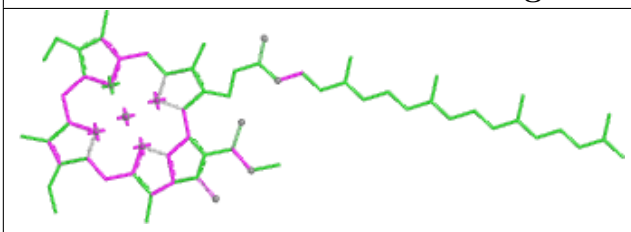

Bond lengths

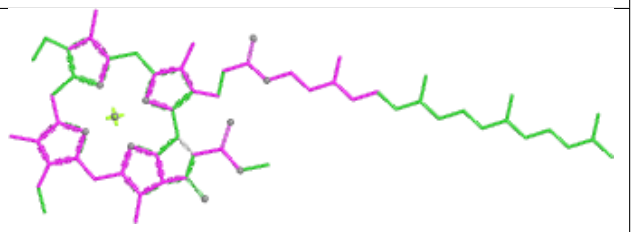

Bond angles

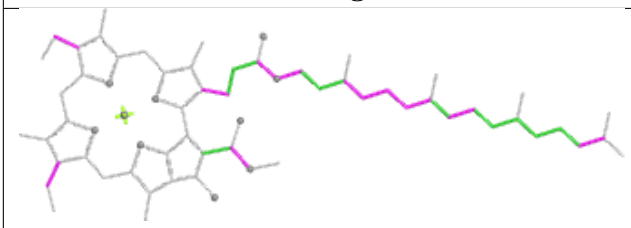

Torsions

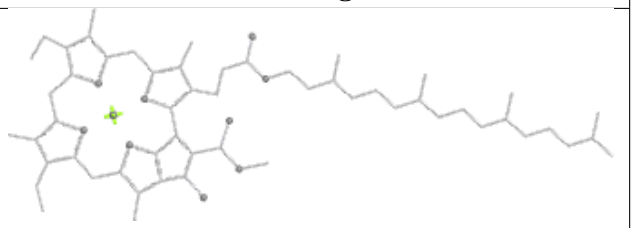

Rings

Ligand CLA B 837

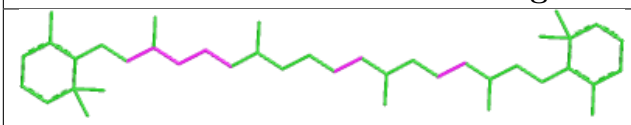

Bond lengths

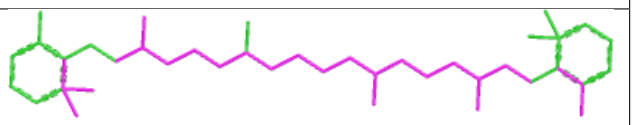

Bond angles

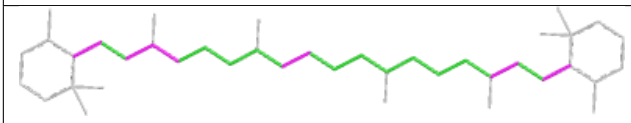

Torsions


Rings

Ligand BCR i 102


Bond lengths


Bond angles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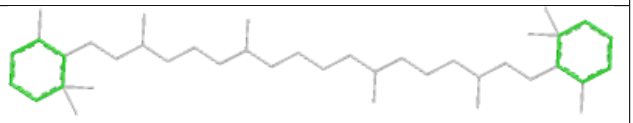
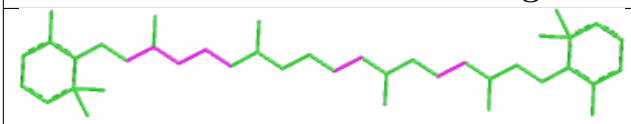
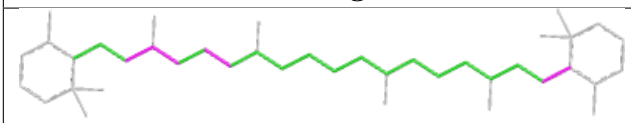
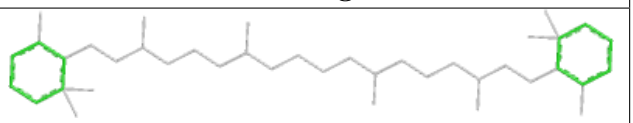

Rings

Ligand BCR A 845

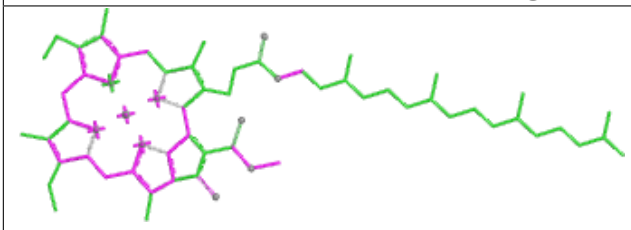

Bond lengths

Bond angles


Torsions


Rings

Ligand CLA B 829



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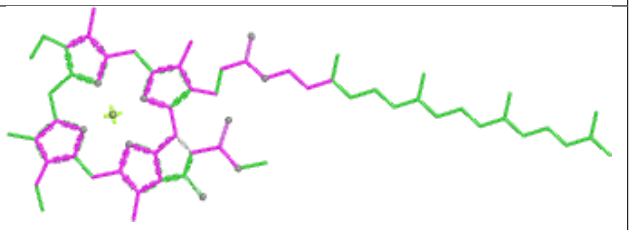
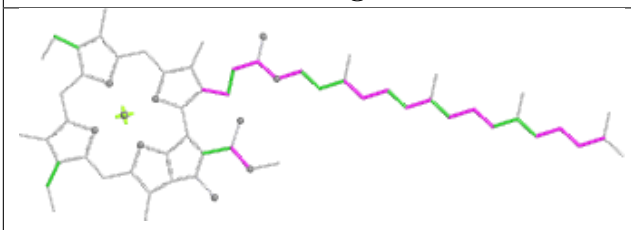


Bond angles



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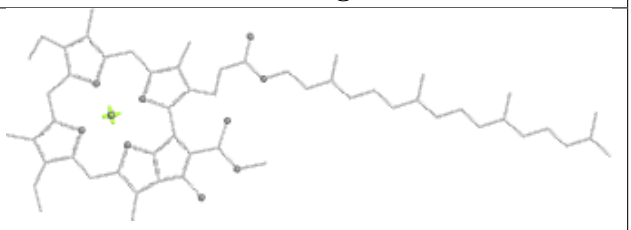
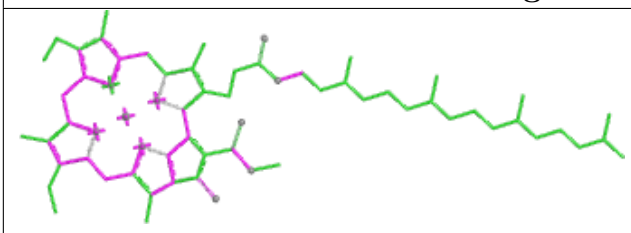


Rings

Ligand CLA H 823



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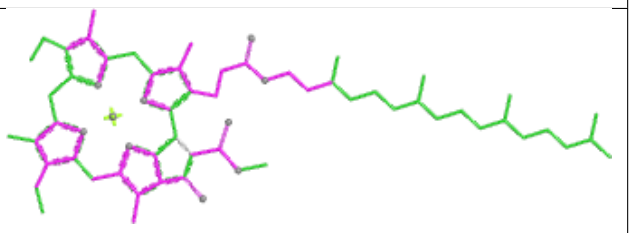
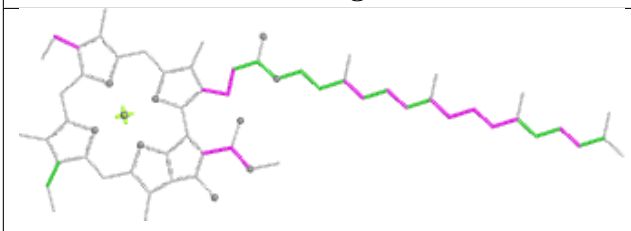
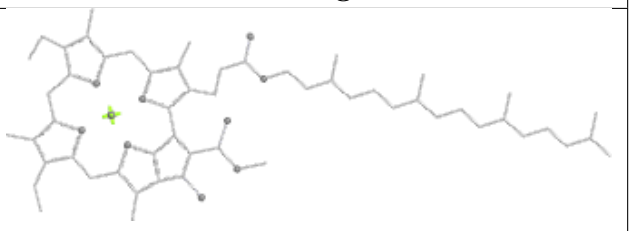


Bond angles

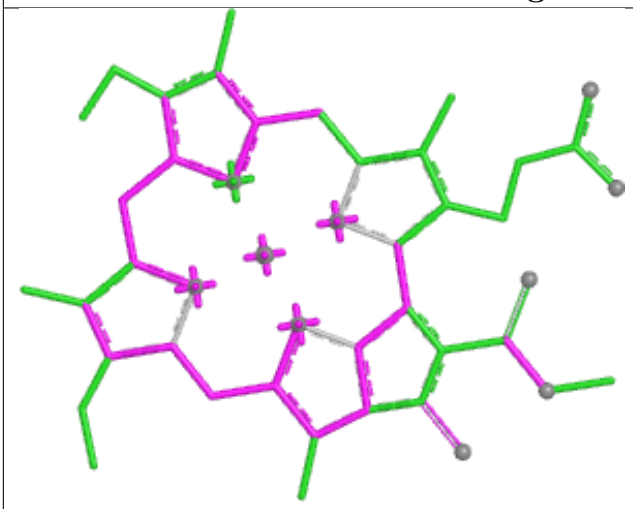


Torsions

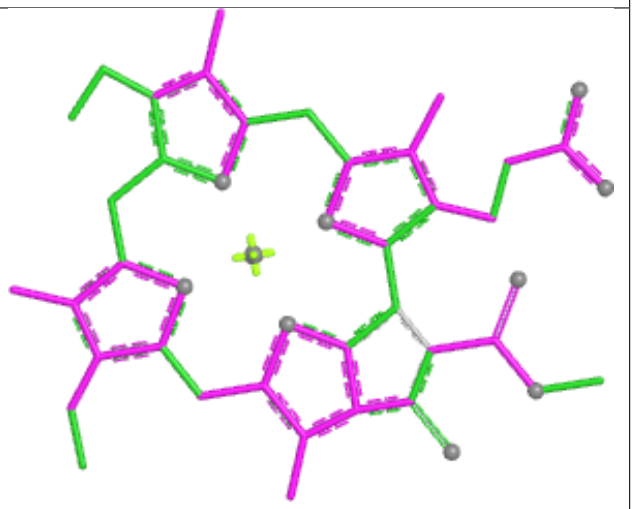


Rings

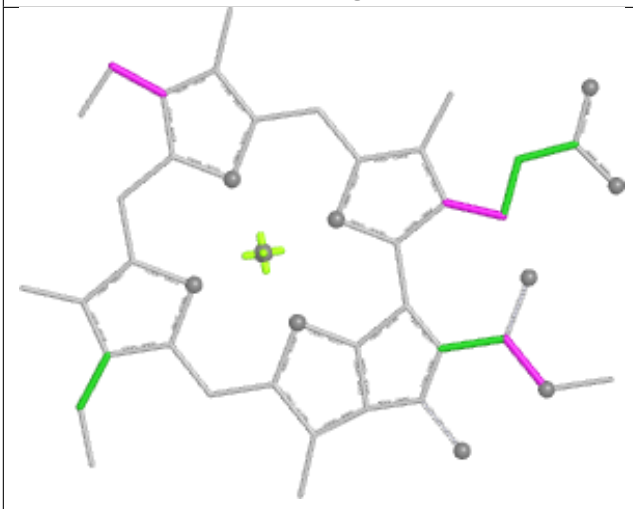
Ligand CLA b 818



Bond lengths



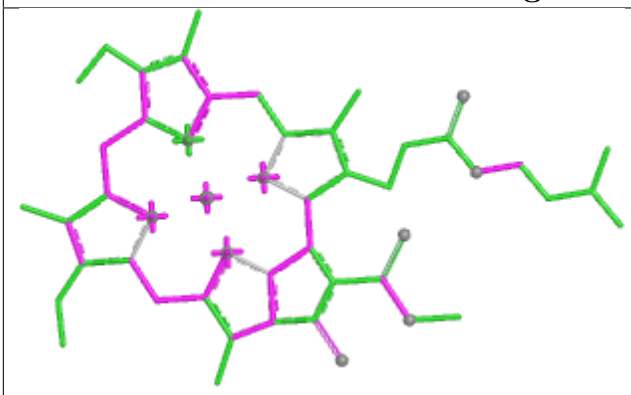
Bond angles



Torsions

Rings

Ligand CLA A 840



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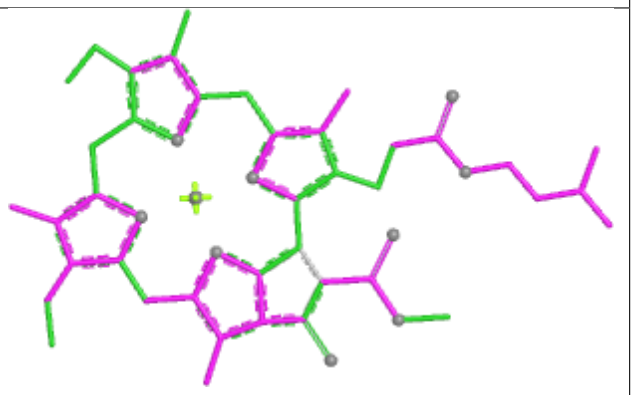

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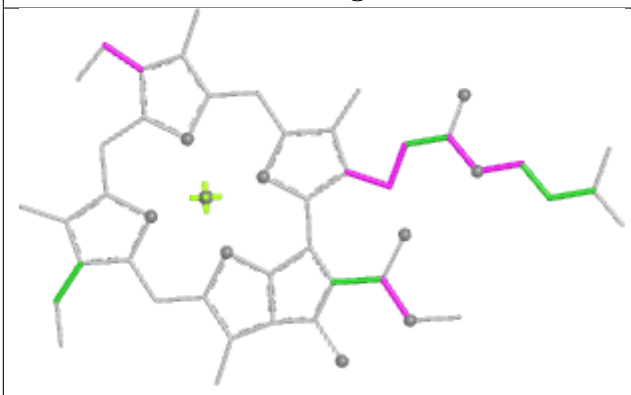

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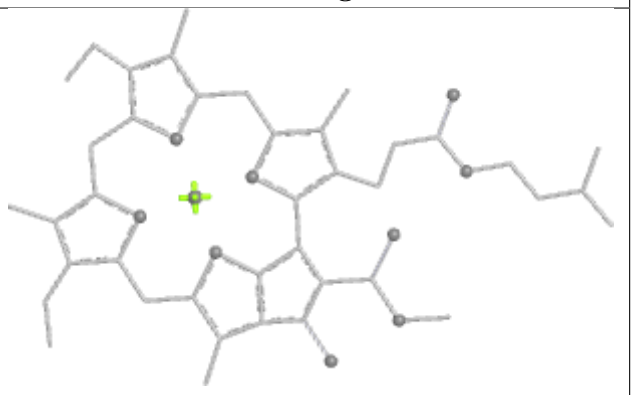
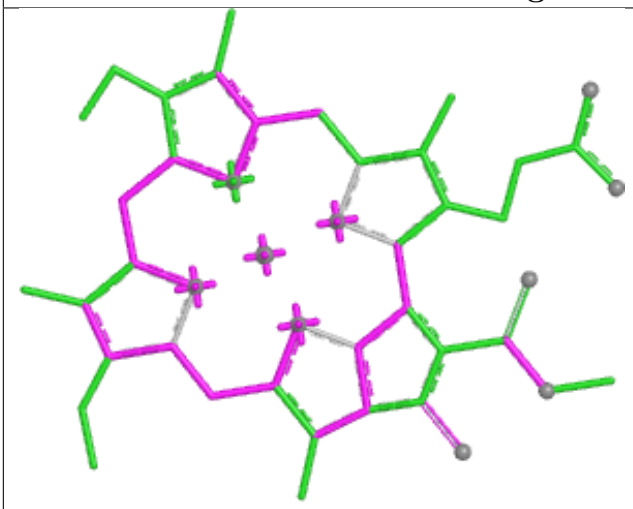


Rings

Ligand CLA b 812



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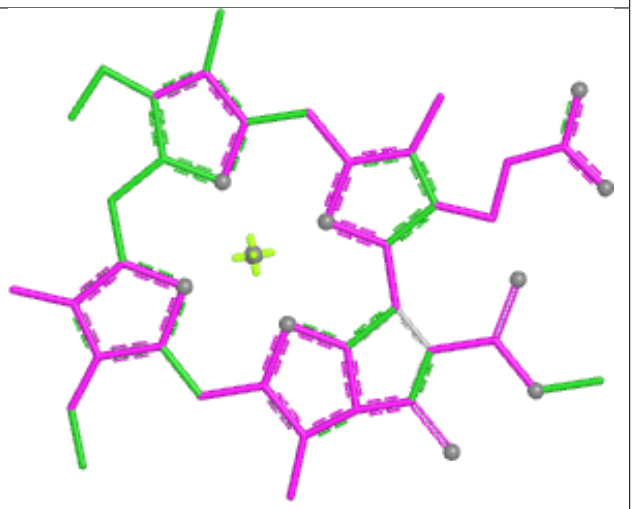

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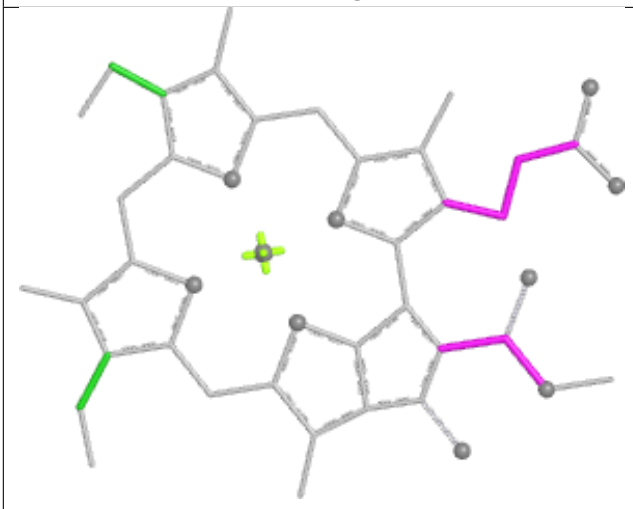
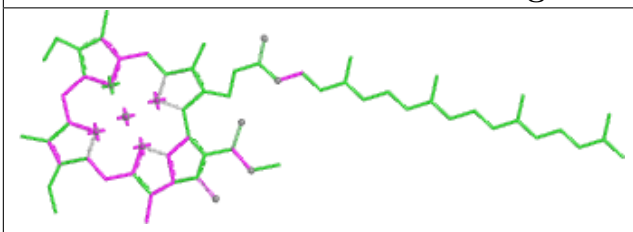


Torsions

Rings

Ligand CL0 G 801



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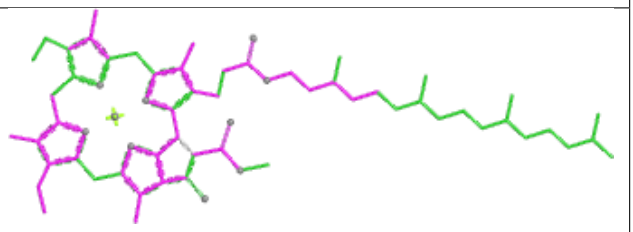
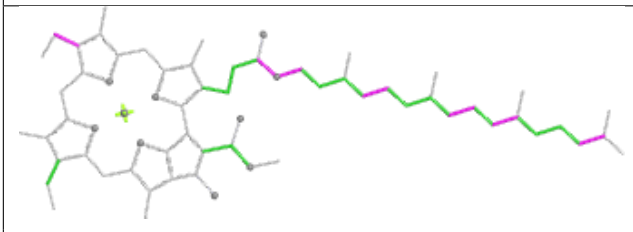


Bond angles



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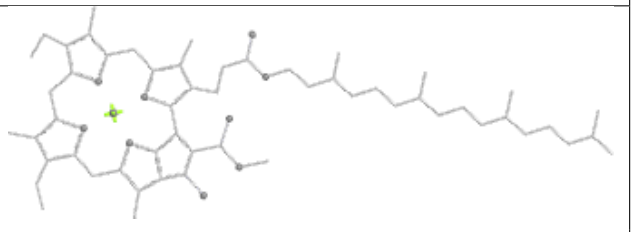
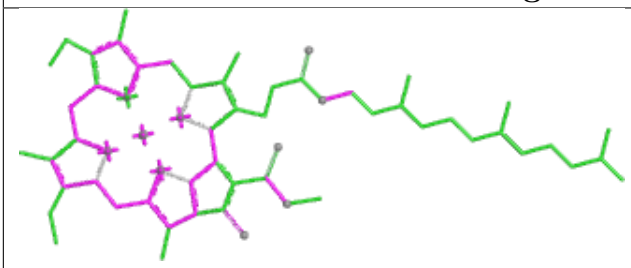
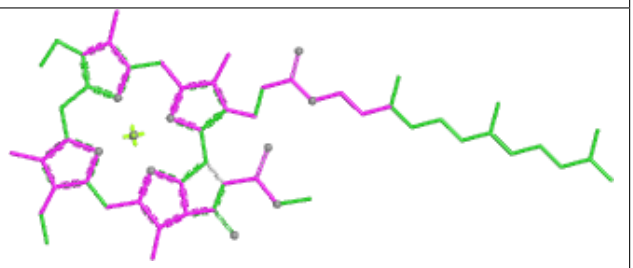


Rings

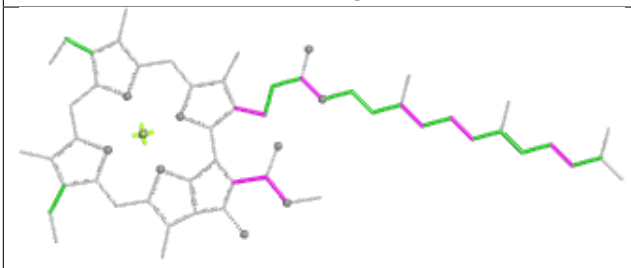
Ligand CLA H 812



Bond lengths



Bond angles



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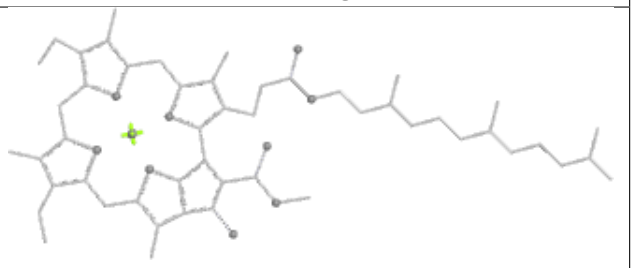
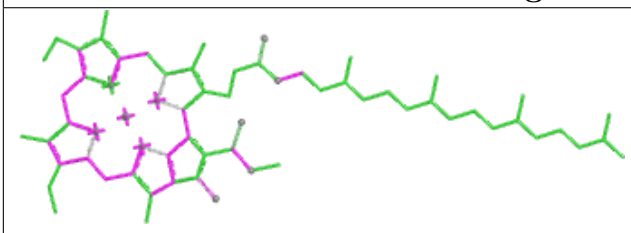


Rings

Ligand CLA P 201



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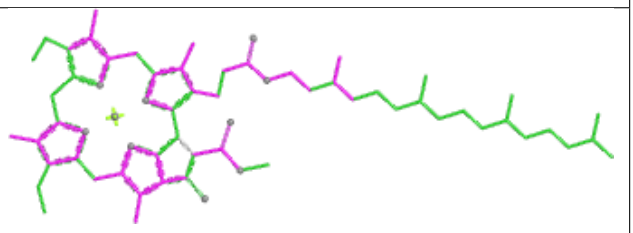
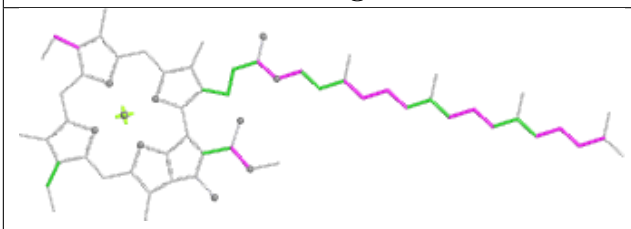


Bond angles



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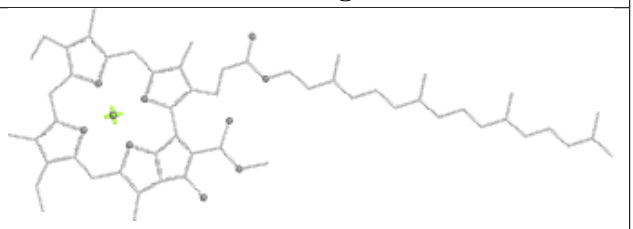
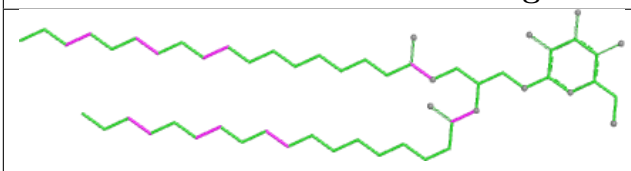


Rings

Ligand LMG b 845



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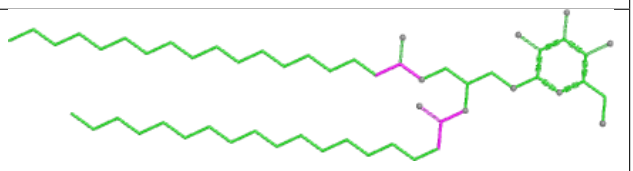
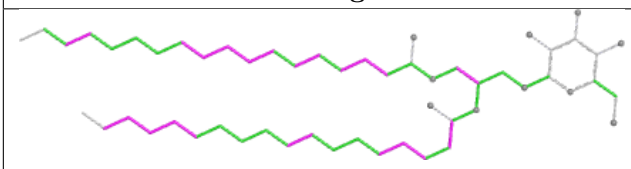


Bond angles



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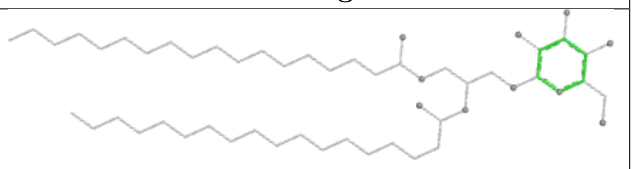
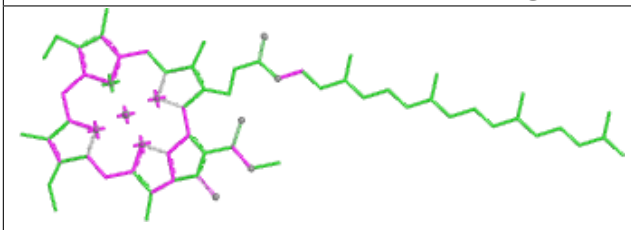


Rings

Ligand CLA B 821



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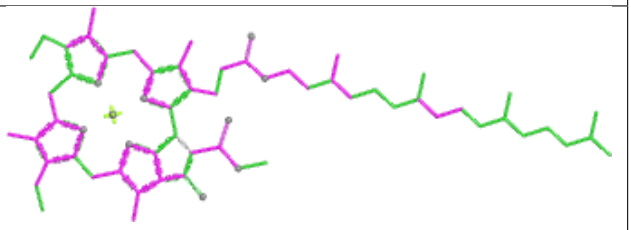
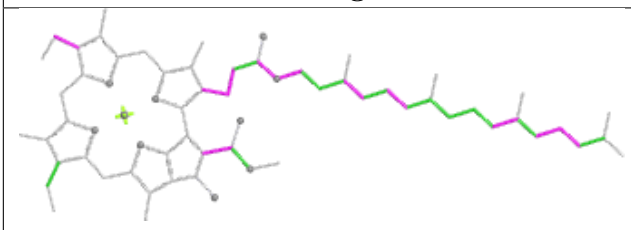
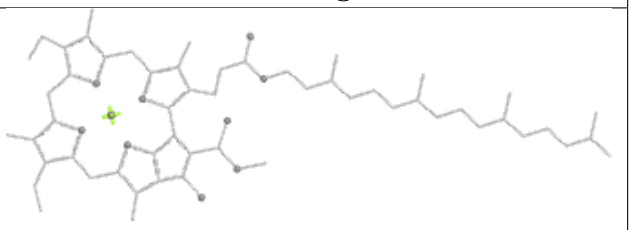


Bond angles

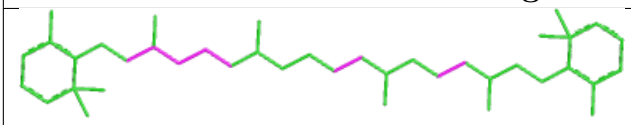


Torsions



Rings

Ligand BCR R 102



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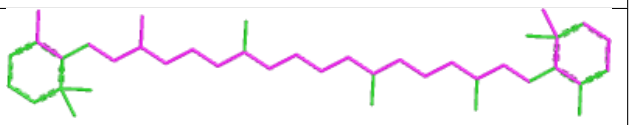
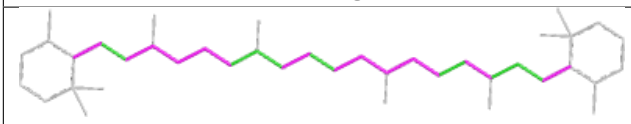


Bond angles



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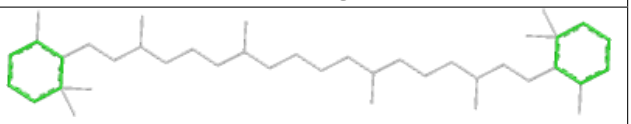
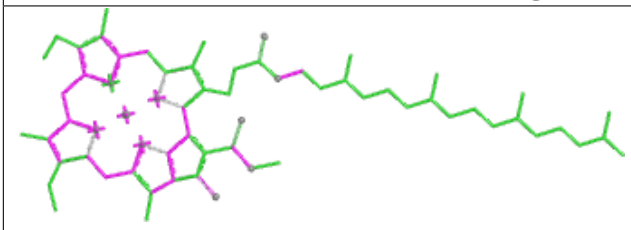
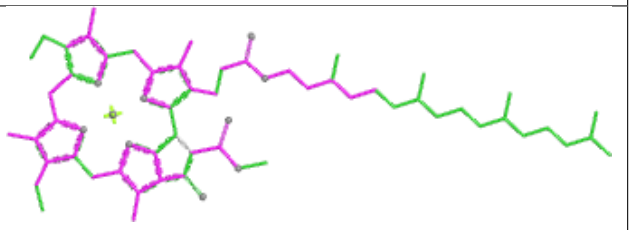


Rings

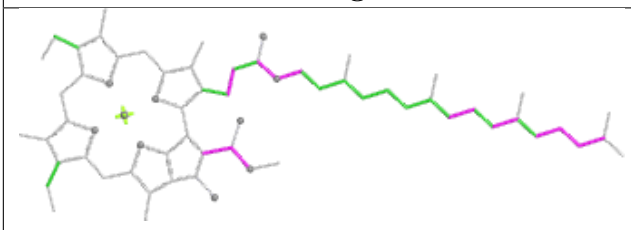
Ligand CLA b 837



Bond lengths



Bond angles



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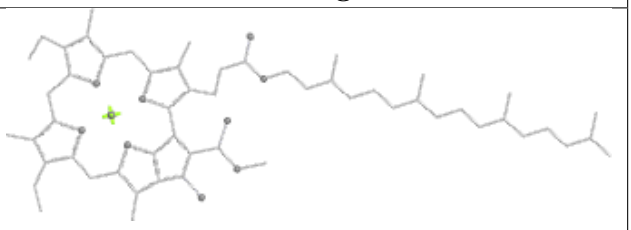
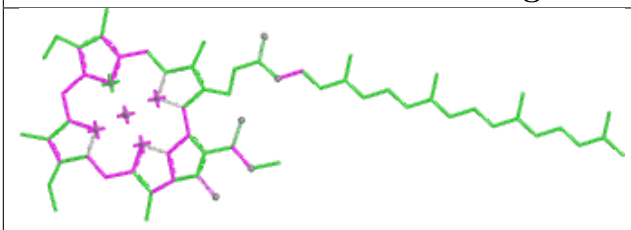
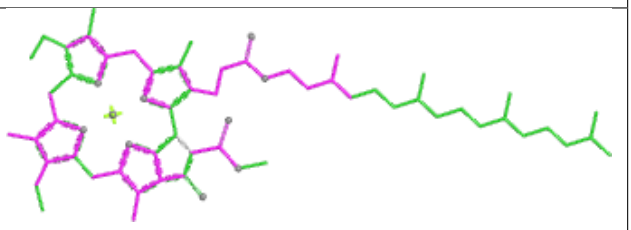


Rings

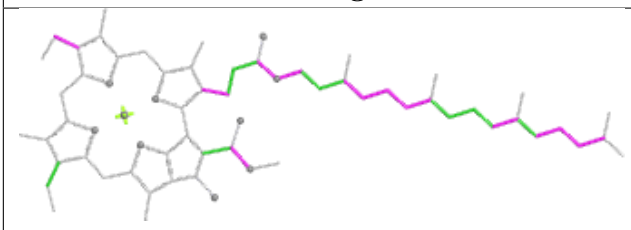
Ligand CLA G 834



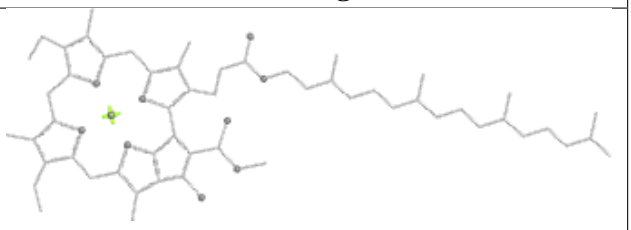
Bond lengths



Bond angles

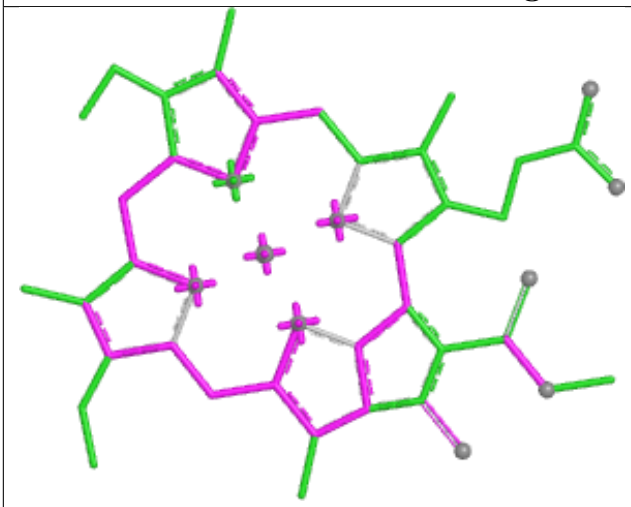


Torsions

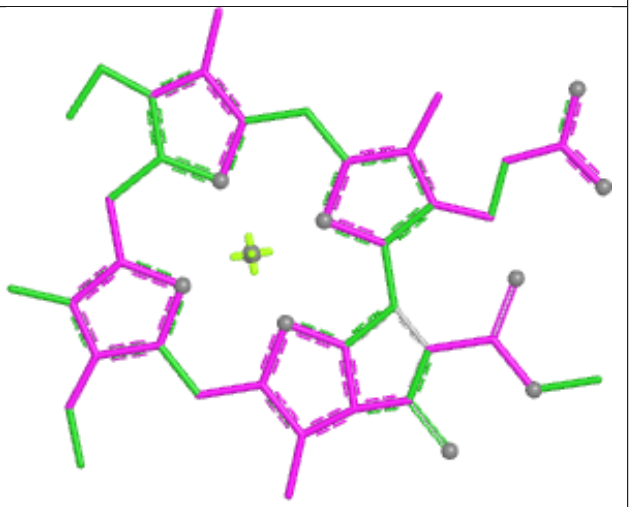


Rings

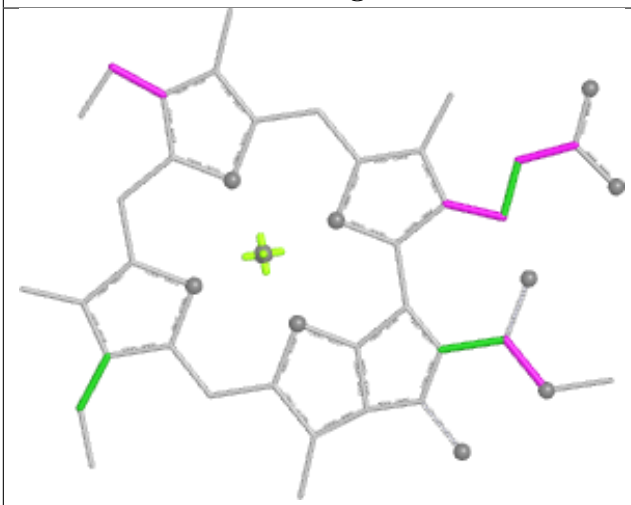
Ligand CLA H 833



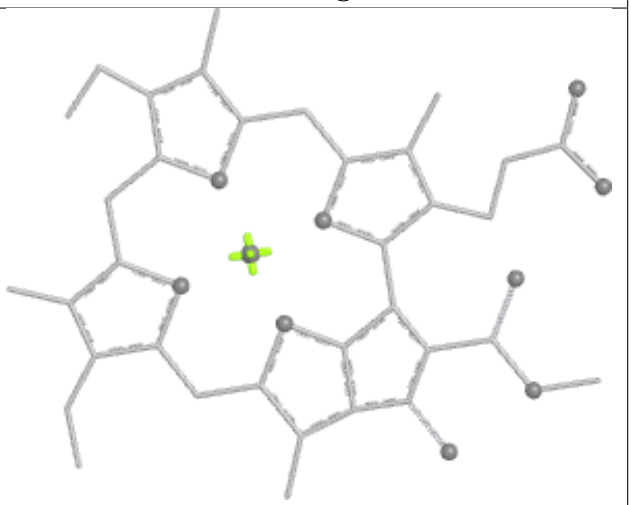
Bond lengths



Bond angles

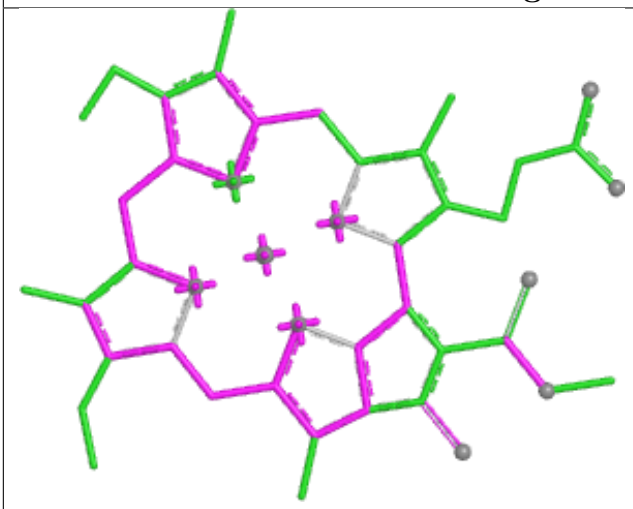


Torsions

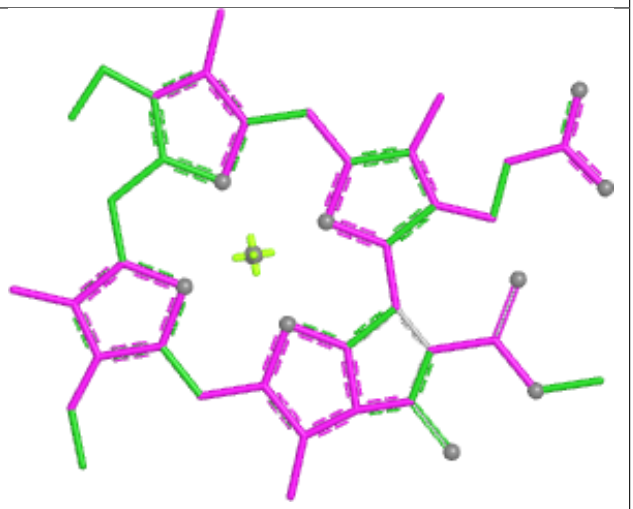


Rings

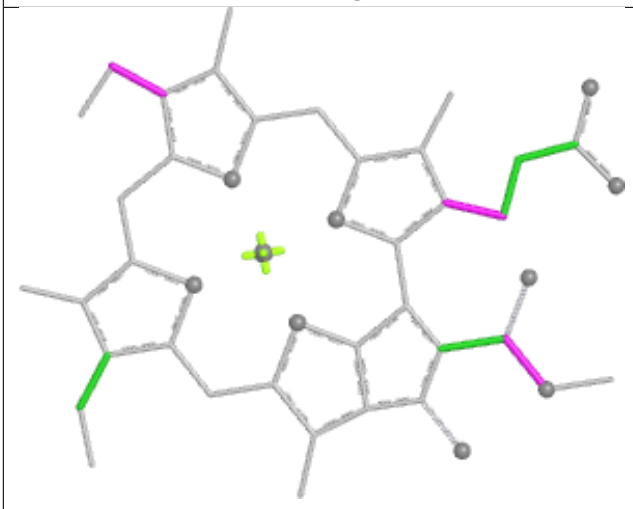
Ligand CLA A 815



Bond lengths



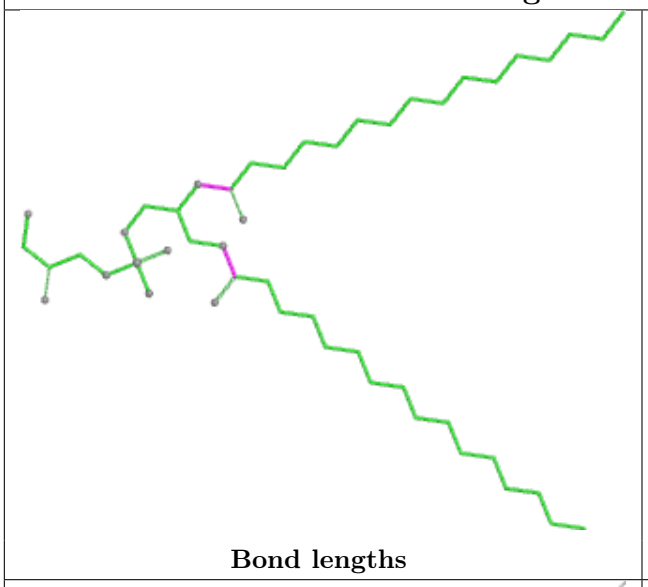
Bond angles



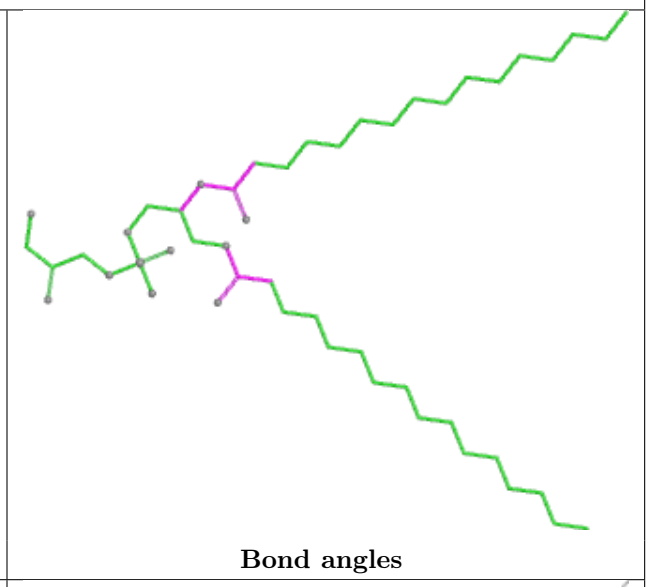
Torsions

Rings

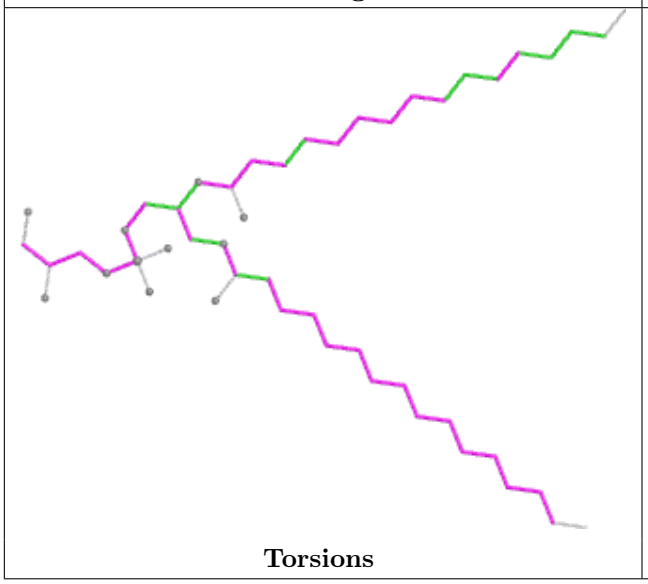
Ligand LHG A 853



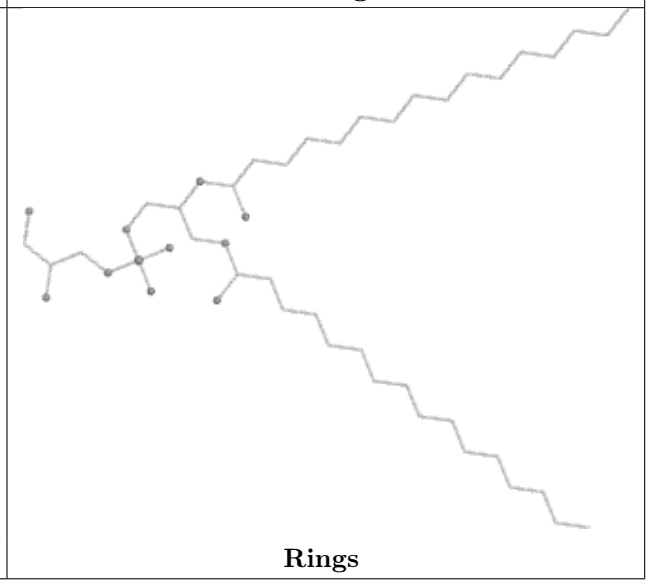
Bond lengths



Bond angles

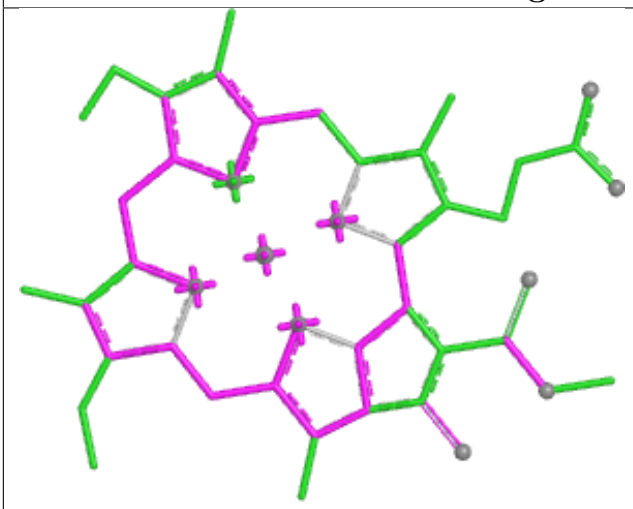


Torsions

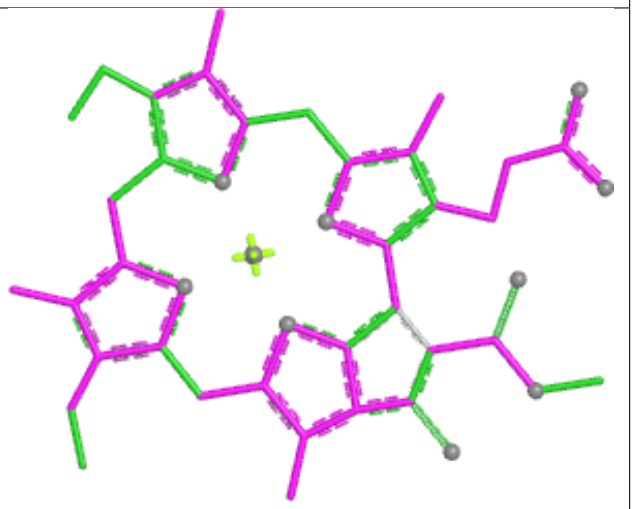


Rings

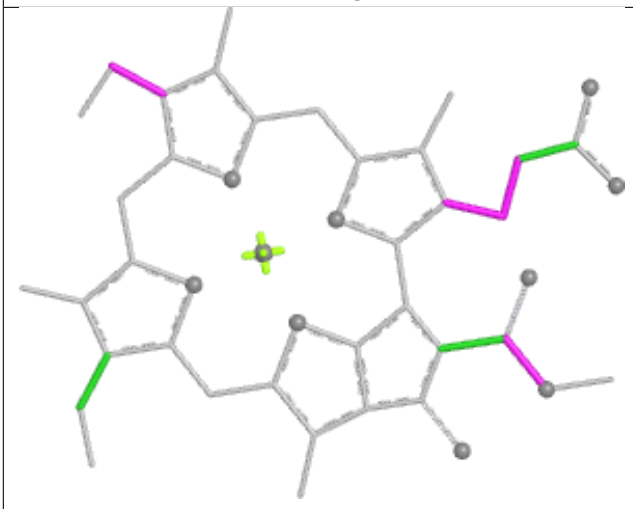
Ligand CLA a 835



Bond lengths



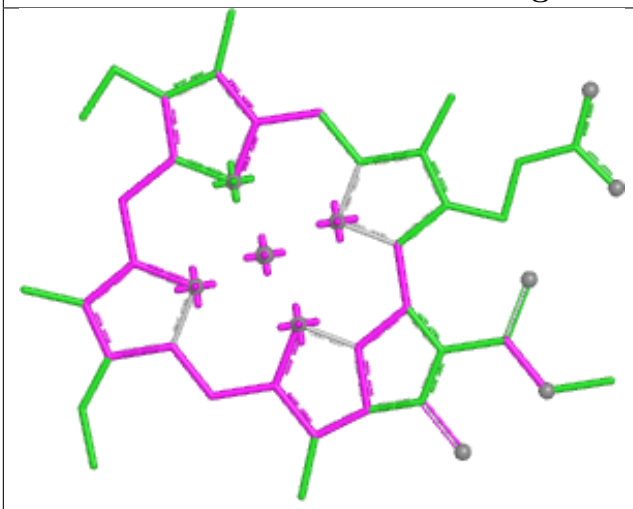
Bond angles



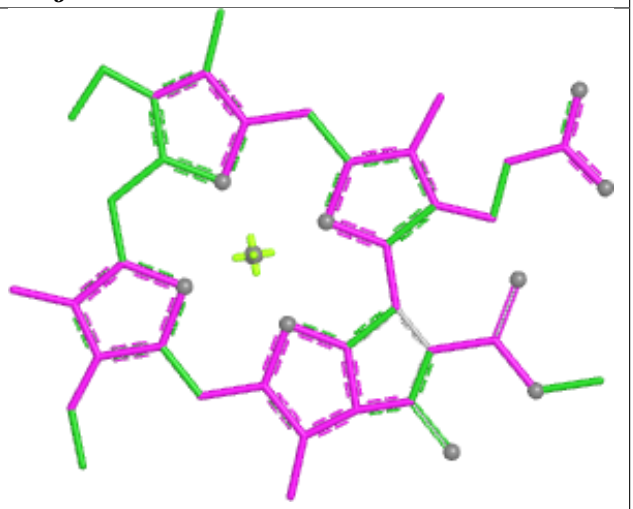
Torsions

Rings

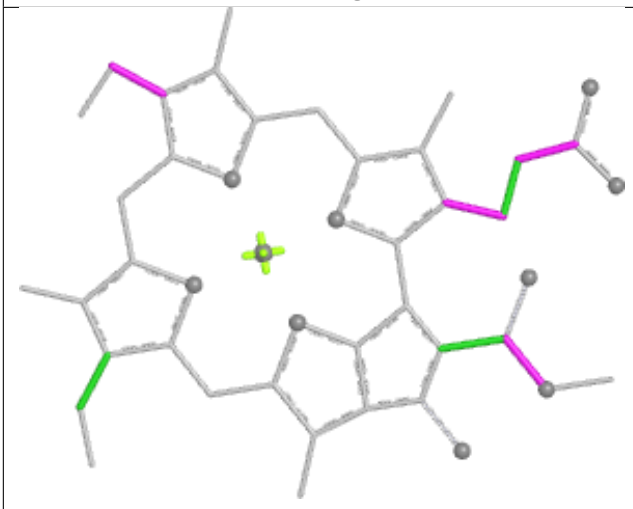
Ligand CLA j 104



Bond lengths



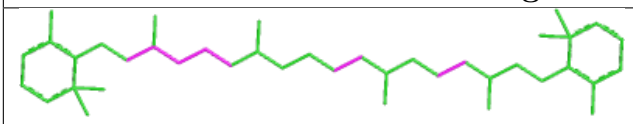
Bond angles



Torsions

Rings

Ligand BCR Q 101



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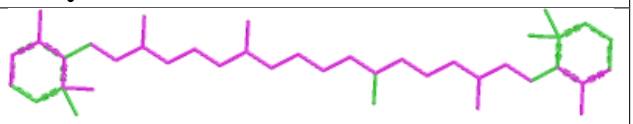
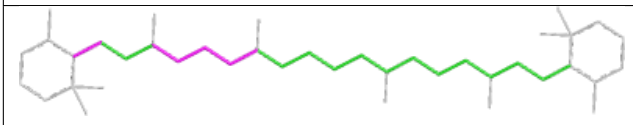
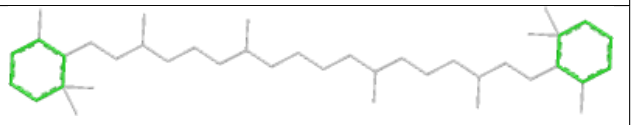


Bond angles

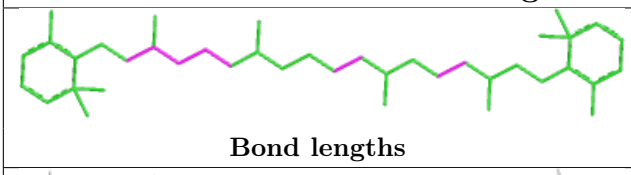


Torsions

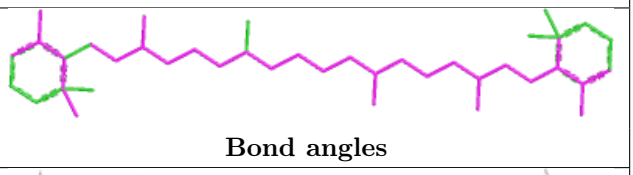


Rings

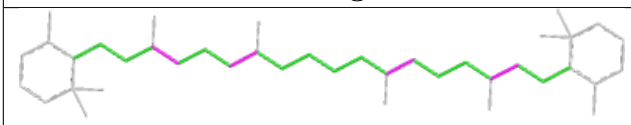
Ligand BCR H 842



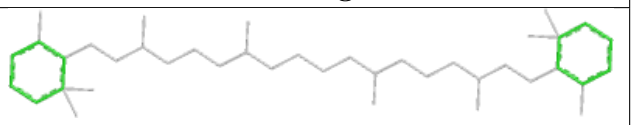
Bond lengths



Bond angles

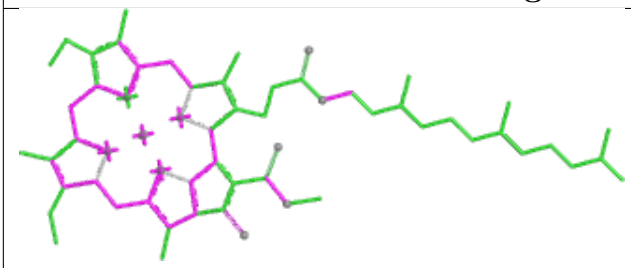


Torsions



Rings

Ligand CLA B 815



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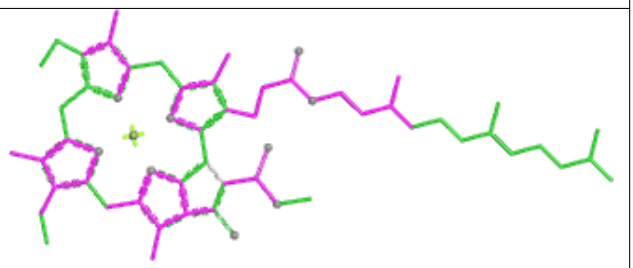
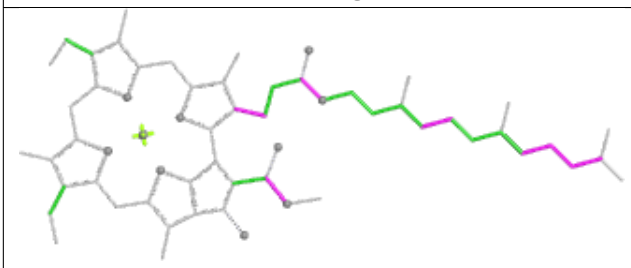
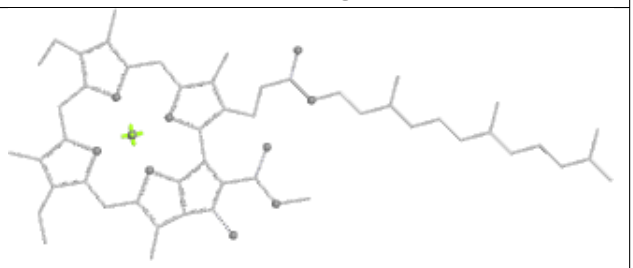


Bond angles

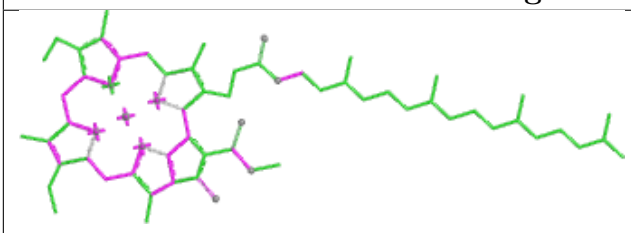


Torsions

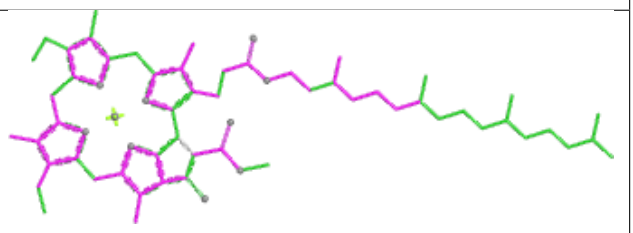


Rings

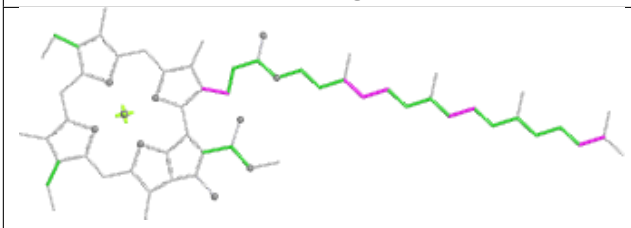
Ligand CLA B 807



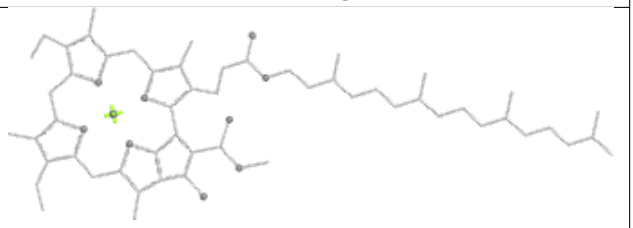
Bond lengths



Bond angles

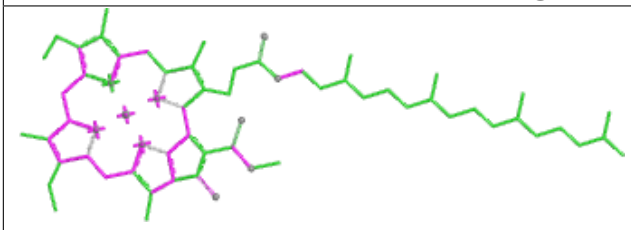


Torsions

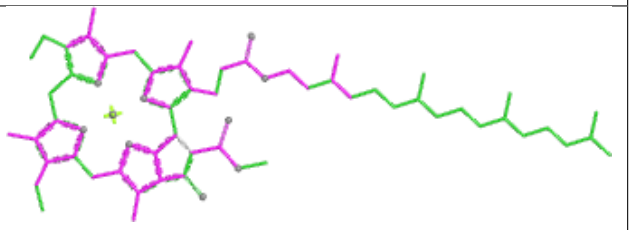


Rings

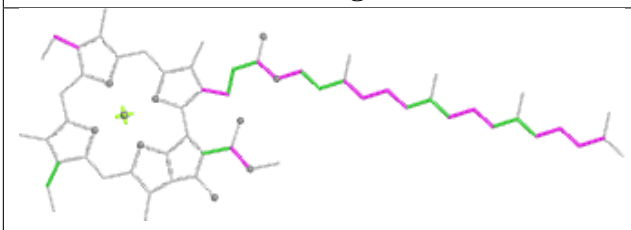
Ligand CLA f 201



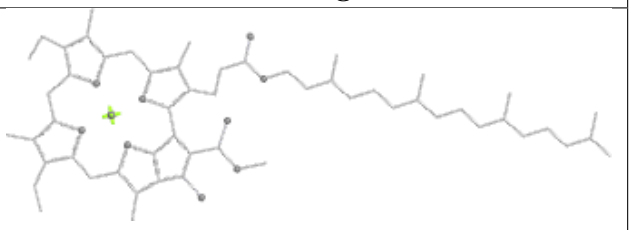
Bond lengths



Bond angles

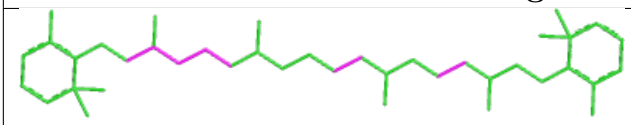


Torsions



Rings

Ligand BCR a 846



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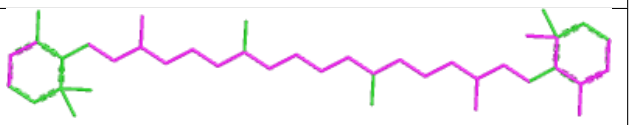
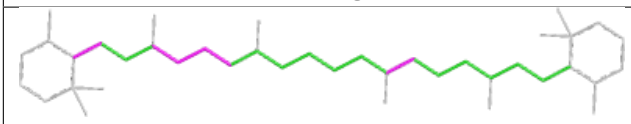
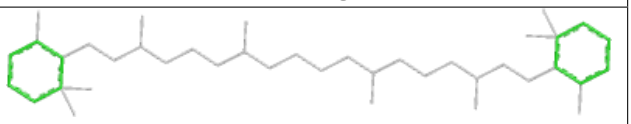


Bond angles

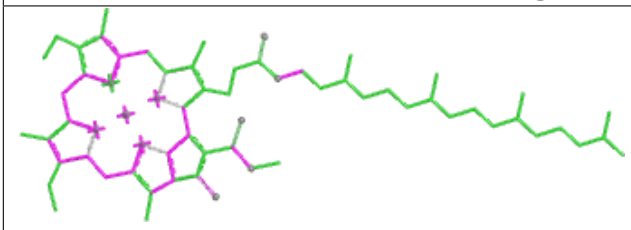


Torsions

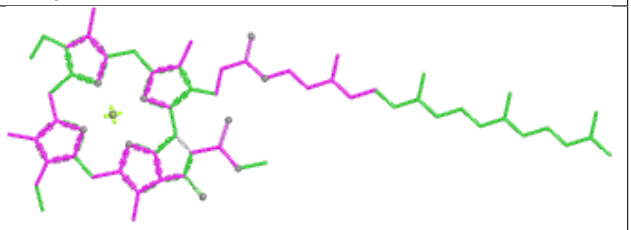


Rings

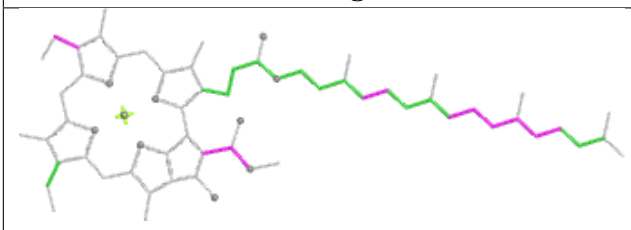
Ligand CLA j 102



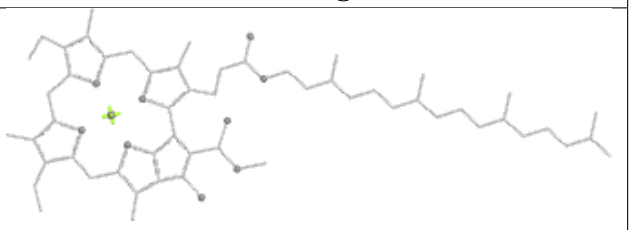
Bond lengths



Bond angles

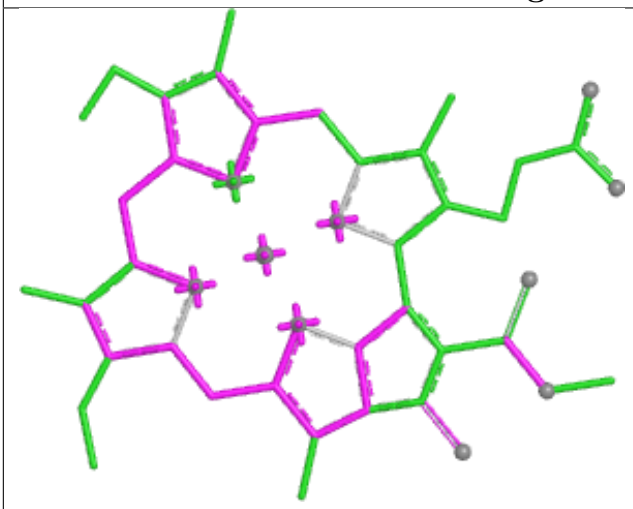


Torsions

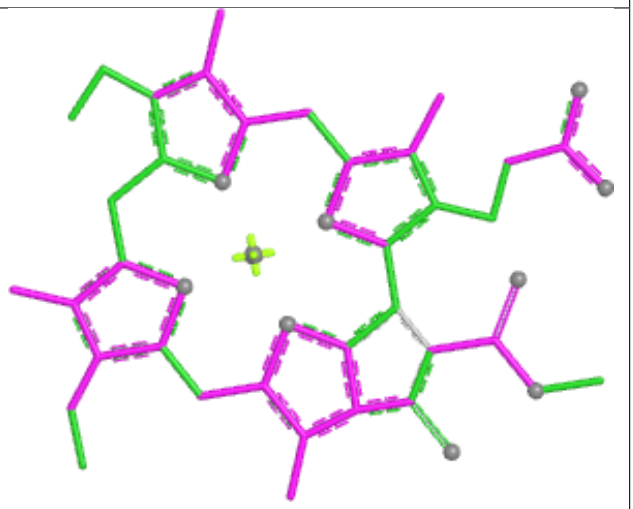


Rings

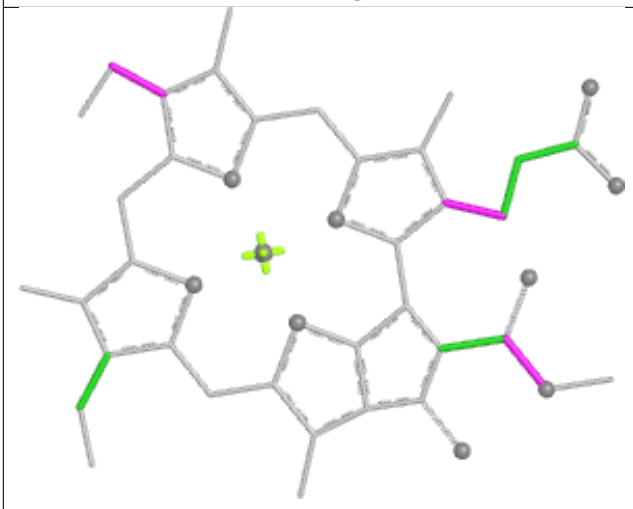
Ligand CLA b 827



Bond lengths



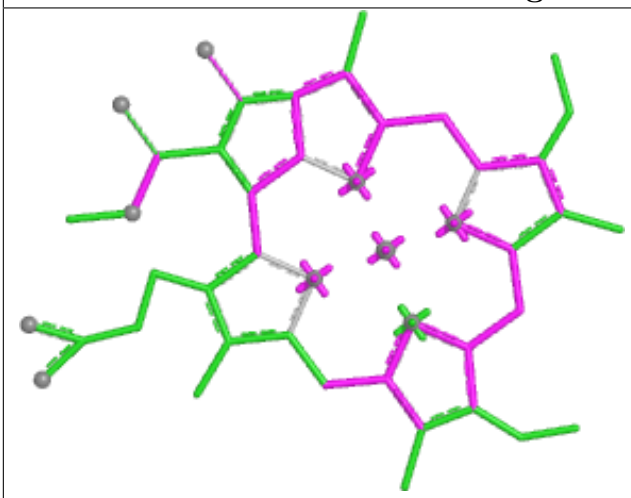
Bond angles



Torsions

Rings

Ligand CLA F 203



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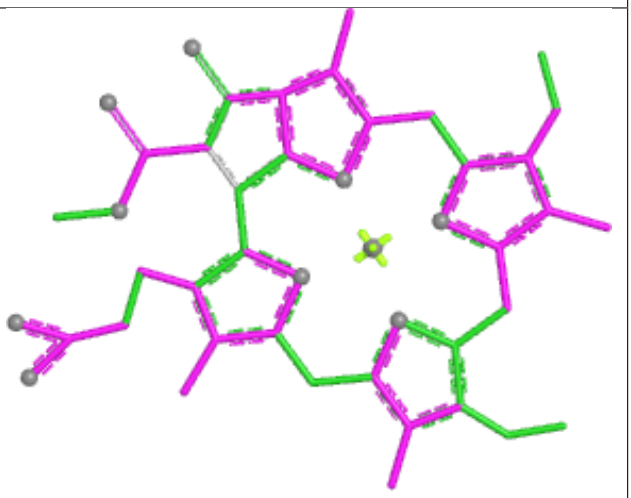
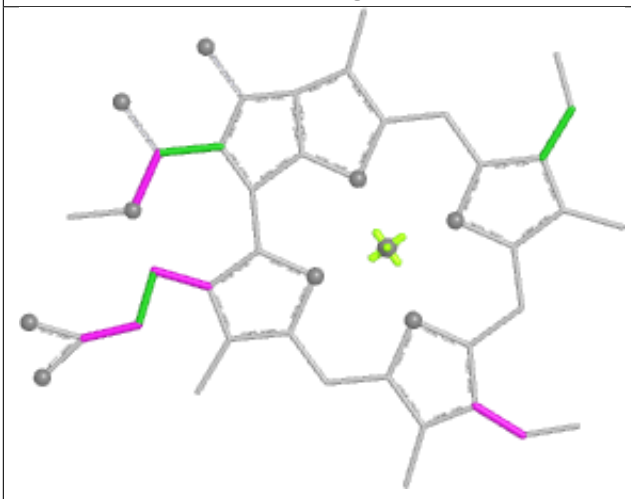
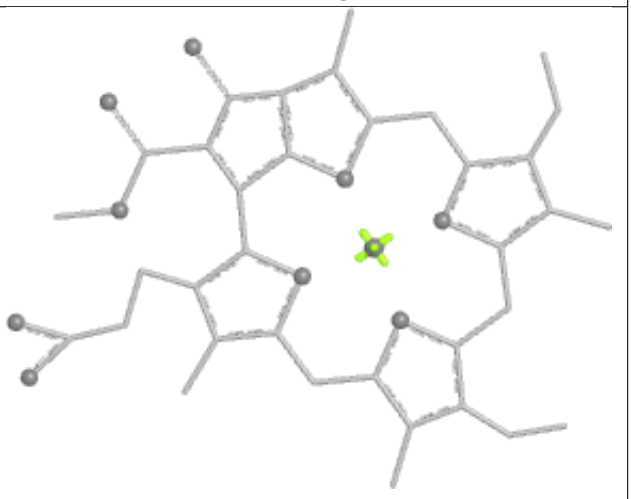


Bond angles

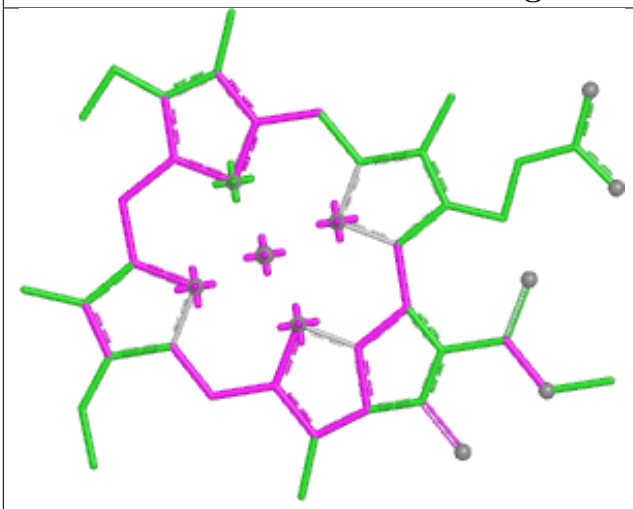


Torsions

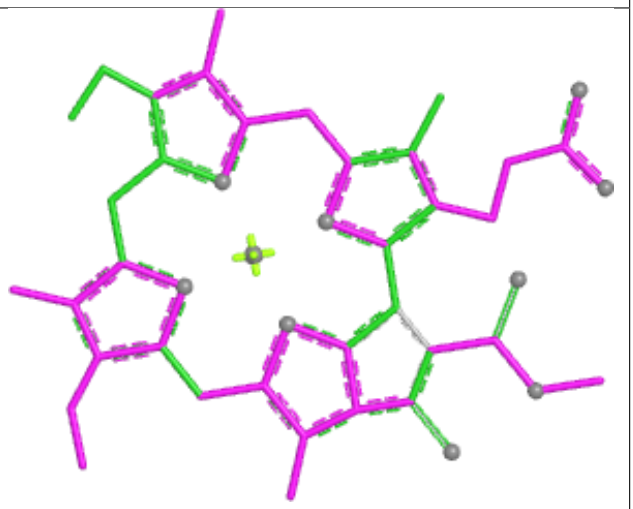


Rings

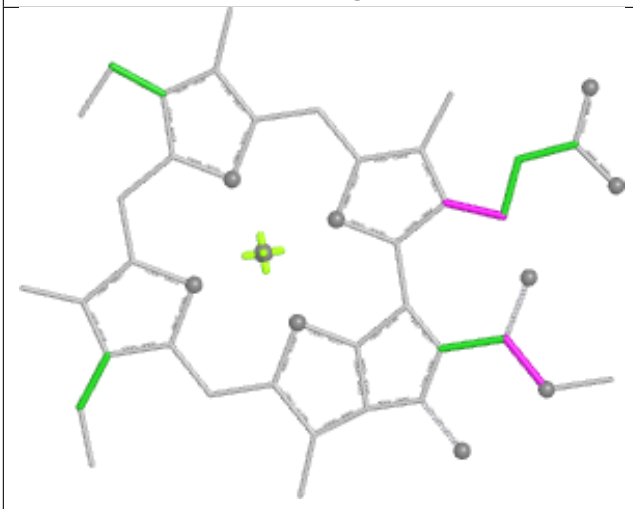
Ligand CLA B 820



Bond lengths



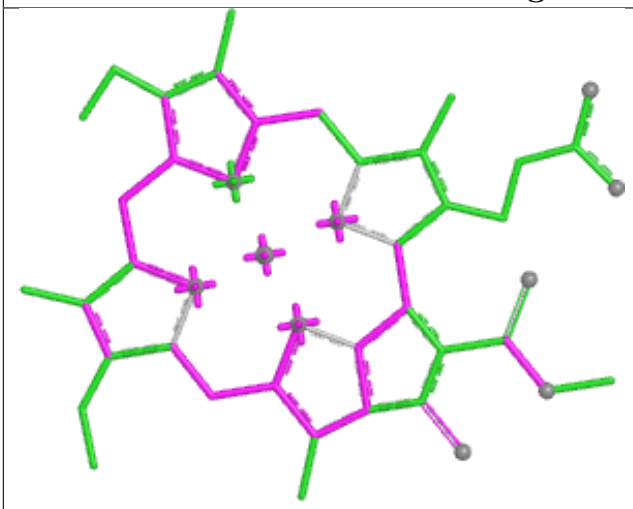
Bond angles



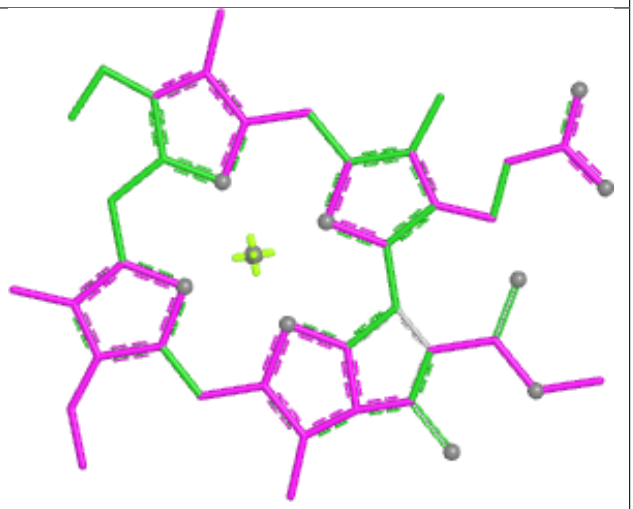
Torsions

Rings

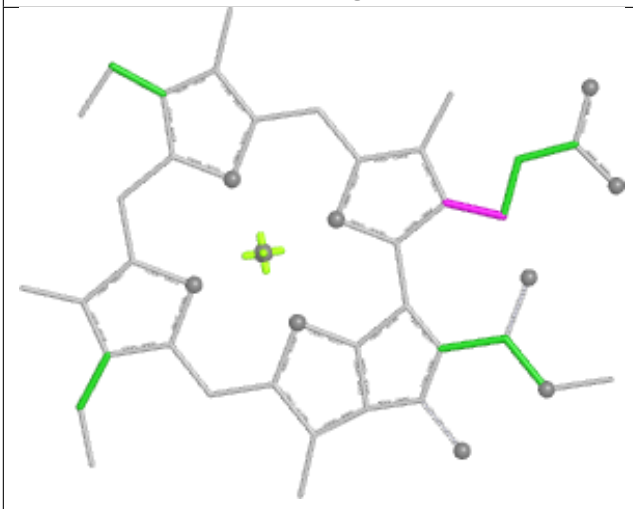
Ligand CLA b 820



Bond lengths



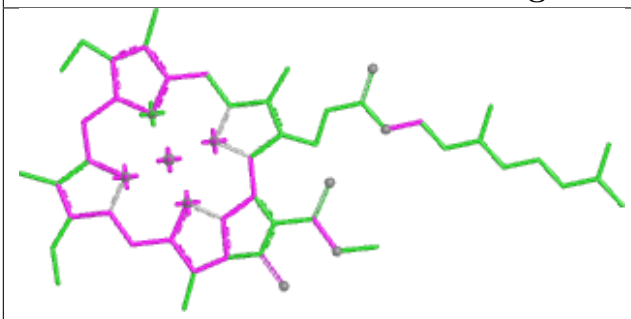
Bond angles



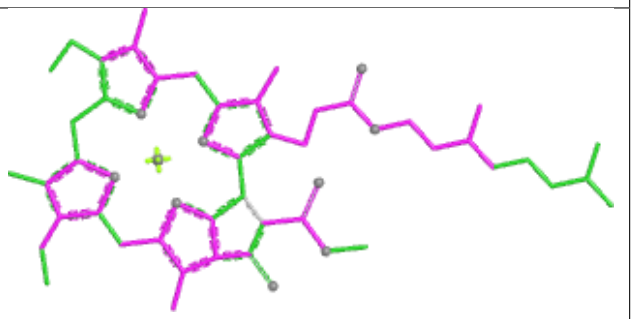
Torsions

Rings

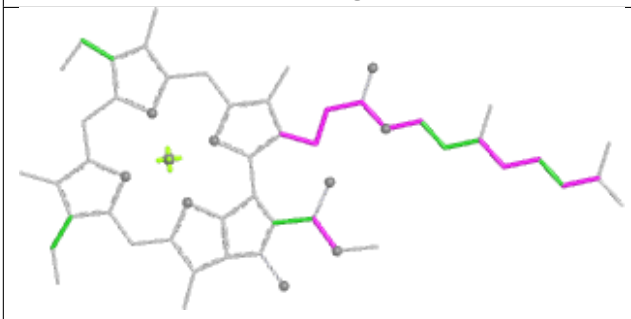
Ligand CLA a 817



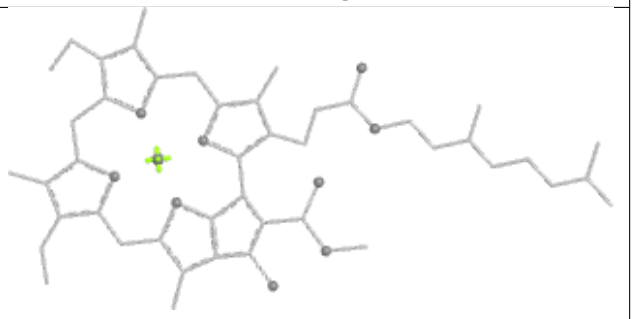
Bond lengths



Bond angles

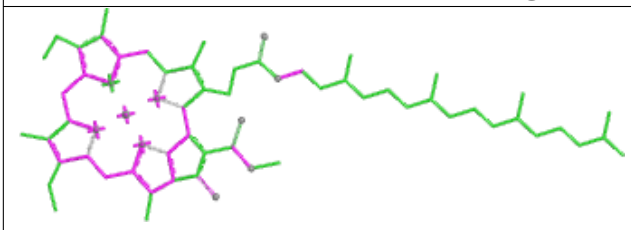


Torsions



Rings

Ligand CLA G 832



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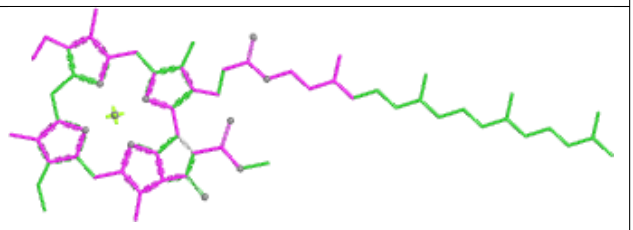
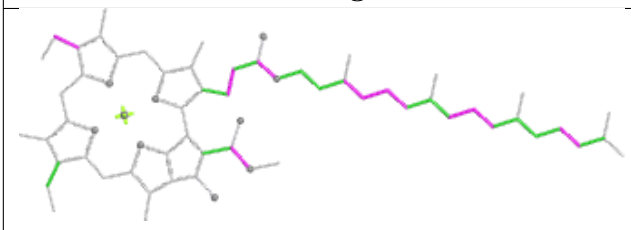
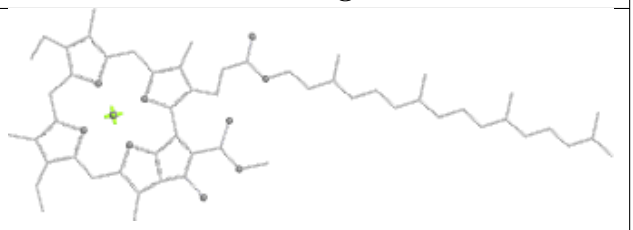


Bond angles

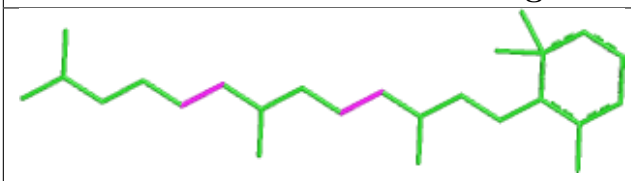


Torsions

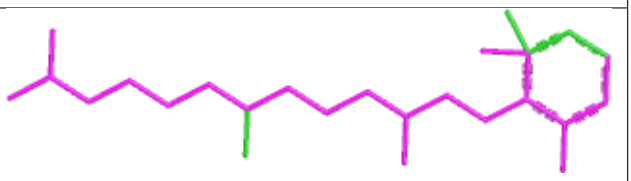


Rings

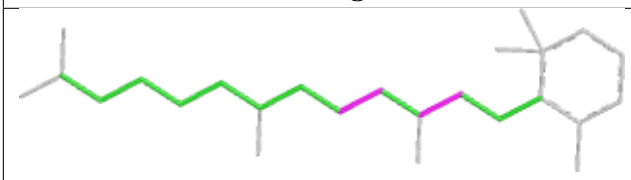
Ligand BCR b 842



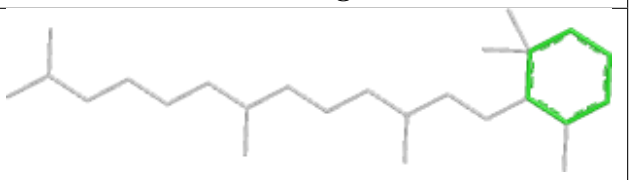
Bond lengths



Bond angles

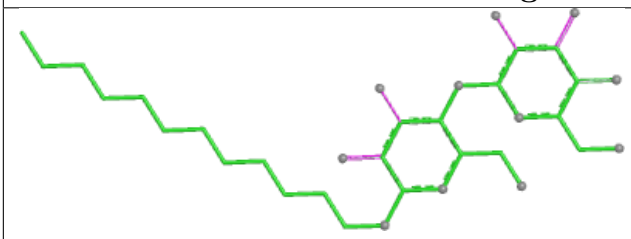


Torsions

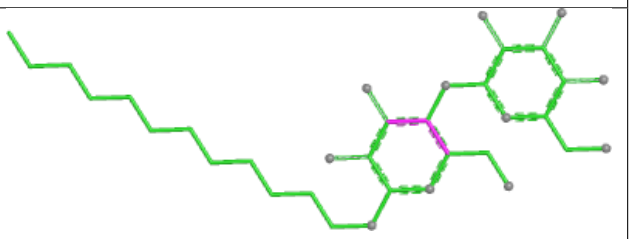


Rings

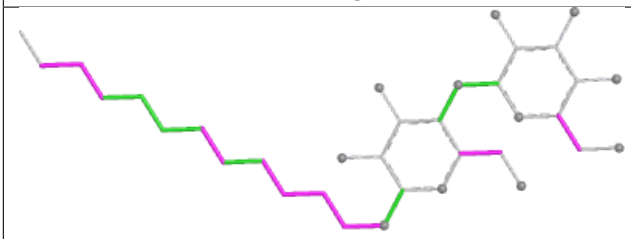
Ligand LMT H 848



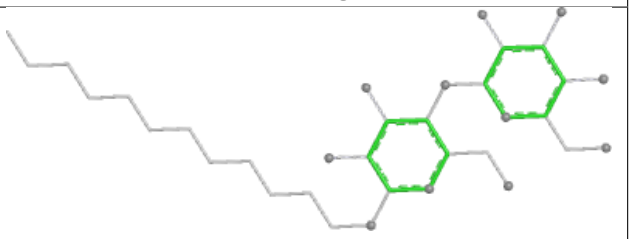
Bond lengths



Bond angles

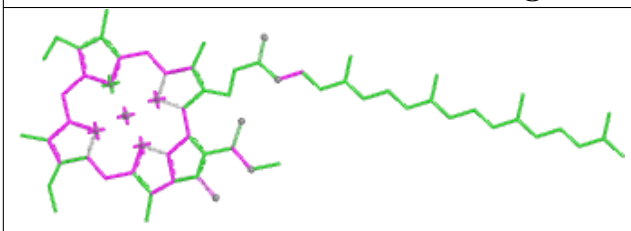


Torsions

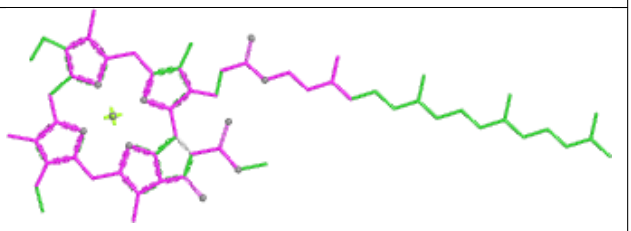


Rings

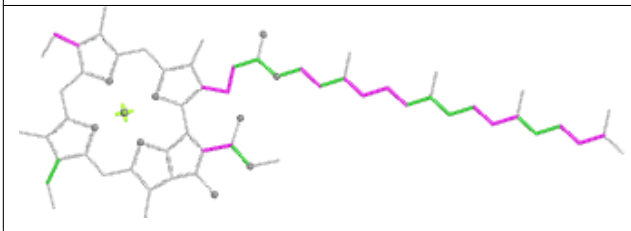
Ligand CLA A 854



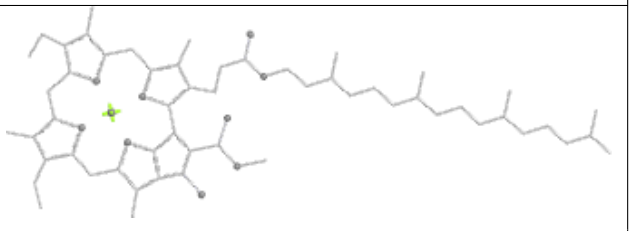
Bond lengths



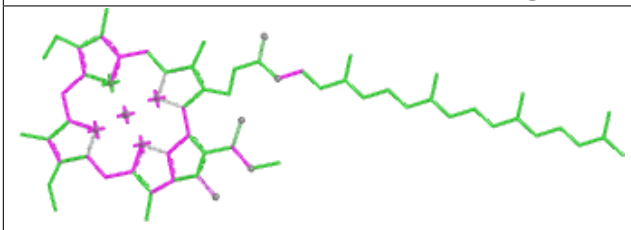
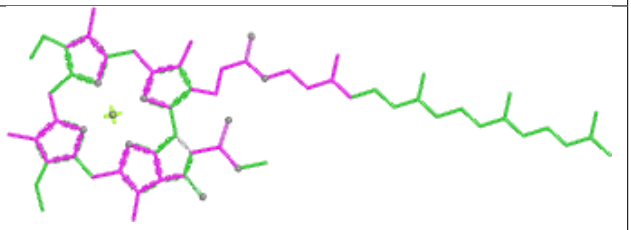
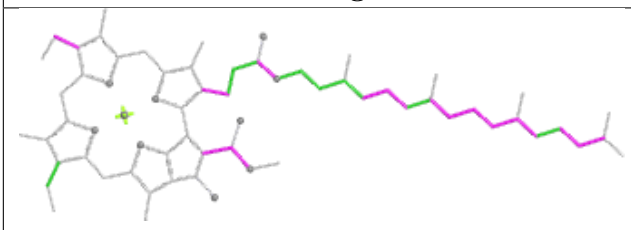
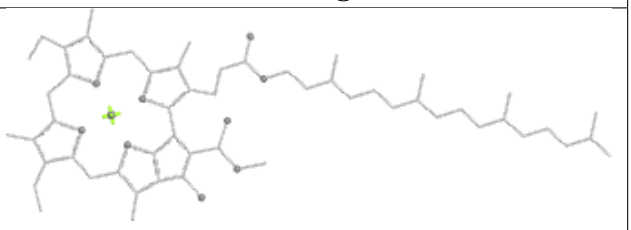
Bond angles

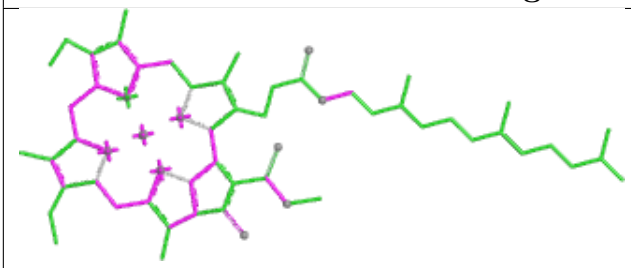
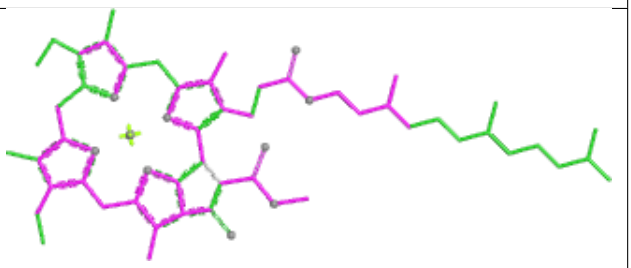
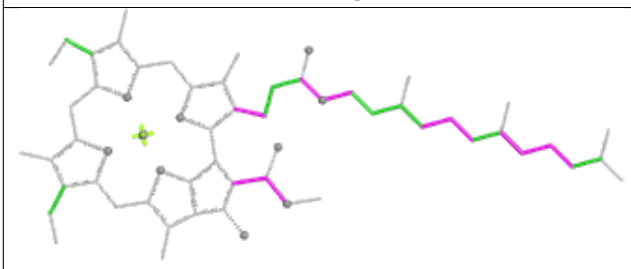
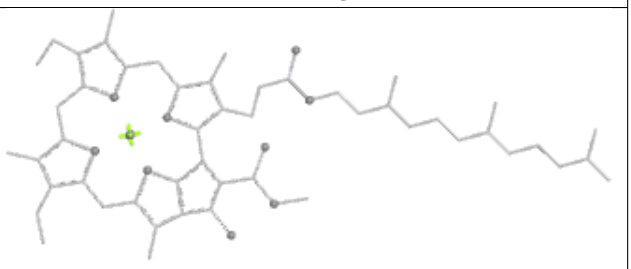


Torsions

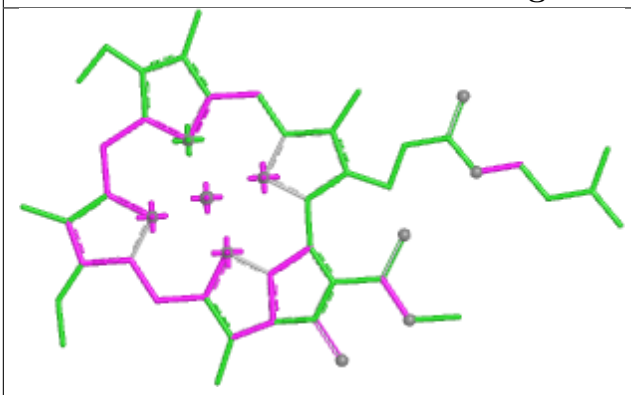


Rings

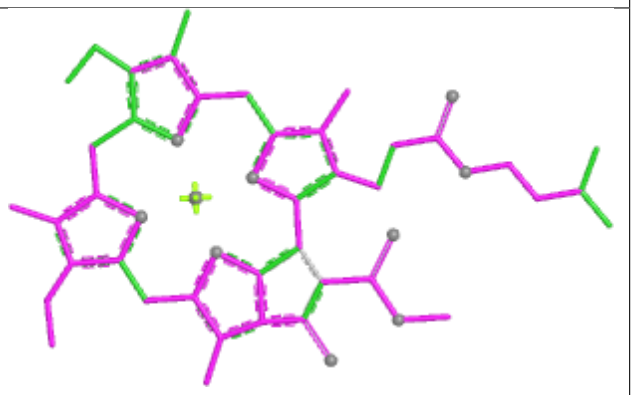
Ligand CLA A 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

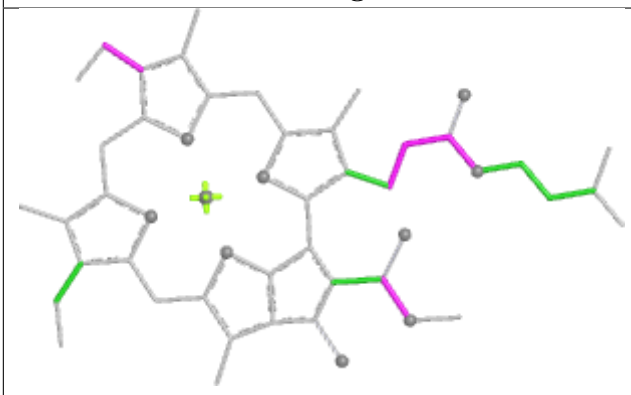
Ligand CLA a 816



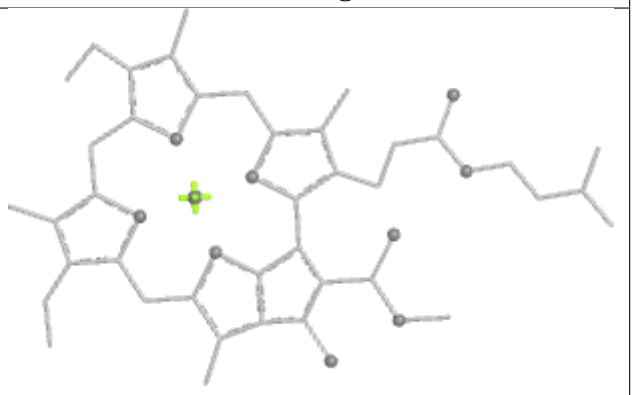
Bond lengths



Bond angles

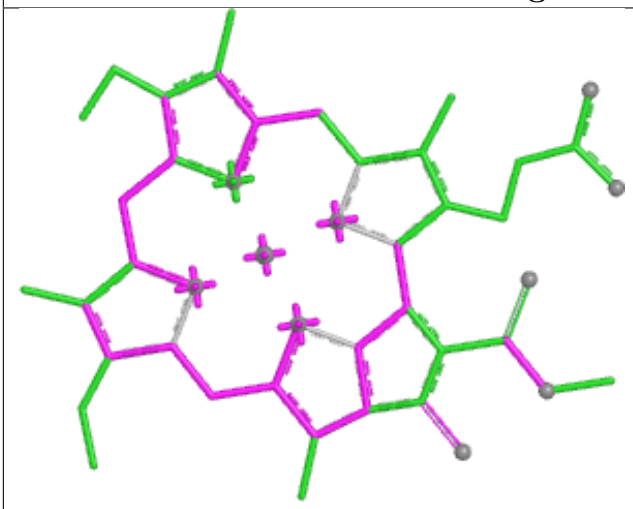


Torsions



Rings

Ligand CLA a 815



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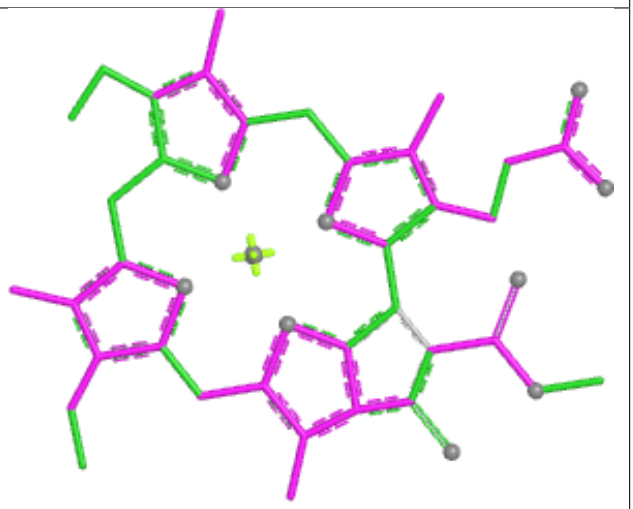
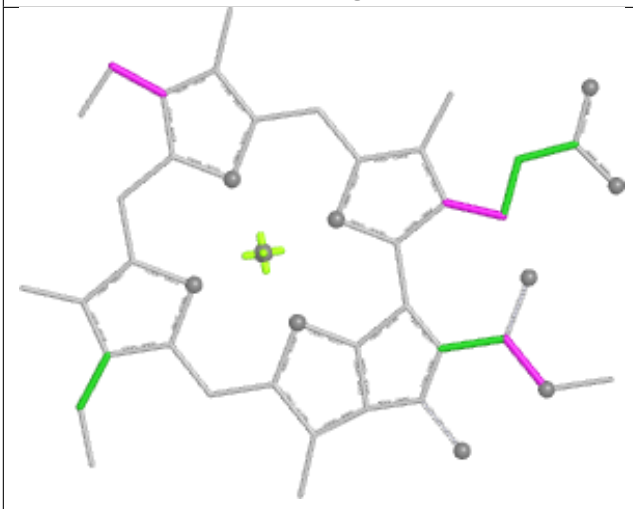


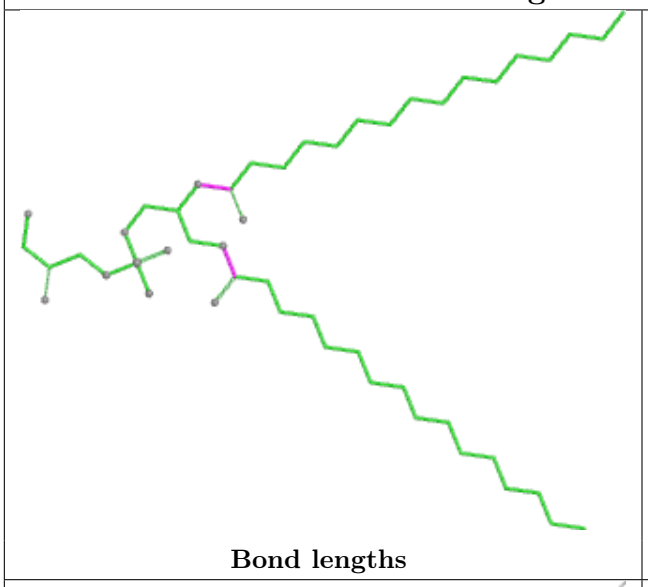
Bond angles



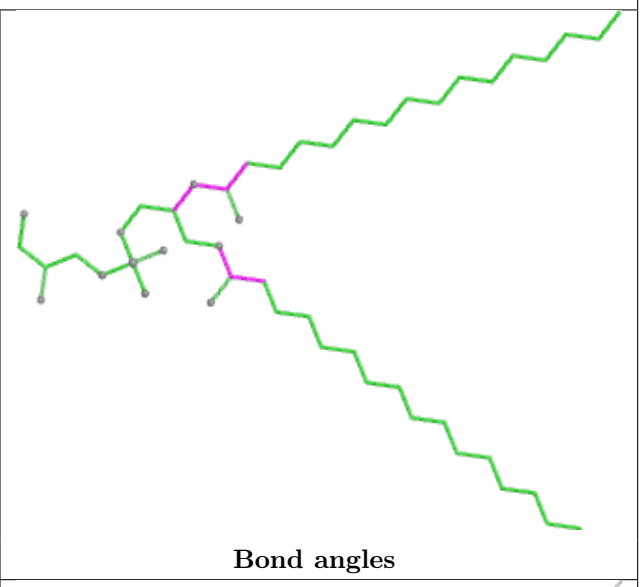
Torsions

Rings

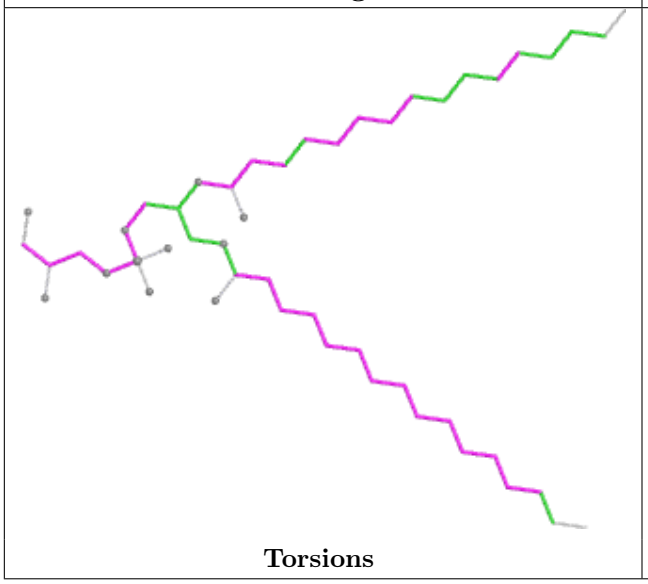
Ligand LHG a 853



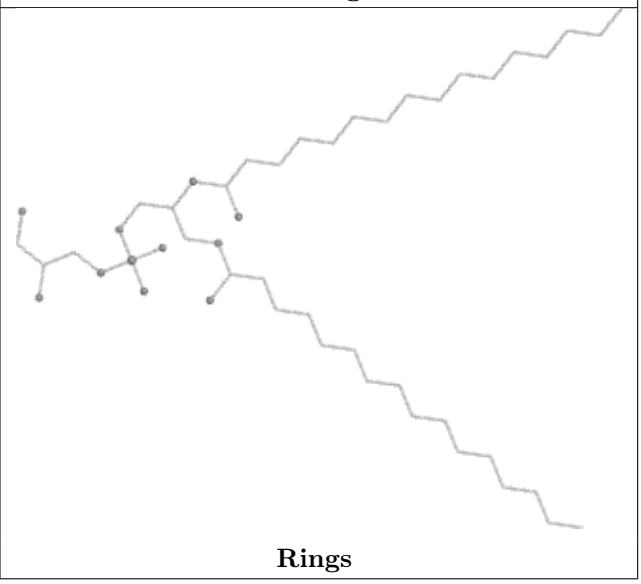
Bond lengths



Bond angles

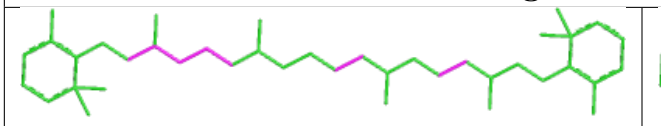


Torsions



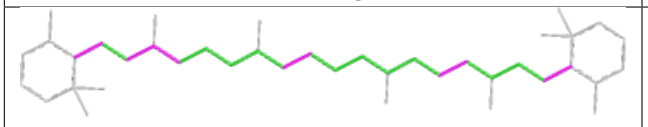
Rings

Ligand BCR G 845

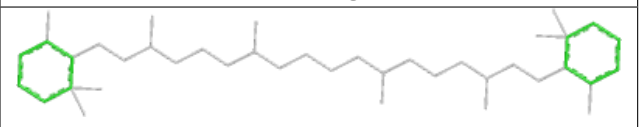


Bond lengths

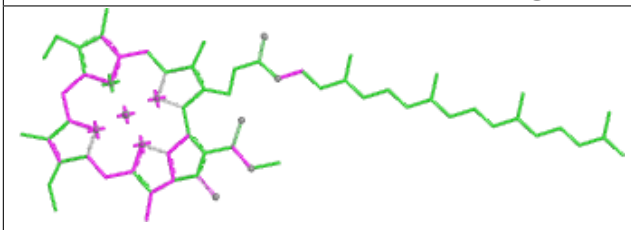
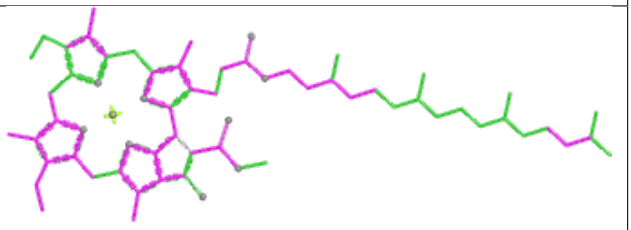
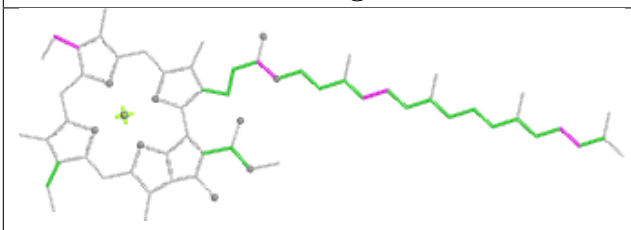
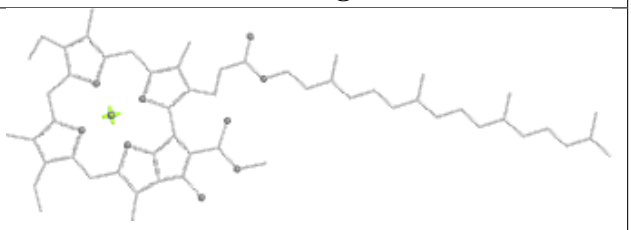
Bond angles

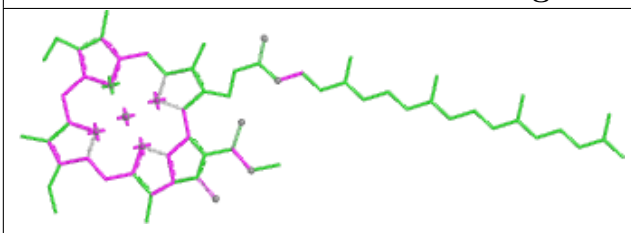
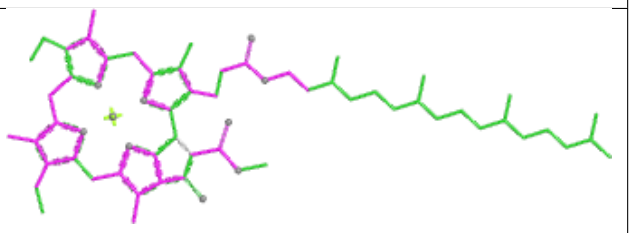
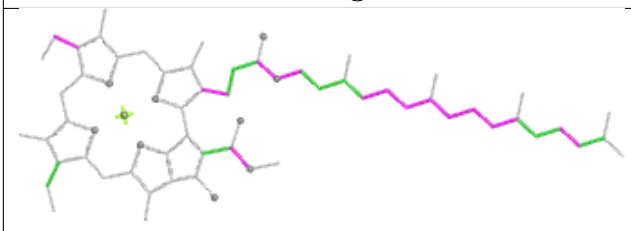
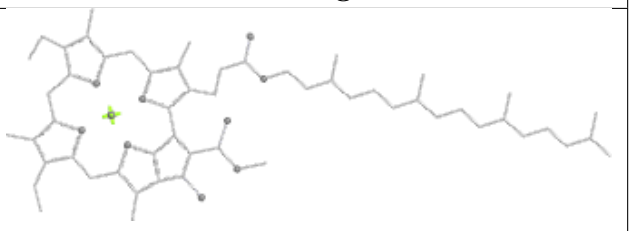


Torsions

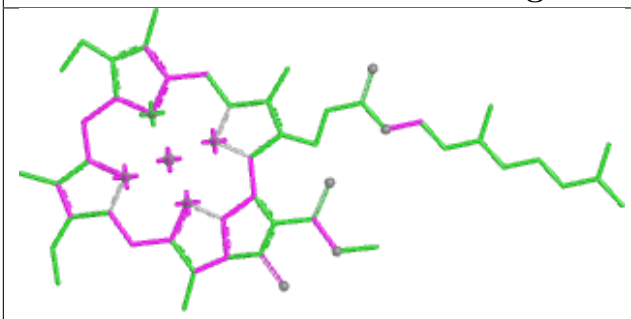


Rings

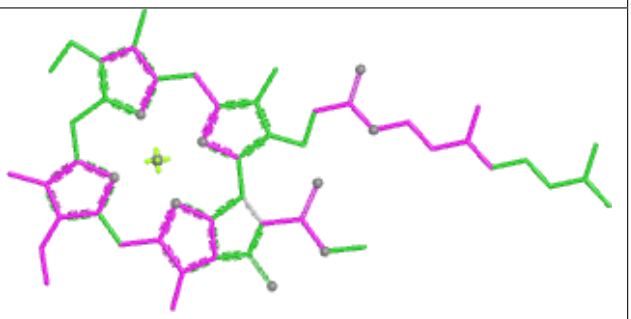
Ligand CL0 A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

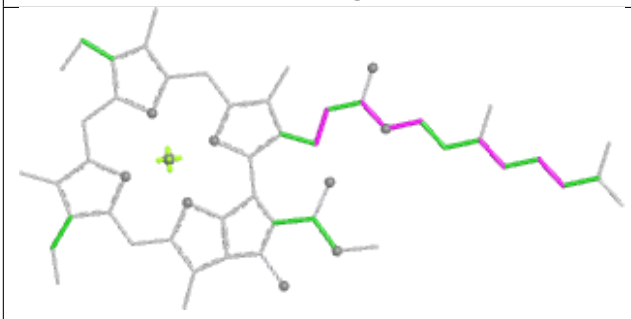
Ligand CLA L 204



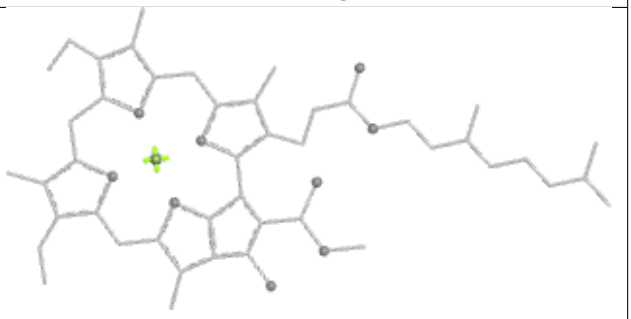
Bond lengths



Bond angles

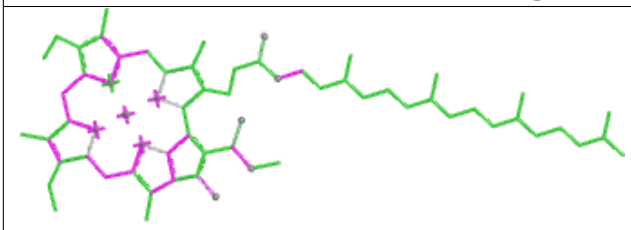


Torsions



Rings

Ligand CLA a 806



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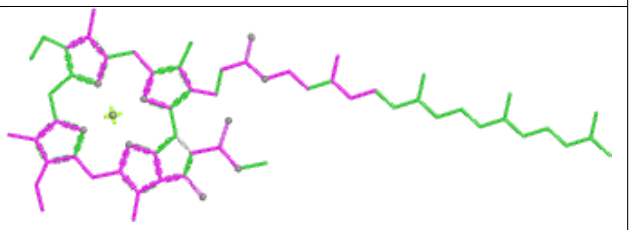
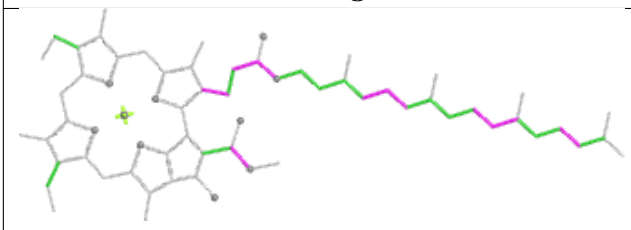
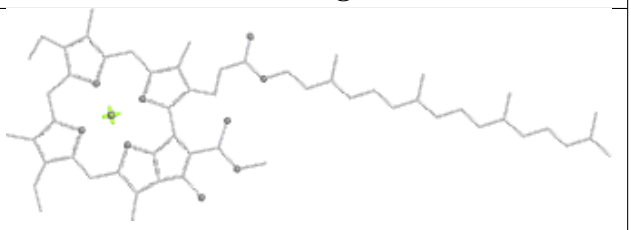


Bond angles

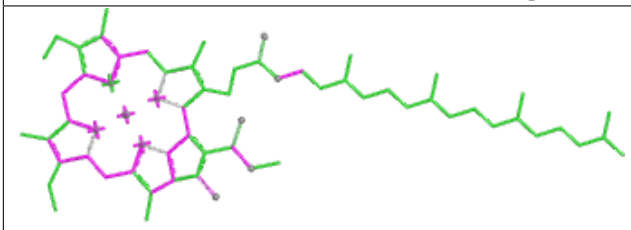


Torsions



Rings

Ligand CLA G 830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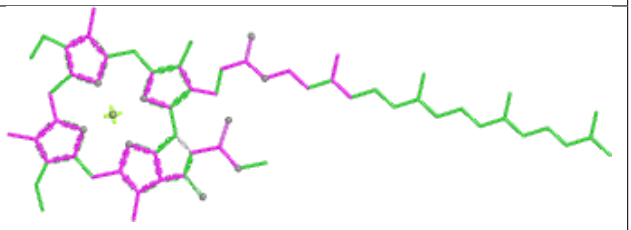
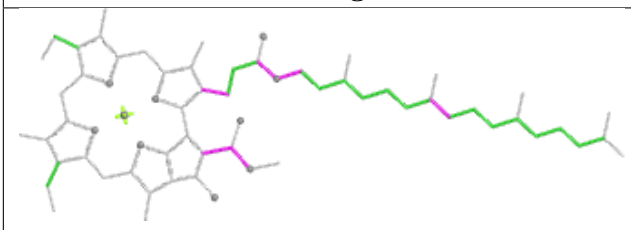

Bond angles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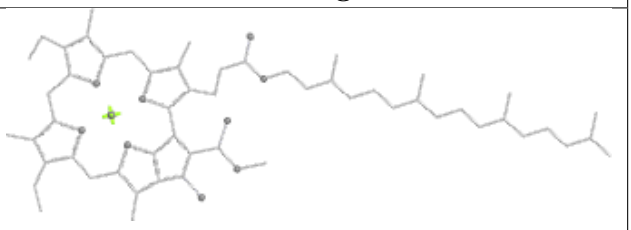
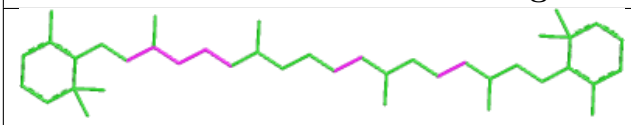
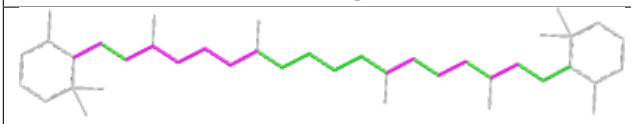
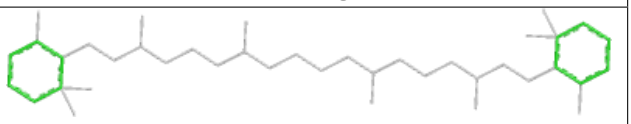

Rings

Ligand BCR f 202

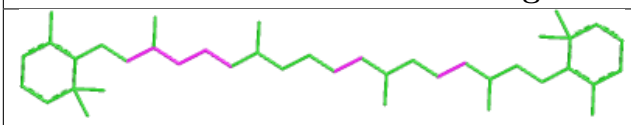

Bond lengths

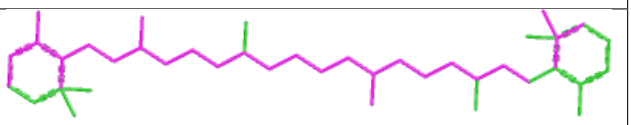
Bond angles

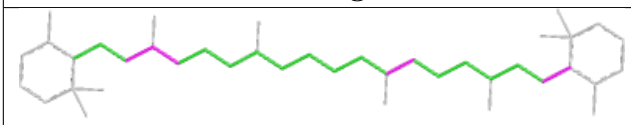

Torsions

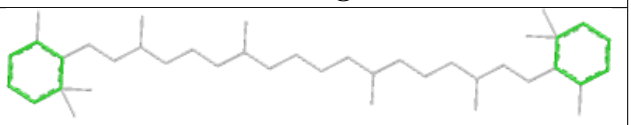

Rings

Ligand BCR B 844

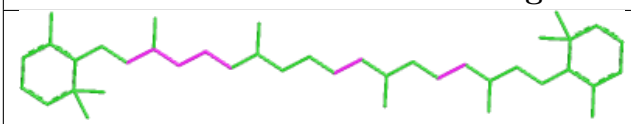

Bond lengths


Bond angles

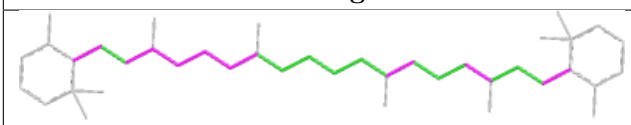

Torsions

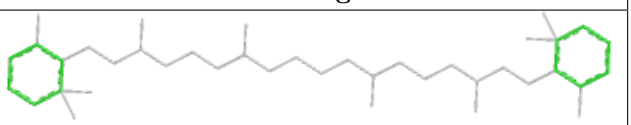

Rings

Ligand BCR S 201

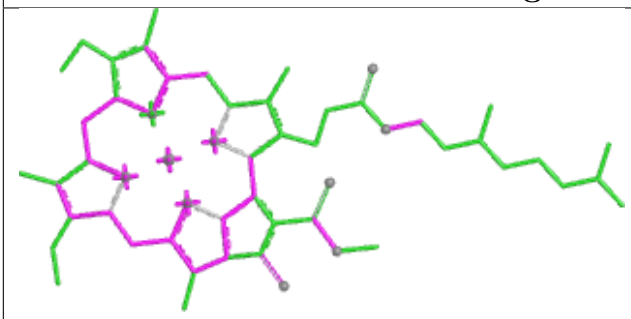

Bond lengths

Bond angles

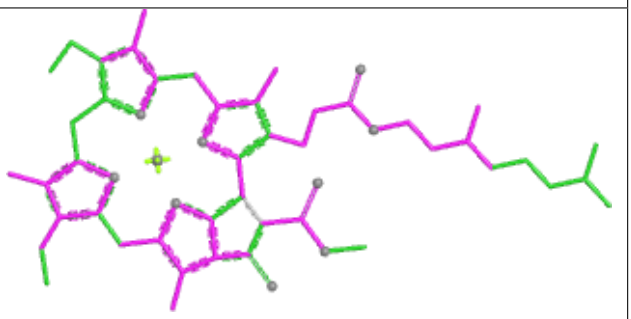

Torsions


Rings

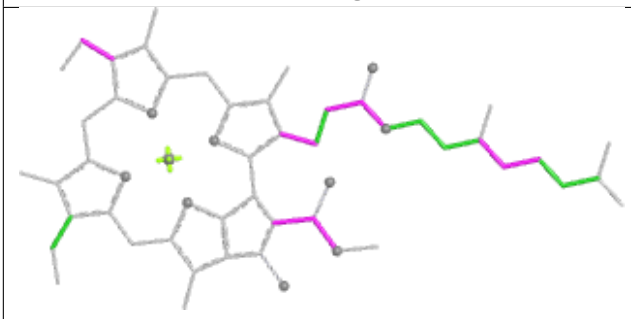
Ligand CLA A 804



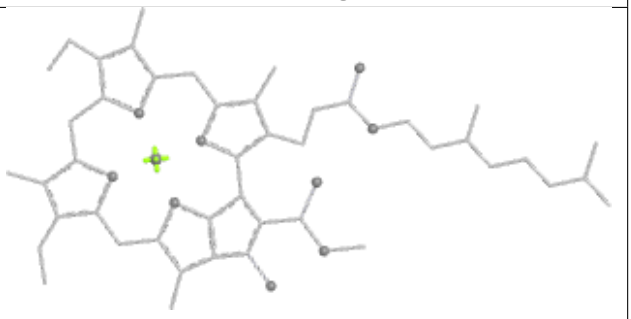
Bond lengths



Bond angles

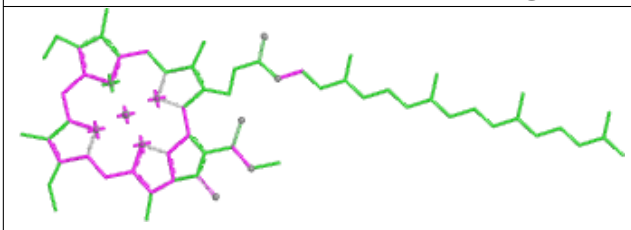


Torsions

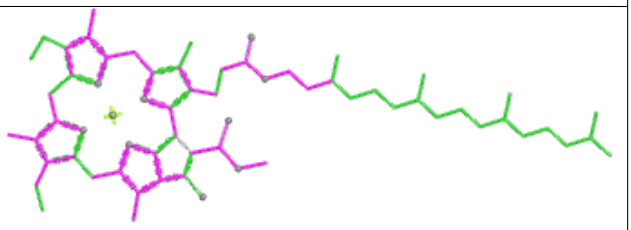


Rings

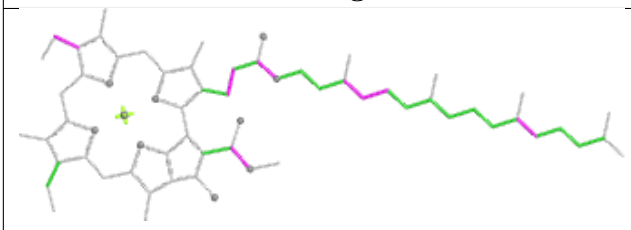
Ligand CLA G 821



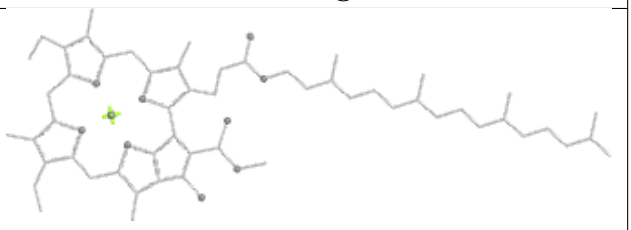
Bond lengths



Bond angles

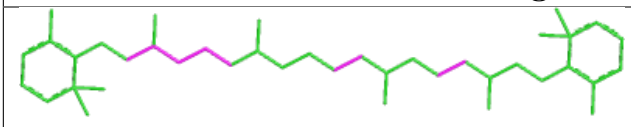


Torsions



Rings

Ligand BCR l 203



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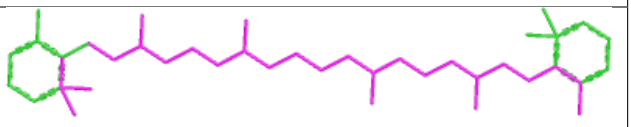
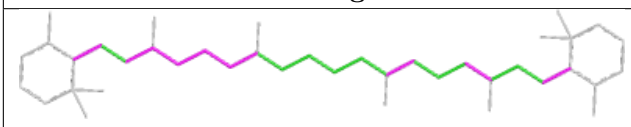
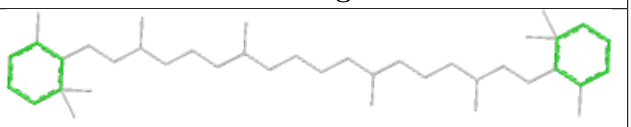


Bond angles

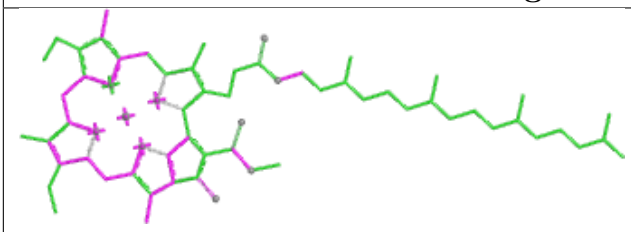


Torsions



Rings

Ligand CLA B 826



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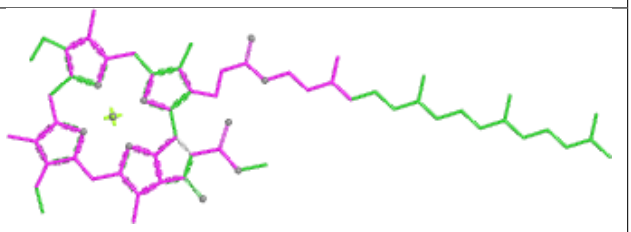
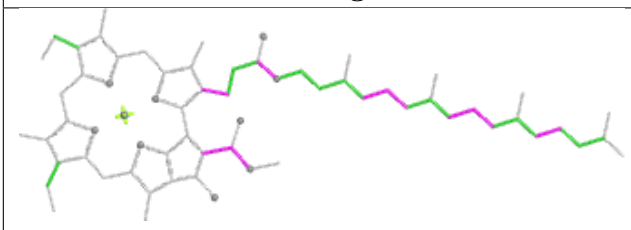


Bond angles



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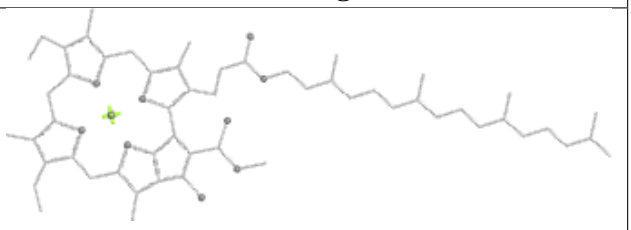
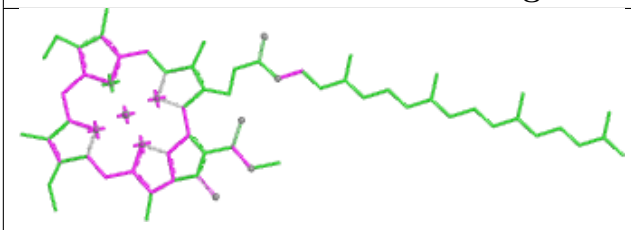


Rings

Ligand CLA G 837



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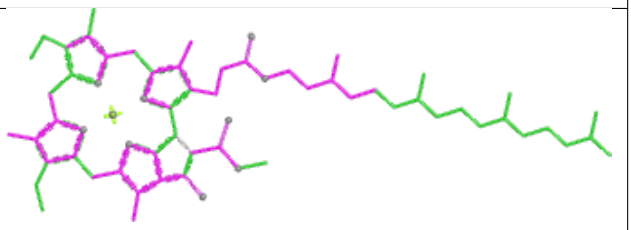

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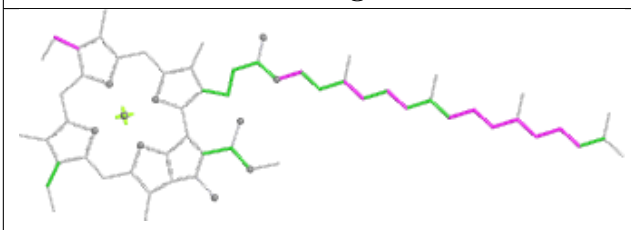

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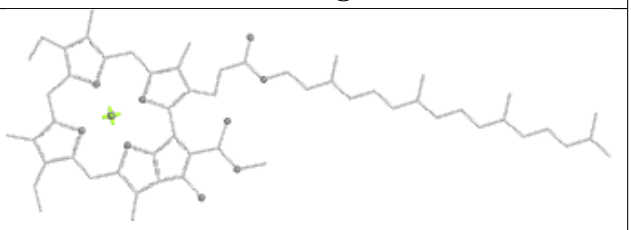
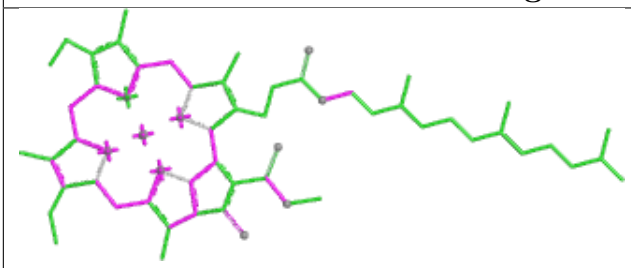


Rings

Ligand CLA B 801



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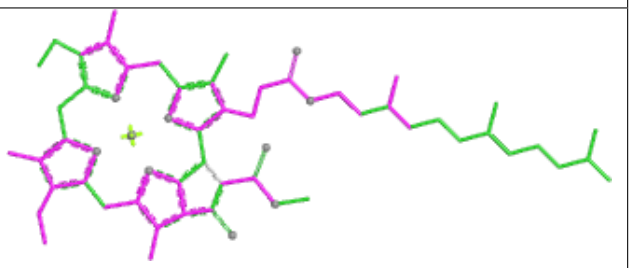
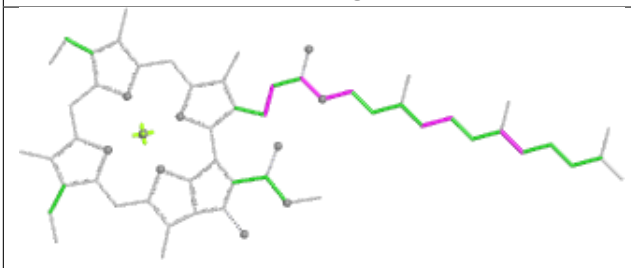
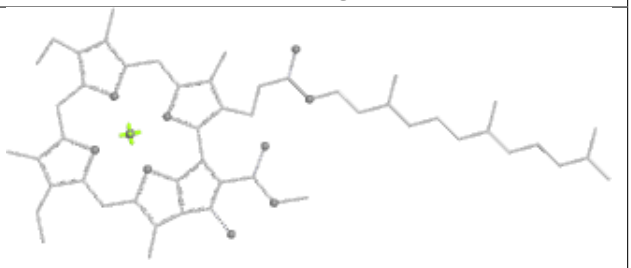


Bond angles

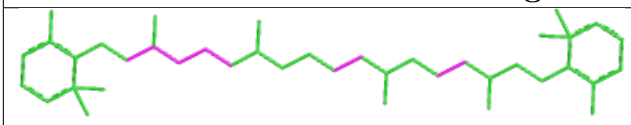


Torsions

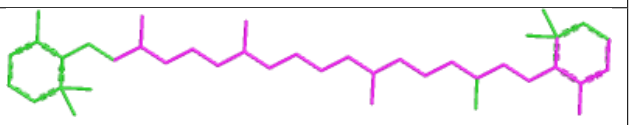


Rings

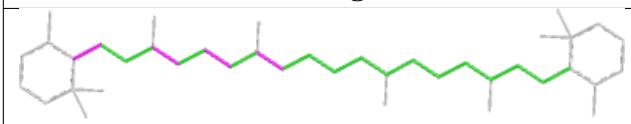
Ligand BCR F 204



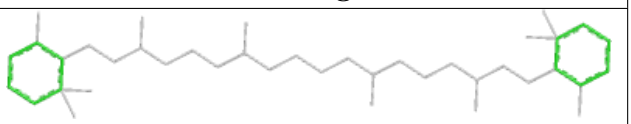
Bond lengths



Bond angles

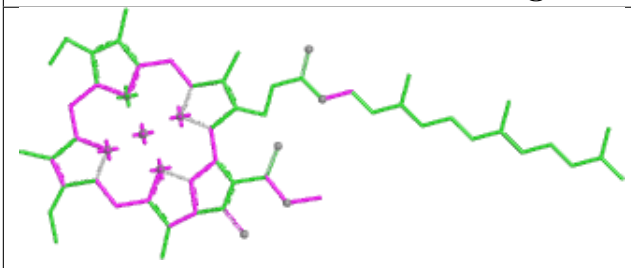


Torsions

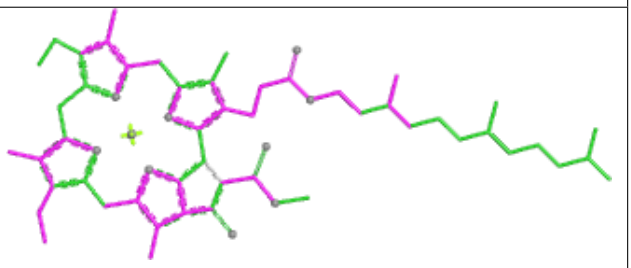


Rings

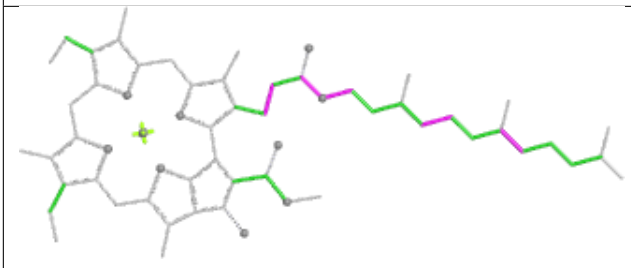
Ligand CLA b 801



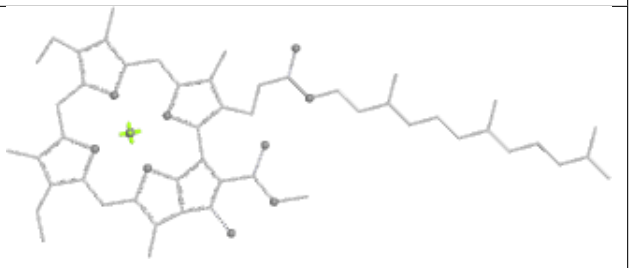
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

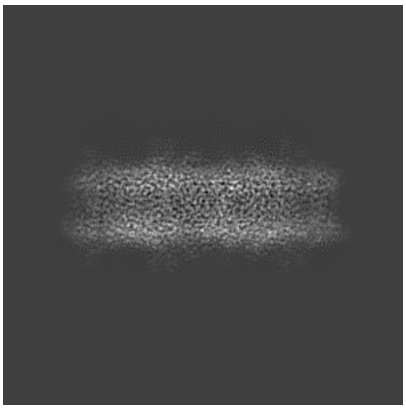
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47359. These allow visual inspection of the internal detail of the map and identification of artifacts.

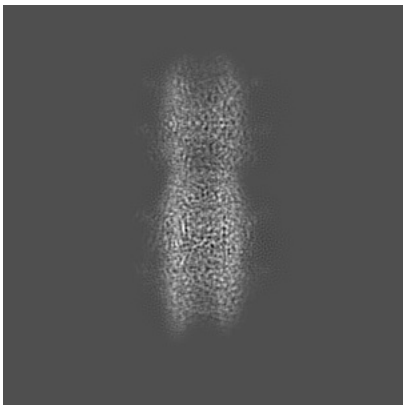
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

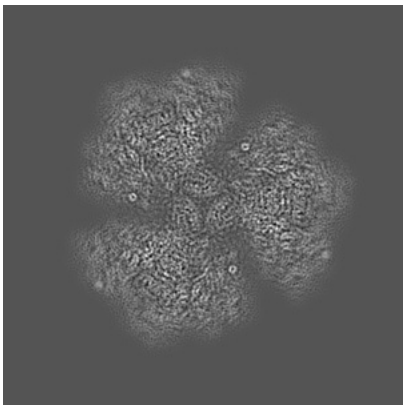
6.1.1 Primary map



X

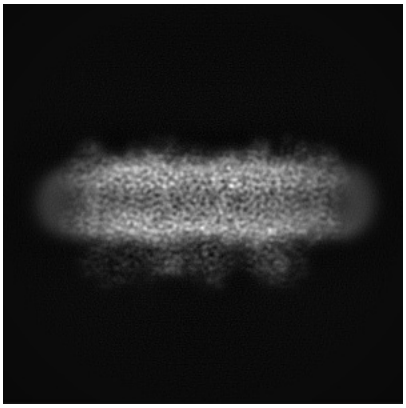


Y

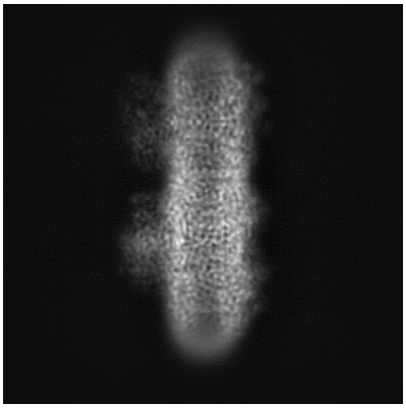


Z

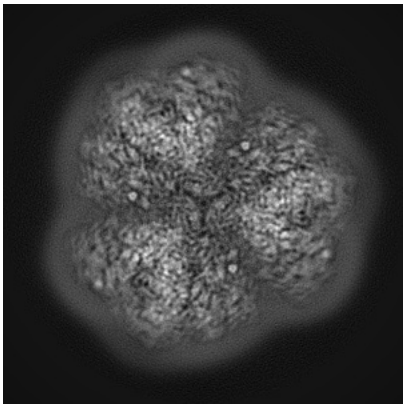
6.1.2 Raw map



X



Y



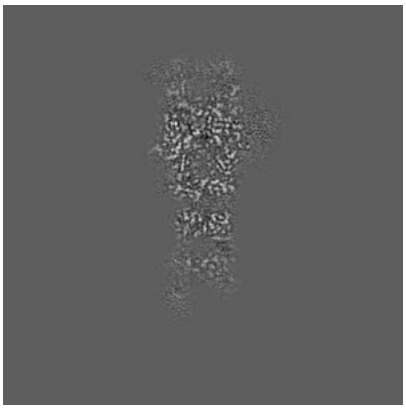
Z

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

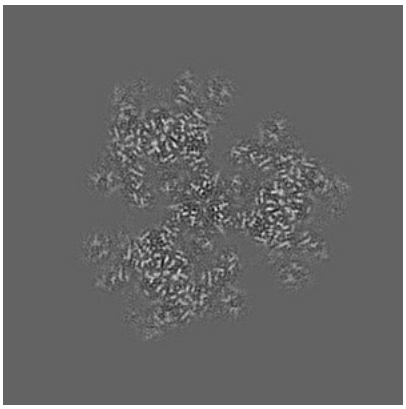
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160

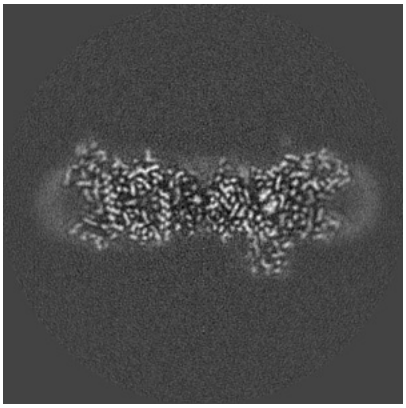


Y Index: 160

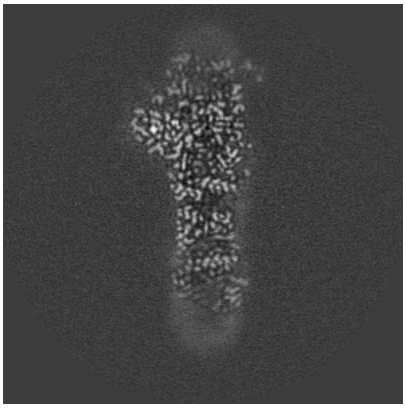


Z Index: 160

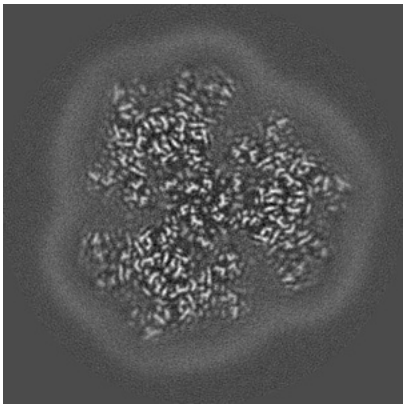
6.2.2 Raw map



X Index: 160



Y Index: 160

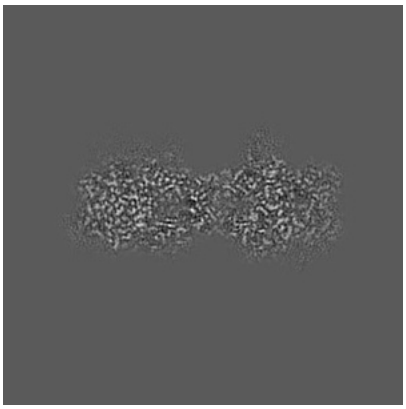


Z Index: 160

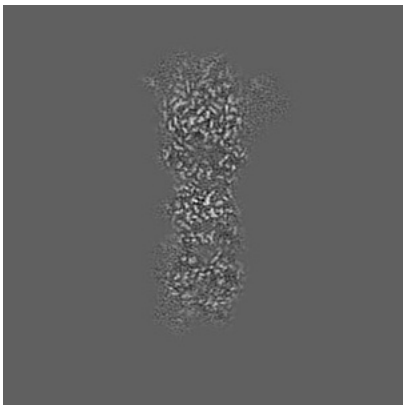
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

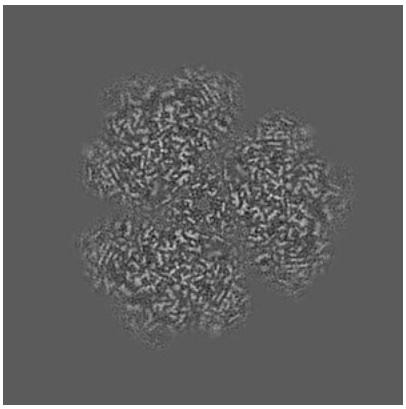
6.3.1 Primary map



X Index: 142

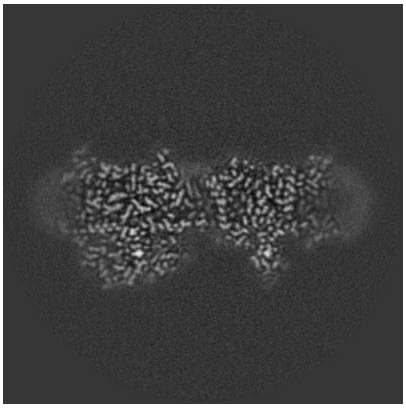


Y Index: 175

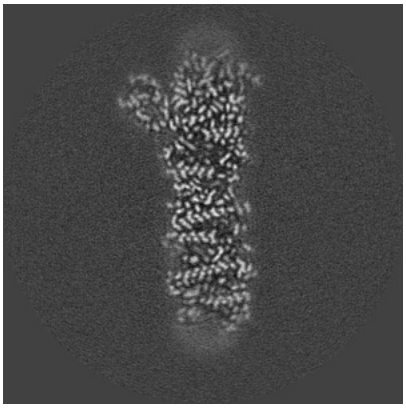


Z Index: 174

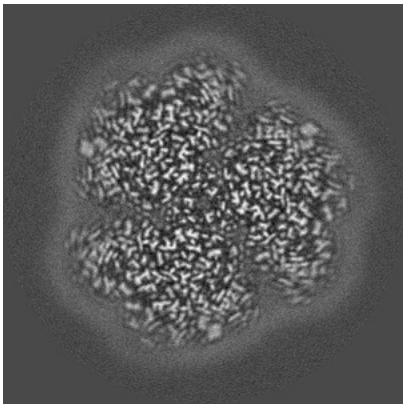
6.3.2 Raw map



X Index: 131



Y Index: 175

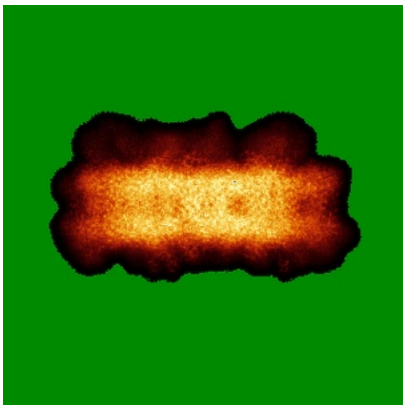


Z Index: 175

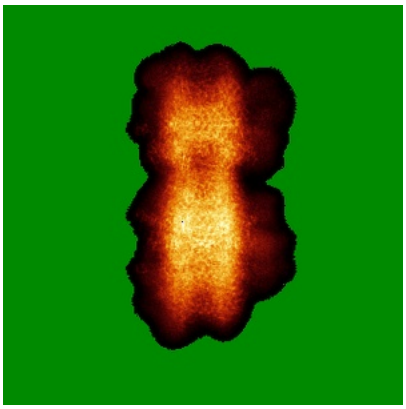
The images above show the largest variance slices of the map in three orthogonal directions.

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

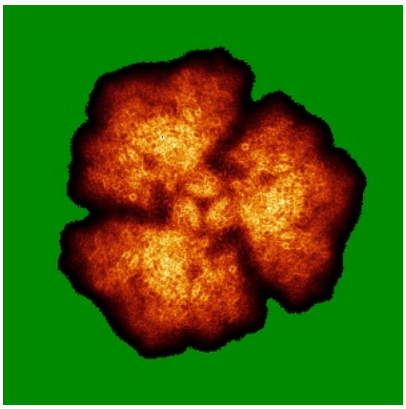
6.4.1 Primary map



X

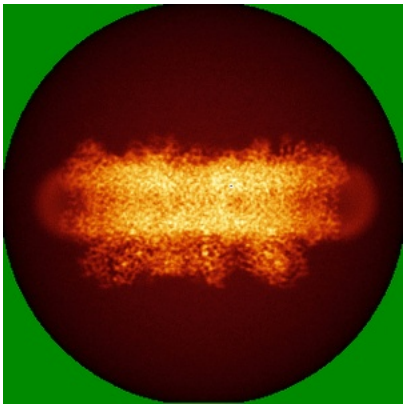


Y

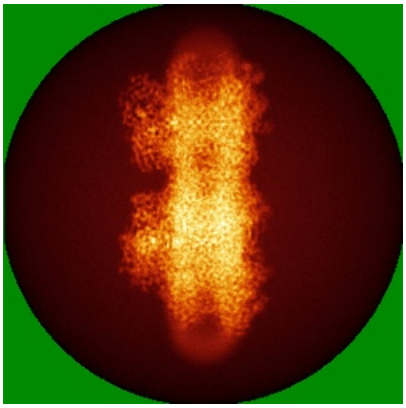


Z

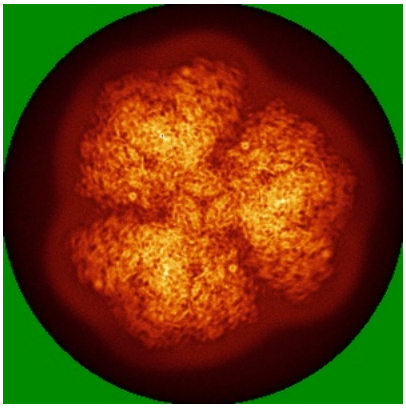
6.4.2 Raw map



X



Y

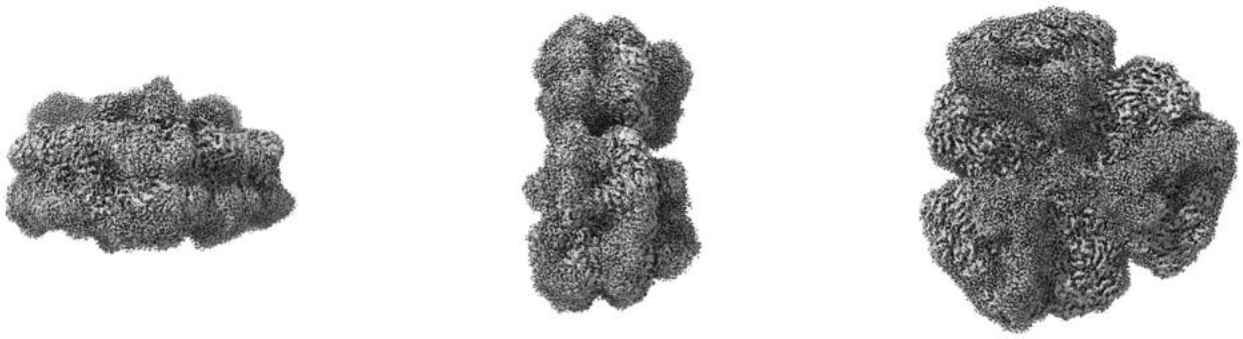


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

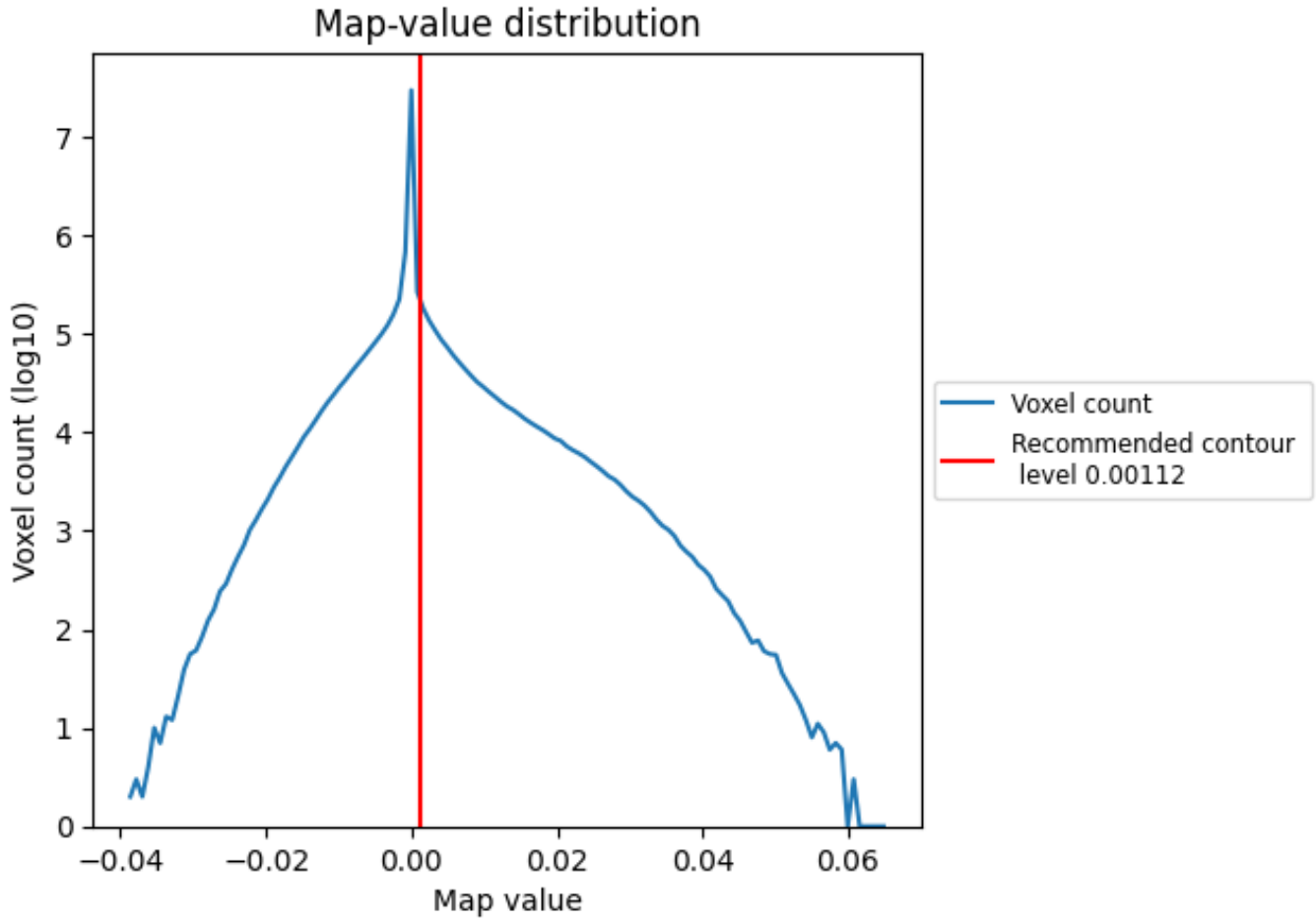
6.6 Mask visualisation (i)

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

7 Map analysis

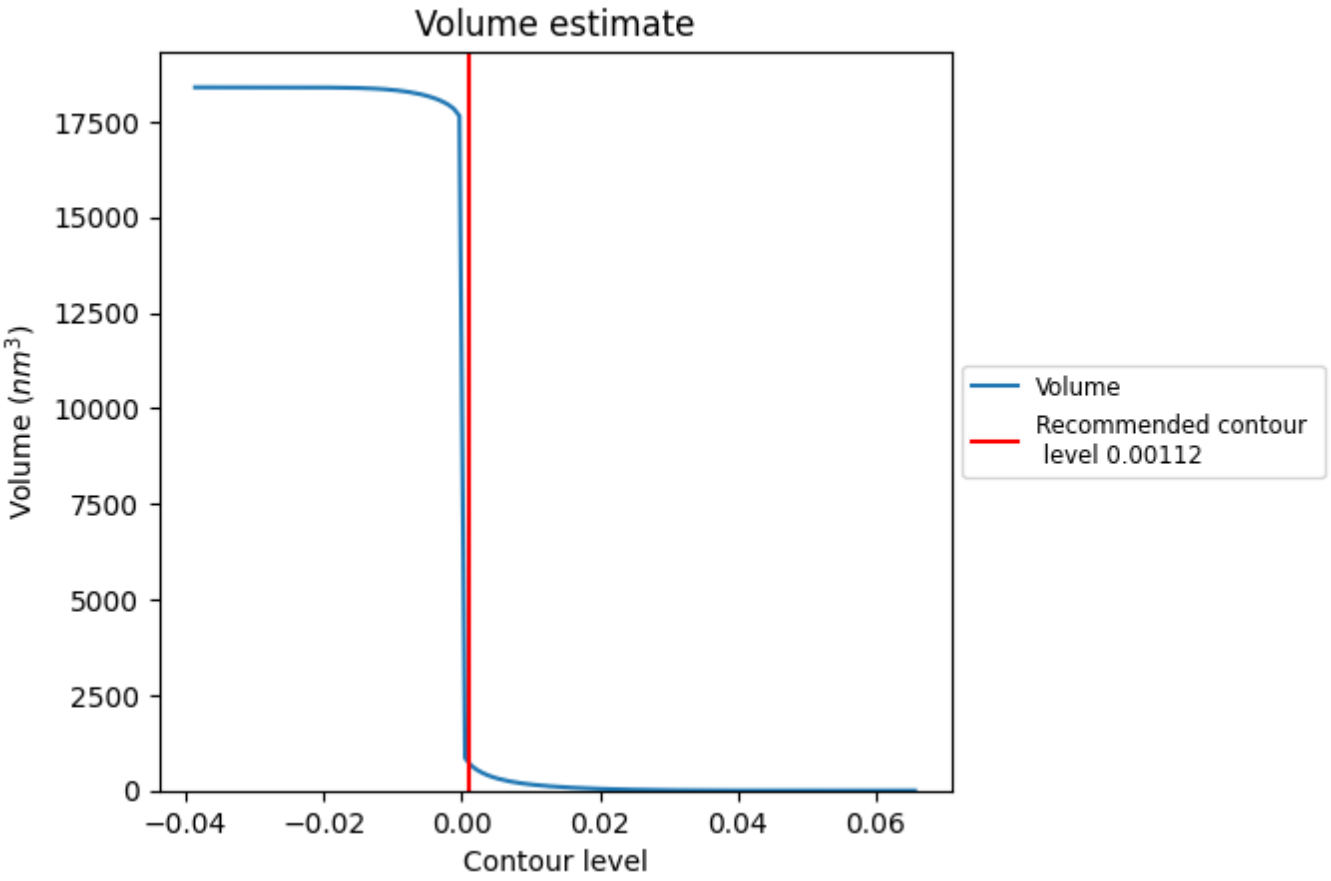
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

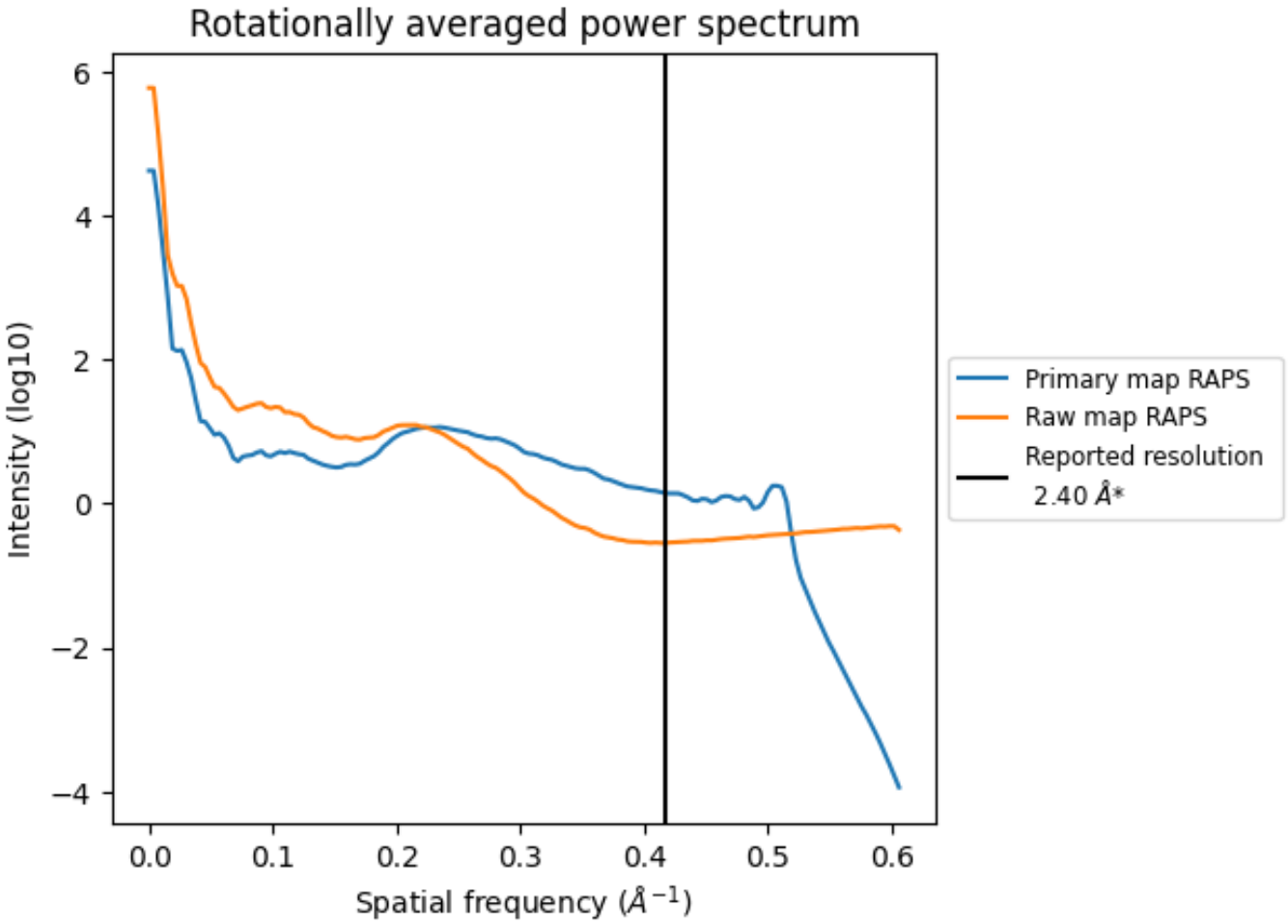
7.2 Volume estimate



The volume at the recommended contour level is 708 nm^3; this corresponds to an approximate mass of 640 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)

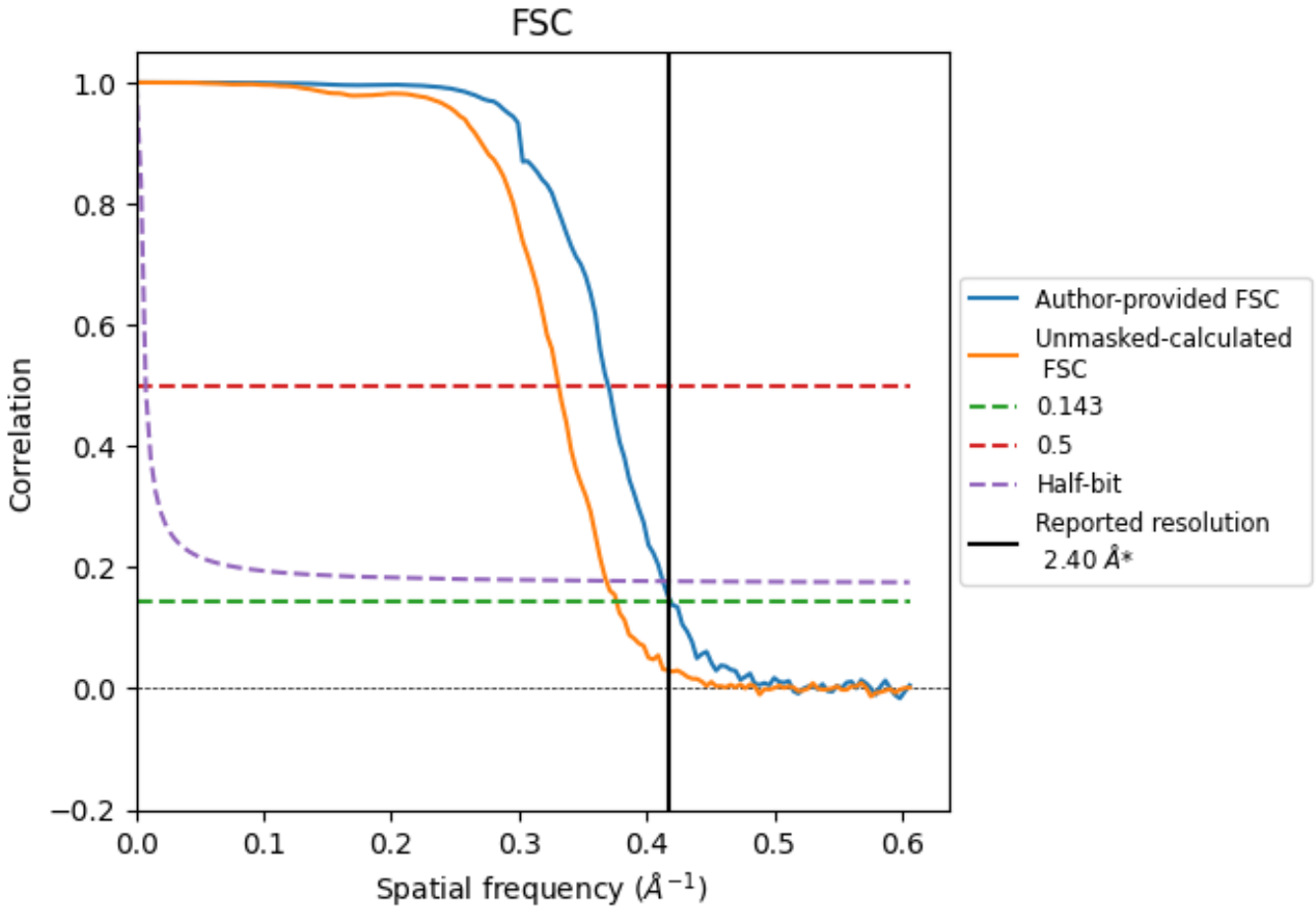


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

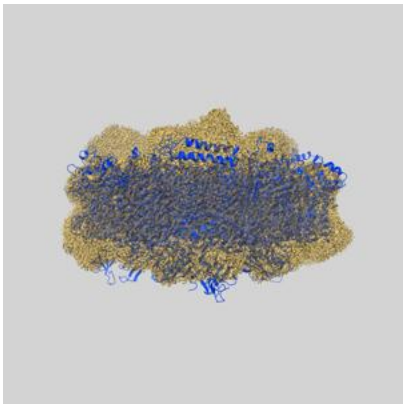
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.70	2.42
Unmasked-calculated*	2.66	3.02	2.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.66 differs from the reported value 2.4 by more than 10 %

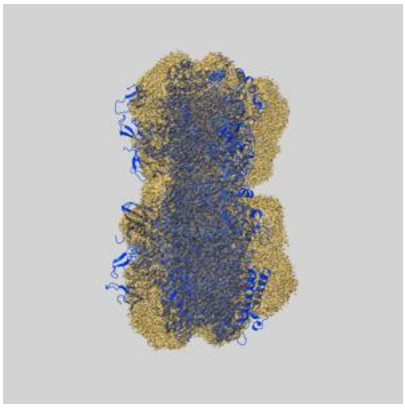
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47359 and PDB model 9E0J. Per-residue inclusion information can be found in section 3 on page 30.

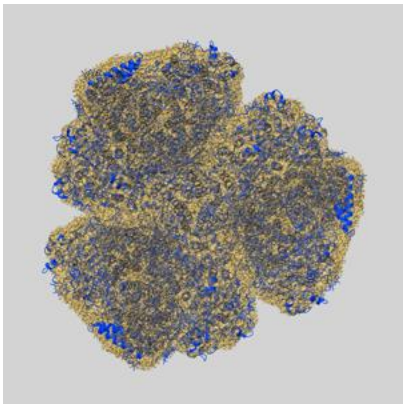
9.1 Map-model overlay



X



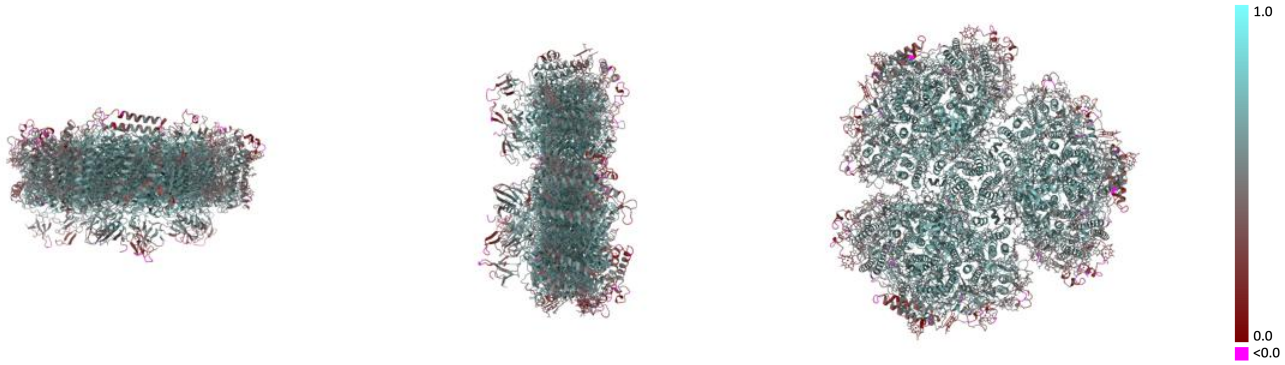
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00112 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.

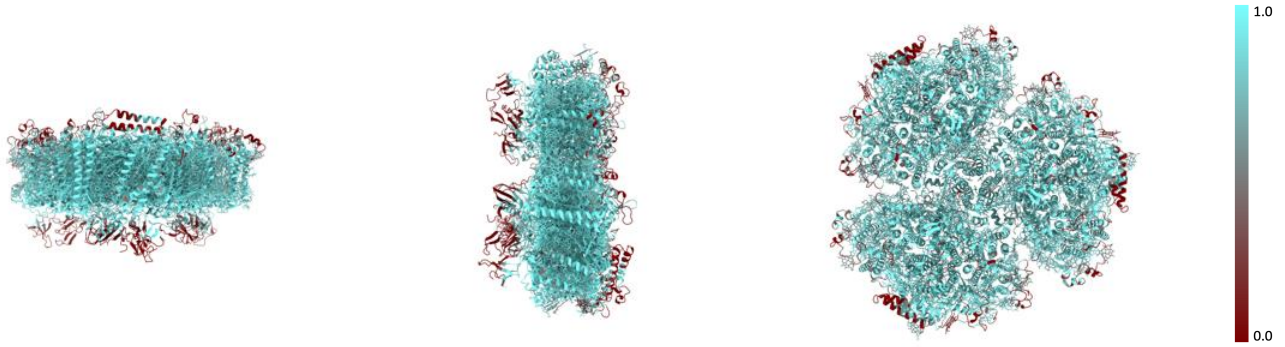
9.2 Q-score mapped to coordinate model



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.

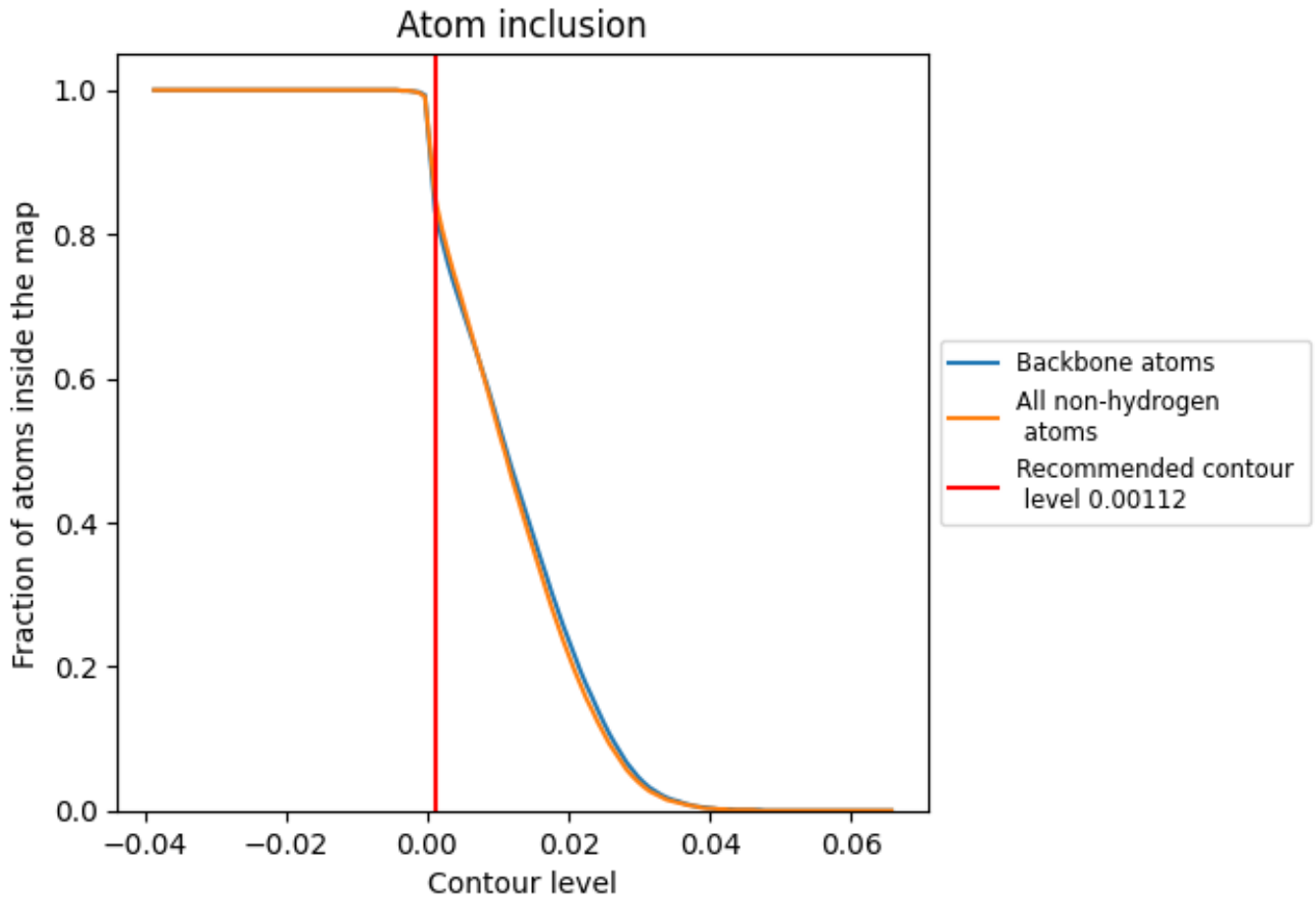
9.3 Atom inclusion mapped to coordinate model



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 (0.00112).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.5700
A	0.9120	0.5760
B	0.9030	0.6090
C	0.3140	0.4450
D	0.4860	0.4910
E	0.4120	0.3990
F	0.6840	0.4230
G	0.9130	0.5760
H	0.8980	0.6030
I	0.9590	0.6510
J	0.7760	0.4280
K	0.3120	0.4410
L	0.9010	0.6240
M	0.9370	0.6550
N	0.4850	0.5060
O	0.4290	0.4260
P	0.6600	0.4140
Q	0.9450	0.6480
R	0.7480	0.3910
S	0.8980	0.6210
T	0.9400	0.6400
a	0.9100	0.5760
b	0.9000	0.6050
c	0.3170	0.4490
d	0.4840	0.4930
e	0.4100	0.4110
f	0.6690	0.4100
i	0.9670	0.6570
j	0.7930	0.4330
l	0.9000	0.6200
m	0.9370	0.6320