Full wwPDB EM Validation Report

Sep 15, 2026 – 08:30 AM JST

PDB ID	:	9KC5 / pdb_00009kc5
EMDB ID	:	EMD-62242
Title	:	PSI-LHCI of the red alga Galdieria sulphuraria NIES-3638
Authors	:	Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on	:	2024-11-01
Resolution	:	2.19 Å(reported)
Based on initial model	:	.

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

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

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

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

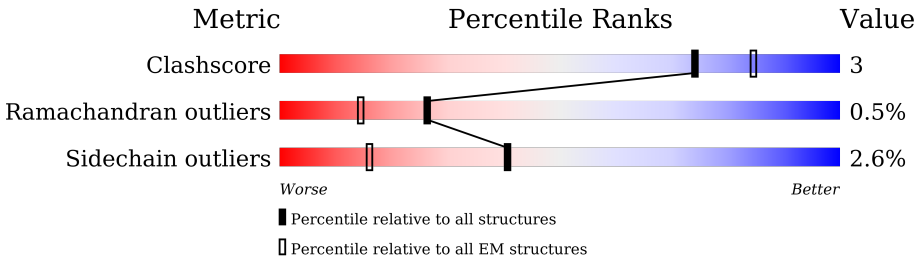
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

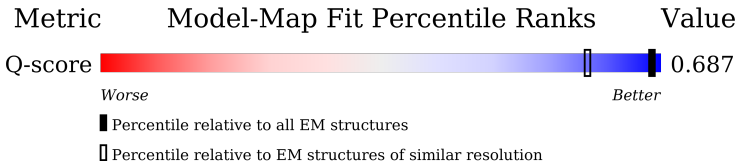
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 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	2745 (1.70 - 2.69)

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	739	95%
2	B	732	96%
3	C	80	96%
4	D	138	93% 7%

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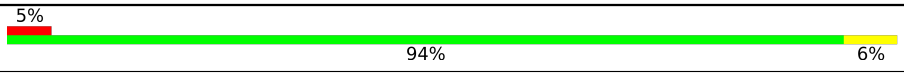
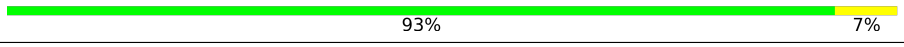
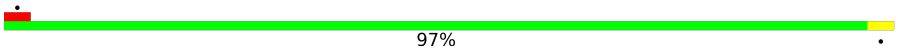
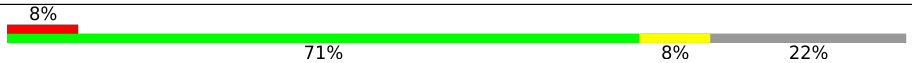
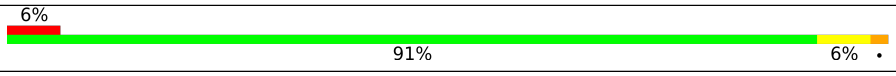
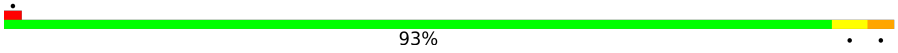
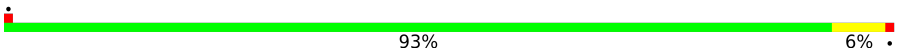
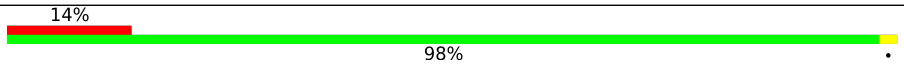
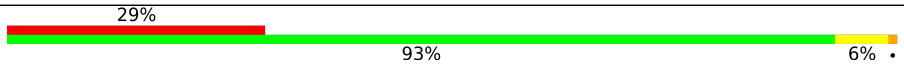
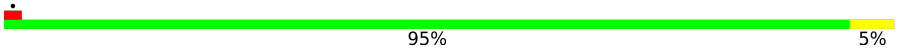
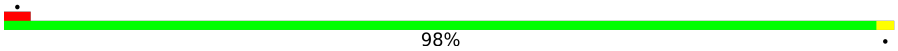
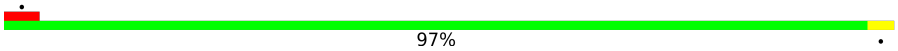
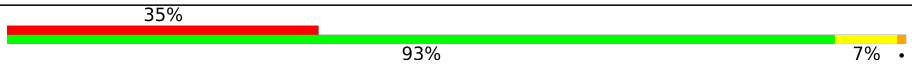
Mol	Chain	Length	Quality of chain
5	E	64	
6	F	161	
7	I	34	
8	J	42	
9	K	65	
10	L	139	
11	M	28	
12	O	95	
13	Z	84	
14	1	177	
15	2	162	
16	3	131	
17	4	178	
18	5	178	
19	6	178	
20	7	168	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	5X6	1	311	-	X	-	-
29	5X6	1	316	-	X	-	-
29	5X6	7	315	-	X	-	-
29	5X6	M	101	-	X	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 41435 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
			Total	C	N	O	S		
1	A	739	5844	3827	1001	990	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5859	3864	988	993	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	600	369	104	115	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	138	1103	706	188	205	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	64	516	333	85	97	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1285	832	216	232	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			273	189	35	47	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	S	0	0
			337	230	50	56	1		

- Molecule 9 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	51	Total	C	N	O	S	0	0
			368	239	59	68	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	139	Total	C	N	O	S	0	0
			1076	707	174	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	28	Total	C	N	O	S	0	0
			214	143	34	36	1		

- Molecule 12 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	95	Total	C	N	O	S	0	0
			748	504	115	128	1		

- Molecule 13 is a protein called Psa28.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	84	Total	C	N	O	S	0	0
			637	423	98	114	2		

- Molecule 14 is a protein called RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	177	Total	C	N	O	S	0	0
			1370	889	235	241	5		

- Molecule 15 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	162	Total	C	N	O	S	0	0
			1286	834	219	229	4		

- Molecule 16 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	99	Total	C	N	O	S	0	0
			772	508	126	132	6		

- Molecule 17 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	178	Total	C	N	O	S	0	0
			1407	926	233	240	8		

- Molecule 18 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	178	Total	C	N	O	S	0	0
			1402	912	238	245	7		

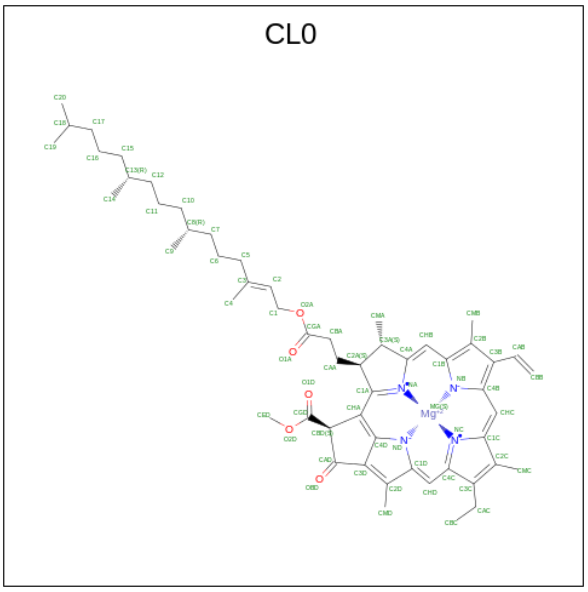
- Molecule 19 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	178	Total	C	N	O	S	0	0
			1450	965	235	241	9		

- Molecule 20 is a protein called Light-harvesting complex protein.

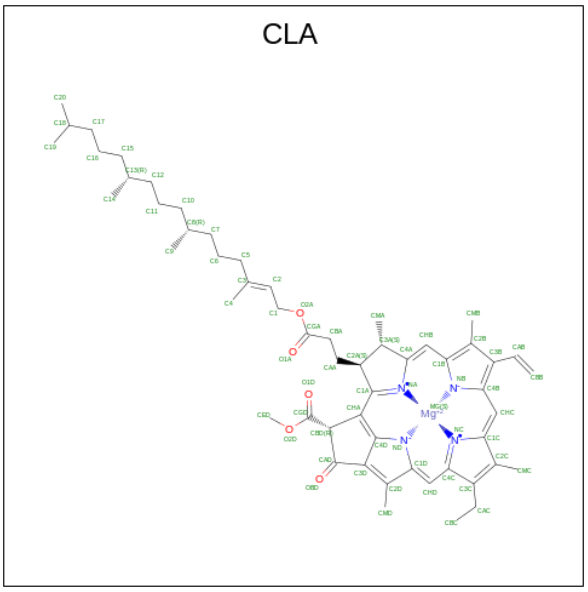
Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	168	Total	C	N	O	S	0	0
			1322	860	220	234	8		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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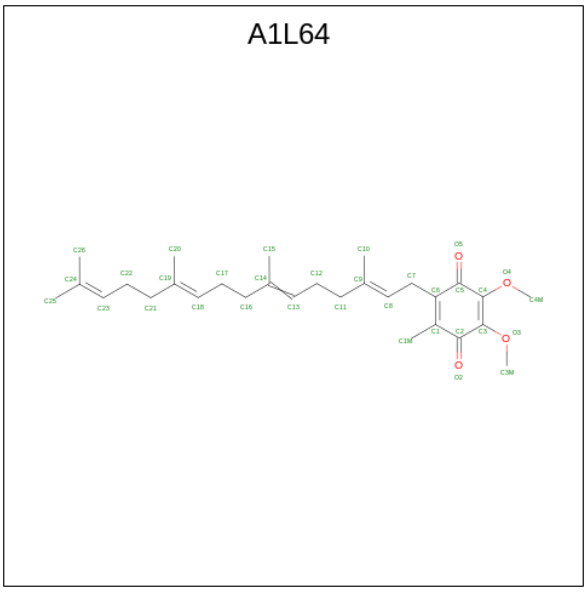
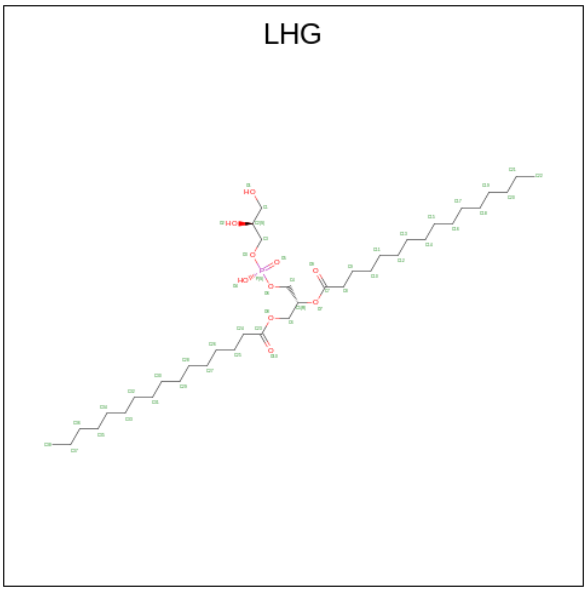
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 23 is Coenzyme Q4 (CCD ID: A1L64) (formula: $C_{29}H_{42}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 33 29 4	0
23	B	1	Total C O 33 29 4	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O P 49 38 10 1	0

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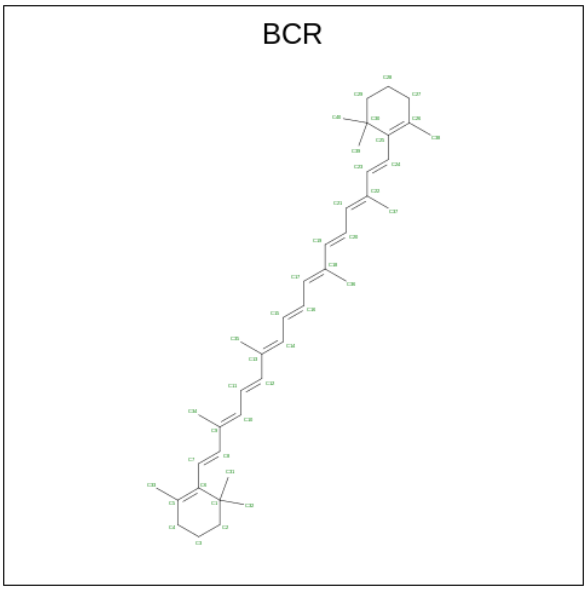
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			40	29	10	1	
24	A	1	Total	C	O	P	0
			33	22	10	1	
24	B	1	Total	C	O	P	0
			33	22	10	1	
24	J	1	Total	C	O	P	0
			33	22	10	1	
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	4	1	Total	C	O	P	0
			32	21	10	1	
24	5	1	Total	C	O	P	0
			25	14	10	1	
24	6	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	4	1	Total C 40 40	0

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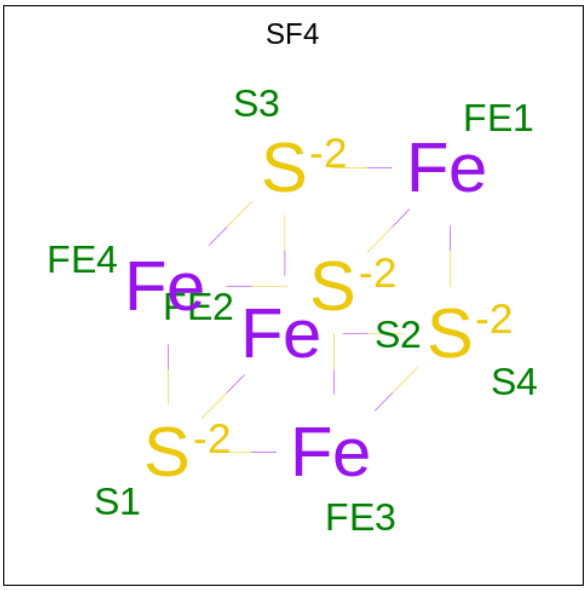
Mol	Chain	Residues	Atoms	AltConf
25	5	1	Total C 40 40	0

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	AltConf
27	A	10	Total C 110 110	0
27	B	2	Total C 18 18	0
27	F	3	Total C 35 35	0
27	I	2	Total C 21 21	0
27	J	2	Total C 22 22	0

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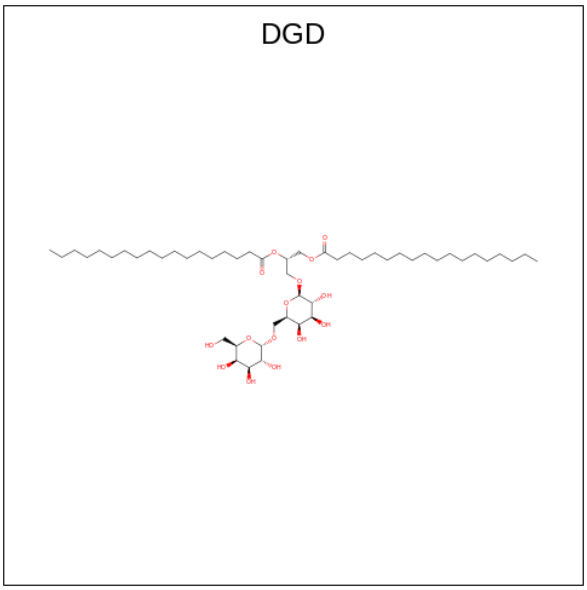
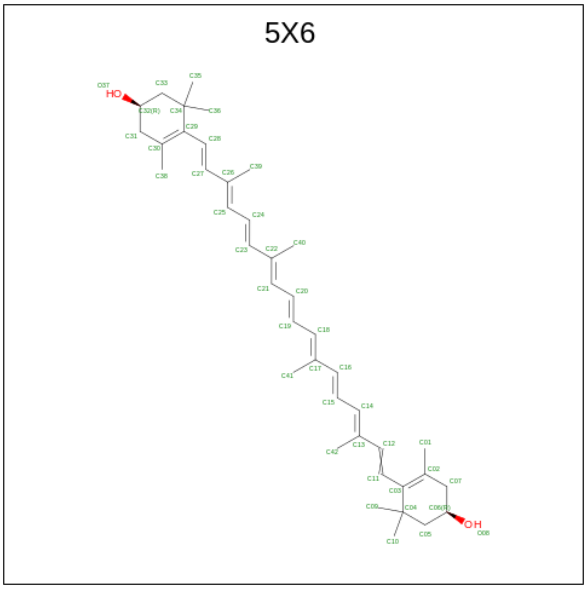
Mol	Chain	Residues	Atoms	AltConf
27	K	1	Total C 11 11	0
27	L	3	Total C 33 33	0
27	M	1	Total C 9 9	0
27	O	3	Total C 24 24	0
27	Z	5	Total C 45 45	0
27	1	3	Total C 33 33	0
27	4	3	Total C 27 27	0
27	5	3	Total C 27 27	0
27	6	7	Total C 73 73	0
27	7	4	Total C 42 42	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C O 66 51 15	0

- Molecule 29 is Zeaxanthin (CCD ID: 5X6) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C O 42 40 2	0
29	J	1	Total C O 42 40 2	0
29	M	1	Total C O 42 40 2	0
29	O	1	Total C O 42 40 2	0
29	O	1	Total C O 42 40 2	0
29	Z	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	2	1	Total C O 42 40 2	0

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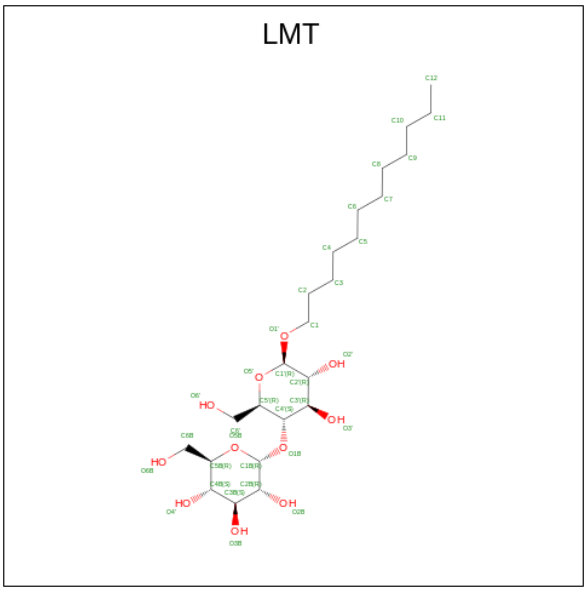
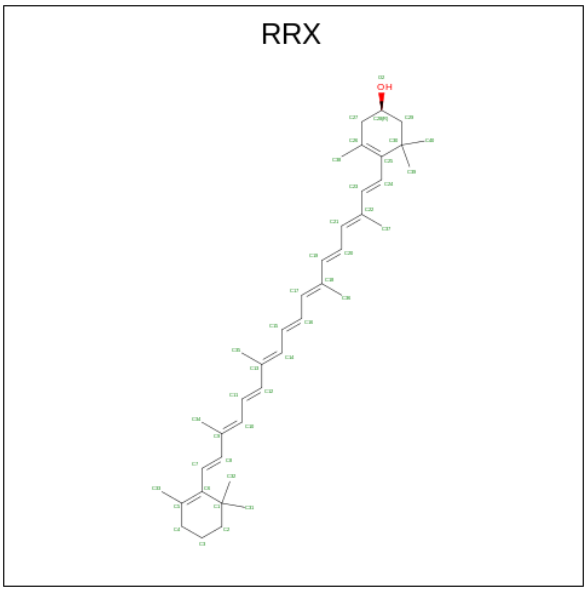
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
30	F	1	Total C O 35 24 11	0
30	O	1	Total C O 35 24 11	0
30	4	1	Total C O 35 24 11	0
30	5	1	Total C O 35 24 11	0

- Molecule 31 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
31	1	1	Total C O 41 40 1	0
31	4	1	Total C O 41 40 1	0
31	5	1	Total C O 41 40 1	0
31	6	1	Total C O 41 40 1	0

- Molecule 32 is water.

Mol	Chain	Residues	Atoms	AltConf
32	A	189	Total O 189 189	0
32	B	220	Total O 220 220	0
32	C	44	Total O 44 44	0
32	D	29	Total O 29 29	0
32	E	18	Total O 18 18	0
32	F	32	Total O 32 32	0
32	I	3	Total O 3 3	0
32	J	5	Total O 5 5	0
32	K	2	Total O 2 2	0
32	L	15	Total O 15 15	0
32	M	3	Total O 3 3	0
32	O	2	Total O 2 2	0
32	Z	5	Total O 5 5	0
32	1	4	Total O 4 4	0
32	2	6	Total O 6 6	0
32	4	10	Total O 10 10	0

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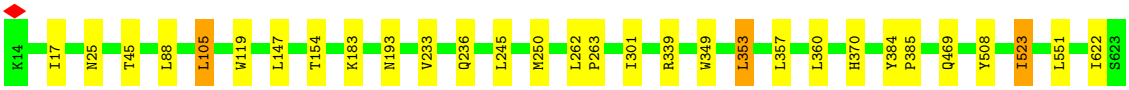
Mol	Chain	Residues	Atoms	AltConf
32	5	11	Total O 11 11	0
32	6	10	Total O 10 10	0

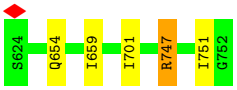
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

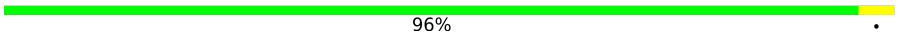
Chain A:

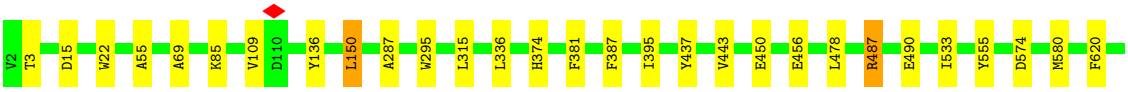




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

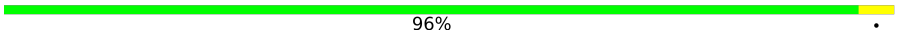
Chain B:

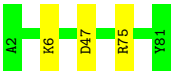




• Molecule 3: Photosystem I iron-sulfur center

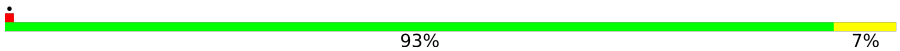
Chain C:

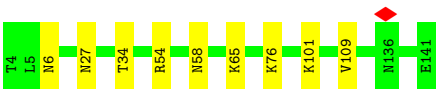




• Molecule 4: Photosystem I reaction center subunit II

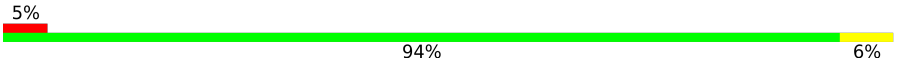
Chain D:





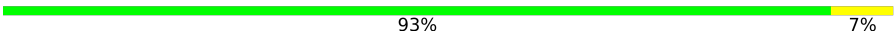
• Molecule 5: Photosystem I subunit IV

Chain E:



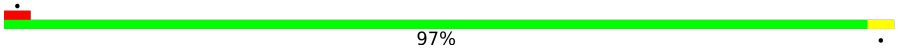
• Molecule 6: Photosystem I reaction center subunit III

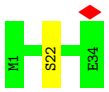
Chain F:



• Molecule 7: Photosystem I reaction center subunit VIII

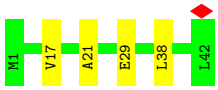
Chain I:





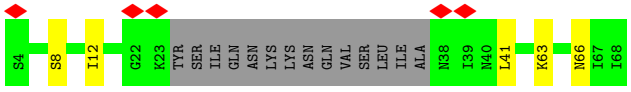
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



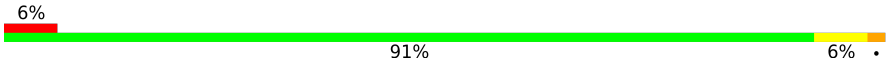
• Molecule 9: PSI-K

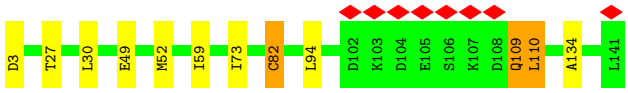
Chain K:



• Molecule 10: Photosystem I reaction center subunit XI

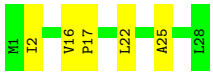
Chain L:





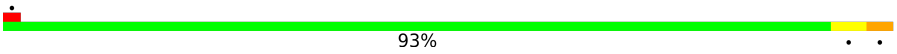
• Molecule 11: Photosystem I reaction center subunit XII

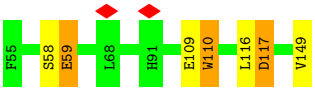
Chain M:



• Molecule 12: Photosystem I subunit O

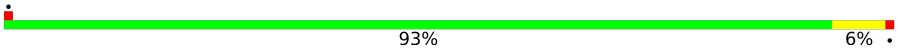
Chain O:

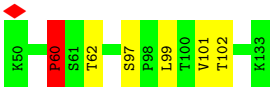




• Molecule 13: Psa28

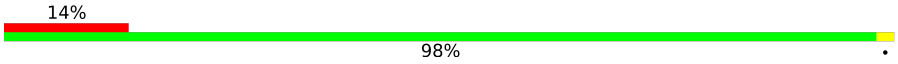
Chain Z:

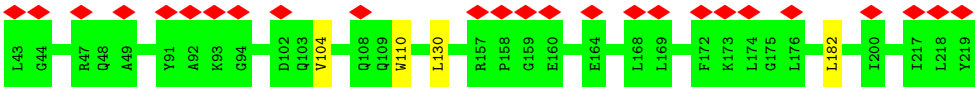




• Molecule 14: RedCAP

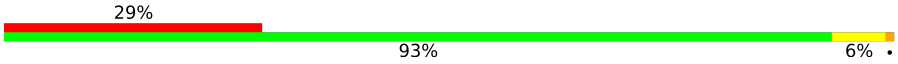
Chain 1:

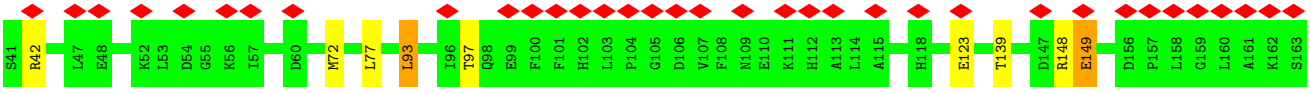


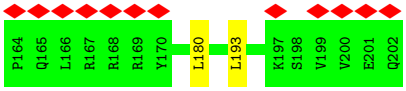


• Molecule 15: Light-harvesting complex protein

Chain 2:

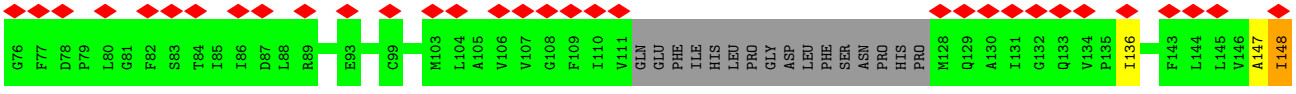


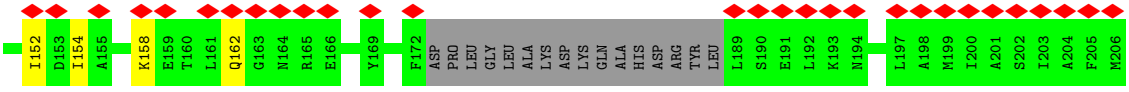




• Molecule 16: Light-harvesting complex protein

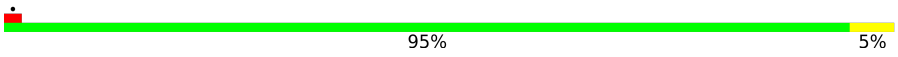
Chain 3:

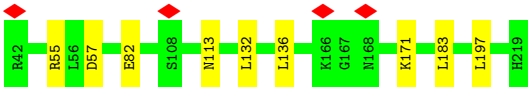




• Molecule 17: Light-harvesting complex protein

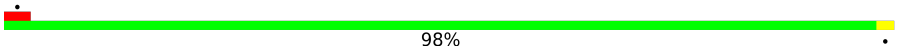
Chain 4:

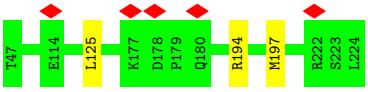




• Molecule 18: Light-harvesting complex protein

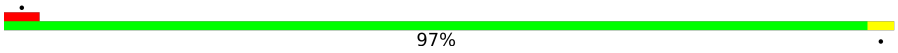
Chain 5:

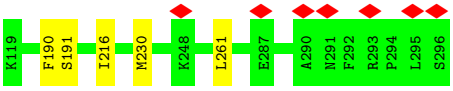




• Molecule 19: Light-harvesting complex protein

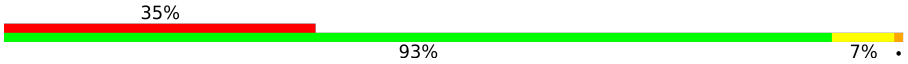
Chain 6:

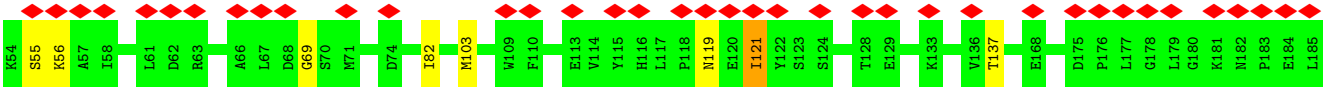


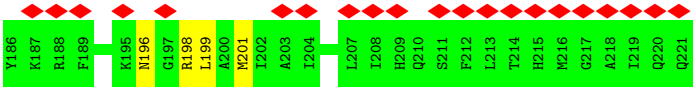


• Molecule 20: Light-harvesting complex protein

Chain 7:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110313	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	240.63998, 240.63998, 240.63998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, DGD, BCR, CL0, UNL, SF4, 5X6, LHG, A1L64, LMT, RRX

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	0.50	0/6038	0.84	0/8223
2	B	0.50	0/6072	0.85	1/8286 (0.0%)
3	C	0.52	0/610	0.84	0/826
4	D	0.47	0/1128	0.89	0/1521
5	E	0.46	0/525	0.76	0/708
6	F	0.48	0/1314	0.86	0/1771
7	I	0.51	0/281	0.80	0/383
8	J	0.49	0/346	0.84	0/472
9	K	0.48	0/368	0.95	0/497
10	L	0.46	0/1102	0.96	1/1495 (0.1%)
11	M	0.47	0/215	0.91	0/291
12	O	0.50	0/775	0.93	0/1065
13	Z	0.49	0/655	0.87	0/900
14	1	0.46	0/1400	0.93	0/1898
15	2	0.47	0/1316	0.98	0/1779
16	3	0.46	0/784	0.97	0/1053
17	4	0.48	0/1450	0.89	0/1963
18	5	0.48	0/1438	0.89	0/1943
19	6	0.47	0/1500	0.89	0/2033
20	7	0.48	0/1358	0.96	0/1841
All	All	0.49	0/28675	0.88	2/38948 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	82	CYS	CB-CA-C	-5.30	102.56	110.88
2	B	15	ASP	CA-CB-CG	5.06	117.66	112.60

There are no chirality outliers.

There are no planarity outliers.

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	5844	0	5739	14	0
2	B	5859	0	5679	19	0
3	C	600	0	580	1	0
4	D	1103	0	1105	3	0
5	E	516	0	528	0	0
6	F	1285	0	1313	4	0
7	I	273	0	282	1	0
8	J	337	0	358	2	0
9	K	368	0	410	1	0
10	L	1076	0	1087	7	0
11	M	214	0	246	4	0
12	O	748	0	745	4	0
13	Z	637	0	661	2	0
14	1	1370	0	1400	1	0
15	2	1286	0	1298	7	0
16	3	772	0	804	4	0
17	4	1407	0	1414	1	0
18	5	1402	0	1413	1	0
19	6	1450	0	1435	2	0
20	7	1322	0	1328	7	0
21	A	65	0	72	1	0
22	1	472	0	428	7	0
22	2	496	0	417	16	0
22	3	255	0	220	4	0
22	4	572	0	510	11	0
22	5	575	0	516	7	0
22	6	610	0	537	10	0
22	7	517	0	403	15	0
22	A	2546	0	2628	29	0
22	B	2528	0	2657	45	0
22	F	147	0	123	4	0
22	J	42	0	31	1	0
22	K	97	0	80	2	0
22	L	163	0	147	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	195	0	156	3	0
22	Z	110	0	105	5	0
23	A	33	0	0	0	0
23	B	33	0	0	0	0
24	1	49	0	74	0	0
24	2	32	0	34	0	0
24	4	32	0	34	1	0
24	5	25	0	20	0	0
24	6	32	0	34	0	0
24	A	122	0	163	0	0
24	B	33	0	36	0	0
24	J	33	0	36	1	0
25	1	40	0	56	2	0
25	2	40	0	56	0	0
25	4	40	0	56	2	0
25	5	40	0	56	1	0
25	A	240	0	336	11	0
25	B	160	0	224	10	0
25	F	80	0	112	5	0
25	I	40	0	56	1	0
25	J	40	0	56	1	0
25	K	40	0	56	4	0
25	L	120	0	168	3	0
25	Z	80	0	112	4	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	1	33	0	0	0	0
27	4	27	0	0	0	0
27	5	27	0	0	0	0
27	6	73	0	0	0	0
27	7	42	0	0	0	0
27	A	110	0	0	0	0
27	B	18	0	0	0	0
27	F	35	0	0	0	0
27	I	21	0	0	0	0
27	J	22	0	0	0	0
27	K	11	0	0	0	0
27	L	33	0	0	0	0
27	M	9	0	0	0	0
27	O	24	0	0	0	0
27	Z	45	0	0	0	0
28	B	66	0	96	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1	210	0	0	0	0
29	2	126	0	0	0	0
29	3	42	0	0	0	0
29	4	126	0	0	0	0
29	5	168	0	0	0	0
29	6	126	0	0	0	0
29	7	210	0	0	0	0
29	B	42	0	0	0	0
29	J	42	0	0	0	0
29	M	42	0	0	0	0
29	O	84	0	0	0	0
29	Z	42	0	0	0	0
30	4	35	0	46	0	0
30	5	35	0	46	0	0
30	F	35	0	46	0	0
30	O	35	0	46	1	0
31	1	41	0	56	3	0
31	4	41	0	56	6	0
31	5	41	0	56	2	0
31	6	41	0	56	3	0
32	1	4	0	0	0	0
32	2	6	0	0	0	0
32	4	10	0	0	0	0
32	5	11	0	0	0	0
32	6	10	0	0	0	0
32	A	189	0	0	0	0
32	B	220	0	0	1	0
32	C	44	0	0	0	0
32	D	29	0	0	0	0
32	E	18	0	0	0	0
32	F	32	0	0	0	0
32	I	3	0	0	0	0
32	J	5	0	0	0	0
32	K	2	0	0	0	0
32	L	15	0	0	0	0
32	M	3	0	0	0	0
32	O	2	0	0	0	0
32	Z	5	0	0	0	0
All	All	41435	0	39134	254	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 3.

All (254) 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)
20:7:56:LYS:CB	22:7:303:CLA:HED1	2.22	0.69
20:7:56:LYS:HB3	22:7:303:CLA:HED1	1.77	0.67
10:L:73:ILE:HD13	14:1:110:TRP:CE3	2.30	0.66
25:B:843:BCR:H311	25:B:843:BCR:HC8	1.79	0.65
22:B:804:CLA:HBD	22:B:804:CLA:HBA1	1.81	0.62
25:A:846:BCR:H382	25:A:846:BCR:H23C	1.83	0.60
15:2:93:LEU:HD22	22:2:305:CLA:HBC2	1.83	0.59
22:B:850:CLA:HHC	22:B:850:CLA:HBB1	1.85	0.59
22:L:203:CLA:HHC	22:L:203:CLA:HBB1	1.84	0.59
22:A:830:CLA:H41	10:L:30:LEU:HD23	1.86	0.58
22:B:838:CLA:HHC	22:B:838:CLA:HBB1	1.85	0.58
25:F:201:BCR:H331	25:F:201:BCR:C8	2.35	0.56
22:A:830:CLA:H42	10:L:27:THR:HG23	1.86	0.56
22:B:801:CLA:H3A	22:B:801:CLA:CGA	2.36	0.56
22:F:206:CLA:HHC	22:F:206:CLA:HBB1	1.88	0.56
22:A:816:CLA:HHC	22:A:816:CLA:HBB1	1.88	0.56
15:2:180:LEU:HD21	22:2:310:CLA:HBC3	1.88	0.55
22:A:808:CLA:HHC	22:A:808:CLA:HBB1	1.87	0.55
25:A:861:BCR:H331	25:A:861:BCR:C8	2.37	0.55
13:Z:60:PRO:O	13:Z:62:THR:N	2.36	0.54
25:Z:205:BCR:H383	25:Z:205:BCR:H23C	1.90	0.54
2:B:533:ILE:HG12	22:B:801:CLA:HMD3	1.90	0.53
25:F:201:BCR:H383	25:F:201:BCR:H23C	1.90	0.53
22:K:102:CLA:HHC	22:K:102:CLA:HBB1	1.90	0.53
22:B:822:CLA:HHC	22:B:839:CLA:HED1	1.90	0.53
25:A:843:BCR:H23C	25:A:843:BCR:H403	1.90	0.53
2:B:55:ALA:CB	2:B:150:LEU:HD13	2.39	0.53
22:B:812:CLA:HHC	22:B:812:CLA:HBB1	1.91	0.53
20:7:56:LYS:HB2	22:7:303:CLA:HED1	1.89	0.53
20:7:199:LEU:HD21	22:7:311:CLA:HBC3	1.90	0.53
22:A:814:CLA:HHC	22:A:814:CLA:HBB1	1.89	0.53
22:B:806:CLA:H102	22:B:806:CLA:H171	1.91	0.53
22:6:307:CLA:HBB1	22:6:307:CLA:HHC	1.90	0.53
22:6:312:CLA:HHC	22:6:312:CLA:HBB1	1.91	0.53
25:B:841:BCR:H311	25:B:841:BCR:HC8	1.90	0.52
22:4:310:CLA:HHC	22:4:310:CLA:HBB1	1.90	0.52
22:B:825:CLA:H43	22:B:833:CLA:HBB2	1.90	0.52
22:B:833:CLA:HHC	22:B:833:CLA:HBB1	1.91	0.52
22:A:837:CLA:HHC	22:A:837:CLA:HBB1	1.91	0.52
25:A:861:BCR:H383	25:A:861:BCR:H23C	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:842:BCR:H382	25:B:842:BCR:H23C	1.91	0.52
31:5:322:RRX:H17	31:5:322:RRX:H21	1.92	0.52
22:B:817:CLA:HHC	22:B:817:CLA:HBB1	1.92	0.52
22:6:303:CLA:HHC	22:6:303:CLA:HBB1	1.91	0.52
2:B:450:GLU:OE2	6:F:80:ARG:NH2	2.40	0.52
22:O:205:CLA:HHC	22:O:205:CLA:HBB1	1.91	0.52
15:2:72:MET:HE3	15:2:77:LEU:HD21	1.90	0.52
22:1:309:CLA:HHC	22:1:309:CLA:HBB1	1.92	0.51
22:2:302:CLA:HBC2	16:3:152:ILE:HD11	1.91	0.51
31:5:322:RRX:H17	31:5:322:RRX:C23	2.40	0.51
22:A:822:CLA:HHC	22:A:822:CLA:HBB1	1.92	0.51
22:A:833:CLA:HHC	22:A:833:CLA:HBB1	1.92	0.51
22:6:308:CLA:HHC	22:6:308:CLA:HBB1	1.92	0.51
22:4:311:CLA:CBB	31:4:317:RRX:H29	2.41	0.51
1:A:659:ILE:HD11	2:B:620:PHE:CD2	2.46	0.51
25:J:103:BCR:C8	25:J:103:BCR:H331	2.41	0.50
22:5:309:CLA:HHC	22:5:309:CLA:HBB1	1.93	0.50
1:A:353:LEU:HD22	1:A:357:LEU:HG	1.92	0.50
22:1:302:CLA:HHC	22:1:302:CLA:HBB1	1.93	0.50
22:B:802:CLA:HAA2	22:B:802:CLA:HBD	1.93	0.50
25:L:202:BCR:H383	25:L:202:BCR:H23C	1.93	0.50
22:5:301:CLA:HHC	22:5:301:CLA:HBB1	1.93	0.50
22:5:308:CLA:HHC	22:5:308:CLA:HBB1	1.92	0.50
2:B:295:TRP:HA	16:3:158:LYS:HD2	1.93	0.50
31:1:315:RRX:H46	31:1:315:RRX:H51	1.93	0.50
15:2:97:THR:HG21	22:2:305:CLA:HBC3	1.94	0.50
22:A:838:CLA:HHC	22:A:838:CLA:HBB1	1.93	0.50
22:B:811:CLA:H43	22:B:812:CLA:C4C	2.42	0.50
22:J:102:CLA:HHC	22:J:102:CLA:HBB1	1.94	0.50
22:B:810:CLA:HHC	22:B:810:CLA:HBB1	1.94	0.50
22:7:310:CLA:HBB1	22:7:310:CLA:HHC	1.94	0.49
25:Z:205:BCR:HC8	25:Z:205:BCR:H331	1.94	0.49
22:B:820:CLA:HHC	22:B:820:CLA:HBB1	1.93	0.49
22:2:309:CLA:HHC	22:2:309:CLA:HBB1	1.95	0.49
25:F:201:BCR:H331	25:F:201:BCR:HC8	1.94	0.49
22:4:309:CLA:HHC	22:4:309:CLA:HBB1	1.95	0.49
22:B:827:CLA:HBD	22:B:827:CLA:HAA1	1.94	0.49
12:O:116:LEU:O	12:O:117:ASP:HB3	2.13	0.49
22:5:305:CLA:HHC	22:5:305:CLA:HBB1	1.95	0.49
2:B:287:ALA:HB2	22:B:819:CLA:HBC2	1.94	0.49
22:A:839:CLA:HHC	22:A:839:CLA:HBB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:205:BCR:H331	25:Z:205:BCR:C8	2.43	0.49
31:4:317:RRX:H6	24:4:318:LHG:HC41	1.94	0.49
25:K:103:BCR:H382	25:K:103:BCR:H23C	1.95	0.49
22:2:306:CLA:HHC	22:2:306:CLA:HBB1	1.95	0.48
22:2:307:CLA:HHC	22:2:307:CLA:HBB1	1.95	0.48
25:I:102:BCR:H382	25:I:102:BCR:H23C	1.95	0.48
22:7:306:CLA:C1A	22:7:306:CLA:CGA	2.91	0.48
22:A:802:CLA:HAB	22:A:809:CLA:H142	1.94	0.48
22:F:205:CLA:HHC	22:F:205:CLA:HBB1	1.94	0.48
22:2:302:CLA:HHC	22:2:302:CLA:HBB1	1.94	0.48
31:4:317:RRX:C23	31:4:317:RRX:H17	2.42	0.48
22:K:102:CLA:HMC2	25:K:103:BCR:H332	1.96	0.48
31:1:315:RRX:C23	31:1:315:RRX:H17	2.42	0.48
25:F:207:BCR:H23C	25:F:207:BCR:H383	1.95	0.48
22:Z:204:CLA:NC	22:Z:204:CLA:H52	2.29	0.48
22:3:303:CLA:HHC	22:3:303:CLA:HBB1	1.95	0.48
22:7:311:CLA:HHC	22:7:311:CLA:HBB1	1.96	0.48
25:A:846:BCR:H331	25:A:846:BCR:C8	2.43	0.48
1:A:105:LEU:HD11	1:A:154:THR:HA	1.96	0.48
1:A:360:LEU:HD21	22:A:804:CLA:HBB1	1.96	0.48
22:1:308:CLA:HHC	22:1:308:CLA:HBB1	1.96	0.47
22:7:312:CLA:HBB1	22:7:312:CLA:HHC	1.96	0.47
22:6:314:CLA:HHC	22:6:314:CLA:HBB1	1.96	0.47
22:1:305:CLA:HBB1	22:1:305:CLA:HHC	1.97	0.47
22:B:802:CLA:HMB1	22:B:802:CLA:HBB1	1.96	0.47
22:B:834:CLA:HMB1	22:B:834:CLA:HBB1	1.97	0.47
22:3:304:CLA:HHC	22:3:304:CLA:HBB1	1.96	0.47
22:5:304:CLA:CGA	22:5:304:CLA:C1A	2.93	0.47
16:3:147:ALA:O	16:3:148:ILE:HB	2.14	0.47
22:F:205:CLA:HAA2	22:F:205:CLA:HBD	1.97	0.47
22:O:204:CLA:HHC	22:O:204:CLA:HBB1	1.97	0.47
22:3:305:CLA:HHC	22:3:305:CLA:HBB1	1.97	0.47
31:4:317:RRX:H17	31:4:317:RRX:H21	1.97	0.47
22:7:306:CLA:HHC	22:7:306:CLA:HBB1	1.97	0.47
2:B:381:PHE:CE2	2:B:580:MET:HE1	2.50	0.47
22:2:310:CLA:HBB1	22:2:310:CLA:HHC	1.96	0.47
22:A:821:CLA:HHC	22:A:821:CLA:HBB1	1.97	0.47
22:4:305:CLA:C1A	22:4:305:CLA:CGA	2.93	0.46
22:4:306:CLA:HHC	22:4:306:CLA:HBB1	1.96	0.46
13:Z:101:VAL:HG13	13:Z:102:THR:HG23	1.96	0.46
31:6:318:RRX:C23	31:6:318:RRX:H17	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:806:CLA:H72	22:B:806:CLA:H41	1.97	0.46
22:B:822:CLA:HBC2	22:B:823:CLA:HBA1	1.96	0.46
22:7:307:CLA:HHC	22:7:307:CLA:HBB1	1.96	0.46
1:A:349:TRP:HB3	22:A:803:CLA:HAC1	1.97	0.46
10:L:59:ILE:HA	10:L:82:CYS:SG	2.56	0.46
22:F:204:CLA:HHC	22:F:204:CLA:HBB1	1.98	0.46
22:2:305:CLA:C1A	22:2:305:CLA:CGA	2.94	0.46
2:B:136:TYR:HB2	11:M:2:ILE:HD11	1.96	0.45
22:B:821:CLA:HHC	22:B:821:CLA:HBB1	1.98	0.45
22:7:313:CLA:HHC	22:7:313:CLA:HBB1	1.97	0.45
22:2:311:CLA:HHC	22:2:311:CLA:HBB1	1.98	0.45
1:A:245:LEU:HD21	22:A:814:CLA:HBC1	1.99	0.45
22:A:809:CLA:HHC	22:A:809:CLA:HBB1	1.97	0.45
25:B:841:BCR:H311	25:B:841:BCR:C8	2.47	0.45
6:F:164:TRP:N	6:F:165:PRO:CD	2.80	0.45
2:B:69:ALA:HB1	11:M:2:ILE:CD1	2.46	0.45
2:B:574:ASP:OD2	32:B:901:HOH:O	2.20	0.45
25:4:316:BCR:H382	25:4:316:BCR:H23C	1.97	0.45
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.34	0.45
22:2:304:CLA:HHC	22:2:304:CLA:HBB1	1.98	0.45
22:B:849:CLA:HBB1	22:B:849:CLA:HMB3	1.99	0.45
17:4:136:LEU:HD22	22:4:307:CLA:CBB	2.46	0.45
22:4:311:CLA:HHC	22:4:311:CLA:HBB1	1.99	0.45
22:6:311:CLA:HMC1	22:6:311:CLA:HBC3	1.99	0.45
20:7:121:ILE:HD12	20:7:137:THR:HG21	1.98	0.45
15:2:42:ARG:CB	22:2:302:CLA:HED1	2.46	0.45
18:5:194:ARG:HA	18:5:197:MET:HE3	1.97	0.45
1:A:508:TYR:HB2	1:A:523:ILE:HG23	1.99	0.44
22:L:205:CLA:HHC	22:L:205:CLA:HBB1	1.98	0.44
22:7:303:CLA:H2A	22:7:303:CLA:HED2	1.98	0.44
22:A:829:CLA:CBB	22:A:837:CLA:CBB	2.95	0.44
25:B:844:BCR:H11C	25:B:844:BCR:H341	1.86	0.44
22:A:817:CLA:CAD	22:A:827:CLA:H41	2.48	0.44
4:D:34:THR:HA	4:D:58:ASN:O	2.18	0.44
22:6:313:CLA:CAB	31:6:318:RRX:H29	2.47	0.44
2:B:717:TYR:CE2	22:B:803:CLA:HED1	2.52	0.44
22:B:812:CLA:H41	22:B:812:CLA:C7	2.48	0.44
22:B:812:CLA:C1A	22:B:812:CLA:CGA	2.96	0.44
15:2:148:ARG:O	15:2:149:GLU:CB	2.66	0.44
1:A:301:ILE:CD1	22:A:816:CLA:HBC2	2.47	0.44
22:5:307:CLA:CGA	22:5:307:CLA:H3A	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:857:CLA:OBD	22:B:803:CLA:HMB2	2.18	0.44
10:L:49:GLU:HA	10:L:52:MET:HE3	1.99	0.44
11:M:25:ALA:HB2	25:1:301:BCR:H312	2.00	0.44
12:O:58:SER:O	12:O:59:GLU:C	2.61	0.44
22:O:203:CLA:HAA2	22:O:203:CLA:HBD	1.98	0.44
25:Z:205:BCR:H11C	25:Z:205:BCR:H341	1.86	0.44
22:4:312:CLA:HHC	22:4:312:CLA:HBB1	1.99	0.44
22:B:809:CLA:H201	7:I:22:SER:HB2	2.00	0.43
11:M:16:VAL:HB	11:M:17:PRO:HD3	2.00	0.43
22:Z:201:CLA:HAA1	22:Z:201:CLA:HBD	2.00	0.43
22:Z:204:CLA:H12	22:Z:204:CLA:NA	2.33	0.43
1:A:370:HIS:ND1	22:A:816:CLA:OBD	2.50	0.43
22:B:818:CLA:CGA	22:B:818:CLA:H3A	2.49	0.43
22:B:836:CLA:HBB1	22:B:836:CLA:HMB3	1.99	0.43
25:B:844:BCR:H382	25:B:844:BCR:H23C	2.00	0.43
22:A:859:CLA:H142	8:J:21:ALA:HA	2.01	0.43
22:B:812:CLA:H43	22:B:812:CLA:C3B	2.48	0.43
25:B:841:BCR:H383	25:B:841:BCR:H23C	2.00	0.43
15:2:42:ARG:HB3	22:2:302:CLA:HED1	2.00	0.43
22:6:306:CLA:CGA	22:6:306:CLA:C1A	2.97	0.43
25:A:843:BCR:H11C	25:A:843:BCR:H341	1.91	0.43
2:B:395:ILE:HD13	2:B:555:TYR:HA	2.00	0.43
2:B:437:TYR:CD1	22:B:803:CLA:H203	2.53	0.43
22:2:308:CLA:HHC	22:2:308:CLA:HBB1	2.01	0.43
22:A:831:CLA:H12	22:B:837:CLA:H93	2.00	0.42
22:B:808:CLA:HHC	22:B:808:CLA:HBB1	2.01	0.42
22:1:307:CLA:HBA1	22:1:307:CLA:HBD	2.00	0.42
19:6:216:ILE:HG12	22:6:309:CLA:CBB	2.49	0.42
22:1:303:CLA:HHC	22:1:303:CLA:HBB1	2.01	0.42
22:B:835:CLA:H41	22:B:835:CLA:H71	2.00	0.42
24:J:106:LHG:HC5	19:6:230:MET:HB3	2.01	0.42
25:1:301:BCR:H403	25:1:301:BCR:H23C	2.02	0.42
1:A:701:ILE:HD13	22:A:858:CLA:HMD2	2.01	0.42
2:B:374:HIS:HE2	22:B:828:CLA:C1B	2.33	0.42
1:A:654:GLN:HB3	1:A:747:ARG:HD2	2.00	0.42
2:B:487:ARG:NH1	2:B:490:GLU:OE1	2.52	0.42
25:L:206:BCR:H11C	25:L:206:BCR:H341	1.89	0.42
22:B:828:CLA:C4A	22:B:828:CLA:HBA1	2.50	0.42
25:B:842:BCR:H15C	25:B:842:BCR:H351	1.92	0.42
31:1:315:RRX:H51	31:1:315:RRX:C8	2.50	0.42
25:F:207:BCR:H11C	25:F:207:BCR:H341	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:109:GLU:O	12:O:110:TRP:C	2.62	0.42
12:O:116:LEU:O	12:O:117:ASP:CB	2.68	0.42
2:B:387:PHE:CE1	25:B:843:BCR:H373	2.55	0.42
25:K:103:BCR:H24C	25:K:103:BCR:H371	1.88	0.42
22:7:304:CLA:HBB1	22:7:304:CLA:HHC	2.02	0.42
25:A:844:BCR:C40	25:A:844:BCR:H23C	2.50	0.42
2:B:456:GLU:OE2	6:F:98:HIS:ND1	2.53	0.42
3:C:47:ASP:OD2	4:D:65:LYS:NZ	2.51	0.42
22:B:824:CLA:HAA2	22:B:824:CLA:HBD	2.02	0.41
10:L:134:ALA:HB1	22:L:205:CLA:HED1	2.02	0.41
22:B:806:CLA:H43	28:B:845:DGD:HB72	2.00	0.41
2:B:657:TRP:CD2	22:B:803:CLA:HMA2	2.55	0.41
25:5:315:BCR:H382	25:5:315:BCR:H23C	2.01	0.41
20:7:198:ARG:HA	20:7:201:MET:HE3	2.03	0.41
22:A:837:CLA:H202	30:O:201:LMT:H122	2.01	0.41
25:A:861:BCR:H331	25:A:861:BCR:HC8	2.01	0.41
25:K:103:BCR:H331	25:K:103:BCR:C8	2.51	0.41
22:A:859:CLA:H8	8:J:17:VAL:HG22	2.03	0.41
22:B:831:CLA:H11	6:F:172:TYR:CE1	2.56	0.41
25:4:316:BCR:H20C	25:4:316:BCR:H361	1.91	0.41
1:A:262:LEU:N	1:A:263:PRO:CD	2.84	0.41
21:A:801:CL0:H12	22:B:802:CLA:OBD	2.21	0.41
10:L:109:GLN:O	10:L:110:LEU:CB	2.69	0.41
20:7:103:MET:HE1	22:7:309:CLA:CBB	2.51	0.41
1:A:119:TRP:CD2	22:A:807:CLA:HED3	2.56	0.41
25:A:861:BCR:H311	25:A:861:BCR:HC7	1.90	0.41
25:A:862:BCR:H20C	25:A:862:BCR:H361	1.94	0.41
25:B:841:BCR:H331	25:B:841:BCR:HC7	1.79	0.41
22:1:306:CLA:HBB1	22:1:306:CLA:HMB3	2.03	0.41
22:4:309:CLA:HBC2	22:4:310:CLA:HBC3	2.03	0.41
31:4:317:RRX:H56	31:4:317:RRX:H46	2.01	0.41
22:Z:201:CLA:HHC	22:Z:201:CLA:HBB1	2.03	0.41
22:Z:204:CLA:H62	22:4:307:CLA:HAB	2.03	0.41
22:3:301:CLA:HHC	22:3:301:CLA:HBB1	2.03	0.41
22:5:310:CLA:H43	22:6:307:CLA:C4B	2.51	0.41
22:A:815:CLA:CHD	22:A:816:CLA:HBB2	2.51	0.40
25:A:862:BCR:H11C	25:A:862:BCR:H341	1.97	0.40
22:B:808:CLA:HAA1	22:B:808:CLA:HBD	2.02	0.40
31:4:317:RRX:H26	31:4:317:RRX:H22	1.96	0.40
22:A:857:CLA:HAA2	22:A:857:CLA:HBD	2.02	0.40
22:2:302:CLA:HBC2	16:3:152:ILE:CD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:310:CLA:CBC	22:4:310:CLA:HHD	2.51	0.40
1:A:384:TYR:N	1:A:385:PRO:CD	2.84	0.40
22:B:809:CLA:C17	22:B:838:CLA:H43	2.52	0.40
22:B:813:CLA:H101	22:B:813:CLA:H62	1.94	0.40
4:D:54:ARG:H	4:D:58:ASN:HD21	1.70	0.40
22:7:308:CLA:HHC	22:7:308:CLA:HBB1	2.04	0.40
9:K:8:SER:O	9:K:12:ILE:HG12	2.21	0.40
25:L:201:BCR:H331	25:L:201:BCR:C8	2.52	0.40
31:6:318:RRX:H26	31:6:318:RRX:H22	1.97	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	737/739 (100%)	714 (97%)	23 (3%)	0	100 100
2	B	730/732 (100%)	711 (97%)	19 (3%)	0	100 100
3	C	78/80 (98%)	77 (99%)	1 (1%)	0	100 100
4	D	136/138 (99%)	129 (95%)	6 (4%)	1 (1%)	18 19
5	E	62/64 (97%)	58 (94%)	2 (3%)	2 (3%)	3 1
6	F	159/161 (99%)	155 (98%)	4 (2%)	0	100 100
7	I	32/34 (94%)	32 (100%)	0	0	100 100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100 100
9	K	47/65 (72%)	45 (96%)	2 (4%)	0	100 100
10	L	137/139 (99%)	132 (96%)	3 (2%)	2 (2%)	8 6
11	M	26/28 (93%)	26 (100%)	0	0	100 100
12	O	93/95 (98%)	87 (94%)	3 (3%)	3 (3%)	3 1
13	Z	82/84 (98%)	79 (96%)	1 (1%)	2 (2%)	4 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	1	175/177 (99%)	171 (98%)	4 (2%)	0	100 100
15	2	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	21 23
16	3	93/131 (71%)	89 (96%)	3 (3%)	1 (1%)	11 10
17	4	176/178 (99%)	171 (97%)	5 (3%)	0	100 100
18	5	176/178 (99%)	169 (96%)	7 (4%)	0	100 100
19	6	176/178 (99%)	168 (96%)	6 (3%)	2 (1%)	11 10
20	7	166/168 (99%)	156 (94%)	8 (5%)	2 (1%)	10 8
All	All	3481/3573 (97%)	3364 (97%)	101 (3%)	16 (0%)	26 27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	L	110	LEU
15	2	149	GLU
4	D	6	ASN
5	E	29	LYS
12	O	59	GLU
12	O	117	ASP
16	3	148	ILE
20	7	55	SER
19	6	191	SER
20	7	69	GLY
5	E	30	SER
10	L	109	GLN
13	Z	60	PRO
19	6	190	PHE
13	Z	97	SER
12	O	110	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/610 (100%)	591 (97%)	19 (3%)	35	48
2	B	599/599 (100%)	590 (98%)	9 (2%)	57	73
3	C	67/67 (100%)	65 (97%)	2 (3%)	36	49
4	D	120/120 (100%)	116 (97%)	4 (3%)	33	45
5	E	57/57 (100%)	55 (96%)	2 (4%)	32	43
6	F	142/142 (100%)	136 (96%)	6 (4%)	26	36
7	I	31/31 (100%)	31 (100%)	0	100	100
8	J	36/36 (100%)	34 (94%)	2 (6%)	19	24
9	K	44/57 (77%)	41 (93%)	3 (7%)	14	17
10	L	115/115 (100%)	113 (98%)	2 (2%)	53	69
11	M	24/24 (100%)	23 (96%)	1 (4%)	26	36
12	O	81/81 (100%)	80 (99%)	1 (1%)	63	78
13	Z	73/73 (100%)	71 (97%)	2 (3%)	39	53
14	1	142/142 (100%)	139 (98%)	3 (2%)	47	63
15	2	136/136 (100%)	132 (97%)	4 (3%)	37	51
16	3	81/109 (74%)	78 (96%)	3 (4%)	30	41
17	4	149/149 (100%)	141 (95%)	8 (5%)	20	25
18	5	151/151 (100%)	150 (99%)	1 (1%)	76	87
19	6	152/152 (100%)	151 (99%)	1 (1%)	76	87
20	7	143/143 (100%)	139 (97%)	4 (3%)	38	52
All	All	2953/2994 (99%)	2876 (97%)	77 (3%)	41	55

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	25	ASN
1	A	45	THR
1	A	88	LEU
1	A	105	LEU
1	A	147	LEU
1	A	183	LYS
1	A	193	ASN
1	A	233	VAL
1	A	236	GLN
1	A	250	MET

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Mol	Chain	Res	Type
1	A	339	ARG
1	A	353	LEU
1	A	469	GLN
1	A	523	ILE
1	A	551	LEU
1	A	622	ILE
1	A	747	ARG
1	A	751	ILE
2	B	3	THR
2	B	85	LYS
2	B	109	VAL
2	B	150	LEU
2	B	315	LEU
2	B	336	LEU
2	B	443	VAL
2	B	478	LEU
2	B	487	ARG
3	C	6	LYS
3	C	75	ARG
4	D	27	ASN
4	D	76	LYS
4	D	101	LYS
4	D	109	VAL
5	E	26	THR
5	E	48	VAL
6	F	32	ASN
6	F	117	LEU
6	F	153	LEU
6	F	169	LEU
6	F	179	MET
6	F	189	ARG
8	J	29	GLU
8	J	38	LEU
9	K	41	LEU
9	K	63	LYS
9	K	66	ASN
10	L	3	ASP
10	L	94	LEU
11	M	22	LEU
12	O	149	VAL
13	Z	60	PRO
13	Z	99	LEU

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Mol	Chain	Res	Type
14	1	104	VAL
14	1	130	LEU
14	1	182	LEU
15	2	93	LEU
15	2	123	GLU
15	2	139	THR
15	2	193	LEU
16	3	136	ILE
16	3	154	ILE
16	3	162	GLN
17	4	55	ARG
17	4	57	ASP
17	4	82	GLU
17	4	113	ASN
17	4	132	LEU
17	4	171	LYS
17	4	183	LEU
17	4	197	LEU
18	5	125	LEU
19	6	261	LEU
20	7	82	ILE
20	7	119	ASN
20	7	121	ILE
20	7	196	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	258	ASN
1	A	315	ASN
1	A	469	GLN
1	A	644	ASN
1	A	715	GLN
2	B	80	ASN
2	B	171	ASN
2	B	205	GLN
2	B	294	ASN
2	B	402	GLN
2	B	585	ASN
2	B	607	ASN
3	C	16	GLN

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Mol	Chain	Res	Type
4	D	58	ASN
4	D	96	GLN
4	D	138	GLN
6	F	32	ASN
6	F	43	ASN
10	L	70	ASN
12	O	106	ASN
13	Z	94	ASN
15	2	98	GLN
15	2	112	HIS
15	2	191	GLN
17	4	81	GLN
17	4	122	GLN
17	4	149	HIS
17	4	174	GLN
17	4	219	HIS
18	5	106	GLN
18	5	192	ASN
19	6	166	HIS
19	6	180	GLN
19	6	199	HIS
19	6	263	ASN
20	7	81	ASN
20	7	142	GLN
20	7	196	ASN
20	7	215	HIS
20	7	221	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 298 ligands modelled in this entry, 52 are unknown - leaving 246 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	Z	204	13	69,73,73	1.92	21 (30%)	83,113,113	2.83	33 (39%)
22	CLA	A	830	1	60,64,73	2.09	20 (33%)	72,102,113	2.89	27 (37%)
22	CLA	B	850	-	49,53,73	2.45	20 (40%)	59,89,113	3.17	28 (47%)
22	CLA	7	310	-	45,49,73	2.53	19 (42%)	54,84,113	3.31	28 (51%)
22	CLA	A	834	1	64,68,73	2.09	19 (29%)	77,107,113	2.89	30 (38%)
22	CLA	1	307	14	59,63,73	2.28	20 (33%)	71,101,113	3.10	31 (43%)
29	5X6	2	314	-	43,43,43	2.72	18 (41%)	58,60,60	4.34	30 (51%)
30	LMT	F	202	-	36,36,36	0.31	0	47,47,47	0.78	2 (4%)
31	RRX	4	317	-	42,42,42	1.66	8 (19%)	57,58,58	1.37	8 (14%)
22	CLA	B	805	2	69,73,73	1.88	19 (27%)	83,113,113	2.86	34 (40%)
22	CLA	A	802	22,1	59,63,73	2.07	19 (32%)	71,101,113	2.96	30 (42%)
22	CLA	A	818	1	69,73,73	1.87	19 (27%)	83,113,113	2.83	30 (36%)
29	5X6	3	306	-	43,43,43	2.74	17 (39%)	58,60,60	4.32	31 (53%)
25	BCR	A	845	-	41,41,41	1.64	11 (26%)	56,56,56	1.62	12 (21%)
24	LHG	4	318	22	31,31,48	0.32	0	34,37,54	0.58	0
22	CLA	1	302	32	69,73,73	2.00	21 (30%)	83,113,113	2.77	29 (34%)
29	5X6	4	315	-	43,43,43	2.73	18 (41%)	58,60,60	4.23	30 (51%)
25	BCR	B	842	-	41,41,41	1.64	8 (19%)	56,56,56	1.39	8 (14%)
24	LHG	2	315	22	31,31,48	0.35	0	34,37,54	0.62	0
22	CLA	6	312	19	46,50,73	2.38	19 (41%)	55,85,113	3.28	28 (50%)
22	CLA	1	303	14	69,73,73	2.06	19 (27%)	83,113,113	2.76	34 (40%)
22	CLA	B	819	32	69,73,73	1.97	19 (27%)	83,113,113	2.62	28 (33%)
22	CLA	4	311	17	49,53,73	2.44	21 (42%)	59,89,113	3.27	27 (45%)
25	BCR	F	201	-	41,41,41	1.69	10 (24%)	56,56,56	1.43	8 (14%)
29	5X6	7	315	-	43,43,43	2.74	16 (37%)	58,60,60	4.12	33 (56%)
29	5X6	7	316	-	43,43,43	2.72	18 (41%)	58,60,60	4.31	29 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	7	311	-	45,49,73	2.55	19 (42%)	54,84,113	3.32	27 (50%)
21	CL0	A	801	1	69,73,73	1.73	18 (26%)	83,113,113	2.70	34 (40%)
22	CLA	7	307	20	49,53,73	2.49	21 (42%)	59,89,113	3.18	28 (47%)
22	CLA	A	806	1	69,73,73	1.86	20 (28%)	83,113,113	2.71	28 (33%)
22	CLA	A	829	1	54,58,73	2.12	18 (33%)	65,95,113	2.95	31 (47%)
22	CLA	F	204	32	65,69,73	1.90	18 (27%)	78,108,113	2.77	27 (34%)
25	BCR	L	202	-	41,41,41	1.66	7 (17%)	56,56,56	1.51	9 (16%)
22	CLA	A	821	1	49,53,73	2.19	20 (40%)	59,89,113	3.26	25 (42%)
29	5X6	6	317	-	43,43,43	2.61	19 (44%)	58,60,60	4.20	34 (58%)
31	RRX	5	322	-	42,42,42	1.63	8 (19%)	57,58,58	1.35	9 (15%)
22	CLA	A	836	1	60,64,73	2.05	21 (35%)	72,102,113	3.02	32 (44%)
22	CLA	B	829	2	69,73,73	1.82	19 (27%)	83,113,113	3.01	30 (36%)
22	CLA	5	304	18	59,63,73	2.22	20 (33%)	71,101,113	3.00	28 (39%)
25	BCR	4	316	-	41,41,41	1.67	8 (19%)	56,56,56	1.40	8 (14%)
29	5X6	1	313	-	43,43,43	2.64	19 (44%)	58,60,60	4.23	29 (50%)
22	CLA	1	306	14	49,53,73	2.46	21 (42%)	59,89,113	3.16	29 (49%)
24	LHG	6	319	22	31,31,48	0.34	0	34,37,54	0.48	0
29	5X6	B	851	-	43,43,43	2.60	17 (39%)	58,60,60	4.07	32 (55%)
29	5X6	4	314	-	43,43,43	2.77	18 (41%)	58,60,60	3.91	32 (55%)
22	CLA	B	811	2	69,73,73	2.02	19 (27%)	83,113,113	2.70	27 (32%)
22	CLA	4	303	17	69,73,73	2.02	18 (26%)	83,113,113	2.87	31 (37%)
22	CLA	2	308	15	59,63,73	2.30	20 (33%)	71,101,113	3.02	30 (42%)
22	CLA	A	825	1	69,73,73	1.89	19 (27%)	83,113,113	2.78	27 (32%)
25	BCR	B	841	-	41,41,41	1.71	8 (19%)	56,56,56	1.49	9 (16%)
29	5X6	6	315	-	43,43,43	2.70	18 (41%)	58,60,60	4.09	28 (48%)
25	BCR	J	103	-	41,41,41	1.78	8 (19%)	56,56,56	1.66	12 (21%)
22	CLA	7	313	20	49,53,73	2.51	20 (40%)	59,89,113	3.21	28 (47%)
22	CLA	A	858	1	69,73,73	1.83	20 (28%)	83,113,113	2.76	31 (37%)
22	CLA	B	838	2	69,73,73	1.80	17 (24%)	83,113,113	2.93	31 (37%)
29	5X6	M	101	-	43,43,43	2.52	16 (37%)	58,60,60	4.79	33 (56%)
24	LHG	A	860	-	32,32,48	0.33	0	35,38,54	0.48	0
25	BCR	2	301	-	41,41,41	1.62	7 (17%)	56,56,56	1.41	7 (12%)
22	CLA	A	837	1	69,73,73	1.85	18 (26%)	83,113,113	2.85	29 (34%)
22	CLA	A	827	1	69,73,73	1.89	18 (26%)	83,113,113	2.55	26 (31%)
22	CLA	2	310	15	46,50,73	2.50	20 (43%)	55,85,113	3.27	26 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	5X6	1	314	-	43,43,43	2.72	17 (39%)	58,60,60	4.33	30 (51%)
22	CLA	B	825	32	69,73,73	1.88	18 (26%)	83,113,113	2.83	29 (34%)
22	CLA	B	826	2	69,73,73	1.83	19 (27%)	83,113,113	2.73	31 (37%)
22	CLA	B	828	2	69,73,73	1.79	17 (24%)	83,113,113	2.81	29 (34%)
22	CLA	5	306	18	69,73,73	2.00	20 (28%)	83,113,113	2.60	27 (32%)
22	CLA	B	833	32	69,73,73	1.92	18 (26%)	83,113,113	2.64	28 (33%)
29	5X6	5	314	-	43,43,43	2.68	18 (41%)	58,60,60	4.46	28 (48%)
22	CLA	B	830	2	69,73,73	1.92	18 (26%)	83,113,113	2.70	29 (34%)
22	CLA	2	309	24	45,49,73	2.52	19 (42%)	54,84,113	3.27	29 (53%)
25	BCR	Z	202	-	41,41,41	1.68	8 (19%)	56,56,56	1.42	10 (17%)
22	CLA	A	832	1	69,73,73	1.91	17 (24%)	83,113,113	2.79	28 (33%)
31	RRX	1	315	-	42,42,42	1.66	7 (16%)	57,58,58	1.45	8 (14%)
25	BCR	1	301	-	41,41,41	1.63	8 (19%)	56,56,56	1.40	9 (16%)
29	5X6	1	316	-	43,43,43	2.79	18 (41%)	58,60,60	4.35	32 (55%)
22	CLA	6	308	19	49,53,73	2.35	18 (36%)	59,89,113	3.20	30 (50%)
24	LHG	B	846	22	32,32,48	0.30	0	35,38,54	0.43	0
25	BCR	A	846	-	41,41,41	1.62	10 (24%)	56,56,56	1.47	9 (16%)
22	CLA	2	303	15	62,66,73	2.23	20 (32%)	74,104,113	2.90	30 (40%)
22	CLA	2	306	15	49,53,73	2.52	21 (42%)	59,89,113	3.22	29 (49%)
22	CLA	B	831	2	69,73,73	1.90	20 (28%)	83,113,113	2.74	27 (32%)
22	CLA	F	206	6	45,49,73	2.30	20 (44%)	54,84,113	3.39	29 (53%)
22	CLA	A	814	32	49,53,73	2.27	20 (40%)	59,89,113	3.08	27 (45%)
29	5X6	7	314	-	43,43,43	2.82	16 (37%)	58,60,60	4.34	32 (55%)
22	CLA	O	204	-	45,49,73	2.53	20 (44%)	54,84,113	3.29	28 (51%)
22	CLA	B	820	2	49,53,73	2.29	18 (36%)	59,89,113	3.12	28 (47%)
22	CLA	A	835	1	55,59,73	2.08	20 (36%)	66,96,113	3.07	29 (43%)
22	CLA	A	819	32	69,73,73	1.96	19 (27%)	83,113,113	2.62	28 (33%)
22	CLA	L	203	10	61,65,73	2.19	21 (34%)	73,103,113	2.89	30 (41%)
22	CLA	5	310	18	56,60,73	2.29	21 (37%)	67,97,113	2.99	27 (40%)
22	CLA	5	311	18	49,53,73	2.41	21 (42%)	59,89,113	3.23	28 (47%)
29	5X6	5	312	-	43,43,43	2.67	17 (39%)	58,60,60	4.12	30 (51%)
22	CLA	A	848	-	69,73,73	1.83	19 (27%)	83,113,113	2.53	28 (33%)
22	CLA	1	304	14	49,53,73	2.38	21 (42%)	59,89,113	3.15	28 (47%)
22	CLA	B	801	-	69,73,73	1.87	17 (24%)	83,113,113	2.55	30 (36%)
22	CLA	1	305	14	49,53,73	2.43	20 (40%)	59,89,113	3.17	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	831	1	69,73,73	1.86	19 (27%)	83,113,113	2.66	27 (32%)
22	CLA	A	816	1	69,73,73	1.85	19 (27%)	83,113,113	2.61	28 (33%)
25	BCR	K	103	-	41,41,41	1.81	6 (14%)	56,56,56	1.70	9 (16%)
24	LHG	A	841	-	48,48,48	0.33	0	51,54,54	0.38	0
30	LMT	O	201	-	36,36,36	0.19	0	47,47,47	0.34	0
29	5X6	7	317	-	43,43,43	2.65	16 (37%)	58,60,60	4.67	29 (50%)
22	CLA	A	805	1	54,58,73	2.24	20 (37%)	65,95,113	3.07	27 (41%)
29	5X6	7	318	-	43,43,43	2.72	18 (41%)	58,60,60	4.30	31 (53%)
24	LHG	J	106	-	32,32,48	0.32	0	35,38,54	0.50	0
22	CLA	3	304	16	49,53,73	2.52	20 (40%)	59,89,113	3.17	28 (47%)
22	CLA	5	303	18	69,73,73	2.01	20 (28%)	83,113,113	2.71	30 (36%)
22	CLA	6	306	19	59,63,73	2.20	19 (32%)	71,101,113	3.10	31 (43%)
22	CLA	5	305	18	49,53,73	2.49	20 (40%)	59,89,113	3.18	27 (45%)
25	BCR	Z	205	-	41,41,41	1.73	7 (17%)	56,56,56	1.59	10 (17%)
22	CLA	O	203	24	50,54,73	2.27	19 (38%)	60,90,113	3.19	28 (46%)
22	CLA	7	306	20	59,63,73	2.29	21 (35%)	71,101,113	3.09	30 (42%)
22	CLA	3	301	16	69,73,73	2.13	21 (30%)	83,113,113	2.81	29 (34%)
22	CLA	B	839	24	69,73,73	1.91	19 (27%)	83,113,113	2.78	29 (34%)
22	CLA	Z	201	32	49,53,73	2.28	17 (34%)	59,89,113	3.10	27 (45%)
25	BCR	L	206	-	41,41,41	1.76	7 (17%)	56,56,56	1.64	12 (21%)
22	CLA	6	311	24	45,49,73	2.49	20 (44%)	54,84,113	3.35	28 (51%)
29	5X6	O	207	-	43,43,43	2.61	19 (44%)	58,60,60	4.46	31 (53%)
29	5X6	2	313	-	43,43,43	2.79	17 (39%)	58,60,60	3.92	27 (46%)
22	CLA	B	821	2	50,54,73	2.30	18 (36%)	60,90,113	3.19	26 (43%)
25	BCR	A	844	-	41,41,41	1.69	9 (21%)	56,56,56	1.62	13 (23%)
22	CLA	6	313	19	49,53,73	2.46	20 (40%)	59,89,113	3.19	26 (44%)
22	CLA	A	822	1	59,63,73	2.06	19 (32%)	71,101,113	2.89	29 (40%)
22	CLA	K	102	9	46,50,73	2.33	20 (43%)	55,85,113	3.24	27 (49%)
22	CLA	A	823	32	69,73,73	1.91	21 (30%)	83,113,113	2.68	26 (31%)
22	CLA	L	204	10	65,69,73	2.09	20 (30%)	78,108,113	2.86	27 (34%)
22	CLA	3	305	16	59,63,73	2.30	20 (33%)	71,101,113	3.01	29 (40%)
22	CLA	A	803	1	69,73,73	1.90	19 (27%)	83,113,113	2.79	28 (33%)
22	CLA	4	308	17	59,63,73	2.23	19 (32%)	71,101,113	3.02	30 (42%)
22	CLA	4	310	17	46,50,73	2.39	19 (41%)	55,85,113	3.51	29 (52%)
22	CLA	A	810	1	58,62,73	2.09	21 (36%)	69,99,113	2.93	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SF4	C	101	3	0,12,12	-	-	-		
22	CLA	A	815	1	66,70,73	1.94	19 (28%)	79,109,113	2.87	29 (36%)
25	BCR	A	862	-	41,41,41	1.62	9 (21%)	56,56,56	1.37	10 (17%)
22	CLA	5	302	18	69,73,73	2.00	20 (28%)	83,113,113	2.79	31 (37%)
22	CLA	A	811	1	69,73,73	1.84	20 (28%)	83,113,113	2.71	27 (32%)
22	CLA	B	849	2	62,66,73	2.00	18 (29%)	74,104,113	2.95	29 (39%)
23	A1L64	B	840	-	33,33,33	1.04	4 (12%)	40,43,43	1.17	4 (10%)
25	BCR	B	843	-	41,41,41	1.62	9 (21%)	56,56,56	1.40	9 (16%)
22	CLA	A	813	1	46,50,73	2.32	20 (43%)	55,85,113	3.37	29 (52%)
24	LHG	5	316	22	24,24,48	0.35	0	27,30,54	0.51	0
22	CLA	4	307	17	49,53,73	2.36	21 (42%)	59,89,113	2.98	26 (44%)
25	BCR	B	844	-	41,41,41	1.65	7 (17%)	56,56,56	1.71	12 (21%)
22	CLA	B	803	2	69,73,73	1.78	19 (27%)	83,113,113	2.79	36 (43%)
22	CLA	4	306	17	49,53,73	2.50	20 (40%)	59,89,113	3.18	28 (47%)
24	LHG	1	317	-	48,48,48	0.26	0	51,54,54	0.30	0
22	CLA	B	810	2	69,73,73	1.84	19 (27%)	83,113,113	2.78	30 (36%)
22	CLA	B	824	32	69,73,73	1.89	19 (27%)	83,113,113	2.69	26 (31%)
29	5X6	2	312	-	43,43,43	2.80	18 (41%)	58,60,60	4.30	30 (51%)
22	CLA	B	817	2	63,67,73	1.96	19 (30%)	75,105,113	2.91	31 (41%)
25	BCR	5	315	-	41,41,41	1.73	8 (19%)	56,56,56	1.42	10 (17%)
22	CLA	6	310	19	59,63,73	2.21	20 (33%)	71,101,113	2.93	30 (42%)
25	BCR	I	102	-	41,41,41	1.65	9 (21%)	56,56,56	1.36	8 (14%)
29	5X6	Z	206	-	43,43,43	2.81	21 (48%)	58,60,60	3.58	27 (46%)
31	RRX	6	318	-	42,42,42	1.70	8 (19%)	57,58,58	1.41	12 (21%)
22	CLA	B	813	2	69,73,73	1.90	21 (30%)	83,113,113	2.76	26 (31%)
22	CLA	A	804	1	69,73,73	1.95	20 (28%)	83,113,113	2.68	29 (34%)
22	CLA	1	310	32	69,73,73	2.07	21 (30%)	83,113,113	2.88	33 (39%)
24	LHG	A	842	22	39,39,48	0.28	0	42,45,54	0.40	0
26	SF4	A	847	2,1	0,12,12	-	-	-		
22	CLA	B	827	2	69,73,73	1.82	20 (28%)	83,113,113	2.79	29 (34%)
22	CLA	B	836	2	51,55,73	2.10	21 (41%)	61,91,113	3.28	28 (45%)
29	5X6	J	104	-	43,43,43	2.65	18 (41%)	58,60,60	4.23	27 (46%)
22	CLA	A	824	32	59,63,73	2.01	19 (32%)	71,101,113	2.91	30 (42%)
22	CLA	A	820	1	69,73,73	1.94	20 (28%)	83,113,113	2.90	31 (37%)
26	SF4	C	102	3	0,12,12	-	-	-		
22	CLA	A	857	32	69,73,73	1.75	18 (26%)	83,113,113	2.80	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	6	303	19	49,53,73	2.41	21 (42%)	59,89,113	3.11	25 (42%)
22	CLA	6	304	19	69,73,73	1.98	20 (28%)	83,113,113	2.73	26 (31%)
29	5X6	O	208	-	43,43,43	2.77	17 (39%)	58,60,60	4.04	31 (53%)
22	CLA	A	807	1	69,73,73	1.85	21 (30%)	83,113,113	2.75	31 (37%)
22	CLA	B	808	2	69,73,73	1.86	21 (30%)	83,113,113	2.91	34 (40%)
22	CLA	4	302	17	49,53,73	2.46	20 (40%)	59,89,113	3.11	27 (45%)
22	CLA	B	832	2	69,73,73	1.80	19 (27%)	83,113,113	2.89	28 (33%)
22	CLA	3	302	16	49,53,73	2.48	20 (40%)	59,89,113	3.21	26 (44%)
22	CLA	7	309	20	59,63,73	2.31	18 (30%)	71,101,113	3.04	31 (43%)
22	CLA	B	818	2	64,68,73	1.91	19 (29%)	77,107,113	2.85	29 (37%)
22	CLA	2	307	15	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
22	CLA	B	806	2	69,73,73	1.92	21 (30%)	83,113,113	2.57	27 (32%)
30	LMT	4	319	-	36,36,36	0.20	0	47,47,47	0.40	0
22	CLA	2	304	15	69,73,73	2.11	21 (30%)	83,113,113	2.85	33 (39%)
22	CLA	B	835	2	69,73,73	1.90	19 (27%)	83,113,113	2.92	33 (39%)
22	CLA	2	305	15	59,63,73	2.28	21 (35%)	71,101,113	3.05	32 (45%)
22	CLA	3	303	16	49,53,73	2.50	21 (42%)	59,89,113	3.15	27 (45%)
22	CLA	1	308	14	46,50,73	2.48	19 (41%)	55,85,113	3.23	27 (49%)
22	CLA	7	303	20	49,53,73	2.48	21 (42%)	59,89,113	3.24	26 (44%)
22	CLA	7	308	20	49,53,73	2.49	20 (40%)	59,89,113	3.15	26 (44%)
22	CLA	B	812	2	59,63,73	2.11	20 (33%)	71,101,113	2.89	30 (42%)
22	CLA	B	807	2	69,73,73	1.93	18 (26%)	83,113,113	2.77	30 (36%)
22	CLA	7	312	-	49,53,73	2.49	20 (40%)	59,89,113	3.19	25 (42%)
29	5X6	1	312	-	43,43,43	2.67	18 (41%)	58,60,60	4.41	31 (53%)
22	CLA	B	816	2	69,73,73	1.86	20 (28%)	83,113,113	2.96	32 (38%)
25	BCR	A	861	-	41,41,41	1.60	8 (19%)	56,56,56	1.39	8 (14%)
28	DGD	B	845	-	67,67,67	0.86	2 (2%)	81,81,81	0.99	5 (6%)
22	CLA	A	859	1	69,73,73	1.88	21 (30%)	83,113,113	2.91	32 (38%)
22	CLA	B	837	32	69,73,73	1.87	20 (28%)	83,113,113	2.71	26 (31%)
22	CLA	7	305	20	49,53,73	2.48	20 (40%)	59,89,113	3.14	27 (45%)
30	LMT	5	320	-	36,36,36	0.18	0	47,47,47	0.43	0
22	CLA	4	304	17	69,73,73	1.99	20 (28%)	83,113,113	2.82	33 (39%)
22	CLA	A	817	1	69,73,73	1.90	20 (28%)	83,113,113	2.74	30 (36%)
22	CLA	L	205	32	49,53,73	2.43	20 (40%)	59,89,113	3.11	25 (42%)
22	CLA	5	307	18	59,63,73	2.20	21 (35%)	71,101,113	2.99	30 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	A	812	1	69,73,73	1.92	20 (28%)	83,113,113	2.69	24 (28%)
22	CLA	4	309	24	69,73,73	2.04	20 (28%)	83,113,113	2.74	29 (34%)
22	CLA	7	304	20	59,63,73	2.27	20 (33%)	71,101,113	2.96	26 (36%)
22	CLA	6	309	19	49,53,73	2.38	20 (40%)	59,89,113	3.10	27 (45%)
22	CLA	1	309	14	49,53,73	2.52	21 (42%)	59,89,113	3.15	26 (44%)
22	CLA	5	301	18	49,53,73	2.37	21 (42%)	59,89,113	3.04	26 (44%)
25	BCR	L	201	-	41,41,41	1.65	8 (19%)	56,56,56	1.40	8 (14%)
22	CLA	B	822	2	69,73,73	1.89	19 (27%)	83,113,113	2.76	25 (30%)
22	CLA	B	823	2	59,63,73	2.11	19 (32%)	71,101,113	2.93	32 (45%)
22	CLA	K	101	32	59,63,73	2.21	20 (33%)	71,101,113	2.92	29 (40%)
22	CLA	6	314	19	46,50,73	2.42	20 (43%)	55,85,113	3.27	26 (47%)
25	BCR	F	207	-	41,41,41	1.74	7 (17%)	56,56,56	1.45	9 (16%)
22	CLA	4	312	17	49,53,73	2.44	20 (40%)	59,89,113	3.24	31 (52%)
22	CLA	A	826	1	69,73,73	1.85	20 (28%)	83,113,113	2.75	28 (33%)
22	CLA	A	828	1	69,73,73	1.80	17 (24%)	83,113,113	2.76	27 (32%)
22	CLA	B	815	2	69,73,73	1.93	19 (27%)	83,113,113	2.74	34 (40%)
22	CLA	5	308	24	45,49,73	2.40	21 (46%)	54,84,113	3.32	27 (50%)
22	CLA	4	305	32	59,63,73	2.17	21 (35%)	71,101,113	2.99	28 (39%)
23	A1L64	A	840	-	33,33,33	0.92	2 (6%)	40,43,43	0.99	4 (10%)
29	5X6	4	313	-	43,43,43	2.74	18 (41%)	58,60,60	3.98	27 (46%)
29	5X6	5	321	-	43,43,43	2.73	17 (39%)	58,60,60	4.17	33 (56%)
22	CLA	A	809	22,1	69,73,73	1.89	19 (27%)	83,113,113	2.91	32 (38%)
22	CLA	2	311	15	49,53,73	2.50	20 (40%)	59,89,113	3.21	27 (45%)
25	BCR	A	843	-	41,41,41	1.70	8 (19%)	56,56,56	1.53	8 (14%)
22	CLA	B	804	2	69,73,73	1.92	19 (27%)	83,113,113	2.98	31 (37%)
22	CLA	F	205	32	49,53,73	2.22	19 (38%)	59,89,113	3.13	27 (45%)
22	CLA	A	838	1	69,73,73	1.87	19 (27%)	83,113,113	2.90	32 (38%)
22	CLA	A	839	32	69,73,73	1.94	19 (27%)	83,113,113	2.67	30 (36%)
22	CLA	B	834	2	55,59,73	2.11	19 (34%)	66,96,113	2.97	27 (40%)
22	CLA	J	102	8	46,50,73	2.42	19 (41%)	55,85,113	3.18	29 (52%)
22	CLA	A	808	1	59,63,73	2.07	17 (28%)	71,101,113	2.98	32 (45%)
22	CLA	O	205	12	54,58,73	2.33	21 (38%)	65,95,113	3.10	31 (47%)
22	CLA	2	302	15	49,53,73	2.49	20 (40%)	59,89,113	3.20	27 (45%)
22	CLA	5	309	18	46,50,73	2.32	19 (41%)	55,85,113	3.25	26 (47%)
29	5X6	6	316	-	43,43,43	2.74	18 (41%)	58,60,60	3.97	33 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	802	32	69,73,73	1.77	20 (28%)	83,113,113	2.81	27 (32%)
22	CLA	6	305	19	69,73,73	2.00	21 (30%)	83,113,113	2.74	30 (36%)
22	CLA	B	809	2	69,73,73	1.86	19 (27%)	83,113,113	2.67	28 (33%)
29	5X6	1	311	-	43,43,43	2.64	17 (39%)	58,60,60	4.51	32 (55%)
29	5X6	5	313	-	43,43,43	2.73	19 (44%)	58,60,60	3.81	29 (50%)
22	CLA	O	206	32	62,66,73	2.19	20 (32%)	74,104,113	2.92	30 (40%)
22	CLA	B	814	2	61,65,73	2.02	21 (34%)	73,103,113	2.88	28 (38%)
22	CLA	6	307	19	69,73,73	2.04	22 (31%)	83,113,113	2.73	29 (34%)
22	CLA	A	833	1	69,73,73	1.96	20 (28%)	83,113,113	2.67	28 (33%)

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
22	CLA	Z	204	13	-	15/39/115/115	-
22	CLA	A	830	1	-	4/29/105/115	-
22	CLA	B	850	-	-	6/15/91/115	-
22	CLA	7	310	-	-	7/10/86/115	-
22	CLA	A	834	1	-	12/33/109/115	-
22	CLA	1	307	14	-	11/27/103/115	-
29	5X6	2	314	-	-	15/29/67/67	0/2/2/2
30	LMT	F	202	-	-	7/21/61/61	0/2/2/2
31	RRX	4	317	-	-	0/29/65/65	0/2/2/2
22	CLA	B	805	2	-	11/39/115/115	-
22	CLA	A	802	22,1	-	7/27/103/115	-
22	CLA	A	818	1	-	12/39/115/115	-
29	5X6	3	306	-	-	17/29/67/67	0/2/2/2
25	BCR	A	845	-	-	2/29/63/63	0/2/2/2
24	LHG	4	318	22	-	13/36/36/53	-
22	CLA	1	302	32	-	12/39/115/115	-
29	5X6	4	315	-	-	18/29/67/67	0/2/2/2
25	BCR	B	842	-	-	3/29/63/63	0/2/2/2
24	LHG	2	315	22	-	17/36/36/53	-
22	CLA	6	312	19	-	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	303	14	-	13/39/115/115	-
22	CLA	B	819	32	-	6/39/115/115	-
22	CLA	4	311	17	-	0/15/91/115	-
25	BCR	F	201	-	-	0/29/63/63	0/2/2/2
29	5X6	7	315	-	-	21/29/67/67	0/2/2/2
29	5X6	7	316	-	-	17/29/67/67	0/2/2/2
22	CLA	7	311	-	-	2/10/86/115	-
21	CL0	A	801	1	-	3/39/115/115	-
22	CLA	7	307	20	-	4/15/91/115	-
22	CLA	A	806	1	-	10/39/115/115	-
22	CLA	A	829	1	-	4/21/97/115	-
22	CLA	F	204	32	-	6/35/111/115	-
25	BCR	L	202	-	-	4/29/63/63	0/2/2/2
22	CLA	A	821	1	-	3/15/91/115	-
29	5X6	6	317	-	-	15/29/67/67	0/2/2/2
31	RRX	5	322	-	-	2/29/65/65	0/2/2/2
22	CLA	A	836	1	-	4/29/105/115	-
22	CLA	B	829	2	-	12/39/115/115	-
22	CLA	5	304	18	-	6/27/103/115	-
25	BCR	4	316	-	-	2/29/63/63	0/2/2/2
29	5X6	1	313	-	-	18/29/67/67	0/2/2/2
22	CLA	1	306	14	-	6/15/91/115	-
24	LHG	6	319	22	-	15/36/36/53	-
29	5X6	B	851	-	-	11/29/67/67	0/2/2/2
29	5X6	4	314	-	-	14/29/67/67	0/2/2/2
22	CLA	B	811	2	-	15/39/115/115	-
22	CLA	4	303	17	-	12/39/115/115	-
22	CLA	2	308	15	-	7/27/103/115	-
22	CLA	A	825	1	-	7/39/115/115	-
25	BCR	B	841	-	-	0/29/63/63	0/2/2/2
29	5X6	6	315	-	-	15/29/67/67	0/2/2/2
25	BCR	J	103	-	-	2/29/63/63	0/2/2/2
22	CLA	7	313	20	-	5/15/91/115	-
22	CLA	A	858	1	-	9/39/115/115	-
22	CLA	B	838	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	5X6	M	101	-	-	22/29/67/67	0/2/2/2
24	LHG	A	860	-	-	13/37/37/53	-
25	BCR	2	301	-	-	4/29/63/63	0/2/2/2
22	CLA	A	837	1	-	6/39/115/115	-
22	CLA	A	827	1	-	7/39/115/115	-
22	CLA	2	310	15	-	3/12/88/115	-
29	5X6	1	314	-	-	18/29/67/67	0/2/2/2
22	CLA	B	825	32	-	11/39/115/115	-
22	CLA	B	826	2	-	2/39/115/115	-
22	CLA	B	828	2	-	3/39/115/115	-
22	CLA	5	306	18	-	7/39/115/115	-
22	CLA	B	833	32	-	5/39/115/115	-
29	5X6	5	314	-	-	18/29/67/67	0/2/2/2
22	CLA	B	830	2	-	12/39/115/115	-
22	CLA	2	309	24	-	3/10/86/115	-
25	BCR	Z	202	-	-	2/29/63/63	0/2/2/2
22	CLA	A	832	1	-	10/39/115/115	-
31	RRX	1	315	-	-	3/29/65/65	0/2/2/2
25	BCR	1	301	-	-	4/29/63/63	0/2/2/2
29	5X6	1	316	-	-	20/29/67/67	0/2/2/2
22	CLA	6	308	19	-	3/15/91/115	-
24	LHG	B	846	22	-	6/37/37/53	-
25	BCR	A	846	-	-	5/29/63/63	0/2/2/2
22	CLA	2	303	15	-	8/31/107/115	-
22	CLA	2	306	15	-	8/15/91/115	-
22	CLA	B	831	2	-	11/39/115/115	-
22	CLA	F	206	6	-	4/10/86/115	-
22	CLA	A	814	32	-	3/15/91/115	-
29	5X6	7	314	-	-	19/29/67/67	0/2/2/2
22	CLA	O	204	-	-	5/10/86/115	-
22	CLA	B	820	2	-	2/15/91/115	-
22	CLA	A	835	1	-	5/23/99/115	-
22	CLA	A	819	32	-	9/39/115/115	-
22	CLA	L	203	10	-	12/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	310	18	-	8/24/100/115	-
22	CLA	5	311	18	-	5/15/91/115	-
29	5X6	5	312	-	-	12/29/67/67	0/2/2/2
22	CLA	A	848	-	-	7/39/115/115	-
22	CLA	1	304	14	-	4/15/91/115	-
22	CLA	B	801	-	-	2/39/115/115	-
22	CLA	1	305	14	-	5/15/91/115	-
22	CLA	A	831	1	-	9/39/115/115	-
22	CLA	A	816	1	-	8/39/115/115	-
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	LHG	A	841	-	-	18/53/53/53	-
30	LMT	O	201	-	-	5/21/61/61	0/2/2/2
29	5X6	7	317	-	-	22/29/67/67	0/2/2/2
22	CLA	A	805	1	-	4/21/97/115	-
29	5X6	7	318	-	-	19/29/67/67	0/2/2/2
24	LHG	J	106	-	-	4/37/37/53	-
22	CLA	3	304	16	-	2/15/91/115	-
22	CLA	5	303	18	-	15/39/115/115	-
22	CLA	6	306	19	-	9/27/103/115	-
22	CLA	5	305	18	-	7/15/91/115	-
25	BCR	Z	205	-	-	2/29/63/63	0/2/2/2
22	CLA	O	203	24	-	6/17/93/115	-
22	CLA	7	306	20	-	12/27/103/115	-
22	CLA	3	301	16	-	10/39/115/115	-
22	CLA	B	839	24	-	4/39/115/115	-
22	CLA	Z	201	32	-	6/15/91/115	-
25	BCR	L	206	-	-	2/29/63/63	0/2/2/2
22	CLA	6	311	24	-	6/10/86/115	-
29	5X6	O	207	-	-	15/29/67/67	0/2/2/2
29	5X6	2	313	-	-	15/29/67/67	0/2/2/2
22	CLA	B	821	2	-	3/17/93/115	-
25	BCR	A	844	-	-	2/29/63/63	0/2/2/2
22	CLA	6	313	19	-	8/15/91/115	-
22	CLA	A	822	1	-	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	102	9	-	3/12/88/115	-
22	CLA	A	823	32	-	9/39/115/115	-
22	CLA	L	204	10	-	10/35/111/115	-
22	CLA	3	305	16	-	9/27/103/115	-
22	CLA	A	803	1	-	7/39/115/115	-
22	CLA	4	308	17	-	8/27/103/115	-
22	CLA	4	310	17	-	4/12/88/115	-
22	CLA	A	810	1	-	7/26/102/115	-
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	A	815	1	-	10/36/112/115	-
25	BCR	A	862	-	-	2/29/63/63	0/2/2/2
22	CLA	5	302	18	-	10/39/115/115	-
22	CLA	A	811	1	-	5/39/115/115	-
22	CLA	B	849	2	-	6/31/107/115	-
23	A1L64	B	840	-	-	6/27/51/51	0/1/1/1
25	BCR	B	843	-	-	4/29/63/63	0/2/2/2
22	CLA	A	813	1	-	4/12/88/115	-
24	LHG	5	316	22	-	3/29/29/53	-
22	CLA	4	307	17	-	0/15/91/115	-
25	BCR	B	844	-	-	3/29/63/63	0/2/2/2
22	CLA	B	803	2	-	5/39/115/115	-
22	CLA	4	306	17	-	6/15/91/115	-
24	LHG	1	317	-	-	16/53/53/53	-
22	CLA	B	810	2	-	5/39/115/115	-
22	CLA	B	824	32	-	6/39/115/115	-
29	5X6	2	312	-	-	18/29/67/67	0/2/2/2
22	CLA	B	817	2	-	10/32/108/115	-
25	BCR	5	315	-	-	0/29/63/63	0/2/2/2
22	CLA	6	310	19	-	8/27/103/115	-
25	BCR	I	102	-	-	0/29/63/63	0/2/2/2
29	5X6	Z	206	-	-	12/29/67/67	0/2/2/2
31	RRX	6	318	-	-	1/29/65/65	0/2/2/2
22	CLA	B	813	2	-	11/39/115/115	-
22	CLA	A	804	1	-	11/39/115/115	-
22	CLA	1	310	32	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	A	842	22	-	12/44/44/53	-
26	SF4	A	847	2,1	-	-	0/6/5/5
22	CLA	B	827	2	-	5/39/115/115	-
22	CLA	B	836	2	-	3/18/94/115	-
29	5X6	J	104	-	-	16/29/67/67	0/2/2/2
22	CLA	A	824	32	-	5/27/103/115	-
22	CLA	A	820	1	-	20/39/115/115	-
26	SF4	C	102	3	-	-	0/6/5/5
22	CLA	A	857	32	-	2/39/115/115	-
22	CLA	6	303	19	-	6/15/91/115	-
22	CLA	6	304	19	-	10/39/115/115	-
29	5X6	O	208	-	-	18/29/67/67	0/2/2/2
22	CLA	A	807	1	-	10/39/115/115	-
22	CLA	B	808	2	-	10/39/115/115	-
22	CLA	4	302	17	-	2/15/91/115	-
22	CLA	B	832	2	-	7/39/115/115	-
22	CLA	3	302	16	-	4/15/91/115	-
22	CLA	7	309	20	-	7/27/103/115	-
22	CLA	B	818	2	-	4/33/109/115	-
22	CLA	2	307	15	-	1/15/91/115	-
22	CLA	B	806	2	-	13/39/115/115	-
30	LMT	4	319	-	-	5/21/61/61	0/2/2/2
22	CLA	2	304	15	-	13/39/115/115	-
22	CLA	B	835	2	-	6/39/115/115	-
22	CLA	2	305	15	-	11/27/103/115	-
22	CLA	3	303	16	-	6/15/91/115	-
22	CLA	1	308	14	-	4/12/88/115	-
22	CLA	7	303	20	-	8/15/91/115	-
22	CLA	7	308	20	-	0/15/91/115	-
22	CLA	B	812	2	-	9/27/103/115	-
22	CLA	B	807	2	-	7/39/115/115	-
22	CLA	7	312	-	-	5/15/91/115	-
29	5X6	1	312	-	-	15/29/67/67	0/2/2/2
22	CLA	B	816	2	-	8/39/115/115	-
25	BCR	A	861	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	B	845	-	-	22/55/95/95	0/2/2/2
22	CLA	A	859	1	-	20/39/115/115	-
22	CLA	B	837	32	-	10/39/115/115	-
22	CLA	7	305	20	-	4/15/91/115	-
30	LMT	5	320	-	-	5/21/61/61	0/2/2/2
22	CLA	4	304	17	-	15/39/115/115	-
22	CLA	A	817	1	-	7/39/115/115	-
22	CLA	L	205	32	-	6/15/91/115	-
22	CLA	5	307	18	-	2/27/103/115	-
22	CLA	A	812	1	-	12/39/115/115	-
22	CLA	4	309	24	-	11/39/115/115	-
22	CLA	7	304	20	-	7/27/103/115	-
22	CLA	6	309	19	-	0/15/91/115	-
22	CLA	1	309	14	-	6/15/91/115	-
22	CLA	5	301	18	-	4/15/91/115	-
25	BCR	L	201	-	-	0/29/63/63	0/2/2/2
22	CLA	B	822	2	-	12/39/115/115	-
22	CLA	B	823	2	-	9/27/103/115	-
22	CLA	K	101	32	-	10/27/103/115	-
22	CLA	6	314	19	-	4/12/88/115	-
25	BCR	F	207	-	-	2/29/63/63	0/2/2/2
22	CLA	4	312	17	-	4/15/91/115	-
22	CLA	A	826	1	-	8/39/115/115	-
22	CLA	A	828	1	-	12/39/115/115	-
22	CLA	B	815	2	-	13/39/115/115	-
22	CLA	5	308	24	-	0/10/86/115	-
22	CLA	4	305	32	-	8/27/103/115	-
23	A1L64	A	840	-	-	9/27/51/51	0/1/1/1
29	5X6	4	313	-	-	13/29/67/67	0/2/2/2
29	5X6	5	321	-	-	14/29/67/67	0/2/2/2
22	CLA	A	809	22,1	-	7/39/115/115	-
22	CLA	2	311	15	-	6/15/91/115	-
25	BCR	A	843	-	-	3/29/63/63	0/2/2/2
22	CLA	B	804	2	-	15/39/115/115	-
22	CLA	F	205	32	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	838	1	-	7/39/115/115	-
22	CLA	A	839	32	-	12/39/115/115	-
22	CLA	B	834	2	-	5/23/99/115	-
22	CLA	J	102	8	-	1/12/88/115	-
22	CLA	A	808	1	-	11/27/103/115	-
22	CLA	O	205	12	-	4/21/97/115	-
22	CLA	2	302	15	-	4/15/91/115	-
22	CLA	5	309	18	-	2/12/88/115	-
29	5X6	6	316	-	-	13/29/67/67	0/2/2/2
22	CLA	B	802	32	-	8/39/115/115	-
22	CLA	6	305	19	-	11/39/115/115	-
22	CLA	B	809	2	-	11/39/115/115	-
29	5X6	1	311	-	-	21/29/67/67	0/2/2/2
29	5X6	5	313	-	-	14/29/67/67	0/2/2/2
22	CLA	O	206	32	-	14/31/107/115	-
22	CLA	B	814	2	-	9/30/106/115	-
22	CLA	6	307	19	-	9/39/115/115	-
22	CLA	A	833	1	-	10/39/115/115	-

All (4064) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	311	CLA	C3C-C2C	5.81	1.49	1.36
22	7	306	CLA	C3C-C2C	5.61	1.48	1.36
22	1	309	CLA	C3C-C2C	5.55	1.48	1.36
22	L	203	CLA	C3C-C2C	5.55	1.48	1.36
22	7	311	CLA	C3C-C2C	5.52	1.48	1.36
22	3	305	CLA	C3C-C2C	5.52	1.48	1.36
22	7	309	CLA	C3C-C2C	5.51	1.48	1.36
29	7	314	5X6	C27-C26	5.47	1.57	1.45
22	3	304	CLA	C3C-C2C	5.47	1.48	1.36
22	2	310	CLA	C3C-C2C	5.47	1.48	1.36
22	1	308	CLA	C3C-C2C	5.46	1.48	1.36
22	2	304	CLA	C3C-C2C	5.46	1.48	1.36
22	2	311	CLA	C3C-C2C	5.45	1.48	1.36
22	4	303	CLA	CHC-C1C	5.45	1.49	1.38
22	2	308	CLA	C3C-C2C	5.45	1.48	1.36
22	7	313	CLA	C3C-C2C	5.44	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	309	CLA	C3C-C2C	5.42	1.48	1.36
29	2	314	5X6	C27-C26	5.41	1.57	1.45
22	7	310	CLA	C3C-C2C	5.41	1.48	1.36
22	J	102	CLA	C3C-C2C	5.40	1.48	1.36
22	K	101	CLA	C3C-C2C	5.40	1.48	1.36
22	7	308	CLA	C3C-C2C	5.40	1.48	1.36
22	2	307	CLA	C3C-C2C	5.40	1.48	1.36
22	7	307	CLA	C3C-C2C	5.40	1.48	1.36
22	3	302	CLA	C3C-C2C	5.40	1.48	1.36
22	2	304	CLA	O2D-CGD	5.39	1.46	1.33
22	2	306	CLA	C3C-C2C	5.39	1.48	1.36
29	5	314	5X6	C27-C26	5.39	1.57	1.45
22	4	311	CLA	C3C-C2C	5.39	1.48	1.36
22	4	302	CLA	C3C-C2C	5.38	1.48	1.36
29	2	312	5X6	C27-C26	5.38	1.57	1.45
22	B	811	CLA	C3C-C2C	5.38	1.48	1.36
22	4	306	CLA	C3C-C2C	5.38	1.48	1.36
22	5	305	CLA	C3C-C2C	5.37	1.48	1.36
22	3	303	CLA	C3C-C2C	5.37	1.48	1.36
22	7	303	CLA	C1D-ND	5.37	1.44	1.37
22	O	204	CLA	C3C-C2C	5.36	1.48	1.36
22	2	303	CLA	C3C-C2C	5.36	1.48	1.36
22	2	305	CLA	C3C-C2C	5.35	1.48	1.36
22	6	306	CLA	C3C-C2C	5.35	1.48	1.36
22	2	310	CLA	C1D-ND	5.34	1.44	1.37
29	6	316	5X6	C27-C26	5.34	1.57	1.45
22	7	311	CLA	C1D-ND	5.34	1.44	1.37
29	3	306	5X6	C27-C26	5.34	1.57	1.45
22	7	307	CLA	C1D-ND	5.34	1.44	1.37
29	Z	206	5X6	C12-C13	5.34	1.57	1.45
22	1	307	CLA	C3C-C2C	5.34	1.48	1.36
29	4	315	5X6	C27-C26	5.33	1.57	1.45
22	7	309	CLA	O2D-CGD	5.32	1.46	1.33
22	O	206	CLA	C3C-C2C	5.32	1.48	1.36
22	1	305	CLA	C3C-C2C	5.32	1.48	1.36
22	7	304	CLA	CHC-C1C	5.31	1.49	1.38
22	7	312	CLA	C3C-C2C	5.30	1.48	1.36
22	6	306	CLA	O2D-CGD	5.30	1.46	1.33
22	B	823	CLA	C3C-C2C	5.30	1.48	1.36
22	4	308	CLA	O2D-CGD	5.30	1.46	1.33
22	L	203	CLA	O2D-CGD	5.30	1.46	1.33
22	3	301	CLA	C3C-C2C	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	321	5X6	C27-C26	5.29	1.57	1.45
22	2	302	CLA	C1D-ND	5.29	1.44	1.37
22	7	305	CLA	C3C-C2C	5.29	1.48	1.36
29	7	316	5X6	C27-C26	5.29	1.57	1.45
22	7	309	CLA	CHC-C1C	5.29	1.49	1.38
22	3	301	CLA	O2D-CGD	5.29	1.46	1.33
22	3	302	CLA	C1D-ND	5.28	1.44	1.37
22	5	307	CLA	O2D-CGD	5.28	1.46	1.33
22	B	850	CLA	O2D-CGD	5.28	1.46	1.33
22	7	310	CLA	O2D-CGD	5.27	1.46	1.33
22	5	310	CLA	C3C-C2C	5.27	1.47	1.36
29	2	313	5X6	C27-C26	5.27	1.57	1.45
22	7	303	CLA	C3C-C2C	5.27	1.47	1.36
22	7	311	CLA	O2D-CGD	5.27	1.46	1.33
22	2	304	CLA	C1D-ND	5.27	1.44	1.37
22	7	304	CLA	C3C-C2C	5.26	1.47	1.36
22	7	312	CLA	O2D-CGD	5.26	1.46	1.33
22	2	308	CLA	O2D-CGD	5.26	1.46	1.33
22	3	305	CLA	O2D-CGD	5.25	1.46	1.33
22	4	308	CLA	CHC-C1C	5.25	1.49	1.38
22	3	303	CLA	O2D-CGD	5.25	1.46	1.33
22	1	303	CLA	CHC-C1C	5.25	1.49	1.38
22	O	205	CLA	C3C-C2C	5.25	1.47	1.36
22	2	302	CLA	C3C-C2C	5.24	1.47	1.36
22	1	303	CLA	O2D-CGD	5.24	1.46	1.33
22	4	303	CLA	C3C-C2C	5.24	1.47	1.36
29	O	208	5X6	C27-C26	5.24	1.57	1.45
22	2	306	CLA	C1D-ND	5.23	1.44	1.37
22	7	313	CLA	C1D-ND	5.23	1.44	1.37
29	5	313	5X6	C27-C26	5.23	1.57	1.45
22	O	204	CLA	C1D-ND	5.23	1.44	1.37
22	4	312	CLA	C3C-C2C	5.23	1.47	1.36
22	2	309	CLA	O2D-CGD	5.23	1.46	1.33
22	6	312	CLA	C1D-ND	5.23	1.44	1.37
22	1	308	CLA	C1D-ND	5.22	1.44	1.37
22	1	309	CLA	O2D-CGD	5.22	1.45	1.33
22	7	313	CLA	O2D-CGD	5.22	1.45	1.33
29	4	313	5X6	C27-C26	5.22	1.57	1.45
22	2	303	CLA	O2D-CGD	5.22	1.45	1.33
22	1	306	CLA	C3C-C2C	5.21	1.47	1.36
22	3	303	CLA	C1D-ND	5.21	1.44	1.37
22	3	304	CLA	C1D-ND	5.21	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	304	CLA	O2D-CGD	5.21	1.45	1.33
22	2	310	CLA	O2D-CGD	5.21	1.45	1.33
22	O	204	CLA	O2D-CGD	5.21	1.45	1.33
22	2	306	CLA	O2D-CGD	5.20	1.45	1.33
22	3	301	CLA	CHC-C1C	5.20	1.49	1.38
22	L	205	CLA	C3C-C2C	5.20	1.47	1.36
29	1	316	5X6	C27-C26	5.20	1.57	1.45
29	J	104	5X6	C27-C26	5.19	1.57	1.45
22	O	205	CLA	O2D-CGD	5.19	1.45	1.33
22	3	305	CLA	CHC-C1C	5.18	1.49	1.38
22	1	308	CLA	O2D-CGD	5.18	1.45	1.33
22	B	839	CLA	C3C-C2C	5.18	1.47	1.36
22	7	305	CLA	O2D-CGD	5.18	1.45	1.33
25	J	103	BCR	C21-C22	5.18	1.42	1.35
22	3	301	CLA	C1D-ND	5.18	1.44	1.37
29	Z	206	5X6	C27-C26	5.17	1.57	1.45
22	2	311	CLA	O2D-CGD	5.17	1.45	1.33
22	A	812	CLA	C3C-C2C	5.16	1.47	1.36
22	A	828	CLA	C3C-C2C	5.16	1.47	1.36
22	5	304	CLA	C3C-C2C	5.16	1.47	1.36
22	1	307	CLA	O2D-CGD	5.16	1.45	1.33
22	4	306	CLA	C1D-ND	5.15	1.44	1.37
22	6	307	CLA	C3C-C2C	5.15	1.47	1.36
22	4	306	CLA	O2D-CGD	5.15	1.45	1.33
22	7	307	CLA	O2D-CGD	5.15	1.45	1.33
22	1	305	CLA	O2D-CGD	5.15	1.45	1.33
22	5	303	CLA	O2D-CGD	5.15	1.45	1.33
22	6	314	CLA	C3C-C2C	5.14	1.47	1.36
22	5	308	CLA	C3C-C2C	5.14	1.47	1.36
22	6	303	CLA	C3C-C2C	5.14	1.47	1.36
22	5	309	CLA	O2D-CGD	5.13	1.45	1.33
22	7	308	CLA	CHC-C1C	5.13	1.48	1.38
22	O	203	CLA	C3C-C2C	5.13	1.47	1.36
22	3	302	CLA	O2D-CGD	5.13	1.45	1.33
29	5	312	5X6	C27-C26	5.13	1.57	1.45
22	7	306	CLA	CHC-C1C	5.13	1.48	1.38
22	B	811	CLA	O2D-CGD	5.13	1.45	1.33
22	1	304	CLA	C3C-C2C	5.13	1.47	1.36
22	A	825	CLA	C3C-C2C	5.12	1.47	1.36
22	A	826	CLA	C3C-C2C	5.12	1.47	1.36
22	5	303	CLA	C3C-C2C	5.12	1.47	1.36
22	6	308	CLA	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	306	CLA	O2D-CGD	5.11	1.45	1.33
22	6	310	CLA	C3C-C2C	5.11	1.47	1.36
22	1	310	CLA	C3C-C2C	5.11	1.47	1.36
22	B	850	CLA	C1D-ND	5.11	1.44	1.37
29	1	312	5X6	C27-C26	5.10	1.56	1.45
22	2	308	CLA	CHC-C1C	5.10	1.48	1.38
22	6	312	CLA	O2D-CGD	5.10	1.45	1.33
22	O	206	CLA	O2D-CGD	5.10	1.45	1.33
22	5	311	CLA	C3C-C2C	5.10	1.47	1.36
29	5	321	5X6	C12-C13	5.10	1.56	1.45
22	1	307	CLA	C1D-ND	5.10	1.44	1.37
22	K	102	CLA	O2D-CGD	5.09	1.45	1.33
29	Z	206	5X6	C14-C13	5.09	1.42	1.35
22	6	310	CLA	O2D-CGD	5.09	1.45	1.33
22	6	313	CLA	C3C-C2C	5.09	1.47	1.36
22	B	850	CLA	C3C-C2C	5.09	1.47	1.36
29	1	313	5X6	C27-C26	5.09	1.56	1.45
22	4	304	CLA	C3C-C2C	5.09	1.47	1.36
22	2	307	CLA	C1D-ND	5.09	1.44	1.37
22	2	311	CLA	C1D-ND	5.08	1.44	1.37
22	6	303	CLA	O2D-CGD	5.08	1.45	1.33
22	O	203	CLA	O2D-CGD	5.08	1.45	1.33
25	K	103	BCR	C10-C9	5.08	1.42	1.35
22	L	203	CLA	C1D-ND	5.08	1.44	1.37
29	6	315	5X6	C27-C26	5.07	1.56	1.45
22	J	102	CLA	O2D-CGD	5.07	1.45	1.33
22	6	309	CLA	C3C-C2C	5.07	1.47	1.36
29	7	318	5X6	C14-C13	5.07	1.42	1.35
29	4	313	5X6	C12-C13	5.07	1.56	1.45
22	6	313	CLA	O2D-CGD	5.07	1.45	1.33
29	7	315	5X6	C27-C26	5.06	1.56	1.45
22	6	305	CLA	O2D-CGD	5.06	1.45	1.33
22	A	834	CLA	C3C-C2C	5.06	1.47	1.36
22	7	312	CLA	C1D-ND	5.06	1.44	1.37
22	1	304	CLA	O2D-CGD	5.06	1.45	1.33
22	B	802	CLA	C3C-C2C	5.06	1.47	1.36
22	K	101	CLA	C1D-ND	5.06	1.44	1.37
22	1	303	CLA	C3C-C2C	5.06	1.47	1.36
22	2	307	CLA	CHC-C1C	5.05	1.48	1.38
22	1	302	CLA	C1D-ND	5.05	1.44	1.37
22	2	307	CLA	O2D-CGD	5.05	1.45	1.33
22	5	304	CLA	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	302	CLA	C3C-C2C	5.04	1.47	1.36
22	1	306	CLA	O2D-CGD	5.04	1.45	1.33
22	2	302	CLA	O2D-CGD	5.04	1.45	1.33
22	B	801	CLA	C3C-C2C	5.04	1.47	1.36
22	4	308	CLA	C3C-C2C	5.04	1.47	1.36
22	1	310	CLA	O2D-CGD	5.04	1.45	1.33
22	2	305	CLA	O2D-CGD	5.04	1.45	1.33
22	B	811	CLA	C1D-ND	5.04	1.44	1.37
22	7	304	CLA	O2D-CGD	5.04	1.45	1.33
22	4	309	CLA	C3C-C2C	5.04	1.47	1.36
22	5	305	CLA	C1D-ND	5.03	1.44	1.37
22	B	825	CLA	C3C-C2C	5.03	1.47	1.36
29	O	207	5X6	C27-C26	5.03	1.56	1.45
22	3	305	CLA	C1D-ND	5.03	1.44	1.37
29	7	315	5X6	C21-C22	5.03	1.42	1.35
22	6	311	CLA	CHC-C1C	5.03	1.48	1.38
29	4	314	5X6	C27-C26	5.02	1.56	1.45
22	4	312	CLA	O2D-CGD	5.02	1.45	1.33
22	6	313	CLA	C1D-ND	5.02	1.44	1.37
22	4	307	CLA	C3C-C2C	5.02	1.47	1.36
22	5	306	CLA	C3C-C2C	5.02	1.47	1.36
22	5	305	CLA	O2D-CGD	5.02	1.45	1.33
22	6	304	CLA	C3C-C2C	5.01	1.47	1.36
22	K	102	CLA	C3C-C2C	5.01	1.47	1.36
22	B	819	CLA	C3C-C2C	5.01	1.47	1.36
29	2	313	5X6	C12-C13	5.01	1.56	1.45
22	O	206	CLA	C1D-ND	5.00	1.43	1.37
22	B	804	CLA	C3C-C2C	5.00	1.47	1.36
22	7	308	CLA	O2D-CGD	5.00	1.45	1.33
22	7	312	CLA	CHC-C1C	5.00	1.48	1.38
22	6	305	CLA	C1D-ND	5.00	1.43	1.37
22	5	307	CLA	C3C-C2C	5.00	1.47	1.36
22	7	305	CLA	C1D-ND	4.99	1.43	1.37
22	A	833	CLA	C3C-C2C	4.99	1.47	1.36
22	5	310	CLA	C1D-ND	4.99	1.43	1.37
22	A	833	CLA	O2A-CGA	4.99	1.47	1.33
22	1	309	CLA	C1D-ND	4.99	1.43	1.37
22	2	303	CLA	C1D-ND	4.99	1.43	1.37
22	4	310	CLA	O2D-CGD	4.99	1.45	1.33
29	7	316	5X6	C12-C13	4.98	1.56	1.45
22	2	309	CLA	C1D-ND	4.98	1.43	1.37
29	7	314	5X6	C23-C22	4.98	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	824	CLA	C3C-C2C	4.98	1.47	1.36
22	B	823	CLA	CHC-C1C	4.98	1.48	1.38
29	6	315	5X6	C12-C13	4.98	1.56	1.45
22	A	805	CLA	C3C-C2C	4.98	1.47	1.36
22	2	311	CLA	CHC-C1C	4.97	1.48	1.38
22	6	311	CLA	O2D-CGD	4.97	1.45	1.33
29	2	313	5X6	C25-C26	4.97	1.42	1.35
22	B	838	CLA	C3C-C2C	4.97	1.47	1.36
22	A	816	CLA	C3C-C2C	4.97	1.47	1.36
22	1	306	CLA	C1D-ND	4.97	1.43	1.37
22	5	311	CLA	O2D-CGD	4.97	1.45	1.33
22	6	307	CLA	O2D-CGD	4.97	1.45	1.33
22	6	308	CLA	C3C-C2C	4.96	1.47	1.36
29	1	314	5X6	C14-C13	4.96	1.42	1.35
22	5	309	CLA	C3C-C2C	4.96	1.47	1.36
22	A	838	CLA	C3C-C2C	4.96	1.47	1.36
22	L	204	CLA	C3C-C2C	4.96	1.47	1.36
22	7	313	CLA	CHC-C1C	4.95	1.48	1.38
29	3	306	5X6	C21-C22	4.95	1.42	1.35
22	4	305	CLA	C3C-C2C	4.95	1.47	1.36
22	A	818	CLA	C3C-C2C	4.94	1.47	1.36
22	7	310	CLA	C1D-ND	4.94	1.43	1.37
22	J	102	CLA	C1D-ND	4.94	1.43	1.37
22	4	311	CLA	O2D-CGD	4.94	1.45	1.33
25	L	206	BCR	C10-C9	4.94	1.42	1.35
22	B	832	CLA	C3C-C2C	4.94	1.47	1.36
22	Z	201	CLA	C3C-C2C	4.94	1.47	1.36
22	A	814	CLA	C3C-C2C	4.94	1.47	1.36
22	7	306	CLA	C1D-ND	4.93	1.43	1.37
22	3	304	CLA	CHC-C1C	4.93	1.48	1.38
22	A	809	CLA	CHC-C1C	4.93	1.48	1.38
22	A	829	CLA	C3C-C2C	4.93	1.47	1.36
22	6	312	CLA	C3C-C2C	4.93	1.47	1.36
22	A	804	CLA	O2D-CGD	4.93	1.45	1.33
22	4	310	CLA	C3C-C2C	4.93	1.47	1.36
22	O	204	CLA	CHC-C1C	4.93	1.48	1.38
22	A	832	CLA	C3C-C2C	4.92	1.47	1.36
22	A	836	CLA	C3C-C2C	4.92	1.47	1.36
22	O	205	CLA	C1D-ND	4.92	1.43	1.37
29	7	318	5X6	C12-C13	4.92	1.56	1.45
22	7	311	CLA	CHC-C1C	4.92	1.48	1.38
29	2	314	5X6	C12-C13	4.91	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	807	CLA	C3C-C2C	4.91	1.47	1.36
22	B	829	CLA	C3C-C2C	4.91	1.47	1.36
22	5	304	CLA	C1D-ND	4.91	1.43	1.37
22	F	205	CLA	C3C-C2C	4.91	1.47	1.36
29	4	314	5X6	C14-C13	4.91	1.42	1.35
29	1	311	5X6	C27-C26	4.91	1.56	1.45
22	A	821	CLA	C3C-C2C	4.91	1.47	1.36
22	7	308	CLA	C1D-ND	4.91	1.43	1.37
22	4	302	CLA	C1D-ND	4.91	1.43	1.37
22	4	309	CLA	O2D-CGD	4.91	1.45	1.33
22	5	301	CLA	O2D-CGD	4.90	1.45	1.33
22	B	830	CLA	O2D-CGD	4.90	1.45	1.33
22	B	821	CLA	CHC-C1C	4.90	1.48	1.38
29	7	317	5X6	C12-C13	4.90	1.56	1.45
22	2	305	CLA	C1D-ND	4.90	1.43	1.37
29	2	312	5X6	C25-C26	4.89	1.42	1.35
29	1	314	5X6	C27-C26	4.89	1.56	1.45
29	5	314	5X6	C12-C13	4.89	1.56	1.45
29	1	316	5X6	C18-C17	4.89	1.42	1.35
22	L	205	CLA	C1D-ND	4.89	1.43	1.37
29	3	306	5X6	C25-C26	4.88	1.42	1.35
29	6	316	5X6	C14-C13	4.88	1.42	1.35
22	5	310	CLA	O2D-CGD	4.88	1.45	1.33
22	B	817	CLA	O2A-CGA	4.87	1.47	1.33
22	B	849	CLA	C3C-C2C	4.87	1.47	1.36
29	7	318	5X6	C27-C26	4.87	1.56	1.45
22	5	309	CLA	C1D-ND	4.87	1.43	1.37
22	1	302	CLA	C3C-C2C	4.87	1.47	1.36
22	L	204	CLA	O2D-CGD	4.87	1.45	1.33
22	2	306	CLA	CHC-C1C	4.86	1.48	1.38
22	4	311	CLA	CHC-C1C	4.86	1.48	1.38
22	B	821	CLA	O2D-CGD	4.86	1.45	1.33
22	B	806	CLA	O2D-CGD	4.86	1.45	1.33
22	7	309	CLA	O2A-CGA	4.86	1.47	1.33
29	B	851	5X6	C21-C22	4.86	1.42	1.35
22	1	310	CLA	O2A-CGA	4.86	1.47	1.33
29	5	321	5X6	C18-C17	4.86	1.42	1.35
29	O	207	5X6	C12-C13	4.85	1.56	1.45
29	7	314	5X6	C21-C22	4.85	1.42	1.35
22	2	305	CLA	CHC-C1C	4.85	1.48	1.38
22	7	309	CLA	C1D-ND	4.85	1.43	1.37
22	F	206	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	310	CLA	CHC-C1C	4.85	1.48	1.38
22	6	304	CLA	O2D-CGD	4.85	1.45	1.33
22	2	310	CLA	CHC-C1C	4.84	1.48	1.38
29	2	312	5X6	C21-C22	4.84	1.42	1.35
22	A	807	CLA	C3C-C2C	4.84	1.47	1.36
22	1	305	CLA	C1D-ND	4.84	1.43	1.37
22	A	815	CLA	C3C-C2C	4.84	1.47	1.36
22	7	305	CLA	CHC-C1C	4.84	1.48	1.38
22	B	815	CLA	C3C-C2C	4.84	1.47	1.36
29	7	315	5X6	C12-C13	4.84	1.56	1.45
22	6	309	CLA	O2D-CGD	4.83	1.45	1.33
22	6	304	CLA	C1D-ND	4.83	1.43	1.37
29	Z	206	5X6	C21-C22	4.83	1.42	1.35
22	4	312	CLA	CHC-C1C	4.83	1.48	1.38
29	4	315	5X6	C12-C13	4.83	1.56	1.45
22	L	205	CLA	CHC-C1C	4.83	1.48	1.38
22	1	308	CLA	CHC-C1C	4.83	1.48	1.38
22	2	309	CLA	CHC-C1C	4.83	1.48	1.38
29	1	313	5X6	C12-C13	4.83	1.56	1.45
29	1	316	5X6	C25-C26	4.82	1.42	1.35
22	A	813	CLA	O2D-CGD	4.82	1.45	1.33
22	4	305	CLA	O2D-CGD	4.82	1.45	1.33
22	7	310	CLA	CHC-C1C	4.82	1.48	1.38
22	B	835	CLA	C3C-C2C	4.82	1.47	1.36
22	6	307	CLA	C1D-ND	4.82	1.43	1.37
22	B	833	CLA	C3C-C2C	4.82	1.47	1.36
29	7	314	5X6	C12-C13	4.82	1.56	1.45
22	4	306	CLA	CHC-C1C	4.81	1.48	1.38
22	B	837	CLA	O2D-CGD	4.81	1.44	1.33
22	4	312	CLA	C1D-ND	4.81	1.43	1.37
29	O	208	5X6	C18-C17	4.81	1.42	1.35
22	B	819	CLA	CHC-C1C	4.81	1.48	1.38
22	4	311	CLA	C1D-ND	4.81	1.43	1.37
22	Z	204	CLA	C3C-C2C	4.80	1.46	1.36
29	7	314	5X6	C25-C26	4.80	1.42	1.35
22	2	308	CLA	C1D-ND	4.80	1.43	1.37
22	B	820	CLA	O2A-CGA	4.80	1.46	1.30
22	A	804	CLA	C4B-NB	-4.80	1.31	1.37
22	4	302	CLA	CHC-C1C	4.80	1.48	1.38
22	5	305	CLA	CHC-C1C	4.79	1.48	1.38
22	A	834	CLA	O2A-CGA	4.79	1.47	1.33
29	4	314	5X6	C18-C17	4.79	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	208	5X6	C14-C13	4.79	1.42	1.35
22	B	813	CLA	C3C-C2C	4.79	1.46	1.36
22	B	831	CLA	C3C-C2C	4.79	1.46	1.36
22	A	817	CLA	C3C-C2C	4.78	1.46	1.36
29	2	313	5X6	C18-C17	4.78	1.42	1.35
22	1	303	CLA	C1D-ND	4.78	1.43	1.37
29	4	313	5X6	C18-C17	4.78	1.42	1.35
22	A	830	CLA	C3C-C2C	4.78	1.46	1.36
22	B	814	CLA	C3C-C2C	4.78	1.46	1.36
22	2	302	CLA	CHC-C1C	4.77	1.48	1.38
22	2	303	CLA	CHC-C1C	4.77	1.48	1.38
29	M	101	5X6	C27-C26	4.77	1.56	1.45
22	2	304	CLA	CHC-C1C	4.77	1.48	1.38
22	A	820	CLA	O2D-CGD	4.77	1.44	1.33
22	6	314	CLA	O2D-CGD	4.77	1.44	1.33
29	4	314	5X6	C16-C17	4.77	1.56	1.45
22	A	817	CLA	O2D-CGD	4.77	1.44	1.33
22	B	837	CLA	C3C-C2C	4.77	1.46	1.36
22	5	302	CLA	CHC-C1C	4.77	1.48	1.38
29	4	313	5X6	C25-C26	4.76	1.42	1.35
29	O	208	5X6	C12-C13	4.76	1.56	1.45
22	B	839	CLA	O2D-CGD	4.76	1.44	1.33
22	5	308	CLA	O2D-CGD	4.76	1.44	1.33
22	7	307	CLA	CHC-C1C	4.76	1.48	1.38
22	B	805	CLA	C3C-C2C	4.76	1.46	1.36
29	7	317	5X6	C27-C26	4.76	1.56	1.45
29	1	316	5X6	C12-C13	4.76	1.56	1.45
29	5	313	5X6	C23-C22	4.76	1.56	1.45
22	B	810	CLA	O2D-CGD	4.76	1.44	1.33
22	O	205	CLA	CHC-C1C	4.75	1.48	1.38
22	B	804	CLA	O2D-CGD	4.75	1.44	1.33
22	3	303	CLA	CHC-C1C	4.75	1.48	1.38
22	5	301	CLA	C3C-C2C	4.75	1.46	1.36
29	Z	206	5X6	C16-C17	4.75	1.56	1.45
22	O	206	CLA	CHC-C1C	4.75	1.48	1.38
25	K	103	BCR	C14-C13	4.75	1.42	1.35
22	F	206	CLA	O2D-CGD	4.75	1.44	1.33
22	6	313	CLA	CHC-C1C	4.75	1.48	1.38
29	7	314	5X6	C14-C13	4.75	1.42	1.35
25	A	843	BCR	C10-C9	4.75	1.42	1.35
22	A	810	CLA	O2A-CGA	4.75	1.47	1.33
22	4	307	CLA	O2A-CGA	4.74	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	302	CLA	CHC-C1C	4.74	1.48	1.38
22	6	304	CLA	CHC-C1C	4.74	1.48	1.38
22	1	307	CLA	CHC-C1C	4.74	1.48	1.38
22	5	311	CLA	C1D-ND	4.74	1.43	1.37
22	B	816	CLA	C3C-C2C	4.74	1.46	1.36
22	4	302	CLA	O2D-CGD	4.73	1.44	1.33
22	A	811	CLA	C3C-C2C	4.73	1.46	1.36
22	A	831	CLA	C3C-C2C	4.73	1.46	1.36
22	6	305	CLA	CHC-C1C	4.73	1.48	1.38
29	1	314	5X6	C18-C17	4.73	1.42	1.35
22	6	309	CLA	CHC-C1C	4.73	1.48	1.38
22	A	819	CLA	C3C-C2C	4.73	1.46	1.36
22	B	821	CLA	C3C-C2C	4.73	1.46	1.36
22	A	837	CLA	C3C-C2C	4.72	1.46	1.36
22	A	814	CLA	O2D-CGD	4.72	1.44	1.33
22	6	305	CLA	C3C-C2C	4.72	1.46	1.36
22	L	205	CLA	O2D-CGD	4.72	1.44	1.33
29	2	312	5X6	C23-C22	4.72	1.56	1.45
29	B	851	5X6	C27-C26	4.72	1.56	1.45
22	A	805	CLA	C1D-ND	4.72	1.43	1.37
22	B	849	CLA	O2D-CGD	4.71	1.44	1.33
22	A	820	CLA	C3C-C2C	4.71	1.46	1.36
22	A	833	CLA	O2D-CGD	4.71	1.44	1.33
22	B	806	CLA	C1B-NB	-4.71	1.32	1.37
22	6	314	CLA	C1D-ND	4.71	1.43	1.37
22	5	302	CLA	O2D-CGD	4.71	1.44	1.33
22	A	839	CLA	O2D-CGD	4.71	1.44	1.33
29	2	312	5X6	C18-C17	4.71	1.42	1.35
22	6	306	CLA	C1D-ND	4.70	1.43	1.37
22	1	307	CLA	O2A-CGA	4.70	1.47	1.33
22	A	808	CLA	CHC-C1C	4.70	1.48	1.38
29	1	311	5X6	C14-C13	4.70	1.42	1.35
29	2	312	5X6	C12-C13	4.70	1.56	1.45
22	5	303	CLA	O2A-CGA	4.70	1.47	1.33
22	A	802	CLA	C3C-C2C	4.69	1.46	1.36
22	A	827	CLA	C1D-ND	4.69	1.43	1.37
29	7	315	5X6	C25-C26	4.69	1.42	1.35
22	5	307	CLA	C1D-ND	4.69	1.43	1.37
22	1	309	CLA	CHC-C1C	4.69	1.48	1.38
22	B	830	CLA	C3C-C2C	4.69	1.46	1.36
29	6	315	5X6	C25-C26	4.69	1.42	1.35
29	O	208	5X6	C25-C26	4.68	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	313	5X6	C25-C26	4.68	1.42	1.35
22	B	826	CLA	C3C-C2C	4.68	1.46	1.36
22	B	819	CLA	O2D-CGD	4.68	1.44	1.33
22	Z	204	CLA	O2D-CGD	4.68	1.44	1.33
22	1	302	CLA	O2D-CGD	4.68	1.44	1.33
25	Z	205	BCR	C10-C9	4.68	1.42	1.35
22	Z	201	CLA	O2A-CGA	4.67	1.46	1.30
22	A	804	CLA	O2A-CGA	4.67	1.47	1.33
29	7	314	5X6	C18-C17	4.67	1.42	1.35
22	4	307	CLA	O2D-CGD	4.66	1.44	1.33
22	A	835	CLA	C3C-C2C	4.66	1.46	1.36
22	7	303	CLA	CHC-C1C	4.66	1.48	1.38
22	B	823	CLA	O2D-CGD	4.66	1.44	1.33
22	A	819	CLA	C1B-NB	-4.66	1.32	1.37
22	L	204	CLA	C1D-ND	4.66	1.43	1.37
29	2	313	5X6	C23-C22	4.66	1.56	1.45
22	1	310	CLA	C1D-ND	4.66	1.43	1.37
22	6	310	CLA	CHC-C1C	4.66	1.48	1.38
22	K	101	CLA	CHC-C1C	4.66	1.48	1.38
22	A	808	CLA	C3C-C2C	4.65	1.46	1.36
22	5	301	CLA	O2A-CGA	4.65	1.46	1.30
29	4	314	5X6	C25-C26	4.65	1.42	1.35
22	A	834	CLA	O2D-CGD	4.65	1.44	1.33
22	L	205	CLA	O2A-CGA	4.65	1.46	1.30
22	A	859	CLA	O2D-CGD	4.65	1.44	1.33
22	A	819	CLA	O2A-CGA	4.65	1.46	1.33
29	4	315	5X6	C16-C17	4.64	1.55	1.45
29	7	315	5X6	C14-C13	4.64	1.41	1.35
22	A	848	CLA	C3C-C2C	4.64	1.46	1.36
22	A	813	CLA	C1D-ND	4.64	1.43	1.37
29	6	317	5X6	C12-C13	4.64	1.55	1.45
29	3	306	5X6	C12-C13	4.64	1.55	1.45
22	B	820	CLA	C3C-C2C	4.64	1.46	1.36
22	B	836	CLA	C3C-C2C	4.64	1.46	1.36
29	7	318	5X6	C16-C17	4.63	1.55	1.45
29	4	313	5X6	C14-C13	4.63	1.41	1.35
22	6	303	CLA	C1D-ND	4.63	1.43	1.37
22	5	304	CLA	CHC-C1C	4.63	1.47	1.38
22	4	309	CLA	CHC-C1C	4.63	1.47	1.38
22	6	309	CLA	O2A-CGA	4.63	1.46	1.30
22	A	830	CLA	O2D-CGD	4.63	1.44	1.33
22	5	311	CLA	O2A-CGA	4.63	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	822	CLA	O2D-CGD	4.63	1.44	1.33
29	5	321	5X6	C14-C13	4.62	1.41	1.35
22	A	839	CLA	C3C-C2C	4.62	1.46	1.36
29	6	315	5X6	C21-C22	4.62	1.41	1.35
29	3	306	5X6	C23-C22	4.62	1.55	1.45
22	5	303	CLA	C1D-ND	4.62	1.43	1.37
22	A	814	CLA	O2A-CGA	4.62	1.46	1.30
29	6	315	5X6	C23-C22	4.62	1.55	1.45
29	O	208	5X6	C21-C22	4.62	1.41	1.35
22	4	302	CLA	O2A-CGA	4.62	1.46	1.30
29	6	317	5X6	C25-C26	4.61	1.41	1.35
22	5	309	CLA	CHC-C1C	4.61	1.47	1.38
22	4	312	CLA	O2A-CGA	4.61	1.46	1.30
22	7	308	CLA	O2A-CGA	4.61	1.46	1.30
22	7	304	CLA	C1D-ND	4.61	1.43	1.37
29	1	314	5X6	C16-C17	4.61	1.55	1.45
22	4	311	CLA	O2A-CGA	4.61	1.46	1.30
22	2	308	CLA	O2A-CGA	4.61	1.46	1.33
29	4	315	5X6	C18-C17	4.61	1.41	1.35
22	6	308	CLA	O2A-CGA	4.60	1.46	1.30
22	A	812	CLA	CHC-C1C	4.60	1.47	1.38
22	7	305	CLA	O2A-CGA	4.60	1.46	1.30
22	4	308	CLA	O2A-CGA	4.60	1.46	1.33
29	1	316	5X6	C14-C13	4.60	1.41	1.35
22	A	812	CLA	O2A-CGA	4.60	1.46	1.33
22	2	307	CLA	O2A-CGA	4.60	1.46	1.30
22	A	808	CLA	O2D-CGD	4.59	1.44	1.33
22	5	306	CLA	O2D-CGD	4.59	1.44	1.33
29	5	312	5X6	C12-C13	4.59	1.55	1.45
22	1	302	CLA	CHC-C1C	4.59	1.47	1.38
22	A	821	CLA	O2A-CGA	4.59	1.46	1.30
22	A	810	CLA	C3C-C2C	4.59	1.46	1.36
22	A	805	CLA	C1B-NB	-4.59	1.32	1.37
29	6	316	5X6	C16-C17	4.59	1.55	1.45
22	A	815	CLA	O2D-CGD	4.58	1.44	1.33
22	1	304	CLA	O2A-CGA	4.58	1.46	1.30
22	6	307	CLA	CHD-C1D	4.58	1.47	1.38
29	1	314	5X6	C12-C13	4.58	1.55	1.45
22	B	810	CLA	C3C-C2C	4.58	1.46	1.36
22	6	303	CLA	O2A-CGA	4.58	1.46	1.30
22	A	813	CLA	C3C-C2C	4.58	1.46	1.36
22	7	303	CLA	O2D-CGD	4.58	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	808	CLA	O2D-CGD	4.58	1.44	1.33
22	B	820	CLA	O2D-CGD	4.57	1.44	1.33
29	5	313	5X6	C16-C17	4.57	1.55	1.45
22	5	308	CLA	CHC-C1C	4.57	1.47	1.38
29	1	316	5X6	C23-C22	4.57	1.55	1.45
29	J	104	5X6	C14-C13	4.57	1.41	1.35
29	6	316	5X6	C25-C26	4.57	1.41	1.35
29	7	317	5X6	C18-C17	4.57	1.41	1.35
22	A	834	CLA	CHC-C1C	4.57	1.47	1.38
22	3	302	CLA	O2A-CGA	4.57	1.46	1.30
22	4	304	CLA	C1D-ND	4.57	1.43	1.37
29	J	104	5X6	C16-C17	4.57	1.55	1.45
29	1	316	5X6	C16-C17	4.57	1.55	1.45
22	3	304	CLA	O2A-CGA	4.57	1.46	1.30
22	1	305	CLA	O2A-CGA	4.57	1.46	1.30
22	F	204	CLA	O2D-CGD	4.57	1.44	1.33
22	Z	201	CLA	O2D-CGD	4.57	1.44	1.33
22	A	817	CLA	C1D-ND	4.56	1.43	1.37
22	6	314	CLA	CHC-C1C	4.56	1.47	1.38
29	5	313	5X6	C14-C13	4.56	1.41	1.35
22	B	815	CLA	O2A-CGA	4.56	1.46	1.33
22	5	307	CLA	CHC-C1C	4.56	1.47	1.38
22	B	812	CLA	C3C-C2C	4.56	1.46	1.36
29	4	314	5X6	C12-C13	4.56	1.55	1.45
22	4	309	CLA	C1D-ND	4.56	1.43	1.37
22	B	822	CLA	C3C-C2C	4.56	1.46	1.36
22	1	306	CLA	CHC-C1C	4.56	1.47	1.38
22	6	306	CLA	O2A-CGA	4.56	1.46	1.33
22	1	306	CLA	O2A-CGA	4.56	1.46	1.30
29	2	312	5X6	C16-C17	4.56	1.55	1.45
29	5	312	5X6	C14-C13	4.55	1.41	1.35
22	5	310	CLA	O2A-CGA	4.55	1.46	1.33
22	A	829	CLA	O2D-CGD	4.55	1.44	1.33
22	B	819	CLA	C1B-NB	-4.55	1.32	1.37
29	5	313	5X6	C18-C17	4.55	1.41	1.35
29	Z	206	5X6	C23-C22	4.55	1.55	1.45
22	7	306	CLA	O2A-CGA	4.55	1.46	1.33
29	5	312	5X6	C18-C17	4.55	1.41	1.35
25	F	207	BCR	C10-C9	4.55	1.41	1.35
29	7	317	5X6	C14-C13	4.55	1.41	1.35
22	2	302	CLA	O2A-CGA	4.55	1.46	1.30
22	B	804	CLA	CHC-C1C	4.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	318	5X6	C25-C26	4.54	1.41	1.35
29	5	313	5X6	C12-C13	4.54	1.55	1.45
22	2	306	CLA	CHD-C1D	4.54	1.47	1.38
29	1	311	5X6	C23-C22	4.54	1.55	1.45
29	1	314	5X6	C25-C26	4.54	1.41	1.35
29	7	317	5X6	C23-C22	4.54	1.55	1.45
29	6	317	5X6	C27-C26	4.54	1.55	1.45
29	1	311	5X6	C25-C26	4.54	1.41	1.35
22	1	309	CLA	O2A-CGA	4.54	1.46	1.30
29	3	306	5X6	C14-C13	4.53	1.41	1.35
22	1	303	CLA	O2A-CGA	4.53	1.46	1.33
22	5	311	CLA	CHD-C1D	4.53	1.47	1.38
22	2	311	CLA	O2A-CGA	4.53	1.46	1.30
22	A	830	CLA	O2A-CGA	4.53	1.46	1.33
22	7	307	CLA	O2A-CGA	4.53	1.46	1.30
29	1	314	5X6	C23-C22	4.53	1.55	1.45
22	5	305	CLA	O2A-CGA	4.53	1.46	1.30
29	2	313	5X6	C14-C13	4.53	1.41	1.35
22	4	306	CLA	O2A-CGA	4.53	1.46	1.30
22	F	205	CLA	O2D-CGD	4.53	1.44	1.33
22	A	806	CLA	O2D-CGD	4.52	1.44	1.33
25	J	103	BCR	C10-C9	4.52	1.41	1.35
22	7	313	CLA	O2A-CGA	4.52	1.46	1.30
22	B	801	CLA	C1B-NB	-4.52	1.32	1.37
29	1	311	5X6	C18-C17	4.52	1.41	1.35
22	A	835	CLA	O2D-CGD	4.52	1.44	1.33
22	3	304	CLA	CHD-C1D	4.52	1.47	1.38
29	5	313	5X6	C21-C22	4.52	1.41	1.35
29	7	316	5X6	C18-C17	4.52	1.41	1.35
22	2	304	CLA	CHD-C1D	4.51	1.47	1.38
22	B	834	CLA	C3C-C2C	4.51	1.46	1.36
22	2	306	CLA	O2A-CGA	4.51	1.45	1.30
25	F	207	BCR	C21-C22	4.51	1.41	1.35
29	1	313	5X6	C16-C17	4.51	1.55	1.45
22	A	836	CLA	O2D-CGD	4.51	1.44	1.33
22	4	303	CLA	O2D-CGD	4.51	1.44	1.33
29	4	314	5X6	C21-C22	4.51	1.41	1.35
22	3	303	CLA	O2A-CGA	4.51	1.45	1.30
22	4	310	CLA	C1D-ND	4.51	1.43	1.37
22	A	819	CLA	O2D-CGD	4.51	1.44	1.33
22	F	205	CLA	O2A-CGA	4.50	1.45	1.30
22	B	812	CLA	CHC-C1C	4.50	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	305	CLA	O2A-CGA	4.50	1.46	1.33
22	A	804	CLA	C3C-C2C	4.50	1.46	1.36
29	7	316	5X6	C14-C13	4.50	1.41	1.35
22	7	304	CLA	O2A-CGA	4.50	1.46	1.33
22	B	828	CLA	O2D-CGD	4.50	1.44	1.33
22	6	308	CLA	C1D-ND	4.49	1.43	1.37
29	2	314	5X6	C23-C22	4.49	1.55	1.45
22	3	301	CLA	O2A-CGA	4.49	1.46	1.33
22	2	305	CLA	O2A-CGA	4.49	1.46	1.33
22	5	310	CLA	CHC-C1C	4.49	1.47	1.38
29	5	312	5X6	C21-C22	4.49	1.41	1.35
22	B	830	CLA	O2A-CGA	4.49	1.46	1.33
22	1	305	CLA	CHC-C1C	4.49	1.47	1.38
22	L	204	CLA	CHC-C1C	4.49	1.47	1.38
22	4	305	CLA	CHC-C1C	4.49	1.47	1.38
22	B	829	CLA	O2A-CGA	4.49	1.46	1.33
22	7	312	CLA	O2A-CGA	4.49	1.45	1.30
22	A	808	CLA	O2A-CGA	4.49	1.46	1.33
22	1	309	CLA	CHD-C1D	4.49	1.47	1.38
25	Z	205	BCR	C21-C22	4.49	1.41	1.35
22	7	303	CLA	O2A-CGA	4.49	1.45	1.30
29	6	316	5X6	C12-C13	4.48	1.55	1.45
22	A	815	CLA	O2A-CGA	4.48	1.46	1.33
29	5	314	5X6	C23-C22	4.48	1.55	1.45
22	A	832	CLA	O2D-CGD	4.48	1.44	1.33
29	J	104	5X6	C12-C13	4.48	1.55	1.45
22	A	858	CLA	CHC-C1C	4.48	1.47	1.38
22	7	303	CLA	CHD-C1D	4.48	1.47	1.38
22	B	850	CLA	O2A-CGA	4.48	1.45	1.30
22	B	804	CLA	O2A-CGA	4.48	1.46	1.33
29	B	851	5X6	C25-C26	4.48	1.41	1.35
29	O	208	5X6	C23-C22	4.47	1.55	1.45
29	4	315	5X6	C23-C22	4.47	1.55	1.45
29	2	313	5X6	C21-C22	4.47	1.41	1.35
22	B	818	CLA	C3C-C2C	4.47	1.46	1.36
29	6	317	5X6	C21-C22	4.47	1.41	1.35
29	1	312	5X6	C23-C22	4.47	1.55	1.45
29	2	312	5X6	C14-C13	4.47	1.41	1.35
31	1	315	RRX	C21-C22	4.47	1.41	1.35
22	2	303	CLA	O2A-CGA	4.47	1.46	1.33
22	A	814	CLA	CHC-C1C	4.46	1.47	1.38
22	A	812	CLA	O2D-CGD	4.46	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	310	CLA	O2A-CGA	4.46	1.46	1.33
22	B	822	CLA	C1B-NB	-4.46	1.32	1.37
22	4	307	CLA	C1D-ND	4.46	1.43	1.37
22	2	304	CLA	O2A-CGA	4.46	1.46	1.33
29	4	315	5X6	C14-C13	4.46	1.41	1.35
22	O	205	CLA	O2A-CGA	4.46	1.46	1.33
22	4	304	CLA	O2D-CGD	4.46	1.44	1.33
22	A	831	CLA	O2A-CGA	4.46	1.46	1.33
22	5	310	CLA	CHD-C1D	4.46	1.47	1.38
29	2	314	5X6	C18-C17	4.46	1.41	1.35
22	1	306	CLA	CHD-C1D	4.46	1.47	1.38
22	B	817	CLA	C3C-C2C	4.46	1.46	1.36
22	L	203	CLA	CHC-C1C	4.45	1.47	1.38
29	1	316	5X6	C24-C25	4.45	1.57	1.43
22	B	817	CLA	CHC-C1C	4.45	1.47	1.38
29	4	313	5X6	C23-C22	4.45	1.55	1.45
22	5	303	CLA	CHC-C1C	4.45	1.47	1.38
31	4	317	RRX	C21-C22	4.45	1.41	1.35
29	6	316	5X6	C18-C17	4.45	1.41	1.35
22	4	309	CLA	O2A-CGA	4.45	1.46	1.33
22	6	313	CLA	O2A-CGA	4.44	1.45	1.30
29	O	207	5X6	C23-C22	4.44	1.55	1.45
29	1	314	5X6	C21-C22	4.44	1.41	1.35
22	A	858	CLA	C3C-C2C	4.44	1.46	1.36
29	5	312	5X6	C23-C22	4.44	1.55	1.45
22	7	305	CLA	CHD-C1D	4.44	1.47	1.38
22	A	803	CLA	O2D-CGD	4.44	1.44	1.33
22	A	822	CLA	O2A-CGA	4.44	1.46	1.33
22	6	303	CLA	CHC-C1C	4.44	1.47	1.38
29	1	312	5X6	C18-C17	4.44	1.41	1.35
29	4	315	5X6	C21-C22	4.44	1.41	1.35
22	A	810	CLA	O2D-CGD	4.44	1.44	1.33
22	B	806	CLA	O2A-CGA	4.43	1.46	1.33
29	5	321	5X6	C16-C17	4.43	1.55	1.45
25	A	844	BCR	C21-C22	4.43	1.41	1.35
22	A	834	CLA	C1D-ND	4.43	1.43	1.37
29	6	315	5X6	C18-C17	4.43	1.41	1.35
29	2	314	5X6	C25-C26	4.43	1.41	1.35
29	Z	206	5X6	C18-C17	4.43	1.41	1.35
29	7	316	5X6	C16-C17	4.43	1.55	1.45
22	B	815	CLA	O2D-CGD	4.43	1.44	1.33
29	6	316	5X6	C23-C22	4.43	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	803	CLA	O2A-CGA	4.42	1.46	1.33
22	A	838	CLA	O2A-CGA	4.42	1.46	1.33
22	3	303	CLA	CHD-C1D	4.42	1.47	1.38
29	J	104	5X6	C25-C26	4.42	1.41	1.35
22	A	822	CLA	C3C-C2C	4.42	1.46	1.36
29	2	314	5X6	C21-C22	4.42	1.41	1.35
22	A	815	CLA	CHC-C1C	4.42	1.47	1.38
22	A	818	CLA	O2A-CGA	4.42	1.46	1.33
22	B	817	CLA	O2D-CGD	4.42	1.44	1.33
22	A	857	CLA	C3C-C2C	4.42	1.46	1.36
22	B	849	CLA	O2A-CGA	4.42	1.46	1.33
21	A	801	CL0	C3C-C2C	4.42	1.46	1.36
22	1	308	CLA	CHD-C1D	4.42	1.47	1.38
22	5	307	CLA	O2A-CGA	4.41	1.46	1.33
22	B	827	CLA	O2D-CGD	4.41	1.44	1.33
22	1	304	CLA	C1D-ND	4.41	1.43	1.37
22	A	805	CLA	O2A-CGA	4.41	1.46	1.33
22	6	306	CLA	CHC-C1C	4.41	1.47	1.38
22	Z	201	CLA	CHC-C1C	4.41	1.47	1.38
29	M	101	5X6	C12-C13	4.41	1.55	1.45
22	A	802	CLA	C1B-NB	-4.40	1.32	1.37
29	5	321	5X6	C23-C22	4.40	1.55	1.45
29	7	315	5X6	C23-C22	4.40	1.55	1.45
22	4	307	CLA	CHC-C1C	4.40	1.47	1.38
22	Z	201	CLA	C1B-NB	-4.40	1.32	1.37
22	K	101	CLA	O2A-CGA	4.40	1.46	1.33
29	6	317	5X6	C14-C13	4.40	1.41	1.35
22	B	809	CLA	O2D-CGD	4.40	1.43	1.33
22	B	838	CLA	O2D-CGD	4.40	1.43	1.33
22	B	835	CLA	O2D-CGD	4.40	1.43	1.33
29	1	312	5X6	C21-C22	4.40	1.41	1.35
22	A	839	CLA	C1D-ND	4.39	1.43	1.37
29	7	316	5X6	C21-C22	4.39	1.41	1.35
22	A	823	CLA	C3C-C2C	4.39	1.46	1.36
25	K	103	BCR	C21-C22	4.39	1.41	1.35
22	7	307	CLA	CHD-C1D	4.39	1.46	1.38
22	B	808	CLA	C3C-C2C	4.39	1.46	1.36
22	B	823	CLA	O2A-CGA	4.38	1.46	1.33
22	7	303	CLA	CHD-C4C	4.38	1.49	1.39
22	2	310	CLA	CHD-C1D	4.38	1.46	1.38
29	7	318	5X6	C21-C22	4.38	1.41	1.35
22	B	850	CLA	CHC-C1C	4.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	829	CLA	CHC-C1C	4.38	1.47	1.38
22	6	312	CLA	CHC-C1C	4.38	1.47	1.38
22	6	310	CLA	C1D-ND	4.38	1.43	1.37
22	A	820	CLA	O2A-CGA	4.38	1.46	1.33
22	B	831	CLA	O2D-CGD	4.37	1.43	1.33
22	4	305	CLA	C1D-ND	4.37	1.43	1.37
22	L	203	CLA	O2A-CGA	4.37	1.46	1.33
22	B	812	CLA	O2A-CGA	4.37	1.46	1.33
22	B	821	CLA	C1D-ND	4.37	1.43	1.37
22	B	806	CLA	C3C-C2C	4.37	1.46	1.36
29	1	316	5X6	C21-C22	4.37	1.41	1.35
22	A	821	CLA	O2D-CGD	4.37	1.43	1.33
29	7	318	5X6	C18-C17	4.37	1.41	1.35
22	2	308	CLA	CHD-C1D	4.37	1.46	1.38
22	B	824	CLA	O2D-CGD	4.37	1.43	1.33
22	K	101	CLA	O2D-CGD	4.37	1.43	1.33
29	5	314	5X6	C16-C17	4.36	1.55	1.45
22	A	827	CLA	O2D-CGD	4.36	1.43	1.33
29	1	311	5X6	C16-C17	4.36	1.55	1.45
22	2	304	CLA	CHD-C4C	4.36	1.49	1.39
22	2	311	CLA	CHD-C1D	4.36	1.46	1.38
22	B	833	CLA	O2D-CGD	4.36	1.43	1.33
22	A	859	CLA	C3C-C2C	4.36	1.46	1.36
22	4	305	CLA	O2A-CGA	4.36	1.46	1.33
22	B	820	CLA	CHC-C1C	4.36	1.47	1.38
22	B	812	CLA	C1D-ND	4.36	1.43	1.37
22	B	814	CLA	CHC-C1C	4.36	1.47	1.38
22	F	204	CLA	O2A-CGA	4.36	1.46	1.33
22	K	102	CLA	CHC-C1C	4.35	1.47	1.38
22	A	828	CLA	O2A-CGA	4.35	1.46	1.33
22	3	305	CLA	CHC-C4B	4.35	1.49	1.39
22	6	308	CLA	CHC-C1C	4.35	1.47	1.38
29	6	317	5X6	C23-C22	4.35	1.55	1.45
29	O	208	5X6	C16-C17	4.35	1.55	1.45
22	1	302	CLA	O2A-CGA	4.35	1.46	1.33
29	7	314	5X6	C16-C17	4.35	1.55	1.45
22	2	302	CLA	CHD-C1D	4.35	1.46	1.38
29	1	313	5X6	C21-C22	4.35	1.41	1.35
22	B	820	CLA	C1D-ND	4.35	1.43	1.37
22	5	311	CLA	CHC-C1C	4.35	1.47	1.38
22	4	304	CLA	CHC-C1C	4.34	1.47	1.38
22	7	304	CLA	CHC-C4B	4.34	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	312	5X6	C12-C13	4.34	1.55	1.45
29	7	318	5X6	C23-C22	4.34	1.55	1.45
22	A	827	CLA	C3C-C2C	4.34	1.46	1.36
22	O	206	CLA	CHD-C1D	4.34	1.46	1.38
29	7	316	5X6	C23-C22	4.34	1.55	1.45
22	B	807	CLA	O2D-CGD	4.34	1.43	1.33
22	A	829	CLA	O2A-CGA	4.34	1.46	1.33
29	4	314	5X6	C23-C22	4.34	1.55	1.45
22	F	204	CLA	C3C-C2C	4.34	1.45	1.36
22	5	304	CLA	O2A-CGA	4.34	1.46	1.33
22	5	305	CLA	CHD-C1D	4.33	1.46	1.38
29	2	314	5X6	C14-C13	4.33	1.41	1.35
22	B	824	CLA	O2A-CGA	4.33	1.46	1.33
29	7	315	5X6	C16-C17	4.33	1.55	1.45
22	F	205	CLA	CHC-C1C	4.33	1.47	1.38
22	7	309	CLA	CHC-C4B	4.33	1.49	1.39
22	A	832	CLA	CHD-C1D	4.33	1.46	1.38
22	B	830	CLA	CHC-C1C	4.33	1.47	1.38
25	K	103	BCR	C17-C18	4.33	1.41	1.35
22	A	833	CLA	CHC-C1C	4.33	1.47	1.38
22	6	314	CLA	CHD-C1D	4.33	1.46	1.38
29	5	314	5X6	C21-C22	4.33	1.41	1.35
25	B	842	BCR	C10-C9	4.33	1.41	1.35
22	6	311	CLA	C1D-ND	4.32	1.43	1.37
29	7	315	5X6	C18-C17	4.32	1.41	1.35
25	B	841	BCR	C17-C18	4.32	1.41	1.35
25	L	202	BCR	C10-C9	4.32	1.41	1.35
22	B	818	CLA	CHD-C1D	4.32	1.46	1.38
22	B	811	CLA	CHD-C1D	4.32	1.46	1.38
22	7	306	CLA	CHD-C4C	4.32	1.49	1.39
22	2	305	CLA	CHD-C1D	4.32	1.46	1.38
22	K	102	CLA	C1D-ND	4.31	1.43	1.37
22	7	311	CLA	CHD-C1D	4.31	1.46	1.38
22	B	825	CLA	C1B-NB	-4.31	1.32	1.37
22	B	828	CLA	C3C-C2C	4.31	1.45	1.36
29	5	312	5X6	C16-C17	4.31	1.55	1.45
29	2	313	5X6	C16-C17	4.31	1.55	1.45
22	3	302	CLA	CHD-C1D	4.31	1.46	1.38
22	A	809	CLA	C3C-C2C	4.31	1.45	1.36
22	1	307	CLA	CHD-C1D	4.31	1.46	1.38
22	B	807	CLA	CHC-C1C	4.31	1.47	1.38
22	7	313	CLA	CHD-C1D	4.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	303	CLA	CHD-C1D	4.31	1.46	1.38
22	2	307	CLA	CHD-C4C	4.31	1.49	1.39
22	4	310	CLA	CHD-C4C	4.31	1.49	1.39
22	B	812	CLA	O2D-CGD	4.31	1.43	1.33
22	5	301	CLA	C1D-ND	4.31	1.43	1.37
22	A	823	CLA	O2D-CGD	4.31	1.43	1.33
29	5	314	5X6	C18-C17	4.30	1.41	1.35
25	L	206	BCR	C17-C18	4.30	1.41	1.35
22	6	307	CLA	O2A-CGA	4.30	1.45	1.33
22	4	303	CLA	O2A-CGA	4.30	1.45	1.33
29	4	313	5X6	C21-C22	4.30	1.41	1.35
22	7	308	CLA	CHD-C1D	4.30	1.46	1.38
29	2	314	5X6	C16-C17	4.30	1.55	1.45
22	B	835	CLA	CHC-C1C	4.30	1.47	1.38
22	2	306	CLA	CHD-C4C	4.30	1.49	1.39
22	A	819	CLA	CHC-C1C	4.29	1.47	1.38
29	1	311	5X6	C12-C13	4.29	1.55	1.45
22	6	307	CLA	CHC-C1C	4.29	1.47	1.38
29	5	321	5X6	C25-C26	4.29	1.41	1.35
22	2	307	CLA	CHD-C1D	4.29	1.46	1.38
22	A	802	CLA	O2A-CGA	4.29	1.45	1.33
22	J	102	CLA	CHC-C1C	4.29	1.47	1.38
22	A	825	CLA	O2D-CGD	4.29	1.43	1.33
29	1	312	5X6	C16-C17	4.29	1.55	1.45
22	B	833	CLA	CHC-C1C	4.29	1.47	1.38
22	A	816	CLA	O2A-CGA	4.28	1.45	1.33
22	7	309	CLA	CHD-C1D	4.28	1.46	1.38
22	6	309	CLA	C1D-ND	4.28	1.43	1.37
22	B	822	CLA	O2D-CGD	4.28	1.43	1.33
22	B	837	CLA	O2A-CGA	4.28	1.45	1.33
31	6	318	RRX	C10-C9	4.28	1.41	1.35
25	5	315	BCR	C10-C9	4.28	1.41	1.35
31	6	318	RRX	C14-C13	4.28	1.41	1.35
22	A	830	CLA	C1D-ND	4.28	1.43	1.37
22	5	306	CLA	C1D-ND	4.28	1.43	1.37
22	B	813	CLA	O2D-CGD	4.28	1.43	1.33
29	J	104	5X6	C23-C22	4.28	1.55	1.45
22	B	824	CLA	C3C-C2C	4.28	1.45	1.36
22	B	827	CLA	C3C-C2C	4.28	1.45	1.36
22	3	301	CLA	CHC-C4B	4.28	1.49	1.39
22	A	809	CLA	O2D-CGD	4.28	1.43	1.33
29	4	315	5X6	C25-C26	4.27	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	850	CLA	CHD-C1D	4.27	1.46	1.38
25	L	206	BCR	C21-C22	4.27	1.41	1.35
22	1	304	CLA	CHC-C1C	4.27	1.47	1.38
29	1	313	5X6	C14-C13	4.27	1.41	1.35
22	5	301	CLA	CHC-C1C	4.27	1.47	1.38
22	B	816	CLA	O2D-CGD	4.27	1.43	1.33
22	3	303	CLA	CHD-C4C	4.26	1.49	1.39
25	B	844	BCR	C17-C18	4.26	1.41	1.35
22	3	304	CLA	CHD-C4C	4.26	1.49	1.39
22	A	837	CLA	O2D-CGD	4.26	1.43	1.33
29	B	851	5X6	C12-C13	4.26	1.55	1.45
22	7	306	CLA	CHD-C1D	4.26	1.46	1.38
22	B	805	CLA	O2D-CGD	4.26	1.43	1.33
22	O	206	CLA	CHD-C4C	4.26	1.49	1.39
22	5	305	CLA	CHD-C4C	4.26	1.48	1.39
22	A	820	CLA	CHC-C1C	4.25	1.47	1.38
22	7	310	CLA	CHD-C1D	4.25	1.46	1.38
22	A	834	CLA	C1B-NB	-4.25	1.32	1.37
22	A	824	CLA	O2D-CGD	4.25	1.43	1.33
29	B	851	5X6	C16-C17	4.25	1.55	1.45
29	6	316	5X6	C21-C22	4.25	1.41	1.35
29	B	851	5X6	C23-C22	4.25	1.55	1.45
22	4	304	CLA	O2A-CGA	4.25	1.45	1.33
22	2	305	CLA	CHD-C4C	4.24	1.48	1.39
22	A	809	CLA	O2A-CGA	4.24	1.45	1.33
22	7	307	CLA	CHD-C4C	4.24	1.48	1.39
29	7	317	5X6	C21-C22	4.24	1.41	1.35
22	B	834	CLA	C1D-ND	4.24	1.43	1.37
22	5	304	CLA	CHD-C1D	4.24	1.46	1.38
22	B	834	CLA	O2A-CGA	4.24	1.45	1.33
25	J	103	BCR	C14-C13	4.24	1.41	1.35
22	A	837	CLA	O2A-CGA	4.24	1.45	1.33
29	4	313	5X6	C16-C17	4.24	1.55	1.45
29	1	313	5X6	C23-C22	4.23	1.55	1.45
22	3	301	CLA	CHD-C1D	4.23	1.46	1.38
22	A	832	CLA	O2A-CGA	4.23	1.45	1.33
22	A	838	CLA	C1B-NB	-4.23	1.32	1.37
22	A	839	CLA	CHC-C1C	4.23	1.47	1.38
22	Z	204	CLA	C1D-ND	4.23	1.43	1.37
22	1	309	CLA	CHD-C4C	4.23	1.48	1.39
22	B	839	CLA	O2A-CGA	4.23	1.45	1.33
22	A	803	CLA	C4B-NB	-4.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	303	CLA	CHC-C4B	4.23	1.48	1.39
31	6	318	RRX	C17-C18	4.23	1.41	1.35
22	4	306	CLA	CHD-C1D	4.23	1.46	1.38
29	3	306	5X6	C16-C17	4.23	1.55	1.45
22	B	849	CLA	C1B-NB	-4.22	1.32	1.37
21	A	801	CL0	C1B-NB	-4.22	1.32	1.37
22	A	836	CLA	C1D-ND	4.22	1.43	1.37
25	Z	202	BCR	C10-C9	4.22	1.41	1.35
22	B	816	CLA	O2A-CGA	4.22	1.45	1.33
22	B	825	CLA	CHC-C4B	4.22	1.48	1.39
22	6	305	CLA	O2A-CGA	4.22	1.45	1.33
22	B	805	CLA	CHC-C1C	4.22	1.47	1.38
22	7	312	CLA	CHD-C1D	4.22	1.46	1.38
29	5	321	5X6	C21-C22	4.21	1.41	1.35
22	A	858	CLA	O2D-CGD	4.21	1.43	1.33
22	6	307	CLA	CHD-C4C	4.21	1.48	1.39
25	4	316	BCR	C10-C9	4.21	1.41	1.35
22	B	827	CLA	O2A-CGA	4.21	1.45	1.33
22	A	826	CLA	C4B-NB	-4.21	1.32	1.37
29	7	316	5X6	C25-C26	4.21	1.41	1.35
22	2	308	CLA	CHD-C4C	4.20	1.48	1.39
22	4	310	CLA	CHC-C1C	4.20	1.47	1.38
22	6	308	CLA	CHD-C1D	4.20	1.46	1.38
22	A	831	CLA	O2D-CGD	4.20	1.43	1.33
22	B	832	CLA	CHC-C1C	4.20	1.47	1.38
22	3	305	CLA	CHD-C4C	4.20	1.48	1.39
22	B	850	CLA	CHD-C4C	4.20	1.48	1.39
22	A	827	CLA	CHC-C1C	4.20	1.47	1.38
29	M	101	5X6	C16-C17	4.19	1.55	1.45
25	B	841	BCR	C10-C9	4.19	1.41	1.35
22	6	311	CLA	CHD-C4C	4.19	1.48	1.39
22	7	313	CLA	CHD-C4C	4.19	1.48	1.39
22	3	301	CLA	CHD-C4C	4.19	1.48	1.39
22	B	823	CLA	C1D-ND	4.19	1.42	1.37
29	6	315	5X6	C16-C17	4.19	1.54	1.45
22	A	837	CLA	CHC-C1C	4.19	1.47	1.38
22	1	308	CLA	CHD-C4C	4.19	1.48	1.39
22	B	809	CLA	C3C-C2C	4.19	1.45	1.36
22	K	101	CLA	CHD-C1D	4.19	1.46	1.38
22	B	835	CLA	O2A-CGA	4.18	1.45	1.33
22	B	820	CLA	CHD-C4C	4.18	1.48	1.39
22	A	806	CLA	C3C-C2C	4.18	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C3C-C2C	4.18	1.45	1.36
22	2	308	CLA	CHC-C4B	4.18	1.48	1.39
29	1	313	5X6	C18-C17	4.18	1.41	1.35
22	O	203	CLA	C1D-ND	4.18	1.42	1.37
22	4	312	CLA	CHD-C1D	4.18	1.46	1.38
22	7	305	CLA	CHD-C4C	4.18	1.48	1.39
22	A	802	CLA	O2D-CGD	4.18	1.43	1.33
22	2	309	CLA	CHD-C1D	4.18	1.46	1.38
22	2	303	CLA	CHD-C4C	4.18	1.48	1.39
29	3	306	5X6	C18-C17	4.17	1.41	1.35
22	2	311	CLA	CHD-C4C	4.17	1.48	1.39
22	4	306	CLA	CHD-C4C	4.17	1.48	1.39
22	A	818	CLA	O2D-CGD	4.17	1.43	1.33
22	5	306	CLA	CHC-C1C	4.17	1.47	1.38
22	B	809	CLA	O2A-CGA	4.17	1.45	1.33
22	A	803	CLA	C1B-NB	-4.17	1.32	1.37
25	5	315	BCR	C17-C18	4.17	1.41	1.35
22	B	836	CLA	O2A-CGA	4.17	1.45	1.33
22	4	302	CLA	CHD-C1D	4.17	1.46	1.38
22	5	302	CLA	O2A-CGA	4.16	1.45	1.33
22	2	302	CLA	CHD-C4C	4.16	1.48	1.39
22	B	835	CLA	C1D-ND	4.16	1.42	1.37
22	B	836	CLA	O2D-CGD	4.16	1.43	1.33
22	B	815	CLA	CHC-C1C	4.16	1.47	1.38
29	O	207	5X6	C16-C17	4.16	1.54	1.45
22	A	825	CLA	CHC-C1C	4.16	1.47	1.38
22	B	814	CLA	O2A-CGA	4.16	1.45	1.33
22	4	304	CLA	C1B-NB	-4.16	1.32	1.37
22	4	309	CLA	CHD-C1D	4.16	1.46	1.38
29	M	101	5X6	C18-C17	4.16	1.41	1.35
25	L	206	BCR	C14-C13	4.15	1.41	1.35
22	B	807	CLA	O2A-CGA	4.15	1.45	1.33
22	1	306	CLA	CHD-C4C	4.15	1.48	1.39
22	A	826	CLA	O2D-CGD	4.15	1.43	1.33
29	7	314	5X6	C24-C25	4.15	1.56	1.43
22	2	310	CLA	CHD-C4C	4.15	1.48	1.39
29	1	312	5X6	C25-C26	4.15	1.41	1.35
22	4	311	CLA	CHD-C1D	4.15	1.46	1.38
22	1	303	CLA	CHD-C4C	4.15	1.48	1.39
22	3	302	CLA	CHD-C4C	4.15	1.48	1.39
22	7	310	CLA	CHD-C4C	4.14	1.48	1.39
22	4	307	CLA	C3D-C2D	4.14	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	308	CLA	CHC-C4B	4.14	1.48	1.39
29	1	312	5X6	C33-C32	4.14	1.58	1.52
25	F	201	BCR	C10-C9	4.14	1.41	1.35
22	4	308	CLA	C1D-ND	4.14	1.42	1.37
22	7	312	CLA	CHC-C4B	4.14	1.48	1.39
22	B	811	CLA	O2A-CGA	4.14	1.45	1.33
22	A	816	CLA	O2D-CGD	4.14	1.43	1.33
22	B	825	CLA	CHC-C1C	4.14	1.46	1.38
22	A	839	CLA	C1B-NB	-4.14	1.32	1.37
22	7	311	CLA	CHD-C4C	4.13	1.48	1.39
22	2	309	CLA	CHD-C4C	4.13	1.48	1.39
29	Z	206	5X6	C25-C26	4.13	1.41	1.35
22	B	829	CLA	C4B-NB	-4.13	1.32	1.37
22	3	305	CLA	CHD-C1D	4.13	1.46	1.38
22	J	102	CLA	CHD-C1D	4.13	1.46	1.38
22	A	811	CLA	O2D-CGD	4.13	1.43	1.33
22	O	204	CLA	CHD-C4C	4.13	1.48	1.39
22	B	824	CLA	C1B-NB	-4.13	1.32	1.37
25	A	843	BCR	C21-C22	4.13	1.41	1.35
22	5	304	CLA	CHD-C4C	4.13	1.48	1.39
22	J	102	CLA	CHD-C4C	4.13	1.48	1.39
29	O	207	5X6	C18-C17	4.13	1.41	1.35
29	O	207	5X6	C14-C13	4.13	1.41	1.35
22	B	801	CLA	O2D-CGD	4.12	1.43	1.33
22	B	811	CLA	CHC-C1C	4.12	1.46	1.38
29	2	313	5X6	C24-C25	4.12	1.56	1.43
22	L	205	CLA	CHD-C1D	4.12	1.46	1.38
22	B	828	CLA	O2A-CGA	4.12	1.45	1.33
22	5	306	CLA	O2A-CGA	4.12	1.45	1.33
22	B	839	CLA	CHC-C1C	4.12	1.46	1.38
22	F	206	CLA	CHC-C1C	4.12	1.46	1.38
22	B	810	CLA	O2A-CGA	4.12	1.45	1.33
29	5	314	5X6	C25-C26	4.12	1.41	1.35
22	A	805	CLA	CHD-C1D	4.12	1.46	1.38
22	O	204	CLA	CHD-C1D	4.12	1.46	1.38
22	A	828	CLA	O2D-CGD	4.12	1.43	1.33
22	B	813	CLA	C1B-NB	-4.12	1.32	1.37
22	B	803	CLA	C1B-NB	-4.11	1.32	1.37
25	A	862	BCR	C10-C9	4.11	1.41	1.35
22	5	308	CLA	C1D-ND	4.11	1.42	1.37
29	1	312	5X6	C14-C13	4.11	1.41	1.35
22	B	838	CLA	O2A-CGA	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	302	CLA	CHD-C1D	4.11	1.46	1.38
29	M	101	5X6	C23-C22	4.11	1.54	1.45
22	2	311	CLA	CHC-C4B	4.11	1.48	1.39
22	A	833	CLA	C1B-NB	-4.11	1.32	1.37
22	4	310	CLA	C1B-NB	-4.11	1.32	1.37
22	4	302	CLA	CHC-C4B	4.10	1.48	1.39
29	7	317	5X6	C16-C17	4.10	1.54	1.45
22	O	203	CLA	O2A-CGA	4.10	1.46	1.33
29	4	314	5X6	C19-C18	4.10	1.56	1.43
22	7	312	CLA	CHD-C4C	4.10	1.48	1.39
22	B	803	CLA	O2A-CGA	4.10	1.45	1.33
22	A	806	CLA	C4B-NB	-4.10	1.32	1.37
22	4	312	CLA	CHD-C4C	4.10	1.48	1.39
22	A	859	CLA	O2A-CGA	4.10	1.45	1.33
22	B	826	CLA	O2D-CGD	4.10	1.43	1.33
22	6	312	CLA	CHD-C1D	4.10	1.46	1.38
22	B	821	CLA	O2A-CGA	4.10	1.46	1.33
22	O	204	CLA	CHC-C4B	4.10	1.48	1.39
22	7	308	CLA	CHC-C4B	4.10	1.48	1.39
29	7	314	5X6	C15-C14	4.10	1.56	1.43
22	A	825	CLA	CHC-C4B	4.09	1.48	1.39
22	A	824	CLA	O2A-CGA	4.09	1.45	1.33
29	5	313	5X6	C24-C25	4.09	1.56	1.43
22	A	839	CLA	O2A-CGA	4.09	1.45	1.33
22	B	832	CLA	O2A-CGA	4.09	1.45	1.33
25	2	301	BCR	C21-C22	4.09	1.41	1.35
22	B	811	CLA	C1B-NB	-4.09	1.32	1.37
22	7	308	CLA	CHD-C4C	4.09	1.48	1.39
25	F	207	BCR	C17-C18	4.09	1.41	1.35
25	1	301	BCR	C21-C22	4.09	1.41	1.35
29	5	314	5X6	C14-C13	4.08	1.41	1.35
22	6	313	CLA	CHD-C1D	4.08	1.46	1.38
22	B	809	CLA	C1D-ND	4.08	1.42	1.37
22	A	835	CLA	O2A-CGA	4.08	1.45	1.33
31	4	317	RRX	C17-C18	4.08	1.41	1.35
22	A	823	CLA	O2A-CGA	4.08	1.45	1.33
22	B	838	CLA	C4B-NB	-4.08	1.32	1.37
29	5	312	5X6	C15-C14	4.07	1.56	1.43
22	O	205	CLA	CHD-C4C	4.07	1.48	1.39
25	B	844	BCR	C10-C9	4.07	1.41	1.35
22	A	804	CLA	C1B-NB	-4.07	1.32	1.37
29	7	315	5X6	C19-C18	4.07	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	301	CLA	CHD-C1D	4.07	1.46	1.38
31	6	318	RRX	C21-C22	4.07	1.41	1.35
22	B	836	CLA	CHC-C1C	4.07	1.46	1.38
22	4	304	CLA	CHD-C1D	4.07	1.46	1.38
31	4	317	RRX	C10-C9	4.07	1.41	1.35
22	B	849	CLA	C4B-NB	-4.07	1.32	1.37
29	M	101	5X6	C21-C22	4.07	1.41	1.35
29	3	306	5X6	C15-C14	4.07	1.56	1.43
22	A	834	CLA	CHD-C4C	4.06	1.48	1.39
22	B	834	CLA	CHC-C1C	4.06	1.46	1.38
22	6	308	CLA	CHD-C4C	4.06	1.48	1.39
29	3	306	5X6	C24-C25	4.06	1.56	1.43
22	A	859	CLA	C1B-NB	-4.06	1.32	1.37
22	4	311	CLA	CHC-C4B	4.06	1.48	1.39
22	O	203	CLA	C4B-NB	-4.06	1.32	1.37
22	B	812	CLA	CHD-C1D	4.06	1.46	1.38
29	1	316	5X6	C19-C18	4.06	1.56	1.43
22	7	309	CLA	CHD-C4C	4.06	1.48	1.39
31	1	315	RRX	C14-C13	4.06	1.41	1.35
22	A	823	CLA	C1D-ND	4.06	1.42	1.37
22	6	313	CLA	CHD-C4C	4.06	1.48	1.39
29	6	317	5X6	C16-C17	4.06	1.54	1.45
31	1	315	RRX	C10-C9	4.06	1.41	1.35
22	5	302	CLA	C1D-ND	4.05	1.42	1.37
22	1	305	CLA	CHD-C1D	4.05	1.46	1.38
29	O	208	5X6	C24-C25	4.05	1.56	1.43
25	5	315	BCR	C14-C13	4.05	1.41	1.35
29	2	313	5X6	C19-C18	4.05	1.56	1.43
22	B	814	CLA	C1D-ND	4.05	1.42	1.37
29	O	207	5X6	C25-C26	4.05	1.41	1.35
22	B	837	CLA	CHC-C1C	4.05	1.46	1.38
22	B	819	CLA	O2A-CGA	4.05	1.45	1.33
29	2	312	5X6	C19-C18	4.05	1.56	1.43
22	1	303	CLA	CHD-C1D	4.05	1.46	1.38
22	7	313	CLA	CHC-C4B	4.05	1.48	1.39
29	4	315	5X6	C24-C25	4.05	1.56	1.43
22	B	818	CLA	O2D-CGD	4.05	1.43	1.33
29	2	314	5X6	C24-C25	4.05	1.56	1.43
29	5	313	5X6	C15-C14	4.04	1.56	1.43
22	A	848	CLA	O2D-CGD	4.04	1.43	1.33
22	F	206	CLA	C1D-ND	4.04	1.42	1.37
22	O	206	CLA	O2A-CGA	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	306	CLA	CHD-C1D	4.04	1.46	1.38
22	L	204	CLA	CHD-C1D	4.04	1.46	1.38
22	A	859	CLA	CHB-C1B	4.04	1.48	1.39
22	B	834	CLA	C1B-NB	-4.04	1.32	1.37
22	6	309	CLA	CHD-C4C	4.04	1.48	1.39
22	B	807	CLA	C1D-ND	4.04	1.42	1.37
29	Z	206	5X6	C15-C14	4.03	1.55	1.43
22	4	312	CLA	CHC-C4B	4.03	1.48	1.39
22	A	820	CLA	C1D-ND	4.03	1.42	1.37
22	A	813	CLA	CHC-C1C	4.03	1.46	1.38
22	2	307	CLA	CHC-C4B	4.03	1.48	1.39
22	7	304	CLA	CHD-C4C	4.03	1.48	1.39
25	Z	205	BCR	C14-C13	4.03	1.41	1.35
22	6	310	CLA	CHD-C1D	4.03	1.46	1.38
22	L	205	CLA	CHC-C4B	4.03	1.48	1.39
22	4	303	CLA	C1D-ND	4.03	1.42	1.37
22	7	311	CLA	CHC-C4B	4.03	1.48	1.39
29	6	315	5X6	C14-C13	4.02	1.41	1.35
22	A	811	CLA	O2A-CGA	4.02	1.45	1.33
22	A	809	CLA	CHD-C4C	4.02	1.48	1.39
29	2	312	5X6	C24-C25	4.02	1.55	1.43
22	6	303	CLA	CHD-C4C	4.02	1.48	1.39
22	2	309	CLA	CHC-C4B	4.02	1.48	1.39
22	2	310	CLA	CHC-C4B	4.01	1.48	1.39
22	L	204	CLA	CHD-C4C	4.01	1.48	1.39
22	B	822	CLA	O2A-CGA	4.01	1.45	1.33
29	2	312	5X6	C15-C14	4.01	1.55	1.43
25	5	315	BCR	C21-C22	4.01	1.41	1.35
22	B	809	CLA	CHD-C1D	4.01	1.46	1.38
22	4	311	CLA	CHD-C4C	4.01	1.48	1.39
22	6	304	CLA	O2A-CGA	4.01	1.45	1.33
25	A	861	BCR	C10-C9	4.01	1.41	1.35
29	1	316	5X6	C20-C21	4.01	1.55	1.43
29	7	314	5X6	C19-C18	4.01	1.55	1.43
29	7	316	5X6	C24-C25	4.01	1.55	1.43
29	1	314	5X6	C19-C18	4.01	1.55	1.43
22	A	823	CLA	C1B-NB	-4.01	1.32	1.37
22	2	303	CLA	CHC-C4B	4.00	1.48	1.39
22	L	204	CLA	O2A-CGA	4.00	1.45	1.33
29	2	314	5X6	C19-C18	4.00	1.55	1.43
22	B	830	CLA	C3D-C2D	4.00	1.50	1.39
29	J	104	5X6	C21-C22	4.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	304	CLA	CHC-C4B	4.00	1.48	1.39
22	A	825	CLA	C1D-ND	4.00	1.42	1.37
22	L	205	CLA	C3D-C2D	4.00	1.50	1.39
22	B	833	CLA	CHD-C1D	4.00	1.46	1.38
29	4	313	5X6	C19-C18	4.00	1.55	1.43
25	A	845	BCR	C17-C18	4.00	1.41	1.35
22	6	303	CLA	CHD-C1D	4.00	1.46	1.38
22	6	312	CLA	CHD-C4C	3.99	1.48	1.39
29	6	316	5X6	C24-C25	3.99	1.55	1.43
22	6	314	CLA	CHD-C4C	3.99	1.48	1.39
22	A	831	CLA	CHC-C1C	3.99	1.46	1.38
22	A	836	CLA	O2A-CGA	3.99	1.45	1.33
22	A	817	CLA	C3D-C2D	3.99	1.50	1.39
22	Z	204	CLA	CHC-C1C	3.99	1.46	1.38
22	7	309	CLA	C3B-C4B	3.99	1.52	1.42
22	A	838	CLA	O2D-CGD	3.99	1.42	1.33
22	A	819	CLA	C4B-NB	-3.99	1.32	1.37
29	7	318	5X6	C19-C18	3.99	1.55	1.43
22	3	301	CLA	C3B-C4B	3.99	1.52	1.42
22	5	311	CLA	CHD-C4C	3.98	1.48	1.39
22	A	826	CLA	O2A-CGA	3.98	1.45	1.33
22	4	305	CLA	CHD-C1D	3.98	1.46	1.38
22	1	305	CLA	CHC-C4B	3.98	1.48	1.39
22	A	804	CLA	C1D-ND	3.98	1.42	1.37
29	7	317	5X6	C19-C18	3.98	1.55	1.43
22	A	816	CLA	CHC-C1C	3.98	1.46	1.38
22	A	803	CLA	C3C-C2C	3.98	1.45	1.36
22	4	307	CLA	CHD-C4C	3.98	1.48	1.39
25	Z	205	BCR	C17-C18	3.98	1.41	1.35
29	1	316	5X6	C15-C14	3.98	1.55	1.43
29	7	316	5X6	C19-C18	3.98	1.55	1.43
22	A	815	CLA	C1D-ND	3.98	1.42	1.37
22	A	807	CLA	O2A-CGA	3.98	1.45	1.33
29	B	851	5X6	C14-C13	3.98	1.41	1.35
29	6	315	5X6	C33-C32	3.97	1.58	1.52
22	A	802	CLA	C4B-NB	-3.97	1.32	1.37
22	A	825	CLA	O2A-CGA	3.97	1.44	1.33
22	A	805	CLA	O2D-CGD	3.97	1.42	1.33
22	A	811	CLA	C1B-NB	-3.97	1.32	1.37
29	O	208	5X6	C19-C18	3.97	1.55	1.43
22	A	805	CLA	CHC-C1C	3.97	1.46	1.38
22	A	830	CLA	CHC-C1C	3.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	814	CLA	O2D-CGD	3.97	1.42	1.33
31	5	322	RRX	C10-C9	3.97	1.41	1.35
22	B	803	CLA	CHC-C1C	3.97	1.46	1.38
29	7	315	5X6	C20-C21	3.97	1.55	1.43
28	B	845	DGD	O1G-C1A	3.97	1.44	1.33
22	5	302	CLA	CHC-C4B	3.97	1.48	1.39
22	4	305	CLA	CHB-C1B	3.96	1.48	1.39
22	1	305	CLA	CHD-C4C	3.96	1.48	1.39
22	K	102	CLA	CHD-C1D	3.96	1.46	1.38
22	B	815	CLA	CHD-C1D	3.96	1.46	1.38
22	B	818	CLA	O2A-CGA	3.96	1.44	1.33
22	A	818	CLA	CHC-C1C	3.96	1.46	1.38
22	6	304	CLA	CHC-C4B	3.96	1.48	1.39
22	B	831	CLA	C1B-NB	-3.96	1.32	1.37
29	2	312	5X6	C20-C21	3.96	1.55	1.43
22	5	307	CLA	CHD-C4C	3.96	1.48	1.39
22	B	822	CLA	CHC-C1C	3.96	1.46	1.38
22	4	310	CLA	CHD-C1D	3.96	1.46	1.38
22	A	820	CLA	CHB-C1B	3.96	1.48	1.39
22	B	827	CLA	CHC-C1C	3.96	1.46	1.38
22	2	303	CLA	C3D-C2D	3.96	1.49	1.39
22	1	304	CLA	CHD-C1D	3.96	1.46	1.38
22	B	807	CLA	C1B-NB	-3.96	1.32	1.37
22	B	826	CLA	O2A-CGA	3.96	1.44	1.33
22	B	833	CLA	O2A-CGA	3.96	1.44	1.33
22	A	806	CLA	O2A-CGA	3.96	1.44	1.33
22	B	831	CLA	C1D-ND	3.95	1.42	1.37
22	B	813	CLA	CHB-C1B	3.95	1.48	1.39
22	L	203	CLA	CHD-C1D	3.95	1.46	1.38
25	A	862	BCR	C21-C22	3.95	1.41	1.35
22	4	311	CLA	C3B-C4B	3.95	1.52	1.42
29	4	314	5X6	C15-C14	3.95	1.55	1.43
22	J	102	CLA	C1B-NB	-3.95	1.32	1.37
29	4	315	5X6	C19-C18	3.95	1.55	1.43
29	O	208	5X6	C20-C21	3.95	1.55	1.43
22	B	817	CLA	C1B-NB	-3.95	1.32	1.37
29	5	314	5X6	C24-C25	3.95	1.55	1.43
29	5	312	5X6	C24-C25	3.95	1.55	1.43
22	A	823	CLA	CHC-C1C	3.95	1.46	1.38
22	1	307	CLA	CHC-C4B	3.95	1.48	1.39
22	4	306	CLA	CHC-C4B	3.95	1.48	1.39
22	5	303	CLA	CHD-C1D	3.95	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	818	CLA	C1D-ND	3.95	1.42	1.37
25	L	201	BCR	C14-C13	3.95	1.41	1.35
22	6	306	CLA	CHD-C4C	3.95	1.48	1.39
22	A	825	CLA	CHB-C1B	3.95	1.48	1.39
29	7	318	5X6	C15-C14	3.95	1.55	1.43
22	1	302	CLA	CHD-C4C	3.94	1.48	1.39
29	5	314	5X6	C19-C18	3.94	1.55	1.43
22	A	832	CLA	C1D-ND	3.94	1.42	1.37
29	1	312	5X6	C19-C18	3.94	1.55	1.43
22	7	304	CLA	OBD-CAD	3.94	1.29	1.22
29	2	312	5X6	C33-C32	3.94	1.58	1.52
29	7	317	5X6	C25-C26	3.94	1.41	1.35
29	M	101	5X6	C19-C18	3.94	1.55	1.43
22	A	809	CLA	CHC-C4B	3.94	1.48	1.39
22	A	839	CLA	C3D-C2D	3.94	1.49	1.39
22	7	306	CLA	CHC-C4B	3.94	1.48	1.39
22	B	833	CLA	C1B-NB	-3.94	1.32	1.37
31	5	322	RRX	C14-C13	3.94	1.41	1.35
29	4	313	5X6	C20-C21	3.94	1.55	1.43
29	6	316	5X6	C19-C18	3.93	1.55	1.43
29	7	315	5X6	C15-C14	3.93	1.55	1.43
28	B	845	DGD	O2G-C1B	3.93	1.45	1.34
22	5	305	CLA	CHC-C4B	3.93	1.48	1.39
22	4	304	CLA	CHD-C4C	3.93	1.48	1.39
22	B	831	CLA	O2A-CGA	3.93	1.44	1.33
29	J	104	5X6	C18-C17	3.93	1.41	1.35
22	A	802	CLA	CHC-C1C	3.93	1.46	1.38
22	4	302	CLA	OBD-CAD	3.93	1.29	1.22
22	2	306	CLA	CHC-C4B	3.93	1.48	1.39
22	B	810	CLA	CHC-C1C	3.93	1.46	1.38
22	4	309	CLA	CHD-C4C	3.93	1.48	1.39
29	6	315	5X6	C24-C25	3.93	1.55	1.43
29	5	312	5X6	C19-C18	3.93	1.55	1.43
22	B	816	CLA	C1D-ND	3.93	1.42	1.37
22	Z	204	CLA	C1B-NB	-3.93	1.33	1.37
22	2	307	CLA	C3B-C4B	3.92	1.51	1.42
22	Z	201	CLA	C1D-ND	3.92	1.42	1.37
22	5	310	CLA	CHD-C4C	3.92	1.48	1.39
22	5	304	CLA	CHB-C1B	3.92	1.48	1.39
22	A	822	CLA	CHC-C1C	3.92	1.46	1.38
22	B	805	CLA	O2A-CGA	3.92	1.44	1.33
22	B	808	CLA	O2A-CGA	3.92	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	317	5X6	C18-C17	3.92	1.41	1.35
22	6	306	CLA	CHB-C1B	3.92	1.48	1.39
29	2	313	5X6	C15-C14	3.92	1.55	1.43
25	J	103	BCR	C17-C18	3.92	1.41	1.35
22	B	808	CLA	OBD-CAD	3.92	1.29	1.22
29	1	311	5X6	C19-C18	3.92	1.55	1.43
29	1	314	5X6	C20-C21	3.92	1.55	1.43
22	B	826	CLA	CHB-C1B	3.92	1.48	1.39
22	4	302	CLA	CHB-C1B	3.91	1.48	1.39
22	A	848	CLA	C1B-NB	-3.91	1.33	1.37
22	1	308	CLA	CHC-C4B	3.91	1.48	1.39
29	6	317	5X6	C24-C25	3.91	1.55	1.43
29	7	317	5X6	C15-C14	3.91	1.55	1.43
22	B	830	CLA	C1D-ND	3.91	1.42	1.37
29	5	321	5X6	C15-C14	3.91	1.55	1.43
29	7	316	5X6	C15-C14	3.91	1.55	1.43
22	3	305	CLA	C3B-C4B	3.91	1.51	1.42
22	A	832	CLA	CHC-C4B	3.91	1.48	1.39
22	A	835	CLA	C3D-C2D	3.91	1.49	1.39
29	J	104	5X6	C15-C14	3.91	1.55	1.43
25	A	844	BCR	C10-C9	3.91	1.41	1.35
25	I	102	BCR	C10-C9	3.91	1.41	1.35
22	1	307	CLA	CHD-C4C	3.91	1.48	1.39
22	A	823	CLA	C4B-NB	-3.91	1.33	1.37
29	7	314	5X6	C20-C21	3.91	1.55	1.43
22	A	848	CLA	CHC-C1C	3.91	1.46	1.38
22	B	825	CLA	C4B-NB	-3.91	1.33	1.37
22	7	310	CLA	C3D-C2D	3.90	1.49	1.39
29	4	313	5X6	C24-C25	3.90	1.55	1.43
29	4	315	5X6	C15-C14	3.90	1.55	1.43
22	J	102	CLA	C3D-C2D	3.90	1.49	1.39
22	B	829	CLA	CHC-C1C	3.90	1.46	1.38
29	M	101	5X6	C14-C13	3.90	1.41	1.35
22	B	824	CLA	C4B-NB	-3.90	1.33	1.37
22	B	834	CLA	O2D-CGD	3.90	1.42	1.33
22	3	302	CLA	CHC-C4B	3.90	1.48	1.39
29	1	313	5X6	C24-C25	3.90	1.55	1.43
22	1	310	CLA	C3D-C2D	3.90	1.49	1.39
29	O	208	5X6	C15-C14	3.90	1.55	1.43
22	B	831	CLA	CHD-C1D	3.90	1.46	1.38
22	A	808	CLA	CHD-C1D	3.90	1.46	1.38
22	6	313	CLA	CHC-C4B	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	314	5X6	C15-C14	3.90	1.55	1.43
22	6	312	CLA	C1B-NB	-3.90	1.33	1.37
22	4	308	CLA	CHD-C4C	3.89	1.48	1.39
22	B	813	CLA	CHC-C1C	3.89	1.46	1.38
22	4	303	CLA	C3B-C4B	3.89	1.51	1.42
29	5	321	5X6	C19-C18	3.89	1.55	1.43
25	A	846	BCR	C21-C22	3.89	1.40	1.35
25	B	842	BCR	C21-C22	3.89	1.40	1.35
29	O	207	5X6	C21-C22	3.89	1.40	1.35
22	O	205	CLA	CHC-C4B	3.89	1.48	1.39
22	B	805	CLA	C1B-NB	-3.89	1.33	1.37
22	A	807	CLA	O2D-CGD	3.89	1.42	1.33
22	B	821	CLA	CHD-C1D	3.89	1.45	1.38
22	O	205	CLA	CHD-C1D	3.89	1.45	1.38
29	1	312	5X6	C24-C25	3.89	1.55	1.43
22	2	311	CLA	C3B-C4B	3.89	1.51	1.42
22	A	831	CLA	C1B-NB	-3.89	1.33	1.37
22	A	857	CLA	CHC-C1C	3.89	1.46	1.38
22	B	833	CLA	OBD-CAD	3.89	1.29	1.22
22	A	836	CLA	C1B-NB	-3.88	1.33	1.37
22	4	309	CLA	CHC-C4B	3.88	1.48	1.39
22	3	303	CLA	CHC-C4B	3.88	1.48	1.39
25	B	841	BCR	C21-C22	3.88	1.40	1.35
22	K	101	CLA	CHD-C4C	3.88	1.48	1.39
22	A	805	CLA	CHB-C1B	3.88	1.48	1.39
29	1	313	5X6	C19-C18	3.88	1.55	1.43
22	7	310	CLA	CHC-C4B	3.88	1.48	1.39
25	L	202	BCR	C14-C13	3.88	1.40	1.35
22	3	304	CLA	C3D-C2D	3.88	1.49	1.39
22	O	203	CLA	CHB-C1B	3.88	1.48	1.39
22	B	801	CLA	C4B-NB	-3.87	1.33	1.37
29	J	104	5X6	C24-C25	3.87	1.55	1.43
22	F	205	CLA	CHB-C1B	3.87	1.48	1.39
25	2	301	BCR	C10-C9	3.87	1.40	1.35
22	1	310	CLA	CHD-C1D	3.87	1.45	1.38
22	A	828	CLA	CHC-C1C	3.87	1.46	1.38
22	A	809	CLA	OBD-CAD	3.87	1.29	1.22
22	A	824	CLA	CHC-C1C	3.87	1.46	1.38
29	3	306	5X6	C19-C18	3.87	1.55	1.43
22	B	804	CLA	C1D-ND	3.87	1.42	1.37
22	7	304	CLA	CHD-C1D	3.87	1.45	1.38
29	J	104	5X6	C33-C32	3.87	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	302	CLA	CHC-C4B	3.87	1.48	1.39
29	5	321	5X6	C24-C25	3.87	1.55	1.43
29	Z	206	5X6	C19-C18	3.87	1.55	1.43
22	B	809	CLA	C4B-NB	-3.87	1.33	1.37
22	5	307	CLA	CHD-C1D	3.87	1.45	1.38
22	A	836	CLA	CHC-C1C	3.87	1.46	1.38
22	A	812	CLA	C1B-NB	-3.87	1.33	1.37
22	7	303	CLA	CHC-C4B	3.87	1.48	1.39
22	7	312	CLA	C3B-C4B	3.87	1.51	1.42
29	4	315	5X6	C20-C21	3.87	1.55	1.43
22	A	848	CLA	C4B-NB	-3.87	1.33	1.37
31	4	317	RRX	C14-C13	3.86	1.40	1.35
22	A	827	CLA	O2A-CGA	3.86	1.44	1.33
29	7	318	5X6	C24-C25	3.86	1.55	1.43
22	B	835	CLA	CHC-C4B	3.86	1.48	1.39
22	2	308	CLA	OBD-CAD	3.86	1.29	1.22
22	B	801	CLA	CHC-C1C	3.86	1.46	1.38
29	5	321	5X6	C20-C21	3.86	1.55	1.43
22	F	206	CLA	C1B-NB	-3.86	1.33	1.37
22	B	805	CLA	CHD-C1D	3.86	1.45	1.38
29	6	316	5X6	C15-C14	3.86	1.55	1.43
29	1	313	5X6	C15-C14	3.86	1.55	1.43
22	B	824	CLA	C1D-ND	3.86	1.42	1.37
29	Z	206	5X6	C20-C21	3.86	1.55	1.43
22	L	203	CLA	CHD-C4C	3.86	1.48	1.39
25	B	841	BCR	C14-C13	3.86	1.40	1.35
29	6	316	5X6	C33-C32	3.86	1.57	1.52
22	6	309	CLA	CHC-C4B	3.86	1.48	1.39
22	4	307	CLA	CHD-C1D	3.86	1.45	1.38
22	2	305	CLA	CHC-C4B	3.86	1.48	1.39
22	5	307	CLA	C1B-NB	-3.85	1.33	1.37
22	B	839	CLA	C1B-NB	-3.85	1.33	1.37
22	A	810	CLA	C1D-ND	3.85	1.42	1.37
22	A	802	CLA	CHC-C4B	3.85	1.48	1.39
22	A	804	CLA	CHB-C1B	3.85	1.48	1.39
29	4	314	5X6	C20-C21	3.85	1.55	1.43
22	6	309	CLA	CHD-C1D	3.85	1.45	1.38
29	7	315	5X6	C24-C25	3.85	1.55	1.43
22	A	830	CLA	CHD-C1D	3.85	1.45	1.38
22	A	820	CLA	C4B-NB	-3.85	1.33	1.37
22	4	302	CLA	C3D-C2D	3.85	1.49	1.39
22	1	305	CLA	C3D-C2D	3.85	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	305	CLA	CHC-C4B	3.85	1.48	1.39
22	K	102	CLA	C1B-NB	-3.84	1.33	1.37
22	L	204	CLA	C1B-NB	-3.84	1.33	1.37
29	1	314	5X6	C24-C25	3.84	1.55	1.43
22	B	819	CLA	CHD-C1D	3.84	1.45	1.38
22	6	309	CLA	C3D-C2D	3.84	1.49	1.39
22	4	302	CLA	CHD-C4C	3.84	1.48	1.39
22	A	811	CLA	CHB-C1B	3.84	1.48	1.39
29	1	313	5X6	C25-C26	3.84	1.40	1.35
29	B	851	5X6	C24-C25	3.84	1.55	1.43
22	2	309	CLA	C3D-C2D	3.84	1.49	1.39
22	6	311	CLA	C3D-C2D	3.84	1.49	1.39
22	6	305	CLA	CHD-C4C	3.84	1.48	1.39
25	1	301	BCR	C10-C9	3.84	1.40	1.35
22	3	303	CLA	C3D-C2D	3.84	1.49	1.39
29	1	311	5X6	C24-C25	3.84	1.55	1.43
22	3	305	CLA	C3D-C2D	3.84	1.49	1.39
22	O	203	CLA	CHC-C1C	3.84	1.46	1.38
29	M	101	5X6	C15-C14	3.84	1.55	1.43
29	4	313	5X6	C15-C14	3.84	1.55	1.43
25	L	201	BCR	C10-C9	3.84	1.40	1.35
22	7	313	CLA	OBD-CAD	3.84	1.29	1.22
22	6	310	CLA	CHC-C4B	3.83	1.48	1.39
22	A	814	CLA	C1D-ND	3.83	1.42	1.37
22	A	836	CLA	C4B-NB	-3.83	1.33	1.37
22	1	303	CLA	CHC-C4B	3.83	1.48	1.39
22	Z	204	CLA	CHD-C1D	3.83	1.45	1.38
22	A	812	CLA	C3D-C2D	3.83	1.49	1.39
22	6	314	CLA	CHC-C4B	3.83	1.48	1.39
22	2	310	CLA	C3D-C2D	3.83	1.49	1.39
22	B	823	CLA	CHD-C1D	3.83	1.45	1.38
22	A	834	CLA	CHC-C4B	3.83	1.48	1.39
22	B	806	CLA	C1D-ND	3.83	1.42	1.37
22	B	826	CLA	C1B-NB	-3.83	1.33	1.37
22	B	849	CLA	CHB-C1B	3.83	1.48	1.39
22	7	307	CLA	CHC-C4B	3.83	1.48	1.39
29	7	318	5X6	C20-C21	3.83	1.55	1.43
22	B	801	CLA	O2A-CGA	3.83	1.44	1.33
22	7	304	CLA	C3B-C4B	3.82	1.51	1.42
25	I	102	BCR	C14-C13	3.82	1.40	1.35
22	A	823	CLA	CHB-C1B	3.82	1.48	1.39
29	2	313	5X6	C20-C21	3.82	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	306	CLA	CHD-C1D	3.82	1.45	1.38
22	7	312	CLA	C3D-C2D	3.82	1.49	1.39
25	Z	202	BCR	C14-C13	3.82	1.40	1.35
22	A	819	CLA	C3D-C2D	3.82	1.49	1.39
22	7	306	CLA	C3B-C4B	3.82	1.51	1.42
29	7	317	5X6	C24-C25	3.82	1.55	1.43
29	1	311	5X6	C15-C14	3.82	1.55	1.43
22	B	850	CLA	CHC-C4B	3.82	1.48	1.39
22	F	206	CLA	CHC-C4B	3.82	1.48	1.39
22	A	813	CLA	C4B-NB	-3.81	1.33	1.37
29	5	313	5X6	C19-C18	3.81	1.55	1.43
22	7	313	CLA	C3B-C4B	3.81	1.51	1.42
22	4	308	CLA	CHD-C1D	3.81	1.45	1.38
22	O	204	CLA	CHB-C1B	3.81	1.48	1.39
29	2	314	5X6	C20-C21	3.81	1.55	1.43
22	B	811	CLA	C4B-NB	-3.81	1.33	1.37
22	1	306	CLA	CHC-C4B	3.81	1.48	1.39
22	4	308	CLA	C3B-C4B	3.81	1.51	1.42
22	B	831	CLA	CHC-C1C	3.81	1.46	1.38
22	A	814	CLA	C1B-NB	-3.81	1.33	1.37
22	2	304	CLA	CHC-C4B	3.81	1.48	1.39
22	2	308	CLA	C3D-C2D	3.81	1.49	1.39
29	7	316	5X6	C20-C21	3.81	1.55	1.43
22	B	815	CLA	C1D-ND	3.81	1.42	1.37
22	B	826	CLA	CHC-C1C	3.81	1.46	1.38
22	5	305	CLA	C3D-C2D	3.81	1.49	1.39
22	6	303	CLA	CHC-C4B	3.81	1.48	1.39
22	5	302	CLA	C3D-C2D	3.81	1.49	1.39
22	5	306	CLA	C3D-C2D	3.81	1.49	1.39
22	O	206	CLA	CHC-C4B	3.81	1.47	1.39
29	3	306	5X6	C20-C21	3.81	1.55	1.43
29	1	313	5X6	C20-C21	3.81	1.55	1.43
29	6	317	5X6	C20-C21	3.80	1.55	1.43
22	B	806	CLA	C3D-C2D	3.80	1.49	1.39
22	B	817	CLA	C1D-ND	3.80	1.42	1.37
22	5	311	CLA	C3D-C2D	3.80	1.49	1.39
22	A	817	CLA	CHC-C1C	3.80	1.46	1.38
22	7	309	CLA	C3D-C2D	3.80	1.49	1.39
22	7	313	CLA	C3D-C2D	3.80	1.49	1.39
29	Z	206	5X6	C28-C29	3.80	1.58	1.45
22	A	831	CLA	C3D-C2D	3.80	1.49	1.39
22	A	834	CLA	CHD-C1D	3.80	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	316	BCR	C17-C18	3.80	1.40	1.35
31	5	322	RRX	C21-C22	3.80	1.40	1.35
22	5	306	CLA	CHB-C1B	3.80	1.47	1.39
22	5	306	CLA	CHD-C4C	3.80	1.47	1.39
22	7	311	CLA	OBD-CAD	3.80	1.29	1.22
22	1	307	CLA	CHB-C1B	3.80	1.47	1.39
22	A	822	CLA	C1D-ND	3.79	1.42	1.37
29	7	317	5X6	C33-C32	3.79	1.57	1.52
22	A	833	CLA	C3D-C2D	3.79	1.49	1.39
22	B	849	CLA	CHD-C1D	3.79	1.45	1.38
22	B	820	CLA	CHD-C1D	3.79	1.45	1.38
22	7	311	CLA	C3D-C2D	3.79	1.49	1.39
22	2	306	CLA	C3D-C2D	3.79	1.49	1.39
22	B	811	CLA	CHD-C4C	3.79	1.47	1.39
22	B	850	CLA	CHB-C1B	3.79	1.47	1.39
22	1	308	CLA	CHB-C1B	3.79	1.47	1.39
22	A	810	CLA	CHB-C1B	3.79	1.47	1.39
29	2	314	5X6	C15-C14	3.79	1.55	1.43
25	A	843	BCR	C14-C13	3.79	1.40	1.35
22	2	308	CLA	C3B-C4B	3.79	1.51	1.42
22	2	305	CLA	C3D-C2D	3.79	1.49	1.39
25	B	843	BCR	C10-C9	3.79	1.40	1.35
22	4	306	CLA	C3D-C2D	3.79	1.49	1.39
22	B	832	CLA	C1B-NB	-3.79	1.33	1.37
22	5	306	CLA	CHC-C4B	3.79	1.47	1.39
22	1	309	CLA	C3D-C2D	3.79	1.49	1.39
22	B	850	CLA	OBD-CAD	3.79	1.29	1.22
22	A	839	CLA	CHB-C1B	3.79	1.47	1.39
22	B	805	CLA	CHB-C1B	3.79	1.47	1.39
22	A	822	CLA	C3D-C2D	3.79	1.49	1.39
22	2	302	CLA	OBD-CAD	3.78	1.29	1.22
22	3	302	CLA	CHB-C1B	3.78	1.47	1.39
22	4	306	CLA	C3B-C4B	3.78	1.51	1.42
22	B	830	CLA	C4B-NB	-3.78	1.33	1.37
22	1	306	CLA	CHB-C1B	3.78	1.47	1.39
29	B	851	5X6	C15-C14	3.78	1.55	1.43
22	1	306	CLA	C3D-C2D	3.78	1.49	1.39
22	O	204	CLA	OBD-CAD	3.78	1.29	1.22
22	2	306	CLA	OBD-CAD	3.78	1.29	1.22
22	7	308	CLA	C3B-C4B	3.78	1.51	1.42
22	7	310	CLA	OBD-CAD	3.78	1.29	1.22
22	L	205	CLA	CHD-C4C	3.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	307	CLA	C3D-C2D	3.78	1.49	1.39
22	A	807	CLA	C1D-ND	3.78	1.42	1.37
22	A	836	CLA	C3D-C2D	3.78	1.49	1.39
29	M	101	5X6	C24-C25	3.78	1.55	1.43
22	A	822	CLA	CHD-C1D	3.78	1.45	1.38
22	A	821	CLA	CHC-C1C	3.78	1.46	1.38
22	4	303	CLA	C1B-NB	-3.78	1.33	1.37
22	5	302	CLA	CHB-C1B	3.78	1.47	1.39
22	B	814	CLA	C1B-NB	-3.78	1.33	1.37
22	B	819	CLA	C1D-ND	3.78	1.42	1.37
22	F	204	CLA	CHB-C1B	3.78	1.47	1.39
22	3	305	CLA	OBD-CAD	3.78	1.29	1.22
22	4	308	CLA	C1B-NB	-3.78	1.33	1.37
22	A	835	CLA	C1B-NB	-3.77	1.33	1.37
22	A	816	CLA	CHC-C4B	3.77	1.47	1.39
22	O	204	CLA	C3D-C2D	3.77	1.49	1.39
22	A	848	CLA	CHC-C4B	3.77	1.47	1.39
29	6	315	5X6	C15-C14	3.77	1.55	1.43
22	4	306	CLA	OBD-CAD	3.77	1.29	1.22
22	1	308	CLA	OBD-CAD	3.77	1.29	1.22
22	1	309	CLA	OBD-CAD	3.77	1.29	1.22
22	2	302	CLA	C3D-C2D	3.77	1.49	1.39
22	B	822	CLA	C4B-NB	-3.77	1.33	1.37
22	6	312	CLA	C3D-C2D	3.77	1.49	1.39
22	B	821	CLA	CHC-C4B	3.77	1.47	1.39
22	B	824	CLA	C3D-C2D	3.77	1.49	1.39
22	A	838	CLA	CHC-C1C	3.77	1.46	1.38
22	6	310	CLA	C3D-C2D	3.77	1.49	1.39
22	B	839	CLA	CHC-C4B	3.77	1.47	1.39
29	2	313	5X6	C33-C32	3.77	1.57	1.52
22	F	204	CLA	CHC-C1C	3.77	1.46	1.38
21	A	801	CL0	O2A-CGA	3.77	1.44	1.33
22	A	823	CLA	OBD-CAD	3.77	1.29	1.22
22	2	311	CLA	OBD-CAD	3.77	1.29	1.22
22	6	303	CLA	OBD-CAD	3.77	1.29	1.22
22	7	303	CLA	CHB-C1B	3.77	1.47	1.39
22	2	310	CLA	C3B-C4B	3.77	1.51	1.42
29	1	312	5X6	C20-C21	3.77	1.55	1.43
22	O	205	CLA	OBD-CAD	3.77	1.29	1.22
29	M	101	5X6	C25-C26	3.76	1.40	1.35
22	B	832	CLA	C4B-NB	-3.76	1.33	1.37
29	5	314	5X6	C15-C14	3.76	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	824	CLA	C4B-NB	-3.76	1.33	1.37
22	B	827	CLA	C1D-ND	3.76	1.42	1.37
22	B	816	CLA	CHC-C1C	3.76	1.46	1.38
22	5	308	CLA	CHC-C4B	3.76	1.47	1.39
22	3	304	CLA	C3B-C4B	3.76	1.51	1.42
25	2	301	BCR	C14-C13	3.76	1.40	1.35
29	J	104	5X6	C19-C18	3.76	1.55	1.43
22	1	304	CLA	CHD-C4C	3.76	1.47	1.39
29	1	311	5X6	C21-C22	3.76	1.40	1.35
22	3	301	CLA	C3D-C2D	3.76	1.49	1.39
29	6	316	5X6	C20-C21	3.76	1.55	1.43
25	B	843	BCR	C21-C22	3.76	1.40	1.35
29	5	313	5X6	C20-C21	3.76	1.55	1.43
22	B	834	CLA	CHB-C1B	3.76	1.47	1.39
29	Z	206	5X6	C24-C25	3.76	1.55	1.43
21	A	801	CL0	C3D-C2D	3.76	1.49	1.39
31	5	322	RRX	C17-C18	3.76	1.40	1.35
22	5	310	CLA	CHC-C4B	3.76	1.47	1.39
22	A	859	CLA	C1D-ND	3.75	1.42	1.37
29	3	306	5X6	C33-C32	3.75	1.57	1.52
22	B	802	CLA	CHC-C4B	3.75	1.47	1.39
22	B	827	CLA	CHB-C1B	3.75	1.47	1.39
31	1	315	RRX	C17-C18	3.75	1.40	1.35
22	A	827	CLA	C4B-NB	-3.75	1.33	1.37
22	J	102	CLA	OBD-CAD	3.75	1.28	1.22
22	B	809	CLA	CHC-C1C	3.75	1.46	1.38
22	A	809	CLA	C1B-NB	-3.75	1.33	1.37
22	1	309	CLA	CHC-C4B	3.75	1.47	1.39
22	1	310	CLA	CHD-C4C	3.75	1.47	1.39
22	B	803	CLA	O2D-CGD	3.75	1.42	1.33
29	6	315	5X6	C19-C18	3.75	1.55	1.43
29	6	317	5X6	C15-C14	3.75	1.55	1.43
22	O	205	CLA	C3D-C2D	3.75	1.49	1.39
22	Z	201	CLA	CHD-C1D	3.75	1.45	1.38
22	5	308	CLA	CHD-C1D	3.75	1.45	1.38
22	5	307	CLA	CHB-C1B	3.75	1.47	1.39
22	A	803	CLA	CHC-C1C	3.75	1.46	1.38
29	5	314	5X6	C20-C21	3.74	1.55	1.43
22	4	305	CLA	CHD-C4C	3.74	1.47	1.39
25	A	846	BCR	C10-C9	3.74	1.40	1.35
22	B	805	CLA	C1D-ND	3.74	1.42	1.37
22	6	305	CLA	CHD-C1D	3.74	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	314	CLA	OBD-CAD	3.74	1.28	1.22
22	B	850	CLA	C3D-C2D	3.74	1.49	1.39
29	7	317	5X6	C20-C21	3.74	1.55	1.43
22	A	827	CLA	C3D-C2D	3.74	1.49	1.39
22	A	833	CLA	CHD-C1D	3.74	1.45	1.38
22	7	311	CLA	C3B-C4B	3.74	1.51	1.42
22	5	301	CLA	CHD-C4C	3.74	1.47	1.39
22	A	813	CLA	C3D-C2D	3.74	1.49	1.39
29	1	312	5X6	C15-C14	3.73	1.55	1.43
22	4	309	CLA	C3B-C4B	3.73	1.51	1.42
29	M	101	5X6	C20-C21	3.73	1.55	1.43
22	3	301	CLA	OBD-CAD	3.73	1.28	1.22
22	L	203	CLA	C3D-C2D	3.73	1.49	1.39
22	3	303	CLA	CHB-C1B	3.73	1.47	1.39
22	A	816	CLA	CHB-C1B	3.73	1.47	1.39
29	6	315	5X6	C20-C21	3.73	1.55	1.43
22	1	302	CLA	C3D-C2D	3.73	1.49	1.39
22	B	831	CLA	CHD-C4C	3.73	1.47	1.39
25	A	844	BCR	C8-C9	-3.73	1.37	1.45
22	A	808	CLA	C1B-NB	-3.73	1.33	1.37
22	5	305	CLA	OBD-CAD	3.73	1.28	1.22
29	5	314	5X6	C33-C32	3.73	1.57	1.52
22	1	308	CLA	C3D-C2D	3.73	1.49	1.39
22	6	313	CLA	C3D-C2D	3.73	1.49	1.39
22	F	205	CLA	CHC-C4B	3.73	1.47	1.39
22	A	815	CLA	C3B-C4B	3.73	1.51	1.42
22	2	310	CLA	OBD-CAD	3.73	1.28	1.22
22	Z	201	CLA	CHC-C4B	3.73	1.47	1.39
22	B	821	CLA	CHD-C4C	3.72	1.47	1.39
29	4	314	5X6	C24-C25	3.72	1.55	1.43
22	6	306	CLA	C3D-C2D	3.72	1.49	1.39
22	B	828	CLA	C4B-NB	-3.72	1.33	1.37
29	O	207	5X6	C24-C25	3.72	1.55	1.43
22	A	857	CLA	CHC-C4B	3.72	1.47	1.39
29	5	312	5X6	C20-C21	3.72	1.55	1.43
25	L	202	BCR	C21-C22	3.72	1.40	1.35
22	A	858	CLA	O2A-CGA	3.72	1.44	1.33
22	B	818	CLA	C4B-NB	-3.72	1.33	1.37
22	5	307	CLA	CHC-C4B	3.72	1.47	1.39
22	7	304	CLA	C3D-C2D	3.72	1.49	1.39
22	7	309	CLA	OBD-CAD	3.72	1.28	1.22
22	5	309	CLA	CHD-C1D	3.72	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	309	CLA	CHB-C1B	3.72	1.47	1.39
22	6	307	CLA	OBD-CAD	3.72	1.28	1.22
22	K	101	CLA	CHC-C4B	3.72	1.47	1.39
22	6	303	CLA	C3D-C2D	3.72	1.49	1.39
22	O	206	CLA	C3D-C2D	3.72	1.49	1.39
22	B	827	CLA	C4B-NB	-3.72	1.33	1.37
22	A	813	CLA	CHD-C1D	3.71	1.45	1.38
22	5	311	CLA	OBD-CAD	3.71	1.28	1.22
22	6	310	CLA	OBD-CAD	3.71	1.28	1.22
22	O	204	CLA	C3B-C4B	3.71	1.51	1.42
29	B	851	5X6	C20-C21	3.71	1.54	1.43
22	6	310	CLA	CHD-C4C	3.71	1.47	1.39
22	A	804	CLA	C3D-C2D	3.71	1.49	1.39
22	2	306	CLA	C3B-C4B	3.71	1.51	1.42
22	1	305	CLA	OBD-CAD	3.71	1.28	1.22
22	A	838	CLA	C4B-NB	-3.71	1.33	1.37
22	2	309	CLA	C3B-C4B	3.71	1.51	1.42
22	7	305	CLA	C3D-C2D	3.71	1.49	1.39
29	1	311	5X6	C33-C32	3.71	1.57	1.52
22	2	304	CLA	C3B-C4B	3.71	1.51	1.42
22	5	305	CLA	C3B-C4B	3.71	1.51	1.42
22	5	304	CLA	CHC-C4B	3.71	1.47	1.39
22	A	811	CLA	CHC-C1C	3.71	1.46	1.38
22	B	838	CLA	CHC-C4B	3.71	1.47	1.39
22	A	808	CLA	C1D-ND	3.71	1.42	1.37
22	7	312	CLA	OBD-CAD	3.71	1.28	1.22
22	6	314	CLA	C3D-C2D	3.71	1.49	1.39
22	A	829	CLA	CHC-C4B	3.71	1.47	1.39
22	A	807	CLA	C1B-NB	-3.71	1.33	1.37
22	B	814	CLA	C3D-C2D	3.70	1.49	1.39
22	A	826	CLA	CHB-C1B	3.70	1.47	1.39
22	L	203	CLA	CHC-C4B	3.70	1.47	1.39
22	B	831	CLA	C3D-C2D	3.70	1.49	1.39
22	7	311	CLA	CHB-C1B	3.70	1.47	1.39
22	A	832	CLA	C3D-C2D	3.70	1.49	1.39
22	L	203	CLA	OBD-CAD	3.70	1.28	1.22
22	K	101	CLA	C3D-C2D	3.70	1.49	1.39
22	5	301	CLA	C3D-C2D	3.70	1.49	1.39
22	B	832	CLA	O2D-CGD	3.70	1.42	1.33
29	1	316	5X6	C33-C32	3.70	1.57	1.52
29	O	207	5X6	C19-C18	3.70	1.54	1.43
22	6	307	CLA	CHC-C4B	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	308	CLA	C3D-C2D	3.70	1.49	1.39
22	B	807	CLA	CHC-C4B	3.70	1.47	1.39
22	5	309	CLA	CHD-C4C	3.69	1.47	1.39
22	6	305	CLA	CHB-C1B	3.69	1.47	1.39
22	A	858	CLA	OBD-CAD	3.69	1.28	1.22
22	A	813	CLA	CHB-C1B	3.69	1.47	1.39
22	A	830	CLA	CHC-C4B	3.69	1.47	1.39
22	A	803	CLA	CHD-C1D	3.69	1.45	1.38
22	1	310	CLA	CHC-C4B	3.69	1.47	1.39
22	7	310	CLA	C3B-C4B	3.69	1.51	1.42
22	5	308	CLA	OBD-CAD	3.69	1.28	1.22
22	B	809	CLA	CHB-C1B	3.69	1.47	1.39
22	B	833	CLA	CHC-C4B	3.69	1.47	1.39
22	B	801	CLA	CHD-C1D	3.69	1.45	1.38
22	1	304	CLA	CHB-C1B	3.69	1.47	1.39
22	3	303	CLA	OBD-CAD	3.69	1.28	1.22
22	O	205	CLA	C3B-C4B	3.69	1.51	1.42
22	2	302	CLA	CHB-C1B	3.69	1.47	1.39
22	A	816	CLA	C1B-NB	-3.69	1.33	1.37
22	F	206	CLA	CHD-C1D	3.68	1.45	1.38
29	O	207	5X6	C15-C14	3.68	1.54	1.43
22	A	813	CLA	C1B-NB	-3.68	1.33	1.37
21	A	801	CL0	O2D-CGD	3.68	1.42	1.33
22	3	303	CLA	C3B-C4B	3.68	1.51	1.42
22	6	311	CLA	CHC-C4B	3.68	1.47	1.39
22	B	820	CLA	C3D-C2D	3.68	1.49	1.39
22	B	821	CLA	C3D-C2D	3.68	1.49	1.39
22	B	822	CLA	C1D-ND	3.68	1.42	1.37
22	B	802	CLA	O2D-CGD	3.68	1.42	1.33
22	5	307	CLA	C3D-C2D	3.68	1.49	1.39
22	A	837	CLA	C1B-NB	-3.68	1.33	1.37
22	B	834	CLA	C3D-C2D	3.68	1.49	1.39
22	1	307	CLA	C3D-C2D	3.68	1.49	1.39
22	3	302	CLA	C3D-C2D	3.68	1.49	1.39
22	4	308	CLA	C3D-C2D	3.68	1.49	1.39
22	6	304	CLA	C3D-C2D	3.68	1.49	1.39
22	5	304	CLA	C3D-C2D	3.68	1.49	1.39
22	B	824	CLA	CHB-C1B	3.68	1.47	1.39
22	F	205	CLA	C1B-NB	-3.68	1.33	1.37
22	6	313	CLA	C1B-NB	-3.68	1.33	1.37
25	1	301	BCR	C17-C18	3.68	1.40	1.35
22	2	302	CLA	C3B-C4B	3.67	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	809	CLA	C1B-NB	-3.67	1.33	1.37
22	A	830	CLA	C3D-C2D	3.67	1.49	1.39
22	5	302	CLA	OBD-CAD	3.67	1.28	1.22
22	2	305	CLA	CHB-C1B	3.67	1.47	1.39
22	F	205	CLA	C1D-ND	3.67	1.42	1.37
29	B	851	5X6	C19-C18	3.67	1.54	1.43
22	B	808	CLA	CHC-C1C	3.67	1.46	1.38
22	A	857	CLA	C3D-C2D	3.67	1.49	1.39
22	5	308	CLA	C1B-NB	-3.67	1.33	1.37
22	B	807	CLA	CHD-C1D	3.67	1.45	1.38
29	4	313	5X6	C33-C32	3.67	1.57	1.52
22	A	815	CLA	CHD-C1D	3.67	1.45	1.38
22	B	811	CLA	C3D-C2D	3.67	1.49	1.39
22	4	307	CLA	CHC-C4B	3.67	1.47	1.39
22	7	307	CLA	C3D-C2D	3.67	1.49	1.39
22	B	814	CLA	CHD-C1D	3.67	1.45	1.38
22	2	303	CLA	CHB-C1B	3.67	1.47	1.39
22	B	833	CLA	C3D-C2D	3.67	1.49	1.39
25	Z	202	BCR	C17-C18	3.67	1.40	1.35
22	4	305	CLA	CHC-C4B	3.66	1.47	1.39
22	6	305	CLA	CHC-C4B	3.66	1.47	1.39
22	7	310	CLA	CHB-C1B	3.66	1.47	1.39
22	A	857	CLA	CHB-C1B	3.66	1.47	1.39
29	2	314	5X6	C28-C29	3.66	1.58	1.45
22	4	303	CLA	CHD-C4C	3.66	1.47	1.39
22	B	802	CLA	C4B-NB	-3.66	1.33	1.37
29	6	317	5X6	C19-C18	3.66	1.54	1.43
22	A	817	CLA	CHB-C1B	3.66	1.47	1.39
22	A	836	CLA	CHC-C4B	3.66	1.47	1.39
22	O	206	CLA	OBD-CAD	3.66	1.28	1.22
22	L	203	CLA	CHB-C1B	3.66	1.47	1.39
22	2	311	CLA	C3D-C2D	3.66	1.49	1.39
22	B	804	CLA	C1B-NB	-3.66	1.33	1.37
22	5	305	CLA	CHB-C1B	3.66	1.47	1.39
22	6	303	CLA	CHB-C1B	3.66	1.47	1.39
22	A	827	CLA	CHD-C1D	3.66	1.45	1.38
22	A	825	CLA	C1B-NB	-3.66	1.33	1.37
22	O	206	CLA	CHB-C1B	3.66	1.47	1.39
22	5	301	CLA	OBD-CAD	3.66	1.28	1.22
22	7	306	CLA	OBD-CAD	3.65	1.28	1.22
22	Z	204	CLA	CHB-C1B	3.65	1.47	1.39
29	O	208	5X6	C33-C32	3.65	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	306	CLA	OBD-CAD	3.65	1.28	1.22
22	A	822	CLA	C1B-NB	-3.65	1.33	1.37
22	A	806	CLA	CHB-C1B	3.65	1.47	1.39
22	A	807	CLA	CHB-C1B	3.65	1.47	1.39
22	7	306	CLA	C3D-C2D	3.65	1.49	1.39
22	A	820	CLA	C1B-NB	-3.65	1.33	1.37
29	5	312	5X6	C25-C26	3.65	1.40	1.35
29	7	314	5X6	C33-C32	3.65	1.57	1.52
22	4	310	CLA	C4C-C3C	3.65	1.51	1.45
22	1	308	CLA	C3B-C4B	3.65	1.51	1.42
22	B	807	CLA	C3D-C2D	3.65	1.49	1.39
22	A	832	CLA	CHC-C1C	3.65	1.45	1.38
22	Z	204	CLA	CHC-C4B	3.64	1.47	1.39
29	1	311	5X6	C20-C21	3.64	1.54	1.43
22	1	309	CLA	CHB-C1B	3.64	1.47	1.39
22	5	309	CLA	C3D-C2D	3.64	1.49	1.39
22	1	307	CLA	OBD-CAD	3.64	1.28	1.22
22	B	828	CLA	C1B-NB	-3.64	1.33	1.37
22	B	807	CLA	CHD-C4C	3.64	1.47	1.39
22	6	311	CLA	OBD-CAD	3.64	1.28	1.22
22	6	314	CLA	C1B-NB	-3.64	1.33	1.37
29	7	316	5X6	C28-C29	3.64	1.58	1.45
22	B	803	CLA	CHD-C1D	3.64	1.45	1.38
22	1	304	CLA	C4B-NB	-3.64	1.33	1.37
22	A	805	CLA	C3D-C2D	3.64	1.49	1.39
22	A	835	CLA	C4B-NB	-3.64	1.33	1.37
22	A	820	CLA	C3D-C2D	3.64	1.49	1.39
22	5	310	CLA	C3D-C2D	3.64	1.49	1.39
22	A	836	CLA	CHD-C1D	3.64	1.45	1.38
22	K	101	CLA	CHB-C1B	3.64	1.47	1.39
22	B	812	CLA	C3D-C2D	3.63	1.49	1.39
22	A	834	CLA	C3D-C2D	3.63	1.49	1.39
22	O	203	CLA	CHD-C1D	3.63	1.45	1.38
22	J	102	CLA	CHC-C4B	3.63	1.47	1.39
22	6	311	CLA	CHB-C1B	3.63	1.47	1.39
22	K	102	CLA	CHB-C1B	3.63	1.47	1.39
22	6	310	CLA	C1B-NB	-3.63	1.33	1.37
22	4	309	CLA	C3D-C2D	3.63	1.49	1.39
22	4	312	CLA	C3D-C2D	3.63	1.49	1.39
22	7	312	CLA	CHB-C1B	3.63	1.47	1.39
22	6	309	CLA	C1B-NB	-3.63	1.33	1.37
22	5	302	CLA	CHD-C4C	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	308	CLA	CHD-C4C	3.63	1.47	1.39
22	A	831	CLA	CHC-C4B	3.63	1.47	1.39
22	4	305	CLA	C3D-C2D	3.63	1.49	1.39
22	A	810	CLA	CHC-C1C	3.63	1.45	1.38
22	B	813	CLA	C4B-NB	-3.63	1.33	1.37
22	A	810	CLA	CHD-C1D	3.63	1.45	1.38
29	6	316	5X6	C28-C29	3.63	1.58	1.45
22	A	803	CLA	C1D-ND	3.63	1.42	1.37
22	F	204	CLA	C1B-NB	-3.62	1.33	1.37
22	2	310	CLA	CHB-C1B	3.62	1.47	1.39
29	1	314	5X6	C33-C32	3.62	1.57	1.52
22	A	808	CLA	C3D-C2D	3.62	1.49	1.39
22	L	205	CLA	C3B-C4B	3.62	1.51	1.42
22	5	301	CLA	C1B-NB	-3.62	1.33	1.37
22	5	303	CLA	CHD-C4C	3.62	1.47	1.39
29	J	104	5X6	C20-C21	3.62	1.54	1.43
22	6	313	CLA	CHB-C1B	3.62	1.47	1.39
22	A	806	CLA	CHC-C1C	3.62	1.45	1.38
22	A	808	CLA	CHD-C4C	3.62	1.47	1.39
22	5	308	CLA	C3D-C2D	3.62	1.49	1.39
22	6	308	CLA	C3D-C2D	3.62	1.49	1.39
22	A	816	CLA	CHD-C1D	3.62	1.45	1.38
22	A	814	CLA	C3D-C2D	3.62	1.49	1.39
22	A	819	CLA	CHB-C1B	3.62	1.47	1.39
22	B	816	CLA	CHC-C4B	3.62	1.47	1.39
22	2	303	CLA	OBD-CAD	3.62	1.28	1.22
22	L	204	CLA	C4B-NB	-3.62	1.33	1.37
22	B	818	CLA	CHC-C1C	3.62	1.45	1.38
22	B	824	CLA	CHC-C1C	3.62	1.45	1.38
21	A	801	CL0	C4B-NB	-3.61	1.33	1.37
22	A	821	CLA	C3D-C2D	3.61	1.49	1.39
22	F	206	CLA	CHB-C1B	3.61	1.47	1.39
22	A	814	CLA	CHD-C4C	3.61	1.47	1.39
22	4	312	CLA	C3B-C4B	3.61	1.51	1.42
22	B	819	CLA	CHD-C4C	3.61	1.47	1.39
22	1	303	CLA	C3B-C4B	3.61	1.51	1.42
22	B	820	CLA	CHB-C1B	3.61	1.47	1.39
22	A	827	CLA	CHB-C1B	3.61	1.47	1.39
22	A	837	CLA	C1D-ND	3.61	1.42	1.37
22	4	303	CLA	C3D-C2D	3.61	1.49	1.39
29	O	207	5X6	C33-C32	3.61	1.57	1.52
22	B	822	CLA	C3D-C2D	3.61	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	311	CLA	OBD-CAD	3.61	1.28	1.22
22	1	303	CLA	C3D-C2D	3.61	1.49	1.39
22	L	204	CLA	CHC-C4B	3.61	1.47	1.39
22	A	817	CLA	C1B-NB	-3.61	1.33	1.37
25	F	201	BCR	C14-C13	3.61	1.40	1.35
22	5	302	CLA	C1B-NB	-3.61	1.33	1.37
22	A	819	CLA	CHC-C4B	3.61	1.47	1.39
25	A	846	BCR	C14-C13	3.61	1.40	1.35
22	B	808	CLA	CHB-C1B	3.61	1.47	1.39
29	1	312	5X6	C28-C29	3.61	1.57	1.45
22	A	812	CLA	CHB-C1B	3.61	1.47	1.39
29	4	314	5X6	C33-C32	3.61	1.57	1.52
22	A	823	CLA	CHD-C1D	3.60	1.45	1.38
22	K	102	CLA	CHC-C4B	3.60	1.47	1.39
29	Z	206	5X6	C33-C32	3.60	1.57	1.52
22	1	303	CLA	OBD-CAD	3.60	1.28	1.22
22	A	807	CLA	C4B-NB	-3.60	1.33	1.37
22	5	311	CLA	C4B-NB	-3.60	1.33	1.37
25	F	207	BCR	C14-C13	3.60	1.40	1.35
22	7	305	CLA	CHB-C1B	3.60	1.47	1.39
22	7	307	CLA	C3B-C4B	3.60	1.51	1.42
29	2	314	5X6	C33-C32	3.60	1.57	1.52
22	A	827	CLA	CHD-C4C	3.60	1.47	1.39
22	B	825	CLA	O2A-CGA	3.60	1.43	1.33
22	5	301	CLA	CHC-C4B	3.60	1.47	1.39
22	5	308	CLA	C3B-C4B	3.60	1.51	1.42
25	I	102	BCR	C21-C22	3.60	1.40	1.35
29	B	851	5X6	C33-C32	3.60	1.57	1.52
29	2	313	5X6	C28-C29	3.60	1.57	1.45
29	5	312	5X6	C33-C32	3.59	1.57	1.52
22	1	310	CLA	CHB-C1B	3.59	1.47	1.39
22	3	301	CLA	CHB-C1B	3.59	1.47	1.39
22	B	815	CLA	C3D-C2D	3.59	1.48	1.39
22	6	308	CLA	OBD-CAD	3.59	1.28	1.22
22	5	309	CLA	CHC-C4B	3.59	1.47	1.39
22	A	818	CLA	C1D-ND	3.59	1.42	1.37
29	7	314	5X6	C28-C29	3.59	1.57	1.45
22	1	304	CLA	CHC-C4B	3.59	1.47	1.39
29	4	314	5X6	C28-C29	3.59	1.57	1.45
22	1	304	CLA	OBD-CAD	3.59	1.28	1.22
22	A	835	CLA	CHC-C1C	3.59	1.45	1.38
25	4	316	BCR	C14-C13	3.59	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	305	CLA	OBD-CAD	3.59	1.28	1.22
22	6	308	CLA	CHC-C4B	3.59	1.47	1.39
22	2	304	CLA	C3D-C2D	3.59	1.48	1.39
22	F	205	CLA	C3D-C2D	3.59	1.48	1.39
22	A	813	CLA	CHD-C4C	3.58	1.47	1.39
22	A	830	CLA	C4B-NB	-3.58	1.33	1.37
22	F	206	CLA	OBD-CAD	3.58	1.28	1.22
22	7	307	CLA	CHB-C1B	3.58	1.47	1.39
22	B	812	CLA	C1B-NB	-3.58	1.33	1.37
22	B	802	CLA	CHD-C1D	3.58	1.45	1.38
22	K	102	CLA	C3D-C2D	3.58	1.48	1.39
29	7	316	5X6	C33-C32	3.58	1.57	1.52
22	A	826	CLA	C1D-ND	3.58	1.42	1.37
22	5	301	CLA	CHB-C1B	3.58	1.47	1.39
22	1	309	CLA	C3B-C4B	3.58	1.51	1.42
22	4	308	CLA	OBD-CAD	3.58	1.28	1.22
22	6	306	CLA	CHC-C4B	3.58	1.47	1.39
29	O	207	5X6	C20-C21	3.58	1.54	1.43
22	6	313	CLA	OBD-CAD	3.58	1.28	1.22
22	A	832	CLA	C4B-NB	-3.57	1.33	1.37
22	4	310	CLA	C3D-C2D	3.57	1.48	1.39
22	4	306	CLA	CHB-C1B	3.57	1.47	1.39
29	4	315	5X6	C28-C29	3.57	1.57	1.45
22	2	307	CLA	OBD-CAD	3.57	1.28	1.22
22	B	828	CLA	CHC-C1C	3.57	1.45	1.38
22	B	826	CLA	CHC-C4B	3.57	1.47	1.39
22	B	835	CLA	C3D-C2D	3.57	1.48	1.39
22	4	304	CLA	CHC-C4B	3.57	1.47	1.39
25	F	201	BCR	C21-C22	3.57	1.40	1.35
22	2	306	CLA	CHB-C1B	3.57	1.47	1.39
22	F	205	CLA	CHD-C1D	3.57	1.45	1.38
22	4	304	CLA	C3D-C2D	3.57	1.48	1.39
25	1	301	BCR	C14-C13	3.57	1.40	1.35
22	O	205	CLA	CHB-C1B	3.57	1.47	1.39
29	2	312	5X6	C28-C29	3.57	1.57	1.45
22	6	305	CLA	C3D-C2D	3.56	1.48	1.39
22	B	849	CLA	CHC-C1C	3.56	1.45	1.38
22	A	818	CLA	C4B-NB	-3.56	1.33	1.37
22	A	824	CLA	C1D-ND	3.56	1.42	1.37
29	3	306	5X6	C28-C29	3.56	1.57	1.45
22	4	303	CLA	CHD-C1D	3.56	1.45	1.38
22	B	825	CLA	O2D-CGD	3.56	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	305	CLA	C4B-NB	-3.56	1.33	1.37
22	A	806	CLA	CHD-C1D	3.56	1.45	1.38
22	A	815	CLA	CHD-C4C	3.56	1.47	1.39
25	A	862	BCR	C14-C13	3.56	1.40	1.35
29	4	315	5X6	C33-C32	3.56	1.57	1.52
22	A	814	CLA	CHC-C4B	3.56	1.47	1.39
22	A	857	CLA	C1B-NB	-3.56	1.33	1.37
22	A	822	CLA	CHC-C4B	3.56	1.47	1.39
22	6	304	CLA	CHB-C1B	3.56	1.47	1.39
22	4	305	CLA	OBD-CAD	3.56	1.28	1.22
25	A	843	BCR	C17-C18	3.55	1.40	1.35
22	L	204	CLA	OBD-CAD	3.55	1.28	1.22
22	A	803	CLA	CHB-C1B	3.55	1.47	1.39
22	A	857	CLA	CHD-C1D	3.55	1.45	1.38
22	A	830	CLA	C1B-NB	-3.55	1.33	1.37
22	A	839	CLA	CHC-C4B	3.55	1.47	1.39
22	3	304	CLA	OBD-CAD	3.55	1.28	1.22
22	6	314	CLA	C3B-C4B	3.55	1.51	1.42
22	6	307	CLA	C3D-C2D	3.55	1.48	1.39
22	B	829	CLA	O2D-CGD	3.55	1.41	1.33
22	A	826	CLA	CHC-C1C	3.55	1.45	1.38
25	A	845	BCR	C14-C13	3.55	1.40	1.35
22	B	815	CLA	CHD-C4C	3.55	1.47	1.39
22	A	829	CLA	C1B-NB	-3.55	1.33	1.37
22	4	309	CLA	OBD-CAD	3.55	1.28	1.22
22	L	204	CLA	C3D-C2D	3.55	1.48	1.39
22	7	305	CLA	C1B-NB	-3.55	1.33	1.37
22	6	310	CLA	CHB-C1B	3.55	1.47	1.39
22	B	804	CLA	CHD-C4C	3.54	1.47	1.39
22	5	304	CLA	OBD-CAD	3.54	1.28	1.22
22	7	303	CLA	C3D-C2D	3.54	1.48	1.39
22	1	302	CLA	C1B-NB	-3.54	1.33	1.37
22	A	823	CLA	C3D-C2D	3.54	1.48	1.39
22	2	309	CLA	OBD-CAD	3.54	1.28	1.22
22	2	308	CLA	C1B-NB	-3.54	1.33	1.37
22	B	828	CLA	CHD-C1D	3.54	1.45	1.38
22	B	813	CLA	CHC-C4B	3.54	1.47	1.39
29	B	851	5X6	C18-C17	3.54	1.40	1.35
22	A	817	CLA	C4B-NB	-3.54	1.33	1.37
22	1	305	CLA	CHB-C1B	3.53	1.47	1.39
22	6	303	CLA	C1B-NB	-3.53	1.33	1.37
22	4	310	CLA	CHC-C4B	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	815	CLA	C3D-C2D	3.53	1.48	1.39
22	B	850	CLA	C3B-C4B	3.53	1.51	1.42
29	5	321	5X6	C28-C29	3.53	1.57	1.45
22	B	819	CLA	CHC-C4B	3.53	1.47	1.39
22	B	822	CLA	CHC-C4B	3.53	1.47	1.39
22	A	829	CLA	CHD-C1D	3.53	1.45	1.38
22	3	304	CLA	CHB-C1B	3.53	1.47	1.39
22	Z	201	CLA	CHD-C4C	3.53	1.47	1.39
22	B	808	CLA	CHC-C4B	3.53	1.47	1.39
25	B	843	BCR	C17-C18	3.53	1.40	1.35
22	A	858	CLA	CHC-C4B	3.53	1.47	1.39
22	6	305	CLA	C1B-NB	-3.53	1.33	1.37
29	6	315	5X6	C28-C29	3.53	1.57	1.45
22	A	832	CLA	C1B-NB	-3.53	1.33	1.37
22	7	306	CLA	CHB-C1B	3.52	1.47	1.39
22	6	312	CLA	OBD-CAD	3.52	1.28	1.22
22	A	817	CLA	O2A-CGA	3.52	1.43	1.33
22	B	801	CLA	CHB-C1B	3.52	1.47	1.39
22	L	204	CLA	CHB-C1B	3.52	1.47	1.39
22	6	311	CLA	CHD-C1D	3.52	1.45	1.38
22	A	828	CLA	CHB-C1B	3.52	1.47	1.39
22	A	812	CLA	OBD-CAD	3.52	1.28	1.22
22	A	808	CLA	CHC-C4B	3.52	1.47	1.39
22	B	817	CLA	C3D-C2D	3.52	1.48	1.39
25	A	846	BCR	C23-C22	-3.52	1.38	1.45
22	A	814	CLA	CHD-C1D	3.52	1.45	1.38
22	A	836	CLA	CHB-C1B	3.52	1.47	1.39
22	B	830	CLA	CHD-C1D	3.52	1.45	1.38
22	1	305	CLA	C3B-C4B	3.52	1.51	1.42
22	2	308	CLA	CHB-C1B	3.51	1.47	1.39
22	4	304	CLA	CHB-C1B	3.51	1.47	1.39
22	1	304	CLA	C1B-NB	-3.51	1.33	1.37
22	O	203	CLA	C1B-NB	-3.51	1.33	1.37
22	B	820	CLA	CHC-C4B	3.51	1.47	1.39
22	B	837	CLA	CHD-C1D	3.51	1.45	1.38
22	5	310	CLA	OBD-CAD	3.51	1.28	1.22
22	4	311	CLA	C3D-C2D	3.51	1.48	1.39
22	A	837	CLA	CHD-C4C	3.51	1.47	1.39
22	L	203	CLA	C1B-NB	-3.51	1.33	1.37
22	B	816	CLA	C3D-C2D	3.51	1.48	1.39
22	B	812	CLA	CHB-C1B	3.51	1.47	1.39
22	A	837	CLA	CHD-C1D	3.51	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	813	CLA	O2A-CGA	3.51	1.43	1.33
22	A	830	CLA	CHD-C4C	3.51	1.47	1.39
22	7	308	CLA	OBD-CAD	3.50	1.28	1.22
22	B	837	CLA	C3D-C2D	3.50	1.48	1.39
29	O	208	5X6	C28-C29	3.50	1.57	1.45
22	B	812	CLA	CHC-C4B	3.50	1.47	1.39
22	A	811	CLA	C4B-NB	-3.50	1.33	1.37
22	A	857	CLA	O2D-CGD	3.50	1.41	1.33
22	4	312	CLA	CHB-C1B	3.50	1.47	1.39
22	A	818	CLA	CHD-C1D	3.50	1.45	1.38
22	B	805	CLA	C3D-C2D	3.50	1.48	1.39
22	Z	204	CLA	C3D-C2D	3.50	1.48	1.39
22	B	835	CLA	CHD-C1D	3.50	1.45	1.38
22	4	312	CLA	C1B-NB	-3.50	1.33	1.37
22	B	806	CLA	CHC-C4B	3.50	1.47	1.39
22	A	818	CLA	OBD-CAD	3.50	1.28	1.22
22	B	825	CLA	CHD-C1D	3.50	1.45	1.38
22	B	803	CLA	CHB-C1B	3.50	1.47	1.39
22	A	826	CLA	C1B-NB	-3.50	1.33	1.37
22	B	821	CLA	C3B-C4B	3.50	1.50	1.42
22	B	814	CLA	CHC-C4B	3.50	1.47	1.39
29	1	316	5X6	C28-C29	3.49	1.57	1.45
22	5	309	CLA	C3B-C4B	3.49	1.50	1.42
22	A	824	CLA	C1B-NB	-3.49	1.33	1.37
22	6	304	CLA	C1B-NB	-3.49	1.33	1.37
22	F	204	CLA	C3D-C2D	3.49	1.48	1.39
22	A	829	CLA	C4B-NB	-3.49	1.33	1.37
22	7	304	CLA	CHB-C1B	3.49	1.47	1.39
22	B	802	CLA	CHC-C1C	3.49	1.45	1.38
22	A	824	CLA	CHC-C4B	3.49	1.47	1.39
29	J	104	5X6	C28-C29	3.49	1.57	1.45
22	4	305	CLA	C1B-NB	-3.49	1.33	1.37
22	B	831	CLA	CHB-C1B	3.49	1.47	1.39
22	A	859	CLA	CHC-C1C	3.49	1.45	1.38
22	5	307	CLA	OBD-CAD	3.49	1.28	1.22
22	B	821	CLA	CHB-C1B	3.48	1.47	1.39
25	L	202	BCR	C17-C18	3.48	1.40	1.35
22	4	309	CLA	CHB-C1B	3.48	1.47	1.39
22	B	810	CLA	C1B-NB	-3.48	1.33	1.37
22	7	303	CLA	OBD-CAD	3.48	1.28	1.22
22	6	303	CLA	C3B-C4B	3.48	1.50	1.42
22	A	833	CLA	CHB-C1B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	810	CLA	C3D-C2D	3.48	1.48	1.39
22	1	310	CLA	OBD-CAD	3.48	1.28	1.22
22	A	802	CLA	C3D-C2D	3.48	1.48	1.39
22	A	806	CLA	C3D-C2D	3.48	1.48	1.39
22	7	304	CLA	C1B-NB	-3.48	1.33	1.37
22	6	314	CLA	CHB-C1B	3.48	1.47	1.39
22	B	823	CLA	OBD-CAD	3.48	1.28	1.22
22	1	302	CLA	CHC-C4B	3.48	1.47	1.39
29	7	315	5X6	C28-C29	3.48	1.57	1.45
22	L	205	CLA	OBD-CAD	3.48	1.28	1.22
25	4	316	BCR	C21-C22	3.48	1.40	1.35
22	A	829	CLA	C1D-ND	3.48	1.42	1.37
22	7	307	CLA	OBD-CAD	3.48	1.28	1.22
22	5	303	CLA	CHB-C1B	3.48	1.47	1.39
22	A	821	CLA	CHC-C4B	3.47	1.47	1.39
22	6	304	CLA	CHD-C4C	3.47	1.47	1.39
22	A	807	CLA	CHC-C1C	3.47	1.45	1.38
29	4	314	5X6	C05-C06	3.47	1.57	1.52
22	B	837	CLA	CHB-C1B	3.47	1.47	1.39
22	A	814	CLA	CHB-C1B	3.47	1.47	1.39
29	7	315	5X6	C33-C32	3.47	1.57	1.52
22	4	303	CLA	OBD-CAD	3.47	1.28	1.22
22	B	819	CLA	C3D-C2D	3.47	1.48	1.39
25	B	842	BCR	C8-C9	-3.47	1.38	1.45
22	6	307	CLA	CHB-C1B	3.47	1.47	1.39
29	B	851	5X6	C05-C06	3.47	1.57	1.52
22	B	804	CLA	C4B-NB	-3.47	1.33	1.37
22	B	836	CLA	C3D-C2D	3.47	1.48	1.39
22	B	831	CLA	C4B-NB	-3.47	1.33	1.37
22	B	819	CLA	C3B-C4B	3.47	1.50	1.42
22	Z	204	CLA	C4B-NB	-3.47	1.33	1.37
22	B	810	CLA	OBD-CAD	3.46	1.28	1.22
22	A	812	CLA	C1D-ND	3.46	1.42	1.37
22	B	849	CLA	CHC-C4B	3.46	1.47	1.39
22	1	302	CLA	OBD-CAD	3.46	1.28	1.22
22	B	809	CLA	CHD-C4C	3.46	1.47	1.39
22	5	309	CLA	CHB-C1B	3.46	1.47	1.39
22	B	822	CLA	CHD-C1D	3.46	1.45	1.38
22	A	805	CLA	CHD-C4C	3.46	1.47	1.39
22	5	309	CLA	C1B-NB	-3.46	1.33	1.37
22	3	305	CLA	CHB-C1B	3.46	1.47	1.39
22	A	810	CLA	C4B-NB	-3.46	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	835	CLA	CHB-C1B	3.46	1.47	1.39
22	A	830	CLA	CHB-C1B	3.45	1.47	1.39
22	A	820	CLA	CHD-C1D	3.45	1.45	1.38
22	B	815	CLA	C1B-NB	-3.45	1.33	1.37
22	B	837	CLA	CHD-C4C	3.45	1.47	1.39
22	5	310	CLA	CHB-C1B	3.45	1.47	1.39
22	B	836	CLA	C1D-ND	3.45	1.42	1.37
22	A	832	CLA	CHD-C4C	3.45	1.47	1.39
22	5	303	CLA	C3D-C2D	3.45	1.48	1.39
22	B	818	CLA	CHB-C1B	3.45	1.47	1.39
22	B	823	CLA	CHC-C4B	3.45	1.47	1.39
22	O	203	CLA	CHC-C4B	3.45	1.47	1.39
22	7	313	CLA	CHB-C1B	3.45	1.47	1.39
22	A	815	CLA	CHC-C4B	3.45	1.47	1.39
22	4	312	CLA	OBD-CAD	3.45	1.28	1.22
22	Z	204	CLA	CHD-C4C	3.45	1.47	1.39
22	A	838	CLA	CHC-C4B	3.45	1.47	1.39
22	A	833	CLA	OBD-CAD	3.45	1.28	1.22
22	A	832	CLA	CHB-C1B	3.45	1.47	1.39
22	A	833	CLA	C1D-ND	3.45	1.42	1.37
22	A	837	CLA	C3D-C2D	3.44	1.48	1.39
22	B	836	CLA	CHD-C4C	3.44	1.47	1.39
22	A	826	CLA	C3D-C2D	3.44	1.48	1.39
22	O	203	CLA	CHD-C4C	3.44	1.47	1.39
22	4	311	CLA	CHB-C1B	3.44	1.47	1.39
22	K	102	CLA	CHD-C4C	3.44	1.47	1.39
22	B	806	CLA	CHC-C1C	3.44	1.45	1.38
22	1	309	CLA	C1B-NB	-3.44	1.33	1.37
22	B	806	CLA	CHB-C1B	3.44	1.47	1.39
22	B	826	CLA	OBD-CAD	3.44	1.28	1.22
22	B	830	CLA	CHC-C4B	3.44	1.47	1.39
22	A	806	CLA	CHC-C4B	3.44	1.47	1.39
22	A	825	CLA	C3D-C2D	3.44	1.48	1.39
22	A	805	CLA	CHC-C4B	3.44	1.47	1.39
22	5	311	CLA	CHC-C4B	3.44	1.47	1.39
22	A	806	CLA	OBD-CAD	3.44	1.28	1.22
22	A	818	CLA	CHB-C1B	3.44	1.47	1.39
22	A	859	CLA	OBD-CAD	3.43	1.28	1.22
22	A	811	CLA	C3D-C2D	3.43	1.48	1.39
22	B	830	CLA	C1B-NB	-3.43	1.33	1.37
22	5	306	CLA	C1B-NB	-3.43	1.33	1.37
22	B	834	CLA	CHD-C1D	3.43	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	818	CLA	C1B-NB	-3.43	1.33	1.37
22	5	301	CLA	C3B-C4B	3.43	1.50	1.42
22	F	206	CLA	C3D-C2D	3.43	1.48	1.39
29	1	311	5X6	C28-C29	3.43	1.57	1.45
22	F	204	CLA	C4B-NB	-3.43	1.33	1.37
22	B	812	CLA	CHD-C4C	3.43	1.47	1.39
22	A	858	CLA	C3D-C2D	3.43	1.48	1.39
22	A	857	CLA	O2A-CGA	3.43	1.43	1.33
22	7	309	CLA	C1B-NB	-3.43	1.33	1.37
22	A	828	CLA	C1B-NB	-3.43	1.33	1.37
22	A	838	CLA	OBD-CAD	3.43	1.28	1.22
22	2	311	CLA	CHB-C1B	3.43	1.47	1.39
22	B	839	CLA	C4B-NB	-3.43	1.33	1.37
22	B	824	CLA	CHD-C1D	3.43	1.45	1.38
22	A	828	CLA	C4B-NB	-3.42	1.33	1.37
22	B	809	CLA	C3D-C2D	3.42	1.48	1.39
25	B	844	BCR	C14-C13	3.42	1.40	1.35
22	A	835	CLA	C1D-ND	3.42	1.42	1.37
22	2	307	CLA	CHB-C1B	3.42	1.47	1.39
22	3	303	CLA	C1B-NB	-3.42	1.33	1.37
22	B	805	CLA	CHC-C4B	3.42	1.47	1.39
22	B	813	CLA	C1D-ND	3.42	1.42	1.37
22	B	839	CLA	C3D-C2D	3.42	1.48	1.39
22	B	839	CLA	CHD-C1D	3.42	1.45	1.38
22	A	857	CLA	C1D-ND	3.42	1.42	1.37
22	A	822	CLA	CHB-C1B	3.42	1.47	1.39
22	A	803	CLA	C1C-NC	-3.42	1.32	1.37
22	4	310	CLA	C3B-C4B	3.42	1.50	1.42
22	B	829	CLA	CHC-C4B	3.41	1.47	1.39
22	4	306	CLA	C1B-NB	-3.41	1.33	1.37
22	A	848	CLA	CHD-C1D	3.41	1.45	1.38
22	2	305	CLA	C1B-NB	-3.41	1.33	1.37
29	5	314	5X6	C28-C29	3.41	1.57	1.45
22	B	826	CLA	C3D-C2D	3.41	1.48	1.39
22	5	302	CLA	CHD-C1D	3.41	1.45	1.38
22	B	827	CLA	C1B-NB	-3.41	1.33	1.37
22	A	810	CLA	C1B-NB	-3.41	1.33	1.37
22	B	834	CLA	CHD-C4C	3.41	1.47	1.39
29	5	321	5X6	C33-C32	3.41	1.57	1.52
22	6	312	CLA	CHC-C4B	3.41	1.47	1.39
22	B	849	CLA	CHD-C4C	3.41	1.47	1.39
22	B	839	CLA	CHD-C4C	3.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	313	5X6	C28-C29	3.41	1.57	1.45
22	A	831	CLA	C1D-ND	3.41	1.42	1.37
22	A	804	CLA	CHD-C1D	3.41	1.45	1.38
22	A	827	CLA	C1B-NB	-3.40	1.33	1.37
22	2	303	CLA	C1B-NB	-3.40	1.33	1.37
22	A	819	CLA	CHD-C1D	3.40	1.45	1.38
22	A	820	CLA	CHD-C4C	3.40	1.47	1.39
22	B	816	CLA	CHD-C1D	3.40	1.45	1.38
22	A	824	CLA	C3D-C2D	3.40	1.48	1.39
22	B	806	CLA	CHD-C4C	3.40	1.47	1.39
22	6	304	CLA	CHD-C1D	3.40	1.45	1.38
22	A	859	CLA	CHC-C4B	3.40	1.47	1.39
22	B	833	CLA	C1D-ND	3.40	1.42	1.37
22	B	837	CLA	C4B-NB	-3.40	1.33	1.37
22	2	307	CLA	C1B-NB	-3.40	1.33	1.37
22	A	848	CLA	O2A-CGA	3.40	1.43	1.33
22	B	836	CLA	CHB-C1B	3.40	1.47	1.39
22	B	812	CLA	OBD-CAD	3.39	1.28	1.22
22	B	825	CLA	CHB-C1B	3.39	1.47	1.39
22	B	829	CLA	C1B-NB	-3.39	1.33	1.37
22	A	818	CLA	CHC-C4B	3.39	1.47	1.39
22	B	812	CLA	C3B-C4B	3.39	1.50	1.42
22	B	836	CLA	CHC-C4B	3.39	1.47	1.39
22	7	313	CLA	C1B-NB	-3.39	1.33	1.37
22	A	807	CLA	C3D-C2D	3.39	1.48	1.39
29	7	317	5X6	C05-C06	3.39	1.57	1.52
22	B	832	CLA	C1D-ND	3.39	1.41	1.37
22	4	304	CLA	C4B-NB	-3.39	1.33	1.37
29	5	312	5X6	C28-C29	3.38	1.57	1.45
22	B	802	CLA	CHB-C1B	3.38	1.47	1.39
22	B	835	CLA	CHB-C1B	3.38	1.47	1.39
22	B	839	CLA	CHB-C1B	3.38	1.47	1.39
22	4	307	CLA	C4B-NB	-3.38	1.33	1.37
22	6	306	CLA	OBD-CAD	3.38	1.28	1.22
29	5	313	5X6	C28-C29	3.38	1.57	1.45
29	7	318	5X6	C28-C29	3.38	1.57	1.45
22	1	304	CLA	C3D-C2D	3.38	1.48	1.39
22	4	308	CLA	CHB-C1B	3.38	1.47	1.39
22	A	834	CLA	OBD-CAD	3.38	1.28	1.22
22	A	812	CLA	CHD-C4C	3.38	1.46	1.39
22	2	304	CLA	C1B-NB	-3.38	1.33	1.37
22	B	849	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	303	CLA	C1B-NB	-3.37	1.33	1.37
22	B	814	CLA	CHB-C1B	3.37	1.47	1.39
22	A	813	CLA	CHC-C4B	3.37	1.47	1.39
22	B	820	CLA	C3B-C4B	3.37	1.50	1.42
22	2	306	CLA	C1B-NB	-3.37	1.33	1.37
22	4	309	CLA	C1B-NB	-3.37	1.33	1.37
29	1	314	5X6	C28-C29	3.37	1.57	1.45
22	B	839	CLA	C1D-ND	3.37	1.41	1.37
22	A	802	CLA	CHD-C1D	3.37	1.44	1.38
29	1	313	5X6	C28-C29	3.37	1.57	1.45
22	A	817	CLA	CHD-C1D	3.37	1.44	1.38
22	6	309	CLA	OBD-CAD	3.36	1.28	1.22
22	5	311	CLA	CHB-C1B	3.36	1.47	1.39
22	B	806	CLA	CHD-C1D	3.36	1.44	1.38
22	A	829	CLA	CHB-C1B	3.36	1.46	1.39
22	B	817	CLA	CHC-C4B	3.36	1.46	1.39
29	O	207	5X6	C28-C29	3.36	1.57	1.45
22	A	818	CLA	C3D-C2D	3.36	1.48	1.39
22	A	804	CLA	CHC-C4B	3.36	1.46	1.39
22	A	858	CLA	CHB-C1B	3.36	1.46	1.39
22	B	814	CLA	CHD-C4C	3.36	1.46	1.39
22	6	311	CLA	C1B-NB	-3.36	1.33	1.37
22	B	820	CLA	OBD-CAD	3.36	1.28	1.22
22	B	835	CLA	C4B-NB	-3.36	1.33	1.37
22	A	819	CLA	C1D-ND	3.36	1.41	1.37
22	B	826	CLA	C1D-ND	3.36	1.41	1.37
25	L	201	BCR	C17-C18	3.36	1.40	1.35
22	J	102	CLA	C3B-C4B	3.35	1.50	1.42
22	B	850	CLA	C1B-NB	-3.35	1.33	1.37
22	K	101	CLA	OBD-CAD	3.35	1.28	1.22
22	B	804	CLA	CHD-C1D	3.35	1.44	1.38
22	A	821	CLA	C1D-ND	3.35	1.41	1.37
22	B	823	CLA	C3D-C2D	3.35	1.48	1.39
22	B	813	CLA	OBD-CAD	3.35	1.28	1.22
22	3	305	CLA	C1B-NB	-3.35	1.33	1.37
29	1	313	5X6	C33-C32	3.35	1.57	1.52
29	M	101	5X6	C33-C32	3.35	1.57	1.52
22	7	308	CLA	C1B-NB	-3.35	1.33	1.37
22	B	828	CLA	CHB-C1B	3.35	1.46	1.39
22	A	802	CLA	CHB-C1B	3.35	1.46	1.39
22	B	822	CLA	CHB-C1B	3.35	1.46	1.39
22	B	836	CLA	C1B-NB	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	206	CLA	CHD-C4C	3.35	1.46	1.39
22	1	310	CLA	C4B-NB	-3.34	1.33	1.37
22	B	816	CLA	CHB-C1B	3.34	1.46	1.39
25	B	844	BCR	C21-C22	3.34	1.40	1.35
22	A	831	CLA	CHD-C1D	3.34	1.44	1.38
22	A	810	CLA	CHC-C4B	3.34	1.46	1.39
22	L	205	CLA	C1B-NB	-3.34	1.33	1.37
22	B	801	CLA	OBD-CAD	3.34	1.28	1.22
22	5	311	CLA	C1B-NB	-3.34	1.33	1.37
22	A	814	CLA	OBD-CAD	3.34	1.28	1.22
22	B	826	CLA	C4B-NB	-3.34	1.33	1.37
22	A	821	CLA	C1C-NC	-3.34	1.32	1.37
22	1	302	CLA	C3B-C4B	3.34	1.50	1.42
22	A	848	CLA	CHB-C1B	3.34	1.46	1.39
22	6	312	CLA	CHB-C1B	3.33	1.46	1.39
22	3	304	CLA	C1B-NB	-3.33	1.33	1.37
22	B	828	CLA	C3D-C2D	3.33	1.48	1.39
22	3	302	CLA	OBD-CAD	3.33	1.28	1.22
22	A	838	CLA	C1C-NC	-3.33	1.32	1.37
22	B	838	CLA	CHB-C1B	3.33	1.46	1.39
22	A	825	CLA	CHD-C1D	3.33	1.44	1.38
25	L	201	BCR	C8-C9	-3.33	1.38	1.45
22	Z	201	CLA	C3D-C2D	3.33	1.48	1.39
25	A	862	BCR	C23-C22	-3.33	1.38	1.45
22	5	306	CLA	OBD-CAD	3.33	1.28	1.22
22	B	802	CLA	O2A-CGA	3.33	1.43	1.33
22	A	809	CLA	CHD-C1D	3.33	1.44	1.38
22	A	820	CLA	CHC-C4B	3.33	1.46	1.39
22	4	307	CLA	CHB-C1B	3.33	1.46	1.39
22	B	838	CLA	C1B-NB	-3.33	1.33	1.37
22	A	822	CLA	CHD-C4C	3.32	1.46	1.39
22	A	829	CLA	CHD-C4C	3.32	1.46	1.39
22	B	801	CLA	CHD-C4C	3.32	1.46	1.39
25	F	201	BCR	C17-C18	3.32	1.40	1.35
22	B	826	CLA	CHD-C1D	3.32	1.44	1.38
22	6	308	CLA	CHB-C1B	3.32	1.46	1.39
22	A	838	CLA	CHD-C1D	3.32	1.44	1.38
22	A	816	CLA	C1D-ND	3.32	1.41	1.37
22	B	838	CLA	CHC-C1C	3.32	1.45	1.38
22	5	303	CLA	OBD-CAD	3.32	1.28	1.22
22	1	302	CLA	CHB-C1B	3.32	1.46	1.39
22	A	859	CLA	C4B-NB	-3.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	802	CLA	C1D-ND	3.32	1.41	1.37
22	A	822	CLA	C4B-NB	-3.32	1.33	1.37
22	F	204	CLA	CHD-C1D	3.32	1.44	1.38
29	B	851	5X6	C28-C29	3.32	1.56	1.45
22	6	312	CLA	C3B-C4B	3.32	1.50	1.42
22	6	309	CLA	C3B-C4B	3.32	1.50	1.42
22	B	808	CLA	C1B-NB	-3.32	1.33	1.37
22	B	801	CLA	C3D-C2D	3.31	1.48	1.39
22	A	817	CLA	CHC-C4B	3.31	1.46	1.39
22	A	809	CLA	C1D-ND	3.31	1.41	1.37
22	1	305	CLA	C1B-NB	-3.31	1.33	1.37
25	Z	202	BCR	C21-C22	3.31	1.40	1.35
22	B	802	CLA	C3D-C2D	3.31	1.48	1.39
22	B	816	CLA	OBD-CAD	3.31	1.28	1.22
22	Z	204	CLA	O2A-CGA	3.31	1.43	1.33
22	A	824	CLA	CHD-C4C	3.31	1.46	1.39
22	6	310	CLA	C3B-C4B	3.31	1.50	1.42
22	A	826	CLA	CHD-C1D	3.31	1.44	1.38
22	B	805	CLA	C4B-NB	-3.31	1.33	1.37
22	7	310	CLA	C1B-NB	-3.31	1.33	1.37
22	B	815	CLA	C4B-NB	-3.30	1.33	1.37
22	2	311	CLA	C1B-NB	-3.30	1.33	1.37
22	Z	201	CLA	OBD-CAD	3.30	1.28	1.22
29	7	317	5X6	C28-C29	3.30	1.56	1.45
22	B	832	CLA	CHC-C4B	3.30	1.46	1.39
22	B	810	CLA	CHC-C4B	3.30	1.46	1.39
22	B	835	CLA	C1B-NB	-3.30	1.33	1.37
22	A	802	CLA	OBD-CAD	3.30	1.28	1.22
22	5	308	CLA	CHB-C1B	3.30	1.46	1.39
22	O	205	CLA	C1B-NB	-3.30	1.33	1.37
22	A	828	CLA	C3D-C2D	3.30	1.48	1.39
22	A	824	CLA	CHD-C1D	3.29	1.44	1.38
25	A	845	BCR	C21-C22	3.29	1.40	1.35
22	B	817	CLA	CHD-C1D	3.29	1.44	1.38
22	A	838	CLA	C3D-C2D	3.29	1.48	1.39
22	5	304	CLA	C1B-NB	-3.29	1.33	1.37
22	7	312	CLA	C1B-NB	-3.29	1.33	1.37
25	A	861	BCR	C21-C22	3.29	1.40	1.35
22	A	833	CLA	CHD-C4C	3.29	1.46	1.39
22	B	829	CLA	CHB-C1B	3.29	1.46	1.39
22	2	304	CLA	CHB-C1B	3.29	1.46	1.39
22	B	829	CLA	C1D-ND	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	807	CLA	CHD-C1D	3.29	1.44	1.38
22	5	303	CLA	CHC-C4B	3.29	1.46	1.39
22	4	311	CLA	C1B-NB	-3.29	1.33	1.37
22	7	306	CLA	C1B-NB	-3.29	1.33	1.37
22	B	827	CLA	CHC-C4B	3.29	1.46	1.39
22	2	309	CLA	C1B-NB	-3.29	1.33	1.37
29	7	315	5X6	C05-C06	3.29	1.57	1.52
25	A	844	BCR	C14-C13	3.29	1.40	1.35
22	B	807	CLA	OBD-CAD	3.29	1.28	1.22
22	A	815	CLA	OBD-CAD	3.28	1.28	1.22
22	6	308	CLA	C1B-NB	-3.28	1.33	1.37
22	A	812	CLA	CHD-C1D	3.28	1.44	1.38
22	7	309	CLA	CHB-C1B	3.28	1.46	1.39
22	B	816	CLA	C4B-NB	-3.28	1.33	1.37
22	6	308	CLA	C3B-C4B	3.28	1.50	1.42
22	2	302	CLA	C1B-NB	-3.28	1.33	1.37
22	B	833	CLA	CHB-C1B	3.28	1.46	1.39
22	B	835	CLA	CHD-C4C	3.28	1.46	1.39
29	7	318	5X6	C33-C32	3.28	1.57	1.52
22	B	833	CLA	CHD-C4C	3.28	1.46	1.39
22	O	203	CLA	C3D-C2D	3.28	1.48	1.39
22	B	829	CLA	C3D-C2D	3.28	1.48	1.39
22	B	824	CLA	CHD-C4C	3.27	1.46	1.39
22	B	813	CLA	C3D-C2D	3.27	1.48	1.39
22	B	804	CLA	CHC-C4B	3.27	1.46	1.39
22	L	205	CLA	CHB-C1B	3.27	1.46	1.39
29	6	317	5X6	C05-C06	3.27	1.57	1.52
22	A	833	CLA	CHC-C4B	3.27	1.46	1.39
22	5	310	CLA	C1B-NB	-3.27	1.33	1.37
22	2	310	CLA	C1B-NB	-3.27	1.33	1.37
22	4	310	CLA	CHB-C1B	3.27	1.46	1.39
22	B	813	CLA	CHD-C1D	3.27	1.44	1.38
22	A	834	CLA	CHB-C1B	3.26	1.46	1.39
22	4	302	CLA	C1B-NB	-3.26	1.33	1.37
22	B	807	CLA	CHB-C1B	3.26	1.46	1.39
22	B	836	CLA	CHD-C1D	3.26	1.44	1.38
22	A	857	CLA	C4B-NB	-3.26	1.33	1.37
22	A	837	CLA	CHC-C4B	3.26	1.46	1.39
22	1	303	CLA	CHB-C1B	3.26	1.46	1.39
22	B	810	CLA	CHB-C1B	3.26	1.46	1.39
22	B	830	CLA	CHD-C4C	3.26	1.46	1.39
22	B	815	CLA	CHC-C4B	3.26	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	804	CLA	C3D-C2D	3.26	1.48	1.39
22	7	307	CLA	C1B-NB	-3.26	1.33	1.37
22	A	838	CLA	CHB-C1B	3.26	1.46	1.39
22	A	803	CLA	C3D-C2D	3.26	1.48	1.39
22	B	838	CLA	OBD-CAD	3.26	1.28	1.22
22	5	305	CLA	C1B-NB	-3.26	1.33	1.37
22	A	817	CLA	CHD-C4C	3.26	1.46	1.39
22	A	811	CLA	CHC-C4B	3.26	1.46	1.39
25	I	102	BCR	C17-C18	3.26	1.40	1.35
22	7	311	CLA	C1B-NB	-3.26	1.33	1.37
22	B	827	CLA	CHD-C1D	3.26	1.44	1.38
22	F	205	CLA	CHD-C4C	3.25	1.46	1.39
22	A	824	CLA	CHB-C1B	3.25	1.46	1.39
22	A	809	CLA	C3D-C2D	3.25	1.48	1.39
22	B	831	CLA	CHC-C4B	3.25	1.46	1.39
22	A	812	CLA	CHC-C4B	3.25	1.46	1.39
29	5	313	5X6	C33-C32	3.25	1.57	1.52
22	A	829	CLA	C3D-C2D	3.25	1.48	1.39
22	B	807	CLA	C4B-NB	-3.25	1.33	1.37
22	B	811	CLA	CHB-C1B	3.25	1.46	1.39
22	4	303	CLA	CHB-C1B	3.25	1.46	1.39
22	A	858	CLA	CHD-C1D	3.25	1.44	1.38
25	A	845	BCR	C8-C9	-3.25	1.39	1.45
22	B	810	CLA	CHD-C1D	3.25	1.44	1.38
22	A	858	CLA	C1B-NB	-3.25	1.33	1.37
22	B	824	CLA	CHC-C4B	3.24	1.46	1.39
22	5	310	CLA	C4B-NB	-3.24	1.33	1.37
22	A	859	CLA	CHD-C1D	3.24	1.44	1.38
22	B	823	CLA	C3B-C4B	3.24	1.50	1.42
29	M	101	5X6	C28-C29	3.24	1.56	1.45
22	B	849	CLA	C3D-C2D	3.24	1.48	1.39
22	6	304	CLA	OBD-CAD	3.24	1.28	1.22
22	A	823	CLA	CHC-C4B	3.24	1.46	1.39
22	A	821	CLA	C3B-C4B	3.24	1.50	1.42
22	O	206	CLA	C1B-NB	-3.24	1.33	1.37
22	A	836	CLA	CHD-C4C	3.24	1.46	1.39
22	6	306	CLA	C1B-NB	-3.24	1.33	1.37
22	A	835	CLA	CHD-C4C	3.24	1.46	1.39
22	1	310	CLA	C3B-C4B	3.24	1.50	1.42
22	B	830	CLA	CHB-C1B	3.24	1.46	1.39
22	B	834	CLA	CHC-C4B	3.24	1.46	1.39
25	2	301	BCR	C17-C18	3.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	CLA	C3B-C4B	3.24	1.50	1.42
22	A	807	CLA	CHC-C4B	3.23	1.46	1.39
22	B	823	CLA	CHB-C1B	3.23	1.46	1.39
22	5	306	CLA	C4B-NB	-3.23	1.33	1.37
22	6	311	CLA	C4B-NB	-3.23	1.33	1.37
21	A	801	CL0	CHC-C1C	3.23	1.45	1.38
22	B	808	CLA	C1D-ND	3.23	1.41	1.37
22	3	302	CLA	C1B-NB	-3.23	1.33	1.37
22	5	303	CLA	C1B-NB	-3.23	1.33	1.37
22	B	818	CLA	C1B-NB	-3.23	1.33	1.37
22	F	204	CLA	CHC-C4B	3.23	1.46	1.39
22	A	809	CLA	C3B-C4B	3.22	1.50	1.42
22	B	832	CLA	CHB-C1B	3.22	1.46	1.39
22	A	816	CLA	OBD-CAD	3.22	1.28	1.22
22	B	832	CLA	CHD-C1D	3.22	1.44	1.38
22	B	804	CLA	OBD-CAD	3.22	1.28	1.22
22	A	859	CLA	CHD-C4C	3.22	1.46	1.39
22	B	808	CLA	CHD-C4C	3.22	1.46	1.39
22	J	102	CLA	CHB-C1B	3.22	1.46	1.39
22	B	811	CLA	OBD-CAD	3.21	1.28	1.22
22	K	102	CLA	OBD-CAD	3.21	1.28	1.22
22	4	307	CLA	C1B-NB	-3.21	1.33	1.37
22	A	826	CLA	CHC-C4B	3.20	1.46	1.39
22	A	805	CLA	C4B-NB	-3.20	1.33	1.37
29	6	317	5X6	C28-C29	3.20	1.56	1.45
29	2	313	5X6	C05-C06	3.20	1.56	1.52
22	A	858	CLA	CHD-C4C	3.20	1.46	1.39
22	A	837	CLA	CHB-C1B	3.20	1.46	1.39
22	A	806	CLA	C1B-NB	-3.20	1.33	1.37
22	3	301	CLA	C1B-NB	-3.20	1.33	1.37
22	Z	204	CLA	OBD-CAD	3.19	1.28	1.22
22	A	810	CLA	CHD-C4C	3.19	1.46	1.39
25	A	861	BCR	C14-C13	3.19	1.40	1.35
22	L	203	CLA	C3B-C4B	3.19	1.50	1.42
22	B	818	CLA	C3D-C2D	3.19	1.47	1.39
29	O	208	5X6	C05-C06	3.19	1.56	1.52
22	4	307	CLA	OBD-CAD	3.18	1.28	1.22
22	2	304	CLA	OBD-CAD	3.18	1.28	1.22
22	K	101	CLA	C4B-NB	-3.18	1.33	1.37
22	A	859	CLA	C3D-C2D	3.18	1.47	1.39
29	6	316	5X6	C11-C03	3.18	1.56	1.45
22	B	805	CLA	OBD-CAD	3.18	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	305	CLA	C3B-C4B	3.18	1.50	1.42
22	B	827	CLA	C3D-C2D	3.17	1.47	1.39
22	B	811	CLA	CHC-C4B	3.17	1.46	1.39
22	O	203	CLA	OBD-CAD	3.17	1.27	1.22
22	B	838	CLA	C3D-C2D	3.17	1.47	1.39
22	A	834	CLA	C3B-C4B	3.17	1.50	1.42
22	A	826	CLA	C1C-NC	-3.17	1.33	1.37
22	A	816	CLA	C3D-C2D	3.17	1.47	1.39
22	A	811	CLA	C1D-ND	3.17	1.41	1.37
22	7	305	CLA	C4B-NB	-3.16	1.33	1.37
22	1	307	CLA	C1B-NB	-3.16	1.33	1.37
22	6	311	CLA	C3B-C4B	3.16	1.50	1.42
22	B	821	CLA	OBD-CAD	3.16	1.27	1.22
22	6	313	CLA	C3B-C4B	3.16	1.50	1.42
22	A	808	CLA	CHB-C1B	3.16	1.46	1.39
22	1	310	CLA	C1B-NB	-3.16	1.33	1.37
22	A	828	CLA	CHD-C1D	3.16	1.44	1.38
22	B	837	CLA	C1B-NB	-3.16	1.33	1.37
22	2	303	CLA	C3B-C4B	3.16	1.50	1.42
22	1	309	CLA	C4C-C3C	3.16	1.50	1.45
22	A	835	CLA	CHD-C1D	3.16	1.44	1.38
22	O	204	CLA	C1B-NB	-3.16	1.33	1.37
22	A	808	CLA	OBD-CAD	3.15	1.27	1.22
22	B	832	CLA	CHD-C4C	3.15	1.46	1.39
22	A	811	CLA	CHD-C4C	3.15	1.46	1.39
22	B	826	CLA	CHD-C4C	3.15	1.46	1.39
25	A	844	BCR	C17-C18	3.15	1.40	1.35
22	A	816	CLA	CHD-C4C	3.15	1.46	1.39
22	3	302	CLA	C3B-C4B	3.15	1.50	1.42
22	A	821	CLA	CHD-C1D	3.15	1.44	1.38
22	K	102	CLA	C3B-C4B	3.15	1.50	1.42
22	B	829	CLA	CHD-C1D	3.15	1.44	1.38
22	A	835	CLA	C1C-NC	-3.15	1.33	1.37
22	A	815	CLA	CHB-C1B	3.15	1.46	1.39
22	B	810	CLA	C3B-C4B	3.14	1.50	1.42
22	O	206	CLA	C4B-NB	-3.14	1.33	1.37
22	B	815	CLA	CHB-C1B	3.14	1.46	1.39
22	B	803	CLA	C3D-C2D	3.14	1.47	1.39
22	Z	201	CLA	CHB-C1B	3.14	1.46	1.39
22	A	818	CLA	CHD-C4C	3.14	1.46	1.39
22	A	825	CLA	CHD-C4C	3.13	1.46	1.39
22	B	818	CLA	CHC-C4B	3.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	202	BCR	C8-C9	-3.13	1.39	1.45
22	6	307	CLA	C1B-NB	-3.13	1.33	1.37
22	7	308	CLA	CHB-C1B	3.13	1.46	1.39
22	A	858	CLA	C4B-NB	-3.13	1.33	1.37
22	B	803	CLA	C4B-NB	-3.13	1.33	1.37
22	B	837	CLA	C1D-ND	3.13	1.41	1.37
22	B	838	CLA	C3B-C4B	3.12	1.50	1.42
22	B	818	CLA	CHD-C4C	3.12	1.46	1.39
22	K	101	CLA	C3B-C4B	3.12	1.50	1.42
22	A	831	CLA	CHD-C4C	3.12	1.46	1.39
22	4	302	CLA	C3B-C4B	3.12	1.50	1.42
22	A	810	CLA	OBD-CAD	3.12	1.27	1.22
22	B	817	CLA	OBD-CAD	3.12	1.27	1.22
22	B	817	CLA	CHB-C1B	3.12	1.46	1.39
29	Z	206	5X6	C11-C03	3.12	1.56	1.45
22	A	831	CLA	CHB-C1B	3.12	1.46	1.39
22	B	804	CLA	CHB-C1B	3.12	1.46	1.39
22	B	803	CLA	CHD-C4C	3.12	1.46	1.39
22	A	808	CLA	C4B-NB	-3.11	1.34	1.37
22	F	204	CLA	OBD-CAD	3.11	1.27	1.22
22	A	831	CLA	C4B-NB	-3.11	1.34	1.37
22	A	812	CLA	C4B-NB	-3.11	1.34	1.37
22	B	815	CLA	OBD-CAD	3.11	1.27	1.22
25	L	201	BCR	C21-C22	3.11	1.39	1.35
22	B	834	CLA	C3B-C4B	3.11	1.50	1.42
25	F	201	BCR	C23-C22	-3.11	1.39	1.45
22	F	205	CLA	C3B-C4B	3.10	1.50	1.42
22	B	822	CLA	CHD-C4C	3.10	1.46	1.39
22	B	817	CLA	CHD-C4C	3.10	1.46	1.39
22	6	310	CLA	C4B-NB	-3.10	1.34	1.37
22	A	839	CLA	CHD-C1D	3.10	1.44	1.38
22	A	838	CLA	C1D-ND	3.10	1.41	1.37
25	B	843	BCR	C14-C13	3.09	1.39	1.35
22	A	848	CLA	C3D-C2D	3.09	1.47	1.39
22	B	801	CLA	CHC-C4B	3.09	1.46	1.39
22	B	816	CLA	C1B-NB	-3.09	1.34	1.37
22	B	808	CLA	C3B-C4B	3.09	1.50	1.42
22	A	820	CLA	OBD-CAD	3.09	1.27	1.22
22	B	833	CLA	C4B-NB	-3.09	1.34	1.37
25	A	845	BCR	C23-C22	-3.09	1.39	1.45
25	F	207	BCR	C8-C9	-3.09	1.39	1.45
22	A	828	CLA	OBD-CAD	3.09	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	310	CLA	C3B-C4B	3.09	1.50	1.42
25	4	316	BCR	C8-C9	-3.09	1.39	1.45
22	5	309	CLA	OBD-CAD	3.09	1.27	1.22
25	L	202	BCR	C23-C22	-3.08	1.39	1.45
22	A	830	CLA	OBD-CAD	3.08	1.27	1.22
29	6	317	5X6	C33-C32	3.08	1.56	1.52
22	B	810	CLA	C3D-C2D	3.08	1.47	1.39
29	5	312	5X6	C05-C06	3.08	1.56	1.52
22	B	838	CLA	C1D-ND	3.08	1.41	1.37
29	2	314	5X6	C11-C03	3.08	1.56	1.45
22	B	808	CLA	C3D-C2D	3.08	1.47	1.39
22	B	827	CLA	CHD-C4C	3.07	1.46	1.39
22	6	313	CLA	C4B-NB	-3.07	1.34	1.37
22	B	816	CLA	CHD-C4C	3.07	1.46	1.39
22	A	821	CLA	CHD-C4C	3.07	1.46	1.39
22	B	820	CLA	C1B-NB	-3.07	1.34	1.37
22	A	821	CLA	C1B-NB	-3.07	1.34	1.37
22	1	307	CLA	C3B-C4B	3.07	1.49	1.42
21	A	801	CL0	CHC-C4B	3.07	1.46	1.39
22	6	306	CLA	C4B-NB	-3.07	1.34	1.37
22	7	303	CLA	C3B-C4B	3.07	1.49	1.42
25	B	843	BCR	C23-C22	-3.07	1.39	1.45
29	5	314	5X6	C05-C06	3.07	1.56	1.52
22	A	803	CLA	CHD-C4C	3.06	1.46	1.39
22	7	305	CLA	OBD-CAD	3.06	1.27	1.22
22	B	837	CLA	CHC-C4B	3.06	1.46	1.39
22	6	305	CLA	OBD-CAD	3.06	1.27	1.22
22	O	206	CLA	C3B-C4B	3.06	1.49	1.42
22	B	849	CLA	OBD-CAD	3.06	1.27	1.22
29	1	312	5X6	C05-C06	3.06	1.56	1.52
29	6	315	5X6	C11-C03	3.05	1.55	1.45
29	7	314	5X6	C11-C03	3.05	1.55	1.45
22	A	825	CLA	OBD-CAD	3.05	1.27	1.22
22	B	806	CLA	OBD-CAD	3.04	1.27	1.22
22	B	825	CLA	C1D-ND	3.04	1.41	1.37
22	1	306	CLA	C4B-NB	-3.04	1.34	1.37
22	A	821	CLA	CHB-C1B	3.04	1.46	1.39
22	B	810	CLA	C4B-NB	-3.04	1.34	1.37
22	B	809	CLA	OBD-CAD	3.04	1.27	1.22
22	B	825	CLA	C3D-C2D	3.04	1.47	1.39
25	A	861	BCR	C17-C18	3.03	1.39	1.35
22	A	828	CLA	CHC-C4B	3.03	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	303	CLA	C4B-NB	-3.03	1.34	1.37
22	A	839	CLA	C3B-C4B	3.03	1.49	1.42
29	2	312	5X6	C05-C06	3.03	1.56	1.52
22	A	815	CLA	C1B-NB	-3.03	1.34	1.37
29	5	313	5X6	C11-C03	3.03	1.55	1.45
22	7	303	CLA	C1B-NB	-3.03	1.34	1.37
22	6	305	CLA	C4B-NB	-3.03	1.34	1.37
22	F	204	CLA	C3B-C4B	3.03	1.49	1.42
29	4	315	5X6	C11-C03	3.03	1.55	1.45
22	7	304	CLA	C1C-C2C	3.02	1.50	1.44
22	4	310	CLA	OBD-CAD	3.02	1.27	1.22
22	B	819	CLA	CHB-C1B	3.02	1.46	1.39
22	B	837	CLA	OBD-CAD	3.02	1.27	1.22
22	1	308	CLA	C1B-NB	-3.02	1.34	1.37
29	5	312	5X6	C11-C03	3.02	1.55	1.45
22	A	806	CLA	C1D-ND	3.02	1.41	1.37
22	5	304	CLA	C4B-NB	-3.02	1.34	1.37
22	B	839	CLA	OBD-CAD	3.02	1.27	1.22
22	2	305	CLA	C4B-NB	-3.02	1.34	1.37
29	O	207	5X6	C05-C06	3.01	1.56	1.52
22	7	305	CLA	C3B-C4B	3.01	1.49	1.42
29	4	314	5X6	C11-C03	3.01	1.55	1.45
22	7	303	CLA	C4B-NB	-3.01	1.34	1.37
22	B	823	CLA	CHD-C4C	3.01	1.46	1.39
22	B	814	CLA	OBD-CAD	3.01	1.27	1.22
29	1	311	5X6	C05-C06	3.01	1.56	1.52
22	1	306	CLA	C1B-NB	-3.01	1.34	1.37
29	7	316	5X6	C05-C06	3.01	1.56	1.52
22	A	813	CLA	OBD-CAD	3.00	1.27	1.22
22	A	831	CLA	OBD-CAD	3.00	1.27	1.22
22	A	806	CLA	CHD-C4C	3.00	1.46	1.39
22	A	837	CLA	C1C-NC	-3.00	1.33	1.37
22	A	819	CLA	CHD-C4C	3.00	1.46	1.39
22	B	810	CLA	CHD-C4C	3.00	1.46	1.39
25	B	844	BCR	C8-C9	-3.00	1.39	1.45
22	A	848	CLA	C1D-ND	3.00	1.41	1.37
22	F	206	CLA	C3B-C4B	2.99	1.49	1.42
22	K	101	CLA	C1B-NB	-2.99	1.34	1.37
22	5	307	CLA	C4B-NB	-2.99	1.34	1.37
22	B	825	CLA	CHD-C4C	2.99	1.46	1.39
25	B	843	BCR	C8-C9	-2.99	1.39	1.45
22	B	822	CLA	C1C-NC	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	316	5X6	C05-C06	2.99	1.56	1.52
29	7	318	5X6	C05-C06	2.98	1.56	1.52
22	B	823	CLA	C1B-NB	-2.98	1.34	1.37
22	A	839	CLA	CHD-C4C	2.98	1.46	1.39
22	A	858	CLA	C1D-ND	2.97	1.41	1.37
22	B	827	CLA	C1C-NC	-2.97	1.33	1.37
22	A	822	CLA	C3B-C4B	2.97	1.49	1.42
22	2	306	CLA	C4C-C3C	2.97	1.50	1.45
22	B	803	CLA	CHC-C4B	2.97	1.46	1.39
22	A	811	CLA	CHD-C1D	2.97	1.44	1.38
22	B	807	CLA	C3B-C4B	2.97	1.49	1.42
29	4	315	5X6	C05-C06	2.96	1.56	1.52
22	B	817	CLA	C3B-C4B	2.96	1.49	1.42
22	F	205	CLA	OBD-CAD	2.96	1.27	1.22
22	A	827	CLA	CHC-C4B	2.96	1.46	1.39
29	2	312	5X6	C11-C03	2.96	1.55	1.45
29	1	314	5X6	C11-C03	2.96	1.55	1.45
22	B	828	CLA	CHC-C4B	2.96	1.46	1.39
22	6	306	CLA	C3B-C4B	2.96	1.49	1.42
25	F	201	BCR	C8-C9	-2.96	1.39	1.45
22	5	302	CLA	C4B-NB	-2.96	1.34	1.37
22	4	307	CLA	C3B-C4B	2.95	1.49	1.42
22	Z	201	CLA	C3B-C4B	2.95	1.49	1.42
22	B	818	CLA	OBD-CAD	2.95	1.27	1.22
21	A	801	CL0	CHB-C1B	2.95	1.46	1.39
29	1	316	5X6	C11-C03	2.94	1.55	1.45
29	3	306	5X6	C05-C06	2.94	1.56	1.52
22	A	811	CLA	OBD-CAD	2.94	1.27	1.22
29	7	315	5X6	C11-C03	2.94	1.55	1.45
22	1	306	CLA	C3B-C4B	2.94	1.49	1.42
22	B	821	CLA	C4B-NB	-2.94	1.34	1.37
22	A	835	CLA	CHC-C4B	2.94	1.46	1.39
22	2	303	CLA	C4B-NB	-2.94	1.34	1.37
22	B	836	CLA	C4B-NB	-2.94	1.34	1.37
29	J	104	5X6	C05-C06	2.93	1.56	1.52
29	7	316	5X6	C11-C03	2.93	1.55	1.45
25	A	844	BCR	C23-C22	-2.93	1.39	1.45
22	1	307	CLA	C4B-NB	-2.93	1.34	1.37
22	B	819	CLA	OBD-CAD	2.93	1.27	1.22
29	5	321	5X6	C05-C06	2.93	1.56	1.52
22	A	814	CLA	C3B-C4B	2.92	1.49	1.42
22	B	835	CLA	OBD-CAD	2.92	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	206	5X6	C05-C06	2.92	1.56	1.52
22	A	848	CLA	MG-ND	-2.92	2.00	2.05
29	5	321	5X6	C11-C03	2.92	1.55	1.45
22	A	804	CLA	OBD-CAD	2.92	1.27	1.22
29	6	316	5X6	C05-C06	2.91	1.56	1.52
22	B	813	CLA	CHD-C4C	2.91	1.45	1.39
25	B	842	BCR	C14-C13	2.91	1.39	1.35
22	A	821	CLA	C4B-NB	-2.91	1.34	1.37
22	A	802	CLA	C3B-C4B	2.91	1.49	1.42
22	7	310	CLA	C4C-C3C	2.91	1.50	1.45
22	B	801	CLA	C1D-ND	2.91	1.41	1.37
22	B	808	CLA	CHD-C1D	2.91	1.44	1.38
22	A	837	CLA	C3B-C4B	2.91	1.49	1.42
29	3	306	5X6	C11-C03	2.90	1.55	1.45
22	B	808	CLA	C3D-C4D	-2.90	1.37	1.44
25	I	102	BCR	C23-C22	-2.90	1.39	1.45
29	7	318	5X6	C11-C03	2.90	1.55	1.45
29	5	313	5X6	C05-C06	2.90	1.56	1.52
22	A	823	CLA	CHD-C4C	2.90	1.45	1.39
22	6	304	CLA	C3B-C4B	2.90	1.49	1.42
25	A	846	BCR	C17-C18	2.90	1.39	1.35
22	B	806	CLA	C1B-C2B	2.89	1.50	1.43
29	O	208	5X6	C11-C03	2.89	1.55	1.45
22	B	802	CLA	C1C-C2C	2.89	1.50	1.44
22	6	309	CLA	CHB-C1B	2.89	1.45	1.39
22	7	303	CLA	C4C-C3C	2.89	1.50	1.45
29	4	313	5X6	C11-C03	2.89	1.55	1.45
29	O	207	5X6	C11-C03	2.89	1.55	1.45
22	5	305	CLA	C4C-C3C	2.89	1.50	1.45
22	4	302	CLA	C4B-NB	-2.89	1.34	1.37
22	B	828	CLA	C1D-ND	2.88	1.41	1.37
25	B	842	BCR	C17-C18	2.88	1.39	1.35
25	F	207	BCR	C23-C22	-2.87	1.39	1.45
22	A	802	CLA	CHD-C4C	2.87	1.45	1.39
22	A	809	CLA	CHB-C1B	2.87	1.45	1.39
22	B	825	CLA	OBD-CAD	2.87	1.27	1.22
25	4	316	BCR	C23-C22	-2.87	1.39	1.45
29	4	313	5X6	C05-C06	2.87	1.56	1.52
31	5	322	RRX	C23-C22	-2.87	1.39	1.45
22	6	306	CLA	C1B-C2B	2.87	1.50	1.43
22	7	307	CLA	C4C-C3C	2.87	1.50	1.45
22	4	310	CLA	C4B-NB	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	829	CLA	CHD-C4C	2.86	1.45	1.39
29	J	104	5X6	C11-C03	2.86	1.55	1.45
22	B	824	CLA	OBD-CAD	2.86	1.27	1.22
25	Z	205	BCR	C8-C9	-2.86	1.39	1.45
21	A	801	CL0	CHD-C1D	2.86	1.43	1.38
22	B	814	CLA	C4B-NB	-2.86	1.34	1.37
22	A	848	CLA	OBD-CAD	2.86	1.27	1.22
22	5	307	CLA	C3B-C4B	2.85	1.49	1.42
22	B	834	CLA	C4B-NB	-2.85	1.34	1.37
22	A	835	CLA	OBD-CAD	2.85	1.27	1.22
22	A	804	CLA	CHD-C4C	2.85	1.45	1.39
22	B	805	CLA	CHD-C4C	2.85	1.45	1.39
22	A	802	CLA	C1D-ND	2.85	1.41	1.37
22	B	810	CLA	C1D-ND	2.85	1.41	1.37
22	6	304	CLA	C1C-C2C	2.84	1.50	1.44
22	A	839	CLA	C4B-NB	-2.84	1.34	1.37
25	A	861	BCR	C12-C13	-2.84	1.39	1.45
25	A	845	BCR	C12-C13	-2.84	1.39	1.45
22	B	825	CLA	C3B-C4B	2.84	1.49	1.42
22	6	309	CLA	C4B-NB	-2.84	1.34	1.37
22	5	306	CLA	C1B-C2B	2.84	1.49	1.43
22	A	848	CLA	CHD-C4C	2.84	1.45	1.39
22	1	306	CLA	C1B-C2B	2.84	1.49	1.43
22	A	806	CLA	C1C-NC	-2.83	1.33	1.37
22	3	302	CLA	C4B-NB	-2.83	1.34	1.37
22	A	808	CLA	C3B-C4B	2.83	1.49	1.42
22	5	304	CLA	C3B-C4B	2.83	1.49	1.42
22	B	806	CLA	C4B-NB	-2.83	1.34	1.37
22	A	824	CLA	OBD-CAD	2.83	1.27	1.22
22	A	807	CLA	CHD-C4C	2.83	1.45	1.39
29	7	317	5X6	C11-C03	2.83	1.55	1.45
29	1	314	5X6	C05-C06	2.83	1.56	1.52
22	2	307	CLA	C1C-C2C	2.83	1.50	1.44
22	L	204	CLA	C3B-C4B	2.82	1.49	1.42
22	B	802	CLA	C1B-NB	-2.82	1.34	1.37
22	A	833	CLA	C3B-C4B	2.82	1.49	1.42
22	A	807	CLA	C3B-C4B	2.82	1.49	1.42
22	A	807	CLA	C1B-C2B	2.82	1.49	1.43
22	A	839	CLA	OBD-CAD	2.82	1.27	1.22
23	B	840	A1L64	C3-C2	-2.81	1.40	1.48
25	A	861	BCR	C8-C9	-2.81	1.39	1.45
29	2	313	5X6	C11-C03	2.81	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	204	CLA	C1C-C2C	2.81	1.50	1.44
22	B	831	CLA	OBD-CAD	2.81	1.27	1.22
22	B	809	CLA	CHC-C4B	2.81	1.45	1.39
22	4	305	CLA	C3B-C4B	2.80	1.49	1.42
22	B	813	CLA	C1B-C2B	2.80	1.49	1.43
22	L	205	CLA	C1C-C2C	2.80	1.50	1.44
25	A	862	BCR	C8-C9	-2.80	1.39	1.45
22	3	305	CLA	C1C-C2C	2.80	1.50	1.44
22	3	303	CLA	C4C-C3C	2.80	1.49	1.45
22	B	839	CLA	C3B-C4B	2.79	1.49	1.42
22	A	826	CLA	CHD-C4C	2.79	1.45	1.39
22	A	804	CLA	CHC-C1C	2.79	1.44	1.38
22	A	820	CLA	C1C-NC	-2.79	1.33	1.37
22	2	309	CLA	C4C-C3C	2.79	1.49	1.45
29	5	314	5X6	C11-C03	2.79	1.55	1.45
22	A	803	CLA	CHC-C4B	2.79	1.45	1.39
25	B	844	BCR	C23-C22	-2.79	1.40	1.45
22	A	810	CLA	C3B-C4B	2.79	1.49	1.42
22	A	838	CLA	CHD-C4C	2.79	1.45	1.39
22	3	301	CLA	C1C-C2C	2.79	1.50	1.44
29	1	311	5X6	C11-C03	2.79	1.55	1.45
29	1	312	5X6	C11-C03	2.78	1.55	1.45
22	1	307	CLA	C1B-C2B	2.78	1.49	1.43
22	B	810	CLA	C1C-NC	-2.78	1.33	1.37
22	A	811	CLA	C4C-C3C	2.78	1.49	1.45
22	4	308	CLA	C1C-C2C	2.78	1.49	1.44
22	A	828	CLA	C1D-ND	2.78	1.41	1.37
22	B	832	CLA	C3D-C2D	2.78	1.46	1.39
22	B	824	CLA	C3B-C4B	2.78	1.49	1.42
29	1	313	5X6	C11-C03	2.78	1.55	1.45
22	A	828	CLA	CHD-C4C	2.78	1.45	1.39
23	A	840	A1L64	C3-C2	-2.77	1.40	1.48
22	B	821	CLA	C1B-NB	-2.77	1.34	1.37
22	A	802	CLA	C3D-C4D	-2.77	1.37	1.44
21	A	801	CL0	CHD-C4C	2.76	1.45	1.39
25	5	315	BCR	C8-C9	-2.76	1.40	1.45
22	4	304	CLA	C3B-C4B	2.76	1.49	1.42
25	Z	202	BCR	C23-C22	-2.76	1.40	1.45
22	A	830	CLA	C3B-C4B	2.76	1.49	1.42
22	A	829	CLA	C3B-C4B	2.76	1.49	1.42
22	A	833	CLA	C4B-NB	-2.76	1.34	1.37
22	A	825	CLA	C1B-C2B	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	303	CLA	C1B-C2B	2.76	1.49	1.43
22	5	302	CLA	C3B-C4B	2.75	1.49	1.42
22	5	303	CLA	C3B-C4B	2.75	1.49	1.42
22	B	830	CLA	OBD-CAD	2.75	1.27	1.22
29	1	313	5X6	C05-C06	2.75	1.56	1.52
22	B	823	CLA	C1C-NC	-2.75	1.33	1.37
21	A	801	CL0	C1B-C2B	2.74	1.49	1.43
22	B	832	CLA	OBD-CAD	2.74	1.27	1.22
25	1	301	BCR	C23-C22	-2.74	1.40	1.45
25	L	201	BCR	C19-C18	-2.74	1.40	1.45
22	A	819	CLA	OBD-CAD	2.73	1.27	1.22
22	A	807	CLA	C1C-NC	-2.73	1.33	1.37
25	A	845	BCR	C19-C18	-2.73	1.40	1.45
22	A	832	CLA	C3B-C4B	2.73	1.49	1.42
22	7	308	CLA	C1C-C2C	2.73	1.49	1.44
22	A	836	CLA	OBD-CAD	2.73	1.27	1.22
22	B	806	CLA	C1C-NC	-2.73	1.33	1.37
22	6	305	CLA	C3B-C4B	2.72	1.49	1.42
25	A	843	BCR	C23-C22	-2.72	1.40	1.45
22	A	859	CLA	C1B-C2B	2.72	1.49	1.43
29	M	101	5X6	C05-C06	2.72	1.56	1.52
25	A	846	BCR	C12-C13	-2.72	1.40	1.45
22	A	830	CLA	C1B-C2B	2.72	1.49	1.43
22	B	828	CLA	C1C-NC	-2.72	1.33	1.37
22	A	825	CLA	C3D-C4D	-2.72	1.38	1.44
22	A	822	CLA	C1C-NC	-2.72	1.33	1.37
22	A	823	CLA	C1B-C2B	2.72	1.49	1.43
22	7	312	CLA	C1C-C2C	2.72	1.49	1.44
25	Z	202	BCR	C12-C13	-2.71	1.40	1.45
25	B	842	BCR	C23-C22	-2.71	1.40	1.45
22	2	308	CLA	C1C-C2C	2.71	1.49	1.44
22	2	311	CLA	C1C-C2C	2.71	1.49	1.44
25	A	843	BCR	C8-C9	-2.71	1.40	1.45
31	5	322	RRX	C8-C9	-2.71	1.40	1.45
22	Z	201	CLA	C4B-NB	-2.71	1.34	1.37
22	B	810	CLA	C1C-C2C	2.71	1.49	1.44
22	B	834	CLA	OBD-CAD	2.71	1.27	1.22
23	B	840	A1L64	C4-C5	-2.70	1.41	1.48
22	B	821	CLA	C1C-C2C	2.70	1.49	1.44
22	A	805	CLA	C1C-NC	-2.70	1.33	1.37
22	4	303	CLA	C1C-C2C	2.70	1.49	1.44
29	7	314	5X6	C05-C06	2.70	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C1D-ND	2.70	1.41	1.37
22	2	302	CLA	C4C-C3C	2.69	1.49	1.45
25	F	201	BCR	C19-C18	-2.69	1.40	1.45
22	7	306	CLA	C1C-C2C	2.69	1.49	1.44
22	2	305	CLA	C4C-C3C	2.69	1.49	1.45
22	5	303	CLA	C1B-C2B	2.69	1.49	1.43
22	A	848	CLA	C1B-C2B	2.69	1.49	1.43
31	1	315	RRX	C23-C22	-2.69	1.40	1.45
22	A	838	CLA	C3B-C4B	2.69	1.49	1.42
22	5	306	CLA	C3B-C4B	2.69	1.49	1.42
22	L	204	CLA	C1B-C2B	2.68	1.49	1.43
22	B	804	CLA	C3B-C4B	2.68	1.49	1.42
22	4	306	CLA	C4C-C3C	2.68	1.49	1.45
22	6	311	CLA	C1B-C2B	2.68	1.49	1.43
25	Z	202	BCR	C19-C18	-2.68	1.40	1.45
22	B	819	CLA	C4B-NB	-2.68	1.34	1.37
22	A	803	CLA	OBD-CAD	2.68	1.27	1.22
29	6	317	5X6	C11-C03	2.68	1.54	1.45
22	6	311	CLA	C1C-C2C	2.68	1.49	1.44
29	2	314	5X6	C05-C06	2.68	1.56	1.52
25	5	315	BCR	C23-C22	-2.68	1.40	1.45
22	2	302	CLA	C4D-CHA	2.68	1.47	1.38
22	A	857	CLA	CHD-C4C	2.68	1.45	1.39
22	B	815	CLA	C3B-C4B	2.68	1.49	1.42
22	6	307	CLA	C4B-NB	-2.67	1.34	1.37
22	B	837	CLA	C3B-C4B	2.67	1.49	1.42
25	2	301	BCR	C8-C9	-2.67	1.40	1.45
31	6	318	RRX	C8-C9	-2.67	1.40	1.45
22	5	304	CLA	C1B-C2B	2.67	1.49	1.43
22	A	839	CLA	C1C-NC	-2.67	1.33	1.37
25	B	843	BCR	C12-C13	-2.67	1.40	1.45
29	M	101	5X6	C11-C03	2.67	1.54	1.45
22	4	305	CLA	C1B-C2B	2.67	1.49	1.43
22	Z	204	CLA	C1B-C2B	2.67	1.49	1.43
22	A	836	CLA	C1B-C2B	2.67	1.49	1.43
22	K	101	CLA	C3B-C2B	2.67	1.50	1.41
22	B	803	CLA	OBD-CAD	2.67	1.27	1.22
22	B	814	CLA	C1C-C2C	2.66	1.49	1.44
22	A	805	CLA	OBD-CAD	2.66	1.27	1.22
22	B	808	CLA	C1C-NC	-2.66	1.33	1.37
29	6	315	5X6	C05-C06	2.66	1.56	1.52
22	5	302	CLA	C1C-C2C	2.66	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	851	5X6	C11-C03	2.66	1.54	1.45
22	A	822	CLA	OBD-CAD	2.66	1.27	1.22
22	A	824	CLA	C1C-NC	-2.66	1.33	1.37
22	6	314	CLA	C4B-NB	-2.66	1.34	1.37
22	4	302	CLA	C1B-C2B	2.66	1.49	1.43
22	B	831	CLA	C1C-NC	-2.65	1.33	1.37
22	A	819	CLA	C3D-C4D	-2.65	1.38	1.44
22	A	817	CLA	OBD-CAD	2.65	1.27	1.22
22	B	828	CLA	OBD-CAD	2.65	1.27	1.22
22	B	836	CLA	C1B-C2B	2.65	1.49	1.43
22	2	310	CLA	C4C-C3C	2.65	1.49	1.45
22	7	309	CLA	C1C-C2C	2.65	1.49	1.44
25	F	201	BCR	C12-C13	-2.65	1.40	1.45
22	A	832	CLA	C1C-NC	-2.64	1.33	1.37
22	A	813	CLA	C3B-C4B	2.64	1.48	1.42
22	A	825	CLA	C3B-C4B	2.64	1.48	1.42
22	O	204	CLA	C1C-C2C	2.64	1.49	1.44
22	B	819	CLA	C3D-C4D	-2.64	1.38	1.44
22	A	848	CLA	C3B-C4B	2.64	1.48	1.42
22	B	838	CLA	CHD-C4C	2.64	1.45	1.39
22	A	816	CLA	C3B-C4B	2.64	1.48	1.42
22	A	809	CLA	C4B-NB	-2.64	1.34	1.37
22	A	858	CLA	C3D-C4D	-2.64	1.38	1.44
25	A	845	BCR	C10-C9	2.63	1.39	1.35
25	L	201	BCR	C23-C22	-2.63	1.40	1.45
22	Z	201	CLA	C3D-C4D	-2.63	1.38	1.44
22	A	821	CLA	OBD-CAD	2.63	1.27	1.22
22	B	804	CLA	C4D-CHA	2.62	1.47	1.38
22	F	204	CLA	CHD-C4C	2.62	1.45	1.39
22	B	824	CLA	C4D-CHA	2.62	1.47	1.38
25	A	861	BCR	C19-C18	-2.62	1.40	1.45
22	7	311	CLA	C4C-C3C	2.62	1.49	1.45
22	A	831	CLA	C1C-C2C	2.62	1.49	1.44
22	A	824	CLA	C1B-C2B	2.62	1.49	1.43
22	5	308	CLA	C3A-C2A	-2.62	1.52	1.54
22	B	828	CLA	CHD-C4C	2.62	1.45	1.39
22	B	833	CLA	C1C-C2C	2.61	1.49	1.44
22	O	203	CLA	C3B-C4B	2.61	1.48	1.42
22	7	313	CLA	C1C-C2C	2.61	1.49	1.44
22	A	817	CLA	C3B-C4B	2.61	1.48	1.42
22	A	816	CLA	C3D-C4D	-2.61	1.38	1.44
22	1	304	CLA	C3D-C4D	-2.61	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	302	CLA	C3B-C2B	2.61	1.50	1.41
22	B	807	CLA	C3D-C4D	-2.61	1.38	1.44
22	A	837	CLA	OBD-CAD	2.61	1.27	1.22
22	7	308	CLA	C4C-C3C	2.60	1.49	1.45
22	B	815	CLA	C1C-NC	-2.60	1.33	1.37
25	I	102	BCR	C8-C9	-2.60	1.40	1.45
22	7	307	CLA	C4D-CHA	2.60	1.47	1.38
31	6	318	RRX	C23-C22	-2.60	1.40	1.45
22	5	303	CLA	C4D-CHA	2.60	1.47	1.38
22	A	825	CLA	C4B-NB	-2.60	1.34	1.37
31	4	317	RRX	C8-C9	-2.60	1.40	1.45
22	4	309	CLA	C4B-NB	-2.60	1.34	1.37
22	A	807	CLA	C4D-CHA	2.60	1.47	1.38
22	7	306	CLA	C4C-C3C	2.60	1.49	1.45
22	3	304	CLA	C1C-C2C	2.60	1.49	1.44
22	A	813	CLA	C1C-C2C	2.59	1.49	1.44
22	3	302	CLA	C1B-C2B	2.59	1.49	1.43
31	1	315	RRX	C8-C9	-2.59	1.40	1.45
22	7	311	CLA	C1C-C2C	2.59	1.49	1.44
22	O	206	CLA	C4D-CHA	2.59	1.47	1.38
22	B	833	CLA	C3B-C4B	2.59	1.48	1.42
22	6	309	CLA	C1C-C2C	2.59	1.49	1.44
22	7	310	CLA	C4D-CHA	2.59	1.47	1.38
22	J	102	CLA	C4C-C3C	2.59	1.49	1.45
22	2	305	CLA	C3B-C2B	2.59	1.50	1.41
22	A	804	CLA	C1C-NC	-2.59	1.33	1.37
22	L	204	CLA	C1C-NC	-2.59	1.33	1.37
25	I	102	BCR	C19-C18	-2.59	1.40	1.45
22	2	303	CLA	C1B-C2B	2.59	1.49	1.43
22	A	838	CLA	C3D-C4D	-2.59	1.38	1.44
22	F	204	CLA	C1C-NC	-2.59	1.33	1.37
22	A	858	CLA	C3B-C4B	2.59	1.48	1.42
22	2	309	CLA	C1C-C2C	2.59	1.49	1.44
22	B	830	CLA	C1C-NC	-2.59	1.33	1.37
22	B	816	CLA	C4D-CHA	2.58	1.47	1.38
22	6	313	CLA	C1C-C2C	2.58	1.49	1.44
25	B	841	BCR	C23-C22	-2.58	1.40	1.45
22	1	305	CLA	C4D-CHA	2.58	1.47	1.38
25	A	844	BCR	C12-C13	-2.58	1.40	1.45
22	6	304	CLA	C4B-NB	-2.58	1.34	1.37
22	7	305	CLA	C4D-CHA	2.58	1.47	1.38
22	F	206	CLA	C1C-C2C	2.58	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	816	CLA	C3B-C4B	2.58	1.48	1.42
22	F	204	CLA	C1D-ND	2.58	1.41	1.37
22	A	813	CLA	C1B-C2B	2.57	1.49	1.43
22	3	302	CLA	C1C-C2C	2.57	1.49	1.44
22	B	824	CLA	C1C-NC	-2.57	1.34	1.37
25	L	206	BCR	C8-C9	-2.57	1.40	1.45
25	L	202	BCR	C8-C9	-2.57	1.40	1.45
22	B	829	CLA	OBD-CAD	2.57	1.26	1.22
22	K	102	CLA	C4B-NB	-2.57	1.34	1.37
22	B	822	CLA	C3B-C4B	2.57	1.48	1.42
22	A	848	CLA	C3D-C4D	-2.57	1.38	1.44
22	1	308	CLA	C1B-C2B	2.57	1.49	1.43
22	2	306	CLA	C4D-CHA	2.57	1.47	1.38
22	7	313	CLA	C4D-CHA	2.57	1.47	1.38
22	A	833	CLA	C1C-C2C	2.57	1.49	1.44
22	B	830	CLA	C3B-C4B	2.57	1.48	1.42
22	2	309	CLA	C4D-CHA	2.57	1.47	1.38
25	A	861	BCR	C23-C22	-2.57	1.40	1.45
22	B	803	CLA	C1C-NC	-2.57	1.34	1.37
22	K	102	CLA	C1C-NC	-2.56	1.34	1.37
22	A	827	CLA	C3B-C4B	2.56	1.48	1.42
21	A	801	CL0	C1D-ND	2.56	1.40	1.37
22	6	314	CLA	C1C-C2C	2.56	1.49	1.44
22	B	836	CLA	C1C-NC	-2.56	1.34	1.37
22	4	306	CLA	C4D-CHA	2.56	1.47	1.38
22	6	307	CLA	C4D-CHA	2.56	1.47	1.38
22	B	834	CLA	C1B-C2B	2.56	1.49	1.43
22	B	850	CLA	C1B-C2B	2.56	1.49	1.43
22	B	813	CLA	C3D-C4D	-2.56	1.38	1.44
22	2	303	CLA	C3B-C2B	2.56	1.49	1.41
22	A	803	CLA	C1B-C2B	2.55	1.49	1.43
22	Z	204	CLA	C3B-C4B	2.55	1.48	1.42
22	1	304	CLA	C1B-C2B	2.55	1.49	1.43
22	B	817	CLA	C4B-NB	-2.55	1.34	1.37
22	4	311	CLA	C4B-NB	-2.55	1.34	1.37
25	A	843	BCR	C19-C18	-2.55	1.40	1.45
22	3	303	CLA	C4D-CHA	2.55	1.47	1.38
22	7	313	CLA	C4C-C3C	2.55	1.49	1.45
22	B	832	CLA	C3B-C4B	2.55	1.48	1.42
22	F	206	CLA	C3A-C2A	-2.55	1.52	1.54
22	A	817	CLA	C4C-C3C	2.55	1.49	1.45
22	B	818	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	CLA	C1B-C2B	2.55	1.49	1.43
22	A	834	CLA	C3D-C4D	-2.55	1.38	1.44
22	5	311	CLA	C4D-CHA	2.55	1.47	1.38
22	O	206	CLA	C1B-C2B	2.55	1.49	1.43
22	4	304	CLA	OBD-CAD	2.55	1.26	1.22
22	K	102	CLA	C4D-CHA	2.55	1.47	1.38
22	A	818	CLA	C3B-C4B	2.55	1.48	1.42
22	1	307	CLA	C1C-C2C	2.55	1.49	1.44
22	1	310	CLA	C1C-C2C	2.55	1.49	1.44
22	5	306	CLA	C4D-CHA	2.55	1.47	1.38
22	B	815	CLA	C3D-C4D	-2.55	1.38	1.44
22	O	206	CLA	C4C-C3C	2.55	1.49	1.45
22	7	310	CLA	C1C-C2C	2.54	1.49	1.44
22	B	821	CLA	C4D-CHA	2.54	1.47	1.38
22	B	813	CLA	C3B-C4B	2.54	1.48	1.42
22	2	305	CLA	C1B-C2B	2.54	1.49	1.43
22	6	308	CLA	C4B-NB	-2.54	1.34	1.37
25	1	301	BCR	C8-C9	-2.54	1.40	1.45
22	1	306	CLA	C3B-C2B	2.54	1.49	1.41
22	B	833	CLA	C3D-C4D	-2.54	1.38	1.44
22	L	204	CLA	C1C-C2C	2.54	1.49	1.44
22	3	304	CLA	C4C-C3C	2.54	1.49	1.45
22	A	821	CLA	C3D-C4D	-2.54	1.38	1.44
25	4	316	BCR	C19-C18	-2.54	1.40	1.45
25	B	844	BCR	C19-C18	-2.54	1.40	1.45
22	A	822	CLA	C3D-C4D	-2.54	1.38	1.44
22	B	802	CLA	C4C-C3C	2.54	1.49	1.45
22	7	308	CLA	C4B-NB	-2.54	1.34	1.37
22	O	205	CLA	C1C-C2C	2.54	1.49	1.44
22	7	305	CLA	C1C-C2C	2.53	1.49	1.44
22	1	309	CLA	C4D-CHA	2.53	1.47	1.38
22	A	818	CLA	C1B-C2B	2.53	1.49	1.43
22	B	823	CLA	C4B-NB	-2.53	1.34	1.37
22	L	205	CLA	C4B-NB	-2.53	1.34	1.37
22	6	313	CLA	C4D-CHA	2.53	1.47	1.38
22	4	307	CLA	C4D-CHA	2.53	1.47	1.38
22	A	803	CLA	C3D-C4D	-2.53	1.38	1.44
22	7	303	CLA	C4D-CHA	2.53	1.47	1.38
22	5	307	CLA	C1B-C2B	2.53	1.49	1.43
22	5	301	CLA	C4D-CHA	2.53	1.47	1.38
22	O	203	CLA	C4D-CHA	2.53	1.47	1.38
22	L	203	CLA	C4D-CHA	2.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	819	CLA	C4D-CHA	2.53	1.47	1.38
22	5	310	CLA	C3B-C2B	2.52	1.49	1.41
22	B	829	CLA	C3B-C4B	2.52	1.48	1.42
22	5	310	CLA	C1C-C2C	2.52	1.49	1.44
25	L	201	BCR	C12-C13	-2.52	1.40	1.45
22	A	829	CLA	C1C-NC	-2.52	1.34	1.37
22	2	311	CLA	C4D-CHA	2.52	1.47	1.38
22	5	305	CLA	C4D-CHA	2.52	1.47	1.38
22	B	829	CLA	C4D-CHA	2.52	1.47	1.38
25	Z	205	BCR	C23-C22	-2.52	1.40	1.45
22	K	101	CLA	C4C-C3C	2.52	1.49	1.45
22	B	825	CLA	C3D-C4D	-2.52	1.38	1.44
22	2	310	CLA	C1C-C2C	2.51	1.49	1.44
22	2	304	CLA	C1C-C2C	2.51	1.49	1.44
22	B	817	CLA	C1C-NC	-2.51	1.34	1.37
22	1	308	CLA	C4D-CHA	2.51	1.47	1.38
22	6	304	CLA	C1B-C2B	2.51	1.49	1.43
22	6	312	CLA	C4B-NB	-2.51	1.34	1.37
22	B	839	CLA	C4D-CHA	2.51	1.47	1.38
22	1	307	CLA	C4C-C3C	2.51	1.49	1.45
22	3	304	CLA	C4D-CHA	2.51	1.47	1.38
22	2	303	CLA	C1C-C2C	2.51	1.49	1.44
22	2	304	CLA	C4C-C3C	2.51	1.49	1.45
22	B	835	CLA	C1C-NC	-2.51	1.34	1.37
22	L	204	CLA	C4D-CHA	2.51	1.47	1.38
22	6	307	CLA	C4C-C3C	2.51	1.49	1.45
22	3	302	CLA	C3B-C2B	2.51	1.49	1.41
22	B	837	CLA	C3D-C4D	-2.51	1.38	1.44
22	B	812	CLA	C1C-C2C	2.51	1.49	1.44
22	7	311	CLA	C4D-CHA	2.51	1.47	1.38
22	A	811	CLA	C3D-C4D	-2.51	1.38	1.44
22	K	101	CLA	C1C-C2C	2.51	1.49	1.44
22	A	824	CLA	C4D-CHA	2.51	1.47	1.38
22	5	302	CLA	C3B-C2B	2.51	1.49	1.41
22	2	303	CLA	C4C-C3C	2.51	1.49	1.45
22	2	307	CLA	C4D-CHA	2.51	1.47	1.38
22	2	305	CLA	C1C-C2C	2.51	1.49	1.44
22	6	313	CLA	C1B-C2B	2.51	1.49	1.43
22	B	806	CLA	C4D-CHA	2.50	1.47	1.38
22	B	820	CLA	C4D-CHA	2.50	1.47	1.38
22	A	859	CLA	C3D-C4D	-2.50	1.38	1.44
22	A	839	CLA	C1C-C2C	2.50	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	802	CLA	CHD-C4C	2.50	1.44	1.39
22	2	310	CLA	C4D-CHA	2.50	1.47	1.38
22	3	302	CLA	C4D-CHA	2.50	1.47	1.38
22	B	812	CLA	C4D-CHA	2.50	1.47	1.38
21	A	801	CL0	C1C-NC	-2.50	1.34	1.37
22	B	830	CLA	C3D-C4D	-2.50	1.38	1.44
22	L	205	CLA	C4D-CHA	2.50	1.47	1.38
22	4	311	CLA	C1C-C2C	2.50	1.49	1.44
22	7	308	CLA	C4D-CHA	2.50	1.47	1.38
22	A	805	CLA	C1B-C2B	2.50	1.49	1.43
22	A	810	CLA	C1C-NC	-2.50	1.34	1.37
22	4	304	CLA	C4D-CHA	2.50	1.47	1.38
22	5	310	CLA	C4C-C3C	2.50	1.49	1.45
22	7	307	CLA	C1C-C2C	2.50	1.49	1.44
22	5	301	CLA	C3D-C4D	-2.50	1.38	1.44
22	B	850	CLA	C4D-CHA	2.50	1.47	1.38
22	A	804	CLA	C4D-CHA	2.50	1.47	1.38
22	B	815	CLA	C4D-CHA	2.49	1.47	1.38
22	A	814	CLA	C3D-C4D	-2.49	1.38	1.44
22	2	304	CLA	C4D-CHA	2.49	1.47	1.38
22	A	815	CLA	C1B-C2B	2.49	1.49	1.43
22	A	859	CLA	C4C-C3C	2.49	1.49	1.45
22	4	304	CLA	C4C-C3C	2.49	1.49	1.45
22	O	204	CLA	C4D-CHA	2.49	1.47	1.38
22	7	312	CLA	C4D-CHA	2.49	1.47	1.38
22	F	206	CLA	C4D-CHA	2.49	1.47	1.38
22	B	836	CLA	C3D-C4D	-2.49	1.38	1.44
25	B	841	BCR	C8-C9	-2.49	1.40	1.45
22	6	313	CLA	C3B-C2B	2.49	1.49	1.41
22	Z	201	CLA	C1C-C2C	2.49	1.49	1.44
22	B	819	CLA	C4D-CHA	2.49	1.47	1.38
22	1	304	CLA	C3B-C2B	2.49	1.49	1.41
22	Z	204	CLA	C4D-CHA	2.49	1.47	1.38
22	1	309	CLA	C4B-NB	-2.49	1.34	1.37
22	A	811	CLA	C1B-C2B	2.49	1.49	1.43
22	6	308	CLA	C4D-CHA	2.49	1.47	1.38
22	6	305	CLA	C1C-C2C	2.48	1.49	1.44
22	5	304	CLA	C3B-C2B	2.48	1.49	1.41
25	L	206	BCR	C23-C22	-2.48	1.40	1.45
22	A	823	CLA	C1C-NC	-2.48	1.34	1.37
22	3	302	CLA	C4C-C3C	2.48	1.49	1.45
22	1	304	CLA	C4C-C3C	2.48	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	305	CLA	C3D-C4D	-2.48	1.38	1.44
22	1	309	CLA	C1C-C2C	2.48	1.49	1.44
22	A	834	CLA	C4D-CHA	2.48	1.47	1.38
22	1	307	CLA	C4D-CHA	2.48	1.47	1.38
22	1	306	CLA	C4D-CHA	2.48	1.47	1.38
22	A	857	CLA	C1B-C2B	2.48	1.49	1.43
22	B	804	CLA	C1B-C2B	2.48	1.49	1.43
25	2	301	BCR	C12-C13	-2.47	1.40	1.45
22	5	303	CLA	C3D-C4D	-2.47	1.38	1.44
22	7	305	CLA	C3B-C2B	2.47	1.49	1.41
22	B	810	CLA	C3D-C4D	-2.47	1.38	1.44
22	3	303	CLA	C1C-C2C	2.47	1.49	1.44
22	5	301	CLA	C1C-C2C	2.47	1.49	1.44
22	B	826	CLA	C1C-NC	-2.47	1.34	1.37
22	2	307	CLA	C4C-C3C	2.47	1.49	1.45
22	6	311	CLA	C3B-C2B	2.47	1.49	1.41
22	B	809	CLA	C1C-NC	-2.47	1.34	1.37
22	B	849	CLA	C1C-NC	-2.47	1.34	1.37
22	4	310	CLA	C4D-CHA	2.47	1.47	1.38
22	2	303	CLA	C4D-CHA	2.47	1.47	1.38
22	A	803	CLA	C3B-C4B	2.47	1.48	1.42
22	4	309	CLA	C4D-CHA	2.46	1.47	1.38
22	5	311	CLA	C3B-C4B	2.46	1.48	1.42
22	2	302	CLA	C1C-C2C	2.46	1.49	1.44
22	6	303	CLA	C4D-CHA	2.46	1.47	1.38
22	A	829	CLA	OBD-CAD	2.46	1.26	1.22
22	A	834	CLA	C1C-C2C	2.46	1.49	1.44
22	B	814	CLA	C4C-C3C	2.46	1.49	1.45
22	A	829	CLA	C4D-CHA	2.46	1.47	1.38
22	4	306	CLA	C1C-C2C	2.46	1.49	1.44
22	B	830	CLA	C4D-CHA	2.46	1.47	1.38
22	B	802	CLA	C3B-C4B	2.46	1.48	1.42
22	B	828	CLA	C4D-CHA	2.46	1.47	1.38
22	7	309	CLA	C4D-CHA	2.46	1.47	1.38
22	A	858	CLA	C1B-C2B	2.46	1.49	1.43
22	5	305	CLA	C1C-C2C	2.46	1.49	1.44
22	7	303	CLA	C3B-C2B	2.46	1.49	1.41
22	A	810	CLA	C4C-C3C	2.46	1.49	1.45
22	1	303	CLA	C4D-CHA	2.46	1.47	1.38
22	7	308	CLA	C3D-C4D	-2.46	1.38	1.44
22	O	205	CLA	C4B-NB	-2.46	1.34	1.37
22	A	832	CLA	OBD-CAD	2.46	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	802	CLA	C4D-CHA	2.46	1.47	1.38
22	6	305	CLA	C4C-C3C	2.46	1.49	1.45
22	B	814	CLA	C3B-C2B	2.46	1.49	1.41
22	1	303	CLA	C4B-NB	-2.45	1.34	1.37
22	5	303	CLA	C4C-C3C	2.45	1.49	1.45
22	F	204	CLA	C3D-C4D	-2.45	1.38	1.44
22	B	814	CLA	C4D-CHA	2.45	1.47	1.38
22	6	314	CLA	C4D-CHA	2.45	1.47	1.38
22	A	837	CLA	C4B-NB	-2.45	1.34	1.37
22	J	102	CLA	C4B-NB	-2.45	1.34	1.37
22	A	810	CLA	C1B-C2B	2.45	1.49	1.43
22	O	203	CLA	C1B-C2B	2.45	1.49	1.43
22	5	301	CLA	C4B-NB	-2.45	1.34	1.37
22	5	308	CLA	C1C-C2C	2.45	1.49	1.44
22	1	307	CLA	C3B-C2B	2.44	1.49	1.41
22	6	310	CLA	C1B-C2B	2.44	1.49	1.43
22	4	312	CLA	C1C-C2C	2.44	1.49	1.44
22	B	849	CLA	C1B-C2B	2.44	1.49	1.43
22	4	309	CLA	C1C-C2C	2.44	1.49	1.44
22	5	306	CLA	C3D-C4D	-2.44	1.38	1.44
22	7	305	CLA	C4C-C3C	2.44	1.49	1.45
21	A	801	CL0	C3D-C4D	-2.44	1.38	1.44
22	1	304	CLA	C4D-CHA	2.44	1.47	1.38
22	A	819	CLA	C3B-C4B	2.44	1.48	1.42
22	O	204	CLA	C4C-C3C	2.44	1.49	1.45
22	3	301	CLA	C4D-CHA	2.44	1.47	1.38
22	4	302	CLA	C4D-CHA	2.44	1.47	1.38
22	2	311	CLA	C4C-C3C	2.44	1.49	1.45
22	A	823	CLA	C3B-C4B	2.44	1.48	1.42
22	A	837	CLA	C4D-CHA	2.44	1.47	1.38
22	B	803	CLA	C4D-CHA	2.44	1.47	1.38
22	B	838	CLA	C4C-C3C	2.44	1.49	1.45
22	7	310	CLA	C1B-C2B	2.44	1.49	1.43
22	K	101	CLA	C3D-C4D	-2.44	1.38	1.44
22	5	311	CLA	C3B-C2B	2.44	1.49	1.41
22	B	850	CLA	C1C-C2C	2.44	1.49	1.44
22	2	306	CLA	C1C-C2C	2.44	1.49	1.44
22	6	309	CLA	C4D-CHA	2.44	1.47	1.38
22	B	831	CLA	C4D-CHA	2.43	1.47	1.38
22	B	826	CLA	C3D-C4D	-2.43	1.38	1.44
22	5	311	CLA	C1B-C2B	2.43	1.49	1.43
22	7	305	CLA	C1B-C2B	2.43	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	840	A1L64	C4-C5	-2.43	1.41	1.48
22	A	830	CLA	C3D-C4D	-2.43	1.38	1.44
22	4	312	CLA	C4D-CHA	2.43	1.47	1.38
22	L	203	CLA	C4B-NB	-2.43	1.34	1.37
22	6	311	CLA	C4C-C3C	2.43	1.49	1.45
22	5	310	CLA	C4D-CHA	2.43	1.47	1.38
22	1	308	CLA	C1C-C2C	2.43	1.49	1.44
25	I	102	BCR	C12-C13	-2.43	1.40	1.45
22	B	805	CLA	C3B-C4B	2.43	1.48	1.42
22	5	304	CLA	C4D-CHA	2.43	1.47	1.38
22	4	303	CLA	C3D-C4D	-2.43	1.38	1.44
22	B	811	CLA	C4D-CHA	2.42	1.47	1.38
22	A	805	CLA	C3D-C4D	-2.42	1.38	1.44
22	A	807	CLA	OBD-CAD	2.42	1.26	1.22
22	B	816	CLA	C3B-C2B	2.42	1.49	1.41
22	A	810	CLA	C3B-C2B	2.42	1.49	1.41
22	A	804	CLA	C3D-C4D	-2.42	1.38	1.44
22	B	812	CLA	C4B-NB	-2.42	1.34	1.37
22	K	101	CLA	C4D-CHA	2.42	1.47	1.38
25	B	843	BCR	C19-C18	-2.42	1.40	1.45
22	A	858	CLA	C3B-C2B	2.42	1.49	1.41
22	B	837	CLA	C4C-C3C	2.42	1.49	1.45
22	A	857	CLA	C3B-C4B	2.42	1.48	1.42
22	A	831	CLA	C3D-C4D	-2.42	1.38	1.44
22	A	808	CLA	C1C-NC	-2.42	1.34	1.37
22	B	805	CLA	C4D-CHA	2.42	1.47	1.38
22	4	305	CLA	C4D-CHA	2.42	1.47	1.38
22	K	102	CLA	C1B-C2B	2.42	1.48	1.43
22	6	310	CLA	C3D-C4D	-2.42	1.38	1.44
22	A	822	CLA	C4D-CHA	2.42	1.47	1.38
22	1	305	CLA	C1C-C2C	2.42	1.49	1.44
22	A	806	CLA	C3D-C4D	-2.42	1.38	1.44
22	O	206	CLA	C3B-C2B	2.41	1.49	1.41
22	7	307	CLA	C1B-C2B	2.41	1.48	1.43
22	6	310	CLA	C3B-C2B	2.41	1.49	1.41
22	5	308	CLA	C4B-NB	-2.41	1.34	1.37
22	A	858	CLA	C1C-C2C	2.41	1.49	1.44
22	J	102	CLA	C4D-CHA	2.41	1.47	1.38
22	5	303	CLA	C1C-C2C	2.41	1.49	1.44
22	1	308	CLA	C4C-C3C	2.41	1.49	1.45
25	K	103	BCR	C8-C9	-2.41	1.40	1.45
22	B	836	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	304	CLA	C3B-C2B	2.41	1.49	1.41
22	5	308	CLA	C4D-CHA	2.41	1.47	1.38
22	2	308	CLA	C4D-CHA	2.41	1.47	1.38
29	1	312	5X6	C01-C02	2.41	1.54	1.50
22	4	311	CLA	C4D-CHA	2.41	1.47	1.38
22	1	310	CLA	C3B-C2B	2.41	1.49	1.41
22	B	827	CLA	OBD-CAD	2.41	1.26	1.22
22	2	304	CLA	C4B-NB	-2.41	1.34	1.37
22	B	831	CLA	C1B-C2B	2.40	1.48	1.43
22	B	825	CLA	C1B-C2B	2.40	1.48	1.43
22	1	303	CLA	C1C-C2C	2.40	1.49	1.44
22	1	305	CLA	C4C-C3C	2.40	1.49	1.45
22	1	304	CLA	C3B-C4B	2.40	1.48	1.42
22	5	306	CLA	C3B-C2B	2.40	1.49	1.41
22	6	306	CLA	C3B-C2B	2.40	1.49	1.41
22	1	302	CLA	C4C-C3C	2.40	1.49	1.45
22	A	825	CLA	C1C-C2C	2.40	1.49	1.44
22	B	839	CLA	C1B-C2B	2.40	1.48	1.43
25	A	862	BCR	C16-C17	-2.40	1.36	1.43
22	B	837	CLA	C1C-NC	-2.40	1.34	1.37
22	O	203	CLA	C3B-C2B	2.40	1.49	1.41
22	A	833	CLA	C3D-C4D	-2.40	1.38	1.44
22	B	817	CLA	C1C-C2C	2.40	1.49	1.44
22	A	814	CLA	C4D-CHA	2.40	1.46	1.38
25	5	315	BCR	C12-C13	-2.39	1.40	1.45
22	1	310	CLA	C1B-C2B	2.39	1.48	1.43
22	3	305	CLA	C4D-CHA	2.39	1.46	1.38
22	6	311	CLA	C3A-C2A	-2.39	1.52	1.54
22	6	313	CLA	C4C-C3C	2.39	1.49	1.45
22	B	820	CLA	C3D-C4D	-2.39	1.38	1.44
25	B	841	BCR	C12-C13	-2.39	1.40	1.45
22	L	205	CLA	C3D-C4D	-2.39	1.38	1.44
22	2	305	CLA	C4D-CHA	2.39	1.46	1.38
22	K	101	CLA	C1B-C2B	2.39	1.48	1.43
22	O	204	CLA	C1B-C2B	2.39	1.48	1.43
31	4	317	RRX	C23-C22	-2.39	1.40	1.45
22	B	803	CLA	C3D-C4D	-2.39	1.38	1.44
22	B	837	CLA	C1B-C2B	2.39	1.48	1.43
22	5	308	CLA	C3D-C4D	-2.39	1.38	1.44
25	K	103	BCR	C23-C22	-2.39	1.40	1.45
22	B	822	CLA	OBD-CAD	2.39	1.26	1.22
22	3	304	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	816	CLA	C4B-NB	-2.38	1.34	1.37
22	A	811	CLA	C1C-C2C	2.38	1.49	1.44
22	B	818	CLA	C3D-C4D	-2.38	1.38	1.44
22	B	815	CLA	C3B-C2B	2.38	1.49	1.41
22	B	824	CLA	C1B-C2B	2.38	1.48	1.43
22	L	203	CLA	C1C-C2C	2.38	1.49	1.44
22	A	820	CLA	C3B-C4B	2.38	1.48	1.42
22	A	806	CLA	C4D-CHA	2.38	1.46	1.38
22	A	858	CLA	C4D-CHA	2.38	1.46	1.38
22	5	309	CLA	C4D-CHA	2.38	1.46	1.38
22	1	302	CLA	C4B-NB	-2.38	1.34	1.37
22	B	814	CLA	C1B-C2B	2.38	1.48	1.43
22	5	301	CLA	C1C-NC	-2.38	1.34	1.37
22	1	302	CLA	C1C-C2C	2.38	1.49	1.44
22	5	307	CLA	C4D-CHA	2.38	1.46	1.38
29	B	851	5X6	C01-C02	2.38	1.54	1.50
25	1	301	BCR	C12-C13	-2.38	1.40	1.45
22	5	310	CLA	C1B-C2B	2.38	1.48	1.43
22	B	807	CLA	C1C-C2C	2.38	1.49	1.44
22	4	304	CLA	C3D-C4D	-2.38	1.38	1.44
22	B	835	CLA	C3B-C2B	2.38	1.49	1.41
22	B	816	CLA	C1C-C2C	2.38	1.49	1.44
22	A	837	CLA	C3D-C4D	-2.37	1.38	1.44
22	A	813	CLA	C1C-NC	-2.37	1.34	1.37
22	B	819	CLA	C1C-NC	-2.37	1.34	1.37
22	4	306	CLA	C4B-NB	-2.37	1.34	1.37
22	A	824	CLA	C3B-C4B	2.37	1.48	1.42
22	5	303	CLA	C3B-C2B	2.37	1.49	1.41
22	L	203	CLA	C3B-C2B	2.37	1.49	1.41
22	B	812	CLA	C3D-C4D	-2.37	1.38	1.44
22	B	821	CLA	C3D-C4D	-2.37	1.38	1.44
22	A	832	CLA	C4D-CHA	2.37	1.46	1.38
22	B	823	CLA	C1C-C2C	2.37	1.49	1.44
31	5	322	RRX	C12-C13	-2.37	1.40	1.45
22	2	309	CLA	C1B-C2B	2.37	1.48	1.43
22	7	311	CLA	C1B-C2B	2.37	1.48	1.43
22	6	305	CLA	C3B-C2B	2.37	1.49	1.41
22	B	822	CLA	C4D-CHA	2.37	1.46	1.38
22	A	805	CLA	C3B-C4B	2.37	1.48	1.42
22	A	831	CLA	C1C-NC	-2.37	1.34	1.37
22	B	839	CLA	C1C-C2C	2.37	1.49	1.44
22	B	806	CLA	C1C-C2C	2.36	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	814	CLA	C4B-NB	-2.36	1.34	1.37
22	A	821	CLA	C1C-C2C	2.36	1.49	1.44
22	6	308	CLA	C3D-C4D	-2.36	1.38	1.44
22	A	830	CLA	C3B-C2B	2.36	1.49	1.41
22	A	823	CLA	C4D-CHA	2.36	1.46	1.38
22	4	306	CLA	C1B-C2B	2.36	1.48	1.43
22	4	308	CLA	C4D-CHA	2.36	1.46	1.38
22	5	305	CLA	C4B-NB	-2.36	1.34	1.37
22	A	811	CLA	C3B-C4B	2.36	1.48	1.42
29	4	314	5X6	C38-C30	2.36	1.54	1.50
22	1	309	CLA	C1B-C2B	2.36	1.48	1.43
22	7	304	CLA	C4D-CHA	2.36	1.46	1.38
22	7	307	CLA	C4B-NB	-2.36	1.34	1.37
31	5	322	RRX	C19-C18	-2.36	1.40	1.45
22	A	817	CLA	C4D-CHA	2.36	1.46	1.38
22	A	827	CLA	C4D-CHA	2.36	1.46	1.38
22	2	302	CLA	C1B-C2B	2.36	1.48	1.43
22	B	826	CLA	C3B-C2B	2.36	1.49	1.41
22	6	311	CLA	C4D-CHA	2.35	1.46	1.38
22	6	306	CLA	C4D-CHA	2.35	1.46	1.38
22	B	836	CLA	C3B-C4B	2.35	1.48	1.42
22	B	850	CLA	C4B-NB	-2.35	1.34	1.37
22	6	314	CLA	C4C-C3C	2.35	1.49	1.45
22	7	303	CLA	C1C-C2C	2.35	1.49	1.44
22	3	302	CLA	C3D-C4D	-2.35	1.38	1.44
22	4	310	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	827	CLA	C3D-C4D	-2.35	1.38	1.44
22	2	310	CLA	C1B-C2B	2.35	1.48	1.43
22	A	833	CLA	C4D-CHA	2.35	1.46	1.38
22	4	302	CLA	C4C-C3C	2.35	1.49	1.45
22	4	308	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	802	CLA	C1B-C2B	2.35	1.48	1.43
22	A	820	CLA	C3B-C2B	2.35	1.49	1.41
22	7	304	CLA	C3D-C4D	-2.35	1.38	1.44
22	2	303	CLA	C3D-C4D	-2.35	1.38	1.44
22	2	304	CLA	C3D-C4D	-2.35	1.38	1.44
22	7	303	CLA	C3D-C4D	-2.35	1.38	1.44
22	7	306	CLA	C3D-C4D	-2.35	1.38	1.44
22	6	312	CLA	C4D-CHA	2.35	1.46	1.38
22	B	815	CLA	C1B-C2B	2.34	1.48	1.43
22	4	312	CLA	C4C-C3C	2.34	1.49	1.45
29	2	314	5X6	C01-C02	2.34	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	205	CLA	C4D-CHA	2.34	1.46	1.38
22	A	822	CLA	C4C-C3C	2.34	1.49	1.45
22	B	801	CLA	C3D-C4D	-2.34	1.38	1.44
22	2	305	CLA	C3D-C4D	-2.34	1.38	1.44
22	6	305	CLA	C4D-CHA	2.34	1.46	1.38
22	A	804	CLA	C4C-C3C	2.34	1.49	1.45
22	2	307	CLA	C1B-C2B	2.34	1.48	1.43
22	A	826	CLA	C3B-C4B	2.34	1.48	1.42
22	L	203	CLA	C4C-C3C	2.34	1.49	1.45
22	1	302	CLA	C4D-CHA	2.34	1.46	1.38
22	K	102	CLA	C3D-C4D	-2.34	1.38	1.44
22	5	305	CLA	C1B-C2B	2.34	1.48	1.43
22	B	802	CLA	C4D-CHA	2.33	1.46	1.38
22	B	805	CLA	C3B-C2B	2.33	1.49	1.41
22	6	303	CLA	C1C-C2C	2.33	1.49	1.44
22	B	820	CLA	C1C-NC	-2.33	1.34	1.37
22	6	309	CLA	C4C-C3C	2.33	1.49	1.45
22	5	309	CLA	C1B-C2B	2.33	1.48	1.43
25	2	301	BCR	C23-C22	-2.33	1.40	1.45
22	B	850	CLA	C3B-C2B	2.33	1.49	1.41
29	6	316	5X6	C41-C17	2.33	1.55	1.50
22	7	312	CLA	C4C-C3C	2.33	1.49	1.45
22	B	809	CLA	C4D-CHA	2.33	1.46	1.38
22	B	818	CLA	C4C-C3C	2.33	1.49	1.45
22	7	310	CLA	C4B-NB	-2.33	1.34	1.37
22	B	803	CLA	C1B-C2B	2.33	1.48	1.43
22	A	809	CLA	C4D-CHA	2.33	1.46	1.38
29	1	311	5X6	C41-C17	2.33	1.55	1.50
22	2	306	CLA	C4B-NB	-2.33	1.34	1.37
22	A	859	CLA	C3B-C4B	2.33	1.48	1.42
22	B	834	CLA	C4D-CHA	2.33	1.46	1.38
22	7	309	CLA	C3D-C4D	-2.33	1.38	1.44
22	B	832	CLA	C1C-C2C	2.33	1.49	1.44
22	A	809	CLA	C3D-C4D	-2.33	1.38	1.44
22	B	837	CLA	C4D-CHA	2.32	1.46	1.38
22	B	827	CLA	C3D-C4D	-2.32	1.38	1.44
22	B	811	CLA	C1B-C2B	2.32	1.48	1.43
22	4	312	CLA	C1B-C2B	2.32	1.48	1.43
22	A	813	CLA	C4D-CHA	2.32	1.46	1.38
22	A	859	CLA	C1C-NC	-2.32	1.34	1.37
22	1	305	CLA	C4B-NB	-2.32	1.34	1.37
22	6	305	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	308	CLA	C4C-C3C	2.32	1.49	1.45
22	A	821	CLA	C4D-CHA	2.32	1.46	1.38
22	A	812	CLA	C1B-C2B	2.32	1.48	1.43
22	4	303	CLA	C4D-CHA	2.32	1.46	1.38
22	4	312	CLA	C4B-NB	-2.32	1.34	1.37
22	B	810	CLA	C4D-CHA	2.32	1.46	1.38
22	B	816	CLA	C3D-C4D	-2.32	1.38	1.44
22	5	302	CLA	C3D-C4D	-2.32	1.38	1.44
29	Z	206	5X6	C41-C17	2.32	1.55	1.50
22	A	837	CLA	C1B-C2B	2.32	1.48	1.43
22	A	810	CLA	C1C-C2C	2.32	1.49	1.44
22	A	806	CLA	C3B-C4B	2.32	1.48	1.42
22	L	203	CLA	C1B-C2B	2.32	1.48	1.43
22	B	823	CLA	C3D-C4D	-2.32	1.38	1.44
22	4	304	CLA	C1C-C2C	2.32	1.49	1.44
22	4	311	CLA	C3D-C4D	-2.32	1.38	1.44
22	6	303	CLA	C4B-NB	-2.32	1.34	1.37
21	A	801	CL0	C4D-CHA	2.32	1.46	1.38
22	A	827	CLA	OBD-CAD	2.31	1.26	1.22
22	5	302	CLA	C1B-C2B	2.31	1.48	1.43
29	1	313	5X6	C01-C02	2.31	1.54	1.50
22	A	804	CLA	C1B-C2B	2.31	1.48	1.43
22	A	834	CLA	C4C-C3C	2.31	1.49	1.45
22	6	312	CLA	C1B-C2B	2.31	1.48	1.43
22	6	310	CLA	C4D-CHA	2.31	1.46	1.38
22	7	311	CLA	C3B-C2B	2.31	1.49	1.41
22	5	304	CLA	C1C-C2C	2.31	1.49	1.44
22	4	309	CLA	C1B-C2B	2.31	1.48	1.43
22	B	813	CLA	C4D-CHA	2.31	1.46	1.38
22	5	311	CLA	C3D-C4D	-2.31	1.39	1.44
22	7	307	CLA	C3B-C2B	2.31	1.49	1.41
22	A	815	CLA	C4D-CHA	2.31	1.46	1.38
22	A	831	CLA	C4D-CHA	2.31	1.46	1.38
22	5	308	CLA	C1B-C2B	2.31	1.48	1.43
22	B	831	CLA	C3B-C4B	2.31	1.48	1.42
22	6	303	CLA	C1B-C2B	2.31	1.48	1.43
22	6	313	CLA	C3D-C4D	-2.30	1.39	1.44
22	A	829	CLA	C3D-C4D	-2.30	1.39	1.44
22	4	305	CLA	C3D-C4D	-2.30	1.39	1.44
22	F	204	CLA	C4D-CHA	2.30	1.46	1.38
22	B	805	CLA	C1C-C2C	2.30	1.49	1.44
22	2	306	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	835	CLA	C3B-C4B	2.30	1.48	1.42
22	2	309	CLA	C3B-C2B	2.30	1.49	1.41
22	A	820	CLA	C4D-CHA	2.30	1.46	1.38
22	3	305	CLA	C4C-C3C	2.30	1.49	1.45
25	A	862	BCR	C17-C18	2.30	1.38	1.35
29	5	321	5X6	C41-C17	2.30	1.55	1.50
22	4	305	CLA	C3B-C2B	2.30	1.49	1.41
22	B	816	CLA	C1C-NC	-2.30	1.34	1.37
22	6	307	CLA	C3B-C2B	2.30	1.49	1.41
22	7	310	CLA	C3B-C2B	2.30	1.49	1.41
22	4	304	CLA	C1B-C2B	2.30	1.48	1.43
22	O	206	CLA	C3D-C4D	-2.30	1.39	1.44
22	B	827	CLA	C3B-C2B	2.30	1.49	1.41
22	A	826	CLA	C3D-C4D	-2.30	1.39	1.44
22	6	307	CLA	C1C-NC	-2.30	1.34	1.37
22	A	828	CLA	C3B-C4B	2.30	1.48	1.42
25	4	316	BCR	C12-C13	-2.30	1.41	1.45
22	B	808	CLA	C4B-NB	-2.29	1.35	1.37
22	A	825	CLA	C4D-CHA	2.29	1.46	1.38
22	A	834	CLA	C4B-NB	-2.29	1.35	1.37
22	B	817	CLA	C3D-C4D	-2.29	1.39	1.44
25	J	103	BCR	C8-C9	-2.29	1.41	1.45
22	4	307	CLA	C1C-C2C	2.29	1.49	1.44
22	A	839	CLA	C4D-CHA	2.29	1.46	1.38
22	A	815	CLA	C3D-C4D	-2.29	1.39	1.44
22	A	813	CLA	C3B-C2B	2.29	1.48	1.41
22	A	828	CLA	C4D-CHA	2.29	1.46	1.38
31	4	317	RRX	C19-C18	-2.29	1.41	1.45
22	4	307	CLA	C3D-C4D	-2.29	1.39	1.44
22	5	310	CLA	C3D-C4D	-2.29	1.39	1.44
22	O	204	CLA	C3B-C2B	2.29	1.48	1.41
22	7	313	CLA	C1B-C2B	2.29	1.48	1.43
22	B	807	CLA	C1C-NC	-2.29	1.34	1.37
22	A	859	CLA	C1C-C2C	2.29	1.49	1.44
22	5	309	CLA	C1C-C2C	2.29	1.49	1.44
22	B	822	CLA	C1B-C2B	2.29	1.48	1.43
22	A	819	CLA	C1C-NC	-2.29	1.34	1.37
22	4	312	CLA	C3D-C4D	-2.29	1.39	1.44
22	B	811	CLA	C1C-NC	-2.29	1.34	1.37
22	J	102	CLA	C3D-C4D	-2.29	1.39	1.44
31	6	318	RRX	C19-C18	-2.29	1.41	1.45
22	1	308	CLA	C4B-NB	-2.29	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	307	CLA	C1C-C2C	2.29	1.49	1.44
22	3	301	CLA	C3D-C4D	-2.29	1.39	1.44
22	A	823	CLA	C3B-C2B	2.29	1.48	1.41
22	Z	204	CLA	C1C-C2C	2.29	1.49	1.44
22	B	825	CLA	C4D-CHA	2.29	1.46	1.38
22	B	839	CLA	C3D-C4D	-2.28	1.39	1.44
22	A	839	CLA	C3D-C4D	-2.28	1.39	1.44
29	6	316	5X6	C38-C30	2.28	1.54	1.50
22	3	301	CLA	C4C-C3C	2.28	1.49	1.45
22	6	303	CLA	C3D-C4D	-2.28	1.39	1.44
22	Z	204	CLA	C3B-C2B	2.28	1.48	1.41
22	A	832	CLA	C3D-C4D	-2.28	1.39	1.44
22	7	312	CLA	C1B-C2B	2.28	1.48	1.43
25	L	202	BCR	C19-C18	-2.28	1.41	1.45
22	A	826	CLA	C4D-CHA	2.28	1.46	1.38
22	7	304	CLA	C4B-NB	-2.28	1.35	1.37
22	B	818	CLA	C3B-C2B	2.28	1.48	1.41
22	A	848	CLA	C4D-CHA	2.28	1.46	1.38
22	O	205	CLA	C3D-C4D	-2.28	1.39	1.44
22	A	858	CLA	C1C-NC	-2.28	1.34	1.37
29	1	313	5X6	C41-C17	2.28	1.55	1.50
22	B	829	CLA	C1C-NC	-2.28	1.34	1.37
22	4	307	CLA	C4C-C3C	2.28	1.49	1.45
29	6	317	5X6	C41-C17	2.28	1.55	1.50
22	B	804	CLA	C1C-C2C	2.28	1.49	1.44
29	1	316	5X6	C24-C23	2.28	1.40	1.34
22	A	828	CLA	C1B-C2B	2.28	1.48	1.43
22	A	816	CLA	C1C-C2C	2.28	1.49	1.44
22	6	312	CLA	C1C-NC	-2.28	1.34	1.37
22	1	309	CLA	C3D-C4D	-2.27	1.39	1.44
22	4	302	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	836	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	835	CLA	C4D-CHA	2.27	1.46	1.38
22	B	817	CLA	C4D-CHA	2.27	1.46	1.38
22	A	810	CLA	C3D-C4D	-2.27	1.39	1.44
22	2	302	CLA	C3B-C2B	2.27	1.48	1.41
22	1	310	CLA	C4C-C3C	2.27	1.49	1.45
22	1	304	CLA	C1C-C2C	2.27	1.49	1.44
22	5	307	CLA	C3B-C2B	2.27	1.48	1.41
22	5	301	CLA	C4C-C3C	2.27	1.49	1.45
22	F	206	CLA	C3D-C4D	-2.27	1.39	1.44
22	2	304	CLA	C1D-C2D	2.27	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	316	5X6	C41-C17	2.27	1.55	1.50
22	B	827	CLA	C3B-C4B	2.27	1.48	1.42
22	2	306	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	812	CLA	C3B-C4B	2.27	1.48	1.42
22	4	305	CLA	C1C-C2C	2.27	1.49	1.44
22	A	816	CLA	C1C-NC	-2.27	1.34	1.37
23	B	840	A1L64	C6-C1	2.27	1.39	1.35
22	3	301	CLA	C1B-C2B	2.27	1.48	1.43
22	3	304	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	835	CLA	C1C-C2C	2.27	1.48	1.44
22	B	829	CLA	C1B-C2B	2.27	1.48	1.43
22	O	205	CLA	C3B-C2B	2.27	1.48	1.41
22	B	823	CLA	C4D-CHA	2.27	1.46	1.38
22	6	304	CLA	C4D-CHA	2.27	1.46	1.38
22	A	836	CLA	C3B-C4B	2.26	1.48	1.42
25	A	862	BCR	C12-C13	-2.26	1.41	1.45
22	2	306	CLA	C3B-C2B	2.26	1.48	1.41
29	O	207	5X6	C41-C17	2.26	1.55	1.50
22	A	814	CLA	C1C-C2C	2.26	1.48	1.44
22	A	808	CLA	C4D-CHA	2.26	1.46	1.38
22	A	826	CLA	OBD-CAD	2.26	1.26	1.22
22	1	309	CLA	C3B-C2B	2.26	1.48	1.41
22	4	306	CLA	C3B-C2B	2.26	1.48	1.41
22	A	806	CLA	C1B-C2B	2.26	1.48	1.43
22	7	307	CLA	C3D-C4D	-2.26	1.39	1.44
22	A	857	CLA	C1C-NC	-2.26	1.34	1.37
22	A	831	CLA	C3B-C4B	2.26	1.48	1.42
22	3	303	CLA	C1B-C2B	2.26	1.48	1.43
22	5	309	CLA	C4B-NB	-2.26	1.35	1.37
25	F	207	BCR	C19-C18	-2.26	1.41	1.45
22	1	308	CLA	C3D-C4D	-2.26	1.39	1.44
22	O	205	CLA	C4D-CHA	2.26	1.46	1.38
22	B	831	CLA	C3B-C2B	2.26	1.48	1.41
22	2	310	CLA	C3B-C2B	2.26	1.48	1.41
22	A	816	CLA	C1B-C2B	2.26	1.48	1.43
22	A	820	CLA	C1B-C2B	2.25	1.48	1.43
22	2	311	CLA	C3D-C4D	-2.25	1.39	1.44
22	B	813	CLA	C1C-C2C	2.25	1.48	1.44
22	A	828	CLA	C3D-C4D	-2.25	1.39	1.44
22	5	304	CLA	C3D-C4D	-2.25	1.39	1.44
22	F	206	CLA	C4B-NB	-2.25	1.35	1.37
22	5	308	CLA	C3B-C2B	2.25	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	313	CLA	C3B-C2B	2.25	1.48	1.41
22	5	305	CLA	C3B-C2B	2.25	1.48	1.41
22	A	812	CLA	C4D-CHA	2.25	1.46	1.38
22	6	305	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	818	CLA	C4D-CHA	2.25	1.46	1.38
25	J	103	BCR	C23-C22	-2.25	1.41	1.45
22	B	827	CLA	C1B-C2B	2.25	1.48	1.43
22	6	307	CLA	C3D-C4D	-2.25	1.39	1.44
22	B	838	CLA	C4D-CHA	2.25	1.46	1.38
22	A	802	CLA	C1C-C2C	2.25	1.48	1.44
22	2	308	CLA	C4C-C3C	2.25	1.48	1.45
22	B	835	CLA	C3D-C4D	-2.25	1.39	1.44
22	1	307	CLA	C3D-C4D	-2.25	1.39	1.44
22	1	305	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	839	CLA	C1B-C2B	2.25	1.48	1.43
22	B	804	CLA	C1C-NC	-2.25	1.34	1.37
22	A	807	CLA	C3D-C4D	-2.25	1.39	1.44
22	F	205	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	820	CLA	C3D-C4D	-2.25	1.39	1.44
29	1	314	5X6	C41-C17	2.25	1.55	1.50
22	B	849	CLA	C3B-C4B	2.25	1.48	1.42
22	O	205	CLA	C1B-C2B	2.24	1.48	1.43
22	5	301	CLA	C1B-C2B	2.24	1.48	1.43
22	A	817	CLA	C1C-C2C	2.24	1.48	1.44
22	B	801	CLA	C4D-CHA	2.24	1.46	1.38
21	A	801	CL0	C3B-C4B	2.24	1.48	1.42
22	3	305	CLA	C3D-C4D	-2.24	1.39	1.44
22	4	311	CLA	C1B-C2B	2.24	1.48	1.43
22	B	834	CLA	C3D-C4D	-2.24	1.39	1.44
22	Z	201	CLA	C4D-CHA	2.24	1.46	1.38
22	O	206	CLA	C1C-C2C	2.24	1.48	1.44
22	A	857	CLA	C4D-CHA	2.24	1.46	1.38
22	1	306	CLA	C1C-C2C	2.24	1.48	1.44
29	6	317	5X6	C38-C30	2.24	1.54	1.50
22	L	203	CLA	C3D-C4D	-2.24	1.39	1.44
22	5	305	CLA	C3D-C4D	-2.24	1.39	1.44
22	5	310	CLA	C1C-NC	-2.24	1.34	1.37
22	B	805	CLA	C1B-C2B	2.24	1.48	1.43
22	A	830	CLA	C4D-CHA	2.24	1.46	1.38
22	B	828	CLA	C3B-C4B	2.24	1.48	1.42
22	1	303	CLA	C4C-C3C	2.24	1.48	1.45
22	4	309	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	308	CLA	C1C-C2C	2.24	1.48	1.44
22	6	312	CLA	C4C-C3C	2.24	1.48	1.45
22	B	802	CLA	C1B-C2B	2.24	1.48	1.43
22	6	314	CLA	C3D-C4D	-2.23	1.39	1.44
22	O	203	CLA	C1C-NC	-2.23	1.34	1.37
22	B	831	CLA	C3D-C4D	-2.23	1.39	1.44
22	Z	204	CLA	O2A-C1	-2.23	1.39	1.46
22	A	807	CLA	C3B-C2B	2.23	1.48	1.41
22	5	304	CLA	C4C-C3C	2.23	1.48	1.45
22	B	838	CLA	CHD-C1D	2.23	1.42	1.38
22	B	806	CLA	C3D-C4D	-2.23	1.39	1.44
22	B	835	CLA	C4D-CHA	2.23	1.46	1.38
22	O	204	CLA	C3D-C4D	-2.23	1.39	1.44
22	2	309	CLA	C3D-C4D	-2.23	1.39	1.44
22	6	307	CLA	C1B-C2B	2.23	1.48	1.43
22	5	306	CLA	C4C-C3C	2.23	1.48	1.45
22	B	820	CLA	C4B-NB	-2.23	1.35	1.37
22	3	303	CLA	C3D-C4D	-2.23	1.39	1.44
22	6	306	CLA	C3D-C4D	-2.23	1.39	1.44
25	B	842	BCR	C19-C18	-2.23	1.41	1.45
22	1	306	CLA	C4C-C3C	2.23	1.48	1.45
22	B	808	CLA	C1C-C2C	2.23	1.48	1.44
22	2	310	CLA	C3D-C4D	-2.23	1.39	1.44
22	6	310	CLA	C1C-C2C	2.23	1.48	1.44
22	A	827	CLA	C1B-C2B	2.23	1.48	1.43
25	A	845	BCR	C15-C14	-2.23	1.36	1.43
22	B	850	CLA	C3D-C4D	-2.23	1.39	1.44
22	A	835	CLA	C1B-C2B	2.23	1.48	1.43
22	3	304	CLA	C4B-NB	-2.23	1.35	1.37
22	7	312	CLA	C4B-NB	-2.22	1.35	1.37
22	A	819	CLA	C1C-C2C	2.22	1.48	1.44
29	7	318	5X6	C41-C17	2.22	1.55	1.50
22	A	809	CLA	C1C-NC	-2.22	1.34	1.37
22	B	827	CLA	C4D-CHA	2.22	1.46	1.38
22	B	850	CLA	C4C-C3C	2.22	1.48	1.45
22	1	305	CLA	C3B-C2B	2.22	1.48	1.41
22	5	307	CLA	C3D-C4D	-2.22	1.39	1.44
22	A	803	CLA	C4D-CHA	2.22	1.46	1.38
22	B	814	CLA	C3B-C4B	2.22	1.48	1.42
22	2	304	CLA	C3B-C2B	2.22	1.48	1.41
22	6	303	CLA	C4C-C3C	2.22	1.48	1.45
29	J	104	5X6	C41-C17	2.22	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	312	CLA	C3B-C2B	2.22	1.48	1.41
22	3	301	CLA	C3B-C2B	2.22	1.48	1.41
22	6	303	CLA	C3B-C2B	2.22	1.48	1.41
22	B	832	CLA	C3B-C2B	2.22	1.48	1.41
22	A	813	CLA	C4C-C3C	2.22	1.48	1.45
22	B	836	CLA	C3B-C2B	2.22	1.48	1.41
22	A	819	CLA	C4C-C3C	2.21	1.48	1.45
29	6	315	5X6	C41-C17	2.21	1.55	1.50
25	B	841	BCR	C19-C18	-2.21	1.41	1.45
22	B	836	CLA	C4D-CHA	2.21	1.46	1.38
22	A	823	CLA	C1C-C2C	2.21	1.48	1.44
22	B	809	CLA	C1B-C2B	2.21	1.48	1.43
22	F	205	CLA	C1B-C2B	2.21	1.48	1.43
22	B	808	CLA	C4C-C3C	2.21	1.48	1.45
22	B	819	CLA	C1C-C2C	2.21	1.48	1.44
22	4	304	CLA	C3B-C2B	2.21	1.48	1.41
22	4	306	CLA	C3D-C4D	-2.21	1.39	1.44
22	3	304	CLA	C3B-C2B	2.21	1.48	1.41
22	F	205	CLA	C1C-C2C	2.21	1.48	1.44
22	B	808	CLA	C1B-C2B	2.21	1.48	1.43
25	5	315	BCR	C19-C18	-2.21	1.41	1.45
22	B	813	CLA	C4C-C3C	2.21	1.48	1.45
22	7	306	CLA	C4D-CHA	2.21	1.46	1.38
22	2	311	CLA	C1B-C2B	2.21	1.48	1.43
22	A	835	CLA	C3B-C4B	2.21	1.47	1.42
22	B	836	CLA	OBD-CAD	2.21	1.26	1.22
22	B	849	CLA	C4D-CHA	2.20	1.46	1.38
22	A	811	CLA	C4D-CHA	2.20	1.46	1.38
22	1	310	CLA	C3D-C4D	-2.20	1.39	1.44
22	B	813	CLA	C1C-NC	-2.20	1.34	1.37
22	3	303	CLA	C3B-C2B	2.20	1.48	1.41
31	1	315	RRX	C12-C13	-2.20	1.41	1.45
22	A	836	CLA	C3B-C2B	2.20	1.48	1.41
22	A	805	CLA	C1C-C2C	2.20	1.48	1.44
22	2	307	CLA	C4B-NB	-2.20	1.35	1.37
22	A	838	CLA	C1C-C2C	2.20	1.48	1.44
22	4	307	CLA	C1C-NC	-2.20	1.34	1.37
31	4	317	RRX	C12-C13	-2.20	1.41	1.45
22	B	818	CLA	C3B-C4B	2.20	1.47	1.42
22	5	302	CLA	C4D-CHA	2.20	1.46	1.38
22	B	823	CLA	C1B-C2B	2.20	1.48	1.43
22	B	835	CLA	C1B-C2B	2.20	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	808	CLA	C3D-C4D	-2.20	1.39	1.44
22	5	308	CLA	C4C-C3C	2.19	1.48	1.45
22	1	308	CLA	C3B-C2B	2.19	1.48	1.41
22	J	102	CLA	C1C-C2C	2.19	1.48	1.44
22	K	102	CLA	C1C-C2C	2.19	1.48	1.44
22	B	809	CLA	C1C-C2C	2.19	1.48	1.44
22	F	205	CLA	C4B-NB	-2.19	1.35	1.37
22	A	830	CLA	C4C-C3C	2.19	1.48	1.45
22	A	818	CLA	C3B-C2B	2.19	1.48	1.41
22	B	801	CLA	C3B-C4B	2.19	1.47	1.42
22	1	305	CLA	C1B-C2B	2.19	1.48	1.43
29	6	315	5X6	C01-C02	2.19	1.54	1.50
22	A	823	CLA	C3D-C4D	-2.19	1.39	1.44
22	7	312	CLA	C3D-C4D	-2.19	1.39	1.44
22	B	833	CLA	C4D-CHA	2.19	1.46	1.38
22	B	833	CLA	C4C-C3C	2.19	1.48	1.45
22	5	311	CLA	C4C-C3C	2.19	1.48	1.45
25	J	103	BCR	C12-C13	-2.19	1.41	1.45
29	Z	206	5X6	C38-C30	2.19	1.54	1.50
22	4	308	CLA	C4B-NB	-2.19	1.35	1.37
22	B	807	CLA	C4D-CHA	2.18	1.46	1.38
22	7	313	CLA	C4B-NB	-2.18	1.35	1.37
22	B	839	CLA	C3B-C2B	2.18	1.48	1.41
25	A	846	BCR	C16-C17	-2.18	1.36	1.43
22	B	829	CLA	C3B-C2B	2.18	1.48	1.41
22	A	821	CLA	C3B-C2B	2.18	1.48	1.41
22	A	812	CLA	C3B-C2B	2.18	1.48	1.41
29	7	318	5X6	C01-C02	2.18	1.54	1.50
22	A	826	CLA	C1C-C2C	2.18	1.48	1.44
25	L	206	BCR	C19-C18	-2.18	1.41	1.45
22	2	302	CLA	C4B-NB	-2.18	1.35	1.37
22	J	102	CLA	C3B-C2B	2.18	1.48	1.41
22	2	309	CLA	C4B-NB	-2.18	1.35	1.37
22	B	808	CLA	C4D-CHA	2.18	1.46	1.38
22	L	205	CLA	C4C-C3C	2.18	1.48	1.45
22	7	309	CLA	C4C-C3C	2.18	1.48	1.45
22	B	834	CLA	C1C-NC	-2.17	1.34	1.37
22	7	306	CLA	C4B-NB	-2.17	1.35	1.37
25	J	103	BCR	C29-C28	-2.17	1.47	1.52
29	5	313	5X6	C41-C17	2.17	1.55	1.50
22	A	817	CLA	C1B-C2B	2.17	1.48	1.43
22	B	838	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	310	CLA	C1B-C2B	2.17	1.48	1.43
22	5	308	CLA	C1C-NC	-2.17	1.34	1.37
22	6	312	CLA	C3D-C4D	-2.17	1.39	1.44
22	5	306	CLA	C1C-C2C	2.17	1.48	1.44
22	L	204	CLA	C3D-C4D	-2.17	1.39	1.44
22	B	819	CLA	CHB-C4A	-2.17	1.32	1.37
22	3	303	CLA	C4B-NB	-2.17	1.35	1.37
22	6	304	CLA	C3D-C4D	-2.17	1.39	1.44
29	2	313	5X6	C38-C30	2.16	1.54	1.50
22	7	313	CLA	C3D-C4D	-2.16	1.39	1.44
22	B	802	CLA	C3B-C2B	2.16	1.48	1.41
22	6	306	CLA	C1C-C2C	2.16	1.48	1.44
22	A	826	CLA	C1B-C2B	2.16	1.48	1.43
22	6	314	CLA	C1B-C2B	2.16	1.48	1.43
22	4	302	CLA	C1C-C2C	2.16	1.48	1.44
22	1	302	CLA	C1B-C2B	2.16	1.48	1.43
22	3	305	CLA	C4B-NB	-2.16	1.35	1.37
22	2	307	CLA	C3B-C2B	2.16	1.48	1.41
22	2	302	CLA	C3D-C4D	-2.16	1.39	1.44
22	A	806	CLA	C1C-C2C	2.16	1.48	1.44
22	A	820	CLA	C1C-C2C	2.16	1.48	1.44
29	O	208	5X6	C41-C17	2.16	1.55	1.50
22	4	311	CLA	C4C-C3C	2.16	1.48	1.45
25	I	102	BCR	C20-C21	-2.16	1.36	1.43
22	7	311	CLA	C3D-C4D	-2.16	1.39	1.44
22	B	832	CLA	C3D-C4D	-2.16	1.39	1.44
29	J	104	5X6	C38-C30	2.16	1.54	1.50
22	A	804	CLA	MG-ND	-2.16	2.01	2.05
22	O	204	CLA	C4B-NB	-2.16	1.35	1.37
22	3	305	CLA	C3B-C2B	2.16	1.48	1.41
25	A	846	BCR	C8-C9	-2.16	1.41	1.45
22	B	809	CLA	C4C-C3C	2.16	1.48	1.45
22	1	304	CLA	C1C-NC	-2.16	1.34	1.37
22	A	835	CLA	C3D-C4D	-2.16	1.39	1.44
22	1	303	CLA	C3D-C4D	-2.15	1.39	1.44
22	B	830	CLA	C1C-C2C	2.15	1.48	1.44
22	B	826	CLA	C4D-CHA	2.15	1.46	1.38
29	4	315	5X6	C41-C17	2.15	1.55	1.50
22	7	304	CLA	C3B-C2B	2.15	1.48	1.41
25	B	843	BCR	C16-C17	-2.15	1.36	1.43
25	Z	205	BCR	C19-C18	-2.15	1.41	1.45
22	B	805	CLA	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	C3D-C4D	-2.15	1.39	1.44
22	5	309	CLA	C3D-C4D	-2.15	1.39	1.44
22	A	848	CLA	C1C-NC	-2.15	1.34	1.37
22	4	303	CLA	C4B-NB	-2.15	1.35	1.37
22	L	204	CLA	C3B-C2B	2.15	1.48	1.41
22	O	204	CLA	C3A-C2A	-2.15	1.52	1.54
22	2	304	CLA	C1B-C2B	2.15	1.48	1.43
22	7	306	CLA	C1B-C2B	2.14	1.48	1.43
22	A	815	CLA	C1C-NC	-2.14	1.34	1.37
29	2	312	5X6	C41-C17	2.14	1.55	1.50
22	1	303	CLA	C1B-C2B	2.14	1.48	1.43
22	A	833	CLA	C4C-C3C	2.14	1.48	1.45
22	2	308	CLA	C3D-C4D	-2.14	1.39	1.44
22	5	311	CLA	C1C-NC	-2.14	1.34	1.37
22	A	824	CLA	C3B-C2B	2.14	1.48	1.41
22	2	307	CLA	C3D-C4D	-2.14	1.39	1.44
29	5	313	5X6	C38-C30	2.14	1.54	1.50
31	6	318	RRX	C12-C13	-2.14	1.41	1.45
29	7	316	5X6	C41-C17	2.14	1.55	1.50
22	B	812	CLA	C3B-C2B	2.14	1.48	1.41
22	B	831	CLA	C1C-C2C	2.14	1.48	1.44
22	A	836	CLA	C1C-NC	-2.14	1.34	1.37
22	B	824	CLA	C1C-C2C	2.14	1.48	1.44
22	A	802	CLA	C4C-C3C	2.14	1.48	1.45
22	A	833	CLA	C1C-NC	-2.13	1.34	1.37
22	A	838	CLA	C4D-CHA	2.13	1.46	1.38
22	B	821	CLA	C4C-C3C	2.13	1.48	1.45
22	2	310	CLA	C4B-NB	-2.13	1.35	1.37
22	B	826	CLA	C1C-C2C	2.13	1.48	1.44
22	4	309	CLA	C4C-C3C	2.13	1.48	1.45
22	7	311	CLA	C4B-NB	-2.13	1.35	1.37
22	A	816	CLA	C4D-CHA	2.13	1.46	1.38
22	6	311	CLA	C3D-C4D	-2.13	1.39	1.44
22	B	812	CLA	C1C-NC	-2.13	1.34	1.37
22	A	805	CLA	C3B-C2B	2.13	1.48	1.41
22	7	303	CLA	C1D-C2D	2.13	1.49	1.45
22	B	828	CLA	C3B-C2B	2.13	1.48	1.41
29	2	314	5X6	C41-C17	2.13	1.55	1.50
22	B	837	CLA	C1C-C2C	2.13	1.48	1.44
25	A	845	BCR	C11-C10	-2.13	1.36	1.43
22	1	306	CLA	C3D-C4D	-2.13	1.39	1.44
22	7	306	CLA	C3B-C2B	2.13	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	311	CLA	C3B-C2B	2.13	1.48	1.41
22	A	812	CLA	C3D-C4D	-2.13	1.39	1.44
22	A	806	CLA	C3B-C2B	2.13	1.48	1.41
22	4	309	CLA	C3B-C2B	2.12	1.48	1.41
22	A	805	CLA	C4D-CHA	2.12	1.46	1.38
22	1	310	CLA	C4D-CHA	2.12	1.46	1.38
25	B	842	BCR	C12-C13	-2.12	1.41	1.45
22	2	308	CLA	C1B-C2B	2.12	1.48	1.43
22	7	310	CLA	C3D-C4D	-2.12	1.39	1.44
22	A	818	CLA	C3D-C4D	-2.12	1.39	1.44
25	A	843	BCR	C16-C17	-2.12	1.36	1.43
29	1	313	5X6	C38-C30	2.12	1.54	1.50
22	F	206	CLA	C3B-C2B	2.12	1.48	1.41
22	A	823	CLA	C4C-C3C	2.12	1.48	1.45
22	6	305	CLA	C1C-NC	-2.12	1.34	1.37
29	5	314	5X6	C41-C17	2.12	1.55	1.50
22	O	205	CLA	C1C-NC	-2.12	1.34	1.37
22	6	314	CLA	C1C-NC	-2.12	1.34	1.37
22	A	827	CLA	C4C-C3C	2.12	1.48	1.45
22	A	807	CLA	MG-ND	-2.11	2.01	2.05
22	7	304	CLA	C4C-C3C	2.11	1.48	1.45
22	A	809	CLA	C3B-C2B	2.11	1.48	1.41
22	A	803	CLA	C3B-C2B	2.11	1.48	1.41
29	4	315	5X6	C01-C02	2.11	1.54	1.50
22	A	829	CLA	C1C-C2C	2.11	1.48	1.44
22	6	309	CLA	C3D-C4D	-2.11	1.39	1.44
22	F	205	CLA	C1C-NC	-2.11	1.34	1.37
22	A	836	CLA	C1C-C2C	2.11	1.48	1.44
22	L	205	CLA	C1B-C2B	2.11	1.48	1.43
22	A	812	CLA	C1C-NC	-2.11	1.34	1.37
22	A	815	CLA	C1C-C2C	2.11	1.48	1.44
22	L	205	CLA	C1C-NC	-2.11	1.34	1.37
22	1	310	CLA	C1C-NC	-2.10	1.34	1.37
22	A	804	CLA	C3B-C2B	2.10	1.48	1.41
25	A	844	BCR	C15-C14	-2.10	1.36	1.43
22	B	806	CLA	C4C-C3C	2.10	1.48	1.45
22	B	822	CLA	C4C-C3C	2.10	1.48	1.45
22	6	310	CLA	C4C-C3C	2.10	1.48	1.45
22	4	305	CLA	C4C-C3C	2.10	1.48	1.45
22	A	812	CLA	C1C-C2C	2.10	1.48	1.44
22	4	308	CLA	CHB-C4A	-2.10	1.32	1.37
22	3	301	CLA	C4B-NB	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	825	CLA	C3B-C2B	2.10	1.48	1.41
22	A	818	CLA	C1C-NC	-2.10	1.34	1.37
22	B	816	CLA	C1B-C2B	2.10	1.48	1.43
22	B	849	CLA	C3D-C4D	-2.10	1.39	1.44
22	K	102	CLA	C3B-C2B	2.10	1.48	1.41
22	B	806	CLA	C3B-C4B	2.09	1.47	1.42
22	A	824	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	836	CLA	C4C-C3C	2.09	1.48	1.45
25	1	301	BCR	C19-C18	-2.09	1.41	1.45
22	B	829	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	857	CLA	C1C-C2C	2.09	1.48	1.44
22	7	306	CLA	C1D-C2D	2.09	1.49	1.45
22	A	810	CLA	C4D-CHA	2.09	1.45	1.38
29	4	313	5X6	C41-C17	2.09	1.55	1.50
22	5	309	CLA	C3B-C2B	2.08	1.48	1.41
23	B	840	A1L64	C6-C5	-2.08	1.40	1.46
22	J	102	CLA	C1B-C2B	2.08	1.48	1.43
22	B	825	CLA	C1C-NC	-2.08	1.34	1.37
22	2	306	CLA	C1D-C2D	2.08	1.49	1.45
22	2	308	CLA	C1D-C2D	2.08	1.49	1.45
22	4	307	CLA	C3B-C2B	2.08	1.48	1.41
29	5	314	5X6	C01-C02	2.08	1.54	1.50
22	6	304	CLA	C4C-C3C	2.08	1.48	1.45
22	5	302	CLA	C1C-NC	-2.08	1.34	1.37
22	A	821	CLA	C1B-C2B	2.08	1.48	1.43
22	4	307	CLA	C1B-C2B	2.08	1.48	1.43
29	4	314	5X6	C01-C02	2.07	1.54	1.50
22	5	309	CLA	C4C-C3C	2.07	1.48	1.45
22	A	834	CLA	C1C-NC	-2.07	1.34	1.37
22	B	813	CLA	C3B-C2B	2.07	1.48	1.41
22	F	206	CLA	C1B-C2B	2.07	1.48	1.43
25	A	862	BCR	C20-C21	-2.07	1.37	1.43
22	A	811	CLA	C3B-C2B	2.07	1.48	1.41
22	B	832	CLA	C1B-C2B	2.07	1.48	1.43
22	O	205	CLA	C4C-C3C	2.07	1.48	1.45
22	B	826	CLA	C1B-C2B	2.07	1.48	1.43
22	A	814	CLA	C1C-NC	-2.07	1.34	1.37
22	B	822	CLA	C1C-C2C	2.07	1.48	1.44
22	7	307	CLA	C1D-C2D	2.07	1.49	1.45
22	4	303	CLA	C1B-C2B	2.07	1.48	1.43
22	A	813	CLA	C3D-C4D	-2.07	1.39	1.44
22	6	309	CLA	C1C-NC	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	201	BCR	C15-C14	-2.07	1.37	1.43
22	1	302	CLA	C3B-C2B	2.07	1.48	1.41
22	2	311	CLA	C4B-NB	-2.07	1.35	1.37
22	B	812	CLA	C1B-C2B	2.07	1.48	1.43
22	B	802	CLA	OBD-CAD	2.07	1.26	1.22
22	B	804	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	817	CLA	C3B-C2B	2.06	1.48	1.41
22	6	312	CLA	C1D-C2D	2.06	1.49	1.45
22	4	305	CLA	C1C-NC	-2.06	1.34	1.37
29	7	316	5X6	C38-C30	2.06	1.54	1.50
22	B	817	CLA	C1B-C2B	2.06	1.48	1.43
22	A	831	CLA	C4C-C3C	2.06	1.48	1.45
21	A	801	CL0	C3B-C2B	2.06	1.48	1.41
22	5	301	CLA	C3B-C2B	2.06	1.48	1.41
29	O	207	5X6	C42-C13	2.06	1.55	1.50
22	4	312	CLA	C3B-C2B	2.06	1.48	1.41
22	F	206	CLA	C1C-NC	-2.06	1.34	1.37
22	A	835	CLA	C3B-C2B	2.06	1.48	1.41
22	2	308	CLA	C3B-C2B	2.06	1.48	1.41
29	1	312	5X6	C41-C17	2.06	1.55	1.50
22	1	302	CLA	C1C-NC	-2.05	1.34	1.37
22	K	102	CLA	C4C-C3C	2.05	1.48	1.45
22	4	310	CLA	C3B-C2B	2.05	1.48	1.41
22	B	832	CLA	C1C-NC	-2.05	1.34	1.37
22	6	309	CLA	CHB-C4A	-2.05	1.32	1.37
22	B	810	CLA	C1B-C2B	2.05	1.48	1.43
22	A	859	CLA	C4D-CHA	2.05	1.45	1.38
22	6	303	CLA	C1C-NC	-2.05	1.34	1.37
22	B	824	CLA	C3B-C2B	2.05	1.48	1.41
22	Z	204	CLA	C3D-C4D	-2.05	1.39	1.44
22	1	309	CLA	C1D-C2D	2.05	1.49	1.45
22	B	820	CLA	C3B-C2B	2.04	1.48	1.41
29	5	312	5X6	C01-C02	2.04	1.54	1.50
22	A	826	CLA	C3B-C2B	2.04	1.48	1.41
25	A	844	BCR	C19-C18	-2.04	1.41	1.45
22	5	307	CLA	C4C-C3C	2.04	1.48	1.45
22	B	811	CLA	C3B-C2B	2.04	1.48	1.41
22	4	308	CLA	C3B-C2B	2.04	1.48	1.41
25	A	846	BCR	C15-C14	-2.04	1.37	1.43
22	B	818	CLA	C1C-NC	-2.04	1.34	1.37
22	5	307	CLA	C1C-NC	-2.04	1.34	1.37
22	A	836	CLA	C4D-CHA	2.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	CLA	C1D-C2D	2.04	1.49	1.45
22	4	311	CLA	C1C-NC	-2.03	1.34	1.37
22	A	814	CLA	C4C-C3C	2.03	1.48	1.45
22	3	305	CLA	C1B-C2B	2.03	1.48	1.43
25	F	201	BCR	C16-C17	-2.03	1.37	1.43
22	2	307	CLA	C1D-C2D	2.03	1.49	1.45
22	L	203	CLA	C1C-NC	-2.03	1.34	1.37
29	5	313	5X6	C01-C02	2.03	1.54	1.50
29	6	317	5X6	C01-C02	2.03	1.54	1.50
22	A	815	CLA	C4B-NB	-2.03	1.35	1.37
22	B	836	CLA	C4C-C3C	2.03	1.48	1.45
22	B	803	CLA	C3B-C2B	2.03	1.48	1.41
22	B	803	CLA	CHB-C4A	-2.03	1.32	1.37
22	3	301	CLA	C1D-C2D	2.03	1.49	1.45
22	A	814	CLA	C3B-C2B	2.03	1.48	1.41
22	5	311	CLA	C1C-C2C	2.02	1.48	1.44
29	4	313	5X6	C01-C02	2.02	1.54	1.50
22	1	306	CLA	C1C-NC	-2.02	1.34	1.37
29	Z	206	5X6	C42-C13	2.02	1.55	1.50
22	B	814	CLA	C3D-C4D	-2.02	1.39	1.44
22	B	809	CLA	C3D-C4D	-2.02	1.39	1.44
22	O	203	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	807	CLA	C1C-C2C	2.02	1.48	1.44
22	6	307	CLA	C1C-C2C	2.02	1.48	1.44
22	3	303	CLA	C1D-C2D	2.02	1.49	1.45
22	1	302	CLA	C3D-C4D	-2.02	1.39	1.44
25	A	845	BCR	C16-C17	-2.02	1.37	1.43
22	A	809	CLA	C1C-C2C	2.02	1.48	1.44
22	7	308	CLA	CHB-C4A	-2.02	1.32	1.37
22	4	311	CLA	C3B-C2B	2.02	1.48	1.41
22	A	830	CLA	C1C-NC	-2.02	1.34	1.37
22	B	811	CLA	C3B-C4B	2.02	1.47	1.42
22	A	817	CLA	C1C-NC	-2.02	1.34	1.37
22	A	859	CLA	C3B-C2B	2.02	1.48	1.41
29	Z	206	5X6	C01-C02	2.02	1.54	1.50
22	Z	204	CLA	C4C-C3C	2.02	1.48	1.45
22	4	310	CLA	C1C-C2C	2.01	1.48	1.44
22	7	308	CLA	C3B-C2B	2.01	1.48	1.41
22	B	802	CLA	C3D-C4D	-2.01	1.39	1.44
22	2	305	CLA	C1D-C2D	2.01	1.49	1.45
22	B	827	CLA	C1C-C2C	2.01	1.48	1.44
29	3	306	5X6	C38-C30	2.01	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	857	CLA	MG-NA	2.01	2.11	2.06
29	Z	206	5X6	C15-C16	2.01	1.39	1.34
29	2	312	5X6	C01-C02	2.01	1.54	1.50
22	6	314	CLA	C3B-C2B	2.01	1.48	1.41
22	7	309	CLA	C4B-NB	-2.01	1.35	1.37
22	A	833	CLA	C1B-C2B	2.01	1.48	1.43
22	B	834	CLA	C4C-C3C	2.01	1.48	1.45
22	A	822	CLA	C1B-C2B	2.01	1.48	1.43
22	B	814	CLA	C1C-NC	-2.01	1.34	1.37
22	7	304	CLA	C1B-C2B	2.01	1.48	1.43
29	O	207	5X6	C38-C30	2.00	1.54	1.50
22	A	838	CLA	C1B-C2B	2.00	1.48	1.43
22	B	808	CLA	C2A-C1A	-2.00	1.47	1.52
25	A	846	BCR	C19-C18	-2.00	1.41	1.45
22	B	806	CLA	MG-ND	-2.00	2.01	2.05
22	2	310	CLA	C1D-C2D	2.00	1.49	1.45

All (6015) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	317	5X6	C01-C02-C03	-13.80	109.03	124.53
29	7	314	5X6	C38-C30-C29	-12.80	110.15	124.53
29	1	311	5X6	C01-C02-C03	-12.17	110.86	124.53
29	M	101	5X6	C38-C30-C29	-12.08	110.97	124.53
29	3	306	5X6	C01-C02-C03	-11.94	111.12	124.53
29	7	318	5X6	C38-C30-C29	-11.91	111.15	124.53
29	1	311	5X6	C38-C30-C29	-11.71	111.38	124.53
29	2	312	5X6	C38-C30-C29	-11.63	111.47	124.53
29	1	311	5X6	C20-C21-C22	-11.45	110.97	127.31
29	B	851	5X6	C38-C30-C29	-11.37	111.76	124.53
29	O	207	5X6	C38-C30-C29	-11.34	111.80	124.53
29	7	317	5X6	C38-C30-C29	-11.26	111.88	124.53
29	4	315	5X6	C38-C30-C29	-11.19	111.96	124.53
22	B	838	CLA	C1D-ND-C4D	-11.12	98.43	106.33
29	7	316	5X6	C24-C25-C26	-10.93	111.70	127.31
29	M	101	5X6	C01-C02-C03	-10.90	112.29	124.53
29	2	312	5X6	C01-C02-C03	-10.89	112.30	124.53
29	5	314	5X6	C15-C14-C13	-10.85	111.83	127.31
29	1	316	5X6	C01-C02-C03	-10.77	112.44	124.53
22	A	820	CLA	C1D-ND-C4D	-10.75	98.70	106.33
29	1	314	5X6	C24-C25-C26	-10.71	112.02	127.31
22	7	306	CLA	C1D-ND-C4D	-10.67	98.75	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	316	5X6	C38-C30-C29	-10.67	112.55	124.53
22	B	838	CLA	C2D-C1D-ND	10.62	117.93	110.10
22	B	832	CLA	C1D-ND-C4D	-10.55	98.84	106.33
29	5	321	5X6	C24-C25-C26	-10.52	112.29	127.31
22	A	837	CLA	C1D-ND-C4D	-10.46	98.90	106.33
22	B	805	CLA	C1D-ND-C4D	-10.45	98.91	106.33
29	2	314	5X6	C38-C30-C29	-10.44	112.80	124.53
29	1	314	5X6	C01-C02-C03	-10.44	112.81	124.53
29	1	313	5X6	C15-C14-C13	-10.43	112.42	127.31
29	1	312	5X6	C15-C14-C13	-10.43	112.43	127.31
29	7	317	5X6	C24-C25-C26	-10.42	112.43	127.31
22	B	828	CLA	C1D-ND-C4D	-10.41	98.94	106.33
22	A	809	CLA	C1D-ND-C4D	-10.35	98.99	106.33
29	5	313	5X6	C15-C14-C13	-10.35	112.55	127.31
29	M	101	5X6	C24-C25-C26	-10.34	112.56	127.31
29	2	314	5X6	C15-C14-C13	-10.33	112.57	127.31
29	7	316	5X6	C01-C02-C03	-10.31	112.95	124.53
22	4	303	CLA	C1D-ND-C4D	-10.30	99.02	106.33
29	O	208	5X6	C38-C30-C29	-10.30	112.96	124.53
22	A	859	CLA	C1D-ND-C4D	-10.28	99.03	106.33
29	O	207	5X6	C24-C25-C26	-10.27	112.65	127.31
29	3	306	5X6	C38-C30-C29	-10.27	113.00	124.53
22	B	821	CLA	C1D-ND-C4D	-10.25	99.05	106.33
29	2	314	5X6	C01-C02-C03	-10.22	113.05	124.53
22	5	302	CLA	C1D-ND-C4D	-10.20	99.09	106.33
29	4	315	5X6	C15-C14-C13	-10.19	112.76	127.31
29	4	313	5X6	C38-C30-C29	-10.18	113.10	124.53
22	A	818	CLA	C1D-ND-C4D	-10.17	99.11	106.33
22	A	838	CLA	C1D-ND-C4D	-10.16	99.11	106.33
22	L	204	CLA	C1D-ND-C4D	-10.16	99.12	106.33
29	5	314	5X6	C01-C02-C03	-10.16	113.12	124.53
22	B	810	CLA	C1D-ND-C4D	-10.10	99.16	106.33
22	A	820	CLA	C2D-C1D-ND	10.09	117.54	110.10
22	B	829	CLA	C1D-ND-C4D	-10.09	99.17	106.33
22	2	305	CLA	C1D-ND-C4D	-10.08	99.17	106.33
22	4	308	CLA	C1D-ND-C4D	-10.07	99.18	106.33
22	F	206	CLA	C1D-ND-C4D	-10.05	99.19	106.33
29	7	317	5X6	C15-C14-C13	-10.05	112.97	127.31
22	B	829	CLA	C2D-C1D-ND	10.02	117.49	110.10
22	A	834	CLA	C1D-ND-C4D	-10.01	99.23	106.33
22	B	808	CLA	C1D-ND-C4D	-9.99	99.24	106.33
22	3	301	CLA	C1D-ND-C4D	-9.98	99.24	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	304	CLA	C1D-ND-C4D	-9.98	99.25	106.33
22	4	310	CLA	CAC-C3C-C4C	9.97	137.75	124.81
22	B	825	CLA	C1D-ND-C4D	-9.96	99.26	106.33
22	B	828	CLA	C2D-C1D-ND	9.94	117.43	110.10
29	4	314	5X6	C15-C14-C13	-9.93	113.14	127.31
22	1	310	CLA	C1D-ND-C4D	-9.92	99.29	106.33
22	F	205	CLA	C1D-ND-C4D	-9.91	99.30	106.33
29	1	314	5X6	C38-C30-C29	-9.90	113.41	124.53
22	B	849	CLA	C1D-ND-C4D	-9.90	99.30	106.33
22	3	305	CLA	C1D-ND-C4D	-9.89	99.31	106.33
22	6	304	CLA	C1D-ND-C4D	-9.89	99.31	106.33
22	A	838	CLA	C2D-C1D-ND	9.89	117.39	110.10
29	1	316	5X6	C20-C21-C22	-9.88	113.21	127.31
29	1	313	5X6	C24-C25-C26	-9.87	113.22	127.31
22	2	308	CLA	C1D-ND-C4D	-9.87	99.33	106.33
22	B	832	CLA	C2D-C1D-ND	9.86	117.37	110.10
22	1	303	CLA	C1D-ND-C4D	-9.85	99.34	106.33
22	A	809	CLA	C2D-C1D-ND	9.84	117.36	110.10
29	5	314	5X6	C20-C21-C22	-9.84	113.27	127.31
22	1	302	CLA	C1D-ND-C4D	-9.82	99.36	106.33
22	O	205	CLA	C1D-ND-C4D	-9.82	99.36	106.33
22	6	306	CLA	C1D-ND-C4D	-9.81	99.37	106.33
22	B	831	CLA	C1D-ND-C4D	-9.80	99.37	106.33
22	7	304	CLA	C1D-ND-C4D	-9.80	99.37	106.33
29	1	313	5X6	C19-C18-C17	-9.79	113.34	127.31
22	5	307	CLA	C1D-ND-C4D	-9.77	99.39	106.33
22	A	825	CLA	C1D-ND-C4D	-9.77	99.39	106.33
29	7	317	5X6	C28-C27-C26	-9.76	111.49	126.23
29	M	101	5X6	C20-C21-C22	-9.75	113.39	127.31
29	7	318	5X6	C20-C21-C22	-9.72	113.43	127.31
29	5	321	5X6	C01-C02-C03	-9.72	113.61	124.53
22	B	835	CLA	C1D-ND-C4D	-9.72	99.43	106.33
29	M	101	5X6	C19-C18-C17	-9.71	113.45	127.31
22	A	858	CLA	C1D-ND-C4D	-9.71	99.44	106.33
22	7	312	CLA	C1D-ND-C4D	-9.70	99.45	106.33
22	7	309	CLA	C1D-ND-C4D	-9.69	99.45	106.33
22	1	307	CLA	C1D-ND-C4D	-9.68	99.46	106.33
22	A	821	CLA	C1D-ND-C4D	-9.68	99.46	106.33
22	A	833	CLA	C1D-ND-C4D	-9.66	99.47	106.33
22	B	823	CLA	C1D-ND-C4D	-9.65	99.48	106.33
29	1	312	5X6	C19-C18-C17	-9.64	113.55	127.31
22	B	814	CLA	C1D-ND-C4D	-9.64	99.49	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	204	CLA	C2D-C1D-ND	9.63	117.20	110.10
29	M	101	5X6	C15-C14-C13	-9.63	113.57	127.31
22	6	311	CLA	C1D-ND-C4D	-9.62	99.50	106.33
22	7	311	CLA	C1D-ND-C4D	-9.62	99.50	106.33
22	B	822	CLA	C1D-ND-C4D	-9.60	99.51	106.33
22	2	307	CLA	C1D-ND-C4D	-9.59	99.52	106.33
22	A	814	CLA	C1D-ND-C4D	-9.59	99.52	106.33
22	B	808	CLA	C2D-C1D-ND	9.59	117.17	110.10
22	1	308	CLA	C1D-ND-C4D	-9.58	99.53	106.33
22	6	303	CLA	C1D-ND-C4D	-9.57	99.53	106.33
22	O	203	CLA	C1D-ND-C4D	-9.57	99.54	106.33
22	4	311	CLA	C1D-ND-C4D	-9.57	99.54	106.33
22	A	824	CLA	C1D-ND-C4D	-9.56	99.54	106.33
29	J	104	5X6	C19-C18-C17	-9.56	113.67	127.31
22	B	802	CLA	C2D-C1D-ND	9.56	117.15	110.10
22	B	850	CLA	C1D-ND-C4D	-9.55	99.55	106.33
22	4	305	CLA	C1D-ND-C4D	-9.55	99.55	106.33
29	1	312	5X6	C11-C12-C13	-9.55	111.81	126.23
29	4	315	5X6	C24-C25-C26	-9.54	113.69	127.31
22	A	818	CLA	C2D-C1D-ND	9.54	117.14	110.10
22	B	836	CLA	C1D-ND-C4D	-9.54	99.56	106.33
22	2	310	CLA	C1D-ND-C4D	-9.54	99.56	106.33
29	6	317	5X6	C15-C14-C13	-9.54	113.70	127.31
22	4	309	CLA	C1D-ND-C4D	-9.54	99.56	106.33
22	A	835	CLA	C2D-C1D-ND	9.54	117.13	110.10
22	B	805	CLA	C2D-C1D-ND	9.53	117.13	110.10
22	A	837	CLA	C2D-C1D-ND	9.53	117.12	110.10
22	A	803	CLA	C1D-ND-C4D	-9.52	99.57	106.33
22	B	813	CLA	C1D-ND-C4D	-9.52	99.57	106.33
22	B	804	CLA	C1D-ND-C4D	-9.52	99.57	106.33
22	A	828	CLA	C1D-ND-C4D	-9.51	99.58	106.33
22	7	313	CLA	C1D-ND-C4D	-9.50	99.59	106.33
22	A	836	CLA	C1D-ND-C4D	-9.48	99.60	106.33
22	A	813	CLA	C1D-ND-C4D	-9.48	99.60	106.33
22	B	826	CLA	C1D-ND-C4D	-9.47	99.61	106.33
29	3	306	5X6	C19-C18-C17	-9.46	113.80	127.31
22	5	309	CLA	C1D-ND-C4D	-9.46	99.61	106.33
22	O	204	CLA	C1D-ND-C4D	-9.46	99.62	106.33
22	A	812	CLA	C1D-ND-C4D	-9.46	99.62	106.33
22	5	308	CLA	C1D-ND-C4D	-9.46	99.62	106.33
22	B	816	CLA	C2D-C1D-ND	9.46	117.07	110.10
22	A	806	CLA	C1D-ND-C4D	-9.45	99.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	837	CLA	C1D-ND-C4D	-9.44	99.63	106.33
22	B	820	CLA	C1D-ND-C4D	-9.44	99.63	106.33
22	2	311	CLA	C1D-ND-C4D	-9.43	99.63	106.33
22	Z	204	CLA	C1D-ND-C4D	-9.43	99.64	106.33
22	2	309	CLA	C1D-ND-C4D	-9.43	99.64	106.33
22	A	812	CLA	C2D-C1D-ND	9.42	117.05	110.10
29	1	312	5X6	C38-C30-C29	-9.42	113.95	124.53
22	B	849	CLA	C2D-C1D-ND	9.42	117.04	110.10
22	F	204	CLA	C1D-ND-C4D	-9.40	99.66	106.33
29	7	318	5X6	C01-C02-C03	-9.40	113.97	124.53
29	O	208	5X6	C20-C21-C22	-9.40	113.90	127.31
22	K	102	CLA	C1D-ND-C4D	-9.40	99.66	106.33
22	B	819	CLA	C1D-ND-C4D	-9.40	99.66	106.33
22	4	302	CLA	C1D-ND-C4D	-9.39	99.66	106.33
29	6	317	5X6	C28-C27-C26	-9.39	112.05	126.23
22	3	304	CLA	C1D-ND-C4D	-9.38	99.67	106.33
29	B	851	5X6	C24-C25-C26	-9.38	113.92	127.31
22	6	308	CLA	C1D-ND-C4D	-9.38	99.67	106.33
29	7	316	5X6	C15-C14-C13	-9.36	113.94	127.31
22	B	817	CLA	C1D-ND-C4D	-9.36	99.68	106.33
22	A	825	CLA	C2D-C1D-ND	9.36	117.00	110.10
29	J	104	5X6	C20-C21-C22	-9.35	113.97	127.31
29	O	207	5X6	C15-C14-C13	-9.34	113.98	127.31
22	B	816	CLA	C1D-ND-C4D	-9.34	99.70	106.33
22	6	312	CLA	C1D-ND-C4D	-9.34	99.70	106.33
29	2	314	5X6	C24-C25-C26	-9.33	113.99	127.31
22	A	815	CLA	C1D-ND-C4D	-9.33	99.71	106.33
22	A	828	CLA	C2D-C1D-ND	9.33	116.98	110.10
22	B	839	CLA	C1D-ND-C4D	-9.33	99.71	106.33
22	4	312	CLA	C1D-ND-C4D	-9.33	99.71	106.33
22	B	804	CLA	C2D-C1D-ND	9.32	116.97	110.10
22	Z	201	CLA	C1D-ND-C4D	-9.32	99.71	106.33
22	F	205	CLA	C2D-C1D-ND	9.32	116.97	110.10
22	1	306	CLA	C1D-ND-C4D	-9.31	99.72	106.33
22	B	807	CLA	C1D-ND-C4D	-9.31	99.72	106.33
22	A	835	CLA	C1D-ND-C4D	-9.31	99.72	106.33
22	3	303	CLA	C1D-ND-C4D	-9.31	99.72	106.33
29	5	314	5X6	C24-C25-C26	-9.30	114.04	127.31
29	7	318	5X6	C11-C12-C13	-9.29	112.19	126.23
22	A	811	CLA	C1D-ND-C4D	-9.29	99.74	106.33
22	O	206	CLA	C1D-ND-C4D	-9.28	99.75	106.33
22	6	305	CLA	C1D-ND-C4D	-9.27	99.75	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	833	CLA	C1D-ND-C4D	-9.26	99.76	106.33
29	7	314	5X6	C01-C02-C03	-9.26	114.13	124.53
22	A	808	CLA	C1D-ND-C4D	-9.25	99.76	106.33
22	7	310	CLA	C1D-ND-C4D	-9.25	99.76	106.33
22	B	803	CLA	C1D-ND-C4D	-9.25	99.76	106.33
29	5	312	5X6	C01-C02-C03	-9.24	114.15	124.53
22	B	836	CLA	C2D-C1D-ND	9.24	116.91	110.10
22	A	817	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	7	303	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	6	313	CLA	C1D-ND-C4D	-9.22	99.78	106.33
22	L	203	CLA	C1D-ND-C4D	-9.22	99.78	106.33
22	2	304	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	F	206	CLA	C2D-C1D-ND	9.20	116.89	110.10
22	A	830	CLA	C1D-ND-C4D	-9.20	99.80	106.33
29	7	314	5X6	C24-C25-C26	-9.20	114.19	127.31
22	6	314	CLA	C1D-ND-C4D	-9.19	99.81	106.33
22	3	302	CLA	C1D-ND-C4D	-9.19	99.81	106.33
29	5	314	5X6	C38-C30-C29	-9.18	114.22	124.53
22	6	310	CLA	C1D-ND-C4D	-9.18	99.82	106.33
22	1	309	CLA	C1D-ND-C4D	-9.18	99.82	106.33
22	1	305	CLA	C1D-ND-C4D	-9.17	99.82	106.33
22	6	307	CLA	C1D-ND-C4D	-9.17	99.82	106.33
22	5	305	CLA	C1D-ND-C4D	-9.17	99.82	106.33
22	A	805	CLA	C1D-ND-C4D	-9.16	99.83	106.33
22	A	811	CLA	C2D-C1D-ND	9.16	116.86	110.10
22	B	825	CLA	C2D-C1D-ND	9.15	116.85	110.10
22	A	816	CLA	C1D-ND-C4D	-9.15	99.83	106.33
22	B	830	CLA	C1D-ND-C4D	-9.15	99.84	106.33
22	2	303	CLA	C1D-ND-C4D	-9.13	99.85	106.33
22	B	827	CLA	C1D-ND-C4D	-9.13	99.85	106.33
29	7	315	5X6	C19-C18-C17	-9.13	114.28	127.31
22	4	306	CLA	C1D-ND-C4D	-9.13	99.85	106.33
22	2	306	CLA	C1D-ND-C4D	-9.12	99.86	106.33
22	B	803	CLA	C2D-C1D-ND	9.11	116.82	110.10
22	A	807	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	2	302	CLA	C1D-ND-C4D	-9.09	99.88	106.33
22	A	822	CLA	C1D-ND-C4D	-9.09	99.88	106.33
22	5	310	CLA	C1D-ND-C4D	-9.09	99.88	106.33
22	B	818	CLA	C1D-ND-C4D	-9.08	99.88	106.33
29	6	315	5X6	C38-C30-C29	-9.07	114.34	124.53
29	7	318	5X6	C28-C27-C26	-9.07	112.53	126.23
21	A	801	CL0	C2D-C1D-ND	9.07	116.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	312	5X6	C15-C14-C13	-9.06	114.38	127.31
22	A	802	CLA	C1D-ND-C4D	-9.06	99.90	106.33
22	A	857	CLA	C2D-C1D-ND	9.05	116.77	110.10
22	B	810	CLA	C2D-C1D-ND	9.04	116.77	110.10
22	B	802	CLA	C1D-ND-C4D	-9.04	99.92	106.33
22	B	815	CLA	C1D-ND-C4D	-9.03	99.92	106.33
29	B	851	5X6	C28-C27-C26	-9.03	112.59	126.23
22	L	205	CLA	C1D-ND-C4D	-9.03	99.92	106.33
22	A	806	CLA	C2D-C1D-ND	9.03	116.76	110.10
22	K	101	CLA	C1D-ND-C4D	-9.02	99.93	106.33
29	O	207	5X6	C20-C21-C22	-9.02	114.44	127.31
22	B	826	CLA	C2D-C1D-ND	9.01	116.74	110.10
22	B	809	CLA	C1D-ND-C4D	-9.01	99.94	106.33
22	5	303	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	A	832	CLA	C1D-ND-C4D	-8.98	99.95	106.33
22	A	807	CLA	C2D-C1D-ND	8.98	116.72	110.10
22	A	859	CLA	C2D-C1D-ND	8.97	116.72	110.10
29	1	316	5X6	C24-C25-C26	-8.97	114.50	127.31
22	B	813	CLA	C2D-C1D-ND	8.97	116.71	110.10
29	6	315	5X6	C15-C14-C13	-8.97	114.51	127.31
29	J	104	5X6	C38-C30-C29	-8.97	114.46	124.53
22	5	311	CLA	C1D-ND-C4D	-8.97	99.97	106.33
29	7	317	5X6	C20-C21-C22	-8.96	114.52	127.31
22	7	308	CLA	C1D-ND-C4D	-8.96	99.97	106.33
22	A	810	CLA	C1D-ND-C4D	-8.95	99.98	106.33
22	5	302	CLA	C2D-C1D-ND	8.95	116.70	110.10
22	A	815	CLA	C2D-C1D-ND	8.94	116.69	110.10
29	5	312	5X6	C15-C14-C13	-8.94	114.55	127.31
29	7	316	5X6	C19-C18-C17	-8.94	114.55	127.31
22	B	835	CLA	C2D-C1D-ND	8.93	116.68	110.10
22	J	102	CLA	C1D-ND-C4D	-8.91	100.00	106.33
22	B	834	CLA	C1D-ND-C4D	-8.91	100.01	106.33
22	4	303	CLA	C2D-C1D-ND	8.90	116.66	110.10
29	4	313	5X6	C24-C25-C26	-8.88	114.63	127.31
29	6	315	5X6	C24-C25-C26	-8.88	114.64	127.31
22	A	839	CLA	C1D-ND-C4D	-8.87	100.03	106.33
29	2	313	5X6	C19-C18-C17	-8.87	114.66	127.31
22	A	824	CLA	C2D-C1D-ND	8.86	116.63	110.10
22	A	829	CLA	C1D-ND-C4D	-8.85	100.05	106.33
29	1	316	5X6	C15-C14-C13	-8.85	114.68	127.31
22	7	307	CLA	C1D-ND-C4D	-8.85	100.05	106.33
22	4	304	CLA	C1D-ND-C4D	-8.85	100.05	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	836	CLA	C2D-C1D-ND	8.84	116.62	110.10
22	6	311	CLA	C2D-C1D-ND	8.83	116.61	110.10
22	L	204	CLA	C2D-C1D-ND	8.83	116.61	110.10
29	2	314	5X6	C19-C18-C17	-8.83	114.72	127.31
22	B	817	CLA	C2D-C1D-ND	8.82	116.60	110.10
22	B	827	CLA	C2D-C1D-ND	8.81	116.60	110.10
29	Z	206	5X6	C38-C30-C29	-8.80	114.64	124.53
29	O	207	5X6	C19-C18-C17	-8.80	114.75	127.31
22	B	806	CLA	C2D-C1D-ND	8.79	116.58	110.10
29	6	317	5X6	C20-C21-C22	-8.79	114.77	127.31
22	A	831	CLA	C2D-C1D-ND	8.78	116.58	110.10
22	5	301	CLA	C1D-ND-C4D	-8.78	100.10	106.33
22	A	821	CLA	C2D-C1D-ND	8.78	116.58	110.10
22	4	310	CLA	C1D-ND-C4D	-8.78	100.10	106.33
22	1	304	CLA	C1D-ND-C4D	-8.78	100.10	106.33
22	B	814	CLA	C2D-C1D-ND	8.77	116.57	110.10
29	3	306	5X6	C15-C14-C13	-8.77	114.80	127.31
22	A	819	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	O	203	CLA	C2D-C1D-ND	8.75	116.55	110.10
29	J	104	5X6	C01-C02-C03	-8.74	114.71	124.53
22	B	837	CLA	C2D-C1D-ND	8.73	116.54	110.10
22	B	824	CLA	C2D-C1D-ND	8.73	116.54	110.10
22	A	831	CLA	C1D-ND-C4D	-8.71	100.14	106.33
22	A	813	CLA	C2D-C1D-ND	8.70	116.52	110.10
22	A	826	CLA	C2D-C1D-ND	8.70	116.52	110.10
22	B	811	CLA	C1D-ND-C4D	-8.70	100.16	106.33
29	2	313	5X6	C01-C02-C03	-8.70	114.76	124.53
22	A	826	CLA	C1D-ND-C4D	-8.68	100.17	106.33
29	3	306	5X6	C11-C12-C13	-8.67	113.13	126.23
22	A	817	CLA	C2D-C1D-ND	8.67	116.49	110.10
22	6	309	CLA	C1D-ND-C4D	-8.66	100.18	106.33
29	6	315	5X6	C01-C02-C03	-8.65	114.81	124.53
29	4	315	5X6	C20-C21-C22	-8.65	114.96	127.31
22	B	822	CLA	C2D-C1D-ND	8.65	116.48	110.10
22	2	304	CLA	C2B-C1B-NB	8.64	116.02	110.23
29	5	321	5X6	C20-C21-C22	-8.62	115.01	127.31
22	B	821	CLA	C2D-C1D-ND	8.62	116.46	110.10
22	A	833	CLA	C2D-C1D-ND	8.62	116.45	110.10
29	1	311	5X6	C11-C12-C13	-8.62	113.22	126.23
29	5	314	5X6	C28-C27-C26	-8.61	113.22	126.23
29	7	314	5X6	C41-C17-C18	-8.60	110.88	122.92
22	5	306	CLA	C1D-ND-C4D	-8.60	100.23	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	814	CLA	C2D-C1D-ND	8.60	116.44	110.10
29	5	312	5X6	C28-C27-C26	-8.58	113.26	126.23
29	6	315	5X6	C28-C27-C26	-8.58	113.27	126.23
29	6	317	5X6	C24-C25-C26	-8.58	115.07	127.31
22	B	830	CLA	C2D-C1D-ND	8.57	116.42	110.10
22	B	839	CLA	C2D-C1D-ND	8.56	116.41	110.10
22	5	307	CLA	C2D-C1D-ND	8.56	116.41	110.10
22	6	304	CLA	C2D-C1D-ND	8.56	116.41	110.10
29	1	311	5X6	C28-C27-C26	-8.56	113.31	126.23
22	Z	201	CLA	C2D-C1D-ND	8.55	116.41	110.10
22	4	308	CLA	C2D-C1D-ND	8.55	116.41	110.10
22	B	834	CLA	C2D-C1D-ND	8.55	116.40	110.10
22	B	816	CLA	O2D-CGD-CBD	8.55	126.46	111.27
22	A	802	CLA	C2D-C1D-ND	8.54	116.40	110.10
22	A	822	CLA	C2D-C1D-ND	8.54	116.40	110.10
22	A	834	CLA	C2D-C1D-ND	8.54	116.40	110.10
22	B	801	CLA	C1D-ND-C4D	-8.52	100.28	106.33
22	B	812	CLA	C1D-ND-C4D	-8.52	100.28	106.33
29	6	316	5X6	C24-C25-C26	-8.52	115.14	127.31
22	B	829	CLA	O2D-CGD-CBD	8.52	126.41	111.27
22	B	820	CLA	C2D-C1D-ND	8.52	116.38	110.10
21	A	801	CL0	C1D-ND-C4D	-8.51	100.29	106.33
22	A	858	CLA	C2D-C1D-ND	8.50	116.37	110.10
29	7	314	5X6	C20-C21-C22	-8.48	115.21	127.31
22	A	857	CLA	C1D-ND-C4D	-8.47	100.31	106.33
29	1	314	5X6	C19-C18-C17	-8.47	115.22	127.31
22	3	305	CLA	C2B-C1B-NB	8.47	115.91	110.23
22	A	823	CLA	C1D-ND-C4D	-8.47	100.32	106.33
29	2	312	5X6	C19-C18-C17	-8.44	115.26	127.31
22	Z	204	CLA	C2D-C1D-ND	8.44	116.32	110.10
22	B	833	CLA	C2D-C1D-ND	8.44	116.32	110.10
22	1	310	CLA	C2D-C1D-ND	8.41	116.31	110.10
29	1	314	5X6	C15-C14-C13	-8.41	115.30	127.31
22	B	801	CLA	C2D-C1D-ND	8.41	116.30	110.10
22	O	205	CLA	C2D-C1D-ND	8.40	116.29	110.10
22	B	831	CLA	C2D-C1D-ND	8.39	116.29	110.10
22	K	102	CLA	C2D-C1D-ND	8.39	116.29	110.10
22	A	848	CLA	C2D-C1D-ND	8.39	116.29	110.10
22	A	839	CLA	C2D-C1D-ND	8.38	116.28	110.10
29	7	315	5X6	C01-C02-C03	-8.37	115.12	124.53
29	M	101	5X6	C28-C27-C26	-8.37	113.58	126.23
22	4	304	CLA	C2B-C1B-NB	8.37	115.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	809	CLA	C2D-C1D-ND	8.36	116.26	110.10
29	2	313	5X6	C38-C30-C29	-8.35	115.15	124.53
29	7	315	5X6	C38-C30-C29	-8.35	115.15	124.53
29	7	315	5X6	C15-C14-C13	-8.35	115.40	127.31
22	6	305	CLA	C2D-C1D-ND	8.34	116.25	110.10
29	1	311	5X6	C24-C25-C26	-8.34	115.41	127.31
22	4	303	CLA	C2B-C1B-NB	8.34	115.82	110.23
22	A	848	CLA	C1D-ND-C4D	-8.34	100.41	106.33
29	B	851	5X6	C20-C21-C22	-8.33	115.42	127.31
22	7	305	CLA	C2B-C1B-NB	8.33	115.82	110.23
22	4	311	CLA	C2D-C1D-ND	8.33	116.24	110.10
22	1	305	CLA	C2D-C1D-ND	8.33	116.24	110.10
29	5	312	5X6	C38-C30-C29	-8.32	115.18	124.53
22	A	823	CLA	C2D-C1D-ND	8.32	116.24	110.10
22	5	308	CLA	C2D-C1D-ND	8.32	116.23	110.10
22	A	810	CLA	C2D-C1D-ND	8.31	116.23	110.10
29	7	317	5X6	C11-C12-C13	-8.31	113.68	126.23
22	2	307	CLA	C2B-C1B-NB	8.31	115.80	110.23
29	5	314	5X6	C19-C18-C17	-8.29	115.48	127.31
22	7	305	CLA	C1D-ND-C4D	-8.29	100.45	106.33
22	A	830	CLA	C2D-C1D-ND	8.28	116.21	110.10
22	L	203	CLA	C2D-C1D-ND	8.27	116.20	110.10
29	7	314	5X6	C28-C27-C26	-8.26	113.75	126.23
22	7	313	CLA	C2B-C1B-NB	8.26	115.77	110.23
29	4	313	5X6	C15-C14-C13	-8.26	115.52	127.31
22	6	306	CLA	C2D-C1D-ND	8.25	116.19	110.10
22	7	309	CLA	C2B-C1B-NB	8.25	115.76	110.23
22	6	303	CLA	C2D-C1D-ND	8.25	116.18	110.10
29	6	316	5X6	C19-C18-C17	-8.25	115.54	127.31
22	2	305	CLA	C2B-C1B-NB	8.25	115.76	110.23
22	A	804	CLA	C2D-C1D-ND	8.24	116.18	110.10
22	1	302	CLA	C2D-C1D-ND	8.24	116.18	110.10
29	B	851	5X6	C15-C14-C13	-8.24	115.55	127.31
22	A	832	CLA	C2D-C1D-ND	8.23	116.17	110.10
29	7	316	5X6	C38-C30-C29	-8.23	115.29	124.53
29	4	314	5X6	C24-C25-C26	-8.22	115.58	127.31
22	B	824	CLA	C1D-ND-C4D	-8.22	100.50	106.33
22	2	311	CLA	C2B-C1B-NB	8.21	115.74	110.23
22	A	808	CLA	C2D-C1D-ND	8.20	116.15	110.10
22	5	309	CLA	C2D-C1D-ND	8.20	116.15	110.10
22	1	303	CLA	C2D-C1D-ND	8.20	116.15	110.10
22	6	313	CLA	C2D-C1D-ND	8.19	116.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	803	CLA	C2D-C1D-ND	8.19	116.14	110.10
22	5	303	CLA	C2D-C1D-ND	8.19	116.14	110.10
22	7	306	CLA	C2D-C1D-ND	8.18	116.13	110.10
22	B	819	CLA	C2D-C1D-ND	8.18	116.13	110.10
22	5	304	CLA	C2D-C1D-ND	8.18	116.13	110.10
22	A	829	CLA	C2D-C1D-ND	8.17	116.13	110.10
29	7	316	5X6	C20-C21-C22	-8.17	115.66	127.31
22	B	806	CLA	C1D-ND-C4D	-8.16	100.54	106.33
22	4	309	CLA	C2D-C1D-ND	8.16	116.12	110.10
22	7	312	CLA	C2D-C1D-ND	8.15	116.11	110.10
29	6	317	5X6	C11-C12-C13	-8.14	113.94	126.23
22	B	804	CLA	C2B-C1B-NB	8.13	115.69	110.23
22	3	301	CLA	C2D-C1D-ND	8.13	116.10	110.10
29	J	104	5X6	C28-C27-C26	-8.13	113.95	126.23
29	4	313	5X6	C20-C21-C22	-8.13	115.71	127.31
22	2	309	CLA	C2D-C1D-ND	8.13	116.09	110.10
22	1	307	CLA	C2D-C1D-ND	8.13	116.09	110.10
29	6	316	5X6	C20-C21-C22	-8.13	115.71	127.31
22	4	310	CLA	C2B-C1B-NB	8.12	115.67	110.23
29	2	312	5X6	C11-C12-C13	-8.12	113.97	126.23
22	3	305	CLA	C2D-C1D-ND	8.11	116.08	110.10
29	6	315	5X6	C19-C18-C17	-8.11	115.74	127.31
22	A	819	CLA	C2D-C1D-ND	8.11	116.08	110.10
22	7	308	CLA	C2B-C1B-NB	8.10	115.66	110.23
22	2	305	CLA	C2D-C1D-ND	8.08	116.06	110.10
22	6	309	CLA	C2B-C1B-NB	8.08	115.65	110.23
22	6	313	CLA	C2B-C1B-NB	8.08	115.65	110.23
22	4	308	CLA	C2B-C1B-NB	8.07	115.64	110.23
29	2	312	5X6	C20-C21-C22	-8.07	115.80	127.31
22	O	206	CLA	C2B-C1B-NB	8.06	115.63	110.23
29	6	316	5X6	C15-C14-C13	-8.03	115.85	127.31
22	4	305	CLA	C2D-C1D-ND	8.02	116.01	110.10
22	2	306	CLA	C2B-C1B-NB	8.01	115.61	110.23
22	7	309	CLA	C2D-C1D-ND	8.01	116.00	110.10
29	2	313	5X6	C28-C27-C26	-8.01	114.14	126.23
22	4	311	CLA	C2B-C1B-NB	8.00	115.59	110.23
22	A	827	CLA	C1D-ND-C4D	-7.99	100.66	106.33
22	1	303	CLA	C2B-C1B-NB	7.99	115.59	110.23
22	7	310	CLA	C2D-C1D-ND	7.99	115.99	110.10
29	Z	206	5X6	C19-C18-C17	-7.99	115.91	127.31
22	6	308	CLA	C2D-C1D-ND	7.99	115.99	110.10
22	4	306	CLA	C2D-C1D-ND	7.98	115.99	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	308	CLA	C2D-C1D-ND	7.98	115.98	110.10
22	2	302	CLA	C2D-C1D-ND	7.98	115.98	110.10
29	4	315	5X6	C28-C27-C26	-7.97	114.19	126.23
29	1	313	5X6	C20-C21-C22	-7.96	115.94	127.31
29	7	316	5X6	C28-C27-C26	-7.96	114.20	126.23
29	2	312	5X6	C24-C25-C26	-7.96	115.96	127.31
22	5	306	CLA	C2D-C1D-ND	7.95	115.97	110.10
22	7	304	CLA	C2B-C1B-NB	7.95	115.56	110.23
22	4	302	CLA	C2D-C1D-ND	7.95	115.96	110.10
29	5	313	5X6	C24-C25-C26	-7.95	115.97	127.31
22	6	314	CLA	C2D-C1D-ND	7.93	115.95	110.10
22	6	311	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	L	205	CLA	C2D-C1D-ND	7.92	115.94	110.10
22	6	310	CLA	C2D-C1D-ND	7.92	115.94	110.10
29	5	313	5X6	C20-C21-C22	-7.92	116.01	127.31
22	5	311	CLA	C2B-C1B-NB	7.91	115.54	110.23
22	B	807	CLA	C2D-C1D-ND	7.91	115.94	110.10
22	2	303	CLA	C2B-C1B-NB	7.91	115.53	110.23
22	7	307	CLA	C2B-C1B-NB	7.91	115.53	110.23
22	5	308	CLA	C2B-C1B-NB	7.90	115.53	110.23
29	2	314	5X6	C20-C21-C22	-7.89	116.04	127.31
29	6	315	5X6	C20-C21-C22	-7.89	116.05	127.31
22	3	301	CLA	C2B-C1B-NB	7.89	115.52	110.23
29	2	313	5X6	C15-C14-C13	-7.89	116.05	127.31
22	1	310	CLA	C2B-C1B-NB	7.88	115.52	110.23
29	4	314	5X6	C28-C27-C26	-7.88	114.33	126.23
22	O	204	CLA	C2D-C1D-ND	7.88	115.91	110.10
22	2	307	CLA	C2D-C1D-ND	7.88	115.91	110.10
22	3	304	CLA	C2B-C1B-NB	7.88	115.51	110.23
29	4	314	5X6	C11-C12-C13	-7.88	114.33	126.23
29	7	318	5X6	C19-C18-C17	-7.88	116.07	127.31
29	1	312	5X6	C24-C25-C26	-7.87	116.08	127.31
22	7	313	CLA	C2D-C1D-ND	7.87	115.90	110.10
22	6	314	CLA	C2B-C1B-NB	7.87	115.51	110.23
22	2	310	CLA	C2D-C1D-ND	7.86	115.90	110.10
22	B	850	CLA	C2D-C1D-ND	7.86	115.90	110.10
29	7	317	5X6	C19-C18-C17	-7.86	116.09	127.31
22	7	304	CLA	C2D-C1D-ND	7.86	115.89	110.10
22	7	303	CLA	CMD-C2D-C1D	7.84	138.53	124.71
22	7	312	CLA	C2B-C1B-NB	7.84	115.48	110.23
29	M	101	5X6	C42-C13-C14	-7.83	111.95	122.92
29	7	315	5X6	C11-C12-C13	-7.83	114.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	101	CLA	C2B-C1B-NB	7.82	115.47	110.23
22	B	807	CLA	C2B-C1B-NB	7.82	115.47	110.23
22	B	815	CLA	C2D-C1D-ND	7.82	115.86	110.10
29	1	313	5X6	C38-C30-C29	-7.81	115.75	124.53
22	7	311	CLA	C2D-C1D-ND	7.80	115.85	110.10
29	O	208	5X6	C24-C25-C26	-7.78	116.20	127.31
22	7	303	CLA	C2B-C1B-NB	7.78	115.45	110.23
22	5	310	CLA	C2B-C1B-NB	7.77	115.44	110.23
22	4	307	CLA	C1D-ND-C4D	-7.77	100.82	106.33
22	B	823	CLA	C2D-C1D-ND	7.76	115.83	110.10
22	1	306	CLA	C2D-C1D-ND	7.76	115.82	110.10
22	4	302	CLA	C2B-C1B-NB	7.76	115.43	110.23
22	B	812	CLA	C2D-C1D-ND	7.75	115.82	110.10
29	O	207	5X6	C28-C27-C26	-7.75	114.52	126.23
29	5	321	5X6	C15-C14-C13	-7.75	116.25	127.31
22	5	310	CLA	C2D-C1D-ND	7.75	115.82	110.10
22	4	309	CLA	C2B-C1B-NB	7.75	115.43	110.23
22	5	305	CLA	C2D-C1D-ND	7.74	115.81	110.10
29	1	311	5X6	C15-C14-C13	-7.74	116.26	127.31
22	1	308	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	6	307	CLA	C2D-C1D-ND	7.73	115.80	110.10
22	4	306	CLA	C2B-C1B-NB	7.73	115.42	110.23
22	4	310	CLA	C2D-C1D-ND	7.72	115.80	110.10
22	3	302	CLA	C2D-C1D-ND	7.72	115.79	110.10
29	5	312	5X6	C24-C25-C26	-7.71	116.30	127.31
29	4	313	5X6	C28-C27-C26	-7.71	114.58	126.23
29	1	311	5X6	C19-C18-C17	-7.71	116.30	127.31
29	5	313	5X6	C28-C27-C26	-7.71	114.59	126.23
22	1	305	CLA	C2B-C1B-NB	7.71	115.40	110.23
22	L	204	CLA	C2B-C1B-NB	7.70	115.39	110.23
29	1	316	5X6	C11-C12-C13	-7.70	114.60	126.23
29	7	318	5X6	C24-C25-C26	-7.69	116.33	127.31
22	5	301	CLA	C2D-C1D-ND	7.69	115.77	110.10
22	5	305	CLA	C2B-C1B-NB	7.68	115.38	110.23
22	7	306	CLA	C2B-C1B-NB	7.68	115.38	110.23
22	A	816	CLA	C2D-C1D-ND	7.67	115.76	110.10
22	2	311	CLA	C2D-C1D-ND	7.67	115.76	110.10
29	6	316	5X6	C28-C27-C26	-7.67	114.64	126.23
29	1	316	5X6	C19-C18-C17	-7.66	116.38	127.31
22	B	821	CLA	C2B-C1B-NB	7.66	115.37	110.23
22	5	311	CLA	C2D-C1D-ND	7.65	115.74	110.10
22	6	309	CLA	C2D-C1D-ND	7.65	115.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	303	CLA	C2D-C1D-ND	7.63	115.73	110.10
22	3	303	CLA	C2D-C1D-ND	7.63	115.73	110.10
22	3	304	CLA	C2D-C1D-ND	7.63	115.73	110.10
22	4	312	CLA	C2D-C1D-ND	7.63	115.72	110.10
29	B	851	5X6	C19-C18-C17	-7.62	116.44	127.31
22	2	310	CLA	C2B-C1B-NB	7.62	115.34	110.23
22	K	101	CLA	C2D-C1D-ND	7.62	115.72	110.10
22	B	817	CLA	C2B-C1B-NB	7.59	115.32	110.23
22	J	102	CLA	C2D-C1D-ND	7.59	115.69	110.10
29	2	313	5X6	C20-C21-C22	-7.58	116.49	127.31
22	4	307	CLA	C2D-C1D-ND	7.58	115.69	110.10
22	A	827	CLA	C2D-C1D-ND	7.58	115.69	110.10
22	3	302	CLA	C2B-C1B-NB	7.58	115.31	110.23
29	O	207	5X6	C01-C02-C03	-7.57	116.02	124.53
29	7	314	5X6	C15-C14-C13	-7.57	116.50	127.31
22	6	310	CLA	C2B-C1B-NB	7.57	115.31	110.23
22	B	811	CLA	C2B-C1B-NB	7.57	115.31	110.23
22	B	818	CLA	C2D-C1D-ND	7.57	115.68	110.10
29	2	314	5X6	C28-C27-C26	-7.56	114.81	126.23
22	1	309	CLA	C2B-C1B-NB	7.55	115.30	110.23
22	4	312	CLA	C2B-C1B-NB	7.55	115.30	110.23
22	4	304	CLA	C2D-C1D-ND	7.54	115.66	110.10
22	2	308	CLA	C2B-C1B-NB	7.54	115.29	110.23
29	4	314	5X6	C38-C30-C29	-7.54	116.06	124.53
22	J	102	CLA	C2B-C1B-NB	7.54	115.29	110.23
22	A	802	CLA	C2B-C1B-NB	7.54	115.28	110.23
29	1	316	5X6	C28-C27-C26	-7.53	114.85	126.23
22	6	308	CLA	C2B-C1B-NB	7.53	115.28	110.23
22	L	205	CLA	C2B-C1B-NB	7.53	115.28	110.23
22	6	312	CLA	C2B-C1B-NB	7.53	115.28	110.23
29	4	313	5X6	C19-C18-C17	-7.52	116.57	127.31
22	6	312	CLA	C2D-C1D-ND	7.51	115.64	110.10
29	2	312	5X6	C28-C27-C26	-7.51	114.88	126.23
29	1	314	5X6	C20-C21-C22	-7.51	116.59	127.31
29	1	313	5X6	C11-C12-C13	-7.50	114.90	126.23
22	6	307	CLA	C2B-C1B-NB	7.49	115.25	110.23
22	2	302	CLA	C2B-C1B-NB	7.49	115.25	110.23
22	7	310	CLA	C2B-C1B-NB	7.49	115.25	110.23
29	1	312	5X6	C28-C27-C26	-7.47	114.95	126.23
22	1	309	CLA	C2D-C1D-ND	7.46	115.61	110.10
22	O	205	CLA	C2B-C1B-NB	7.46	115.24	110.23
29	O	208	5X6	C19-C18-C17	-7.46	116.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	206	CLA	C2D-C1D-ND	7.46	115.60	110.10
22	7	311	CLA	C2B-C1B-NB	7.45	115.23	110.23
22	A	804	CLA	C1D-ND-C4D	-7.45	101.04	106.33
29	3	306	5X6	C24-C25-C26	-7.45	116.68	127.31
22	7	307	CLA	C2D-C1D-ND	7.44	115.58	110.10
29	O	208	5X6	C28-C27-C26	-7.43	115.01	126.23
22	2	304	CLA	CMD-C2D-C1D	7.42	137.79	124.71
29	3	306	5X6	C41-C17-C18	-7.42	112.53	122.92
22	A	805	CLA	C2D-C1D-ND	7.41	115.56	110.10
22	B	812	CLA	C2B-C1B-NB	7.41	115.20	110.23
22	4	307	CLA	C2B-C1B-NB	7.41	115.20	110.23
29	7	314	5X6	C11-C12-C13	-7.39	115.06	126.23
29	5	313	5X6	C38-C30-C29	-7.39	116.23	124.53
22	1	302	CLA	C2B-C1B-NB	7.38	115.18	110.23
22	1	307	CLA	C2B-C1B-NB	7.38	115.18	110.23
22	2	306	CLA	C2D-C1D-ND	7.37	115.53	110.10
22	A	809	CLA	C2B-C1B-NB	7.36	115.17	110.23
22	2	309	CLA	C2B-C1B-NB	7.35	115.16	110.23
29	1	312	5X6	C20-C21-C22	-7.35	116.82	127.31
22	6	305	CLA	C2B-C1B-NB	7.34	115.15	110.23
22	A	827	CLA	C2B-C1B-NB	7.34	115.15	110.23
22	1	304	CLA	C2D-C1D-ND	7.34	115.51	110.10
22	5	307	CLA	C2B-C1B-NB	7.32	115.14	110.23
22	B	825	CLA	C2B-C1B-NB	7.32	115.14	110.23
22	1	304	CLA	C2B-C1B-NB	7.30	115.13	110.23
22	2	304	CLA	C2D-C1D-ND	7.30	115.48	110.10
22	7	307	CLA	CMD-C2D-C1D	7.28	137.53	124.71
29	J	104	5X6	C41-C17-C18	-7.27	112.73	122.92
29	M	101	5X6	C39-C26-C25	-7.27	112.74	122.92
22	B	831	CLA	C2B-C1B-NB	7.26	115.10	110.23
22	A	804	CLA	C2C-C1C-NC	7.24	116.75	109.97
29	Z	206	5X6	C01-C02-C03	-7.24	116.40	124.53
29	3	306	5X6	C28-C27-C26	-7.22	115.32	126.23
29	5	321	5X6	C19-C18-C17	-7.22	117.00	127.31
22	1	306	CLA	C2B-C1B-NB	7.22	115.07	110.23
22	3	303	CLA	C2B-C1B-NB	7.22	115.07	110.23
29	M	101	5X6	C11-C12-C13	-7.22	115.33	126.23
29	5	313	5X6	C11-C12-C13	-7.22	115.33	126.23
29	1	313	5X6	C28-C27-C26	-7.21	115.34	126.23
22	B	835	CLA	C2B-C1B-NB	7.20	115.06	110.23
29	4	314	5X6	C20-C21-C22	-7.19	117.05	127.31
29	1	313	5X6	C39-C26-C25	-7.19	112.85	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	317	5X6	C38-C30-C29	-7.18	116.46	124.53
22	5	304	CLA	C2B-C1B-NB	7.18	115.04	110.23
22	O	204	CLA	C2B-C1B-NB	7.17	115.04	110.23
22	A	830	CLA	C2B-C1B-NB	7.17	115.04	110.23
22	B	839	CLA	C2B-C1B-NB	7.16	115.03	110.23
29	J	104	5X6	C11-C12-C13	-7.16	115.42	126.23
22	7	305	CLA	C2D-C1D-ND	7.16	115.38	110.10
22	Z	204	CLA	C2B-C1B-NB	7.15	115.03	110.23
29	5	312	5X6	C11-C12-C13	-7.15	115.43	126.23
22	7	308	CLA	C2D-C1D-ND	7.13	115.36	110.10
22	5	303	CLA	C2B-C1B-NB	7.12	115.01	110.23
29	1	314	5X6	C11-C12-C13	-7.12	115.47	126.23
22	B	850	CLA	C2B-C1B-NB	7.12	115.00	110.23
22	6	303	CLA	C2B-C1B-NB	7.12	115.00	110.23
22	4	305	CLA	C2B-C1B-NB	7.12	115.00	110.23
22	6	307	CLA	CMD-C2D-C1D	7.11	137.24	124.71
29	J	104	5X6	C40-C22-C21	-7.10	112.97	122.92
29	6	315	5X6	C11-C12-C13	-7.10	115.51	126.23
22	A	857	CLA	O2D-CGD-CBD	7.09	123.87	111.27
29	Z	206	5X6	C27-C26-C25	-7.08	108.07	118.94
29	J	104	5X6	C24-C25-C26	-7.08	117.20	127.31
22	B	833	CLA	C2B-C1B-NB	7.08	114.98	110.23
22	1	304	CLA	CMD-C2D-C1D	7.08	137.19	124.71
22	A	859	CLA	O2D-CGD-CBD	7.07	123.83	111.27
22	6	306	CLA	C2B-C1B-NB	7.06	114.97	110.23
22	B	804	CLA	O2D-CGD-CBD	7.06	123.81	111.27
22	A	817	CLA	C2B-C1B-NB	7.06	114.96	110.23
29	6	316	5X6	C38-C30-C29	-7.06	116.61	124.53
22	A	810	CLA	C2B-C1B-NB	7.05	114.96	110.23
29	M	101	5X6	C40-C22-C21	-7.04	113.06	122.92
22	7	303	CLA	C2D-C1D-ND	7.04	115.29	110.10
29	O	207	5X6	C39-C26-C25	-7.03	113.07	122.92
29	1	314	5X6	C28-C27-C26	-7.03	115.62	126.23
29	7	315	5X6	C41-C17-C18	-7.02	113.08	122.92
22	1	308	CLA	C2B-C1B-NB	7.02	114.94	110.23
29	2	313	5X6	C11-C12-C13	-7.02	115.63	126.23
29	5	312	5X6	C19-C18-C17	-7.02	117.30	127.31
22	B	810	CLA	C2B-C1B-NB	7.01	114.93	110.23
29	O	208	5X6	C11-C12-C13	-7.00	115.66	126.23
22	A	834	CLA	C2B-C1B-NB	7.00	114.92	110.23
22	A	815	CLA	C2B-C1B-NB	7.00	114.92	110.23
22	B	819	CLA	C2B-C1B-NB	7.00	114.92	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	808	CLA	O2D-CGD-CBD	6.99	123.68	111.27
22	A	836	CLA	C2B-C1B-NB	6.96	114.90	110.23
29	7	315	5X6	C20-C21-C22	-6.95	117.40	127.31
22	2	306	CLA	CMD-C2D-C1D	6.95	136.95	124.71
22	B	832	CLA	O2D-CGD-CBD	6.94	123.60	111.27
29	7	315	5X6	C28-C27-C26	-6.94	115.75	126.23
22	A	825	CLA	C2B-C1B-NB	6.93	114.88	110.23
22	3	302	CLA	CMD-C2D-C1D	6.93	136.92	124.71
29	1	312	5X6	C40-C22-C21	-6.93	113.22	122.92
29	5	314	5X6	C39-C26-C25	-6.92	113.22	122.92
22	1	307	CLA	CMD-C2D-C1D	6.92	136.91	124.71
22	B	816	CLA	C2B-C1B-NB	6.90	114.86	110.23
29	1	312	5X6	C39-C26-C25	-6.90	113.25	122.92
22	B	837	CLA	C2B-C1B-NB	6.90	114.86	110.23
29	1	314	5X6	C39-C26-C25	-6.89	113.28	122.92
22	B	830	CLA	C2B-C1B-NB	6.88	114.85	110.23
22	B	818	CLA	C2B-C1B-NB	6.88	114.84	110.23
22	4	306	CLA	CMD-C2D-C1D	6.87	136.83	124.71
22	2	304	CLA	CHD-C1D-ND	-6.87	118.14	124.45
29	7	318	5X6	C40-C22-C21	-6.87	113.30	122.92
22	5	309	CLA	C2B-C1B-NB	6.86	114.83	110.23
22	1	302	CLA	CMD-C2D-C1D	6.86	136.80	124.71
22	4	311	CLA	CMD-C2D-C1D	6.86	136.80	124.71
22	A	813	CLA	C2B-C1B-NB	6.85	114.83	110.23
22	2	311	CLA	CMD-C2D-C1D	6.84	136.77	124.71
29	5	321	5X6	C28-C27-C26	-6.84	115.90	126.23
29	O	207	5X6	C11-C12-C13	-6.84	115.90	126.23
22	7	306	CLA	CMD-C2D-C1D	6.84	136.76	124.71
22	B	834	CLA	C2B-C1B-NB	6.83	114.81	110.23
22	1	309	CLA	CMD-C2D-C1D	6.83	136.75	124.71
22	5	301	CLA	C2B-C1B-NB	6.83	114.81	110.23
22	3	301	CLA	CMD-C2D-C1D	6.82	136.73	124.71
22	A	822	CLA	C2B-C1B-NB	6.81	114.80	110.23
22	O	203	CLA	C2B-C1B-NB	6.81	114.80	110.23
29	5	321	5X6	C38-C30-C29	-6.81	116.89	124.53
29	2	314	5X6	C39-C26-C25	-6.80	113.39	122.92
22	A	858	CLA	C2B-C1B-NB	6.80	114.79	110.23
22	5	302	CLA	C2B-C1B-NB	6.80	114.79	110.23
22	B	838	CLA	C2B-C1B-NB	6.79	114.79	110.23
22	A	808	CLA	C2B-C1B-NB	6.79	114.79	110.23
29	4	315	5X6	C19-C18-C17	-6.77	117.64	127.31
22	6	304	CLA	C2B-C1B-NB	6.77	114.77	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	820	CLA	C2B-C1B-NB	6.76	114.77	110.23
22	B	828	CLA	C2B-C1B-NB	6.76	114.77	110.23
22	A	803	CLA	CMD-C2D-C1D	6.75	136.61	124.71
29	4	315	5X6	C42-C13-C14	-6.74	113.49	122.92
22	A	821	CLA	O2D-CGD-CBD	6.73	123.22	111.27
22	6	312	CLA	CMD-C2D-C1D	6.72	136.56	124.71
22	O	205	CLA	CMD-C2D-C1D	6.72	136.56	124.71
22	7	306	CLA	CHD-C1D-ND	-6.71	118.29	124.45
22	B	815	CLA	C2B-C1B-NB	6.70	114.72	110.23
29	7	314	5X6	C40-C22-C21	-6.70	113.54	122.92
29	O	207	5X6	C23-C22-C21	-6.69	108.68	118.94
29	5	314	5X6	C41-C17-C18	-6.69	113.56	122.92
29	5	314	5X6	C40-C22-C21	-6.68	113.57	122.92
22	2	302	CLA	CMD-C2D-C1D	6.68	136.48	124.71
29	7	316	5X6	C42-C13-C14	-6.67	113.58	122.92
22	4	312	CLA	CMD-C2D-C1D	6.67	136.47	124.71
29	O	208	5X6	C39-C26-C25	-6.67	113.58	122.92
22	A	832	CLA	C4A-NA-C1A	-6.67	103.71	106.71
22	6	305	CLA	CMD-C2D-C1D	6.66	136.46	124.71
22	7	305	CLA	CMD-C2D-C1D	6.66	136.45	124.71
29	2	314	5X6	C40-C22-C21	-6.66	113.60	122.92
22	A	828	CLA	O2D-CGD-CBD	6.66	123.09	111.27
22	7	313	CLA	CMD-C2D-C1D	6.66	136.44	124.71
22	5	305	CLA	CMD-C2D-C1D	6.65	136.44	124.71
29	1	312	5X6	C23-C22-C21	-6.65	108.74	118.94
22	A	812	CLA	C2B-C1B-NB	6.64	114.68	110.23
29	7	318	5X6	C15-C14-C13	-6.64	117.84	127.31
22	7	311	CLA	CMD-C2D-C1D	6.63	136.40	124.71
22	B	823	CLA	C2B-C1B-NB	6.63	114.68	110.23
22	A	819	CLA	C2B-C1B-NB	6.63	114.68	110.23
22	2	310	CLA	CMD-C2D-C1D	6.63	136.39	124.71
29	7	315	5X6	C24-C25-C26	-6.62	117.86	127.31
29	B	851	5X6	C20-C19-C18	-6.62	109.91	123.47
22	Z	201	CLA	CMD-C2D-C1D	6.62	136.38	124.71
29	O	207	5X6	C19-C20-C21	-6.62	109.91	123.47
22	3	303	CLA	CMD-C2D-C1D	6.62	136.38	124.71
29	5	321	5X6	C11-C12-C13	-6.62	116.23	126.23
22	7	308	CLA	CMD-C2D-C1D	6.62	136.38	124.71
22	L	203	CLA	C2B-C1B-NB	6.61	114.67	110.23
29	4	313	5X6	C01-C02-C03	-6.61	117.10	124.53
22	O	204	CLA	CMD-C2D-C1D	6.61	136.37	124.71
22	5	304	CLA	CMD-C2D-C1D	6.61	136.36	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	824	CLA	C2B-C1B-NB	6.61	114.66	110.23
22	B	829	CLA	C2B-C1B-NB	6.60	114.66	110.23
29	5	312	5X6	C39-C26-C25	-6.60	113.68	122.92
22	B	814	CLA	C2B-C1B-NB	6.60	114.66	110.23
22	1	308	CLA	CMD-C2D-C1D	6.60	136.34	124.71
22	2	308	CLA	CHD-C1D-ND	-6.59	118.40	124.45
29	6	317	5X6	C19-C18-C17	-6.58	117.92	127.31
29	5	312	5X6	C23-C22-C21	-6.58	108.84	118.94
22	4	310	CLA	CMD-C2D-C1D	6.57	136.29	124.71
22	A	834	CLA	CMD-C2D-C1D	6.56	136.28	124.71
22	K	102	CLA	C2B-C1B-NB	6.56	114.63	110.23
22	A	809	CLA	O2D-CGD-CBD	6.56	122.93	111.27
22	4	304	CLA	CMD-C2D-C1D	6.55	136.26	124.71
29	J	104	5X6	C23-C22-C21	-6.55	108.89	118.94
22	B	822	CLA	C2B-C1B-NB	6.54	114.62	110.23
22	A	821	CLA	C2B-C1B-NB	6.54	114.62	110.23
22	A	805	CLA	C2B-C1B-NB	6.54	114.61	110.23
22	3	304	CLA	CMD-C2D-C1D	6.53	136.22	124.71
22	B	802	CLA	O2D-CGD-CBD	6.53	122.87	111.27
29	1	313	5X6	C19-C20-C21	-6.53	110.10	123.47
29	1	313	5X6	C41-C17-C18	-6.52	113.79	122.92
29	4	315	5X6	C39-C26-C25	-6.52	113.79	122.92
29	M	101	5X6	C41-C17-C18	-6.51	113.80	122.92
22	B	849	CLA	O2D-CGD-CBD	6.51	122.84	111.27
22	A	818	CLA	C2B-C1B-NB	6.51	114.60	110.23
22	O	206	CLA	CMD-C2D-C1D	6.51	136.18	124.71
22	6	308	CLA	CMD-C2D-C1D	6.49	136.15	124.71
29	1	316	5X6	C39-C26-C25	-6.49	113.84	122.92
29	7	317	5X6	C39-C26-C25	-6.48	113.84	122.92
22	7	309	CLA	CHD-C1D-ND	-6.48	118.50	124.45
22	2	307	CLA	CMD-C2D-C1D	6.48	136.13	124.71
29	5	314	5X6	C42-C13-C14	-6.47	113.85	122.92
22	2	305	CLA	CHD-C1D-ND	-6.47	118.51	124.45
29	2	314	5X6	C42-C13-C14	-6.47	113.86	122.92
22	B	811	CLA	C2D-C1D-ND	6.47	114.87	110.10
22	A	829	CLA	C2B-C1B-NB	6.46	114.56	110.23
22	7	309	CLA	CMD-C2D-C1D	6.46	136.09	124.71
29	6	315	5X6	C16-C17-C18	-6.45	109.04	118.94
29	6	317	5X6	C16-C17-C18	-6.45	109.04	118.94
29	7	315	5X6	C27-C26-C25	-6.45	109.04	118.94
29	1	312	5X6	C19-C20-C21	-6.44	110.27	123.47
22	K	101	CLA	CMD-C2D-C1D	6.44	136.07	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	314	CLA	CMD-C2D-C1D	6.44	136.07	124.71
22	3	301	CLA	CHD-C1D-ND	-6.44	118.54	124.45
29	O	208	5X6	C12-C13-C14	-6.43	109.07	118.94
22	A	833	CLA	C2B-C1B-NB	6.42	114.54	110.23
22	7	310	CLA	O2D-CGD-CBD	6.42	122.68	111.27
25	B	844	BCR	C8-C9-C10	6.42	128.79	118.94
22	2	308	CLA	CMD-C2D-C1D	6.42	136.03	124.71
22	1	302	CLA	CHD-C1D-ND	-6.42	118.56	124.45
22	A	811	CLA	C2B-C1B-NB	6.42	114.53	110.23
22	2	307	CLA	CHD-C1D-ND	-6.42	118.56	124.45
22	5	309	CLA	CMD-C2D-C1D	6.41	136.01	124.71
22	2	305	CLA	CMD-C2D-C1D	6.41	136.00	124.71
22	L	203	CLA	CMD-C2D-C1D	6.40	136.00	124.71
22	5	304	CLA	CHD-C1D-ND	-6.40	118.57	124.45
22	A	805	CLA	CMD-C2D-C1D	6.39	135.98	124.71
22	B	811	CLA	O2D-CGD-CBD	6.39	122.62	111.27
22	B	828	CLA	CHD-C1D-ND	-6.38	118.59	124.45
29	Z	206	5X6	C24-C25-C26	-6.38	118.20	127.31
29	3	306	5X6	C20-C21-C22	-6.37	118.22	127.31
29	4	315	5X6	C40-C22-C21	-6.37	114.00	122.92
22	B	822	CLA	O2D-CGD-CBD	6.36	122.58	111.27
22	4	310	CLA	C4A-NA-C1A	-6.36	103.85	106.71
22	B	832	CLA	C2B-C1B-NB	6.35	114.49	110.23
29	4	313	5X6	C11-C12-C13	-6.35	116.64	126.23
22	B	805	CLA	C2B-C1B-NB	6.35	114.49	110.23
22	1	306	CLA	CMD-C2D-C1D	6.35	135.90	124.71
29	7	316	5X6	C39-C26-C25	-6.34	114.03	122.92
22	A	837	CLA	C2B-C1B-NB	6.34	114.48	110.23
22	A	832	CLA	O2D-CGD-CBD	6.34	122.54	111.27
22	A	838	CLA	C2B-C1B-NB	6.34	114.48	110.23
22	5	311	CLA	CMD-C2D-C1D	6.33	135.87	124.71
29	1	314	5X6	C19-C20-C21	-6.33	110.50	123.47
29	4	313	5X6	C40-C22-C21	-6.33	114.06	122.92
22	1	309	CLA	CHD-C1D-ND	-6.33	118.64	124.45
22	B	850	CLA	CMD-C2D-C1D	6.32	135.85	124.71
22	1	307	CLA	CHD-C1D-ND	-6.32	118.65	124.45
29	7	318	5X6	C41-C17-C18	-6.31	114.08	122.92
29	2	313	5X6	C40-C22-C21	-6.31	114.08	122.92
22	A	826	CLA	C2B-C1B-NB	6.31	114.46	110.23
22	7	303	CLA	CHD-C1D-ND	-6.31	118.66	124.45
29	5	321	5X6	C16-C17-C18	-6.31	109.26	118.94
22	B	809	CLA	C2C-C1C-NC	6.30	115.88	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	309	CLA	CMD-C2D-C1D	6.30	135.82	124.71
29	7	318	5X6	C20-C19-C18	-6.30	110.57	123.47
22	5	306	CLA	C2B-C1B-NB	6.30	114.45	110.23
29	5	312	5X6	C19-C20-C21	-6.30	110.58	123.47
22	2	306	CLA	CHD-C1D-ND	-6.29	118.67	124.45
22	2	302	CLA	O2D-CGD-CBD	6.29	122.44	111.27
29	O	208	5X6	C01-C02-C03	-6.29	117.47	124.53
22	3	302	CLA	CHD-C1D-ND	-6.29	118.68	124.45
22	A	832	CLA	C2B-C1B-NB	6.28	114.44	110.23
22	B	836	CLA	O2D-CGD-CBD	6.28	122.42	111.27
22	3	304	CLA	CHD-C1D-ND	-6.27	118.69	124.45
22	B	813	CLA	C2B-C1B-NB	6.26	114.43	110.23
22	Z	201	CLA	C2B-C1B-NB	6.26	114.43	110.23
22	6	313	CLA	CMD-C2D-C1D	6.26	135.74	124.71
29	2	314	5X6	C11-C12-C13	-6.26	116.78	126.23
22	A	835	CLA	C2B-C1B-NB	6.25	114.42	110.23
29	5	312	5X6	C20-C21-C22	-6.25	118.39	127.31
22	A	804	CLA	CMD-C2D-C1D	6.25	135.72	124.71
22	7	313	CLA	CHD-C1D-ND	-6.24	118.72	124.45
29	4	315	5X6	C16-C17-C18	-6.24	109.37	118.94
22	A	857	CLA	CHD-C1D-ND	-6.24	118.72	124.45
22	A	809	CLA	CMD-C2D-C1D	6.24	135.71	124.71
22	5	303	CLA	CMD-C2D-C1D	6.24	135.70	124.71
22	B	849	CLA	C2B-C1B-NB	6.24	114.41	110.23
22	B	827	CLA	C2C-C1C-NC	6.23	115.81	109.97
22	3	305	CLA	CMD-C2D-C1D	6.23	135.70	124.71
22	6	306	CLA	CMD-C2D-C1D	6.23	135.70	124.71
22	A	806	CLA	C2B-C1B-NB	6.23	114.41	110.23
22	B	816	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
29	1	312	5X6	C01-C02-C03	-6.23	117.54	124.53
29	6	316	5X6	C39-C26-C25	-6.23	114.20	122.92
22	F	204	CLA	C2B-C1B-NB	6.22	114.40	110.23
29	O	208	5X6	C15-C14-C13	-6.22	118.43	127.31
29	J	104	5X6	C27-C26-C25	-6.22	109.40	118.94
29	6	316	5X6	C11-C12-C13	-6.21	116.85	126.23
29	4	315	5X6	C11-C12-C13	-6.21	116.85	126.23
22	4	308	CLA	CHD-C1D-ND	-6.19	118.77	124.45
22	B	827	CLA	CMD-C2D-C1D	6.19	135.62	124.71
22	3	303	CLA	CHD-C1D-ND	-6.19	118.77	124.45
29	1	313	5X6	C42-C13-C14	-6.19	114.26	122.92
22	A	809	CLA	CHD-C1D-ND	-6.19	118.77	124.45
22	A	820	CLA	C2B-C1B-NB	6.18	114.38	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	813	CLA	O2D-CGD-CBD	6.18	122.25	111.27
22	A	803	CLA	C2C-C1C-NC	6.18	115.76	109.97
29	J	104	5X6	C19-C20-C21	-6.18	110.81	123.47
22	A	859	CLA	C2C-C1C-NC	6.18	115.76	109.97
22	7	307	CLA	CHD-C1D-ND	-6.18	118.78	124.45
22	B	825	CLA	O2D-CGD-CBD	6.17	122.24	111.27
22	2	310	CLA	CHD-C1D-ND	-6.17	118.78	124.45
22	B	802	CLA	C2B-C1B-NB	6.17	114.37	110.23
22	A	825	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
22	2	303	CLA	CMD-C2D-C1D	6.17	135.58	124.71
22	B	815	CLA	O2D-CGD-CBD	6.16	122.22	111.27
22	5	308	CLA	CMD-C2D-C1D	6.16	135.57	124.71
29	1	314	5X6	C39-C26-C27	-6.16	108.38	118.08
22	7	308	CLA	CHD-C1D-ND	-6.15	118.80	124.45
22	5	305	CLA	CHD-C1D-ND	-6.14	118.81	124.45
22	F	205	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
29	2	313	5X6	C19-C20-C21	-6.14	110.89	123.47
29	4	315	5X6	C41-C17-C18	-6.14	114.32	122.92
22	A	824	CLA	C2B-C1B-NB	6.14	114.35	110.23
22	4	306	CLA	CHD-C1D-ND	-6.14	118.81	124.45
22	B	826	CLA	C2B-C1B-NB	6.13	114.34	110.23
22	2	311	CLA	CHD-C1D-ND	-6.13	118.83	124.45
22	1	310	CLA	CMD-C2D-C1D	6.12	135.50	124.71
22	1	308	CLA	CHD-C1D-ND	-6.12	118.83	124.45
22	7	311	CLA	CHD-C1D-ND	-6.12	118.83	124.45
22	7	312	CLA	CMD-C2D-C1D	6.11	135.48	124.71
22	B	819	CLA	CHD-C1D-ND	-6.11	118.84	124.45
22	Z	201	CLA	CHD-C1D-ND	-6.11	118.84	124.45
22	J	102	CLA	CMD-C2D-C1D	6.11	135.48	124.71
22	3	305	CLA	CHD-C1D-ND	-6.11	118.84	124.45
22	6	312	CLA	CHD-C1D-ND	-6.10	118.85	124.45
22	4	312	CLA	O2D-CGD-CBD	6.09	122.08	111.27
29	2	312	5X6	C41-C17-C18	-6.09	114.40	122.92
22	2	303	CLA	CHD-C1D-ND	-6.08	118.86	124.45
22	4	312	CLA	CHD-C1D-ND	-6.08	118.87	124.45
22	2	309	CLA	CMD-C2D-C1D	6.08	135.42	124.71
22	B	812	CLA	CMD-C2D-C1D	6.07	135.41	124.71
22	4	309	CLA	CHD-C1D-ND	-6.07	118.88	124.45
29	7	317	5X6	C28-C29-C30	-6.06	106.77	121.46
22	A	836	CLA	C2C-C1C-NC	6.06	115.64	109.97
22	A	837	CLA	O2D-CGD-CBD	6.05	122.02	111.27
22	5	310	CLA	CMD-C2D-C1D	6.05	135.38	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	206	CLA	C2B-C1B-NB	6.05	114.29	110.23
22	6	307	CLA	CHD-C1D-ND	-6.05	118.89	124.45
22	A	838	CLA	O2D-CGD-CBD	6.05	122.02	111.27
22	B	836	CLA	C2C-C1C-NC	6.05	115.64	109.97
29	6	316	5X6	C42-C13-C12	-6.05	108.55	118.08
22	A	818	CLA	O2D-CGD-CBD	6.04	122.01	111.27
22	B	835	CLA	O2D-CGD-CBD	6.04	122.01	111.27
29	7	316	5X6	C41-C17-C18	-6.04	114.46	122.92
22	B	807	CLA	CMD-C2D-C1D	6.04	135.36	124.71
22	A	834	CLA	CHD-C1D-ND	-6.04	118.91	124.45
22	A	838	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
22	A	823	CLA	C2B-C1B-NB	6.03	114.28	110.23
22	B	839	CLA	O2D-CGD-CBD	6.03	121.98	111.27
29	1	316	5X6	C40-C22-C21	-6.03	114.48	122.92
29	2	314	5X6	C19-C20-C21	-6.02	111.13	123.47
22	O	205	CLA	CHD-C1D-ND	-6.02	118.92	124.45
22	6	314	CLA	CHD-C1D-ND	-6.01	118.93	124.45
22	5	311	CLA	CHD-C1D-ND	-6.01	118.93	124.45
29	1	313	5X6	C40-C22-C21	-6.01	114.50	122.92
22	2	308	CLA	C4A-NA-C1A	-6.01	104.00	106.71
22	O	206	CLA	CHD-C1D-ND	-6.01	118.93	124.45
29	Z	206	5X6	C15-C14-C13	-6.01	118.73	127.31
29	6	316	5X6	C01-C02-C03	-6.01	117.78	124.53
22	1	303	CLA	CMD-C2D-C1D	6.01	135.30	124.71
22	O	204	CLA	CHD-C1D-ND	-6.00	118.94	124.45
29	4	313	5X6	C39-C26-C25	-6.00	114.52	122.92
29	Z	206	5X6	C19-C20-C21	-6.00	111.19	123.47
22	6	306	CLA	CHD-C1D-ND	-5.99	118.95	124.45
22	A	807	CLA	C2B-C1B-NB	5.99	114.25	110.23
22	4	311	CLA	CHD-C1D-ND	-5.99	118.95	124.45
22	A	831	CLA	C2B-C1B-NB	5.99	114.25	110.23
22	5	307	CLA	CHD-C1D-ND	-5.98	118.96	124.45
29	J	104	5X6	C39-C26-C25	-5.98	114.54	122.92
22	A	804	CLA	C2B-C1B-NB	5.97	114.24	110.23
29	7	317	5X6	C19-C20-C21	-5.97	111.24	123.47
22	A	816	CLA	C2B-C1B-NB	5.97	114.23	110.23
22	A	826	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
22	B	850	CLA	CHD-C1D-ND	-5.97	118.97	124.45
29	7	317	5X6	C40-C22-C21	-5.97	114.57	122.92
22	6	306	CLA	O2D-CGD-CBD	5.96	121.87	111.27
22	Z	204	CLA	CMD-C2D-C1D	5.96	135.22	124.71
22	1	305	CLA	CMD-C2D-C1D	5.96	135.22	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	815	CLA	CMD-C2D-C1D	5.96	135.21	124.71
22	B	807	CLA	CHD-C1D-ND	-5.96	118.98	124.45
22	4	303	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
22	B	832	CLA	CMD-C2D-C1D	5.95	135.21	124.71
29	O	207	5X6	C27-C26-C25	-5.94	109.82	118.94
29	7	314	5X6	C19-C18-C17	-5.94	118.83	127.31
22	7	304	CLA	CMD-C2D-C1D	5.94	135.19	124.71
29	5	313	5X6	C40-C22-C21	-5.94	114.60	122.92
22	7	312	CLA	CHD-C1D-ND	-5.94	119.00	124.45
22	B	827	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
29	7	314	5X6	C39-C26-C25	-5.94	114.61	122.92
29	6	315	5X6	C19-C20-C21	-5.94	111.31	123.47
22	6	308	CLA	CHD-C1D-ND	-5.93	119.00	124.45
22	F	206	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
22	B	836	CLA	C2B-C1B-NB	5.93	114.21	110.23
29	5	312	5X6	C42-C13-C14	-5.93	114.62	122.92
22	B	818	CLA	O2D-CGD-CBD	5.92	121.80	111.27
29	O	207	5X6	C42-C13-C14	-5.92	114.64	122.92
29	7	314	5X6	C42-C13-C14	-5.91	114.64	122.92
22	O	203	CLA	CMD-C2D-C1D	5.91	135.13	124.71
22	A	838	CLA	CMD-C2D-C1D	5.91	135.13	124.71
29	1	311	5X6	C16-C17-C18	-5.91	109.88	118.94
29	7	316	5X6	C19-C20-C21	-5.90	111.38	123.47
29	6	316	5X6	C41-C17-C18	-5.90	114.66	122.92
22	5	307	CLA	CMD-C2D-C1D	5.90	135.11	124.71
22	B	822	CLA	C2C-C1C-NC	5.90	115.50	109.97
29	3	306	5X6	C20-C19-C18	-5.90	111.39	123.47
22	A	835	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
29	O	207	5X6	C40-C22-C21	-5.89	114.67	122.92
29	6	317	5X6	C42-C13-C14	-5.89	114.67	122.92
22	B	803	CLA	C2C-C1C-NC	5.89	115.49	109.97
22	K	102	CLA	CMD-C2D-C1D	5.89	135.10	124.71
21	A	801	CL0	C2B-C1B-NB	5.89	114.18	110.23
22	6	309	CLA	CMD-C2D-C1D	5.89	135.09	124.71
22	A	820	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	1	310	CLA	CHD-C1D-ND	-5.88	119.05	124.45
21	A	801	CL0	C2C-C1C-NC	5.88	115.48	109.97
22	J	102	CLA	CHD-C1D-ND	-5.88	119.05	124.45
22	1	306	CLA	CHD-C1D-ND	-5.88	119.05	124.45
29	7	315	5X6	C42-C13-C14	-5.88	114.69	122.92
22	5	308	CLA	CHD-C1D-ND	-5.87	119.06	124.45
29	1	311	5X6	C28-C29-C30	-5.87	107.24	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	816	CLA	CMD-C2D-C1D	5.87	135.05	124.71
22	B	832	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
22	A	825	CLA	O2D-CGD-CBD	5.86	121.68	111.27
22	B	804	CLA	CMD-C2D-C1D	5.86	135.04	124.71
22	7	309	CLA	C4A-NA-C1A	-5.86	104.07	106.71
22	4	308	CLA	CMD-C2D-C1D	5.85	135.02	124.71
22	5	302	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
22	6	304	CLA	CMD-C2D-C1D	5.84	135.01	124.71
22	B	804	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
22	A	831	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
29	7	314	5X6	C20-C19-C18	-5.83	111.53	123.47
22	B	839	CLA	CMD-C2D-C1D	5.82	134.97	124.71
22	A	823	CLA	C2C-C1C-NC	5.82	115.42	109.97
22	4	303	CLA	CMD-C2D-C1D	5.82	134.97	124.71
29	3	306	5X6	C42-C13-C14	-5.82	114.78	122.92
29	5	321	5X6	C19-C20-C21	-5.81	111.56	123.47
22	6	303	CLA	CMD-C2D-C1D	5.81	134.96	124.71
22	A	859	CLA	CMD-C2D-C1D	5.81	134.95	124.71
22	B	826	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
29	5	321	5X6	C40-C22-C21	-5.81	114.79	122.92
29	1	313	5X6	C23-C22-C21	-5.80	110.04	118.94
29	7	316	5X6	C11-C12-C13	-5.80	117.47	126.23
22	F	204	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
22	A	803	CLA	C2B-C1B-NB	5.79	114.12	110.23
22	B	803	CLA	C2B-C1B-NB	5.79	114.12	110.23
29	J	104	5X6	C20-C19-C18	-5.79	111.61	123.47
22	B	837	CLA	CMD-C2D-C1D	5.79	134.92	124.71
22	B	850	CLA	C2C-C1C-NC	5.79	115.39	109.97
22	A	813	CLA	CMD-C2D-C1D	5.79	134.91	124.71
22	2	302	CLA	CHD-C1D-ND	-5.79	119.14	124.45
29	5	321	5X6	C39-C26-C25	-5.79	114.82	122.92
22	B	805	CLA	CHD-C1D-ND	-5.79	119.14	124.45
22	4	302	CLA	CMD-C2D-C1D	5.78	134.91	124.71
22	A	857	CLA	C2C-C1C-NC	5.78	115.39	109.97
22	F	206	CLA	CMD-C2D-C1D	5.78	134.90	124.71
22	B	802	CLA	C2C-C1C-NC	5.78	115.39	109.97
29	1	312	5X6	C27-C26-C25	-5.78	110.08	118.94
22	A	807	CLA	C2C-C1C-NC	5.78	115.38	109.97
22	6	311	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
22	A	823	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
29	Z	206	5X6	C39-C26-C25	-5.77	114.85	122.92
22	4	304	CLA	CHD-C1D-ND	-5.77	119.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	808	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
22	A	802	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
22	B	835	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
29	1	311	5X6	C19-C20-C21	-5.76	111.67	123.47
29	J	104	5X6	C16-C17-C18	-5.76	110.10	118.94
22	A	812	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
22	B	819	CLA	CMD-C2D-C1D	5.76	134.86	124.71
22	B	810	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
29	O	207	5X6	C16-C17-C18	-5.76	110.11	118.94
22	B	824	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
22	A	822	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	6	307	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	A	827	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	B	818	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	B	818	CLA	CMD-C2D-C1D	5.75	134.85	124.71
29	O	208	5X6	C16-C17-C18	-5.75	110.12	118.94
22	B	826	CLA	O2D-CGD-CBD	5.75	121.48	111.27
22	4	311	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
22	1	303	CLA	CHD-C1D-ND	-5.74	119.18	124.45
22	L	204	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
22	A	811	CLA	CMD-C2D-C1D	5.74	134.83	124.71
29	2	312	5X6	C40-C22-C21	-5.74	114.89	122.92
22	6	304	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
29	6	317	5X6	C20-C19-C18	-5.73	111.73	123.47
22	B	801	CLA	C2B-C1B-NB	5.73	114.08	110.23
22	B	836	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
22	A	820	CLA	C2C-C1C-NC	5.73	115.34	109.97
22	A	835	CLA	C2C-C1C-NC	5.72	115.33	109.97
22	6	305	CLA	CHD-C1D-ND	-5.72	119.20	124.45
29	1	312	5X6	C41-C17-C18	-5.71	114.92	122.92
22	B	811	CLA	CMD-C2D-C1D	5.71	134.78	124.71
29	6	315	5X6	C23-C22-C21	-5.71	110.17	118.94
22	6	309	CLA	CHD-C1D-ND	-5.71	119.20	124.45
22	B	827	CLA	C2B-C1B-NB	5.71	114.06	110.23
22	B	838	CLA	O2D-CGD-CBD	5.71	121.41	111.27
22	F	206	CLA	O2D-CGD-CBD	5.71	121.41	111.27
22	A	857	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
29	J	104	5X6	C12-C11-C03	-5.71	111.18	127.20
22	5	309	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
29	Z	206	5X6	C12-C13-C14	-5.70	110.19	118.94
22	7	305	CLA	CHD-C1D-ND	-5.70	119.22	124.45
29	5	313	5X6	C19-C18-C17	-5.70	119.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	839	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
22	B	816	CLA	CMD-C2D-C1D	5.69	134.75	124.71
22	F	205	CLA	CMD-C2D-C1D	5.69	134.75	124.71
22	A	839	CLA	C2B-C1B-NB	5.69	114.05	110.23
22	7	304	CLA	C4A-NA-C1A	-5.69	104.15	106.71
22	A	802	CLA	O2D-CGD-CBD	5.68	121.37	111.27
29	5	314	5X6	C16-C17-C18	-5.68	110.22	118.94
29	6	316	5X6	C19-C20-C21	-5.68	111.84	123.47
29	5	312	5X6	C27-C26-C25	-5.68	110.22	118.94
29	1	316	5X6	C42-C13-C14	-5.68	114.97	122.92
22	4	308	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
22	7	304	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
29	5	321	5X6	C42-C13-C14	-5.67	114.97	122.92
22	A	858	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
22	A	806	CLA	C2C-C1C-NC	5.66	115.28	109.97
22	A	805	CLA	C2C-C1C-NC	5.66	115.28	109.97
22	B	825	CLA	CHD-C1D-ND	-5.66	119.25	124.45
22	L	205	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
22	6	303	CLA	CHD-C1D-ND	-5.66	119.25	124.45
22	7	304	CLA	CHD-C1D-ND	-5.66	119.26	124.45
22	A	828	CLA	C2C-C1C-NC	5.65	115.27	109.97
22	O	203	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
22	A	818	CLA	C2C-C1C-NC	5.65	115.27	109.97
22	B	829	CLA	C2C-C1C-NC	5.65	115.27	109.97
22	B	807	CLA	O2D-CGD-CBD	5.65	121.31	111.27
22	A	837	CLA	CHD-C1D-ND	-5.65	119.27	124.45
22	5	302	CLA	CHD-C1D-ND	-5.65	119.27	124.45
22	A	848	CLA	C2B-C1B-NB	5.64	114.02	110.23
22	A	820	CLA	O2D-CGD-CBD	5.64	121.30	111.27
29	2	313	5X6	C42-C13-C14	-5.64	115.02	122.92
29	6	317	5X6	C40-C22-C21	-5.64	115.02	122.92
22	B	834	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	A	820	CLA	CHD-C1D-ND	-5.64	119.27	124.45
22	K	101	CLA	CHD-C1D-ND	-5.63	119.28	124.45
22	A	826	CLA	CHD-C1D-ND	-5.63	119.28	124.45
29	4	313	5X6	C42-C13-C14	-5.63	115.04	122.92
22	A	826	CLA	C2C-C1C-NC	5.62	115.23	109.97
22	Z	204	CLA	C2C-C1C-NC	5.62	115.23	109.97
22	B	809	CLA	CMD-C2D-C1D	5.62	134.61	124.71
29	Z	206	5X6	C20-C21-C22	-5.61	119.30	127.31
22	L	203	CLA	C2C-C1C-NC	5.61	115.23	109.97
22	7	310	CLA	CMD-C2D-C1D	5.61	134.60	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	848	CLA	CMD-C2D-C1D	5.61	134.59	124.71
22	A	830	CLA	C2C-C1C-NC	5.60	115.22	109.97
22	5	306	CLA	CMD-C2D-C1D	5.60	134.58	124.71
22	B	808	CLA	C2B-C1B-NB	5.60	113.98	110.23
22	A	859	CLA	C2B-C1B-NB	5.60	113.98	110.23
29	2	312	5X6	C42-C13-C14	-5.59	115.09	122.92
22	B	839	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
22	A	823	CLA	O2D-CGD-CBD	5.59	121.21	111.27
29	1	314	5X6	C40-C22-C21	-5.59	115.09	122.92
22	B	832	CLA	CHD-C1D-ND	-5.59	119.32	124.45
22	B	820	CLA	O2D-CGD-CBD	5.59	121.20	111.27
29	M	101	5X6	C12-C11-C03	-5.59	111.52	127.20
22	B	824	CLA	C2C-C1C-NC	5.58	115.20	109.97
22	A	818	CLA	CHD-C1D-ND	-5.58	119.33	124.45
22	7	308	CLA	C4A-NA-C1A	-5.58	104.20	106.71
22	1	305	CLA	CHD-C1D-ND	-5.58	119.33	124.45
22	Z	201	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
29	B	851	5X6	C11-C12-C13	-5.57	117.81	126.23
22	B	815	CLA	CHD-C1D-ND	-5.57	119.33	124.45
22	B	805	CLA	O2D-CGD-CBD	5.57	121.17	111.27
22	4	305	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	4	303	CLA	O2D-CGD-CBD	5.57	121.16	111.27
22	B	806	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
22	6	304	CLA	O2D-CGD-CBD	5.57	121.16	111.27
22	A	822	CLA	CMD-C2D-C1D	5.56	134.52	124.71
22	1	310	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
22	B	808	CLA	CMD-C2D-C1D	5.56	134.52	124.71
22	A	837	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
22	5	311	CLA	O2D-CGD-CBD	5.56	121.15	111.27
22	A	823	CLA	CMD-C2D-C1D	5.56	134.51	124.71
29	2	314	5X6	C41-C17-C18	-5.56	115.14	122.92
29	5	313	5X6	C42-C13-C14	-5.56	115.14	122.92
22	4	303	CLA	C4A-NA-C1A	-5.56	104.21	106.71
29	4	314	5X6	C19-C20-C21	-5.55	112.10	123.47
22	5	301	CLA	C2C-C1C-NC	5.55	115.17	109.97
22	A	818	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
22	4	303	CLA	CHD-C1D-ND	-5.55	119.35	124.45
22	A	808	CLA	C4A-NA-C1A	-5.55	104.21	106.71
22	A	818	CLA	CMD-C2D-C1D	5.55	134.49	124.71
22	3	301	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
22	B	813	CLA	CMD-C2D-C1D	5.55	134.49	124.71
22	B	831	CLA	O2D-CGD-CBD	5.55	121.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	805	CLA	CHD-C1D-ND	-5.54	119.36	124.45
22	Z	204	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
22	6	313	CLA	CHD-C1D-ND	-5.54	119.36	124.45
29	Z	206	5X6	C42-C13-C14	-5.54	115.16	122.92
22	4	307	CLA	C2C-C1C-NC	5.54	115.16	109.97
29	4	314	5X6	C01-C02-C03	-5.54	118.31	124.53
22	A	815	CLA	CMD-C2D-C1D	5.54	134.47	124.71
22	B	838	CLA	C2C-C1C-NC	5.53	115.16	109.97
22	6	303	CLA	C2C-C1C-NC	5.53	115.16	109.97
22	5	307	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
22	5	302	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	B	835	CLA	CMD-C2D-C1D	5.52	134.45	124.71
22	B	834	CLA	O2D-CGD-CBD	5.52	121.08	111.27
22	B	802	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
22	A	821	CLA	C2C-C1C-NC	5.52	115.15	109.97
22	7	305	CLA	C4A-NA-C1A	-5.52	104.22	106.71
22	B	803	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
22	K	102	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
29	4	315	5X6	C19-C20-C21	-5.52	112.16	123.47
22	A	835	CLA	O2D-CGD-CBD	5.52	121.08	111.27
22	A	815	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
22	B	830	CLA	C2C-C1C-NC	5.52	115.14	109.97
22	B	821	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
22	4	302	CLA	CHD-C1D-ND	-5.52	119.38	124.45
29	6	315	5X6	C20-C19-C18	-5.52	112.17	123.47
29	6	316	5X6	C40-C22-C21	-5.52	115.20	122.92
22	B	817	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
22	B	829	CLA	CHD-C1D-ND	-5.52	119.39	124.45
22	5	310	CLA	CHD-C1D-ND	-5.51	119.39	124.45
22	A	826	CLA	CMD-C2D-C1D	5.51	134.43	124.71
22	A	817	CLA	O2D-CGD-CBD	5.51	121.06	111.27
22	A	859	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	A	813	CLA	C2C-C1C-NC	5.51	115.13	109.97
22	A	824	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	A	826	CLA	C3C-C4C-NC	5.51	116.75	110.57
29	6	317	5X6	C27-C28-C29	-5.50	111.75	127.20
22	B	823	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
22	A	810	CLA	C2C-C1C-NC	5.50	115.13	109.97
22	7	303	CLA	O2D-CGD-CBD	5.50	121.04	111.27
22	A	817	CLA	CHD-C1D-ND	-5.50	119.40	124.45
22	A	813	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
29	O	208	5X6	C40-C22-C21	-5.50	115.22	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	819	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
22	L	205	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	A	824	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
29	2	314	5X6	C23-C22-C21	-5.49	110.51	118.94
29	M	101	5X6	C27-C28-C29	-5.49	111.78	127.20
22	B	831	CLA	C2C-C1C-NC	5.49	115.11	109.97
22	7	312	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
22	B	825	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
22	5	309	CLA	CHD-C1D-ND	-5.49	119.41	124.45
22	B	817	CLA	CMD-C2D-C1D	5.48	134.38	124.71
29	2	313	5X6	C24-C25-C26	-5.48	119.48	127.31
29	4	313	5X6	C19-C20-C21	-5.48	112.24	123.47
22	A	805	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
29	4	315	5X6	C01-C02-C03	-5.48	118.38	124.53
22	B	837	CLA	C2C-C1C-NC	5.48	115.10	109.97
22	2	311	CLA	C4A-NA-C1A	-5.48	104.24	106.71
29	1	316	5X6	C19-C20-C21	-5.47	112.26	123.47
22	B	827	CLA	CHD-C1D-ND	-5.47	119.43	124.45
22	A	821	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
22	B	838	CLA	CHD-C1D-ND	-5.47	119.43	124.45
22	A	848	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
22	4	310	CLA	C2C-C1C-NC	5.47	115.09	109.97
22	1	309	CLA	C2C-C1C-NC	5.46	115.09	109.97
22	A	834	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
29	O	207	5X6	C20-C19-C18	-5.46	112.28	123.47
29	5	314	5X6	C19-C20-C21	-5.46	112.29	123.47
29	2	313	5X6	C41-C17-C18	-5.46	115.27	122.92
22	B	837	CLA	CHD-C1D-ND	-5.46	119.44	124.45
22	A	814	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	O	208	5X6	C41-C17-C18	-5.45	115.28	122.92
22	B	811	CLA	CHD-C1D-ND	-5.45	119.44	124.45
22	B	823	CLA	CMD-C2D-C1D	5.45	134.32	124.71
29	O	208	5X6	C27-C26-C25	-5.45	110.58	118.94
22	A	829	CLA	CMD-C2D-C1D	5.45	134.32	124.71
29	4	314	5X6	C23-C22-C21	-5.45	110.58	118.94
22	O	206	CLA	C2C-C1C-NC	5.45	115.07	109.97
22	7	309	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
29	5	314	5X6	C12-C11-C03	-5.45	111.91	127.20
22	B	830	CLA	CHD-C1D-ND	-5.44	119.45	124.45
22	B	836	CLA	CMD-C2D-C1D	5.44	134.30	124.71
22	B	810	CLA	O2D-CGD-CBD	5.44	120.93	111.27
22	A	832	CLA	CMD-C2D-C1D	5.44	134.29	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	306	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
22	A	859	CLA	CHD-C1D-ND	-5.43	119.46	124.45
22	F	205	CLA	C2B-C1B-NB	5.43	113.87	110.23
29	5	313	5X6	C20-C19-C18	-5.43	112.36	123.47
22	B	820	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	1	314	5X6	C27-C28-C29	-5.43	111.96	127.20
22	B	849	CLA	CHD-C1D-ND	-5.43	119.47	124.45
22	L	204	CLA	O2D-CGD-CBD	5.42	120.91	111.27
22	B	824	CLA	O2D-CGD-CBD	5.42	120.90	111.27
22	4	305	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
22	B	818	CLA	CHD-C1D-ND	-5.42	119.48	124.45
22	O	204	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
22	L	203	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	O	203	CLA	C2C-C1C-NC	5.41	115.04	109.97
22	2	306	CLA	O2D-CGD-CBD	5.41	120.88	111.27
22	B	810	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	F	205	CLA	CHD-C1D-ND	-5.41	119.48	124.45
22	A	811	CLA	C2C-C1C-NC	5.41	115.04	109.97
22	5	303	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	O	205	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	B	813	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
22	B	849	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	6	310	CLA	CMD-C2D-C1D	5.40	134.24	124.71
22	6	310	CLA	CHD-C1D-ND	-5.40	119.49	124.45
22	Z	204	CLA	CHD-C1D-ND	-5.40	119.49	124.45
22	L	203	CLA	CHD-C1D-ND	-5.40	119.49	124.45
22	B	830	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
22	1	304	CLA	CHD-C1D-ND	-5.40	119.49	124.45
29	6	317	5X6	C12-C11-C03	-5.40	112.05	127.20
29	4	313	5X6	C27-C26-C25	-5.40	110.66	118.94
22	3	305	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
22	6	305	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
22	A	830	CLA	O2D-CGD-CBD	5.39	120.84	111.27
22	B	814	CLA	C2C-C1C-NC	5.38	115.02	109.97
22	A	824	CLA	CHD-C1D-ND	-5.38	119.51	124.45
22	5	311	CLA	C2C-C1C-NC	5.38	115.01	109.97
22	6	311	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	5	306	CLA	C2C-C1C-NC	5.37	115.00	109.97
22	1	304	CLA	C2C-C1C-NC	5.37	115.00	109.97
22	A	806	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
22	A	833	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
22	A	825	CLA	CMD-C2D-C1D	5.37	134.18	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	812	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
22	7	306	CLA	C4A-NA-C1A	-5.37	104.29	106.71
29	5	312	5X6	C42-C13-C12	-5.36	109.62	118.08
22	3	302	CLA	CHD-C4C-C3C	-5.36	116.95	124.84
22	B	822	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
22	A	829	CLA	O2D-CGD-CBD	5.36	120.80	111.27
29	3	306	5X6	C23-C22-C21	-5.36	110.72	118.94
22	4	304	CLA	C4A-NA-C1A	-5.36	104.30	106.71
22	K	102	CLA	C2C-C1C-NC	5.36	114.99	109.97
22	6	308	CLA	C2C-C1C-NC	5.36	114.99	109.97
22	A	803	CLA	O2D-CGD-CBD	5.36	120.79	111.27
22	A	803	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
22	2	309	CLA	CHD-C1D-ND	-5.35	119.53	124.45
22	1	310	CLA	O2D-CGD-CBD	5.35	120.77	111.27
22	A	822	CLA	CHD-C1D-ND	-5.35	119.54	124.45
22	O	206	CLA	O2D-CGD-CBD	5.35	120.77	111.27
22	B	827	CLA	O2D-CGD-CBD	5.34	120.76	111.27
22	A	808	CLA	C2C-C1C-NC	5.34	114.98	109.97
29	5	314	5X6	C11-C12-C13	-5.34	118.16	126.23
22	B	815	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
22	A	810	CLA	CMD-C2D-C1D	5.34	134.13	124.71
22	5	308	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
29	7	318	5X6	C28-C29-C30	-5.34	108.53	121.46
22	B	825	CLA	CMD-C2D-C1D	5.34	134.12	124.71
22	A	810	CLA	CHD-C1D-ND	-5.34	119.55	124.45
22	A	813	CLA	CHD-C1D-ND	-5.34	119.55	124.45
29	6	315	5X6	C40-C22-C21	-5.33	115.45	122.92
22	A	828	CLA	CMD-C2D-C1D	5.33	134.11	124.71
22	A	836	CLA	CHD-C1D-ND	-5.33	119.55	124.45
22	5	301	CLA	CMD-C2D-C1D	5.33	134.10	124.71
22	A	808	CLA	CHD-C1D-ND	-5.33	119.56	124.45
22	F	204	CLA	C2C-C1C-NC	5.33	114.96	109.97
29	O	207	5X6	C12-C13-C14	-5.32	110.77	118.94
29	1	313	5X6	C01-C02-C03	-5.32	118.55	124.53
22	A	808	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	B	828	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
22	B	808	CLA	C2C-C1C-NC	5.32	114.96	109.97
22	F	204	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	F	204	CLA	C3C-C4C-NC	5.32	116.54	110.57
22	B	820	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
22	6	310	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
29	6	317	5X6	C28-C29-C30	-5.32	108.58	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	832	CLA	CHD-C1D-ND	-5.32	119.57	124.45
29	B	851	5X6	C16-C17-C18	-5.32	110.78	118.94
22	B	811	CLA	C4A-NA-C1A	-5.32	104.32	106.71
22	B	805	CLA	CHD-C4C-C3C	-5.32	117.03	124.84
22	B	838	CLA	CHD-C4C-C3C	-5.32	117.03	124.84
22	2	308	CLA	O2D-CGD-CBD	5.31	120.71	111.27
29	5	313	5X6	C19-C20-C21	-5.31	112.59	123.47
22	A	814	CLA	C2B-C1B-NB	5.31	113.79	110.23
29	4	314	5X6	C42-C13-C14	-5.31	115.48	122.92
22	B	809	CLA	O2D-CGD-CBD	5.31	120.70	111.27
22	7	310	CLA	CHD-C1D-ND	-5.31	119.58	124.45
22	A	821	CLA	CHD-C1D-ND	-5.31	119.58	124.45
29	1	311	5X6	C20-C19-C18	-5.31	112.60	123.47
22	B	834	CLA	C2C-C1C-NC	5.31	114.94	109.97
29	7	317	5X6	C15-C16-C17	-5.31	111.51	126.42
22	2	302	CLA	C2C-C1C-NC	5.31	114.94	109.97
22	A	819	CLA	CHD-C1D-ND	-5.30	119.58	124.45
22	K	101	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
29	7	317	5X6	C42-C13-C14	-5.30	115.49	122.92
22	A	839	CLA	CMD-C2D-C1D	5.30	134.06	124.71
22	B	849	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
22	B	831	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
22	A	857	CLA	C3C-C4C-NC	5.30	116.52	110.57
22	5	303	CLA	C2C-C1C-NC	5.30	114.94	109.97
22	B	802	CLA	C3C-C4C-NC	5.30	116.52	110.57
22	A	829	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
22	4	307	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
22	B	836	CLA	CHD-C1D-ND	-5.30	119.58	124.45
22	A	803	CLA	CHD-C1D-ND	-5.29	119.59	124.45
22	6	314	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
22	A	831	CLA	C2C-C1C-NC	5.29	114.93	109.97
21	A	801	CL0	CHD-C4C-C3C	-5.29	117.06	124.84
29	4	314	5X6	C19-C18-C17	-5.29	119.76	127.31
22	B	824	CLA	C3C-C4C-NC	5.29	116.50	110.57
22	B	826	CLA	CMD-C2D-C1D	5.29	134.03	124.71
22	B	821	CLA	C4A-NA-C1A	-5.28	104.33	106.71
22	2	311	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
22	B	838	CLA	CMD-C2D-C1D	5.28	134.02	124.71
22	7	310	CLA	C2C-C1C-NC	5.28	114.92	109.97
22	7	306	CLA	C3D-C4D-ND	5.28	118.78	110.24
29	2	313	5X6	C23-C22-C21	-5.28	110.84	118.94
22	A	817	CLA	C2C-C1C-NC	5.28	114.92	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	312	5X6	C27-C28-C29	-5.28	112.38	127.20
29	5	312	5X6	C16-C17-C18	-5.27	110.85	118.94
22	B	806	CLA	C2B-C1B-NB	5.27	113.77	110.23
22	B	806	CLA	CMD-C2D-C1D	5.27	134.00	124.71
22	B	832	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
22	2	303	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	B	806	CLA	C2C-C1C-NC	5.27	114.91	109.97
22	A	837	CLA	CMD-C2D-C1D	5.27	134.00	124.71
29	J	104	5X6	C15-C14-C13	-5.27	119.79	127.31
22	1	305	CLA	C2C-C1C-NC	5.27	114.91	109.97
22	B	817	CLA	O2D-CGD-CBD	5.27	120.62	111.27
22	4	305	CLA	CHD-C1D-ND	-5.26	119.62	124.45
22	A	808	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
22	1	305	CLA	O2D-CGD-CBD	5.26	120.62	111.27
22	4	311	CLA	O2D-CGD-CBD	5.26	120.62	111.27
22	1	304	CLA	C3B-C2B-C1B	-5.26	100.81	107.16
29	1	312	5X6	C15-C16-C17	-5.26	111.64	126.42
22	B	833	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
22	6	313	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
22	A	838	CLA	CHD-C1D-ND	-5.25	119.62	124.45
29	3	306	5X6	C39-C26-C25	-5.25	115.56	122.92
29	4	314	5X6	C20-C19-C18	-5.25	112.72	123.47
29	5	313	5X6	C16-C17-C18	-5.25	110.88	118.94
22	A	814	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
22	6	303	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
22	6	310	CLA	O2D-CGD-CBD	5.25	120.60	111.27
22	B	823	CLA	CHD-C1D-ND	-5.25	119.63	124.45
22	A	821	CLA	CMD-C2D-C1D	5.25	133.96	124.71
22	B	829	CLA	CMD-C2D-C1D	5.25	133.96	124.71
22	5	303	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	A	811	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
22	B	812	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	2	308	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	B	833	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	A	836	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	7	311	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	A	816	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	B	831	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	Z	204	CLA	O2D-CGD-CBD	5.24	120.58	111.27
22	2	310	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	A	809	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
25	K	103	BCR	C16-C15-C14	5.24	134.20	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	304	CLA	C2C-C1C-NC	5.24	114.88	109.97
22	1	305	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
22	5	311	CLA	C3B-C2B-C1B	-5.23	100.84	107.16
22	A	802	CLA	CHD-C1D-ND	-5.23	119.65	124.45
22	A	820	CLA	CMD-C2D-C1D	5.23	133.93	124.71
22	1	303	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
29	6	317	5X6	C19-C20-C21	-5.22	112.77	123.47
22	B	825	CLA	C2C-C1C-NC	5.22	114.87	109.97
22	7	303	CLA	C2C-C1C-NC	5.22	114.86	109.97
29	4	314	5X6	C27-C26-C25	-5.22	110.93	118.94
22	5	310	CLA	C2C-C1C-NC	5.22	114.86	109.97
22	5	301	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
22	B	816	CLA	C3C-C4C-NC	5.22	116.42	110.57
22	A	802	CLA	CMD-C2D-C1D	5.22	133.91	124.71
22	A	857	CLA	C2B-C1B-NB	5.22	113.73	110.23
22	4	310	CLA	CHD-C1D-ND	-5.22	119.66	124.45
22	5	310	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
22	7	308	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
22	B	807	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
22	3	305	CLA	C4A-NA-C1A	-5.21	104.36	106.71
22	4	309	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
22	6	309	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
22	7	313	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
22	B	829	CLA	CAA-C2A-C3A	-5.21	98.52	112.78
22	B	805	CLA	CMD-C2D-C1D	5.20	133.88	124.71
22	1	306	CLA	C2C-C1C-NC	5.20	114.84	109.97
22	A	810	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
22	A	857	CLA	CMD-C2D-C1D	5.20	133.87	124.71
22	B	829	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
29	5	313	5X6	C23-C22-C21	-5.19	110.97	118.94
22	A	830	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
22	B	819	CLA	C4A-NA-C1A	-5.19	104.37	106.71
29	7	316	5X6	C12-C11-C03	-5.18	112.64	127.20
22	A	819	CLA	CMD-C2D-C1D	5.18	133.84	124.71
22	6	308	CLA	O2D-CGD-CBD	5.18	120.47	111.27
25	Z	205	BCR	C8-C9-C10	5.17	126.88	118.94
22	A	820	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
22	B	821	CLA	CHD-C1D-ND	-5.17	119.70	124.45
22	B	830	CLA	O2D-CGD-CBD	5.17	120.46	111.27
29	7	315	5X6	C20-C19-C18	-5.17	112.88	123.47
22	B	804	CLA	CHD-C1D-ND	-5.17	119.70	124.45
22	B	833	CLA	C2C-C1C-NC	5.17	114.82	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	807	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
22	A	833	CLA	C2C-C1C-NC	5.17	114.81	109.97
22	L	203	CLA	O2D-CGD-CBD	5.17	120.45	111.27
22	A	825	CLA	CHD-C1D-ND	-5.17	119.71	124.45
22	A	814	CLA	C2C-C1C-NC	5.17	114.81	109.97
22	B	828	CLA	CMD-C2D-C1D	5.17	133.82	124.71
22	B	813	CLA	C2C-C1C-NC	5.17	114.81	109.97
22	5	304	CLA	CHD-C4C-C3C	-5.17	117.25	124.84
22	2	304	CLA	O2D-CGD-CBD	5.16	120.45	111.27
22	O	204	CLA	O2D-CGD-CBD	5.16	120.44	111.27
22	B	839	CLA	CHD-C1D-ND	-5.16	119.71	124.45
22	B	814	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
22	B	828	CLA	C2C-C1C-NC	5.16	114.81	109.97
29	4	313	5X6	C16-C17-C18	-5.16	111.02	118.94
22	K	102	CLA	O2D-CGD-CBD	5.16	120.44	111.27
22	7	305	CLA	C3B-C2B-C1B	-5.16	100.94	107.16
22	5	304	CLA	C2C-C1C-NC	5.16	114.80	109.97
22	B	816	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
29	2	313	5X6	C12-C13-C14	-5.16	111.03	118.94
22	6	304	CLA	CHD-C1D-ND	-5.16	119.72	124.45
22	1	307	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
29	7	318	5X6	C16-C17-C18	-5.15	111.03	118.94
22	L	205	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	F	206	CLA	C2C-C1C-NC	5.15	114.80	109.97
22	3	301	CLA	O2D-CGD-CBD	5.15	120.42	111.27
29	2	312	5X6	C16-C17-C18	-5.15	111.04	118.94
22	B	817	CLA	CHD-C1D-ND	-5.15	119.72	124.45
22	3	303	CLA	C2C-C1C-NC	5.14	114.79	109.97
22	A	822	CLA	CAC-C3C-C4C	5.14	131.48	124.81
22	6	306	CLA	C2C-C1C-NC	5.14	114.79	109.97
22	7	313	CLA	O2D-CGD-CBD	5.14	120.40	111.27
22	A	838	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
22	2	307	CLA	O2D-CGD-CBD	5.14	120.40	111.27
22	A	836	CLA	CMD-C2D-C1D	5.14	133.76	124.71
22	A	834	CLA	C4A-NA-C1A	-5.14	104.40	106.71
22	4	309	CLA	C4A-NA-C1A	-5.14	104.40	106.71
22	A	806	CLA	O2D-CGD-CBD	5.14	120.39	111.27
22	B	802	CLA	C3B-C2B-C1B	-5.13	100.96	107.16
29	1	314	5X6	C12-C11-C03	-5.13	112.78	127.20
29	6	315	5X6	C42-C13-C14	-5.13	115.73	122.92
22	A	858	CLA	C2C-C1C-NC	5.13	114.78	109.97
22	5	306	CLA	CHD-C4C-C3C	-5.13	117.30	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	M	101	5X6	C19-C20-C21	-5.13	112.97	123.47
22	B	819	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
22	7	305	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
22	1	302	CLA	C2C-C1C-NC	5.12	114.77	109.97
22	K	102	CLA	CHD-C1D-ND	-5.12	119.75	124.45
22	A	848	CLA	CHD-C1D-ND	-5.12	119.75	124.45
22	B	835	CLA	C3B-C2B-C1B	-5.12	100.98	107.16
22	B	811	CLA	C3B-C2B-C1B	-5.12	100.98	107.16
22	5	309	CLA	C4A-NA-C1A	-5.12	104.41	106.71
22	A	825	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
22	A	823	CLA	C3C-C4C-NC	5.12	116.31	110.57
22	3	305	CLA	O2D-CGD-CBD	5.11	120.36	111.27
22	A	816	CLA	C2C-C1C-NC	5.11	114.76	109.97
22	4	311	CLA	C4A-NA-C1A	-5.11	104.41	106.71
22	L	204	CLA	CMD-C2D-C1D	5.11	133.72	124.71
22	B	802	CLA	CHD-C1D-ND	-5.11	119.76	124.45
29	7	317	5X6	C11-C03-C02	-5.11	109.09	121.46
22	B	811	CLA	C2C-C1C-NC	5.11	114.75	109.97
22	6	312	CLA	CHD-C4C-C3C	-5.11	117.34	124.84
22	A	838	CLA	C3C-C4C-NC	5.10	116.30	110.57
22	4	305	CLA	C2C-C1C-NC	5.10	114.75	109.97
22	A	837	CLA	C2C-C1C-NC	5.10	114.75	109.97
22	B	820	CLA	CHD-C1D-ND	-5.10	119.77	124.45
22	A	802	CLA	C2C-C1C-NC	5.10	114.75	109.97
29	O	208	5X6	C12-C11-C03	-5.10	112.88	127.20
29	6	317	5X6	C24-C23-C22	-5.10	112.09	126.42
22	6	314	CLA	C2C-C1C-NC	5.10	114.75	109.97
22	A	807	CLA	CMD-C2D-C1D	5.10	133.69	124.71
22	A	832	CLA	CHD-C4C-C3C	-5.09	117.35	124.84
22	1	308	CLA	CHD-C4C-C3C	-5.09	117.35	124.84
22	2	306	CLA	C2C-C1C-NC	5.09	114.74	109.97
29	1	312	5X6	C12-C11-C03	-5.09	112.91	127.20
29	O	208	5X6	C20-C19-C18	-5.09	113.05	123.47
22	5	306	CLA	CHD-C1D-ND	-5.09	119.78	124.45
22	A	815	CLA	C4A-NA-C1A	-5.09	104.42	106.71
22	B	827	CLA	C3C-C4C-NC	5.09	116.28	110.57
22	A	828	CLA	C2B-C1B-NB	5.09	113.64	110.23
22	A	819	CLA	C2C-C1C-NC	5.08	114.73	109.97
22	B	803	CLA	CMD-C2D-C1D	5.08	133.67	124.71
22	1	304	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
29	1	311	5X6	C40-C22-C21	-5.08	115.80	122.92
22	F	204	CLA	C3D-C2D-C1D	-5.08	98.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	302	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
22	B	824	CLA	CMD-C2D-C1D	5.08	133.67	124.71
22	6	311	CLA	CHD-C1D-ND	-5.08	119.78	124.45
22	B	806	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
22	A	832	CLA	C2C-C1C-NC	5.08	114.73	109.97
22	7	306	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	A	812	CLA	C2C-C1C-NC	5.08	114.73	109.97
22	B	810	CLA	C2C-C1C-NC	5.07	114.72	109.97
29	1	316	5X6	C24-C23-C22	-5.07	112.17	126.42
22	B	802	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
22	B	837	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
22	1	307	CLA	C2C-C1C-NC	5.07	114.72	109.97
29	1	311	5X6	C41-C17-C18	-5.07	115.82	122.92
22	B	836	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
22	B	809	CLA	C2B-C1B-NB	5.06	113.62	110.23
22	A	827	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
22	1	306	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
22	A	833	CLA	CHD-C1D-ND	-5.05	119.81	124.45
22	5	307	CLA	C2C-C1C-NC	5.05	114.70	109.97
22	2	307	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
22	3	304	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
25	J	103	BCR	C20-C21-C22	5.05	134.51	127.31
29	7	316	5X6	C24-C23-C22	-5.05	112.24	126.42
29	7	317	5X6	C27-C28-C29	-5.05	113.03	127.20
22	B	813	CLA	CAC-C3C-C4C	5.05	131.36	124.81
22	B	814	CLA	O2D-CGD-CBD	5.04	120.23	111.27
22	5	305	CLA	C2C-C1C-NC	5.04	114.70	109.97
29	2	312	5X6	C27-C26-C25	-5.04	111.20	118.94
22	6	305	CLA	C2C-C1C-NC	5.04	114.70	109.97
22	5	301	CLA	CHD-C1D-ND	-5.04	119.82	124.45
22	O	203	CLA	CHD-C1D-ND	-5.03	119.83	124.45
22	Z	201	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
22	6	314	CLA	O2D-CGD-CBD	5.03	120.20	111.27
22	A	830	CLA	CHD-C1D-ND	-5.03	119.83	124.45
29	5	321	5X6	C23-C22-C21	-5.03	111.23	118.94
22	B	808	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
22	B	802	CLA	CMD-C2D-C1D	5.02	133.57	124.71
29	7	316	5X6	C40-C22-C21	-5.02	115.89	122.92
22	A	804	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
22	3	302	CLA	C4A-NA-C1A	-5.02	104.45	106.71
22	7	305	CLA	C2C-C1C-NC	5.02	114.67	109.97
29	2	312	5X6	C39-C26-C25	-5.02	115.89	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	839	CLA	CHD-C1D-ND	-5.02	119.84	124.45
22	A	858	CLA	CMD-C2D-C1D	5.02	133.55	124.71
22	A	815	CLA	C2C-C1C-NC	5.01	114.67	109.97
22	A	809	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
22	7	307	CLA	C4A-NA-C1A	-5.01	104.45	106.71
22	4	312	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
22	A	808	CLA	O2D-CGD-CBD	5.01	120.17	111.27
22	B	804	CLA	C2C-C1C-NC	5.01	114.66	109.97
29	5	313	5X6	C39-C26-C25	-5.01	115.91	122.92
22	3	302	CLA	C2C-C1C-NC	5.00	114.66	109.97
22	B	826	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
22	B	836	CLA	C3C-C4C-NC	5.00	116.18	110.57
22	A	831	CLA	C3C-C4C-NC	5.00	116.18	110.57
22	A	814	CLA	CHD-C1D-ND	-5.00	119.86	124.45
22	A	815	CLA	CHD-C1D-ND	-5.00	119.86	124.45
22	B	809	CLA	CHD-C1D-ND	-5.00	119.86	124.45
22	K	101	CLA	C2C-C1C-NC	5.00	114.66	109.97
22	7	307	CLA	C2C-C1C-NC	5.00	114.65	109.97
22	B	804	CLA	C3B-C2B-C1B	-5.00	101.13	107.16
29	4	314	5X6	C42-C13-C12	-4.99	110.21	118.08
22	A	837	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
29	6	317	5X6	C39-C26-C27	-4.99	110.21	118.08
22	A	836	CLA	O2D-CGD-CBD	4.99	120.14	111.27
22	A	830	CLA	CMD-C2D-C1D	4.99	133.51	124.71
29	Z	206	5X6	C41-C17-C18	-4.99	115.93	122.92
22	A	817	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
22	B	806	CLA	C3C-C4C-NC	4.99	116.16	110.57
22	A	811	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
29	1	312	5X6	C12-C13-C14	-4.99	111.29	118.94
22	B	838	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
22	4	307	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
22	4	306	CLA	C2C-C1C-NC	4.98	114.64	109.97
29	7	315	5X6	C12-C11-C03	-4.98	113.22	127.20
22	B	821	CLA	CMD-C2D-C1D	4.98	133.49	124.71
22	B	818	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
22	5	302	CLA	O2D-CGD-CBD	4.98	120.11	111.27
22	B	808	CLA	CHD-C1D-ND	-4.98	119.88	124.45
22	1	309	CLA	O2D-CGD-CBD	4.97	120.11	111.27
22	B	809	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
22	1	302	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
22	3	301	CLA	C4A-NA-C1A	-4.97	104.47	106.71
22	1	308	CLA	C2C-C1C-NC	4.97	114.63	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	835	CLA	C3C-C4C-NC	4.97	116.14	110.57
29	4	315	5X6	C12-C11-C03	-4.97	113.25	127.20
29	5	312	5X6	C20-C19-C18	-4.97	113.30	123.47
22	J	102	CLA	C2C-C1C-NC	4.97	114.62	109.97
22	A	807	CLA	C3C-C4C-NC	4.96	116.14	110.57
22	B	826	CLA	C2C-C1C-NC	4.96	114.62	109.97
29	7	315	5X6	C27-C28-C29	-4.96	113.27	127.20
22	2	303	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
29	M	101	5X6	C20-C19-C18	-4.96	113.32	123.47
22	2	302	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
29	M	101	5X6	C24-C23-C22	-4.96	112.49	126.42
22	2	309	CLA	C2C-C1C-NC	4.96	114.61	109.97
22	J	102	CLA	CHD-C4C-C3C	-4.96	117.56	124.84
29	B	851	5X6	C41-C17-C18	-4.96	115.98	122.92
22	O	206	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
29	7	318	5X6	C23-C22-C21	-4.95	111.34	118.94
22	7	311	CLA	C2C-C1C-NC	4.95	114.61	109.97
22	2	305	CLA	C3D-C4D-ND	4.95	118.24	110.24
22	B	850	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
22	B	835	CLA	CHD-C1D-ND	-4.94	119.92	124.45
22	A	811	CLA	CAC-C3C-C4C	4.94	131.22	124.81
29	B	851	5X6	C12-C11-C03	-4.94	113.34	127.20
22	B	804	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
22	A	858	CLA	CHD-C1D-ND	-4.93	119.92	124.45
22	2	303	CLA	C2C-C1C-NC	4.93	114.59	109.97
29	1	313	5X6	C16-C17-C18	-4.92	111.38	118.94
22	B	801	CLA	CHD-C4C-C3C	-4.92	117.60	124.84
22	6	311	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
22	B	822	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	B	851	5X6	C19-C20-C21	-4.92	113.40	123.47
29	7	315	5X6	C23-C22-C21	-4.92	111.39	118.94
22	B	829	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
22	A	817	CLA	CMD-C2D-C1D	4.91	133.37	124.71
29	7	316	5X6	C12-C13-C14	-4.91	111.40	118.94
22	B	827	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
29	1	311	5X6	C12-C11-C03	-4.91	113.41	127.20
22	L	204	CLA	C3B-C2B-C1B	-4.91	101.23	107.16
22	1	310	CLA	C3D-C4D-ND	4.91	118.18	110.24
22	7	304	CLA	O2D-CGD-CBD	4.91	119.99	111.27
29	2	312	5X6	C20-C19-C18	-4.91	113.42	123.47
29	1	314	5X6	C15-C16-C17	-4.91	112.64	126.42
22	2	309	CLA	CHD-C4C-C3C	-4.91	117.63	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	839	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
22	A	811	CLA	CHD-C1D-ND	-4.90	119.95	124.45
22	A	806	CLA	CHD-C1D-ND	-4.90	119.95	124.45
22	4	304	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	2	308	CLA	C3D-C4D-ND	4.90	118.16	110.24
29	1	316	5X6	C27-C26-C25	-4.90	111.43	118.94
22	4	305	CLA	C4-C3-C5	4.90	123.51	115.27
22	B	810	CLA	CHD-C1D-ND	-4.89	119.96	124.45
29	5	321	5X6	C12-C13-C14	-4.89	111.44	118.94
22	1	303	CLA	O2D-CGD-CBD	4.89	119.96	111.27
22	A	830	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
22	7	303	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
22	4	304	CLA	CHD-C4C-C3C	-4.89	117.66	124.84
22	A	818	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
22	O	204	CLA	C2C-C1C-NC	4.88	114.55	109.97
22	A	839	CLA	C2C-C1C-NC	4.88	114.55	109.97
22	3	303	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	A	857	CLA	O2D-CGD-O1D	-4.88	114.30	123.84
22	7	312	CLA	O2D-CGD-CBD	4.88	119.93	111.27
22	B	816	CLA	C2C-C1C-NC	4.87	114.54	109.97
22	B	813	CLA	O2D-CGD-CBD	4.87	119.93	111.27
22	B	813	CLA	C3C-C4C-NC	4.87	116.04	110.57
22	L	204	CLA	C2C-C1C-NC	4.87	114.54	109.97
22	A	815	CLA	C3C-C4C-NC	4.87	116.03	110.57
22	4	308	CLA	C4A-NA-C1A	-4.87	104.52	106.71
22	6	313	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
22	2	304	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
22	B	822	CLA	C3C-C4C-NC	4.87	116.03	110.57
29	5	314	5X6	C23-C22-C21	-4.87	111.47	118.94
22	B	810	CLA	C3C-C4C-NC	4.87	116.03	110.57
22	6	308	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
29	7	316	5X6	C16-C17-C18	-4.86	111.48	118.94
22	2	310	CLA	O2D-CGD-CBD	4.86	119.91	111.27
22	7	309	CLA	O2D-CGD-CBD	4.86	119.91	111.27
22	A	831	CLA	CMD-C2D-C1D	4.86	133.28	124.71
22	A	837	CLA	C3D-C4D-ND	4.86	118.10	110.24
22	6	312	CLA	C2C-C1C-NC	4.86	114.53	109.97
22	3	302	CLA	O2D-CGD-CBD	4.86	119.91	111.27
22	B	822	CLA	CMD-C2D-C1D	4.86	133.27	124.71
22	O	206	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
22	A	836	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
29	6	316	5X6	C27-C26-C25	-4.85	111.49	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	804	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
22	4	306	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
22	2	305	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
22	2	306	CLA	CAC-C3C-C4C	4.85	131.10	124.81
22	5	302	CLA	C3D-C4D-ND	4.85	118.08	110.24
29	B	851	5X6	C01-C02-C03	-4.84	119.09	124.53
22	B	834	CLA	CMD-C2D-C1D	4.84	133.25	124.71
22	L	204	CLA	CHD-C1D-ND	-4.84	120.01	124.45
29	5	321	5X6	C41-C17-C18	-4.84	116.15	122.92
22	A	812	CLA	CHD-C1D-ND	-4.84	120.01	124.45
22	5	311	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
22	Z	204	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
22	6	305	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
22	5	305	CLA	C4A-NA-C1A	-4.84	104.53	106.71
22	A	824	CLA	C2C-C1C-NC	4.84	114.50	109.97
22	A	826	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
29	1	311	5X6	C11-C03-C02	-4.83	109.76	121.46
22	B	831	CLA	CMD-C2D-C1D	4.83	133.22	124.71
22	A	834	CLA	C2C-C1C-NC	4.83	114.50	109.97
22	7	306	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
22	B	814	CLA	CHD-C1D-ND	-4.83	120.02	124.45
22	7	311	CLA	O2D-CGD-CBD	4.83	119.84	111.27
22	K	101	CLA	C3B-C2B-C1B	-4.83	101.34	107.16
22	A	821	CLA	C3C-C4C-NC	4.83	115.98	110.57
22	B	813	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
22	A	829	CLA	C2C-C1C-NC	4.82	114.49	109.97
22	B	816	CLA	CHD-C1D-ND	-4.82	120.02	124.45
29	O	208	5X6	C19-C20-C21	-4.82	113.60	123.47
22	B	835	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
21	A	801	CL0	O2D-CGD-CBD	4.82	119.83	111.27
29	7	318	5X6	C19-C20-C21	-4.82	113.60	123.47
22	3	305	CLA	C3D-C4D-ND	4.82	118.04	110.24
22	L	203	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
29	4	313	5X6	C20-C19-C18	-4.82	113.61	123.47
29	5	314	5X6	C20-C19-C18	-4.81	113.61	123.47
22	B	811	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
29	1	313	5X6	C27-C28-C29	-4.81	113.69	127.20
22	F	205	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
22	A	839	CLA	C3C-C4C-NC	4.81	115.97	110.57
22	F	206	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
22	6	311	CLA	C2C-C1C-NC	4.81	114.48	109.97
29	3	306	5X6	C27-C26-C25	-4.81	111.56	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	313	5X6	C42-C13-C12	-4.81	110.50	118.08
22	A	815	CLA	C4-C3-C5	4.81	123.36	115.27
22	A	858	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
29	2	312	5X6	C19-C20-C21	-4.80	113.63	123.47
22	B	821	CLA	C3D-C4D-ND	4.80	118.01	110.24
22	2	310	CLA	C2C-C1C-NC	4.80	114.47	109.97
22	7	303	CLA	CAC-C3C-C4C	4.80	131.04	124.81
22	B	839	CLA	C2C-C1C-NC	4.80	114.47	109.97
22	A	835	CLA	CHD-C1D-ND	-4.80	120.05	124.45
22	B	805	CLA	C2C-C1C-NC	4.80	114.47	109.97
22	A	836	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
29	2	314	5X6	C15-C16-C17	-4.80	112.94	126.42
29	1	316	5X6	C11-C03-C02	-4.79	109.85	121.46
29	6	315	5X6	C27-C26-C25	-4.79	111.59	118.94
22	1	305	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
22	2	305	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
22	6	305	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
22	B	828	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
22	3	304	CLA	C2C-C1C-NC	4.79	114.46	109.97
22	1	304	CLA	O2D-CGD-CBD	4.79	119.77	111.27
29	5	313	5X6	C12-C11-C03	-4.79	113.76	127.20
22	5	305	CLA	CAC-C3C-C4C	4.78	131.02	124.81
22	B	835	CLA	C3C-C4C-NC	4.78	115.94	110.57
22	B	823	CLA	O2D-CGD-CBD	4.78	119.77	111.27
29	1	314	5X6	C24-C23-C22	-4.78	112.98	126.42
22	2	305	CLA	C2C-C1C-NC	4.78	114.45	109.97
22	B	820	CLA	C2C-C1C-NC	4.78	114.45	109.97
22	5	307	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	F	205	CLA	C3C-C4C-NC	4.78	115.93	110.57
22	7	304	CLA	C3D-C4D-ND	4.78	117.97	110.24
22	A	857	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
22	A	812	CLA	C3C-C4C-NC	4.77	115.92	110.57
22	B	812	CLA	C2C-C1C-NC	4.77	114.44	109.97
22	5	304	CLA	C3D-C4D-ND	4.77	117.96	110.24
22	A	859	CLA	C4-C3-C5	4.77	123.30	115.27
22	1	310	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
22	K	101	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	B	830	CLA	CMD-C2D-C1D	4.77	133.12	124.71
25	K	103	BCR	C15-C16-C17	4.77	133.24	123.47
22	2	310	CLA	C4A-NA-C1A	-4.77	104.56	106.71
22	6	313	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	2	303	CLA	C3B-C2B-C1B	-4.77	101.41	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	815	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	4	311	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	7	308	CLA	O2D-CGD-CBD	4.76	119.73	111.27
22	L	205	CLA	CHD-C1D-ND	-4.76	120.08	124.45
22	5	303	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
29	1	312	5X6	C42-C13-C14	-4.76	116.25	122.92
22	4	306	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	4	302	CLA	C2C-C1C-NC	4.76	114.43	109.97
22	A	813	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
29	4	315	5X6	C23-C22-C21	-4.76	111.64	118.94
22	4	303	CLA	C3D-C4D-ND	4.76	117.93	110.24
22	6	313	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
22	B	850	CLA	O2D-CGD-CBD	4.76	119.72	111.27
22	7	313	CLA	C2C-C1C-NC	4.75	114.43	109.97
29	Z	206	5X6	C28-C27-C26	-4.75	119.05	126.23
22	A	810	CLA	C3C-C4C-NC	4.75	115.90	110.57
22	4	308	CLA	C3D-C4D-ND	4.75	117.92	110.24
22	A	825	CLA	C3C-C4C-NC	4.75	115.90	110.57
22	5	309	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	A	822	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
22	O	205	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	B	824	CLA	C3D-C2D-C1D	-4.75	99.36	105.83
22	3	301	CLA	C3D-C4D-ND	4.74	117.91	110.24
22	A	802	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
22	A	835	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
29	6	316	5X6	C16-C17-C18	-4.74	111.67	118.94
29	1	316	5X6	C20-C19-C18	-4.74	113.77	123.47
22	4	308	CLA	O2D-CGD-CBD	4.74	119.69	111.27
22	A	820	CLA	C3D-C4D-ND	4.74	117.90	110.24
22	A	834	CLA	C3D-C4D-ND	4.74	117.90	110.24
22	6	309	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
22	3	302	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
22	A	806	CLA	C3C-C4C-NC	4.74	115.88	110.57
22	3	303	CLA	C4A-NA-C1A	-4.74	104.58	106.71
22	4	312	CLA	C4A-NA-C1A	-4.74	104.58	106.71
22	5	305	CLA	O2D-CGD-CBD	4.73	119.68	111.27
22	5	310	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
22	B	808	CLA	C3C-C4C-NC	4.73	115.88	110.57
22	4	310	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
29	6	315	5X6	C41-C17-C18	-4.73	116.30	122.92
22	2	302	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
22	3	303	CLA	CHD-C4C-C3C	-4.73	117.89	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	311	CLA	O2D-CGD-CBD	4.73	119.67	111.27
29	4	313	5X6	C23-C22-C21	-4.73	111.69	118.94
22	6	306	CLA	C3D-C4D-ND	4.73	117.88	110.24
22	A	812	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
22	B	834	CLA	C3C-C4C-NC	4.72	115.87	110.57
22	A	838	CLA	C2C-C1C-NC	4.72	114.39	109.97
22	B	801	CLA	CHD-C1D-ND	-4.72	120.12	124.45
22	A	848	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
22	B	821	CLA	O2D-CGD-CBD	4.72	119.65	111.27
22	B	831	CLA	C3D-C4D-ND	4.72	117.87	110.24
22	A	829	CLA	C4A-NA-C1A	-4.72	104.58	106.71
22	1	309	CLA	C4A-NA-C1A	-4.72	104.58	106.71
29	5	321	5X6	C12-C11-C03	-4.72	113.95	127.20
29	7	314	5X6	C11-C03-C02	-4.72	110.04	121.46
22	A	828	CLA	CHD-C4C-C3C	-4.72	117.91	124.84
22	7	312	CLA	C4A-NA-C1A	-4.71	104.59	106.71
22	7	310	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
29	6	316	5X6	C12-C11-C03	-4.71	113.97	127.20
22	F	206	CLA	CHD-C1D-ND	-4.71	120.13	124.45
22	3	304	CLA	C4A-NA-C1A	-4.71	104.59	106.71
22	5	308	CLA	C2C-C1C-NC	4.71	114.38	109.97
22	A	858	CLA	C3D-C4D-ND	4.71	117.85	110.24
22	B	801	CLA	C2C-C1C-NC	4.71	114.38	109.97
29	3	306	5X6	C15-C16-C17	-4.71	113.19	126.42
22	2	309	CLA	C4A-NA-C1A	-4.71	104.59	106.71
22	7	311	CLA	C4A-NA-C1A	-4.70	104.59	106.71
29	4	314	5X6	C40-C22-C21	-4.70	116.33	122.92
22	A	807	CLA	CAC-C3C-C4C	4.70	130.91	124.81
22	2	304	CLA	C2C-C1C-NC	4.70	114.38	109.97
22	A	829	CLA	CHD-C1D-ND	-4.70	120.13	124.45
22	7	309	CLA	C3D-C4D-ND	4.70	117.84	110.24
22	1	308	CLA	O2D-CGD-CBD	4.70	119.62	111.27
22	4	302	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
22	1	307	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
22	B	813	CLA	CHD-C1D-ND	-4.70	120.14	124.45
22	A	828	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
22	A	834	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	K	102	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	6	307	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
22	A	858	CLA	C3C-C4C-NC	4.69	115.83	110.57
22	7	307	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
22	A	839	CLA	C3D-C2D-C1D	-4.69	99.44	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	828	CLA	CHD-C1D-ND	-4.68	120.15	124.45
29	M	101	5X6	C12-C13-C14	-4.68	111.75	118.94
29	6	317	5X6	C12-C13-C14	-4.68	111.75	118.94
22	B	809	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
22	5	307	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
22	A	824	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
22	B	816	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
22	6	309	CLA	C4A-NA-C1A	-4.68	104.60	106.71
22	B	818	CLA	C3B-C2B-C1B	-4.68	101.52	107.16
22	B	834	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
29	5	321	5X6	C27-C28-C29	-4.67	114.07	127.20
22	B	825	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
22	A	859	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
22	A	822	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
29	7	315	5X6	C40-C22-C21	-4.67	116.38	122.92
22	A	827	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
22	3	304	CLA	O2D-CGD-CBD	4.67	119.57	111.27
22	A	814	CLA	CAC-C3C-C4C	4.67	130.87	124.81
22	B	849	CLA	CMD-C2D-C1D	4.67	132.94	124.71
22	6	309	CLA	C2C-C1C-NC	4.67	114.35	109.97
29	4	313	5X6	C41-C17-C18	-4.67	116.39	122.92
22	2	306	CLA	C4A-NA-C1A	-4.66	104.61	106.71
22	L	204	CLA	C3D-C4D-ND	4.66	117.78	110.24
22	B	831	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
22	A	831	CLA	O2D-CGD-CBD	4.66	119.55	111.27
22	B	810	CLA	C3D-C4D-ND	4.66	117.77	110.24
22	1	302	CLA	C3D-C4D-ND	4.66	117.77	110.24
29	B	851	5X6	C24-C23-C22	-4.65	113.34	126.42
22	A	806	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
22	B	805	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
29	7	315	5X6	C39-C26-C25	-4.65	116.41	122.92
29	4	314	5X6	C15-C16-C17	-4.65	113.36	126.42
22	A	804	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	B	805	CLA	C3D-C4D-ND	4.65	117.75	110.24
22	1	306	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	A	833	CLA	C3D-C4D-ND	4.64	117.75	110.24
22	B	849	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
22	5	302	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
22	B	817	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
22	4	307	CLA	CMD-C2D-C1D	4.64	132.89	124.71
29	6	315	5X6	C12-C13-C14	-4.64	111.82	118.94
22	A	819	CLA	C4A-NA-C1A	-4.64	104.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	313	5X6	C16-C17-C18	-4.64	111.82	118.94
22	B	807	CLA	C2C-C1C-NC	4.64	114.32	109.97
22	7	307	CLA	CAC-C3C-C4C	4.64	130.83	124.81
22	6	306	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
22	A	807	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	B	837	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	B	834	CLA	CHD-C1D-ND	-4.64	120.19	124.45
22	K	101	CLA	C4A-NA-C1A	-4.64	104.62	106.71
22	5	301	CLA	O2D-CGD-CBD	4.63	119.50	111.27
22	B	816	CLA	C4A-NA-C1A	-4.63	104.62	106.71
22	A	810	CLA	O2D-CGD-CBD	4.63	119.50	111.27
22	B	832	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
22	6	312	CLA	C3D-C4D-ND	4.63	117.73	110.24
22	5	305	CLA	CHD-C4C-C3C	-4.63	118.04	124.84
22	A	823	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
22	7	311	CLA	C3D-C4D-ND	4.63	117.72	110.24
22	A	804	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
22	A	804	CLA	O2D-CGD-CBD	4.63	119.49	111.27
22	6	312	CLA	C4A-NA-C1A	-4.63	104.63	106.71
22	7	305	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
22	J	102	CLA	O2D-CGD-CBD	4.63	119.49	111.27
22	B	822	CLA	C3D-C4D-ND	4.63	117.72	110.24
22	7	307	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
22	4	309	CLA	C2C-C1C-NC	4.62	114.30	109.97
29	4	314	5X6	C39-C26-C25	-4.62	116.45	122.92
22	A	833	CLA	CMD-C2D-C1D	4.62	132.86	124.71
22	A	806	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
22	B	832	CLA	C2C-C1C-NC	4.62	114.30	109.97
22	L	205	CLA	C2C-C1C-NC	4.62	114.30	109.97
22	K	101	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	B	807	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
22	B	803	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
22	O	205	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
29	1	311	5X6	C27-C28-C29	-4.61	114.25	127.20
22	A	830	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	O	203	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
22	A	824	CLA	O2D-CGD-CBD	4.61	119.46	111.27
22	7	312	CLA	C3D-C4D-ND	4.61	117.69	110.24
22	A	848	CLA	C2C-C1C-NC	4.61	114.29	109.97
22	6	311	CLA	C3C-C4C-NC	4.61	115.74	110.57
29	5	313	5X6	C41-C17-C18	-4.61	116.47	122.92
22	A	859	CLA	C3D-C4D-ND	4.60	117.69	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	307	CLA	C3D-C4D-ND	4.60	117.69	110.24
22	6	311	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
25	A	846	BCR	C34-C9-C10	-4.60	116.47	122.92
22	A	802	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
22	4	305	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
22	5	309	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
22	B	803	CLA	CHD-C1D-ND	-4.60	120.23	124.45
22	A	831	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
22	1	303	CLA	C3D-C4D-ND	4.60	117.68	110.24
22	5	303	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
22	B	815	CLA	C2C-C1C-NC	4.60	114.28	109.97
22	3	301	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
21	A	801	CL0	C3D-C2D-C1D	-4.60	99.56	105.83
22	B	817	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
22	1	308	CLA	C3D-C4D-ND	4.59	117.67	110.24
22	6	307	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
22	B	828	CLA	C3D-C4D-ND	4.59	117.67	110.24
22	6	305	CLA	CAC-C3C-C4C	4.59	130.77	124.81
22	4	305	CLA	C3D-C4D-ND	4.59	117.67	110.24
29	2	314	5X6	C12-C11-C03	-4.59	114.31	127.20
22	1	307	CLA	O2D-CGD-CBD	4.59	119.42	111.27
22	5	308	CLA	C4A-NA-C1A	-4.59	104.64	106.71
22	B	833	CLA	CMD-C2D-C1D	4.59	132.80	124.71
22	2	311	CLA	C2C-C1C-NC	4.59	114.27	109.97
22	3	304	CLA	C3D-C4D-ND	4.59	117.66	110.24
22	B	836	CLA	O2D-CGD-O1D	-4.58	114.87	123.84
22	A	805	CLA	C3D-C4D-ND	4.58	117.65	110.24
29	1	313	5X6	C27-C26-C25	-4.58	111.91	118.94
22	3	302	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	1	310	CLA	C2C-C1C-NC	4.58	114.26	109.97
22	B	812	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	B	810	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	B	807	CLA	C3D-C4D-ND	4.58	117.64	110.24
22	B	850	CLA	C3D-C4D-ND	4.58	117.64	110.24
22	2	310	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	6	313	CLA	C2C-C1C-NC	4.57	114.26	109.97
29	4	315	5X6	C20-C19-C18	-4.57	114.11	123.47
22	2	310	CLA	C3D-C4D-ND	4.57	117.64	110.24
22	B	804	CLA	C3C-C4C-NC	4.57	115.70	110.57
22	B	837	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
22	O	205	CLA	C3D-C4D-ND	4.57	117.63	110.24
22	1	307	CLA	C3B-C2B-C1B	-4.57	101.64	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	310	CLA	O2D-CGD-CBD	4.57	119.39	111.27
22	B	815	CLA	C4A-NA-C1A	-4.57	104.65	106.71
22	A	813	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
22	A	818	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
22	4	306	CLA	CAC-C3C-C4C	4.57	130.73	124.81
22	A	810	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
29	1	314	5X6	C28-C29-C30	-4.56	110.41	121.46
22	6	314	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
22	B	825	CLA	C3B-C2B-C1B	-4.56	101.65	107.16
22	5	307	CLA	C3D-C4D-ND	4.56	117.61	110.24
29	4	314	5X6	C01-C02-C07	-4.56	105.91	114.36
22	5	304	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	O	206	CLA	C3D-C4D-ND	4.56	117.61	110.24
22	A	825	CLA	C2C-C1C-NC	4.56	114.24	109.97
22	A	825	CLA	C3B-C2B-C1B	-4.55	101.66	107.16
22	B	820	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	B	823	CLA	C3C-C4C-NC	4.55	115.68	110.57
22	6	310	CLA	C2C-C1C-NC	4.55	114.24	109.97
22	A	819	CLA	C3C-C4C-NC	4.55	115.68	110.57
22	L	204	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
29	4	315	5X6	C38-C30-C31	-4.55	105.92	114.36
22	1	302	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	B	814	CLA	C3C-C4C-NC	4.55	115.67	110.57
22	5	311	CLA	C4A-NA-C1A	-4.55	104.66	106.71
29	5	312	5X6	C40-C22-C21	-4.55	116.55	122.92
22	A	808	CLA	C4-C3-C5	4.55	122.92	115.27
22	4	312	CLA	C2C-C1C-NC	4.55	114.23	109.97
22	A	803	CLA	C3D-C4D-ND	4.54	117.59	110.24
22	A	802	CLA	C3C-C4C-NC	4.54	115.67	110.57
22	6	306	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
22	A	824	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
29	2	313	5X6	C41-C17-C16	-4.54	110.92	118.08
22	1	309	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	Z	204	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
22	2	304	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
29	B	851	5X6	C27-C26-C25	-4.54	111.97	118.94
22	B	826	CLA	C3C-C4C-NC	4.54	115.66	110.57
22	7	309	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
22	A	821	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	B	812	CLA	C3C-C4C-NC	4.54	115.66	110.57
22	A	839	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	B	814	CLA	CMD-C2D-C1D	4.54	132.71	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	205	CLA	C4A-NA-C1A	-4.53	104.67	106.71
22	6	308	CLA	C4A-NA-C1A	-4.53	104.67	106.71
29	2	312	5X6	C11-C03-C02	-4.53	110.48	121.46
29	7	318	5X6	C27-C28-C29	-4.53	114.47	127.20
22	5	305	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	2	305	CLA	C4A-NA-C1A	-4.53	104.67	106.71
22	5	304	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	A	820	CLA	C3C-C4C-NC	4.53	115.65	110.57
22	A	810	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	B	839	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	L	205	CLA	C3C-C4C-NC	4.53	115.65	110.57
22	4	310	CLA	CAC-C3C-C2C	-4.53	119.78	127.53
22	B	823	CLA	C3D-C4D-ND	4.53	117.56	110.24
22	7	312	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	B	807	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	2	309	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	B	835	CLA	C2C-C1C-NC	4.53	114.21	109.97
22	1	307	CLA	C3D-C4D-ND	4.53	117.56	110.24
22	2	306	CLA	CHD-C4C-C3C	-4.53	118.19	124.84
22	O	203	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
29	Z	206	5X6	C16-C17-C18	-4.52	112.00	118.94
22	5	311	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	4	309	CLA	C3D-C4D-ND	4.52	117.56	110.24
22	B	807	CLA	C4A-NA-C1A	-4.52	104.67	106.71
22	2	305	CLA	O2D-CGD-CBD	4.52	119.31	111.27
22	B	829	CLA	C3C-C4C-NC	4.52	115.64	110.57
22	A	812	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
22	1	310	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	A	814	CLA	C4A-NA-C1A	-4.52	104.67	106.71
22	6	310	CLA	C3D-C4D-ND	4.52	117.55	110.24
22	A	824	CLA	C3C-C4C-NC	4.52	115.64	110.57
22	F	204	CLA	CHD-C1D-ND	-4.52	120.30	124.45
29	3	306	5X6	C11-C03-C02	-4.52	110.52	121.46
29	B	851	5X6	C39-C26-C25	-4.52	116.60	122.92
22	A	814	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
22	7	313	CLA	C3D-C4D-ND	4.52	117.54	110.24
22	3	303	CLA	C3D-C4D-ND	4.51	117.54	110.24
22	1	302	CLA	O2D-CGD-CBD	4.51	119.29	111.27
22	2	309	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
22	B	824	CLA	CAC-C3C-C4C	4.51	130.67	124.81
22	2	303	CLA	C3D-C4D-ND	4.51	117.54	110.24
22	4	302	CLA	C3D-C4D-ND	4.51	117.54	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	304	CLA	C3D-C4D-ND	4.51	117.54	110.24
29	5	321	5X6	C01-C02-C07	-4.51	106.00	114.36
22	1	306	CLA	C3D-C4D-ND	4.51	117.53	110.24
22	A	811	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
22	6	312	CLA	O2D-CGD-CBD	4.51	119.28	111.27
22	7	303	CLA	C3D-C4D-ND	4.51	117.53	110.24
25	2	301	BCR	C37-C22-C21	-4.51	116.61	122.92
22	2	311	CLA	C3D-C4D-ND	4.51	117.53	110.24
22	B	825	CLA	C3C-C4C-NC	4.50	115.62	110.57
22	B	814	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
29	4	313	5X6	C12-C13-C14	-4.50	112.03	118.94
22	B	832	CLA	C3C-C4C-NC	4.50	115.62	110.57
22	6	314	CLA	C4A-NA-C1A	-4.50	104.68	106.71
22	5	310	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	A	821	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	B	824	CLA	CHD-C1D-ND	-4.50	120.32	124.45
22	A	814	CLA	C3D-C4D-ND	4.50	117.51	110.24
22	2	307	CLA	C4A-NA-C1A	-4.50	104.68	106.71
22	A	816	CLA	C3C-C4C-NC	4.50	115.61	110.57
22	B	838	CLA	C3D-C4D-ND	4.50	117.51	110.24
22	5	308	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
29	2	312	5X6	C12-C11-C03	-4.49	114.58	127.20
22	A	821	CLA	CAC-C3C-C4C	4.49	130.64	124.81
22	3	305	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
22	B	817	CLA	C2C-C1C-NC	4.49	114.18	109.97
22	6	308	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
22	4	309	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
22	B	833	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
22	B	833	CLA	C3D-C4D-ND	4.49	117.50	110.24
29	5	312	5X6	C12-C11-C03	-4.49	114.60	127.20
22	B	839	CLA	C3D-C4D-ND	4.48	117.49	110.24
22	6	303	CLA	C3D-C4D-ND	4.48	117.49	110.24
22	B	806	CLA	CHD-C1D-ND	-4.48	120.33	124.45
22	A	832	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	A	811	CLA	C3C-C4C-NC	4.48	115.60	110.57
22	A	816	CLA	CHD-C1D-ND	-4.48	120.33	124.45
22	7	313	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	4	303	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
22	B	811	CLA	C3D-C4D-ND	4.48	117.49	110.24
22	2	304	CLA	C4-C3-C5	4.48	122.81	115.27
22	A	827	CLA	CHD-C1D-ND	-4.48	120.34	124.45
22	3	305	CLA	C3D-C2D-C1D	-4.48	99.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	851	5X6	C23-C22-C21	-4.48	112.07	118.94
22	7	307	CLA	O2D-CGD-CBD	4.48	119.22	111.27
22	B	814	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
22	O	204	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
22	B	836	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
22	A	834	CLA	O2D-CGD-CBD	4.48	119.22	111.27
22	2	306	CLA	C3D-C4D-ND	4.47	117.48	110.24
22	6	303	CLA	C3D-C2D-C1D	-4.47	99.72	105.83
22	B	821	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
22	Z	201	CLA	C2C-C1C-NC	4.47	114.16	109.97
22	A	806	CLA	CMD-C2D-C1D	4.47	132.60	124.71
22	A	826	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
22	2	305	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
22	6	308	CLA	C3D-C4D-ND	4.47	117.47	110.24
22	B	826	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
22	L	205	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
22	A	829	CLA	C3C-C4C-NC	4.47	115.58	110.57
22	B	850	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
22	A	818	CLA	C3D-C4D-ND	4.47	117.46	110.24
22	4	312	CLA	C3D-C4D-ND	4.47	117.46	110.24
22	B	833	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
29	O	207	5X6	C15-C16-C17	-4.46	113.88	126.42
22	B	819	CLA	C3D-C4D-ND	4.46	117.45	110.24
22	B	832	CLA	O2D-CGD-O1D	-4.46	115.12	123.84
22	A	824	CLA	C3D-C4D-ND	4.46	117.45	110.24
22	4	304	CLA	CAC-C3C-C4C	4.46	130.59	124.81
22	5	302	CLA	C2C-C1C-NC	4.46	114.15	109.97
22	A	826	CLA	O2D-CGD-CBD	4.46	119.19	111.27
22	B	829	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
22	A	831	CLA	CHD-C1D-ND	-4.46	120.36	124.45
22	B	814	CLA	C3D-C4D-ND	4.46	117.45	110.24
22	A	814	CLA	O2D-CGD-CBD	4.46	119.19	111.27
22	B	830	CLA	C3B-C2B-C1B	-4.45	101.78	107.16
22	4	304	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
29	6	316	5X6	C15-C16-C17	-4.45	113.91	126.42
22	2	303	CLA	C4A-NA-C1A	-4.45	104.70	106.71
29	7	316	5X6	C23-C22-C21	-4.45	112.11	118.94
22	O	204	CLA	C3D-C4D-ND	4.45	117.44	110.24
29	O	208	5X6	C24-C23-C22	-4.45	113.91	126.42
22	B	815	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
22	6	311	CLA	C3D-C4D-ND	4.45	117.44	110.24
22	7	310	CLA	CAC-C3C-C4C	4.45	130.58	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	832	CLA	C3D-C4D-ND	4.45	117.44	110.24
22	2	304	CLA	C3D-C4D-ND	4.45	117.44	110.24
22	4	304	CLA	O2D-CGD-CBD	4.45	119.17	111.27
22	2	309	CLA	CAC-C3C-C4C	4.45	130.58	124.81
29	2	314	5X6	C16-C17-C18	-4.45	112.12	118.94
29	Z	206	5X6	C11-C12-C13	-4.45	119.52	126.23
22	1	308	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
22	5	311	CLA	C3D-C4D-ND	4.45	117.43	110.24
22	B	830	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	A	809	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
22	B	830	CLA	C3C-C4C-NC	4.44	115.55	110.57
29	4	314	5X6	C12-C11-C03	-4.44	114.73	127.20
29	M	101	5X6	C15-C16-C17	-4.44	113.94	126.42
22	A	808	CLA	C3D-C4D-ND	4.44	117.42	110.24
22	B	849	CLA	C3D-C4D-ND	4.44	117.42	110.24
22	A	805	CLA	C3C-C4C-NC	4.44	115.55	110.57
22	6	310	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	3	303	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	2	304	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
22	B	826	CLA	CHD-C1D-ND	-4.44	120.38	124.45
29	5	312	5X6	C11-C03-C02	-4.44	110.71	121.46
22	2	307	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
22	5	306	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
22	A	805	CLA	O2D-CGD-CBD	4.43	119.14	111.27
22	2	304	CLA	C4A-NA-C1A	-4.43	104.71	106.71
22	A	819	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
22	7	308	CLA	C3D-C4D-ND	4.43	117.40	110.24
22	B	835	CLA	C4-C3-C2	-4.43	112.32	123.68
22	5	305	CLA	C3D-C4D-ND	4.43	117.40	110.24
29	4	313	5X6	C12-C11-C03	-4.43	114.77	127.20
25	L	206	BCR	C8-C9-C10	4.43	125.73	118.94
22	B	829	CLA	O2D-CGD-O1D	-4.43	115.19	123.84
22	B	837	CLA	C3D-C4D-ND	4.42	117.39	110.24
22	7	311	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
22	A	815	CLA	O2D-CGD-CBD	4.42	119.13	111.27
29	1	313	5X6	C20-C19-C18	-4.42	114.42	123.47
29	1	311	5X6	C15-C16-C17	-4.42	114.00	126.42
29	M	101	5X6	C27-C26-C25	-4.42	112.16	118.94
22	B	850	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
22	1	309	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
29	6	315	5X6	C39-C26-C25	-4.42	116.73	122.92
29	1	314	5X6	C11-C03-C02	-4.42	110.76	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	307	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
22	J	102	CLA	C3D-C2D-C1D	-4.42	99.81	105.83
22	4	308	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
22	A	817	CLA	C3D-C4D-ND	4.41	117.38	110.24
22	B	818	CLA	C3D-C4D-ND	4.41	117.38	110.24
22	Z	204	CLA	C3D-C4D-ND	4.41	117.38	110.24
29	1	314	5X6	C23-C22-C21	-4.41	112.17	118.94
22	4	306	CLA	C4A-NA-C1A	-4.41	104.72	106.71
22	7	306	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
22	7	307	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
29	5	321	5X6	C24-C23-C22	-4.41	114.03	126.42
22	4	307	CLA	CHD-C1D-ND	-4.41	120.40	124.45
22	B	828	CLA	O2D-CGD-CBD	4.41	119.10	111.27
22	K	102	CLA	C3C-C4C-NC	4.40	115.51	110.57
22	2	309	CLA	C3D-C4D-ND	4.40	117.36	110.24
22	2	311	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
22	5	301	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
22	1	304	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	1	303	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	F	205	CLA	C3D-C4D-ND	4.40	117.36	110.24
22	A	809	CLA	C3D-C4D-ND	4.40	117.35	110.24
22	7	308	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
22	B	802	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
22	5	309	CLA	C3D-C4D-ND	4.40	117.35	110.24
22	A	848	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
22	2	306	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
22	1	306	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
29	7	315	5X6	C19-C20-C21	-4.39	114.47	123.47
22	A	803	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
22	A	823	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
22	A	831	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
22	3	304	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
29	6	316	5X6	C24-C23-C22	-4.39	114.08	126.42
22	F	206	CLA	C3D-C4D-ND	4.39	117.34	110.24
22	5	308	CLA	C3D-C4D-ND	4.39	117.34	110.24
22	F	205	CLA	C2C-C1C-NC	4.39	114.08	109.97
29	O	208	5X6	C42-C13-C14	-4.39	116.78	122.92
29	2	312	5X6	C24-C23-C22	-4.39	114.09	126.42
22	7	310	CLA	C3D-C4D-ND	4.39	117.33	110.24
22	A	836	CLA	C3D-C4D-ND	4.38	117.33	110.24
22	6	304	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	A	805	CLA	C4A-NA-C1A	-4.38	104.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	314	CLA	C3D-C4D-ND	4.38	117.33	110.24
22	6	312	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	2	303	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	A	832	CLA	C3D-C4D-ND	4.38	117.32	110.24
22	B	801	CLA	CMD-C2D-C1D	4.38	132.43	124.71
22	6	309	CLA	C3D-C4D-ND	4.38	117.32	110.24
22	A	816	CLA	C3D-C4D-ND	4.37	117.31	110.24
22	B	830	CLA	C3D-C4D-ND	4.37	117.31	110.24
21	A	801	CL0	C3B-C2B-C1B	-4.37	101.88	107.16
22	A	832	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
22	1	303	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
22	1	309	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
29	5	314	5X6	C12-C13-C14	-4.37	112.24	118.94
22	B	822	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
22	A	805	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
22	7	310	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
22	6	310	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
29	7	317	5X6	C23-C22-C21	-4.37	112.24	118.94
22	4	303	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
22	A	827	CLA	CMD-C2D-C1D	4.36	132.40	124.71
22	B	849	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
29	1	316	5X6	C27-C28-C29	-4.36	114.95	127.20
22	B	819	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	J	102	CLA	C3D-C4D-ND	4.36	117.29	110.24
22	7	303	CLA	CHD-C4C-C3C	-4.36	118.43	124.84
22	2	307	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
29	3	306	5X6	C19-C20-C21	-4.36	114.55	123.47
22	4	302	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	A	820	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
22	5	306	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
22	L	204	CLA	C3C-C4C-NC	4.35	115.45	110.57
22	1	302	CLA	C4A-NA-C1A	-4.35	104.75	106.71
22	B	838	CLA	C3B-C2B-C1B	-4.35	101.91	107.16
22	4	311	CLA	C3D-C4D-ND	4.35	117.28	110.24
22	A	819	CLA	C3D-C4D-ND	4.35	117.27	110.24
22	B	801	CLA	C3B-C2B-C1B	-4.35	101.91	107.16
22	4	311	CLA	C3B-C2B-C1B	-4.35	101.91	107.16
22	6	304	CLA	C2C-C1C-NC	4.35	114.04	109.97
22	B	822	CLA	CAC-C3C-C4C	4.35	130.45	124.81
22	B	813	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	A	817	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	A	817	CLA	C3D-C2D-C1D	-4.34	99.91	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	308	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
22	6	307	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	L	205	CLA	C3D-C4D-ND	4.34	117.26	110.24
22	B	803	CLA	C3C-C4C-NC	4.34	115.44	110.57
22	B	835	CLA	C3D-C4D-ND	4.34	117.25	110.24
29	6	317	5X6	C01-C02-C03	-4.34	119.66	124.53
29	5	314	5X6	C15-C16-C17	-4.33	114.24	126.42
22	6	307	CLA	O2D-CGD-CBD	4.33	118.97	111.27
22	B	821	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
22	A	837	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
22	K	102	CLA	C3D-C4D-ND	4.33	117.25	110.24
29	1	312	5X6	C25-C24-C23	-4.33	109.70	123.22
22	A	812	CLA	CMD-C2D-C1D	4.33	132.34	124.71
22	B	826	CLA	C3D-C4D-ND	4.33	117.24	110.24
22	K	101	CLA	C3D-C4D-ND	4.33	117.24	110.24
22	A	833	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
22	A	835	CLA	CMD-C2D-C1D	4.33	132.34	124.71
22	6	313	CLA	C4A-NA-C1A	-4.32	104.76	106.71
22	2	302	CLA	CAC-C3C-C4C	4.32	130.42	124.81
29	J	104	5X6	C11-C03-C02	-4.32	110.99	121.46
22	B	823	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
22	A	831	CLA	C4A-NA-C1A	-4.32	104.76	106.71
22	5	310	CLA	C3D-C4D-ND	4.32	117.23	110.24
22	B	839	CLA	C3C-C4C-NC	4.32	115.42	110.57
22	4	311	CLA	C3C-C4C-NC	4.32	115.42	110.57
22	A	813	CLA	C3D-C4D-ND	4.32	117.22	110.24
22	O	203	CLA	O2D-CGD-CBD	4.32	118.94	111.27
22	F	206	CLA	C3C-C4C-NC	4.31	115.41	110.57
22	5	307	CLA	C3B-C2B-C1B	-4.31	101.95	107.16
22	4	312	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
22	O	206	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
29	7	315	5X6	C15-C16-C17	-4.31	114.30	126.42
22	A	835	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
22	B	820	CLA	C4A-NA-C1A	-4.31	104.77	106.71
22	5	302	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
22	B	809	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
25	B	844	BCR	C34-C9-C10	-4.31	116.89	122.92
22	A	828	CLA	C3C-C4C-NC	4.31	115.40	110.57
22	3	302	CLA	C3D-C4D-ND	4.31	117.20	110.24
22	7	312	CLA	C2C-C1C-NC	4.31	114.01	109.97
22	B	820	CLA	C3D-C4D-ND	4.30	117.20	110.24
29	J	104	5X6	C25-C24-C23	-4.30	109.79	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	828	CLA	C4-C3-C5	4.30	122.51	115.27
22	7	304	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
22	A	803	CLA	C3B-C4B-NB	4.30	114.50	110.52
22	A	828	CLA	C3D-C4D-ND	4.30	117.19	110.24
22	B	813	CLA	C3D-C4D-ND	4.30	117.19	110.24
29	7	314	5X6	C38-C30-C31	-4.30	106.39	114.36
22	B	801	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
22	A	832	CLA	C3C-C4C-NC	4.30	115.39	110.57
22	A	808	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
29	1	314	5X6	C42-C13-C12	-4.29	111.32	118.08
29	5	314	5X6	C27-C26-C25	-4.29	112.36	118.94
22	4	310	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
22	B	815	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
22	A	804	CLA	CHD-C1D-ND	-4.28	120.52	124.45
22	7	308	CLA	C2C-C1C-NC	4.28	113.98	109.97
22	F	204	CLA	CAC-C3C-C4C	4.28	130.36	124.81
22	6	304	CLA	C3B-C2B-C1B	-4.27	102.00	107.16
22	6	307	CLA	C3D-C4D-ND	4.27	117.15	110.24
22	4	304	CLA	C3D-C4D-ND	4.27	117.14	110.24
22	B	803	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
22	2	307	CLA	C2C-C1C-NC	4.27	113.97	109.97
22	7	303	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
22	7	313	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
22	B	815	CLA	C3D-C4D-ND	4.27	117.14	110.24
29	7	315	5X6	C16-C17-C18	-4.27	112.39	118.94
22	A	812	CLA	O2D-CGD-CBD	4.27	118.85	111.27
22	B	821	CLA	C2C-C1C-NC	4.27	113.97	109.97
22	2	311	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
22	B	835	CLA	C4A-NA-C1A	-4.26	104.79	106.71
22	B	822	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
22	4	311	CLA	C2C-C1C-NC	4.26	113.97	109.97
29	1	316	5X6	C12-C11-C03	-4.26	115.23	127.20
22	A	823	CLA	CAC-C3C-C4C	4.26	130.34	124.81
25	A	861	BCR	C37-C22-C21	-4.26	116.95	122.92
22	A	829	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
22	A	812	CLA	C3D-C4D-ND	4.26	117.13	110.24
22	4	310	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	4	305	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
22	1	305	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
22	6	305	CLA	C4A-NA-C1A	-4.26	104.79	106.71
22	4	305	CLA	O2D-CGD-CBD	4.25	118.83	111.27
22	A	837	CLA	C3C-C4C-NC	4.25	115.34	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	822	CLA	C3D-C4D-ND	4.25	117.12	110.24
22	7	303	CLA	C4A-NA-C1A	-4.25	104.80	106.71
22	B	828	CLA	C3C-C4C-NC	4.25	115.34	110.57
22	L	205	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
22	A	838	CLA	C3D-C4D-ND	4.25	117.11	110.24
22	B	816	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
22	A	829	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
22	6	314	CLA	C3C-C4C-NC	4.25	115.33	110.57
22	3	304	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
22	4	306	CLA	C3D-C4D-ND	4.25	117.11	110.24
22	A	816	CLA	O2D-CGD-CBD	4.24	118.81	111.27
22	B	837	CLA	C3C-C4C-NC	4.24	115.33	110.57
22	5	310	CLA	C3C-C4C-NC	4.24	115.33	110.57
22	A	830	CLA	C3D-C4D-ND	4.24	117.10	110.24
22	A	828	CLA	C4A-NA-C1A	-4.24	104.80	106.71
22	F	205	CLA	C4A-NA-C1A	-4.23	104.80	106.71
22	A	811	CLA	C3D-C4D-ND	4.23	117.08	110.24
22	6	306	CLA	C4-C3-C5	4.23	122.39	115.27
22	A	806	CLA	C3D-C4D-ND	4.23	117.08	110.24
22	B	849	CLA	C3C-C4C-NC	4.23	115.31	110.57
22	6	314	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
22	4	307	CLA	C3C-C4C-NC	4.23	115.31	110.57
22	B	836	CLA	C3D-C4D-ND	4.23	117.07	110.24
22	A	804	CLA	C3C-C4C-NC	4.22	115.31	110.57
29	6	316	5X6	C20-C19-C18	-4.22	114.82	123.47
22	5	301	CLA	C3D-C4D-ND	4.22	117.07	110.24
22	1	310	CLA	C4A-NA-C1A	-4.22	104.81	106.71
22	7	306	CLA	C2C-C1C-NC	4.22	113.93	109.97
22	A	859	CLA	C3C-C4C-NC	4.22	115.31	110.57
22	A	858	CLA	O2D-CGD-CBD	4.22	118.77	111.27
22	2	308	CLA	C2C-C1C-NC	4.22	113.92	109.97
22	3	305	CLA	C2C-C1C-NC	4.22	113.92	109.97
22	7	310	CLA	C4A-NA-C1A	-4.22	104.81	106.71
22	B	828	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
29	6	316	5X6	C42-C13-C14	-4.21	117.02	122.92
22	7	313	CLA	C4A-NA-C1A	-4.21	104.81	106.71
22	4	302	CLA	CAC-C3C-C4C	4.21	130.28	124.81
22	Z	204	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
22	F	205	CLA	O2D-CGD-CBD	4.21	118.75	111.27
22	B	838	CLA	C4-C3-C5	4.21	122.36	115.27
22	A	819	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
22	6	313	CLA	CAC-C3C-C4C	4.21	130.27	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	203	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
22	B	825	CLA	C3D-C4D-ND	4.21	117.05	110.24
29	7	316	5X6	C15-C16-C17	-4.21	114.60	126.42
22	A	858	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
22	O	203	CLA	C4A-NA-C1A	-4.20	104.82	106.71
22	1	304	CLA	C3D-C4D-ND	4.20	117.04	110.24
22	B	824	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	B	831	CLA	C3C-C4C-NC	4.20	115.28	110.57
29	4	313	5X6	C24-C23-C22	-4.20	114.61	126.42
29	7	314	5X6	C19-C20-C21	-4.20	114.87	123.47
22	B	817	CLA	C3D-C4D-ND	4.20	117.03	110.24
22	A	807	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	5	308	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	B	837	CLA	C4A-NA-C1A	-4.20	104.82	106.71
22	1	305	CLA	C3D-C4D-ND	4.20	117.03	110.24
22	A	807	CLA	CHD-C1D-ND	-4.20	120.60	124.45
22	6	308	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	A	857	CLA	C4A-NA-C1A	-4.20	104.82	106.71
22	7	308	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
22	A	822	CLA	C3B-C2B-C1B	-4.20	102.10	107.16
22	1	303	CLA	C4A-NA-C1A	-4.20	104.82	106.71
22	B	827	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
22	A	803	CLA	C3C-C4C-NC	4.19	115.27	110.57
22	3	301	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
22	1	307	CLA	C4-C3-C5	4.19	122.31	115.27
22	6	309	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
22	O	205	CLA	C4A-NA-C1A	-4.18	104.83	106.71
22	4	309	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
22	6	311	CLA	O2D-CGD-CBD	4.18	118.70	111.27
29	5	312	5X6	C25-C24-C23	-4.18	110.17	123.22
22	A	826	CLA	CAC-C3C-C4C	4.18	130.23	124.81
22	A	802	CLA	C3D-C4D-ND	4.18	117.00	110.24
22	Z	201	CLA	C3D-C4D-ND	4.18	117.00	110.24
22	5	306	CLA	C3C-C4C-NC	4.18	115.25	110.57
22	7	312	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
22	B	804	CLA	CAA-C2A-C3A	-4.17	101.36	112.78
22	4	312	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
22	A	837	CLA	CAC-C3C-C4C	4.17	130.22	124.81
25	L	201	BCR	C37-C22-C21	-4.17	117.08	122.92
22	B	829	CLA	C3D-C4D-ND	4.17	116.98	110.24
22	B	812	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
22	O	205	CLA	O2D-CGD-CBD	4.16	118.67	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	321	5X6	C20-C19-C18	-4.16	114.95	123.47
22	B	808	CLA	C3D-C4D-ND	4.16	116.97	110.24
29	2	313	5X6	C12-C11-C03	-4.16	115.53	127.20
29	5	321	5X6	C11-C03-C02	-4.16	111.39	121.46
29	5	321	5X6	C27-C26-C25	-4.16	112.56	118.94
22	4	303	CLA	C3C-C4C-NC	4.16	115.23	110.57
22	4	310	CLA	C3D-C4D-ND	4.16	116.96	110.24
25	Z	205	BCR	C34-C9-C10	-4.16	117.10	122.92
22	B	818	CLA	C4A-NA-C1A	-4.15	104.84	106.71
22	B	809	CLA	C3D-C4D-ND	4.15	116.96	110.24
22	A	810	CLA	C3D-C4D-ND	4.15	116.96	110.24
29	1	311	5X6	C24-C23-C22	-4.15	114.75	126.42
29	Z	206	5X6	C20-C19-C18	-4.15	114.97	123.47
29	6	317	5X6	C27-C26-C25	-4.15	112.57	118.94
22	A	816	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	6	313	CLA	C3D-C4D-ND	4.15	116.95	110.24
29	7	314	5X6	C41-C17-C16	-4.15	111.54	118.08
22	A	836	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
22	A	815	CLA	C3D-C4D-ND	4.15	116.95	110.24
22	1	307	CLA	CAA-C2A-C3A	-4.15	101.43	112.78
29	4	314	5X6	C41-C17-C18	-4.15	117.12	122.92
29	5	314	5X6	C01-C02-C07	-4.15	106.67	114.36
21	A	801	CL0	C3C-C4C-NC	4.14	115.22	110.57
29	6	317	5X6	C23-C22-C21	-4.14	112.58	118.94
29	2	313	5X6	C14-C15-C16	-4.14	110.30	123.22
22	A	839	CLA	CAC-C3C-C4C	4.14	130.18	124.81
22	A	812	CLA	C4A-NA-C1A	-4.14	104.84	106.71
22	2	306	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
29	1	313	5X6	C12-C13-C14	-4.14	112.59	118.94
29	4	314	5X6	C24-C23-C22	-4.13	114.80	126.42
21	A	801	CL0	CAA-C2A-C3A	-4.13	101.46	112.78
22	A	823	CLA	CHD-C1D-ND	-4.13	120.66	124.45
29	3	306	5X6	C42-C13-C12	-4.13	111.57	118.08
22	7	309	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
22	A	839	CLA	C3D-C4D-ND	4.13	116.92	110.24
29	O	207	5X6	C41-C17-C18	-4.13	117.14	122.92
22	A	822	CLA	C3C-C4C-NC	4.13	115.20	110.57
22	L	203	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	A	809	CLA	C4A-NA-C1A	-4.13	104.85	106.71
25	L	202	BCR	C34-C9-C10	-4.13	117.14	122.92
22	B	829	CLA	C4A-NA-C1A	-4.13	104.85	106.71
29	1	312	5X6	C20-C19-C18	-4.13	115.02	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	822	CLA	O2D-CGD-O1D	-4.12	115.77	123.84
22	4	307	CLA	O2D-CGD-CBD	4.12	118.60	111.27
22	A	857	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
22	5	310	CLA	C4A-NA-C1A	-4.12	104.85	106.71
22	A	833	CLA	C3C-C4C-NC	4.12	115.19	110.57
22	Z	201	CLA	C3C-C4C-NC	4.12	115.19	110.57
25	A	845	BCR	C34-C9-C8	4.12	124.57	118.08
29	4	314	5X6	C27-C28-C29	-4.12	115.62	127.20
22	B	833	CLA	C3C-C4C-NC	4.12	115.19	110.57
21	A	801	CL0	CHD-C1D-ND	-4.12	120.67	124.45
22	A	827	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
25	F	201	BCR	C34-C9-C8	4.12	124.56	118.08
29	O	207	5X6	C01-C02-C07	-4.11	106.73	114.36
22	B	812	CLA	O2D-CGD-CBD	4.11	118.58	111.27
22	1	305	CLA	C4A-NA-C1A	-4.11	104.86	106.71
25	K	103	BCR	C37-C22-C21	-4.11	117.16	122.92
22	A	808	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
22	5	301	CLA	C3C-C4C-NC	4.11	115.18	110.57
29	1	313	5X6	C24-C23-C22	-4.11	114.87	126.42
22	B	807	CLA	C3C-C4C-NC	4.11	115.18	110.57
22	F	204	CLA	C3D-C4D-ND	4.11	116.88	110.24
22	A	836	CLA	C3C-C4C-NC	4.11	115.18	110.57
29	O	208	5X6	C14-C15-C16	-4.11	110.41	123.22
22	A	832	CLA	O2D-CGD-O1D	-4.10	115.81	123.84
22	5	302	CLA	C3C-C4C-NC	4.10	115.17	110.57
22	B	831	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
22	A	813	CLA	C3C-C4C-NC	4.10	115.17	110.57
22	A	818	CLA	C3C-C4C-NC	4.10	115.17	110.57
22	B	823	CLA	C4A-NA-C1A	-4.10	104.86	106.71
22	A	822	CLA	O2D-CGD-CBD	4.10	118.55	111.27
29	Z	206	5X6	C27-C28-C29	-4.10	115.69	127.20
22	A	848	CLA	C3C-C4C-NC	4.10	115.17	110.57
22	A	827	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
22	O	205	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
29	7	317	5X6	C12-C11-C03	-4.10	115.70	127.20
22	2	302	CLA	C3D-C4D-ND	4.10	116.86	110.24
29	1	311	5X6	C27-C26-C25	-4.09	112.66	118.94
22	O	203	CLA	C3D-C4D-ND	4.09	116.86	110.24
22	A	809	CLA	C2C-C1C-NC	4.09	113.81	109.97
22	B	818	CLA	C3C-C4C-NC	4.09	115.16	110.57
22	J	102	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
22	B	812	CLA	CAC-C3C-C4C	4.09	130.12	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	308	CLA	C3C-C4C-NC	4.09	115.16	110.57
29	6	316	5X6	C01-C02-C07	-4.09	106.78	114.36
22	B	809	CLA	C3C-C4C-NC	4.09	115.15	110.57
22	6	304	CLA	C3C-C4C-NC	4.09	115.15	110.57
22	5	309	CLA	O2D-CGD-CBD	4.09	118.53	111.27
22	6	305	CLA	C3D-C4D-ND	4.08	116.84	110.24
22	1	310	CLA	C3C-C4C-NC	4.08	115.15	110.57
22	B	837	CLA	CAC-C3C-C4C	4.08	130.10	124.81
22	7	307	CLA	C3D-C4D-ND	4.08	116.83	110.24
22	B	817	CLA	C3C-C4C-NC	4.08	115.14	110.57
22	2	305	CLA	CAC-C3C-C4C	4.08	130.10	124.81
25	L	202	BCR	C37-C22-C23	4.07	124.50	118.08
29	6	317	5X6	C15-C16-C17	-4.07	114.97	126.42
22	B	818	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
22	4	306	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
29	7	314	5X6	C42-C13-C12	-4.07	111.66	118.08
22	A	857	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
22	B	803	CLA	C3D-C4D-ND	4.07	116.82	110.24
22	A	830	CLA	C3C-C4C-NC	4.07	115.13	110.57
29	B	851	5X6	C40-C22-C21	-4.07	117.23	122.92
22	7	310	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
22	4	306	CLA	O2D-CGD-CBD	4.07	118.49	111.27
22	7	304	CLA	C3D-C2D-C1D	-4.06	100.28	105.83
22	3	303	CLA	CAC-C3C-C4C	4.06	130.08	124.81
29	7	314	5X6	C05-C06-C07	-4.06	104.74	110.30
22	A	829	CLA	C3D-C4D-ND	4.06	116.81	110.24
25	B	843	BCR	C16-C15-C14	4.06	131.79	123.47
22	A	832	CLA	CAC-C3C-C4C	4.06	130.08	124.81
22	6	310	CLA	C3C-C4C-NC	4.06	115.12	110.57
22	A	825	CLA	C3D-C4D-ND	4.06	116.80	110.24
29	7	314	5X6	C12-C13-C14	-4.05	112.72	118.94
22	5	305	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
29	5	313	5X6	C15-C16-C17	-4.05	115.03	126.42
22	A	859	CLA	C1C-C2C-C3C	-4.05	102.69	106.96
29	B	851	5X6	C12-C13-C14	-4.05	112.72	118.94
22	B	838	CLA	C3C-C4C-NC	4.05	115.12	110.57
29	7	315	5X6	C42-C13-C12	-4.05	111.69	118.08
22	B	805	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
22	A	803	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
22	B	810	CLA	C4A-NA-C1A	-4.05	104.89	106.71
22	B	819	CLA	C3C-C4C-NC	4.05	115.11	110.57
22	5	306	CLA	O2D-CGD-CBD	4.05	118.46	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	309	CLA	C3C-C4C-NC	4.05	115.11	110.57
29	3	306	5X6	C16-C17-C18	-4.05	112.73	118.94
22	A	808	CLA	C3C-C4C-NC	4.05	115.11	110.57
22	A	817	CLA	C3C-C4C-NC	4.05	115.11	110.57
22	A	805	CLA	C3B-C4B-NB	4.04	114.27	110.52
29	B	851	5X6	C14-C15-C16	-4.04	110.60	123.22
22	5	307	CLA	C4A-NA-C1A	-4.04	104.89	106.71
22	6	303	CLA	C4A-NA-C1A	-4.04	104.89	106.71
29	7	317	5X6	C20-C19-C18	-4.04	115.20	123.47
22	5	303	CLA	C3C-C4C-NC	4.04	115.10	110.57
22	B	821	CLA	C3C-C4C-NC	4.04	115.10	110.57
22	A	805	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
22	2	310	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
29	7	316	5X6	C01-C02-C07	-4.03	106.88	114.36
29	6	316	5X6	C11-C03-C02	-4.03	111.69	121.46
22	B	813	CLA	C4A-NA-C1A	-4.03	104.89	106.71
29	1	311	5X6	C39-C26-C25	-4.03	117.28	122.92
22	A	810	CLA	CAC-C3C-C4C	4.03	130.04	124.81
22	B	810	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
22	L	203	CLA	C3C-C4C-NC	4.03	115.08	110.57
22	4	308	CLA	C3B-C2B-C1B	-4.02	102.30	107.16
22	A	820	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
22	A	805	CLA	O2D-CGD-O1D	-4.02	115.97	123.84
25	B	841	BCR	C37-C22-C21	-4.02	117.29	122.92
22	O	204	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
22	B	802	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
29	3	306	5X6	C12-C11-C03	-4.02	115.91	127.20
29	2	312	5X6	C23-C22-C21	-4.02	112.77	118.94
22	O	203	CLA	C3C-C4C-NC	4.02	115.08	110.57
22	5	301	CLA	C4A-NA-C1A	-4.02	104.90	106.71
22	A	811	CLA	O2D-CGD-CBD	4.02	118.41	111.27
29	M	101	5X6	C23-C22-C21	-4.02	112.78	118.94
22	4	307	CLA	C4A-NA-C1A	-4.02	104.90	106.71
22	K	101	CLA	C3C-C4C-NC	4.01	115.07	110.57
22	A	835	CLA	C3D-C4D-ND	4.01	116.73	110.24
22	B	834	CLA	C3B-C2B-C1B	-4.01	102.32	107.16
22	1	303	CLA	CAC-C3C-C4C	4.01	130.01	124.81
22	B	818	CLA	CAC-C3C-C4C	4.01	130.01	124.81
29	M	101	5X6	C40-C22-C23	-4.01	111.76	118.08
22	B	834	CLA	C3D-C4D-ND	4.01	116.72	110.24
22	5	304	CLA	O2D-CGD-CBD	4.01	118.39	111.27
22	A	838	CLA	C4C-C3C-C2C	-4.01	101.06	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	311	5X6	C12-C13-C14	-4.01	112.79	118.94
22	A	837	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
22	A	859	CLA	C3B-C4B-NB	4.00	114.23	110.52
25	4	316	BCR	C37-C22-C21	-4.00	117.31	122.92
22	B	803	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
22	5	306	CLA	C3D-C4D-ND	4.00	116.71	110.24
29	7	316	5X6	C11-C03-C02	-4.00	111.77	121.46
22	O	206	CLA	C4A-NA-C1A	-4.00	104.91	106.71
22	2	309	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
22	5	309	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
22	B	819	CLA	C2C-C1C-NC	4.00	113.72	109.97
29	2	313	5X6	C15-C16-C17	-4.00	115.19	126.42
29	5	313	5X6	C27-C26-C25	-4.00	112.81	118.94
22	1	309	CLA	CAC-C3C-C4C	4.00	129.99	124.81
22	B	827	CLA	C1C-C2C-C3C	-4.00	102.76	106.96
22	7	306	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	B	829	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
22	1	308	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
22	B	850	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
22	1	307	CLA	O2A-CGA-CBA	3.98	124.41	111.91
22	6	311	CLA	C4A-NA-C1A	-3.98	104.92	106.71
22	6	312	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
29	Z	206	5X6	C25-C24-C23	-3.98	110.79	123.22
22	1	302	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
29	4	315	5X6	C24-C23-C22	-3.98	115.23	126.42
22	6	313	CLA	C3C-C4C-NC	3.98	115.03	110.57
22	A	818	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
22	K	102	CLA	CAC-C3C-C4C	3.98	129.97	124.81
22	B	835	CLA	O2D-CGD-O1D	-3.98	116.07	123.84
25	A	845	BCR	C30-C25-C26	-3.97	117.02	122.61
22	7	305	CLA	C3D-C4D-ND	3.97	116.67	110.24
22	B	805	CLA	CAC-C3C-C4C	3.97	129.97	124.81
22	1	309	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	1	304	CLA	CAC-C3C-C4C	3.97	129.96	124.81
22	7	310	CLA	C3C-C4C-NC	3.97	115.02	110.57
22	Z	204	CLA	C3C-C4C-NC	3.97	115.02	110.57
22	L	203	CLA	C3B-C2B-C1B	-3.97	102.38	107.16
22	7	311	CLA	C3B-C2B-C1B	-3.97	102.38	107.16
22	B	806	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
22	B	812	CLA	C3D-C4D-ND	3.96	116.65	110.24
22	6	308	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
29	Z	206	5X6	C23-C22-C21	-3.96	112.87	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	838	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
22	A	816	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	A	815	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
22	J	102	CLA	CAC-C3C-C4C	3.95	129.94	124.81
29	B	851	5X6	C27-C28-C29	-3.95	116.11	127.20
22	B	827	CLA	CAC-C3C-C4C	3.95	129.93	124.81
22	6	303	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
22	A	803	CLA	C3B-C2B-C1B	-3.95	102.40	107.16
22	B	801	CLA	C3C-C4C-NC	3.94	114.99	110.57
29	6	316	5X6	C12-C13-C14	-3.94	112.89	118.94
29	1	313	5X6	C25-C24-C23	-3.94	110.92	123.22
22	1	304	CLA	C3C-C4C-NC	3.94	114.99	110.57
29	7	318	5X6	C27-C26-C25	-3.94	112.90	118.94
29	1	316	5X6	C41-C17-C18	-3.94	117.41	122.92
22	B	815	CLA	C3C-C4C-NC	3.94	114.98	110.57
22	7	306	CLA	CAC-C3C-C4C	3.94	129.92	124.81
22	A	805	CLA	CAC-C3C-C4C	3.93	129.91	124.81
22	2	308	CLA	C3B-C2B-C1B	-3.93	102.41	107.16
22	B	802	CLA	C3D-C4D-ND	3.93	116.60	110.24
22	B	816	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
22	2	302	CLA	C3B-C2B-C1B	-3.93	102.42	107.16
22	1	307	CLA	C3C-C4C-NC	3.93	114.98	110.57
22	B	821	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
22	4	307	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
22	B	823	CLA	C4C-C3C-C2C	-3.93	101.17	106.90
29	7	315	5X6	C12-C13-C14	-3.93	112.91	118.94
22	B	830	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
22	A	813	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
22	2	309	CLA	C3C-C4C-NC	3.93	114.97	110.57
22	B	831	CLA	C4A-NA-C1A	-3.93	104.94	106.71
29	7	314	5X6	C01-C02-C07	-3.92	107.09	114.36
22	A	807	CLA	C3D-C4D-ND	3.92	116.58	110.24
22	B	808	CLA	CAC-C3C-C4C	3.92	129.89	124.81
29	B	851	5X6	C40-C22-C23	-3.92	111.91	118.08
22	A	831	CLA	C3D-C4D-ND	3.91	116.57	110.24
22	6	305	CLA	C3C-C4C-NC	3.91	114.96	110.57
25	A	844	BCR	C37-C22-C23	3.91	124.24	118.08
22	A	821	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
22	A	807	CLA	CAA-C2A-C3A	-3.91	102.07	112.78
22	1	305	CLA	C3C-C4C-NC	3.91	114.95	110.57
22	1	303	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
22	1	302	CLA	CAC-C3C-C4C	3.90	129.88	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	311	5X6	C42-C13-C12	-3.90	111.93	118.08
29	6	317	5X6	C41-C17-C18	-3.90	117.46	122.92
22	B	834	CLA	CAC-C3C-C4C	3.90	129.87	124.81
22	B	838	CLA	CAC-C3C-C4C	3.90	129.87	124.81
22	B	827	CLA	CMC-C2C-C1C	3.90	130.98	125.04
22	O	204	CLA	C3C-C4C-NC	3.90	114.94	110.57
29	3	306	5X6	C12-C13-C14	-3.90	112.96	118.94
22	F	204	CLA	C3B-C2B-C1B	-3.90	102.46	107.16
29	6	315	5X6	C15-C16-C17	-3.90	115.47	126.42
22	B	835	CLA	CAC-C3C-C4C	3.90	129.87	124.81
22	B	812	CLA	C4A-NA-C1A	-3.89	104.95	106.71
22	6	306	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
21	A	801	CL0	CMD-C2D-C1D	3.89	131.57	124.71
29	O	207	5X6	C27-C28-C29	-3.89	116.27	127.20
22	A	802	CLA	C4A-NA-C1A	-3.89	104.96	106.71
22	A	811	CLA	CMC-C2C-C1C	3.89	130.96	125.04
22	Z	201	CLA	O2D-CGD-CBD	3.89	118.18	111.27
25	B	841	BCR	C34-C9-C10	-3.89	117.48	122.92
22	6	310	CLA	C4A-NA-C1A	-3.89	104.96	106.71
22	6	312	CLA	C3B-C2B-C1B	-3.89	102.47	107.16
25	4	316	BCR	C15-C16-C17	3.89	131.44	123.47
22	B	804	CLA	C3D-C4D-ND	3.89	116.52	110.24
22	7	312	CLA	C3C-C4C-NC	3.89	114.93	110.57
22	A	831	CLA	CAC-C3C-C4C	3.88	129.85	124.81
21	A	801	CL0	C3D-C4D-ND	3.88	116.51	110.24
22	F	206	CLA	CMC-C2C-C1C	3.88	130.95	125.04
29	O	207	5X6	C24-C23-C22	-3.88	115.52	126.42
25	A	843	BCR	C34-C9-C10	-3.87	117.50	122.92
22	6	309	CLA	C3C-C4C-NC	3.87	114.91	110.57
29	1	316	5X6	C16-C17-C18	-3.87	113.00	118.94
22	B	805	CLA	C3C-C4C-NC	3.87	114.91	110.57
29	1	314	5X6	C41-C17-C18	-3.87	117.50	122.92
22	O	204	CLA	C4A-NA-C1A	-3.87	104.97	106.71
29	1	312	5X6	C16-C17-C18	-3.87	113.01	118.94
22	F	206	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
22	4	307	CLA	C3D-C4D-ND	3.87	116.49	110.24
21	A	801	CL0	C1C-C2C-C3C	-3.87	102.89	106.96
29	7	317	5X6	C27-C26-C25	-3.87	113.01	118.94
22	B	834	CLA	C4A-NA-C1A	-3.86	104.97	106.71
22	4	302	CLA	C4A-NA-C1A	-3.86	104.97	106.71
29	7	315	5X6	C11-C03-C02	-3.86	112.11	121.46
22	5	303	CLA	C3D-C4D-ND	3.86	116.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	816	CLA	C3D-C4D-ND	3.86	116.48	110.24
22	B	814	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
31	1	315	RRX	C34-C9-C10	-3.85	117.52	122.92
28	B	845	DGD	O2G-C1B-C2B	3.85	119.81	111.50
22	A	859	CLA	C3B-C2B-C1B	-3.85	102.51	107.16
22	B	808	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
29	2	314	5X6	C24-C23-C22	-3.85	115.60	126.42
22	B	827	CLA	C3D-C4D-ND	3.85	116.47	110.24
25	2	301	BCR	C34-C9-C10	-3.85	117.53	122.92
22	3	301	CLA	C2C-C1C-NC	3.85	113.58	109.97
29	2	313	5X6	C20-C19-C18	-3.85	115.59	123.47
22	1	306	CLA	C3B-C4B-NB	3.85	114.08	110.52
22	5	304	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
25	A	843	BCR	C30-C25-C26	-3.85	117.19	122.61
22	A	836	CLA	C3B-C4B-NB	3.85	114.08	110.52
22	A	826	CLA	C4C-C3C-C2C	-3.85	101.29	106.90
22	5	303	CLA	C4-C3-C5	3.84	121.74	115.27
22	A	804	CLA	C3B-C4B-NB	3.84	114.08	110.52
22	5	308	CLA	O2D-CGD-CBD	3.84	118.09	111.27
22	2	302	CLA	C3C-C4C-NC	3.84	114.88	110.57
22	B	833	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
25	A	846	BCR	C37-C22-C21	-3.84	117.54	122.92
22	A	827	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
22	A	830	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	7	311	CLA	C3C-C4C-NC	3.84	114.87	110.57
22	B	802	CLA	C4A-NA-C1A	-3.83	104.98	106.71
29	7	315	5X6	C41-C17-C16	-3.83	112.04	118.08
29	6	315	5X6	C24-C23-C22	-3.83	115.65	126.42
22	2	311	CLA	C3C-C4C-NC	3.83	114.87	110.57
31	4	317	RRX	C37-C22-C21	-3.83	117.56	122.92
22	6	303	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
22	A	821	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
22	A	817	CLA	CAC-C3C-C4C	3.83	129.78	124.81
22	L	203	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
22	6	304	CLA	CMC-C2C-C1C	3.83	130.87	125.04
22	B	839	CLA	C4A-NA-C1A	-3.82	104.99	106.71
22	B	831	CLA	C3B-C4B-NB	3.82	114.06	110.52
29	2	313	5X6	C27-C26-C25	-3.82	113.08	118.94
22	7	304	CLA	C2C-C1C-NC	3.82	113.55	109.97
22	B	823	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
29	4	313	5X6	C27-C28-C29	-3.82	116.48	127.20
22	A	812	CLA	CAC-C3C-C4C	3.82	129.76	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	308	CLA	C4A-NA-C1A	-3.81	104.99	106.71
22	A	806	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
22	B	817	CLA	CAC-C3C-C4C	3.81	129.76	124.81
22	B	833	CLA	O2D-CGD-CBD	3.81	118.05	111.27
29	4	314	5X6	C11-C03-C02	-3.81	112.22	121.46
31	1	315	RRX	C16-C15-C14	3.81	131.28	123.47
22	6	305	CLA	O2D-CGD-CBD	3.81	118.04	111.27
22	4	312	CLA	CAC-C3C-C4C	3.81	129.75	124.81
22	J	102	CLA	C4A-NA-C1A	-3.81	104.99	106.71
22	6	304	CLA	C4A-NA-C1A	-3.81	104.99	106.71
22	B	850	CLA	C4A-NA-C1A	-3.81	104.99	106.71
29	7	318	5X6	C24-C23-C22	-3.81	115.72	126.42
22	O	206	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
22	B	808	CLA	C4A-NA-C1A	-3.81	105.00	106.71
22	7	309	CLA	C2C-C1C-NC	3.81	113.54	109.97
22	K	102	CLA	C3B-C2B-C1B	-3.81	102.57	107.16
22	L	205	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
22	B	823	CLA	C4-C3-C5	3.80	121.67	115.27
29	1	316	5X6	C38-C30-C31	-3.80	107.31	114.36
22	L	204	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
22	B	836	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
22	B	820	CLA	C3C-C4C-NC	3.80	114.83	110.57
25	I	102	BCR	C37-C22-C21	-3.80	117.60	122.92
29	J	104	5X6	C12-C13-C14	-3.80	113.11	118.94
29	1	313	5X6	C12-C11-C03	-3.80	116.54	127.20
22	4	305	CLA	C3C-C4C-NC	3.80	114.83	110.57
25	L	206	BCR	C37-C22-C21	-3.80	117.61	122.92
22	5	301	CLA	CAC-C3C-C4C	3.79	129.73	124.81
22	B	849	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
22	F	204	CLA	CMC-C2C-C1C	3.79	130.81	125.04
22	B	811	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
22	B	805	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
29	J	104	5X6	C15-C16-C17	-3.79	115.78	126.42
22	A	823	CLA	C3D-C4D-ND	3.79	116.36	110.24
22	F	205	CLA	CAC-C3C-C4C	3.78	129.72	124.81
22	O	205	CLA	C3C-C4C-NC	3.78	114.81	110.57
22	6	307	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
22	A	831	CLA	CMB-C2B-C1B	3.78	131.13	125.37
29	4	315	5X6	C27-C26-C25	-3.78	113.14	118.94
25	L	206	BCR	C34-C9-C10	-3.78	117.62	122.92
29	6	317	5X6	C35-C34-C29	3.78	116.43	110.30
22	A	814	CLA	C3C-C4C-NC	3.78	114.81	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	314	5X6	C20-C19-C18	-3.78	115.74	123.47
22	A	839	CLA	C4A-NA-C1A	-3.77	105.01	106.71
22	5	309	CLA	C3B-C2B-C1B	-3.77	102.61	107.16
29	5	312	5X6	C01-C02-C07	-3.77	107.36	114.36
22	A	813	CLA	C3B-C4B-NB	3.77	114.02	110.52
25	L	206	BCR	C1-C6-C5	-3.77	117.30	122.61
22	B	814	CLA	CAC-C3C-C4C	3.77	129.70	124.81
29	4	315	5X6	C42-C13-C12	-3.77	112.14	118.08
22	O	203	CLA	C3B-C4B-NB	3.77	114.01	110.52
29	Z	206	5X6	C38-C30-C31	-3.77	107.37	114.36
22	A	858	CLA	CAC-C3C-C4C	3.77	129.70	124.81
29	6	317	5X6	C39-C26-C25	-3.77	117.65	122.92
22	B	835	CLA	C4C-C3C-C2C	-3.77	101.41	106.90
22	A	833	CLA	CAC-C3C-C4C	3.77	129.70	124.81
22	B	828	CLA	CAC-C3C-C4C	3.76	129.69	124.81
22	B	801	CLA	C3D-C4D-ND	3.76	116.32	110.24
29	2	312	5X6	C42-C13-C12	-3.76	112.15	118.08
22	A	823	CLA	C3B-C4B-NB	3.76	114.00	110.52
29	2	313	5X6	C39-C26-C25	-3.76	117.66	122.92
22	B	820	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
22	5	308	CLA	CAC-C3C-C4C	3.76	129.69	124.81
22	4	305	CLA	C3B-C4B-NB	3.76	114.00	110.52
22	5	307	CLA	C3B-C4B-NB	3.76	114.00	110.52
29	5	314	5X6	C25-C24-C23	-3.76	111.49	123.22
22	B	816	CLA	C4C-C3C-C2C	-3.76	101.42	106.90
22	B	825	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
22	A	828	CLA	C3B-C4B-NB	3.75	114.00	110.52
22	F	206	CLA	CAC-C3C-C4C	3.75	129.68	124.81
25	B	841	BCR	C15-C16-C17	3.75	131.16	123.47
22	B	809	CLA	C3B-C2B-C1B	-3.75	102.63	107.16
25	1	301	BCR	C34-C9-C10	-3.75	117.67	122.92
29	6	315	5X6	C14-C15-C16	-3.75	111.50	123.22
29	7	314	5X6	C15-C16-C17	-3.75	115.87	126.42
22	6	310	CLA	C4-C3-C5	3.75	121.58	115.27
22	6	308	CLA	CAC-C3C-C4C	3.75	129.68	124.81
22	A	832	CLA	C4C-C3C-C2C	-3.75	101.43	106.90
21	A	801	CL0	O2D-CGD-O1D	-3.75	116.51	123.84
22	1	302	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
22	6	310	CLA	CAC-C3C-C4C	3.75	129.67	124.81
22	A	832	CLA	CMB-C2B-C1B	3.75	131.08	125.37
22	4	305	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
22	5	307	CLA	C1C-C2C-C3C	-3.75	103.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	203	CLA	C4A-NA-C1A	-3.75	105.02	106.71
22	A	804	CLA	CAC-C3C-C4C	3.75	129.67	124.81
22	5	301	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
22	1	310	CLA	CAC-C3C-C4C	3.74	129.67	124.81
22	B	807	CLA	CAC-C3C-C4C	3.74	129.67	124.81
22	3	302	CLA	C3C-C4C-NC	3.74	114.77	110.57
29	O	208	5X6	C27-C28-C29	-3.74	116.69	127.20
29	5	314	5X6	C24-C23-C22	-3.74	115.90	126.42
22	A	828	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
22	1	306	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
25	I	102	BCR	C34-C9-C8	3.74	123.96	118.08
29	4	314	5X6	C16-C17-C18	-3.73	113.21	118.94
25	Z	202	BCR	C34-C9-C8	3.73	123.96	118.08
22	A	857	CLA	C3D-C4D-ND	3.73	116.28	110.24
22	A	809	CLA	C3C-C4C-NC	3.73	114.76	110.57
29	1	313	5X6	C15-C16-C17	-3.73	115.93	126.42
29	Z	206	5X6	C24-C23-C22	-3.73	115.93	126.42
22	A	816	CLA	C4A-NA-C1A	-3.73	105.03	106.71
22	A	826	CLA	C4A-NA-C1A	-3.73	105.03	106.71
22	6	303	CLA	C3C-C4C-NC	3.73	114.75	110.57
29	3	306	5X6	C41-C17-C16	-3.72	112.21	118.08
22	7	304	CLA	C3C-C4C-NC	3.72	114.75	110.57
22	A	848	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
29	4	313	5X6	C14-C15-C16	-3.72	111.61	123.22
22	4	308	CLA	C3C-C4C-NC	3.72	114.74	110.57
29	O	207	5X6	C12-C11-C03	-3.72	116.76	127.20
22	3	301	CLA	C3C-C4C-NC	3.72	114.74	110.57
22	O	206	CLA	CAC-C3C-C4C	3.72	129.63	124.81
22	A	833	CLA	C1-O2A-CGA	3.72	126.19	116.44
29	5	321	5X6	C15-C16-C17	-3.72	115.98	126.42
22	B	813	CLA	C3B-C4B-NB	3.72	113.96	110.52
22	A	833	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
29	7	315	5X6	C24-C23-C22	-3.71	115.99	126.42
25	1	301	BCR	C37-C22-C21	-3.71	117.73	122.92
22	B	804	CLA	CAC-C3C-C4C	3.71	129.62	124.81
31	1	315	RRX	C37-C22-C21	-3.71	117.73	122.92
22	4	302	CLA	C3C-C4C-NC	3.71	114.73	110.57
22	B	839	CLA	CMC-C2C-C1C	3.71	130.69	125.04
25	A	843	BCR	C37-C22-C21	-3.71	117.73	122.92
29	1	314	5X6	C42-C13-C14	-3.71	117.73	122.92
22	1	309	CLA	C3C-C4C-NC	3.71	114.73	110.57
29	1	312	5X6	C39-C26-C27	-3.71	112.24	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	305	CLA	C3C-C4C-NC	3.70	114.72	110.57
22	4	305	CLA	CAC-C3C-C4C	3.70	129.62	124.81
22	B	817	CLA	O2A-CGA-CBA	3.70	123.53	111.91
22	B	819	CLA	C3B-C2B-C1B	-3.70	102.69	107.16
29	O	208	5X6	C41-C17-C16	-3.70	112.25	118.08
22	A	826	CLA	C3D-C4D-ND	3.70	116.22	110.24
22	7	304	CLA	CMC-C2C-C1C	3.70	130.67	125.04
22	7	305	CLA	O2D-CGD-CBD	3.69	117.83	111.27
29	7	316	5X6	C20-C19-C18	-3.69	115.91	123.47
29	3	306	5X6	C27-C28-C29	-3.69	116.83	127.20
22	2	310	CLA	C3C-C4C-NC	3.69	114.71	110.57
22	5	301	CLA	C3B-C2B-C1B	-3.69	102.71	107.16
22	5	304	CLA	C4A-NA-C1A	-3.69	105.05	106.71
22	4	306	CLA	C3C-C4C-NC	3.68	114.70	110.57
22	K	102	CLA	C4A-NA-C1A	-3.68	105.05	106.71
29	7	318	5X6	C12-C11-C03	-3.68	116.86	127.20
22	B	805	CLA	C3B-C4B-NB	3.68	113.93	110.52
22	F	206	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
22	B	809	CLA	CMC-C2C-C1C	3.68	130.65	125.04
22	B	849	CLA	C3B-C4B-NB	3.68	113.93	110.52
22	6	306	CLA	CAC-C3C-C4C	3.68	129.59	124.81
22	K	101	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
31	4	317	RRX	C34-C9-C10	-3.68	117.77	122.92
22	4	308	CLA	CMC-C2C-C1C	3.68	130.64	125.04
22	5	304	CLA	C3B-C4B-NB	3.68	113.93	110.52
22	A	827	CLA	C3C-C4C-NC	3.68	114.69	110.57
29	5	312	5X6	C15-C16-C17	-3.68	116.09	126.42
22	B	812	CLA	C1-O2A-CGA	3.68	126.09	116.44
22	B	809	CLA	C3B-C4B-NB	3.68	113.92	110.52
22	2	303	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
25	B	843	BCR	C37-C22-C21	-3.68	117.78	122.92
29	2	312	5X6	C12-C13-C14	-3.67	113.30	118.94
22	A	813	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
22	A	834	CLA	C3C-C4C-NC	3.67	114.69	110.57
29	7	315	5X6	C01-C02-C07	-3.67	107.55	114.36
22	5	307	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
22	B	806	CLA	C4-C3-C5	3.67	121.45	115.27
29	J	104	5X6	C14-C15-C16	-3.67	111.76	123.22
22	4	302	CLA	O2D-CGD-CBD	3.67	117.79	111.27
22	B	825	CLA	CAA-C2A-C3A	-3.67	102.73	112.78
22	1	307	CLA	C3B-C4B-NB	3.67	113.92	110.52
29	2	314	5X6	C27-C26-C25	-3.67	113.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	310	CLA	CAC-C3C-C4C	3.67	129.57	124.81
22	B	806	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
22	B	804	CLA	CBA-CAA-C2A	3.67	124.68	113.86
22	4	309	CLA	CAC-C3C-C4C	3.67	129.57	124.81
29	1	314	5X6	C20-C19-C18	-3.66	115.97	123.47
25	Z	202	BCR	C37-C22-C21	-3.66	117.79	122.92
29	5	313	5X6	C24-C23-C22	-3.66	116.12	126.42
22	A	828	CLA	CAC-C3C-C4C	3.66	129.56	124.81
25	K	103	BCR	C34-C9-C10	-3.66	117.79	122.92
29	Z	206	5X6	C14-C15-C16	-3.66	111.79	123.22
22	B	833	CLA	C4A-NA-C1A	-3.66	105.06	106.71
22	L	204	CLA	C4A-NA-C1A	-3.66	105.06	106.71
29	7	317	5X6	C41-C17-C18	-3.66	117.80	122.92
22	4	310	CLA	CHC-C1C-C2C	-3.66	116.57	126.73
22	B	819	CLA	CAC-C3C-C4C	3.66	129.56	124.81
22	O	203	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
22	L	203	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
29	6	316	5X6	C41-C17-C16	-3.66	112.32	118.08
22	2	302	CLA	C4A-NA-C1A	-3.65	105.06	106.71
22	A	808	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
29	O	208	5X6	C15-C16-C17	-3.65	116.16	126.42
22	A	807	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
22	A	824	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
22	B	816	CLA	CAC-C3C-C4C	3.65	129.54	124.81
29	6	315	5X6	C12-C11-C03	-3.65	116.95	127.20
22	B	829	CLA	CAC-C3C-C4C	3.65	129.54	124.81
22	A	823	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
29	1	316	5X6	C28-C29-C30	-3.65	112.63	121.46
22	A	813	CLA	C4A-NA-C1A	-3.64	105.07	106.71
29	7	318	5X6	C39-C26-C25	-3.64	117.82	122.92
22	6	311	CLA	C4C-C3C-C2C	-3.64	101.59	106.90
29	2	314	5X6	C41-C17-C16	-3.64	112.34	118.08
22	5	306	CLA	C3B-C4B-NB	3.64	113.89	110.52
29	Z	206	5X6	C12-C11-C03	-3.64	116.98	127.20
22	6	311	CLA	CAA-C2A-C3A	-3.64	107.61	116.10
25	A	862	BCR	C34-C9-C10	-3.64	117.83	122.92
22	A	834	CLA	C3B-C2B-C1B	-3.63	102.78	107.16
22	7	305	CLA	C3C-C4C-NC	3.63	114.64	110.57
25	Z	205	BCR	C37-C22-C21	-3.63	117.84	122.92
22	A	824	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
22	4	305	CLA	C4A-NA-C1A	-3.63	105.07	106.71
22	7	313	CLA	C3C-C4C-NC	3.63	114.64	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	803	CLA	CAC-C3C-C4C	3.63	129.52	124.81
22	B	824	CLA	C4C-C3C-C2C	-3.63	101.61	106.90
22	1	303	CLA	C2C-C1C-NC	3.63	113.37	109.97
22	B	813	CLA	C4C-C3C-C2C	-3.63	101.61	106.90
22	B	824	CLA	C3D-C4D-ND	3.63	116.10	110.24
22	A	835	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
22	F	204	CLA	C4A-NA-C1A	-3.63	105.08	106.71
29	7	315	5X6	C40-C22-C23	-3.63	112.36	118.08
22	F	206	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
22	B	822	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
31	5	322	RRX	C37-C22-C21	-3.62	117.85	122.92
22	3	303	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
22	6	312	CLA	CAC-C3C-C4C	3.62	129.51	124.81
22	A	814	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	A	810	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
22	B	836	CLA	CAC-C3C-C4C	3.62	129.50	124.81
22	5	303	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	7	304	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
22	6	311	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
25	L	201	BCR	C34-C9-C10	-3.61	117.86	122.92
22	4	308	CLA	C2C-C1C-NC	3.61	113.36	109.97
22	B	803	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
29	5	313	5X6	C01-C02-C03	-3.61	120.47	124.53
22	6	306	CLA	C4A-NA-C1A	-3.61	105.08	106.71
22	6	307	CLA	C4A-NA-C1A	-3.61	105.08	106.71
22	A	834	CLA	CAC-C3C-C4C	3.61	129.49	124.81
22	B	823	CLA	O2A-CGA-CBA	3.61	123.23	111.91
22	B	826	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
31	6	318	RRX	C37-C22-C21	-3.61	117.87	122.92
22	5	303	CLA	C3B-C4B-NB	3.61	113.86	110.52
22	B	818	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
22	A	821	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
22	F	205	CLA	C4C-C3C-C2C	-3.60	101.64	106.90
22	2	304	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
22	6	309	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
29	2	314	5X6	C25-C24-C23	-3.60	111.97	123.22
29	7	317	5X6	C25-C24-C23	-3.60	111.98	123.22
22	A	833	CLA	O2D-CGD-CBD	3.60	117.67	111.27
25	5	315	BCR	C34-C9-C10	-3.60	117.88	122.92
22	4	303	CLA	CMC-C2C-C1C	3.60	130.52	125.04
22	1	308	CLA	C3C-C4C-NC	3.60	114.61	110.57
22	B	832	CLA	O2A-CGA-CBA	3.60	123.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	314	5X6	C16-C17-C18	-3.60	113.42	118.94
22	F	205	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
22	A	838	CLA	CAC-C3C-C4C	3.60	129.47	124.81
29	M	101	5X6	C42-C13-C12	-3.59	112.41	118.08
22	B	806	CLA	C3D-C4D-ND	3.59	116.05	110.24
25	A	843	BCR	C37-C22-C23	3.59	123.74	118.08
22	3	302	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	A	826	CLA	CMC-C2C-C1C	3.59	130.51	125.04
22	A	808	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	A	821	CLA	C4A-NA-C1A	-3.59	105.09	106.71
22	B	849	CLA	CBC-CAC-C3C	-3.59	102.53	112.43
22	1	310	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	A	807	CLA	C3B-C4B-NB	3.59	113.84	110.52
22	7	308	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
22	4	311	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	Z	204	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	6	314	CLA	CAC-C3C-C4C	3.58	129.46	124.81
22	B	834	CLA	C4C-C3C-C2C	-3.58	101.68	106.90
25	A	845	BCR	C37-C22-C23	3.58	123.72	118.08
22	B	838	CLA	C4-C3-C2	-3.58	114.49	123.68
22	B	808	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
22	A	838	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
22	A	816	CLA	CAC-C3C-C4C	3.58	129.46	124.81
22	1	305	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
22	A	827	CLA	C3D-C4D-ND	3.58	116.03	110.24
22	L	205	CLA	CAC-C3C-C4C	3.58	129.45	124.81
22	6	305	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
22	5	305	CLA	C3C-C4C-NC	3.58	114.58	110.57
22	4	309	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
22	A	820	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
22	1	305	CLA	CAC-C3C-C4C	3.58	129.45	124.81
22	B	850	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
25	F	207	BCR	C35-C13-C14	-3.57	117.92	122.92
22	B	829	CLA	C3B-C4B-NB	3.57	113.83	110.52
22	A	827	CLA	CMC-C2C-C1C	3.57	130.48	125.04
22	1	306	CLA	O2D-CGD-CBD	3.57	117.62	111.27
22	6	306	CLA	C3C-C4C-NC	3.57	114.58	110.57
21	A	801	CL0	CHB-C4A-NA	3.57	129.45	124.51
22	A	833	CLA	CMC-C2C-C1C	3.57	130.47	125.04
29	6	317	5X6	C14-C15-C16	-3.57	112.08	123.22
22	7	312	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
29	1	316	5X6	C15-C16-C17	-3.57	116.39	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	318	RRX	C34-C9-C10	-3.57	117.92	122.92
22	4	304	CLA	C3C-C4C-NC	3.57	114.57	110.57
22	5	311	CLA	CAC-C3C-C4C	3.57	129.44	124.81
22	5	311	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
22	6	307	CLA	C3C-C4C-NC	3.57	114.57	110.57
25	B	844	BCR	C37-C22-C21	-3.57	117.93	122.92
22	J	102	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
29	1	312	5X6	C28-C29-C30	-3.57	112.82	121.46
22	A	827	CLA	O2D-CGD-CBD	3.57	117.60	111.27
29	5	312	5X6	C41-C17-C18	-3.56	117.93	122.92
22	4	311	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
22	5	306	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
22	A	858	CLA	O2A-CGA-CBA	3.56	123.08	111.91
29	3	306	5X6	C40-C22-C21	-3.56	117.94	122.92
25	I	102	BCR	C37-C22-C23	3.56	123.68	118.08
22	7	309	CLA	C3C-C4C-NC	3.56	114.56	110.57
22	K	102	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
22	5	301	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
22	2	310	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
29	O	207	5X6	C14-C15-C16	-3.55	112.13	123.22
22	A	808	CLA	CAC-C3C-C4C	3.55	129.42	124.81
22	A	828	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
22	1	304	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
22	1	307	CLA	CAC-C3C-C4C	3.55	129.41	124.81
22	B	850	CLA	CBC-CAC-C3C	-3.55	102.65	112.43
22	B	849	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
29	1	314	5X6	C41-C17-C16	-3.54	112.49	118.08
22	A	821	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
22	A	814	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
25	K	103	BCR	C36-C18-C17	-3.54	117.96	122.92
22	4	312	CLA	C3C-C4C-NC	3.54	114.54	110.57
22	6	303	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
25	B	844	BCR	C15-C16-C17	3.54	130.72	123.47
25	J	103	BCR	C34-C9-C10	-3.54	117.97	122.92
25	F	207	BCR	C37-C22-C21	-3.54	117.97	122.92
25	A	861	BCR	C34-C9-C10	-3.54	117.97	122.92
22	4	302	CLA	C3B-C4B-NB	3.54	113.80	110.52
22	A	804	CLA	CHC-C1C-C2C	-3.54	116.91	126.73
22	6	306	CLA	CMC-C2C-C1C	3.53	130.42	125.04
22	6	307	CLA	CAC-C3C-C4C	3.53	129.40	124.81
22	A	833	CLA	C3B-C2B-C1B	-3.53	102.90	107.16
22	4	309	CLA	C3C-C4C-NC	3.53	114.53	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	305	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
22	B	804	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
25	B	842	BCR	C37-C22-C21	-3.53	117.98	122.92
22	A	835	CLA	C4-C3-C5	3.53	120.02	115.98
29	2	314	5X6	C42-C13-C12	-3.53	112.51	118.08
29	2	314	5X6	C38-C30-C31	-3.53	107.81	114.36
29	M	101	5X6	C14-C15-C16	-3.53	112.20	123.22
22	B	820	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
22	6	306	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
22	4	307	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
22	5	311	CLA	C3B-C4B-NB	3.52	113.78	110.52
22	5	302	CLA	C4A-NA-C1A	-3.52	105.12	106.71
22	B	834	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
25	I	102	BCR	C34-C9-C10	-3.52	117.99	122.92
22	5	311	CLA	C3C-C4C-NC	3.52	114.52	110.57
22	B	808	CLA	CMC-C2C-C1C	3.52	130.40	125.04
22	A	802	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
22	6	304	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
22	1	306	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
22	B	836	CLA	O2A-CGA-CBA	3.52	122.94	111.91
25	A	845	BCR	C37-C22-C21	-3.52	118.00	122.92
29	B	851	5X6	C01-C02-C07	-3.51	107.84	114.36
22	O	205	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
22	7	308	CLA	C3C-C4C-NC	3.51	114.51	110.57
22	B	824	CLA	C3B-C4B-NB	3.51	113.78	110.52
22	A	839	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
22	B	831	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
22	6	313	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
21	A	801	CL0	C3B-C4B-NB	3.51	113.77	110.52
22	K	101	CLA	CAC-C3C-C4C	3.51	129.36	124.81
29	2	313	5X6	C25-C24-C23	-3.51	112.27	123.22
22	B	839	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
22	L	204	CLA	C3B-C4B-NB	3.51	113.77	110.52
22	B	808	CLA	C4C-C3C-C2C	-3.50	101.79	106.90
22	6	303	CLA	O2D-CGD-CBD	3.50	117.50	111.27
22	B	809	CLA	CAC-C3C-C4C	3.50	129.36	124.81
22	A	831	CLA	C4C-C3C-C2C	-3.50	101.79	106.90
22	B	815	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
22	B	823	CLA	CAC-C3C-C4C	3.50	129.35	124.81
22	1	305	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
22	A	823	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
22	B	806	CLA	CAC-C3C-C4C	3.50	129.35	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	309	CLA	O2D-CGD-CBD	3.50	117.48	111.27
22	B	813	CLA	C4-C3-C5	3.50	121.15	115.27
22	6	312	CLA	CHC-C1C-C2C	-3.50	117.02	126.73
29	O	208	5X6	C23-C22-C21	-3.50	113.58	118.94
22	B	826	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
22	A	848	CLA	C3D-C4D-ND	3.49	115.89	110.24
22	6	306	CLA	C3B-C4B-NB	3.49	113.76	110.52
22	3	305	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
29	M	101	5X6	C28-C29-C30	-3.49	113.00	121.46
22	B	804	CLA	CMC-C2C-C1C	3.49	130.36	125.04
29	2	313	5X6	C27-C28-C29	-3.49	117.39	127.20
22	5	303	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
22	F	204	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
22	2	305	CLA	C3B-C4B-NB	3.49	113.75	110.52
29	4	315	5X6	C27-C28-C29	-3.49	117.40	127.20
22	2	307	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
22	B	824	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
22	A	835	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
22	B	828	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
22	A	831	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
29	7	318	5X6	C15-C16-C17	-3.49	116.62	126.42
22	B	811	CLA	C3D-C2D-C1D	-3.48	101.08	105.83
22	B	812	CLA	CMC-C2C-C1C	3.48	130.34	125.04
22	A	827	CLA	CAC-C3C-C4C	3.48	129.33	124.81
29	7	318	5X6	C01-C02-C07	-3.48	107.90	114.36
22	4	303	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
22	F	206	CLA	C4A-NA-C1A	-3.48	105.14	106.71
25	F	201	BCR	C37-C22-C21	-3.48	118.05	122.92
22	2	305	CLA	C3C-C4C-NC	3.48	114.47	110.57
29	J	104	5X6	C27-C28-C29	-3.48	117.43	127.20
22	B	805	CLA	CMC-C2C-C1C	3.48	130.34	125.04
22	A	825	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
22	A	824	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
22	6	310	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
22	B	813	CLA	CMC-C2C-C1C	3.47	130.33	125.04
22	B	810	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
29	M	101	5X6	C25-C24-C23	-3.47	112.38	123.22
22	B	801	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
22	4	304	CLA	C3B-C4B-NB	3.47	113.74	110.52
22	A	822	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
22	B	828	CLA	C3B-C4B-NB	3.47	113.73	110.52
22	3	304	CLA	C1C-C2C-C3C	-3.47	103.31	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	301	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
25	J	103	BCR	C37-C22-C23	3.47	123.54	118.08
22	A	836	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
25	B	843	BCR	C34-C9-C10	-3.47	118.07	122.92
22	6	307	CLA	CHC-C1C-C2C	-3.47	117.11	126.73
22	F	204	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
22	6	308	CLA	C1D-CHD-C4C	-3.46	118.58	126.06
25	A	846	BCR	C36-C18-C17	-3.46	118.07	122.92
22	A	826	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
22	B	811	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
22	B	831	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
22	A	824	CLA	C4A-NA-C1A	-3.46	105.15	106.71
22	5	302	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
22	B	838	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
25	B	844	BCR	C37-C22-C23	3.46	123.53	118.08
22	A	806	CLA	CAC-C3C-C4C	3.46	129.30	124.81
22	1	308	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	B	840	A1L64	O4-C4-C3	3.46	136.68	123.64
22	7	303	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	B	840	A1L64	O4-C4-C5	-3.46	104.87	116.56
22	7	311	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
22	L	205	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
22	O	206	CLA	C3C-C4C-NC	3.46	114.45	110.57
22	5	307	CLA	C3C-C4C-NC	3.46	114.45	110.57
29	7	318	5X6	C25-C24-C23	-3.46	112.43	123.22
22	B	806	CLA	C3B-C4B-NB	3.45	113.72	110.52
29	5	312	5X6	C27-C28-C29	-3.45	117.50	127.20
22	7	305	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
22	5	310	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
31	5	322	RRX	C34-C9-C10	-3.45	118.09	122.92
29	1	316	5X6	C14-C15-C16	-3.45	112.45	123.22
25	J	103	BCR	C21-C20-C19	3.45	133.99	123.22
22	F	204	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
22	4	304	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
29	B	851	5X6	C42-C13-C14	-3.45	118.09	122.92
22	B	811	CLA	C3B-C4B-NB	3.45	113.71	110.52
29	2	312	5X6	C27-C28-C29	-3.45	117.52	127.20
22	3	301	CLA	CAC-C3C-C4C	3.45	129.28	124.81
22	3	303	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
29	6	315	5X6	C27-C28-C29	-3.45	117.52	127.20
22	A	835	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
22	B	814	CLA	C4A-NA-C1A	-3.45	105.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	304	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
22	5	306	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
22	1	302	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
22	5	311	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
22	5	306	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
22	A	803	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
22	A	837	CLA	C4C-C3C-C2C	-3.44	101.88	106.90
22	1	306	CLA	C4A-NA-C1A	-3.44	105.16	106.71
22	O	204	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	Z	201	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	A	803	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
22	B	819	CLA	C4C-C3C-C2C	-3.44	101.88	106.90
22	A	828	CLA	C3B-C2B-C1B	-3.44	103.01	107.16
31	5	322	RRX	C34-C9-C8	3.44	123.50	118.08
22	A	805	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
22	B	810	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	2	309	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	A	817	CLA	C3B-C4B-NB	3.44	113.70	110.52
22	7	303	CLA	C3B-C4B-NB	3.44	113.70	110.52
22	O	205	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
22	3	304	CLA	C3C-C4C-NC	3.43	114.42	110.57
22	3	304	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
22	2	303	CLA	CAC-C3C-C4C	3.43	129.26	124.81
22	O	206	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
22	A	819	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
22	2	311	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
22	4	303	CLA	C2C-C1C-NC	3.43	113.19	109.97
22	4	303	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
22	A	832	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
22	5	308	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
29	7	316	5X6	C40-C22-C23	-3.43	112.68	118.08
22	A	807	CLA	CBA-CAA-C2A	3.42	123.97	113.86
22	A	817	CLA	C4A-NA-C1A	-3.42	105.17	106.71
22	B	805	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
22	B	837	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
22	1	306	CLA	C3C-C4C-NC	3.42	114.41	110.57
22	3	303	CLA	C3C-C4C-NC	3.42	114.41	110.57
22	2	306	CLA	C3C-C4C-NC	3.42	114.41	110.57
29	7	315	5X6	C25-C24-C23	-3.42	112.54	123.22
22	B	821	CLA	CAC-C3C-C4C	3.42	129.25	124.81
22	4	302	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
22	3	302	CLA	C1C-C2C-C3C	-3.42	103.36	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	315	5X6	C14-C15-C16	-3.42	112.55	123.22
22	A	807	CLA	O2D-CGD-CBD	3.42	117.34	111.27
29	4	315	5X6	C25-C24-C23	-3.42	112.55	123.22
22	A	830	CLA	CAC-C3C-C4C	3.42	129.25	124.81
22	4	312	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
22	A	802	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
29	M	101	5X6	C16-C17-C18	-3.42	113.70	118.94
22	B	811	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
22	1	307	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
22	Z	204	CLA	C3B-C4B-NB	3.41	113.68	110.52
22	2	308	CLA	C3C-C4C-NC	3.41	114.40	110.57
22	7	307	CLA	C3C-C4C-NC	3.41	114.40	110.57
22	K	102	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
22	B	828	CLA	C1-O2A-CGA	3.41	125.39	116.44
22	A	859	CLA	CAC-C3C-C4C	3.41	129.23	124.81
29	5	314	5X6	C41-C17-C16	-3.41	112.71	118.08
22	A	810	CLA	C3B-C4B-NB	3.41	113.68	110.52
25	Z	205	BCR	C37-C22-C23	3.41	123.45	118.08
22	2	303	CLA	C3C-C4C-NC	3.41	114.39	110.57
22	1	310	CLA	O2A-CGA-CBA	3.41	122.60	111.91
22	1	308	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
29	6	315	5X6	C01-C02-C07	-3.41	108.04	114.36
22	A	836	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
22	5	310	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
22	2	302	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
22	4	309	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
22	B	830	CLA	C4A-NA-C1A	-3.40	105.18	106.71
22	L	204	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
29	2	314	5X6	C27-C28-C29	-3.40	117.66	127.20
22	7	312	CLA	CAC-C3C-C4C	3.40	129.22	124.81
22	L	205	CLA	CMB-C2B-C1B	3.40	130.54	125.37
22	B	808	CLA	CBC-CAC-C3C	-3.39	103.08	112.43
22	A	815	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
22	6	307	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
22	A	834	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
25	A	844	BCR	C37-C22-C21	-3.39	118.17	122.92
22	6	314	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
22	B	815	CLA	CAC-C3C-C4C	3.39	129.21	124.81
22	A	825	CLA	CAC-C3C-C4C	3.39	129.21	124.81
22	J	102	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
22	7	309	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
22	7	313	CLA	C1D-CHD-C4C	-3.39	118.75	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	308	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
22	A	836	CLA	CAC-C3C-C4C	3.39	129.20	124.81
22	B	804	CLA	C3B-C4B-NB	3.39	113.66	110.52
22	A	815	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
29	O	207	5X6	C25-C24-C23	-3.39	112.65	123.22
22	A	812	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
22	B	837	CLA	O2D-CGD-CBD	3.38	117.28	111.27
25	F	207	BCR	C34-C9-C10	-3.38	118.19	122.92
22	A	827	CLA	C4A-NA-C1A	-3.38	105.19	106.71
29	6	316	5X6	C23-C22-C21	-3.38	113.75	118.94
25	K	103	BCR	C35-C13-C14	-3.38	118.19	122.92
22	4	305	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
22	5	304	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
29	3	306	5X6	C01-C02-C07	-3.38	108.09	114.36
22	A	858	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
22	A	859	CLA	CHC-C1C-C2C	-3.38	117.35	126.73
22	B	839	CLA	CAC-C3C-C4C	3.38	129.19	124.81
22	1	309	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
29	3	306	5X6	C14-C15-C16	-3.38	112.68	123.22
22	4	311	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
22	A	829	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
22	A	833	CLA	C4A-NA-C1A	-3.37	105.19	106.71
22	B	830	CLA	CAC-C3C-C4C	3.37	129.19	124.81
29	O	208	5X6	C25-C24-C23	-3.37	112.70	123.22
22	A	839	CLA	C3B-C2B-C1B	-3.37	103.09	107.16
22	4	309	CLA	O2D-CGD-CBD	3.37	117.25	111.27
22	B	822	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
29	5	312	5X6	C14-C15-C16	-3.37	112.71	123.22
22	B	833	CLA	CMB-C2B-C1B	3.37	130.50	125.37
22	B	804	CLA	C4C-C3C-C2C	-3.36	101.99	106.90
22	B	836	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
22	5	306	CLA	CAC-C3C-C4C	3.36	129.17	124.81
22	1	304	CLA	C4A-NA-C1A	-3.36	105.19	106.71
22	B	803	CLA	O2A-C1-C2	-3.36	99.80	108.64
22	B	805	CLA	C6-C5-C3	-3.36	104.64	113.45
22	B	811	CLA	CHC-C1C-C2C	-3.36	117.39	126.73
22	J	102	CLA	C3C-C4C-NC	3.36	114.34	110.57
22	5	304	CLA	C3C-C4C-NC	3.36	114.34	110.57
22	A	818	CLA	O2A-CGA-CBA	3.36	122.45	111.91
22	7	303	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
22	B	802	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
22	7	305	CLA	CAC-C3C-C4C	3.36	129.16	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	817	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
22	A	820	CLA	C3B-C4B-NB	3.35	113.63	110.52
22	A	830	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
22	7	307	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
22	6	309	CLA	CAC-C3C-C4C	3.35	129.16	124.81
22	A	805	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
22	A	809	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
22	A	830	CLA	C3B-C4B-NB	3.35	113.62	110.52
22	A	859	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
22	7	311	CLA	CAC-C3C-C4C	3.35	129.15	124.81
22	A	831	CLA	CMC-C2C-C1C	3.35	130.14	125.04
22	B	809	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
22	2	307	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
22	A	834	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
22	Z	201	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
22	1	310	CLA	C4-C3-C5	3.35	120.90	115.27
22	7	313	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
22	B	810	CLA	C4C-C3C-C2C	-3.34	102.02	106.90
22	O	204	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
22	A	809	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
22	A	838	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
29	J	104	5X6	C24-C23-C22	-3.34	117.04	126.42
22	4	304	CLA	O2A-CGA-CBA	3.34	122.38	111.91
22	B	808	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
22	B	836	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
22	A	807	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
22	2	304	CLA	C1D-CHD-C4C	-3.33	118.86	126.06
22	B	850	CLA	CHC-C1C-C2C	-3.33	117.47	126.73
22	3	302	CLA	C3B-C4B-NB	3.33	113.61	110.52
22	B	818	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
22	7	306	CLA	C2A-C1A-CHA	-3.33	118.03	123.86
29	1	316	5X6	C42-C13-C12	-3.33	112.83	118.08
29	5	321	5X6	C14-C15-C16	-3.33	112.82	123.22
22	3	303	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
22	A	818	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
22	A	835	CLA	C3B-C4B-NB	3.33	113.60	110.52
22	6	311	CLA	C3B-C4B-NB	3.33	113.60	110.52
22	Z	201	CLA	C3B-C2B-C1B	-3.33	103.15	107.16
22	4	304	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
22	A	815	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
22	B	816	CLA	C1-C2-C3	-3.32	120.30	126.04
22	J	102	CLA	CHC-C1C-C2C	-3.32	117.50	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	826	CLA	O2A-CGA-CBA	3.32	122.33	111.91
22	A	835	CLA	CAC-C3C-C4C	3.32	129.12	124.81
22	B	834	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
22	L	203	CLA	CHC-C1C-C2C	-3.32	117.51	126.73
22	5	305	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
22	7	310	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
22	2	303	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
22	B	825	CLA	C3B-C4B-NB	3.32	113.59	110.52
22	2	303	CLA	C3B-C4B-NB	3.32	113.59	110.52
22	A	825	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
22	4	303	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
22	A	836	CLA	CHC-C1C-C2C	-3.31	117.52	126.73
22	A	812	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
22	Z	204	CLA	CMC-C2C-C1C	3.31	130.09	125.04
22	B	827	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
22	6	310	CLA	C3B-C4B-NB	3.31	113.59	110.52
22	A	802	CLA	CMC-C2C-C1C	3.31	130.08	125.04
29	2	313	5X6	C01-C02-C07	-3.31	108.23	114.36
22	6	309	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
25	4	316	BCR	C34-C9-C10	-3.30	118.30	122.92
22	4	306	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
22	7	307	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
29	7	316	5X6	C38-C30-C31	-3.30	108.24	114.36
22	B	807	CLA	CMB-C2B-C1B	3.30	130.40	125.37
25	J	103	BCR	C34-C9-C8	3.30	123.28	118.08
22	B	804	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
22	7	306	CLA	C3C-C4C-NC	3.30	114.27	110.57
22	B	803	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
22	A	816	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
22	2	309	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
29	6	317	5X6	C38-C30-C31	-3.30	108.24	114.36
22	5	302	CLA	CMC-C2C-C1C	3.30	130.06	125.04
22	A	859	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
25	L	202	BCR	C37-C22-C21	-3.30	118.31	122.92
22	A	804	CLA	O2A-C1-C2	3.30	117.30	108.64
22	A	838	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
22	B	827	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
22	A	814	CLA	CHC-C1C-C2C	-3.29	117.58	126.73
22	B	814	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
22	A	839	CLA	CMC-C2C-C1C	3.29	130.05	125.04
22	A	807	CLA	C1-C2-C3	-3.29	120.35	126.04
22	1	302	CLA	CHC-C1C-C2C	-3.29	117.59	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	826	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
22	B	839	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
22	B	837	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
22	2	305	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
22	5	302	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
22	1	309	CLA	CHC-C1C-C2C	-3.29	117.60	126.73
22	5	303	CLA	CAC-C3C-C4C	3.29	129.07	124.81
29	1	312	5X6	C38-C30-C31	-3.29	108.27	114.36
22	A	804	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
22	A	806	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
22	1	307	CLA	C4A-NA-C1A	-3.29	105.23	106.71
22	B	827	CLA	C3B-C4B-NB	3.28	113.56	110.52
22	A	811	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
22	4	308	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
22	7	310	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
22	7	309	CLA	C1-O2A-CGA	3.28	125.05	116.44
22	5	303	CLA	C4A-NA-C1A	-3.28	105.23	106.71
22	A	805	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
22	K	102	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
22	7	308	CLA	CAC-C3C-C4C	3.28	129.06	124.81
22	2	302	CLA	CHC-C1C-C2C	-3.28	117.62	126.73
22	Z	204	CLA	C4-C3-C5	3.28	120.79	115.27
22	A	858	CLA	O2A-CGA-O1A	-3.28	115.32	123.59
22	4	305	CLA	CBA-CAA-C2A	3.28	123.54	113.86
22	2	302	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
22	6	314	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
22	B	818	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
23	B	840	A1L64	O3-C3-C2	-3.28	105.48	116.56
22	A	848	CLA	O2D-CGD-CBD	3.28	117.09	111.27
22	4	305	CLA	C4-C3-C2	-3.27	115.28	123.68
22	B	814	CLA	C4C-C3C-C2C	-3.27	102.12	106.90
31	6	318	RRX	C34-C9-C8	3.27	123.23	118.08
25	A	846	BCR	C37-C22-C23	3.27	123.23	118.08
22	B	838	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	1	302	CLA	CMC-C2C-C1C	3.27	130.02	125.04
25	A	845	BCR	C34-C9-C10	-3.27	118.34	122.92
25	5	315	BCR	C37-C22-C23	3.27	123.23	118.08
22	1	310	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
22	A	837	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
22	7	312	CLA	CMC-C2C-C1C	3.27	130.02	125.04
22	A	819	CLA	CAC-C3C-C4C	3.27	129.05	124.81
22	A	833	CLA	CBC-CAC-C3C	-3.27	103.42	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	811	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
22	A	831	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
22	6	308	CLA	CHC-C1C-C2C	-3.27	117.65	126.73
22	7	311	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
22	5	308	CLA	CAA-C2A-C3A	-3.27	108.47	116.10
22	A	827	CLA	C3B-C4B-NB	3.27	113.55	110.52
22	4	309	CLA	C4-C3-C5	3.27	120.77	115.27
29	5	314	5X6	C27-C28-C29	-3.27	118.03	127.20
22	O	206	CLA	CHC-C1C-C2C	-3.27	117.66	126.73
22	3	301	CLA	CMC-C2C-C1C	3.27	130.01	125.04
22	6	314	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
22	6	303	CLA	CHC-C1C-C2C	-3.27	117.66	126.73
22	3	303	CLA	CHC-C1C-C2C	-3.27	117.66	126.73
22	A	829	CLA	C1C-C2C-C3C	-3.26	103.52	106.96
22	B	801	CLA	C1C-C2C-C3C	-3.26	103.52	106.96
22	2	306	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
22	2	308	CLA	CMC-C2C-C1C	3.26	130.01	125.04
22	B	838	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
25	A	862	BCR	C37-C22-C21	-3.26	118.35	122.92
22	B	833	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
22	4	304	CLA	C1-C2-C3	-3.26	120.41	126.04
22	B	808	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
22	B	835	CLA	C1-O2A-CGA	3.26	124.99	116.44
22	5	306	CLA	C1-O2A-CGA	3.26	124.99	116.44
22	A	858	CLA	CMC-C2C-C1C	3.26	130.00	125.04
22	1	303	CLA	C3C-C4C-NC	3.26	114.22	110.57
22	B	826	CLA	C1C-C2C-C3C	-3.25	103.53	106.96
22	B	808	CLA	C2A-C1A-CHA	-3.25	118.17	123.86
22	A	815	CLA	CMB-C2B-C1B	3.25	130.32	125.37
22	7	306	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
29	1	312	5X6	C41-C17-C16	-3.25	112.95	118.08
22	7	303	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
22	K	101	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
25	L	202	BCR	C34-C9-C8	3.25	123.20	118.08
22	B	808	CLA	C1-C2-C3	-3.25	120.42	126.04
22	B	826	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
22	B	835	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
22	5	308	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
22	B	817	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
22	2	304	CLA	CAC-C3C-C4C	3.25	129.03	124.81
29	2	312	5X6	C15-C16-C17	-3.25	117.29	126.42
22	B	814	CLA	C3B-C4B-NB	3.25	113.53	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	310	CLA	C1-O2A-CGA	3.25	124.96	116.44
22	A	807	CLA	O2A-CGA-CBA	3.25	122.09	111.91
29	5	314	5X6	C38-C30-C31	-3.25	108.34	114.36
22	A	832	CLA	C1-O2A-CGA	3.24	124.95	116.44
22	O	206	CLA	C3B-C4B-NB	3.24	113.52	110.52
22	A	804	CLA	C3D-C4D-ND	3.24	115.48	110.24
25	A	844	BCR	C30-C25-C26	-3.24	118.05	122.61
29	7	316	5X6	C14-C15-C16	-3.24	113.11	123.22
22	B	829	CLA	CMC-C2C-C1C	3.24	129.97	125.04
22	1	307	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
22	2	306	CLA	CHC-C1C-C2C	-3.24	117.73	126.73
22	B	832	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
22	6	308	CLA	C3C-C4C-NC	3.24	114.20	110.57
22	B	801	CLA	O2D-CGD-CBD	3.24	117.02	111.27
22	B	810	CLA	CAC-C3C-C4C	3.24	129.01	124.81
25	A	844	BCR	C34-C9-C10	-3.24	118.39	122.92
22	B	820	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
22	B	812	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
22	A	858	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
22	B	802	CLA	CAC-C3C-C4C	3.24	129.01	124.81
22	A	815	CLA	CAC-C3C-C4C	3.23	129.01	124.81
22	A	805	CLA	CMC-C2C-C1C	3.23	129.96	125.04
22	A	837	CLA	CBC-CAC-C3C	-3.23	103.52	112.43
22	A	825	CLA	CMC-C2C-C1C	3.23	129.96	125.04
22	A	822	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
22	1	309	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
22	2	310	CLA	CAC-C3C-C4C	3.23	129.00	124.81
22	A	818	CLA	C3B-C4B-NB	3.23	113.51	110.52
25	Z	202	BCR	C37-C22-C23	3.23	123.17	118.08
22	A	827	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
25	A	861	BCR	C34-C9-C8	3.23	123.16	118.08
22	5	310	CLA	C3B-C4B-NB	3.23	113.51	110.52
25	L	201	BCR	C16-C15-C14	3.23	130.08	123.47
22	4	305	CLA	CMC-C2C-C1C	3.22	129.95	125.04
22	6	313	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
31	4	317	RRX	C34-C9-C8	3.22	123.16	118.08
22	B	812	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
22	B	825	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
22	A	807	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
22	B	849	CLA	CAC-C3C-C4C	3.22	128.99	124.81
22	B	831	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
22	B	832	CLA	C4C-C3C-C2C	-3.22	102.20	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	312	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
22	6	307	CLA	O2A-CGA-CBA	3.22	122.01	111.91
22	2	306	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
22	A	834	CLA	CHC-C1C-C2C	-3.22	117.79	126.73
22	5	301	CLA	CHC-C1C-C2C	-3.22	117.79	126.73
22	4	304	CLA	CHC-C1C-C2C	-3.22	117.79	126.73
22	2	307	CLA	C3C-C4C-NC	3.22	114.18	110.57
22	A	838	CLA	C2A-C1A-CHA	-3.22	118.23	123.86
22	5	309	CLA	CHC-C1C-C2C	-3.22	117.79	126.73
22	4	307	CLA	CAC-C3C-C4C	3.22	128.98	124.81
22	B	832	CLA	C1C-C2C-C3C	-3.22	103.58	106.96
22	K	102	CLA	CHC-C1C-C2C	-3.21	117.80	126.73
29	1	316	5X6	C23-C22-C21	-3.21	114.01	118.94
22	3	304	CLA	CAC-C3C-C4C	3.21	128.98	124.81
22	O	203	CLA	CMC-C2C-C1C	3.21	129.93	125.04
22	5	307	CLA	CMC-C2C-C1C	3.21	129.93	125.04
22	A	826	CLA	C3B-C4B-NB	3.21	113.50	110.52
22	6	312	CLA	C3B-C4B-NB	3.21	113.50	110.52
22	5	305	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
22	F	206	CLA	CMA-C3A-C2A	-3.21	108.60	116.10
22	2	311	CLA	CAC-C3C-C4C	3.21	128.98	124.81
22	A	829	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
22	B	803	CLA	C3B-C4B-NB	3.21	113.49	110.52
22	A	825	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	A	837	CLA	O2A-CGA-CBA	3.21	121.97	111.91
22	A	816	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
22	B	817	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
22	A	837	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
22	A	819	CLA	C1C-C2C-C3C	-3.21	103.59	106.96
25	5	315	BCR	C37-C22-C21	-3.21	118.43	122.92
22	2	304	CLA	CHC-C1C-C2C	-3.20	117.83	126.73
25	A	843	BCR	C15-C16-C17	3.20	130.04	123.47
22	B	805	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
22	A	830	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
31	6	318	RRX	C37-C22-C23	3.20	123.12	118.08
22	B	827	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	A	803	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
22	A	848	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	A	813	CLA	CAC-C3C-C4C	3.20	128.96	124.81
29	5	313	5X6	C27-C28-C29	-3.20	118.22	127.20
22	5	303	CLA	CED-O2D-CGD	3.20	123.17	115.94
22	A	836	CLA	O2A-CGA-CBA	3.20	121.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	804	CLA	CHB-C4A-NA	3.20	128.93	124.51
21	A	801	CL0	C1D-CHD-C4C	-3.20	119.16	126.06
22	A	857	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	B	807	CLA	CMC-C2C-C1C	3.19	129.90	125.04
22	B	803	CLA	CAC-C3C-C4C	3.19	128.95	124.81
22	1	302	CLA	C3C-C4C-NC	3.19	114.15	110.57
22	B	807	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
22	1	305	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
22	6	304	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
22	B	850	CLA	C3C-C4C-NC	3.19	114.15	110.57
22	B	818	CLA	CHC-C1C-C2C	-3.19	117.87	126.73
22	B	811	CLA	CAC-C3C-C4C	3.19	128.95	124.81
22	2	305	CLA	C1D-CHD-C4C	-3.19	119.18	126.06
31	4	317	RRX	C37-C22-C23	3.19	123.10	118.08
22	1	306	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
22	B	823	CLA	C2A-C1A-CHA	-3.19	118.29	123.86
22	B	820	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
22	5	311	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
22	B	810	CLA	CMC-C2C-C1C	3.18	129.89	125.04
22	A	822	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
22	5	303	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
22	5	309	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	B	823	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
22	B	812	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
22	A	833	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
22	4	306	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
22	4	306	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
22	5	310	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	5	321	5X6	C38-C30-C31	-3.18	108.46	114.36
22	B	837	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
22	7	310	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
22	6	303	CLA	CAC-C3C-C4C	3.18	128.93	124.81
22	B	817	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
25	Z	205	BCR	C15-C16-C17	3.18	129.98	123.47
22	4	302	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
22	B	831	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
25	B	842	BCR	C37-C22-C23	3.18	123.08	118.08
22	5	304	CLA	CAC-C3C-C4C	3.18	128.93	124.81
25	A	844	BCR	C16-C15-C14	3.18	129.98	123.47
22	A	802	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
22	A	857	CLA	CMC-C2C-C1C	3.18	129.88	125.04
22	2	311	CLA	C1C-C2C-C3C	-3.18	103.62	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	308	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
22	6	311	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
22	A	824	CLA	C3B-C4B-NB	3.17	113.46	110.52
22	5	309	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
22	A	812	CLA	C1D-CHD-C4C	-3.17	119.21	126.06
22	7	310	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
22	1	308	CLA	CMB-C2B-C1B	3.17	130.20	125.37
22	A	809	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
25	F	201	BCR	C15-C16-C17	3.17	129.97	123.47
22	B	822	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
22	6	304	CLA	C2A-C1A-CHA	-3.17	118.31	123.86
22	B	836	CLA	CMC-C2C-C1C	3.17	129.87	125.04
22	K	101	CLA	C3B-C4B-NB	3.17	113.46	110.52
29	4	313	5X6	C15-C16-C17	-3.17	117.51	126.42
25	K	103	BCR	C12-C13-C14	3.17	123.81	118.94
22	4	307	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
22	2	308	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
22	A	848	CLA	O2A-CGA-CBA	3.17	121.84	111.91
22	1	310	CLA	CMC-C2C-C1C	3.17	129.86	125.04
29	4	315	5X6	C14-C15-C16	-3.17	113.34	123.22
22	B	816	CLA	O1D-CGD-CBD	-3.16	118.01	124.48
25	L	206	BCR	C16-C15-C14	3.16	129.96	123.47
22	B	837	CLA	CMB-C2B-C1B	3.16	130.19	125.37
22	B	811	CLA	C3C-C4C-NC	3.16	114.12	110.57
29	7	317	5X6	C39-C26-C27	-3.16	113.10	118.08
22	A	810	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
22	6	305	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
29	1	314	5X6	C27-C26-C25	-3.16	114.09	118.94
22	4	312	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
22	A	816	CLA	C1D-CHD-C4C	-3.16	119.25	126.06
22	B	807	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
22	4	308	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
22	L	204	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
22	B	802	CLA	C1D-CHD-C4C	-3.16	119.25	126.06
22	B	807	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	3	305	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
22	A	819	CLA	CED-O2D-CGD	3.15	123.07	115.94
29	Z	206	5X6	C01-C02-C07	-3.15	108.51	114.36
22	A	803	CLA	C4A-NA-C1A	-3.15	105.29	106.71
22	B	815	CLA	C3B-C4B-NB	3.15	113.44	110.52
29	5	312	5X6	C24-C23-C22	-3.15	117.56	126.42
22	6	310	CLA	C4C-C3C-C2C	-3.15	102.30	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	801	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
22	6	311	CLA	CAC-C3C-C2C	3.15	132.92	127.53
22	B	815	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
29	5	321	5X6	C41-C17-C16	-3.15	113.11	118.08
22	5	302	CLA	C3B-C4B-NB	3.15	113.44	110.52
22	A	810	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
22	A	826	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
22	7	307	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
22	B	817	CLA	CBC-CAC-C3C	-3.15	103.76	112.43
22	B	815	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
22	A	811	CLA	C4-C3-C5	3.15	120.56	115.27
22	2	310	CLA	C4C-C3C-C2C	-3.14	102.31	106.90
22	B	822	CLA	C3B-C4B-NB	3.14	113.43	110.52
29	7	316	5X6	C25-C24-C23	-3.14	113.41	123.22
22	1	304	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
22	3	302	CLA	CAC-C3C-C4C	3.14	128.89	124.81
22	5	305	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
22	5	306	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
22	B	836	CLA	C4A-NA-C1A	-3.14	105.29	106.71
22	F	205	CLA	C3B-C2B-C1B	-3.14	103.37	107.16
29	M	101	5X6	C11-C03-C02	-3.14	113.86	121.46
29	1	312	5X6	C24-C23-C22	-3.14	117.60	126.42
22	5	308	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
22	7	312	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
25	B	843	BCR	C34-C9-C8	3.14	123.02	118.08
22	B	813	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
22	A	835	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
22	B	839	CLA	O2A-CGA-CBA	3.14	121.76	111.91
22	A	817	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
22	7	311	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
22	K	101	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
22	A	836	CLA	CBC-CAC-C3C	-3.14	103.79	112.43
22	6	305	CLA	CMC-C2C-C1C	3.13	129.81	125.04
22	B	809	CLA	CHC-C1C-C2C	-3.13	118.02	126.73
22	A	818	CLA	CHC-C1C-C2C	-3.13	118.02	126.73
22	1	304	CLA	CHC-C1C-C2C	-3.13	118.02	126.73
29	5	314	5X6	C14-C15-C16	-3.13	113.44	123.22
22	B	827	CLA	C4A-NA-C1A	-3.13	105.30	106.71
22	1	308	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
22	A	839	CLA	C4-C3-C5	3.13	120.54	115.27
22	Z	204	CLA	CBC-CAC-C3C	-3.13	103.80	112.43
22	A	859	CLA	C6-C7-C8	-3.13	105.80	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	303	CLA	C3C-C4C-NC	3.13	114.08	110.57
22	A	811	CLA	C3B-C4B-NB	3.13	113.42	110.52
22	2	310	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
25	A	845	BCR	C29-C30-C25	3.13	115.30	110.48
22	2	305	CLA	CBA-CAA-C2A	3.13	123.09	113.86
22	A	828	CLA	C1D-CHD-C4C	-3.13	119.32	126.06
22	B	801	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
22	B	814	CLA	C1D-CHD-C4C	-3.12	119.32	126.06
22	Z	204	CLA	CAC-C3C-C4C	3.12	128.86	124.81
22	7	304	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
29	1	313	5X6	C14-C15-C16	-3.12	113.48	123.22
29	7	314	5X6	C14-C15-C16	-3.12	113.48	123.22
22	5	304	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
29	5	314	5X6	C11-C03-C02	-3.12	113.91	121.46
22	B	837	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
22	A	822	CLA	CMC-C2C-C1C	3.12	129.78	125.04
22	B	821	CLA	CMC-C2C-C1C	3.12	129.78	125.04
22	A	839	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
22	5	305	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
22	2	310	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
22	6	306	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
22	A	811	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
22	4	306	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
29	1	312	5X6	C42-C13-C12	-3.11	113.18	118.08
29	4	314	5X6	C05-C06-C07	-3.11	106.05	110.30
25	L	201	BCR	C37-C22-C23	3.11	122.97	118.08
22	A	819	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
22	B	824	CLA	C4A-NA-C1A	-3.11	105.31	106.71
22	2	304	CLA	C3C-C4C-NC	3.11	114.05	110.57
22	A	806	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
22	A	828	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
22	A	848	CLA	CAC-C3C-C4C	3.10	128.84	124.81
22	7	313	CLA	CAC-C3C-C4C	3.10	128.84	124.81
22	A	857	CLA	C1D-CHD-C4C	-3.10	119.36	126.06
22	5	307	CLA	CAC-C3C-C4C	3.10	128.84	124.81
22	2	309	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
22	4	310	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
22	Z	204	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	B	822	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
22	F	204	CLA	O2D-CGD-CBD	3.10	116.78	111.27
22	A	821	CLA	CMC-C2C-C1C	3.10	129.76	125.04
25	J	103	BCR	C16-C15-C14	3.10	129.82	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	801	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	1	306	CLA	CAC-C3C-C4C	3.10	128.83	124.81
22	A	857	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
22	A	823	CLA	O2A-CGA-CBA	3.09	121.62	111.91
22	1	304	CLA	C3B-C4B-NB	3.09	113.38	110.52
22	B	828	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
22	A	814	CLA	CBC-CAC-C3C	-3.09	103.91	112.43
22	B	821	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
29	B	851	5X6	C15-C16-C17	-3.09	117.73	126.42
22	1	310	CLA	C3B-C4B-NB	3.09	113.38	110.52
22	B	806	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
22	6	310	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
22	Z	204	CLA	C4A-NA-C1A	-3.09	105.32	106.71
22	5	306	CLA	C4A-NA-C1A	-3.09	105.32	106.71
22	B	838	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
22	B	823	CLA	CMB-C2B-C1B	3.09	130.07	125.37
25	5	315	BCR	C34-C9-C8	3.09	122.94	118.08
22	A	806	CLA	C3B-C4B-NB	3.09	113.38	110.52
22	A	805	CLA	C2A-C1A-CHA	-3.09	118.46	123.86
22	A	828	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
22	2	311	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
29	4	315	5X6	C15-C16-C17	-3.08	117.75	126.42
22	A	808	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
22	B	801	CLA	C4-C3-C5	3.08	120.46	115.27
22	B	803	CLA	O2D-CGD-CBD	3.08	116.74	111.27
22	3	301	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	5	302	CLA	C1-C2-C3	-3.08	120.71	126.04
29	B	851	5X6	C38-C30-C31	-3.08	108.65	114.36
22	B	817	CLA	CMC-C2C-C1C	3.08	129.73	125.04
22	7	308	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
22	B	831	CLA	CAC-C3C-C4C	3.08	128.81	124.81
22	B	836	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
22	B	804	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
21	A	801	CL0	CMA-C3A-C2A	-3.08	101.41	113.83
22	7	311	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
22	7	313	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
22	B	830	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	1	307	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	O	204	CLA	CAC-C3C-C4C	3.08	128.80	124.81
22	4	311	CLA	CAC-C3C-C4C	3.08	128.80	124.81
22	A	813	CLA	CAA-C2A-C3A	-3.08	106.57	114.26
22	1	309	CLA	C3B-C4B-NB	3.08	113.37	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	313	CLA	C3B-C4B-NB	3.08	113.37	110.52
22	A	821	CLA	C1D-CHD-C4C	-3.08	119.42	126.06
22	B	816	CLA	CMC-C2C-C1C	3.08	129.72	125.04
29	7	316	5X6	C41-C17-C16	-3.08	113.23	118.08
22	A	807	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
22	B	831	CLA	CHC-C1C-C2C	-3.08	118.19	126.73
22	A	859	CLA	C2A-C1A-CHA	-3.08	118.48	123.86
22	A	816	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
22	A	820	CLA	C4C-C3C-C2C	-3.08	102.42	106.90
22	6	305	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
22	A	836	CLA	O2A-CGA-O1A	-3.07	115.83	123.59
22	A	825	CLA	C3B-C4B-NB	3.07	113.37	110.52
22	B	819	CLA	C1D-CHD-C4C	-3.07	119.43	126.06
25	J	103	BCR	C16-C17-C18	3.07	131.69	127.31
29	2	312	5X6	C14-C15-C16	-3.07	113.63	123.22
22	B	850	CLA	CMC-C2C-C1C	3.07	129.72	125.04
25	5	315	BCR	C15-C16-C17	3.07	129.76	123.47
22	B	815	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
25	F	207	BCR	C37-C22-C23	3.07	122.91	118.08
22	4	312	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	1	306	CLA	CHB-C4A-NA	3.06	128.75	124.51
22	B	822	CLA	C4A-NA-C1A	-3.06	105.33	106.71
22	6	314	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
22	A	820	CLA	CMC-C2C-C1C	3.06	129.70	125.04
22	6	309	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
22	B	834	CLA	C3B-C4B-NB	3.06	113.35	110.52
25	L	201	BCR	C34-C9-C8	3.06	122.90	118.08
22	A	858	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
22	5	307	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
22	2	303	CLA	CMC-C2C-C1C	3.06	129.70	125.04
22	B	829	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
22	4	302	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
25	L	206	BCR	C35-C13-C14	-3.06	118.64	122.92
22	B	823	CLA	C2C-C1C-NC	3.06	112.83	109.97
22	2	307	CLA	CMC-C2C-C1C	3.06	129.69	125.04
22	B	802	CLA	CMC-C2C-C1C	3.05	129.69	125.04
22	B	808	CLA	CMB-C2B-C1B	3.05	130.02	125.37
28	B	845	DGD	C2G-O2G-C1B	-3.05	110.27	117.79
22	O	204	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
22	A	825	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	2	302	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
22	A	837	CLA	CMC-C2C-C1C	3.05	129.68	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	203	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
22	5	302	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
25	A	862	BCR	C34-C9-C8	3.05	122.88	118.08
22	A	837	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
29	7	316	5X6	C27-C28-C29	-3.05	118.64	127.20
22	2	309	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	6	312	CLA	C3C-C4C-NC	3.05	113.99	110.57
22	A	835	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
22	B	801	CLA	CAC-C3C-C4C	3.05	128.76	124.81
22	B	828	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
22	B	835	CLA	C5-C3-C2	3.05	127.28	121.12
22	A	848	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	1	310	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	A	831	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	7	306	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	B	814	CLA	O2A-CGA-CBA	3.04	121.46	111.91
22	A	806	CLA	C1-O2A-CGA	3.04	124.43	116.44
22	L	203	CLA	CAC-C3C-C4C	3.04	128.76	124.81
22	B	849	CLA	CMC-C2C-C1C	3.04	129.68	125.04
22	A	807	CLA	C4A-NA-C1A	-3.04	105.34	106.71
22	2	308	CLA	C1-O2A-CGA	3.04	124.42	116.44
22	B	803	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
22	3	302	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
22	4	302	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
22	4	310	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
22	A	830	CLA	C4A-NA-C1A	-3.04	105.34	106.71
22	A	810	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
22	A	823	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
22	4	312	CLA	CHC-C1C-C2C	-3.04	118.30	126.73
22	1	308	CLA	CAC-C3C-C4C	3.04	128.75	124.81
29	6	317	5X6	C40-C22-C23	-3.04	113.29	118.08
25	F	207	BCR	C16-C15-C14	3.04	129.69	123.47
22	5	303	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
29	6	316	5X6	C27-C28-C29	-3.03	118.68	127.20
22	A	823	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
22	6	313	CLA	CMC-C2C-C1C	3.03	129.66	125.04
22	B	833	CLA	CAC-C3C-C4C	3.03	128.75	124.81
22	B	803	CLA	CMC-C2C-C1C	3.03	129.66	125.04
22	3	304	CLA	CHC-C1C-C2C	-3.03	118.31	126.73
22	B	838	CLA	C1D-CHD-C4C	-3.03	119.52	126.06
29	5	321	5X6	C25-C24-C23	-3.03	113.76	123.22
22	A	838	CLA	C4-C3-C2	-3.03	115.90	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	806	CLA	C4-C3-C2	-3.03	115.91	123.68
22	2	306	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
22	A	857	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
22	2	302	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	A	805	CLA	CHC-C1C-C2C	-3.03	118.33	126.73
22	A	806	CLA	CHC-C1C-C2C	-3.03	118.33	126.73
22	A	848	CLA	CHC-C1C-C2C	-3.03	118.33	126.73
22	1	307	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
22	A	830	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
22	A	810	CLA	O2A-CGA-CBA	3.02	121.39	111.91
22	Z	201	CLA	C4A-NA-C1A	-3.02	105.35	106.71
22	B	835	CLA	C4-C3-C5	3.02	120.35	115.27
22	Z	201	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	O	204	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
25	Z	202	BCR	C34-C9-C10	-3.02	118.69	122.92
22	6	304	CLA	CAC-C3C-C4C	3.02	128.73	124.81
22	3	305	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	B	813	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
25	A	844	BCR	C34-C9-C8	3.02	122.83	118.08
22	A	839	CLA	CMA-C3A-C2A	-3.01	101.67	113.83
22	A	832	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
22	B	815	CLA	CBC-CAC-C3C	-3.01	104.12	112.43
22	7	304	CLA	CAC-C3C-C4C	3.01	128.72	124.81
22	4	304	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
22	4	307	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
22	A	815	CLA	CMC-C2C-C1C	3.01	129.63	125.04
22	1	310	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
22	5	301	CLA	CMC-C2C-C1C	3.01	129.63	125.04
29	7	318	5X6	C42-C13-C14	-3.01	118.70	122.92
22	1	303	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
22	O	203	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
22	A	839	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
22	B	804	CLA	C4-C3-C5	3.01	120.34	115.27
22	A	821	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
22	A	822	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
22	B	830	CLA	CMC-C2C-C1C	3.01	129.62	125.04
22	B	826	CLA	C4A-NA-C1A	-3.01	105.35	106.71
22	B	824	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
22	6	305	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
29	2	313	5X6	C38-C30-C31	-3.01	108.78	114.36
29	B	851	5X6	C28-C29-C30	-3.01	114.18	121.46
25	A	861	BCR	C16-C15-C14	3.01	129.63	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	308	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
22	7	305	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
22	A	813	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
22	A	812	CLA	C3B-C4B-NB	3.00	113.30	110.52
22	A	834	CLA	CMC-C2C-C1C	3.00	129.61	125.04
22	A	839	CLA	C1D-CHD-C4C	-3.00	119.58	126.06
25	B	842	BCR	C34-C9-C10	-3.00	118.72	122.92
22	A	807	CLA	CMC-C2C-C1C	3.00	129.61	125.04
22	6	308	CLA	CMC-C2C-C1C	3.00	129.61	125.04
29	J	104	5X6	C01-C02-C07	-3.00	108.80	114.36
22	A	809	CLA	CAC-C3C-C4C	3.00	128.70	124.81
25	F	201	BCR	C34-C9-C10	-3.00	118.72	122.92
22	2	303	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
29	1	316	5X6	C01-C02-C07	-3.00	108.80	114.36
22	F	205	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
22	5	306	CLA	CHC-C1C-C2C	-2.99	118.41	126.73
31	1	315	RRX	C34-C9-C8	2.99	122.80	118.08
22	B	819	CLA	O2D-CGD-CBD	2.99	116.59	111.27
22	6	308	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
22	B	829	CLA	C1D-CHD-C4C	-2.99	119.60	126.06
22	B	806	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
22	B	820	CLA	CAC-C3C-C4C	2.99	128.69	124.81
22	6	304	CLA	C3B-C4B-NB	2.99	113.29	110.52
22	Z	204	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
29	7	317	5X6	C14-C15-C16	-2.99	113.89	123.22
22	5	310	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
22	B	804	CLA	O1D-CGD-CBD	-2.99	118.37	124.48
29	4	315	5X6	C12-C13-C14	-2.99	114.36	118.94
22	B	825	CLA	CMC-C2C-C1C	2.99	129.59	125.04
22	B	824	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
29	7	318	5X6	C14-C15-C16	-2.99	113.90	123.22
22	A	803	CLA	O2A-CGA-CBA	2.99	121.28	111.91
22	5	302	CLA	C2A-C1A-CHA	-2.98	118.64	123.86
22	5	309	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
22	A	817	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	B	818	CLA	C3B-C4B-NB	2.98	113.28	110.52
22	A	809	CLA	C1-O2A-CGA	2.98	124.27	116.44
22	7	306	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
22	A	833	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
22	1	309	CLA	C1D-CHD-C4C	-2.98	119.63	126.06
22	A	810	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
22	B	807	CLA	C1D-CHD-C4C	-2.98	119.63	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	204	CLA	CMC-C2C-C1C	2.98	129.57	125.04
22	A	836	CLA	C1-O2A-CGA	2.98	124.26	116.44
22	B	817	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
29	2	313	5X6	C24-C23-C22	-2.98	118.05	126.42
22	5	301	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
22	4	309	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
21	A	801	CL0	C4C-C3C-C2C	-2.98	102.56	106.90
22	1	305	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
22	B	830	CLA	C4-C3-C5	2.97	120.28	115.27
22	O	205	CLA	CAC-C3C-C4C	2.97	128.67	124.81
22	L	205	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
22	B	824	CLA	CMC-C2C-C1C	2.97	129.57	125.04
22	B	806	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
22	4	305	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
22	A	834	CLA	C1-O2A-CGA	2.97	124.24	116.44
31	5	322	RRX	C37-C22-C23	2.97	122.76	118.08
22	B	829	CLA	O1D-CGD-CBD	-2.97	118.41	124.48
22	7	306	CLA	CBA-CAA-C2A	2.97	122.63	113.86
22	B	818	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	J	102	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	B	840	A1L64	O3-C3-C4	2.97	134.84	123.64
22	B	803	CLA	C7-C6-C5	-2.97	105.30	113.36
22	4	312	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
29	6	316	5X6	C04-C03-C02	-2.97	118.43	122.61
22	B	814	CLA	CMC-C2C-C1C	2.97	129.56	125.04
29	1	316	5X6	C12-C13-C14	-2.97	114.39	118.94
22	A	808	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	A	833	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	2	305	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
22	A	803	CLA	CMC-C2C-C1C	2.97	129.56	125.04
22	5	304	CLA	CBA-CAA-C2A	2.96	122.61	113.86
21	A	801	CL0	CMA-C3A-C4A	-2.96	103.81	111.77
22	6	309	CLA	CMC-C2C-C1C	2.96	129.55	125.04
22	O	205	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
22	7	307	CLA	CMC-C2C-C1C	2.96	129.55	125.04
29	7	317	5X6	C24-C23-C22	-2.96	118.10	126.42
22	O	205	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	2	311	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
22	B	801	CLA	C1-O2A-CGA	2.96	124.21	116.44
22	B	828	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
22	7	309	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	A	832	CLA	CHC-C1C-C2C	-2.96	118.51	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	816	CLA	O2A-CGA-CBA	2.96	121.19	111.91
22	4	308	CLA	O2A-CGA-CBA	2.96	121.19	111.91
22	5	310	CLA	O2A-CGA-CBA	2.96	121.19	111.91
22	7	309	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
29	O	207	5X6	C41-C17-C16	-2.96	113.42	118.08
22	Z	201	CLA	CMC-C2C-C1C	2.96	129.54	125.04
22	B	850	CLA	C3B-C4B-NB	2.96	113.26	110.52
22	B	828	CLA	CHB-C4A-NA	2.95	128.60	124.51
22	7	313	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
22	B	833	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
29	1	316	5X6	C25-C24-C23	-2.95	114.01	123.22
22	2	305	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
22	B	839	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
22	B	849	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
29	7	314	5X6	C12-C11-C03	-2.95	118.92	127.20
22	6	304	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
22	A	807	CLA	C1-O2A-CGA	2.95	124.18	116.44
22	B	808	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
22	B	833	CLA	CMC-C2C-C1C	2.95	129.53	125.04
25	K	103	BCR	C19-C18-C17	2.95	123.46	118.94
22	O	205	CLA	CMC-C2C-C1C	2.95	129.53	125.04
22	B	804	CLA	C4-C3-C2	-2.95	116.12	123.68
22	6	310	CLA	CMC-C2C-C1C	2.95	129.53	125.04
22	A	803	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
29	B	851	5X6	C25-C24-C23	-2.94	114.03	123.22
22	Z	204	CLA	O2A-CGA-O1A	-2.94	116.16	123.59
29	M	101	5X6	C39-C26-C27	-2.94	113.44	118.08
22	A	848	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
22	A	812	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
22	A	834	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	B	821	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
22	A	830	CLA	CMC-C2C-C1C	2.94	129.52	125.04
25	A	846	BCR	C34-C9-C8	2.94	122.71	118.08
22	2	305	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	A	823	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	A	818	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
29	7	314	5X6	C27-C28-C29	-2.94	118.95	127.20
22	6	306	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
22	3	302	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
22	5	304	CLA	CMC-C2C-C1C	2.94	129.51	125.04
22	4	304	CLA	C4-C3-C5	2.94	120.21	115.27
22	7	307	CLA	C4C-C3C-C2C	-2.94	102.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	809	CLA	C4-C3-C5	2.93	120.21	115.27
22	A	818	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	B	849	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
22	A	820	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
22	7	309	CLA	O2A-CGA-CBA	2.93	121.11	111.91
22	B	810	CLA	CHB-C4A-NA	2.93	128.57	124.51
22	B	826	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
25	B	842	BCR	C35-C13-C14	-2.93	118.82	122.92
25	A	861	BCR	C35-C13-C14	-2.93	118.82	122.92
22	7	312	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
22	A	818	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
22	B	811	CLA	C2A-C1A-CHA	-2.93	118.74	123.86
29	5	313	5X6	C33-C32-C31	-2.93	106.30	110.30
22	5	307	CLA	CHD-C4C-NC	2.93	128.82	124.20
22	A	833	CLA	C3B-C4B-NB	2.93	113.23	110.52
22	A	830	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
22	4	307	CLA	CMB-C2B-C1B	2.93	129.83	125.37
22	O	204	CLA	CAA-C2A-C3A	-2.93	109.27	116.10
22	B	815	CLA	O2A-CGA-CBA	2.93	121.09	111.91
29	3	306	5X6	C38-C30-C31	-2.93	108.93	114.36
22	B	849	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	K	101	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
22	4	303	CLA	O2A-CGA-CBA	2.92	121.08	111.91
22	B	834	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
22	A	809	CLA	CMC-C2C-C1C	2.92	129.49	125.04
22	4	305	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
22	B	830	CLA	C1D-CHD-C4C	-2.92	119.75	126.06
25	4	316	BCR	C36-C18-C17	-2.92	118.83	122.92
22	B	815	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
22	6	307	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
22	A	835	CLA	CMC-C2C-C1C	2.92	129.49	125.04
22	B	809	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	2	307	CLA	CAC-C3C-C4C	2.92	128.60	124.81
22	A	817	CLA	C1-C2-C3	-2.92	121.00	126.04
22	B	820	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
29	7	316	5X6	C27-C26-C25	-2.92	114.47	118.94
22	4	309	CLA	CMC-C2C-C1C	2.92	129.48	125.04
22	O	203	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
22	6	307	CLA	CHB-C4A-NA	2.91	128.54	124.51
25	F	201	BCR	C37-C22-C23	2.91	122.66	118.08
22	7	309	CLA	CAC-C3C-C4C	2.91	128.58	124.81
22	B	825	CLA	CHB-C4A-NA	2.91	128.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	801	CL0	CAC-C3C-C4C	2.91	128.58	124.81
21	A	801	CL0	CMC-C2C-C1C	2.91	129.46	125.04
22	B	830	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
21	A	801	CL0	CHC-C1C-C2C	-2.90	118.66	126.73
22	B	803	CLA	CHB-C4A-NA	2.90	128.53	124.51
29	3	306	5X6	C24-C23-C22	-2.90	118.26	126.42
22	B	825	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
22	6	304	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	A	845	BCR	C30-C25-C24	2.90	123.99	115.78
22	A	814	CLA	CMC-C2C-C1C	2.90	129.46	125.04
22	A	819	CLA	C1-O2A-CGA	2.90	124.06	116.44
22	B	820	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
29	Z	206	5X6	C15-C16-C17	-2.90	118.27	126.42
22	K	102	CLA	C3B-C4B-NB	2.90	113.20	110.52
22	6	306	CLA	CBA-CAA-C2A	2.90	122.41	113.86
22	B	825	CLA	C1-O2A-CGA	2.89	124.04	116.44
22	4	308	CLA	CHD-C4C-NC	2.89	128.76	124.20
22	1	308	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
22	O	203	CLA	CAC-C3C-C4C	2.89	128.56	124.81
22	O	206	CLA	CED-O2D-CGD	2.89	122.48	115.94
22	A	802	CLA	C4-C3-C5	2.89	120.13	115.27
22	B	803	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	1	313	5X6	C40-C22-C23	-2.89	113.52	118.08
22	A	838	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	7	314	5X6	C16-C17-C18	-2.89	114.51	118.94
29	7	314	5X6	C27-C26-C25	-2.89	114.51	118.94
22	A	857	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
22	7	305	CLA	C3B-C4B-NB	2.89	113.19	110.52
22	Z	201	CLA	CBA-CAA-C2A	2.89	122.39	113.86
22	B	814	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
22	B	829	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
25	4	316	BCR	C34-C9-C8	2.89	122.63	118.08
22	7	304	CLA	CHD-C4C-NC	2.89	128.75	124.20
25	B	841	BCR	C36-C18-C17	-2.88	118.88	122.92
22	7	309	CLA	CHB-C1B-C2B	-2.88	119.09	127.24
22	B	826	CLA	C3B-C4B-NB	2.88	113.19	110.52
22	7	306	CLA	CMC-C2C-C1C	2.88	129.43	125.04
22	7	306	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
29	2	312	5X6	C01-C02-C07	-2.88	109.01	114.36
22	A	824	CLA	CAC-C3C-C4C	2.88	128.55	124.81
22	Z	201	CLA	CAC-C3C-C4C	2.88	128.55	124.81
22	B	828	CLA	C1D-CHD-C4C	-2.88	119.85	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	303	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
29	J	104	5X6	C38-C30-C31	-2.88	109.03	114.36
29	M	101	5X6	C01-C02-C07	-2.88	109.03	114.36
22	F	206	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
29	1	314	5X6	C01-C02-C07	-2.87	109.03	114.36
22	B	812	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
22	A	859	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
22	A	803	CLA	CAA-C2A-C1A	-2.87	102.56	111.97
25	B	842	BCR	C1-C6-C5	-2.87	118.57	122.61
22	A	830	CLA	C2A-C1A-CHA	-2.87	118.84	123.86
22	A	816	CLA	CMC-C2C-C1C	2.87	129.41	125.04
22	5	301	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
22	4	303	CLA	CAC-C3C-C4C	2.87	128.53	124.81
29	2	314	5X6	C11-C03-C02	-2.87	114.52	121.46
22	B	812	CLA	C4-C3-C2	-2.87	116.33	123.68
22	7	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	3	303	CLA	C3B-C4B-NB	2.87	113.17	110.52
29	O	208	5X6	C40-C22-C23	-2.86	113.56	118.08
22	5	303	CLA	C1-O2A-CGA	2.86	123.96	116.44
22	B	826	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	A	818	CLA	CAC-C3C-C4C	2.86	128.53	124.81
22	A	811	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	A	815	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	A	817	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	Z	201	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	L	203	CLA	C4-C3-C5	2.86	120.08	115.27
22	6	313	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
22	B	801	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	A	828	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
22	4	304	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
22	A	830	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
22	A	817	CLA	C1D-CHD-C4C	-2.86	119.89	126.06
22	A	836	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
29	4	313	5X6	C25-C24-C23	-2.86	114.30	123.22
22	A	859	CLA	CMC-C2C-C1C	2.86	129.39	125.04
25	B	844	BCR	C35-C13-C14	-2.86	118.92	122.92
22	B	816	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
22	A	824	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
22	B	802	CLA	O2A-CGA-CBA	2.85	120.86	111.91
22	A	807	CLA	O2A-CGA-O1A	-2.85	116.40	123.59
22	B	827	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
22	A	802	CLA	C3B-C4B-NB	2.85	113.16	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	804	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
25	1	301	BCR	C37-C22-C23	2.85	122.56	118.08
25	A	844	BCR	C24-C23-C22	2.85	130.54	126.23
31	1	315	RRX	C35-C13-C14	-2.85	118.94	122.92
25	L	206	BCR	C15-C16-C17	2.85	129.31	123.47
25	A	844	BCR	C35-C13-C14	-2.85	118.94	122.92
31	4	317	RRX	C15-C16-C17	2.84	129.30	123.47
22	7	308	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
22	B	815	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
22	4	303	CLA	CHD-C4C-NC	2.84	128.68	124.20
22	1	303	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
22	5	311	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
25	F	207	BCR	C12-C13-C14	2.84	123.30	118.94
22	A	827	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
22	4	303	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
22	A	820	CLA	CAC-C3C-C4C	2.84	128.50	124.81
22	A	803	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
22	B	803	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	B	833	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
25	A	843	BCR	C36-C18-C17	-2.84	118.95	122.92
22	B	805	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
22	B	824	CLA	C1-O2A-CGA	2.84	123.89	116.44
22	6	311	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
22	A	808	CLA	CMC-C2C-C1C	2.83	129.35	125.04
22	2	307	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
22	6	309	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
22	B	834	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
22	B	828	CLA	CMC-C2C-C1C	2.83	129.35	125.04
22	A	813	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
22	7	304	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
22	B	803	CLA	C20-C18-C19	2.83	123.55	110.51
22	A	814	CLA	C3B-C2B-C1B	-2.83	103.75	107.16
22	6	310	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
22	A	834	CLA	C4-C3-C2	-2.83	116.43	123.68
31	1	315	RRX	C36-C18-C17	-2.83	118.97	122.92
22	B	825	CLA	CAC-C3C-C4C	2.83	128.48	124.81
29	5	312	5X6	C12-C13-C14	-2.82	114.61	118.94
22	3	301	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
22	6	313	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
22	B	823	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	4	310	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
22	A	829	CLA	CAC-C3C-C4C	2.82	128.47	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	310	CLA	C3C-C4C-NC	2.82	113.73	110.57
22	A	839	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
22	B	832	CLA	CMC-C2C-C1C	2.82	129.33	125.04
25	A	844	BCR	C36-C18-C17	-2.82	118.97	122.92
22	A	802	CLA	CAC-C3C-C4C	2.82	128.47	124.81
22	A	814	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
22	2	304	CLA	O2A-CGA-CBA	2.82	120.75	111.91
22	A	812	CLA	CMC-C2C-C1C	2.82	129.33	125.04
25	1	301	BCR	C34-C9-C8	2.82	122.51	118.08
22	4	304	CLA	CMC-C2C-C1C	2.82	129.33	125.04
29	4	313	5X6	C41-C17-C16	-2.81	113.64	118.08
22	B	836	CLA	C3B-C4B-NB	2.81	113.13	110.52
22	4	310	CLA	C3B-C4B-NB	2.81	113.13	110.52
22	7	305	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
22	A	810	CLA	C4A-NA-C1A	-2.81	105.44	106.71
29	1	316	5X6	C06-C07-C02	2.81	117.46	111.85
22	2	306	CLA	C3B-C4B-NB	2.81	113.12	110.52
22	5	302	CLA	CAC-C3C-C4C	2.81	128.46	124.81
22	A	848	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	A	824	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
22	A	848	CLA	C3B-C4B-NB	2.81	113.12	110.52
22	6	306	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
22	7	312	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
22	B	818	CLA	C4-C3-C5	2.81	120.00	115.27
22	A	819	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
22	B	834	CLA	CMC-C2C-C1C	2.81	129.32	125.04
22	A	836	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
22	2	306	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	B	811	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
22	6	312	CLA	CHD-C4C-NC	2.81	128.63	124.20
22	3	304	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
22	A	838	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	2	304	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	4	311	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
22	B	839	CLA	O1D-CGD-CBD	-2.80	118.75	124.48
22	B	837	CLA	C3B-C4B-NB	2.80	113.12	110.52
22	A	829	CLA	CMB-C2B-C1B	2.80	129.64	125.37
22	A	809	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
22	B	808	CLA	O2A-CGA-CBA	2.80	120.70	111.91
22	A	838	CLA	C5-C3-C2	2.80	126.79	121.12
22	A	813	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	B	808	CLA	CHC-C1C-C2C	-2.80	118.95	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	822	CLA	C1-O2A-CGA	2.80	123.80	116.44
22	B	813	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
29	2	314	5X6	C40-C22-C23	-2.80	113.66	118.08
22	5	303	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	A	831	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
22	A	858	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	B	801	CLA	C4A-NA-C1A	-2.80	105.45	106.71
22	6	312	CLA	CHC-C1C-NC	2.80	128.45	124.20
22	B	828	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
22	7	304	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
22	A	838	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
25	B	843	BCR	C35-C13-C14	-2.80	119.01	122.92
22	L	205	CLA	CMC-C2C-C1C	2.80	129.30	125.04
22	4	308	CLA	C4C-C3C-C2C	-2.79	102.82	106.90
22	5	302	CLA	O2A-CGA-CBA	2.79	120.68	111.91
22	4	309	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
22	2	308	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
22	7	309	CLA	CHD-C4C-NC	2.79	128.60	124.20
22	6	312	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
25	2	301	BCR	C34-C9-C8	2.79	122.48	118.08
22	A	808	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	B	833	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	A	833	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	O	207	5X6	C11-C03-C02	-2.79	114.70	121.46
22	6	307	CLA	C4-C3-C5	2.79	119.96	115.27
29	2	314	5X6	C14-C15-C16	-2.79	114.52	123.22
22	2	308	CLA	CAC-C3C-C4C	2.79	128.43	124.81
25	B	842	BCR	C16-C15-C14	2.79	129.19	123.47
22	B	819	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
22	A	858	CLA	C4A-NA-C1A	-2.79	105.45	106.71
22	B	805	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
22	6	303	CLA	CMC-C2C-C1C	2.79	129.28	125.04
22	3	301	CLA	O2A-CGA-CBA	2.79	120.65	111.91
22	A	804	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
22	7	308	CLA	CHB-C1B-C2B	-2.78	119.37	127.24
22	2	307	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	1	311	5X6	C42-C13-C14	-2.78	119.02	122.92
22	A	809	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	4	312	CLA	O2A-CGA-CBA	2.78	122.97	114.03
22	B	807	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
23	A	840	A1L64	O3-C3-C2	-2.78	107.15	116.56
22	B	812	CLA	O2A-CGA-CBA	2.78	120.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	305	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
22	F	206	CLA	CAA-C2A-C3A	-2.78	109.61	116.10
22	B	820	CLA	CMC-C2C-C1C	2.78	129.27	125.04
22	B	833	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
22	A	810	CLA	CMB-C2B-C3B	2.78	133.32	126.59
22	A	815	CLA	C4-C3-C2	-2.78	116.55	123.68
22	4	307	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	5	302	CLA	CHD-C4C-NC	2.78	128.58	124.20
22	7	309	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
25	Z	205	BCR	C35-C13-C14	-2.78	119.03	122.92
22	6	309	CLA	CHB-C1B-C2B	-2.78	119.39	127.24
22	B	805	CLA	C4A-NA-C1A	-2.78	105.46	106.71
22	B	823	CLA	CAA-C2A-C1A	-2.78	102.88	111.97
29	5	313	5X6	C14-C15-C16	-2.78	114.56	123.22
22	A	813	CLA	CMC-C2C-C1C	2.77	129.26	125.04
22	7	304	CLA	O2A-CGA-CBA	2.77	120.62	111.91
22	3	301	CLA	CHD-C4C-NC	2.77	128.57	124.20
22	B	834	CLA	O2A-CGA-CBA	2.77	120.61	111.91
22	A	858	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
22	B	806	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	F	206	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
25	L	206	BCR	C37-C22-C23	2.77	122.44	118.08
29	6	317	5X6	C41-C17-C16	-2.77	113.71	118.08
22	A	809	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
22	B	817	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	L	204	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
22	2	309	CLA	CAA-C2A-C3A	-2.77	109.64	116.10
22	B	830	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	3	301	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	A	806	CLA	CMC-C2C-C1C	2.77	129.25	125.04
22	6	306	CLA	CHD-C4C-NC	2.77	128.56	124.20
22	4	303	CLA	CHC-C4B-NB	-2.76	121.33	124.26
25	B	843	BCR	C37-C22-C23	2.76	122.43	118.08
29	1	311	5X6	C39-C26-C27	-2.76	113.72	118.08
22	A	812	CLA	C1-O2A-CGA	2.76	123.69	116.44
22	2	302	CLA	C3B-C4B-NB	2.76	113.08	110.52
22	6	306	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	4	314	5X6	C38-C30-C31	-2.76	109.24	114.36
22	6	303	CLA	C3B-C4B-NB	2.76	113.08	110.52
22	A	859	CLA	O1D-CGD-CBD	-2.76	118.84	124.48
29	4	314	5X6	C25-C24-C23	-2.76	114.61	123.22
25	4	316	BCR	C37-C22-C23	2.76	122.42	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	827	CLA	C4-C3-C5	2.76	119.91	115.27
22	7	308	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
22	A	818	CLA	C4A-NA-C1A	-2.76	105.47	106.71
22	A	816	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
22	B	835	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
22	7	306	CLA	C4-C3-C5	2.75	119.91	115.27
22	A	816	CLA	C4-C3-C5	2.75	119.90	115.27
22	B	838	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	B	801	CLA	CMA-C3A-C2A	-2.75	102.72	113.83
22	B	817	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
29	5	312	5X6	C41-C17-C16	-2.75	113.74	118.08
29	O	207	5X6	C28-C29-C30	-2.75	114.80	121.46
22	B	803	CLA	C1-C2-C3	-2.75	121.29	126.04
22	B	816	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
22	A	824	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
22	A	838	CLA	C3B-C4B-NB	2.75	113.06	110.52
22	7	309	CLA	CED-O2D-CGD	2.75	122.15	115.94
22	6	304	CLA	O2A-CGA-CBA	2.75	120.53	111.91
22	7	303	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
22	4	308	CLA	CHB-C1B-C2B	-2.75	119.48	127.24
22	7	305	CLA	CMB-C2B-C3B	2.75	133.24	126.59
22	A	837	CLA	C4A-NA-C1A	-2.74	105.47	106.71
29	6	316	5X6	C14-C15-C16	-2.74	114.65	123.22
22	A	838	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
22	B	820	CLA	CBA-CAA-C2A	2.74	121.96	113.86
22	A	810	CLA	C1-O2A-CGA	2.74	123.64	116.44
22	5	305	CLA	C3B-C4B-NB	2.74	113.06	110.52
22	B	821	CLA	O2A-CGA-CBA	2.74	123.07	112.23
22	L	205	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
22	A	808	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	O	207	5X6	C38-C30-C31	-2.74	109.28	114.36
22	B	805	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	A	820	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
22	1	304	CLA	CMB-C2B-C3B	2.74	133.22	126.59
22	4	308	CLA	CHC-C4B-NB	-2.74	121.36	124.26
22	6	303	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
22	B	817	CLA	C4A-NA-C1A	-2.74	105.47	106.71
22	B	801	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	B	818	CLA	O2A-CGA-CBA	2.74	120.50	111.91
22	A	808	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
22	4	308	CLA	CAA-C2A-C3A	-2.74	105.29	112.78
22	2	308	CLA	C4C-C3C-C2C	-2.73	102.91	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	303	CLA	CHD-C4C-NC	2.73	128.51	124.20
22	A	811	CLA	C4A-NA-C1A	-2.73	105.48	106.71
22	Z	201	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
29	1	311	5X6	C14-C15-C16	-2.73	114.69	123.22
22	A	815	CLA	C1-O2A-CGA	2.73	123.61	116.44
22	7	305	CLA	CMC-C2C-C1C	2.73	129.20	125.04
29	1	313	5X6	C28-C29-C30	-2.73	114.85	121.46
22	1	306	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
22	6	307	CLA	C3B-C4B-NB	2.73	113.05	110.52
22	B	838	CLA	CMB-C2B-C1B	2.73	129.52	125.37
22	3	305	CLA	CHB-C1B-C2B	-2.73	119.53	127.24
22	4	309	CLA	C1-O2A-CGA	2.73	123.60	116.44
29	2	312	5X6	C38-C30-C31	-2.73	109.30	114.36
22	O	206	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
22	A	829	CLA	CMC-C2C-C1C	2.73	129.19	125.04
22	A	815	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
22	B	803	CLA	CMA-C3A-C2A	-2.73	102.83	113.83
29	1	312	5X6	C40-C22-C23	-2.72	113.78	118.08
22	B	837	CLA	CMC-C2C-C1C	2.72	129.19	125.04
22	A	804	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	2	303	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
22	B	805	CLA	C4-C3-C5	2.72	119.85	115.27
22	A	817	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
29	5	312	5X6	C38-C30-C31	-2.72	109.31	114.36
22	5	302	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
22	5	303	CLA	O2A-CGA-CBA	2.72	120.44	111.91
31	6	318	RRX	C15-C16-C17	2.72	129.04	123.47
22	B	819	CLA	CHB-C1B-C2B	-2.72	119.56	127.24
22	1	303	CLA	CMC-C2C-C1C	2.72	129.18	125.04
22	F	204	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
29	6	316	5X6	C25-C24-C23	-2.72	114.73	123.22
22	B	809	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	B	810	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
22	A	805	CLA	O2A-CGA-CBA	2.72	120.44	111.91
22	5	303	CLA	O2D-CGD-CBD	2.72	116.09	111.27
29	1	312	5X6	C36-C34-C29	2.72	114.70	110.30
22	2	308	CLA	O2A-CGA-CBA	2.72	120.43	111.91
21	A	801	CL0	C1-O2A-CGA	2.72	123.57	116.44
22	1	306	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
22	B	832	CLA	CGD-CBD-CAD	-2.71	101.94	110.73
22	B	803	CLA	C4A-NA-C1A	-2.71	105.49	106.71
22	4	310	CLA	CHC-C1C-NC	2.71	128.32	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	851	5X6	C11-C03-C02	-2.71	114.89	121.46
22	B	815	CLA	CMC-C2C-C1C	2.71	129.17	125.04
22	B	830	CLA	C3B-C4B-NB	2.71	113.03	110.52
22	A	825	CLA	O2A-CGA-CBA	2.71	120.41	111.91
22	A	835	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	A	818	CLA	CMC-C2C-C1C	2.71	129.16	125.04
22	5	306	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
22	4	310	CLA	CHD-C4C-C3C	-2.71	120.86	124.84
22	4	304	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
29	3	306	5X6	C25-C24-C23	-2.71	114.77	123.22
22	2	305	CLA	C1-O2A-CGA	2.71	123.55	116.44
22	4	305	CLA	CBC-CAC-C3C	-2.71	104.97	112.43
22	B	829	CLA	CBA-CAA-C2A	2.71	121.85	113.86
22	2	308	CLA	CHD-C4C-NC	2.71	128.47	124.20
22	4	311	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
25	L	202	BCR	C35-C13-C14	-2.70	119.14	122.92
22	5	307	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
22	7	310	CLA	C3B-C4B-NB	2.70	113.02	110.52
29	1	311	5X6	C25-C24-C23	-2.70	114.79	123.22
22	A	822	CLA	C4A-NA-C1A	-2.70	105.49	106.71
25	F	207	BCR	C15-C16-C17	2.70	129.00	123.47
22	B	825	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	2	305	CLA	CMC-C2C-C1C	2.70	129.15	125.04
22	A	835	CLA	C1-O2A-CGA	2.70	123.52	116.44
22	B	850	CLA	CAC-C3C-C4C	2.70	128.31	124.81
29	7	315	5X6	C38-C30-C31	-2.70	109.36	114.36
22	B	825	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
22	O	204	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
22	2	307	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
22	B	822	CLA	C4-C3-C5	2.70	119.81	115.27
22	3	304	CLA	CMC-C2C-C1C	2.69	129.14	125.04
22	A	820	CLA	C4-C3-C5	2.69	119.80	115.27
22	1	306	CLA	CED-O2D-CGD	2.69	122.03	115.94
22	4	312	CLA	CMC-C2C-C1C	2.69	129.14	125.04
25	A	861	BCR	C36-C18-C17	-2.69	119.15	122.92
22	2	308	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
22	A	838	CLA	CMC-C2C-C1C	2.69	129.14	125.04
22	5	306	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	A	815	CLA	O2A-CGA-CBA	2.69	120.35	111.91
29	4	315	5X6	C11-C03-C02	-2.69	114.94	121.46
29	M	101	5X6	C38-C30-C31	-2.69	109.37	114.36
22	L	204	CLA	O2D-CGD-O1D	-2.69	118.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	835	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
22	4	305	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
22	L	205	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	F	206	CLA	CHD-C4C-NC	2.69	128.44	124.20
22	5	308	CLA	C3B-C4B-NB	2.69	113.01	110.52
22	4	310	CLA	CMC-C2C-C1C	2.69	129.13	125.04
22	6	304	CLA	CHD-C4C-NC	2.69	128.44	124.20
22	A	817	CLA	CMC-C2C-C1C	2.69	129.13	125.04
22	B	837	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
22	A	858	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
22	A	858	CLA	C3B-C4B-NB	2.68	113.00	110.52
22	3	305	CLA	O2A-CGA-CBA	2.68	120.33	111.91
22	A	802	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
22	1	307	CLA	O2A-C1-C2	2.68	115.69	108.64
22	1	310	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
22	F	205	CLA	CMC-C2C-C1C	2.68	129.12	125.04
25	A	845	BCR	C16-C15-C14	2.68	128.97	123.47
22	1	302	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	O	206	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
22	4	307	CLA	CMC-C2C-C1C	2.68	129.12	125.04
22	B	836	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
29	1	311	5X6	C23-C22-C21	-2.68	114.83	118.94
22	2	305	CLA	CMB-C2B-C3B	2.68	133.08	126.59
22	O	205	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
22	A	809	CLA	O2A-CGA-CBA	2.68	120.31	111.91
22	A	825	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
22	B	808	CLA	OBD-CAD-C3D	-2.68	122.07	128.52
22	3	301	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
22	7	303	CLA	CMC-C2C-C1C	2.68	129.12	125.04
22	L	203	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
25	B	844	BCR	C34-C9-C8	-2.67	113.86	118.08
22	5	304	CLA	C2A-C1A-CHA	-2.67	119.18	123.86
22	Z	204	CLA	C1-C2-C3	-2.67	121.42	126.04
22	7	303	CLA	CMD-C2D-C3D	-2.67	121.46	127.61
25	A	843	BCR	C35-C13-C14	-2.67	119.18	122.92
22	B	849	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
22	1	305	CLA	CMC-C2C-C1C	2.67	129.11	125.04
22	5	304	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	A	816	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
22	B	821	CLA	CMB-C2B-C1B	2.67	129.43	125.37
29	7	314	5X6	C24-C23-C22	-2.67	118.92	126.42
22	B	816	CLA	C2A-C1A-CHA	-2.67	119.19	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	312	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
25	1	301	BCR	C36-C18-C17	-2.67	119.19	122.92
22	5	301	CLA	C3B-C4B-NB	2.67	112.99	110.52
22	4	308	CLA	CAC-C3C-C4C	2.67	128.27	124.81
22	A	831	CLA	C4-C3-C2	-2.67	116.84	123.68
22	B	849	CLA	C4A-NA-C1A	-2.66	105.51	106.71
22	A	809	CLA	C2A-C1A-CHA	-2.66	119.20	123.86
22	2	303	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
22	F	205	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	5	309	CLA	CHD-C4C-NC	2.66	128.40	124.20
22	B	822	CLA	CMC-C2C-C1C	2.66	129.09	125.04
22	B	822	CLA	O2A-CGA-CBA	2.66	120.26	111.91
22	A	824	CLA	C1-O2A-CGA	2.66	123.42	116.44
22	4	303	CLA	C1-O2A-CGA	2.66	123.42	116.44
22	3	305	CLA	CAC-C3C-C4C	2.66	128.26	124.81
22	7	310	CLA	CAA-C2A-C3A	-2.66	109.89	116.10
25	B	841	BCR	C34-C9-C8	2.66	122.27	118.08
25	B	844	BCR	C36-C18-C17	-2.66	119.20	122.92
22	B	819	CLA	CED-O2D-CGD	2.66	121.95	115.94
22	B	813	CLA	O1D-CGD-CBD	-2.66	119.05	124.48
25	5	315	BCR	C36-C18-C17	-2.66	119.20	122.92
22	O	203	CLA	CHD-C4C-NC	2.66	128.39	124.20
29	O	208	5X6	C42-C13-C12	-2.66	113.89	118.08
22	4	306	CLA	C3B-C4B-NB	2.65	112.98	110.52
22	A	834	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	A	806	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
22	A	838	CLA	C1-O2A-CGA	2.65	123.40	116.44
22	2	307	CLA	CHD-C4C-NC	2.65	128.38	124.20
25	1	301	BCR	C16-C15-C14	2.65	128.90	123.47
22	A	808	CLA	O2A-CGA-CBA	2.65	120.23	111.91
31	5	322	RRX	C15-C16-C17	2.65	128.90	123.47
22	5	306	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
22	1	302	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
29	5	313	5X6	C25-C24-C23	-2.65	114.96	123.22
25	L	202	BCR	C16-C15-C14	2.65	128.90	123.47
22	A	858	CLA	C4-C3-C5	2.65	119.72	115.27
22	A	822	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	2	304	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
22	A	806	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
22	A	820	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	1	316	5X6	C39-C26-C27	-2.64	113.91	118.08
22	3	305	CLA	CHD-C4C-NC	2.64	128.37	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	311	5X6	C01-C02-C07	-2.64	109.46	114.36
22	5	309	CLA	CAA-C2A-C1A	2.64	117.99	112.14
22	7	310	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
22	B	807	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	6	312	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
22	A	819	CLA	C3B-C4B-NB	2.64	112.96	110.52
22	5	311	CLA	CHB-C4A-NA	2.64	128.16	124.51
29	6	315	5X6	C25-C24-C23	-2.64	114.99	123.22
22	A	806	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	1	303	CLA	CED-O2D-CGD	2.64	121.90	115.94
22	A	821	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
22	5	309	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
22	A	817	CLA	CED-O2D-CGD	2.63	121.89	115.94
22	B	832	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
29	7	314	5X6	C25-C24-C23	-2.63	115.00	123.22
22	A	819	CLA	O2D-CGD-CBD	2.63	115.94	111.27
22	A	821	CLA	C3B-C4B-NB	2.63	112.95	110.52
22	1	308	CLA	C3B-C4B-NB	2.63	112.95	110.52
22	A	836	CLA	CMC-C2C-C1C	2.63	129.04	125.04
22	O	204	CLA	CMC-C2C-C1C	2.63	129.04	125.04
22	5	307	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
22	A	823	CLA	CMA-C3A-C4A	2.63	118.83	111.77
22	B	821	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
22	B	809	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
22	B	830	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
22	7	309	CLA	CMC-C2C-C1C	2.63	129.04	125.04
22	B	816	CLA	C3B-C4B-NB	2.62	112.95	110.52
22	B	825	CLA	CMA-C3A-C2A	-2.62	103.24	113.83
22	B	809	CLA	O2A-CGA-CBA	2.62	120.14	111.91
25	A	862	BCR	C37-C22-C23	2.62	122.21	118.08
29	1	314	5X6	C40-C22-C23	-2.62	113.94	118.08
29	7	317	5X6	C16-C17-C18	-2.62	114.92	118.94
22	4	303	CLA	CHB-C1B-C2B	-2.62	119.83	127.24
22	A	810	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
22	2	305	CLA	C4-C3-C2	-2.62	116.96	123.68
22	B	823	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	B	831	CLA	CMC-C2C-C1C	2.62	129.03	125.04
25	4	316	BCR	C35-C13-C14	-2.62	119.25	122.92
29	7	317	5X6	C35-C34-C29	2.62	114.55	110.30
23	A	840	A1L64	O3-C3-C4	2.62	133.51	123.64
22	O	206	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	7	304	CLA	CHB-C1B-C2B	-2.62	119.85	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	308	CLA	CMA-C3A-C2A	-2.61	110.00	116.10
22	B	839	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
22	A	820	CLA	C4A-NA-C1A	-2.61	105.53	106.71
29	7	318	5X6	C11-C03-C02	-2.61	115.13	121.46
22	4	308	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
22	5	304	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
25	F	207	BCR	C34-C9-C8	2.61	122.19	118.08
22	4	311	CLA	CHB-C1B-C2B	-2.61	119.87	127.24
22	B	827	CLA	CBA-CAA-C2A	2.61	121.57	113.86
22	A	825	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	A	822	CLA	O2A-CGA-CBA	2.61	120.09	111.91
22	6	306	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
29	4	313	5X6	C38-C30-C31	-2.61	109.53	114.36
22	A	828	CLA	CBC-CAC-C3C	-2.61	105.25	112.43
21	A	801	CL0	CGD-CBD-CAD	-2.61	102.30	110.73
22	A	810	CLA	CMC-C2C-C1C	2.60	129.01	125.04
22	B	825	CLA	C4A-NA-C1A	-2.60	105.53	106.71
22	1	306	CLA	CMC-C2C-C1C	2.60	129.00	125.04
22	A	807	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	3	305	CLA	CHC-C4B-NB	-2.60	121.50	124.26
22	1	306	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
25	L	202	BCR	C36-C18-C17	-2.60	119.28	122.92
22	B	827	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
22	5	311	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	L	204	CLA	CAC-C3C-C4C	2.60	128.19	124.81
22	A	833	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
22	B	807	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
22	B	829	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
29	7	314	5X6	C09-C04-C03	2.60	114.51	110.30
22	1	304	CLA	CMC-C2C-C1C	2.60	129.00	125.04
22	4	312	CLA	CHB-C1B-C2B	-2.60	119.90	127.24
22	B	814	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
22	A	829	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
22	7	312	CLA	CHD-C4C-NC	2.60	128.29	124.20
22	4	303	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	K	101	CLA	O2A-CGA-CBA	2.59	120.05	111.91
22	B	802	CLA	CMB-C2B-C1B	2.59	129.32	125.37
22	Z	204	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	A	816	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	A	837	CLA	CAA-CBA-CGA	-2.59	105.67	113.25
22	5	302	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
22	2	309	CLA	CMC-C2C-C1C	2.59	128.99	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	302	CLA	CMC-C2C-C1C	2.59	128.99	125.04
22	4	305	CLA	CHD-C4C-NC	2.59	128.29	124.20
29	M	101	5X6	C41-C17-C16	-2.59	113.99	118.08
22	6	305	CLA	C3B-C4B-NB	2.59	112.92	110.52
25	A	862	BCR	C36-C18-C17	-2.59	119.29	122.92
22	1	302	CLA	C3B-C4B-NB	2.59	112.92	110.52
22	A	804	CLA	O2A-CGA-CBA	2.59	120.04	111.91
25	L	206	BCR	C36-C18-C17	-2.59	119.30	122.92
22	1	307	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	1	302	CLA	CHD-C4C-NC	2.59	128.28	124.20
22	3	301	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	B	824	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
22	A	808	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
22	1	303	CLA	CMB-C2B-C1B	2.59	129.31	125.37
22	B	839	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
22	A	815	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	6	311	CLA	CED-O2D-CGD	2.59	121.78	115.94
22	B	812	CLA	OBD-CAD-C3D	-2.58	122.30	128.52
22	B	825	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
22	B	850	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	Z	204	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	4	309	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	3	305	CLA	CMC-C2C-C1C	2.58	128.97	125.04
22	B	819	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
22	4	310	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	6	306	CLA	C4-C3-C2	-2.58	117.06	123.68
22	A	810	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	A	829	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	O	205	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	7	308	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	2	307	CLA	CHB-C1B-C2B	-2.58	119.96	127.24
22	K	102	CLA	CMC-C2C-C1C	2.58	128.96	125.04
29	6	317	5X6	C25-C24-C23	-2.58	115.17	123.22
22	B	809	CLA	CMB-C2B-C1B	2.58	129.29	125.37
22	A	809	CLA	CHB-C1B-C2B	-2.58	119.96	127.24
29	1	311	5X6	C41-C17-C16	-2.58	114.02	118.08
22	B	829	CLA	O2A-CGA-CBA	2.58	119.99	111.91
22	3	302	CLA	CHD-C4C-NC	2.57	128.26	124.20
22	6	310	CLA	O2A-CGA-CBA	2.57	119.99	111.91
22	4	306	CLA	CMC-C2C-C1C	2.57	128.96	125.04
22	F	205	CLA	CHD-C4C-NC	2.57	128.26	124.20
22	K	101	CLA	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	307	CLA	O2A-CGA-CBA	2.57	119.97	111.91
22	A	823	CLA	C1-C2-C3	-2.57	121.60	126.04
22	B	826	CLA	CAC-C3C-C4C	2.57	128.14	124.81
22	1	309	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
25	A	862	BCR	C35-C13-C14	-2.57	119.33	122.92
22	F	206	CLA	C2A-C1A-CHA	-2.57	119.37	123.85
22	O	205	CLA	C1-C2-C3	-2.57	122.60	126.75
22	B	807	CLA	C4-C3-C5	2.57	119.59	115.27
29	7	318	5X6	C42-C13-C12	-2.57	114.03	118.08
22	L	203	CLA	C3B-C4B-NB	2.57	112.89	110.52
22	2	304	CLA	CHD-C4C-NC	2.57	128.25	124.20
25	F	207	BCR	C36-C18-C17	-2.56	119.33	122.92
22	5	310	CLA	CMC-C2C-C1C	2.56	128.94	125.04
22	7	311	CLA	C3B-C4B-NB	2.56	112.89	110.52
22	2	303	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	B	819	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
22	A	816	CLA	CMB-C2B-C1B	2.56	129.27	125.37
22	B	808	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
22	4	304	CLA	CBC-CAC-C3C	-2.56	105.38	112.43
22	B	817	CLA	CAA-C2A-C1A	-2.56	103.59	111.97
22	3	301	CLA	CHC-C4B-NB	-2.56	121.55	124.26
22	6	310	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
22	A	832	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
22	3	302	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
22	1	308	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
22	B	816	CLA	CMB-C2B-C3B	2.56	132.78	126.59
25	2	301	BCR	C15-C16-C17	2.55	128.71	123.47
22	1	308	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	3	305	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
25	5	315	BCR	C35-C13-C14	-2.55	119.35	122.92
22	2	304	CLA	C3B-C4B-NB	2.55	112.88	110.52
22	2	308	CLA	CMB-C2B-C1B	2.55	129.26	125.37
22	A	857	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
22	B	818	CLA	CMC-C2C-C1C	2.55	128.93	125.04
22	B	812	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	B	833	CLA	C4-C3-C5	2.55	119.56	115.27
22	5	304	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
22	2	302	CLA	CMC-C2C-C1C	2.55	128.92	125.04
22	4	312	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	6	306	CLA	O2A-CGA-CBA	2.55	119.91	111.91
22	B	831	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
29	6	315	5X6	C38-C30-C31	-2.55	109.63	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	309	CLA	CMB-C2B-C1B	2.55	129.25	125.37
22	B	835	CLA	O2A-CGA-CBA	2.55	119.90	111.91
22	B	827	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	7	307	CLA	C3B-C4B-NB	2.54	112.88	110.52
25	5	315	BCR	C20-C21-C22	2.54	130.94	127.31
22	A	809	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
29	1	313	5X6	C01-C02-C07	-2.54	109.64	114.36
22	O	206	CLA	O2A-CGA-CBA	2.54	119.89	111.91
22	1	302	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
22	F	206	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
22	4	308	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
22	A	814	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
22	B	835	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	O	205	CLA	O2A-CGA-CBA	2.54	119.87	111.91
25	A	846	BCR	C15-C16-C17	2.54	128.67	123.47
29	1	312	5X6	C14-C15-C16	-2.54	115.30	123.22
22	1	305	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	2	304	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
22	2	304	CLA	CMC-C2C-C1C	2.53	128.90	125.04
22	5	307	CLA	C4-C3-C5	2.53	119.53	115.27
22	A	824	CLA	CMB-C2B-C1B	2.53	129.23	125.37
22	1	305	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	A	826	CLA	CHC-C1C-C2C	-2.53	119.70	126.73
22	K	101	CLA	C4-C3-C5	2.53	119.53	115.27
22	1	307	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	2	303	CLA	O2A-CGA-CBA	2.53	119.85	111.91
22	B	805	CLA	O2A-CGA-CBA	2.53	119.85	111.91
22	L	203	CLA	CBA-CAA-C2A	2.53	121.33	113.86
22	5	306	CLA	CMC-C2C-C1C	2.53	128.89	125.04
29	7	318	5X6	C12-C13-C14	-2.53	115.06	118.94
22	A	829	CLA	O2A-CGA-CBA	2.53	119.84	111.91
22	A	809	CLA	CMB-C2B-C1B	2.53	129.22	125.37
22	2	311	CLA	CHB-C1B-C2B	-2.53	120.10	127.24
22	B	807	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
22	5	306	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
22	7	308	CLA	CMC-C2C-C1C	2.53	128.88	125.04
22	6	304	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
22	5	303	CLA	CMC-C2C-C1C	2.52	128.88	125.04
29	1	311	5X6	C36-C34-C29	2.52	114.39	110.30
22	A	814	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
22	A	823	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	5	305	CLA	CMC-C2C-C1C	2.52	128.88	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	304	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
22	A	815	CLA	CHB-C1B-C2B	-2.52	120.11	127.24
22	4	311	CLA	CHD-C4C-NC	2.52	128.18	124.20
22	Z	204	CLA	C7-C6-C5	-2.52	106.51	113.36
22	Z	204	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
22	6	303	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
22	A	839	CLA	C3B-C4B-NB	2.52	112.85	110.52
22	5	307	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
22	6	312	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
29	1	314	5X6	C25-C24-C23	-2.52	115.35	123.22
22	A	839	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	O	204	CLA	CHD-C4C-NC	2.52	128.17	124.20
22	7	313	CLA	CHD-C4C-NC	2.52	128.17	124.20
22	A	820	CLA	CHD-C4C-NC	2.52	128.17	124.20
29	J	104	5X6	C04-C03-C02	-2.52	119.07	122.61
22	A	813	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
22	2	304	CLA	CHB-C1B-C2B	-2.51	120.14	127.24
22	4	302	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	6	313	CLA	CMB-C2B-C3B	2.51	132.68	126.59
22	B	835	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
22	7	313	CLA	CMC-C2C-C1C	2.51	128.87	125.04
22	4	312	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
22	1	310	CLA	CHD-C4C-NC	2.51	128.16	124.20
29	7	318	5X6	C33-C32-C31	-2.51	106.86	110.30
22	A	819	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
22	A	859	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	Z	201	CLA	CHD-C4C-NC	2.51	128.16	124.20
22	1	303	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
22	1	303	CLA	CHB-C1B-C2B	-2.51	120.14	127.24
22	A	839	CLA	O2A-CGA-CBA	2.51	119.79	111.91
22	2	311	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	A	813	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
22	B	832	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
22	B	821	CLA	CHB-C1B-C2B	-2.51	120.15	127.24
22	7	306	CLA	CHB-C1B-C2B	-2.51	120.15	127.24
25	Z	205	BCR	C36-C18-C17	-2.51	119.41	122.92
22	A	818	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	B	832	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	4	308	CLA	CHC-C1C-C2C	-2.50	119.77	126.73
22	A	816	CLA	C1-O2A-CGA	2.50	123.01	116.44
22	1	303	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
22	4	309	CLA	C3B-C4B-NB	2.50	112.84	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	317	RRX	C15-C14-C13	2.50	130.88	127.31
22	7	303	CLA	C2A-C1A-CHA	-2.50	119.48	123.86
22	B	810	CLA	CMB-C2B-C1B	2.50	129.18	125.37
22	3	303	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	A	830	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	I	102	BCR	C15-C16-C17	2.50	128.59	123.47
22	4	311	CLA	CHC-C4B-NB	-2.50	121.61	124.26
22	B	802	CLA	CHC-C1C-C2C	-2.50	119.79	126.73
22	3	304	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	A	819	CLA	CMC-C2C-C1C	2.50	128.84	125.04
22	7	306	CLA	C4-C3-C2	-2.50	117.27	123.68
22	3	303	CLA	CMC-C2C-C1C	2.50	128.84	125.04
22	B	821	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	2	303	CLA	C4-C3-C5	2.50	119.47	115.27
22	6	311	CLA	CMA-C3A-C2A	-2.50	110.27	116.10
23	A	840	A1L64	O4-C4-C3	2.50	133.05	123.64
22	1	306	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	A	813	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
25	A	844	BCR	C2-C1-C6	2.50	114.32	110.48
22	B	820	CLA	CHD-C4C-NC	2.49	128.13	124.20
22	B	849	CLA	C4-C3-C5	2.49	119.47	115.27
22	7	305	CLA	CED-O2D-CGD	2.49	121.58	115.94
22	A	839	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
22	7	309	CLA	CHC-C4B-NB	-2.49	121.62	124.26
22	6	305	CLA	CHD-C4C-NC	2.49	128.13	124.20
22	2	306	CLA	CMC-C2C-C1C	2.49	128.83	125.04
22	6	308	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
22	6	310	CLA	CMB-C2B-C3B	2.49	132.62	126.59
22	2	310	CLA	CHD-C4C-NC	2.49	128.13	124.20
22	B	817	CLA	CHD-C4C-NC	2.49	128.12	124.20
22	B	818	CLA	C1-C2-C3	-2.49	121.74	126.04
22	B	801	CLA	O2A-CGA-CBA	2.49	119.72	111.91
25	L	201	BCR	C35-C13-C14	-2.49	119.44	122.92
25	1	301	BCR	C35-C13-C14	-2.49	119.44	122.92
22	A	826	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
29	5	313	5X6	C12-C13-C14	-2.49	115.12	118.94
22	B	835	CLA	C3B-C4B-NB	2.49	112.82	110.52
22	6	303	CLA	CHD-C4C-NC	2.49	128.12	124.20
22	A	811	CLA	O2A-CGA-CBA	2.49	119.71	111.91
29	6	316	5X6	C38-C30-C31	-2.49	109.75	114.36
22	B	812	CLA	C4-C3-C5	2.49	119.45	115.27
22	7	311	CLA	O2D-CGD-O1D	-2.49	118.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	309	CLA	C3B-C4B-NB	2.49	112.82	110.52
22	B	839	CLA	C16-C15-C13	-2.48	107.89	115.92
22	L	204	CLA	CHD-C4C-NC	2.48	128.12	124.20
22	3	302	CLA	CMC-C2C-C1C	2.48	128.82	125.04
22	L	204	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
22	A	836	CLA	C4A-NA-C1A	-2.48	105.59	106.71
22	A	826	CLA	C4-C3-C5	2.48	119.44	115.27
22	6	304	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	2	303	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
22	A	817	CLA	O2A-CGA-CBA	2.48	119.69	111.91
22	4	310	CLA	CHB-C1B-C2B	-2.48	120.24	127.24
22	3	301	CLA	CHB-C1B-C2B	-2.48	120.24	127.24
22	O	203	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
29	4	315	5X6	C01-C02-C07	-2.48	109.77	114.36
22	A	828	CLA	CMA-C3A-C2A	-2.48	103.84	113.83
22	A	817	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
22	7	313	CLA	C3B-C4B-NB	2.48	112.81	110.52
22	B	807	CLA	O2A-CGA-CBA	2.48	119.68	111.91
22	B	801	CLA	CMC-C2C-C1C	2.48	128.81	125.04
22	A	834	CLA	O2A-CGA-CBA	2.48	119.68	111.91
22	A	834	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
25	A	845	BCR	C27-C26-C25	-2.47	119.14	122.73
22	6	308	CLA	CHD-C4C-NC	2.47	128.10	124.20
22	F	204	CLA	O2A-CGA-CBA	2.47	119.67	111.91
22	B	833	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
22	1	303	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	B	826	CLA	CMC-C2C-C1C	2.47	128.81	125.04
22	7	306	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	Z	204	CLA	CGD-CBD-CAD	-2.47	102.73	110.73
22	2	310	CLA	C3B-C4B-NB	2.47	112.81	110.52
22	7	309	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
22	B	836	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	B	811	CLA	CHD-C4C-NC	2.47	128.09	124.20
22	A	833	CLA	C4-C3-C2	-2.47	117.34	123.68
22	A	824	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	K	101	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
22	B	834	CLA	C4-C3-C5	2.47	118.80	115.98
22	A	804	CLA	OBD-CAD-C3D	-2.47	122.58	128.52
22	7	306	CLA	O2A-CGA-CBA	2.47	119.65	111.91
22	A	858	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	3	305	CLA	C1-C2-C3	-2.47	121.78	126.04
22	2	310	CLA	O2D-CGD-O1D	-2.46	119.02	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	314	CLA	CHB-C1B-C2B	-2.46	120.28	127.24
25	B	841	BCR	C37-C22-C23	2.46	121.96	118.08
22	A	808	CLA	C5-C3-C2	-2.46	116.13	121.12
22	6	305	CLA	CMB-C2B-C3B	2.46	132.55	126.59
22	A	857	CLA	C3B-C4B-NB	2.46	112.80	110.52
22	B	805	CLA	CBA-CAA-C2A	2.46	121.13	113.86
22	B	832	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
23	A	840	A1L64	O4-C4-C5	-2.46	108.23	116.56
22	5	310	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
22	A	822	CLA	CMB-C2B-C1B	2.46	129.12	125.37
22	1	307	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
22	J	102	CLA	CHD-C4C-NC	2.46	128.08	124.20
22	O	203	CLA	O2A-CGA-CBA	2.46	121.96	112.23
25	Z	202	BCR	C16-C15-C14	2.46	128.51	123.47
22	6	310	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	802	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
22	B	811	CLA	CMB-C2B-C1B	2.46	129.11	125.37
22	A	831	CLA	O2A-CGA-CBA	2.46	119.62	111.91
22	4	304	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	J	102	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	4	309	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
22	B	826	CLA	O2A-CGA-CBA	2.46	119.62	111.91
22	4	305	CLA	O2A-CGA-CBA	2.46	119.62	111.91
22	A	859	CLA	CGD-CBD-CAD	-2.46	102.78	110.73
22	B	834	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
22	B	823	CLA	CHC-C1C-C2C	-2.45	119.91	126.73
22	B	801	CLA	C6-C7-C8	-2.45	107.99	115.92
22	B	826	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	L	202	BCR	C7-C8-C9	2.45	129.94	126.23
22	6	314	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	A	814	CLA	CHD-C4C-NC	2.45	128.07	124.20
22	B	815	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	7	303	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	F	206	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
22	A	803	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	805	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
22	A	838	CLA	C4A-NA-C1A	-2.45	105.61	106.71
29	7	314	5X6	C23-C22-C21	-2.45	115.18	118.94
22	1	307	CLA	CBA-CAA-C2A	2.45	121.09	113.86
22	B	850	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
22	B	814	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
25	A	862	BCR	C29-C28-C27	2.44	116.84	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	303	CLA	CHD-C4C-NC	2.44	128.06	124.20
22	6	309	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
22	A	815	CLA	C2A-C3A-C4A	-2.44	97.92	101.87
22	A	857	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
22	5	311	CLA	CMC-C2C-C1C	2.44	128.76	125.04
22	B	838	CLA	CMC-C2C-C1C	2.44	128.76	125.04
22	2	311	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	I	102	BCR	C36-C18-C17	-2.44	119.51	122.92
22	2	304	CLA	CHC-C4B-NB	-2.44	121.67	124.26
22	A	802	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	5	311	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
22	7	305	CLA	CHD-C4C-NC	2.44	128.04	124.20
22	B	824	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	2	311	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	Z	201	CLA	CHB-C1B-C2B	-2.44	120.35	127.24
22	2	308	CLA	CHB-C1B-C2B	-2.44	120.36	127.24
22	A	827	CLA	C4C-C3C-C2C	-2.44	103.35	106.90
22	B	835	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
25	F	201	BCR	C36-C18-C17	-2.44	119.51	122.92
22	A	825	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
22	2	309	CLA	C3B-C4B-NB	2.44	112.77	110.52
22	B	823	CLA	CMA-C3A-C4A	-2.43	105.23	111.77
22	1	310	CLA	CMB-C2B-C3B	2.43	132.48	126.59
22	B	804	CLA	CHD-C4C-NC	2.43	128.04	124.20
22	B	850	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
22	O	203	CLA	CED-O2D-CGD	2.43	121.44	115.94
29	7	318	5X6	C39-C26-C27	-2.43	114.24	118.08
22	1	308	CLA	CHD-C4C-NC	2.43	128.04	124.20
29	7	315	5X6	C39-C26-C27	-2.43	114.25	118.08
22	A	821	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	5	311	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
22	A	809	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	7	304	CLA	CHC-C4B-NB	-2.43	121.68	124.26
22	5	310	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	A	806	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
25	2	301	BCR	C35-C13-C14	-2.43	119.52	122.92
22	7	313	CLA	CHB-C1B-C2B	-2.43	120.38	127.24
22	L	203	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	B	820	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
22	B	805	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	B	810	CLA	C3B-C4B-NB	2.43	112.77	110.52
25	A	861	BCR	C37-C22-C23	2.43	121.90	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	839	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
22	B	828	CLA	C4A-NA-C1A	-2.43	105.61	106.71
22	4	309	CLA	CHB-C1B-C2B	-2.43	120.38	127.24
22	B	817	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
22	A	848	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	B	830	CLA	C1-O2A-CGA	2.43	122.81	116.44
22	B	809	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
22	A	836	CLA	C4-C3-C2	-2.43	117.46	123.68
22	B	819	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
22	A	829	CLA	C1-C2-C3	-2.42	122.83	126.75
22	7	312	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
22	B	826	CLA	CHD-C4C-NC	2.42	128.02	124.20
22	4	303	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	A	802	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
22	A	811	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
22	B	810	CLA	C4-C3-C5	2.42	119.35	115.27
22	5	304	CLA	C4-C3-C2	-2.42	117.46	123.68
22	7	312	CLA	CHB-C1B-C2B	-2.42	120.40	127.24
22	1	303	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
22	5	302	CLA	CMB-C2B-C3B	2.42	132.45	126.59
22	A	819	CLA	CMB-C2B-C3B	2.42	132.45	126.59
22	2	307	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
22	B	838	CLA	C11-C10-C8	-2.42	108.10	115.92
22	4	308	CLA	C1-O2A-CGA	2.42	122.79	116.44
22	7	313	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	3	301	CLA	C1-C2-C3	-2.42	121.86	126.04
22	O	205	CLA	CED-O2D-CGD	2.42	121.40	115.94
22	B	836	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
22	3	303	CLA	C2A-C1A-CHA	-2.42	119.64	123.86
25	A	862	BCR	C16-C15-C14	2.41	128.42	123.47
22	B	817	CLA	CMB-C2B-C1B	2.41	129.05	125.37
22	A	819	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
22	7	311	CLA	C2A-C1A-CHA	-2.41	119.64	123.85
22	B	849	CLA	C1-O2A-CGA	2.41	122.78	116.44
22	B	815	CLA	CHD-C4C-NC	2.41	128.01	124.20
22	B	805	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
22	A	836	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	J	102	CLA	CHC-C1C-NC	2.41	127.86	124.20
22	1	310	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	Z	202	BCR	C15-C16-C17	2.41	128.41	123.47
22	L	203	CLA	O2A-CGA-CBA	2.41	119.47	111.91
22	A	837	CLA	CMB-C2B-C1B	2.41	129.04	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	816	CLA	C7-C6-C5	-2.41	106.81	113.36
22	B	837	CLA	CED-O2D-CGD	2.41	121.39	115.94
29	6	316	5X6	C04-C03-C11	-2.41	108.97	115.78
22	6	314	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	839	CLA	C3B-C4B-NB	2.41	112.75	110.52
29	M	101	5X6	C36-C34-C29	-2.41	106.39	110.30
22	K	101	CLA	CMB-C2B-C3B	2.41	132.42	126.59
22	O	206	CLA	C4-C3-C5	2.41	119.32	115.27
22	7	312	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
22	1	302	CLA	C4-C3-C5	2.41	119.32	115.27
22	B	803	CLA	C4-C3-C5	2.41	119.32	115.27
22	B	829	CLA	C1-O2A-CGA	2.40	122.75	116.44
22	A	837	CLA	CHD-C4C-NC	2.40	127.99	124.20
22	4	302	CLA	CMB-C2B-C3B	2.40	132.41	126.59
31	6	318	RRX	C16-C15-C14	2.40	128.40	123.47
29	O	207	5X6	C32-C31-C30	2.40	116.64	111.85
22	7	306	CLA	CHC-C4B-NB	-2.40	121.71	124.26
22	2	308	CLA	C4-C3-C5	2.40	119.31	115.27
22	5	303	CLA	CHD-C4C-NC	2.40	127.99	124.20
22	2	307	CLA	CHC-C4B-NB	-2.40	121.72	124.26
22	B	809	CLA	C4A-NA-C1A	-2.40	105.63	106.71
22	7	310	CLA	CMC-C2C-C1C	2.40	128.69	125.04
22	7	311	CLA	CHD-C4C-NC	2.40	127.98	124.20
31	4	317	RRX	C36-C18-C17	-2.40	119.56	122.92
22	A	834	CLA	CMB-C2B-C1B	2.40	129.02	125.37
22	4	312	CLA	CHD-C4C-NC	2.40	127.98	124.20
22	6	314	CLA	C3B-C4B-NB	2.40	112.74	110.52
22	O	203	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
22	B	811	CLA	CHC-C1C-NC	2.40	127.84	124.20
22	A	813	CLA	CHD-C4C-NC	2.40	127.98	124.20
25	F	201	BCR	C15-C14-C13	2.40	130.73	127.31
22	B	810	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
29	5	321	5X6	C40-C22-C23	-2.40	114.30	118.08
22	6	313	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	2	311	CLA	CHC-C4B-NB	-2.39	121.72	124.26
22	A	808	CLA	CHB-C1B-C2B	-2.39	120.47	127.24
25	L	202	BCR	C15-C16-C17	2.39	128.38	123.47
29	4	314	5X6	C12-C13-C14	-2.39	115.27	118.94
22	F	204	CLA	CMB-C2B-C1B	2.39	129.01	125.37
22	J	102	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
22	2	307	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
22	B	837	CLA	O2A-CGA-O1A	-2.39	117.56	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	306	CLA	CHD-C4C-NC	2.39	127.97	124.20
22	B	833	CLA	CHB-C1B-C2B	-2.39	120.48	127.24
22	K	102	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
25	J	103	BCR	C24-C23-C22	2.39	129.85	126.23
22	J	102	CLA	C3B-C4B-NB	2.39	112.73	110.52
22	2	306	CLA	CHB-C1B-C2B	-2.39	120.50	127.24
22	A	839	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	5	305	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	A	837	CLA	C4-C3-C5	2.39	119.28	115.27
22	A	824	CLA	C2A-C1A-CHA	-2.39	119.69	123.86
22	J	102	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	A	823	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
22	B	838	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
22	4	308	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	2	304	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
22	A	822	CLA	C3B-C4B-NB	2.38	112.72	110.52
22	B	805	CLA	C11-C10-C8	-2.38	108.22	115.92
22	F	205	CLA	C3B-C4B-NB	2.38	112.72	110.52
22	1	310	CLA	C6-C5-C3	2.38	119.70	113.45
22	4	307	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	6	314	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
22	B	823	CLA	CMA-C3A-C2A	-2.38	104.23	113.83
22	B	804	CLA	O2A-CGA-CBA	2.38	119.37	111.91
22	2	309	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
22	3	304	CLA	C3B-C4B-NB	2.38	112.72	110.52
22	7	313	CLA	CHC-C4B-NB	-2.37	121.74	124.26
22	B	839	CLA	CHD-C4C-NC	2.37	127.94	124.20
22	J	102	CLA	CHB-C1B-C2B	-2.37	120.53	127.24
22	A	825	CLA	C4A-NA-C1A	-2.37	105.64	106.71
22	A	833	CLA	C5-C3-C2	2.37	125.92	121.12
25	2	301	BCR	C36-C18-C17	-2.37	119.60	122.92
22	F	205	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
22	B	817	CLA	C1-O2A-CGA	2.37	122.67	116.44
22	A	828	CLA	C5-C3-C2	-2.37	116.32	121.12
22	4	310	CLA	CMB-C2B-C1B	2.37	128.98	125.37
25	J	103	BCR	C11-C10-C9	2.37	130.69	127.31
22	2	302	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
22	7	307	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	A	859	CLA	CHD-C4C-NC	2.37	127.94	124.20
22	4	309	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
31	6	318	RRX	C36-C18-C17	-2.37	119.61	122.92
25	Z	205	BCR	C10-C11-C12	2.37	130.60	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	303	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	B	815	CLA	C4-C3-C5	2.37	119.25	115.27
22	2	304	CLA	CHC-C1C-NC	2.37	127.79	124.20
22	B	820	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	5	310	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	B	810	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
22	2	303	CLA	CMB-C2B-C3B	2.36	132.31	126.59
22	5	308	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
31	5	322	RRX	C36-C18-C17	-2.36	119.62	122.92
22	4	308	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
22	2	306	CLA	CHC-C4B-NB	-2.36	121.76	124.26
22	7	307	CLA	CHB-C1B-C2B	-2.36	120.58	127.24
22	2	303	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	A	826	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	3	304	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	L	205	CLA	CHB-C1B-C2B	-2.36	120.58	127.24
22	A	808	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
25	A	846	BCR	C19-C18-C17	2.35	122.55	118.94
22	A	848	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
22	5	309	CLA	CHC-C1C-NC	2.35	127.77	124.20
29	7	317	5X6	C41-C17-C16	-2.35	114.37	118.08
22	A	825	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	4	312	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
22	3	304	CLA	CHB-C1B-C2B	-2.35	120.60	127.24
22	A	802	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	6	312	CLA	CMB-C2B-C1B	2.35	128.95	125.37
31	6	318	RRX	C35-C13-C14	-2.35	119.63	122.92
22	B	825	CLA	O2A-CGA-CBA	2.35	119.28	111.91
22	4	306	CLA	CHC-C4B-NB	-2.35	121.77	124.26
22	B	815	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
22	B	831	CLA	CMB-C2B-C3B	2.35	132.27	126.59
22	2	304	CLA	C5-C3-C2	-2.35	116.37	121.12
22	1	303	CLA	CHC-C1C-NC	2.35	127.76	124.20
22	7	311	CLA	CMA-C3A-C2A	-2.35	110.62	116.10
22	1	303	CLA	C1-C2-C3	-2.35	121.98	126.04
22	B	819	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	J	103	BCR	C37-C22-C21	-2.35	119.64	122.92
22	4	311	CLA	CMC-C2C-C1C	2.35	128.61	125.04
29	6	317	5X6	C32-C31-C30	2.35	116.53	111.85
22	B	839	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	B	811	CLA	CMA-C3A-C2A	-2.34	104.37	113.83
29	2	314	5X6	C12-C13-C14	-2.34	115.34	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	306	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
22	4	304	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
22	4	302	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	B	810	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
22	A	832	CLA	CHB-C1B-C2B	-2.34	120.62	127.24
22	K	101	CLA	CMC-C2C-C1C	2.34	128.61	125.04
31	5	322	RRX	C35-C13-C14	-2.34	119.64	122.92
22	A	827	CLA	CHD-C4C-NC	2.34	127.89	124.20
25	A	843	BCR	C30-C25-C24	2.34	122.40	115.78
25	Z	202	BCR	C36-C18-C17	-2.34	119.64	122.92
22	A	857	CLA	CHA-C1A-NA	-2.34	121.04	126.40
25	B	841	BCR	C35-C13-C14	-2.34	119.64	122.92
22	7	309	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
22	6	308	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
22	2	310	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
22	6	305	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
22	B	828	CLA	CMA-C3A-C2A	-2.34	104.40	113.83
22	1	305	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	L	204	CLA	CMB-C2B-C1B	2.34	128.93	125.37
22	B	812	CLA	CHB-C1B-C2B	-2.34	120.64	127.24
29	O	208	5X6	C38-C30-C31	-2.34	110.03	114.36
22	K	101	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	Z	204	CLA	C4-C3-C2	-2.34	117.69	123.68
22	3	304	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
28	B	845	DGD	C1D-C2D-C3D	2.34	114.86	110.00
22	O	204	CLA	CMA-C3A-C2A	-2.34	110.65	116.10
22	A	817	CLA	C6-C5-C3	2.34	119.58	113.45
31	5	322	RRX	C16-C15-C14	2.33	128.26	123.47
29	6	316	5X6	C05-C06-C07	-2.33	107.11	110.30
22	2	310	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
22	A	836	CLA	C5-C3-C2	2.33	125.84	121.12
22	4	303	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
22	A	837	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
22	7	308	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
22	2	307	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	J	102	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	B	807	CLA	CHB-C1B-C2B	-2.33	120.65	127.24
22	B	830	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	6	311	CLA	CHD-C4C-NC	2.33	127.88	124.20
22	B	832	CLA	C6-C7-C8	-2.33	108.39	115.92
22	A	810	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
22	A	813	CLA	CAA-C2A-C1A	-2.33	106.99	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	826	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
22	A	809	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
22	F	206	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	A	829	CLA	C5-C3-C4	2.33	119.74	114.60
22	B	835	CLA	C6-C5-C3	2.33	119.56	113.45
22	6	303	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
22	O	205	CLA	C3B-C4B-NB	2.33	112.67	110.52
22	A	834	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
22	A	808	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
22	F	206	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
22	O	205	CLA	CHB-C1B-C2B	-2.32	120.67	127.24
22	A	820	CLA	CAA-C2A-C3A	2.32	119.14	112.78
22	6	309	CLA	CHD-C4C-NC	2.32	127.86	124.20
22	L	203	CLA	CMC-C2C-C1C	2.32	128.58	125.04
21	A	801	CL0	O2A-CGA-CBA	2.32	119.20	111.91
29	1	311	5X6	C09-C04-C03	2.32	114.07	110.30
22	A	826	CLA	CMA-C3A-C2A	-2.32	104.47	113.83
22	2	308	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	A	830	CLA	C1-O2A-CGA	2.32	122.53	116.44
25	L	201	BCR	C16-C17-C18	2.32	130.62	127.31
22	A	818	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	833	CLA	CHD-C4C-NC	2.32	127.86	124.20
22	5	302	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	L	205	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
22	A	858	CLA	C11-C10-C8	-2.32	108.42	115.92
22	5	305	CLA	CHB-C1B-C2B	-2.32	120.69	127.24
22	A	831	CLA	C5-C3-C2	2.32	125.81	121.12
22	5	301	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	A	824	CLA	CMC-C2C-C1C	2.32	128.57	125.04
22	6	310	CLA	CHD-C4C-NC	2.32	127.86	124.20
25	B	841	BCR	C15-C14-C13	2.32	130.62	127.31
22	6	308	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	B	827	CLA	CMA-C3A-C2A	-2.32	104.48	113.83
22	1	302	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
22	B	802	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	835	CLA	C1-C2-C3	-2.32	122.04	126.04
22	A	804	CLA	CHB-C1B-NB	-2.32	121.81	124.26
22	B	814	CLA	C4-C3-C5	2.32	119.17	115.27
22	7	304	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	A	834	CLA	CHB-C1B-C2B	-2.32	120.70	127.24
22	O	206	CLA	CHD-C4C-NC	2.32	127.85	124.20
22	A	802	CLA	CHB-C4A-NA	2.31	127.71	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	804	CLA	CMC-C2C-C1C	2.31	128.56	125.04
22	6	309	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	J	103	BCR	C35-C13-C14	-2.31	119.68	122.92
22	7	311	CLA	CHB-C1B-C2B	-2.31	120.70	127.24
22	B	823	CLA	CHC-C4B-NB	-2.31	121.81	124.26
22	6	313	CLA	CHD-C4C-NC	2.31	127.85	124.20
22	B	823	CLA	CED-O2D-CGD	2.31	121.17	115.94
22	4	306	CLA	CHB-C1B-C2B	-2.31	120.71	127.24
22	5	308	CLA	CHD-C4C-NC	2.31	127.84	124.20
22	K	102	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	3	304	CLA	CHC-C4B-NB	-2.31	121.81	124.26
22	K	101	CLA	C1-C2-C3	-2.31	122.05	126.04
22	B	823	CLA	CHB-C1B-C2B	-2.31	120.72	127.24
22	A	818	CLA	C4-C3-C5	2.31	119.15	115.27
22	B	805	CLA	CMA-C3A-C2A	-2.30	104.53	113.83
22	O	204	CLA	C2A-C1A-CHA	-2.30	119.83	123.85
22	A	802	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
22	A	813	CLA	CMB-C2B-C3B	2.30	132.17	126.59
22	B	838	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	2	309	CLA	C2A-C1A-CHA	-2.30	119.84	123.85
22	A	829	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
22	6	308	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
22	B	816	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	B	830	CLA	O2A-CGA-CBA	2.30	119.12	111.91
22	Z	204	CLA	O2A-CGA-CBA	2.30	119.12	111.91
22	1	308	CLA	CMC-C2C-C1C	2.30	128.54	125.04
22	6	312	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	6	317	5X6	C42-C13-C12	-2.30	114.46	118.08
22	6	313	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	Z	205	BCR	C16-C15-C14	2.30	128.18	123.47
22	A	809	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
22	4	303	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
22	2	311	CLA	CMB-C2B-C1B	2.30	128.87	125.37
22	2	304	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
31	4	317	RRX	C35-C13-C14	-2.30	119.71	122.92
22	L	205	CLA	CHD-C4C-NC	2.30	127.82	124.20
22	A	829	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
22	B	814	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	2	311	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	5	302	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	3	302	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
22	7	305	CLA	CHB-C1B-C2B	-2.29	120.76	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	312	CLA	CHC-C4B-NB	-2.29	121.83	124.26
29	2	314	5X6	C01-C02-C07	-2.29	110.11	114.36
22	B	832	CLA	C4A-NA-C1A	-2.29	105.67	106.71
22	4	308	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	A	813	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	J	102	CLA	CMB-C2B-C1B	2.29	128.86	125.37
29	2	312	5X6	C06-C07-C02	2.29	116.42	111.85
22	B	803	CLA	CHD-C4C-NC	2.29	127.81	124.20
25	Z	202	BCR	C7-C8-C9	2.29	129.70	126.23
29	O	208	5X6	C28-C29-C30	-2.29	115.91	121.46
22	3	305	CLA	C1-O2A-CGA	2.29	122.45	116.44
22	B	807	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
22	B	817	CLA	CHB-C1B-C2B	-2.29	120.77	127.24
22	A	812	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	3	305	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	5	307	CLA	CMB-C2B-C3B	2.29	132.13	126.59
22	7	307	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	F	202	LMT	C3'-C4'-C5'	2.29	116.17	110.93
22	1	304	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	B	849	CLA	CHB-C1B-NB	-2.29	121.83	124.26
28	B	845	DGD	O1G-C1A-C2A	2.29	119.08	111.91
29	B	851	5X6	C34-C29-C30	2.29	125.83	122.61
29	4	315	5X6	C09-C04-C03	2.28	114.00	110.30
22	B	826	CLA	OBD-CAD-C3D	-2.28	123.02	128.52
22	A	814	CLA	O2A-CGA-CBA	2.28	121.37	114.03
22	7	313	CLA	CHB-C4A-NA	2.28	127.67	124.51
22	O	204	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
29	O	208	5X6	C01-C02-C07	-2.28	110.13	114.36
22	B	838	CLA	O2A-CGA-CBA	2.28	119.07	111.91
22	O	203	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
22	A	834	CLA	C3B-C4B-NB	2.28	112.63	110.52
22	B	801	CLA	C11-C10-C8	-2.28	108.55	115.92
22	1	302	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	O	206	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	4	311	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
22	B	835	CLA	CMB-C2B-C3B	2.28	132.10	126.59
22	1	305	CLA	C3B-C4B-NB	2.28	112.63	110.52
22	1	308	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	B	821	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
22	6	310	CLA	C1-O2A-CGA	2.28	122.41	116.44
22	1	307	CLA	CMC-C2C-C1C	2.28	128.50	125.04
25	1	301	BCR	C15-C16-C17	2.27	128.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	303	CLA	C1-C2-C3	-2.27	122.11	126.04
22	1	304	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
22	3	304	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	5	302	CLA	C4-C3-C5	2.27	119.10	115.27
22	A	859	CLA	C5-C3-C2	-2.27	116.52	121.12
22	5	304	CLA	O2A-CGA-CBA	2.27	119.04	111.91
22	6	311	CLA	CMB-C2B-C3B	2.27	132.09	126.59
22	4	307	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
22	B	831	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
22	4	309	CLA	O2A-CGA-CBA	2.27	119.04	111.91
22	7	308	CLA	CHC-C4B-NB	-2.27	121.85	124.26
22	A	829	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
25	4	316	BCR	C19-C18-C17	2.27	122.43	118.94
25	5	315	BCR	C16-C15-C14	2.27	128.13	123.47
22	A	803	CLA	CED-O2D-CGD	2.27	121.07	115.94
25	F	201	BCR	C11-C10-C9	2.27	130.55	127.31
22	5	303	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
22	B	820	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
22	A	808	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	3	304	CLA	CED-O2D-CGD	2.27	121.07	115.94
22	B	822	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
22	6	311	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	1	305	CLA	CHB-C1B-C2B	-2.27	120.84	127.24
22	4	311	CLA	CAA-C2A-C3A	-2.27	106.58	112.78
22	5	310	CLA	CMB-C2B-C3B	2.26	132.07	126.59
22	2	309	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
22	A	822	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
22	6	305	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
22	B	809	CLA	C4-C3-C5	2.26	119.08	115.27
22	A	835	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
22	1	305	CLA	CMB-C2B-C1B	2.26	128.81	125.37
22	B	832	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	1	310	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
22	B	810	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	B	808	CLA	CMA-C3A-C2A	-2.26	104.72	113.83
22	3	303	CLA	CED-O2D-CGD	2.26	121.05	115.94
22	B	806	CLA	O2A-CGA-CBA	2.26	118.99	111.91
22	1	307	CLA	CHD-C4C-NC	2.26	127.76	124.20
22	4	307	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
22	4	302	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
22	4	304	CLA	CHD-C4C-NC	2.26	127.76	124.20
22	5	305	CLA	CHC-C4B-NB	-2.25	121.87	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	838	CLA	OBD-CAD-C3D	-2.25	123.09	128.52
22	A	822	CLA	CHB-C4A-NA	2.25	127.63	124.51
22	6	305	CLA	CHB-C4A-NA	2.25	127.63	124.51
22	B	830	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
22	A	821	CLA	CMB-C2B-C1B	2.25	128.80	125.37
22	B	808	CLA	CHD-C4C-NC	2.25	127.75	124.20
22	4	310	CLA	CAA-C2A-C1A	2.25	117.13	112.14
22	K	102	CLA	CHD-C4C-NC	2.25	127.75	124.20
22	1	309	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
22	5	311	CLA	CHD-C4C-NC	2.25	127.75	124.20
22	A	827	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
22	A	857	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	A	833	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
22	6	310	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	A	824	CLA	O2A-CGA-CBA	2.25	118.96	111.91
29	6	317	5X6	C33-C32-C31	2.25	113.38	110.30
22	5	302	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
22	2	302	CLA	CHB-C1B-C2B	-2.25	120.89	127.24
22	A	818	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
22	B	832	CLA	CAA-CBA-CGA	-2.25	106.69	113.25
22	A	823	CLA	C4A-NA-C1A	-2.25	105.70	106.71
22	2	305	CLA	CHB-C1B-C2B	-2.25	120.89	127.24
22	F	204	CLA	C1-C2-C3	-2.25	122.16	126.04
22	A	811	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	3	303	CLA	CHB-C1B-C2B	-2.25	120.89	127.24
22	B	834	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
22	7	310	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
22	A	835	CLA	C4A-NA-C1A	-2.24	105.70	106.71
22	6	311	CLA	C2A-C1A-CHA	-2.24	119.94	123.85
22	B	803	CLA	C1-O2A-CGA	2.24	122.33	116.44
22	2	311	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
22	5	308	CLA	CHC-C1C-NC	2.24	127.60	124.20
22	5	301	CLA	CHB-C1B-C2B	-2.24	120.91	127.24
22	L	204	CLA	C4-C3-C5	2.24	119.04	115.27
22	A	814	CLA	CHC-C1C-NC	2.24	127.60	124.20
22	5	301	CLA	O2A-CGA-CBA	2.24	121.23	114.03
22	A	822	CLA	C4-C3-C5	2.24	119.04	115.27
29	Z	206	5X6	C28-C29-C30	-2.24	116.04	121.46
22	7	311	CLA	CMC-C2C-C1C	2.24	128.45	125.04
22	7	310	CLA	CMA-C3A-C2A	-2.24	110.87	116.10
22	A	829	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
25	B	842	BCR	C36-C18-C17	-2.24	119.79	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	848	CLA	C4-C3-C5	2.24	119.03	115.27
22	B	818	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
22	O	205	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	7	303	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
22	4	312	CLA	C3B-C4B-NB	2.24	112.59	110.52
22	A	806	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
22	6	307	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
22	A	819	CLA	CHB-C1B-C2B	-2.23	120.93	127.24
22	Z	201	CLA	C3B-C4B-NB	2.23	112.59	110.52
29	2	312	5X6	C25-C24-C23	-2.23	116.25	123.22
22	1	302	CLA	CHC-C1C-NC	2.23	127.59	124.20
29	2	312	5X6	C41-C17-C16	-2.23	114.56	118.08
22	B	812	CLA	CMB-C2B-C1B	2.23	128.77	125.37
22	F	204	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
22	A	803	CLA	CHD-C4C-NC	2.23	127.72	124.20
22	A	803	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
22	O	205	CLA	C5-C3-C4	2.23	119.53	114.60
22	B	826	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
22	A	859	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
22	A	818	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
22	B	805	CLA	C5-C3-C2	-2.23	116.61	121.12
22	B	810	CLA	CED-O2D-CGD	2.23	120.97	115.94
22	1	309	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
22	2	305	CLA	CHD-C4C-NC	2.23	127.71	124.20
22	B	804	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
22	2	308	CLA	CHC-C4B-NB	-2.22	121.90	124.26
25	L	206	BCR	C12-C13-C14	2.22	122.35	118.94
22	7	308	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	3	304	CLA	CMB-C2B-C1B	2.22	128.75	125.37
29	B	851	5X6	C35-C34-C29	2.22	113.90	110.30
22	B	816	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
22	O	204	CLA	C3B-C4B-NB	2.22	112.57	110.52
22	2	302	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	A	820	CLA	O2A-CGA-CBA	2.22	118.87	111.91
22	K	102	CLA	CHB-C4A-NA	2.22	127.58	124.51
31	6	318	RRX	C2-C1-C6	2.22	113.90	110.48
22	B	829	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	3	303	CLA	CHD-C4C-NC	2.22	127.70	124.20
22	A	835	CLA	CBA-CAA-C2A	-2.22	107.32	113.86
21	A	801	CL0	CHD-C4C-NC	2.22	127.70	124.20
22	B	849	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
22	2	307	CLA	C3B-C4B-NB	2.22	112.57	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	812	CLA	CHD-C4C-NC	2.21	127.69	124.20
22	A	807	CLA	O2A-C1-C2	2.21	114.45	108.64
22	A	838	CLA	CHD-C4C-NC	2.21	127.69	124.20
22	7	305	CLA	CHB-C4A-NA	2.21	127.57	124.51
22	B	824	CLA	C1-C2-C3	-2.21	122.22	126.04
22	B	835	CLA	CHD-C4C-NC	2.21	127.69	124.20
22	O	205	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
31	1	315	RRX	C37-C22-C23	2.21	121.56	118.08
29	1	313	5X6	C38-C30-C31	-2.21	110.26	114.36
22	O	203	CLA	CHB-C4A-NA	2.21	127.57	124.51
31	6	318	RRX	C15-C14-C13	2.21	130.47	127.31
22	B	806	CLA	OBD-CAD-C3D	-2.21	123.20	128.52
22	1	303	CLA	CHC-C4B-NB	-2.21	121.92	124.26
22	A	835	CLA	CHD-C4C-NC	2.21	127.68	124.20
22	B	831	CLA	C4-C3-C5	2.21	118.98	115.27
25	B	844	BCR	C20-C21-C22	2.21	130.46	127.31
22	A	859	CLA	C1-C2-C3	-2.21	122.23	126.04
22	7	308	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	O	206	CLA	CMC-C2C-C1C	2.21	128.40	125.04
22	A	817	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
22	B	833	CLA	CHD-C4C-NC	2.21	127.68	124.20
22	7	310	CLA	C2A-C1A-CHA	-2.21	120.00	123.85
22	6	305	CLA	C1-O2A-CGA	2.20	122.23	116.44
22	3	303	CLA	CHC-C1C-NC	2.20	127.55	124.20
22	A	858	CLA	CMB-C2B-C3B	2.20	131.93	126.59
22	1	304	CLA	CED-O2D-CGD	2.20	120.92	115.94
22	B	813	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
22	B	828	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
22	A	822	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
22	B	837	CLA	C11-C10-C8	-2.20	108.80	115.92
29	4	314	5X6	C41-C17-C16	-2.20	114.61	118.08
22	A	802	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
22	O	205	CLA	C1-O2A-CGA	2.20	122.22	116.44
22	5	308	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	A	819	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	B	808	CLA	C4-C3-C5	2.20	118.97	115.27
22	A	838	CLA	CMB-C2B-C1B	2.20	128.72	125.37
22	A	827	CLA	C1-C2-C3	-2.20	122.24	126.04
22	A	828	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
22	2	308	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
25	A	844	BCR	C30-C25-C24	2.20	121.99	115.78
22	B	805	CLA	CAA-C2A-C1A	-2.19	104.79	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	821	CLA	CHC-C4B-NB	-2.19	121.94	124.26
22	B	803	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
22	1	303	CLA	O2A-CGA-CBA	2.19	118.79	111.91
22	B	824	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
22	A	830	CLA	CHD-C4C-NC	2.19	127.66	124.20
22	2	304	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	A	836	CLA	CHD-C4C-NC	2.19	127.65	124.20
22	5	309	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
22	6	307	CLA	CHC-C1C-NC	2.19	127.52	124.20
22	2	306	CLA	CHC-C1C-NC	2.19	127.52	124.20
22	1	305	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
22	B	818	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
22	B	808	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
22	7	307	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
22	A	834	CLA	CHC-C1C-NC	2.19	127.52	124.20
25	A	846	BCR	C35-C13-C14	-2.19	119.86	122.92
22	1	309	CLA	CHB-C4A-NA	2.19	127.53	124.51
22	5	301	CLA	CHD-C4C-NC	2.19	127.65	124.20
22	6	313	CLA	O2A-CGA-CBA	2.19	121.05	114.03
21	A	801	CL0	CMB-C2B-C1B	2.18	128.70	125.37
29	7	315	5X6	C04-C03-C02	-2.18	119.54	122.61
22	B	806	CLA	C4A-NA-C1A	-2.18	105.72	106.71
22	5	308	CLA	CMC-C2C-C1C	2.18	128.36	125.04
29	5	321	5X6	C06-C07-C02	2.18	116.20	111.85
22	1	304	CLA	CHD-C4C-NC	2.18	127.64	124.20
22	7	307	CLA	CHD-C4C-NC	2.18	127.64	124.20
22	B	810	CLA	O2A-CGA-CBA	2.18	118.76	111.91
22	3	301	CLA	C1-O2A-CGA	2.18	122.17	116.44
22	6	303	CLA	CHB-C1B-C2B	-2.18	121.07	127.24
22	B	828	CLA	CHD-C4C-NC	2.18	127.64	124.20
29	7	318	5X6	C38-C30-C31	-2.18	110.31	114.36
22	A	832	CLA	O2A-CGA-CBA	2.18	118.75	111.91
22	Z	201	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	A	814	CLA	C3B-C4B-NB	2.18	112.54	110.52
22	6	308	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	B	816	CLA	CHB-C1B-C2B	-2.18	121.08	127.24
22	B	831	CLA	CHD-C4C-NC	2.18	127.64	124.20
25	L	201	BCR	C30-C25-C24	2.18	121.94	115.78
22	F	204	CLA	CED-O2D-CGD	2.18	120.87	115.94
25	I	102	BCR	C35-C13-C14	-2.18	119.87	122.92
22	A	805	CLA	CHD-C4C-NC	2.18	127.64	124.20
22	4	312	CLA	CAA-C2A-C3A	-2.18	106.81	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	845	BCR	C36-C18-C17	-2.18	119.87	122.92
22	6	305	CLA	C1-C2-C3	-2.18	122.28	126.04
22	6	307	CLA	CHB-C1B-C2B	-2.18	121.08	127.24
22	A	858	CLA	CHD-C4C-NC	2.18	127.64	124.20
22	1	310	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	B	804	CLA	C6-C7-C8	-2.18	108.88	115.92
29	6	315	5X6	C41-C17-C16	-2.18	114.65	118.08
22	B	807	CLA	CHD-C4C-NC	2.18	127.64	124.20
22	A	832	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
22	2	306	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	7	311	CLA	CAA-C2A-C3A	-2.18	111.02	116.10
22	F	206	CLA	CMB-C2B-C1B	2.18	128.69	125.37
22	5	308	CLA	C2A-C1A-CHA	-2.18	120.05	123.85
22	A	820	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
22	B	806	CLA	CMC-C2C-C1C	2.18	128.35	125.04
22	O	204	CLA	CHC-C4B-NB	-2.18	121.95	124.26
22	A	829	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
22	4	306	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	F	205	CLA	CHC-C1C-NC	2.17	127.50	124.20
22	5	309	CLA	CMB-C2B-C1B	2.17	128.68	125.37
22	B	820	CLA	O2A-CGA-CBA	2.17	121.01	114.03
22	B	849	CLA	CHD-C4C-NC	2.17	127.63	124.20
22	L	203	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	B	806	CLA	O2D-CGD-CBD	2.17	115.13	111.27
22	6	313	CLA	CHB-C1B-C2B	-2.17	121.10	127.24
30	F	202	LMT	C2'-C3'-C4'	2.17	114.64	109.68
22	B	802	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
22	B	850	CLA	C4C-C3C-C2C	-2.17	103.74	106.90
22	A	808	CLA	CHB-C4A-NA	2.17	127.51	124.51
22	B	850	CLA	CHB-C4A-NA	2.17	127.51	124.51
22	B	805	CLA	CMB-C2B-C3B	2.17	131.84	126.59
22	A	820	CLA	CBA-CAA-C2A	2.17	120.26	113.86
22	6	306	CLA	CMB-C2B-C1B	2.17	128.67	125.37
22	2	302	CLA	CHC-C4B-NB	-2.17	121.96	124.26
22	5	305	CLA	CHC-C1C-NC	2.17	127.49	124.20
29	5	313	5X6	C40-C22-C23	-2.17	114.67	118.08
22	A	807	CLA	CHB-C1B-NB	-2.16	121.97	124.26
22	3	303	CLA	CHC-C4B-NB	-2.16	121.97	124.26
22	A	804	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
29	7	315	5X6	C33-C32-C31	-2.16	107.34	110.30
22	A	820	CLA	C1-O2A-CGA	2.16	122.12	116.44
22	B	827	CLA	CHD-C4C-NC	2.16	127.61	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	321	5X6	C35-C34-C29	2.16	113.81	110.30
22	B	819	CLA	CMC-C2C-C1C	2.16	128.33	125.04
22	3	302	CLA	CMB-C2B-C3B	2.16	131.82	126.59
22	B	802	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	B	811	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
22	6	314	CLA	CHD-C4C-NC	2.16	127.61	124.20
22	4	309	CLA	CMB-C2B-C1B	2.16	128.66	125.37
22	7	309	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	806	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
22	L	204	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
29	1	314	5X6	C14-C15-C16	-2.16	116.48	123.22
22	A	802	CLA	O2A-CGA-CBA	2.16	118.68	111.91
22	4	303	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
22	A	836	CLA	CMB-C2B-C1B	2.16	128.66	125.37
22	F	204	CLA	C3B-C4B-NB	2.16	112.52	110.52
22	4	312	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
22	A	838	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
22	B	814	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
22	4	312	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
25	I	102	BCR	C16-C15-C14	2.15	127.89	123.47
21	A	801	CL0	O2A-C1-C2	-2.15	102.98	108.64
25	Z	205	BCR	C20-C21-C22	2.15	130.38	127.31
22	B	810	CLA	CHD-C4C-NC	2.15	127.59	124.20
22	4	312	CLA	CHC-C1C-NC	2.15	127.47	124.20
22	A	832	CLA	CED-O2D-CGD	2.15	120.80	115.94
22	1	310	CLA	CHB-C4A-NA	2.15	127.48	124.51
22	B	804	CLA	CMB-C2B-C1B	2.15	128.64	125.37
22	A	806	CLA	C4-C3-C5	2.15	118.89	115.27
22	7	304	CLA	C1-O2A-CGA	2.15	122.08	116.44
29	4	314	5X6	C39-C26-C27	-2.15	114.69	118.08
22	3	305	CLA	CED-O2D-CGD	2.15	120.80	115.94
22	B	816	CLA	C6-C5-C3	2.15	119.09	113.45
22	A	848	CLA	CMC-C2C-C1C	2.15	128.31	125.04
22	4	307	CLA	CHD-C4C-NC	2.15	127.59	124.20
22	5	311	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
25	B	841	BCR	C1-C6-C7	2.15	121.85	115.78
22	B	805	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	7	312	CLA	C3B-C4B-NB	2.15	112.51	110.52
29	7	317	5X6	C01-C02-C07	-2.15	110.38	114.36
22	4	306	CLA	CHD-C4C-NC	2.15	127.58	124.20
22	B	818	CLA	C7-C6-C5	-2.15	107.53	113.36
22	1	310	CLA	O1D-CGD-CBD	-2.15	120.09	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	311	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
22	K	102	CLA	CMB-C2B-C1B	2.14	128.63	125.37
22	A	805	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
22	A	858	CLA	C6-C7-C8	-2.14	108.99	115.92
22	B	819	CLA	CHC-C4B-NB	-2.14	121.99	124.26
22	B	811	CLA	CHB-C4A-NA	2.14	127.48	124.51
22	O	204	CLA	CHB-C4A-NA	2.14	127.48	124.51
22	5	305	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
22	B	850	CLA	CED-O2D-CGD	2.14	120.79	115.94
22	4	311	CLA	CMB-C2B-C1B	2.14	128.63	125.37
29	O	207	5X6	C10-C04-C03	2.14	113.78	110.30
22	4	306	CLA	CHC-C1C-NC	2.14	127.45	124.20
22	B	819	CLA	CHD-C4C-NC	2.14	127.58	124.20
22	B	815	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
22	A	820	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
25	A	844	BCR	C4-C5-C6	-2.14	119.62	122.73
22	5	307	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
22	1	304	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
22	1	309	CLA	CHC-C4B-NB	-2.14	121.99	124.26
22	6	307	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
31	6	318	RRX	C11-C10-C9	2.14	130.36	127.31
22	B	809	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
22	7	309	CLA	CHC-C1C-NC	2.14	127.45	124.20
22	6	307	CLA	CMB-C2B-C1B	2.14	128.62	125.37
22	F	205	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
22	A	839	CLA	CHD-C4C-NC	2.14	127.57	124.20
22	B	818	CLA	CMB-C2B-C3B	2.14	131.76	126.59
22	B	826	CLA	C1-C2-C3	-2.14	122.35	126.04
22	7	310	CLA	CHC-C4B-NB	-2.13	122.00	124.26
22	O	205	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
22	4	306	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
22	A	858	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
22	B	823	CLA	CHD-C4C-NC	2.13	127.57	124.20
22	3	301	CLA	C4-C3-C5	2.13	118.86	115.27
22	B	818	CLA	CHB-C4A-NA	2.13	127.46	124.51
22	7	303	CLA	CHC-C1C-NC	2.13	127.44	124.20
22	7	313	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
25	B	844	BCR	C10-C11-C12	2.13	129.87	123.22
22	6	305	CLA	CED-O2D-CGD	2.13	120.76	115.94
22	2	310	CLA	CHC-C1C-NC	2.13	127.44	124.20
22	B	834	CLA	CHD-C4C-NC	2.13	127.56	124.20
22	6	305	CLA	C4-C3-C5	2.13	118.86	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	813	CLA	O2A-CGA-CBA	2.13	118.59	111.91
22	5	307	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	A	845	BCR	C15-C16-C17	2.13	127.83	123.47
22	A	831	CLA	CHD-C4C-NC	2.13	127.56	124.20
22	2	302	CLA	CHD-C4C-NC	2.13	127.56	124.20
29	4	314	5X6	C14-C15-C16	-2.13	116.58	123.22
22	7	307	CLA	CED-O2D-CGD	2.13	120.75	115.94
22	6	308	CLA	O2A-CGA-CBA	2.13	120.86	114.03
22	6	304	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
22	A	807	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	F	205	CLA	CED-O2D-CGD	2.13	120.74	115.94
22	L	204	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	A	802	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
22	A	806	CLA	CMA-C3A-C2A	-2.12	105.26	113.83
22	4	304	CLA	CMB-C2B-C3B	2.12	131.73	126.59
22	B	825	CLA	CHD-C4C-NC	2.12	127.55	124.20
22	A	837	CLA	C3B-C4B-NB	2.12	112.48	110.52
22	6	309	CLA	CED-O2D-CGD	2.12	120.74	115.94
22	5	304	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	L	205	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	4	303	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
29	Z	206	5X6	C40-C22-C21	-2.12	119.95	122.92
22	A	812	CLA	O2A-CGA-CBA	2.12	118.56	111.91
22	B	803	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
22	L	203	CLA	CED-O2D-CGD	2.12	120.73	115.94
22	4	310	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
22	2	309	CLA	CED-O2D-CGD	2.12	120.73	115.94
22	4	311	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	J	102	CLA	CAA-C2A-C3A	-2.12	108.97	114.26
22	B	816	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	B	817	CLA	C1-C2-C3	-2.12	122.38	126.04
22	A	859	CLA	CAA-CBA-CGA	-2.12	107.07	113.25
22	6	312	CLA	CHB-C1B-C2B	-2.12	121.26	127.24
22	2	302	CLA	CHC-C1C-NC	2.12	127.41	124.20
22	1	307	CLA	C5-C3-C2	-2.12	116.83	121.12
22	4	305	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	7	311	CLA	CHC-C4B-NB	-2.12	122.02	124.26
22	B	822	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	A	819	CLA	CHD-C4C-NC	2.12	127.54	124.20
22	B	830	CLA	CHD-C4C-NC	2.12	127.54	124.20
22	B	831	CLA	CBA-CAA-C2A	2.12	120.11	113.86
22	B	801	CLA	O2A-CGA-O1A	-2.12	118.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	809	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
22	A	825	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
29	5	313	5X6	C38-C30-C31	-2.11	110.44	114.36
22	4	302	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	A	831	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
22	6	310	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
31	1	315	RRX	C1-C6-C7	2.11	121.75	115.78
29	6	317	5X6	C11-C03-C02	-2.11	116.35	121.46
22	B	839	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	B	826	CLA	CMB-C2B-C3B	2.11	131.70	126.59
22	A	824	CLA	CHD-C4C-NC	2.11	127.53	124.20
22	5	307	CLA	C1-C2-C3	-2.11	122.39	126.04
22	B	849	CLA	CAA-C2A-C1A	-2.11	105.06	111.97
22	B	803	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
22	B	828	CLA	CMB-C2B-C3B	2.11	131.69	126.59
29	6	316	5X6	C33-C32-C31	-2.11	107.42	110.30
22	O	206	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
22	A	804	CLA	C1-C2-C3	-2.11	122.40	126.04
22	4	304	CLA	CHB-C1B-C2B	-2.11	121.29	127.24
29	5	313	5X6	C41-C17-C16	-2.11	114.76	118.08
22	B	815	CLA	C1-C2-C3	-2.11	122.40	126.04
22	1	306	CLA	CMA-C3A-C2A	-2.11	105.34	113.83
22	7	313	CLA	CHC-C1C-NC	2.10	127.40	124.20
22	6	306	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	2	310	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	5	301	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	7	313	CLA	CED-O2D-CGD	2.10	120.69	115.94
22	7	306	CLA	C3B-C4B-NB	2.10	112.46	110.52
22	A	836	CLA	CHB-C1B-NB	-2.10	122.03	124.26
22	6	314	CLA	CHC-C4B-NB	-2.10	122.03	124.26
25	2	301	BCR	C37-C22-C23	2.10	121.39	118.08
22	1	303	CLA	C16-C15-C13	-2.10	109.13	115.92
29	4	315	5X6	C40-C22-C23	-2.10	114.77	118.08
22	2	306	CLA	CED-O2D-CGD	2.10	120.69	115.94
22	A	824	CLA	CAA-C2A-C1A	-2.10	105.09	111.97
22	1	302	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
22	6	312	CLA	CMC-C2C-C1C	2.10	128.24	125.04
29	3	306	5X6	C28-C29-C30	-2.10	116.38	121.46
22	2	310	CLA	CHC-C4B-NB	-2.10	122.03	124.26
22	4	306	CLA	CAA-C2A-C1A	2.10	118.85	111.97
22	B	838	CLA	C1-C2-C3	-2.10	122.42	126.04
22	A	825	CLA	C1-C2-C3	-2.10	122.42	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	820	CLA	CMB-C2B-C3B	2.10	131.67	126.59
21	A	801	CL0	C4-C3-C5	2.10	118.80	115.27
22	B	820	CLA	CMB-C2B-C1B	2.10	128.56	125.37
22	7	310	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	B	823	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
21	A	801	CL0	CHB-C1B-NB	-2.10	122.04	124.26
22	A	804	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
22	B	833	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
22	B	836	CLA	CHB-C1B-NB	-2.09	122.04	124.26
22	A	848	CLA	CMA-C3A-C2A	-2.09	105.38	113.83
22	F	204	CLA	CHB-C1B-C2B	-2.09	121.32	127.24
29	1	313	5X6	C10-C04-C03	2.09	113.69	110.30
29	5	321	5X6	C34-C29-C30	-2.09	119.67	122.61
22	5	310	CLA	CHD-C4C-NC	2.09	127.50	124.20
22	F	206	CLA	C3B-C4B-NB	2.09	112.46	110.52
31	6	318	RRX	C16-C17-C18	2.09	130.30	127.31
22	A	827	CLA	CHB-C4A-NA	2.09	127.41	124.51
22	A	832	CLA	CMC-C2C-C1C	2.09	128.22	125.04
22	5	309	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
22	B	803	CLA	CMB-C2B-C1B	2.09	128.56	125.37
22	2	305	CLA	CHB-C4A-NA	2.09	127.40	124.51
22	B	829	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
22	A	804	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
22	O	203	CLA	CMB-C2B-C3B	2.09	131.65	126.59
22	A	835	CLA	CMB-C2B-C3B	2.09	131.64	126.59
22	6	303	CLA	CHB-C4A-NA	2.09	127.40	124.51
22	K	101	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
29	B	851	5X6	C36-C34-C29	-2.09	106.92	110.30
22	B	824	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	A	857	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
22	1	303	CLA	C1-O2A-CGA	2.09	121.92	116.44
22	1	310	CLA	C7-C6-C5	-2.09	107.69	113.36
25	B	843	BCR	C36-C18-C17	-2.09	120.00	122.92
22	J	102	CLA	CED-O2D-CGD	2.09	120.65	115.94
22	A	818	CLA	CMB-C2B-C1B	2.08	128.54	125.37
22	A	816	CLA	CBA-CAA-C2A	2.08	120.02	113.86
22	6	308	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
22	6	308	CLA	CED-O2D-CGD	2.08	120.65	115.94
22	A	857	CLA	O2A-CGA-CBA	2.08	118.44	111.91
22	5	311	CLA	CMB-C2B-C3B	2.08	131.63	126.59
22	A	826	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	A	846	BCR	C16-C15-C14	2.08	127.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	308	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
22	A	815	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
22	5	303	CLA	OBD-CAD-C3D	-2.08	123.51	128.52
22	7	303	CLA	CHD-C4C-NC	2.08	127.48	124.20
22	A	814	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
22	5	307	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
22	Z	204	CLA	C6-C5-C3	2.08	118.90	113.45
22	B	828	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
25	B	843	BCR	C16-C17-C18	2.08	130.28	127.31
22	2	311	CLA	O2A-CGA-CBA	2.08	120.70	114.03
22	1	306	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
22	B	820	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
22	7	307	CLA	CHC-C1C-NC	2.08	127.35	124.20
25	A	845	BCR	C35-C13-C14	-2.08	120.02	122.92
22	K	102	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
22	2	305	CLA	C4-C3-C5	2.07	118.76	115.27
22	A	829	CLA	CMA-C3A-C2A	-2.07	105.47	113.83
22	B	832	CLA	C3B-C4B-NB	2.07	112.44	110.52
29	1	316	5X6	C40-C22-C23	-2.07	114.81	118.08
22	1	308	CLA	CHC-C1C-NC	2.07	127.35	124.20
22	1	307	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
22	5	303	CLA	C6-C5-C3	2.07	118.89	113.45
22	B	803	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
25	A	861	BCR	C12-C13-C14	2.07	122.11	118.94
22	6	307	CLA	CHD-C4C-NC	2.07	127.46	124.20
22	A	832	CLA	C11-C12-C13	-2.07	109.24	115.92
25	B	842	BCR	C16-C17-C18	2.07	130.26	127.31
22	B	815	CLA	CMA-C3A-C2A	-2.07	105.49	113.83
22	1	306	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	1	309	CLA	CMC-C2C-C1C	2.07	128.19	125.04
22	6	309	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
22	A	810	CLA	OBD-CAD-C3D	-2.06	123.55	128.52
22	7	309	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
22	B	827	CLA	O2A-CGA-CBA	2.06	118.38	111.91
22	6	311	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
25	A	862	BCR	C16-C17-C18	2.06	130.25	127.31
22	A	808	CLA	C1-O2A-CGA	2.06	121.85	116.44
25	A	862	BCR	C29-C30-C25	2.06	113.65	110.48
22	4	307	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
22	4	303	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	4	310	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	A	844	BCR	C12-C13-C14	2.06	122.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	305	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
22	B	834	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	3	305	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
22	B	817	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
22	B	816	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
22	1	303	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
22	1	302	CLA	O2A-CGA-CBA	2.05	118.36	111.91
22	A	831	CLA	CGD-CBD-CAD	-2.05	104.08	110.73
22	2	305	CLA	O2A-CGA-CBA	2.05	118.35	111.91
25	J	103	BCR	C15-C14-C13	2.05	130.24	127.31
22	B	838	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
22	L	203	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
22	2	303	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
25	5	315	BCR	C15-C14-C13	2.05	130.24	127.31
22	A	807	CLA	C4-C3-C5	2.05	118.72	115.27
22	6	308	CLA	C3B-C4B-NB	2.05	112.42	110.52
22	7	306	CLA	CHC-C1C-NC	2.05	127.31	124.20
22	B	815	CLA	CMB-C2B-C3B	2.05	131.55	126.59
22	5	303	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
25	B	844	BCR	C19-C18-C17	2.05	122.09	118.94
22	B	812	CLA	CHB-C4A-NA	2.05	127.35	124.51
22	2	308	CLA	CED-O2D-CGD	2.05	120.57	115.94
21	A	801	CL0	C2A-C1A-CHA	-2.05	120.28	123.86
22	B	833	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	836	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
22	A	839	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
22	3	301	CLA	CMB-C2B-C1B	2.05	128.49	125.37
22	1	304	CLA	CHB-C1B-C2B	-2.05	121.45	127.24
22	5	305	CLA	CHB-C4A-NA	2.05	127.34	124.51
22	A	818	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
25	Z	202	BCR	C35-C13-C14	-2.05	120.06	122.92
22	1	309	CLA	CHC-C1C-NC	2.05	127.31	124.20
22	A	848	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	B	813	CLA	CHA-C1A-NA	-2.04	121.72	126.40
22	A	828	CLA	CMC-C2C-C1C	2.04	128.15	125.04
22	A	823	CLA	CHA-C1A-NA	-2.04	121.72	126.40
22	2	305	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	1	301	BCR	C16-C17-C18	2.04	130.22	127.31
22	A	859	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	4	304	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	6	308	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	5	306	CLA	CHD-C4C-NC	2.04	127.42	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	322	RRX	C15-C14-C13	2.04	130.22	127.31
22	4	309	CLA	CHC-C4B-NB	-2.04	122.10	124.26
22	B	808	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
22	B	819	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	4	306	CLA	CED-O2D-CGD	2.04	120.55	115.94
22	B	835	CLA	CMC-C2C-C1C	2.04	128.14	125.04
22	A	830	CLA	OBD-CAD-C3D	-2.04	123.62	128.52
22	B	819	CLA	CHC-C1C-NC	2.04	127.29	124.20
22	6	305	CLA	O2A-CGA-CBA	2.04	118.30	111.91
22	2	304	CLA	CED-O2D-CGD	2.04	120.55	115.94
22	B	850	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
22	A	848	CLA	CED-O2D-CGD	2.04	120.54	115.94
22	A	824	CLA	CMA-C3A-C2A	-2.04	105.62	113.83
22	O	206	CLA	CHB-C1B-C2B	-2.04	121.49	127.24
22	A	811	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
25	B	844	BCR	C15-C14-C13	2.03	130.21	127.31
22	3	302	CLA	CHB-C1B-C2B	-2.03	121.49	127.24
22	5	311	CLA	CHB-C1B-C2B	-2.03	121.49	127.24
29	5	312	5X6	C04-C03-C11	-2.03	110.02	115.78
22	A	809	CLA	CHB-C4A-NA	2.03	127.33	124.51
22	A	827	CLA	CMB-C2B-C3B	2.03	131.51	126.59
22	B	839	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	B	850	CLA	CMB-C2B-C1B	2.03	128.47	125.37
22	L	203	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
22	A	826	CLA	CHB-C4A-NA	2.03	127.32	124.51
22	2	309	CLA	CHC-C4B-NB	-2.03	122.11	124.26
22	B	821	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
22	B	836	CLA	CHD-C4C-NC	2.03	127.40	124.20
22	2	306	CLA	CHD-C4C-NC	2.03	127.40	124.20
22	2	306	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
22	7	307	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
22	Z	201	CLA	CMB-C2B-C1B	2.03	128.46	125.37
22	6	314	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
22	A	805	CLA	CED-O2D-CGD	2.03	120.53	115.94
22	7	305	CLA	O2A-CGA-CBA	2.03	120.55	114.03
22	5	304	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
22	6	307	CLA	CMC-C2C-C1C	2.03	128.13	125.04
22	4	302	CLA	CHC-C1C-NC	2.03	127.28	124.20
22	A	816	CLA	C5-C3-C2	-2.03	117.02	121.12
22	B	806	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
22	5	302	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
25	Z	202	BCR	C2-C1-C6	2.03	113.60	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	306	5X6	C09-C04-C03	2.03	113.58	110.30
21	A	801	CL0	O2A-CGA-O1A	-2.02	118.48	123.59
22	A	817	CLA	CHB-C1B-C2B	-2.02	121.52	127.24
22	A	811	CLA	CHB-C1B-NB	-2.02	122.11	124.26
22	B	812	CLA	C3B-C4B-NB	2.02	112.39	110.52
28	B	845	DGD	C4D-C3D-C2D	2.02	114.36	110.82
25	L	206	BCR	C10-C11-C12	2.02	129.53	123.22
22	B	837	CLA	C1-O2A-CGA	2.02	121.75	116.44
25	B	843	BCR	C12-C13-C14	2.02	122.04	118.94
22	B	838	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
29	4	313	5X6	C01-C02-C07	-2.02	110.61	114.36
29	4	314	5X6	C04-C03-C02	-2.02	119.77	122.61
25	K	103	BCR	C23-C22-C21	2.02	122.04	118.94
22	4	304	CLA	C1-O2A-CGA	2.02	121.74	116.44
22	F	204	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
22	F	205	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
22	O	206	CLA	CHC-C1C-NC	2.02	127.27	124.20
22	2	309	CLA	CHD-C4C-NC	2.02	127.39	124.20
22	B	827	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
22	B	812	CLA	CHD-C4C-NC	2.02	127.39	124.20
22	B	839	CLA	CMB-C2B-C1B	2.02	128.44	125.37
22	3	302	CLA	CHB-C4A-NA	2.02	127.30	124.51
29	7	314	5X6	C34-C29-C30	2.02	125.46	122.61
22	B	835	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
22	B	826	CLA	C7-C6-C5	-2.02	107.88	113.36
22	L	203	CLA	CHC-C1C-NC	2.02	127.26	124.20
22	A	817	CLA	CHD-C4C-NC	2.02	127.38	124.20
22	B	815	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
22	1	306	CLA	CHC-C1C-NC	2.02	127.26	124.20
22	B	830	CLA	CED-O2D-CGD	2.02	120.50	115.94
22	Z	201	CLA	O2D-CGD-O1D	-2.02	119.90	123.84
22	4	310	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	5	305	CLA	CHD-C4C-NC	2.02	127.38	124.20
29	O	208	5X6	C11-C03-C02	-2.01	116.58	121.46
29	5	321	5X6	C28-C29-C30	-2.01	116.58	121.46
22	B	829	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
22	2	309	CLA	CHC-C1C-NC	2.01	127.26	124.20
22	1	304	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
22	B	802	CLA	C11-C10-C8	-2.01	109.42	115.92
22	F	205	CLA	O2A-CGA-CBA	2.01	120.49	114.03
22	B	813	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	Z	204	CLA	C2A-C1A-CHA	-2.01	120.34	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	L	206	BCR	C16-C17-C18	2.01	130.18	127.31
29	6	315	5X6	C28-C29-C30	-2.01	116.59	121.46
22	A	834	CLA	CHB-C4A-NA	2.01	127.29	124.51
22	B	823	CLA	CHC-C1C-NC	2.01	127.25	124.20
22	2	305	CLA	CAA-CBA-CGA	2.01	119.13	113.25
22	B	825	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
22	7	309	CLA	CMB-C2B-C1B	2.01	128.43	125.37
22	B	801	CLA	CHD-C4C-NC	2.01	127.37	124.20
22	B	815	CLA	C1-O2A-CGA	2.01	121.71	116.44
22	A	804	CLA	CMB-C2B-C1B	2.01	128.43	125.37
22	6	310	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
22	B	814	CLA	CMB-C2B-C1B	2.01	128.43	125.37
22	K	102	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
22	A	829	CLA	CHD-C4C-NC	2.01	127.36	124.20
22	B	838	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
22	A	821	CLA	CBC-CAC-C3C	-2.00	106.90	112.43
22	A	837	CLA	C5-C3-C2	-2.00	117.06	121.12
22	2	306	CLA	O2A-CGA-CBA	2.00	120.47	114.03
22	B	807	CLA	C1-O2A-CGA	2.00	121.70	116.44
22	2	309	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	A	811	CLA	C5-C3-C2	-2.00	117.06	121.12
22	4	302	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
22	B	808	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	A	822	CLA	C1-C2-C3	-2.00	122.58	126.04
22	K	101	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	B	802	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
22	A	806	CLA	C4A-NA-C1A	-2.00	105.81	106.71
22	6	309	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
22	5	310	CLA	CHB-C1B-C2B	-2.00	121.59	127.24

There are no chirality outliers.

All (1948) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	816	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	822	CLA	CHA-CBD-CGD-O1D
22	A	822	CLA	CHA-CBD-CGD-O2D
22	A	828	CLA	CHA-CBD-CGD-O1D
22	A	828	CLA	CHA-CBD-CGD-O2D
22	A	832	CLA	CHA-CBD-CGD-O1D
22	A	832	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	835	CLA	C4-C3-C5-C6
22	A	837	CLA	CHA-CBD-CGD-O2D
22	A	848	CLA	C11-C12-C13-C14
22	A	859	CLA	C1A-C2A-CAA-CBA
22	A	859	CLA	C2-C3-C5-C6
22	A	859	CLA	C4-C3-C5-C6
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C14-C13-C15-C16
22	B	811	CLA	CHA-CBD-CGD-O2D
22	B	816	CLA	CHA-CBD-CGD-O2D
22	B	820	CLA	C3A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	834	CLA	C4-C3-C5-C6
22	B	838	CLA	CBD-CGD-O2D-CED
22	B	838	CLA	C2-C3-C5-C6
22	B	838	CLA	C4-C3-C5-C6
22	B	850	CLA	C1A-C2A-CAA-CBA
22	B	850	CLA	C3A-C2A-CAA-CBA
22	K	102	CLA	CBD-CGD-O2D-CED
22	L	204	CLA	C2A-CAA-CBA-CGA
22	O	203	CLA	CHA-CBD-CGD-O1D
22	O	203	CLA	CHA-CBD-CGD-O2D
22	Z	201	CLA	C1A-C2A-CAA-CBA
22	Z	201	CLA	C3A-C2A-CAA-CBA
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	305	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	C1A-C2A-CAA-CBA
22	1	307	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	O2A-C1-C2-C3
22	1	307	CLA	C4-C3-C5-C6
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	310	CLA	C1A-C2A-CAA-CBA
22	1	310	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	2	304	CLA	C4-C3-C5-C6
22	2	305	CLA	C1A-C2A-CAA-CBA
22	2	311	CLA	CBD-CGD-O2D-CED
22	4	304	CLA	CBD-CGD-O2D-CED
22	4	304	CLA	C11-C12-C13-C14
22	4	305	CLA	C2-C3-C5-C6
22	4	305	CLA	C4-C3-C5-C6
22	4	306	CLA	C2A-CAA-CBA-CGA
22	4	310	CLA	C2C-C3C-CAC-CBC
22	4	310	CLA	C4C-C3C-CAC-CBC
22	4	312	CLA	CBD-CGD-O2D-CED
22	5	311	CLA	C3A-C2A-CAA-CBA
22	6	303	CLA	C3A-C2A-CAA-CBA
22	6	306	CLA	C1A-C2A-CAA-CBA
22	6	306	CLA	C4-C3-C5-C6
22	6	311	CLA	CHA-CBD-CGD-O1D
22	6	311	CLA	CHA-CBD-CGD-O2D
22	6	312	CLA	C1A-C2A-CAA-CBA
22	6	312	CLA	C3A-C2A-CAA-CBA
22	6	313	CLA	CHA-CBD-CGD-O1D
22	6	313	CLA	CHA-CBD-CGD-O2D
22	6	313	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	C1A-C2A-CAA-CBA
22	7	306	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CHA-CBD-CGD-O2D
22	7	311	CLA	CBD-CGD-O2D-CED
23	A	840	A1L64	C12-C13-C14-C15
24	A	841	LHG	C3-O3-P-O5
24	B	846	LHG	C3-O3-P-O5
24	J	106	LHG	C2-C3-O3-P
24	J	106	LHG	C4-O6-P-O3
24	2	315	LHG	C3-O3-P-O5
24	2	315	LHG	C3-O3-P-O6
24	2	315	LHG	C4-O6-P-O3
24	2	315	LHG	C4-O6-P-O5
24	4	318	LHG	C3-O3-P-O5
24	4	318	LHG	C4-O6-P-O5
24	5	316	LHG	C3-O3-P-O4
24	5	316	LHG	C3-O3-P-O5
24	6	319	LHG	C4-O6-P-O4
24	6	319	LHG	C4-O6-P-O5
25	A	844	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	B	843	BCR	C1-C6-C7-C8
25	B	843	BCR	C5-C6-C7-C8
25	B	843	BCR	C21-C22-C23-C24
25	B	843	BCR	C37-C22-C23-C24
25	L	202	BCR	C7-C8-C9-C34
25	Z	202	BCR	C37-C22-C23-C24
25	1	301	BCR	C21-C22-C23-C24
25	1	301	BCR	C37-C22-C23-C24
25	1	301	BCR	C23-C24-C25-C26
25	1	301	BCR	C23-C24-C25-C30
25	2	301	BCR	C7-C8-C9-C10
25	2	301	BCR	C7-C8-C9-C34
25	4	316	BCR	C7-C8-C9-C10
25	4	316	BCR	C7-C8-C9-C34
28	B	845	DGD	C2B-C1B-O2G-C2G
29	B	851	5X6	C41-C17-C18-C19
29	B	851	5X6	C15-C16-C17-C41
29	B	851	5X6	C39-C26-C27-C28
29	B	851	5X6	C24-C25-C26-C39
29	B	851	5X6	C11-C12-C13-C14
29	B	851	5X6	C42-C13-C14-C15
29	B	851	5X6	C20-C21-C22-C40
29	B	851	5X6	C40-C22-C23-C24
29	J	104	5X6	C41-C17-C18-C19
29	J	104	5X6	C39-C26-C27-C28
29	J	104	5X6	C02-C03-C11-C12
29	J	104	5X6	C12-C13-C14-C15
29	J	104	5X6	C42-C13-C14-C15
29	J	104	5X6	C20-C21-C22-C40
29	J	104	5X6	C40-C22-C23-C24
29	M	101	5X6	C41-C17-C18-C19
29	M	101	5X6	C15-C16-C17-C18
29	M	101	5X6	C17-C18-C19-C20
29	M	101	5X6	C14-C15-C16-C17
29	M	101	5X6	C24-C25-C26-C39
29	M	101	5X6	C18-C19-C20-C21
29	M	101	5X6	C11-C12-C13-C42
29	M	101	5X6	C12-C13-C14-C15
29	M	101	5X6	C26-C27-C28-C29
29	M	101	5X6	C20-C21-C22-C40
29	M	101	5X6	C20-C21-C22-C23
29	M	101	5X6	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	M	101	5X6	C22-C23-C24-C25
29	O	207	5X6	C41-C17-C18-C19
29	O	207	5X6	C15-C16-C17-C41
29	O	207	5X6	C25-C26-C27-C28
29	O	207	5X6	C24-C25-C26-C39
29	O	207	5X6	C11-C12-C13-C42
29	O	207	5X6	C42-C13-C14-C15
29	O	207	5X6	C20-C21-C22-C40
29	O	208	5X6	C41-C17-C18-C19
29	O	208	5X6	C39-C26-C27-C28
29	O	208	5X6	C24-C25-C26-C39
29	O	208	5X6	C42-C13-C14-C15
29	O	208	5X6	C20-C21-C22-C40
29	Z	206	5X6	C41-C17-C18-C19
29	Z	206	5X6	C25-C26-C27-C28
29	Z	206	5X6	C24-C25-C26-C39
29	Z	206	5X6	C42-C13-C14-C15
29	Z	206	5X6	C40-C22-C23-C24
29	Z	206	5X6	C22-C23-C24-C25
29	1	311	5X6	C15-C16-C17-C41
29	1	311	5X6	C17-C18-C19-C20
29	1	311	5X6	C25-C26-C27-C28
29	1	311	5X6	C18-C19-C20-C21
29	1	311	5X6	C03-C11-C12-C13
29	1	311	5X6	C11-C12-C13-C14
29	1	311	5X6	C12-C13-C14-C15
29	1	311	5X6	C27-C28-C29-C34
29	1	311	5X6	C20-C21-C22-C40
29	1	311	5X6	C20-C21-C22-C23
29	1	311	5X6	C40-C22-C23-C24
29	1	312	5X6	C41-C17-C18-C19
29	1	312	5X6	C15-C16-C17-C41
29	1	312	5X6	C24-C25-C26-C39
29	1	312	5X6	C11-C12-C13-C42
29	1	312	5X6	C42-C13-C14-C15
29	1	312	5X6	C27-C28-C29-C30
29	1	312	5X6	C20-C21-C22-C40
29	1	313	5X6	C41-C17-C18-C19
29	1	313	5X6	C15-C16-C17-C18
29	1	313	5X6	C14-C15-C16-C17
29	1	313	5X6	C25-C26-C27-C28
29	1	313	5X6	C24-C25-C26-C39

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Mol	Chain	Res	Type	Atoms
29	1	313	5X6	C24-C25-C26-C27
29	1	313	5X6	C11-C12-C13-C14
29	1	313	5X6	C42-C13-C14-C15
29	1	313	5X6	C27-C28-C29-C30
29	1	313	5X6	C20-C21-C22-C40
29	1	314	5X6	C41-C17-C18-C19
29	1	314	5X6	C39-C26-C27-C28
29	1	314	5X6	C24-C25-C26-C39
29	1	314	5X6	C03-C11-C12-C13
29	1	314	5X6	C02-C03-C11-C12
29	1	314	5X6	C04-C03-C11-C12
29	1	314	5X6	C27-C28-C29-C30
29	1	314	5X6	C20-C21-C22-C40
29	1	316	5X6	C15-C16-C17-C41
29	1	316	5X6	C39-C26-C27-C28
29	1	316	5X6	C24-C25-C26-C39
29	1	316	5X6	C42-C13-C14-C15
29	1	316	5X6	C27-C28-C29-C30
29	1	316	5X6	C20-C21-C22-C40
29	2	312	5X6	C41-C17-C18-C19
29	2	312	5X6	C15-C16-C17-C41
29	2	312	5X6	C14-C15-C16-C17
29	2	312	5X6	C39-C26-C27-C28
29	2	312	5X6	C24-C25-C26-C39
29	2	312	5X6	C42-C13-C14-C15
29	2	312	5X6	C26-C27-C28-C29
29	2	312	5X6	C20-C21-C22-C40
29	2	313	5X6	C41-C17-C18-C19
29	2	313	5X6	C15-C16-C17-C18
29	2	313	5X6	C24-C25-C26-C27
29	2	313	5X6	C04-C03-C11-C12
29	2	313	5X6	C11-C12-C13-C14
29	2	313	5X6	C42-C13-C14-C15
29	2	313	5X6	C27-C28-C29-C34
29	2	313	5X6	C20-C21-C22-C40
29	2	314	5X6	C41-C17-C18-C19
29	2	314	5X6	C24-C25-C26-C39
29	2	314	5X6	C24-C25-C26-C27
29	2	314	5X6	C18-C19-C20-C21
29	2	314	5X6	C11-C12-C13-C42
29	2	314	5X6	C42-C13-C14-C15
29	2	314	5X6	C20-C21-C22-C40

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Mol	Chain	Res	Type	Atoms
29	2	314	5X6	C21-C22-C23-C24
29	3	306	5X6	C41-C17-C18-C19
29	3	306	5X6	C15-C16-C17-C18
29	3	306	5X6	C15-C16-C17-C41
29	3	306	5X6	C14-C15-C16-C17
29	3	306	5X6	C39-C26-C27-C28
29	3	306	5X6	C11-C12-C13-C14
29	3	306	5X6	C11-C12-C13-C42
29	3	306	5X6	C42-C13-C14-C15
29	3	306	5X6	C27-C28-C29-C34
29	3	306	5X6	C20-C21-C22-C40
29	3	306	5X6	C40-C22-C23-C24
29	3	306	5X6	C22-C23-C24-C25
29	4	313	5X6	C41-C17-C18-C19
29	4	313	5X6	C15-C16-C17-C41
29	4	313	5X6	C14-C15-C16-C17
29	4	313	5X6	C39-C26-C27-C28
29	4	313	5X6	C24-C25-C26-C39
29	4	313	5X6	C42-C13-C14-C15
29	4	313	5X6	C20-C21-C22-C40
29	4	313	5X6	C40-C22-C23-C24
29	4	313	5X6	C22-C23-C24-C25
29	4	314	5X6	C16-C17-C18-C19
29	4	314	5X6	C15-C16-C17-C18
29	4	314	5X6	C11-C12-C13-C14
29	4	314	5X6	C42-C13-C14-C15
29	4	314	5X6	C20-C21-C22-C40
29	4	314	5X6	C40-C22-C23-C24
29	4	315	5X6	C41-C17-C18-C19
29	4	315	5X6	C15-C16-C17-C18
29	4	315	5X6	C14-C15-C16-C17
29	4	315	5X6	C24-C25-C26-C39
29	4	315	5X6	C24-C25-C26-C27
29	4	315	5X6	C18-C19-C20-C21
29	4	315	5X6	C03-C11-C12-C13
29	4	315	5X6	C02-C03-C11-C12
29	4	315	5X6	C11-C12-C13-C42
29	4	315	5X6	C42-C13-C14-C15
29	4	315	5X6	C20-C21-C22-C40
29	4	315	5X6	C22-C23-C24-C25
29	5	312	5X6	C41-C17-C18-C19
29	5	312	5X6	C15-C16-C17-C41

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Mol	Chain	Res	Type	Atoms
29	5	312	5X6	C39-C26-C27-C28
29	5	312	5X6	C24-C25-C26-C39
29	5	312	5X6	C11-C12-C13-C14
29	5	312	5X6	C42-C13-C14-C15
29	5	312	5X6	C20-C21-C22-C40
29	5	312	5X6	C40-C22-C23-C24
29	5	313	5X6	C39-C26-C27-C28
29	5	313	5X6	C24-C25-C26-C39
29	5	313	5X6	C03-C11-C12-C13
29	5	313	5X6	C11-C12-C13-C14
29	5	313	5X6	C42-C13-C14-C15
29	5	313	5X6	C20-C21-C22-C40
29	5	313	5X6	C40-C22-C23-C24
29	5	314	5X6	C41-C17-C18-C19
29	5	314	5X6	C39-C26-C27-C28
29	5	314	5X6	C24-C25-C26-C39
29	5	314	5X6	C18-C19-C20-C21
29	5	314	5X6	C03-C11-C12-C13
29	5	314	5X6	C02-C03-C11-C12
29	5	314	5X6	C11-C12-C13-C14
29	5	314	5X6	C12-C13-C14-C15
29	5	314	5X6	C42-C13-C14-C15
29	5	314	5X6	C20-C21-C22-C40
29	5	314	5X6	C22-C23-C24-C25
29	5	321	5X6	C41-C17-C18-C19
29	5	321	5X6	C24-C25-C26-C39
29	5	321	5X6	C24-C25-C26-C27
29	5	321	5X6	C02-C03-C11-C12
29	5	321	5X6	C11-C12-C13-C42
29	5	321	5X6	C42-C13-C14-C15
29	5	321	5X6	C20-C21-C22-C40
29	5	321	5X6	C22-C23-C24-C25
29	6	315	5X6	C41-C17-C18-C19
29	6	315	5X6	C15-C16-C17-C41
29	6	315	5X6	C39-C26-C27-C28
29	6	315	5X6	C24-C25-C26-C39
29	6	315	5X6	C42-C13-C14-C15
29	6	315	5X6	C20-C21-C22-C40
29	6	315	5X6	C40-C22-C23-C24
29	6	315	5X6	C22-C23-C24-C25
29	6	316	5X6	C41-C17-C18-C19
29	6	316	5X6	C39-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	6	316	5X6	C24-C25-C26-C39
29	6	316	5X6	C11-C12-C13-C14
29	6	316	5X6	C42-C13-C14-C15
29	6	316	5X6	C20-C21-C22-C40
29	6	317	5X6	C41-C17-C18-C19
29	6	317	5X6	C15-C16-C17-C41
29	6	317	5X6	C25-C26-C27-C28
29	6	317	5X6	C42-C13-C14-C15
29	6	317	5X6	C27-C28-C29-C30
29	6	317	5X6	C20-C21-C22-C40
29	6	317	5X6	C23-C24-C25-C26
29	7	314	5X6	C16-C17-C18-C19
29	7	314	5X6	C14-C15-C16-C17
29	7	314	5X6	C24-C25-C26-C39
29	7	314	5X6	C18-C19-C20-C21
29	7	314	5X6	C03-C11-C12-C13
29	7	314	5X6	C11-C12-C13-C42
29	7	314	5X6	C42-C13-C14-C15
29	7	314	5X6	C20-C21-C22-C23
29	7	314	5X6	C21-C22-C23-C24
29	7	314	5X6	C22-C23-C24-C25
29	7	315	5X6	C41-C17-C18-C19
29	7	315	5X6	C24-C25-C26-C39
29	7	315	5X6	C18-C19-C20-C21
29	7	315	5X6	C02-C03-C11-C12
29	7	315	5X6	C11-C12-C13-C14
29	7	315	5X6	C42-C13-C14-C15
29	7	315	5X6	C23-C24-C25-C26
29	7	316	5X6	C41-C17-C18-C19
29	7	316	5X6	C25-C26-C27-C28
29	7	316	5X6	C24-C25-C26-C39
29	7	316	5X6	C24-C25-C26-C27
29	7	316	5X6	C18-C19-C20-C21
29	7	316	5X6	C02-C03-C11-C12
29	7	316	5X6	C11-C12-C13-C42
29	7	316	5X6	C12-C13-C14-C15
29	7	316	5X6	C42-C13-C14-C15
29	7	316	5X6	C20-C21-C22-C40
29	7	316	5X6	C40-C22-C23-C24
29	7	316	5X6	C21-C22-C23-C24
29	7	317	5X6	C16-C17-C18-C19
29	7	317	5X6	C41-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	7	317	5X6	C15-C16-C17-C41
29	7	317	5X6	C39-C26-C27-C28
29	7	317	5X6	C24-C25-C26-C39
29	7	317	5X6	C03-C11-C12-C13
29	7	317	5X6	C11-C12-C13-C14
29	7	317	5X6	C42-C13-C14-C15
29	7	317	5X6	C20-C21-C22-C40
29	7	317	5X6	C20-C21-C22-C23
29	7	317	5X6	C22-C23-C24-C25
29	7	318	5X6	C41-C17-C18-C19
29	7	318	5X6	C15-C16-C17-C18
29	7	318	5X6	C14-C15-C16-C17
29	7	318	5X6	C24-C25-C26-C27
29	7	318	5X6	C12-C13-C14-C15
29	7	318	5X6	C27-C28-C29-C30
29	7	318	5X6	C26-C27-C28-C29
29	7	318	5X6	C20-C21-C22-C40
31	1	315	RRX	C1-C6-C7-C8
31	1	315	RRX	C5-C6-C7-C8
31	5	322	RRX	C7-C8-C9-C10
22	1	307	CLA	O1D-CGD-O2D-CED
22	1	309	CLA	O1D-CGD-O2D-CED
22	2	310	CLA	O1D-CGD-O2D-CED
22	4	304	CLA	O1D-CGD-O2D-CED
22	5	310	CLA	O1D-CGD-O2D-CED
22	L	203	CLA	O1D-CGD-O2D-CED
22	1	303	CLA	O1D-CGD-O2D-CED
22	2	311	CLA	O1D-CGD-O2D-CED
22	7	311	CLA	O1D-CGD-O2D-CED
22	A	808	CLA	CBD-CGD-O2D-CED
22	A	814	CLA	CBD-CGD-O2D-CED
22	A	821	CLA	CBD-CGD-O2D-CED
22	L	203	CLA	CBD-CGD-O2D-CED
22	O	204	CLA	CBD-CGD-O2D-CED
22	O	206	CLA	CBD-CGD-O2D-CED
22	1	302	CLA	CBD-CGD-O2D-CED
22	1	309	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CBD-CGD-O2D-CED
22	2	306	CLA	CBD-CGD-O2D-CED
22	2	308	CLA	CBD-CGD-O2D-CED
22	2	310	CLA	CBD-CGD-O2D-CED
22	3	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	3	303	CLA	CBD-CGD-O2D-CED
22	4	302	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	CBD-CGD-O2D-CED
22	5	310	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	CBD-CGD-O2D-CED
22	7	312	CLA	CBD-CGD-O2D-CED
22	Z	204	CLA	O1A-CGA-O2A-C1
22	4	304	CLA	O1A-CGA-O2A-C1
24	2	315	LHG	O10-C23-O8-C6
22	6	311	CLA	C2C-C3C-CAC-CBC
22	K	102	CLA	O1D-CGD-O2D-CED
22	O	204	CLA	O1D-CGD-O2D-CED
22	2	306	CLA	O1D-CGD-O2D-CED
22	3	301	CLA	O1D-CGD-O2D-CED
30	F	202	LMT	O5B-C1B-O1B-C4'
22	B	838	CLA	O1D-CGD-O2D-CED
22	4	312	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	A	813	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	CBD-CGD-O2D-CED
22	B	811	CLA	CBD-CGD-O2D-CED
22	B	815	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	CBD-CGD-O2D-CED
22	1	306	CLA	CBD-CGD-O2D-CED
22	2	309	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBD-CGD-O2D-CED
22	5	305	CLA	CBD-CGD-O2D-CED
22	5	311	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	CBD-CGD-O2D-CED
22	6	314	CLA	CBD-CGD-O2D-CED
22	7	304	CLA	CBD-CGD-O2D-CED
22	7	313	CLA	CBD-CGD-O2D-CED
22	6	311	CLA	C4C-C3C-CAC-CBC
22	A	810	CLA	O1A-CGA-O2A-C1
22	A	834	CLA	O1A-CGA-O2A-C1
22	A	836	CLA	O1A-CGA-O2A-C1
22	B	804	CLA	O1A-CGA-O2A-C1
22	B	830	CLA	O1A-CGA-O2A-C1
22	L	203	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	310	CLA	O1D-CGD-O2D-CED
22	5	309	CLA	CBD-CGD-O2D-CED
22	6	305	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	C13-C15-C16-C17
22	6	313	CLA	O1D-CGD-O2D-CED
28	B	845	DGD	O1B-C1B-O2G-C2G
22	A	818	CLA	C3-C5-C6-C7
22	A	819	CLA	C3-C5-C6-C7
22	A	834	CLA	C3-C5-C6-C7
22	B	808	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	822	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	B	849	CLA	C3-C5-C6-C7
22	L	204	CLA	C3-C5-C6-C7
22	4	303	CLA	C3-C5-C6-C7
22	5	302	CLA	C3-C5-C6-C7
22	5	303	CLA	C3-C5-C6-C7
22	6	310	CLA	C3-C5-C6-C7
22	A	810	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	CBA-CGA-O2A-C1
22	A	838	CLA	CBA-CGA-O2A-C1
22	B	804	CLA	CBA-CGA-O2A-C1
22	B	836	CLA	CBA-CGA-O2A-C1
22	Z	204	CLA	CBA-CGA-O2A-C1
22	4	304	CLA	CBA-CGA-O2A-C1
24	2	315	LHG	C24-C23-O8-C6
22	7	303	CLA	O1D-CGD-O2D-CED
22	B	804	CLA	CBD-CGD-O2D-CED
22	1	309	CLA	C2C-C3C-CAC-CBC
22	5	310	CLA	C3-C5-C6-C7
22	4	309	CLA	C4-C3-C5-C6
22	2	304	CLA	C2-C3-C5-C6
22	B	822	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	CBD-CGD-O2D-CED
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	821	CLA	C2A-CAA-CBA-CGA
22	A	827	CLA	C2A-CAA-CBA-CGA
22	B	837	CLA	C2A-CAA-CBA-CGA
22	2	305	CLA	C2A-CAA-CBA-CGA
22	4	305	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	5	304	CLA	C2A-CAA-CBA-CGA
22	6	306	CLA	C2A-CAA-CBA-CGA
22	7	306	CLA	C2A-CAA-CBA-CGA
22	B	807	CLA	C3-C5-C6-C7
22	B	809	CLA	C3-C5-C6-C7
22	B	829	CLA	C3-C5-C6-C7
22	5	307	CLA	C3-C5-C6-C7
22	7	306	CLA	C3-C5-C6-C7
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	809	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBA-CGA-O2A-C1
22	B	830	CLA	CBA-CGA-O2A-C1
22	L	203	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	CBA-CGA-O2A-C1
22	3	303	CLA	O1D-CGD-O2D-CED
22	4	302	CLA	O1D-CGD-O2D-CED
22	6	306	CLA	CBD-CGD-O2D-CED
22	7	305	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	C2-C1-O2A-CGA
22	A	814	CLA	O1D-CGD-O2D-CED
22	O	206	CLA	O1D-CGD-O2D-CED
22	1	302	CLA	O1D-CGD-O2D-CED
22	4	310	CLA	O1D-CGD-O2D-CED
23	A	840	A1L64	C12-C13-C14-C16
22	A	807	CLA	O1A-CGA-O2A-C1
22	A	809	CLA	O1A-CGA-O2A-C1
22	A	838	CLA	O1A-CGA-O2A-C1
22	B	838	CLA	O1A-CGA-O2A-C1
25	J	103	BCR	C19-C20-C21-C22
29	1	311	5X6	C23-C24-C25-C26
29	5	321	5X6	C17-C18-C19-C20
29	7	316	5X6	C17-C18-C19-C20
30	5	320	LMT	O5B-C5B-C6B-O6B
22	A	834	CLA	CBD-CGD-O2D-CED
22	B	806	CLA	CBD-CGD-O2D-CED
22	Z	201	CLA	CBD-CGD-O2D-CED
22	4	303	CLA	CBD-CGD-O2D-CED
22	7	312	CLA	O1D-CGD-O2D-CED
24	1	317	LHG	O2-C2-C3-O3
22	A	833	CLA	C3-C5-C6-C7
22	A	839	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	838	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	O1A-CGA-O2A-C1
22	B	836	CLA	O1A-CGA-O2A-C1
22	2	308	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	CBD-CGD-O2D-CED
30	O	201	LMT	O5B-C5B-C6B-O6B
30	4	319	LMT	O5B-C5B-C6B-O6B
22	6	307	CLA	C13-C15-C16-C17
30	5	320	LMT	C4B-C5B-C6B-O6B
22	1	309	CLA	C4C-C3C-CAC-CBC
22	B	814	CLA	C3-C5-C6-C7
22	4	309	CLA	C3-C5-C6-C7
22	B	816	CLA	CBA-CGA-O2A-C1
22	O	203	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	C4-C3-C5-C6
22	A	815	CLA	C4-C3-C5-C6
22	B	806	CLA	C4-C3-C5-C6
22	A	808	CLA	C2-C3-C5-C6
22	A	815	CLA	C2-C3-C5-C6
22	B	806	CLA	C2-C3-C5-C6
22	1	307	CLA	C2-C3-C5-C6
22	6	306	CLA	C2-C3-C5-C6
22	2	311	CLA	C2A-CAA-CBA-CGA
22	2	302	CLA	O1D-CGD-O2D-CED
22	A	839	CLA	O1A-CGA-O2A-C1
22	B	816	CLA	O1A-CGA-O2A-C1
23	A	840	A1L64	C9-C11-C12-C13
23	A	840	A1L64	C19-C21-C22-C23
22	B	817	CLA	C3-C5-C6-C7
22	A	808	CLA	CBA-CGA-O2A-C1
30	4	319	LMT	C4'-C5'-C6'-O6'
22	A	808	CLA	O1D-CGD-O2D-CED
22	A	821	CLA	O1D-CGD-O2D-CED
22	B	811	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	O1D-CGD-O2D-CED
22	A	813	CLA	O1D-CGD-O2D-CED
22	A	817	CLA	O1D-CGD-O2D-CED
22	1	306	CLA	O1D-CGD-O2D-CED
22	3	302	CLA	O1D-CGD-O2D-CED
24	1	317	LHG	C1-C2-C3-O3
22	2	304	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	829	CLA	CBA-CGA-O2A-C1
22	A	830	CLA	CBA-CGA-O2A-C1
22	B	814	CLA	CBA-CGA-O2A-C1
22	B	831	CLA	CBA-CGA-O2A-C1
22	2	304	CLA	CBA-CGA-O2A-C1
22	4	309	CLA	CBA-CGA-O2A-C1
22	A	832	CLA	CBD-CGD-O2D-CED
30	O	201	LMT	C4B-C5B-C6B-O6B
22	7	304	CLA	O1D-CGD-O2D-CED
22	5	302	CLA	C15-C16-C17-C18
22	4	309	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	C2-C3-C5-C6
22	4	309	CLA	C2-C3-C5-C6
22	A	804	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C10-C8-C9
22	A	834	CLA	C11-C10-C8-C9
22	A	839	CLA	C11-C10-C8-C9
22	A	859	CLA	C11-C10-C8-C9
22	B	808	CLA	C6-C7-C8-C9
22	B	809	CLA	C11-C12-C13-C14
22	B	810	CLA	C11-C12-C13-C14
22	B	811	CLA	C6-C7-C8-C9
22	B	811	CLA	C11-C10-C8-C9
22	B	813	CLA	C14-C13-C15-C16
22	B	817	CLA	C11-C10-C8-C9
22	B	822	CLA	C11-C12-C13-C14
22	B	829	CLA	C6-C7-C8-C9
22	B	838	CLA	C6-C7-C8-C9
22	L	204	CLA	C11-C10-C8-C9
22	O	206	CLA	C6-C7-C8-C9
22	1	310	CLA	C6-C7-C8-C9
22	4	303	CLA	C6-C7-C8-C9
22	B	815	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	O1D-CGD-O2D-CED
22	7	313	CLA	O1D-CGD-O2D-CED
22	A	816	CLA	C15-C16-C17-C18
25	L	206	BCR	C7-C8-C9-C34
25	Z	205	BCR	C7-C8-C9-C34
29	J	104	5X6	C15-C16-C17-C41
29	J	104	5X6	C11-C12-C13-C42
29	O	208	5X6	C15-C16-C17-C41
29	O	208	5X6	C11-C12-C13-C42

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Mol	Chain	Res	Type	Atoms
29	1	311	5X6	C39-C26-C27-C28
29	1	312	5X6	C39-C26-C27-C28
29	1	312	5X6	C40-C22-C23-C24
29	1	313	5X6	C40-C22-C23-C24
29	1	314	5X6	C11-C12-C13-C42
29	1	316	5X6	C11-C12-C13-C42
29	2	312	5X6	C40-C22-C23-C24
29	2	313	5X6	C15-C16-C17-C41
29	2	313	5X6	C39-C26-C27-C28
29	2	313	5X6	C40-C22-C23-C24
29	2	314	5X6	C39-C26-C27-C28
29	2	314	5X6	C40-C22-C23-C24
29	4	314	5X6	C15-C16-C17-C41
29	4	314	5X6	C39-C26-C27-C28
29	5	314	5X6	C40-C22-C23-C24
29	5	321	5X6	C15-C16-C17-C41
29	6	316	5X6	C15-C16-C17-C41
29	6	316	5X6	C40-C22-C23-C24
29	6	317	5X6	C40-C22-C23-C24
29	7	314	5X6	C15-C16-C17-C41
29	7	315	5X6	C15-C16-C17-C41
29	7	315	5X6	C39-C26-C27-C28
29	7	315	5X6	C40-C22-C23-C24
29	7	318	5X6	C39-C26-C27-C28
29	7	318	5X6	C11-C12-C13-C42
29	7	318	5X6	C40-C22-C23-C24
25	L	206	BCR	C7-C8-C9-C10
25	Z	205	BCR	C7-C8-C9-C10
29	M	101	5X6	C11-C12-C13-C14
29	1	311	5X6	C21-C22-C23-C24
29	1	312	5X6	C11-C12-C13-C14
29	1	316	5X6	C15-C16-C17-C18
29	2	312	5X6	C11-C12-C13-C14
29	7	314	5X6	C11-C12-C13-C14
29	7	317	5X6	C15-C16-C17-C18
29	7	317	5X6	C21-C22-C23-C24
22	A	829	CLA	O1A-CGA-O2A-C1
22	B	833	CLA	C10-C11-C12-C13
22	6	314	CLA	O1D-CGD-O2D-CED
22	5	311	CLA	O1D-CGD-O2D-CED
22	6	312	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	812	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	C10-C11-C12-C13
22	B	807	CLA	C8-C10-C11-C12
22	B	811	CLA	C15-C16-C17-C18
22	B	830	CLA	C5-C6-C7-C8
22	B	835	CLA	C5-C6-C7-C8
22	B	837	CLA	C10-C11-C12-C13
22	B	837	CLA	C13-C15-C16-C17
22	B	838	CLA	C15-C16-C17-C18
22	4	309	CLA	C13-C15-C16-C17
22	5	303	CLA	C10-C11-C12-C13
22	6	303	CLA	O1D-CGD-O2D-CED
22	1	308	CLA	CBD-CGD-O2D-CED
22	A	809	CLA	C10-C11-C12-C13
22	A	820	CLA	C10-C11-C12-C13
22	A	820	CLA	C15-C16-C17-C18
22	A	831	CLA	C15-C16-C17-C18
22	A	837	CLA	C10-C11-C12-C13
22	B	812	CLA	C5-C6-C7-C8
22	B	831	CLA	C8-C10-C11-C12
22	6	307	CLA	C8-C10-C11-C12
22	2	309	CLA	O1D-CGD-O2D-CED
24	A	842	LHG	O1-C1-C2-O2
22	A	825	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
24	4	318	LHG	C23-C24-C25-C26
30	4	319	LMT	C4B-C5B-C6B-O6B
22	6	305	CLA	C13-C15-C16-C17
22	B	811	CLA	CBA-CGA-O2A-C1
22	4	308	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	O1D-CGD-O2D-CED
30	F	202	LMT	O1'-C1-C2-C3
22	B	813	CLA	C10-C11-C12-C13
22	7	306	CLA	C5-C6-C7-C8
24	1	317	LHG	C23-C24-C25-C26
28	B	845	DGD	C1B-C2B-C3B-C4B
22	B	814	CLA	C8-C10-C11-C12
22	A	806	CLA	C13-C15-C16-C17
22	A	848	CLA	C11-C10-C8-C7
22	A	859	CLA	C11-C12-C13-C15
22	B	808	CLA	C12-C13-C15-C16
22	4	304	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	5	303	CLA	C6-C7-C8-C10
22	B	813	CLA	C3-C5-C6-C7
29	M	101	5X6	C23-C24-C25-C26
29	2	313	5X6	C23-C24-C25-C26
29	7	318	5X6	C17-C18-C19-C20
22	O	203	CLA	C2A-CAA-CBA-CGA
22	7	310	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	C15-C16-C17-C18
22	A	826	CLA	C15-C16-C17-C18
22	B	815	CLA	C5-C6-C7-C8
22	B	827	CLA	C15-C16-C17-C18
22	Z	204	CLA	C10-C11-C12-C13
30	4	319	LMT	O5'-C5'-C6'-O6'
29	O	207	5X6	C26-C27-C28-C29
29	6	316	5X6	C03-C11-C12-C13
29	7	315	5X6	C03-C11-C12-C13
22	A	802	CLA	O1A-CGA-O2A-C1
22	A	827	CLA	C5-C6-C7-C8
22	A	834	CLA	C10-C11-C12-C13
22	5	309	CLA	O1D-CGD-O2D-CED
23	A	840	A1L64	C14-C16-C17-C18
23	B	840	A1L64	C19-C21-C22-C23
29	O	207	5X6	C22-C23-C24-C25
29	1	311	5X6	C22-C23-C24-C25
29	1	316	5X6	C14-C15-C16-C17
29	1	316	5X6	C22-C23-C24-C25
29	2	312	5X6	C22-C23-C24-C25
29	2	314	5X6	C22-C23-C24-C25
29	4	314	5X6	C22-C23-C24-C25
29	7	315	5X6	C14-C15-C16-C17
29	7	315	5X6	C22-C23-C24-C25
22	A	827	CLA	C15-C16-C17-C18
22	B	810	CLA	C15-C16-C17-C18
22	B	815	CLA	C13-C15-C16-C17
22	B	819	CLA	C8-C10-C11-C12
22	B	822	CLA	C8-C10-C11-C12
22	F	204	CLA	C8-C10-C11-C12
22	L	203	CLA	C5-C6-C7-C8
22	1	310	CLA	C13-C15-C16-C17
22	6	304	CLA	C10-C11-C12-C13
22	A	808	CLA	O1A-CGA-O2A-C1
22	A	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	831	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	C10-C11-C12-C13
22	A	820	CLA	C8-C10-C11-C12
22	B	811	CLA	C5-C6-C7-C8
22	B	813	CLA	C5-C6-C7-C8
22	B	825	CLA	C10-C11-C12-C13
22	F	204	CLA	C10-C11-C12-C13
22	1	302	CLA	C15-C16-C17-C18
22	2	305	CLA	C5-C6-C7-C8
22	4	305	CLA	C5-C6-C7-C8
22	4	308	CLA	C5-C6-C7-C8
22	B	812	CLA	O1A-CGA-O2A-C1
22	4	308	CLA	O1A-CGA-O2A-C1
22	A	826	CLA	C10-C11-C12-C13
22	A	827	CLA	C13-C15-C16-C17
22	B	809	CLA	C8-C10-C11-C12
22	K	101	CLA	C5-C6-C7-C8
22	1	310	CLA	C10-C11-C12-C13
22	4	304	CLA	C8-C10-C11-C12
22	6	305	CLA	C5-C6-C7-C8
24	B	846	LHG	C3-O3-P-O6
24	5	316	LHG	C3-O3-P-O6
24	6	319	LHG	C3-O3-P-O6
24	6	319	LHG	C4-O6-P-O3
22	4	308	CLA	CBD-CGD-O2D-CED
22	A	826	CLA	C8-C10-C11-C12
22	B	804	CLA	C13-C15-C16-C17
22	B	825	CLA	C13-C15-C16-C17
24	A	842	LHG	C7-C8-C9-C10
22	2	304	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	O1D-CGD-O2D-CED
22	1	310	CLA	C4-C3-C5-C6
22	4	309	CLA	C8-C10-C11-C12
22	B	817	CLA	C2A-CAA-CBA-CGA
22	1	305	CLA	C2A-CAA-CBA-CGA
22	4	312	CLA	C2A-CAA-CBA-CGA
22	A	859	CLA	C16-C17-C18-C19
22	5	303	CLA	C16-C17-C18-C19
22	O	206	CLA	C3-C5-C6-C7
22	1	310	CLA	C3-C5-C6-C7
22	B	835	CLA	CBA-CGA-O2A-C1
28	B	845	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
29	1	316	5X6	C18-C19-C20-C21
29	2	312	5X6	C18-C19-C20-C21
22	B	804	CLA	O1D-CGD-O2D-CED
29	5	314	5X6	C17-C18-C19-C20
22	3	305	CLA	CBD-CGD-O2D-CED
22	1	310	CLA	C15-C16-C17-C18
29	J	104	5X6	C24-C25-C26-C39
29	1	311	5X6	C41-C17-C18-C19
29	1	311	5X6	C24-C25-C26-C39
29	1	314	5X6	C42-C13-C14-C15
29	1	316	5X6	C41-C17-C18-C19
29	3	306	5X6	C24-C25-C26-C39
29	4	314	5X6	C24-C25-C26-C39
29	5	313	5X6	C41-C17-C18-C19
29	6	317	5X6	C24-C25-C26-C39
29	7	315	5X6	C20-C21-C22-C40
29	7	318	5X6	C24-C25-C26-C39
22	Z	204	CLA	C3-C5-C6-C7
24	A	860	LHG	C25-C26-C27-C28
30	F	202	LMT	C6-C7-C8-C9
22	B	813	CLA	C16-C17-C18-C20
22	K	101	CLA	C6-C7-C8-C10
22	3	305	CLA	CBA-CGA-O2A-C1
22	7	305	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	C10-C11-C12-C13
22	O	206	CLA	C10-C11-C12-C13
24	A	841	LHG	C11-C10-C9-C8
22	B	822	CLA	O1D-CGD-O2D-CED
22	Z	201	CLA	O1D-CGD-O2D-CED
28	B	845	DGD	CAA-CBA-CCA-CDA
22	B	849	CLA	C5-C6-C7-C8
28	B	845	DGD	CEA-CFA-CGA-CHA
22	A	831	CLA	C3-C5-C6-C7
22	A	834	CLA	O1D-CGD-O2D-CED
25	L	202	BCR	C11-C10-C9-C8
29	J	104	5X6	C16-C17-C18-C19
29	M	101	5X6	C24-C25-C26-C27
29	Z	206	5X6	C20-C21-C22-C23
29	1	312	5X6	C24-C25-C26-C27
29	1	313	5X6	C16-C17-C18-C19
29	1	313	5X6	C12-C13-C14-C15
29	1	314	5X6	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	1	316	5X6	C20-C21-C22-C23
29	3	306	5X6	C16-C17-C18-C19
29	5	314	5X6	C24-C25-C26-C27
29	5	314	5X6	C20-C21-C22-C23
29	6	315	5X6	C12-C13-C14-C15
29	7	314	5X6	C24-C25-C26-C27
29	7	315	5X6	C16-C17-C18-C19
29	7	315	5X6	C20-C21-C22-C23
29	7	317	5X6	C24-C25-C26-C27
29	7	317	5X6	C12-C13-C14-C15
29	7	318	5X6	C16-C17-C18-C19
22	B	805	CLA	CBA-CGA-O2A-C1
22	B	837	CLA	CBA-CGA-O2A-C1
22	K	101	CLA	CBA-CGA-O2A-C1
24	A	841	LHG	C29-C30-C31-C32
22	O	203	CLA	O1A-CGA-O2A-C1
22	5	303	CLA	C16-C17-C18-C20
22	6	306	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	C4-C3-C5-C6
28	B	845	DGD	C7A-C8A-C9A-CAA
22	B	828	CLA	C2-C3-C5-C6
22	A	848	CLA	C11-C10-C8-C9
22	B	802	CLA	C6-C7-C8-C9
22	B	822	CLA	C14-C13-C15-C16
22	B	830	CLA	C11-C10-C8-C9
22	1	303	CLA	C11-C12-C13-C14
22	3	301	CLA	C6-C7-C8-C9
22	4	303	CLA	O1D-CGD-O2D-CED
28	B	845	DGD	C4A-C5A-C6A-C7A
22	A	818	CLA	C2A-CAA-CBA-CGA
22	2	306	CLA	C2A-CAA-CBA-CGA
22	B	811	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	O1A-CGA-O2A-C1
29	O	207	5X6	C40-C22-C23-C24
29	O	208	5X6	C40-C22-C23-C24
29	1	314	5X6	C15-C16-C17-C41
29	1	314	5X6	C40-C22-C23-C24
29	1	316	5X6	C40-C22-C23-C24
29	2	314	5X6	C15-C16-C17-C41
29	4	315	5X6	C40-C22-C23-C24
29	5	313	5X6	C15-C16-C17-C41
29	5	313	5X6	C11-C12-C13-C42

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Mol	Chain	Res	Type	Atoms
29	5	314	5X6	C15-C16-C17-C41
29	5	321	5X6	C40-C22-C23-C24
29	6	317	5X6	C39-C26-C27-C28
29	6	317	5X6	C11-C12-C13-C42
29	7	315	5X6	C11-C12-C13-C42
29	7	316	5X6	C15-C16-C17-C41
29	7	317	5X6	C11-C12-C13-C42
24	A	842	LHG	O1-C1-C2-C3
25	B	844	BCR	C7-C8-C9-C10
29	M	101	5X6	C25-C26-C27-C28
29	7	317	5X6	C25-C26-C27-C28
29	7	318	5X6	C25-C26-C27-C28
22	3	301	CLA	C3-C5-C6-C7
22	A	831	CLA	C10-C11-C12-C13
22	B	831	CLA	C5-C6-C7-C8
22	7	309	CLA	C5-C6-C7-C8
24	6	319	LHG	C8-C7-O7-C5
30	5	320	LMT	C5-C6-C7-C8
22	A	832	CLA	C16-C17-C18-C19
22	A	859	CLA	C16-C17-C18-C20
30	F	202	LMT	C2-C3-C4-C5
22	B	837	CLA	C15-C16-C17-C18
24	2	315	LHG	C24-C25-C26-C27
22	A	831	CLA	C3A-C2A-CAA-CBA
22	A	859	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	C3A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	7	306	CLA	C3A-C2A-CAA-CBA
29	4	315	5X6	C17-C18-C19-C20
22	2	305	CLA	CBD-CGD-O2D-CED
22	B	831	CLA	O2A-C1-C2-C3
29	O	207	5X6	C18-C19-C20-C21
29	O	208	5X6	C18-C19-C20-C21
29	2	313	5X6	C18-C19-C20-C21
29	4	314	5X6	C18-C19-C20-C21
29	5	313	5X6	C18-C19-C20-C21
22	B	806	CLA	O1D-CGD-O2D-CED
22	7	309	CLA	C3-C5-C6-C7
22	A	812	CLA	C4-C3-C5-C6
22	A	825	CLA	C4-C3-C5-C6
22	1	303	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	825	CLA	C2-C3-C5-C6
24	2	315	LHG	C8-C7-O7-C5
22	L	203	CLA	C8-C10-C11-C12
24	2	315	LHG	C7-C8-C9-C10
22	3	305	CLA	O1A-CGA-O2A-C1
28	B	845	DGD	O1A-C1A-O1G-C1G
22	B	839	CLA	C15-C16-C17-C18
28	B	845	DGD	C2A-C3A-C4A-C5A
22	A	807	CLA	C2-C1-O2A-CGA
22	1	302	CLA	C2-C1-O2A-CGA
22	A	839	CLA	C10-C11-C12-C13
22	B	805	CLA	O1A-CGA-O2A-C1
22	B	837	CLA	O1A-CGA-O2A-C1
28	B	845	DGD	CDA-CEA-CFA-CGA
22	B	813	CLA	C16-C17-C18-C19
22	B	850	CLA	CBD-CGD-O2D-CED
25	A	844	BCR	C23-C24-C25-C26
25	A	845	BCR	C23-C24-C25-C30
25	B	842	BCR	C1-C6-C7-C8
25	B	842	BCR	C23-C24-C25-C26
29	B	851	5X6	C27-C28-C29-C30
29	J	104	5X6	C27-C28-C29-C34
29	M	101	5X6	C02-C03-C11-C12
29	M	101	5X6	C27-C28-C29-C30
29	O	207	5X6	C04-C03-C11-C12
29	O	208	5X6	C02-C03-C11-C12
29	Z	206	5X6	C27-C28-C29-C30
29	1	312	5X6	C02-C03-C11-C12
29	1	312	5X6	C04-C03-C11-C12
29	1	316	5X6	C02-C03-C11-C12
29	2	312	5X6	C02-C03-C11-C12
29	2	313	5X6	C02-C03-C11-C12
29	3	306	5X6	C02-C03-C11-C12
29	4	314	5X6	C02-C03-C11-C12
29	4	315	5X6	C04-C03-C11-C12
29	5	312	5X6	C02-C03-C11-C12
29	5	312	5X6	C27-C28-C29-C34
29	5	313	5X6	C02-C03-C11-C12
29	5	314	5X6	C27-C28-C29-C34
29	5	321	5X6	C27-C28-C29-C30
29	6	316	5X6	C02-C03-C11-C12
29	6	317	5X6	C02-C03-C11-C12

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Mol	Chain	Res	Type	Atoms
29	7	315	5X6	C27-C28-C29-C30
29	7	317	5X6	C02-C03-C11-C12
29	7	317	5X6	C27-C28-C29-C30
29	7	318	5X6	C02-C03-C11-C12
21	A	801	CL0	CBA-CGA-O2A-C1
22	A	828	CLA	CBA-CGA-O2A-C1
22	A	859	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	B	801	CLA	C15-C16-C17-C18
22	B	804	CLA	C8-C10-C11-C12
22	6	306	CLA	C5-C6-C7-C8
22	4	306	CLA	CBD-CGD-O2D-CED
22	A	859	CLA	C15-C16-C17-C18
22	B	819	CLA	C5-C6-C7-C8
22	2	304	CLA	C8-C10-C11-C12
22	4	309	CLA	C5-C6-C7-C8
22	B	832	CLA	C4-C3-C5-C6
23	B	840	A1L64	C20-C19-C21-C22
22	A	815	CLA	C11-C10-C8-C7
22	A	817	CLA	C11-C10-C8-C7
22	A	832	CLA	C2-C3-C5-C6
22	A	834	CLA	C11-C10-C8-C7
22	A	839	CLA	C11-C12-C13-C15
22	B	809	CLA	C11-C10-C8-C7
22	B	818	CLA	C11-C10-C8-C7
22	B	822	CLA	C11-C12-C13-C15
22	B	830	CLA	C11-C10-C8-C7
22	B	832	CLA	C2-C3-C5-C6
22	B	849	CLA	C11-C10-C8-C7
22	1	303	CLA	C11-C12-C13-C15
22	3	301	CLA	C6-C7-C8-C10
22	4	303	CLA	C11-C10-C8-C7
22	5	302	CLA	C6-C7-C8-C10
21	A	801	CL0	O1A-CGA-O2A-C1
22	A	859	CLA	O1A-CGA-O2A-C1
22	K	101	CLA	O1A-CGA-O2A-C1
22	1	303	CLA	O1A-CGA-O2A-C1
29	1	316	5X6	C13-C14-C15-C16
22	A	820	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	C15-C16-C17-C18
30	5	320	LMT	C11-C10-C9-C8
22	A	832	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	842	LHG	C16-C17-C18-C19
24	1	317	LHG	C17-C18-C19-C20
22	A	833	CLA	C10-C11-C12-C13
22	7	304	CLA	C3-C5-C6-C7
29	O	208	5X6	C26-C27-C28-C29
22	B	825	CLA	CBA-CGA-O2A-C1
22	A	820	CLA	C5-C6-C7-C8
22	3	305	CLA	C5-C6-C7-C8
22	B	823	CLA	O1D-CGD-O2D-CED
28	B	845	DGD	CBA-CCA-CDA-CEA
24	4	318	LHG	C8-C7-O7-C5
22	B	824	CLA	C13-C15-C16-C17
24	4	318	LHG	C24-C25-C26-C27
22	A	824	CLA	CBA-CGA-O2A-C1
24	1	317	LHG	C16-C17-C18-C19
22	B	803	CLA	C16-C17-C18-C20
22	K	101	CLA	C6-C7-C8-C9
28	B	845	DGD	O6E-C5E-C6E-O5E
22	A	833	CLA	C8-C10-C11-C12
22	B	823	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
23	B	840	A1L64	C18-C19-C21-C22
22	A	823	CLA	C11-C10-C8-C9
22	A	839	CLA	C11-C12-C13-C14
22	B	809	CLA	C11-C10-C8-C9
22	B	822	CLA	C6-C7-C8-C9
22	B	849	CLA	C11-C10-C8-C9
22	4	303	CLA	C11-C10-C8-C9
22	4	304	CLA	C14-C13-C15-C16
22	5	302	CLA	C6-C7-C8-C9
22	5	303	CLA	C6-C7-C8-C9
22	6	304	CLA	C11-C10-C8-C9
22	A	802	CLA	C3-C5-C6-C7
22	2	304	CLA	C3-C5-C6-C7
22	1	307	CLA	C2A-CAA-CBA-CGA
29	1	316	5X6	C11-C12-C13-C14
29	4	315	5X6	C25-C26-C27-C28
29	6	315	5X6	C11-C12-C13-C14
29	7	318	5X6	C11-C12-C13-C14
22	A	828	CLA	O1A-CGA-O2A-C1
22	B	829	CLA	O1A-CGA-O2A-C1
22	A	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	B	820	CLA	C1A-C2A-CAA-CBA
22	O	206	CLA	C1A-C2A-CAA-CBA
22	1	306	CLA	C1A-C2A-CAA-CBA
22	3	301	CLA	C1A-C2A-CAA-CBA
22	3	305	CLA	C1A-C2A-CAA-CBA
22	4	305	CLA	C1A-C2A-CAA-CBA
22	5	304	CLA	C1A-C2A-CAA-CBA
22	5	311	CLA	C1A-C2A-CAA-CBA
22	6	303	CLA	C1A-C2A-CAA-CBA
22	6	308	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C16-C17-C18-C19
29	O	207	5X6	C17-C18-C19-C20
29	7	315	5X6	C19-C20-C21-C22
22	2	308	CLA	C5-C6-C7-C8
24	1	317	LHG	C19-C20-C21-C22
22	A	807	CLA	C3-C5-C6-C7
22	2	305	CLA	C3-C5-C6-C7
22	A	828	CLA	C10-C11-C12-C13
24	A	841	LHG	C31-C32-C33-C34
22	Z	204	CLA	C16-C17-C18-C19
22	1	308	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	C2C-C3C-CAC-CBC
22	A	828	CLA	C4-C3-C5-C6
22	A	832	CLA	C4-C3-C5-C6
24	1	317	LHG	C14-C15-C16-C17
22	5	306	CLA	C8-C10-C11-C12
22	A	820	CLA	O1A-CGA-O2A-C1
22	B	816	CLA	C16-C17-C18-C20
22	B	811	CLA	C10-C11-C12-C13
22	A	824	CLA	O1A-CGA-O2A-C1
22	B	816	CLA	C10-C11-C12-C13
22	F	204	CLA	C14-C13-C15-C16
22	B	849	CLA	C10-C11-C12-C13
22	A	830	CLA	C5-C6-C7-C8
22	2	304	CLA	C13-C15-C16-C17
22	A	824	CLA	C5-C6-C7-C8
22	A	859	CLA	C10-C11-C12-C13
25	L	202	BCR	C11-C10-C9-C34
22	B	814	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	6	319	LHG	C24-C25-C26-C27
22	6	311	CLA	CBD-CGD-O2D-CED
22	B	831	CLA	C13-C15-C16-C17
22	1	302	CLA	C13-C15-C16-C17
22	1	303	CLA	C8-C10-C11-C12
22	A	812	CLA	C2-C1-O2A-CGA
22	B	812	CLA	C2-C1-O2A-CGA
22	B	827	CLA	C2-C1-O2A-CGA
22	5	310	CLA	CBA-CGA-O2A-C1
23	A	840	A1L64	C22-C23-C24-C25
23	A	840	A1L64	C22-C23-C24-C26
22	A	826	CLA	C13-C15-C16-C17
22	2	305	CLA	O1D-CGD-O2D-CED
22	4	308	CLA	O1D-CGD-O2D-CED
22	A	817	CLA	C15-C16-C17-C18
22	A	833	CLA	C15-C16-C17-C18
22	A	839	CLA	C13-C15-C16-C17
22	B	805	CLA	C15-C16-C17-C18
29	6	317	5X6	C24-C25-C26-C27
22	A	816	CLA	CAA-CBA-CGA-O2A
24	6	319	LHG	O9-C7-O7-C5
22	B	825	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	C11-C10-C8-C7
22	A	816	CLA	C12-C13-C15-C16
22	A	820	CLA	C11-C10-C8-C7
22	A	823	CLA	C11-C10-C8-C7
22	A	839	CLA	C11-C10-C8-C7
22	A	859	CLA	C11-C10-C8-C7
22	B	806	CLA	C11-C12-C13-C15
22	B	814	CLA	C6-C7-C8-C10
22	B	815	CLA	C11-C10-C8-C7
22	B	817	CLA	C11-C10-C8-C7
22	B	825	CLA	C6-C7-C8-C10
22	B	837	CLA	C11-C10-C8-C7
22	B	838	CLA	C6-C7-C8-C10
22	L	204	CLA	C6-C7-C8-C10
22	Z	204	CLA	C12-C13-C15-C16
22	1	303	CLA	C12-C13-C15-C16
22	4	304	CLA	C6-C7-C8-C10
22	5	303	CLA	C2-C3-C5-C6
22	K	101	CLA	C3-C5-C6-C7
22	A	812	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	815	CLA	C11-C10-C8-C9
22	A	818	CLA	C11-C12-C13-C14
22	A	859	CLA	C11-C12-C13-C14
22	B	806	CLA	C11-C12-C13-C14
22	B	814	CLA	C6-C7-C8-C9
22	B	815	CLA	C11-C10-C8-C9
22	B	819	CLA	C11-C12-C13-C14
22	B	825	CLA	C6-C7-C8-C9
22	B	837	CLA	C11-C10-C8-C9
22	B	838	CLA	C11-C12-C13-C14
22	L	204	CLA	C6-C7-C8-C9
22	4	304	CLA	C6-C7-C8-C9
22	6	305	CLA	C11-C10-C8-C9
22	1	304	CLA	CBD-CGD-O2D-CED
22	B	810	CLA	CBA-CGA-O2A-C1
22	A	858	CLA	C5-C6-C7-C8
22	F	204	CLA	C5-C6-C7-C8
22	4	306	CLA	O1D-CGD-O2D-CED
29	M	101	5X6	C39-C26-C27-C28
29	2	312	5X6	C11-C12-C13-C42
29	7	314	5X6	C39-C26-C27-C28
22	A	820	CLA	C16-C17-C18-C19
25	Z	202	BCR	C21-C22-C23-C24
29	1	314	5X6	C25-C26-C27-C28
29	1	314	5X6	C11-C12-C13-C14
29	4	315	5X6	C11-C12-C13-C14
29	5	321	5X6	C25-C26-C27-C28
29	7	315	5X6	C15-C16-C17-C18
31	6	318	RRX	C7-C8-C9-C10
22	A	828	CLA	C13-C15-C16-C17
22	A	839	CLA	C8-C10-C11-C12
22	A	836	CLA	C5-C6-C7-C8
29	1	311	5X6	C26-C27-C28-C29
29	4	313	5X6	C26-C27-C28-C29
30	5	320	LMT	C3-C4-C5-C6
22	B	806	CLA	C5-C6-C7-C8
22	B	817	CLA	C11-C12-C13-C14
22	A	819	CLA	C4-C3-C5-C6
22	5	303	CLA	C4-C3-C5-C6
22	B	814	CLA	C2-C3-C5-C6
30	O	201	LMT	C1-C2-C3-C4
22	A	805	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	L	205	CLA	CBD-CGD-O2D-CED
22	B	850	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	C3A-C2A-CAA-CBA
22	L	204	CLA	C3A-C2A-CAA-CBA
22	1	306	CLA	C3A-C2A-CAA-CBA
22	6	313	CLA	C3A-C2A-CAA-CBA
22	B	838	CLA	C5-C6-C7-C8
29	2	314	5X6	C17-C18-C19-C20
29	7	318	5X6	C19-C20-C21-C22
30	O	201	LMT	C2-C1-O1'-C1'
24	A	841	LHG	C23-C24-C25-C26
22	1	307	CLA	CBA-CGA-O2A-C1
22	A	828	CLA	C5-C6-C7-C8
22	A	833	CLA	C13-C15-C16-C17
24	2	315	LHG	C27-C28-C29-C30
28	B	845	DGD	CCB-CDB-CEB-CFB
22	6	306	CLA	C3-C5-C6-C7
24	4	318	LHG	C27-C28-C29-C30
22	A	817	CLA	C16-C17-C18-C20
28	B	845	DGD	C9A-CAA-CBA-CCA
22	B	805	CLA	C3-C5-C6-C7
22	5	306	CLA	C3-C5-C6-C7
22	B	822	CLA	C5-C6-C7-C8
22	B	810	CLA	O1A-CGA-O2A-C1
22	7	304	CLA	C6-C7-C8-C10
24	4	318	LHG	C28-C29-C30-C31
22	5	310	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	C3-C5-C6-C7
22	7	306	CLA	C4C-C3C-CAC-CBC
28	B	845	DGD	O2G-C2G-C3G-O3G
24	4	318	LHG	C30-C31-C32-C33
24	A	860	LHG	C8-C7-O7-C5
22	3	305	CLA	O1D-CGD-O2D-CED
22	Z	204	CLA	C16-C17-C18-C20
22	2	304	CLA	C16-C17-C18-C20
24	2	315	LHG	O9-C7-O7-C5
22	1	303	CLA	C4-C3-C5-C6
22	A	832	CLA	C2-C1-O2A-CGA
22	A	833	CLA	C2-C1-O2A-CGA
22	3	305	CLA	C2-C1-O2A-CGA
22	5	306	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	826	CLA	C14-C13-C15-C16
22	A	834	CLA	C6-C7-C8-C9
22	B	830	CLA	C11-C12-C13-C14
22	O	206	CLA	C11-C10-C8-C9
22	5	302	CLA	C14-C13-C15-C16
22	6	307	CLA	C6-C7-C8-C9
22	5	301	CLA	CBD-CGD-O2D-CED
22	A	807	CLA	C8-C10-C11-C12
24	A	860	LHG	C2-C3-O3-P
24	2	315	LHG	C2-C3-O3-P
24	1	317	LHG	C32-C33-C34-C35
22	B	816	CLA	C16-C17-C18-C19
25	A	845	BCR	C23-C24-C25-C26
29	O	208	5X6	C04-C03-C11-C12
29	Z	206	5X6	C04-C03-C11-C12
29	1	311	5X6	C02-C03-C11-C12
29	1	312	5X6	C27-C28-C29-C34
29	5	313	5X6	C27-C28-C29-C34
29	6	315	5X6	C04-C03-C11-C12
29	6	315	5X6	C27-C28-C29-C34
22	1	303	CLA	C15-C16-C17-C18
25	A	843	BCR	C7-C8-C9-C34
29	6	316	5X6	C11-C12-C13-C42
22	B	821	CLA	CBA-CGA-O2A-C1
22	J	102	CLA	C1A-C2A-CAA-CBA
22	K	102	CLA	C1A-C2A-CAA-CBA
22	2	310	CLA	C1A-C2A-CAA-CBA
25	L	202	BCR	C7-C8-C9-C10
29	O	208	5X6	C21-C22-C23-C24
29	1	316	5X6	C21-C22-C23-C24
31	1	315	RRX	C7-C8-C9-C10
24	1	317	LHG	C31-C32-C33-C34
29	B	851	5X6	C18-C19-C20-C21
24	1	317	LHG	C15-C16-C17-C18
22	A	832	CLA	C16-C17-C18-C20
22	A	838	CLA	C16-C17-C18-C20
22	7	304	CLA	C6-C7-C8-C9
22	2	308	CLA	C3-C5-C6-C7
22	A	820	CLA	C13-C15-C16-C17
30	4	319	LMT	C5-C6-C7-C8
22	B	802	CLA	C4-C3-C5-C6
22	5	306	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	806	CLA	C11-C12-C13-C15
22	A	815	CLA	C12-C13-C15-C16
22	A	818	CLA	C11-C12-C13-C15
22	A	848	CLA	C11-C12-C13-C15
22	A	859	CLA	C6-C7-C8-C10
22	B	802	CLA	C6-C7-C8-C10
22	B	808	CLA	C6-C7-C8-C10
22	B	809	CLA	C11-C12-C13-C15
22	B	819	CLA	C11-C12-C13-C15
22	B	822	CLA	C6-C7-C8-C10
22	B	829	CLA	C6-C7-C8-C10
22	B	832	CLA	C12-C13-C15-C16
22	Z	204	CLA	C11-C12-C13-C15
22	1	310	CLA	C6-C7-C8-C10
22	4	303	CLA	C6-C7-C8-C10
22	4	304	CLA	C11-C12-C13-C15
22	5	302	CLA	C12-C13-C15-C16
22	6	304	CLA	C12-C13-C15-C16
22	A	820	CLA	C3-C5-C6-C7
22	A	822	CLA	C3-C5-C6-C7
28	B	845	DGD	C8A-C9A-CAA-CBA
29	O	207	5X6	C23-C24-C25-C26
29	O	208	5X6	C17-C18-C19-C20
29	2	312	5X6	C19-C20-C21-C22
29	2	312	5X6	C23-C24-C25-C26
29	2	313	5X6	C17-C18-C19-C20
29	7	317	5X6	C19-C20-C21-C22
22	A	820	CLA	C16-C17-C18-C20
22	4	303	CLA	C16-C17-C18-C19
24	4	318	LHG	O9-C7-O7-C5
22	A	818	CLA	C8-C10-C11-C12
22	5	305	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C16-C17-C18-C19
22	B	804	CLA	C16-C17-C18-C19
22	A	857	CLA	C15-C16-C17-C18
24	A	842	LHG	C24-C25-C26-C27
22	B	807	CLA	C13-C15-C16-C17
22	B	832	CLA	C5-C6-C7-C8
22	1	307	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	CAD-CBD-CGD-O2D
22	A	815	CLA	CAD-CBD-CGD-O2D
22	A	820	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	831	CLA	CAD-CBD-CGD-O2D
22	B	810	CLA	CAD-CBD-CGD-O2D
22	B	815	CLA	CAD-CBD-CGD-O2D
22	B	826	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	L	205	CLA	CAD-CBD-CGD-O2D
22	1	308	CLA	CAD-CBD-CGD-O2D
22	2	305	CLA	CAD-CBD-CGD-O2D
22	2	308	CLA	CAD-CBD-CGD-O2D
22	4	309	CLA	CAD-CBD-CGD-O2D
22	5	303	CLA	CAD-CBD-CGD-O2D
22	5	311	CLA	CAD-CBD-CGD-O2D
22	6	312	CLA	CAD-CBD-CGD-O2D
22	6	314	CLA	CAD-CBD-CGD-O2D
22	B	831	CLA	C15-C16-C17-C18
29	J	104	5X6	C03-C11-C12-C13
29	2	312	5X6	C03-C11-C12-C13
29	5	312	5X6	C03-C11-C12-C13
29	7	314	5X6	C26-C27-C28-C29
29	7	317	5X6	C26-C27-C28-C29
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	CBA-CGA-O2A-C1
22	A	817	CLA	C16-C17-C18-C19
22	A	826	CLA	C16-C17-C18-C20
22	B	824	CLA	C16-C17-C18-C19
22	6	307	CLA	C16-C17-C18-C19
24	1	317	LHG	C30-C31-C32-C33
22	A	819	CLA	C2-C3-C5-C6
22	B	802	CLA	C2-C3-C5-C6
22	1	303	CLA	C2-C3-C5-C6
24	A	842	LHG	C4-C5-C6-O8
24	6	319	LHG	C4-C5-C6-O8
24	2	315	LHG	O6-C4-C5-O7
22	B	817	CLA	CAA-CBA-CGA-O2A
22	F	206	CLA	O1D-CGD-O2D-CED
22	A	803	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	812	CLA	CHA-CBD-CGD-O1D
22	A	813	CLA	CHA-CBD-CGD-O1D
22	A	813	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	858	CLA	CHA-CBD-CGD-O2D
22	A	859	CLA	CHA-CBD-CGD-O1D
22	A	859	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	811	CLA	CHA-CBD-CGD-O1D
22	B	816	CLA	CHA-CBD-CGD-O1D
22	B	824	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O2D
22	B	834	CLA	CHA-CBD-CGD-O1D
22	F	206	CLA	CHA-CBD-CGD-O1D
22	F	206	CLA	CHA-CBD-CGD-O2D
22	L	203	CLA	CHA-CBD-CGD-O1D
22	L	203	CLA	CHA-CBD-CGD-O2D
22	L	205	CLA	CHA-CBD-CGD-O1D
22	O	204	CLA	CHA-CBD-CGD-O1D
22	2	302	CLA	CHA-CBD-CGD-O1D
22	7	303	CLA	CHA-CBD-CGD-O1D
22	7	303	CLA	CHA-CBD-CGD-O2D
22	7	309	CLA	CHA-CBD-CGD-O1D
22	7	309	CLA	CHA-CBD-CGD-O2D
22	7	310	CLA	CHA-CBD-CGD-O1D
29	4	313	5X6	C23-C24-C25-C26
22	A	848	CLA	O1D-CGD-O2D-CED
22	F	206	CLA	CBD-CGD-O2D-CED
29	J	104	5X6	C24-C25-C26-C27
29	1	316	5X6	C12-C13-C14-C15
24	A	860	LHG	O7-C5-C6-O8
24	B	846	LHG	O7-C5-C6-O8
24	1	317	LHG	O7-C5-C6-O8
22	1	310	CLA	C8-C10-C11-C12
22	A	805	CLA	O1A-CGA-O2A-C1
22	B	811	CLA	C3-C5-C6-C7
22	B	824	CLA	C3-C5-C6-C7
22	6	305	CLA	C4-C3-C5-C6
22	A	835	CLA	O1A-CGA-O2A-C1
22	B	832	CLA	C14-C13-C15-C16
22	B	833	CLA	C11-C10-C8-C9
22	B	838	CLA	C11-C10-C8-C9
22	6	304	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	6	311	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1A-CGA-O2A-C1
25	B	844	BCR	C7-C8-C9-C34
29	1	311	5X6	C11-C12-C13-C42
29	4	314	5X6	C11-C12-C13-C42
29	5	312	5X6	C11-C12-C13-C42
29	1	313	5X6	C21-C22-C23-C24
29	2	314	5X6	C11-C12-C13-C14
29	6	316	5X6	C15-C16-C17-C18
22	A	858	CLA	C3-C5-C6-C7
22	7	303	CLA	C1A-C2A-CAA-CBA
22	7	309	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C11-C12-C13-C14
22	A	810	CLA	C5-C6-C7-C8
22	B	823	CLA	C2-C1-O2A-CGA
24	A	841	LHG	C3-O3-P-O6
24	4	318	LHG	C3-O3-P-O6
22	B	839	CLA	CAA-CBA-CGA-O2A
22	B	823	CLA	C2-C3-C5-C6
28	B	845	DGD	CAB-CBB-CCB-CDB
24	J	106	LHG	C4-O6-P-O4
24	6	319	LHG	C3-O3-P-O5
22	B	806	CLA	C16-C17-C18-C19
22	7	310	CLA	C2C-C3C-CAC-CBC
22	B	835	CLA	C8-C10-C11-C12
22	O	206	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	C3-C5-C6-C7
22	A	839	CLA	C3-C5-C6-C7
22	A	833	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C6-C7-C8-C9
22	A	803	CLA	CAD-CBD-CGD-O1D
22	B	805	CLA	CAD-CBD-CGD-O1D
22	B	834	CLA	CAD-CBD-CGD-O1D
22	B	834	CLA	C2-C3-C5-C6
22	L	203	CLA	CAD-CBD-CGD-O1D
22	O	204	CLA	CAD-CBD-CGD-O1D
22	5	304	CLA	CAD-CBD-CGD-O1D
22	A	848	CLA	C15-C16-C17-C18
24	A	860	LHG	C30-C31-C32-C33
22	A	806	CLA	C15-C16-C17-C18
22	O	205	CLA	CBA-CGA-O2A-C1
22	6	304	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	B	804	CLA	C4-C3-C5-C6
22	L	205	CLA	O1D-CGD-O2D-CED
22	A	804	CLA	C6-C7-C8-C10
22	A	807	CLA	C12-C13-C15-C16
22	A	820	CLA	C11-C12-C13-C15
22	B	805	CLA	C11-C10-C8-C7
22	B	811	CLA	C11-C10-C8-C7
22	B	813	CLA	C12-C13-C15-C16
22	B	835	CLA	C11-C10-C8-C7
22	6	307	CLA	C11-C12-C13-C15
24	6	319	LHG	C23-C24-C25-C26
22	O	206	CLA	O1A-CGA-O2A-C1
22	7	309	CLA	O1A-CGA-O2A-C1
22	A	815	CLA	C13-C15-C16-C17
22	B	818	CLA	C10-C11-C12-C13
22	A	820	CLA	C2A-CAA-CBA-CGA
22	A	826	CLA	C16-C17-C18-C19
24	A	860	LHG	C4-C5-C6-O8
24	B	846	LHG	C4-C5-C6-O8
22	A	858	CLA	C15-C16-C17-C18
22	O	205	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	C4-C3-C5-C6
22	B	821	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	C11-C12-C13-C14
22	A	815	CLA	C14-C13-C15-C16
22	B	815	CLA	C11-C12-C13-C14
22	Z	204	CLA	C11-C12-C13-C14
22	1	302	CLA	C14-C13-C15-C16
22	5	303	CLA	C11-C10-C8-C9
29	1	313	5X6	C03-C11-C12-C13
29	3	306	5X6	C03-C11-C12-C13
22	4	303	CLA	C8-C10-C11-C12
29	M	101	5X6	C19-C20-C21-C22
24	6	319	LHG	C7-C8-C9-C10
25	A	862	BCR	C7-C8-C9-C34
22	A	823	CLA	C8-C10-C11-C12
22	A	828	CLA	C16-C17-C18-C19
29	Z	206	5X6	C15-C16-C17-C18
29	Z	206	5X6	C11-C12-C13-C14
22	O	206	CLA	C5-C6-C7-C8
22	1	302	CLA	C10-C11-C12-C13
25	B	844	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
22	O	206	CLA	C4-C3-C5-C6
22	A	816	CLA	C13-C15-C16-C17
22	1	307	CLA	CAA-CBA-CGA-O2A
22	B	826	CLA	C2-C1-O2A-CGA
22	O	205	CLA	C2-C1-O2A-CGA
22	1	310	CLA	C2-C1-O2A-CGA
22	B	804	CLA	C16-C17-C18-C20
22	1	304	CLA	O1D-CGD-O2D-CED
22	7	309	CLA	CBA-CGA-O2A-C1
22	L	204	CLA	O1A-CGA-O2A-C1
22	B	833	CLA	C16-C17-C18-C19
25	B	842	BCR	C5-C6-C7-C8
29	1	314	5X6	C27-C28-C29-C34
29	2	312	5X6	C27-C28-C29-C34
29	4	313	5X6	C27-C28-C29-C34
29	6	316	5X6	C27-C28-C29-C34
29	7	315	5X6	C27-C28-C29-C34
29	7	316	5X6	C04-C03-C11-C12
22	6	305	CLA	C2-C3-C5-C6
22	B	803	CLA	C8-C10-C11-C12
29	1	311	5X6	C16-C17-C18-C19
29	5	313	5X6	C16-C17-C18-C19
24	A	842	LHG	C3-O3-P-O6
24	A	860	LHG	C3-O3-P-O6
24	4	318	LHG	C4-O6-P-O3
22	A	817	CLA	C8-C10-C11-C12
24	6	319	LHG	C28-C29-C30-C31
22	A	804	CLA	C4-C3-C5-C6
22	B	807	CLA	C4-C3-C5-C6
22	B	830	CLA	C11-C12-C13-C15
22	5	306	CLA	C11-C10-C8-C7
22	A	816	CLA	C14-C13-C15-C16
22	A	859	CLA	C6-C7-C8-C9
22	B	818	CLA	C11-C10-C8-C9
22	Z	204	CLA	C14-C13-C15-C16
22	6	307	CLA	C11-C12-C13-C14
22	L	204	CLA	C5-C6-C7-C8
29	1	316	5X6	C23-C24-C25-C26
29	7	314	5X6	C13-C14-C15-C16
29	7	318	5X6	C13-C14-C15-C16
22	B	812	CLA	C6-C7-C8-C10
22	L	204	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	806	CLA	C16-C17-C18-C20
22	7	310	CLA	C4C-C3C-CAC-CBC
22	A	828	CLA	C8-C10-C11-C12
22	4	304	CLA	C13-C15-C16-C17
29	4	313	5X6	C11-C12-C13-C14
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	858	CLA	C13-C15-C16-C17
22	A	806	CLA	C8-C10-C11-C12
22	A	857	CLA	C2A-CAA-CBA-CGA
22	B	830	CLA	C16-C17-C18-C20
29	O	208	5X6	C13-C14-C15-C16
29	1	314	5X6	C23-C24-C25-C26
29	7	314	5X6	C19-C20-C21-C22
24	2	315	LHG	O6-C4-C5-C6
22	B	827	CLA	C3-C5-C6-C7
22	6	304	CLA	C3-C5-C6-C7
22	A	819	CLA	O1A-CGA-O2A-C1
22	2	303	CLA	C4-C3-C5-C6
22	B	809	CLA	C15-C16-C17-C18
24	A	841	LHG	C17-C18-C19-C20
22	A	802	CLA	C2-C1-O2A-CGA
22	B	805	CLA	C2-C1-O2A-CGA
22	B	835	CLA	C2-C1-O2A-CGA
22	1	303	CLA	C2-C1-O2A-CGA
22	2	305	CLA	C2C-C3C-CAC-CBC
22	B	808	CLA	C8-C10-C11-C12
22	B	822	CLA	C13-C15-C16-C17
22	B	832	CLA	C13-C15-C16-C17
22	3	301	CLA	C10-C11-C12-C13
22	6	303	CLA	CAA-CBA-CGA-O1A
30	F	202	LMT	C4'-C5'-C6'-O6'
22	A	816	CLA	CAA-CBA-CGA-O1A
22	5	301	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	C3A-C2A-CAA-CBA
22	B	802	CLA	C3A-C2A-CAA-CBA
22	7	307	CLA	C3A-C2A-CAA-CBA
22	2	306	CLA	CAA-CBA-CGA-O1A
22	2	304	CLA	C16-C17-C18-C19
23	A	840	A1L64	C5-C4-O4-C4M
22	A	819	CLA	C11-C10-C8-C9
22	A	820	CLA	C11-C12-C13-C14
22	5	306	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	6	305	CLA	C11-C12-C13-C14
24	1	317	LHG	C34-C35-C36-C37
22	1	305	CLA	CAA-CBA-CGA-O1A
22	1	305	CLA	CAA-CBA-CGA-O2A
22	5	301	CLA	CAA-CBA-CGA-O1A
25	A	846	BCR	C11-C10-C9-C34
25	A	846	BCR	C16-C17-C18-C36
25	2	301	BCR	C20-C21-C22-C37
28	B	845	DGD	C1G-C2G-C3G-O3G
29	M	101	5X6	C42-C13-C14-C15
29	7	314	5X6	C41-C17-C18-C19
29	7	314	5X6	C20-C21-C22-C40
22	3	305	CLA	C3-C5-C6-C7
22	2	311	CLA	CAA-CBA-CGA-O1A
22	3	303	CLA	CAA-CBA-CGA-O1A
24	A	841	LHG	C30-C31-C32-C33
22	A	859	CLA	O2A-C1-C2-C3
22	B	817	CLA	O2A-C1-C2-C3
22	1	309	CLA	CAA-CBA-CGA-O1A
22	6	303	CLA	CAA-CBA-CGA-O2A
22	7	307	CLA	CAA-CBA-CGA-O1A
29	Z	206	5X6	C11-C12-C13-C42
31	5	322	RRX	C7-C8-C9-C34
22	5	301	CLA	CAA-CBA-CGA-O2A
22	5	305	CLA	CAA-CBA-CGA-O1A
24	J	106	LHG	C4-C5-O7-C7
24	2	315	LHG	C4-C5-O7-C7
22	B	830	CLA	C4-C3-C5-C6
22	Z	204	CLA	C4-C3-C5-C6
22	6	310	CLA	C4-C3-C5-C6
22	B	815	CLA	C1A-C2A-CAA-CBA
22	K	101	CLA	C1A-C2A-CAA-CBA
22	L	204	CLA	C1A-C2A-CAA-CBA
22	O	205	CLA	C1A-C2A-CAA-CBA
22	2	303	CLA	C1A-C2A-CAA-CBA
22	3	303	CLA	C1A-C2A-CAA-CBA
22	5	302	CLA	C1A-C2A-CAA-CBA
22	7	304	CLA	C1A-C2A-CAA-CBA
22	7	307	CLA	C1A-C2A-CAA-CBA
22	7	312	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C16-C17-C18-C19
22	A	811	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	A	833	CLA	C11-C12-C13-C15
22	A	837	CLA	C6-C7-C8-C10
22	A	838	CLA	C11-C10-C8-C7
22	B	807	CLA	C6-C7-C8-C10
22	B	833	CLA	C6-C7-C8-C10
22	Z	204	CLA	C2-C3-C5-C6
22	5	303	CLA	C11-C10-C8-C7
22	5	305	CLA	CAA-CBA-CGA-O2A
22	B	817	CLA	C10-C11-C12-C13
22	7	307	CLA	CAA-CBA-CGA-O2A
22	B	825	CLA	C15-C16-C17-C18
24	1	317	LHG	O6-C4-C5-C6
22	A	838	CLA	C3-C5-C6-C7
22	A	808	CLA	C6-C7-C8-C10
22	1	302	CLA	C16-C17-C18-C20
22	A	802	CLA	C4-C3-C5-C6
22	F	204	CLA	C4-C3-C5-C6
22	A	808	CLA	C5-C6-C7-C8
23	B	840	A1L64	C2-C3-O3-C3M
23	B	840	A1L64	C5-C4-O4-C4M
25	A	846	BCR	C11-C10-C9-C8
25	A	846	BCR	C16-C17-C18-C19
25	F	207	BCR	C12-C13-C14-C15
25	2	301	BCR	C20-C21-C22-C23
30	F	202	LMT	C3-C4-C5-C6
29	1	312	5X6	C18-C19-C20-C21
22	A	831	CLA	CBA-CGA-O2A-C1
21	A	801	CL0	CAA-CBA-CGA-O2A
22	B	813	CLA	C4C-C3C-CAC-CBC
29	O	208	5X6	C23-C24-C25-C26
29	1	313	5X6	C13-C14-C15-C16
29	6	317	5X6	C17-C18-C19-C20
22	2	311	CLA	CAA-CBA-CGA-O2A
29	6	315	5X6	C26-C27-C28-C29
22	A	831	CLA	O1A-CGA-O2A-C1
22	1	309	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C4-C3-C5-C6
22	5	302	CLA	C4-C3-C5-C6
22	A	824	CLA	C2-C1-O2A-CGA
22	A	829	CLA	C2-C1-O2A-CGA
22	B	803	CLA	C2-C1-O2A-CGA
22	B	807	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	O	206	CLA	C2-C3-C5-C6
29	6	317	5X6	C14-C15-C16-C17
22	3	303	CLA	CAA-CBA-CGA-O2A
22	4	306	CLA	CAA-CBA-CGA-O2A
22	7	305	CLA	CAA-CBA-CGA-O1A
22	A	836	CLA	C6-C7-C8-C9
22	B	806	CLA	C6-C7-C8-C9
24	A	841	LHG	C33-C34-C35-C36
22	B	813	CLA	C2C-C3C-CAC-CBC
24	A	841	LHG	C11-C12-C13-C14
28	B	845	DGD	C3A-C4A-C5A-C6A
22	7	305	CLA	CAA-CBA-CGA-O2A
22	4	304	CLA	C10-C11-C12-C13
22	B	815	CLA	C2A-CAA-CBA-CGA
22	6	310	CLA	C6-C7-C8-C10
22	2	306	CLA	CAA-CBA-CGA-O2A
22	A	815	CLA	O1A-CGA-O2A-C1
25	A	843	BCR	C23-C24-C25-C30
25	A	846	BCR	C23-C24-C25-C26
29	J	104	5X6	C04-C03-C11-C12
29	O	208	5X6	C27-C28-C29-C34
29	1	313	5X6	C02-C03-C11-C12
29	1	313	5X6	C27-C28-C29-C34
29	5	314	5X6	C04-C03-C11-C12
29	5	321	5X6	C04-C03-C11-C12
29	7	316	5X6	C27-C28-C29-C34
22	7	303	CLA	CAA-CBA-CGA-O1A
22	A	807	CLA	C13-C15-C16-C17
29	7	317	5X6	C13-C14-C15-C16
29	O	208	5X6	C15-C16-C17-C18
22	A	818	CLA	C2-C3-C5-C6
22	B	821	CLA	O1A-CGA-O2A-C1
22	B	816	CLA	C13-C15-C16-C17
29	3	306	5X6	C18-C19-C20-C21
29	6	315	5X6	C18-C19-C20-C21
22	4	304	CLA	C16-C17-C18-C20
24	A	842	LHG	O6-C4-C5-O7
22	4	306	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	C2A-CAA-CBA-CGA
23	A	840	A1L64	C2-C3-O3-C3M
22	A	858	CLA	C8-C10-C11-C12
22	7	313	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	B	811	CLA	C16-C17-C18-C19
22	A	827	CLA	C4-C3-C5-C6
22	A	804	CLA	C2-C3-C5-C6
22	B	804	CLA	C6-C7-C8-C10
22	B	822	CLA	C12-C13-C15-C16
22	B	830	CLA	C2-C3-C5-C6
22	F	204	CLA	C2-C3-C5-C6
22	1	302	CLA	C12-C13-C15-C16
22	2	303	CLA	C2-C3-C5-C6
22	4	304	CLA	C11-C10-C8-C7
22	B	850	CLA	CAA-CBA-CGA-O1A
22	B	831	CLA	C3-C5-C6-C7
29	6	315	5X6	C19-C20-C21-C22
24	A	841	LHG	C1-C2-C3-O3
30	O	201	LMT	O1'-C1-C2-C3
22	B	850	CLA	CAA-CBA-CGA-O2A
22	3	302	CLA	CAA-CBA-CGA-O2A
24	A	860	LHG	C26-C27-C28-C29
25	F	207	BCR	C35-C13-C14-C15
25	K	103	BCR	C16-C17-C18-C36
22	B	809	CLA	CAA-CBA-CGA-O2A
22	B	837	CLA	C4-C3-C5-C6
22	B	849	CLA	C4-C3-C5-C6
22	L	203	CLA	C4-C3-C5-C6
22	5	302	CLA	C2-C3-C5-C6
22	6	310	CLA	C2-C3-C5-C6
22	A	818	CLA	C5-C6-C7-C8
22	A	804	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C14-C13-C15-C16
22	A	833	CLA	C11-C12-C13-C14
22	A	858	CLA	C11-C10-C8-C9
22	B	805	CLA	C11-C10-C8-C9
22	1	303	CLA	C14-C13-C15-C16
22	A	823	CLA	C3A-C2A-CAA-CBA
22	6	306	CLA	C3A-C2A-CAA-CBA
22	A	823	CLA	CAA-CBA-CGA-O2A
22	7	312	CLA	CAA-CBA-CGA-O2A
22	A	804	CLA	CAD-CBD-CGD-O2D
22	A	805	CLA	CAD-CBD-CGD-O2D
22	A	810	CLA	CAD-CBD-CGD-O2D
22	A	818	CLA	CAD-CBD-CGD-O2D
22	A	824	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	829	CLA	CAD-CBD-CGD-O2D
22	A	835	CLA	CAD-CBD-CGD-O2D
22	B	812	CLA	CAD-CBD-CGD-O2D
22	B	814	CLA	CAD-CBD-CGD-O2D
22	B	837	CLA	CAD-CBD-CGD-O2D
22	B	839	CLA	CAD-CBD-CGD-O2D
22	F	205	CLA	CAD-CBD-CGD-O2D
22	O	206	CLA	CAD-CBD-CGD-O2D
22	Z	204	CLA	CAD-CBD-CGD-O2D
22	2	307	CLA	CAD-CBD-CGD-O2D
22	3	305	CLA	CAD-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O2D
22	4	312	CLA	CAD-CBD-CGD-O2D
22	5	302	CLA	CAD-CBD-CGD-O2D
22	5	306	CLA	CAD-CBD-CGD-O2D
22	7	306	CLA	CAD-CBD-CGD-O2D
24	A	860	LHG	C4-C5-O7-C7
22	7	306	CLA	C6-C7-C8-C10
22	5	305	CLA	C2C-C3C-CAC-CBC
22	A	833	CLA	CBD-CGD-O2D-CED
22	2	308	CLA	C2-C1-O2A-CGA
22	1	304	CLA	CAA-CBA-CGA-O2A
22	K	101	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	C13-C15-C16-C17
22	A	830	CLA	C4-C3-C5-C6
22	B	817	CLA	C4-C3-C5-C6
22	A	802	CLA	C6-C7-C8-C9
22	B	802	CLA	C16-C17-C18-C19
22	A	802	CLA	C2-C3-C5-C6
22	A	827	CLA	C2-C3-C5-C6
22	B	815	CLA	CAA-CBA-CGA-O2A
22	5	303	CLA	CAA-CBA-CGA-O2A
29	J	104	5X6	C11-C12-C13-C14
29	O	207	5X6	C21-C22-C23-C24
29	4	315	5X6	C21-C22-C23-C24
22	L	205	CLA	CAA-CBA-CGA-O2A
22	1	306	CLA	CAA-CBA-CGA-O1A
22	7	313	CLA	CAA-CBA-CGA-O1A
22	A	823	CLA	O1A-CGA-O2A-C1
22	1	306	CLA	CAA-CBA-CGA-O2A
22	A	804	CLA	O2A-C1-C2-C3
22	A	808	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	B	815	CLA	O2A-C1-C2-C3
22	L	203	CLA	O2A-C1-C2-C3
22	1	302	CLA	O2A-C1-C2-C3
22	4	309	CLA	O2A-C1-C2-C3
22	5	310	CLA	O2A-C1-C2-C3
22	6	305	CLA	O2A-C1-C2-C3
22	A	815	CLA	CBA-CGA-O2A-C1
22	A	810	CLA	C2A-CAA-CBA-CGA
22	A	811	CLA	O1A-CGA-O2A-C1
22	3	302	CLA	CAA-CBA-CGA-O1A
22	7	312	CLA	CAA-CBA-CGA-O1A
22	A	803	CLA	CHA-CBD-CGD-O2D
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	858	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	805	CLA	CHA-CBD-CGD-O1D
22	B	809	CLA	CHA-CBD-CGD-O1D
22	B	809	CLA	CHA-CBD-CGD-O2D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	834	CLA	CHA-CBD-CGD-O2D
22	O	204	CLA	CHA-CBD-CGD-O2D
22	2	303	CLA	CHA-CBD-CGD-O2D
22	2	306	CLA	CHA-CBD-CGD-O1D
22	2	306	CLA	CHA-CBD-CGD-O2D
22	4	303	CLA	CHA-CBD-CGD-O2D
22	5	304	CLA	CHA-CBD-CGD-O1D
22	5	307	CLA	CHA-CBD-CGD-O2D
22	5	310	CLA	CHA-CBD-CGD-O1D
22	5	310	CLA	CHA-CBD-CGD-O2D
22	6	308	CLA	CHA-CBD-CGD-O1D
22	6	308	CLA	CHA-CBD-CGD-O2D
22	6	310	CLA	CHA-CBD-CGD-O1D
22	6	310	CLA	CHA-CBD-CGD-O2D
22	6	314	CLA	CHA-CBD-CGD-O2D
22	7	313	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	C4-C3-C5-C6
25	K	103	BCR	C16-C17-C18-C19
29	4	314	5X6	C24-C25-C26-C27
24	1	317	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
22	A	831	CLA	C16-C17-C18-C19
22	A	803	CLA	CAA-CBA-CGA-O2A
22	A	818	CLA	CAA-CBA-CGA-O2A
22	B	812	CLA	CAA-CBA-CGA-O2A
24	A	860	LHG	O7-C7-C8-C9
22	A	811	CLA	CBA-CGA-O2A-C1
22	5	305	CLA	C4C-C3C-CAC-CBC
22	B	806	CLA	CAA-CBA-CGA-O2A
24	A	841	LHG	O7-C7-C8-C9
22	A	804	CLA	CBD-CGD-O2D-CED
22	A	804	CLA	C5-C6-C7-C8
22	A	832	CLA	C13-C15-C16-C17
22	B	832	CLA	C15-C16-C17-C18
22	2	303	CLA	C3-C5-C6-C7
24	A	860	LHG	C7-C8-C9-C10
24	A	842	LHG	C8-C7-O7-C5
22	A	837	CLA	C4-C3-C5-C6
22	B	818	CLA	C4-C3-C5-C6
22	A	858	CLA	C11-C10-C8-C7
22	B	804	CLA	C2-C3-C5-C6
22	B	806	CLA	C6-C7-C8-C10
22	B	831	CLA	C11-C12-C13-C15
22	O	206	CLA	C6-C7-C8-C10
22	2	304	CLA	C11-C12-C13-C15
22	4	303	CLA	C16-C17-C18-C20
22	7	303	CLA	CAA-CBA-CGA-O2A
22	A	819	CLA	C11-C12-C13-C14
22	A	820	CLA	C6-C7-C8-C9
22	B	804	CLA	C6-C7-C8-C9
22	B	819	CLA	C6-C7-C8-C9
22	2	303	CLA	C6-C7-C8-C9
22	4	309	CLA	C14-C13-C15-C16
22	A	827	CLA	C2B-C3B-CAB-CBB
22	B	828	CLA	C2B-C3B-CAB-CBB
22	K	101	CLA	C2B-C3B-CAB-CBB
22	O	203	CLA	C2B-C3B-CAB-CBB
22	1	307	CLA	C2B-C3B-CAB-CBB
22	6	313	CLA	C2B-C3B-CAB-CBB
22	7	303	CLA	C2B-C3B-CAB-CBB
22	1	304	CLA	CAA-CBA-CGA-O1A
22	A	823	CLA	CBA-CGA-O2A-C1
22	A	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	839	CLA	C5-C6-C7-C8
22	L	205	CLA	CAA-CBA-CGA-O1A
22	B	809	CLA	CAA-CBA-CGA-O1A
22	6	310	CLA	C5-C6-C7-C8
22	A	808	CLA	C6-C7-C8-C9
22	B	824	CLA	C16-C17-C18-C20
22	6	310	CLA	C6-C7-C8-C9
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C1A-C2A-CAA-CBA
22	B	802	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	C1A-C2A-CAA-CBA
22	L	203	CLA	C1A-C2A-CAA-CBA
22	4	303	CLA	C1A-C2A-CAA-CBA
22	4	308	CLA	C1A-C2A-CAA-CBA
22	6	304	CLA	C1A-C2A-CAA-CBA
22	6	313	CLA	C1A-C2A-CAA-CBA
24	6	319	LHG	C1-C2-C3-O3
24	A	841	LHG	C19-C20-C21-C22
24	6	319	LHG	C27-C28-C29-C30
24	A	841	LHG	C32-C33-C34-C35
24	A	842	LHG	C18-C19-C20-C21
22	A	823	CLA	CAA-CBA-CGA-O1A
22	K	101	CLA	CAA-CBA-CGA-O1A
22	5	303	CLA	CAA-CBA-CGA-O1A
22	A	825	CLA	CAA-CBA-CGA-O2A
22	B	830	CLA	C3-C5-C6-C7
22	F	205	CLA	CAA-CBA-CGA-O2A
22	2	306	CLA	C4B-C3B-CAB-CBB
22	2	309	CLA	C4B-C3B-CAB-CBB
22	7	304	CLA	C4B-C3B-CAB-CBB
22	7	310	CLA	C4B-C3B-CAB-CBB
24	A	841	LHG	C4-O6-P-O5
24	A	842	LHG	C3-O3-P-O5
24	A	860	LHG	C4-O6-P-O5
22	A	804	CLA	CAA-CBA-CGA-O1A
22	B	806	CLA	CAA-CBA-CGA-O1A
22	B	801	CLA	CAA-CBA-CGA-O2A
22	3	304	CLA	CAA-CBA-CGA-O2A
22	4	308	CLA	C3-C5-C6-C7
25	A	843	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	J	103	BCR	C1-C6-C7-C8
29	B	851	5X6	C02-C03-C11-C12
22	Z	204	CLA	C15-C16-C17-C18
22	B	815	CLA	CAA-CBA-CGA-O1A
22	A	809	CLA	C16-C17-C18-C20
22	1	302	CLA	C16-C17-C18-C19
28	B	845	DGD	O6D-C5D-C6D-O5D
22	B	812	CLA	CAA-CBA-CGA-O1A
28	B	845	DGD	C3B-C4B-C5B-C6B
22	Z	201	CLA	CAA-CBA-CGA-O2A
24	2	315	LHG	O7-C7-C8-C9
22	6	307	CLA	C4-C3-C5-C6
22	A	808	CLA	CAD-CBD-CGD-O1D
22	A	811	CLA	CAD-CBD-CGD-O1D
22	B	802	CLA	CAD-CBD-CGD-O1D
22	B	807	CLA	CAD-CBD-CGD-O1D
22	B	808	CLA	CAD-CBD-CGD-O1D
22	B	839	CLA	CAD-CBD-CGD-O1D
22	2	304	CLA	CAD-CBD-CGD-O1D
22	2	311	CLA	CAD-CBD-CGD-O1D
22	3	301	CLA	CAD-CBD-CGD-O1D
22	3	303	CLA	CAD-CBD-CGD-O1D
22	4	305	CLA	CAD-CBD-CGD-O1D
22	6	307	CLA	CAD-CBD-CGD-O1D
24	A	860	LHG	C6-C5-O7-C7
24	B	846	LHG	C4-C5-O7-C7
24	B	846	LHG	C6-C5-O7-C7
22	A	803	CLA	CAA-CBA-CGA-O1A
24	A	841	LHG	O8-C23-C24-C25
24	4	318	LHG	O8-C23-C24-C25
22	A	825	CLA	C13-C15-C16-C17
22	5	303	CLA	C13-C15-C16-C17
22	A	819	CLA	C6-C7-C8-C9
22	A	820	CLA	C14-C13-C15-C16
22	A	837	CLA	C6-C7-C8-C9
22	B	829	CLA	C14-C13-C15-C16
24	2	315	LHG	C30-C31-C32-C33
30	F	202	LMT	C11-C10-C9-C8
22	A	818	CLA	CAA-CBA-CGA-O1A
22	A	826	CLA	CAA-CBA-CGA-O2A
22	2	305	CLA	CAA-CBA-CGA-O2A
22	5	304	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	A	841	LHG	C35-C36-C37-C38
22	B	817	CLA	CAA-CBA-CGA-O1A
22	A	810	CLA	CAA-CBA-CGA-O2A
22	A	859	CLA	CAA-CBA-CGA-O2A
22	B	829	CLA	CAA-CBA-CGA-O2A
22	2	308	CLA	CAA-CBA-CGA-O2A
22	3	301	CLA	CAA-CBA-CGA-O2A
22	A	848	CLA	C8-C10-C11-C12
24	4	318	LHG	O10-C23-C24-C25
22	B	825	CLA	C5-C6-C7-C8
22	A	806	CLA	C6-C7-C8-C10
22	A	819	CLA	C11-C12-C13-C15
22	A	828	CLA	C11-C10-C8-C7
22	A	834	CLA	C6-C7-C8-C10
22	B	813	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C3A-C2A-CAA-CBA
22	2	305	CLA	C3A-C2A-CAA-CBA
22	6	307	CLA	C6-C7-C8-C10
22	3	301	CLA	CAA-CBA-CGA-O1A
22	F	205	CLA	CAA-CBA-CGA-O1A
22	A	839	CLA	CAA-CBA-CGA-O2A
22	4	305	CLA	CAA-CBA-CGA-O2A
25	A	862	BCR	C7-C8-C9-C10
29	1	314	5X6	C15-C16-C17-C18
29	2	314	5X6	C25-C26-C27-C28
22	2	305	CLA	CAA-CBA-CGA-O1A
29	7	316	5X6	C13-C14-C15-C16
24	1	317	LHG	C24-C25-C26-C27
22	7	306	CLA	C6-C7-C8-C9
22	2	303	CLA	CAA-CBA-CGA-O2A
22	1	302	CLA	C8-C10-C11-C12
23	B	840	A1L64	C3-C4-O4-C4M
22	A	810	CLA	CAA-CBA-CGA-O1A
22	A	825	CLA	CAA-CBA-CGA-O1A
22	4	305	CLA	CAA-CBA-CGA-O1A
22	5	304	CLA	CAA-CBA-CGA-O1A
24	A	841	LHG	O10-C23-C24-C25
22	Z	201	CLA	CAA-CBA-CGA-O1A
22	6	313	CLA	CAA-CBA-CGA-O2A
22	Z	204	CLA	C8-C10-C11-C12
24	6	319	LHG	O2-C2-C3-O3
22	A	811	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	6	305	CLA	CAA-CBA-CGA-O2A
22	B	804	CLA	C10-C11-C12-C13
22	5	303	CLA	C5-C6-C7-C8
24	A	842	LHG	O9-C7-C8-C9
22	A	838	CLA	C2A-CAA-CBA-CGA
22	3	304	CLA	CAA-CBA-CGA-O1A
22	4	306	CLA	C2C-C3C-CAC-CBC
22	2	303	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

150 monomers are involved in 214 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Z	204	CLA	3	0
22	A	830	CLA	2	0
22	B	850	CLA	1	0
22	7	310	CLA	1	0
22	1	307	CLA	1	0
31	4	317	RRX	6	0
22	A	802	CLA	1	0
24	4	318	LHG	1	0
22	1	302	CLA	1	0
25	B	842	BCR	2	0
22	6	312	CLA	1	0
22	1	303	CLA	1	0
22	B	819	CLA	1	0
22	4	311	CLA	2	0
25	F	201	BCR	3	0
22	7	311	CLA	2	0
21	A	801	CL0	1	0
22	7	307	CLA	1	0
22	A	829	CLA	1	0
22	F	204	CLA	1	0
25	L	202	BCR	1	0
22	A	821	CLA	1	0
31	5	322	RRX	2	0
22	5	304	CLA	1	0
25	4	316	BCR	2	0
22	1	306	CLA	1	0
22	B	811	CLA	1	0
22	2	308	CLA	1	0
25	B	841	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	J	103	BCR	1	0
22	7	313	CLA	1	0
22	A	858	CLA	1	0
22	B	838	CLA	2	0
22	A	837	CLA	3	0
22	A	827	CLA	1	0
22	2	310	CLA	2	0
22	B	825	CLA	1	0
22	B	828	CLA	2	0
22	B	833	CLA	2	0
22	2	309	CLA	1	0
31	1	315	RRX	3	0
25	1	301	BCR	2	0
22	6	308	CLA	1	0
25	A	846	BCR	2	0
22	2	306	CLA	1	0
22	B	831	CLA	1	0
22	F	206	CLA	1	0
22	A	814	CLA	2	0
22	O	204	CLA	1	0
22	B	820	CLA	1	0
22	L	203	CLA	1	0
22	5	310	CLA	1	0
22	B	801	CLA	2	0
22	1	305	CLA	1	0
22	A	831	CLA	1	0
22	A	816	CLA	4	0
25	K	103	BCR	4	0
30	O	201	LMT	1	0
24	J	106	LHG	1	0
22	3	304	CLA	1	0
22	6	306	CLA	1	0
22	5	305	CLA	1	0
25	Z	205	BCR	4	0
22	O	203	CLA	1	0
22	7	306	CLA	2	0
22	3	301	CLA	1	0
22	B	839	CLA	1	0
22	Z	201	CLA	2	0
25	L	206	BCR	1	0
22	6	311	CLA	1	0
22	B	821	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	844	BCR	1	0
22	6	313	CLA	1	0
22	A	822	CLA	1	0
22	K	102	CLA	2	0
22	3	305	CLA	1	0
22	A	803	CLA	1	0
22	4	310	CLA	3	0
22	A	815	CLA	1	0
25	A	862	BCR	2	0
22	B	849	CLA	1	0
25	B	843	BCR	2	0
22	4	307	CLA	2	0
25	B	844	BCR	2	0
22	B	803	CLA	4	0
22	4	306	CLA	1	0
22	B	810	CLA	1	0
22	B	824	CLA	1	0
22	B	817	CLA	1	0
25	5	315	BCR	1	0
25	I	102	BCR	1	0
31	6	318	RRX	3	0
22	B	813	CLA	1	0
22	A	804	CLA	1	0
22	B	827	CLA	1	0
22	B	836	CLA	1	0
22	A	857	CLA	2	0
22	6	303	CLA	1	0
22	A	807	CLA	1	0
22	B	808	CLA	2	0
22	7	309	CLA	1	0
22	B	818	CLA	1	0
22	2	307	CLA	1	0
22	B	806	CLA	3	0
22	2	304	CLA	1	0
22	B	835	CLA	1	0
22	2	305	CLA	3	0
22	3	303	CLA	1	0
22	1	308	CLA	1	0
22	7	303	CLA	4	0
22	7	308	CLA	1	0
22	B	812	CLA	5	0
22	7	312	CLA	1	0

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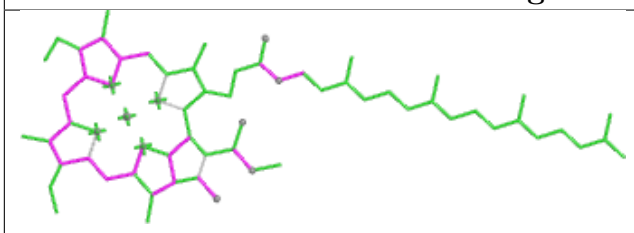
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	861	BCR	4	0
28	B	845	DGD	1	0
22	A	859	CLA	2	0
22	B	837	CLA	1	0
22	A	817	CLA	1	0
22	L	205	CLA	2	0
22	5	307	CLA	1	0
22	4	309	CLA	2	0
22	7	304	CLA	1	0
22	6	309	CLA	1	0
22	1	309	CLA	1	0
22	5	301	CLA	1	0
25	L	201	BCR	1	0
22	B	822	CLA	2	0
22	B	823	CLA	1	0
22	6	314	CLA	1	0
25	F	207	BCR	2	0
22	4	312	CLA	1	0
22	5	308	CLA	1	0
22	4	305	CLA	1	0
22	A	809	CLA	2	0
22	2	311	CLA	1	0
25	A	843	BCR	2	0
22	B	804	CLA	1	0
22	F	205	CLA	2	0
22	A	838	CLA	1	0
22	A	839	CLA	1	0
22	B	834	CLA	1	0
22	J	102	CLA	1	0
22	A	808	CLA	1	0
22	O	205	CLA	1	0
22	2	302	CLA	5	0
22	5	309	CLA	1	0
22	B	802	CLA	3	0
22	B	809	CLA	2	0
22	6	307	CLA	2	0
22	A	833	CLA	1	0

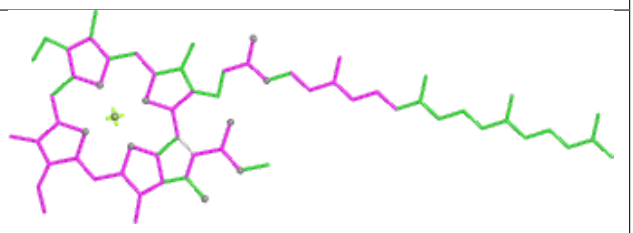
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

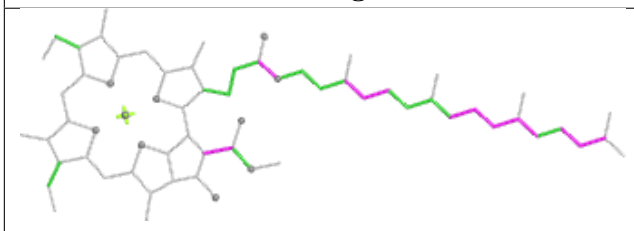
Ligand CLA Z 204



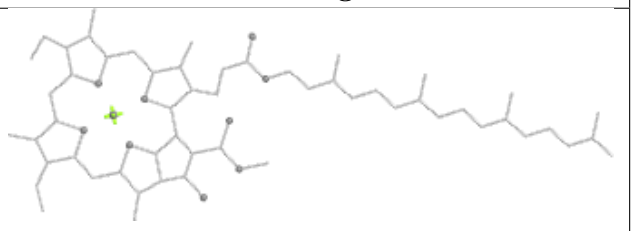
Bond lengths



Bond angles

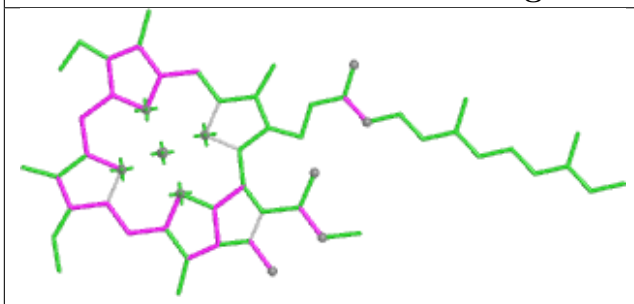


Torsions

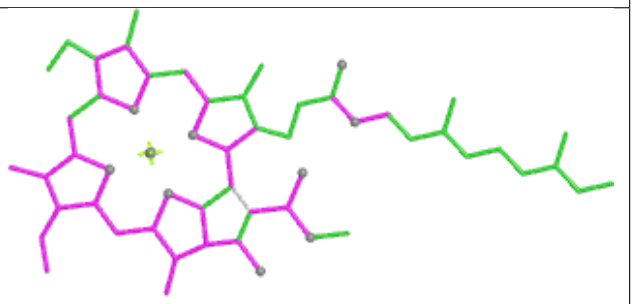


Rings

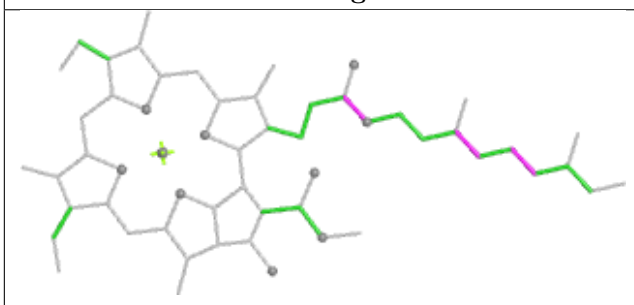
Ligand CLA A 830



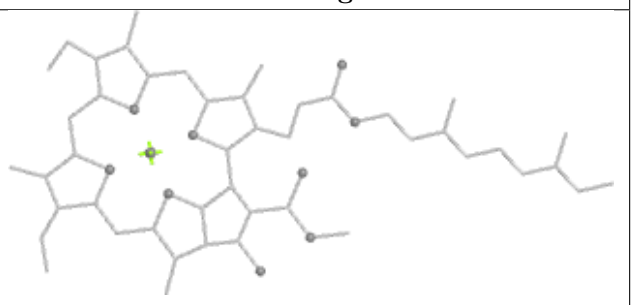
Bond lengths



Bond angles

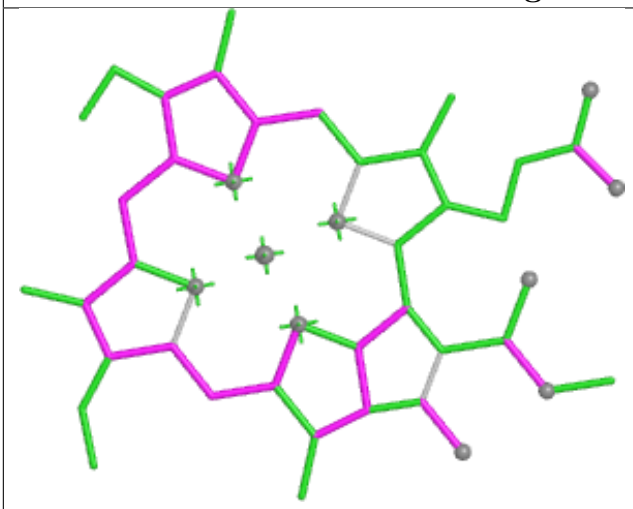


Torsions

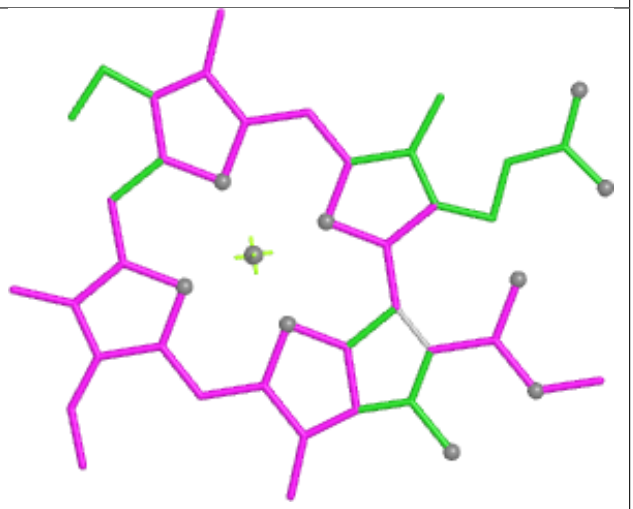


Rings

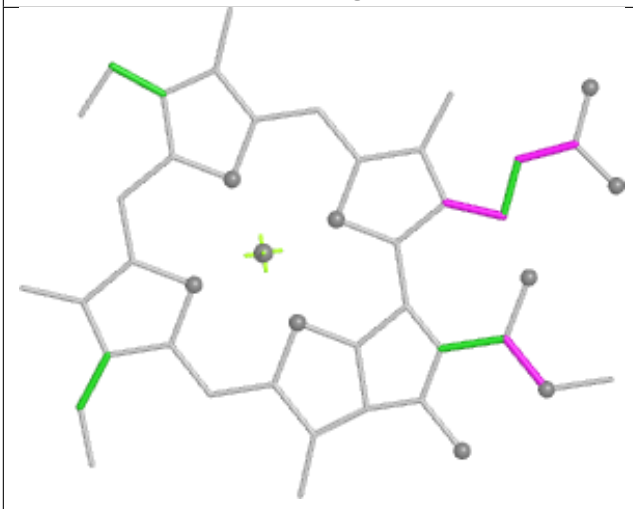
Ligand CLA B 850



Bond lengths



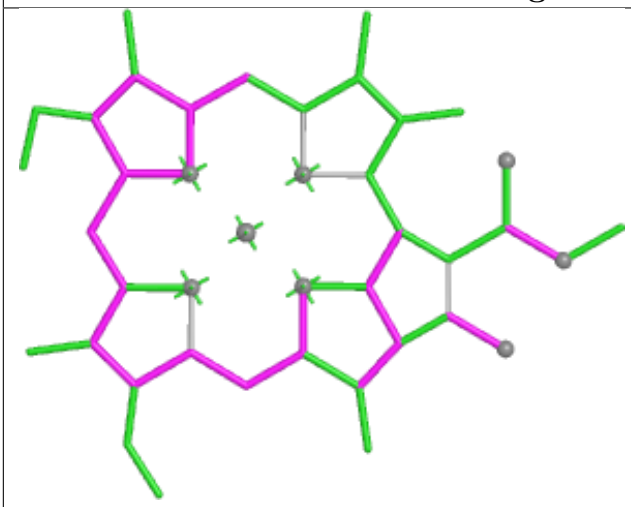
Bond angles



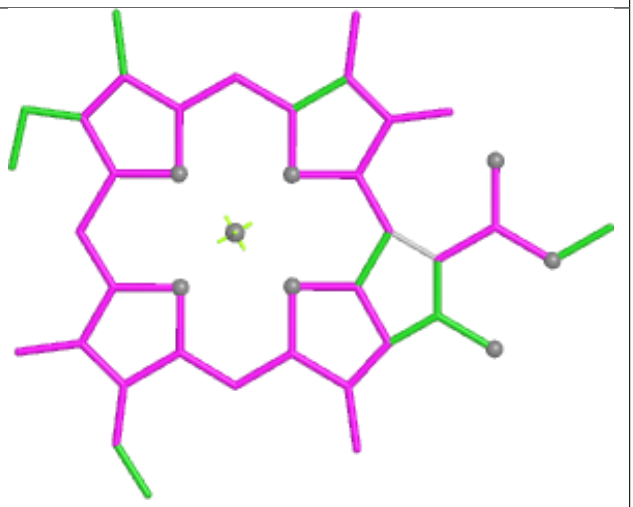
Torsions

Rings

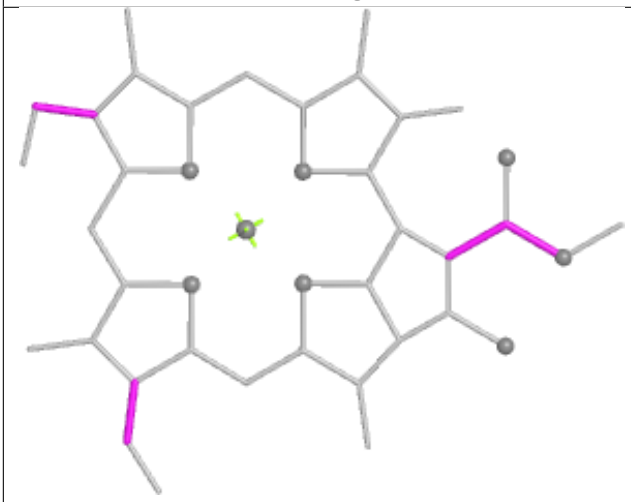
Ligand CLA 7 310



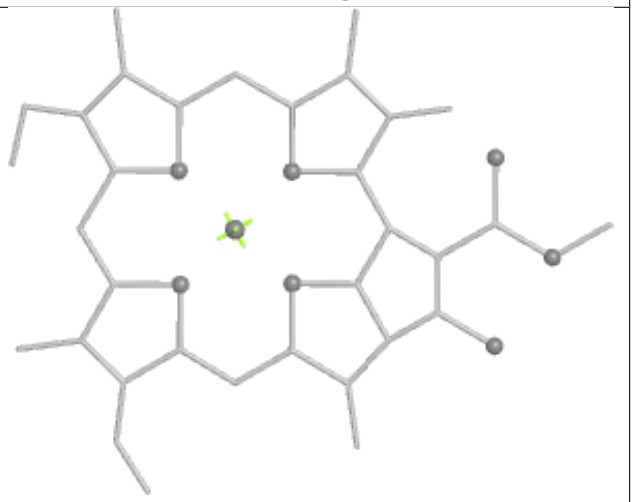
Bond lengths



Bond angles

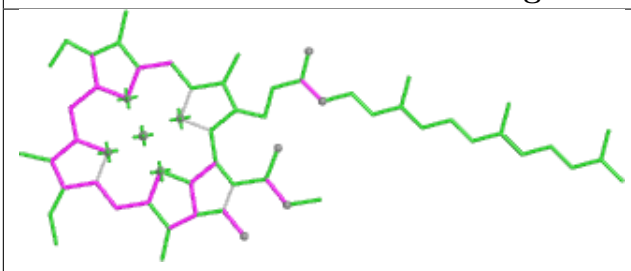


Torsions

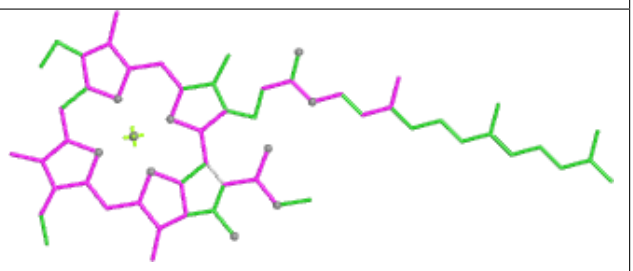


Rings

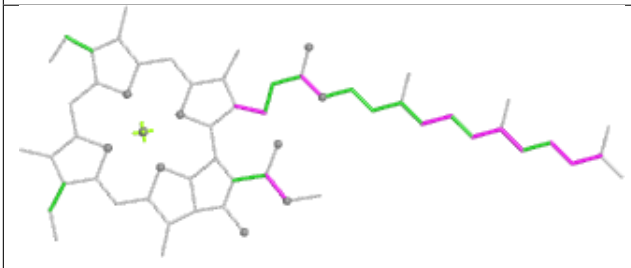
Ligand CLA A 834



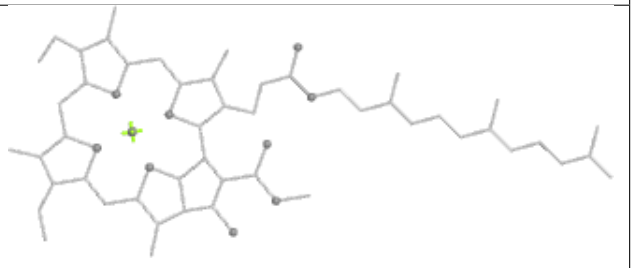
Bond lengths



Bond angles

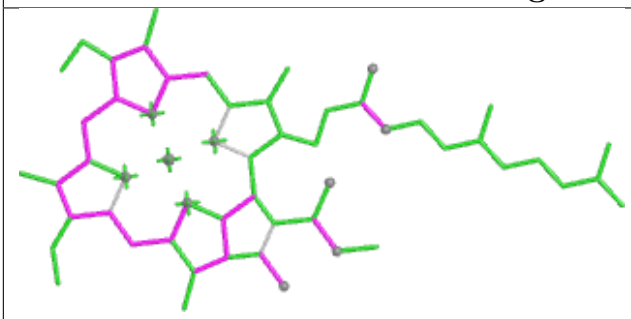


Torsions

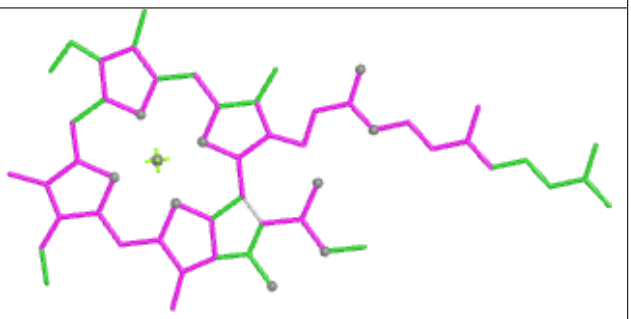


Rings

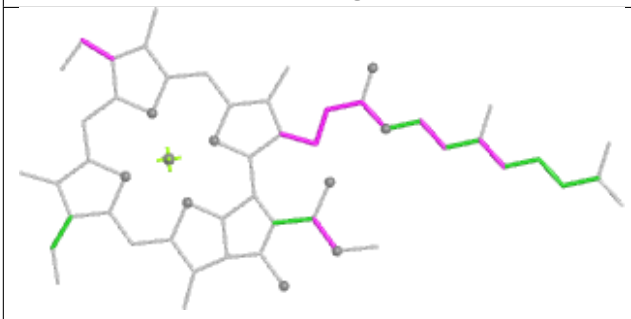
Ligand CLA 1 307



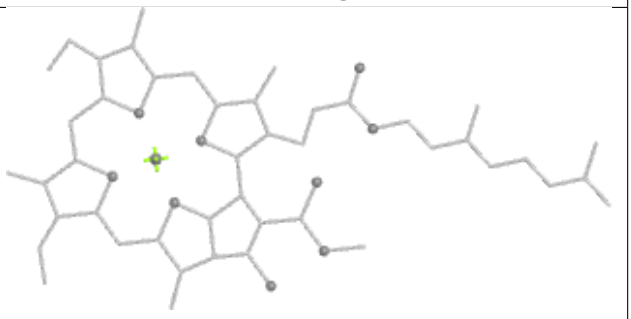
Bond lengths



Bond angles

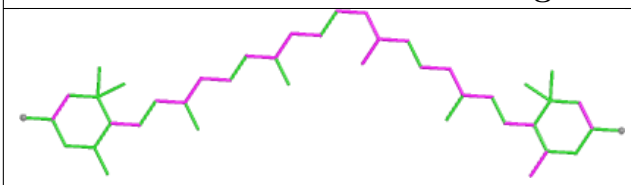


Torsions



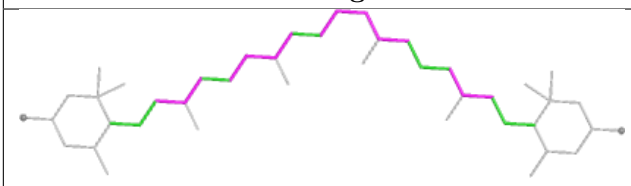
Rings

Ligand 5X6 2 314

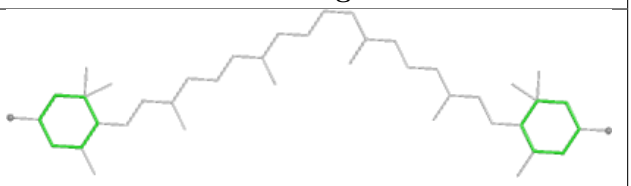


Bond lengths

Bond angles

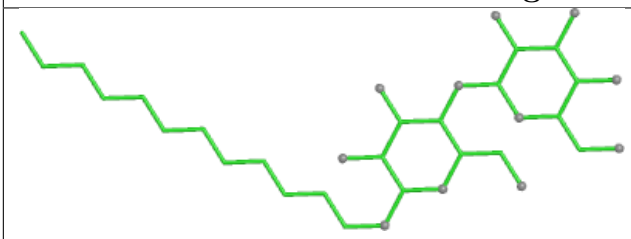


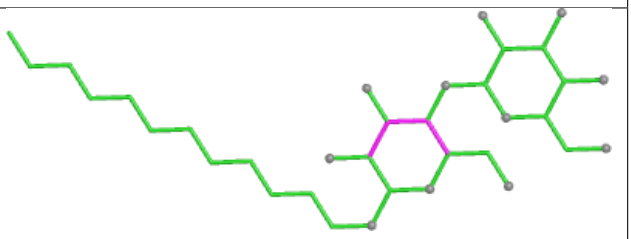
Torsions

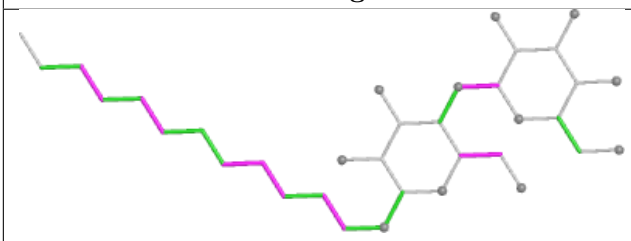


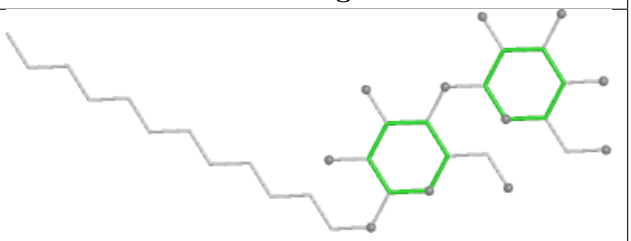
Rings

Ligand LMT F 202

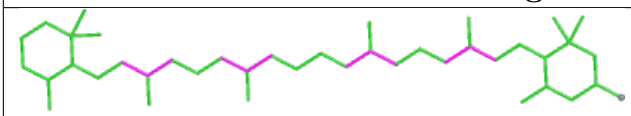

Bond lengths

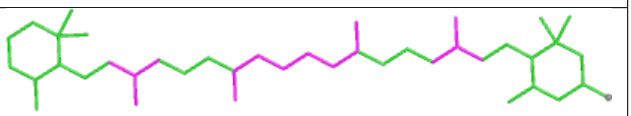

Bond angles

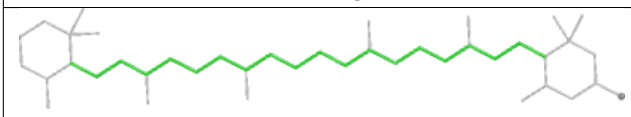

Torsions


Rings

Ligand RRX 4 317


Bond lengths


Bond angles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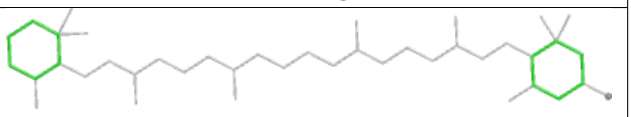
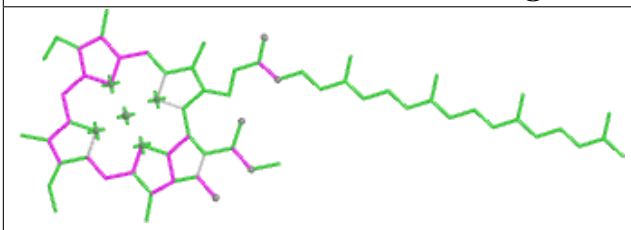
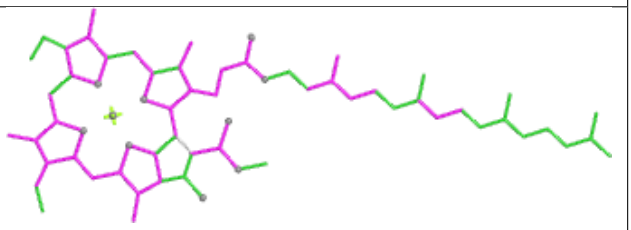
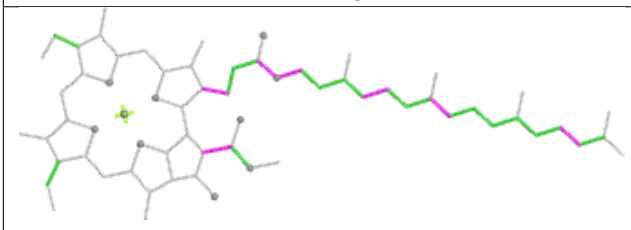
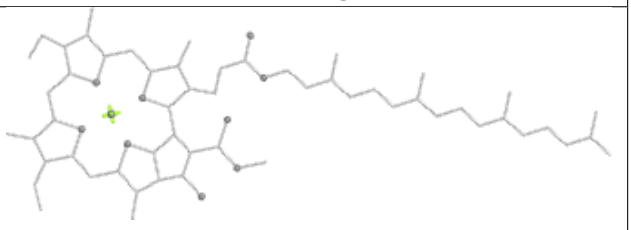

Rings

Ligand CLA B 805

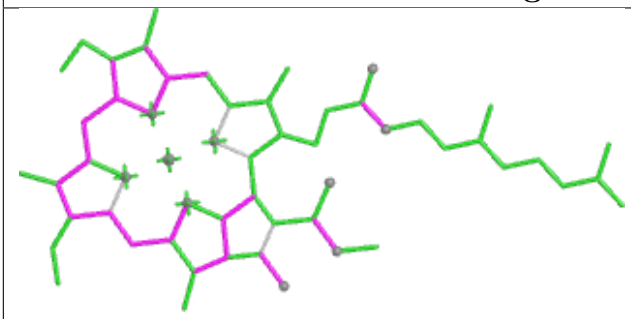

Bond lengths


Bond angles

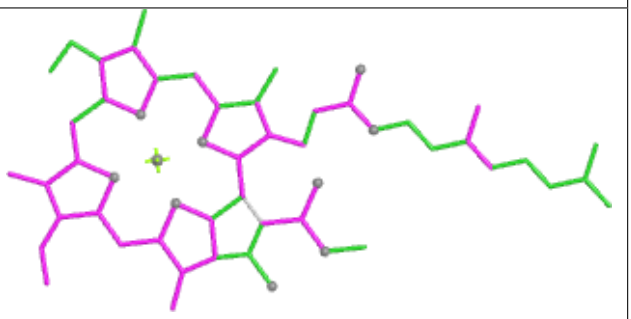

Torsions


Rings

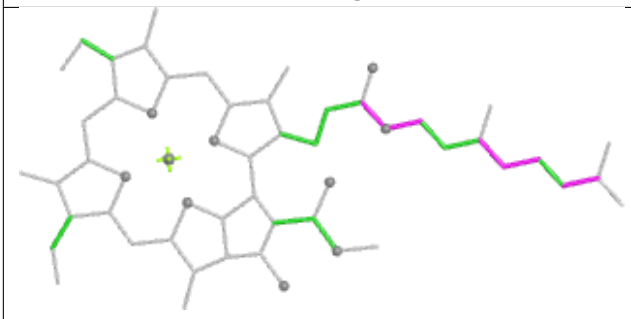
Ligand CLA A 802



Bond lengths



Bond angles



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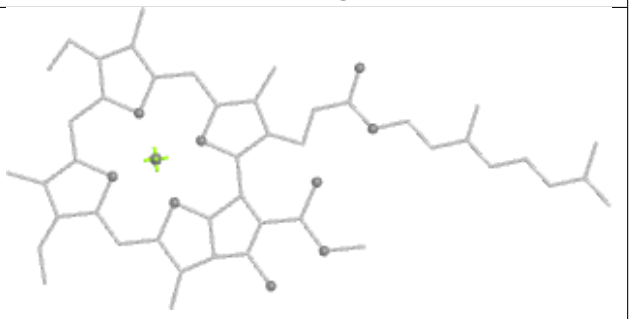
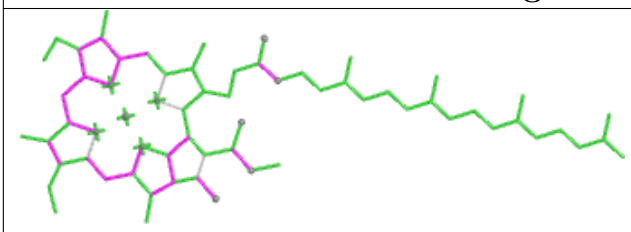
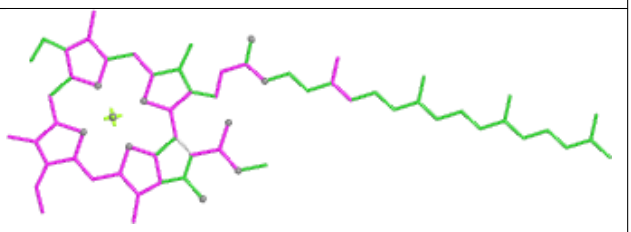


Rings

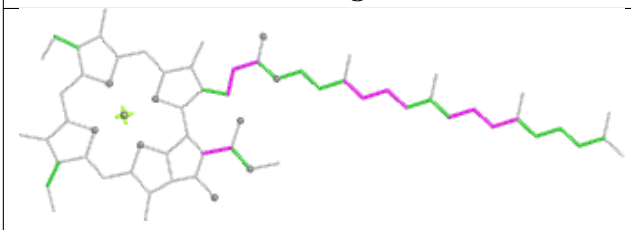
Ligand CLA A 818



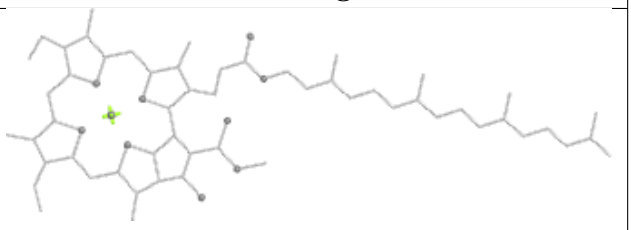
Bond lengths



Bond angles

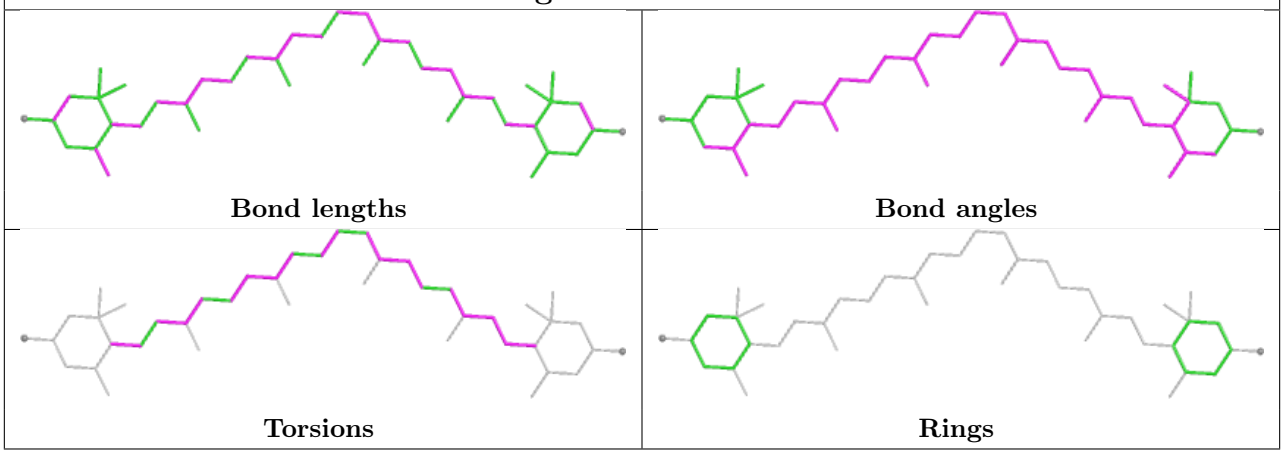


Torsions

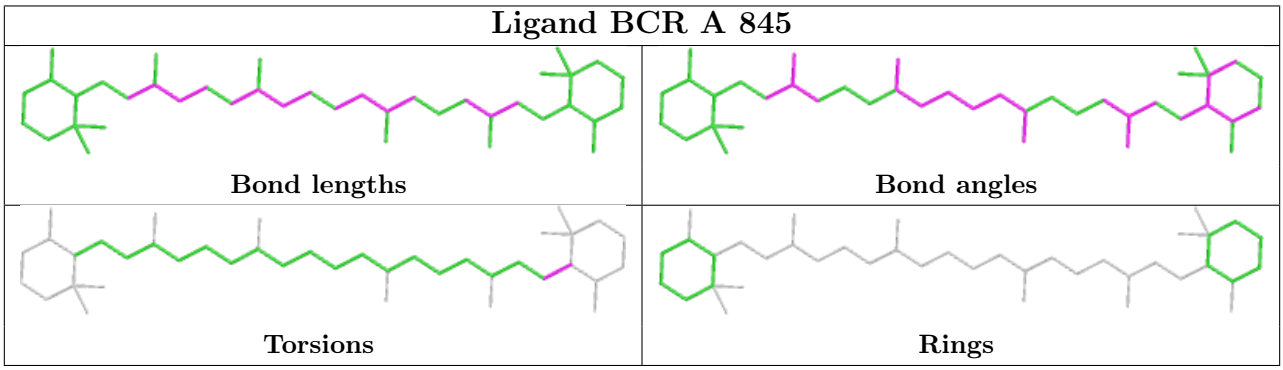


Rings

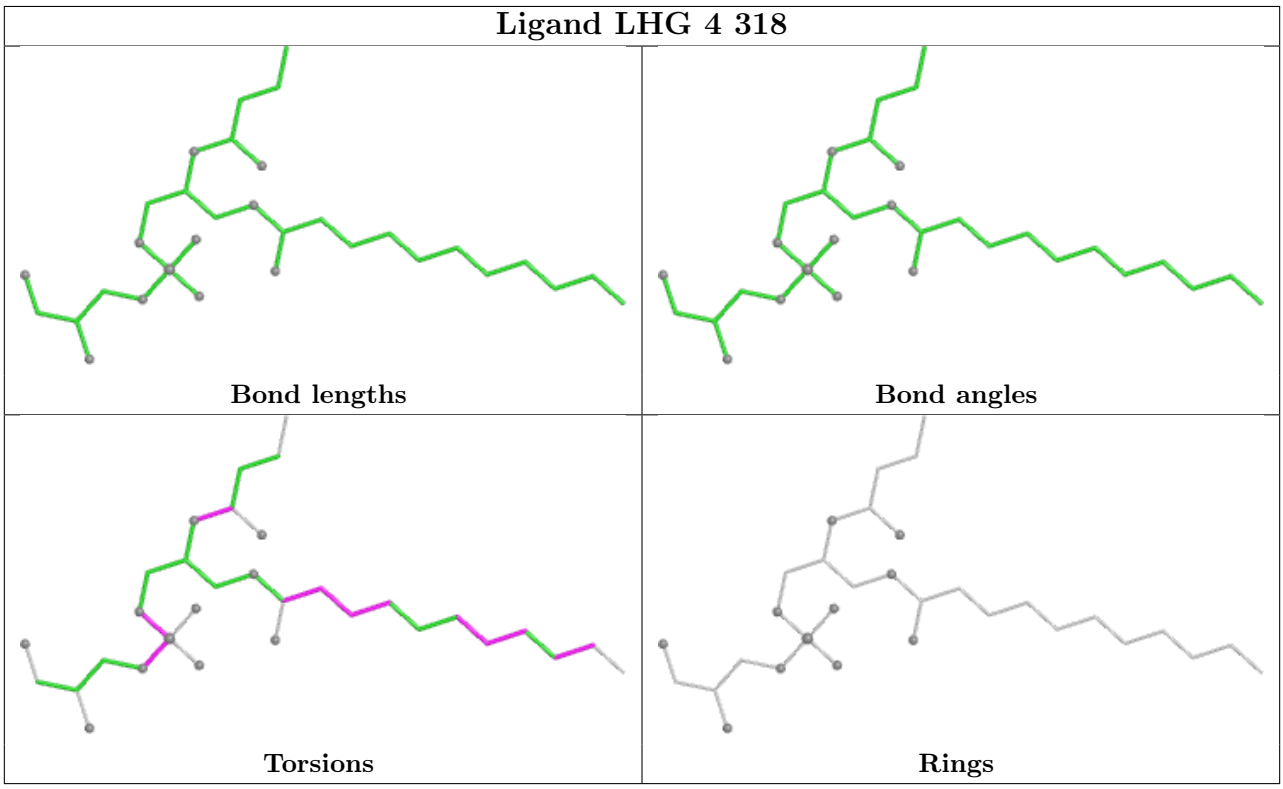
Ligand 5X6 3 306



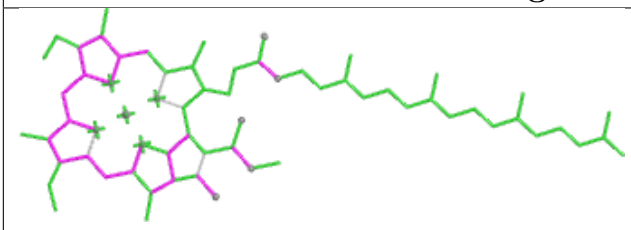
Ligand BCR A 845



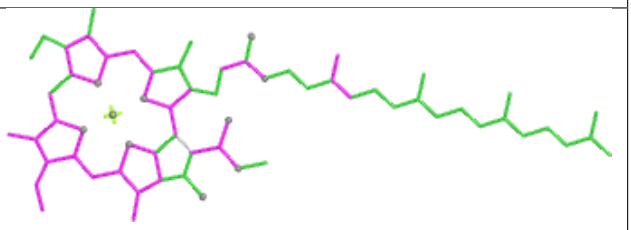
Ligand LHG 4 318



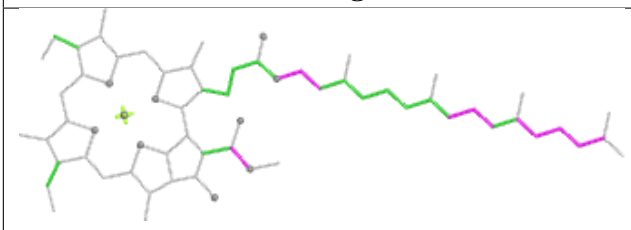
Ligand CLA 1 302



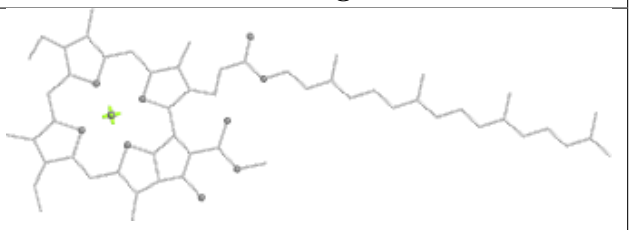
Bond lengths



Bond angles

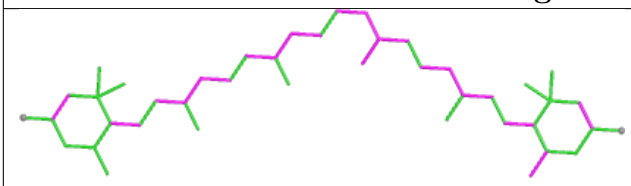


Torsions



Rings

Ligand 5X6 4 315



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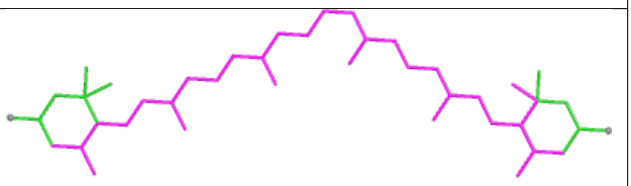
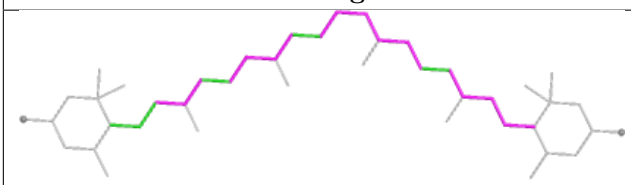
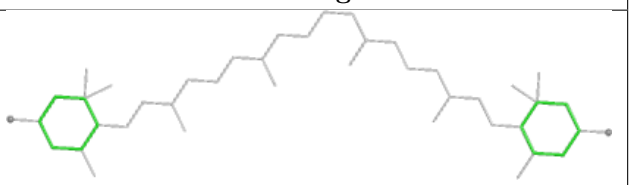


Bond angles

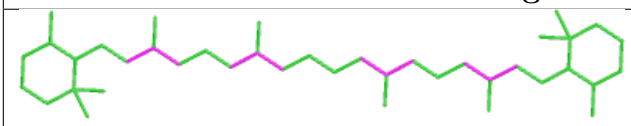


Torsions

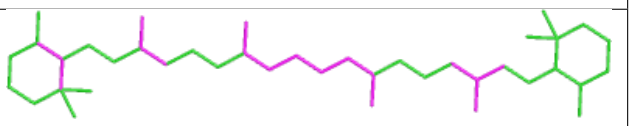


Rings

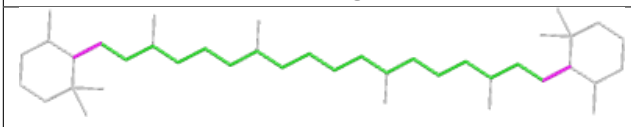
Ligand BCR B 842



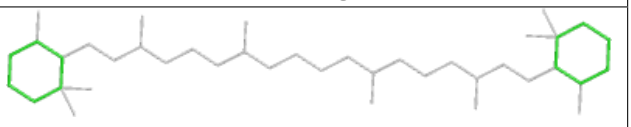
Bond lengths



Bond angles

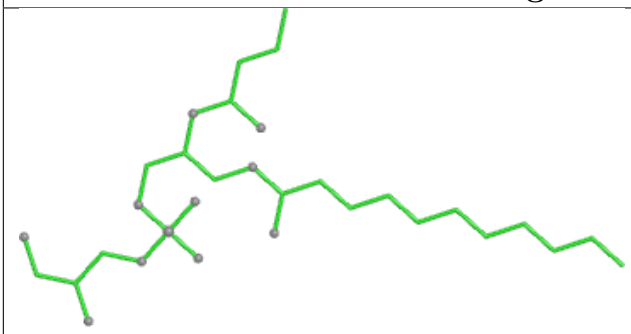


Torsions

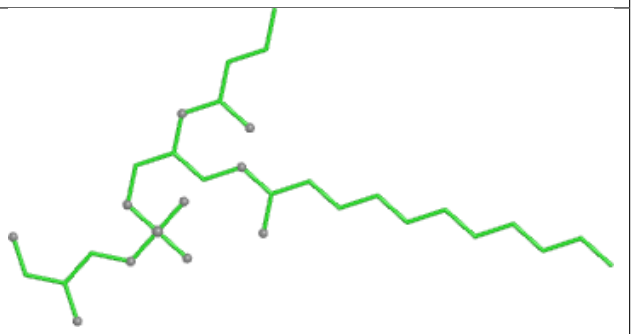


Rings

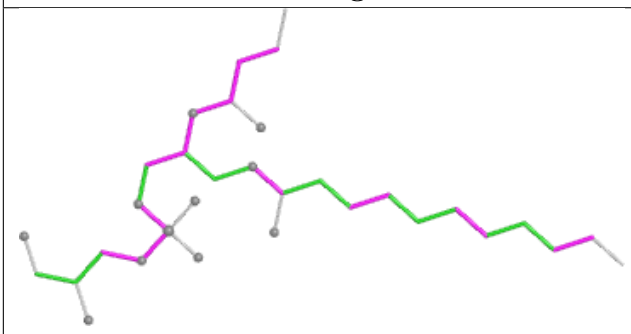
Ligand LHG 2 315



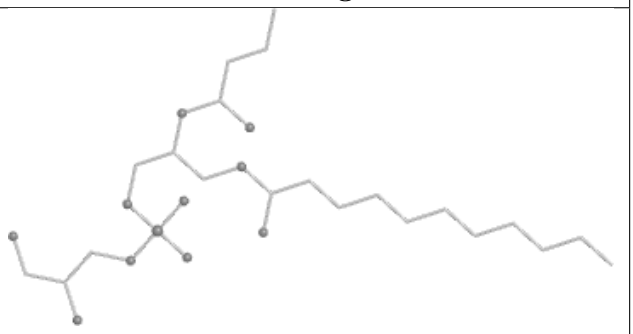
Bond lengths



Bond angles

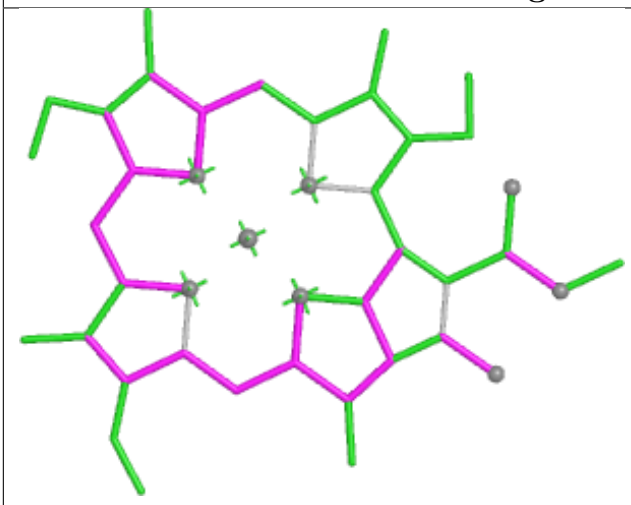


Torsions

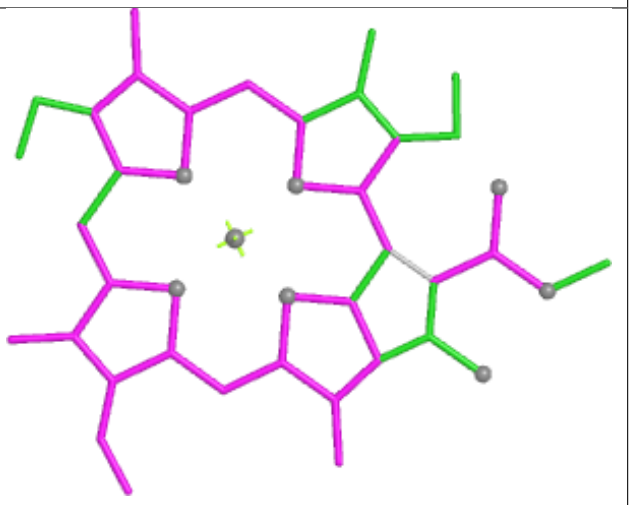


Rings

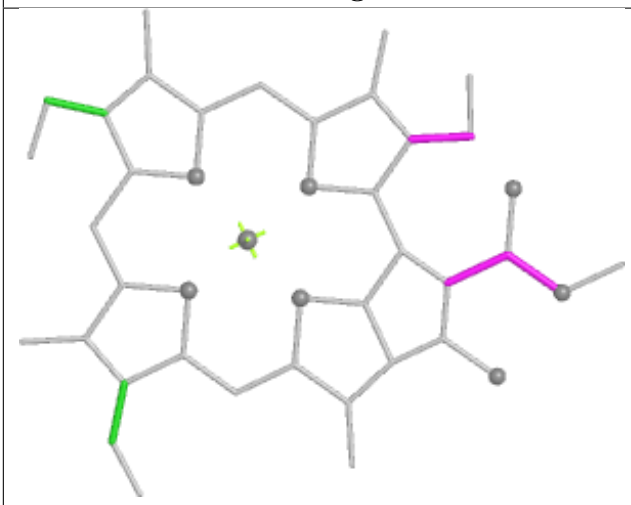
Ligand CLA 6 312



Bond lengths



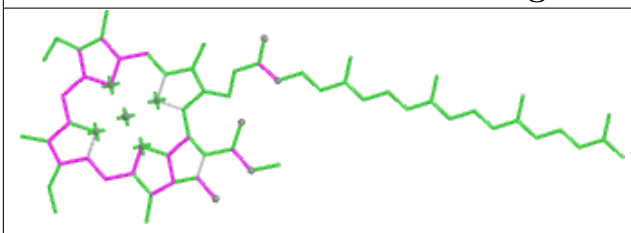
Bond angles



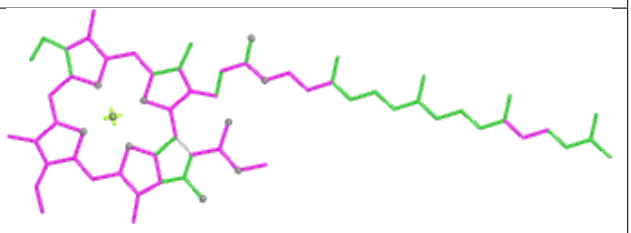
Torsions

Rings

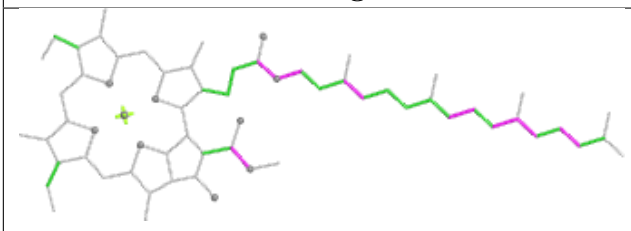
Ligand CLA 1 303



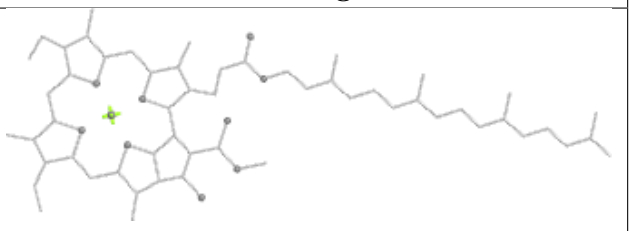
Bond lengths



Bond angles

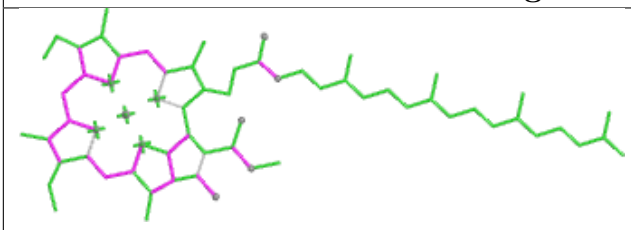


Torsions

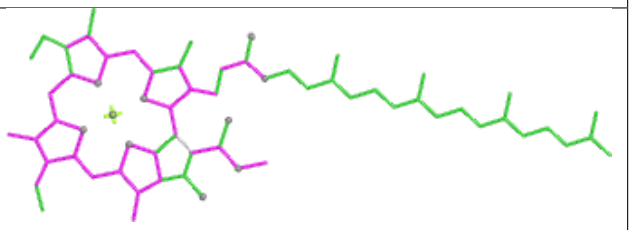


Rings

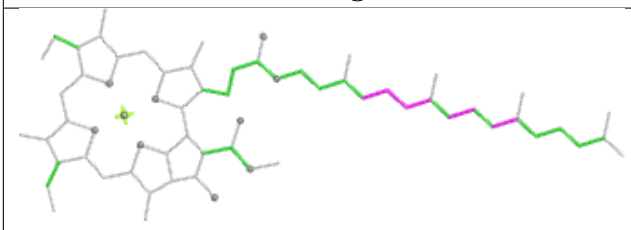
Ligand CLA B 819



Bond lengths



Bond angles



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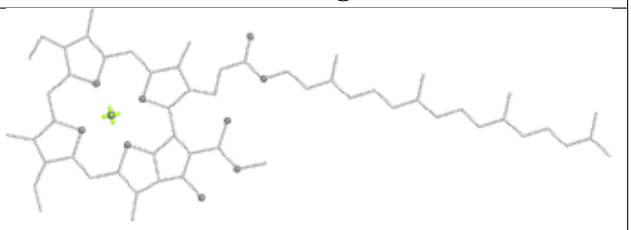
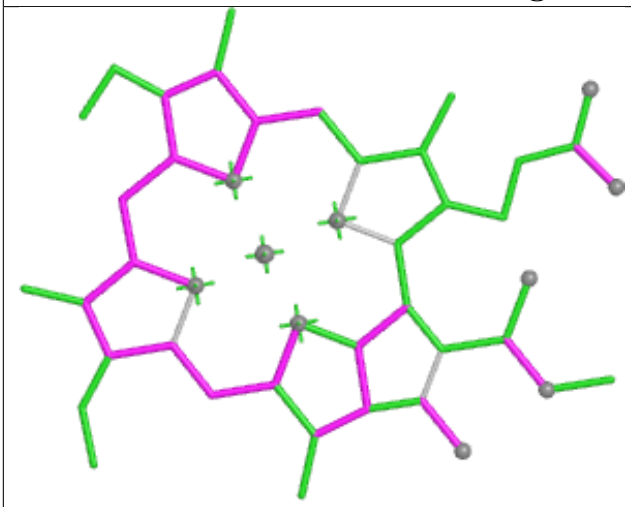


Rings

Ligand CLA 4 311



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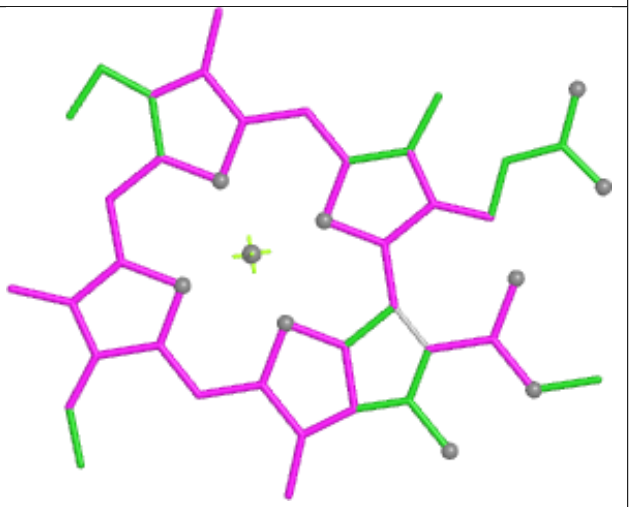
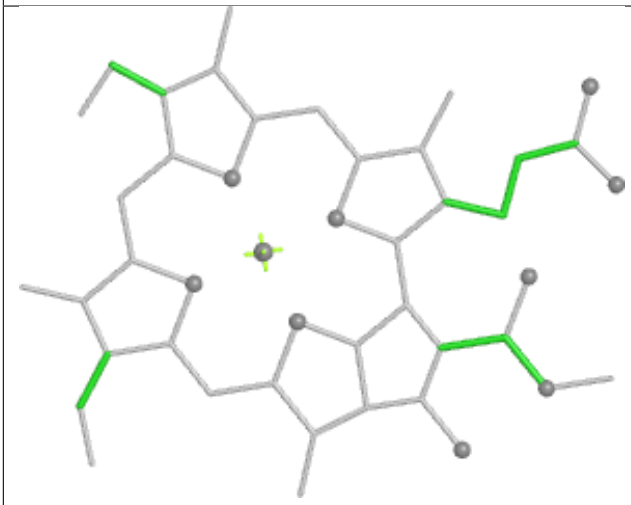
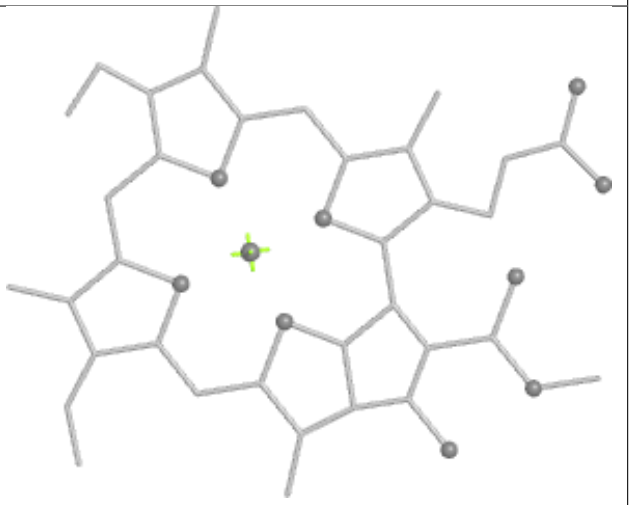


Bond angles

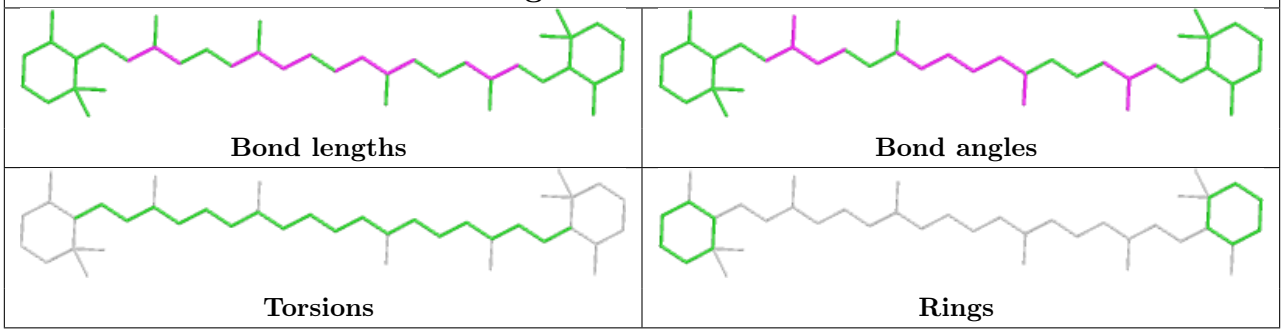


Torsions

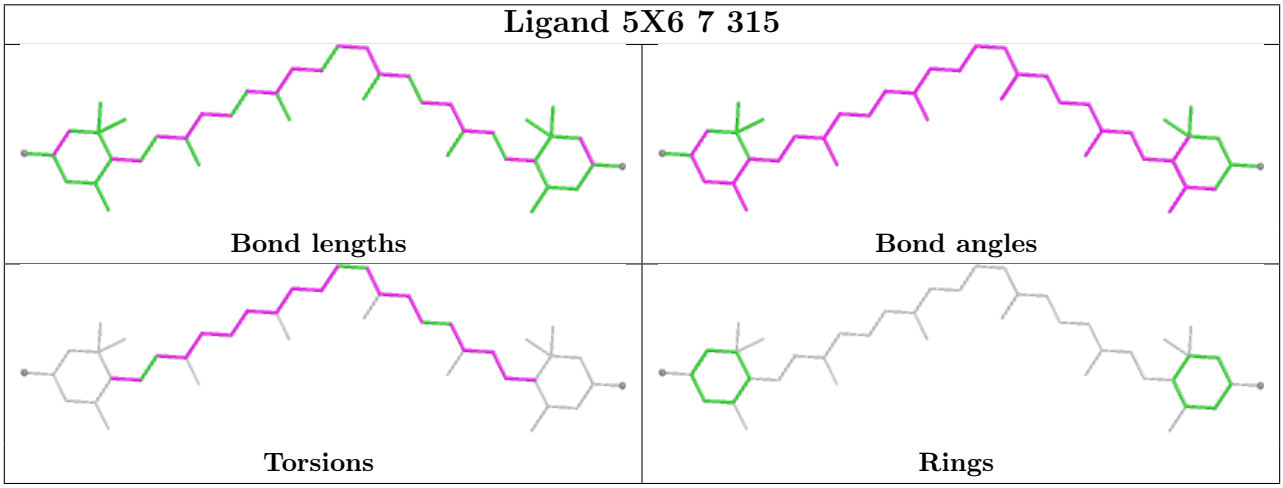


Rings

Ligand BCR F 201



Ligand 5X6 7 315



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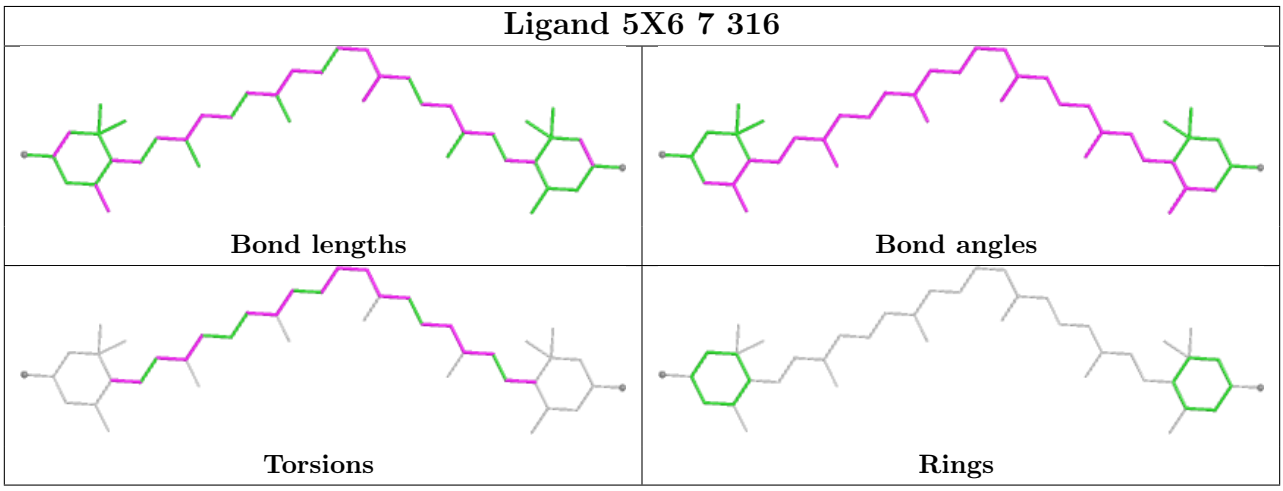
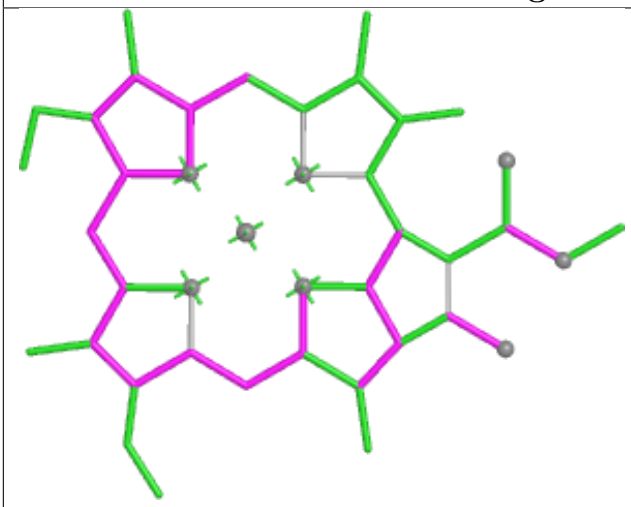
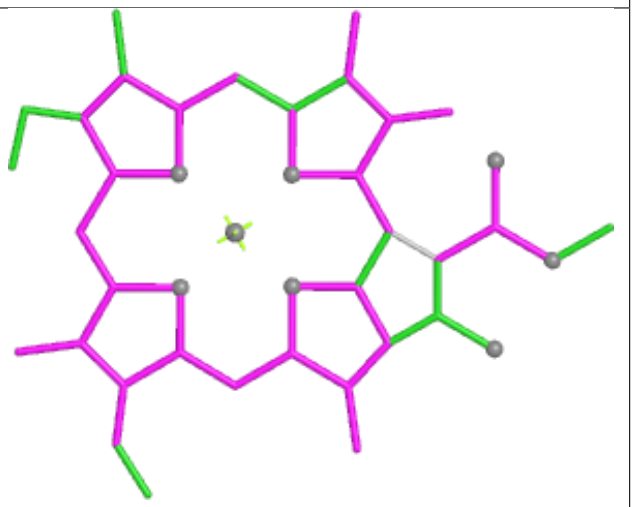


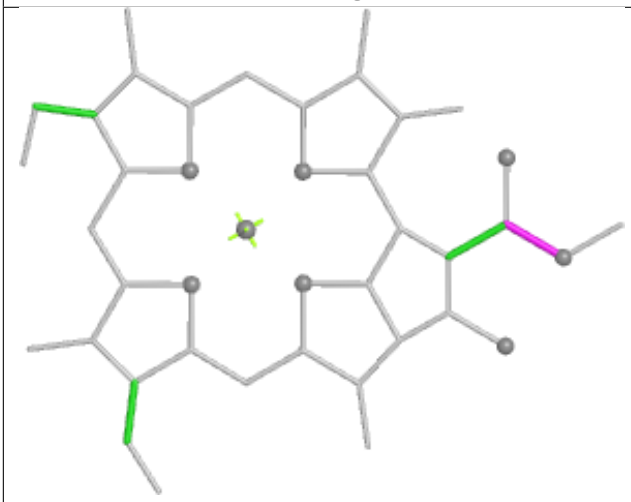
Ligand CLA 7 311



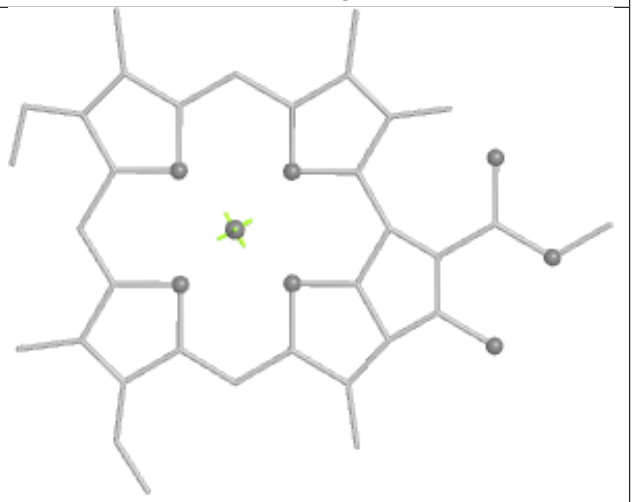
Bond lengths



Bond angles

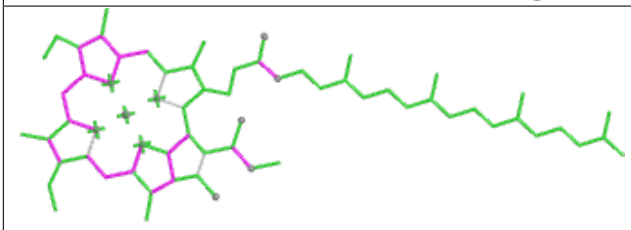


Torsions



Rings

Ligand CL0 A 801



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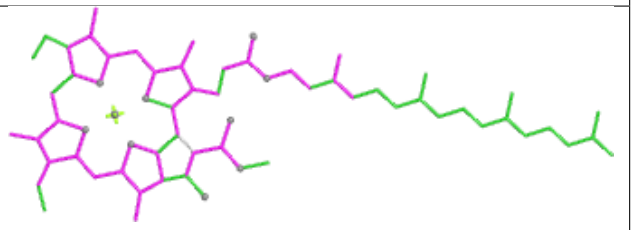
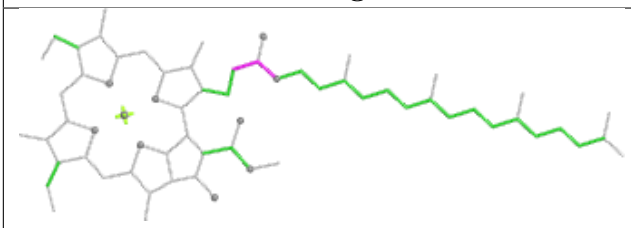
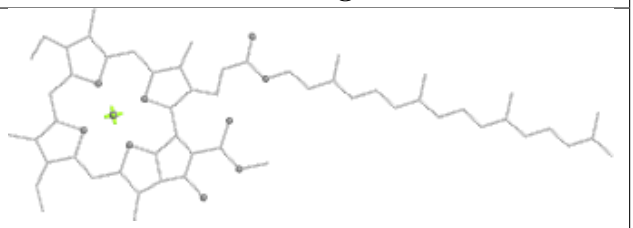


Bond angles

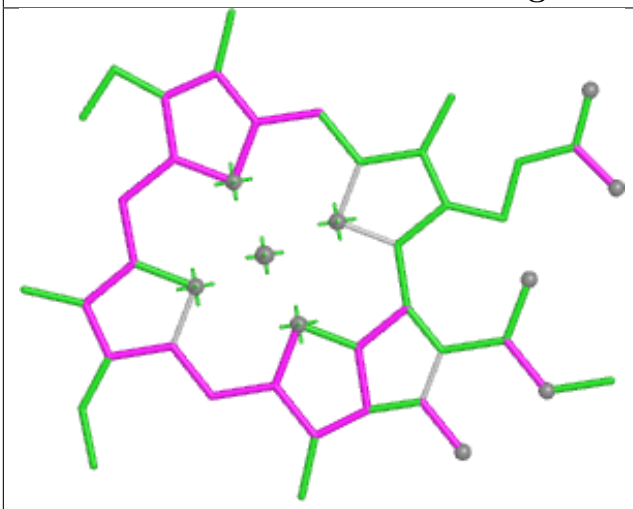


Torsions



Rings

Ligand CLA 7 307



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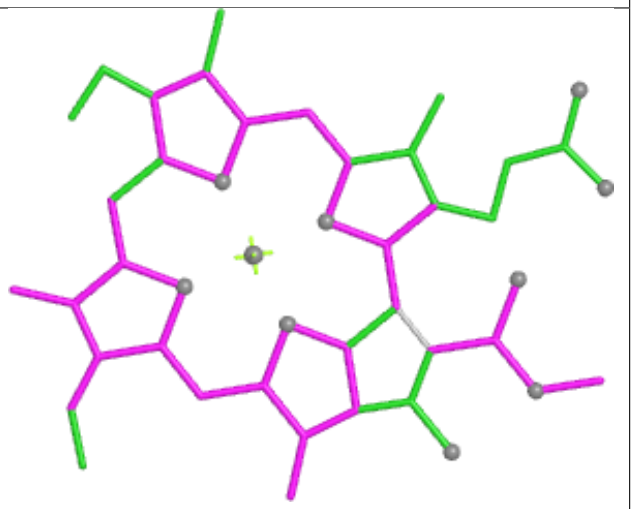
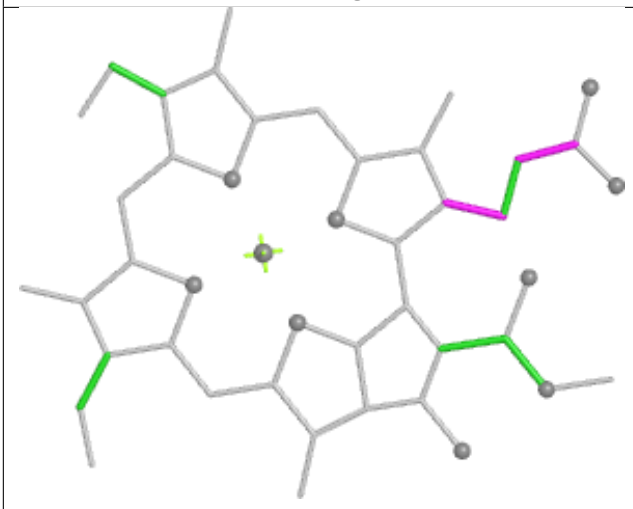


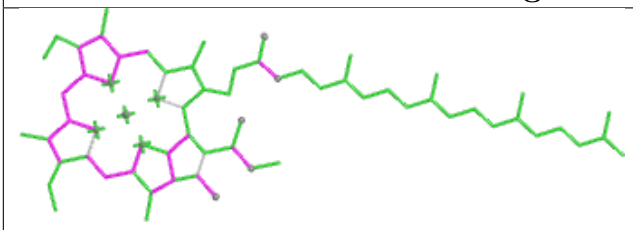
Bond angles



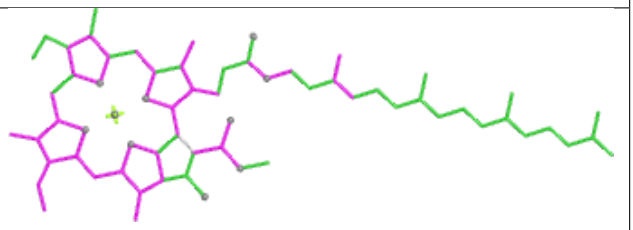
Torsions

Rings

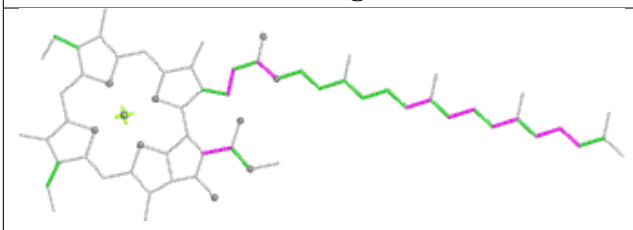
Ligand CLA A 806



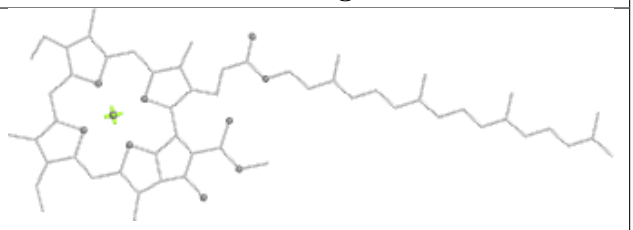
Bond lengths



Bond angles

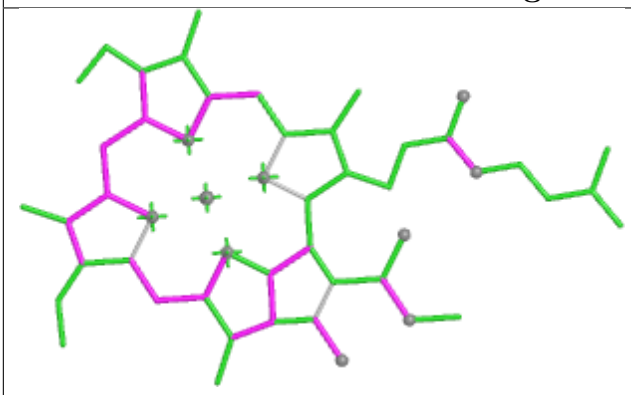


Torsions

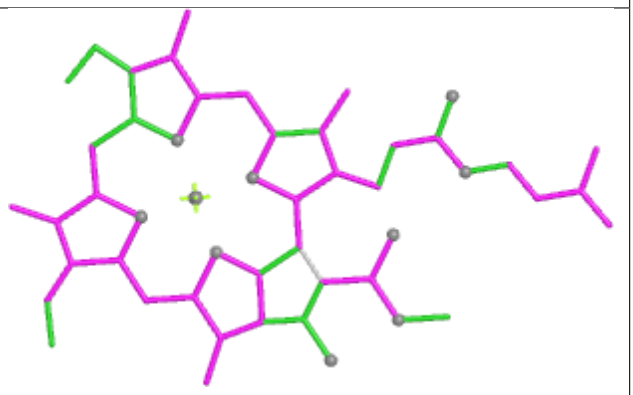


Rings

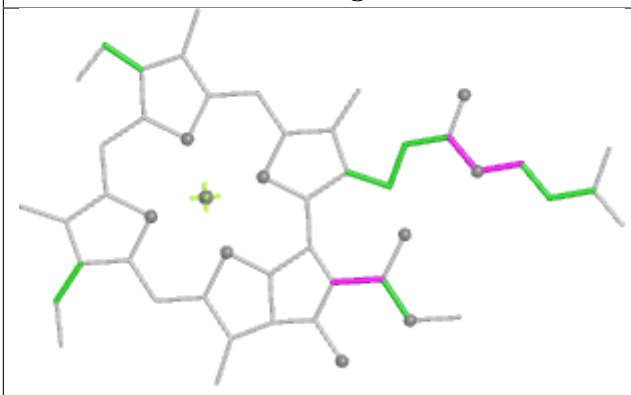
Ligand CLA A 829



Bond lengths



Bond angles



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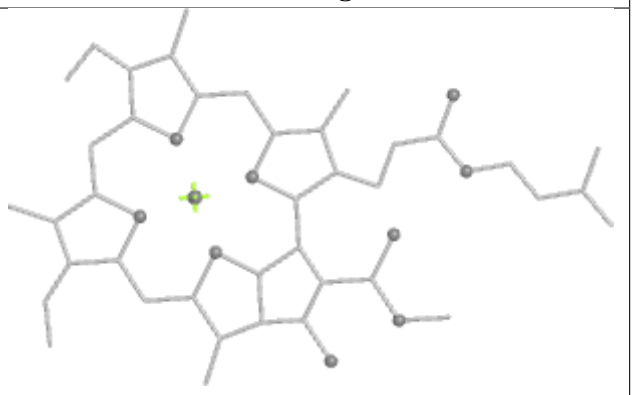
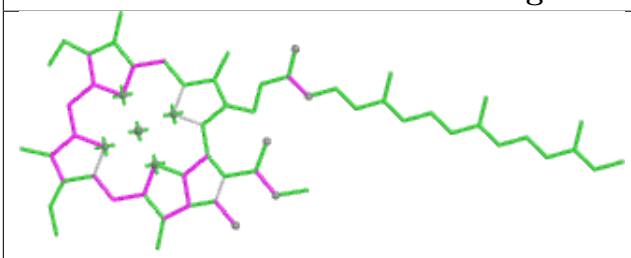


Rings

Ligand CLA F 204



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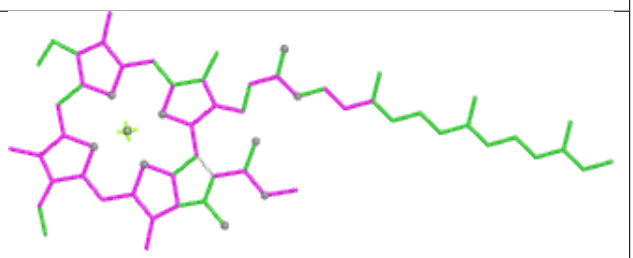
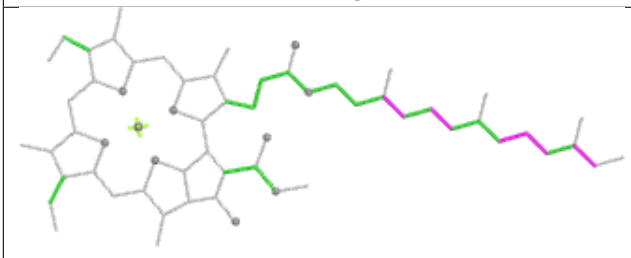


Bond angles



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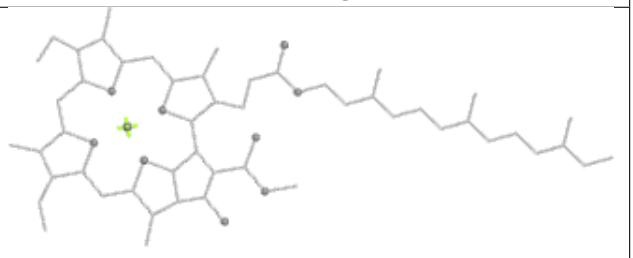
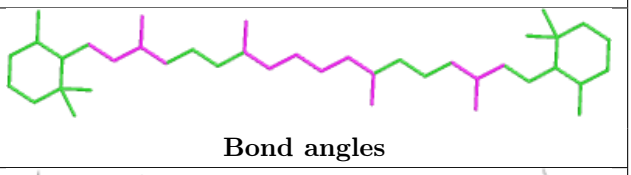


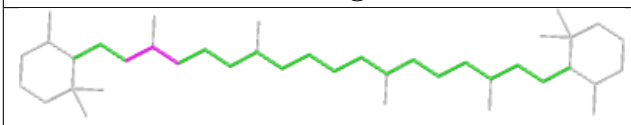
Rings

Ligand BCR L 202

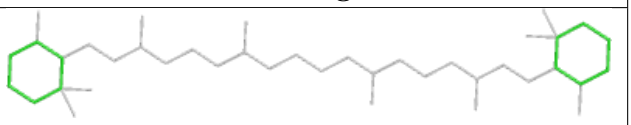
Bond lengths



Bond angles

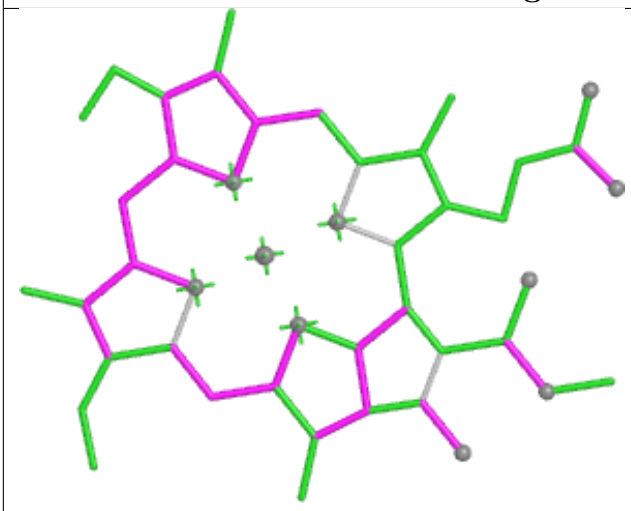


Torsions

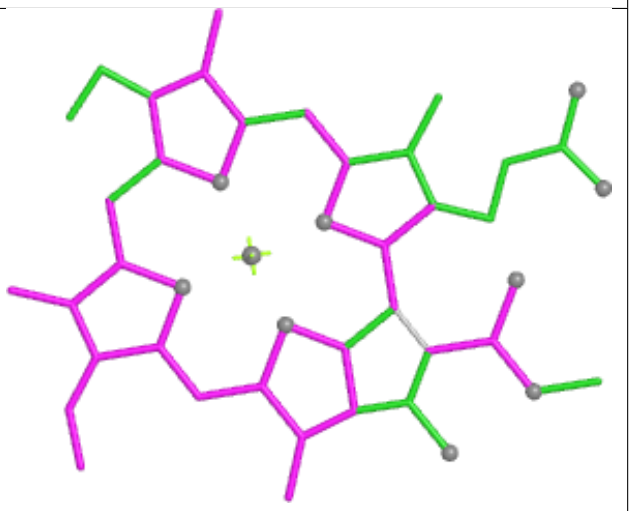


Rings

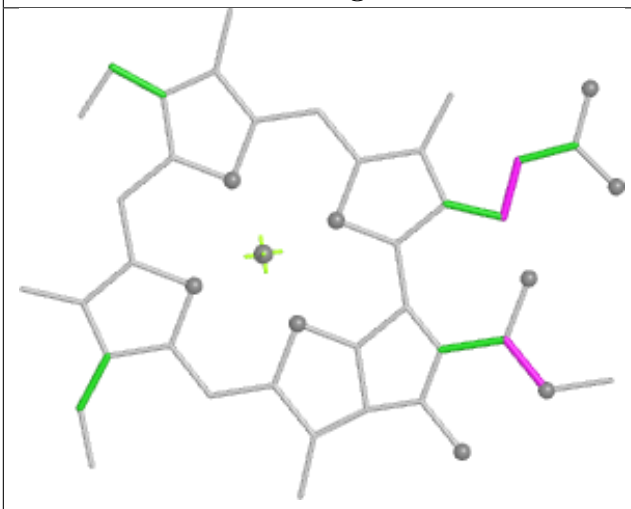
Ligand CLA A 821



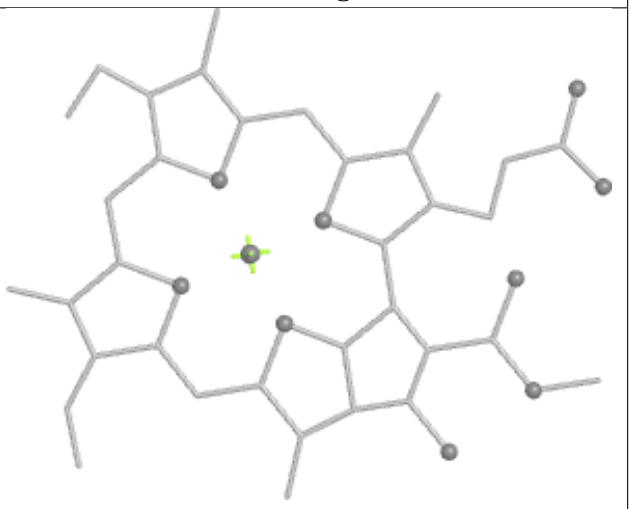
Bond lengths



Bond angles

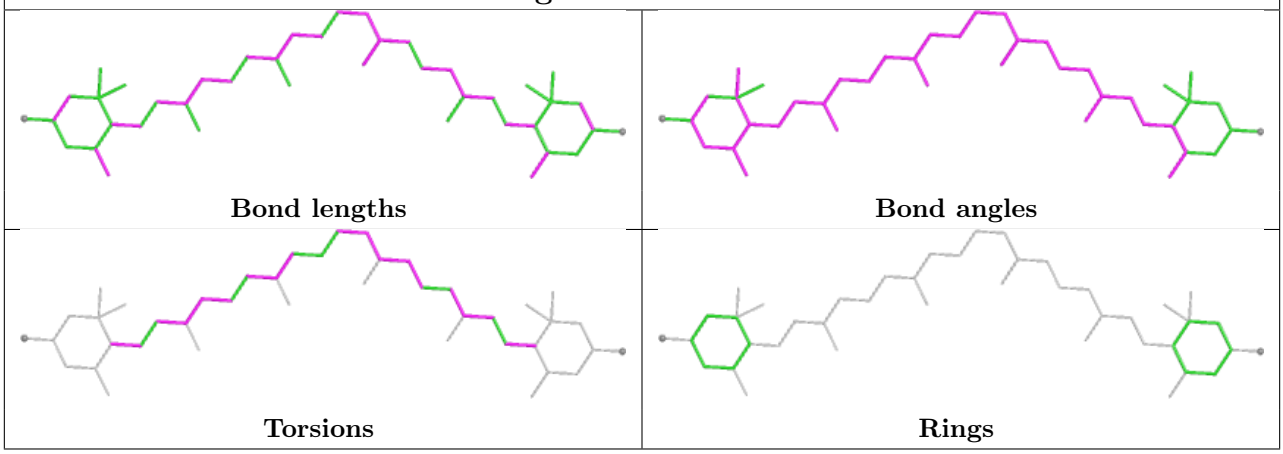


Torsions

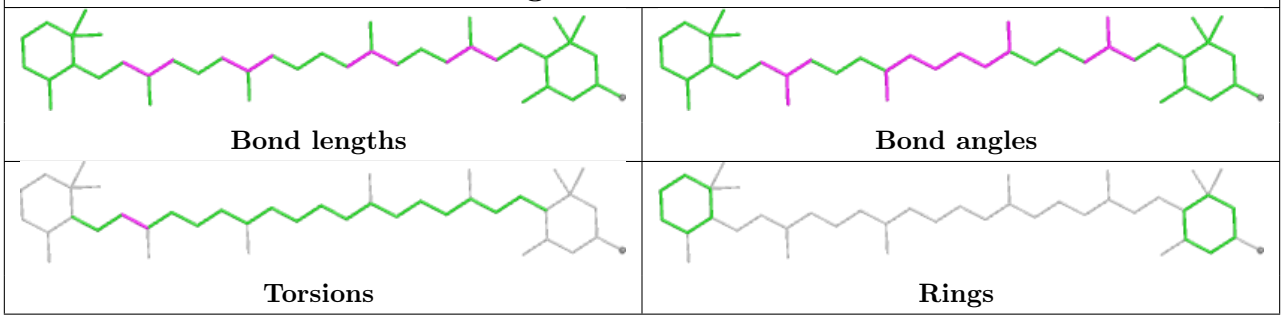


Rings

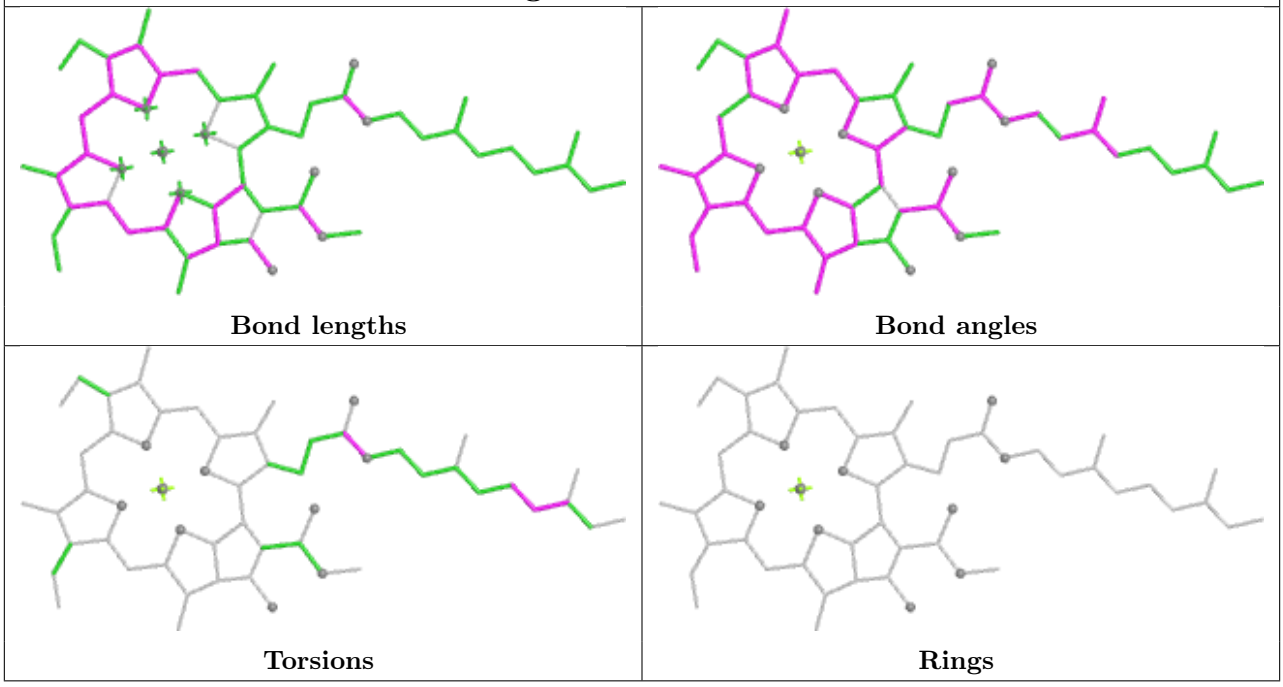
Ligand 5X6 6 317



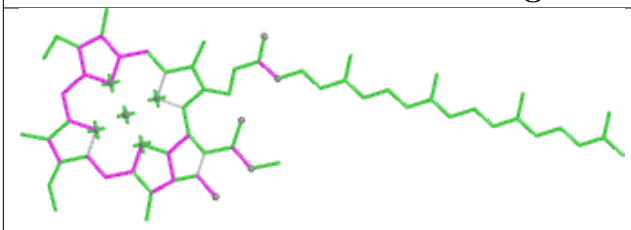
Ligand RRX 5 322



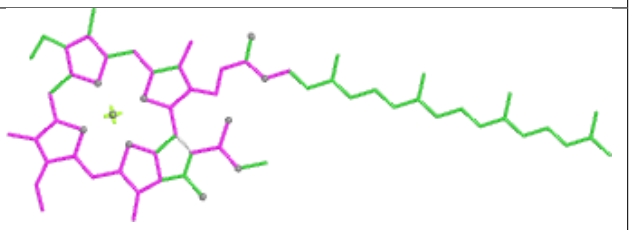
Ligand CLA A 836



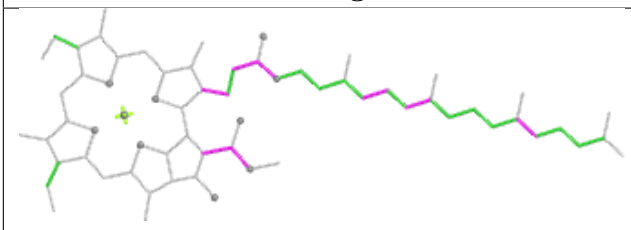
Ligand CLA B 829



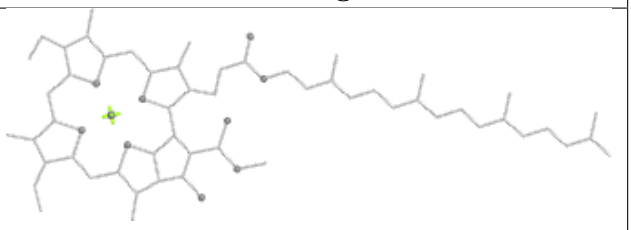
Bond lengths



Bond angles

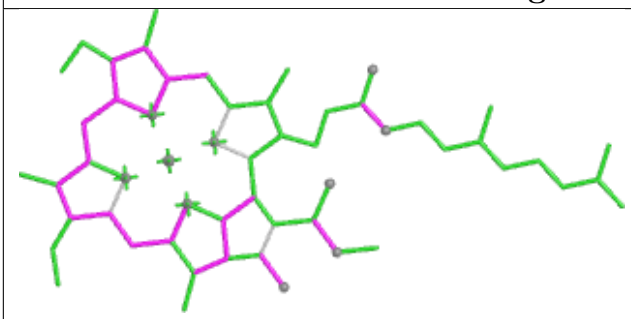


Torsions

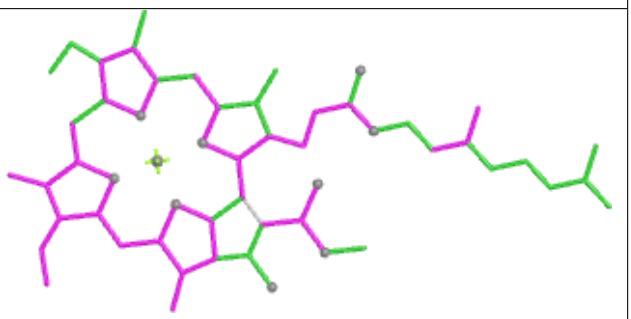


Rings

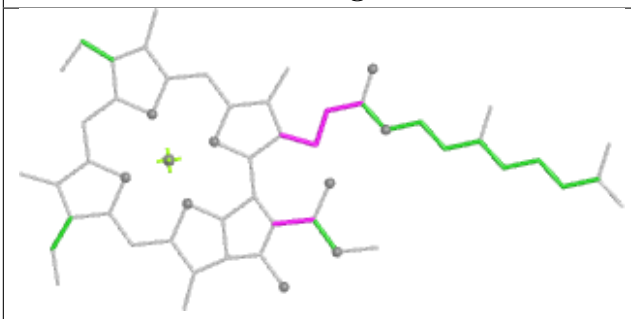
Ligand CLA 5 304



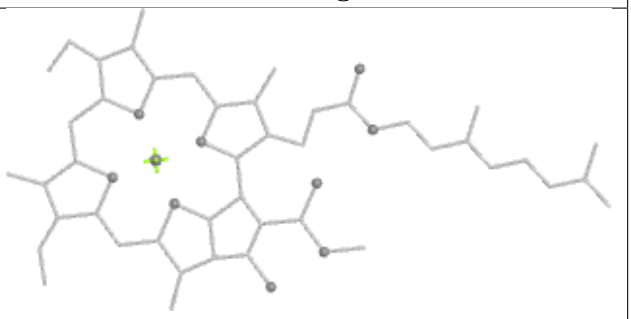
Bond lengths



Bond angles

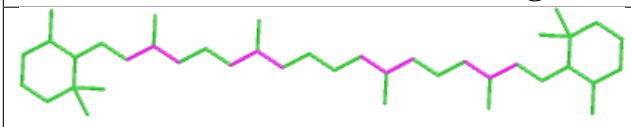


Torsions

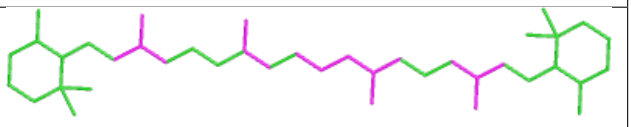


Rings

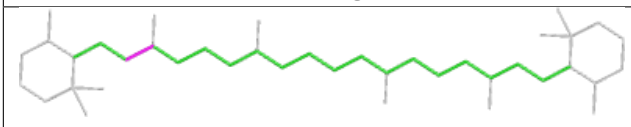
Ligand BCR 4 316



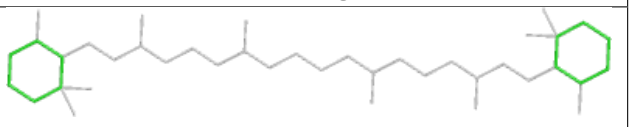
Bond lengths



Bond angles

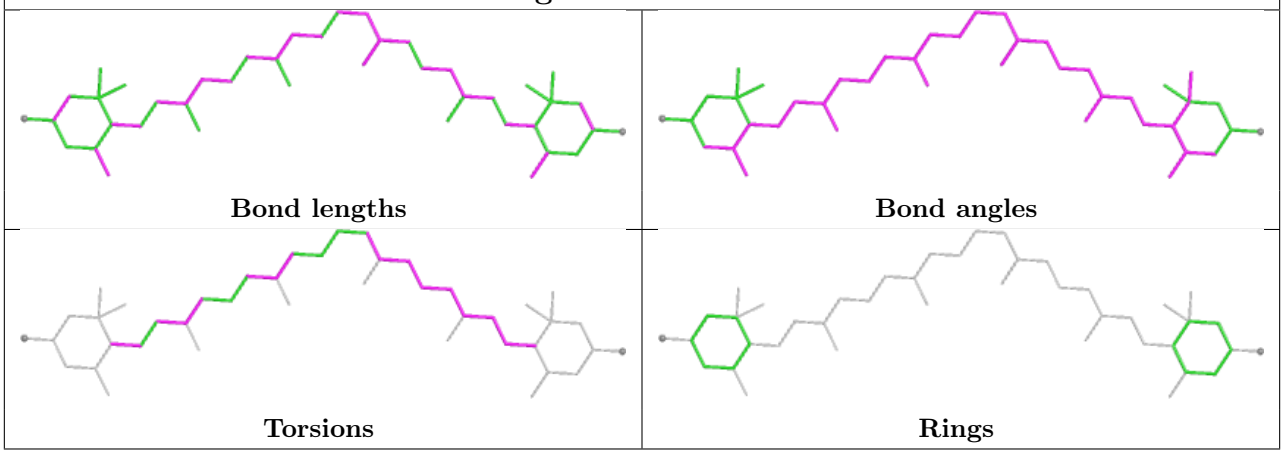


Torsions

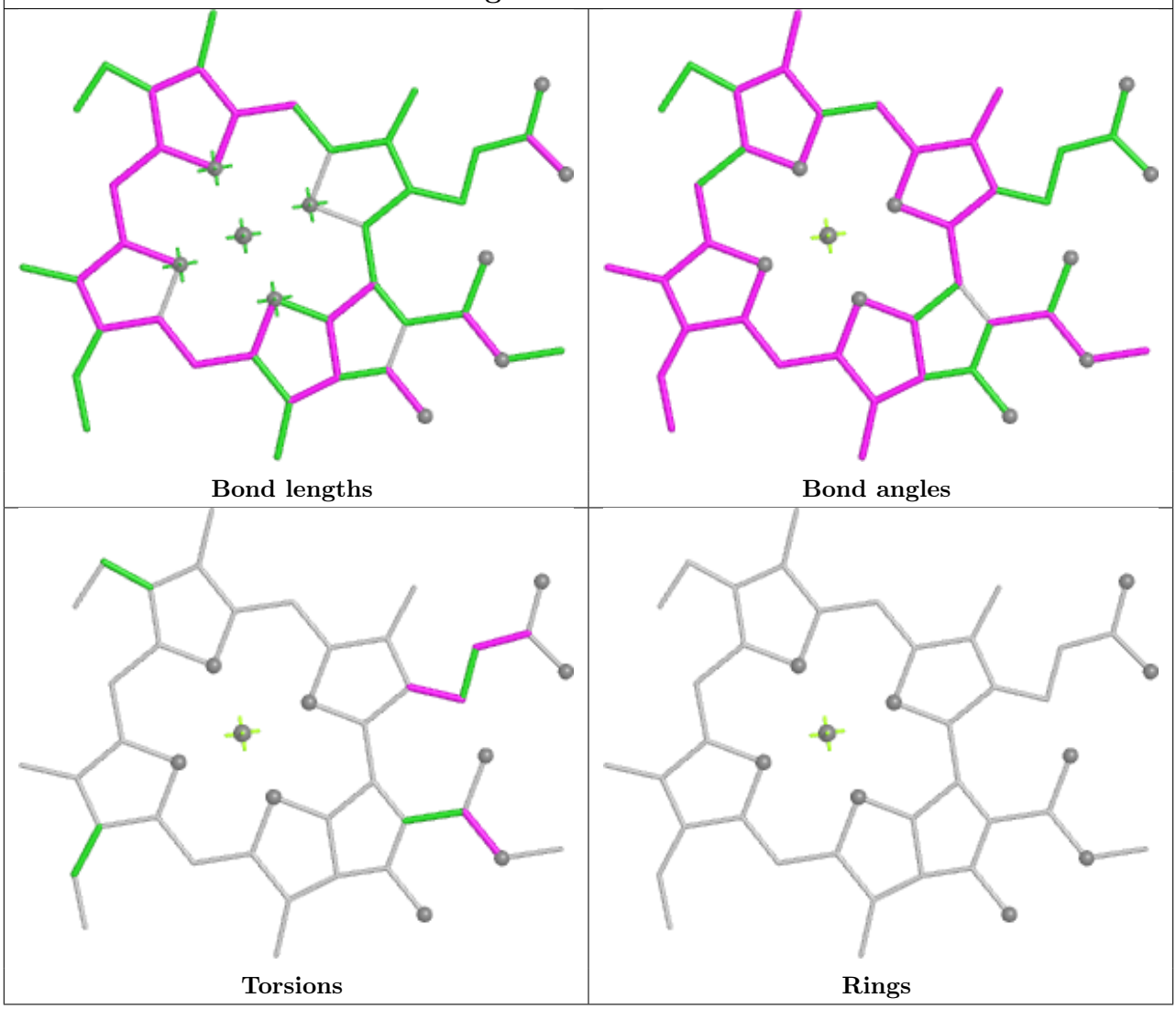


Rings

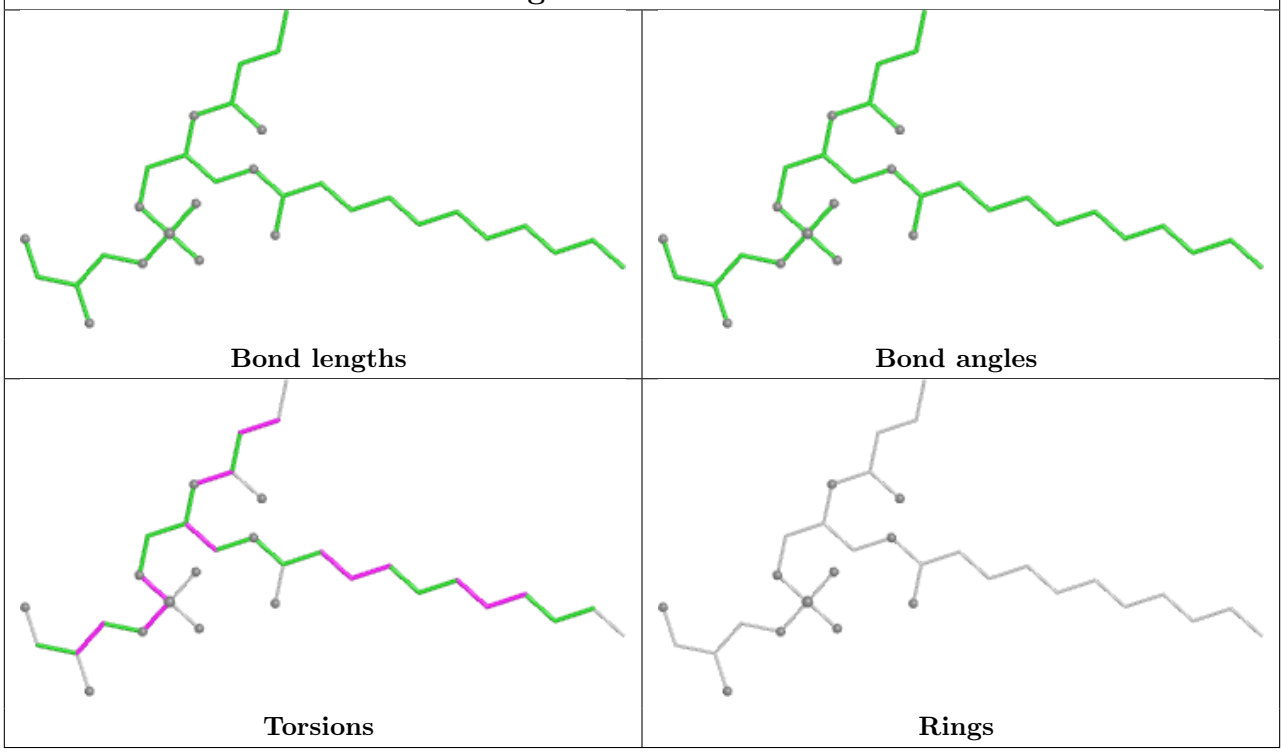
Ligand 5X6 1 313



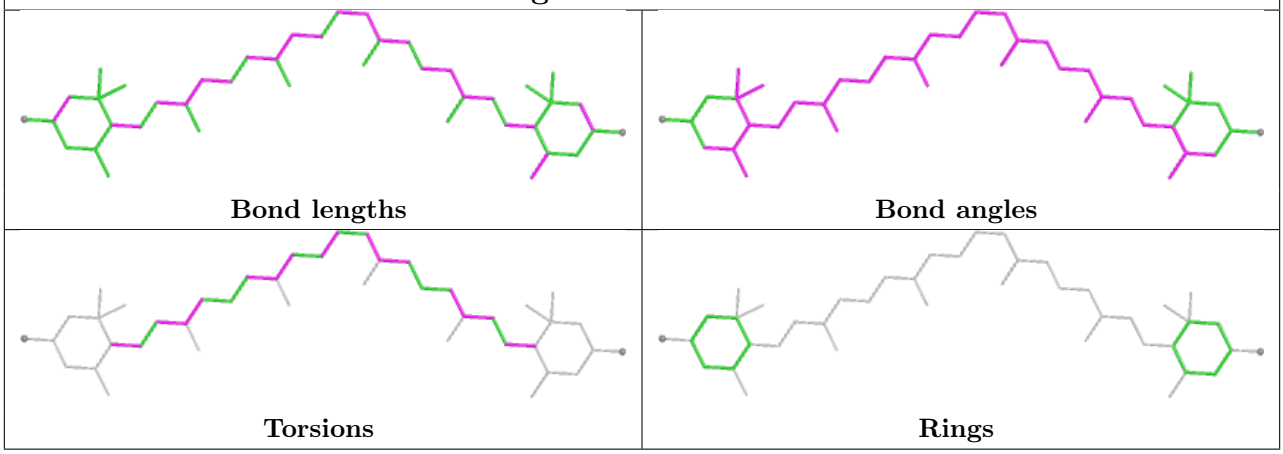
Ligand CLA 1 306



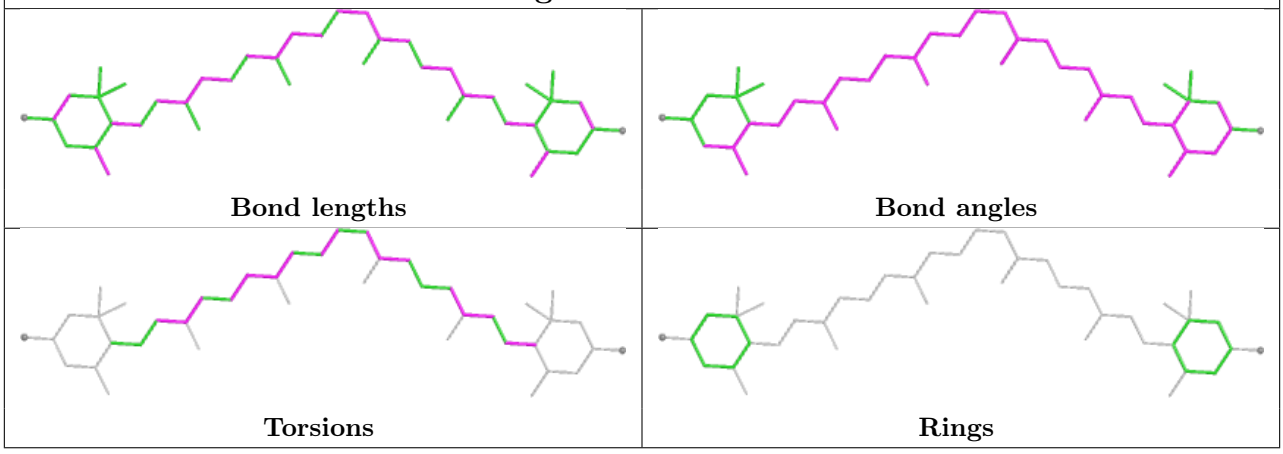
Ligand LHG 6 319

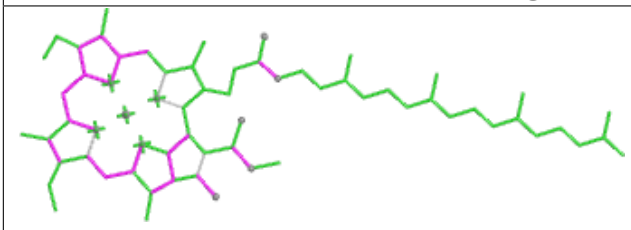
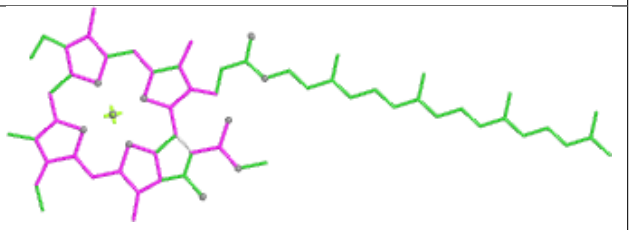
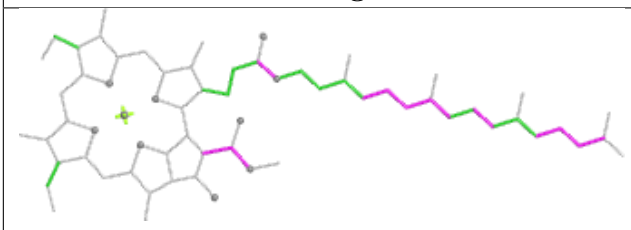
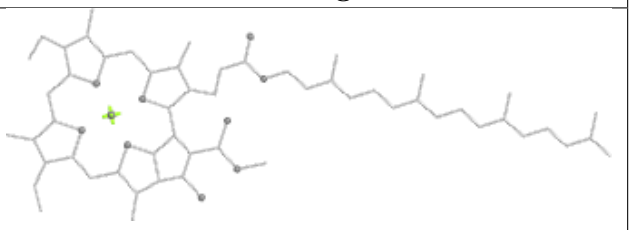


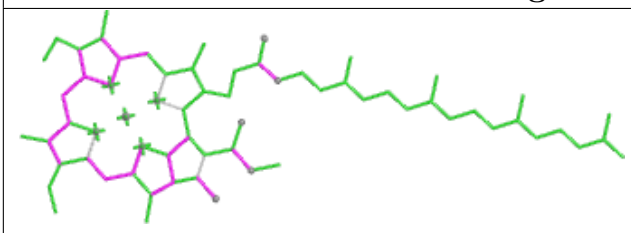
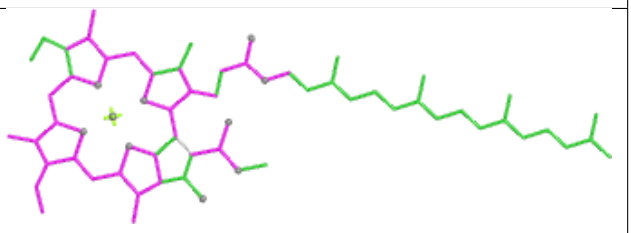
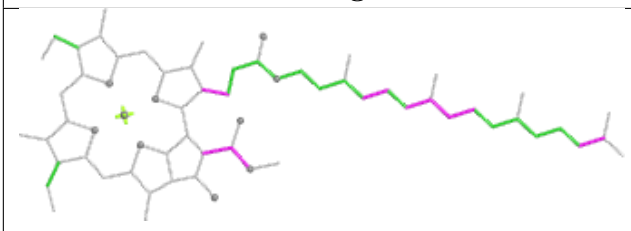
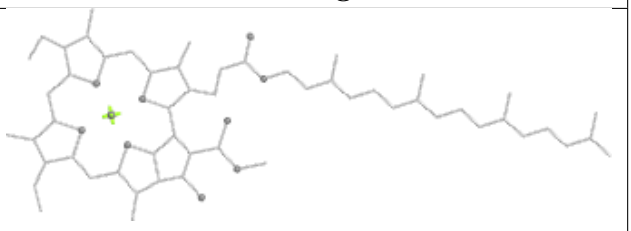
Ligand 5X6 B 851



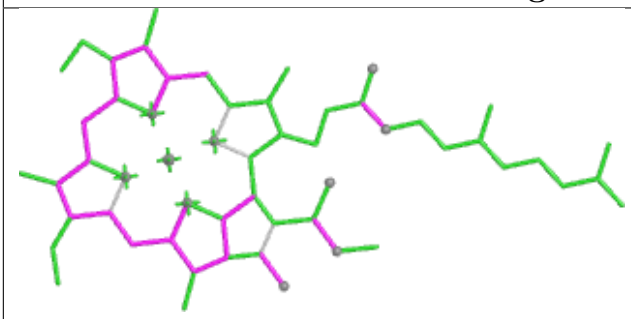
Ligand 5X6 4 314



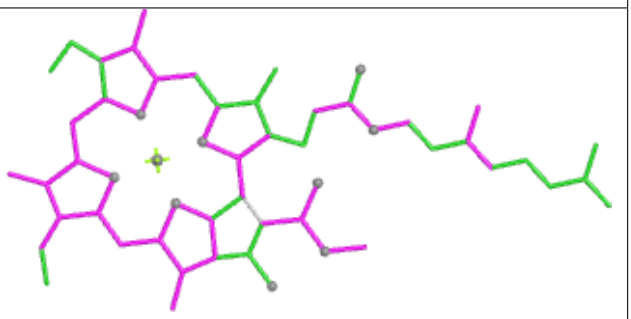
Ligand CLA B 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

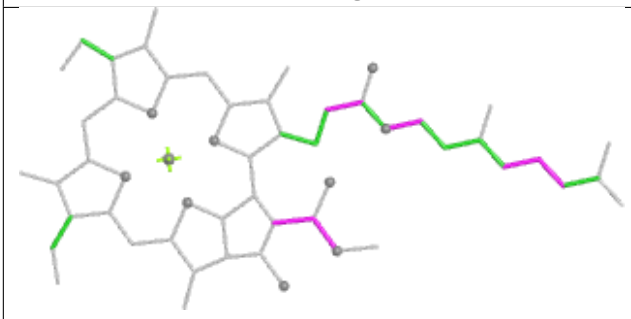
Ligand CLA 2 308



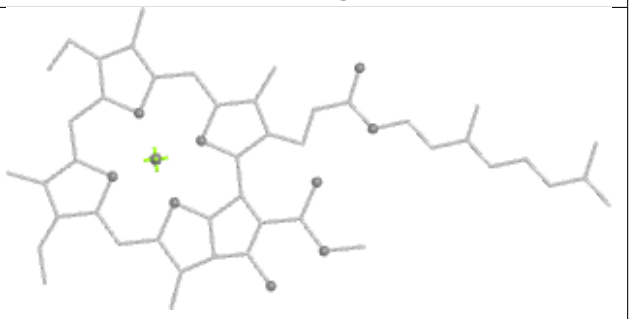
Bond lengths



Bond angles

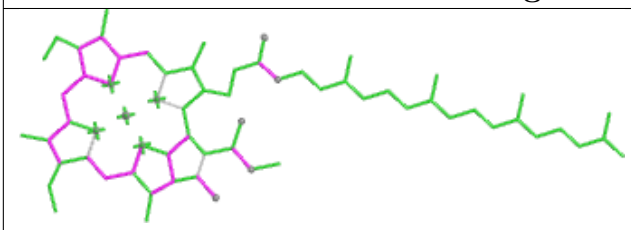


Torsions

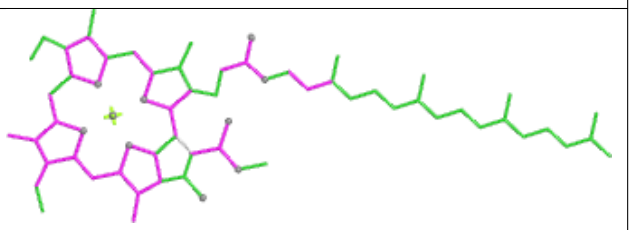


Rings

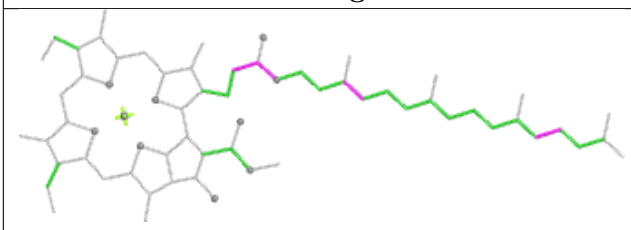
Ligand CLA A 825



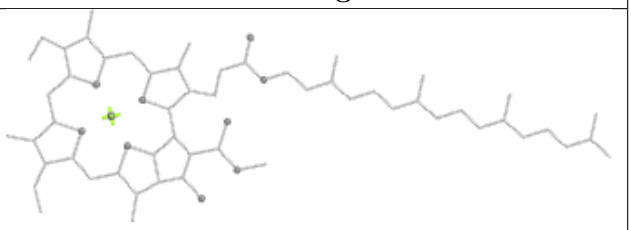
Bond lengths



Bond angles

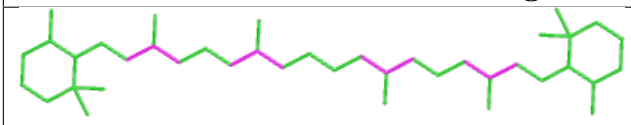


Torsions

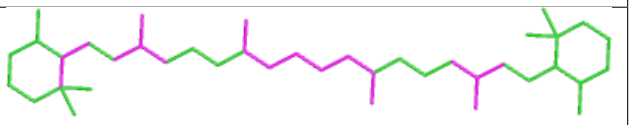


Rings

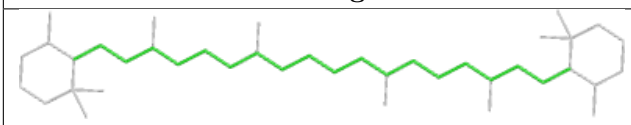
Ligand BCR B 841



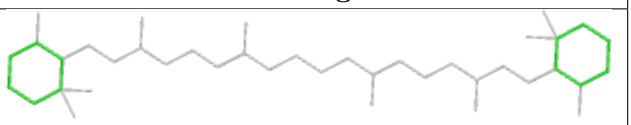
Bond lengths



Bond angles

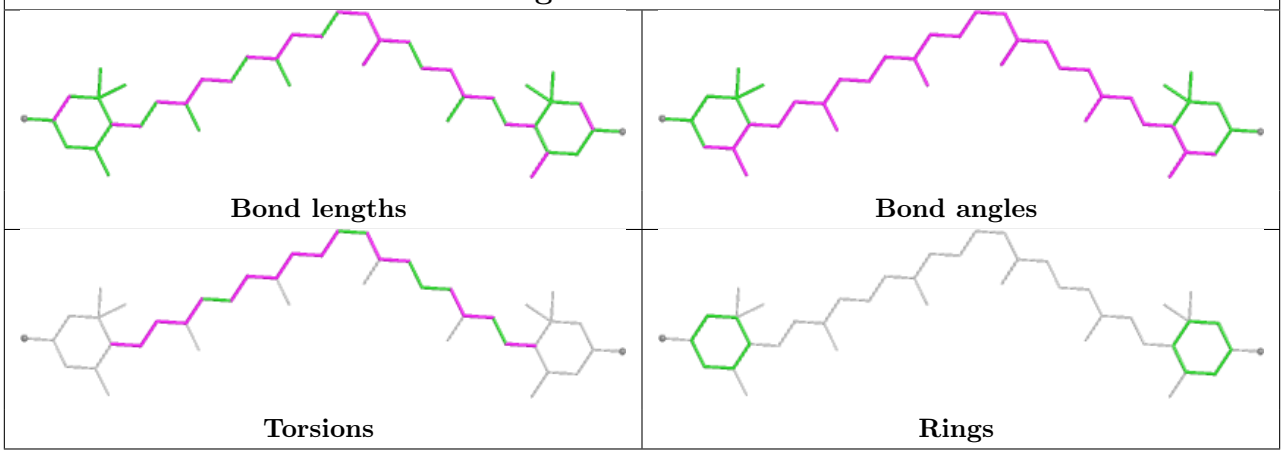


Torsions

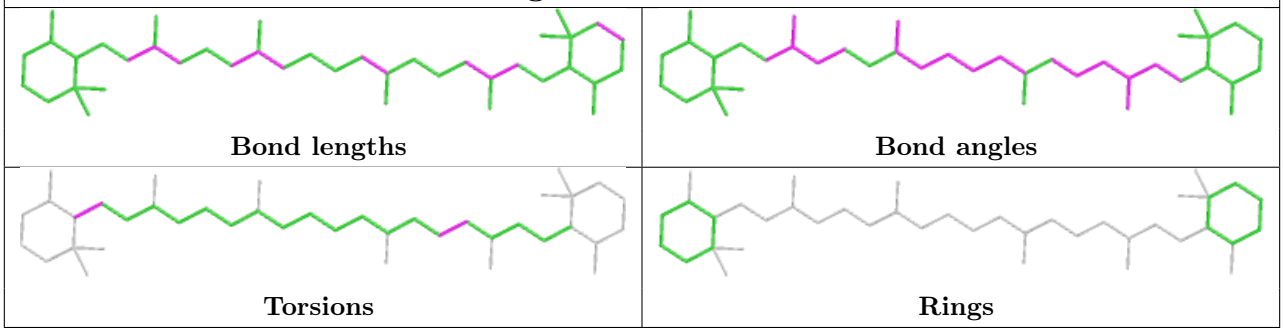


Rings

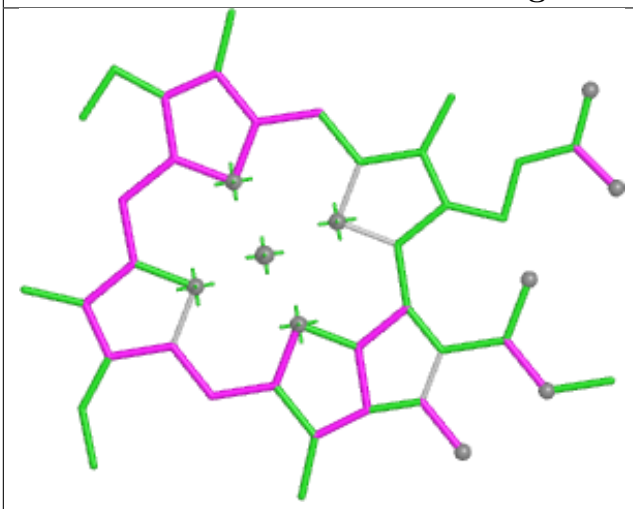
Ligand 5X6 6 315



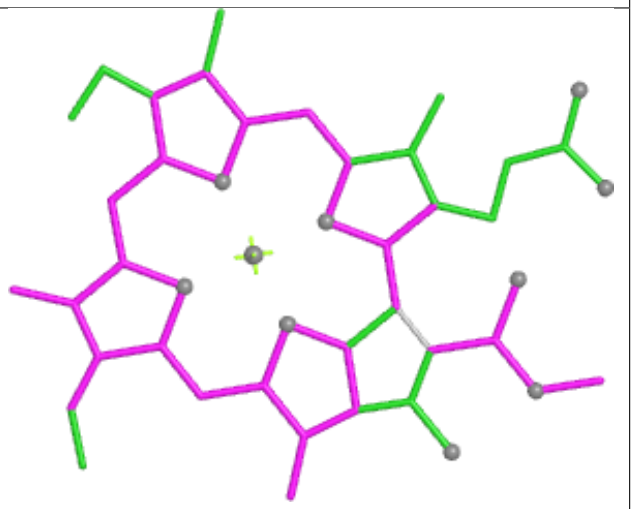
Ligand BCR J 103



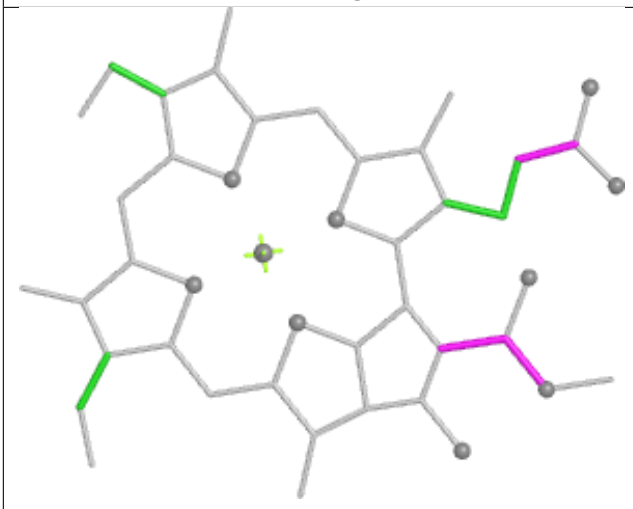
Ligand CLA 7 313



Bond lengths



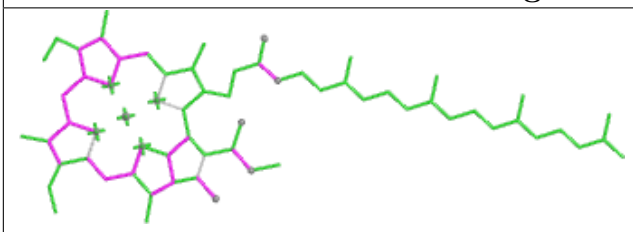
Bond angles



Torsions

Rings

Ligand CLA A 858



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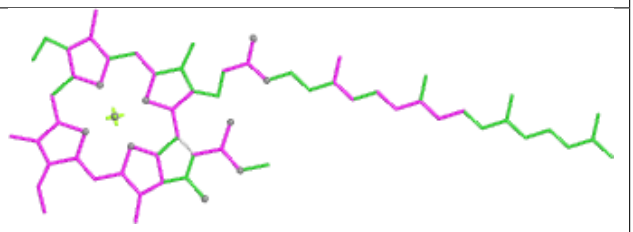
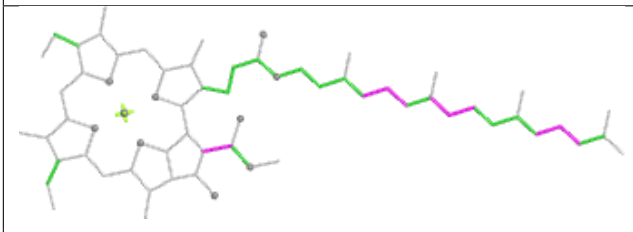
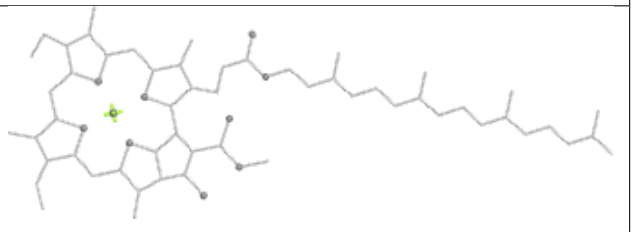


Bond angles

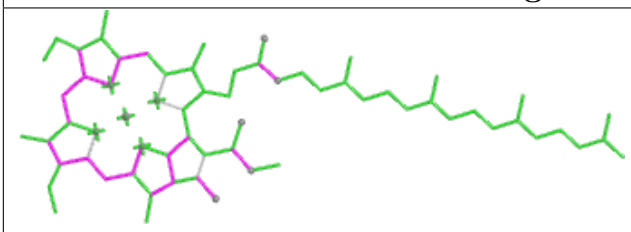


Torsions

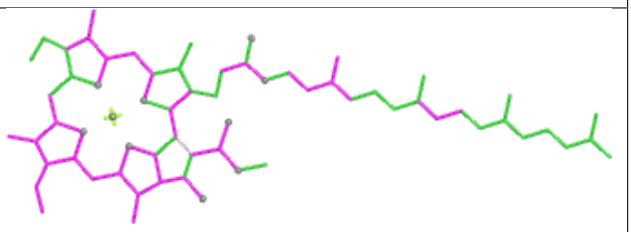


Rings

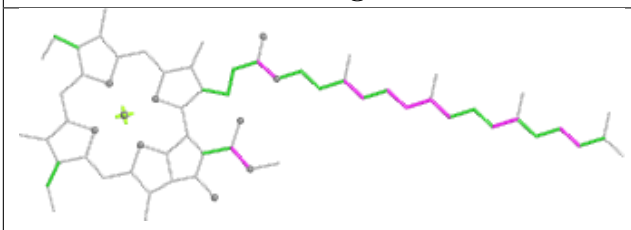
Ligand CLA B 838



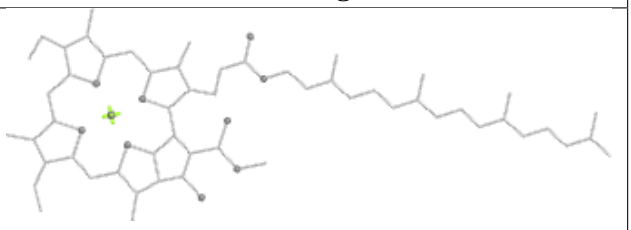
Bond lengths



Bond angles

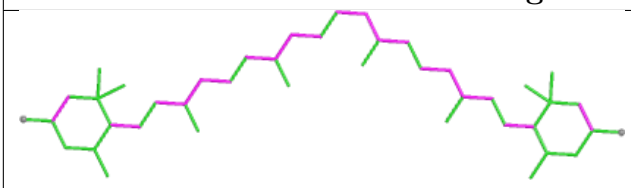


Torsions

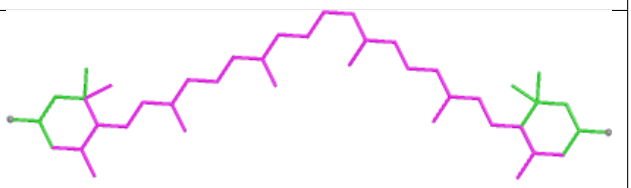


Rings

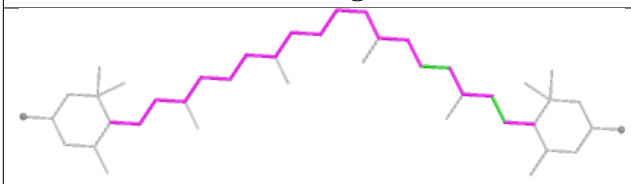
Ligand 5X6 M 101



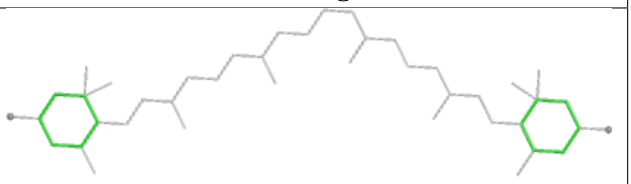
Bond lengths



Bond angles

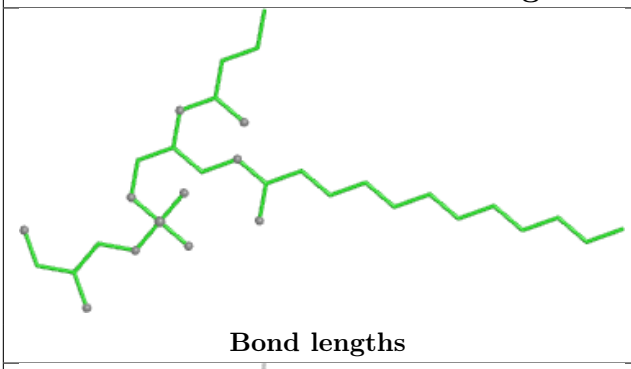


Torsions

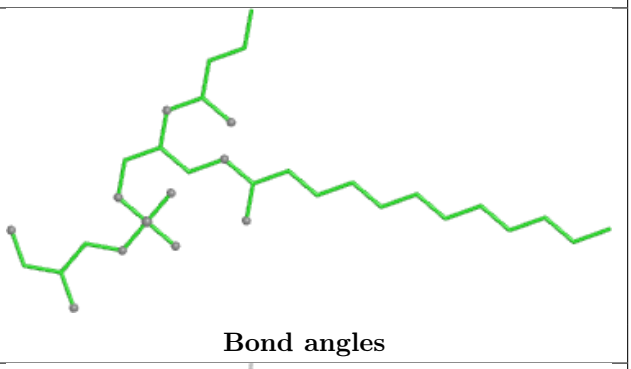


Rings

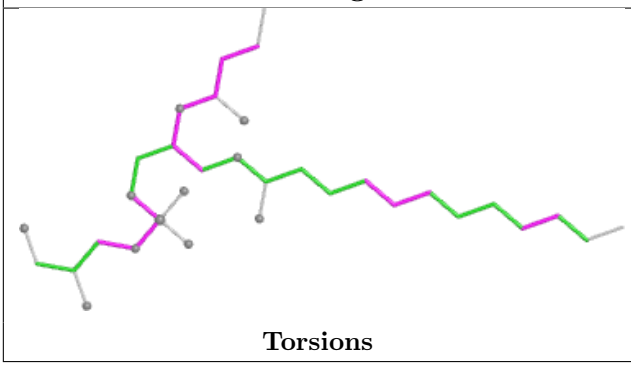
Ligand LHG A 860



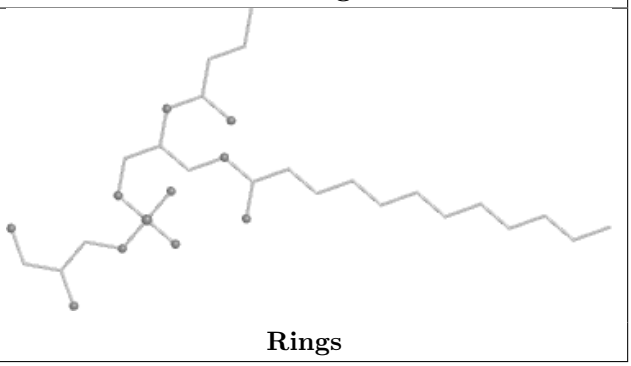
Bond lengths



Bond angles

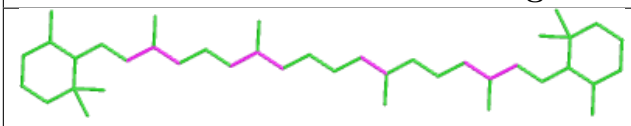


Torsions

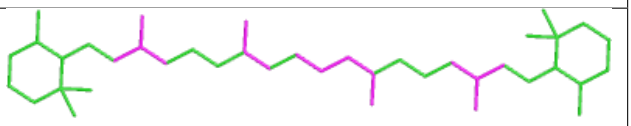


Rings

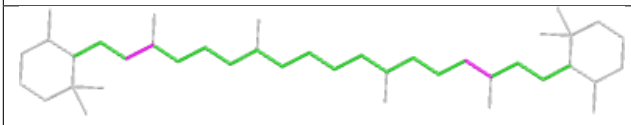
Ligand BCR 2 301



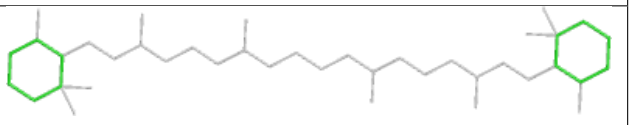
Bond lengths



Bond angles

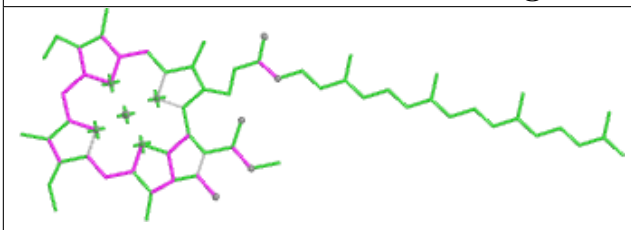


Torsions



Rings

Ligand CLA A 837



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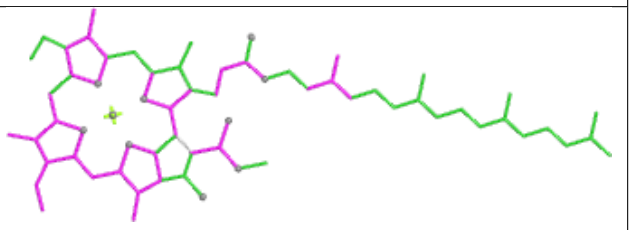

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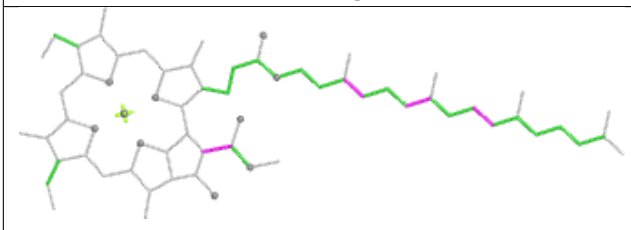

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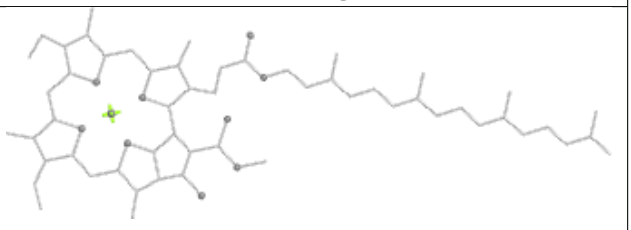
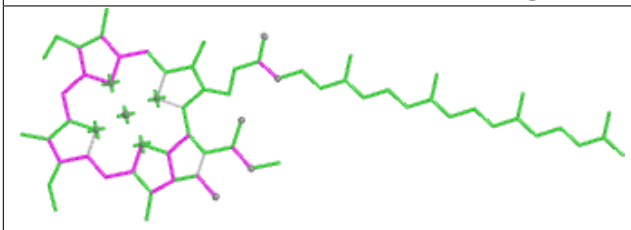


Rings

Ligand CLA A 827



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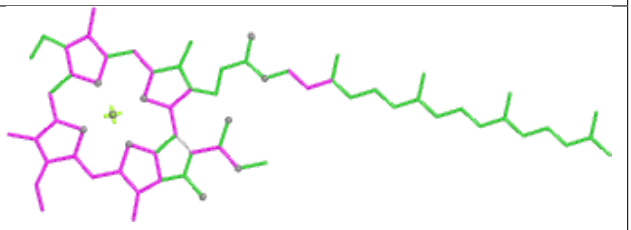

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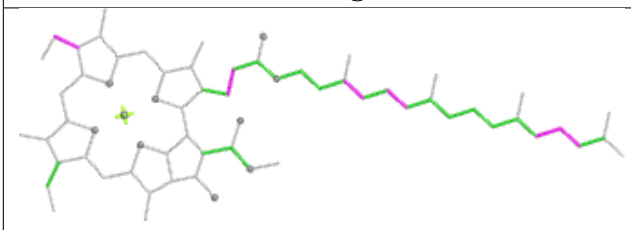

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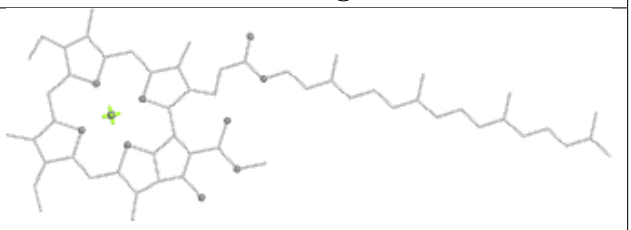
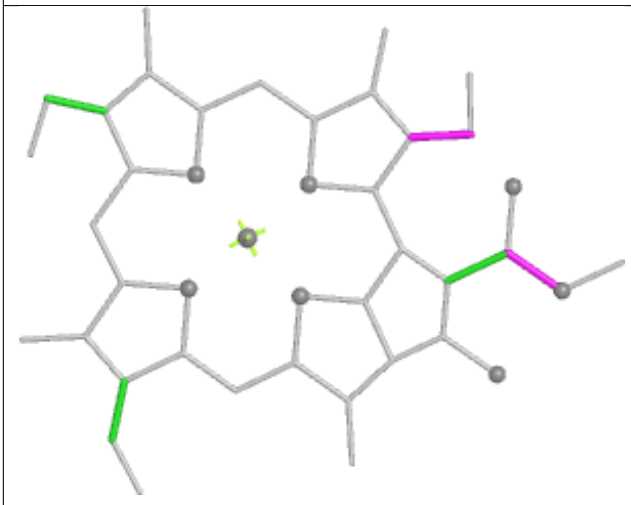


Rings

Ligand CLA 2 310

Bond lengths

Bond angles



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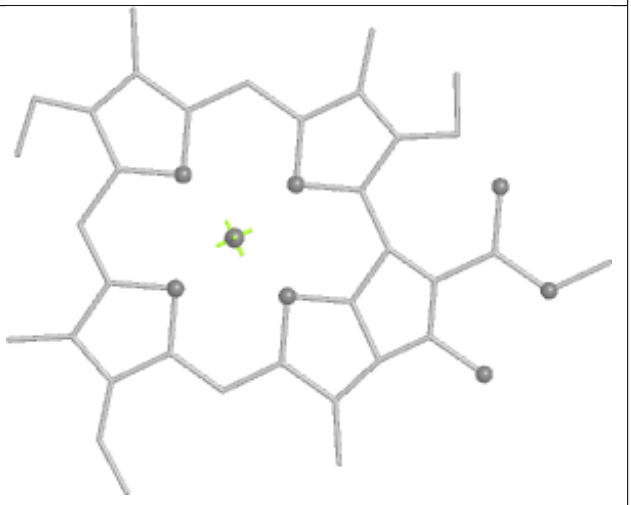
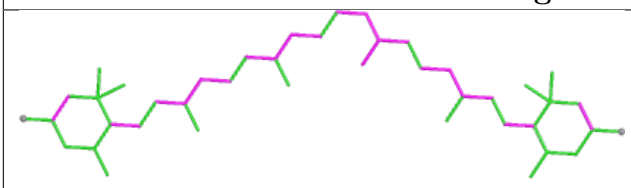


Rings

Ligand 5X6 1 314



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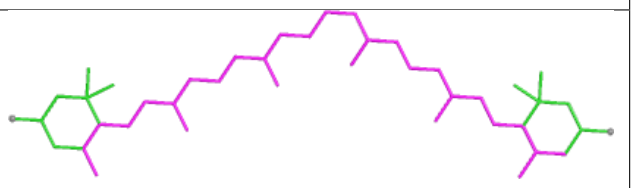
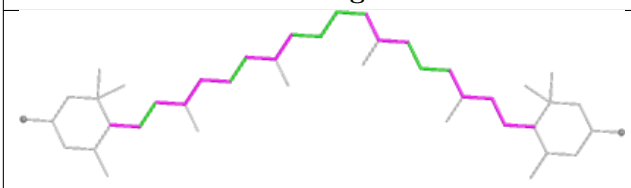


Bond angles



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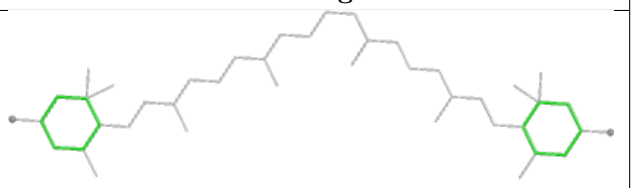
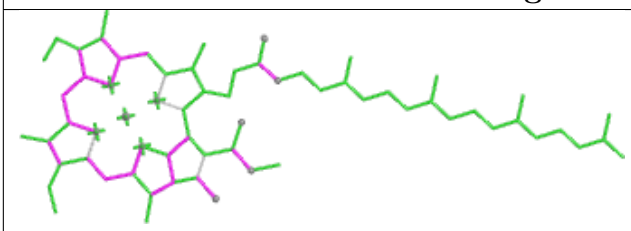


Rings

Ligand CLA B 825



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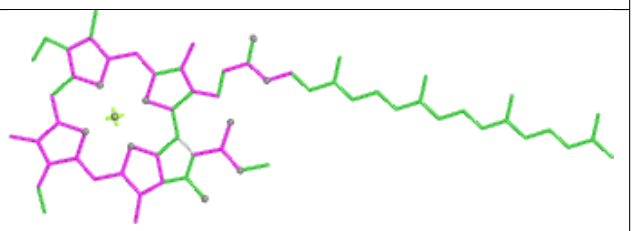
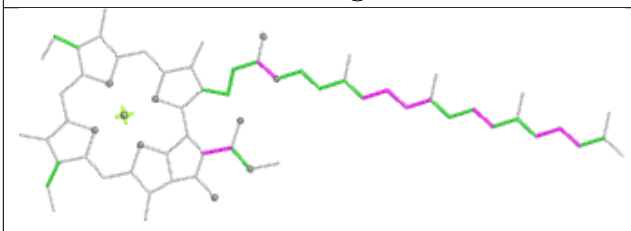


Bond angles



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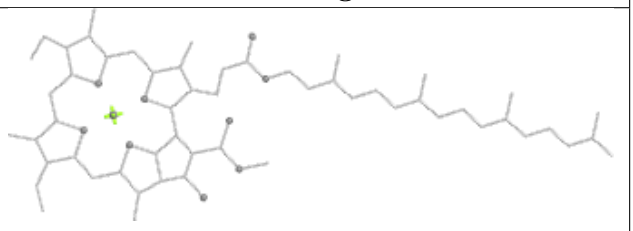
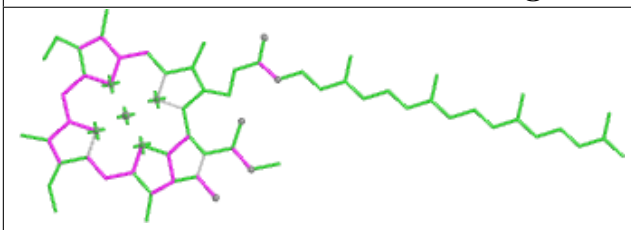


Rings

Ligand CLA B 826



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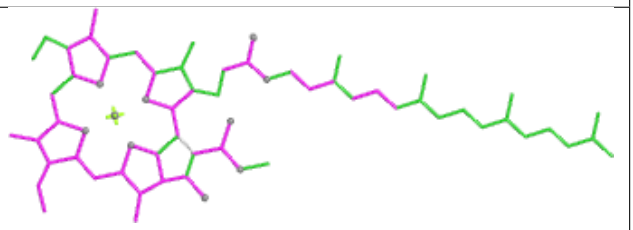
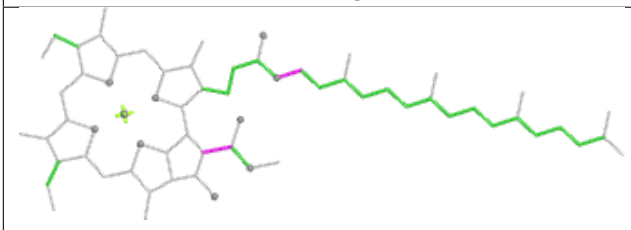


Bond angles



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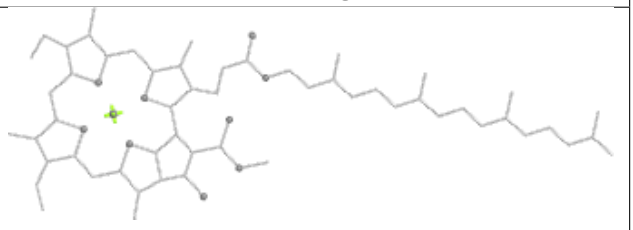
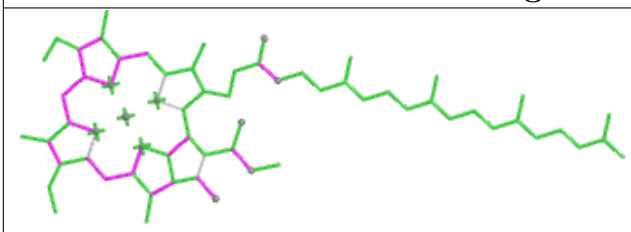


Rings

Ligand CLA B 828



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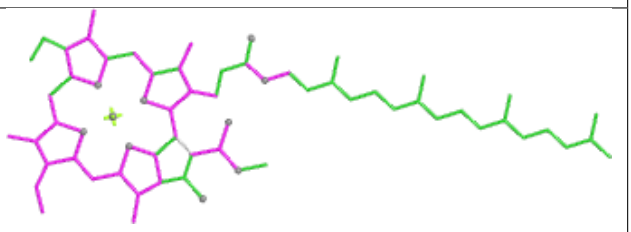
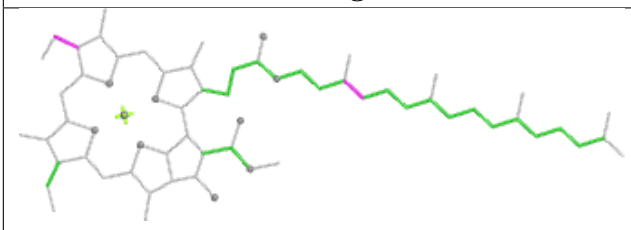


Bond angles



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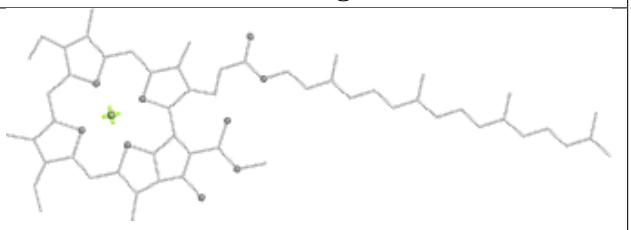
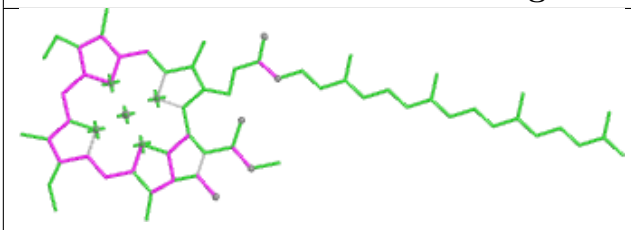


Rings

Ligand CLA 5 306



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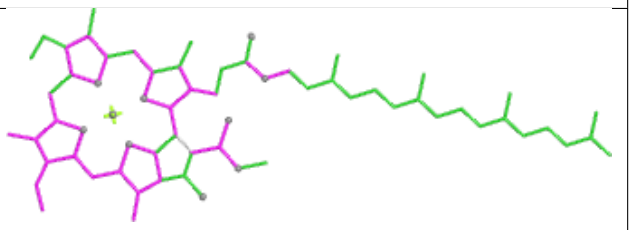
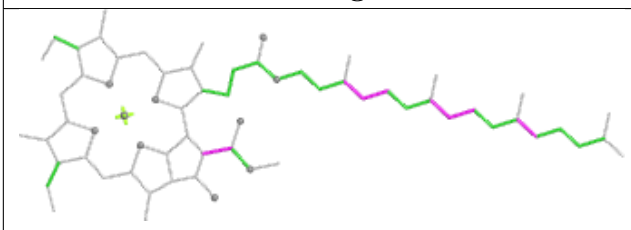


Bond angles



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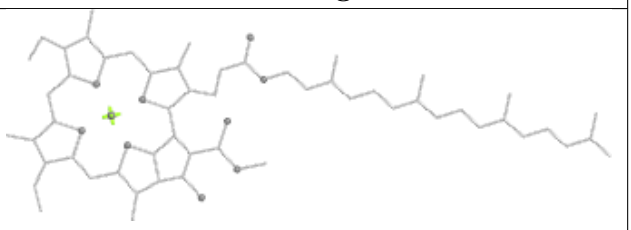
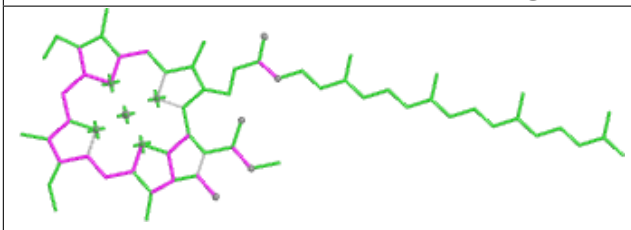


Rings

Ligand CLA B 833



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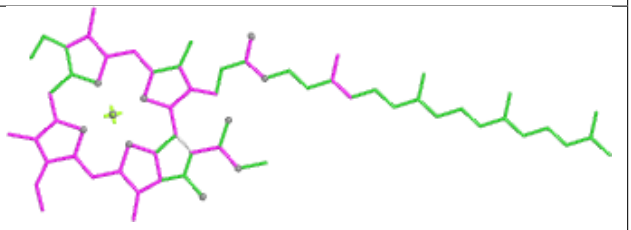
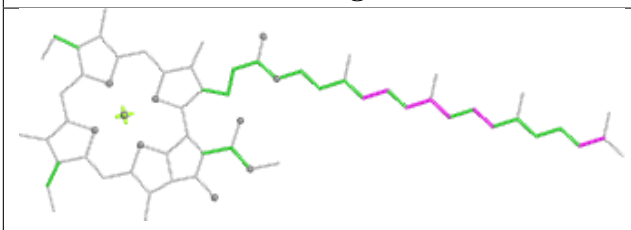


Bond angles



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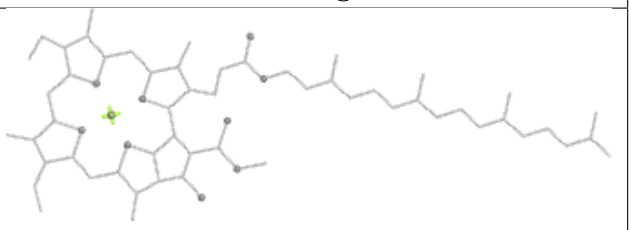
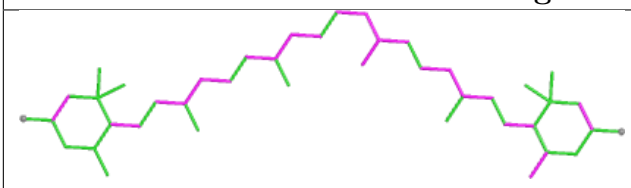


Rings

Ligand 5X6 5 314



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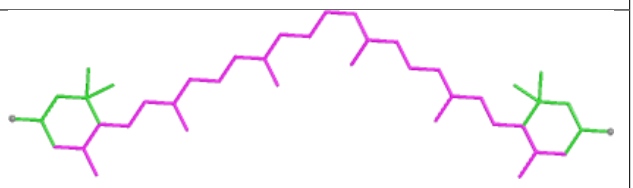
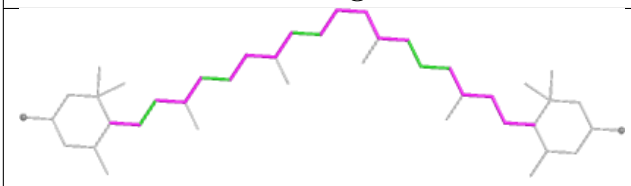


Bond angles



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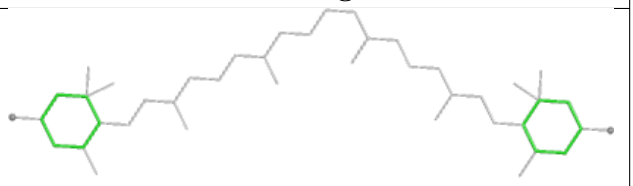
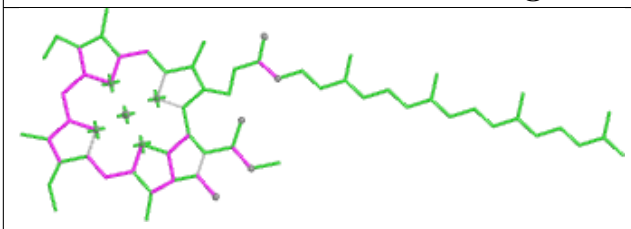


Rings

Ligand CLA B 830



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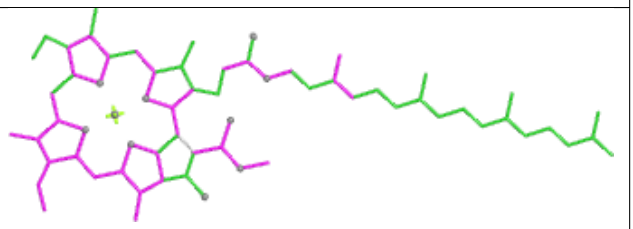
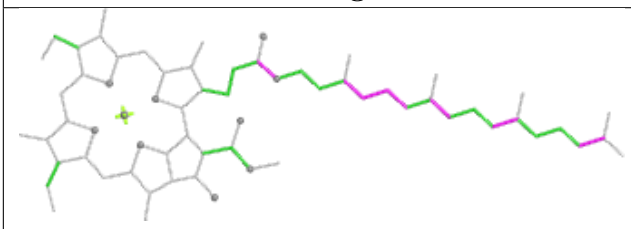
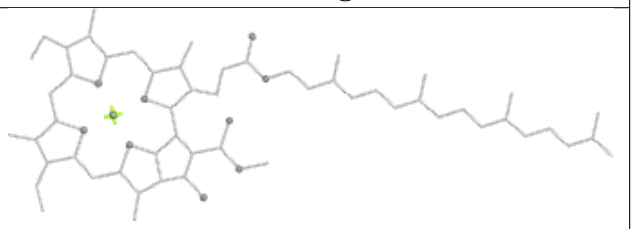


Bond angles

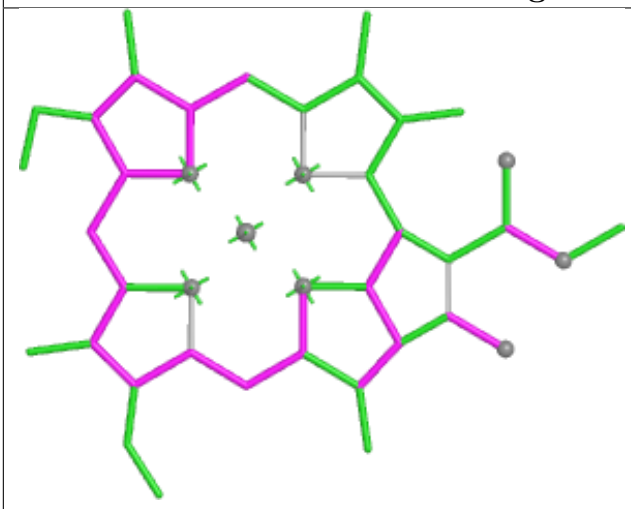


Torsions



Rings

Ligand CLA 2 309



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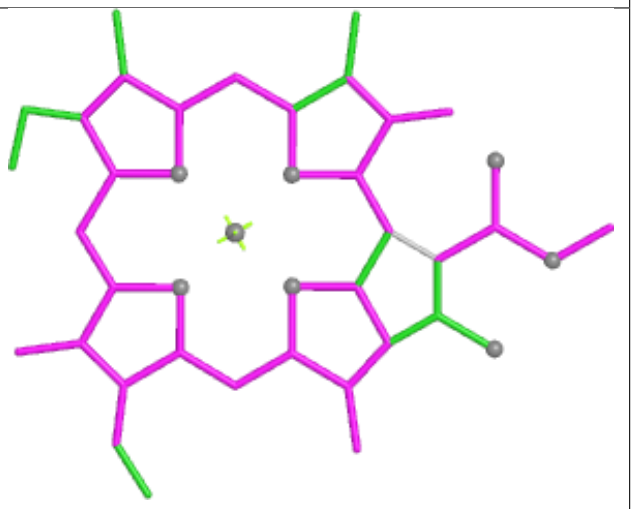
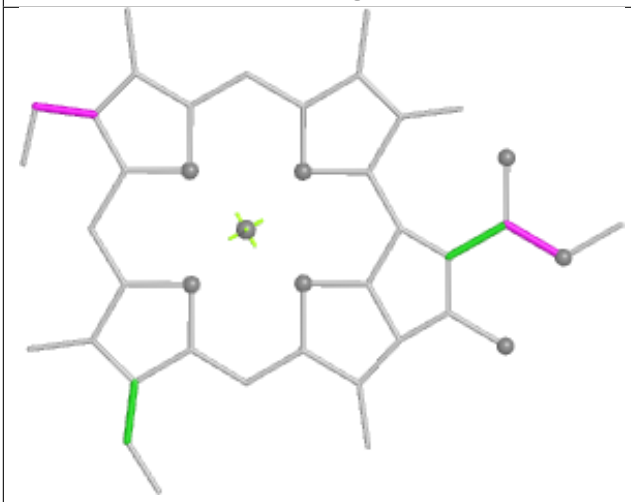


Bond angles



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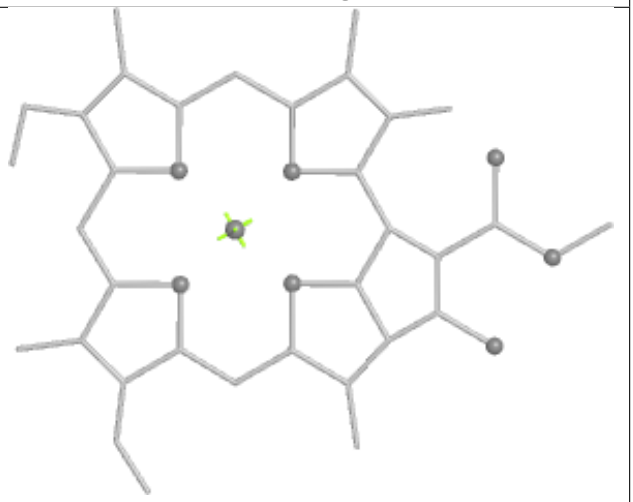
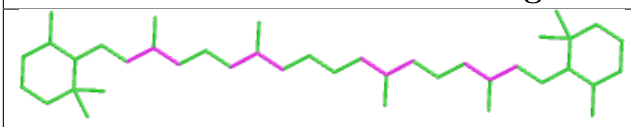


Rings

Ligand BCR Z 202



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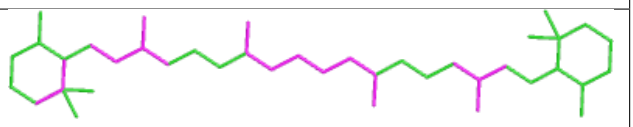
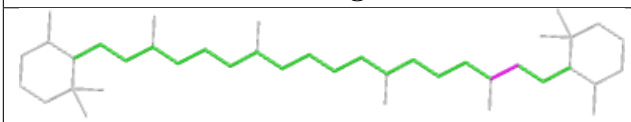
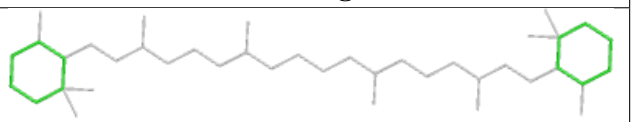


Bond angles

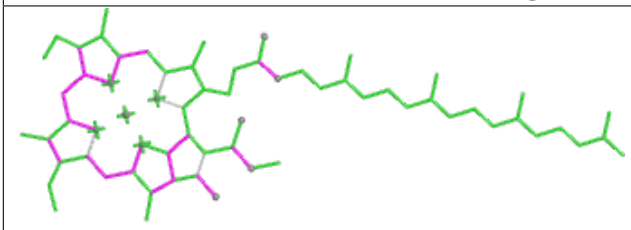


Torsions

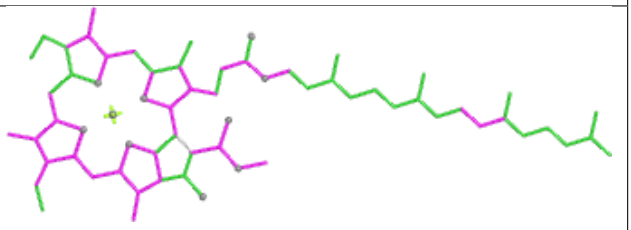


Rings

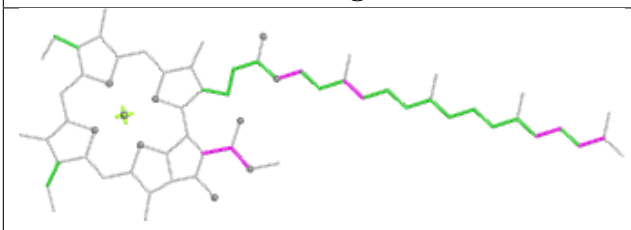
Ligand CLA A 832



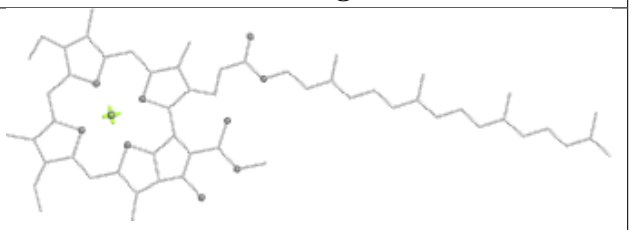
Bond lengths



Bond angles

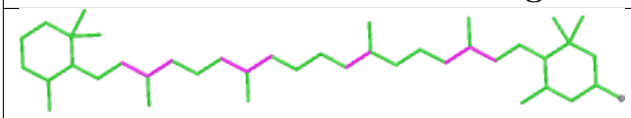


Torsions



Rings

Ligand RRX 1 315



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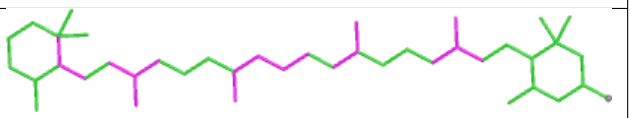
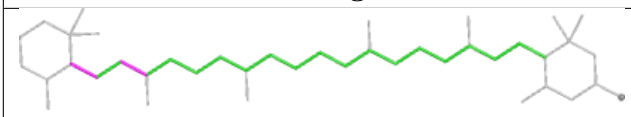
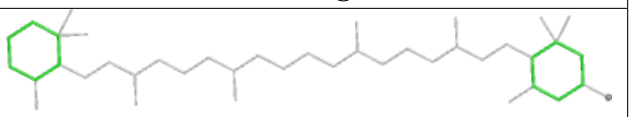


Bond angles

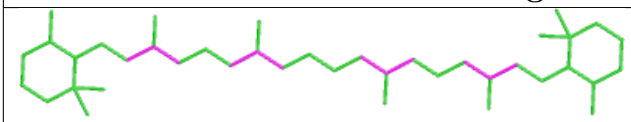


Torsions



Rings

Ligand BCR 1 301



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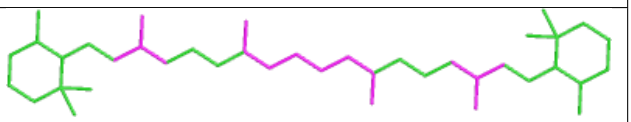
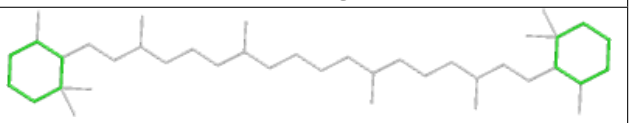


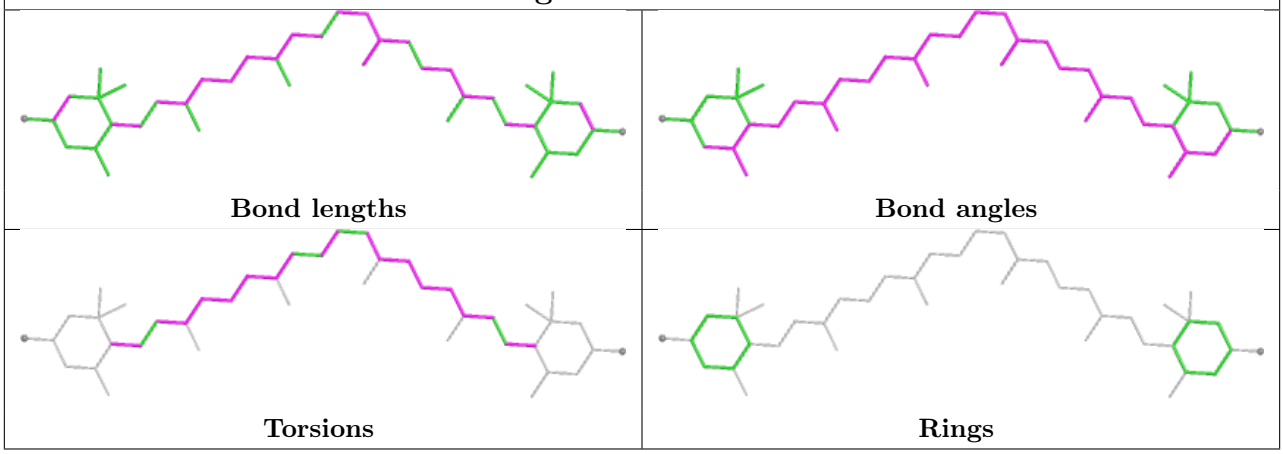
Bond angles

Torsions

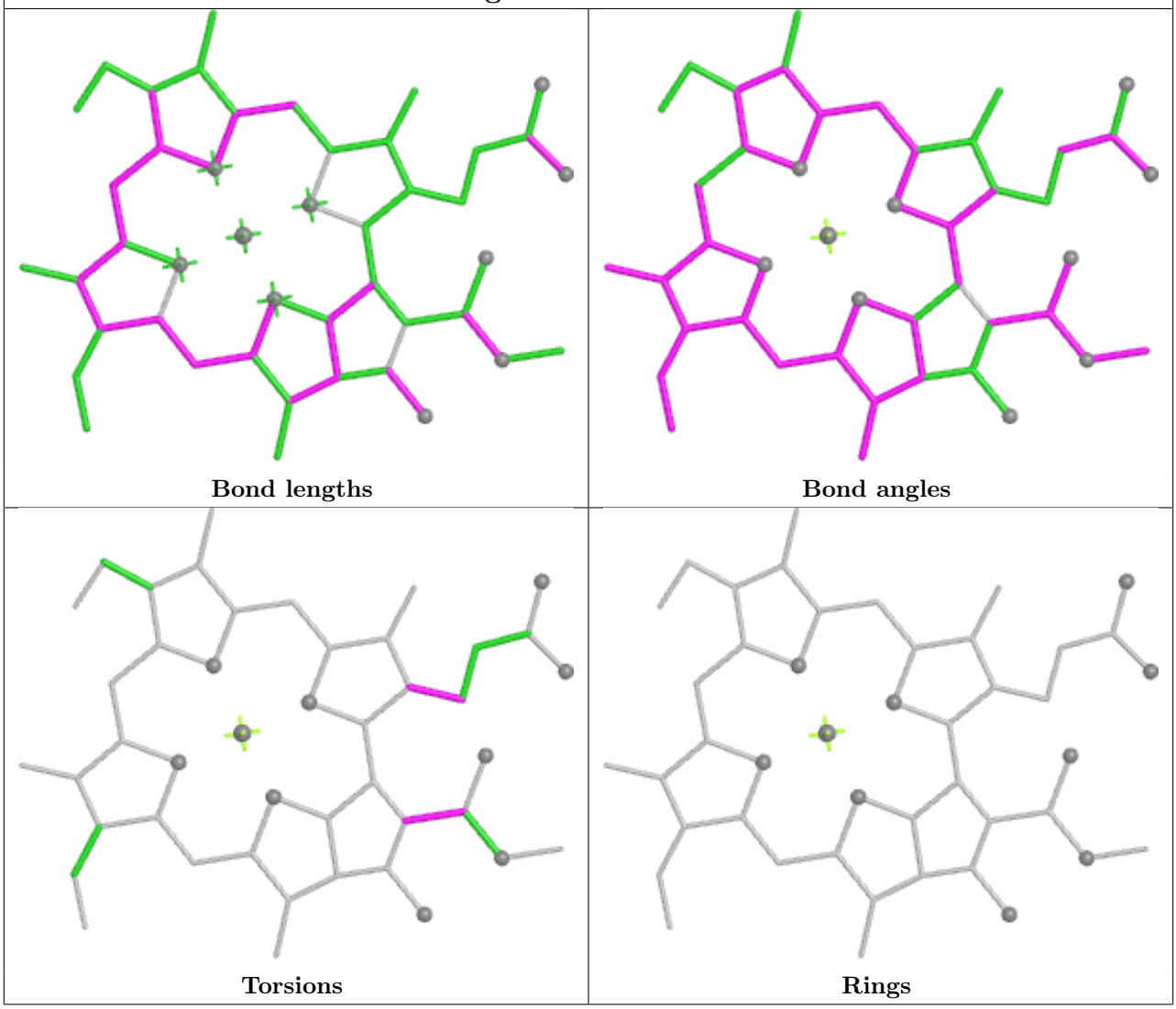


Rings

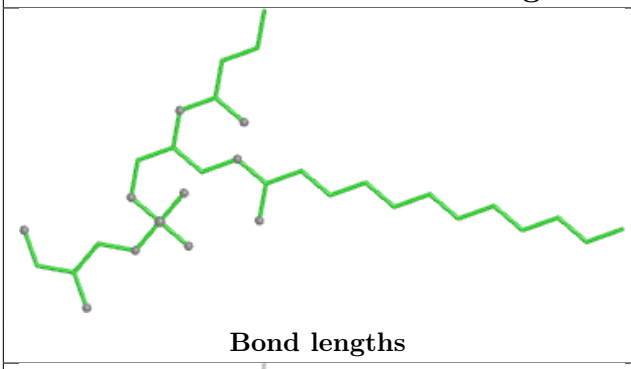
Ligand 5X6 1 316



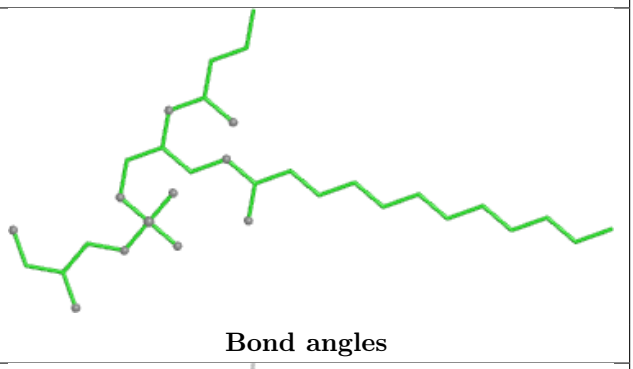
Ligand CLA 6 308



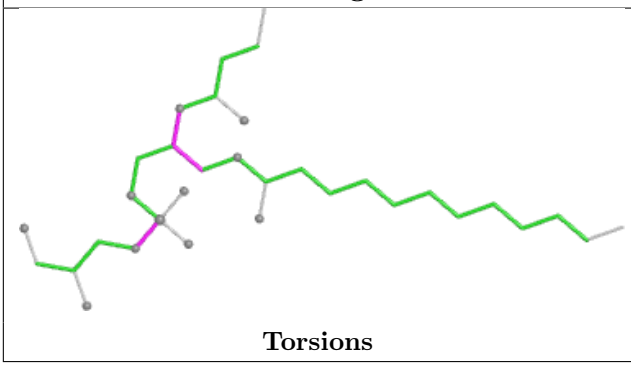
Ligand LHG B 846



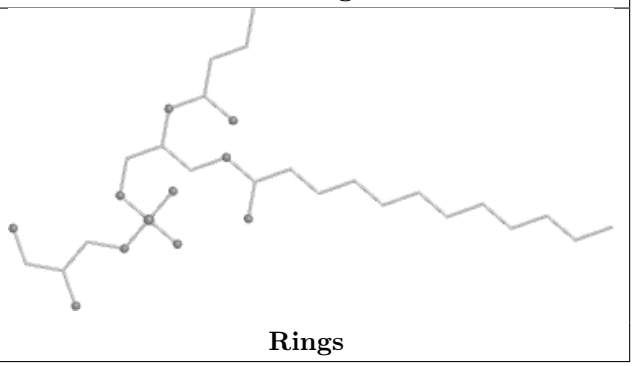
Bond lengths



Bond angles

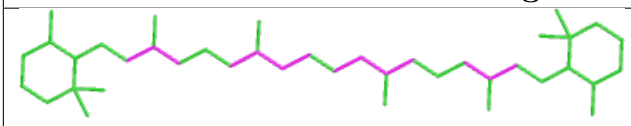


Torsions



Rings

Ligand BCR A 846



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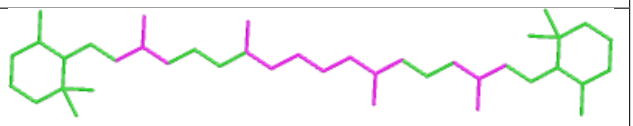
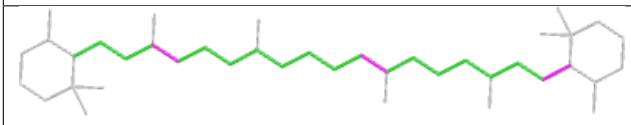


Bond angles



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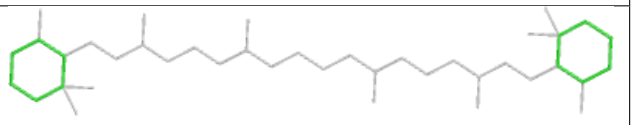
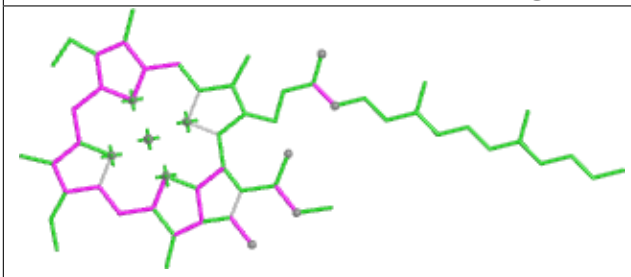
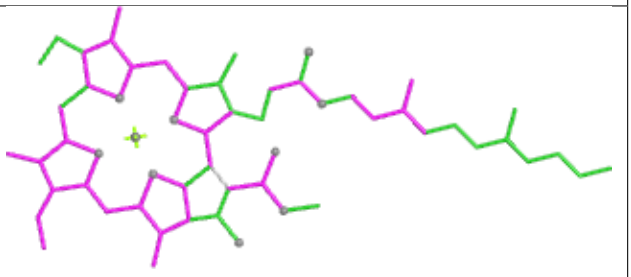


Rings

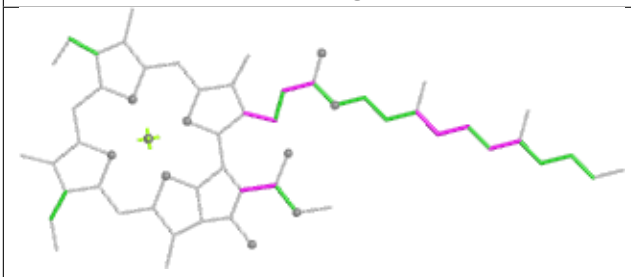
Ligand CLA 2 303



Bond lengths



Bond angles



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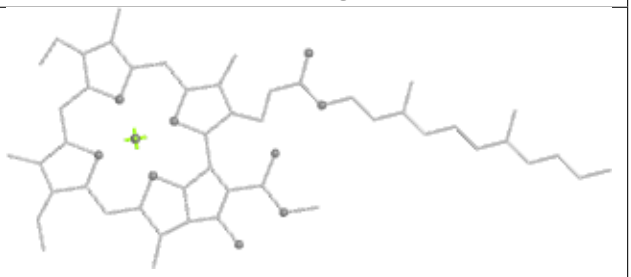
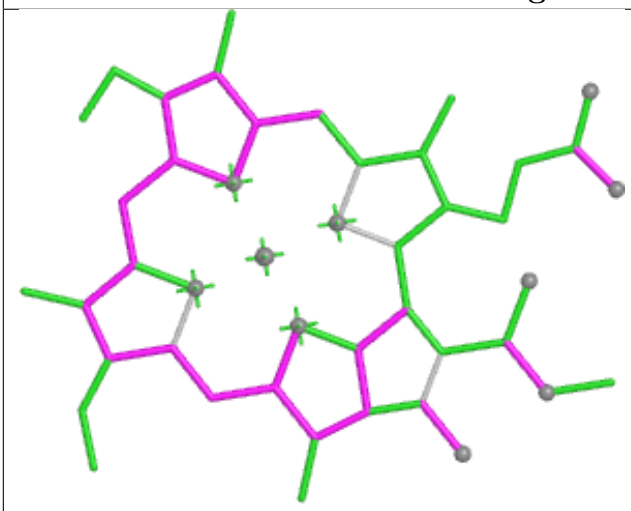


Rings

Ligand CLA 2 306



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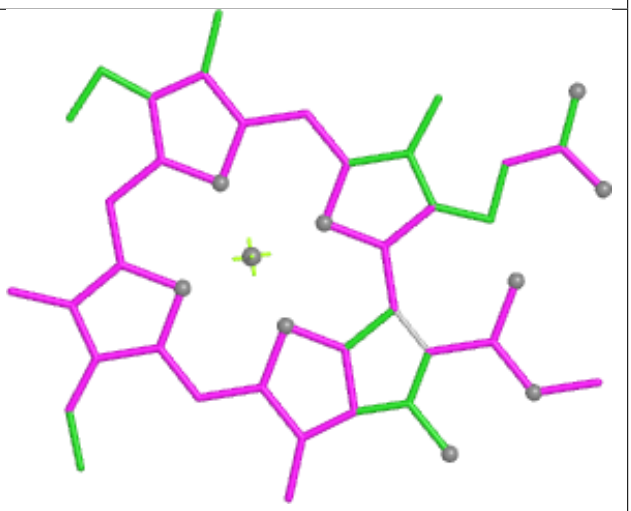
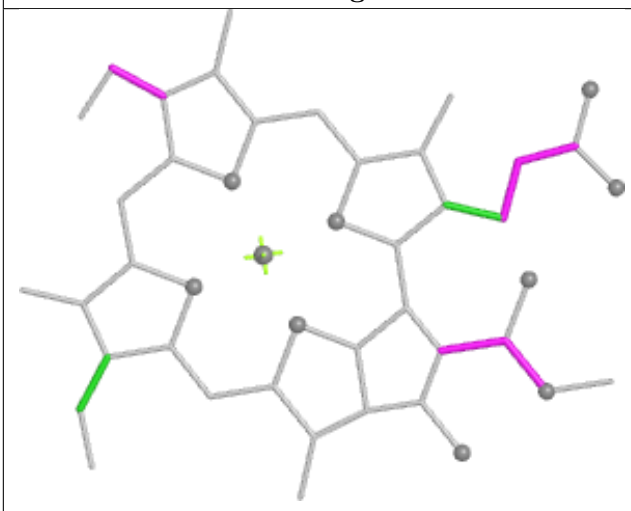


Bond angles



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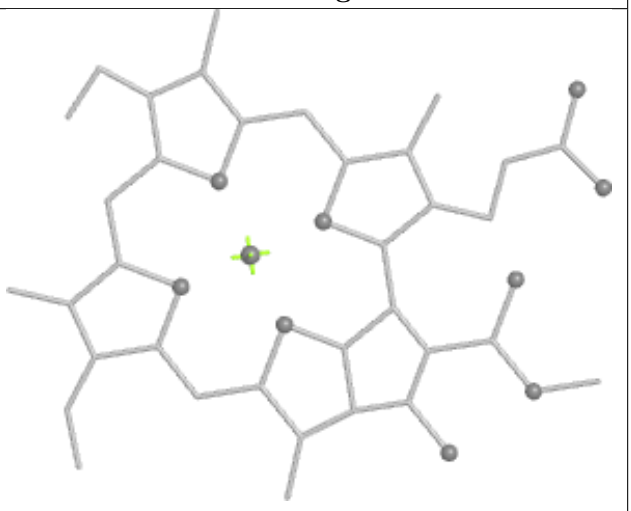
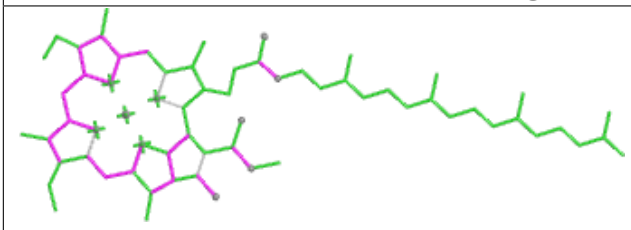


Rings

Ligand CLA B 831



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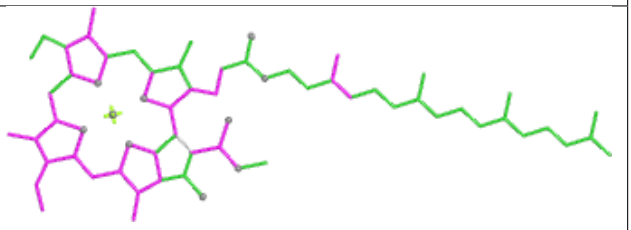
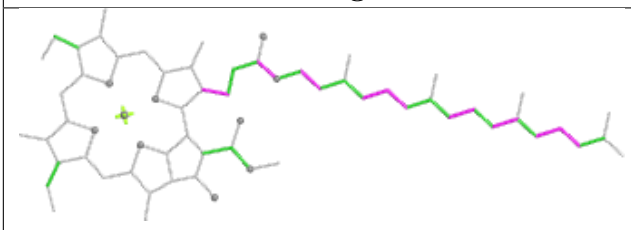
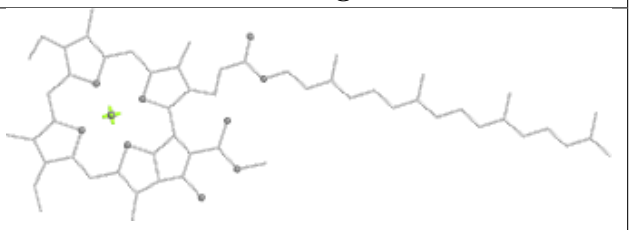


Bond angles

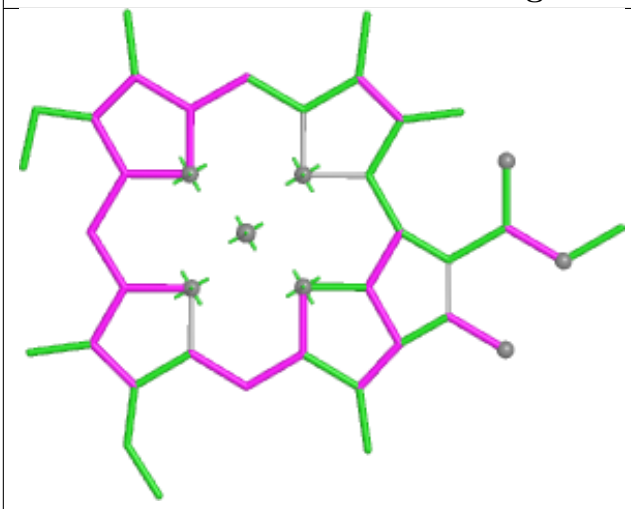


Torsions



Rings

Ligand CLA F 206



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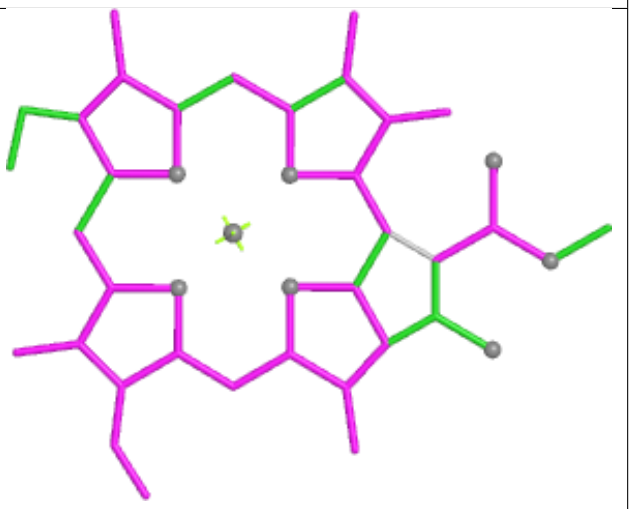
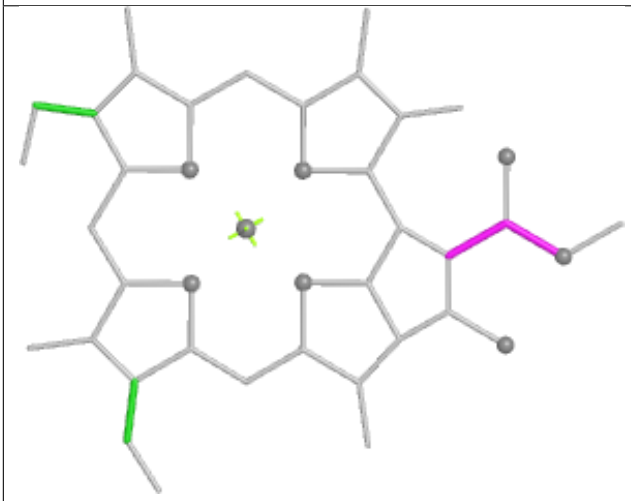


Bond angles



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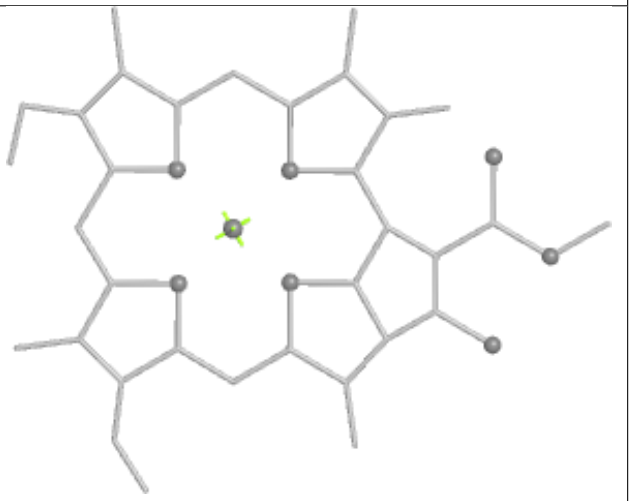
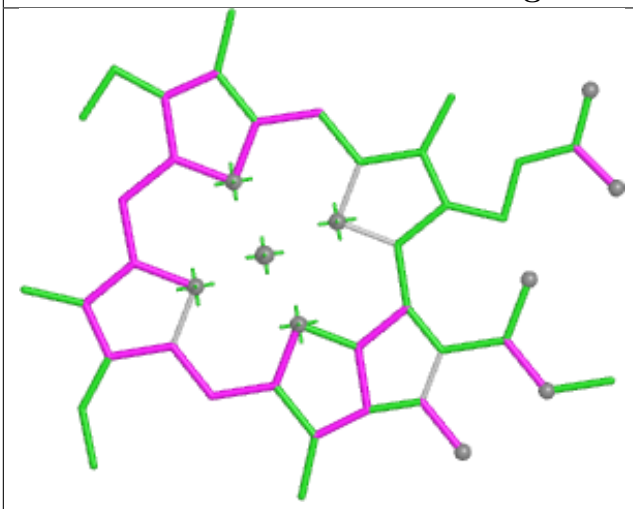


Rings

Ligand CLA A 814



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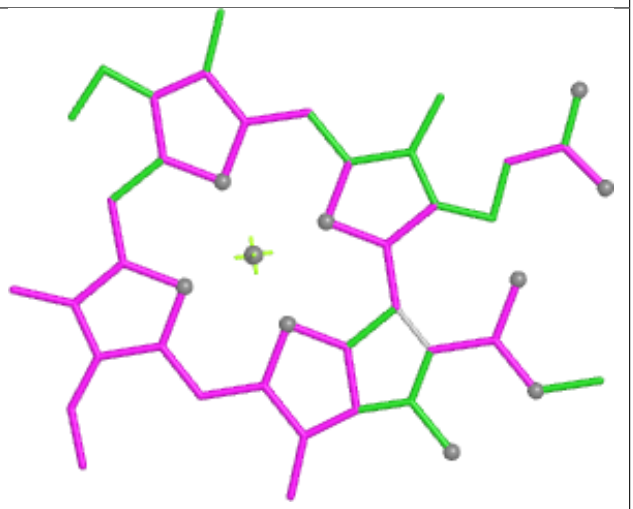
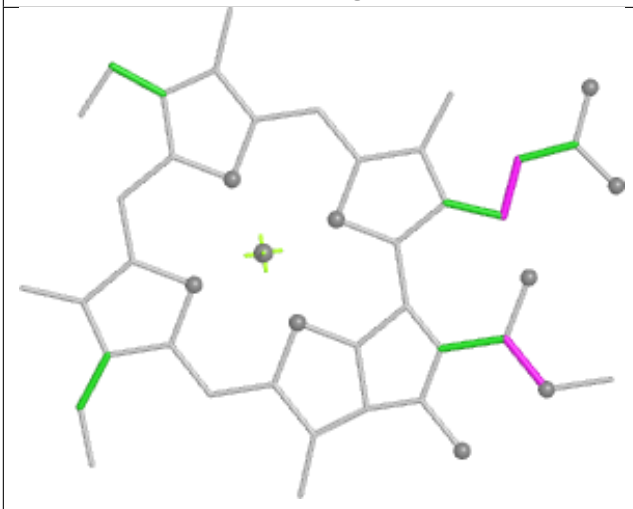


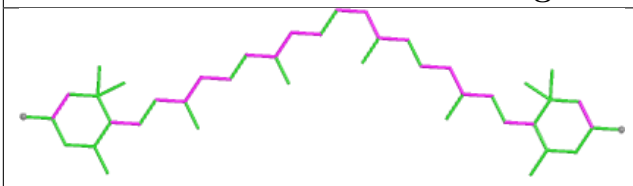
Bond angles



Torsions

Rings

Ligand 5X6 7 314



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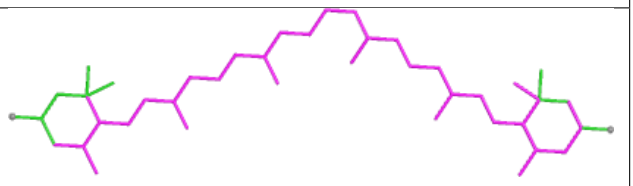
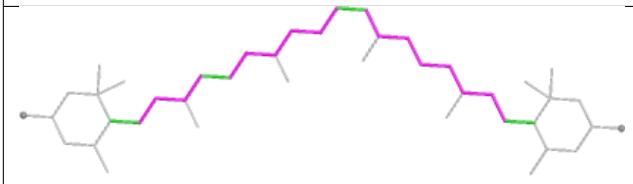
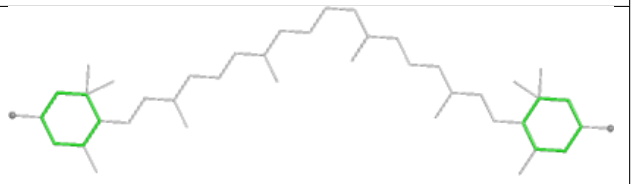


Bond angles

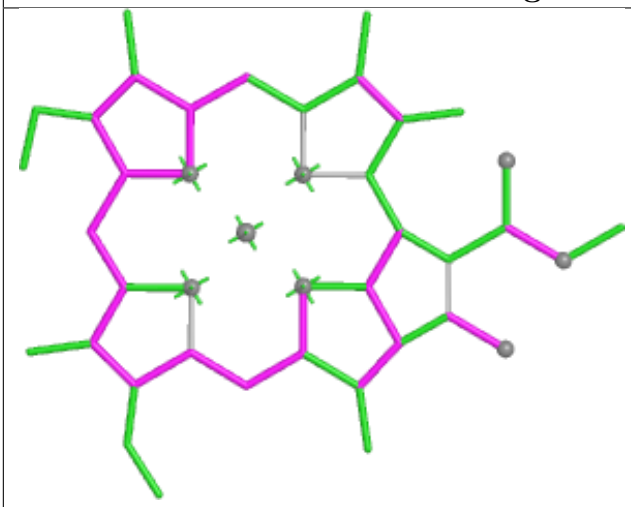


Torsions



Rings

Ligand CLA O 204



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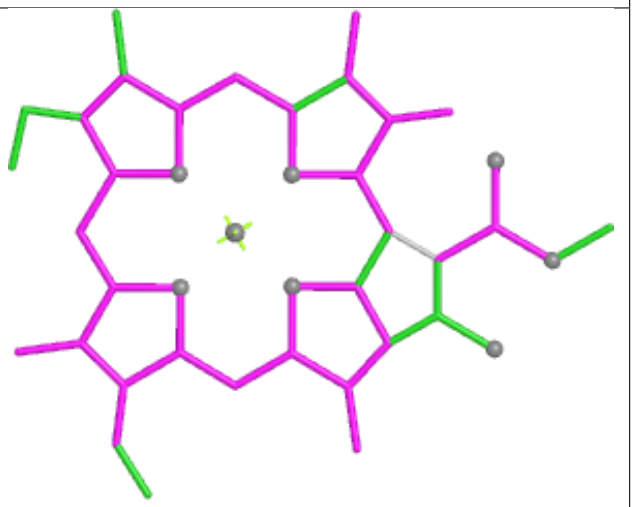
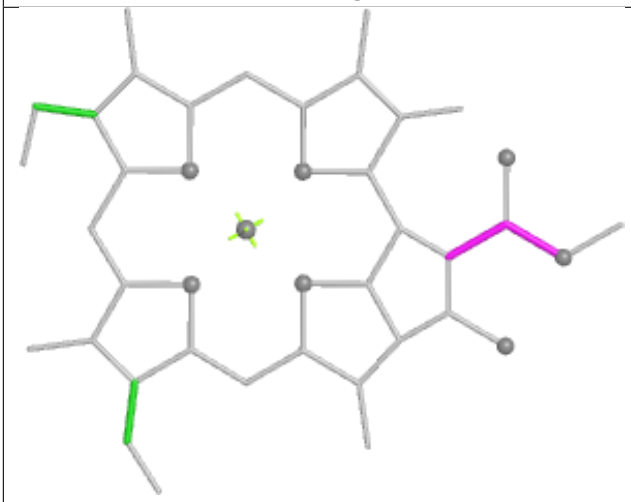
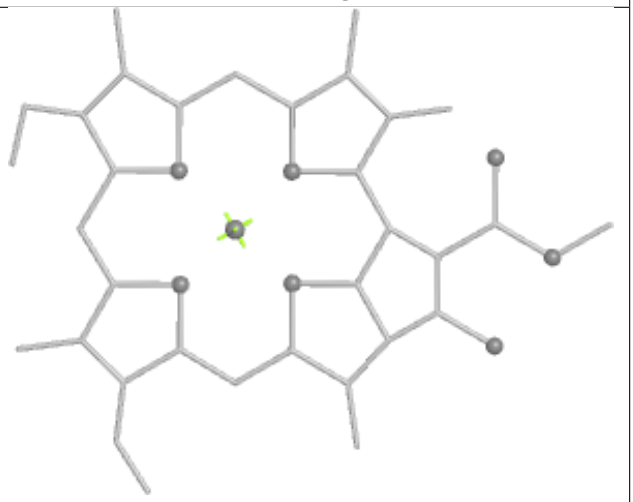


Bond angles

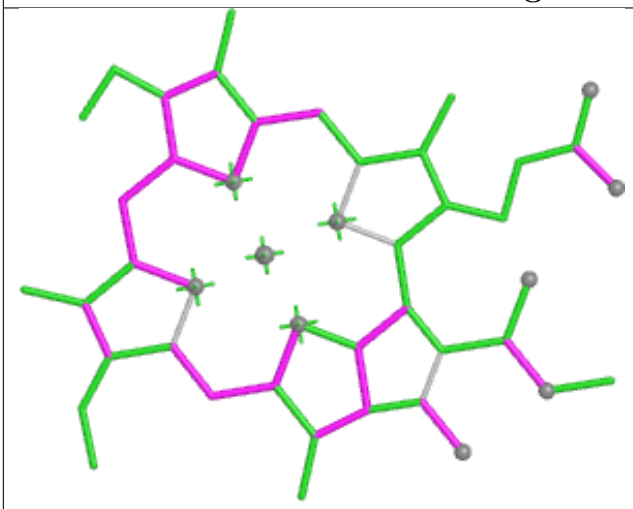


Torsions

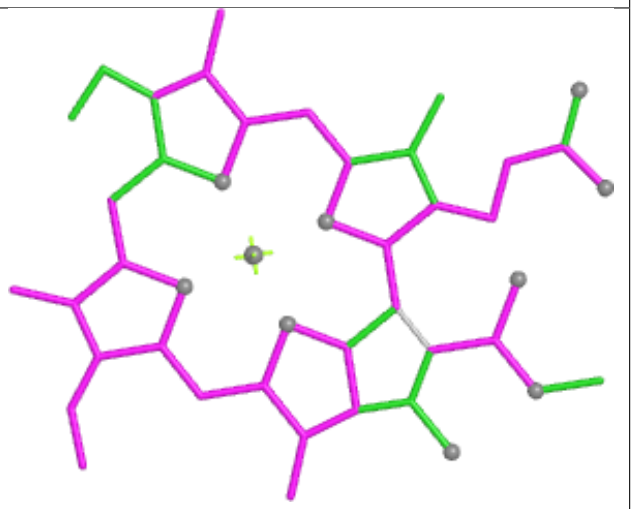


Rings

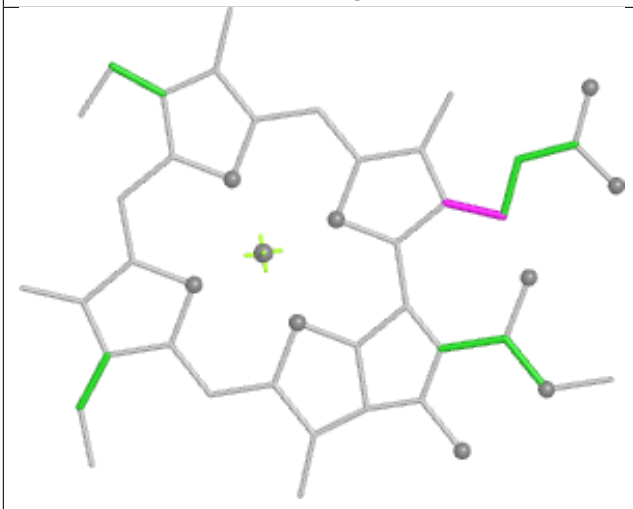
Ligand CLA B 820



Bond lengths



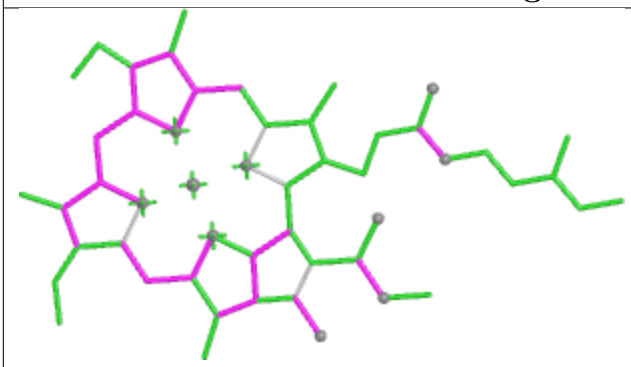
Bond angles



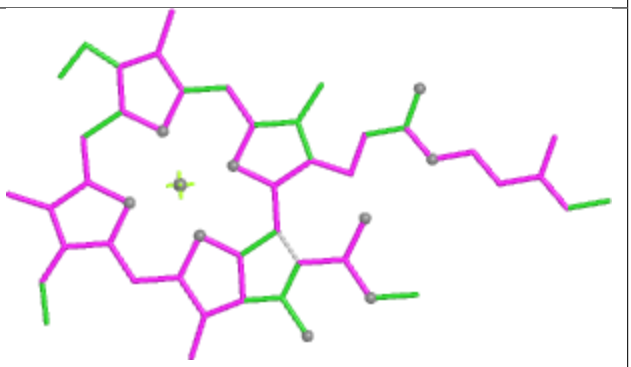
Torsions

Rings

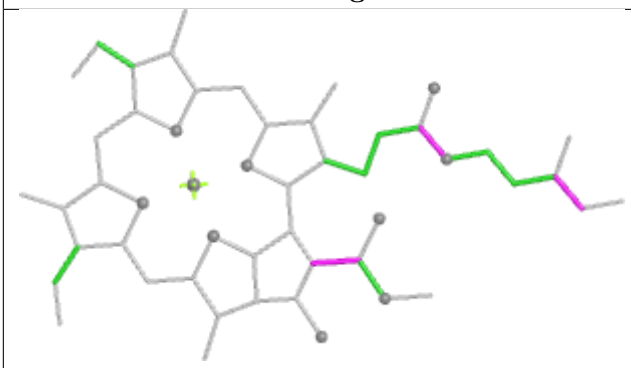
Ligand CLA A 835



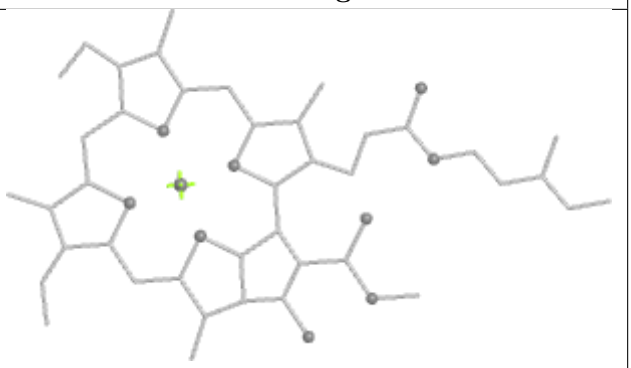
Bond lengths



Bond angles

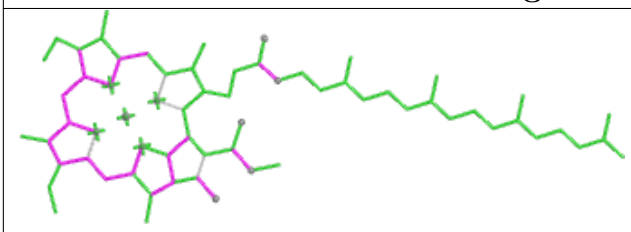


Torsions

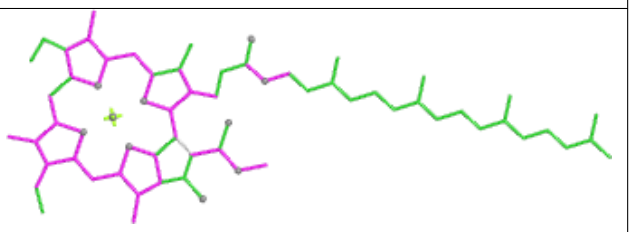


Rings

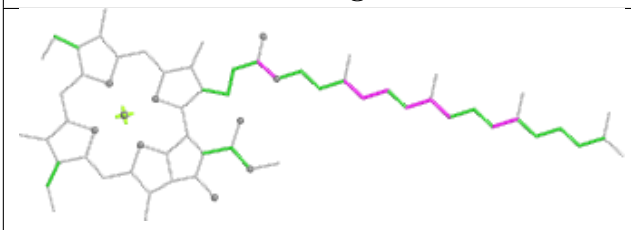
Ligand CLA A 819



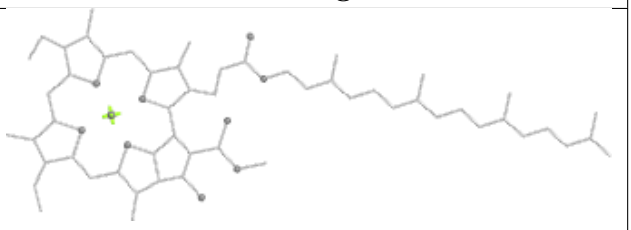
Bond lengths



Bond angles

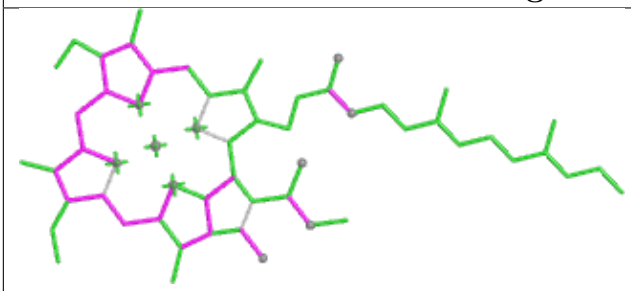


Torsions



Rings

Ligand CLA L 203



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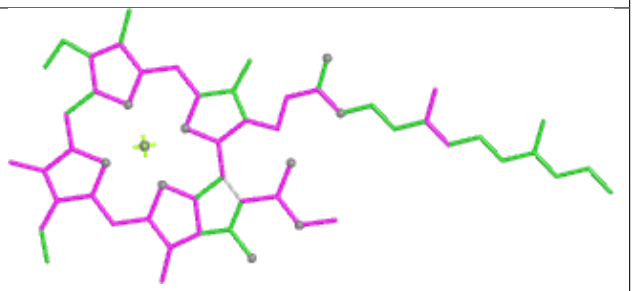
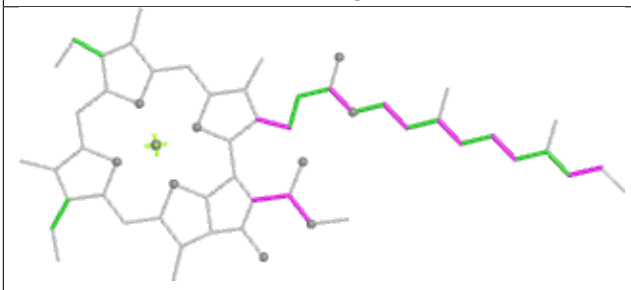
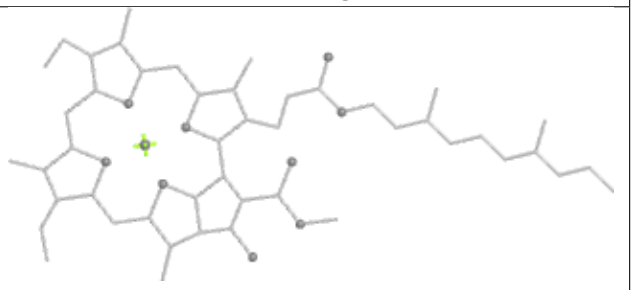


Bond angles

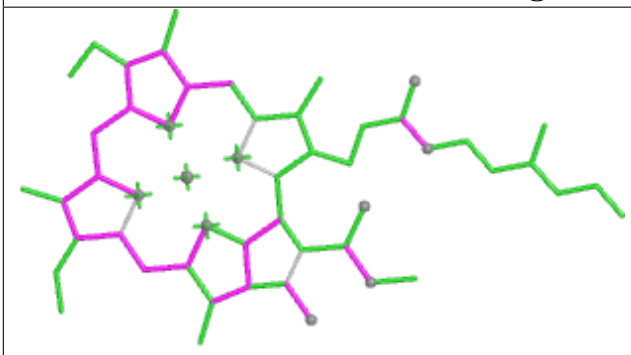


Torsions



Rings

Ligand CLA 5 310



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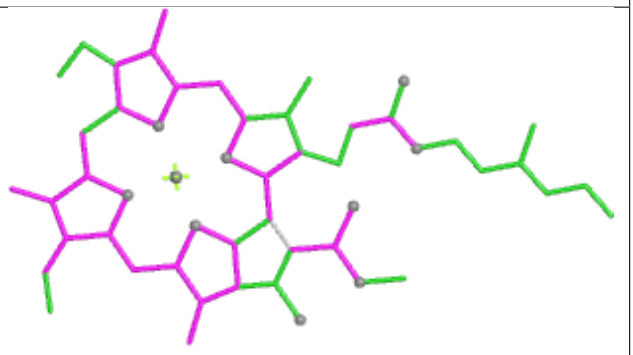
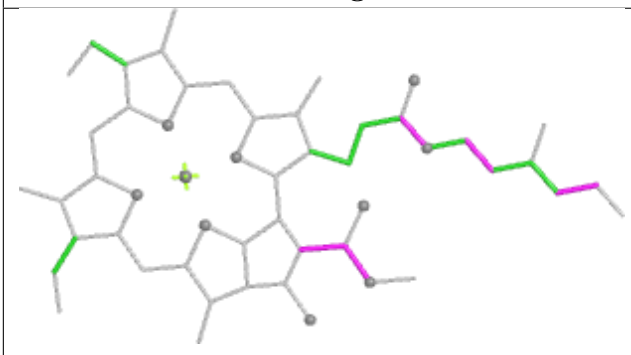


Bond angles



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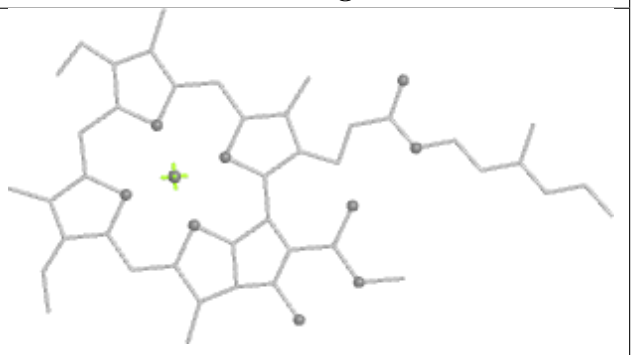
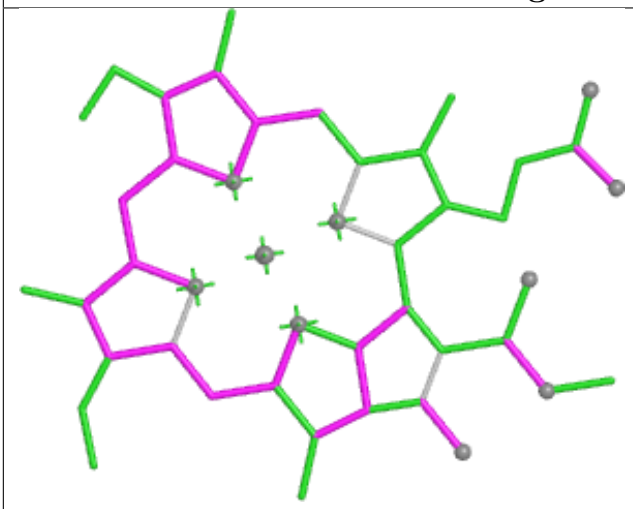


Rings

Ligand CLA 5 311



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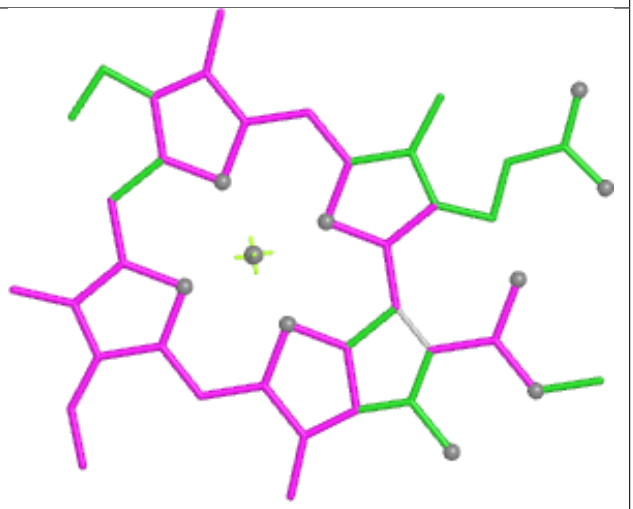
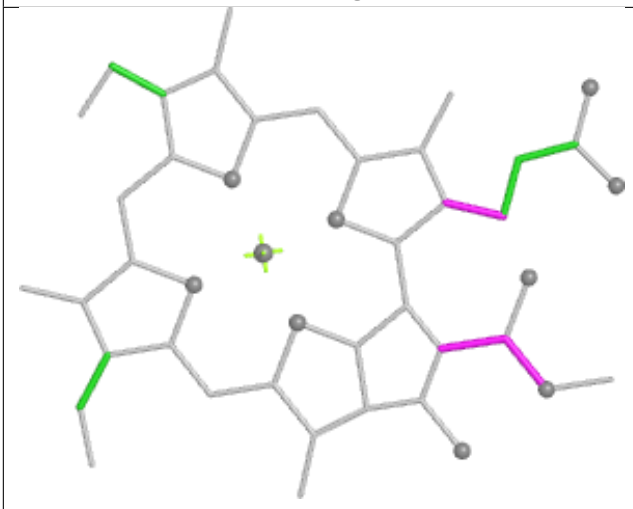


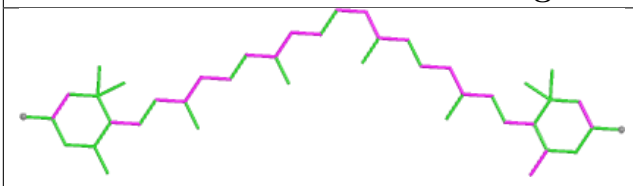
Bond angles



Torsions

Rings

Ligand 5X6 5 312



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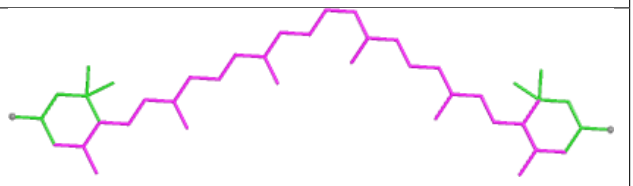
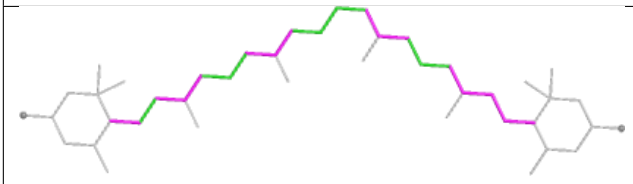


Bond angles



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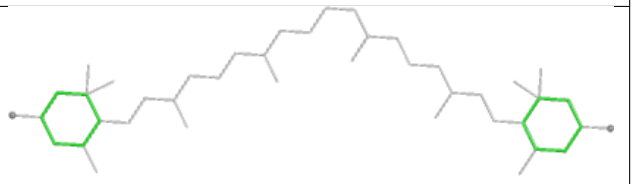
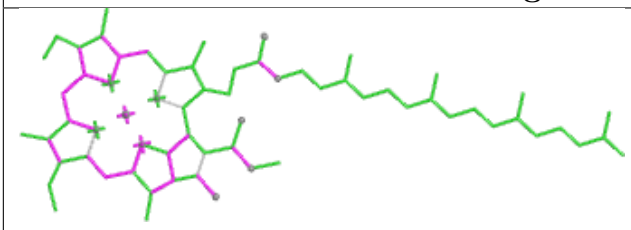


Rings

Ligand CLA A 848



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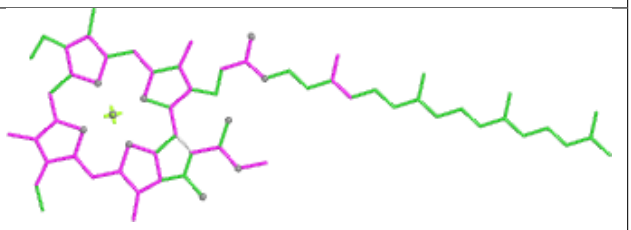
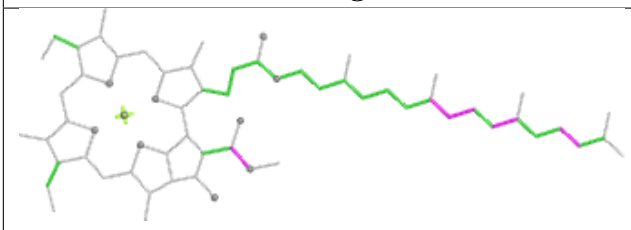


Bond angles



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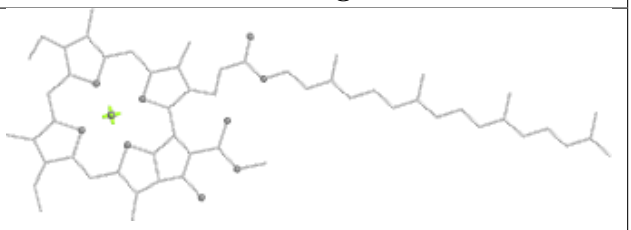
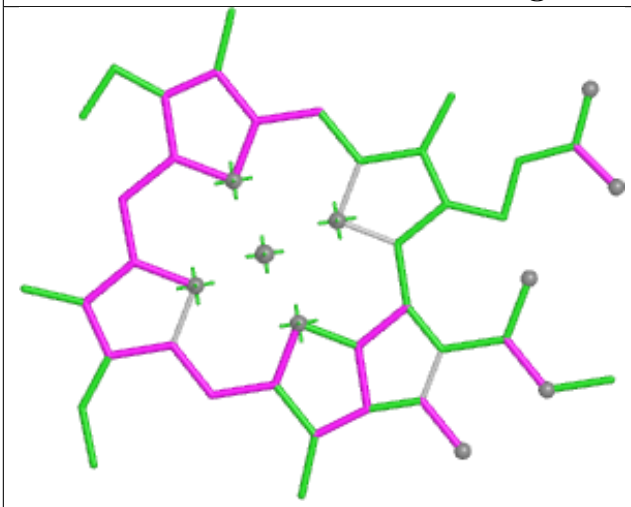


Rings

Ligand CLA 1 304



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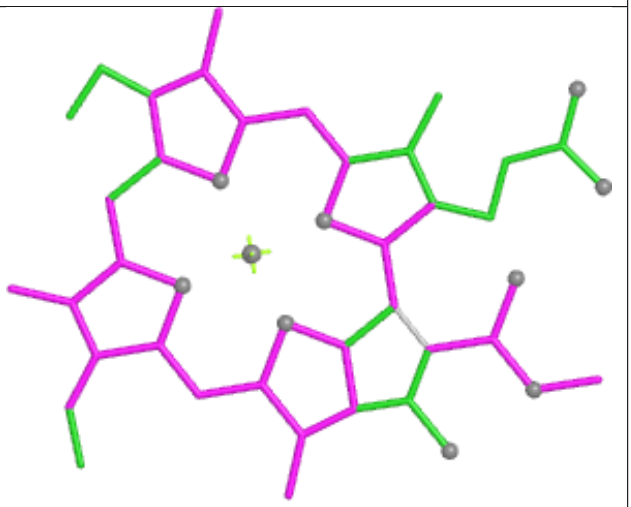
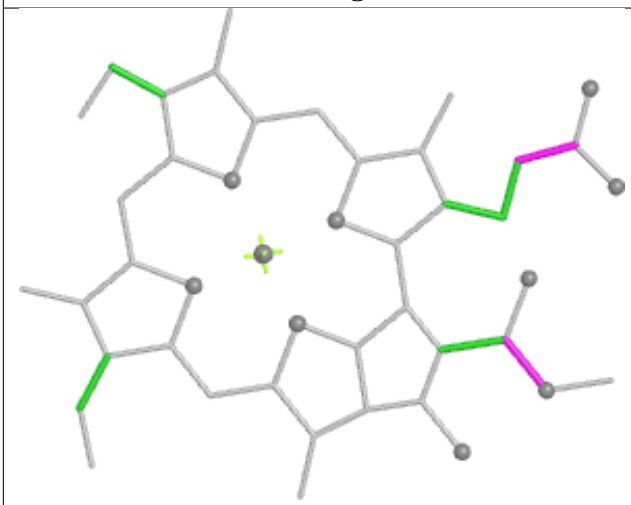


Bond angles



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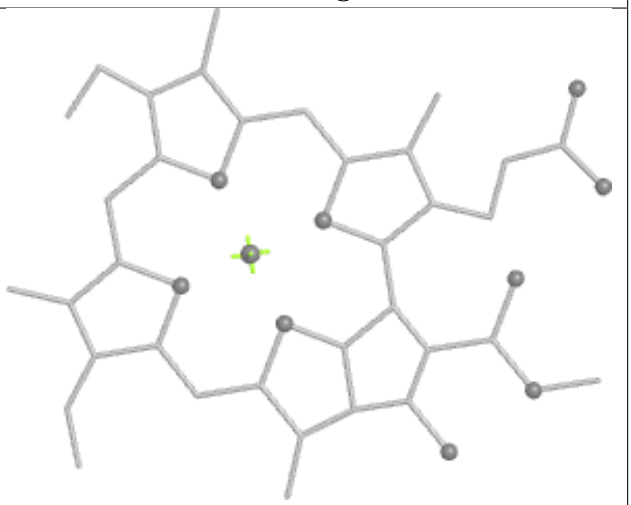
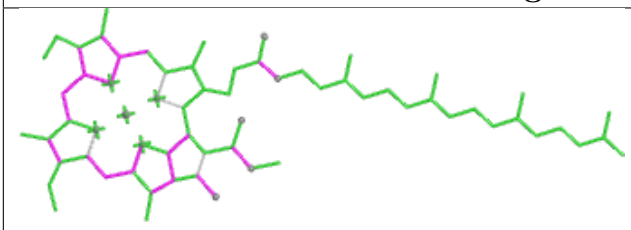


Rings

Ligand CLA B 801



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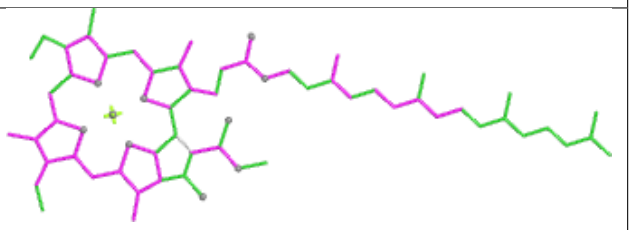
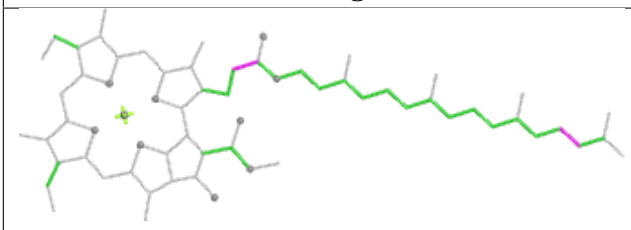
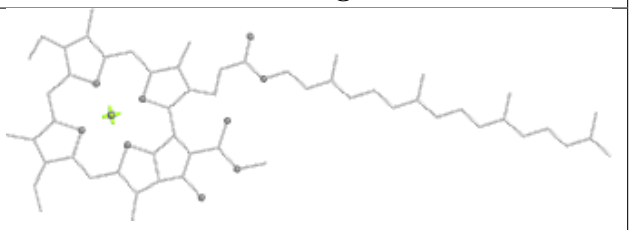


Bond angles

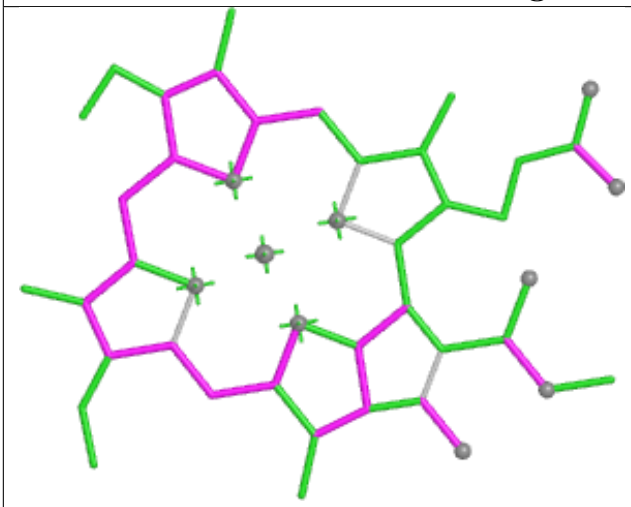


Torsions



Rings

Ligand CLA 1 305



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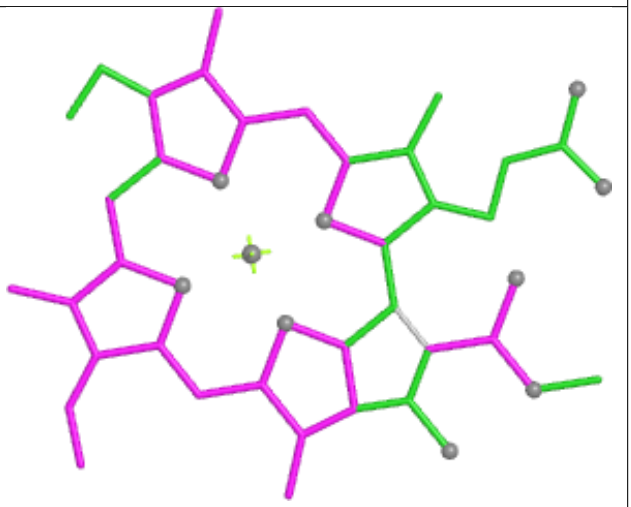
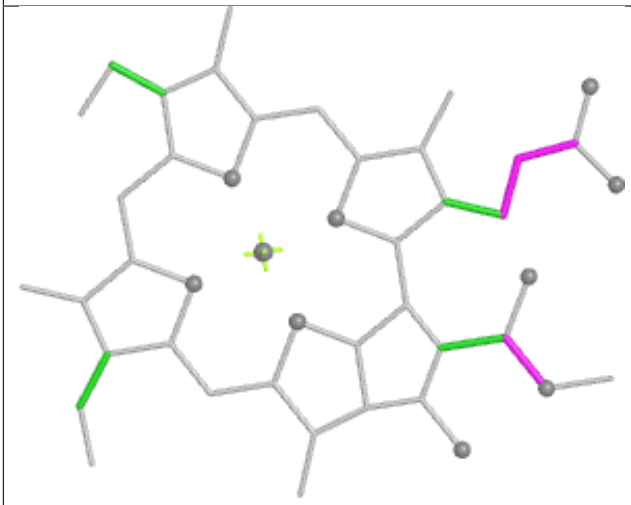
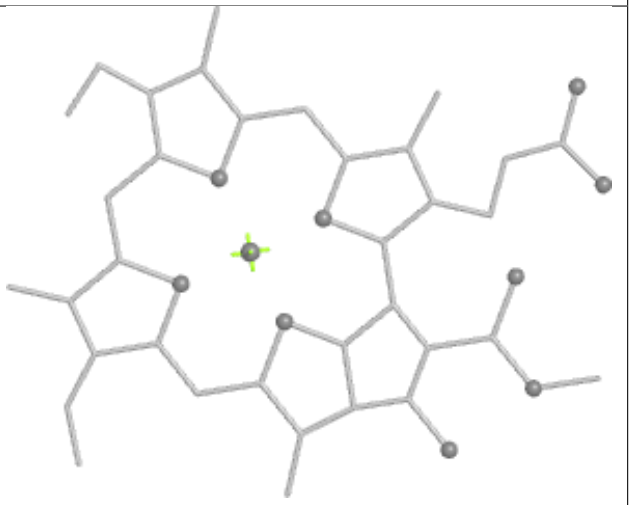


Bond angles

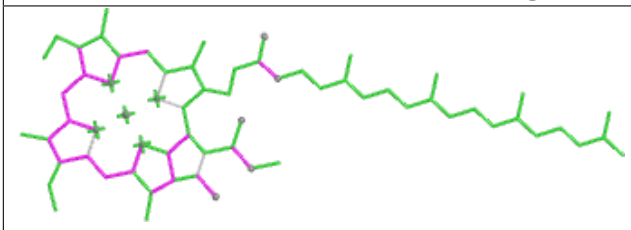


Torsions



Rings

Ligand CLA A 831



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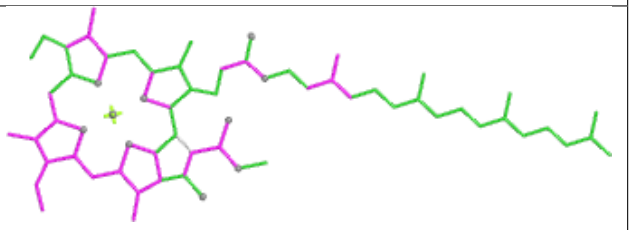
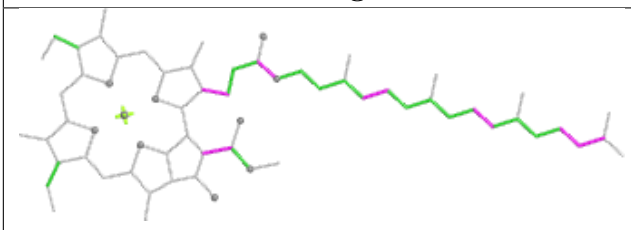


Bond angles



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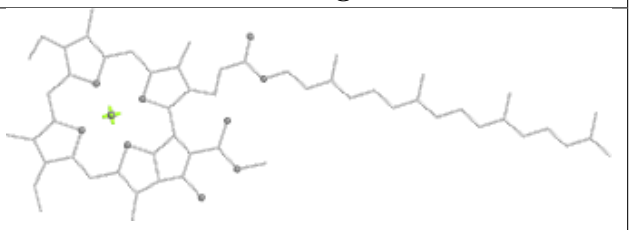
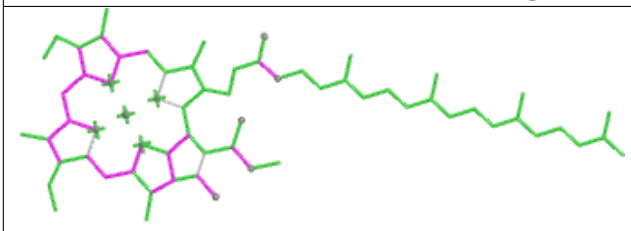


Rings

Ligand CLA A 816



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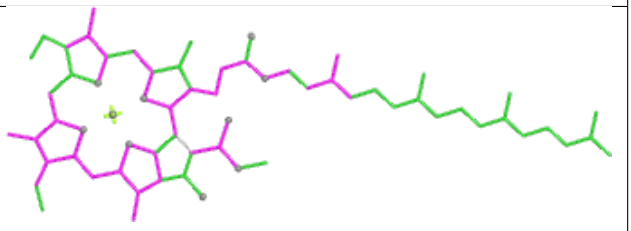
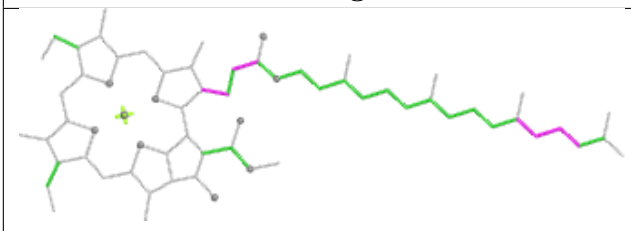


Bond angles



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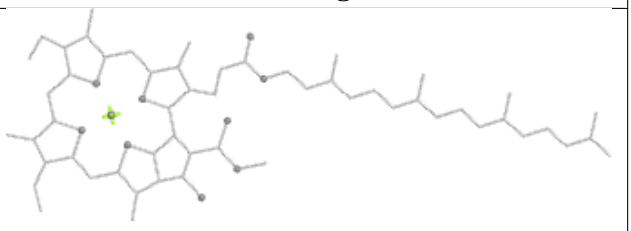
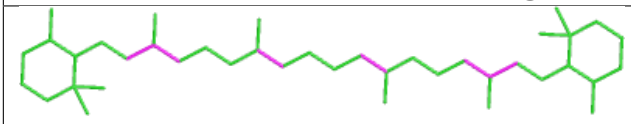
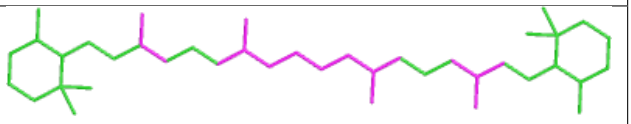


Rings

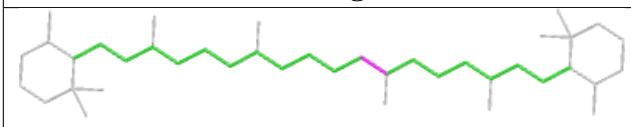
Ligand BCR K 103



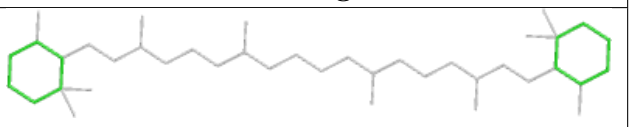
Bond lengths



Bond angles

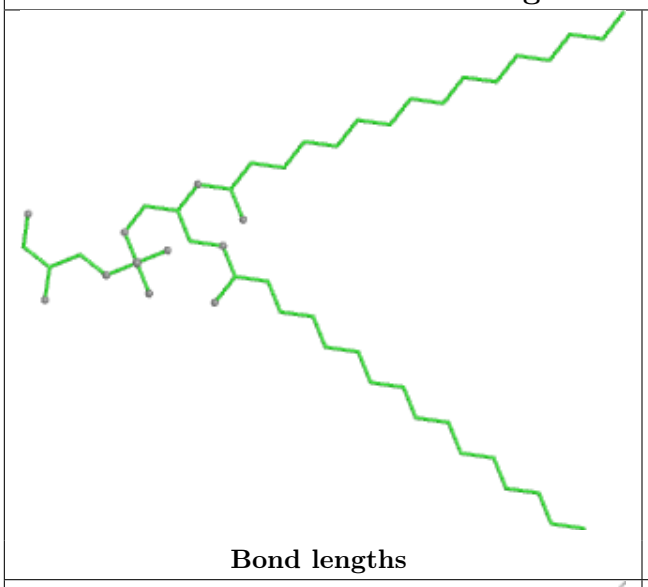


Torsions



Rings

Ligand LHG A 841



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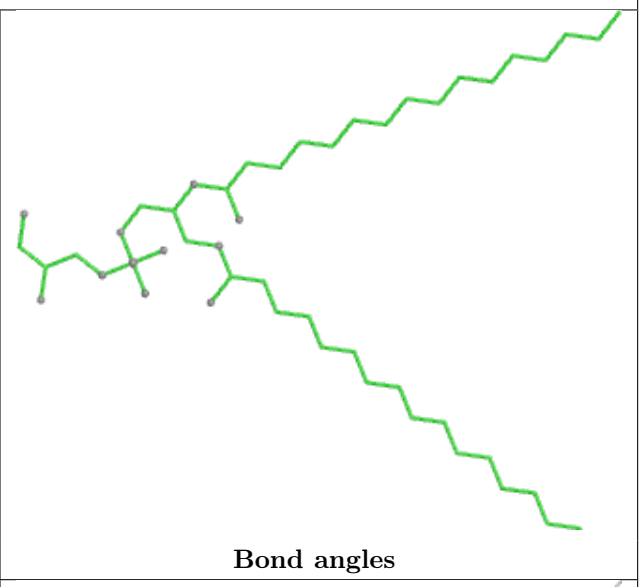
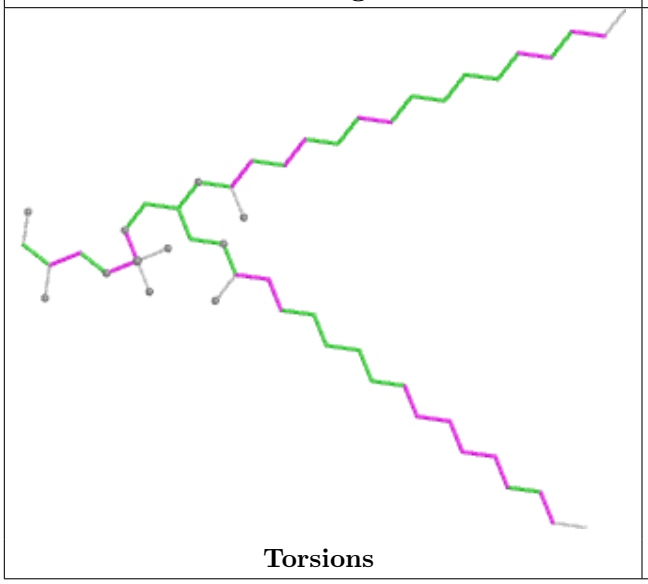
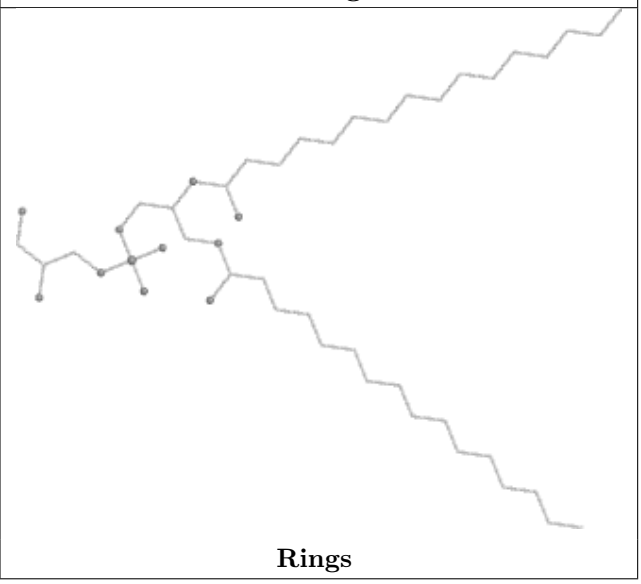


Bond angles

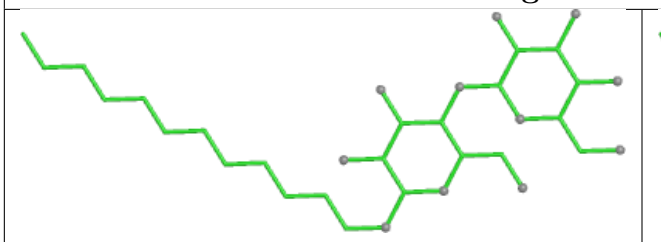


Torsions

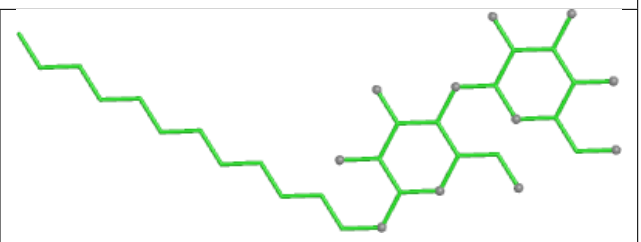


Rings

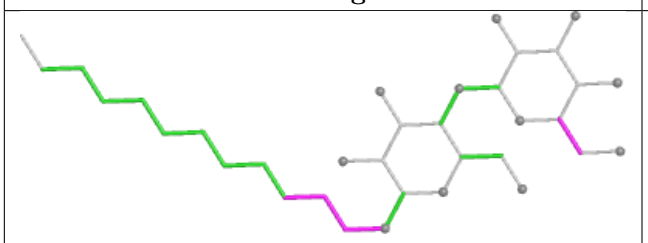
Ligand LMT O 201



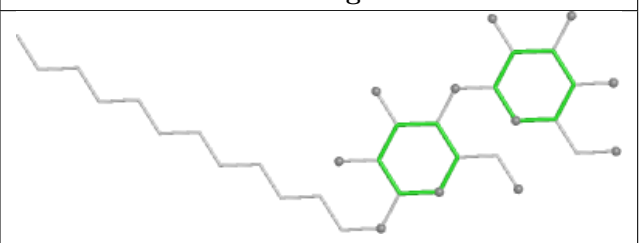
Bond lengths



Bond angles

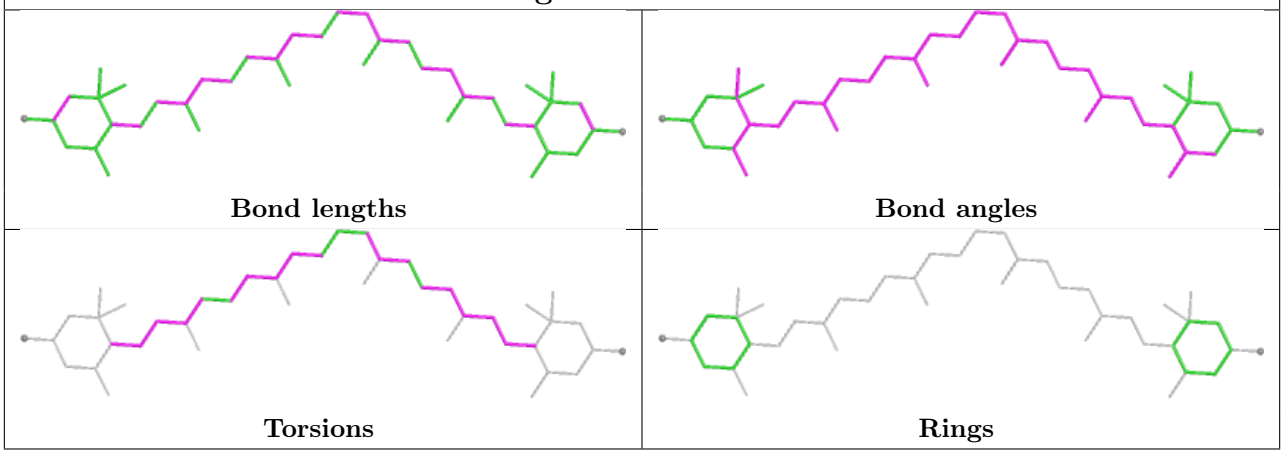


Torsions

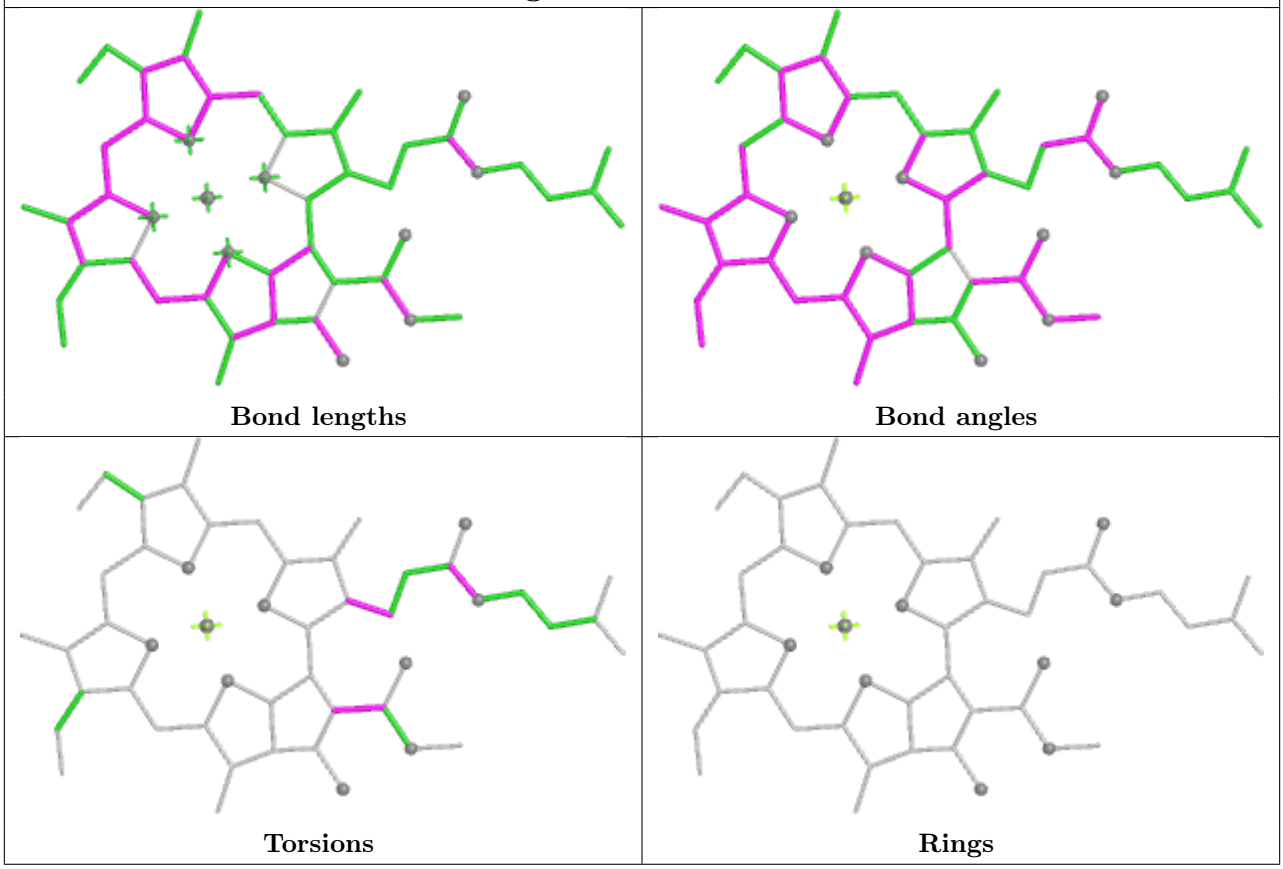


Rings

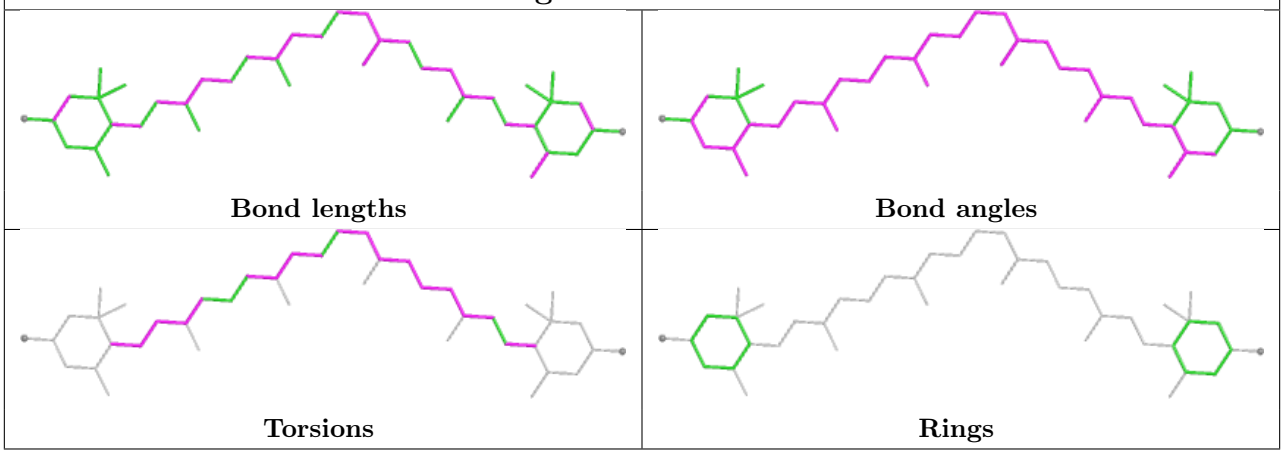
Ligand 5X6 7 317



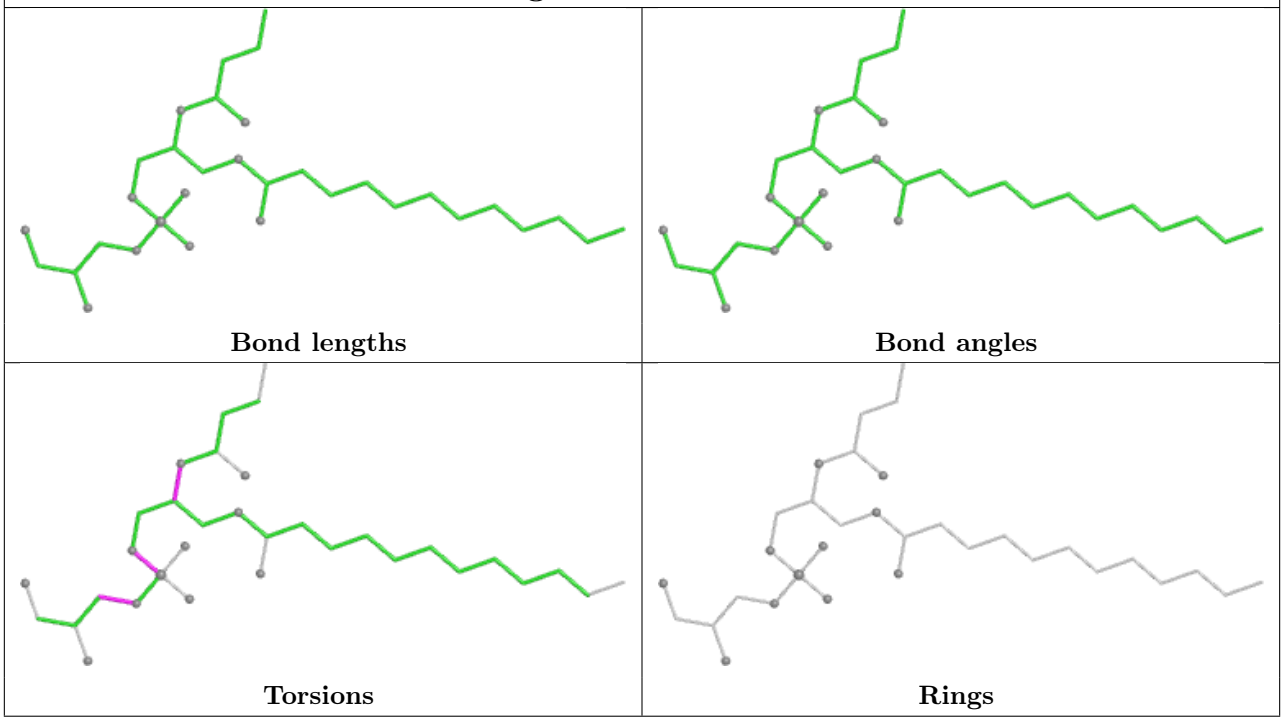
Ligand CLA A 805



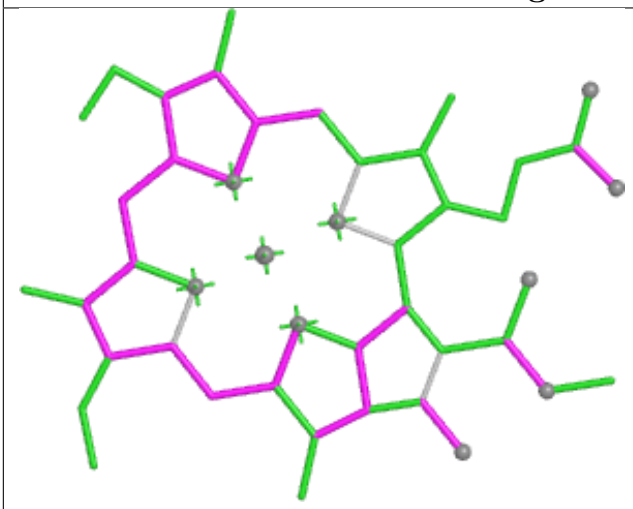
Ligand 5X6 7 318



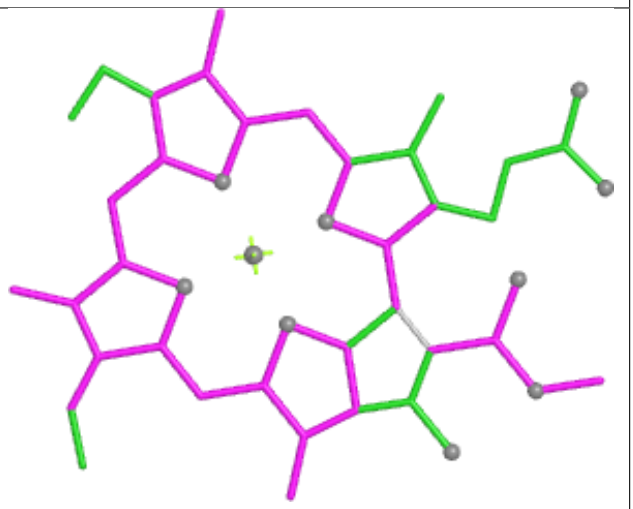
Ligand LHG J 106



Ligand CLA 3 304



Bond lengths



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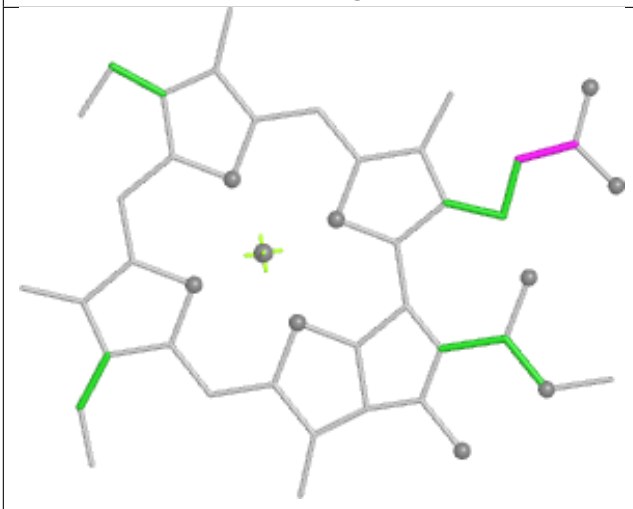
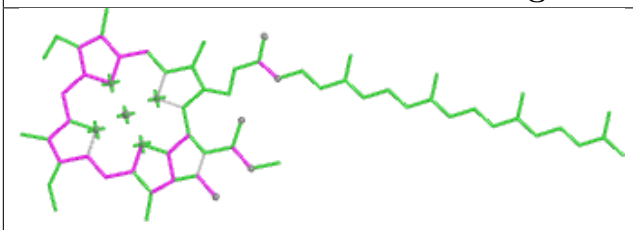


Torsions

Rings

Ligand CLA 5 303



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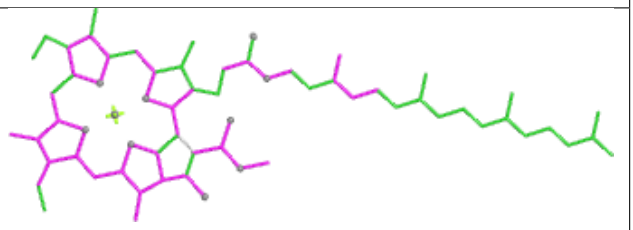
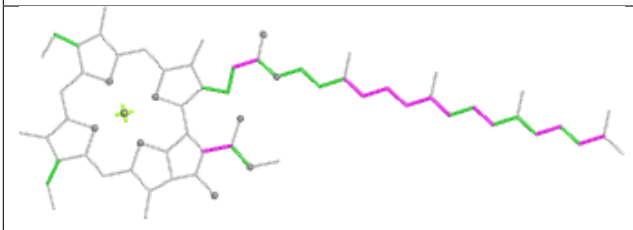
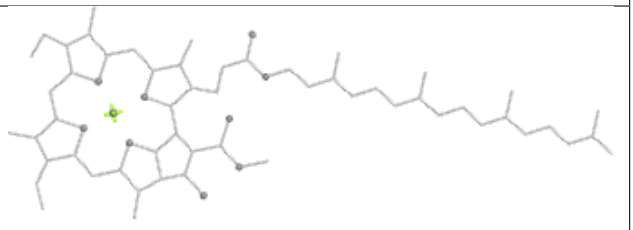


Bond angles

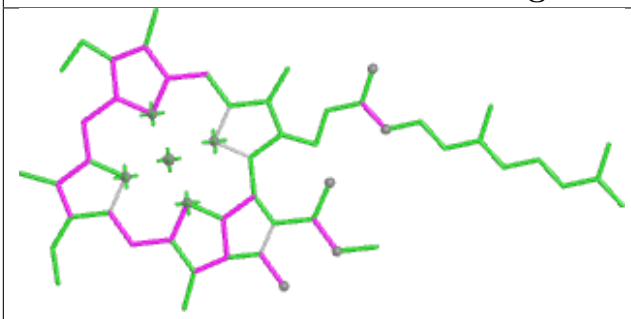


Torsions

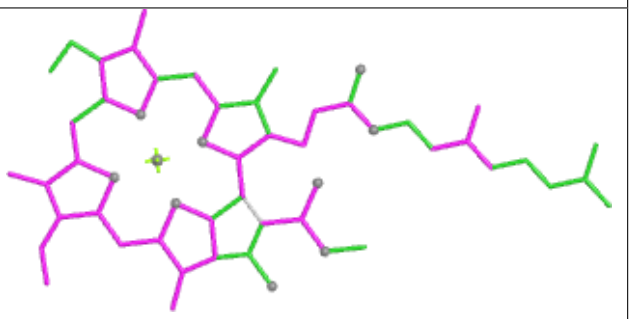


Rings

Ligand CLA 6 306



Bond lengths



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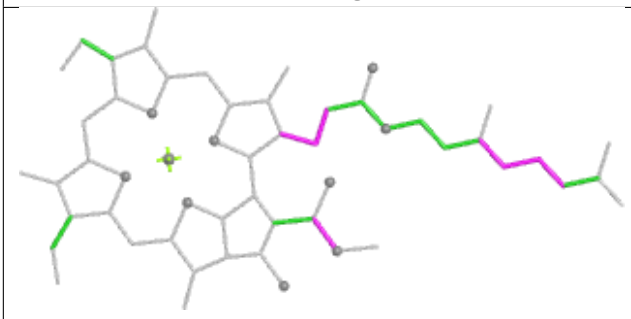

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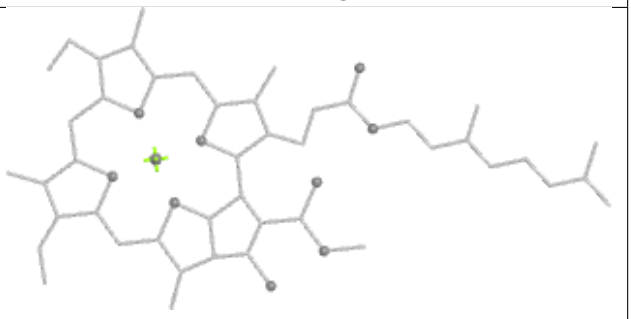
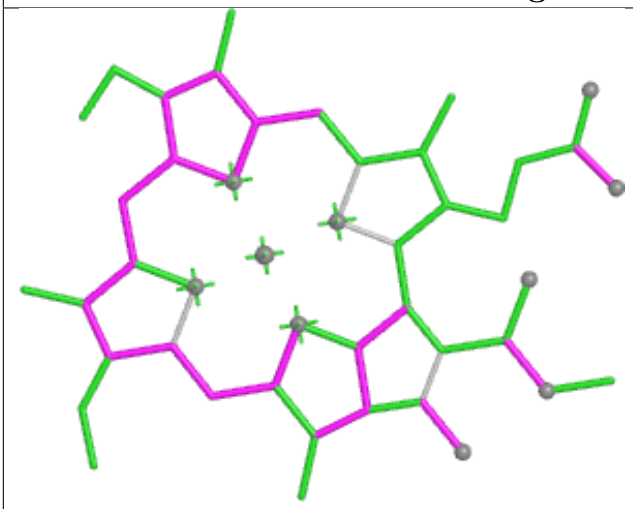


Rings

Ligand CLA 5 305



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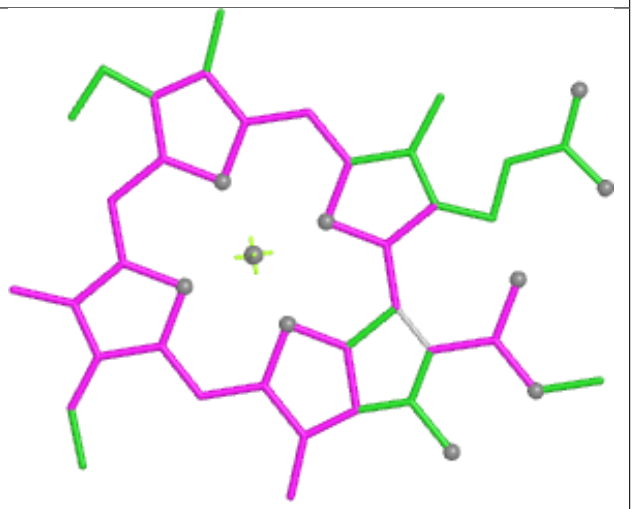
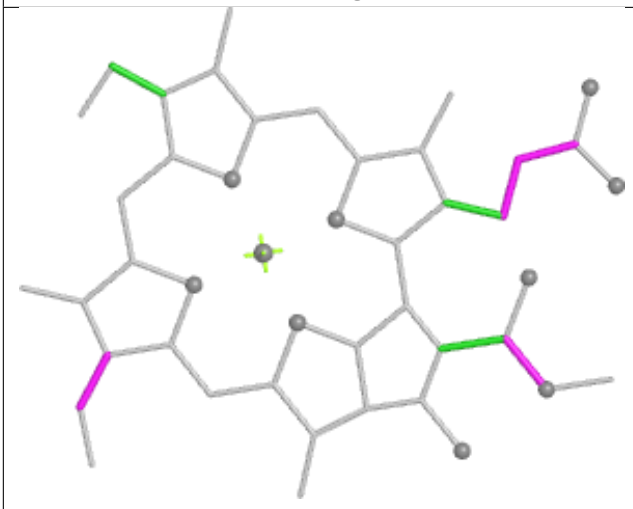


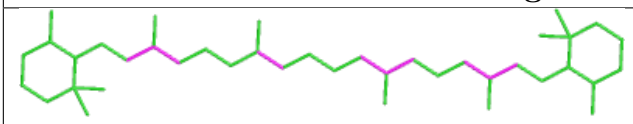
Bond angles



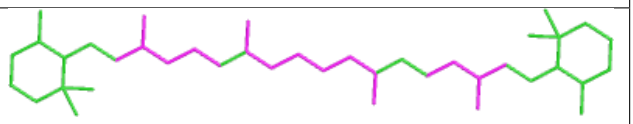
Torsions

Rings

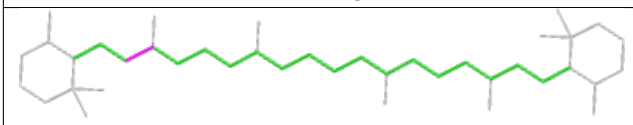
Ligand BCR Z 205



Bond lengths



Bond angles



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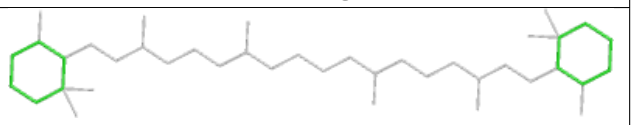
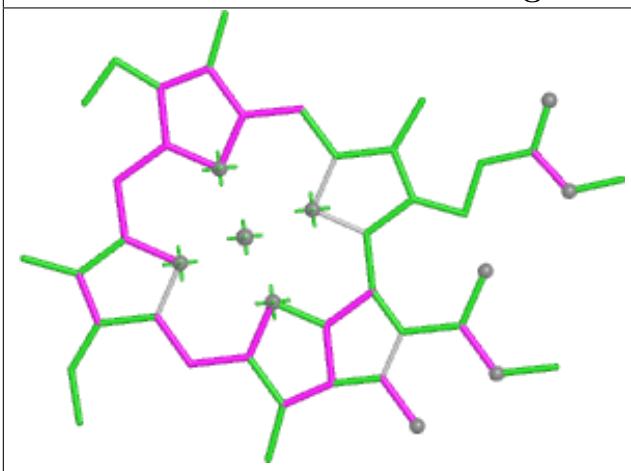


Rings

Ligand CLA O 203



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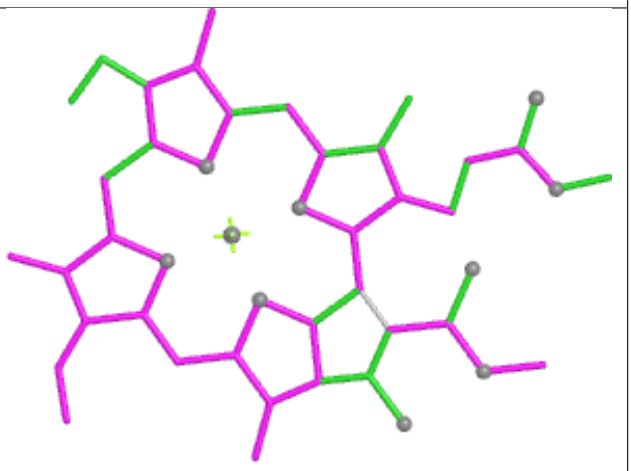

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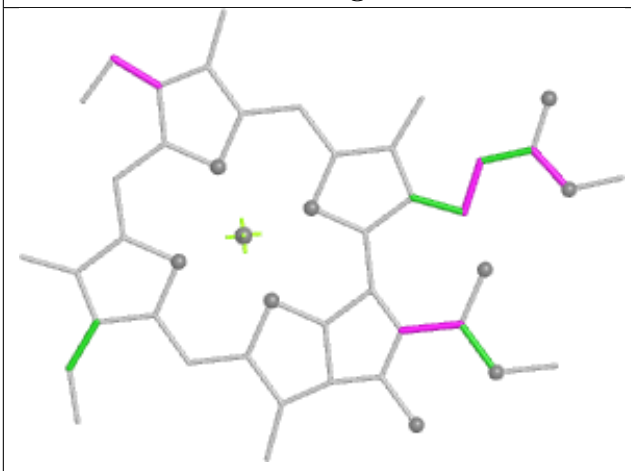

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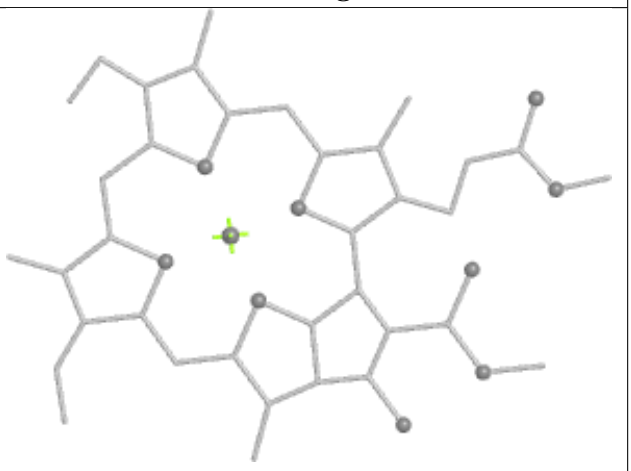
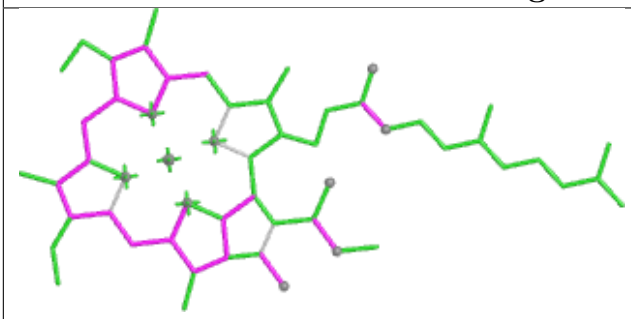
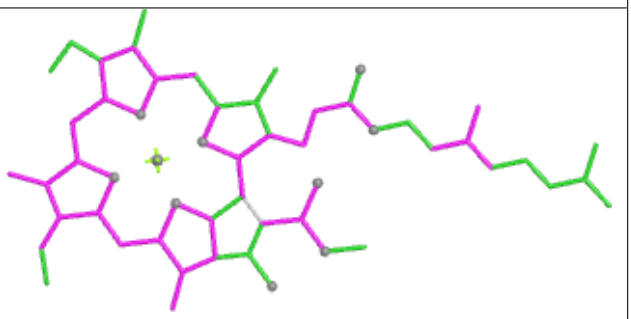
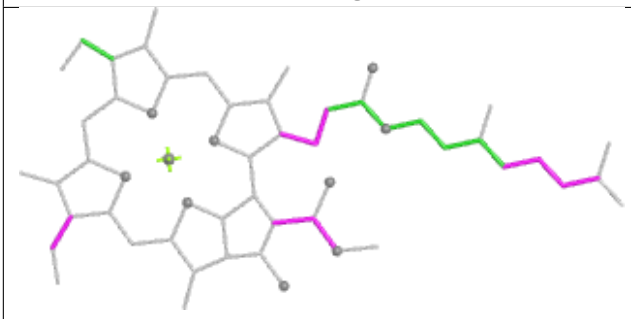
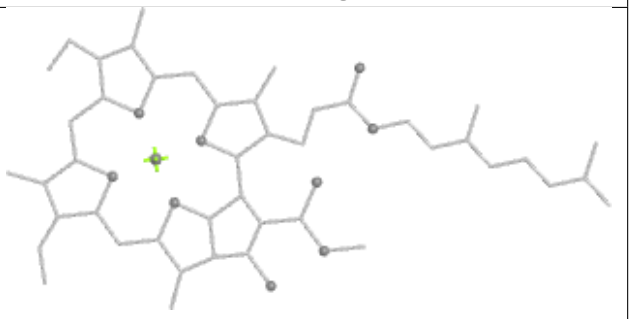
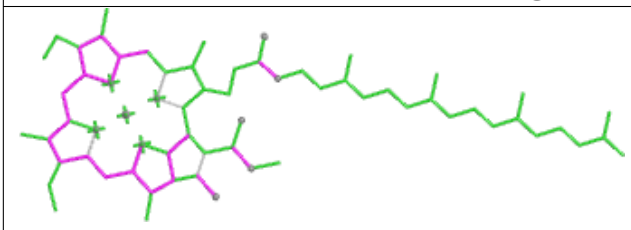
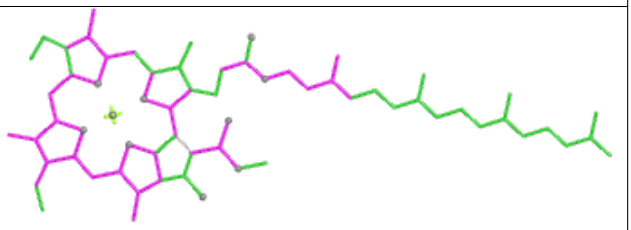
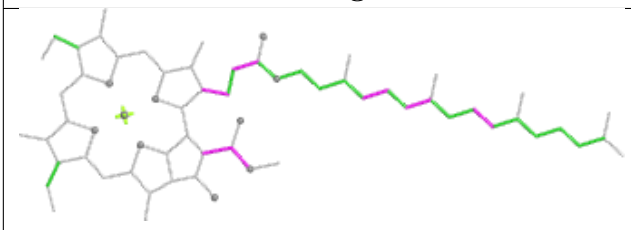
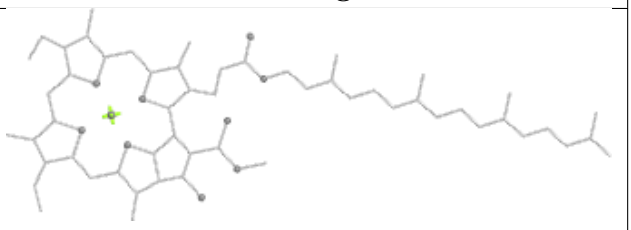
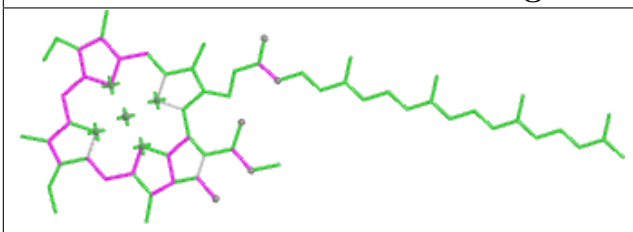


Rings

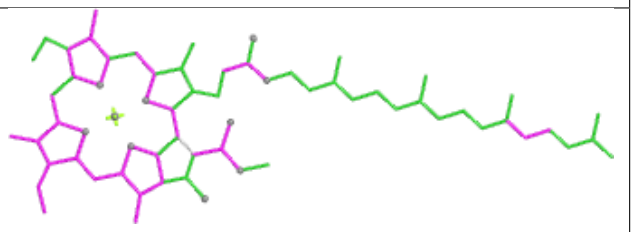
Ligand CLA 7 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

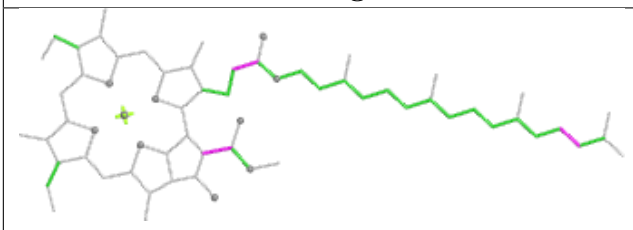
Ligand CLA B 839



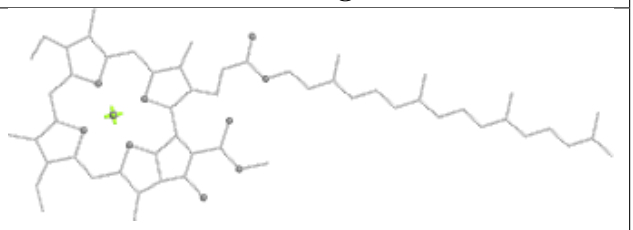
Bond lengths



Bond angles

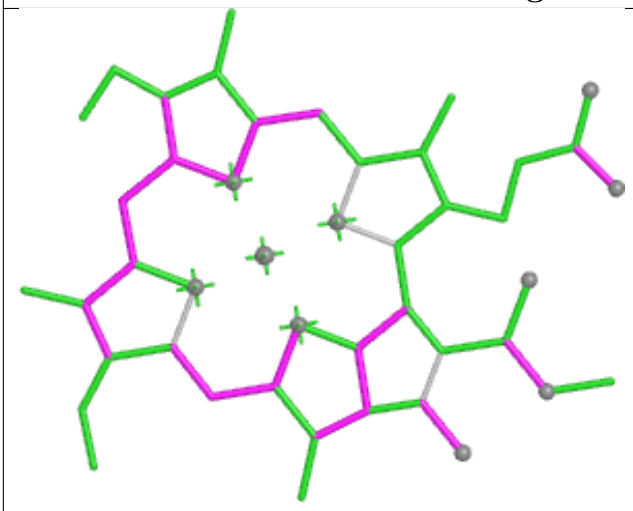


Torsions

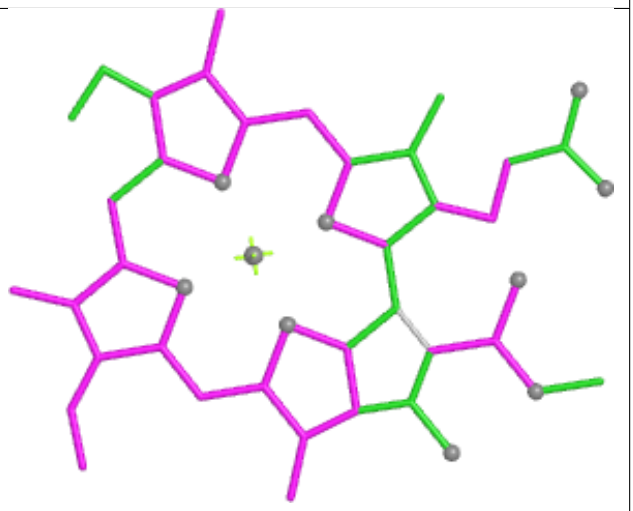


Rings

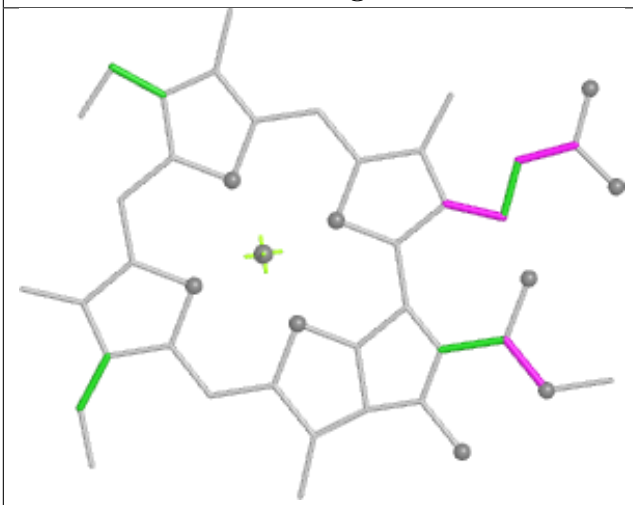
Ligand CLA Z 201



Bond lengths



Bond angles



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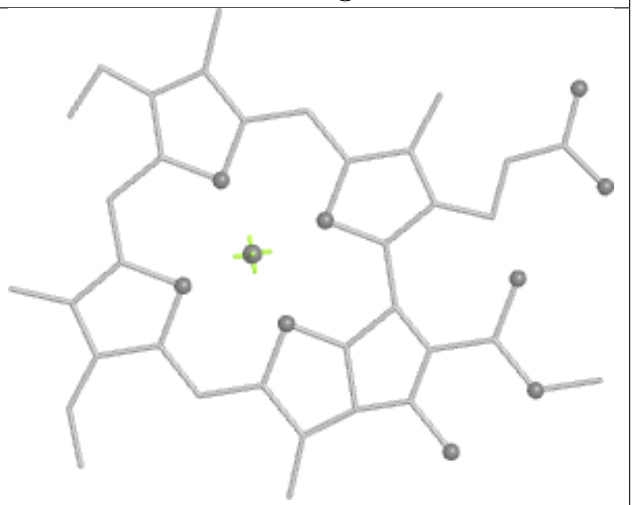
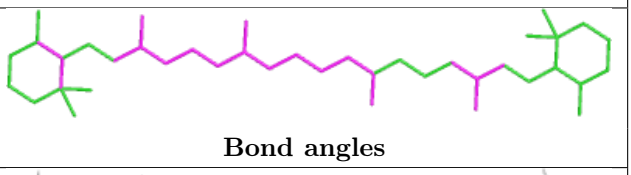


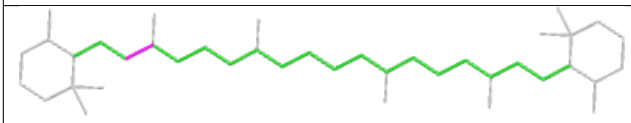
Rings

Ligand BCR L 206

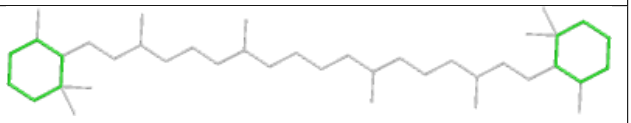
Bond lengths



Bond angles

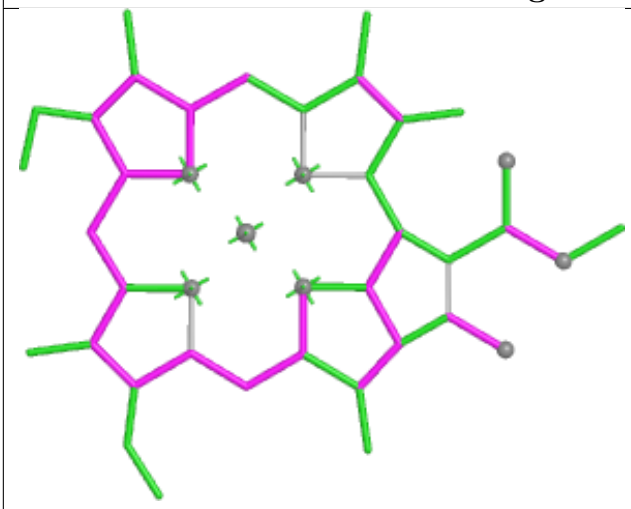


Torsions

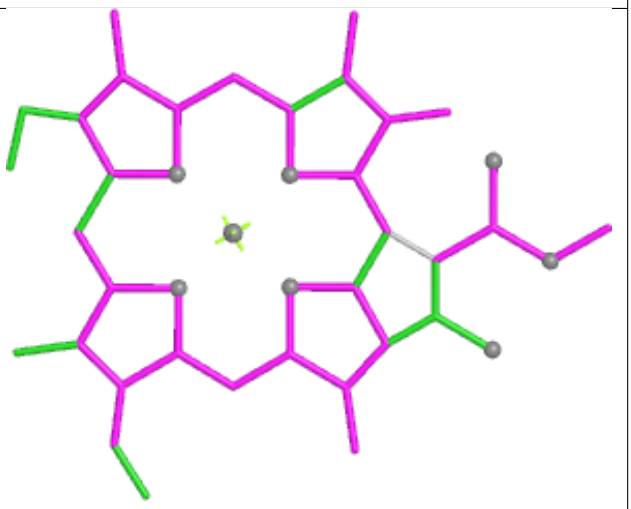


Rings

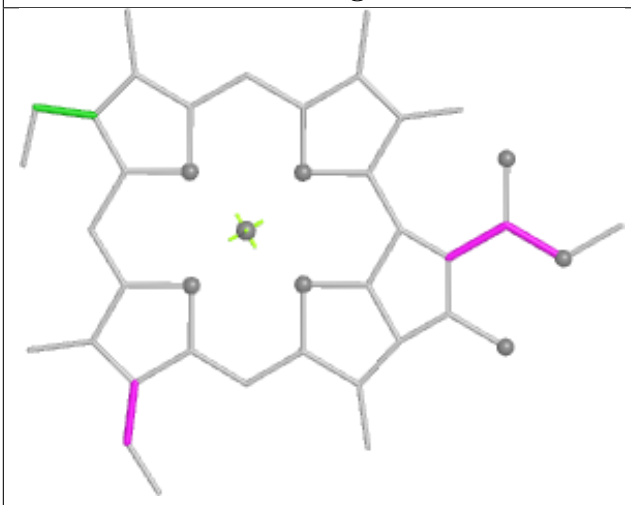
Ligand CLA 6 311



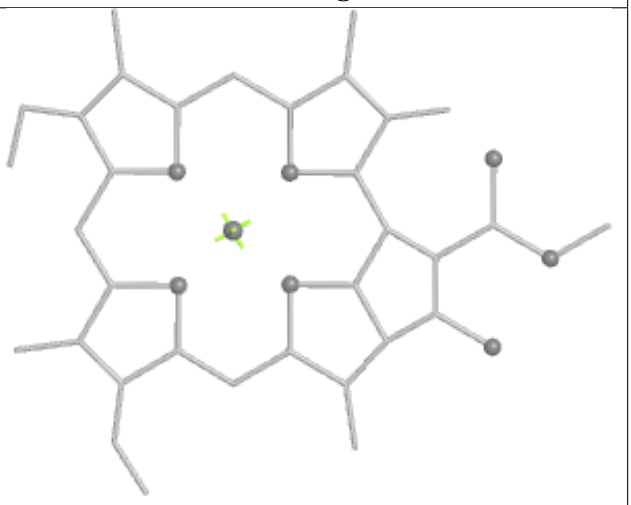
Bond lengths



Bond angles

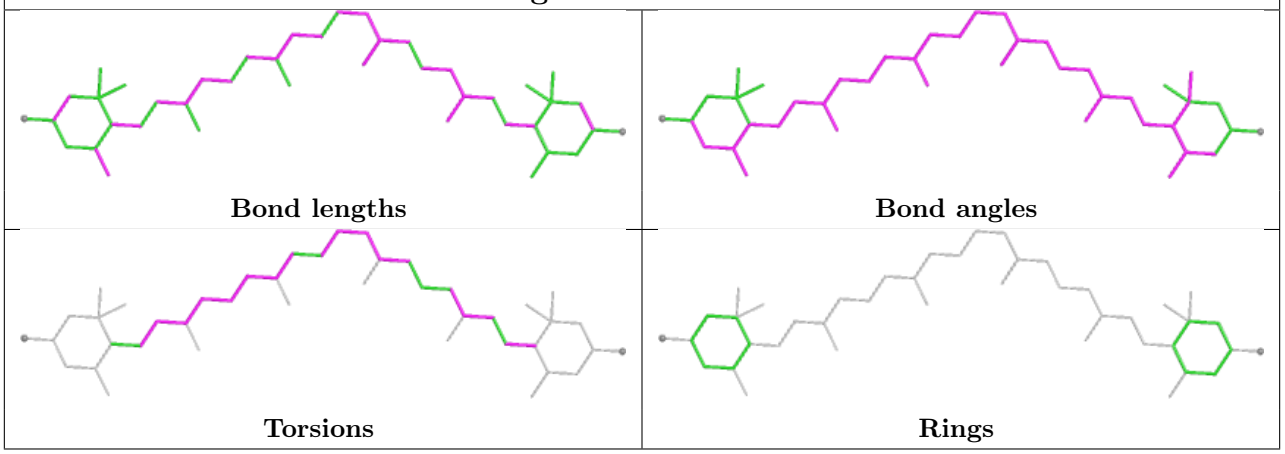


Torsions

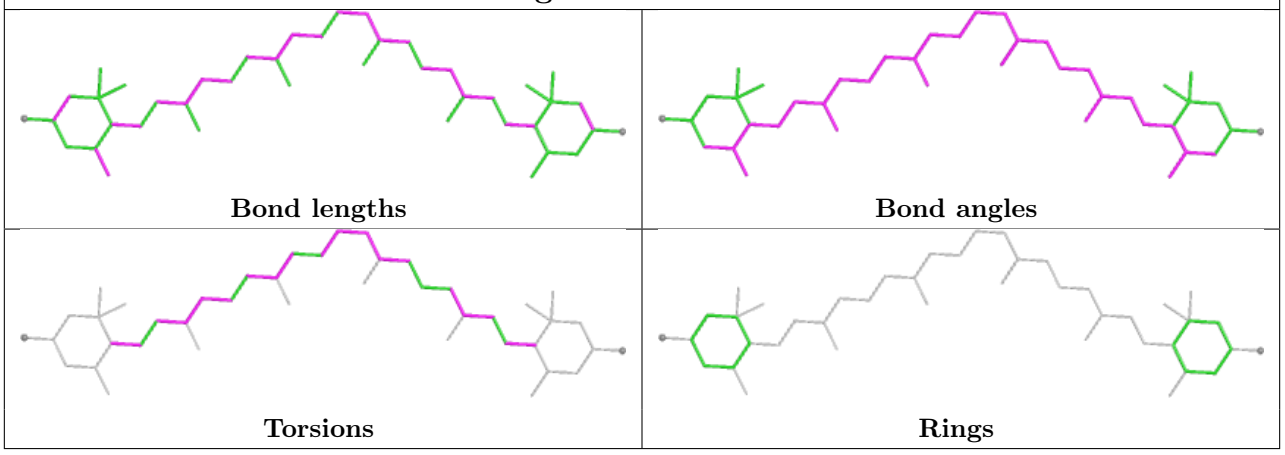


Rings

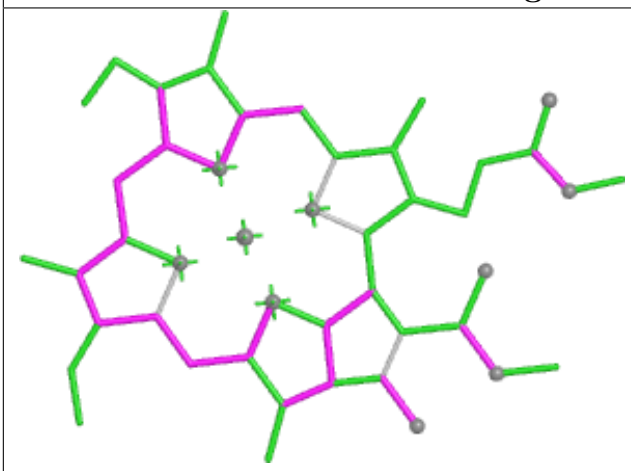
Ligand 5X6 O 207



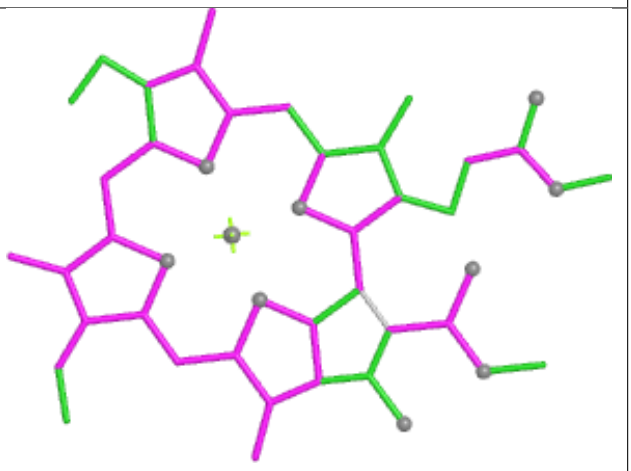
Ligand 5X6 2 313



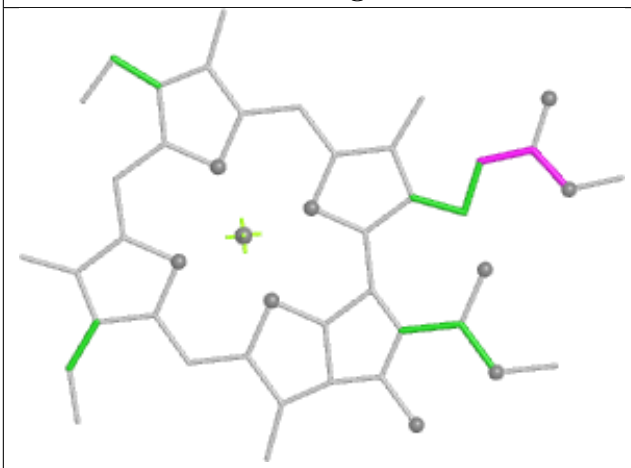
Ligand CLA B 821



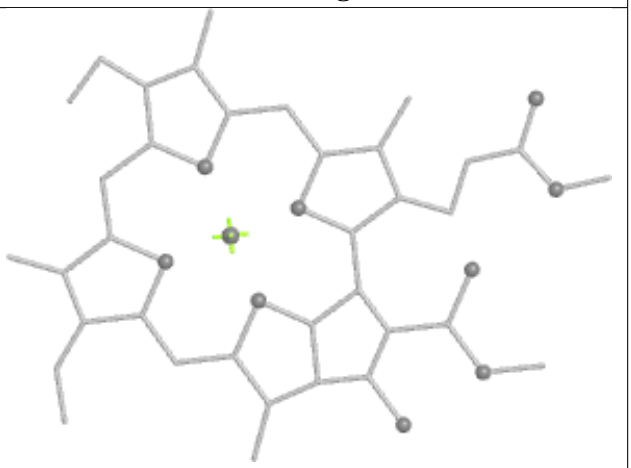
Bond lengths



Bond angles

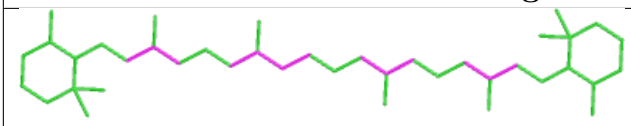


Torsions

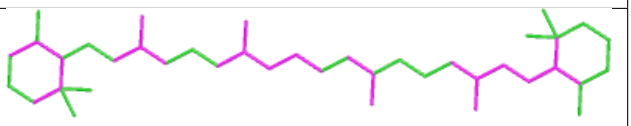


Rings

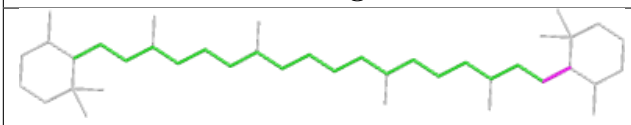
Ligand BCR A 844



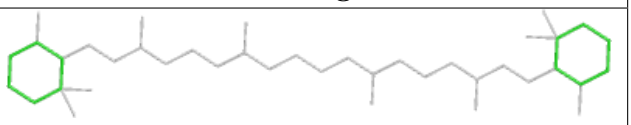
Bond lengths



Bond angles

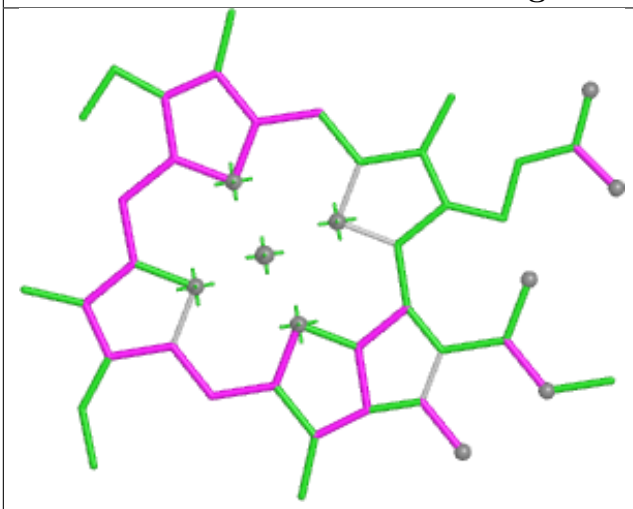


Torsions

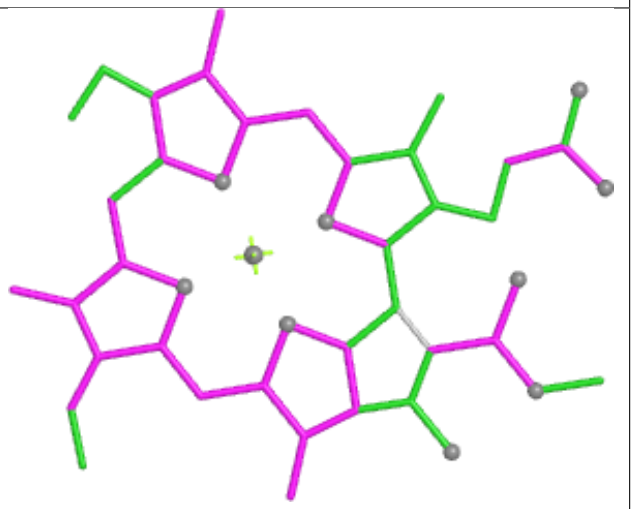


Rings

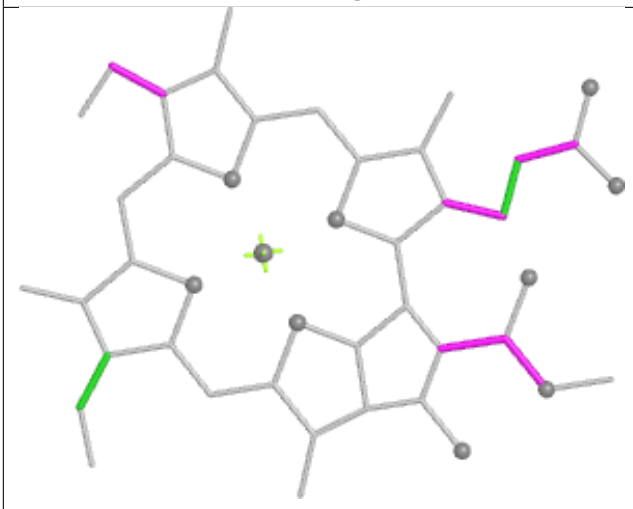
Ligand CLA 6 313



Bond lengths



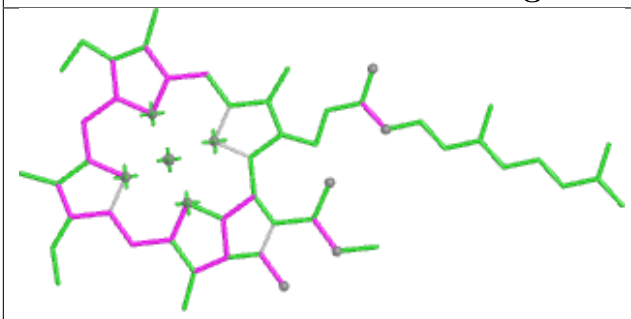
Bond angles



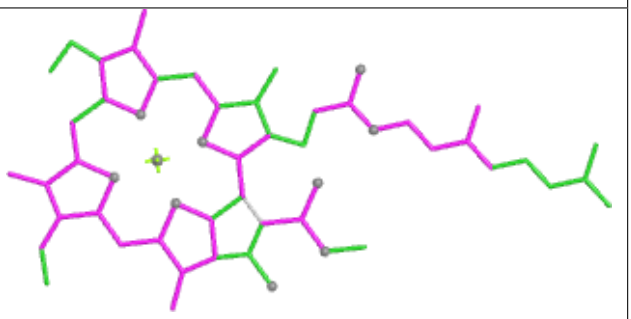
Torsions

Rings

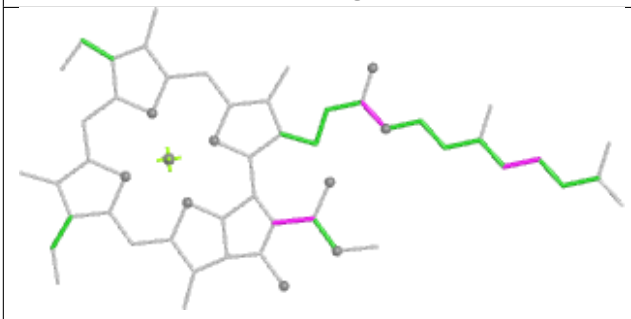
Ligand CLA A 822



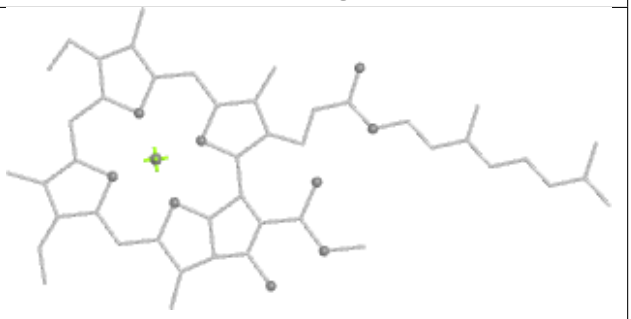
Bond lengths



Bond angles

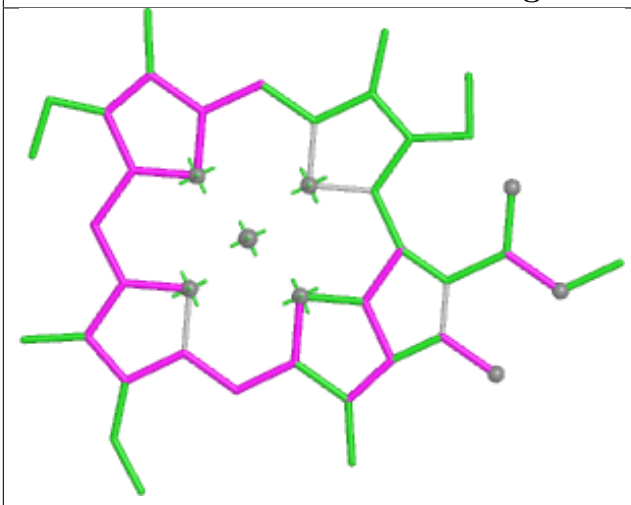


Torsions

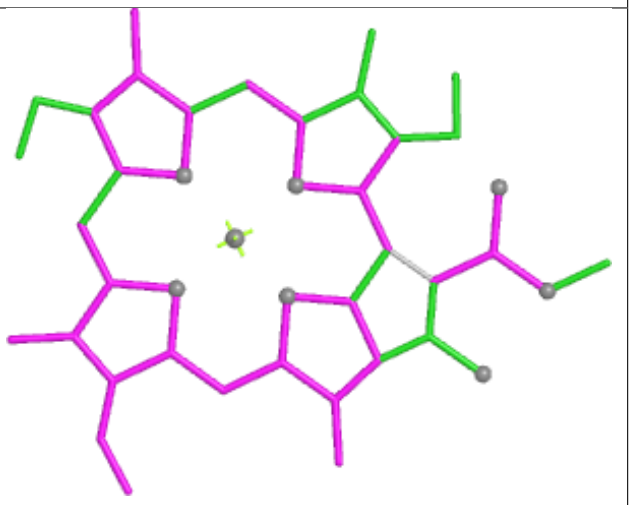


Rings

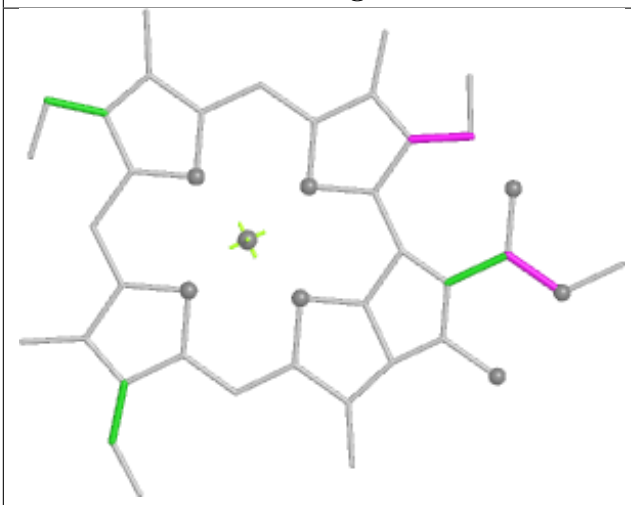
Ligand CLA K 102



Bond lengths



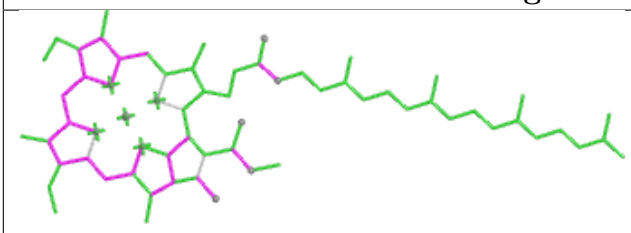
Bond angles



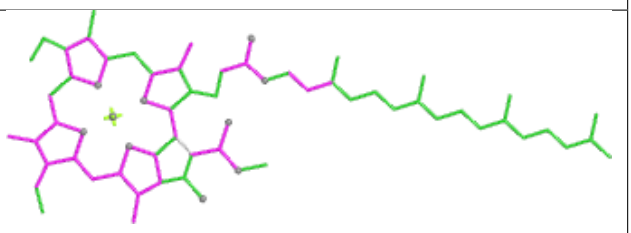
Torsions

Rings

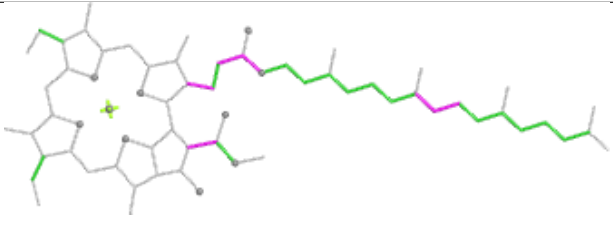
Ligand CLA A 823



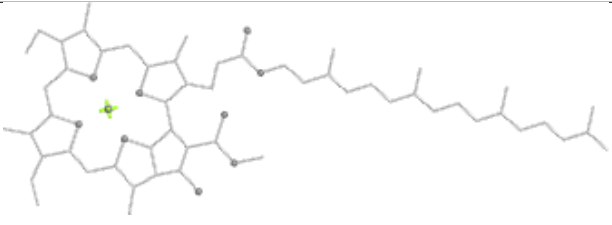
Bond lengths



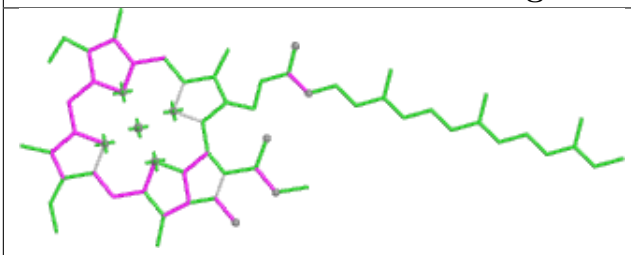
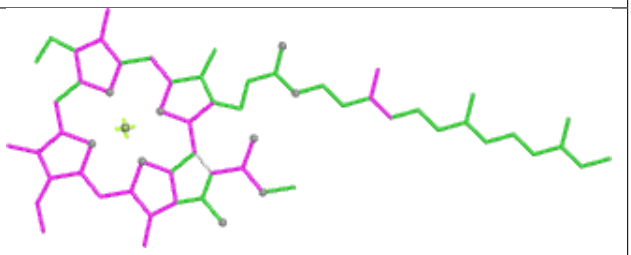
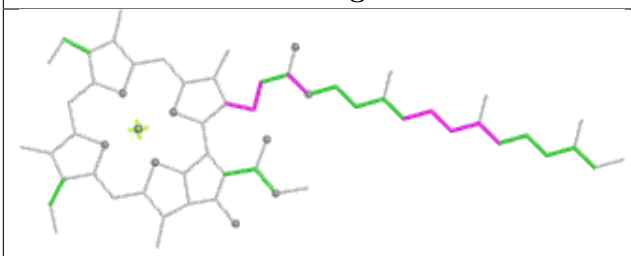
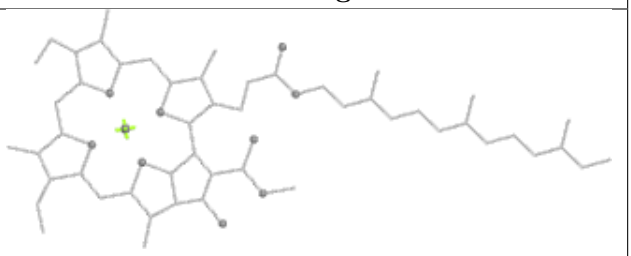
Bond angles

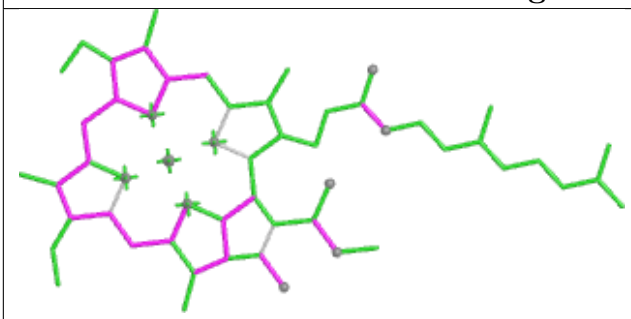
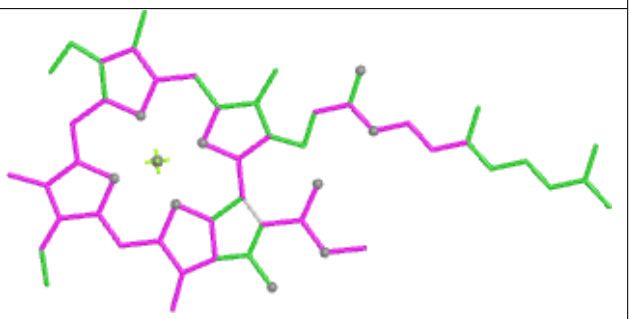
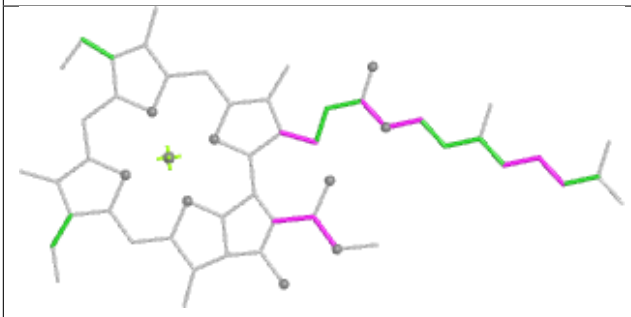
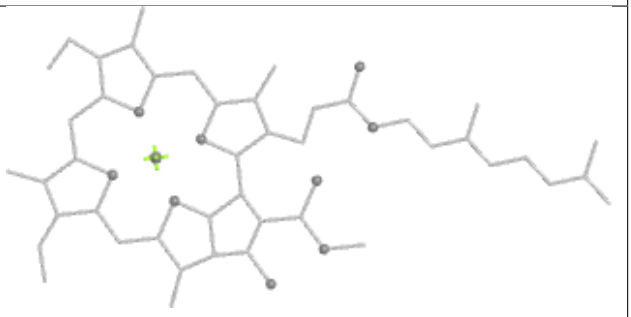


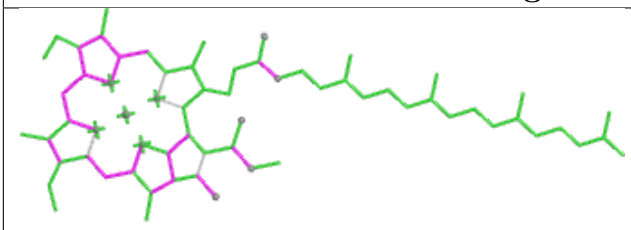
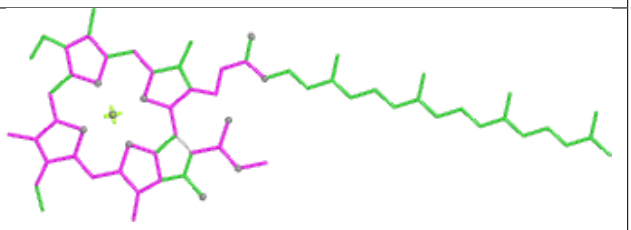
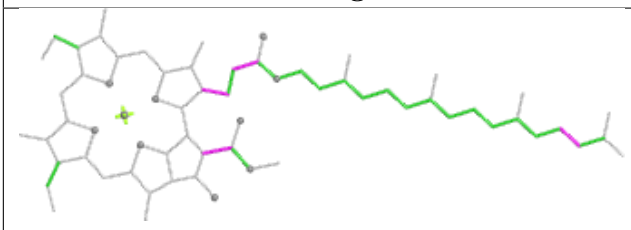
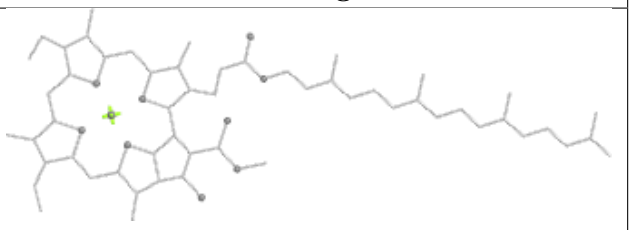
Torsions

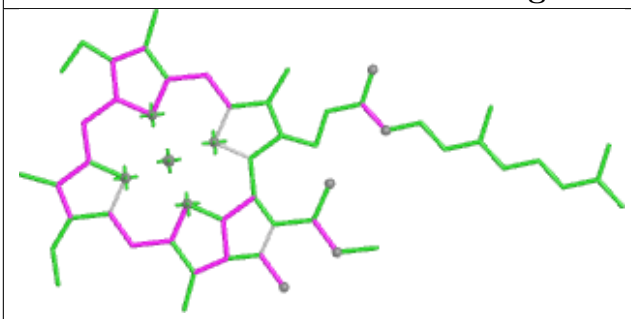
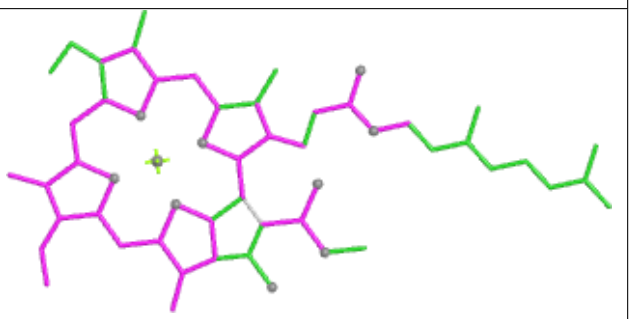
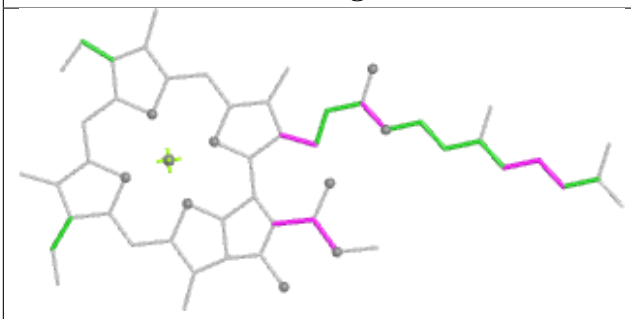
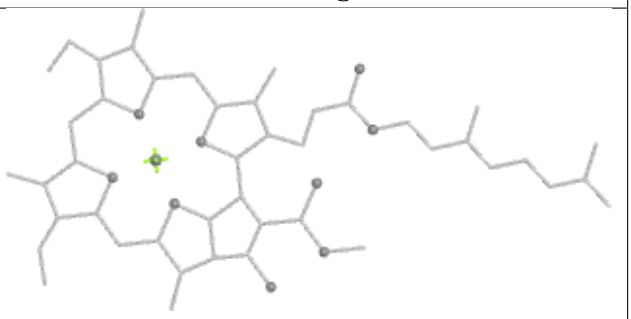


Rings

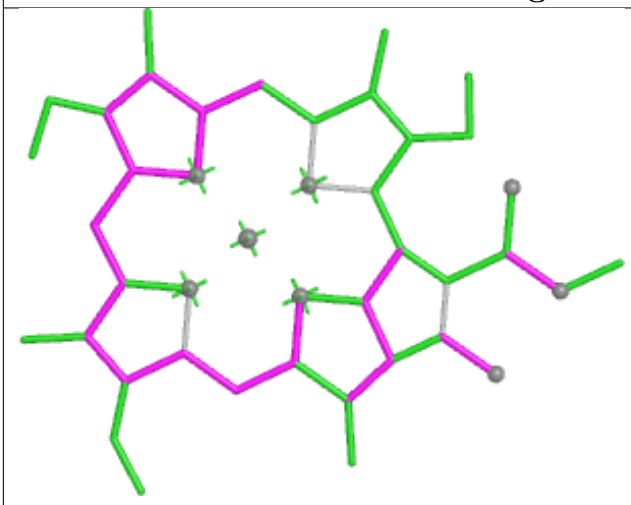
Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

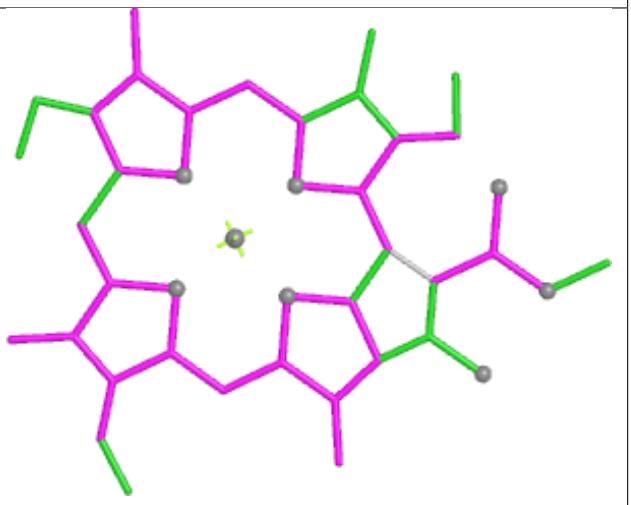
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

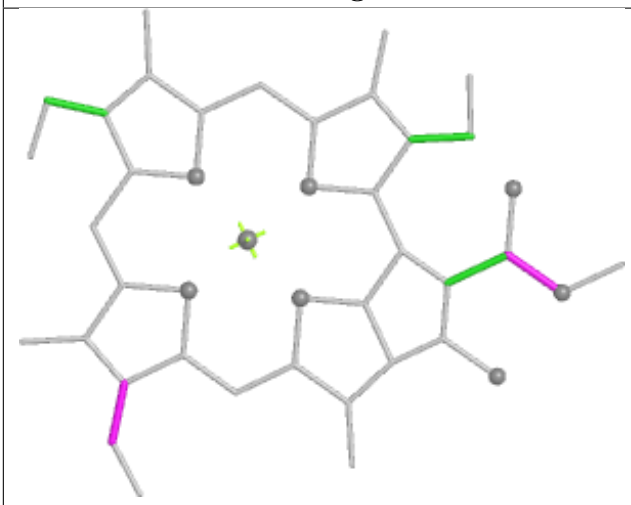
Ligand CLA 4 310



Bond lengths



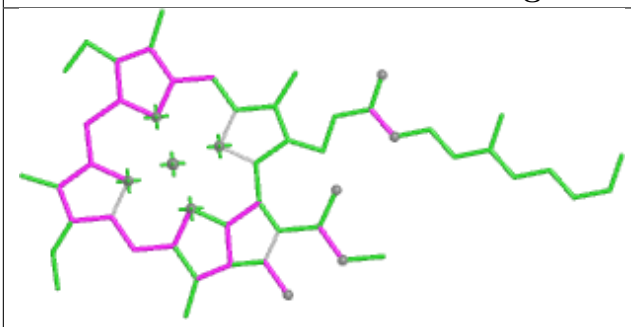
Bond angles



Torsions

Rings

Ligand CLA A 810



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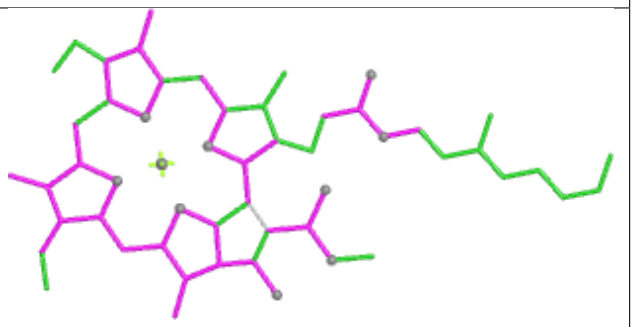
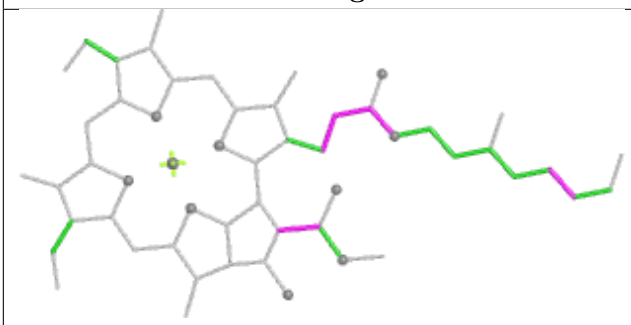
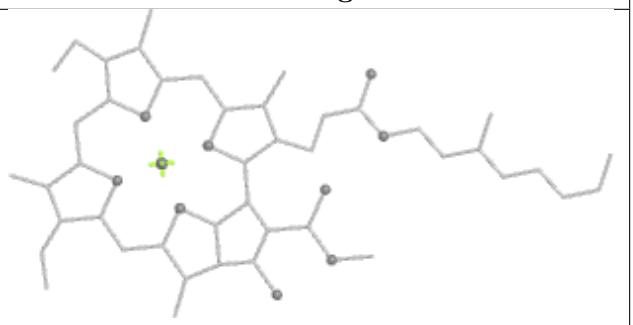


Bond angles

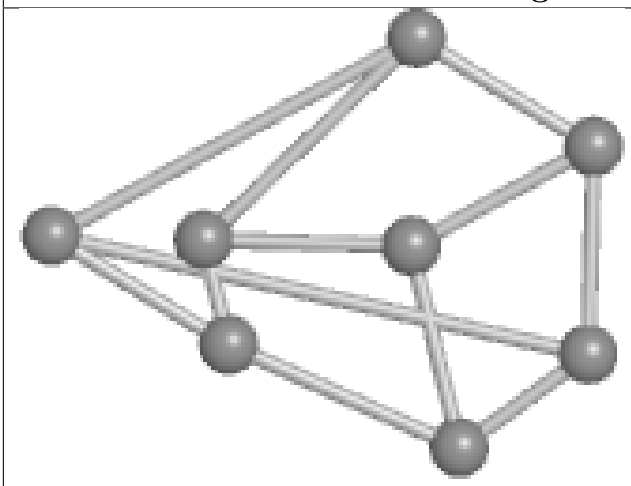


Torsions



Rings

Ligand SF4 C 101



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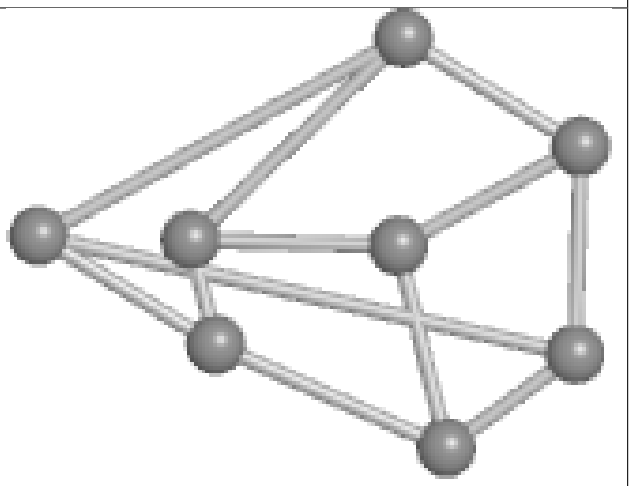
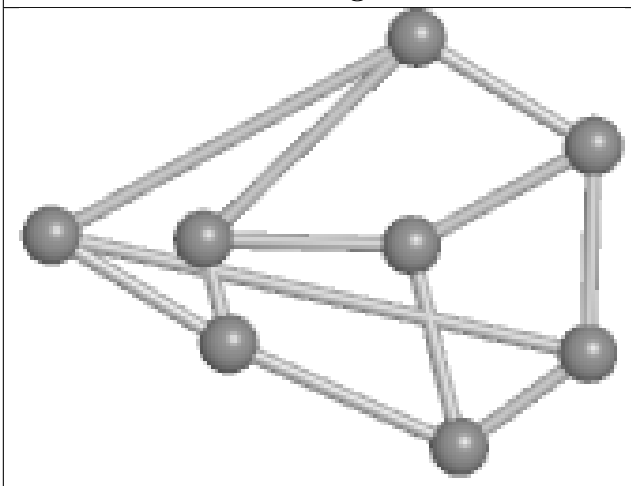
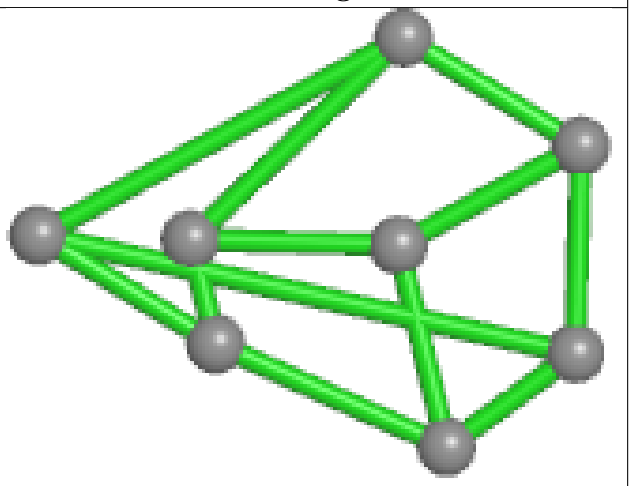


Bond angles

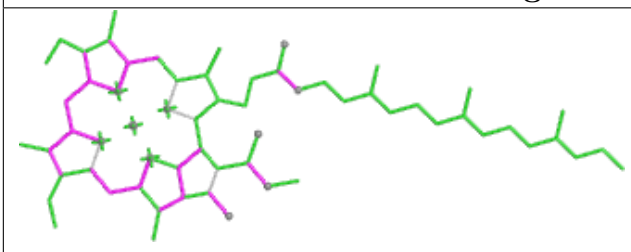


Torsions

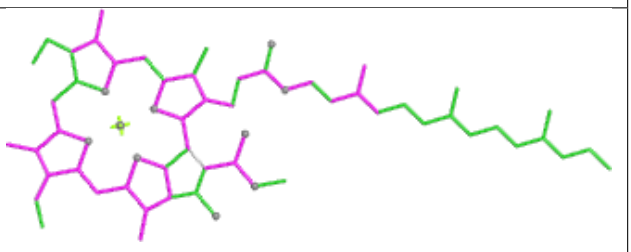


Rings

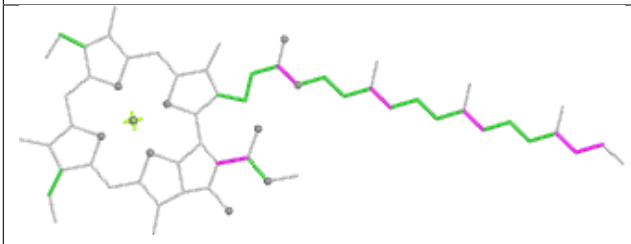
Ligand CLA A 815



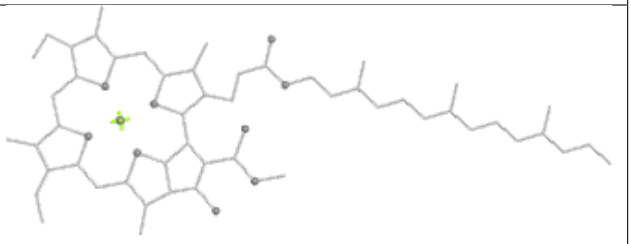
Bond lengths



Bond angles

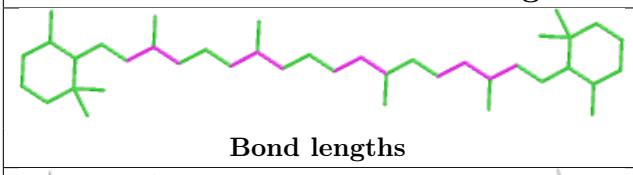


Torsions

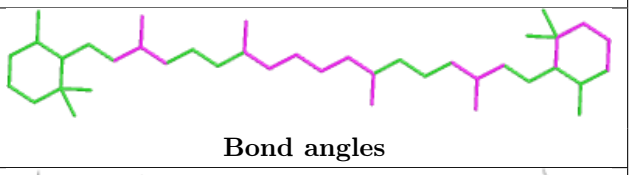


Rings

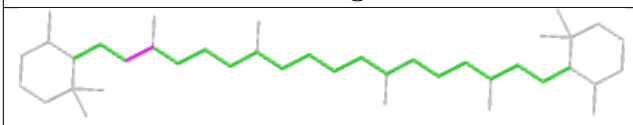
Ligand BCR A 862



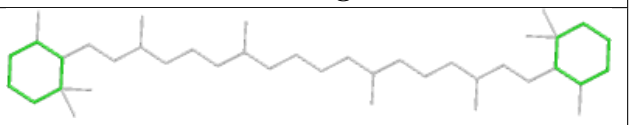
Bond lengths



Bond angles

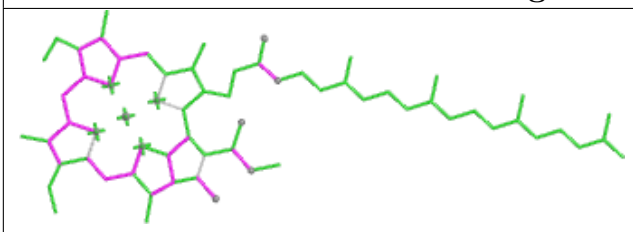


Torsions



Rings

Ligand CLA 5 302



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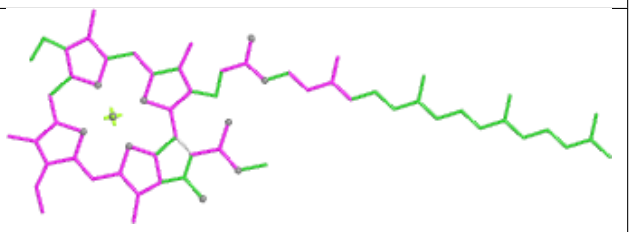
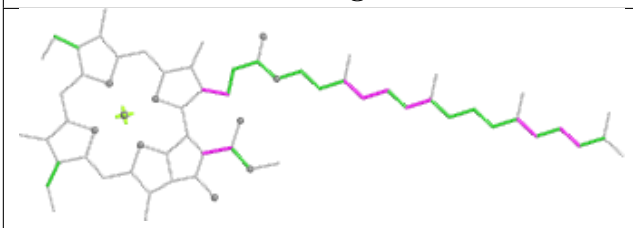


Bond angles



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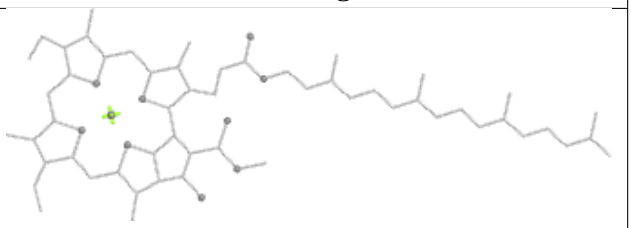
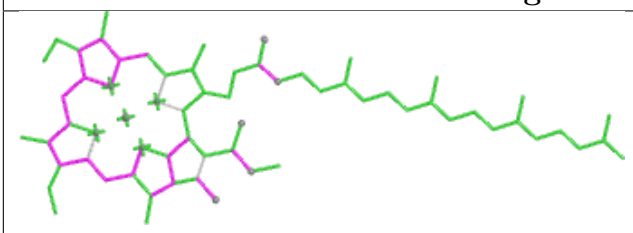


Rings

Ligand CLA A 811



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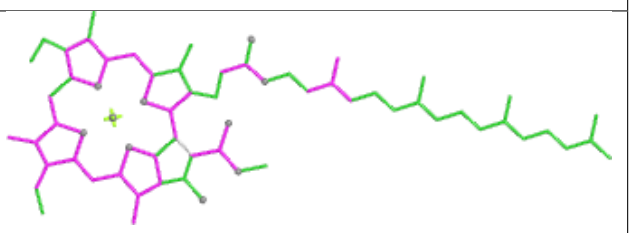
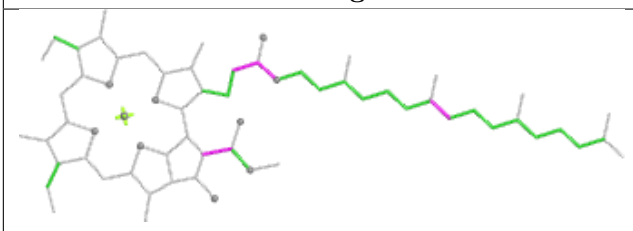
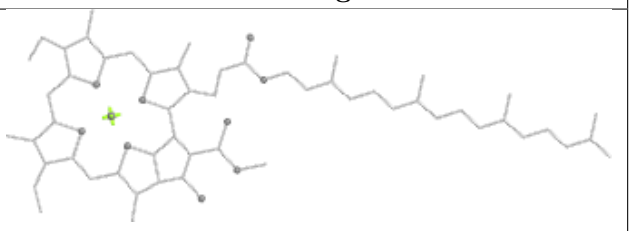


Bond angles

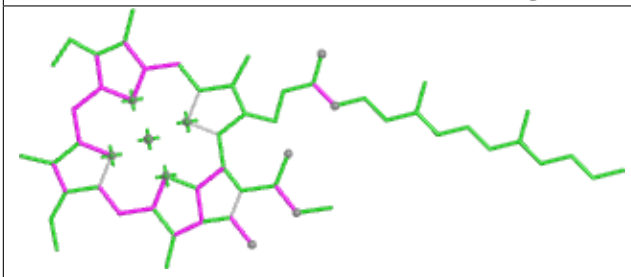


Torsions



Rings

Ligand CLA B 849



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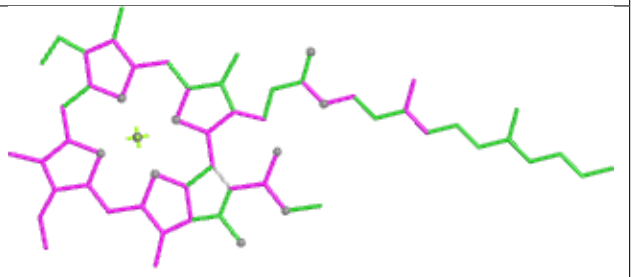
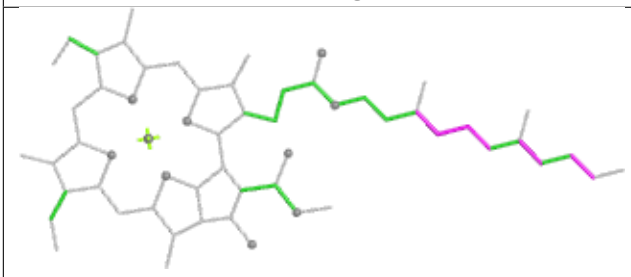
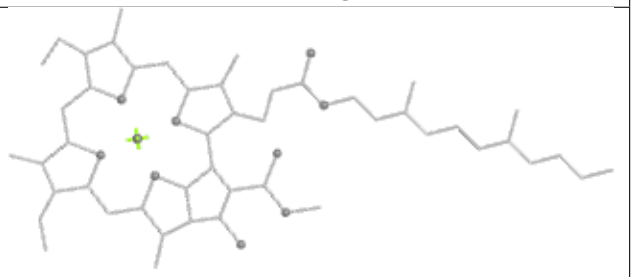


Bond angles

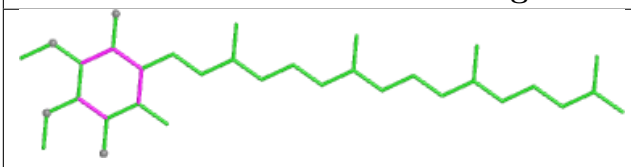


Torsions



Rings

Ligand A1L64 B 840



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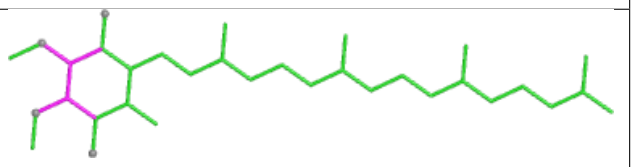
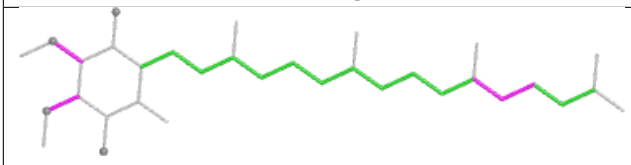


Bond angles



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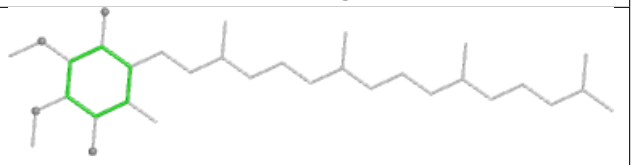
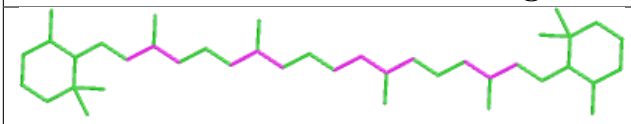


Rings

Ligand BCR B 843



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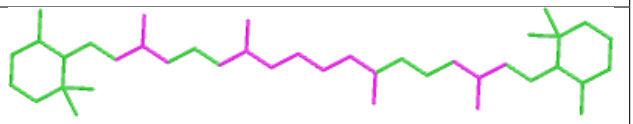
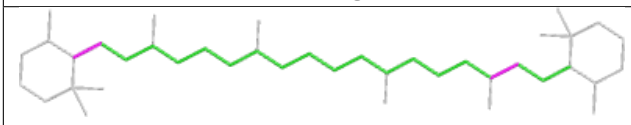


Bond angles



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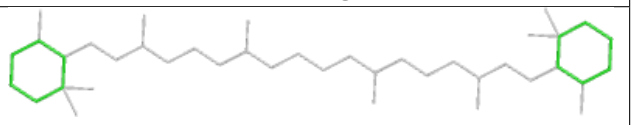
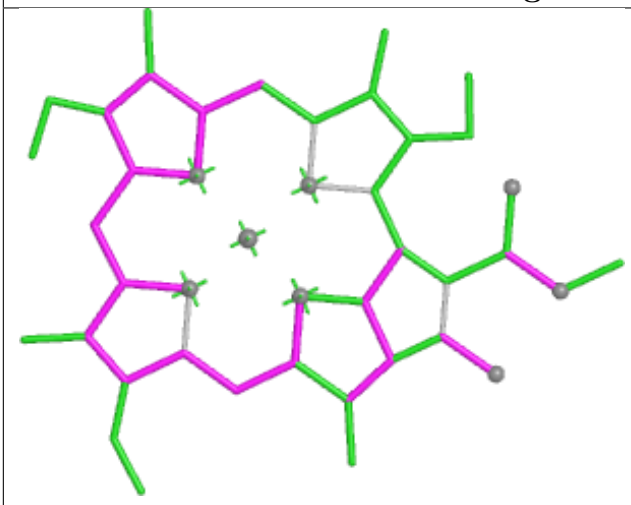


Rings

Ligand CLA A 813



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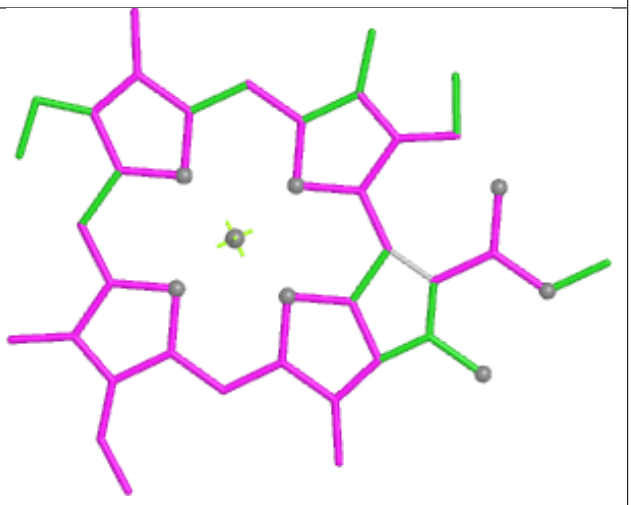
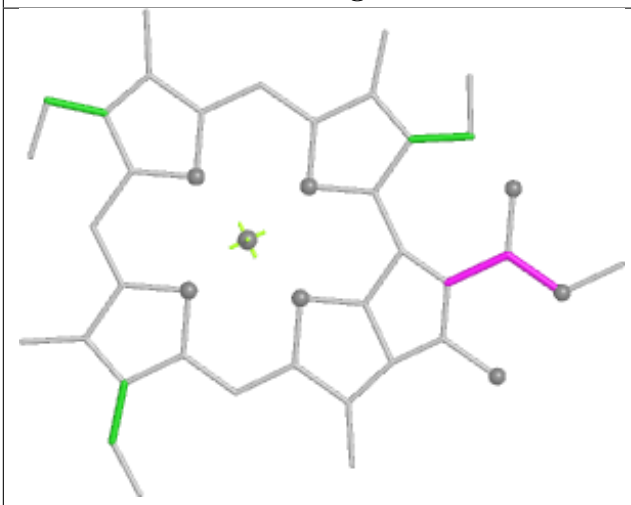


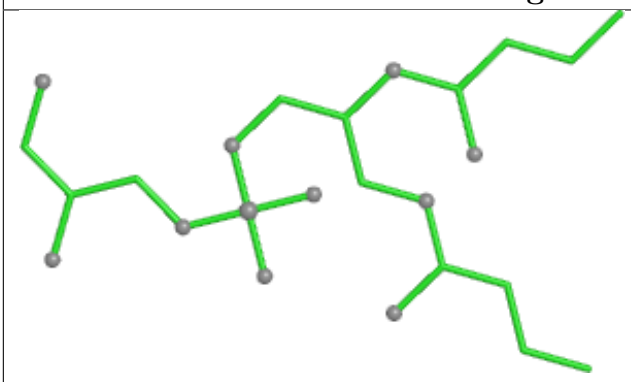
Bond angles



Torsions

Rings

Ligand LHG 5 316



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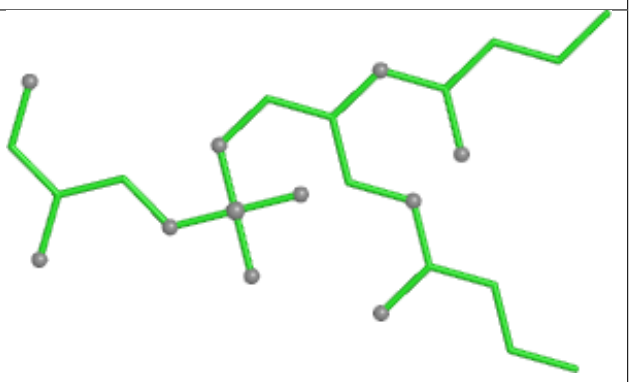
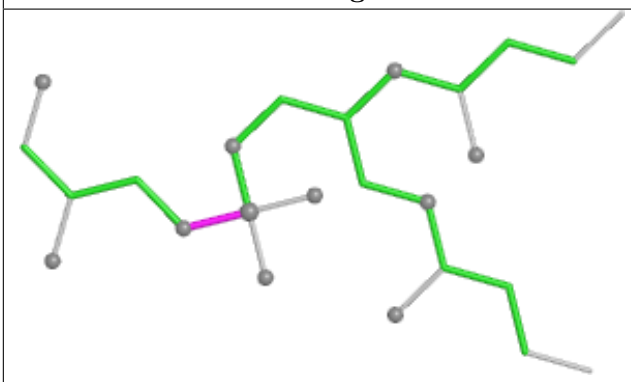


Bond angles



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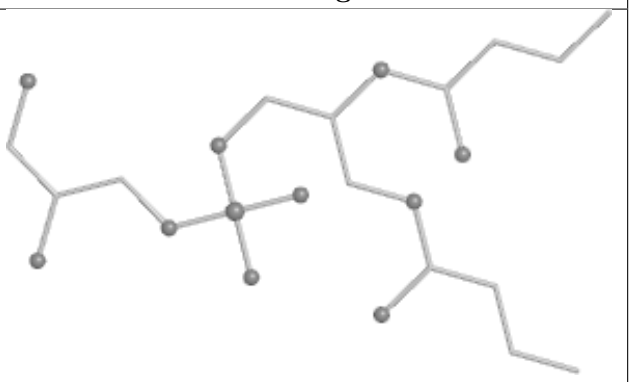
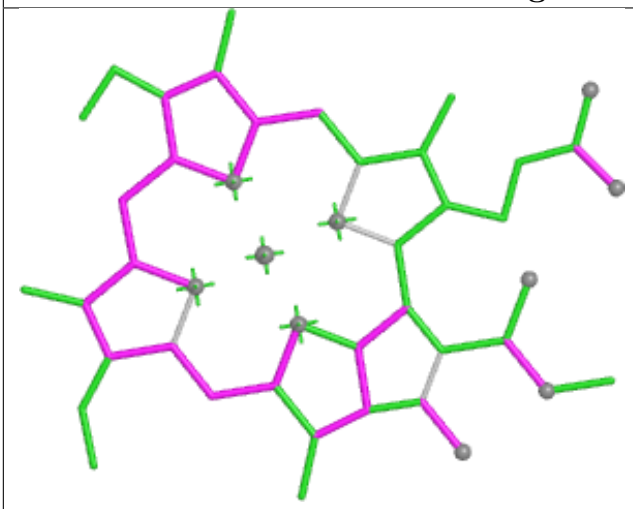


Rings

Ligand CLA 4 307



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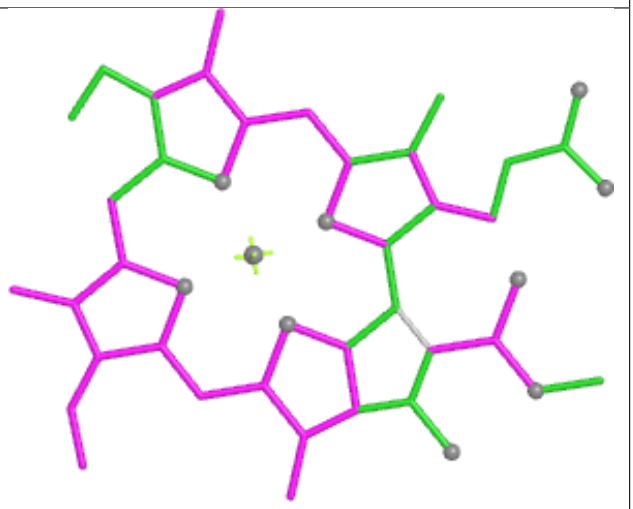
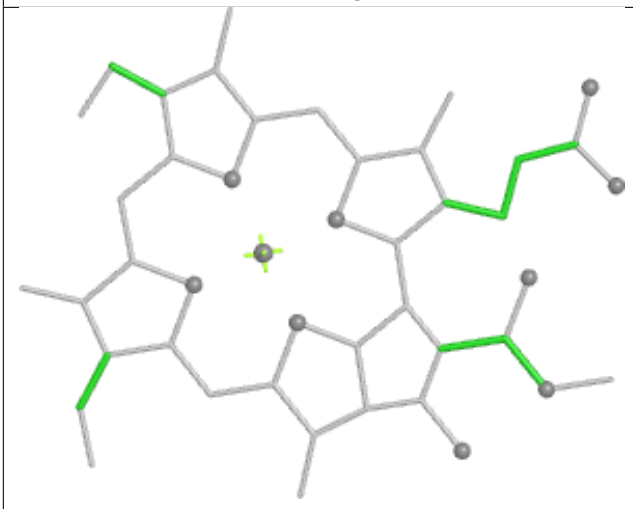


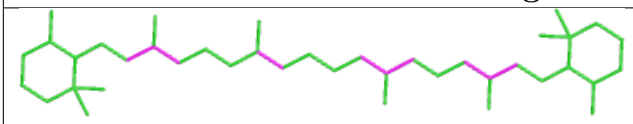
Bond angles



Torsions

Rings

Ligand BCR B 844



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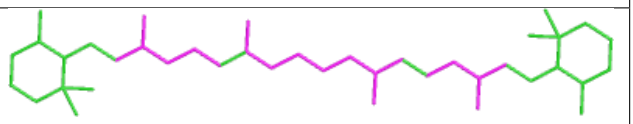
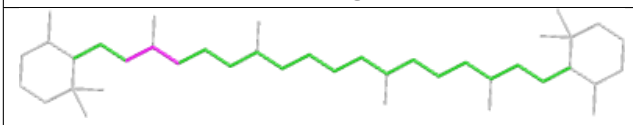
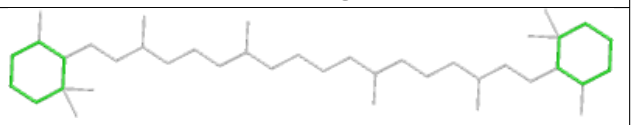


Bond angles

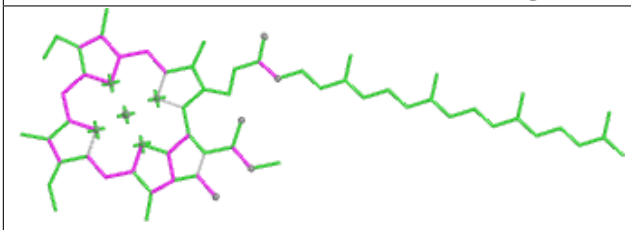


Torsions



Rings

Ligand CLA B 803



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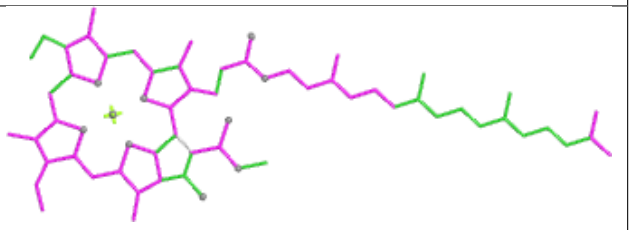
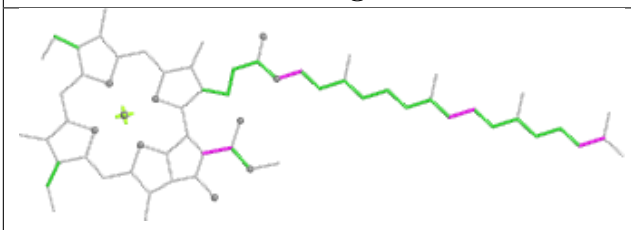


Bond angles



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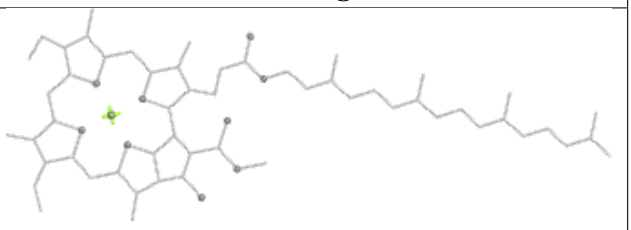
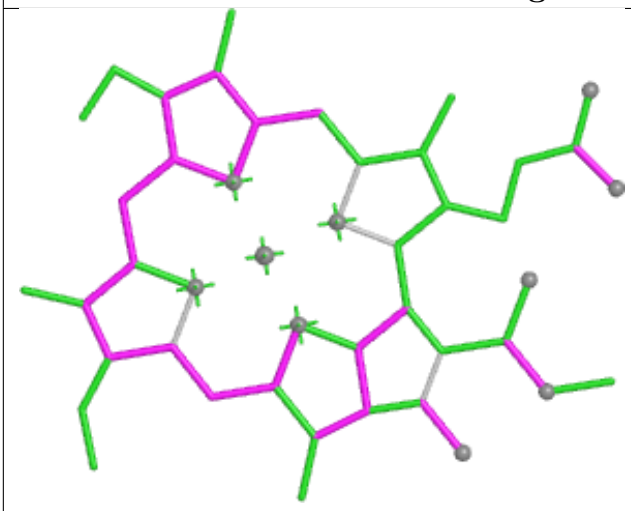


Rings

Ligand CLA 4 306



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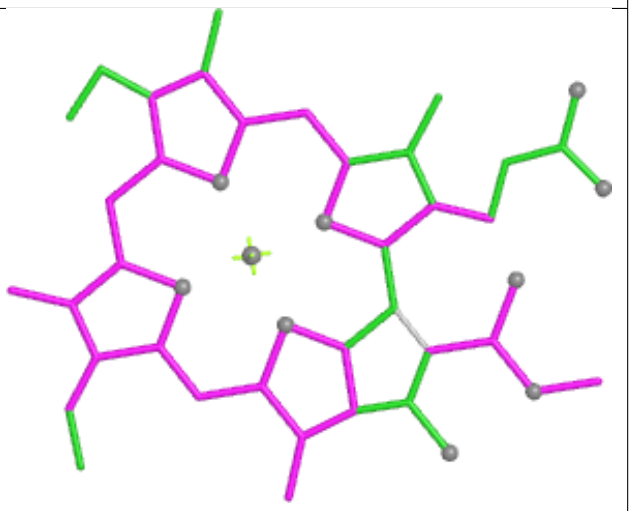
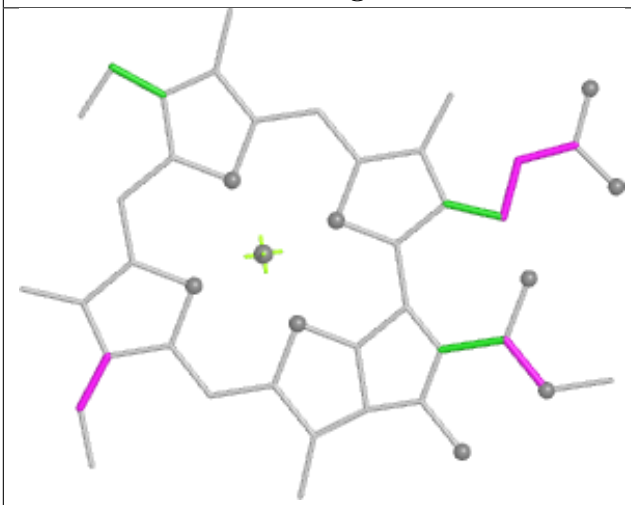
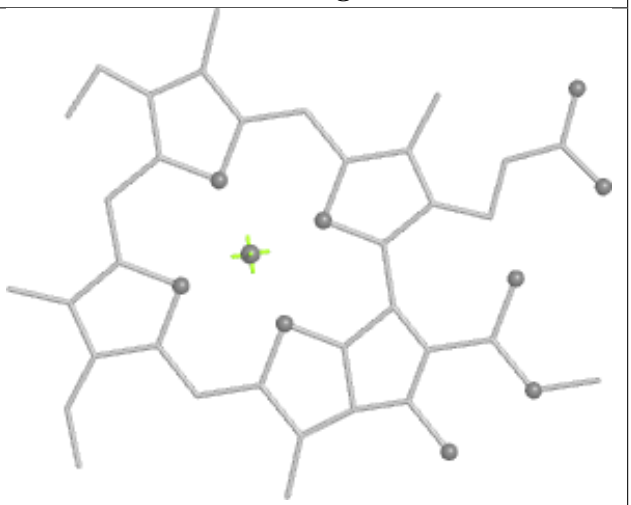


Bond angles

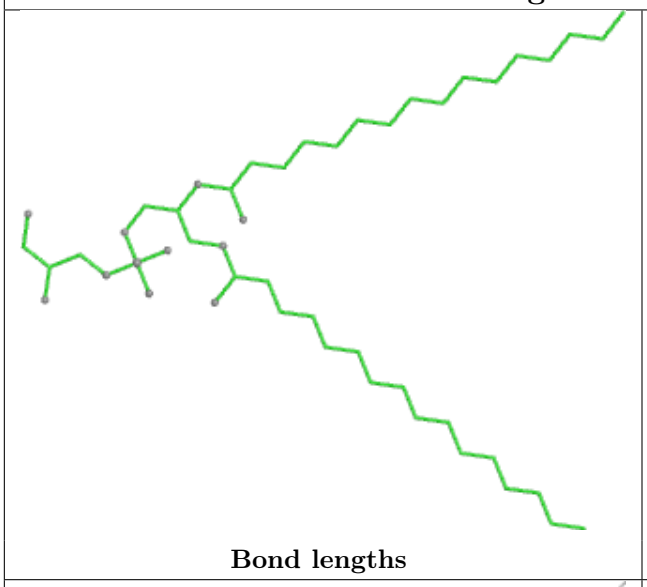


Torsions



Rings

Ligand LHG 1 317



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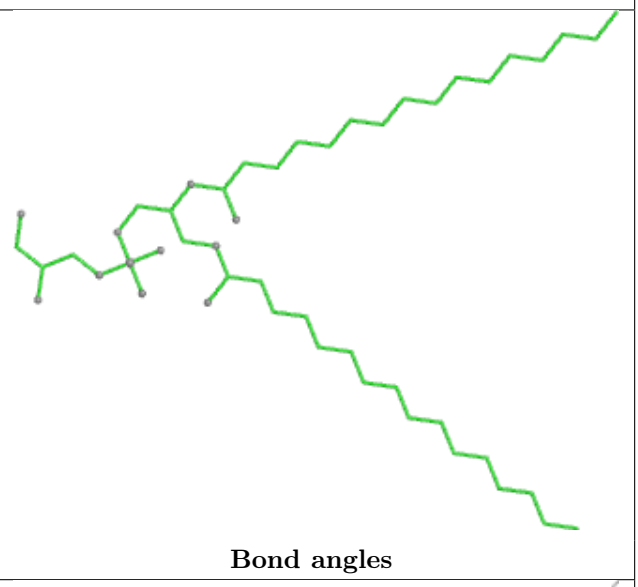
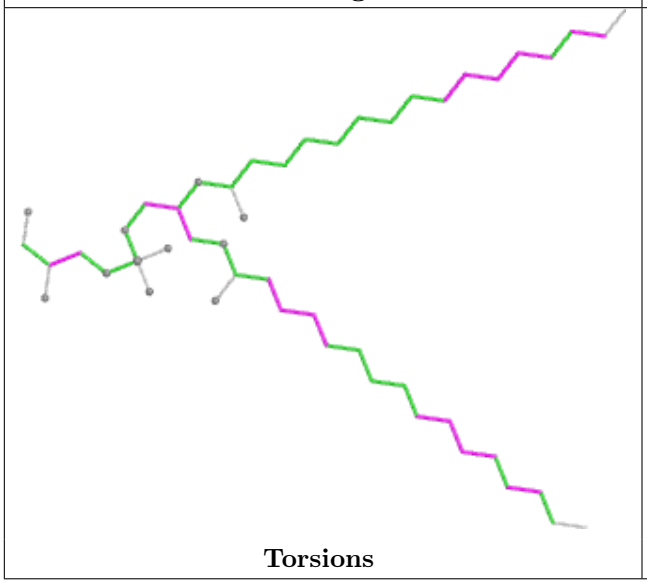
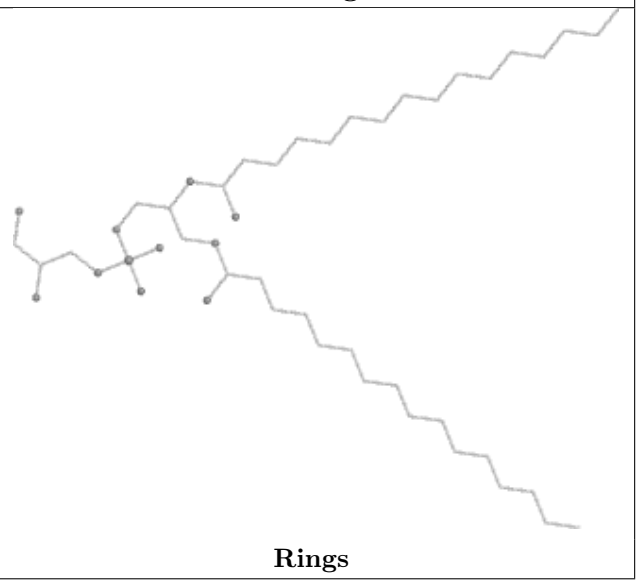


Bond angles

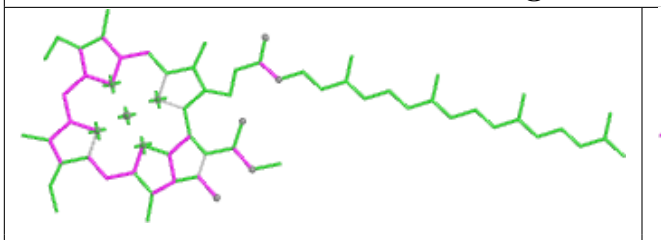


Torsions



Rings

Ligand CLA B 810



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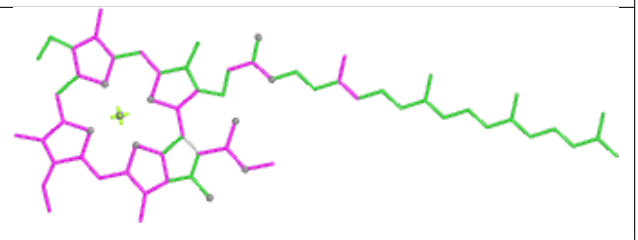
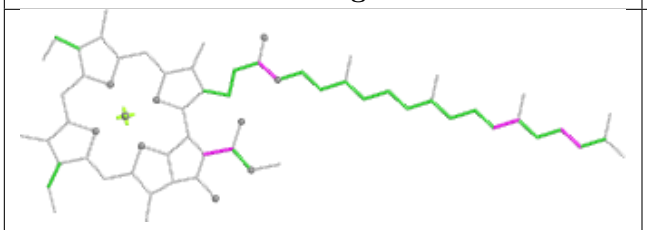
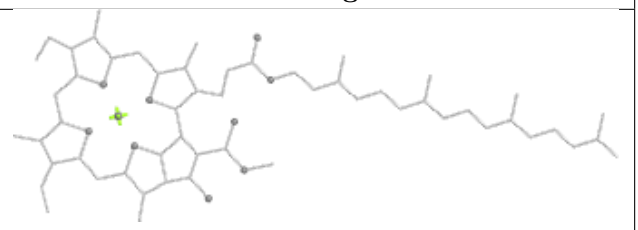


Bond angles

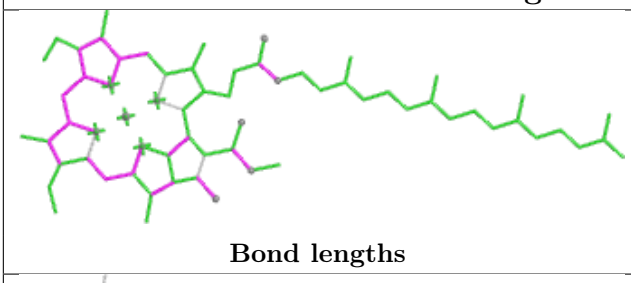


Torsions

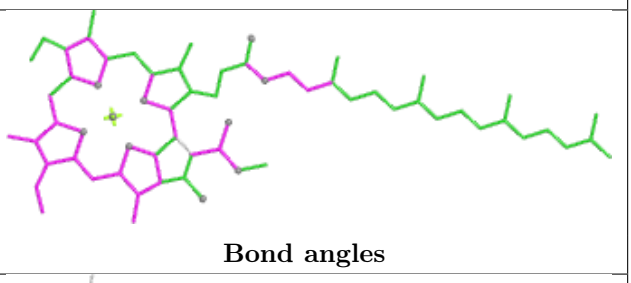


Rings

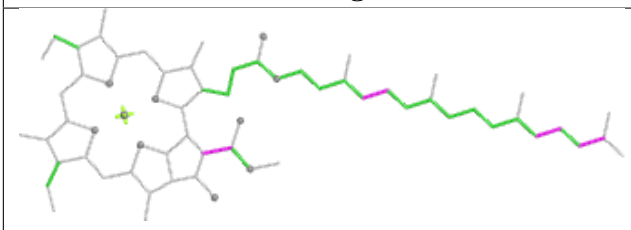
Ligand CLA B 824



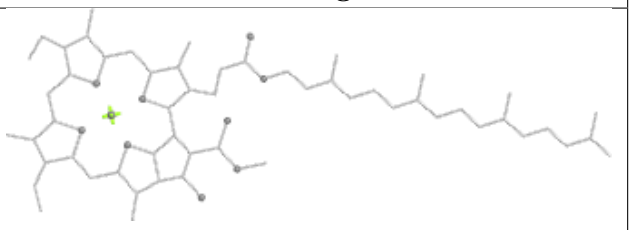
Bond lengths



Bond angles

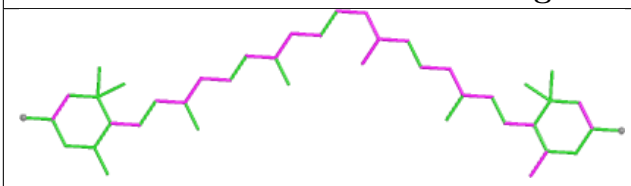


Torsions



Rings

Ligand 5X6 2 312



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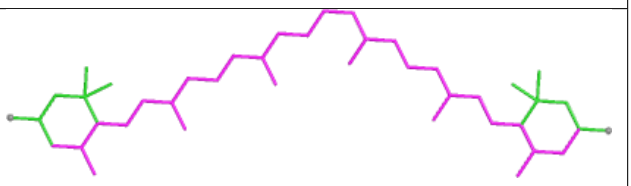
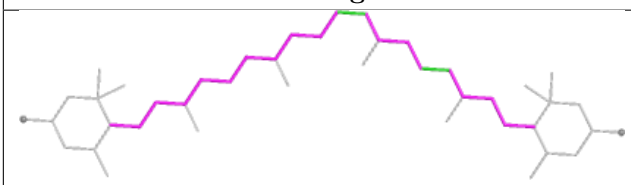
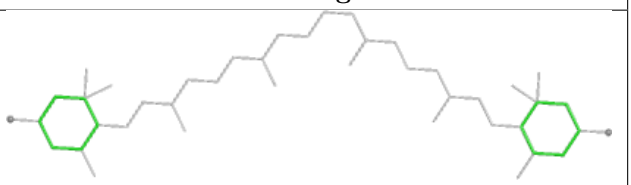


Bond angles

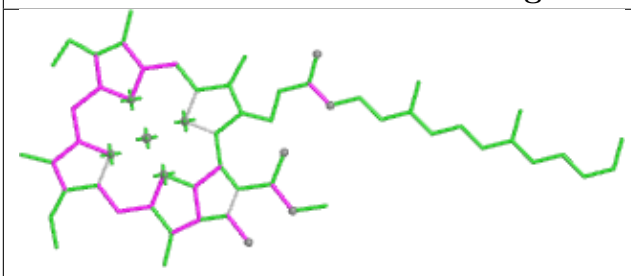


Torsions



Rings

Ligand CLA B 817



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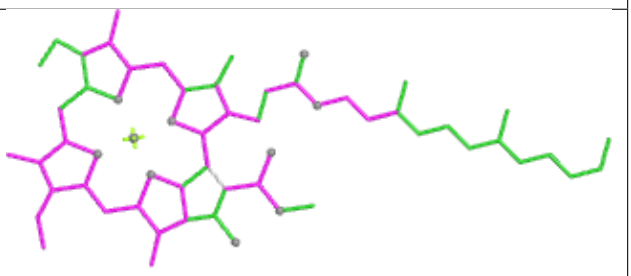

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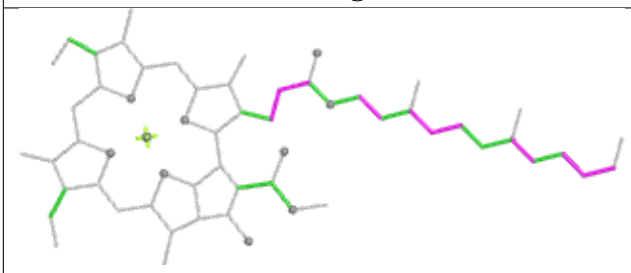

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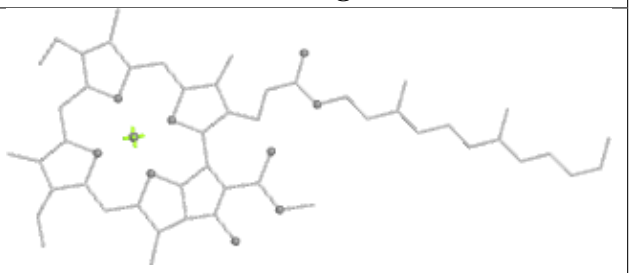
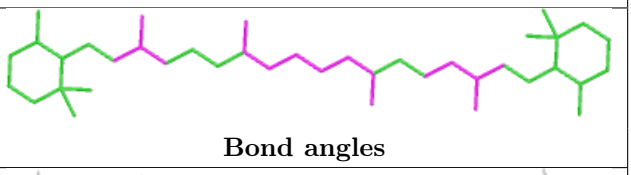


Rings

Ligand BCR 5 315

Bond lengths



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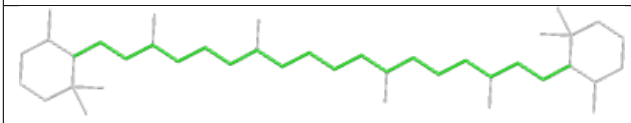

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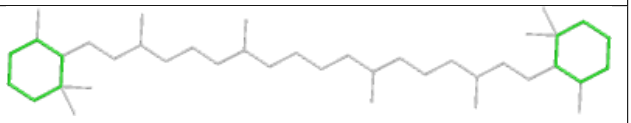
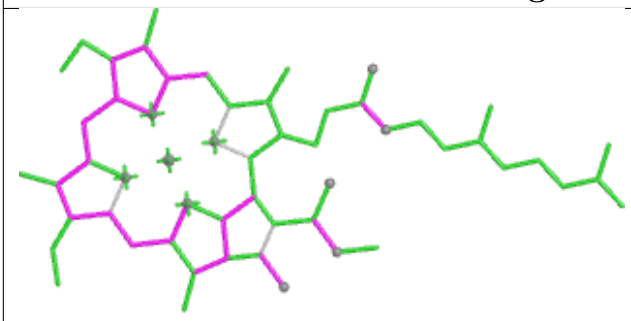


Rings

Ligand CLA 6 310



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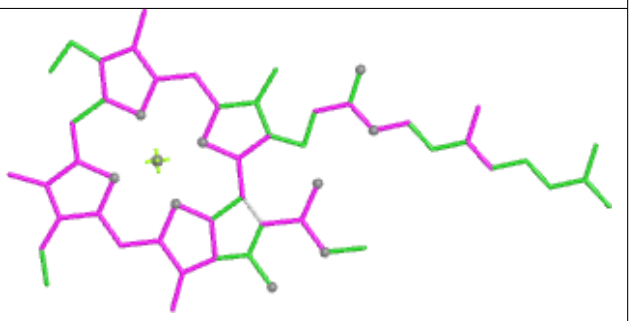
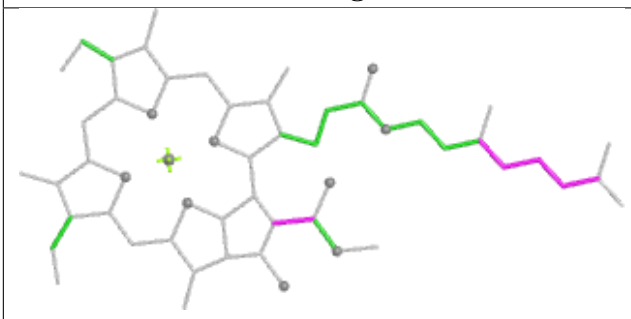


Bond angles



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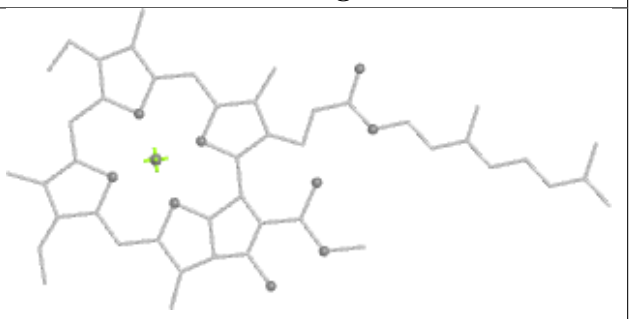
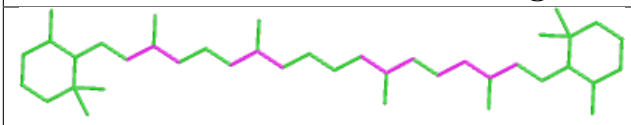


Rings

Ligand BCR I 102



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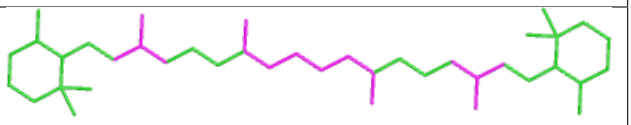
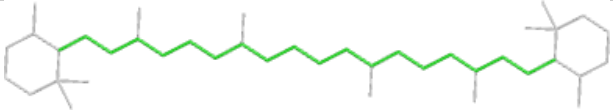


Bond angles



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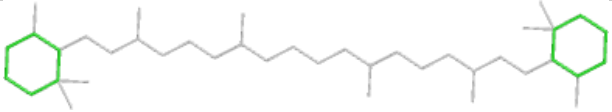
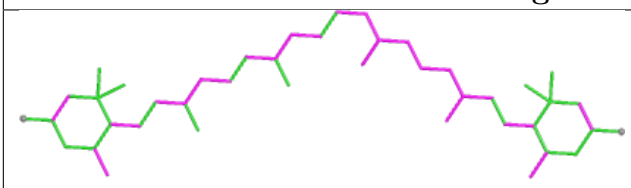


Rings

Ligand 5X6 Z 206



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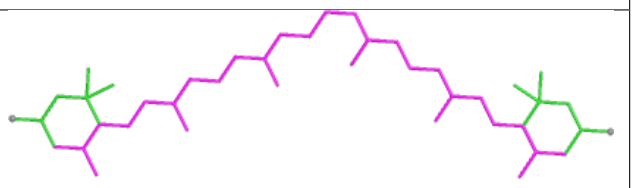
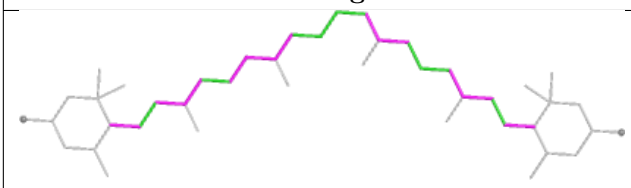


Bond angles



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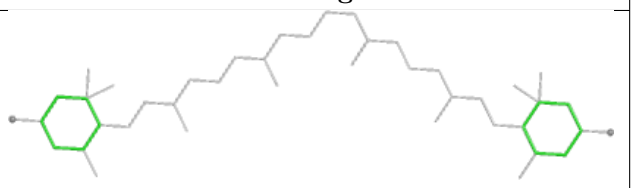
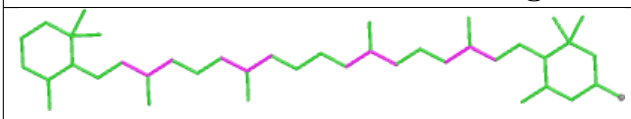


Rings

Ligand RRX 6 318



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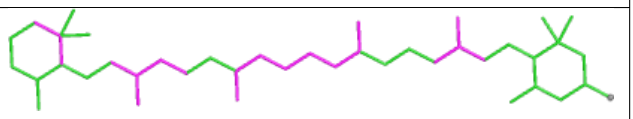
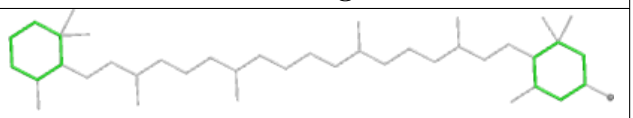


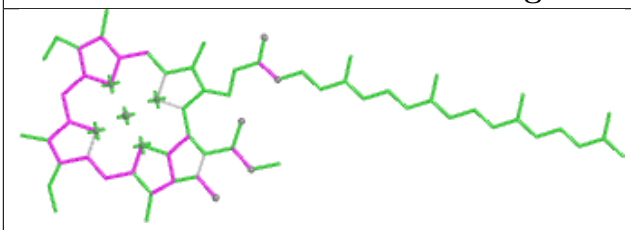
Bond angles

Torsions



Rings

Ligand CLA B 813



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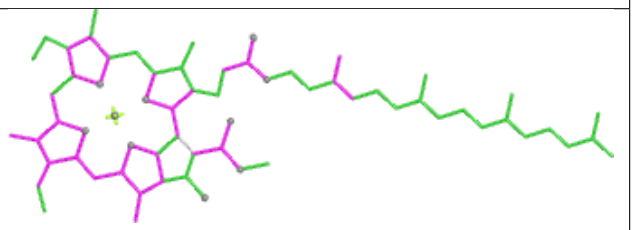
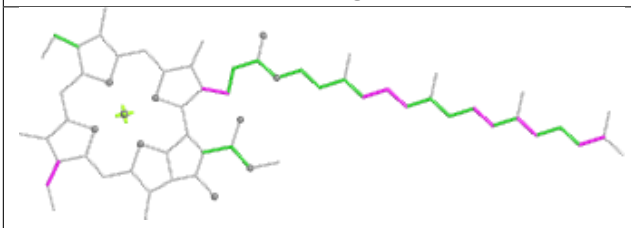
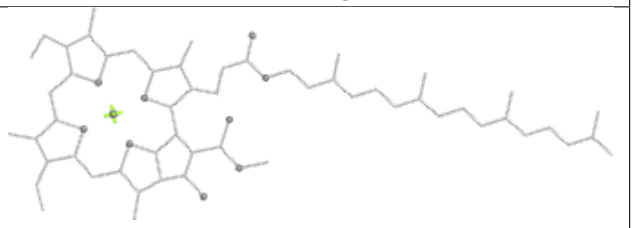


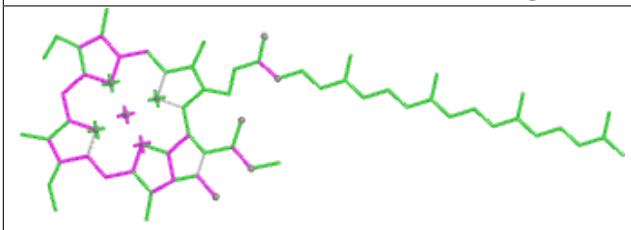
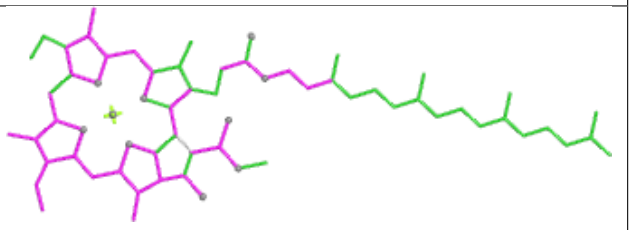
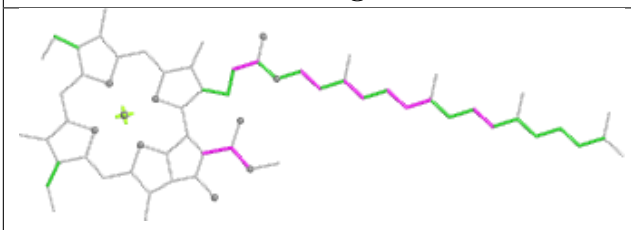
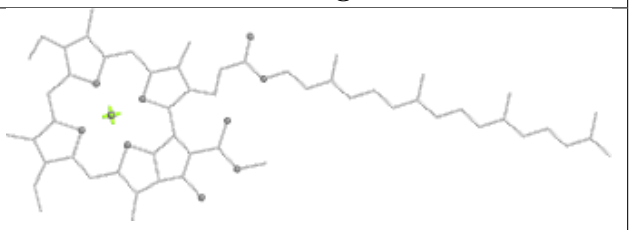
Bond angles

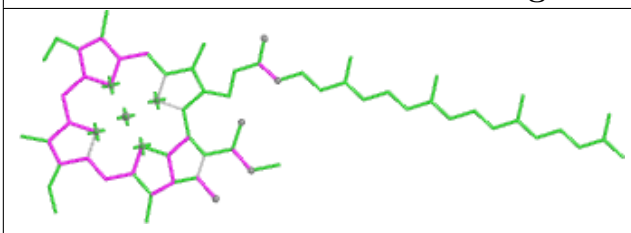
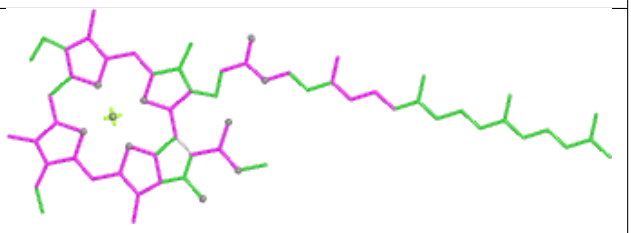
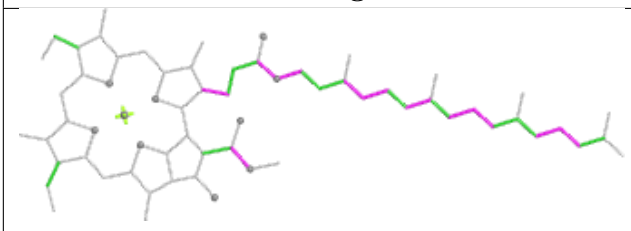
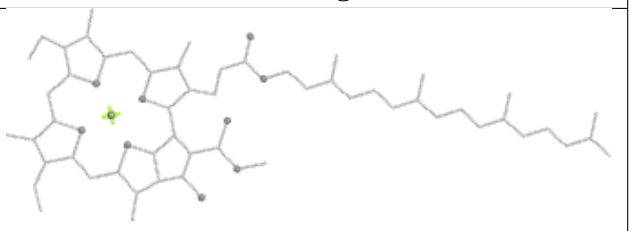


Torsions

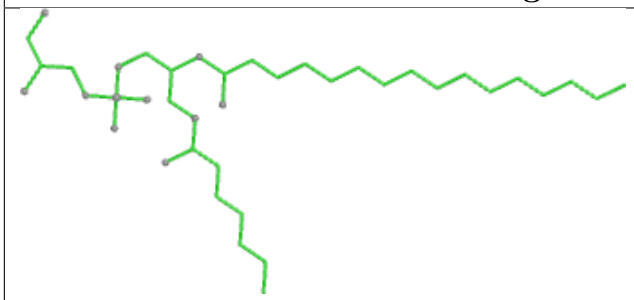


Rings

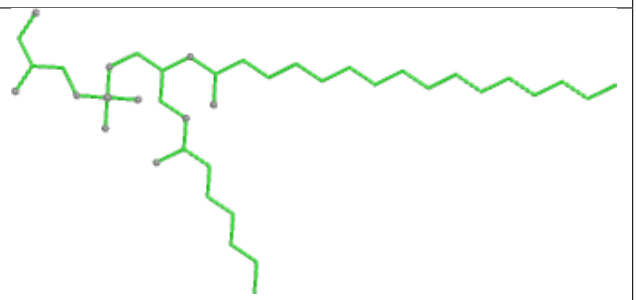
Ligand CLA A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

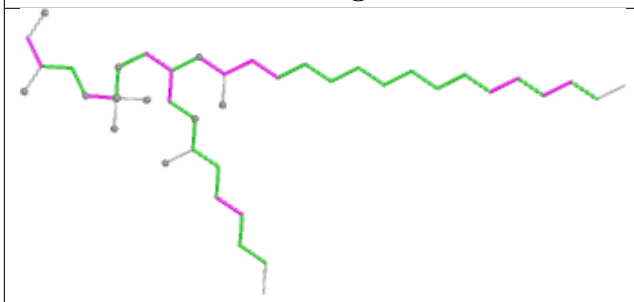
Ligand LHG A 842



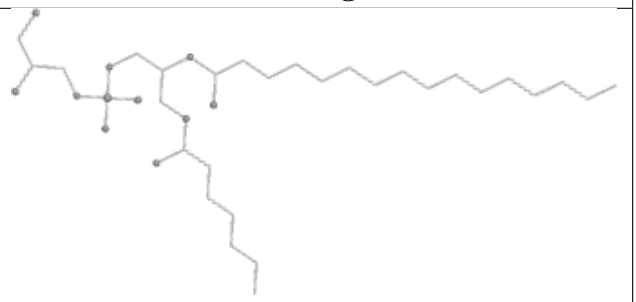
Bond lengths



Bond angles

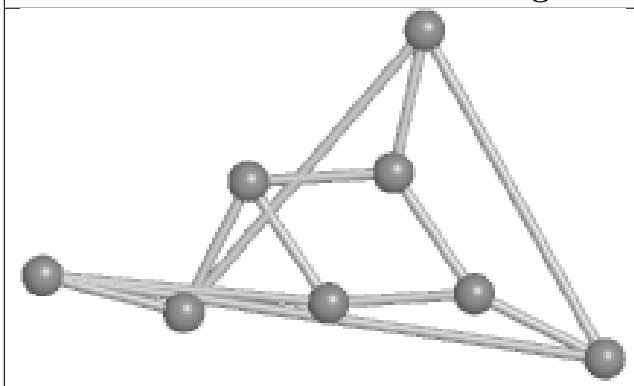


Torsions



Rings

Ligand SF4 A 847



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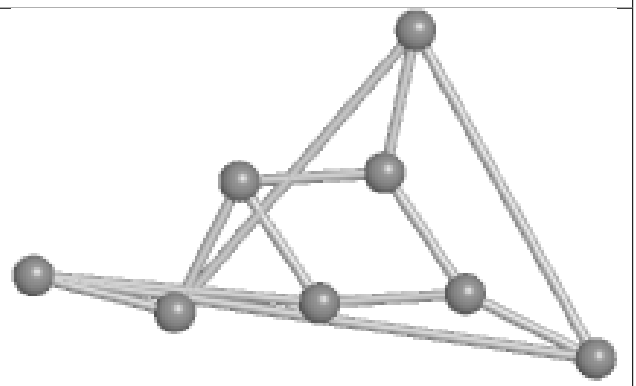
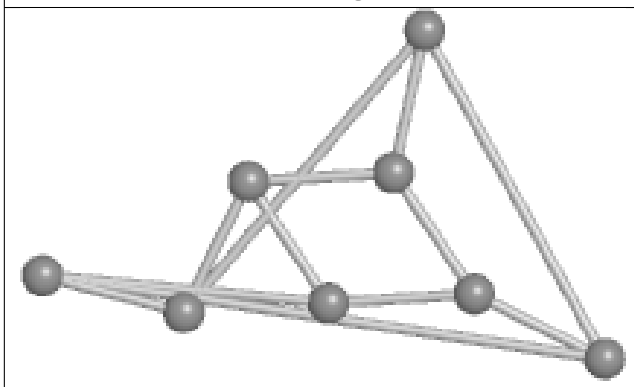
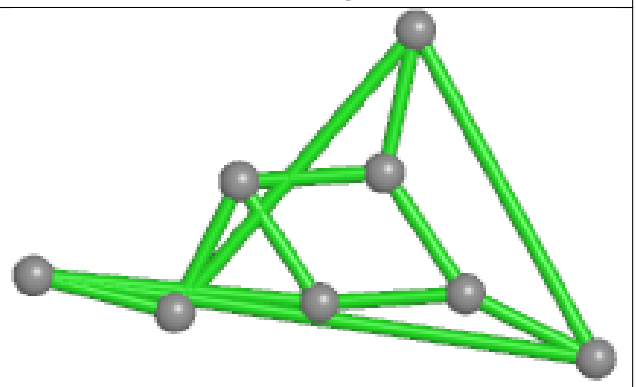


Bond angles

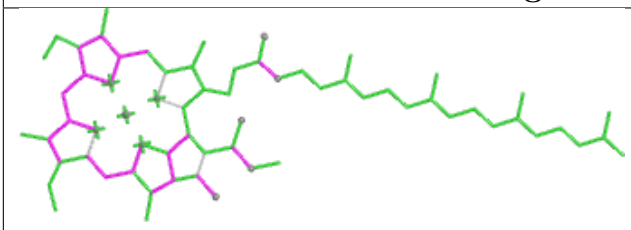


Torsions

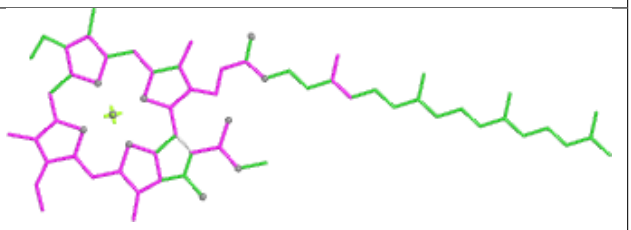


Rings

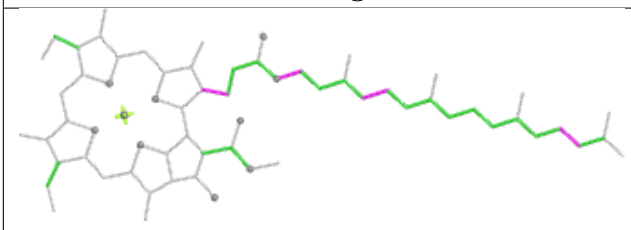
Ligand CLA B 827



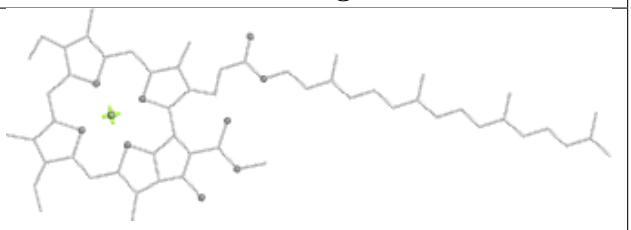
Bond lengths



Bond angles

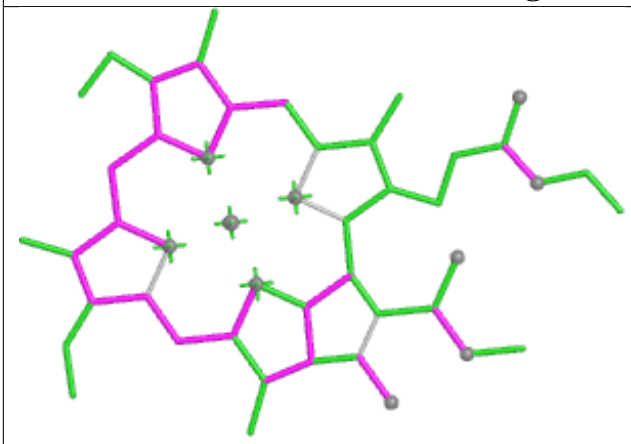


Torsions

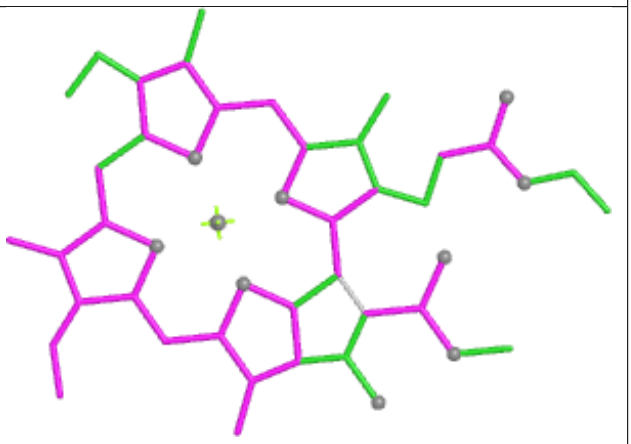


Rings

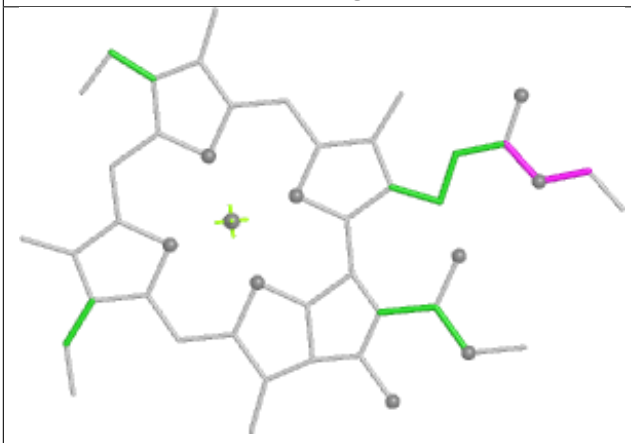
Ligand CLA B 836



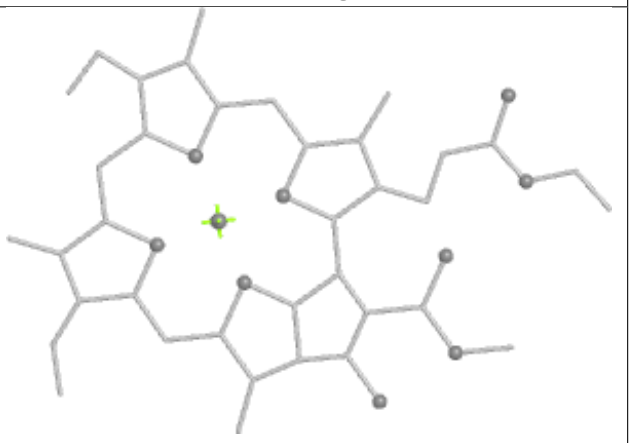
Bond lengths



Bond angles

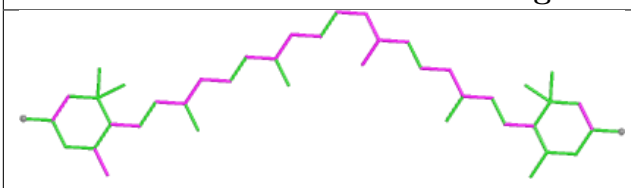


Torsions



Rings

Ligand 5X6 J 104



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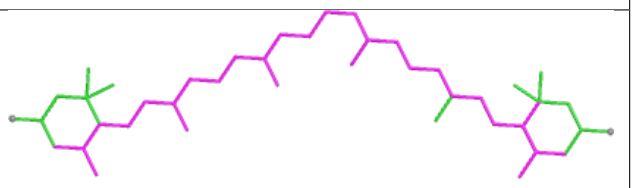
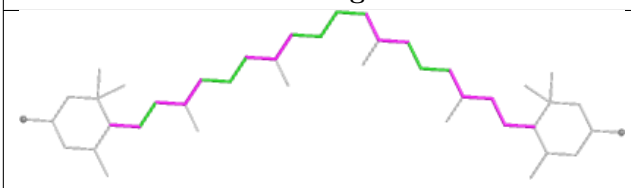
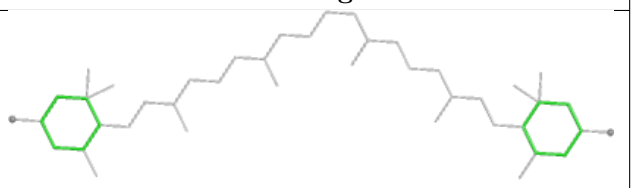


Bond angles

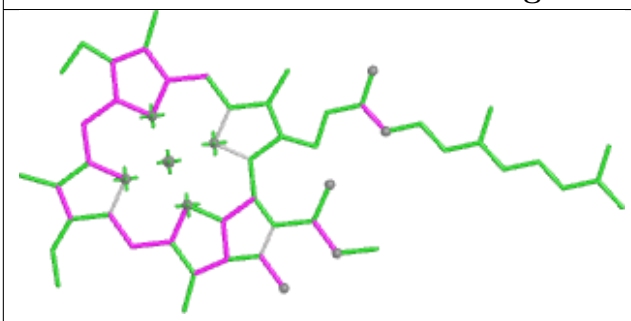


Torsions

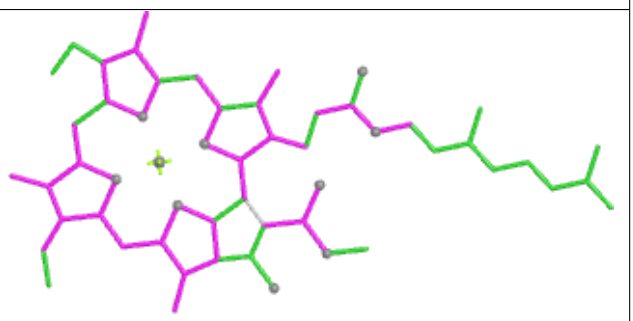


Rings

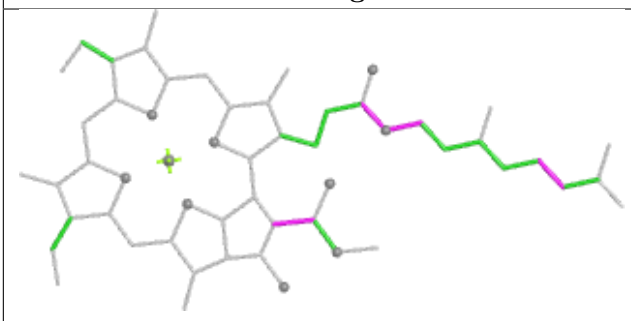
Ligand CLA A 824



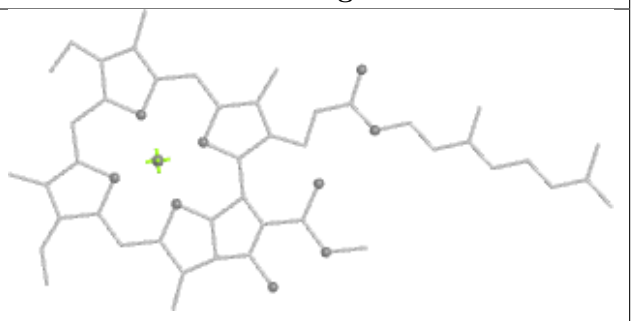
Bond lengths



Bond angles

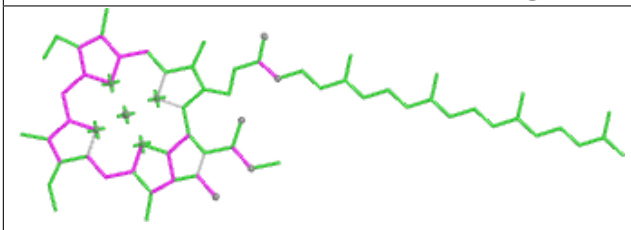


Torsions

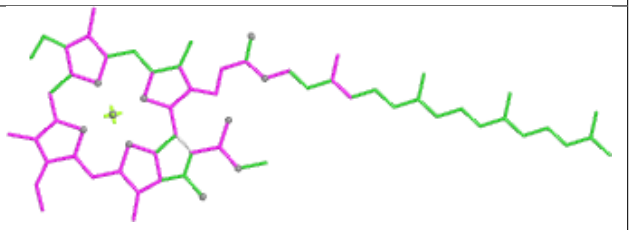


Rings

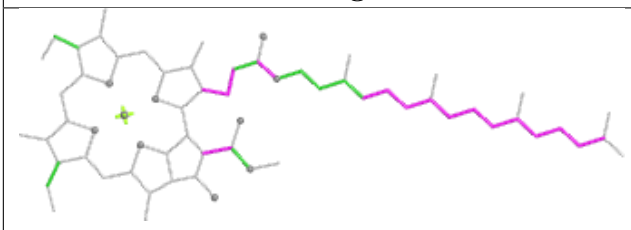
Ligand CLA A 820



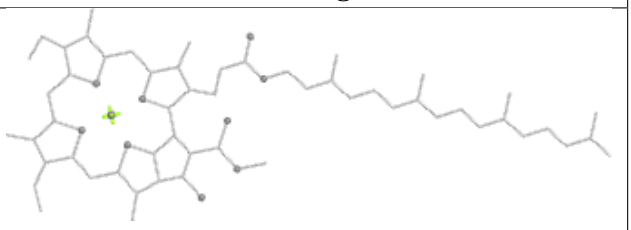
Bond lengths



Bond angles

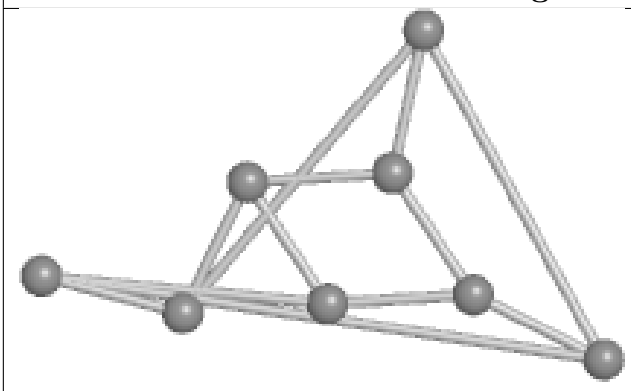


Torsions



Rings

Ligand SF4 C 102



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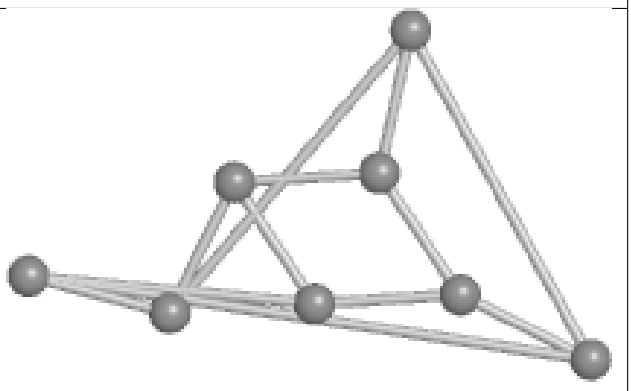
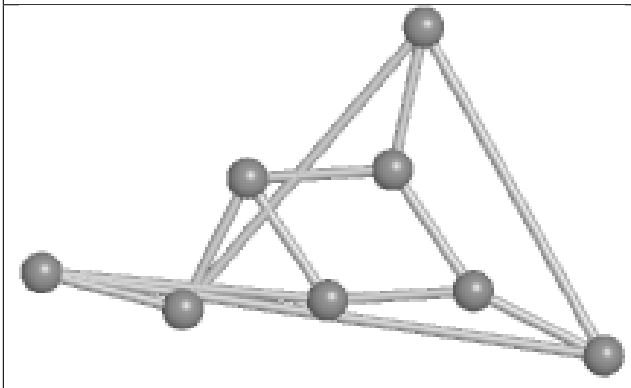


Bond angles



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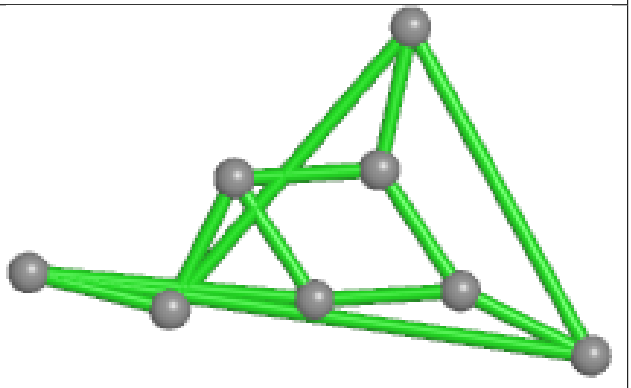
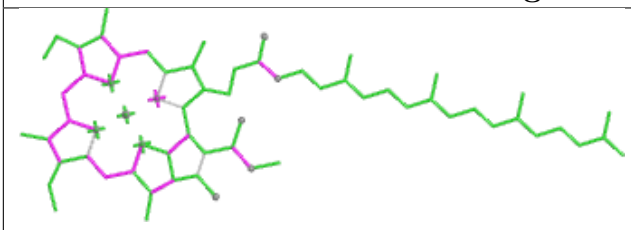
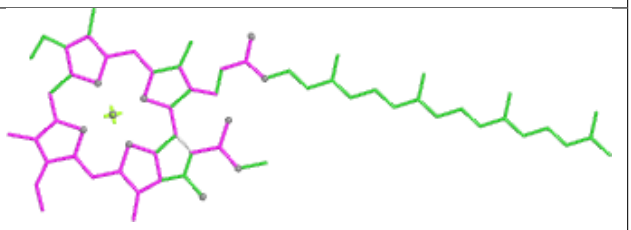


Rings

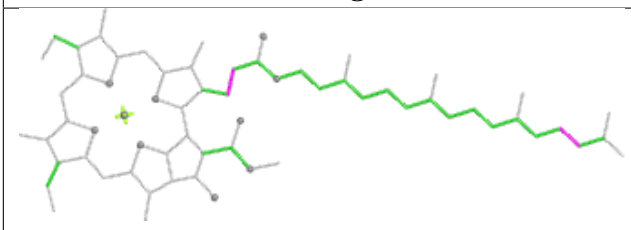
Ligand CLA A 857



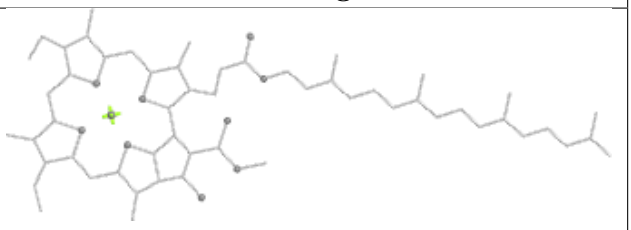
Bond lengths



Bond angles

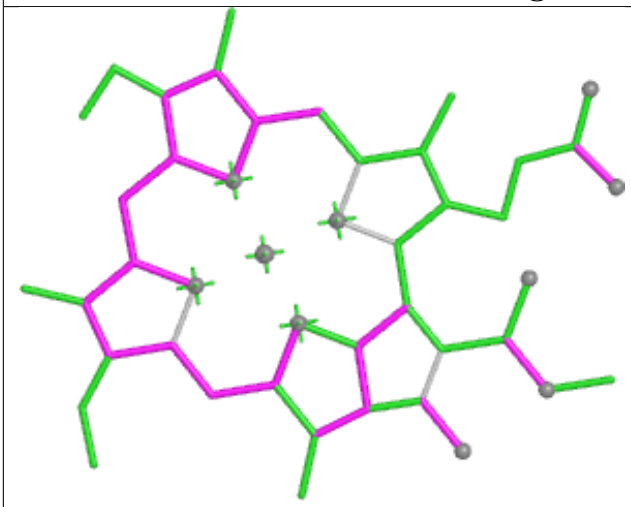


Torsions

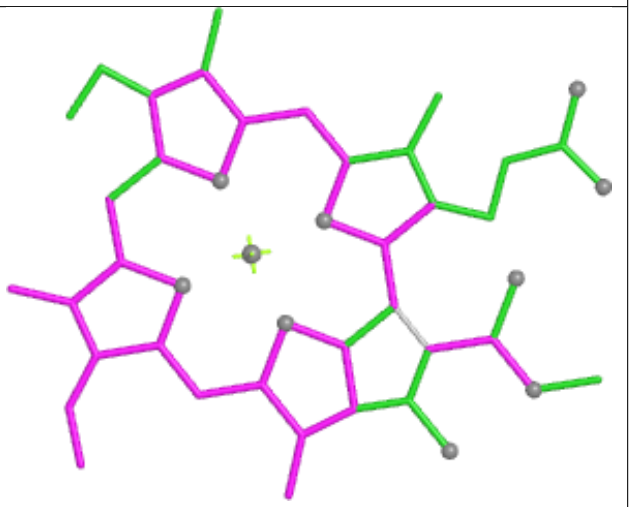


Rings

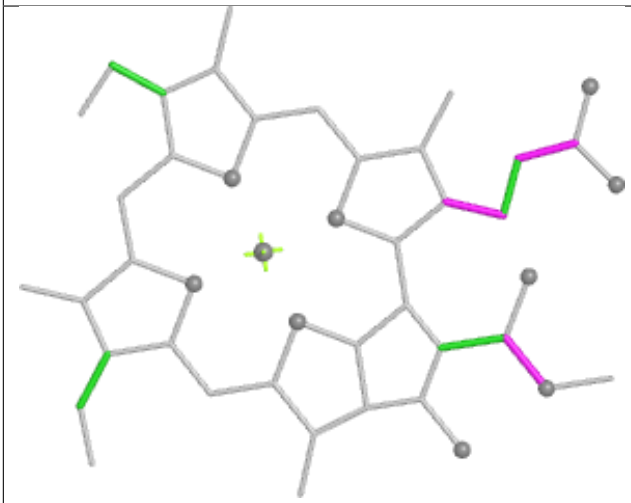
Ligand CLA 6 303



Bond lengths



Bond angles



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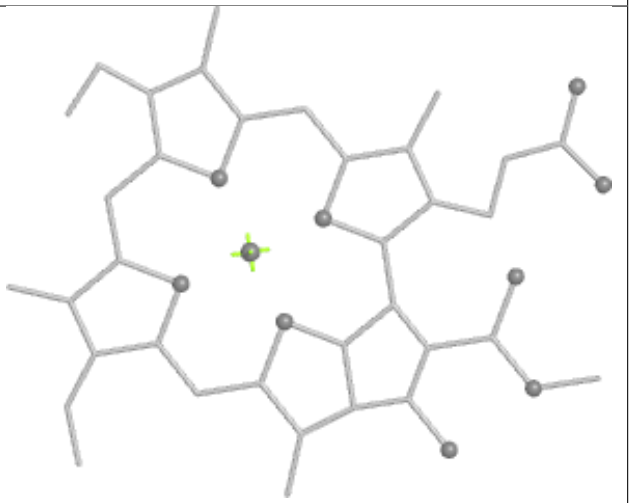
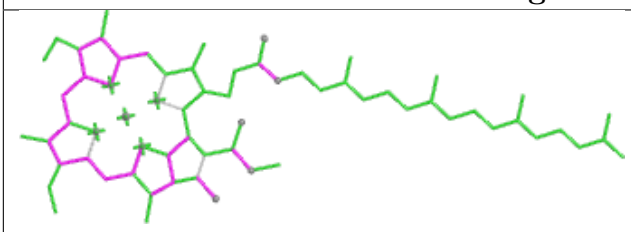
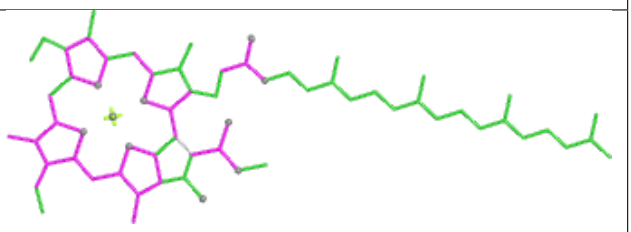


Rings

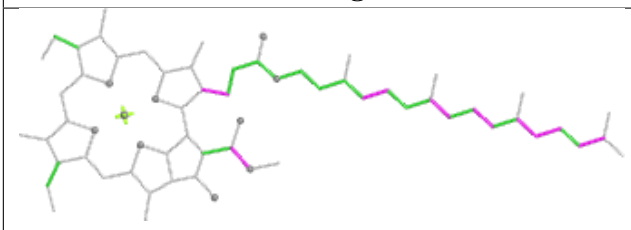
Ligand CLA 6 304



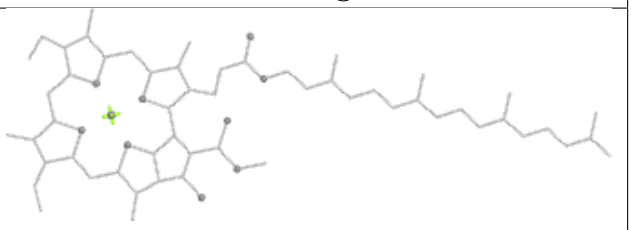
Bond lengths



Bond angles

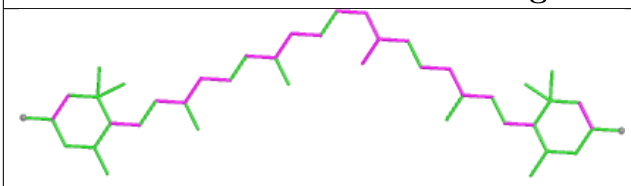


Torsions



Rings

Ligand 5X6 O 208



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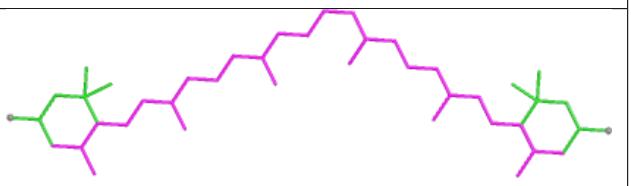
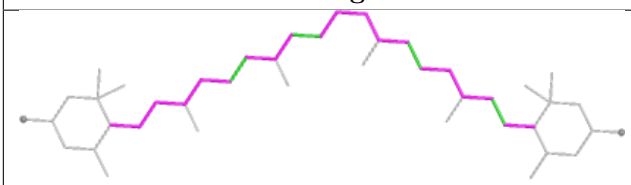


Bond angles



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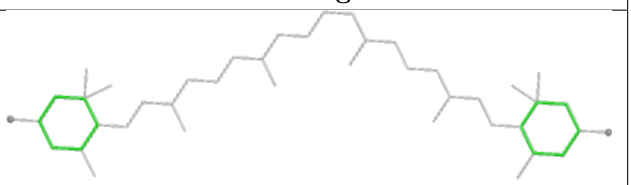
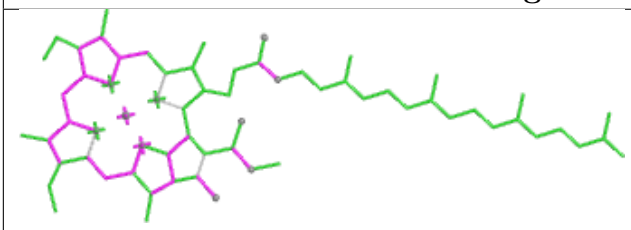


Rings

Ligand CLA A 807



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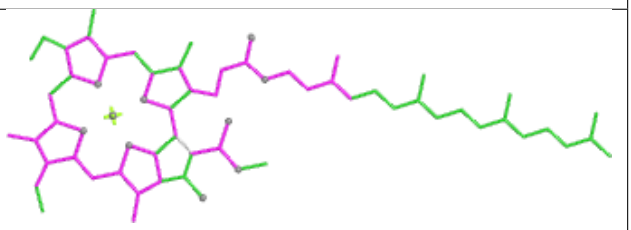
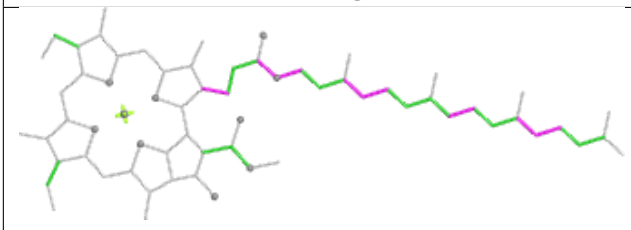
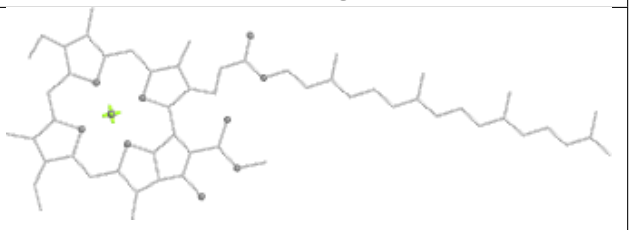


Bond angles

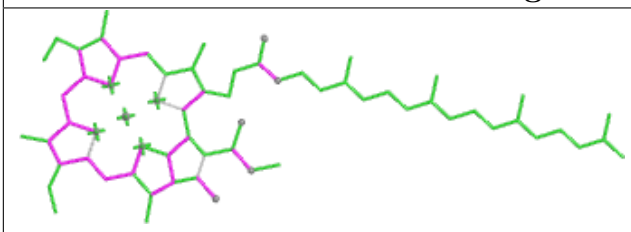


Torsions



Rings

Ligand CLA B 808



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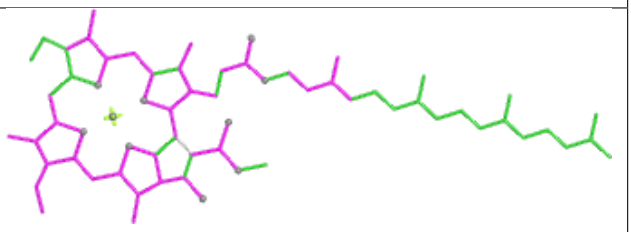
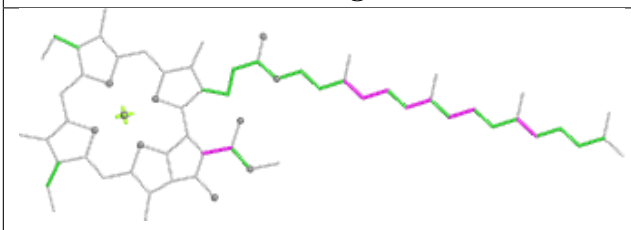


Bond angles



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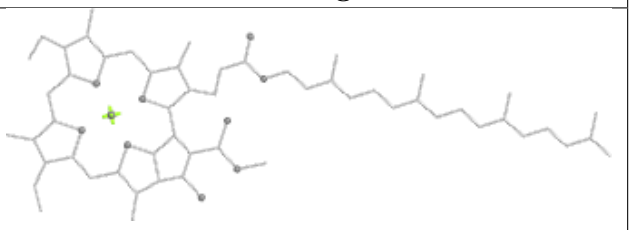
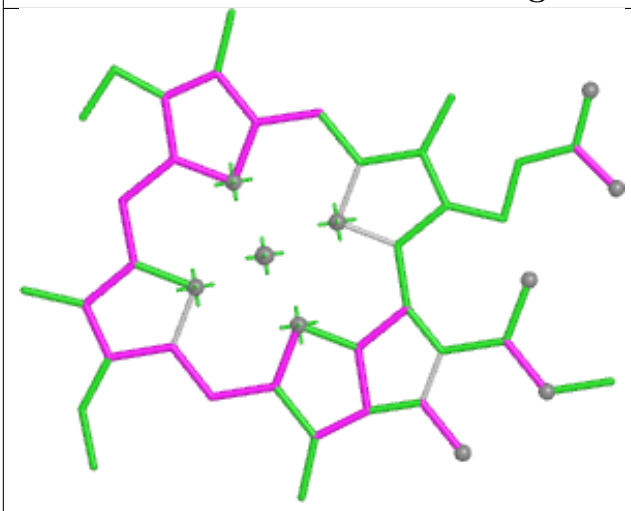
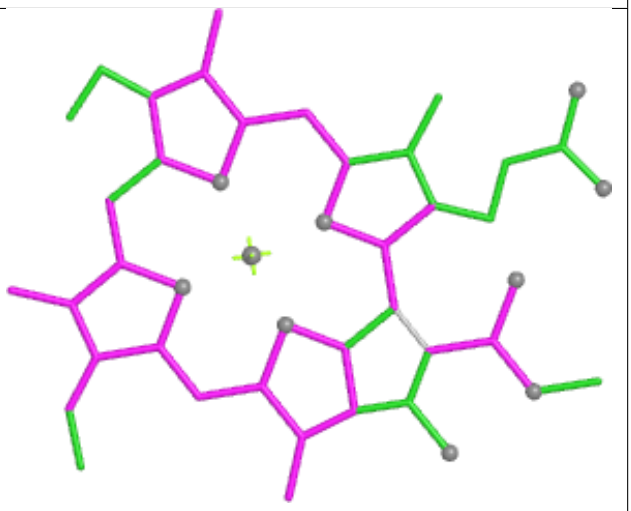


Rings

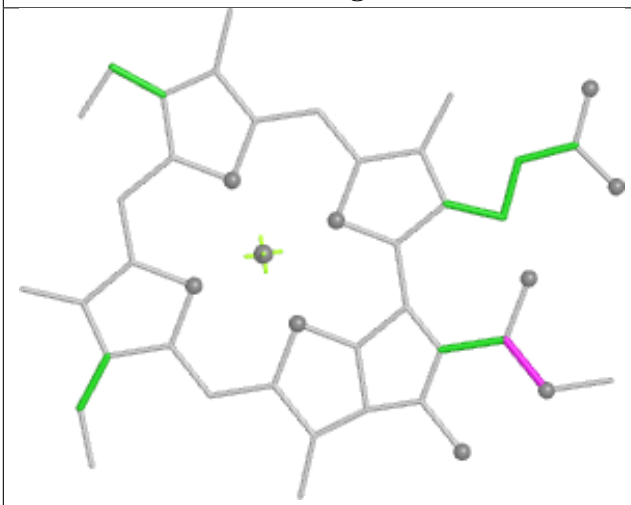
Ligand CLA 4 302



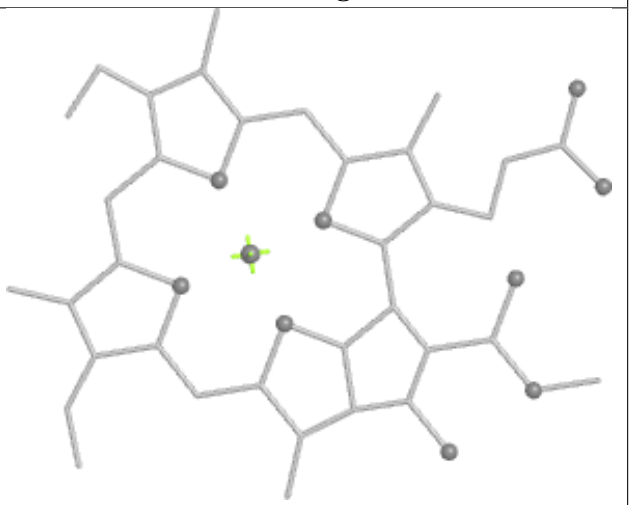
Bond lengths



Bond angles

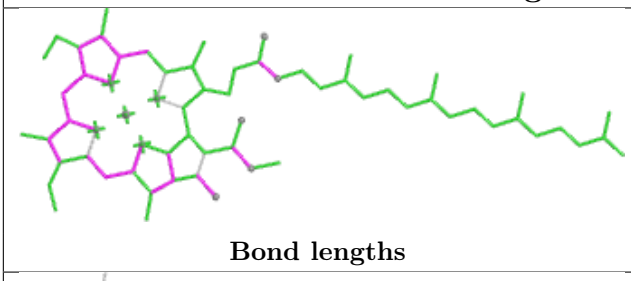


Torsions

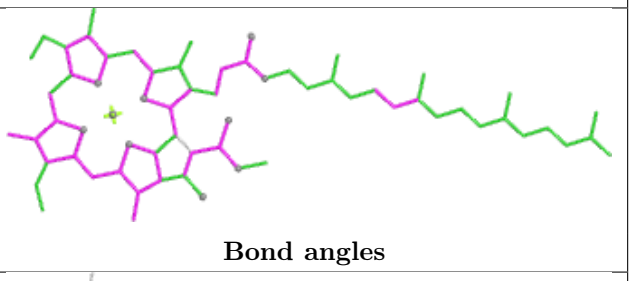


Rings

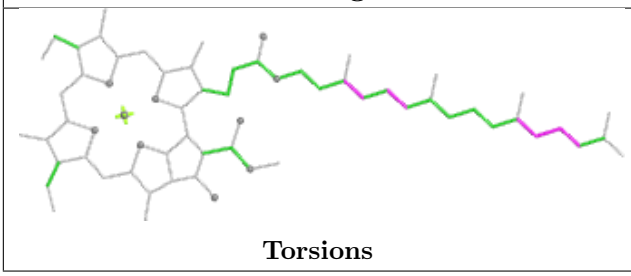
Ligand CLA B 832



Bond lengths



Bond angles



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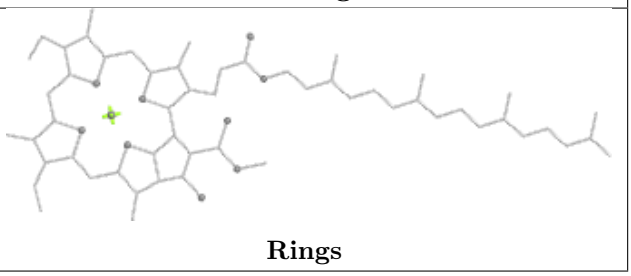
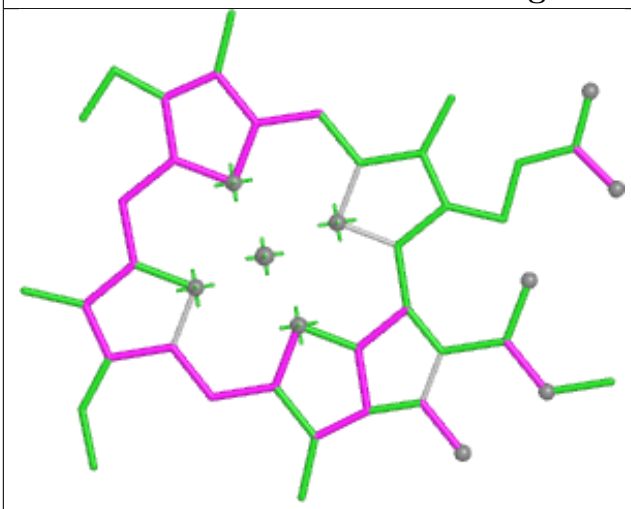
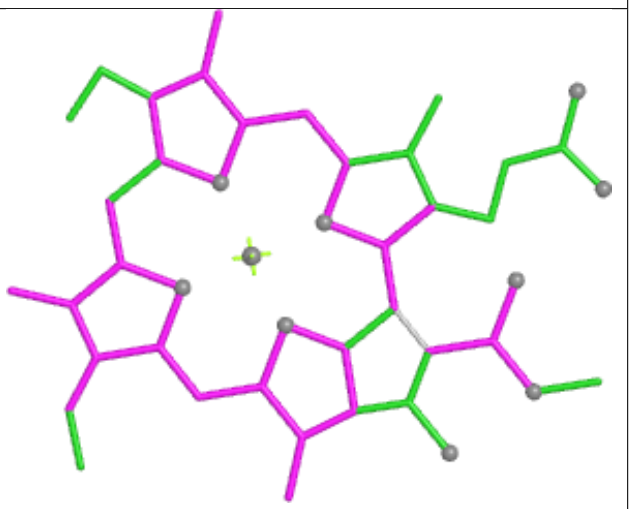


Rings

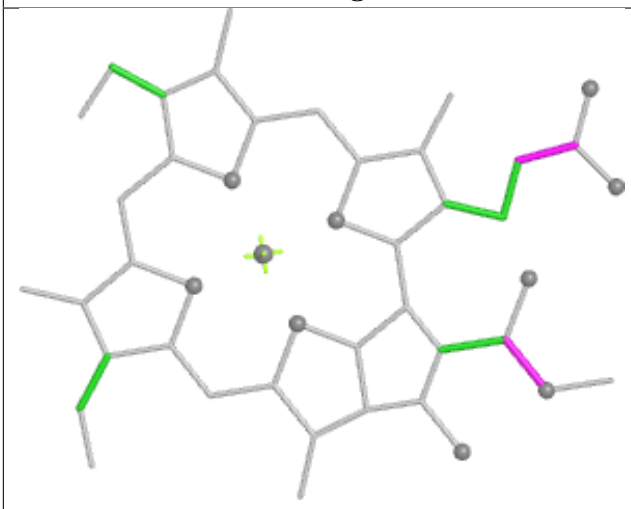
Ligand CLA 3 302



Bond lengths

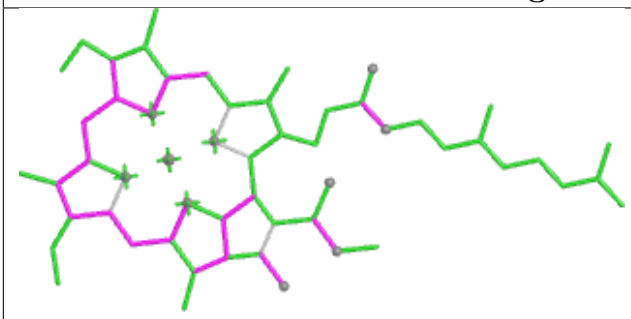
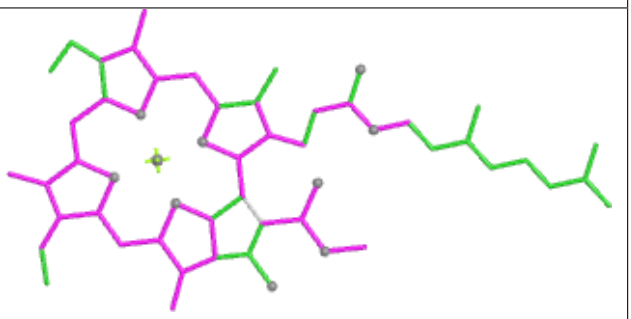
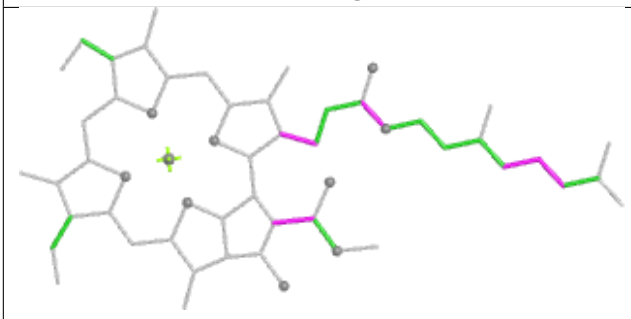
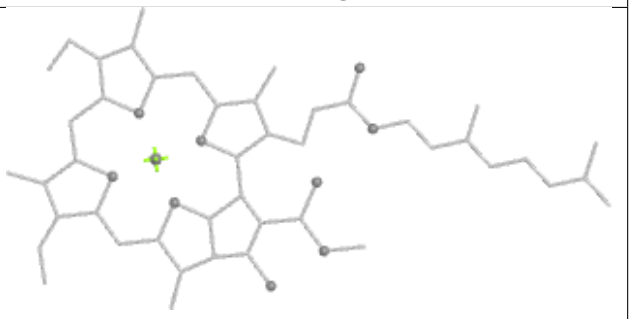


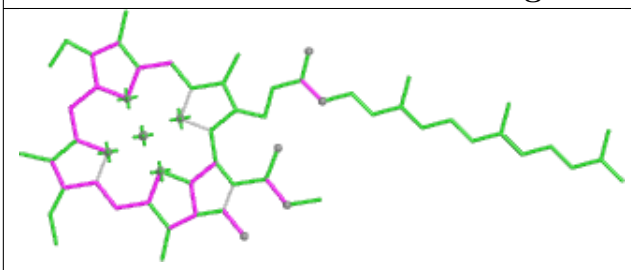
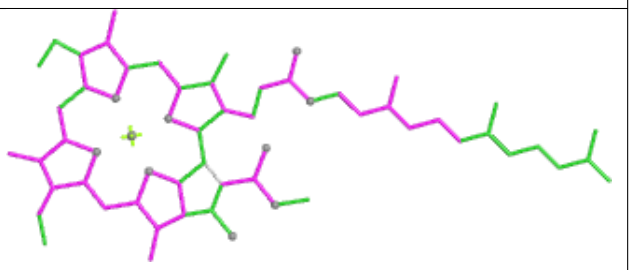
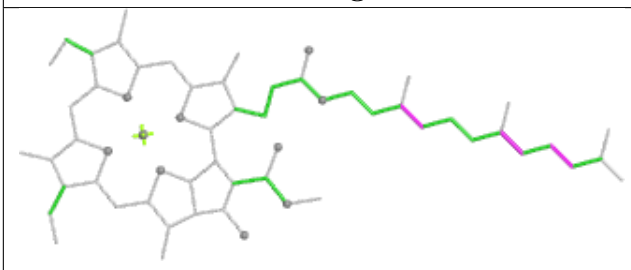
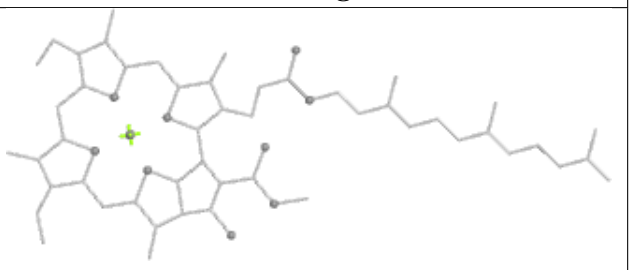
Bond angles



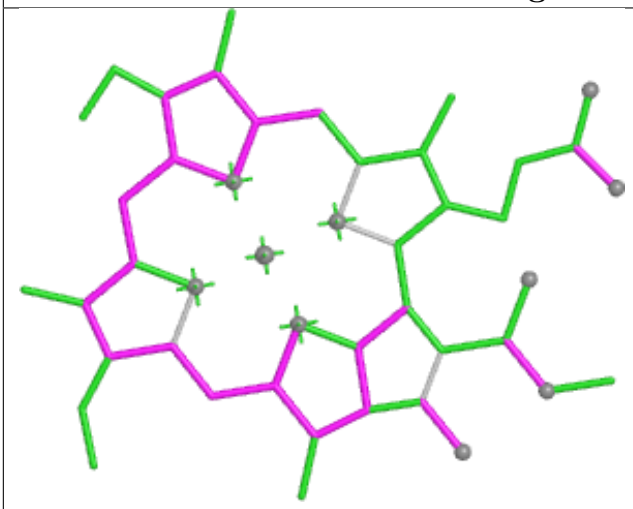
Torsions

Rings

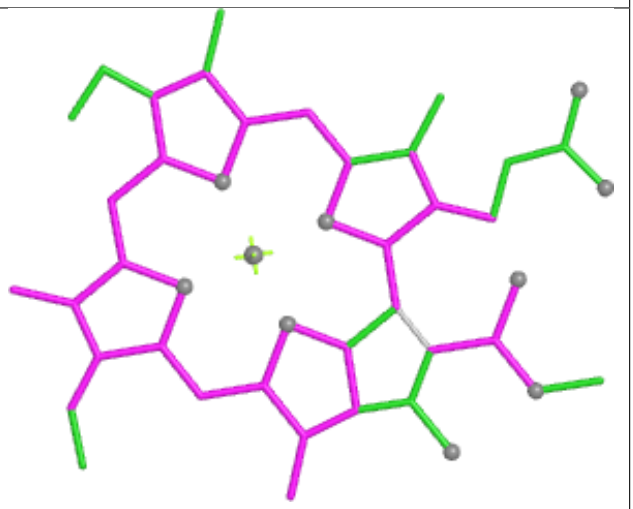
Ligand CLA 7 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

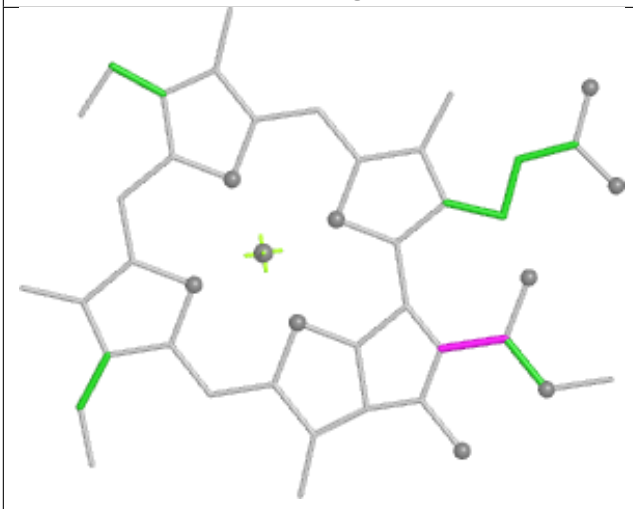
Ligand CLA 2 307



Bond lengths



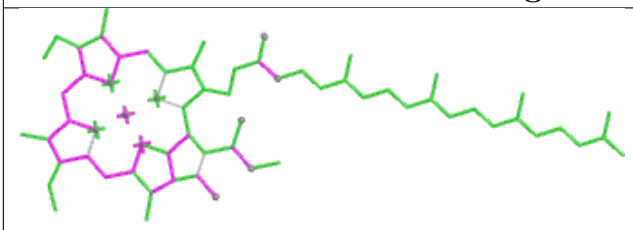
Bond angles



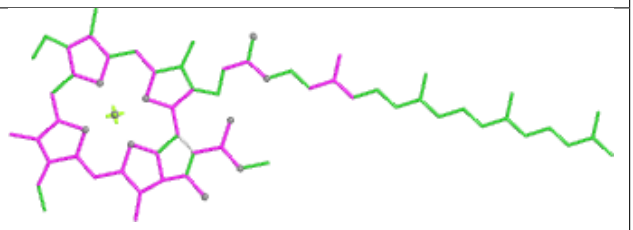
Torsions

Rings

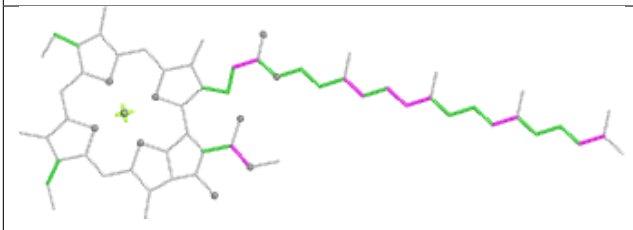
Ligand CLA B 806



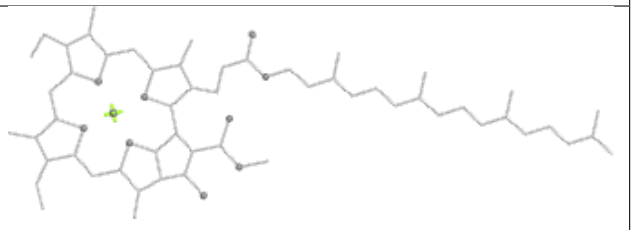
Bond lengths



Bond angles

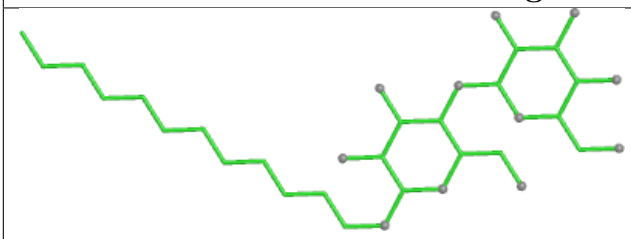


Torsions



Rings

Ligand LMT 4 319



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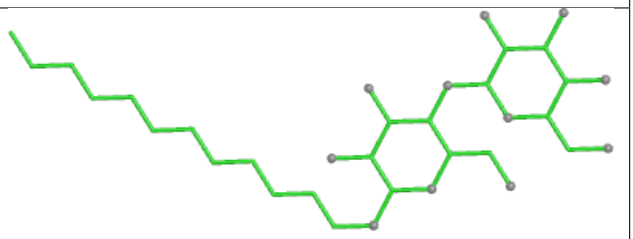
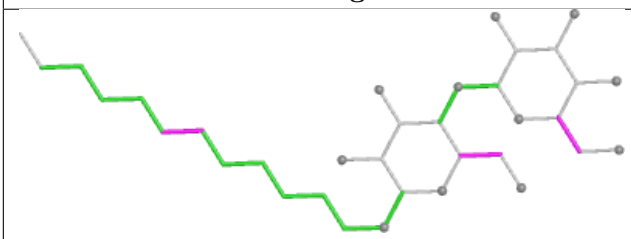


Bond angles



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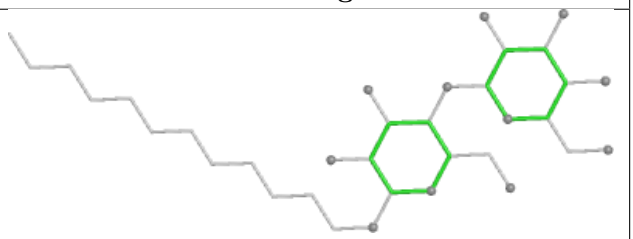
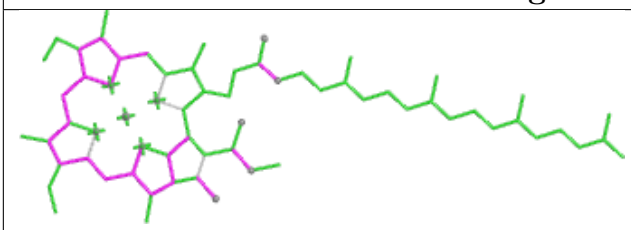


Rings

Ligand CLA 2 304



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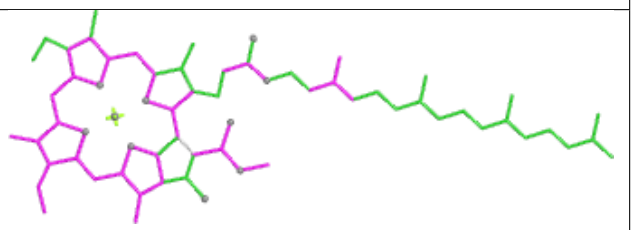
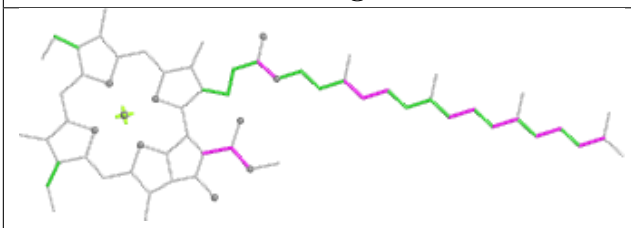


Bond angles



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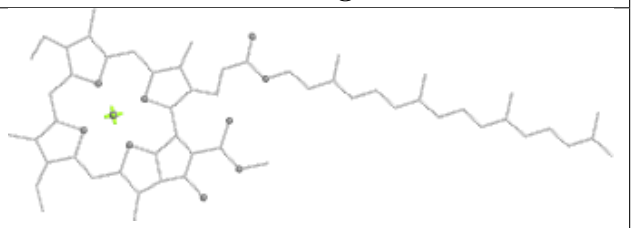
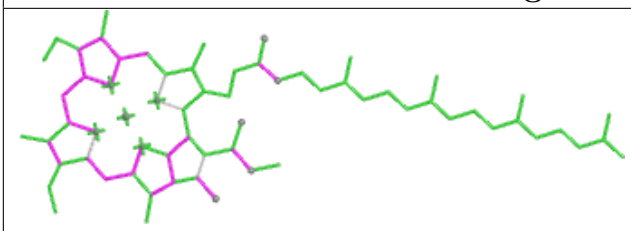


Rings

Ligand CLA B 835



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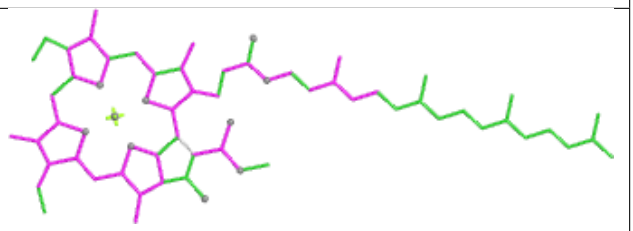
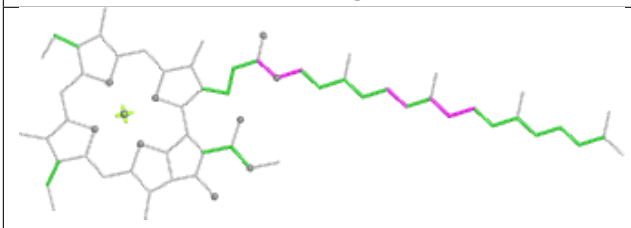


Bond angles



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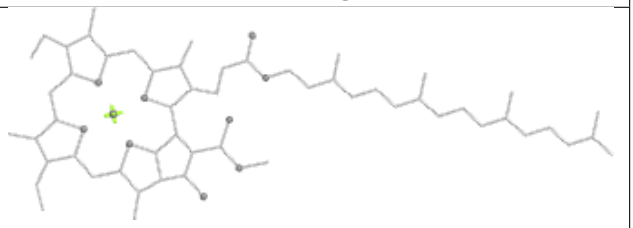
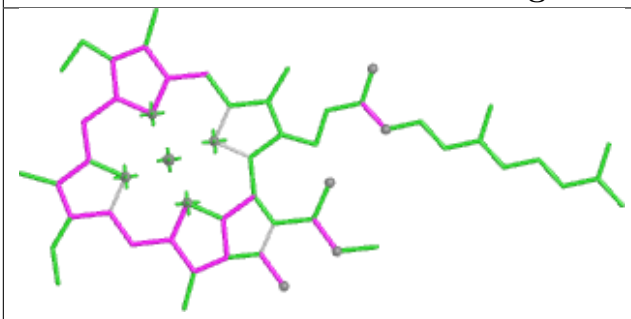


Rings

Ligand CLA 2 305



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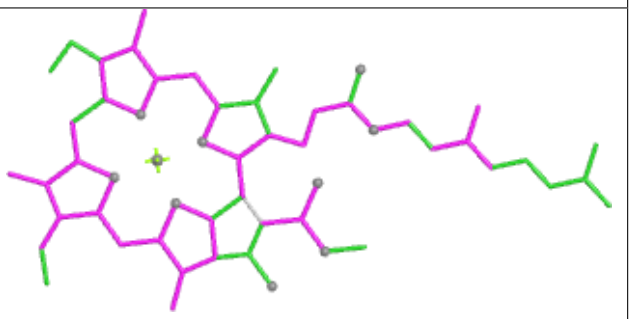
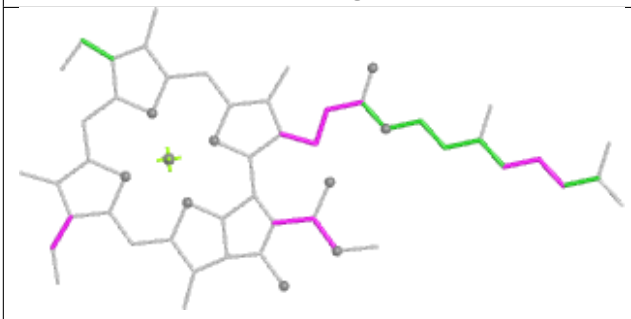
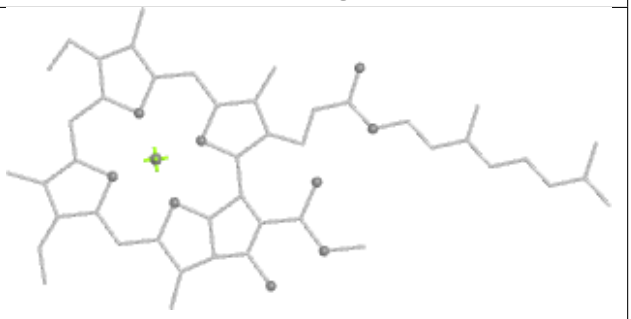


Bond angles

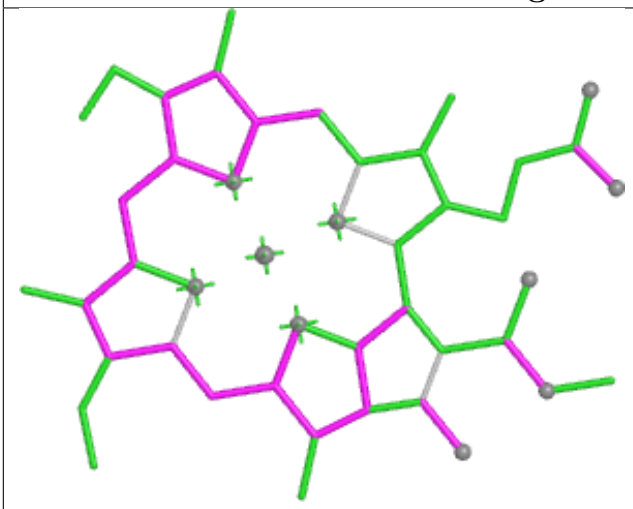


Torsions



Rings

Ligand CLA 3 303



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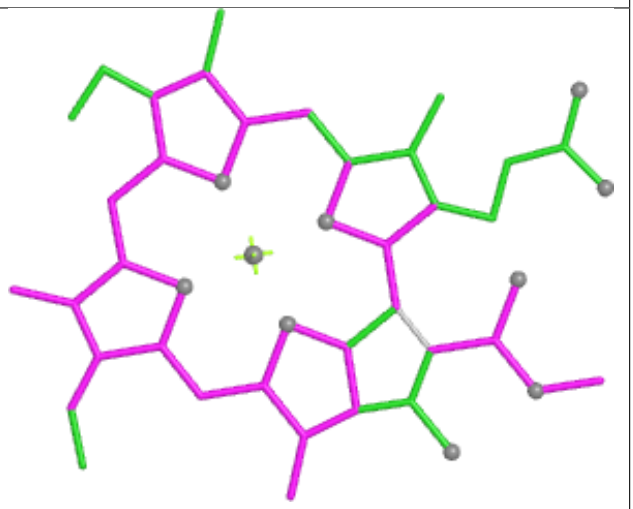
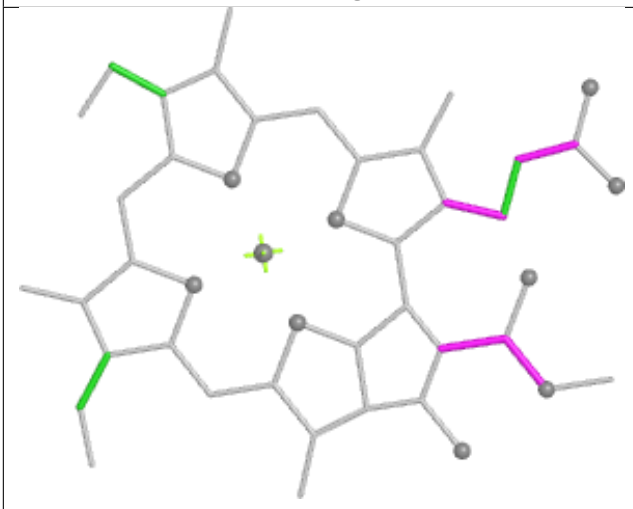


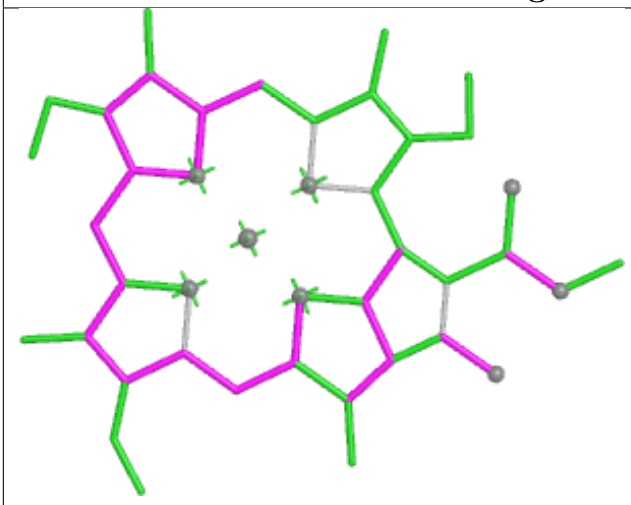
Bond angles



Torsions

Rings

Ligand CLA 1 308



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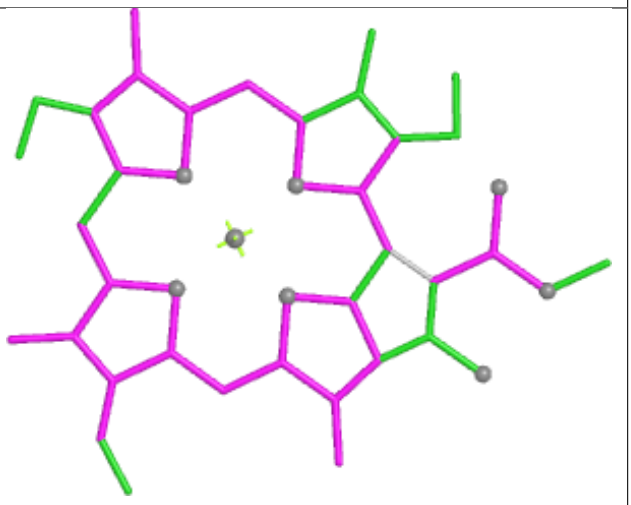
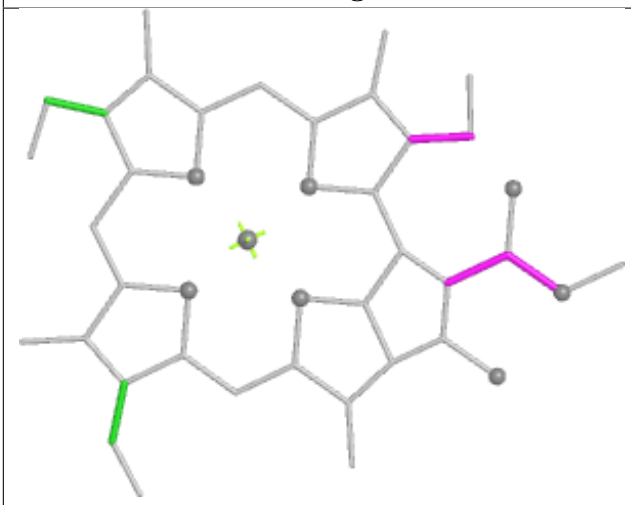


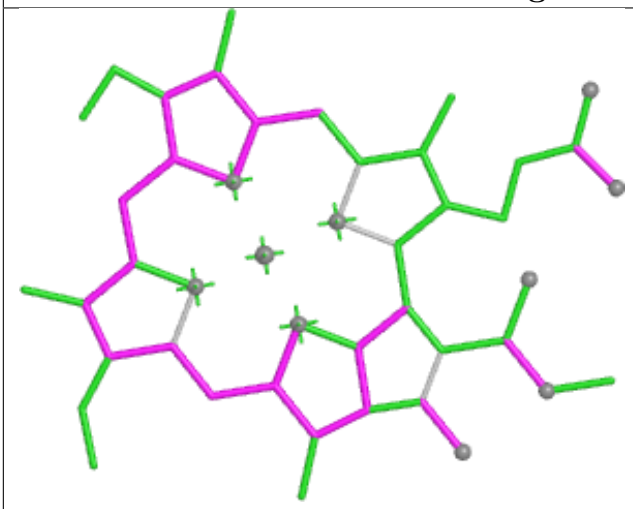
Bond angles



Torsions

Rings

Ligand CLA 7 303



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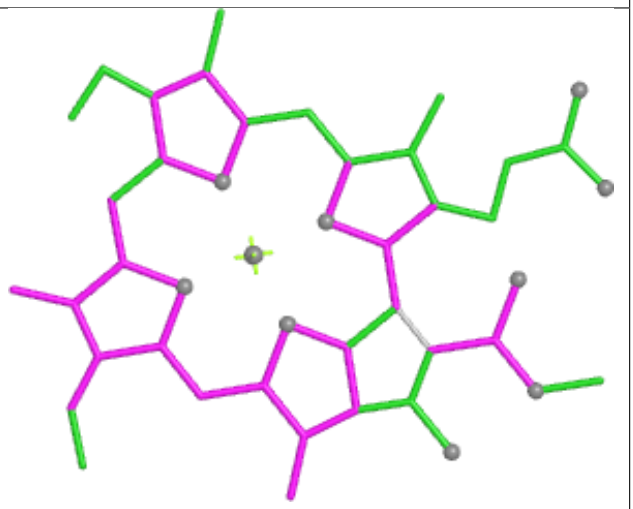

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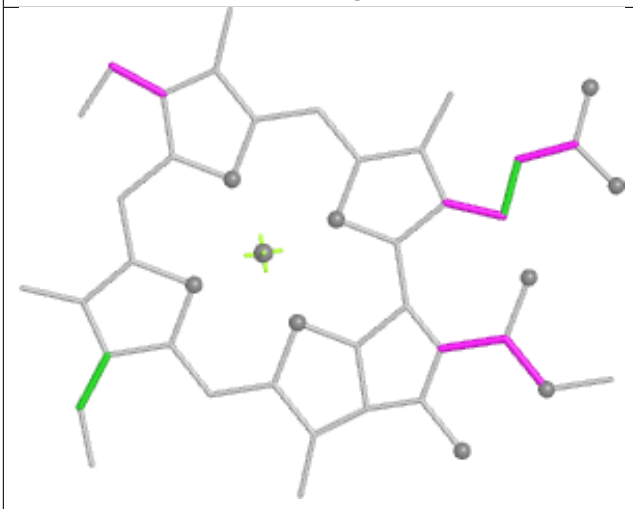
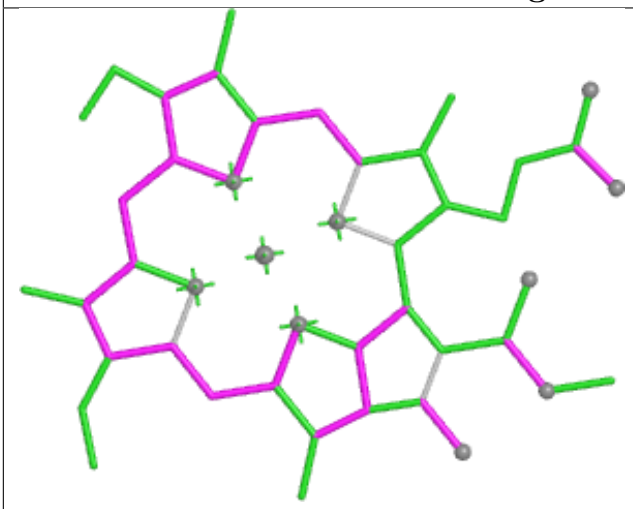


Torsions

Rings

Ligand CLA 7 308



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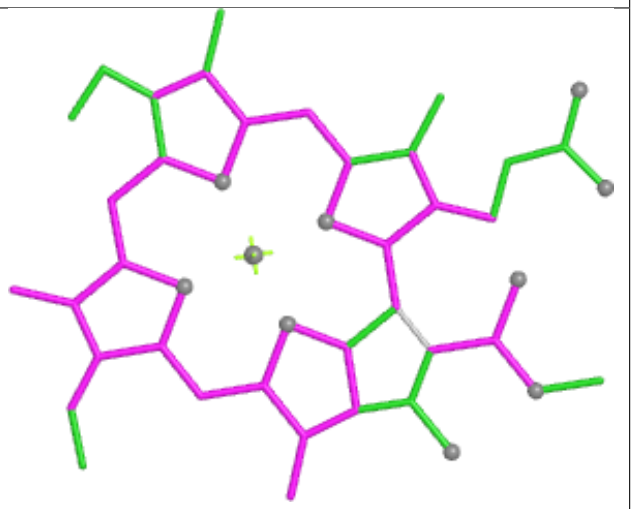
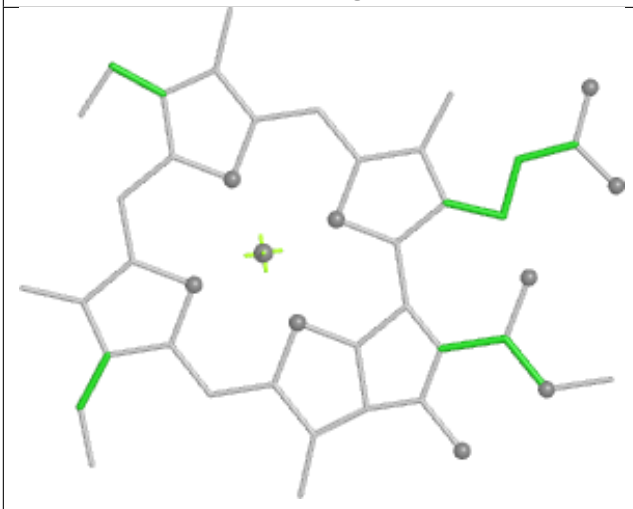


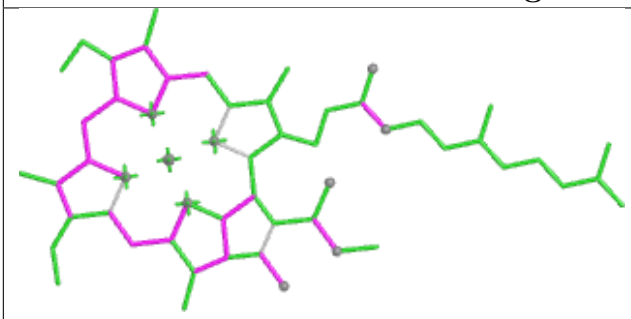
Bond angles



Torsions

Rings

Ligand CLA B 812



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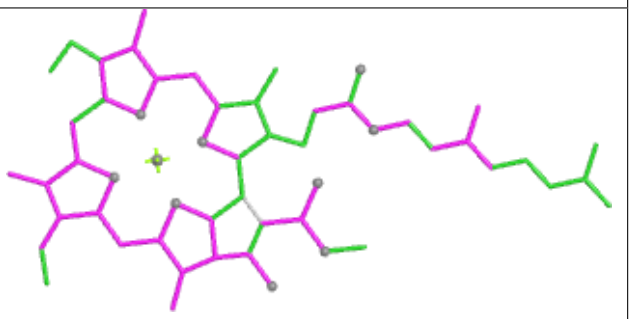
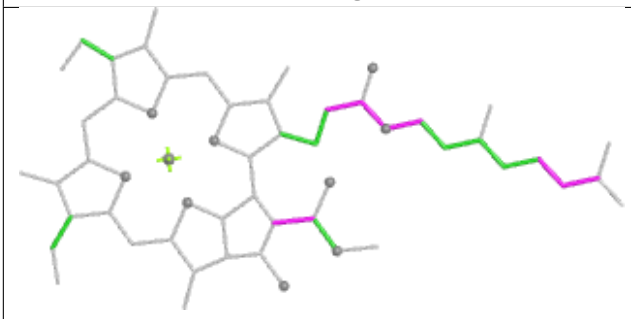
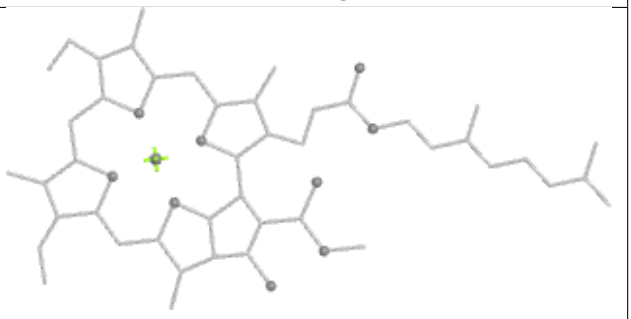


Bond angles

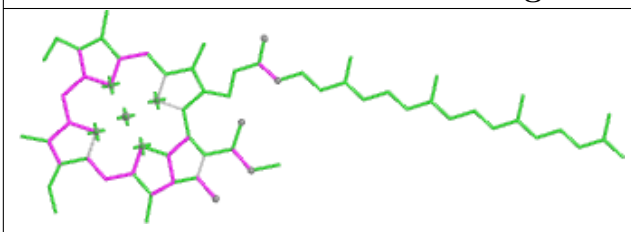


Torsions

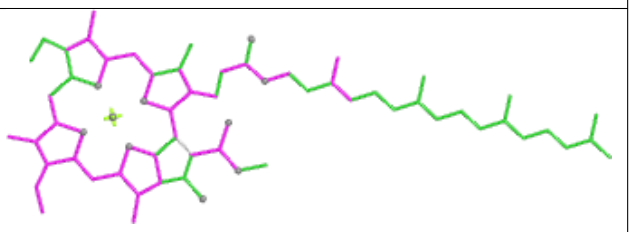


Rings

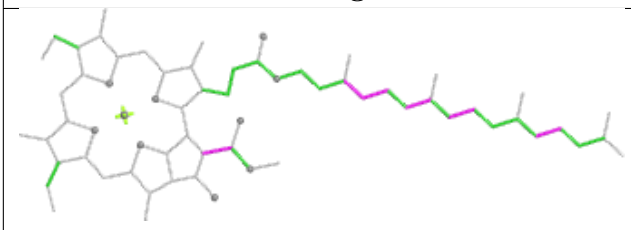
Ligand CLA B 807



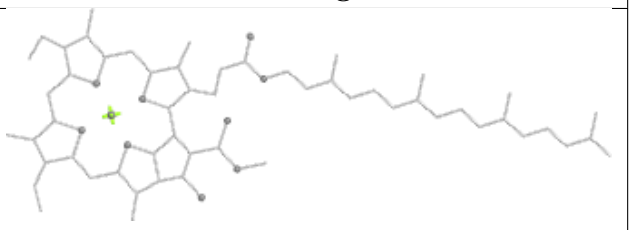
Bond lengths



Bond angles

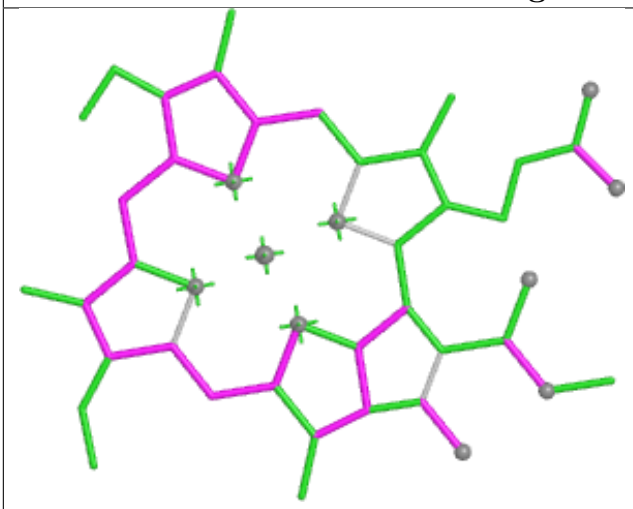


Torsions

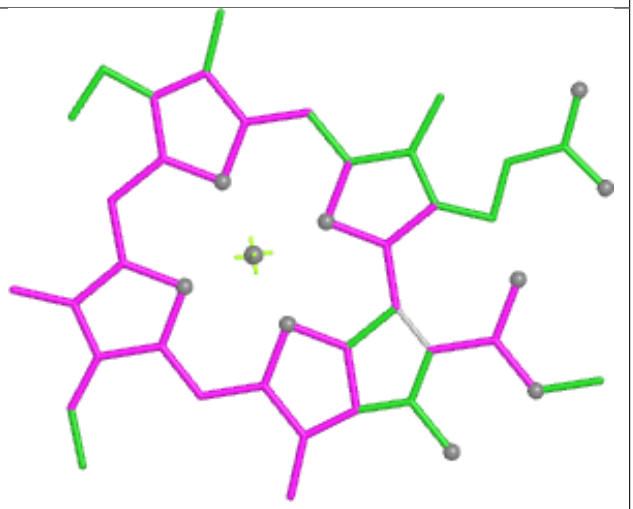


Rings

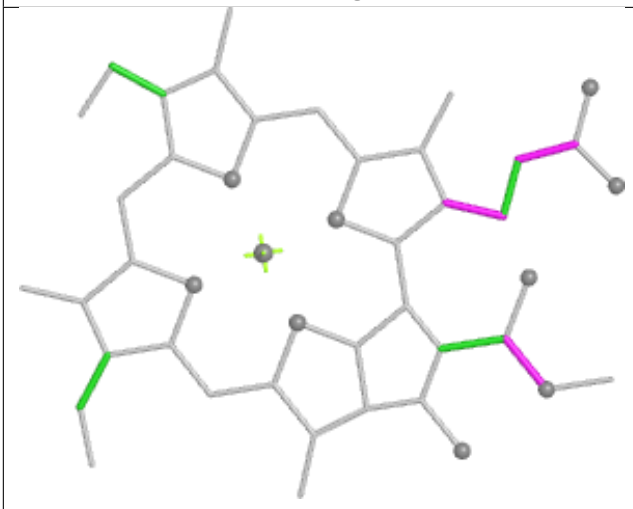
Ligand CLA 7 312



Bond lengths



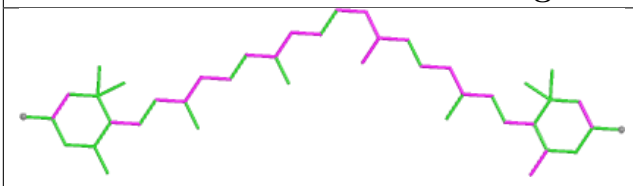
Bond angles



Torsions

Rings

Ligand 5X6 1 312



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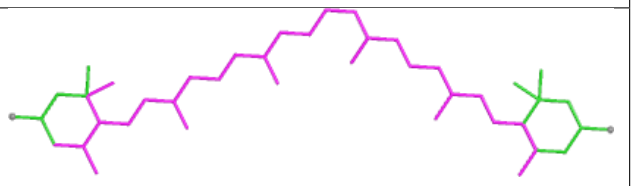
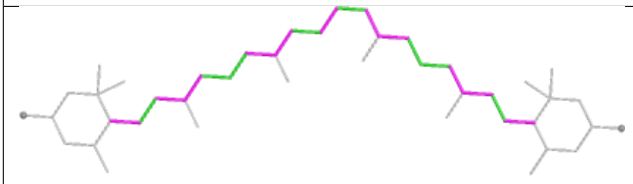
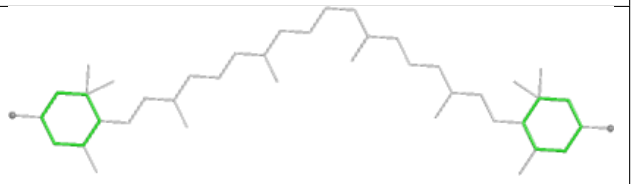


Bond angles

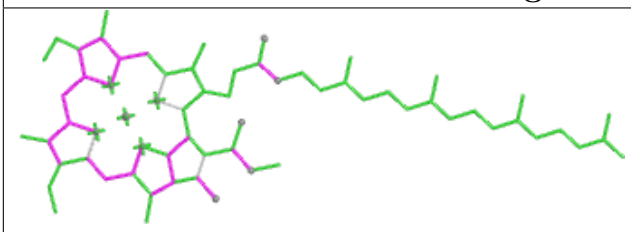


Torsions



Rings

Ligand CLA B 816



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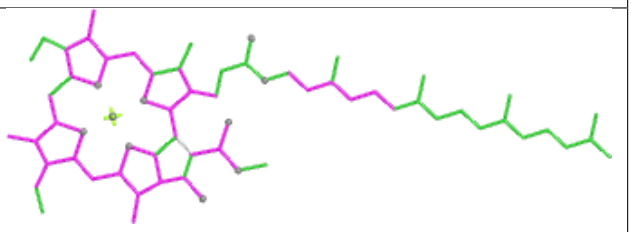

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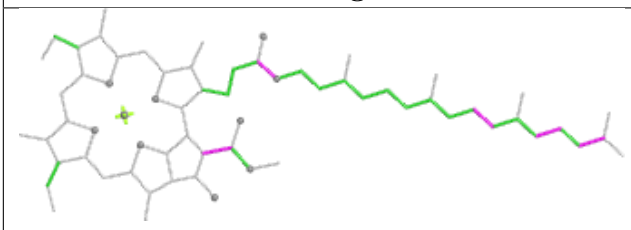

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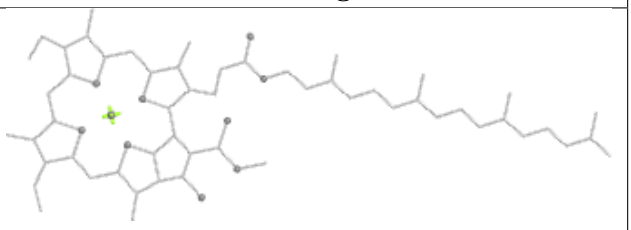
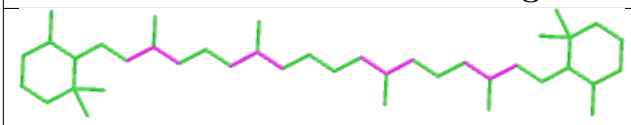


Rings

Ligand BCR A 861



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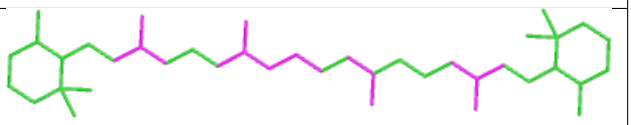
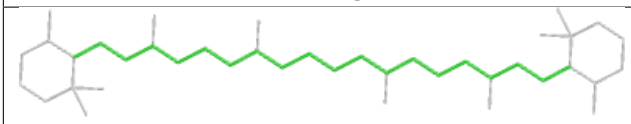


Bond angles



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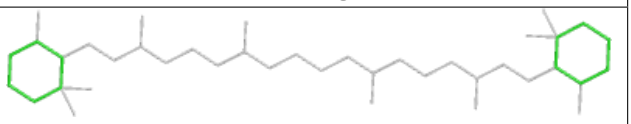
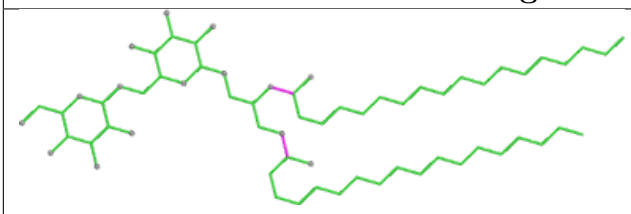
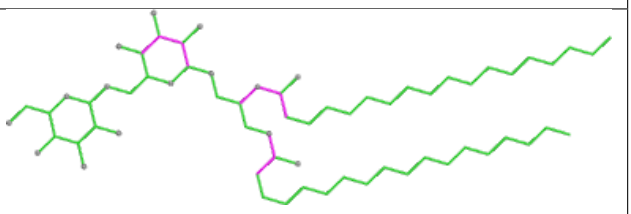


Rings

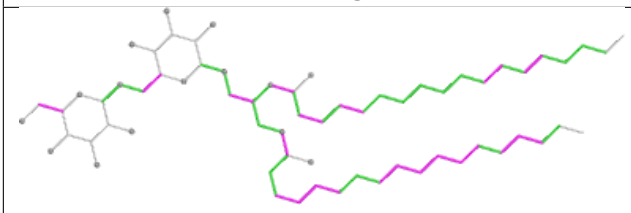
Ligand DGD B 845



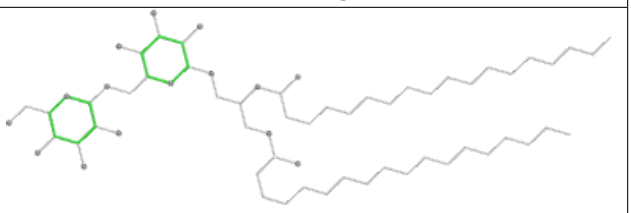
Bond lengths



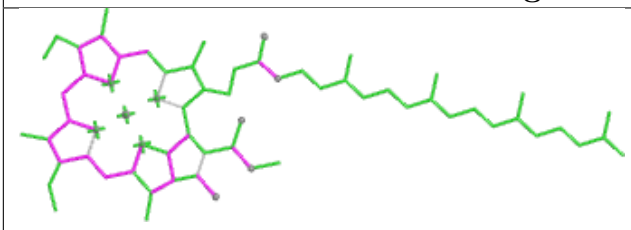
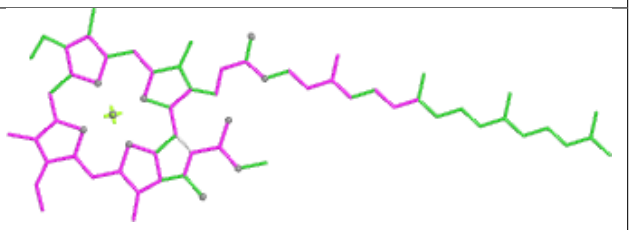
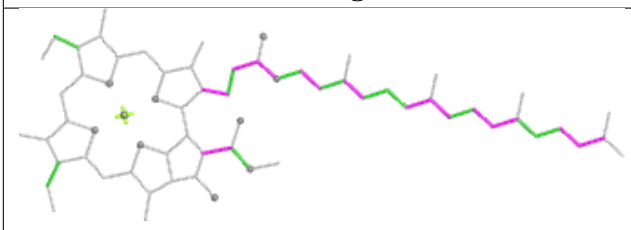
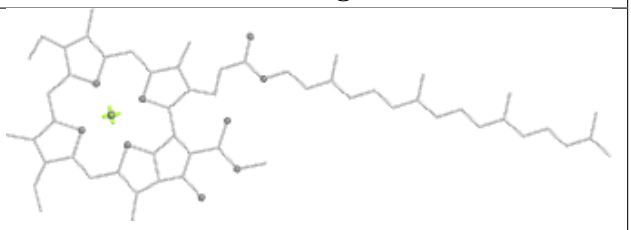
Bond angles



Torsions



Rings

Ligand CLA A 859	
	
Bond lengths	Bond angles
	
Torsions	Rings

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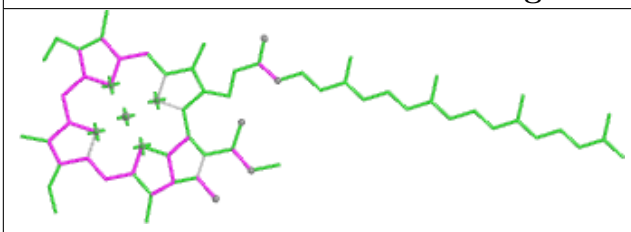
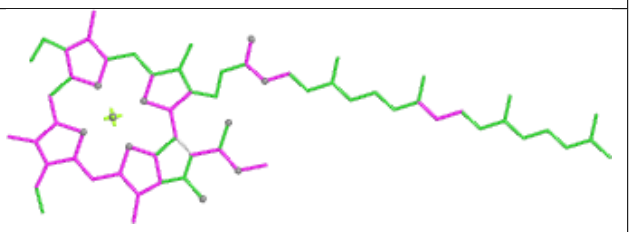
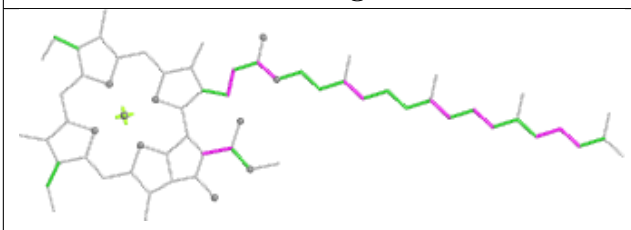
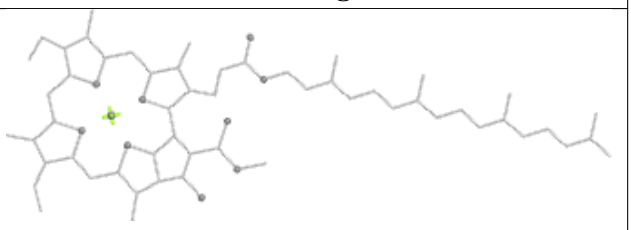
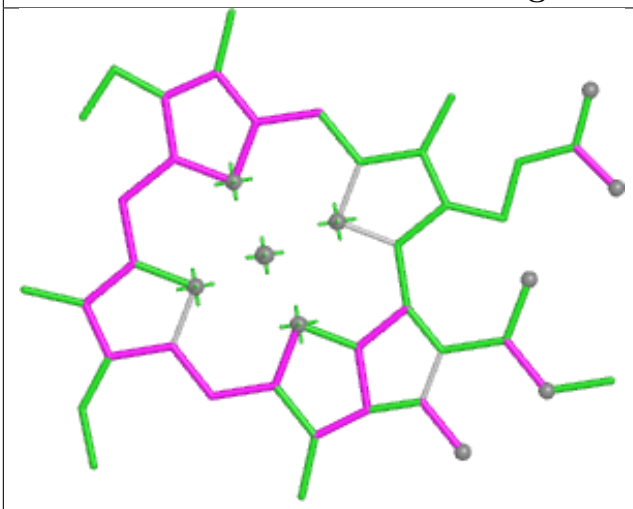
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 305



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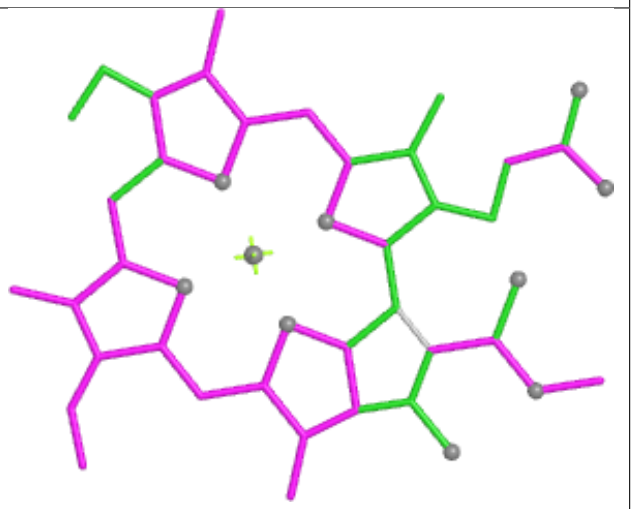
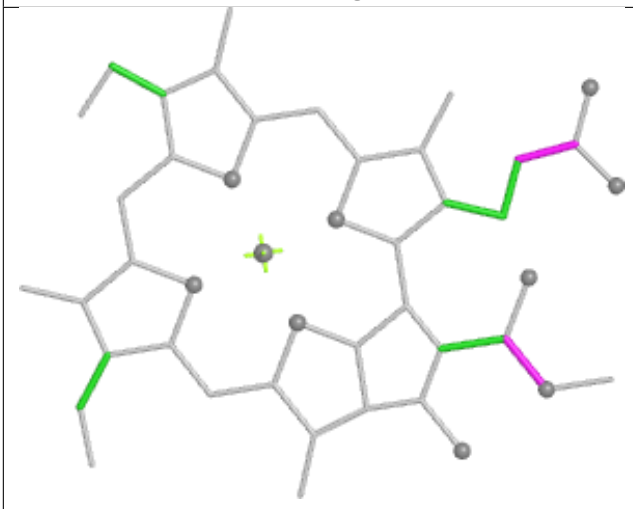


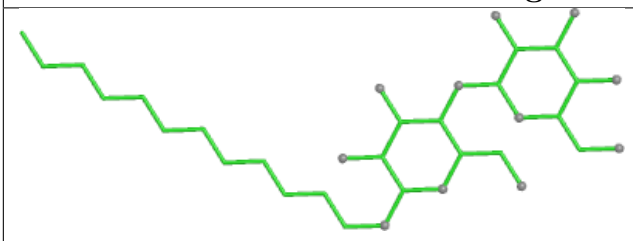
Bond angles



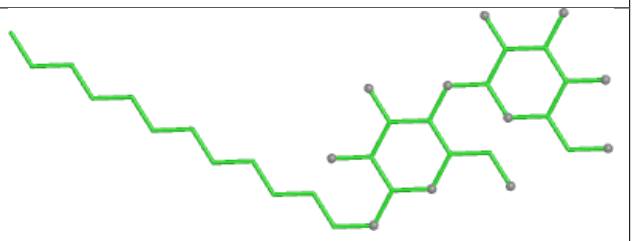
Torsions

Rings

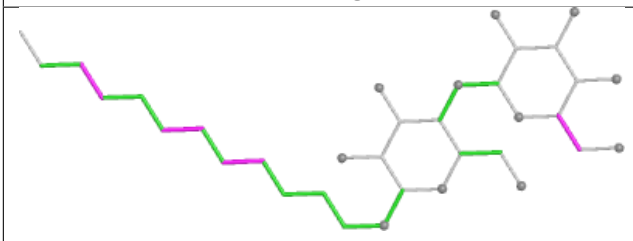
Ligand LMT 5 320



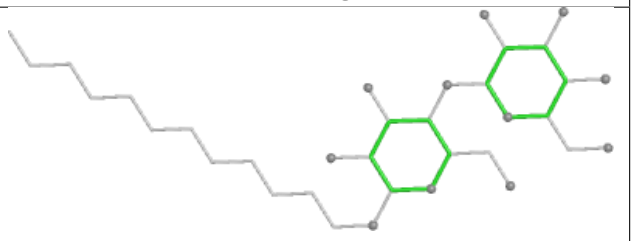
Bond lengths



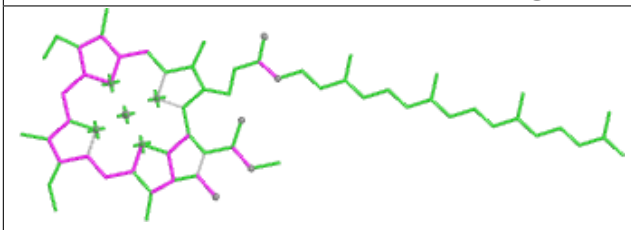
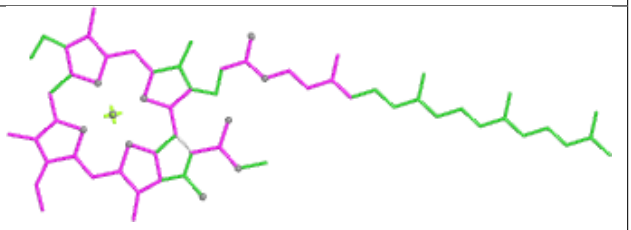
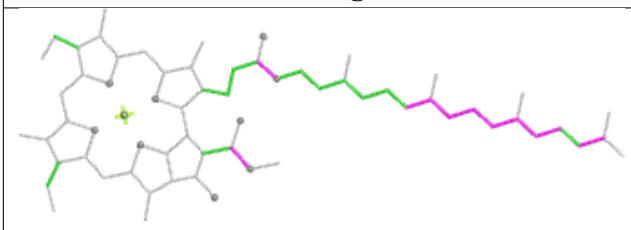
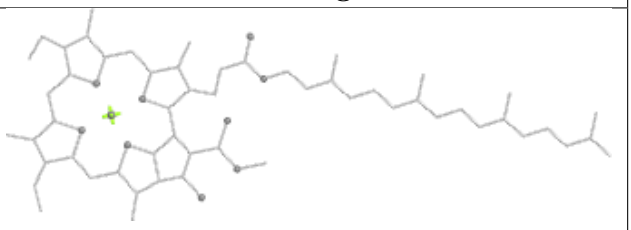
Bond angles

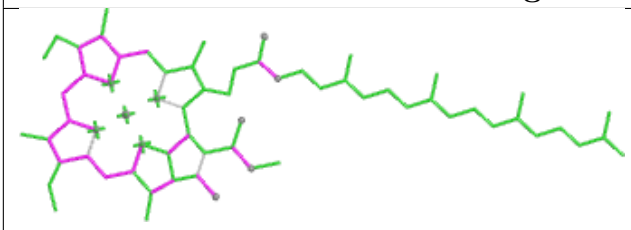
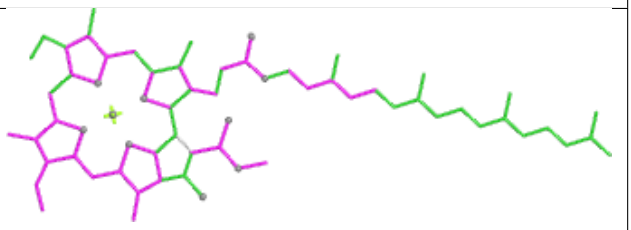
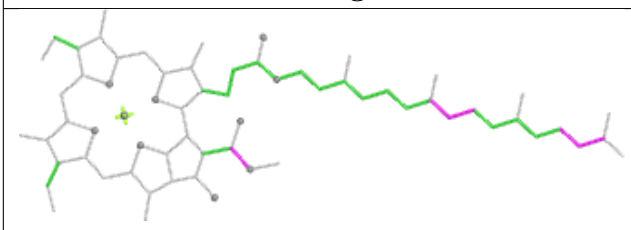
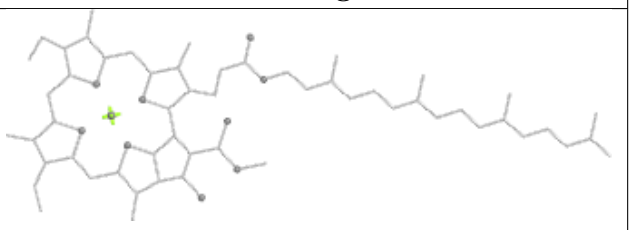


Torsions

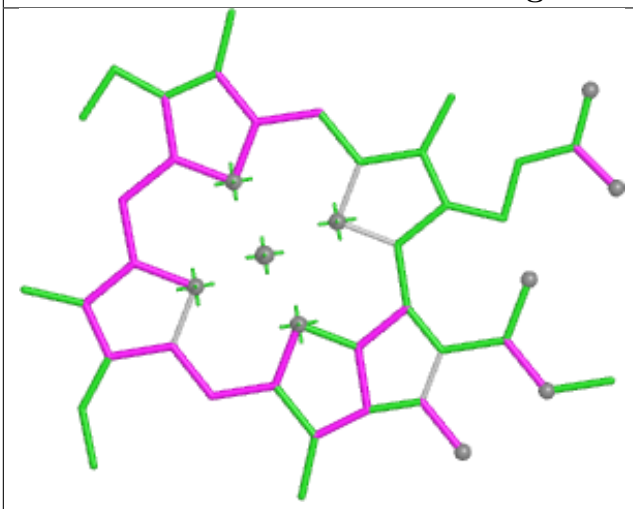


Rings

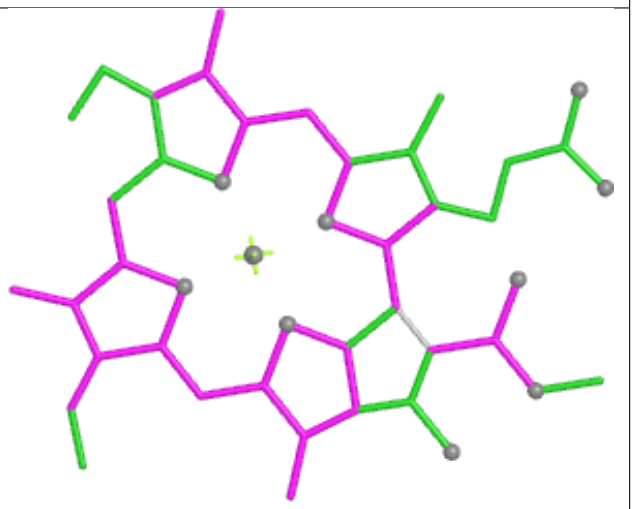
Ligand CLA 4 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

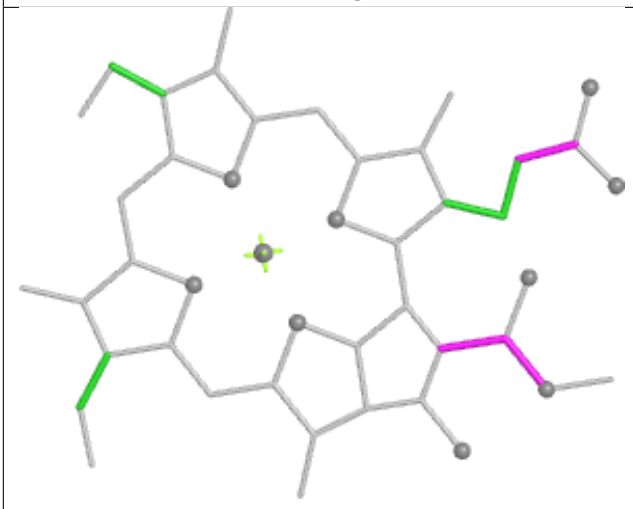
Ligand CLA L 205



Bond lengths

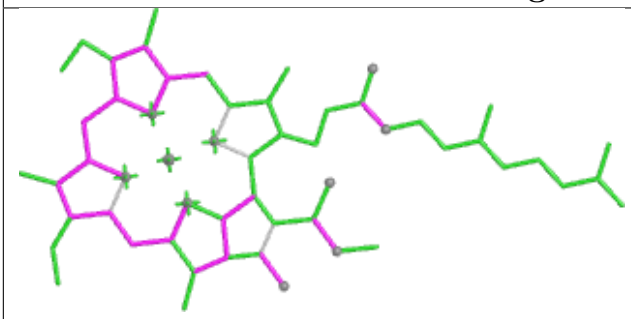
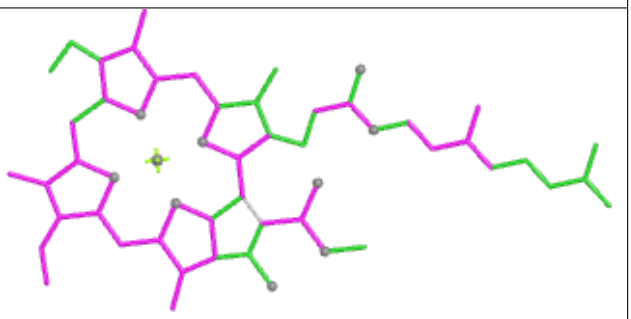
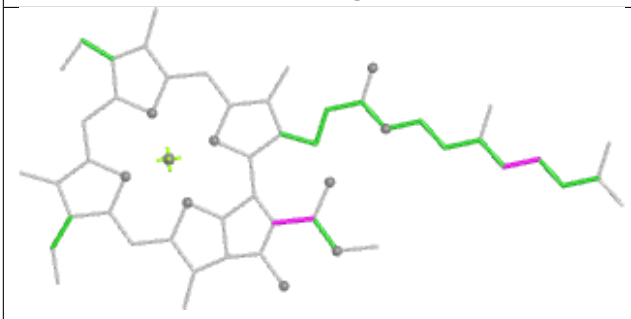
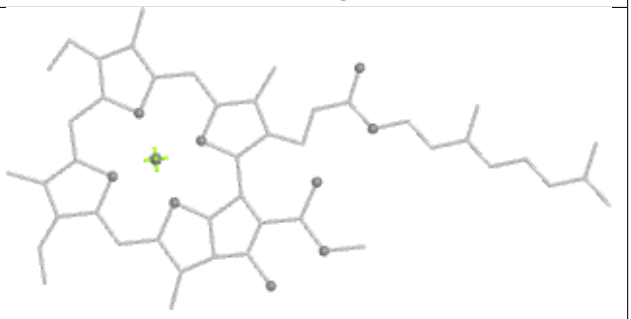


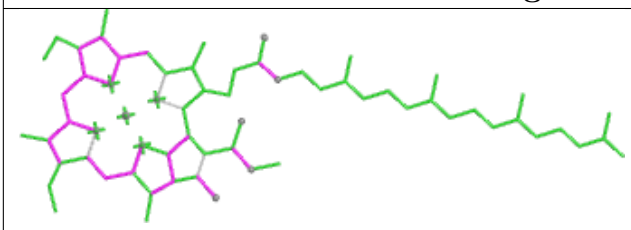
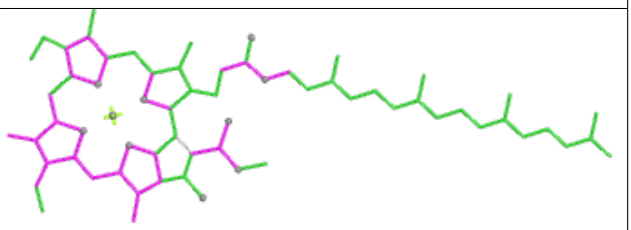
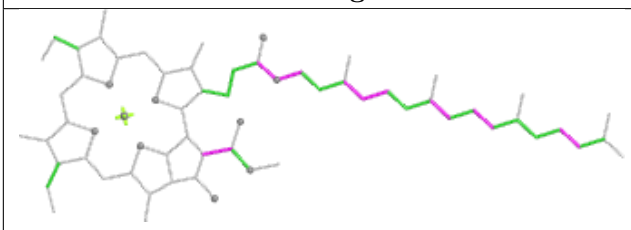
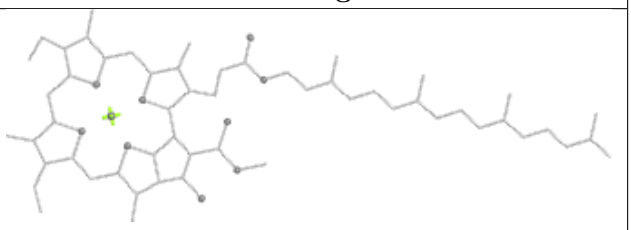
Bond angles



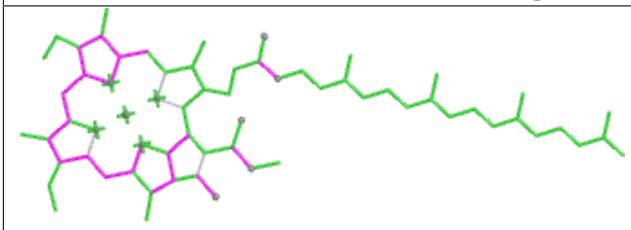
Torsions

Rings

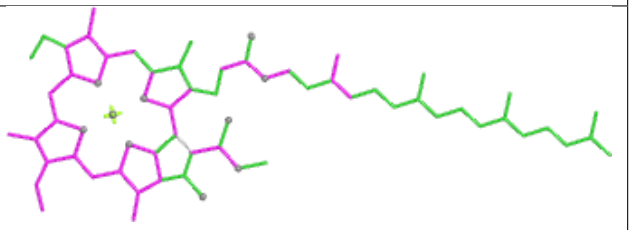
Ligand CLA 5 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

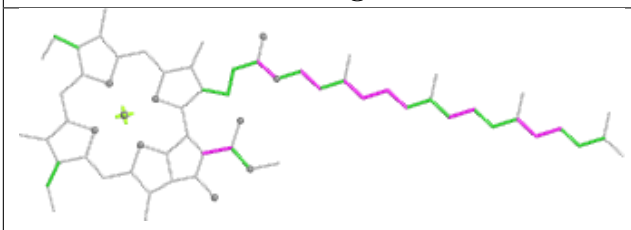
Ligand CLA 4 309



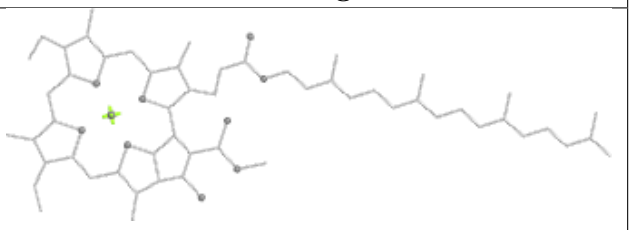
Bond lengths



Bond angles

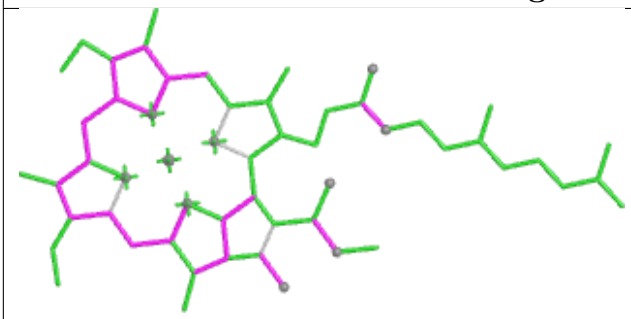


Torsions

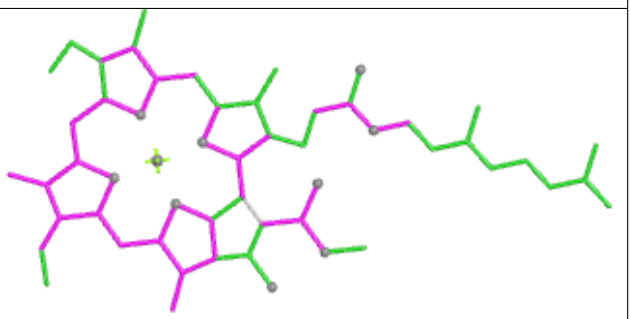


Rings

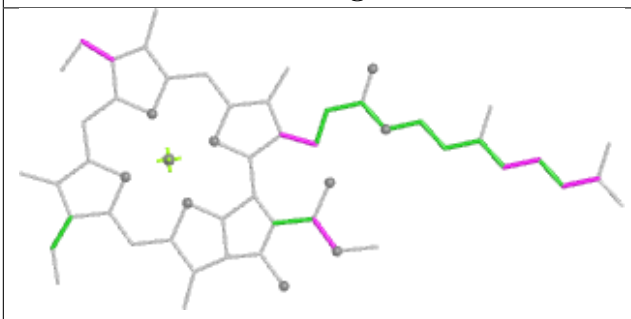
Ligand CLA 7 304



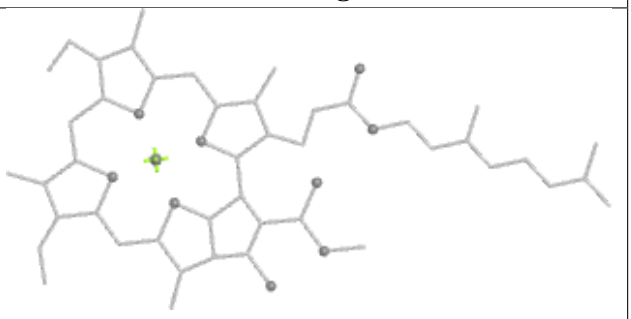
Bond lengths



Bond angles

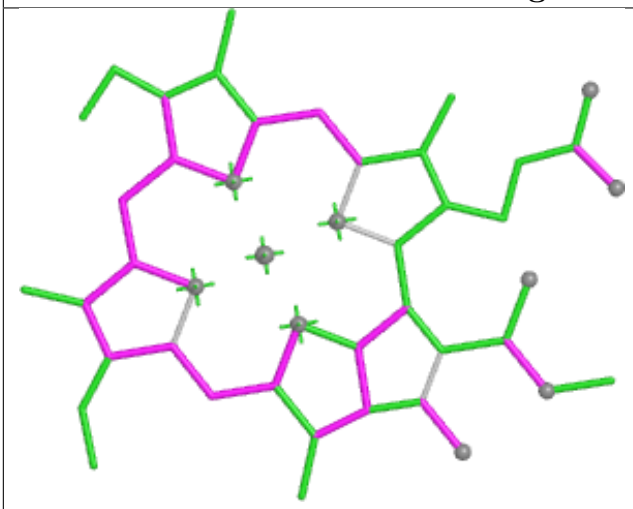


Torsions



Rings

Ligand CLA 6 309



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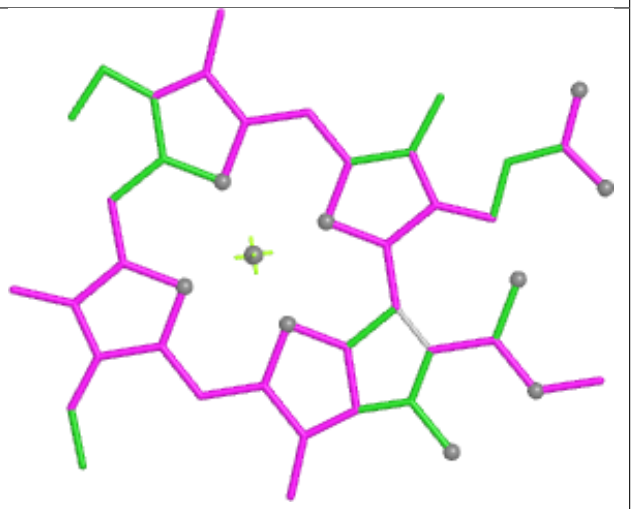
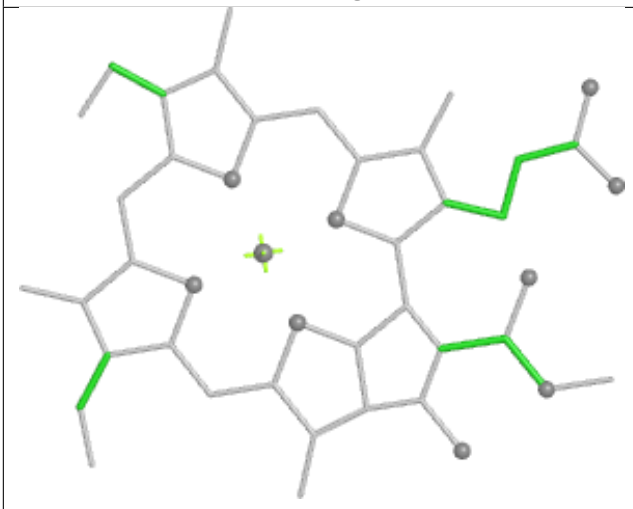


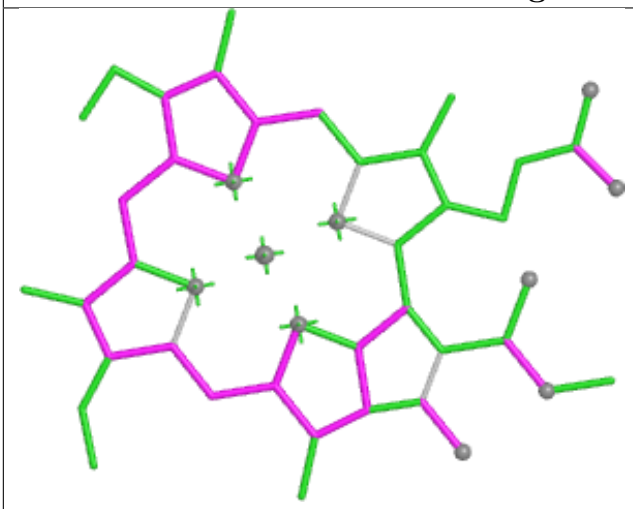
Bond angles



Torsions

Rings

Ligand CLA 1 309



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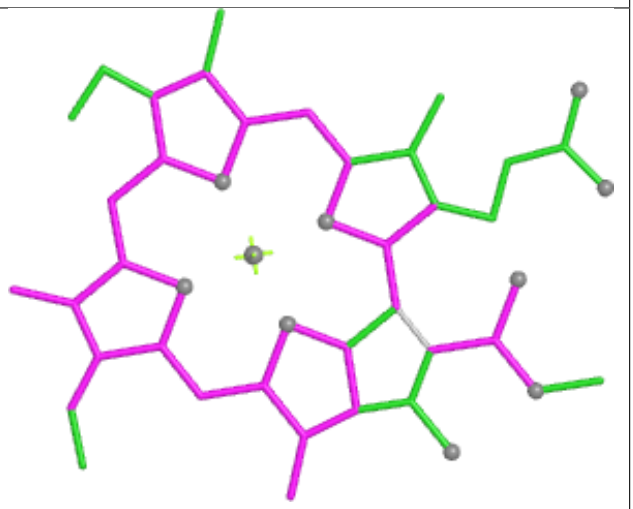
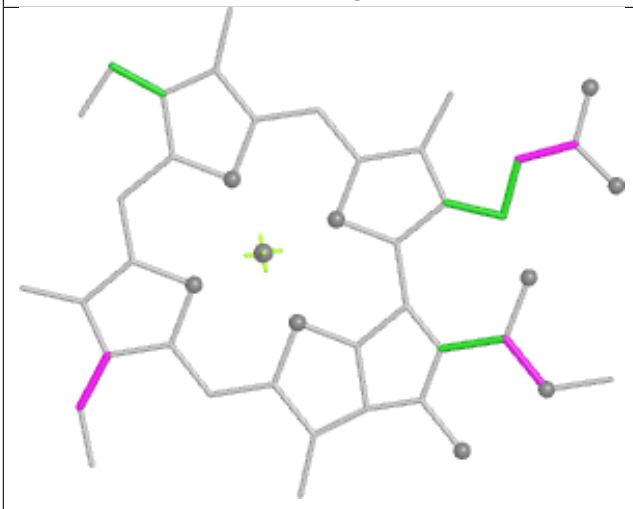


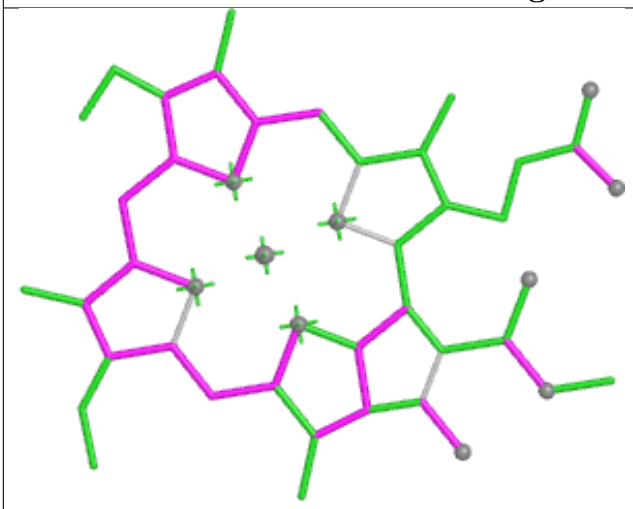
Bond angles



Torsions

Rings

Ligand CLA 5 301



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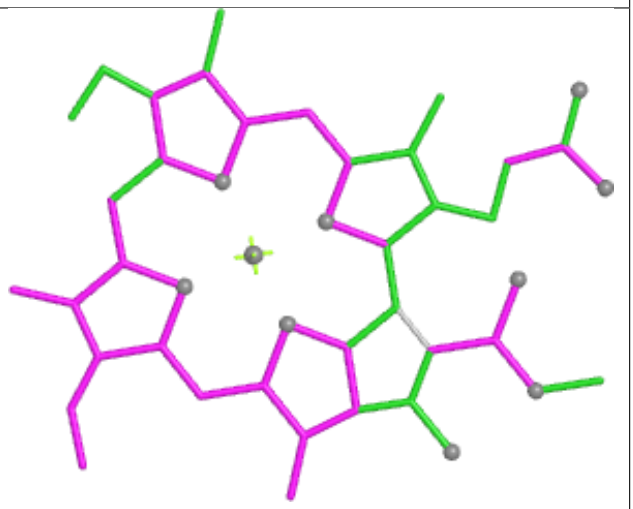
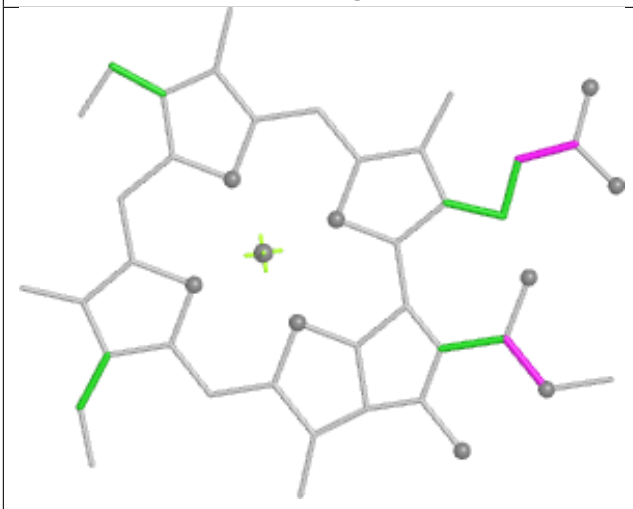


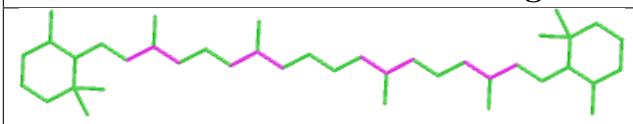
Bond angles



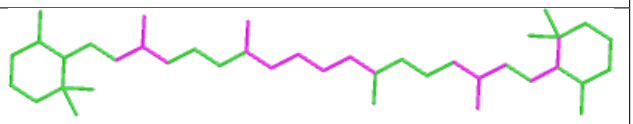
Torsions

Rings

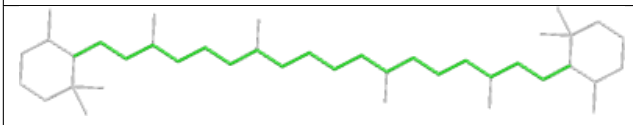
Ligand BCR L 201



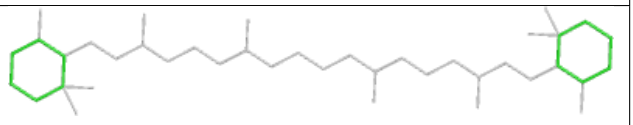
Bond lengths



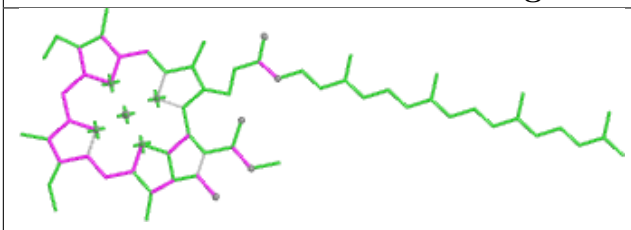
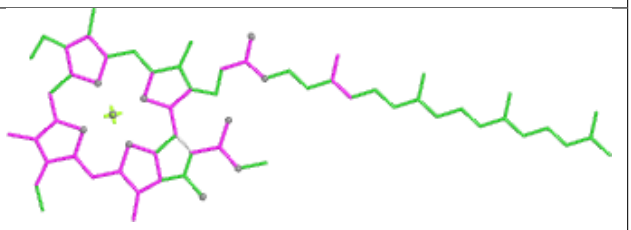
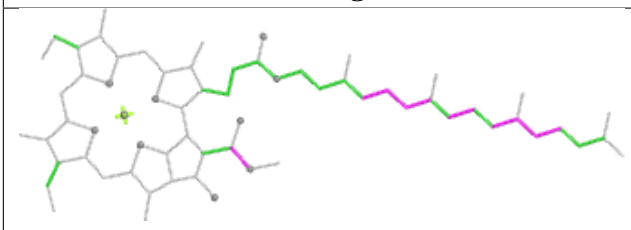
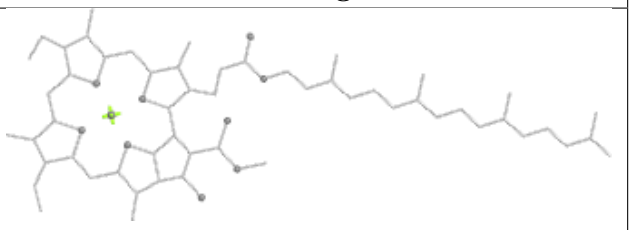
Bond angles

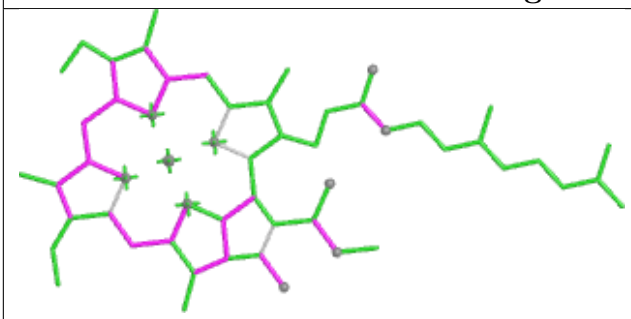
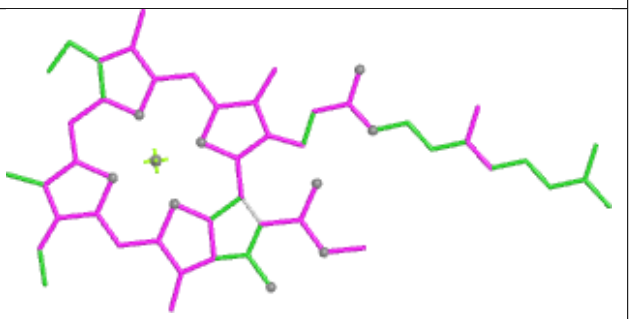
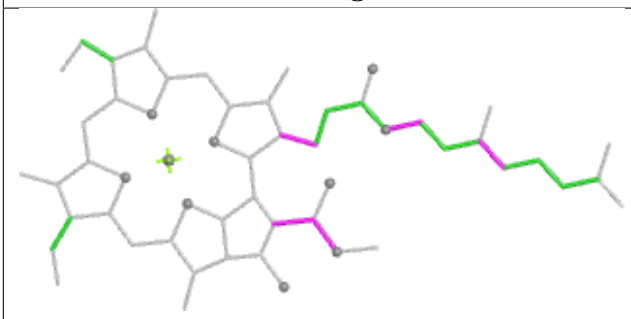
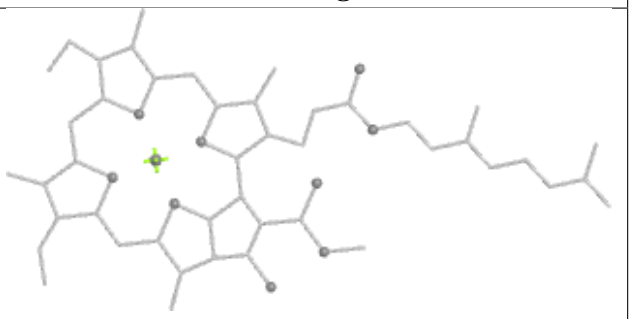


Torsions

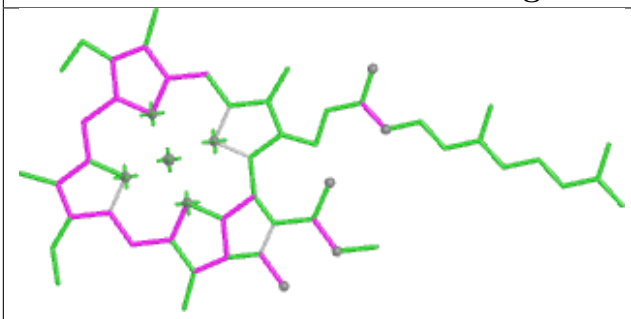


Rings

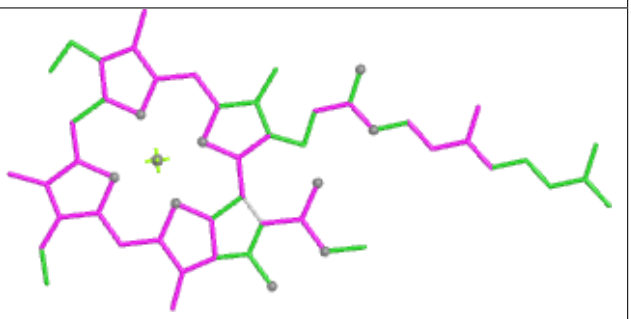
Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

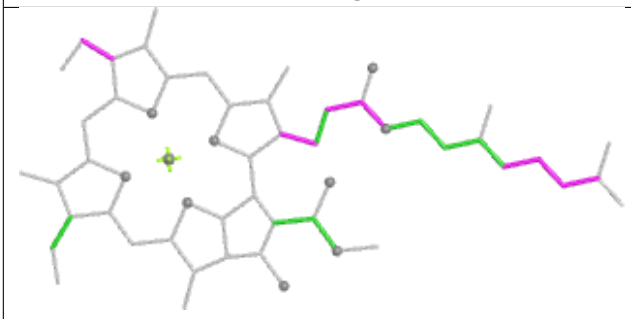
Ligand CLA K 101



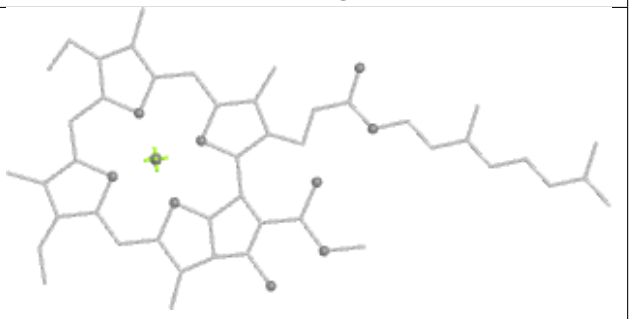
Bond lengths



Bond angles

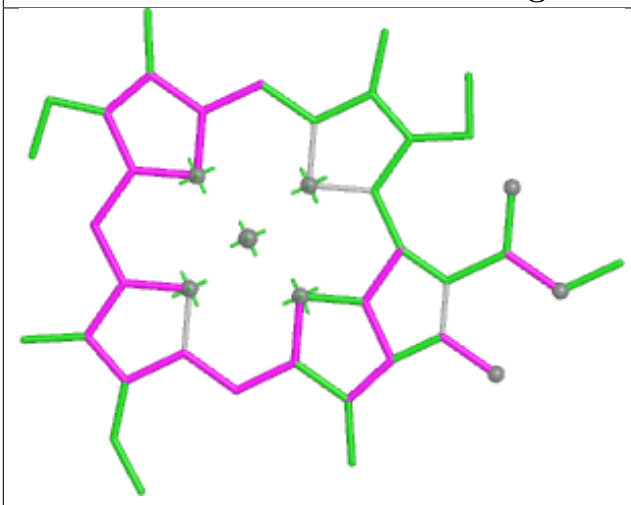


Torsions

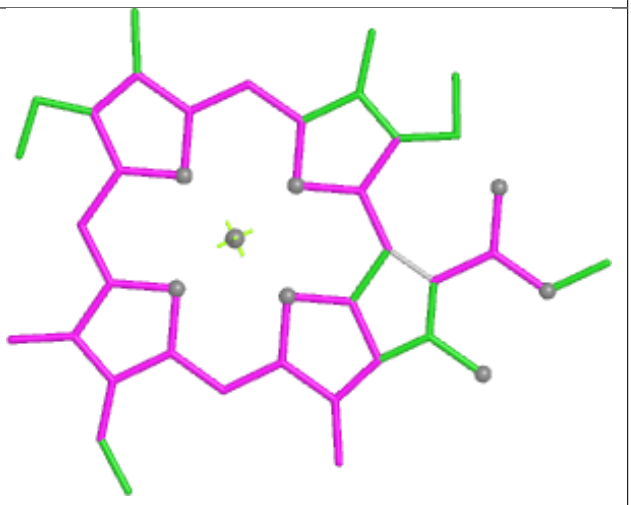


Rings

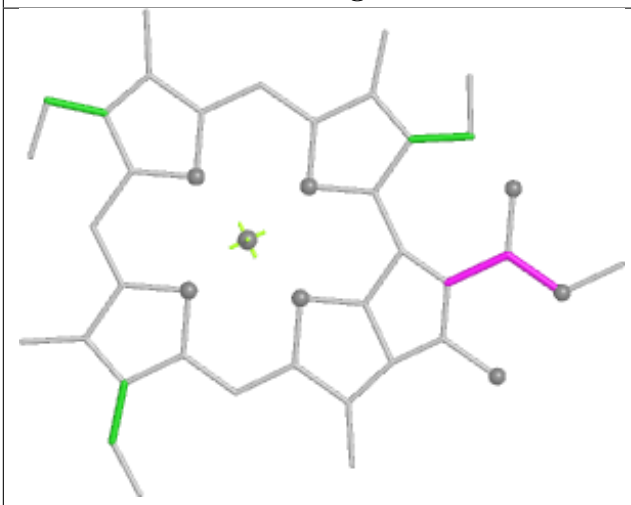
Ligand CLA 6 314



Bond lengths



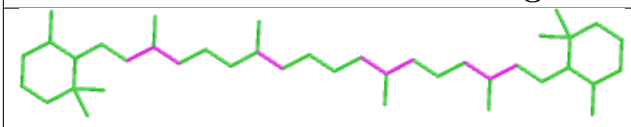
Bond angles



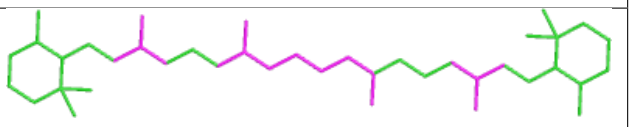
Torsions

Rings

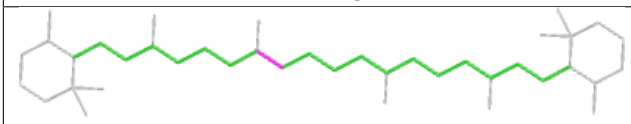
Ligand BCR F 207



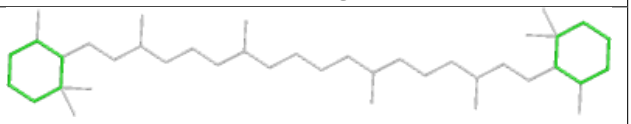
Bond lengths



Bond angles

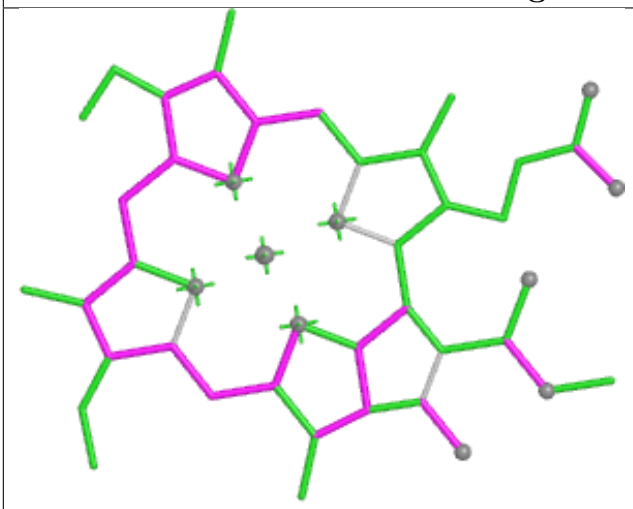


Torsions

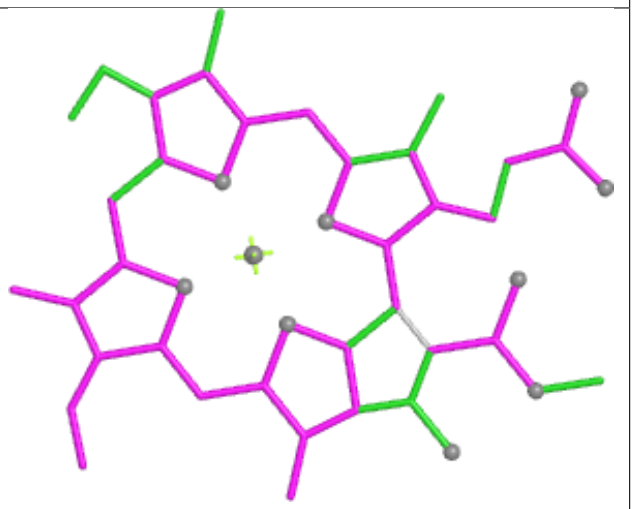


Rings

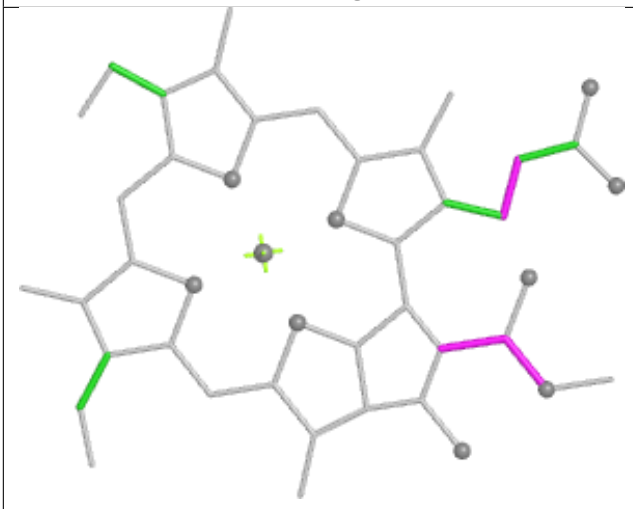
Ligand CLA 4 312



Bond lengths



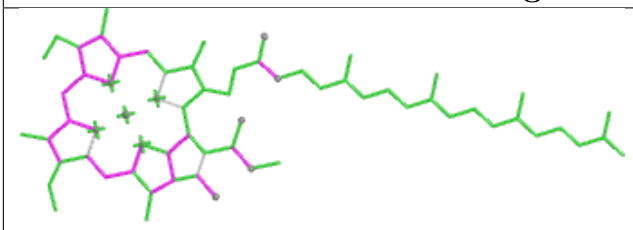
Bond angles



Torsions

Rings

Ligand CLA A 826



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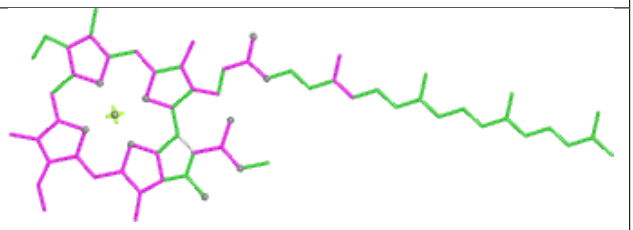
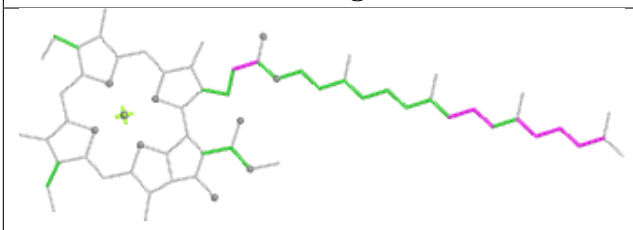
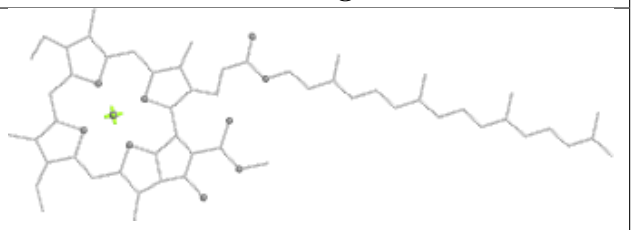


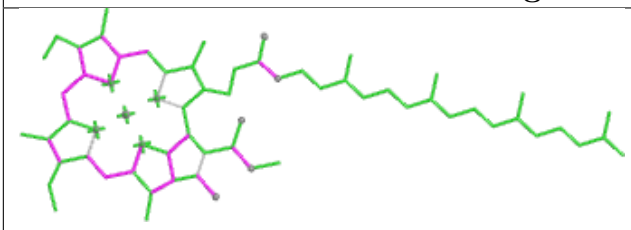
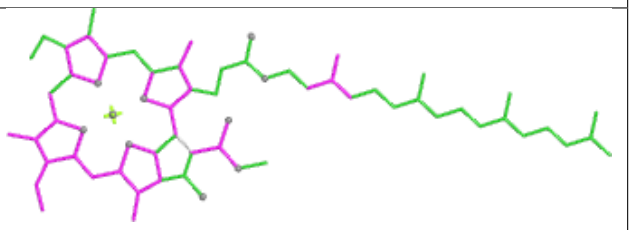
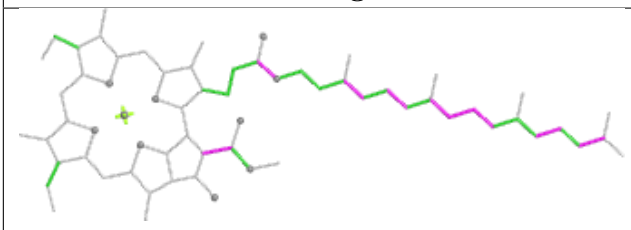
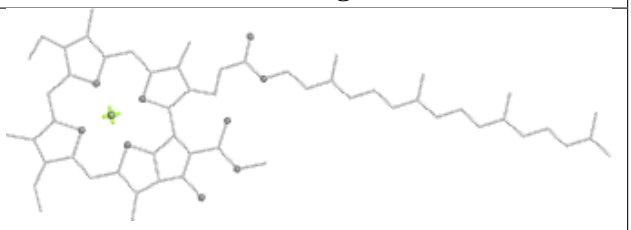
Bond angles

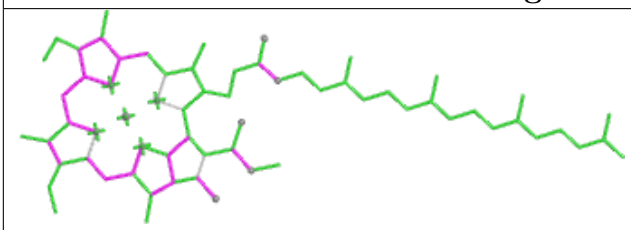
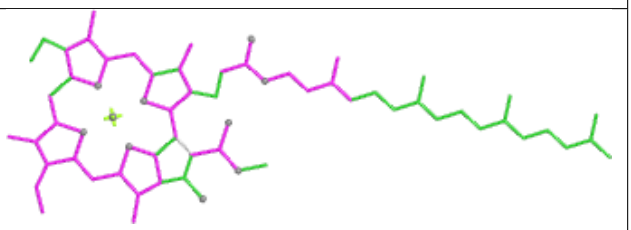
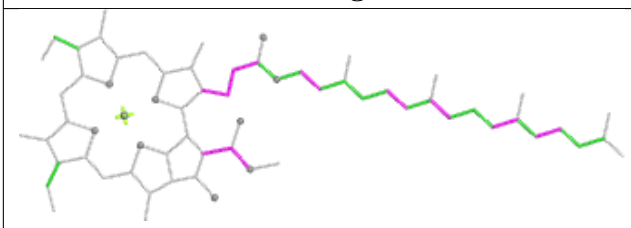
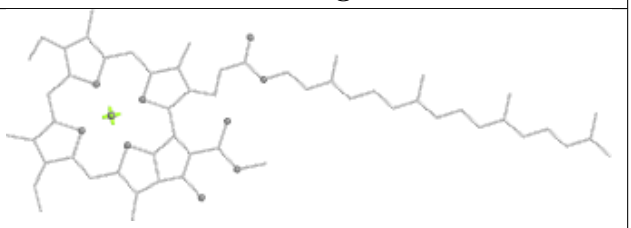


Torsions

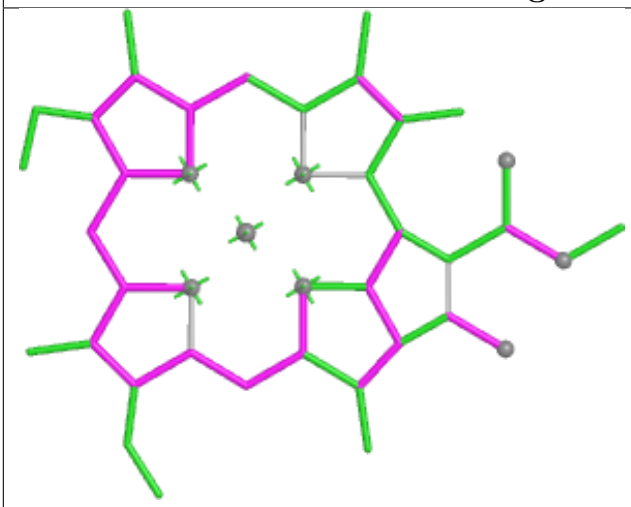


Rings

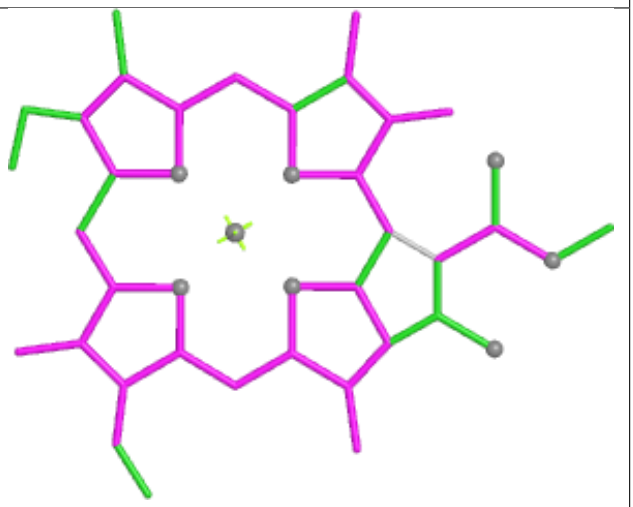
Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

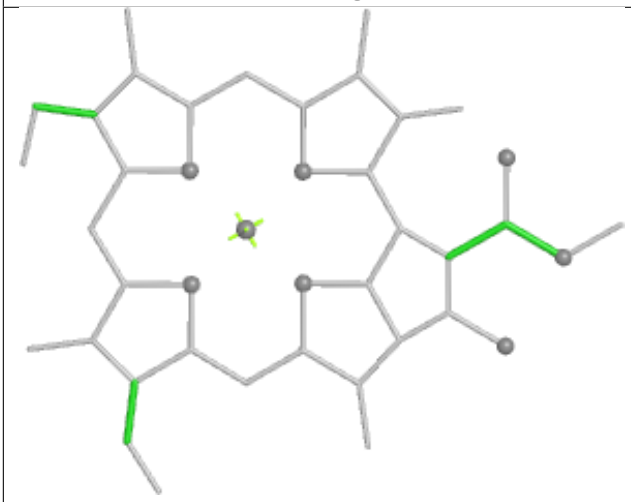
Ligand CLA 5 308



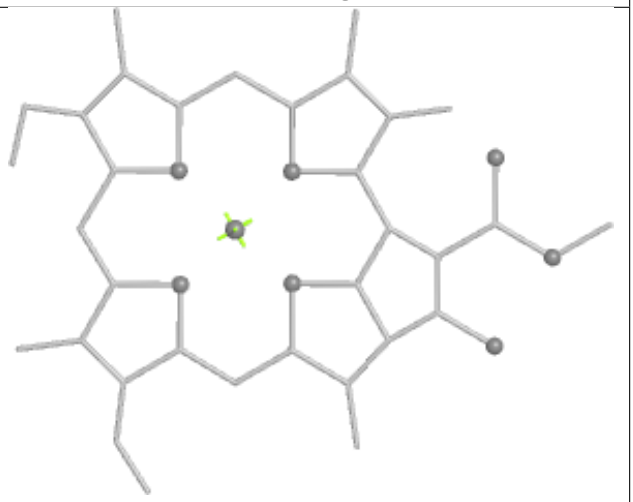
Bond lengths



Bond angles

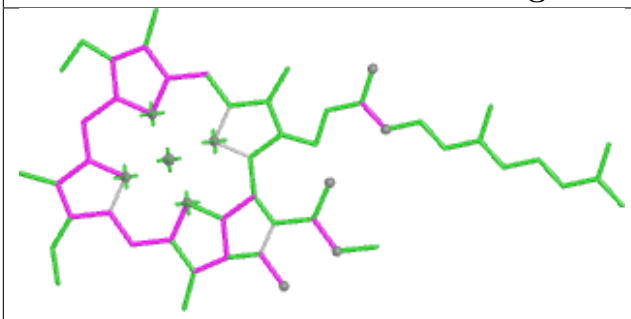


Torsions



Rings

Ligand CLA 4 305



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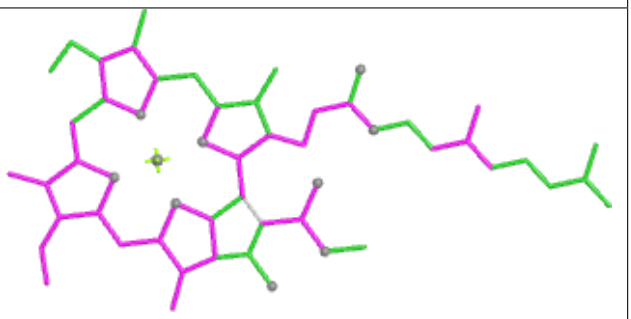
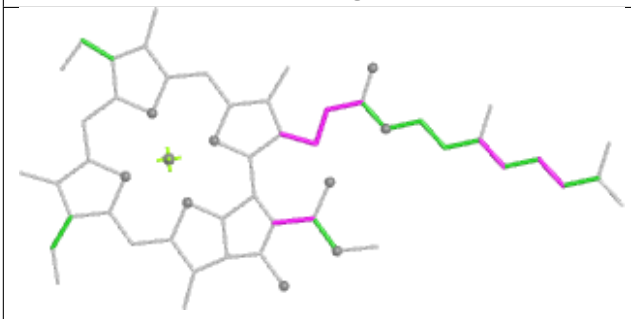
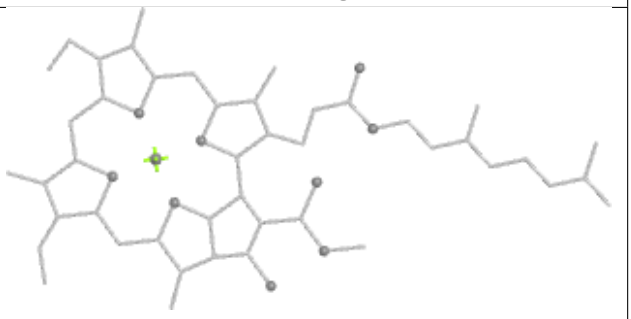


Bond angles

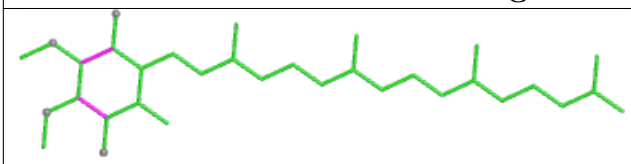


Torsions



Rings

Ligand A1L64 A 840



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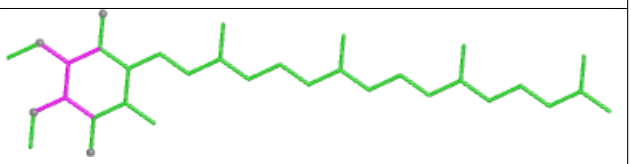
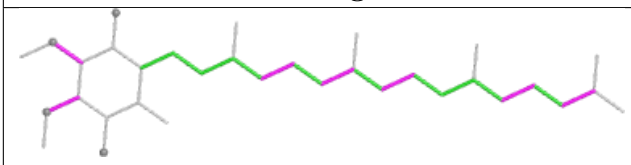
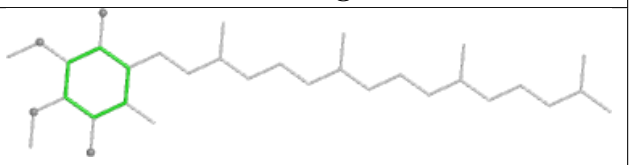


Bond angles

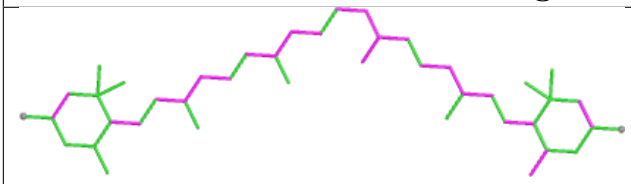


Torsions



Rings

Ligand 5X6 4 313



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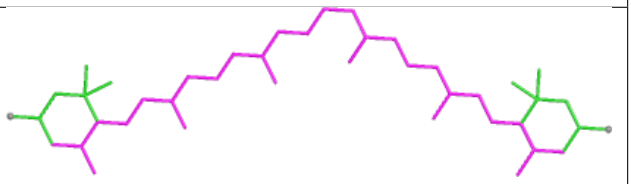
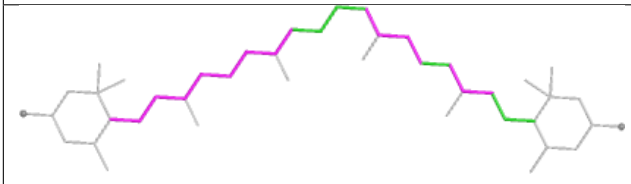
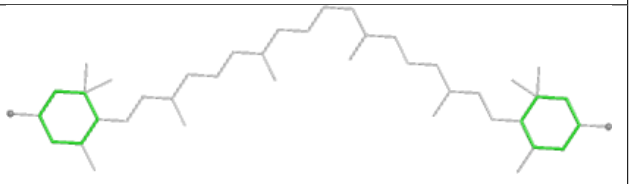


Bond angles

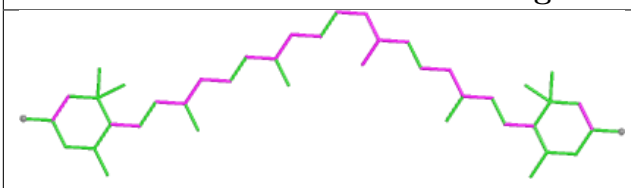


Torsions



Rings

Ligand 5X6 5 321



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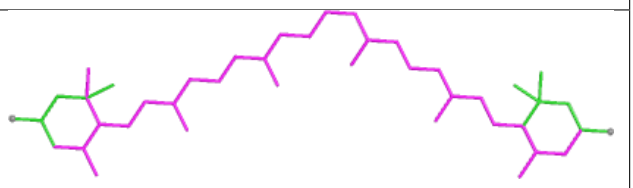
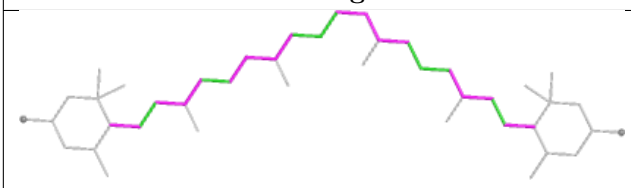


Bond angles



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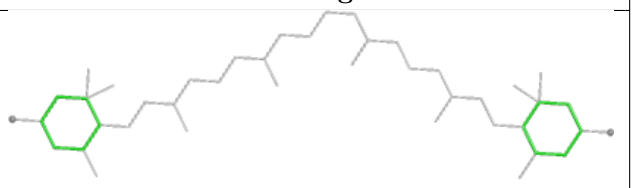
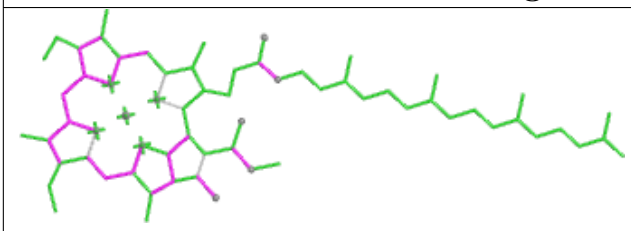


Rings

Ligand CLA A 809



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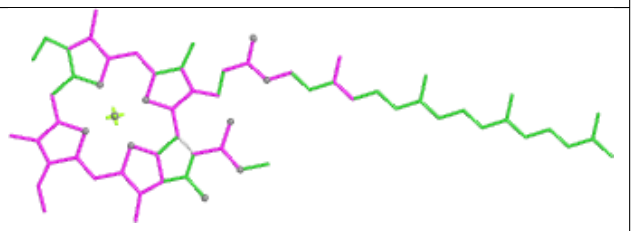
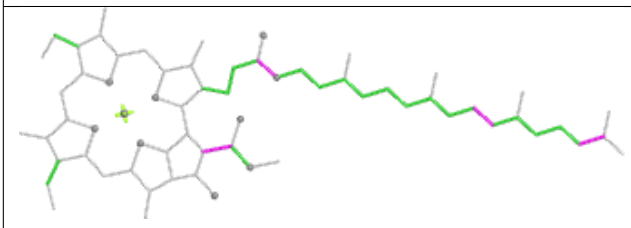


Bond angles



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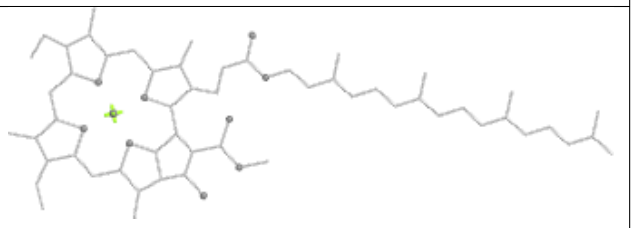
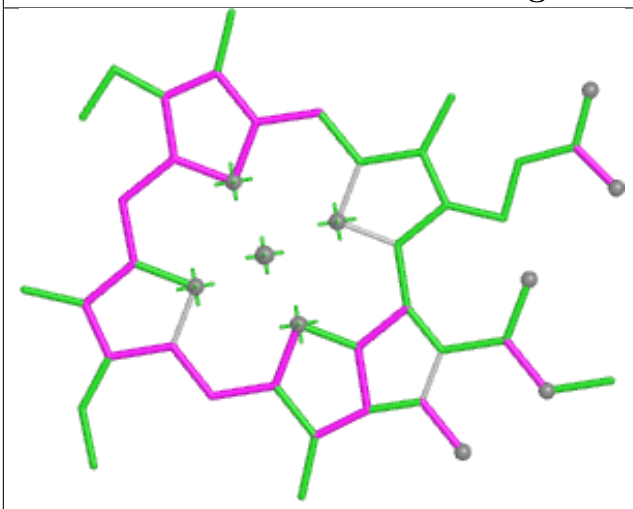


Rings

Ligand CLA 2 311



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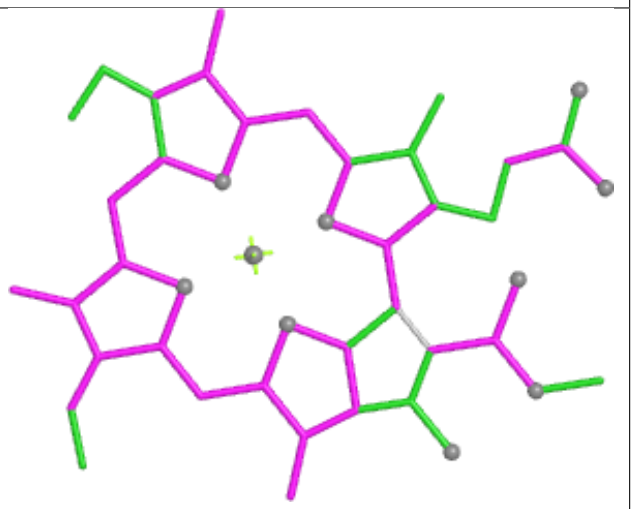
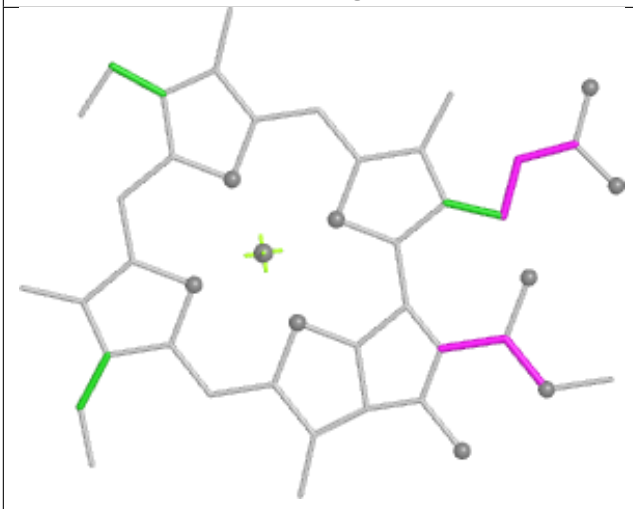


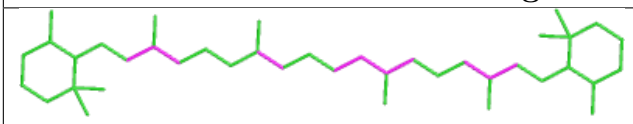
Bond angles



Torsions

Rings

Ligand BCR A 843



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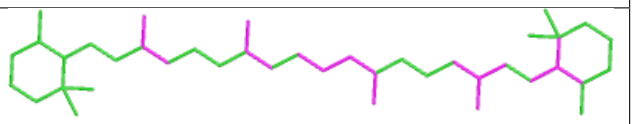
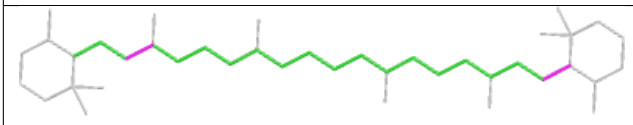
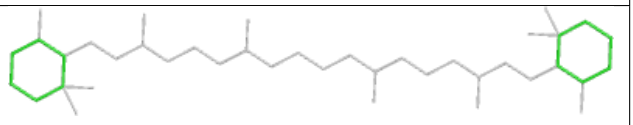


Bond angles

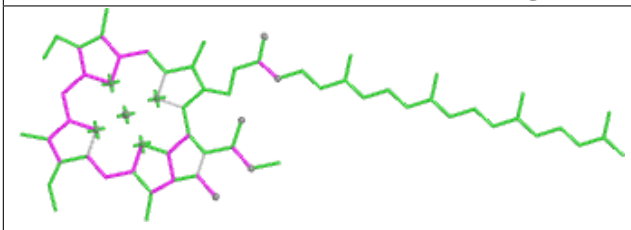


Torsions

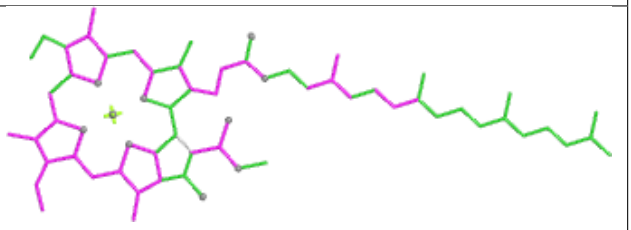


Rings

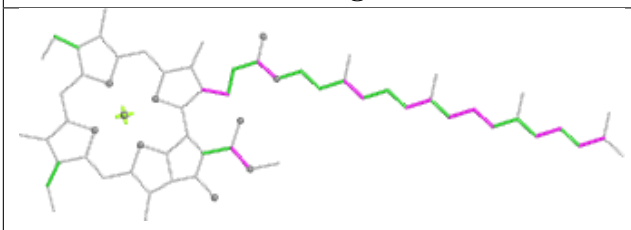
Ligand CLA B 804



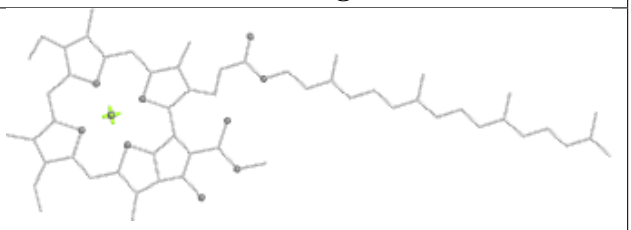
Bond lengths



Bond angles

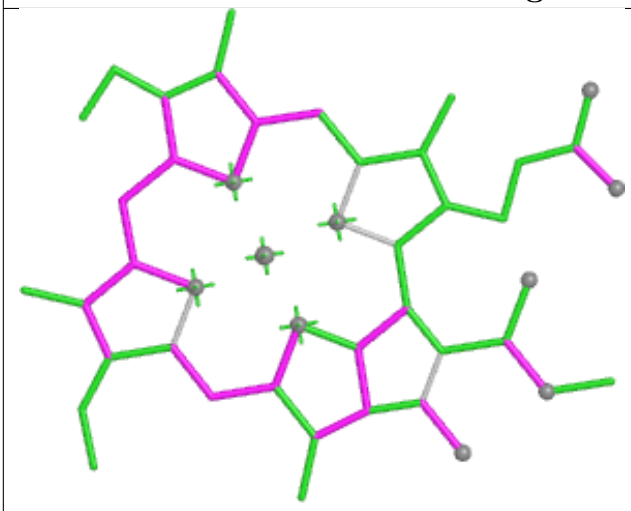


Torsions



Rings

Ligand CLA F 205



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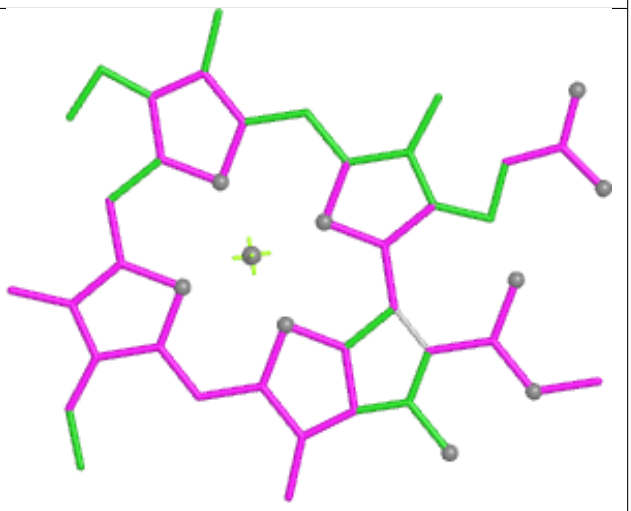
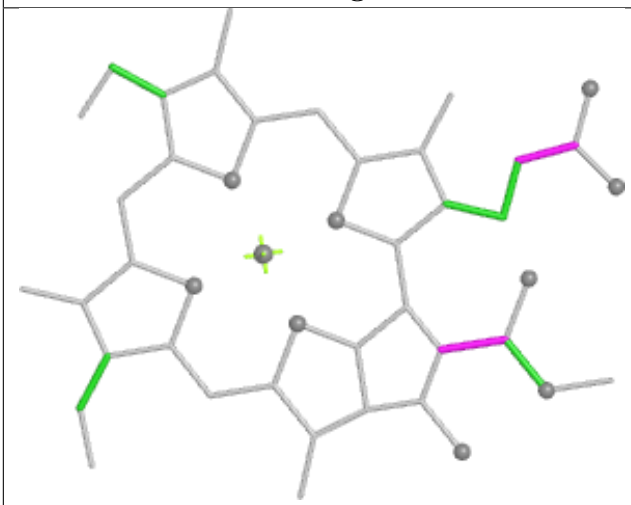


Bond angles



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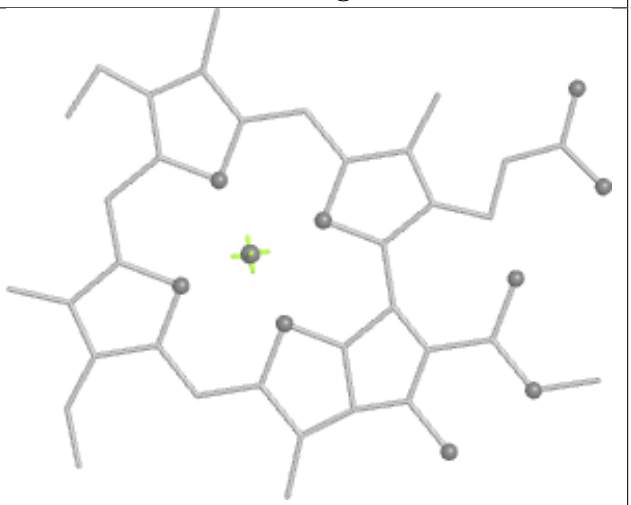
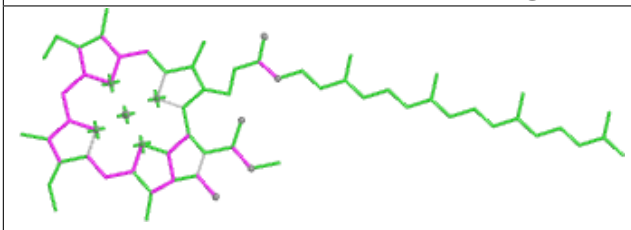
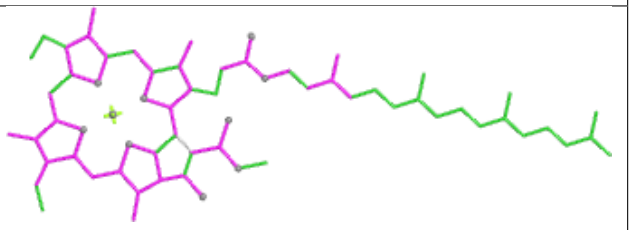
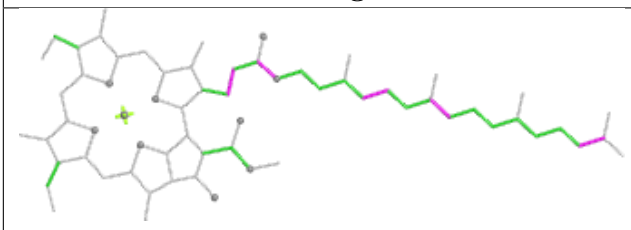
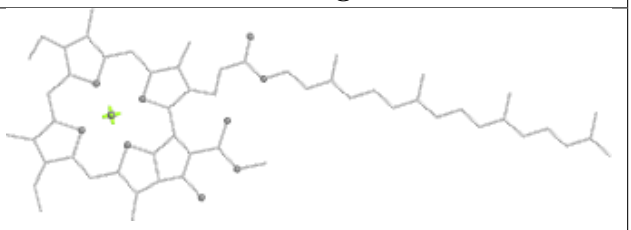
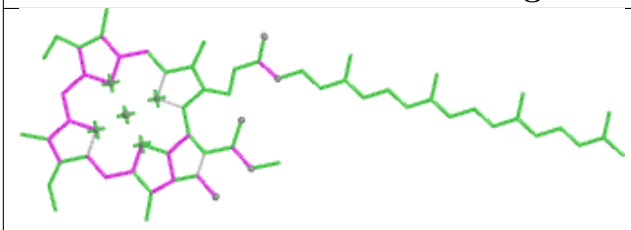
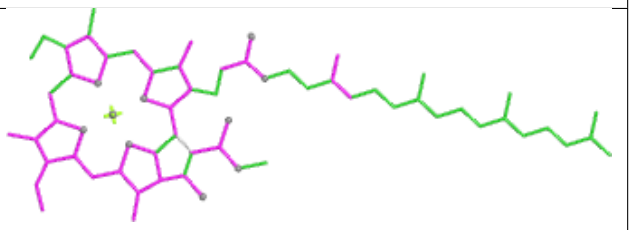
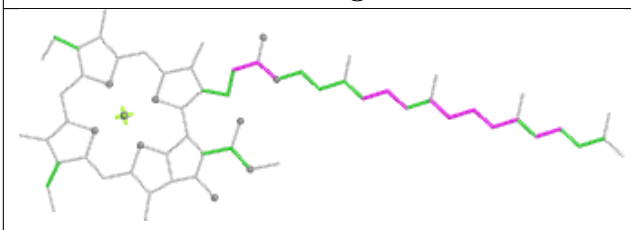
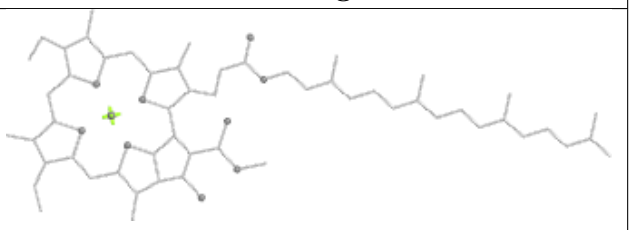
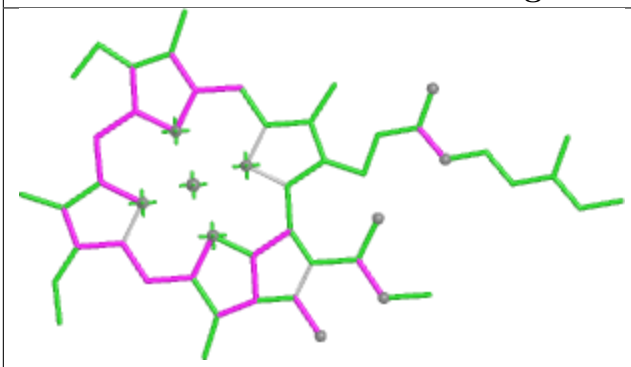


Rings

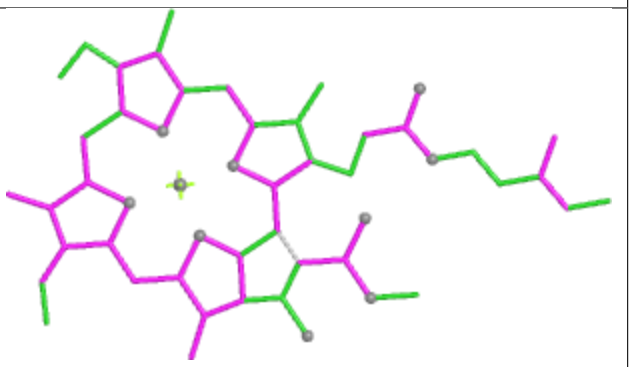
Ligand CLA A 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

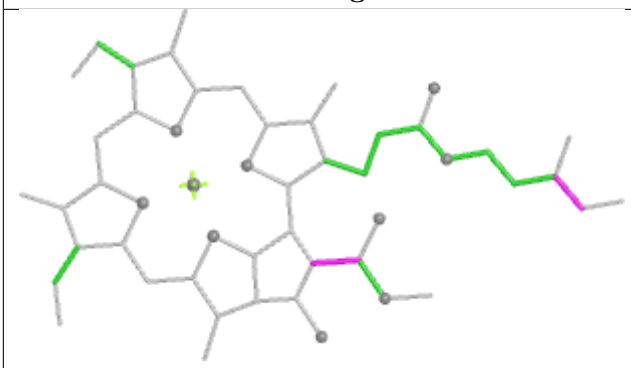
Ligand CLA B 834



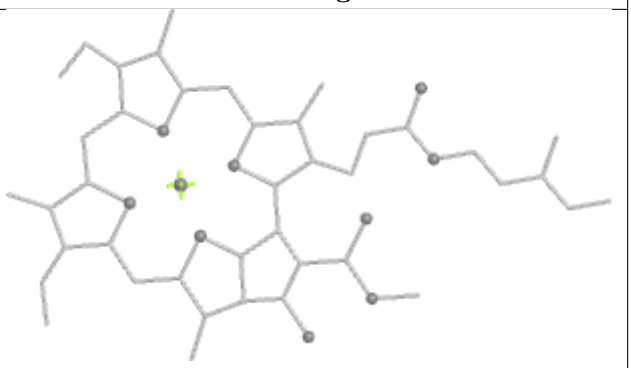
Bond lengths



Bond angles

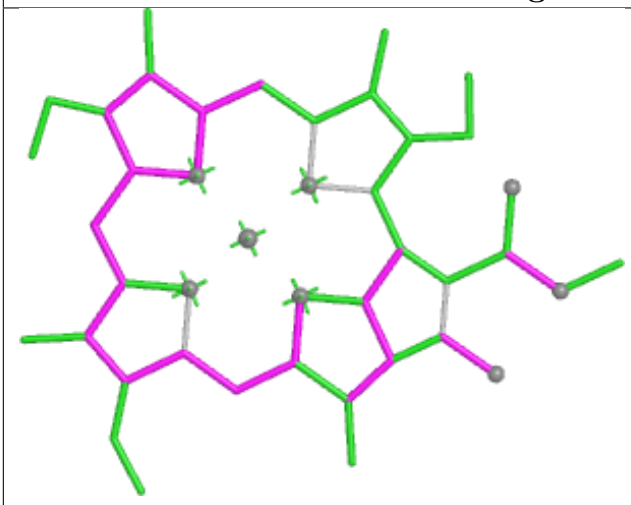


Torsions



Rings

Ligand CLA J 102



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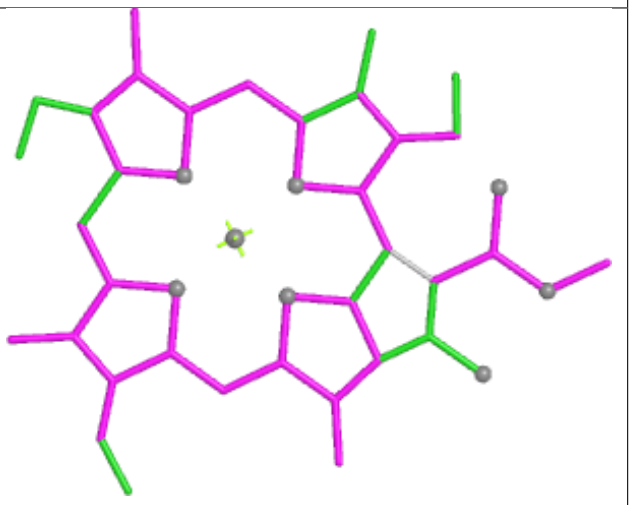
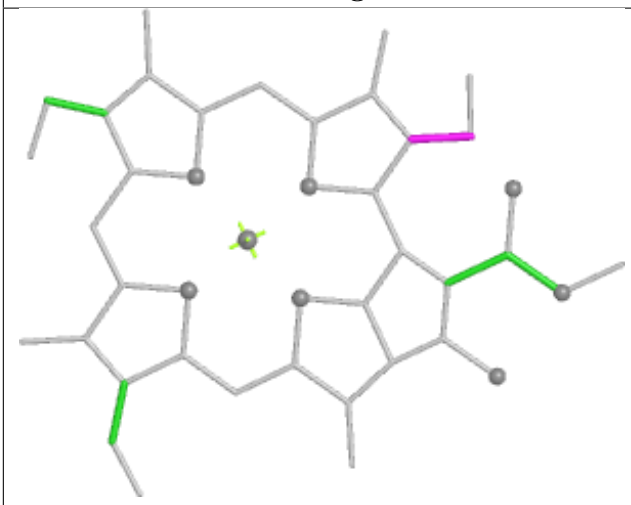


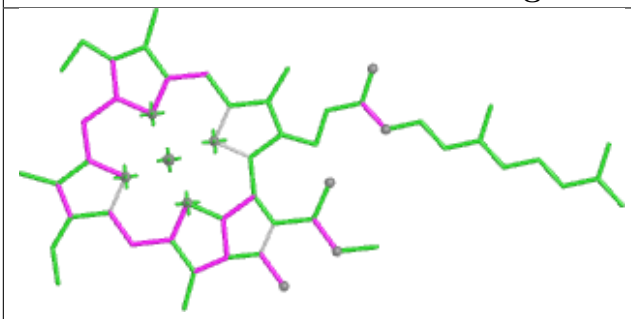
Bond angles



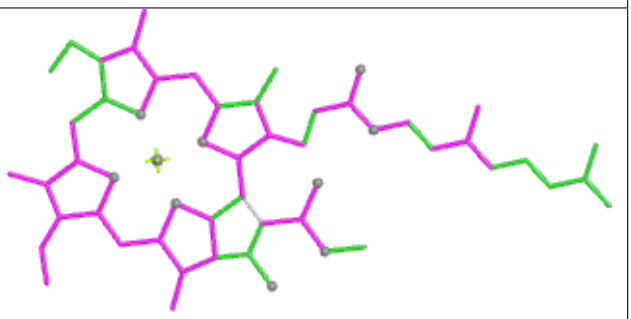
Torsions

Rings

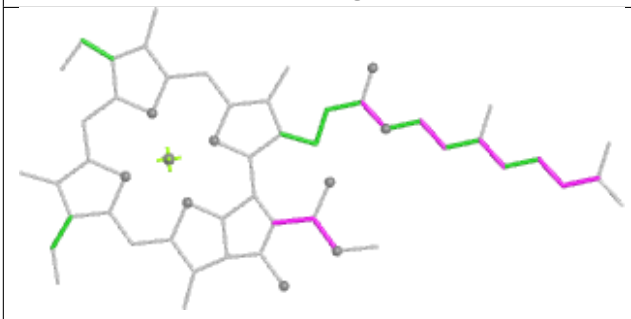
Ligand CLA A 808



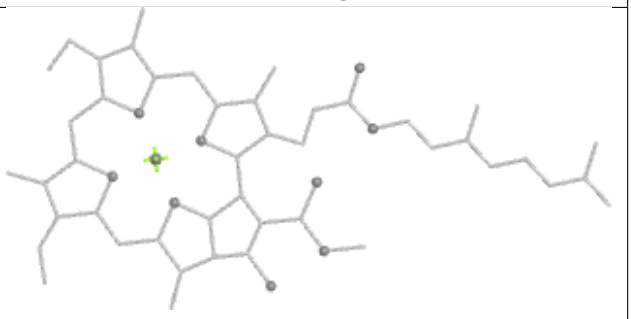
Bond lengths



Bond angles

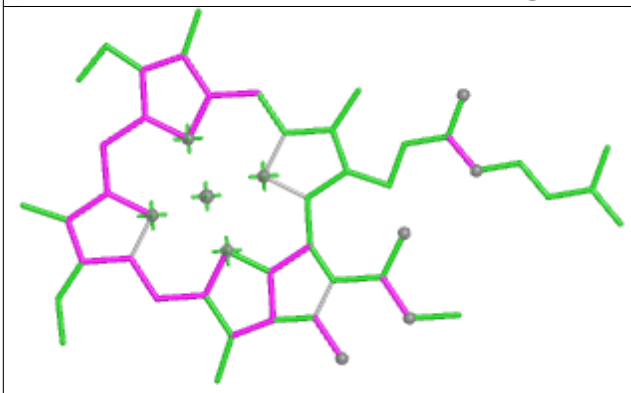


Torsions

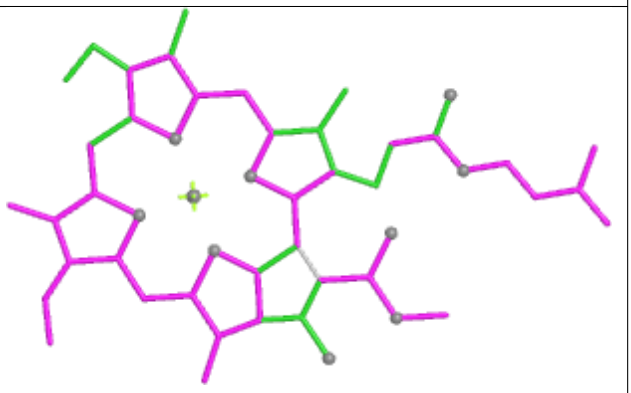


Rings

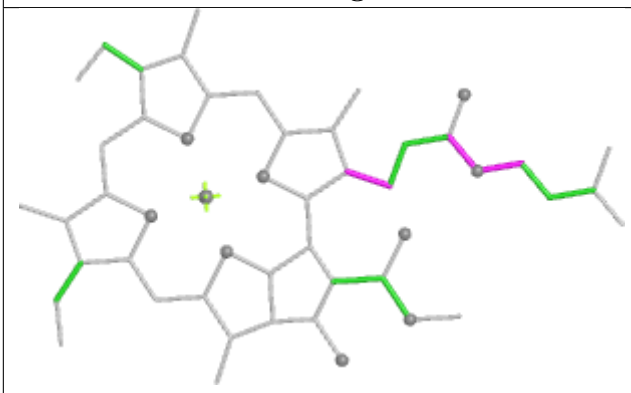
Ligand CLA O 205



Bond lengths



Bond angles



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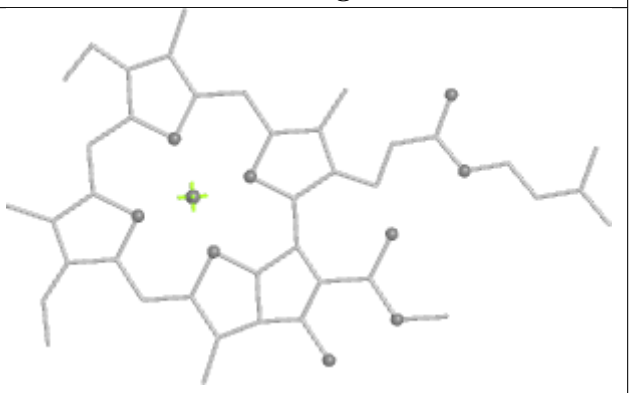
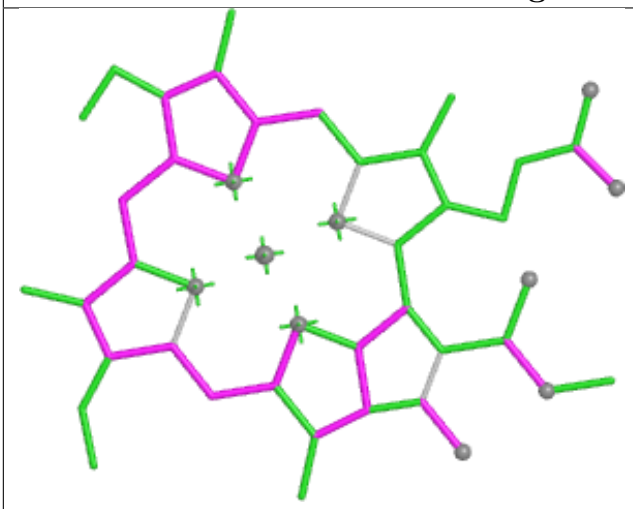
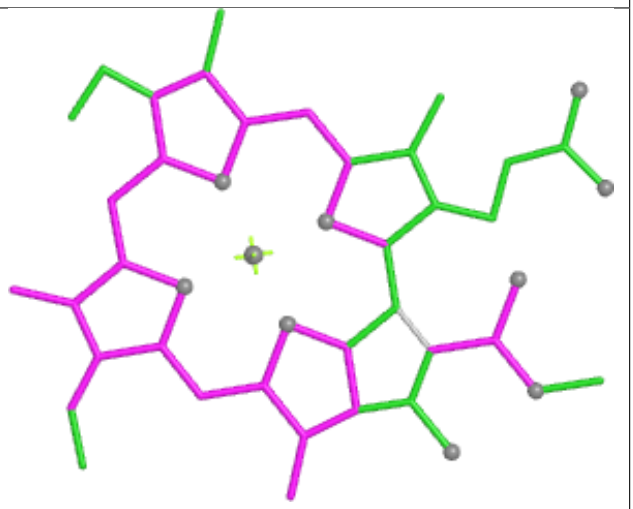


Rings

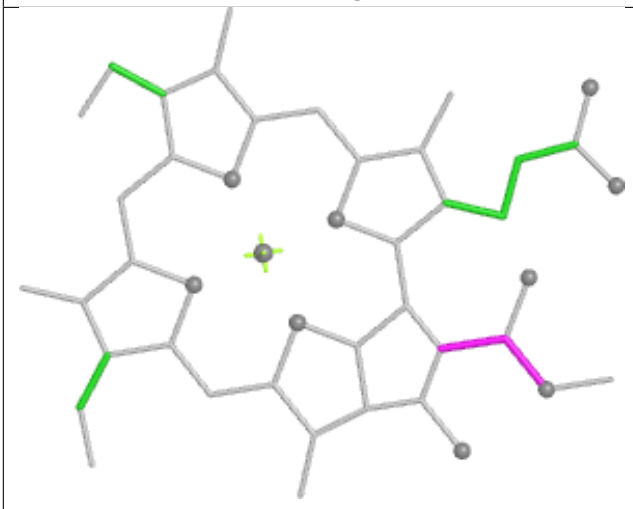
Ligand CLA 2 302



Bond lengths



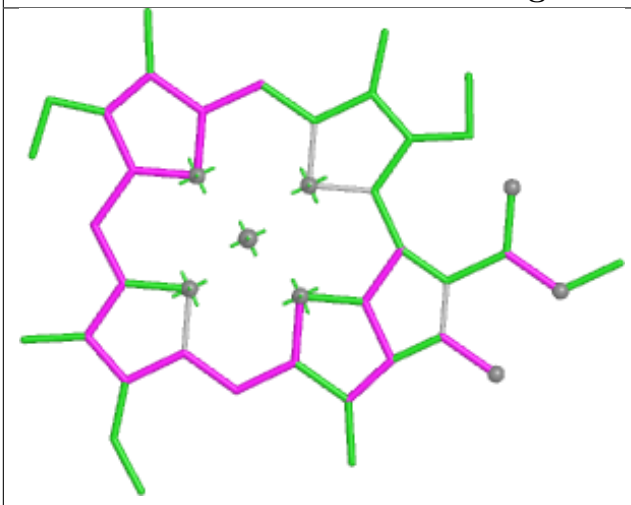
Bond angles



Torsions

Rings

Ligand CLA 5 309



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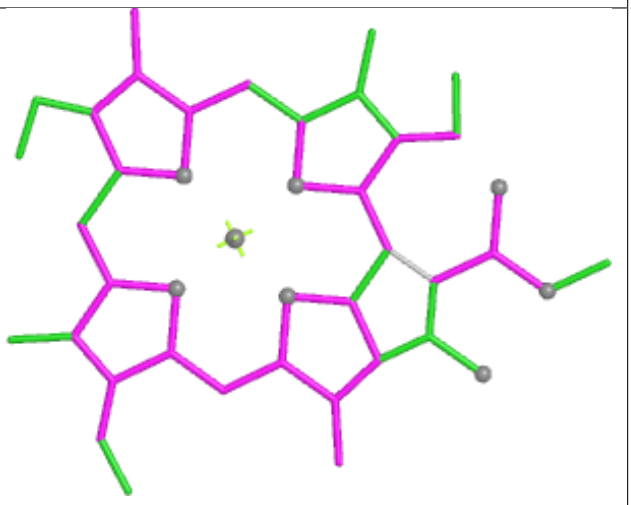
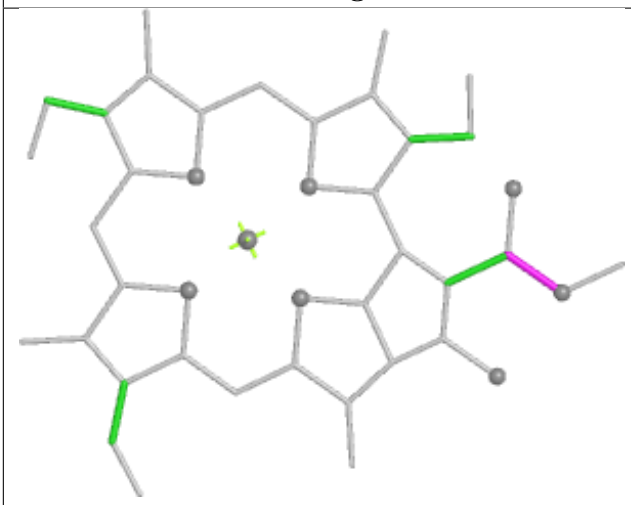


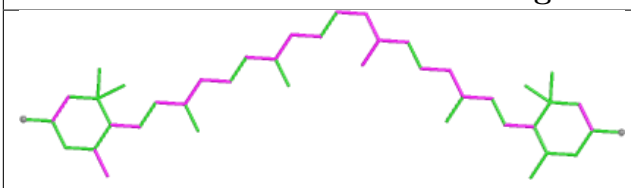
Bond angles



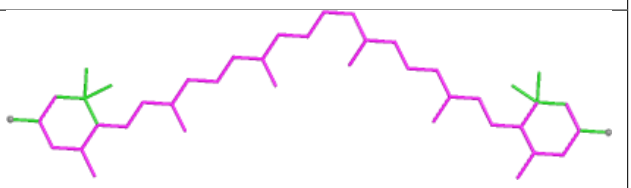
Torsions

Rings

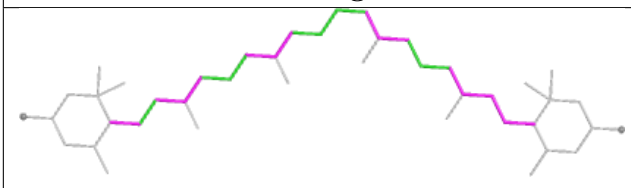
Ligand 5X6 6 316



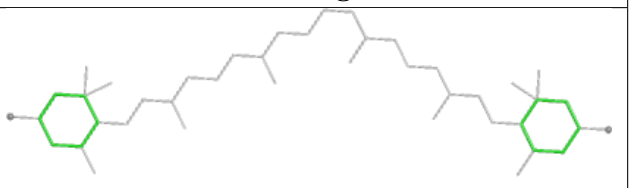
Bond lengths



Bond angles

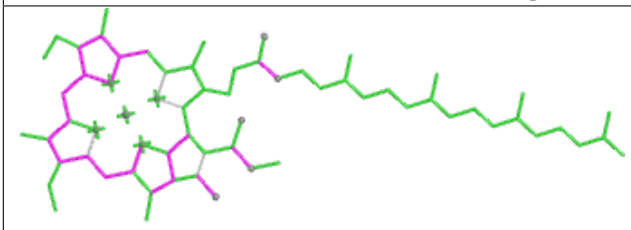


Torsions

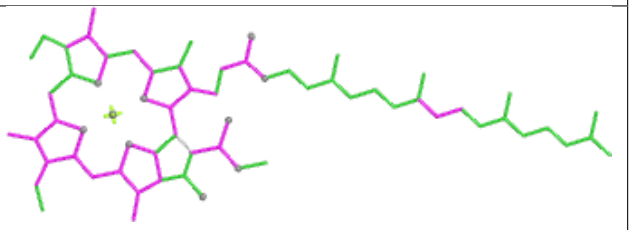


Rings

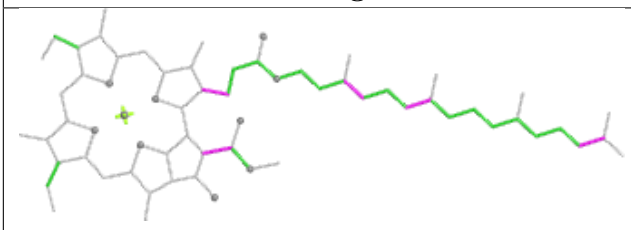
Ligand CLA B 802



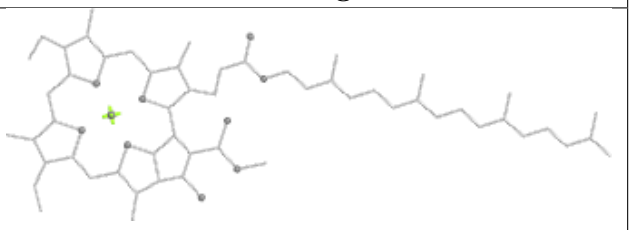
Bond lengths



Bond angles

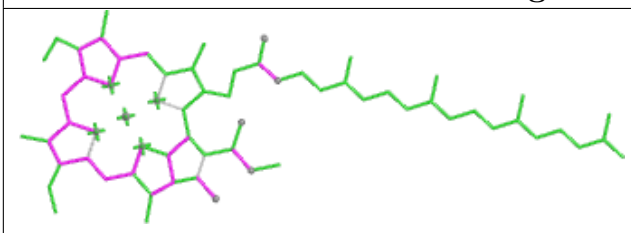


Torsions

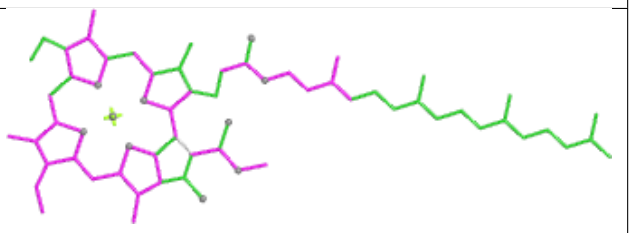


Rings

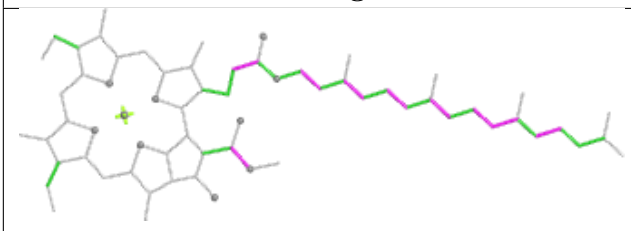
Ligand CLA 6 305



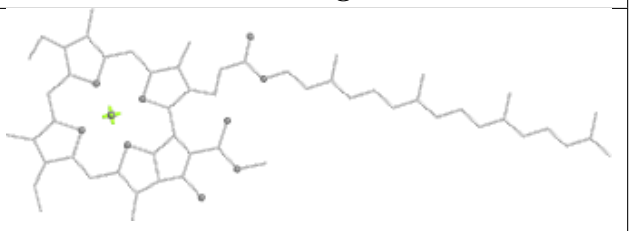
Bond lengths



Bond angles

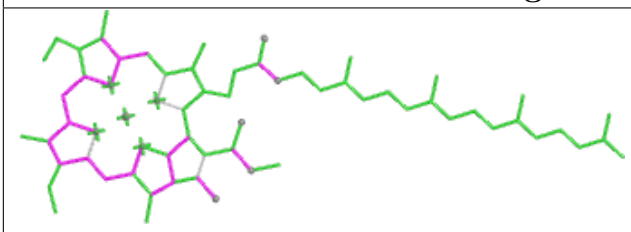


Torsions

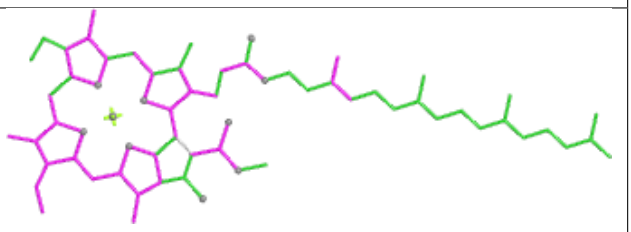


Rings

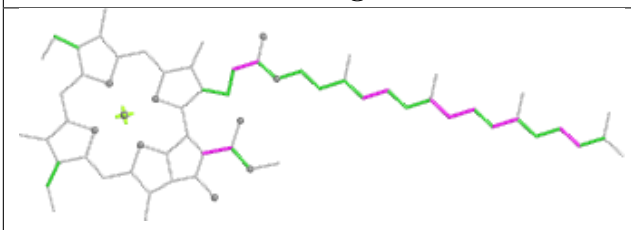
Ligand CLA B 809



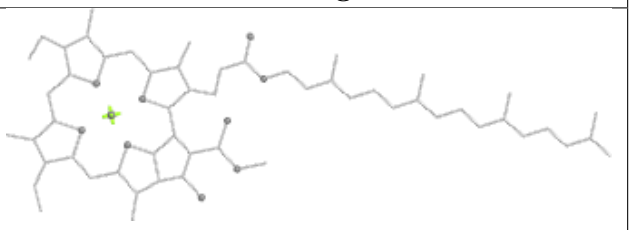
Bond lengths



Bond angles

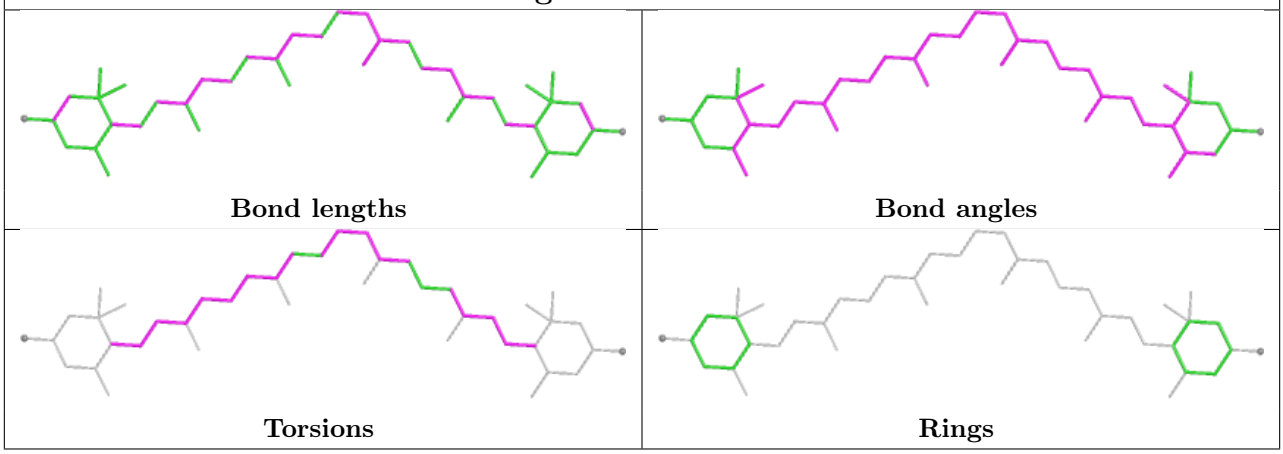


Torsions

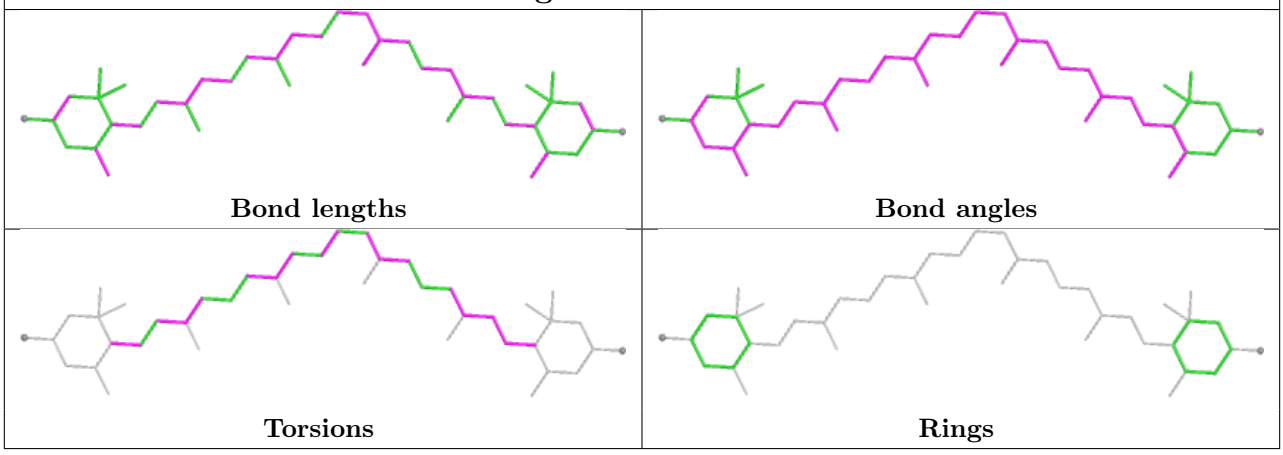


Rings

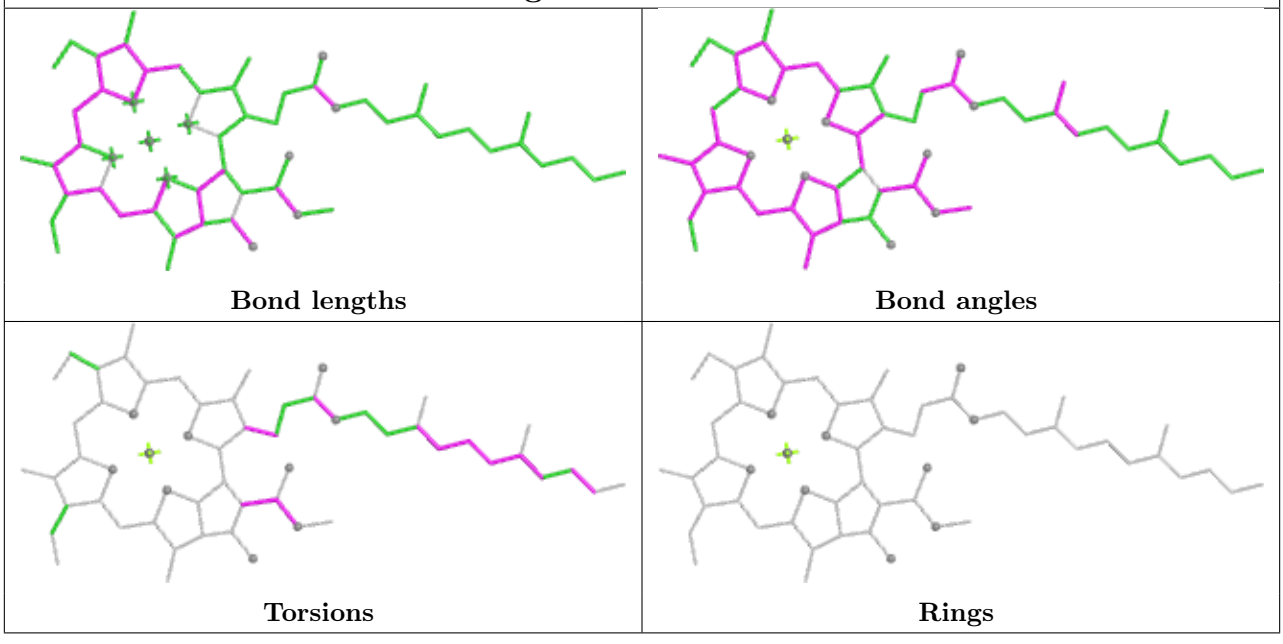
Ligand 5X6 1 311

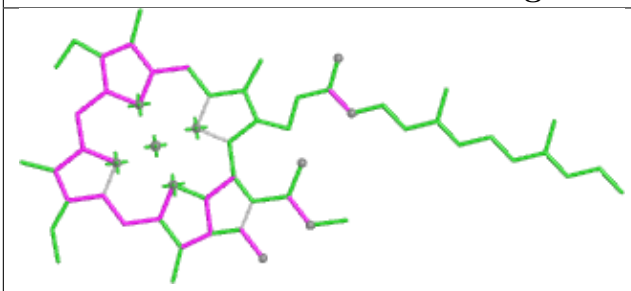
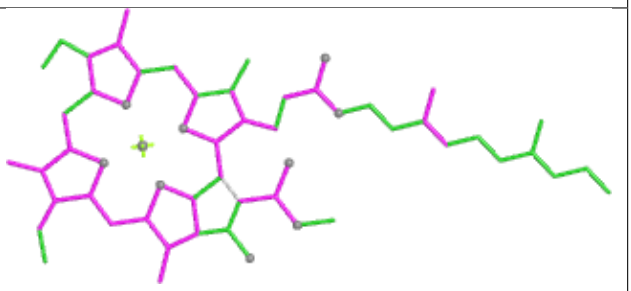
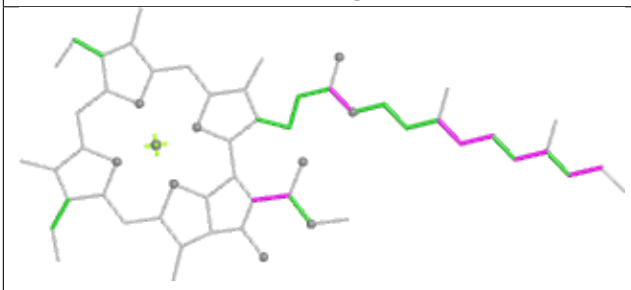
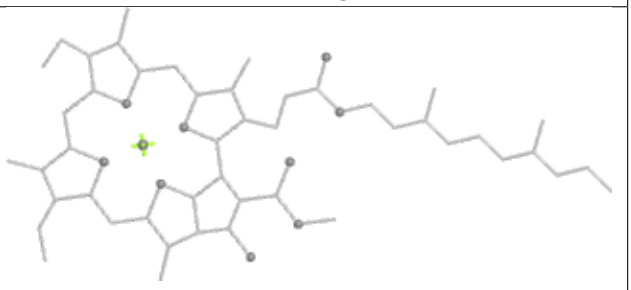


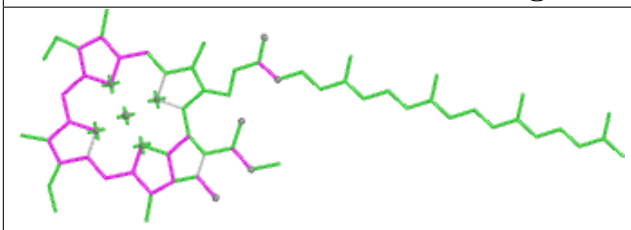
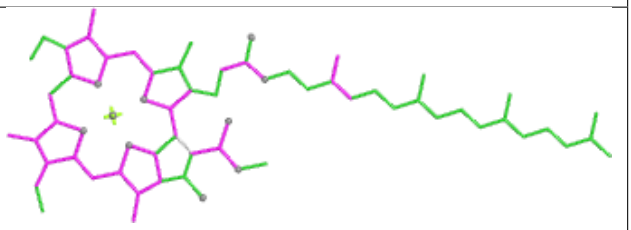
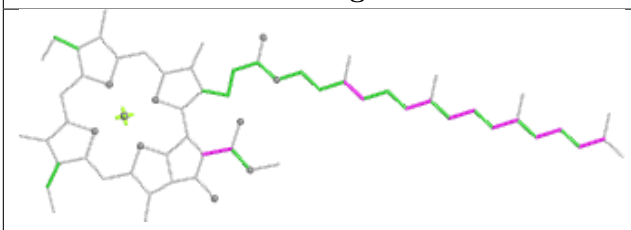
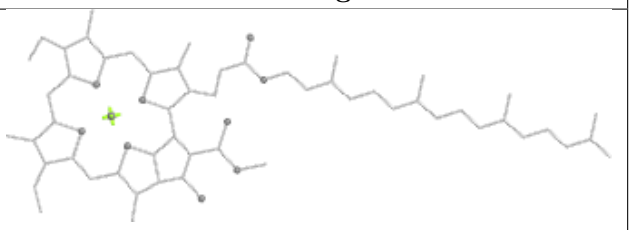
Ligand 5X6 5 313

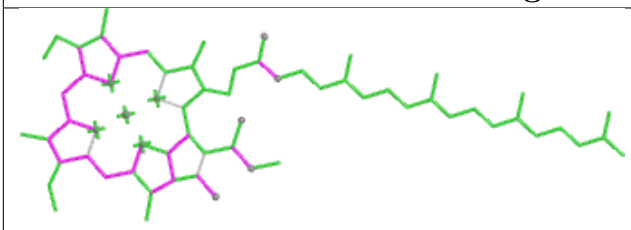
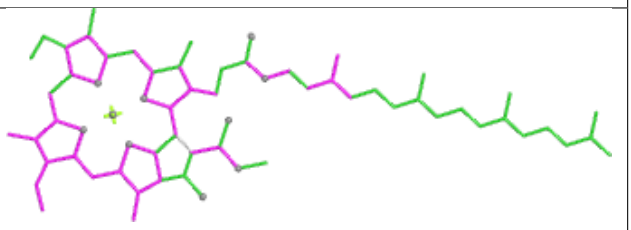
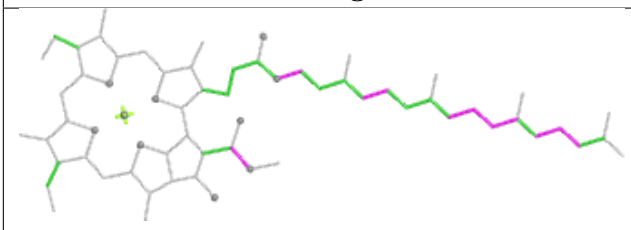
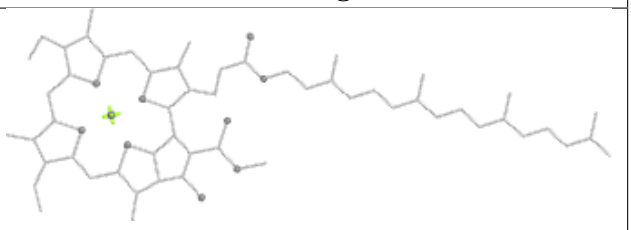


Ligand CLA O 206



Ligand CLA B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 833	
	
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.

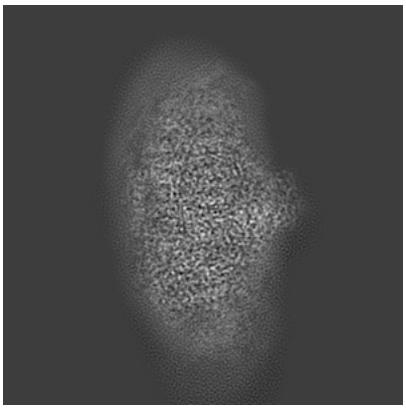
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62242. These allow visual inspection of the internal detail of the map and identification of artifacts.

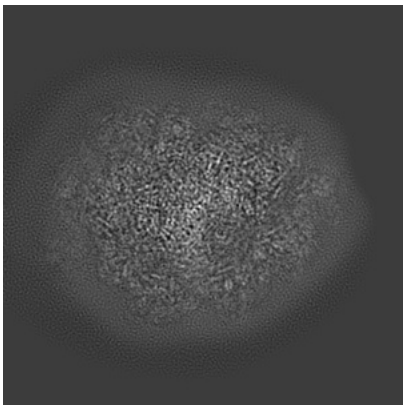
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

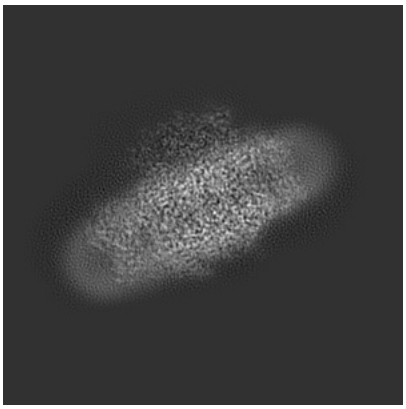
6.1.1 Primary map



X

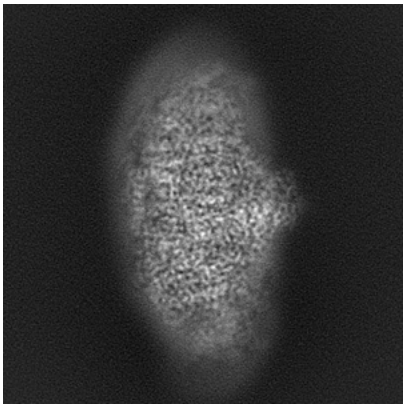


Y

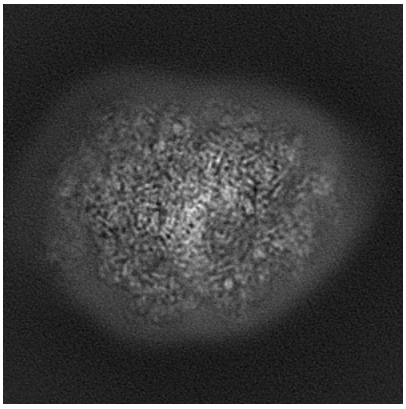


Z

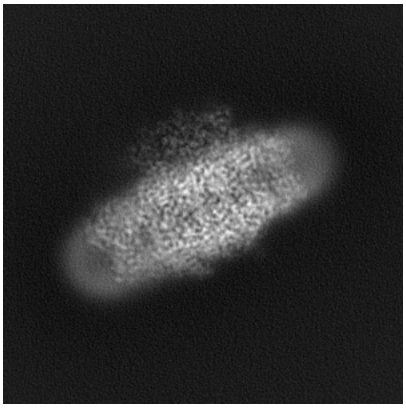
6.1.2 Raw map



X



Y

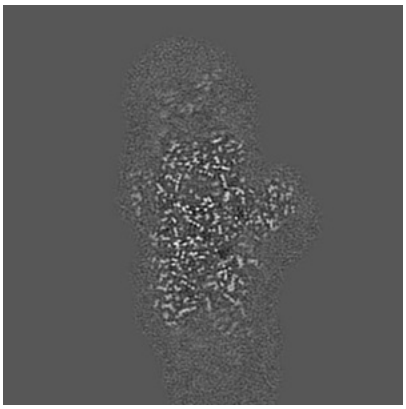


Z

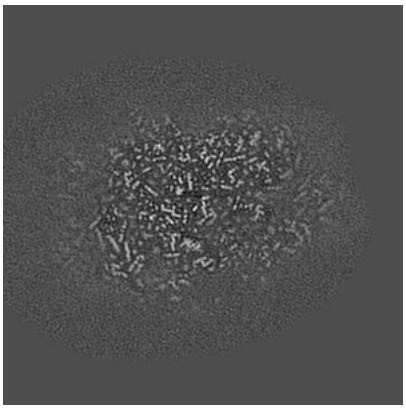
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

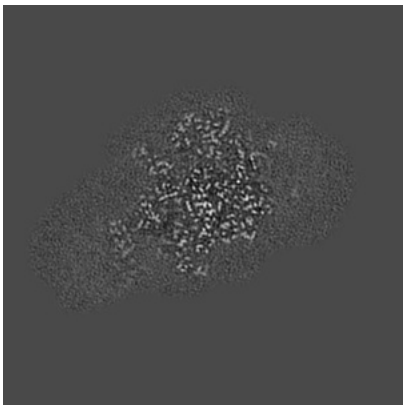
6.2.1 Primary map



X Index: 160

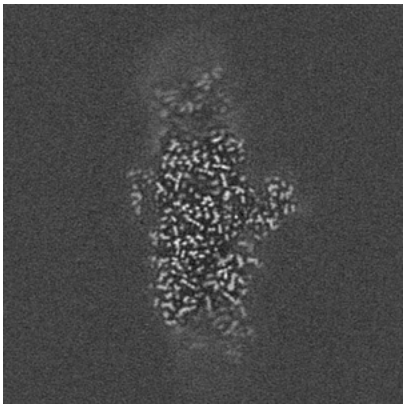


Y Index: 160

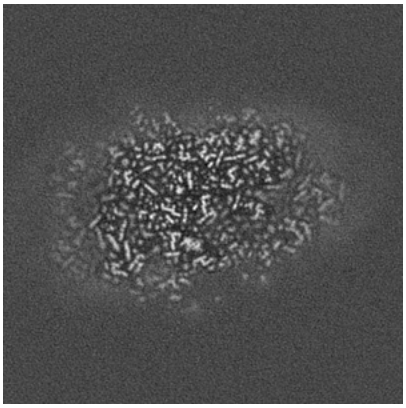


Z Index: 160

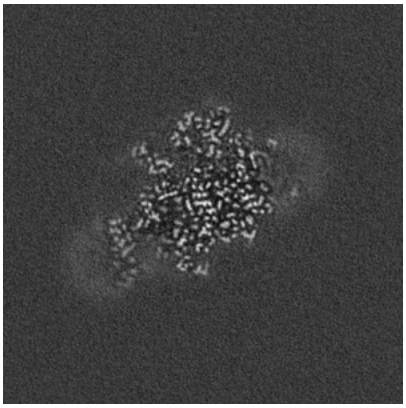
6.2.2 Raw map



X Index: 160



Y Index: 160

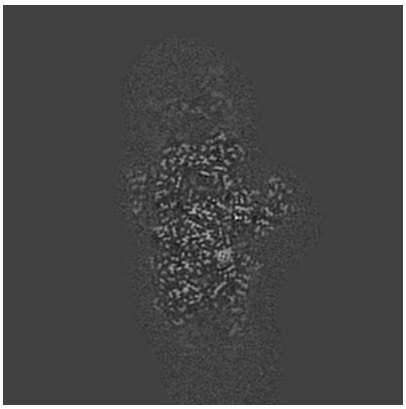


Z Index: 160

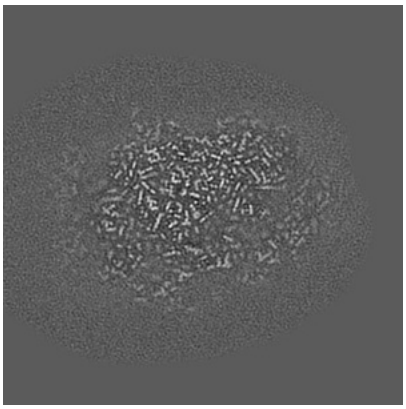
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



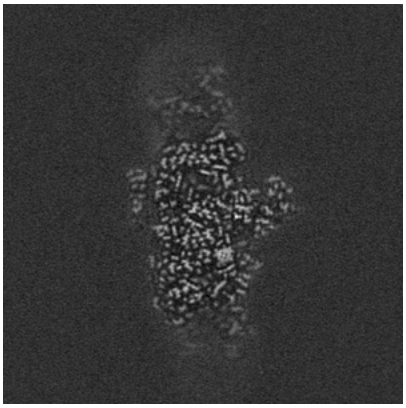
X Index: 158



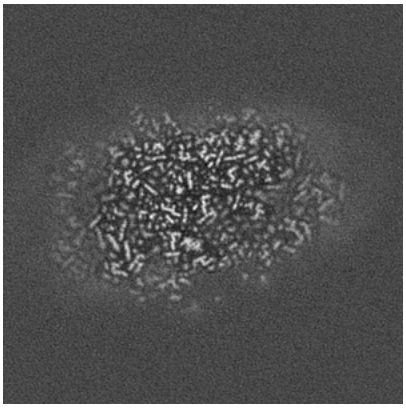
Y Index: 158

Z Index: 147

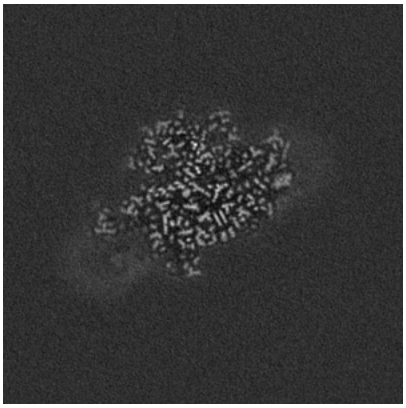
6.3.2 Raw map



X Index: 158



Y Index: 160

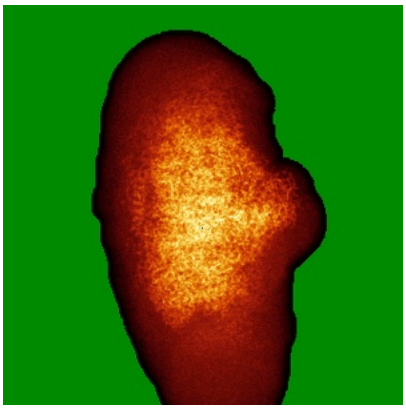


Z Index: 147

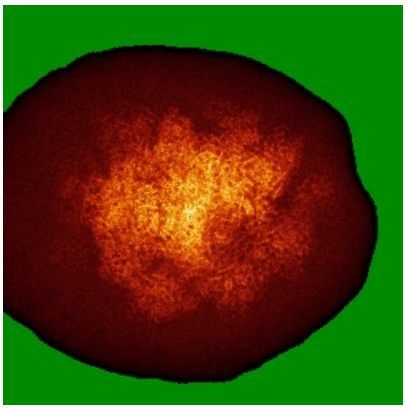
The images above show the largest variance slices of the map in three orthogonal directions.

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

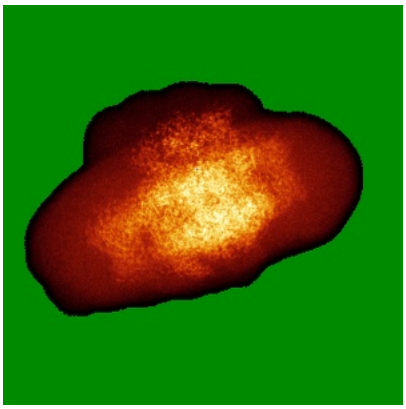
6.4.1 Primary map



X

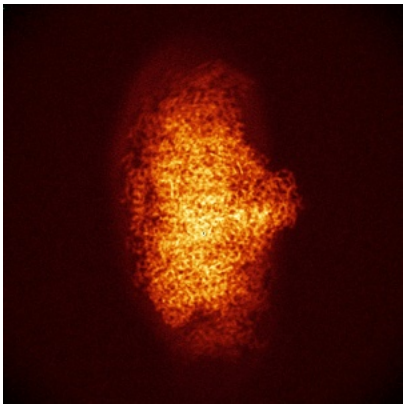


Y

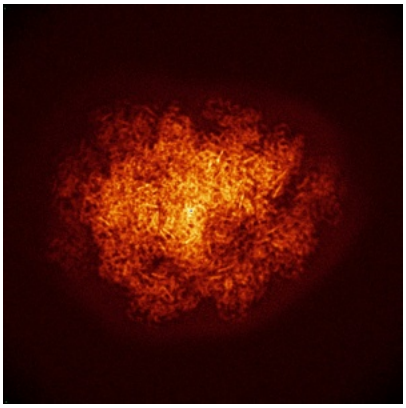


Z

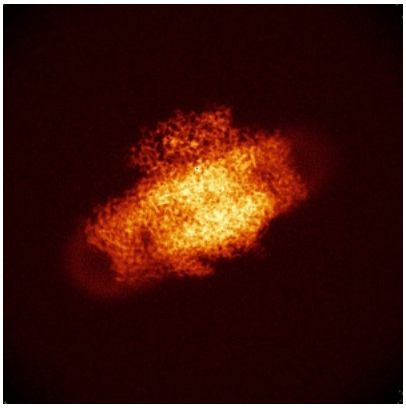
6.4.2 Raw map



X



Y

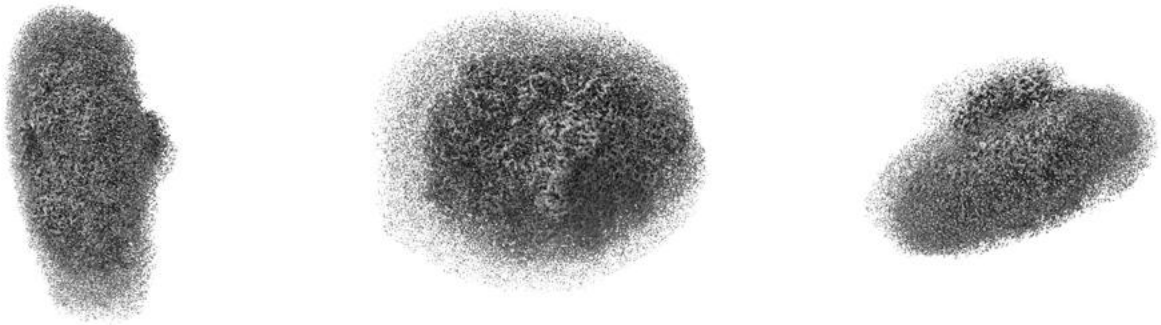


Z

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)

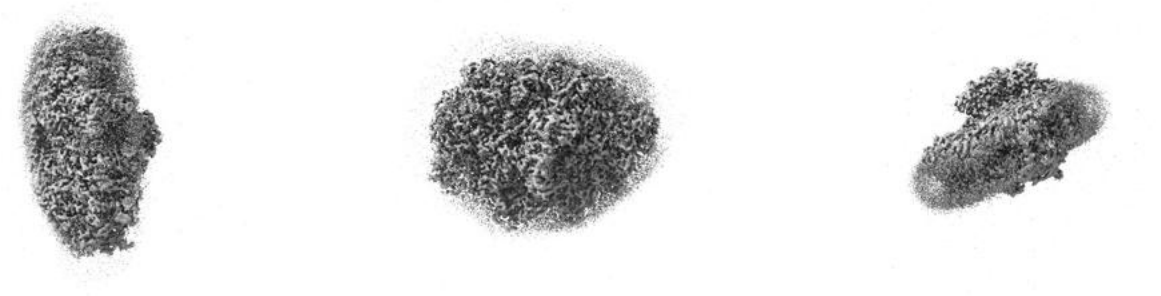
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

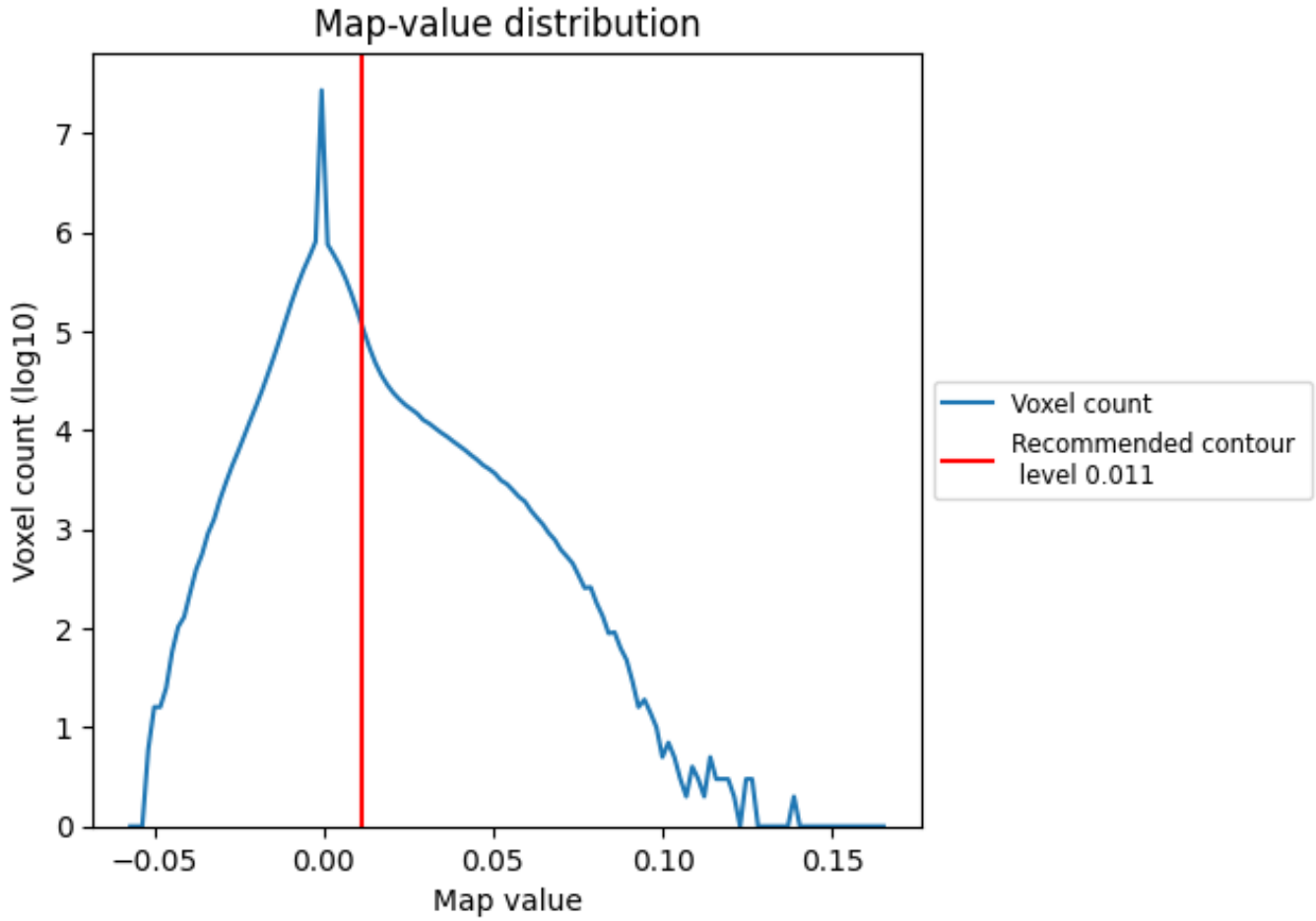
6.6 Mask visualisation (i)

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

7 Map analysis

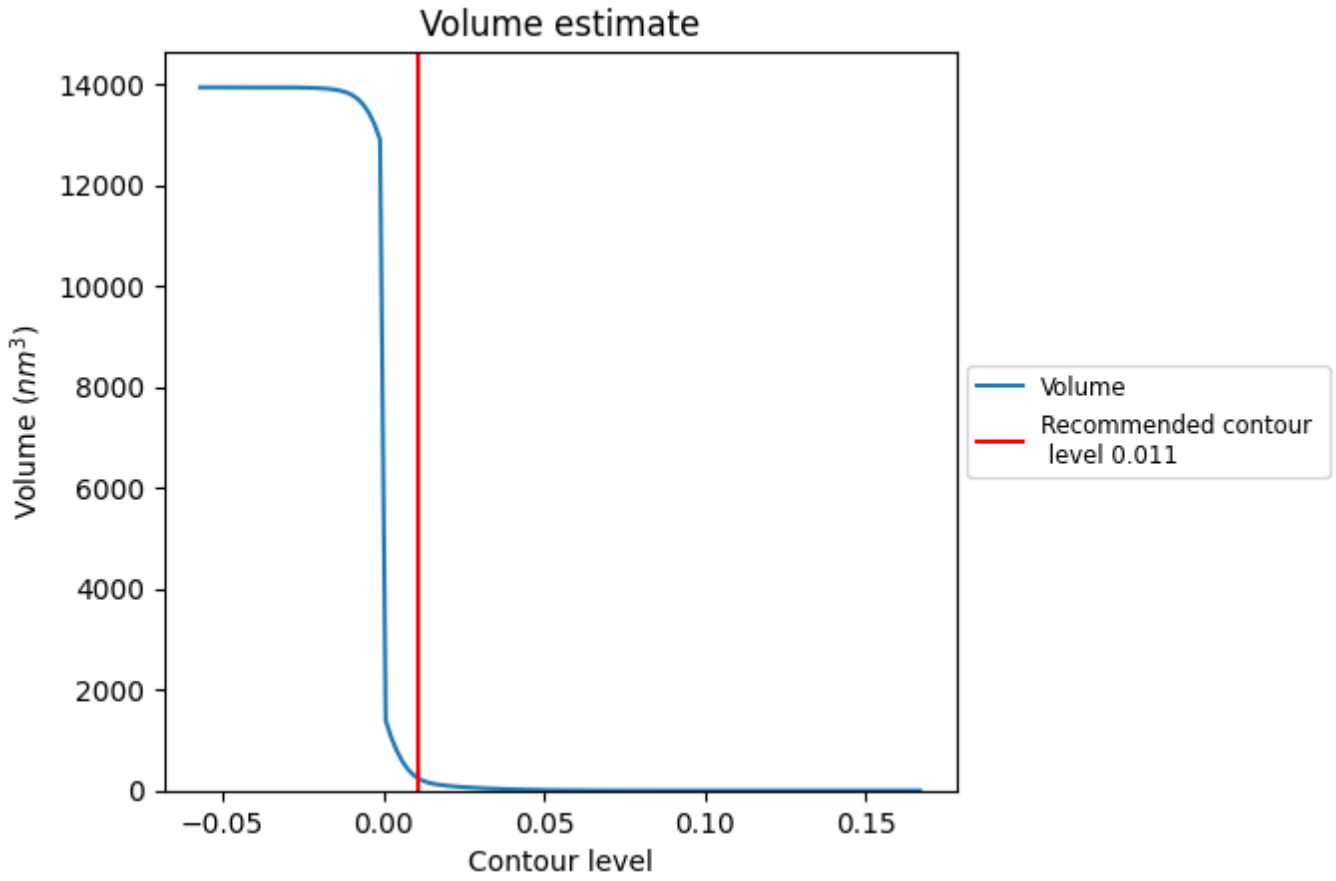
This section contains the results of statistical analysis of the map.

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.

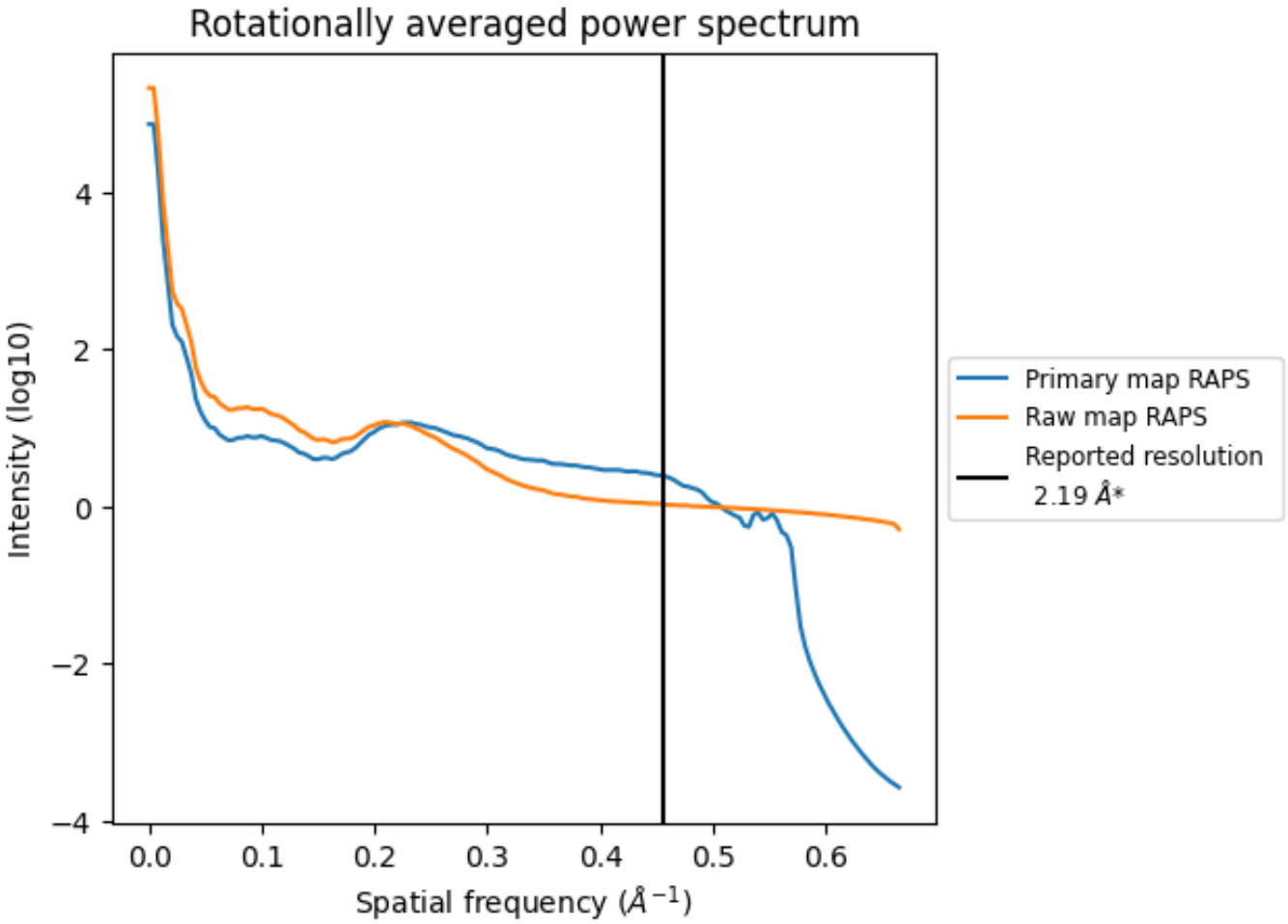
7.2 Volume estimate



The volume at the recommended contour level is 238 nm^3; this corresponds to an approximate mass of 215 kDa.

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

7.3 Rotationally averaged power spectrum (i)

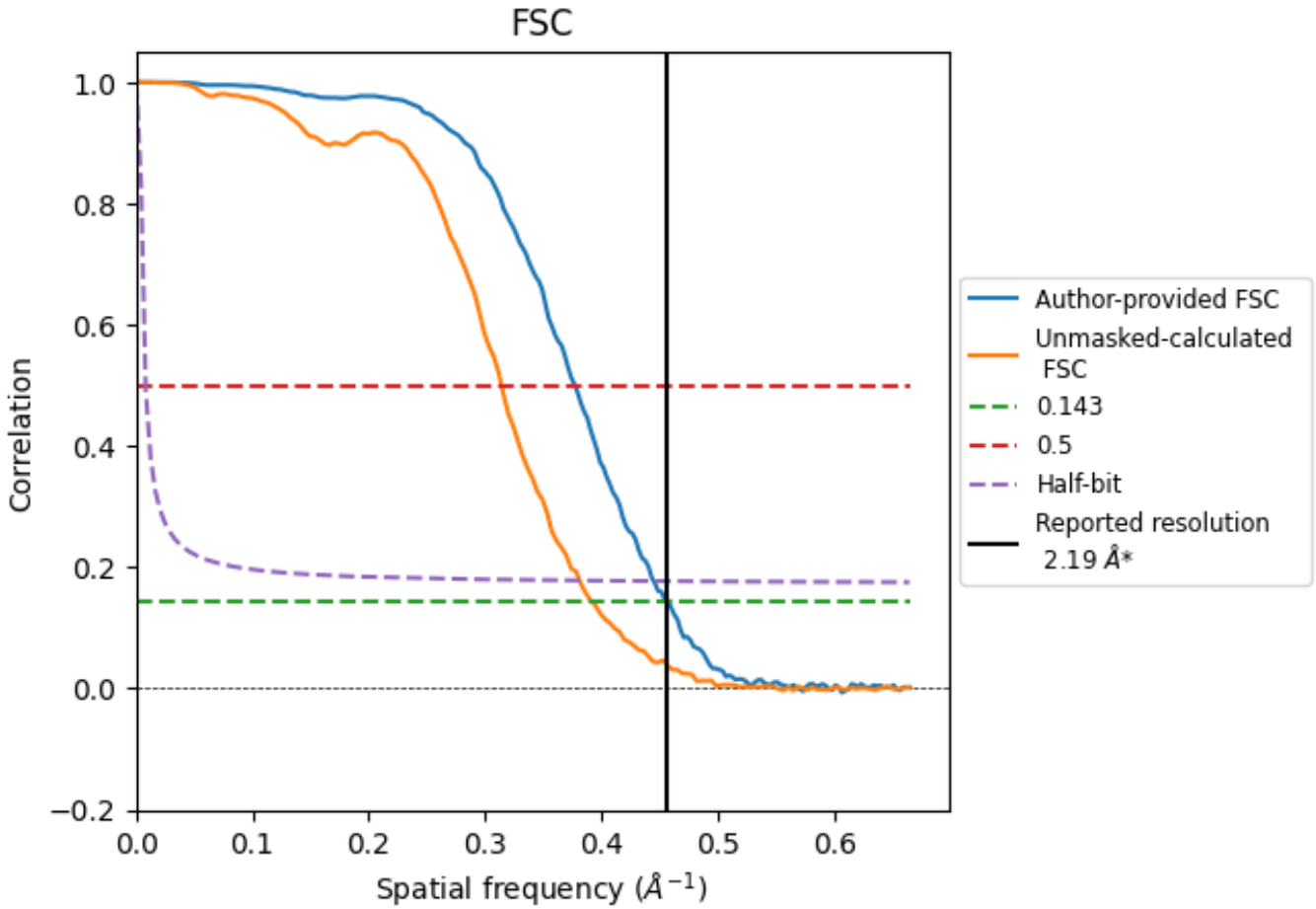


*Reported resolution corresponds to spatial frequency of 0.457 Å^{-1}

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 0.457 Å^{-1}

8.2 Resolution estimates (i)

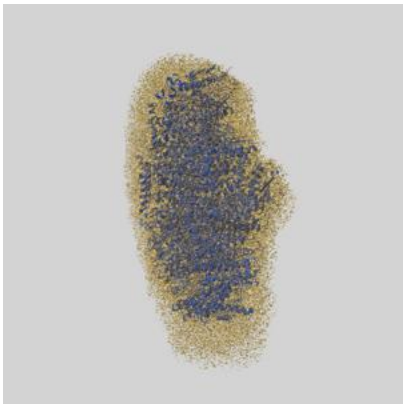
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.65	2.24
Unmasked-calculated*	2.55	3.18	2.62

*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 2.55 differs from the reported value 2.19 by more than 10 %

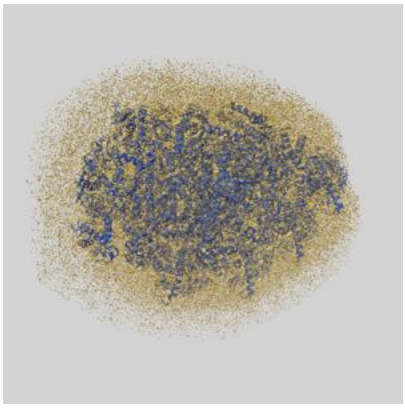
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62242 and PDB model 9KC5. Per-residue inclusion information can be found in section 3 on page 26.

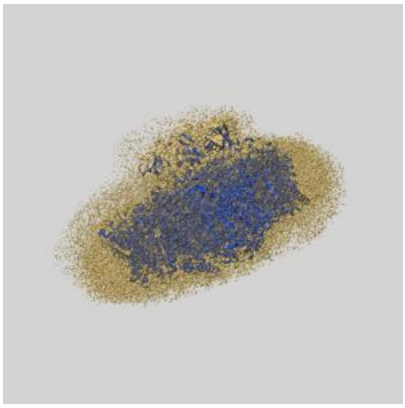
9.1 Map-model overlay



X



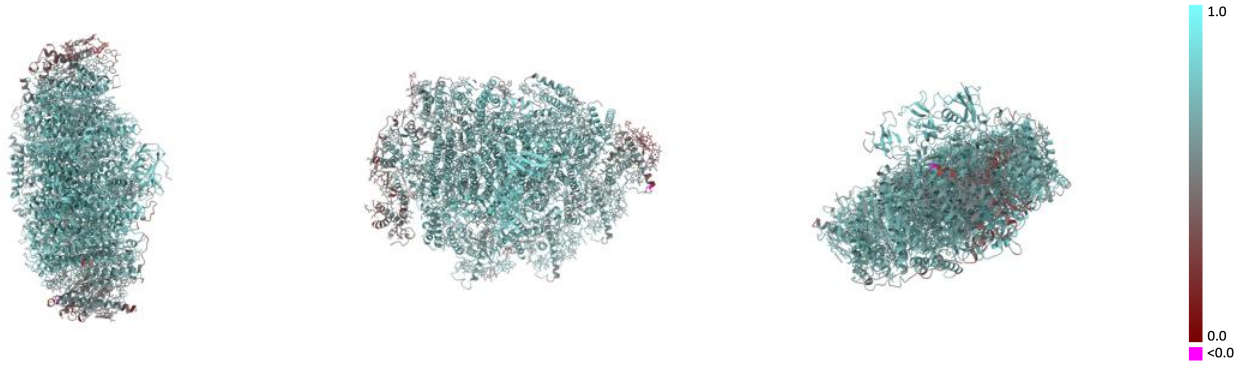
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

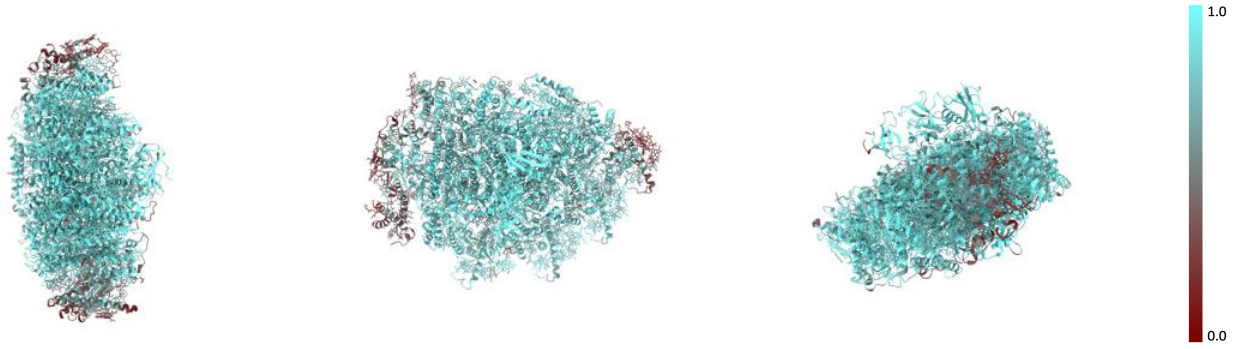
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

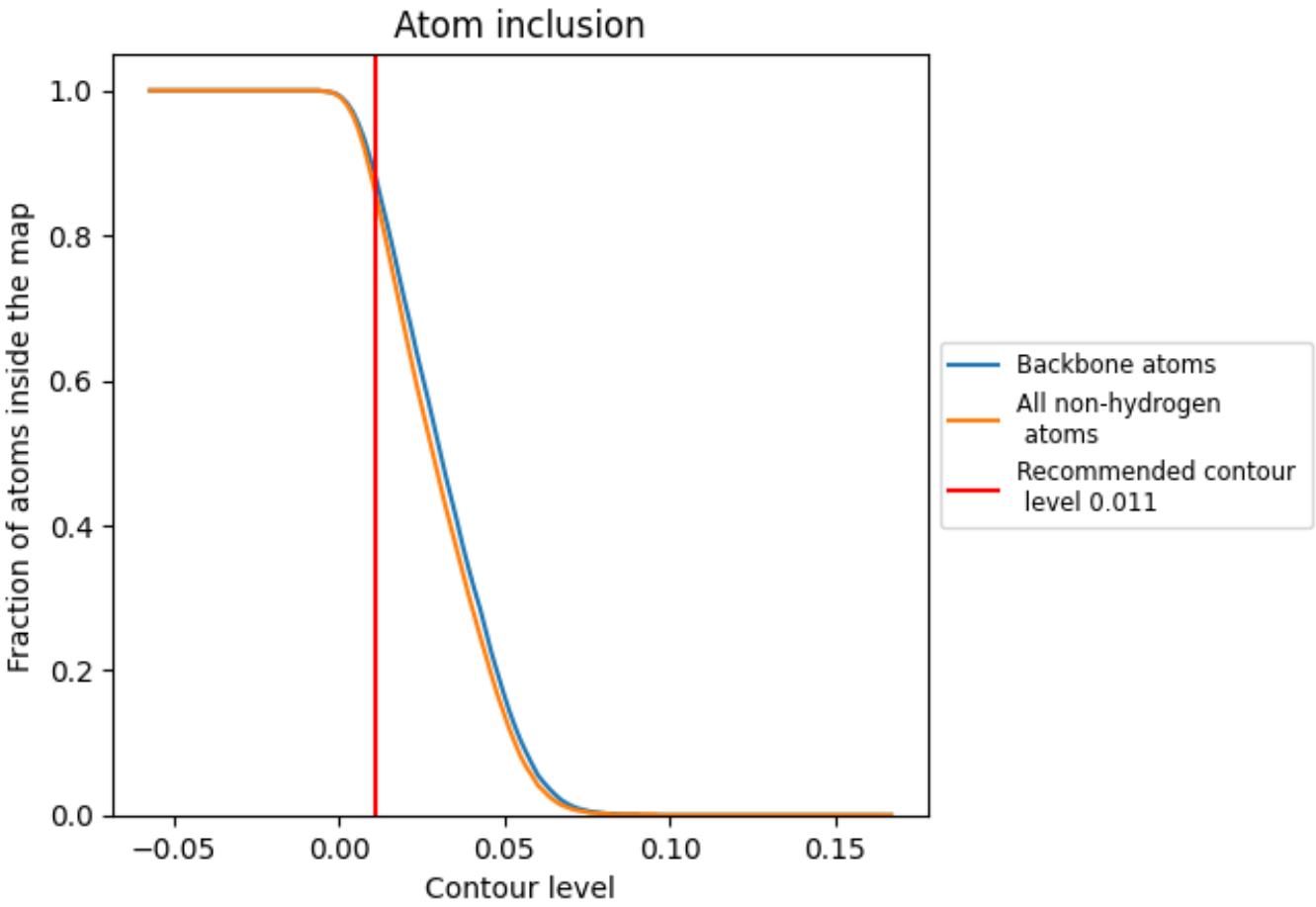
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.6870
1	0.7200	0.6010
2	0.5950	0.5410
3	0.3740	0.4350
4	0.8710	0.6700
5	0.8700	0.6590
6	0.8630	0.6520
7	0.5370	0.4840
A	0.9510	0.7560
B	0.9530	0.7560
C	0.9900	0.7830
D	0.9280	0.7280
E	0.8640	0.6980
F	0.9240	0.7260
I	0.8890	0.6970
J	0.9190	0.7140
K	0.8370	0.6510
L	0.8750	0.6870
M	0.7980	0.6310
O	0.8420	0.6600
Z	0.9320	0.7120