Full wwPDB EM Validation Report ⓘ

Oct 1, 2026 – 12:29 AM JST

PDB ID	:	6JO5 / pdb_00006jo5
EMDB ID	:	EMD-9853
Title	:	Structure of the green algal photosystem I supercomplex with light-harvesting complex I
Authors	:	Suga, M.; Miyazaki, N.; Takahashi, Y.
Deposited on	:	2019-03-20
Resolution	:	2.90 Å(reported)

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

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

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

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

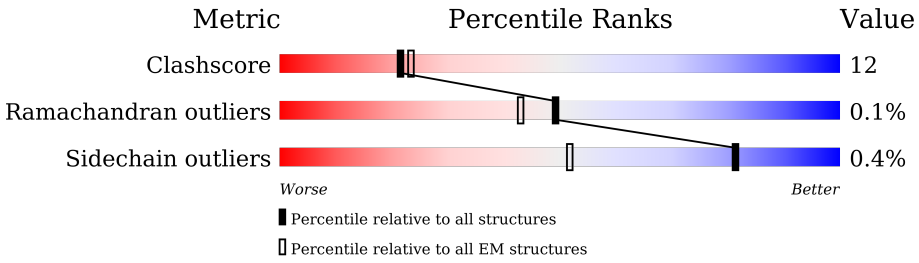
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

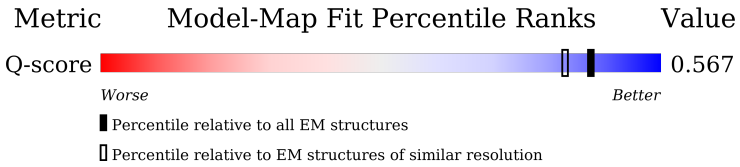
1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	751	83% 15% .
2	B	755	84% 13% .
3	C	81	83% 16% .
4	D	161	75% 14% 11%

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Mol	Chain	Length	Quality of chain
5	E	73	
6	F	165	
7	G	94	
8	I	106	
9	J	41	
10	K	87	
11	L	156	
12	1	194	
12	Z	194	
13	3	268	
14	7	215	
15	8	217	
16	4	236	
17	5	229	
18	6	232	
19	2	221	
20	9	189	

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
22	CLA	A	802	-	-	X	-
22	CLA	A	835	-	-	X	-
25	BCR	4	621	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 48476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	738	Total	C	N	O	S	0	0
			5800	3793	989	996	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5822	3824	978	1002	18		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	insertion	UNP P09144
B	-15	HIS	-	insertion	UNP P09144
B	-14	HIS	-	insertion	UNP P09144
B	-13	HIS	-	insertion	UNP P09144
B	-12	HIS	-	insertion	UNP P09144
B	-11	HIS	-	insertion	UNP P09144
B	-10	HIS	-	insertion	UNP P09144
B	-9	HIS	-	insertion	UNP P09144
B	-8	HIS	-	insertion	UNP P09144
B	-7	HIS	-	insertion	UNP P09144
B	-6	HIS	-	insertion	UNP P09144
B	-5	HIS	-	insertion	UNP P09144
B	-4	HIS	-	insertion	UNP P09144
B	-3	HIS	-	insertion	UNP P09144
B	-2	HIS	-	insertion	UNP P09144
B	-1	HIS	-	insertion	UNP P09144
B	0	HIS	-	insertion	UNP P09144
B	1	HIS	-	insertion	UNP P09144
B	2	HIS	-	insertion	UNP P09144
B	3	HIS	-	insertion	UNP P09144

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1132	725	200	200	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			480	306	85	89		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	68	Total	C	N	O	0	0
			503	327	87	89		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			320	219	45	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	45	Total	C	N	O	S	0	0
			297	190	49	56	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			853	561	136	153	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
12	Z	192	Total	C	N	O	S	0	0
			1436	937	238	258	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	202	Total	C	N	O	S	0	0
			1555	1018	252	277	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	212	Total	C	N	O	S	0	0
			1644	1069	273	296	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	203	Total	C	N	O	S	0	0
			1570	1029	254	282	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	223	Total	C	N	O	S	0	0
			1744	1137	291	308	8		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1765	1164	292	303	6		

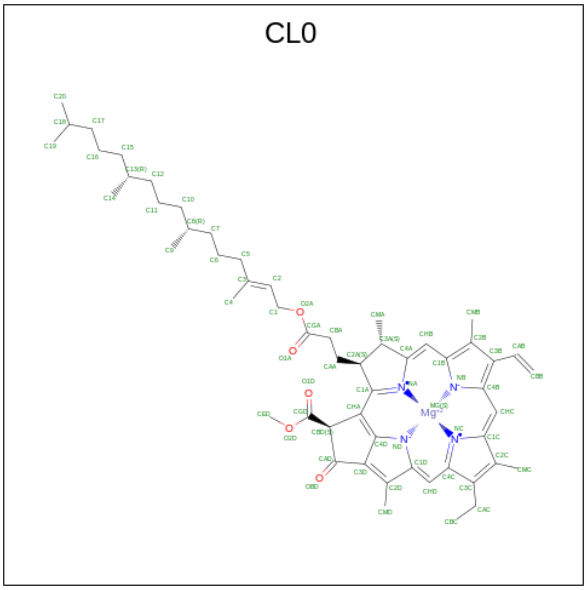
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	119	Total	C	N	O	S	0	0
			838	535	147	151	5		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

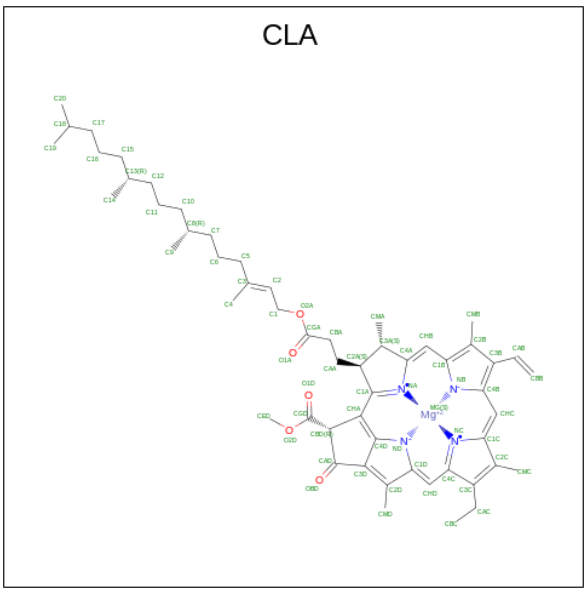
Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	152	Total	C	N	O	S	0	0
			1180	766	195	213	6		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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: $C_{55}H_{72}MgN_4O_5$).



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
			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
			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	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	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			60	50	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
			57	47	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
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			49	39	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
			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
			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
			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	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			50	40	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
			51	41	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
			52	42	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	
22	B	1	Total	C	Mg	N	O	0
			45	35	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
			54	44	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
			60	50	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
			55	45	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
			56	46	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
			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
			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
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			49	39	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	

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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
			45	35	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
			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
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	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
			65	55	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			50	40	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	

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	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
			60	50	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
			52	42	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
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	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
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	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
			41	33	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	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
			52	42	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	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
			52	42	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			56	46	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
			41	33	1	4	3	
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
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	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
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	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
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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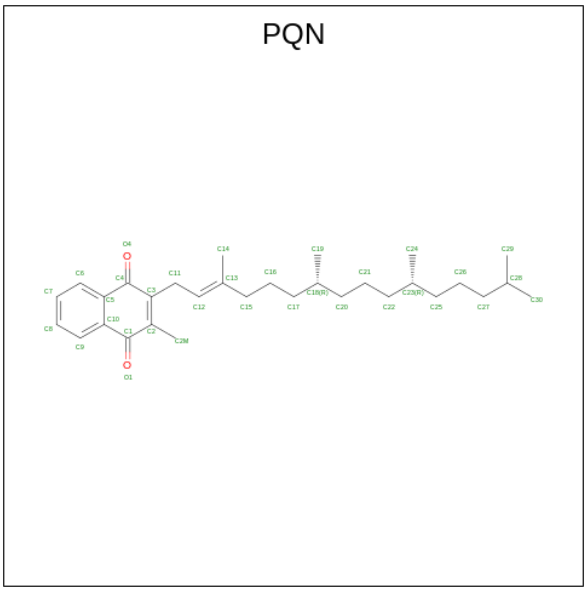
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	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
			52	42	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			56	46	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
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	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
			46	36	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
			50	40	1	4	5	

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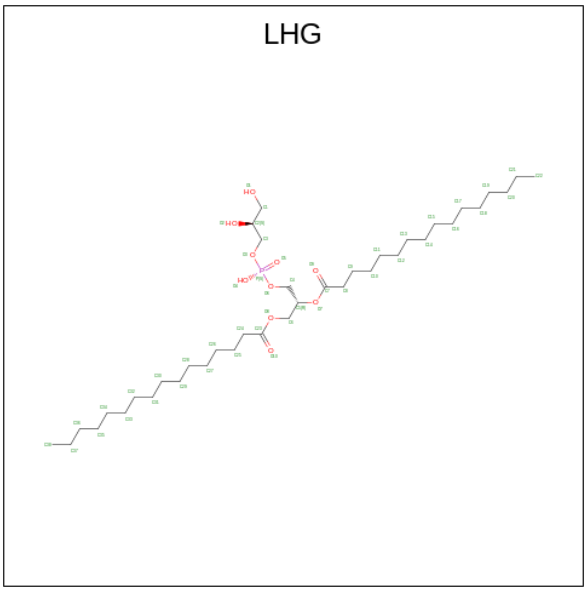
Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



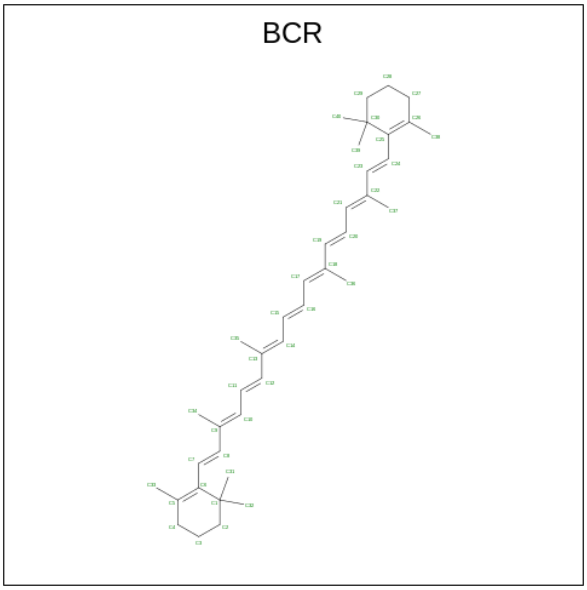
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			38	27	10	1	
24	A	1	Total	C	O	P	0
			30	19	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	1	1	Total	C	O	P	0
			43	32	10	1	
24	7	1	Total	C	O	P	0
			37	26	10	1	
24	8	1	Total	C	O	P	0
			37	26	10	1	
24	Z	1	Total	C	O	P	0
			43	32	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	4	1	Total	C	O	P	0
			32	21	10	1	
24	5	1	Total	C	O	P	0
			37	26	10	1	
24	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



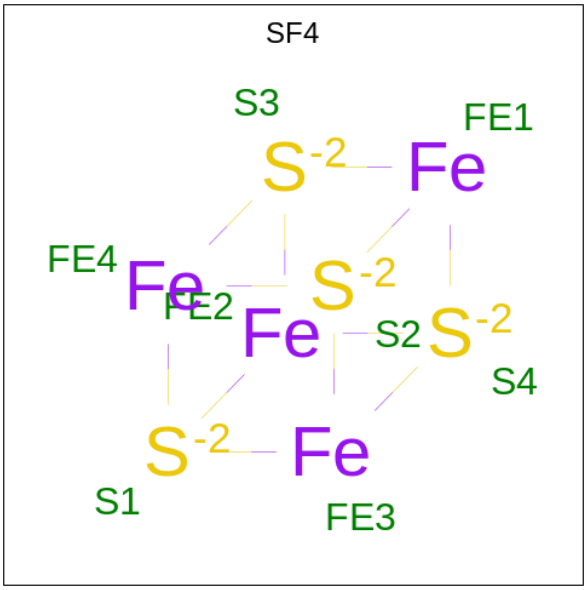
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	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	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	6	1	Total C 40 40	0

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



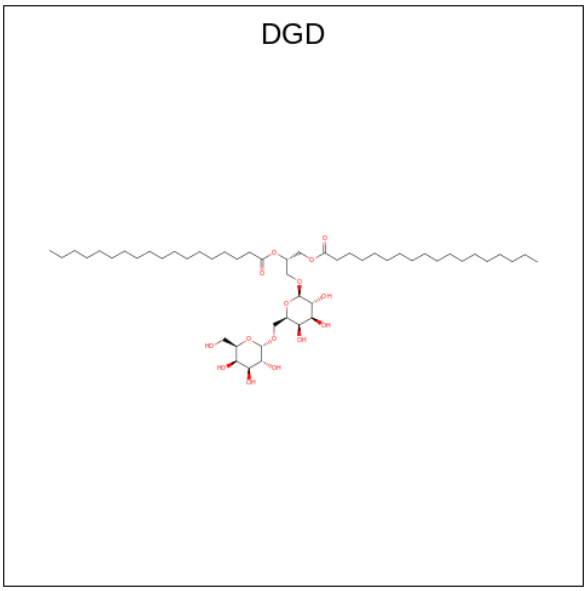
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total Fe S 8 4 4	0

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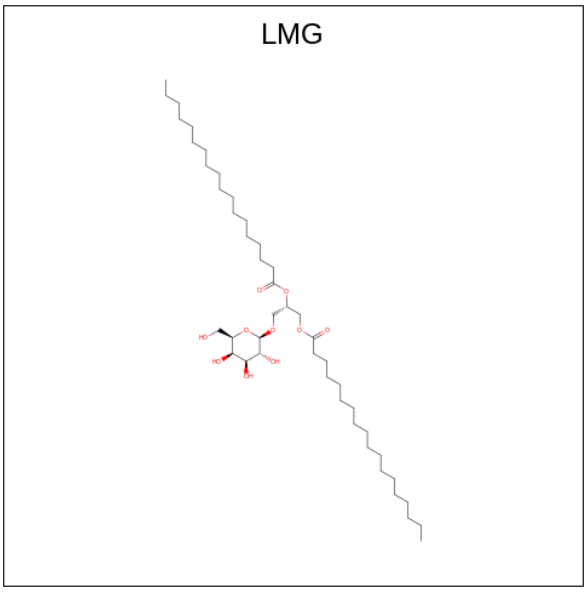
Mol	Chain	Residues	Atoms	AltConf
26	C	1	Total Fe S 8 4 4	0
26	C	1	Total Fe S 8 4 4	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



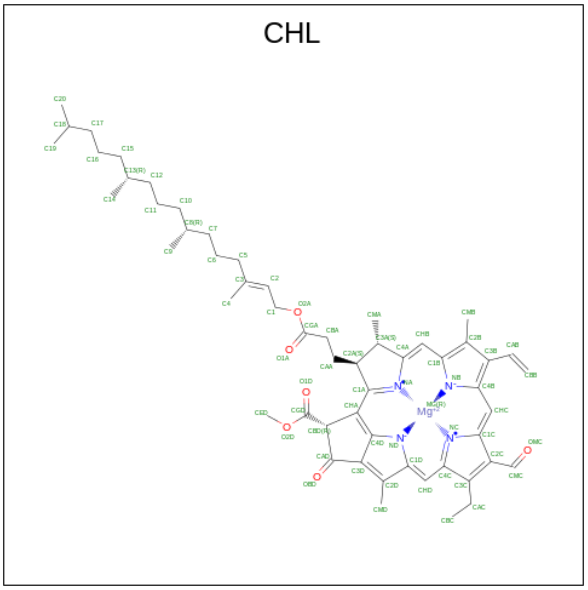
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C O 66 51 15	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total 35	C 25	O 10	0
28	9	1	Total 44	C 34	O 10	0

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



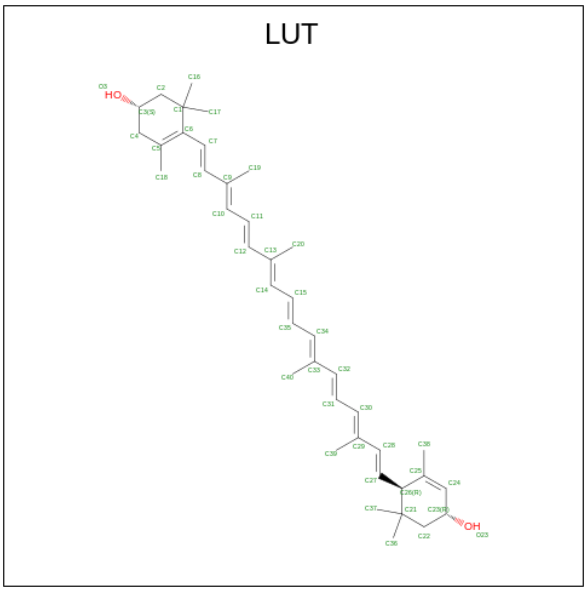
Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total 53	C 42	Mg 1	N 4	O 6	0
29	1	1	Total 48	C 37	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	Z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	Z	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	1	1	Total	C	O	0
			42	40	2	
30	1	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	Z	1	Total	C	O	0
			42	40	2	
30	Z	1	Total	C	O	0
			42	40	2	
30	Z	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	

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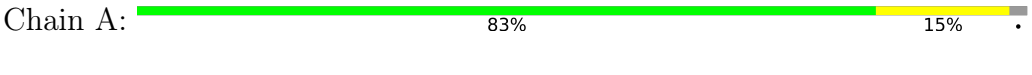
Mol	Chain	Residues	Atoms			AltConf
30	5	1	Total	C	O	0
			42	40	2	
30	5	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	

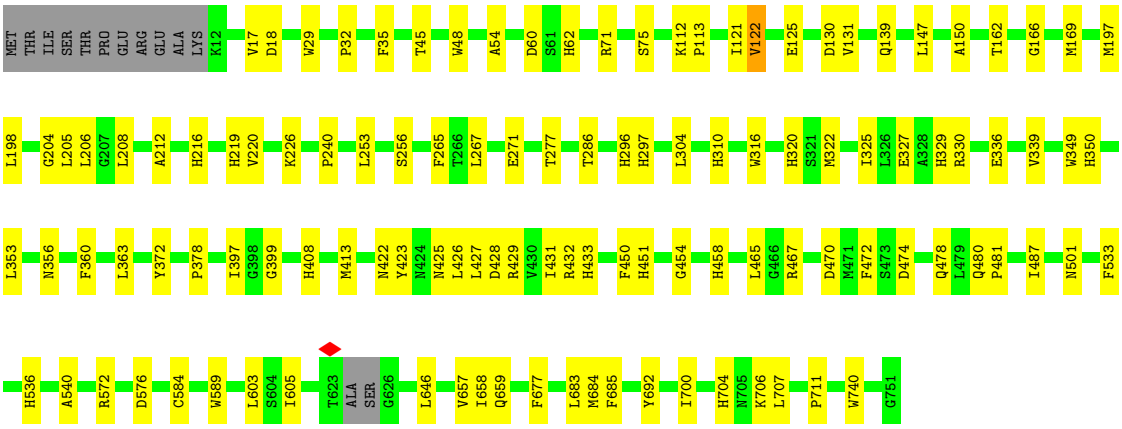
3 Residue-property plots (i)

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

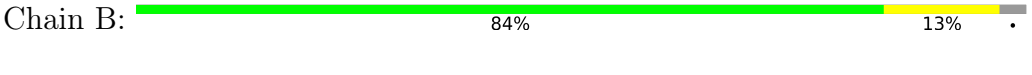
Chain A:

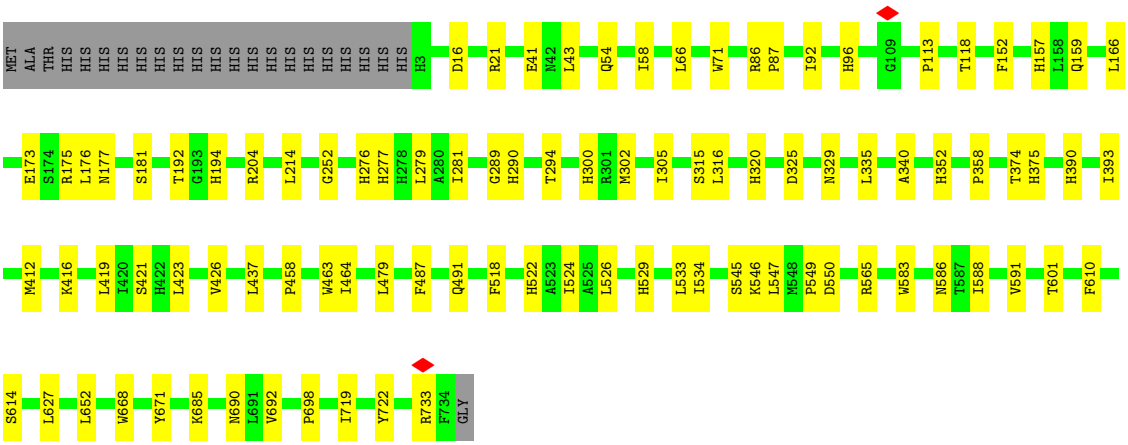




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

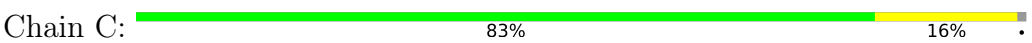
Chain B:

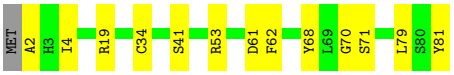




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

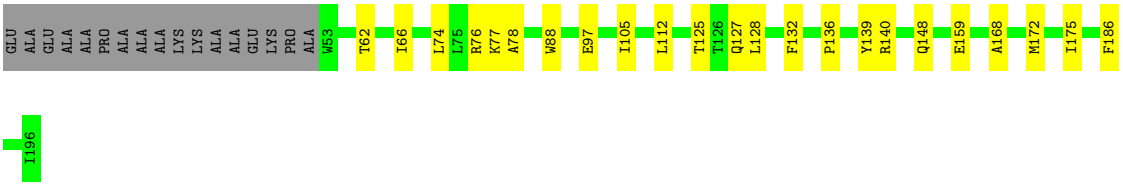




• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:





• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:

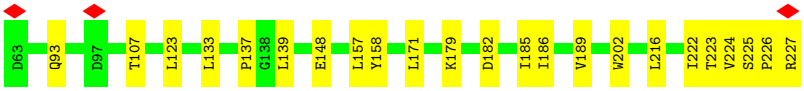




• Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic

Chain F:

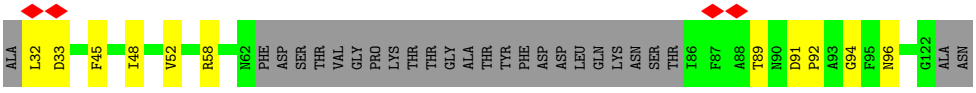




• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:

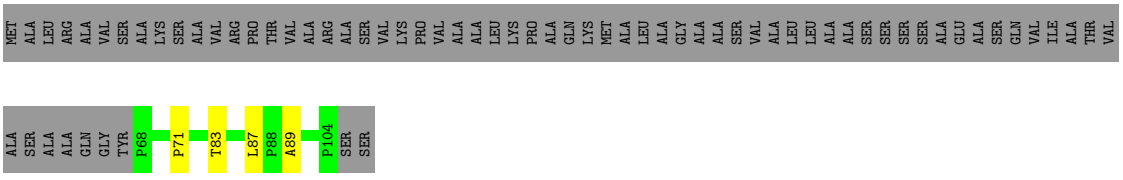




• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:





• Molecule 9: Photosystem I reaction center subunit IX

Chain J:

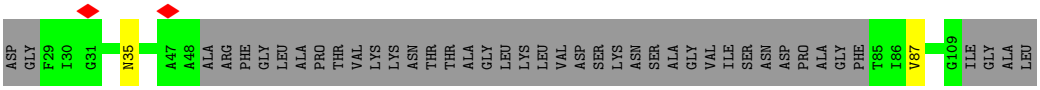




• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

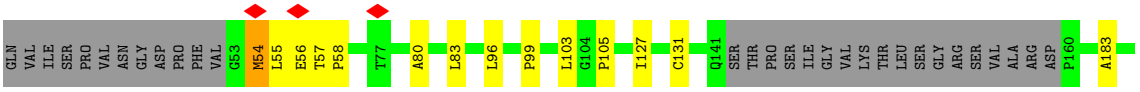




• Molecule 11: Photosystem I reaction center subunit XI

Chain L:

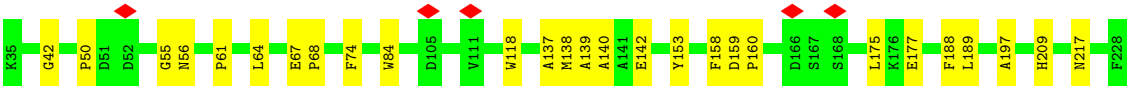




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

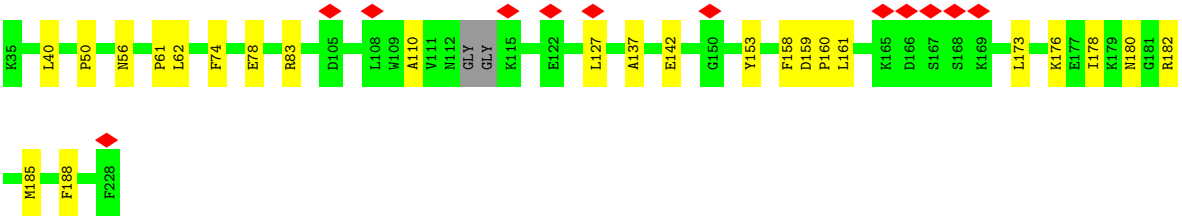




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:

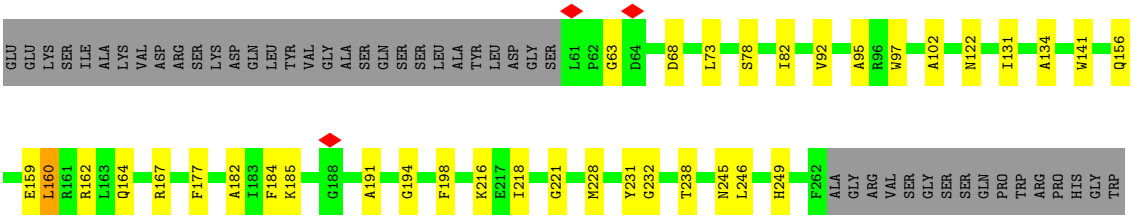




• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



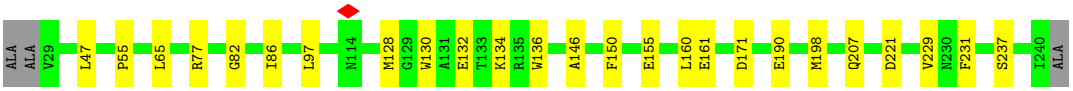




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

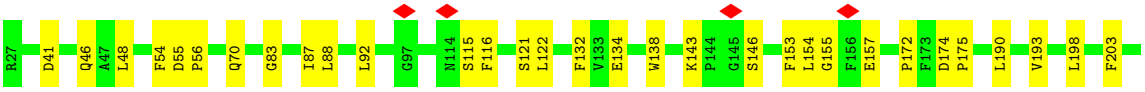




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



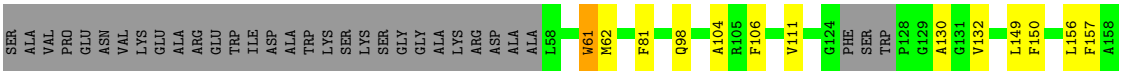




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



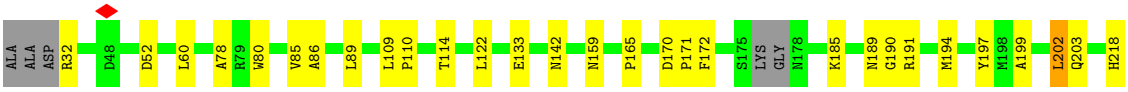


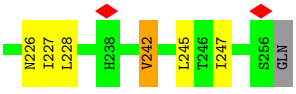


• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



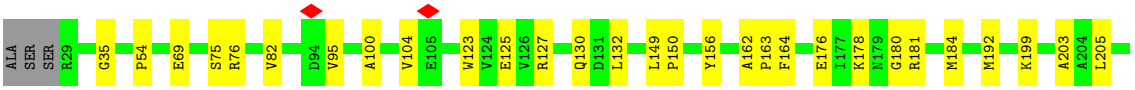


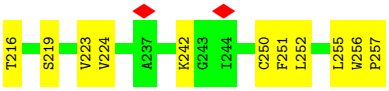


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

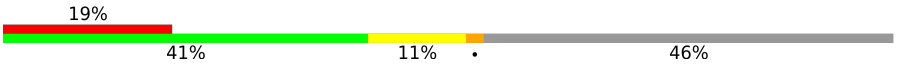


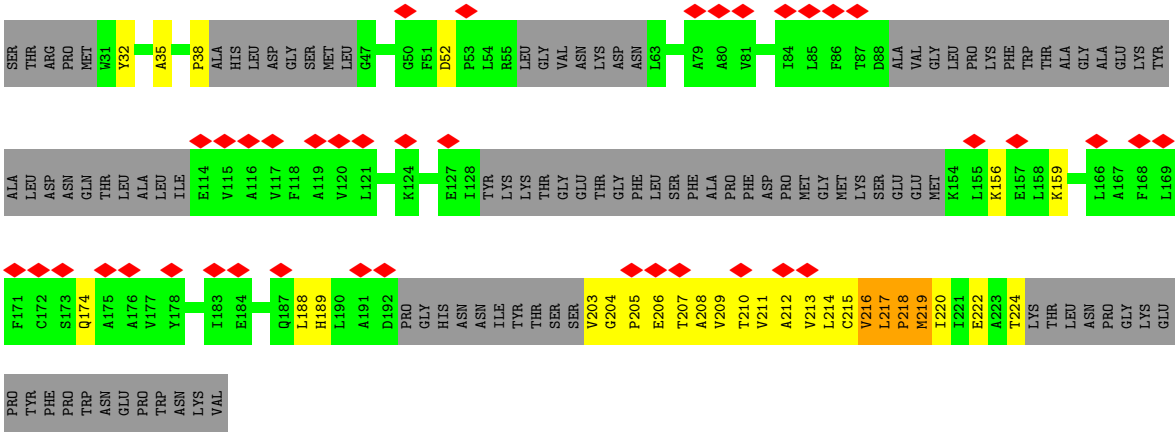




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

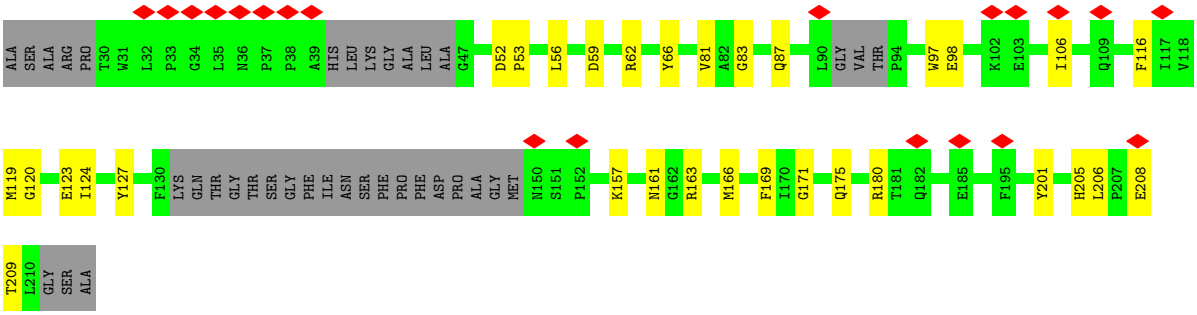




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.34	0/5995	0.69	0/8172
2	B	0.29	0/6035	0.55	0/8240
3	C	0.30	0/610	0.68	0/826
4	D	0.24	0/1160	0.49	0/1567
5	E	0.21	0/490	0.40	0/667
6	F	0.27	0/1291	0.56	0/1747
7	G	0.20	0/513	0.50	0/696
8	I	0.28	0/293	0.57	0/406
9	J	0.27	0/331	0.59	0/454
10	K	0.20	0/297	0.41	0/401
11	L	0.27	0/874	0.56	0/1194
12	1	0.24	0/1490	0.50	0/2028
12	Z	0.24	0/1481	0.53	0/2015
13	3	0.30	0/1601	0.58	1/2173 (0.0%)
14	7	0.27	0/1696	0.57	0/2303
15	8	0.30	0/1700	0.61	0/2315
16	4	0.27	0/1621	0.64	6/2209 (0.3%)
17	5	0.25	0/1798	0.55	2/2450 (0.1%)
18	6	0.22	0/1827	0.49	0/2497
19	2	0.41	1/851 (0.1%)	0.85	6/1154 (0.5%)
20	9	0.29	0/1211	0.60	2/1643 (0.1%)
All	All	0.29	1/33165 (0.0%)	0.59	17/45157 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
14	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	217	LEU	C-N	5.60	1.41	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	4	209	LYS	N-CA-C	-8.43	102.09	111.28
19	2	204	GLY	O-C-N	7.68	123.83	121.07
19	2	218	PRO	CA-N-CD	-7.29	101.79	112.00
19	2	217	LEU	CA-C-N	-7.06	111.52	119.28
19	2	217	LEU	C-N-CA	-7.06	111.52	119.28
19	2	216	VAL	N-CA-C	-6.95	103.53	110.62
16	4	61	TRP	CA-C-N	6.34	129.24	122.26
16	4	61	TRP	C-N-CA	6.34	129.24	122.26
16	4	206	GLY	N-CA-C	-6.05	103.26	112.51
17	5	242	VAL	CA-C-N	5.87	129.63	120.82
17	5	242	VAL	C-N-CA	5.87	129.63	120.82
19	2	217	LEU	C-N-CD	5.26	146.56	125.00
20	9	106	ILE	CA-C-N	5.25	139.59	127.00
20	9	106	ILE	C-N-CA	5.25	139.59	127.00
16	4	238	THR	CA-C-N	5.22	136.09	120.69
16	4	238	THR	C-N-CA	5.22	136.09	120.69
13	3	122	ASN	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	7	150	PHE	Peptide
2	B	668	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5800	0	5646	108	0
2	B	5822	0	5574	97	0
3	C	600	0	581	11	0
4	D	1132	0	1150	17	0
5	E	480	0	476	7	0
6	F	1265	0	1301	52	0
7	G	503	0	496	7	0
8	I	281	0	292	5	0
9	J	320	0	322	7	0
10	K	297	0	319	2	0
11	L	853	0	864	25	0
12	1	1444	0	1395	24	0
12	Z	1436	0	1388	21	0
13	3	1555	0	1522	29	0
14	7	1644	0	1582	22	0
15	8	1649	0	1628	34	0
16	4	1570	0	1526	71	0
17	5	1744	0	1715	40	0
18	6	1765	0	1767	42	0
19	2	838	0	767	65	0
20	9	1180	0	1160	34	0
21	A	65	0	72	3	0
22	1	722	0	735	31	0
22	2	540	0	426	18	0
22	3	696	0	630	23	0
22	4	576	0	490	41	0
22	5	737	0	632	26	0
22	6	696	0	620	40	0
22	7	741	0	658	30	0
22	8	680	0	592	20	0
22	9	514	0	426	15	0
22	A	2689	0	2796	193	0
22	B	2480	0	2545	116	0
22	F	175	0	177	5	0
22	G	96	0	72	0	0
22	J	42	0	31	0	0
22	K	91	0	66	3	0
22	L	115	0	111	0	0
22	Z	714	0	714	22	0
23	A	33	0	46	4	0
23	B	33	0	46	1	0
24	1	43	0	56	2	0
24	4	81	0	106	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	5	37	0	44	0	0
24	6	49	0	74	19	0
24	7	37	0	44	0	0
24	8	37	0	44	1	0
24	A	117	0	153	5	0
24	B	23	0	16	0	0
24	Z	43	0	56	1	0
25	3	120	0	163	12	0
25	4	40	0	56	39	0
25	5	80	0	112	11	0
25	6	80	0	110	10	0
25	7	80	0	112	6	0
25	8	40	0	56	6	0
25	A	240	0	336	24	0
25	B	280	0	392	28	0
25	F	40	0	56	15	0
25	G	40	0	56	3	0
25	I	40	0	56	1	0
25	J	40	0	56	2	0
25	K	80	0	112	5	0
25	L	80	0	112	9	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	2	0
28	9	44	0	61	1	0
28	J	35	0	40	0	0
29	1	101	0	74	5	0
29	3	66	0	70	3	0
29	4	201	0	150	24	0
29	5	145	0	101	5	0
29	6	206	0	159	9	0
29	7	54	0	43	1	0
29	8	56	0	47	0	0
29	9	93	0	64	1	0
29	Z	101	0	73	1	0
30	1	126	0	168	13	0
30	2	84	0	112	6	0
30	3	84	0	112	7	0
30	4	84	0	112	17	0
30	5	84	0	112	20	0
30	6	84	0	112	8	0
30	7	84	0	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	8	84	0	112	12	0
30	9	84	0	112	8	0
30	Z	126	0	168	11	0
All	All	48476	0	47944	1124	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 12.

All (1124) 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)
16:4:257:TRP:CD1	22:4:616:CLA:CBB	1.75	1.60
19:2:32:TYR:CE2	19:2:35:ALA:HB2	1.37	1.59
22:A:802:CLA:C19	22:A:842:CLA:C4	1.79	1.53
19:2:32:TYR:CD2	19:2:35:ALA:HB2	1.41	1.50
1:A:198:LEU:HD23	1:A:322:MET:CE	1.43	1.48
22:A:805:CLA:C4	22:A:812:CLA:HBB1	1.44	1.45
19:2:189:HIS:ND1	22:2:613:CLA:CAA	1.80	1.41
19:2:189:HIS:ND1	22:2:613:CLA:HAA2	1.09	1.39
19:2:189:HIS:CE1	22:2:613:CLA:HAA2	1.63	1.33
2:B:416:LYS:NZ	6:F:226:PRO:CG	1.91	1.33
19:2:32:TYR:CE2	19:2:35:ALA:CB	2.11	1.31
1:A:198:LEU:CD2	1:A:322:MET:HE1	1.58	1.31
22:A:833:CLA:OBD	11:L:57:THR:HG21	1.34	1.22
17:5:185:LYS:O	17:5:189:ASN:ND2	1.76	1.18
2:B:416:LYS:NZ	6:F:226:PRO:HG2	1.50	1.17
2:B:416:LYS:HZ3	6:F:226:PRO:CG	1.51	1.17
1:A:198:LEU:CD2	1:A:322:MET:CE	2.17	1.16
19:2:222:GLU:HG3	20:9:127:TYR:HE2	1.10	1.16
2:B:159:GLN:HE21	19:2:224:THR:HG21	1.09	1.15
17:5:85:VAL:HG11	30:5:620:LUT:H12	1.29	1.14
19:2:222:GLU:CG	20:9:127:TYR:HE2	1.59	1.14
11:L:186:TYR:O	11:L:188:CYS:N	1.80	1.13
22:B:820:CLA:HHC	22:B:820:CLA:HBB1	1.25	1.12
2:B:416:LYS:NZ	6:F:226:PRO:HG3	1.61	1.11
18:6:257:PRO:HB2	22:6:616:CLA:HAB	1.27	1.11
22:B:812:CLA:HBB2	22:B:820:CLA:C7	1.81	1.10
22:B:841:CLA:HHC	22:B:841:CLA:HBB1	1.34	1.08
22:B:812:CLA:HBB2	22:B:820:CLA:H72	1.08	1.07
16:4:207:ASP:HB3	16:4:209:LYS:HE2	1.07	1.06
22:A:805:CLA:HHC	22:A:805:CLA:HBB1	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:805:CLA:H42	22:A:812:CLA:HBB1	1.37	1.04
19:2:209:VAL:O	19:2:213:VAL:HG23	1.56	1.04
22:A:815:CLA:HHC	22:A:815:CLA:HBB1	1.39	1.04
19:2:32:TYR:CD2	19:2:35:ALA:CB	2.34	1.04
6:F:223:THR:OG1	6:F:227:ARG:NH2	1.91	1.03
22:7:620:CLA:CGA	18:6:250:CYS:O	2.06	1.03
17:5:203:GLN:NE2	30:5:620:LUT:O3	1.91	1.03
15:8:242:PHE:CE2	15:8:243:LEU:HG	1.94	1.02
1:A:198:LEU:HD21	1:A:322:MET:HE1	1.35	1.02
22:A:805:CLA:C4	22:A:812:CLA:CBB	2.37	1.01
6:F:223:THR:CB	6:F:227:ARG:HH22	1.74	1.01
19:2:222:GLU:CG	20:9:127:TYR:CE2	2.45	1.00
2:B:159:GLN:NE2	19:2:224:THR:HG21	1.77	1.00
22:B:831:CLA:HBC3	25:F:305:BCR:H362	1.43	1.00
2:B:159:GLN:HE21	19:2:224:THR:CG2	1.73	0.99
22:A:805:CLA:H43	22:A:812:CLA:HBB1	1.45	0.99
6:F:223:THR:CB	6:F:227:ARG:NH2	2.27	0.98
2:B:416:LYS:HZ1	6:F:226:PRO:CG	1.64	0.97
16:4:207:ASP:CB	16:4:209:LYS:HE2	1.95	0.97
22:A:802:CLA:C19	22:A:842:CLA:H41	1.94	0.97
16:4:207:ASP:HB3	16:4:209:LYS:CE	1.93	0.96
11:L:183:ALA:O	11:L:187:VAL:HG23	1.66	0.96
19:2:222:GLU:HG3	20:9:127:TYR:CE2	2.02	0.95
22:4:604:CLA:CHC	25:4:621:BCR:H393	1.96	0.95
16:4:257:TRP:HD1	22:4:616:CLA:CBB	1.65	0.94
11:L:186:TYR:C	11:L:188:CYS:H	1.72	0.94
1:A:212:ALA:HB3	22:A:815:CLA:HBB2	1.47	0.94
22:7:620:CLA:H91	29:6:607:CHL:H42	1.47	0.93
16:4:257:TRP:NE1	22:4:616:CLA:CBB	2.31	0.93
22:4:604:CLA:CHC	25:4:621:BCR:C39	2.46	0.93
20:9:120:GLY:O	20:9:124:ILE:HG12	1.68	0.93
18:6:257:PRO:HB2	22:6:616:CLA:CAB	1.99	0.92
22:7:620:CLA:H111	29:6:607:CHL:H41	1.52	0.92
19:2:189:HIS:ND1	22:2:613:CLA:HAA1	1.84	0.92
19:2:222:GLU:HG2	20:9:127:TYR:CE2	2.05	0.91
24:6:619:LHG:H111	24:6:619:LHG:C27	1.99	0.91
22:B:812:CLA:CBB	22:B:820:CLA:H72	2.00	0.91
19:2:214:LEU:O	19:2:218:PRO:HD3	1.70	0.90
22:A:805:CLA:H41	22:A:812:CLA:HBB1	1.51	0.90
24:6:619:LHG:H111	24:6:619:LHG:H272	1.52	0.90
1:A:198:LEU:HD23	1:A:322:MET:HE3	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:207:GLN:NE2	30:7:621:LUT:O3	2.04	0.90
1:A:198:LEU:HD23	1:A:322:MET:HE2	1.52	0.89
18:6:257:PRO:CB	22:6:616:CLA:HAB	2.01	0.89
19:2:212:ALA:O	19:2:216:VAL:HG23	1.74	0.88
6:F:224:VAL:HG12	6:F:226:PRO:CD	2.05	0.87
16:4:257:TRP:CG	22:4:616:CLA:CBB	2.57	0.87
29:4:618:CHL:HBB2	25:4:621:BCR:H10C	1.54	0.87
1:A:212:ALA:CB	22:A:815:CLA:HBB2	2.04	0.86
6:F:223:THR:CG2	6:F:227:ARG:HH22	1.89	0.84
22:4:604:CLA:C4B	25:4:621:BCR:H393	2.07	0.83
22:6:601:CLA:C3B	24:6:619:LHG:H282	2.07	0.83
6:F:224:VAL:HG12	6:F:226:PRO:HD2	1.58	0.83
18:6:252:LEU:HB2	22:6:622:CLA:HMA2	1.60	0.83
19:2:219:MET:HE3	22:9:609:CLA:H3A	1.60	0.83
16:4:111:VAL:HG11	30:4:619:LUT:H12	1.59	0.83
6:F:226:PRO:O	6:F:227:ARG:HB2	1.76	0.82
13:3:194:GLY:O	13:3:198:PHE:HB2	1.79	0.82
29:4:618:CHL:CBB	25:4:621:BCR:H10C	2.09	0.82
6:F:225:SER:N	6:F:226:PRO:HD2	1.94	0.82
13:3:156:GLN:O	13:3:160:LEU:HB2	1.79	0.82
22:6:601:CLA:H2	24:6:619:LHG:H152	1.62	0.82
19:2:219:MET:HE2	22:9:609:CLA:HMA3	1.63	0.81
20:9:83:GLY:O	20:9:87:GLN:HG3	1.81	0.81
22:B:820:CLA:HBB1	22:B:820:CLA:CHC	2.08	0.81
25:F:305:BCR:H331	25:F:305:BCR:C8	2.11	0.81
22:7:620:CLA:C9	29:6:607:CHL:H42	2.10	0.80
19:2:207:THR:O	19:2:211:VAL:HG13	1.81	0.80
22:B:825:CLA:H72	22:B:841:CLA:H191	1.62	0.80
17:5:203:GLN:HE22	30:5:620:LUT:HO3	1.28	0.80
19:2:219:MET:CE	22:9:609:CLA:HMA3	2.11	0.80
2:B:315:SER:OG	22:B:841:CLA:O1A	2.00	0.80
22:B:803:CLA:HMB1	22:B:803:CLA:HBB1	1.62	0.80
6:F:224:VAL:HG12	6:F:225:SER:H	1.46	0.80
20:9:62:ARG:HD2	20:9:66:TYR:CE2	2.17	0.80
22:A:805:CLA:CBB	22:A:807:CLA:CAD	2.60	0.79
6:F:224:VAL:CG1	6:F:226:PRO:HD2	2.12	0.79
22:A:802:CLA:CGA	22:A:802:CLA:H3A	2.11	0.79
22:6:601:CLA:C4B	24:6:619:LHG:H282	2.11	0.79
22:A:815:CLA:H2	22:A:817:CLA:HMB1	1.64	0.78
6:F:224:VAL:CB	6:F:226:PRO:HD2	2.14	0.78
1:A:212:ALA:CB	22:A:815:CLA:CBB	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:LEU:HD13	25:F:305:BCR:H321	1.65	0.77
19:2:203:VAL:HG13	19:2:206:GLU:OE1	1.85	0.77
2:B:719:ILE:HG23	22:B:827:CLA:HBB1	1.66	0.76
17:5:171:PRO:HD2	30:5:620:LUT:H23	1.66	0.76
19:2:32:TYR:CE2	19:2:35:ALA:CA	2.68	0.76
1:A:212:ALA:HB1	22:A:815:CLA:CBB	2.16	0.76
12:Z:176:LYS:O	12:Z:180:ASN:ND2	2.18	0.75
6:F:223:THR:HG21	6:F:227:ARG:NH2	2.02	0.75
11:L:55:LEU:HD23	11:L:56:GLU:N	2.02	0.75
29:4:606:CHL:HAA1	25:4:621:BCR:H23C	1.70	0.74
6:F:224:VAL:C	6:F:226:PRO:HD2	2.13	0.74
22:2:601:CLA:HBB2	22:2:602:CLA:HHD	1.67	0.74
15:8:138:TRP:CE3	22:8:609:CLA:HMA3	2.22	0.74
19:2:214:LEU:O	19:2:217:LEU:HB3	1.87	0.73
22:3:610:CLA:HBB1	30:3:621:LUT:H32	1.69	0.73
22:A:832:CLA:HED2	11:L:55:LEU:HD11	1.71	0.73
6:F:225:SER:N	6:F:226:PRO:CD	2.51	0.73
22:A:805:CLA:HBB2	22:A:807:CLA:CAD	2.19	0.73
29:4:618:CHL:HAB	25:4:621:BCR:C10	2.19	0.73
22:A:835:CLA:H42	25:L:201:BCR:C36	2.18	0.73
22:B:820:CLA:O1A	22:B:820:CLA:H3A	1.89	0.73
1:A:310:HIS:CE1	25:K:4001:BCR:H363	2.24	0.72
19:2:215:CYS:O	19:2:218:PRO:HD2	1.88	0.72
16:4:208:ILE:CG2	16:4:212:LYS:HE3	2.20	0.72
16:4:156:LEU:HD12	25:4:621:BCR:C15	2.20	0.72
6:F:224:VAL:HG12	6:F:225:SER:N	2.03	0.72
18:6:82:VAL:HG11	30:6:621:LUT:H12	1.71	0.72
14:7:97:LEU:HD23	22:7:620:CLA:H2A	1.71	0.71
19:2:219:MET:HE3	22:9:609:CLA:C3A	2.20	0.71
22:A:832:CLA:HAA2	11:L:57:THR:HG23	1.72	0.71
19:2:219:MET:CE	22:9:609:CLA:CMA	2.68	0.71
6:F:223:THR:HG21	6:F:227:ARG:HH22	1.54	0.71
22:A:806:CLA:H61	25:A:849:BCR:HC8	1.73	0.71
22:B:825:CLA:H52	22:B:841:CLA:H201	1.72	0.71
22:B:818:CLA:HAB	22:B:818:CLA:H8	1.71	0.71
14:7:134:LYS:HG3	22:7:608:CLA:HBB1	1.73	0.71
22:A:835:CLA:O2D	22:A:835:CLA:H2A	1.91	0.70
22:B:806:CLA:HHB	22:B:829:CLA:HAB	1.71	0.70
22:A:806:CLA:H11	22:A:807:CLA:HBB1	1.71	0.70
22:A:835:CLA:H42	25:L:201:BCR:H363	1.74	0.70
2:B:487:PHE:O	2:B:491:GLN:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:219:MET:HE3	22:9:609:CLA:CMA	2.21	0.70
13:3:159:GLU:OE2	13:3:162:ARG:NH2	2.23	0.70
16:4:208:ILE:HD11	22:4:610:CLA:HMA1	1.72	0.70
19:2:189:HIS:CG	22:2:613:CLA:HAA2	2.19	0.70
29:4:618:CHL:CAB	25:4:621:BCR:H10C	2.20	0.70
19:2:222:GLU:HG2	20:9:127:TYR:CD2	2.27	0.69
22:A:802:CLA:H122	25:A:852:BCR:H23C	1.75	0.69
22:3:609:CLA:HBB1	22:3:617:CLA:HBB1	1.75	0.69
2:B:276:HIS:HE1	22:B:816:CLA:C1A	2.05	0.69
6:F:224:VAL:HG12	6:F:226:PRO:HD3	1.75	0.69
19:2:206:GLU:O	19:2:210:THR:HG23	1.92	0.69
22:A:835:CLA:C4	25:L:201:BCR:H363	2.22	0.69
16:4:203:TRP:O	16:4:204:SER:HB2	1.90	0.69
22:A:802:CLA:H121	22:A:802:CLA:H91	1.74	0.69
22:A:835:CLA:HHC	22:A:835:CLA:HBB1	1.74	0.69
2:B:545:SER:HA	6:F:224:VAL:HG11	1.75	0.69
14:7:132:GLU:HG2	22:7:609:CLA:C1B	2.23	0.69
1:A:169:MET:HG3	25:A:848:BCR:H322	1.75	0.68
22:B:812:CLA:CBB	22:B:820:CLA:H102	2.24	0.68
2:B:290:HIS:O	22:B:820:CLA:HED1	1.93	0.68
6:F:223:THR:CG2	6:F:227:ARG:NH2	2.54	0.68
19:2:216:VAL:O	19:2:220:ILE:HG13	1.92	0.68
24:6:619:LHG:H111	24:6:619:LHG:C28	2.23	0.68
22:A:843:CLA:H143	25:L:201:BCR:H17C	1.74	0.68
1:A:297:HIS:HB2	22:A:819:CLA:C1B	2.24	0.68
19:2:208:ALA:O	19:2:211:VAL:HG22	1.95	0.67
22:A:832:CLA:HBB1	24:A:847:LHG:H141	1.76	0.67
24:6:619:LHG:H111	24:6:619:LHG:H281	1.77	0.67
22:6:613:CLA:H52	24:6:619:LHG:H182	1.77	0.67
22:A:805:CLA:HBB2	22:A:807:CLA:C3D	2.25	0.67
29:4:608:CHL:HMA1	25:4:621:BCR:C36	2.25	0.66
1:A:458:HIS:HE1	22:A:835:CLA:C1A	2.08	0.66
18:6:252:LEU:CB	22:6:622:CLA:HMA2	2.26	0.66
22:A:805:CLA:HBB1	22:A:805:CLA:CHC	2.19	0.66
6:F:224:VAL:CG1	6:F:226:PRO:CD	2.71	0.66
6:F:226:PRO:O	6:F:227:ARG:CB	2.43	0.66
2:B:416:LYS:CE	6:F:226:PRO:HG2	2.26	0.66
6:F:224:VAL:HB	6:F:226:PRO:HD2	1.77	0.66
22:A:802:CLA:H191	22:A:842:CLA:C4	2.14	0.66
16:4:232:GLN:HE22	30:4:619:LUT:C3	2.08	0.65
29:4:608:CHL:HMA1	25:4:621:BCR:H362	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:602:CLA:HBB1	30:1:618:LUT:H32	1.79	0.65
16:4:159:TRP:CH2	25:4:621:BCR:H331	2.32	0.65
17:5:245:LEU:HD11	25:5:625:BCR:H352	1.78	0.65
16:4:207:ASP:HB2	16:4:209:LYS:HG2	1.78	0.65
22:7:620:CLA:H111	29:6:607:CHL:C4	2.26	0.65
22:A:802:CLA:H192	22:A:842:CLA:C4	2.15	0.65
18:6:251:PHE:HB2	25:6:625:BCR:H282	1.77	0.65
13:3:238:THR:HG21	13:3:245:ASN:HD21	1.61	0.65
22:A:805:CLA:H41	22:A:812:CLA:CBB	2.18	0.65
22:B:803:CLA:HBB1	22:B:803:CLA:CMB	2.27	0.64
29:4:606:CHL:CBA	25:4:621:BCR:H21C	2.27	0.64
20:9:206:LEU:O	20:9:209:THR:HG22	1.97	0.64
1:A:470:ASP:HB3	22:A:835:CLA:HED3	1.78	0.64
25:F:305:BCR:H383	25:F:305:BCR:H23C	1.79	0.64
1:A:605:ILE:HD12	21:A:801:CL0:H53	1.79	0.64
22:A:809:CLA:HBB2	22:A:829:CLA:H203	1.80	0.64
14:7:132:GLU:HG2	22:7:609:CLA:NB	2.12	0.64
16:4:208:ILE:HD11	22:4:610:CLA:H2A	1.78	0.64
1:A:458:HIS:CE1	22:A:835:CLA:C1A	2.81	0.64
2:B:690:ASN:O	4:D:76:ARG:NH2	2.26	0.64
22:A:815:CLA:HBB1	22:A:815:CLA:CHC	2.20	0.64
1:A:467:ARG:HH22	11:L:105:PRO:HB3	1.61	0.64
2:B:276:HIS:HB3	22:B:817:CLA:HMB2	1.80	0.63
2:B:458:PRO:HG3	2:B:518:PHE:HB2	1.79	0.63
1:A:700:ILE:HD13	22:A:841:CLA:HMD1	1.79	0.63
2:B:416:LYS:HZ3	6:F:226:PRO:CB	2.11	0.63
12:Z:110:ALA:HB1	12:Z:127:LEU:HD12	1.80	0.63
29:4:618:CHL:HAB	25:4:621:BCR:H10C	1.79	0.63
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.79	0.63
22:4:611:CLA:HAB	25:6:623:BCR:H312	1.80	0.63
1:A:454:GLY:HA3	22:A:835:CLA:CBB	2.27	0.63
24:6:619:LHG:H272	24:6:619:LHG:C11	2.28	0.63
20:9:59:ASP:HB3	20:9:62:ARG:HB3	1.79	0.63
1:A:327:GLU:HG2	1:A:339:VAL:HG22	1.81	0.63
2:B:416:LYS:HZ1	6:F:226:PRO:HG2	1.28	0.63
22:A:802:CLA:C1D	2:B:583:TRP:HE1	2.11	0.62
22:A:805:CLA:CBB	22:A:807:CLA:OBD	2.46	0.62
16:4:159:TRP:CH2	25:4:621:BCR:C33	2.82	0.62
9:J:24:GLY:O	9:J:28:GLU:HG2	1.99	0.62
1:A:572:ARG:NH1	24:A:846:LHG:O10	2.32	0.62
9:J:28:GLU:OE1	9:J:28:GLU:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:76:ARG:NE	18:6:176:GLU:OE2	2.29	0.62
22:A:802:CLA:H203	22:A:831:CLA:H191	1.81	0.62
22:B:823:CLA:HBA1	25:B:846:BCR:H16C	1.82	0.62
20:9:119:MET:O	20:9:123:GLU:HG2	1.99	0.61
22:A:803:CLA:H122	25:B:848:BCR:H12C	1.82	0.61
12:Z:158:PHE:CZ	22:Z:608:CLA:NC	2.68	0.61
16:4:208:ILE:HG21	16:4:212:LYS:HE3	1.82	0.61
19:2:189:HIS:CE1	22:2:613:CLA:CAA	2.56	0.61
22:A:833:CLA:OBD	11:L:57:THR:CG2	2.29	0.61
22:B:837:CLA:H151	25:F:305:BCR:H21C	1.83	0.61
11:L:186:TYR:C	11:L:188:CYS:N	2.41	0.61
22:7:610:CLA:HBB1	30:7:621:LUT:H32	1.83	0.61
29:4:606:CHL:HAA1	25:4:621:BCR:H21C	1.82	0.61
17:5:199:ALA:O	17:5:203:GLN:HG3	2.00	0.61
1:A:450:PHE:O	22:A:835:CLA:HBB2	2.01	0.61
1:A:423:TYR:CE1	4:D:105:ILE:HG13	2.36	0.60
1:A:433:HIS:HB3	11:L:55:LEU:CD1	2.31	0.60
2:B:276:HIS:CE1	22:B:816:CLA:NA	2.68	0.60
22:B:839:CLA:H142	25:L:201:BCR:H21C	1.83	0.60
12:1:160:PRO:HD2	30:1:617:LUT:H23	1.83	0.60
22:B:812:CLA:H12	20:9:56:LEU:HD21	1.84	0.60
22:A:815:CLA:H122	22:3:607:CLA:HMC1	1.83	0.60
16:4:207:ASP:O	16:4:208:ILE:HG22	2.01	0.60
1:A:212:ALA:HB1	22:A:815:CLA:HBB1	1.83	0.60
14:7:207:GLN:HE22	30:7:621:LUT:C3	2.14	0.60
1:A:204:GLY:O	1:A:208:LEU:HB2	2.02	0.60
22:B:841:CLA:HBB1	22:B:841:CLA:CHC	2.16	0.60
11:L:187:VAL:HG12	11:L:187:VAL:O	2.00	0.60
14:7:128:MET:O	14:7:132:GLU:HB2	2.02	0.60
22:A:802:CLA:HBB1	22:A:802:CLA:HMB3	1.84	0.59
22:A:816:CLA:H71	25:3:719:BCR:H12C	1.83	0.59
19:2:32:TYR:CZ	19:2:35:ALA:HA	2.38	0.59
19:2:203:VAL:O	19:2:207:THR:HG23	2.00	0.59
20:9:53:PRO:HD2	30:9:617:LUT:H23	1.84	0.59
16:4:209:LYS:N	16:4:209:LYS:HD3	2.17	0.59
1:A:458:HIS:HE1	22:A:835:CLA:CHA	2.14	0.59
22:A:802:CLA:HAA2	22:A:802:CLA:HBD	1.85	0.59
1:A:706:LYS:HE3	6:F:216:LEU:HD22	1.84	0.59
22:B:815:CLA:HBB1	25:B:843:BCR:H382	1.85	0.59
13:3:159:GLU:OE2	13:3:162:ARG:NE	2.35	0.59
19:2:203:VAL:O	19:2:203:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:158:PHE:HZ	22:Z:608:CLA:NC	2.00	0.59
16:4:200:PRO:HD2	30:4:619:LUT:H23	1.84	0.59
18:6:54:PRO:HD2	30:6:624:LUT:H23	1.84	0.59
22:1:610:CLA:HBB1	30:1:617:LUT:H32	1.85	0.58
14:7:97:LEU:HD23	22:7:620:CLA:C2A	2.33	0.58
25:4:621:BCR:H331	25:4:621:BCR:C8	2.32	0.58
19:2:32:TYR:CZ	19:2:35:ALA:CA	2.86	0.58
2:B:374:THR:HG22	22:B:827:CLA:HAB	1.85	0.58
29:1:607:CHL:HBB1	29:1:607:CHL:HMB3	1.85	0.58
16:4:208:ILE:HG23	16:4:212:LYS:HE3	1.83	0.58
22:A:805:CLA:CBB	22:A:812:CLA:H142	2.33	0.58
14:7:97:LEU:CD2	22:7:620:CLA:H2A	2.34	0.58
22:8:604:CLA:HBB1	25:8:619:BCR:H393	1.85	0.58
1:A:130:ASP:OD2	6:F:93:GLN:NE2	2.37	0.58
18:6:75:SER:HB2	18:6:180:GLY:HA3	1.85	0.58
22:B:837:CLA:H162	25:F:305:BCR:H383	1.86	0.58
15:8:172:PRO:HA	12:Z:62:LEU:HD22	1.86	0.58
16:4:208:ILE:CD1	22:4:610:CLA:HMA1	2.33	0.58
15:8:41:ASP:OD1	15:8:46:GLN:NE2	2.36	0.58
15:8:224:HIS:CD2	22:8:614:CLA:NC	2.71	0.58
29:4:606:CHL:HBA2	25:4:621:BCR:H19C	1.86	0.58
22:A:815:CLA:H111	22:3:607:CLA:CBB	2.33	0.58
22:B:838:CLA:HBA2	22:B:841:CLA:H203	1.85	0.58
22:7:620:CLA:HBB1	22:7:620:CLA:H93	1.86	0.57
16:4:213:LEU:HD22	22:4:611:CLA:HED2	1.85	0.57
22:B:826:CLA:H122	25:B:846:BCR:H373	1.86	0.57
22:B:832:CLA:H192	22:B:837:CLA:H121	1.86	0.57
22:B:839:CLA:HBB2	23:B:842:PQN:H141	1.84	0.57
22:B:840:CLA:H191	8:I:89:ALA:HA	1.87	0.57
14:7:55:PRO:HD2	30:7:622:LUT:H23	1.86	0.57
19:2:189:HIS:CG	22:2:613:CLA:CAA	2.80	0.57
15:8:134:GLU:OE1	15:8:134:GLU:HA	2.04	0.57
2:B:547:LEU:O	2:B:565:ARG:NH2	2.38	0.57
1:A:45:THR:HG23	5:E:78:GLN:HE21	1.67	0.57
29:5:607:CHL:H42	25:5:625:BCR:H383	1.85	0.57
19:2:219:MET:HE2	22:9:609:CLA:CMA	2.33	0.57
1:A:125:GLU:OE1	6:F:107:THR:OG1	2.22	0.57
22:A:805:CLA:HAA1	22:A:805:CLA:HBD	1.86	0.57
2:B:152:PHE:CE1	19:2:220:ILE:HD13	2.40	0.57
2:B:546:LYS:HD2	5:E:51:TYR:HA	1.87	0.57
16:4:207:ASP:CB	16:4:209:LYS:HG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:602:CLA:H61	30:6:624:LUT:H28	1.86	0.57
20:9:205:HIS:ND1	20:9:208:GLU:OE2	2.35	0.57
22:A:820:CLA:HAB	22:A:820:CLA:H8	1.86	0.56
15:8:242:PHE:CD2	15:8:243:LEU:HG	2.39	0.56
22:A:802:CLA:H91	22:A:802:CLA:C12	2.35	0.56
2:B:375:HIS:HE2	22:B:828:CLA:C1B	2.18	0.56
12:Z:160:PRO:HD2	30:Z:617:LUT:H23	1.87	0.56
18:6:95:VAL:HG11	22:6:604:CLA:HED2	1.87	0.56
16:4:221:LEU:HD11	22:4:611:CLA:HAC1	1.88	0.56
16:4:106:PHE:CZ	29:4:608:CHL:HED2	2.40	0.56
22:B:822:CLA:HHC	22:B:841:CLA:HED1	1.88	0.56
15:8:198:LEU:HD23	30:8:617:LUT:H11	1.86	0.56
22:A:841:CLA:H2	22:B:832:CLA:H42	1.88	0.56
22:1:610:CLA:H52	30:1:617:LUT:H30	1.87	0.56
16:4:247:HIS:CD2	22:4:614:CLA:NC	2.73	0.56
2:B:281:ILE:HD12	22:B:818:CLA:HBB1	1.88	0.56
25:F:305:BCR:H331	25:F:305:BCR:HC8	1.88	0.56
22:7:601:CLA:H171	22:7:613:CLA:HBC1	1.87	0.56
22:A:835:CLA:H2	11:L:99:PRO:HB2	1.87	0.56
2:B:276:HIS:CE1	22:B:816:CLA:C1A	2.88	0.56
13:3:245:ASN:HD22	22:3:613:CLA:HED2	1.71	0.56
19:2:188:LEU:HD22	22:2:613:CLA:HED1	1.88	0.56
19:2:211:VAL:HG23	19:2:212:ALA:N	2.20	0.56
22:A:802:CLA:H3A	22:A:802:CLA:O2A	2.06	0.55
4:D:140:ARG:HB3	4:D:148:GLN:HB3	1.88	0.55
19:2:217:LEU:O	19:2:217:LEU:HD12	2.06	0.55
1:A:707:LEU:HD12	22:A:841:CLA:HMA2	1.87	0.55
22:A:835:CLA:HHC	22:A:835:CLA:CBB	2.35	0.55
6:F:223:THR:HB	6:F:227:ARG:NH2	2.20	0.55
2:B:54:GLN:HE21	2:B:58:ILE:HG13	1.72	0.55
22:A:815:CLA:HHC	22:A:815:CLA:CBB	2.26	0.55
11:L:57:THR:HG22	11:L:58:PRO:HD2	1.89	0.55
22:9:612:CLA:HMA1	22:9:612:CLA:H2	1.88	0.55
2:B:437:LEU:HD12	22:B:833:CLA:HAB	1.89	0.55
22:4:604:CLA:C1C	25:4:621:BCR:C39	2.85	0.55
17:5:203:GLN:OE1	30:5:620:LUT:H42	2.07	0.55
18:6:216:THR:H	18:6:219:SER:HB2	1.72	0.55
22:B:820:CLA:C1C	22:B:820:CLA:H71	2.37	0.55
12:Z:137:ALA:HB2	22:Z:606:CLA:H52	1.88	0.55
20:9:81:VAL:HG11	30:9:616:LUT:H12	1.89	0.54
22:B:831:CLA:HMD2	22:B:841:CLA:H92	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:226:PHE:CZ	30:4:620:LUT:H10	2.43	0.54
29:4:606:CHL:CAA	25:4:621:BCR:H21C	2.37	0.54
3:C:61:ASP:O	5:E:86:ASN:ND2	2.38	0.54
22:A:802:CLA:CGA	22:A:802:CLA:C3A	2.85	0.54
22:B:813:CLA:H42	25:B:844:BCR:H21C	1.90	0.54
6:F:224:VAL:CG1	6:F:225:SER:H	2.18	0.54
25:F:305:BCR:H383	25:F:305:BCR:C23	2.36	0.54
16:4:232:GLN:HG2	22:4:613:CLA:ND	2.22	0.54
22:5:617:CLA:HED3	24:6:619:LHG:H142	1.89	0.54
20:9:206:LEU:O	20:9:206:LEU:HD23	2.07	0.54
22:A:807:CLA:H151	22:A:830:CLA:HBB2	1.90	0.54
22:A:811:CLA:H12	22:A:813:CLA:H43	1.90	0.54
25:F:305:BCR:C23	25:F:305:BCR:C38	2.85	0.54
22:4:611:CLA:HBC3	24:4:622:LHG:HC62	1.90	0.54
18:6:192:MET:HE1	18:6:251:PHE:HB3	1.89	0.54
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.89	0.54
16:4:81:PHE:CZ	22:4:601:CLA:HAB	2.42	0.54
25:5:622:BCR:HC32	24:6:619:LHG:O9	2.07	0.54
16:4:160:VAL:HG21	25:4:621:BCR:H16C	1.89	0.54
22:1:603:CLA:HBC1	29:1:607:CHL:HBB2	1.90	0.53
18:6:156:TYR:HB3	22:6:610:CLA:HED2	1.90	0.53
1:A:265:PHE:HA	22:K:4003:CLA:HBC3	1.91	0.53
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.90	0.53
18:6:199:LYS:HE2	18:6:203:ALA:HB1	1.91	0.53
29:5:608:CHL:H12	30:5:620:LUT:H383	1.89	0.53
19:2:205:PRO:O	19:2:209:VAL:HG23	2.08	0.53
22:A:804:CLA:HBB2	22:A:812:CLA:H72	1.90	0.53
2:B:352:HIS:ND1	22:B:817:CLA:OBD	2.40	0.53
12:1:158:PHE:CZ	22:1:608:CLA:NC	2.76	0.53
14:7:221:ASP:HB3	14:7:229:VAL:HG11	1.91	0.53
16:4:217:LYS:NZ	22:4:611:CLA:O1D	2.29	0.53
22:4:601:CLA:HBB1	24:4:622:LHG:H272	1.89	0.53
22:A:802:CLA:H91	25:A:852:BCR:C21	2.38	0.53
12:1:118:TRP:NE1	30:1:619:LUT:O3	2.40	0.53
12:1:153:TYR:HE1	12:1:177:GLU:OE1	1.91	0.53
13:3:159:GLU:CD	13:3:162:ARG:HH21	2.14	0.53
22:Z:610:CLA:H52	30:Z:617:LUT:H30	1.90	0.53
22:6:611:CLA:HBC3	24:6:619:LHG:HC62	1.91	0.53
19:2:32:TYR:CE2	19:2:35:ALA:HA	2.43	0.53
2:B:41:GLU:HG2	2:B:166:LEU:HB2	1.90	0.53
22:3:612:CLA:HHC	22:3:612:CLA:HBB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:MET:HB2	22:A:802:CLA:C1C	2.39	0.53
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.91	0.53
22:4:610:CLA:HBB1	30:4:619:LUT:H32	1.91	0.53
17:5:247:ILE:HD11	25:5:625:BCR:H351	1.89	0.53
1:A:458:HIS:CE1	22:A:835:CLA:NA	2.77	0.53
1:A:487:ILE:HD11	22:A:838:CLA:H2	1.91	0.53
1:A:501:ASN:HB2	22:A:837:CLA:HED2	1.89	0.53
22:A:854:CLA:HBC2	2:B:586:ASN:HB2	1.91	0.53
2:B:335:LEU:HD11	22:B:829:CLA:HBB1	1.90	0.53
6:F:179:LYS:HB2	6:F:182:ASP:HB2	1.90	0.53
24:8:620:LHG:H271	24:8:620:LHG:HC91	1.91	0.53
1:A:198:LEU:CD2	1:A:322:MET:HE3	2.21	0.53
1:A:267:LEU:HD13	22:K:4003:CLA:HMD1	1.91	0.53
22:A:815:CLA:H2	22:A:817:CLA:CMB	2.37	0.53
16:4:160:VAL:CG2	25:4:621:BCR:H16C	2.39	0.52
25:4:621:BCR:C33	25:4:621:BCR:C8	2.85	0.52
17:5:133:GLU:OE1	17:5:133:GLU:HA	2.08	0.52
17:5:197:TYR:CD2	30:5:624:LUT:H12	2.44	0.52
1:A:330:ARG:HE	1:A:336:GLU:HA	1.75	0.52
2:B:698:PRO:O	3:C:81:TYR:OH	2.19	0.52
13:3:228:MET:HG2	30:3:622:LUT:H12	1.90	0.52
12:Z:50:PRO:O	12:Z:56:ASN:ND2	2.43	0.52
22:5:613:CLA:HHC	22:5:613:CLA:HBB1	1.90	0.52
22:A:807:CLA:HHB	22:A:831:CLA:HAB	1.91	0.52
22:A:815:CLA:H111	22:3:607:CLA:HBB1	1.90	0.52
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.91	0.52
2:B:671:TYR:OH	22:B:803:CLA:OBD	2.28	0.52
15:8:56:PRO:HD2	30:8:618:LUT:H23	1.91	0.52
15:8:203:PHE:CD2	30:8:618:LUT:H12	2.44	0.52
16:4:150:PHE:HB2	29:4:607:CHL:HBC1	1.90	0.52
25:5:622:BCR:C3	24:6:619:LHG:O9	2.58	0.52
17:5:191:ARG:HA	17:5:194:MET:HE3	1.92	0.52
22:A:805:CLA:HBB1	22:A:807:CLA:OBD	2.08	0.52
22:A:843:CLA:H202	11:L:96:LEU:HD21	1.90	0.52
22:B:831:CLA:HAC1	22:B:838:CLA:HBC3	1.92	0.52
6:F:189:VAL:HG13	22:F:301:CLA:H122	1.90	0.52
12:1:61:PRO:HD2	30:1:618:LUT:H23	1.92	0.52
22:A:802:CLA:C1B	22:A:854:CLA:HAB	2.40	0.52
12:1:74:PHE:HB3	22:1:602:CLA:HHB	1.92	0.52
22:7:604:CLA:C1B	25:7:623:BCR:H281	2.21	0.52
22:A:840:CLA:HBA2	24:A:847:LHG:H221	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:LEU:O	2:B:733:ARG:NH2	2.40	0.52
22:B:840:CLA:HBB1	25:B:848:BCR:H363	1.90	0.52
20:9:175:GLN:OE1	30:9:616:LUT:H42	2.09	0.52
22:A:835:CLA:HAA1	22:A:835:CLA:HBD	1.91	0.52
22:B:826:CLA:H13	25:B:847:BCR:H15C	1.92	0.52
14:7:97:LEU:HD22	22:7:620:CLA:O1D	2.10	0.52
8:I:83:THR:HG22	8:I:87:LEU:HD12	1.92	0.52
12:1:197:ALA:HB2	22:1:616:CLA:HED2	1.90	0.52
22:1:602:CLA:H72	30:1:618:LUT:H28	1.91	0.52
1:A:704:HIS:HE1	22:A:841:CLA:C4D	2.23	0.52
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.91	0.52
22:B:831:CLA:CBC	25:F:305:BCR:H362	2.29	0.52
22:A:802:CLA:H192	22:A:842:CLA:H41	1.86	0.51
22:A:815:CLA:C2	22:A:817:CLA:HMB1	2.37	0.51
22:B:825:CLA:H92	22:B:836:CLA:H41	1.92	0.51
19:2:210:THR:O	19:2:214:LEU:HG	2.10	0.51
19:2:218:PRO:HG3	22:2:601:CLA:CMA	2.41	0.51
22:A:802:CLA:HBC3	22:A:802:CLA:HHD	1.93	0.51
22:3:617:CLA:HBA2	22:7:601:CLA:H72	1.91	0.51
22:7:606:CLA:HHC	22:7:606:CLA:HBB1	1.93	0.51
22:A:805:CLA:HHC	22:A:805:CLA:CBB	2.26	0.51
22:1:611:CLA:HAB	25:8:619:BCR:H312	1.92	0.51
1:A:35:PHE:HB2	1:A:62:HIS:CD2	2.46	0.51
6:F:186:ILE:HG12	9:J:10:THR:HG22	1.92	0.51
2:B:290:HIS:C	22:B:820:CLA:HED1	2.36	0.51
20:9:206:LEU:HD23	20:9:206:LEU:C	2.36	0.51
1:A:147:LEU:HD11	22:A:830:CLA:H42	1.93	0.51
1:A:451:HIS:HA	22:A:835:CLA:HAB	1.93	0.51
22:A:809:CLA:H71	22:A:831:CLA:H171	1.93	0.51
22:A:829:CLA:H121	22:A:854:CLA:H203	1.92	0.51
2:B:358:PRO:HG3	22:B:818:CLA:HBA1	1.93	0.51
7:G:58:ARG:NH2	7:G:94:GLY:O	2.44	0.51
12:Z:83:ARG:NH1	22:Z:608:CLA:OBD	2.40	0.51
25:A:848:BCR:H362	25:A:849:BCR:H21C	1.93	0.51
16:4:62:MET:HE2	18:6:130:GLN:NE2	2.25	0.51
29:6:606:CHL:HHC	29:6:606:CHL:HBB1	1.92	0.51
1:A:363:LEU:HD11	22:A:820:CLA:H71	1.93	0.50
17:5:80:TRP:CE2	29:5:608:CHL:HED2	2.46	0.50
17:5:226:ASN:HD22	17:5:227:ILE:H	1.60	0.50
22:A:816:CLA:H101	25:3:719:BCR:H14C	1.93	0.50
6:F:133:LEU:HD22	6:F:148:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:256:TRP:CG	22:6:622:CLA:HED2	2.46	0.50
19:2:206:GLU:O	19:2:210:THR:OG1	2.29	0.50
2:B:426:VAL:HG21	2:B:529:HIS:HD2	1.75	0.50
6:F:224:VAL:CG1	6:F:225:SER:N	2.73	0.50
13:3:131:ILE:HG22	13:3:134:ALA:H	1.76	0.50
22:3:606:CLA:HHC	22:3:606:CLA:HBB1	1.94	0.50
22:A:802:CLA:CHB	22:A:854:CLA:HAB	2.42	0.50
22:B:820:CLA:CHB	22:B:820:CLA:H12	2.41	0.50
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.92	0.50
25:B:801:BCR:H323	22:B:832:CLA:HBB1	1.93	0.50
3:C:2:ALA:N	3:C:71:SER:O	2.45	0.50
14:7:171:ASP:OD1	30:7:621:LUT:O23	2.29	0.50
17:5:32:ARG:NH2	17:5:52:ASP:O	2.45	0.50
17:5:203:GLN:CD	30:5:620:LUT:O3	2.55	0.50
13:3:63:GLY:HA3	13:3:218:ILE:HG21	1.93	0.50
16:4:260:ASP:OD1	22:4:616:CLA:C4B	2.51	0.50
22:A:841:CLA:HBC1	23:A:844:PQN:H201	1.93	0.50
22:4:604:CLA:C1C	25:4:621:BCR:H391	2.42	0.50
2:B:412:MET:HG3	25:B:846:BCR:H402	1.93	0.50
22:B:805:CLA:HHC	22:B:805:CLA:HBB1	1.94	0.50
3:C:4:ILE:HB	3:C:68:TYR:HB2	1.93	0.50
10:K:35:ASN:ND2	22:K:4003:CLA:OBD	2.45	0.50
13:3:164:GLN:OE1	13:3:167:ARG:NH2	2.43	0.50
15:8:154:LEU:HB2	22:Z:603:CLA:H2	1.93	0.50
16:4:157:PHE:HZ	25:4:621:BCR:H373	1.76	0.50
1:A:18:ASP:OD2	1:A:71:ARG:NH2	2.41	0.50
22:A:835:CLA:H72	25:L:201:BCR:H14C	1.93	0.50
4:D:125:THR:HG23	4:D:136:PRO:HG2	1.93	0.50
13:3:141:TRP:NE1	22:3:606:CLA:OBD	2.34	0.50
17:5:170:ASP:OD1	30:5:620:LUT:O23	2.27	0.50
17:5:245:LEU:HD13	18:6:224:VAL:HG21	1.92	0.50
22:2:610:CLA:HBB1	30:2:616:LUT:H32	1.93	0.50
2:B:340:ALA:HB2	25:B:847:BCR:H372	1.92	0.49
25:5:622:BCR:HC42	24:6:619:LHG:HC82	1.93	0.49
19:2:209:VAL:O	19:2:213:VAL:CG2	2.44	0.49
22:B:821:CLA:HMD2	25:B:843:BCR:HC7	1.94	0.49
3:C:34:CYS:HA	5:E:67:VAL:HG23	1.94	0.49
4:D:128:LEU:HA	4:D:132:PHE:HD2	1.77	0.49
22:F:303:CLA:HHC	22:F:303:CLA:HBB1	1.92	0.49
15:8:233:TYR:CD1	22:8:613:CLA:H12	2.47	0.49
16:4:159:TRP:HH2	25:4:621:BCR:H333	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ILE:HG13	1:A:659:GLN:HG3	1.94	0.49
22:A:832:CLA:HBA2	24:A:847:LHG:HC92	1.94	0.49
12:1:142:GLU:HG3	22:1:609:CLA:C4B	2.43	0.49
22:6:604:CLA:H171	22:6:610:CLA:HBC1	1.93	0.49
22:A:805:CLA:H43	22:A:812:CLA:CBB	2.27	0.49
2:B:277:HIS:HB2	22:B:817:CLA:C1B	2.42	0.49
13:3:102:ALA:HA	13:3:231:TYR:HE2	1.76	0.49
22:B:812:CLA:HHC	22:B:812:CLA:HBB1	1.94	0.49
25:3:717:BCR:HC31	22:7:601:CLA:HBC2	1.94	0.49
12:Z:142:GLU:HA	12:Z:142:GLU:OE1	2.12	0.49
16:4:203:TRP:O	16:4:204:SER:CB	2.61	0.49
16:4:208:ILE:HA	16:4:211:LEU:HB2	1.93	0.49
18:6:123:TRP:CE2	25:6:623:BCR:H10C	2.48	0.49
19:2:156:LYS:HD3	22:2:612:CLA:HAA2	1.95	0.49
22:A:818:CLA:CHD	22:A:819:CLA:HBB2	2.43	0.49
22:B:815:CLA:HMB1	25:B:845:BCR:HC8	1.95	0.49
16:4:130:ALA:HB1	16:4:132:VAL:HG23	1.95	0.49
29:4:606:CHL:CGA	25:4:621:BCR:H21C	2.43	0.49
22:6:614:CLA:HED1	24:6:619:LHG:C22	2.43	0.49
22:A:835:CLA:HBB1	22:A:835:CLA:CHC	2.40	0.49
22:B:807:CLA:H12	8:I:83:THR:HG21	1.95	0.49
6:F:123:LEU:HD21	9:J:38:VAL:HG11	1.94	0.49
22:1:613:CLA:H2	22:1:614:CLA:OBD	2.13	0.49
14:7:47:LEU:HD11	14:7:65:LEU:HD21	1.93	0.49
15:8:115:SER:OG	15:8:116:PHE:N	2.46	0.49
19:2:206:GLU:O	19:2:210:THR:CG2	2.60	0.49
25:A:856:BCR:HC22	9:J:31:ARG:HH11	1.78	0.49
22:B:820:CLA:C4B	22:B:820:CLA:H62	2.42	0.49
20:9:201:TYR:O	20:9:205:HIS:HB2	2.12	0.49
22:A:843:CLA:H121	22:B:839:CLA:H102	1.95	0.48
2:B:545:SER:C	6:F:224:VAL:HG13	2.38	0.48
16:4:106:PHE:CE1	29:4:608:CHL:HED2	2.47	0.48
17:5:226:ASN:ND2	22:5:614:CLA:O1D	2.44	0.48
19:2:32:TYR:HE2	19:2:35:ALA:CB	2.07	0.48
1:A:216:HIS:HB2	22:A:815:CLA:C1C	2.42	0.48
4:D:88:TRP:HB3	4:D:136:PRO:HB3	1.95	0.48
11:L:131:CYS:HB3	25:L:205:BCR:H19C	1.95	0.48
22:A:843:CLA:HAB	2:B:692:VAL:HG11	1.95	0.48
22:B:839:CLA:H151	11:L:127:ILE:HG21	1.95	0.48
12:1:137:ALA:HB2	22:1:606:CLA:H52	1.95	0.48
22:1:613:CLA:H101	24:1:620:LHG:H301	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:198:LEU:HD13	22:8:611:CLA:HMD3	1.95	0.48
29:4:618:CHL:HAB	25:4:621:BCR:C11	2.42	0.48
18:6:127:ARG:HH21	29:6:618:CHL:HMC	1.78	0.48
19:2:32:TYR:CE2	19:2:35:ALA:HB1	2.35	0.48
22:A:821:CLA:HBB1	25:K:4001:BCR:H14C	1.95	0.48
2:B:214:LEU:O	20:9:180:ARG:NH1	2.46	0.48
22:B:811:CLA:O2D	20:9:62:ARG:NH2	2.46	0.48
29:1:607:CHL:HBB1	29:1:607:CHL:CMB	2.43	0.48
14:7:160:LEU:HD23	14:7:161:GLU:HG3	1.94	0.48
16:4:111:VAL:HG11	30:4:619:LUT:H10	1.94	0.48
17:5:242:VAL:HG11	25:5:625:BCR:H353	1.94	0.48
4:D:97:GLU:H	4:D:127:GLN:HE22	1.61	0.48
18:6:256:TRP:O	22:6:622:CLA:O2D	2.30	0.48
1:A:219:HIS:CE1	22:A:816:CLA:ND	2.82	0.48
16:4:263:ARG:HD2	22:4:616:CLA:HMA2	1.95	0.48
20:9:56:LEU:HD13	22:9:602:CLA:H42	1.96	0.48
22:A:808:CLA:H41	22:A:808:CLA:H61	1.57	0.48
12:1:159:ASP:OD1	30:1:617:LUT:O23	2.29	0.48
22:8:610:CLA:H52	30:8:617:LUT:H30	1.95	0.48
16:4:98:GLN:NE2	16:4:191:PRO:O	2.44	0.48
16:4:104:ALA:HB1	16:4:219:GLY:HA3	1.96	0.48
16:4:256:VAL:HG23	22:4:613:CLA:O1A	2.14	0.48
2:B:43:LEU:HD22	4:D:186:PHE:HZ	1.79	0.48
22:1:603:CLA:CBC	29:1:607:CHL:HBB2	2.44	0.48
22:1:606:CLA:H61	22:1:606:CLA:H41	1.63	0.48
29:5:607:CHL:HBB2	22:5:609:CLA:HAC2	1.95	0.48
1:A:75:SER:HB3	22:A:812:CLA:HHD	1.95	0.47
12:1:188:PHE:CD2	30:1:618:LUT:H12	2.49	0.47
22:1:602:CLA:H52	30:1:618:LUT:H28	1.95	0.47
22:A:841:CLA:H92	25:B:801:BCR:H15C	1.96	0.47
17:5:197:TYR:CE2	30:5:624:LUT:H10	2.48	0.47
1:A:422:ASN:HD21	1:A:427:LEU:HD23	1.79	0.47
23:A:844:PQN:H162	25:B:801:BCR:H382	1.95	0.47
22:B:812:CLA:H2	22:B:812:CLA:H61	1.72	0.47
4:D:62:THR:HB	4:D:112:LEU:HD22	1.96	0.47
22:Z:606:CLA:H41	22:Z:606:CLA:H61	1.66	0.47
22:Z:613:CLA:H93	24:Z:620:LHG:H321	1.96	0.47
16:4:156:LEU:HD12	25:4:621:BCR:C14	2.44	0.47
22:5:617:CLA:CMB	22:6:622:CLA:HBC1	2.45	0.47
1:A:353:LEU:HD11	22:A:831:CLA:HBB1	1.97	0.47
22:A:836:CLA:HHC	22:A:836:CLA:HBB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:182:ALA:HA	13:3:185:LYS:HE2	1.96	0.47
12:Z:159:ASP:OD1	30:Z:617:LUT:O23	2.29	0.47
17:5:133:GLU:HG3	22:5:609:CLA:C4B	2.43	0.47
2:B:325:ASP:O	2:B:329:ASN:ND2	2.47	0.47
22:B:832:CLA:H152	6:F:157:LEU:HD22	1.96	0.47
7:G:52:VAL:HG11	12:1:140:ALA:HA	1.96	0.47
22:1:610:CLA:H13	30:1:617:LUT:H403	1.96	0.47
14:7:136:TRP:HB2	22:7:609:CLA:HMA2	1.96	0.47
12:Z:61:PRO:HD2	30:Z:618:LUT:H23	1.96	0.47
17:5:133:GLU:HG3	22:5:609:CLA:NB	2.29	0.47
17:5:202:LEU:HG	22:5:613:CLA:HAC2	1.96	0.47
20:9:123:GLU:HG3	22:9:609:CLA:C4B	2.44	0.47
22:A:835:CLA:C4	25:L:201:BCR:C36	2.86	0.47
22:B:820:CLA:HHC	22:B:820:CLA:CBB	2.16	0.47
11:L:55:LEU:HD23	11:L:55:LEU:C	2.39	0.47
19:2:211:VAL:CG2	19:2:212:ALA:N	2.77	0.47
22:2:611:CLA:H41	22:2:611:CLA:H61	1.66	0.47
22:B:841:CLA:HHC	22:B:841:CLA:CBB	2.23	0.47
13:3:95:ALA:HB1	13:3:221:GLY:HA3	1.97	0.47
30:9:616:LUT:H35	30:9:616:LUT:H401	1.80	0.47
1:A:131:VAL:HG12	1:A:139:GLN:HG2	1.96	0.47
1:A:304:LEU:HD21	22:A:828:CLA:H192	1.97	0.47
2:B:464:ILE:HD11	22:B:836:CLA:H2	1.97	0.47
19:2:218:PRO:CG	22:2:601:CLA:CMA	2.93	0.47
1:A:297:HIS:HB2	22:A:819:CLA:CHB	2.45	0.47
22:A:842:CLA:HAC1	23:A:844:PQN:H172	1.97	0.47
2:B:550:ASP:OD2	4:D:175:ILE:HD11	2.15	0.47
22:5:602:CLA:H122	30:5:624:LUT:H371	1.97	0.47
18:6:162:ALA:HB2	22:6:610:CLA:HBD	1.97	0.47
22:A:811:CLA:H111	22:A:811:CLA:H152	1.76	0.47
25:F:305:BCR:C8	25:F:305:BCR:C33	2.85	0.47
12:Z:40:LEU:HD12	29:Z:601:CHL:HMA3	1.97	0.47
16:4:159:TRP:CH2	25:4:621:BCR:H333	2.49	0.47
22:A:802:CLA:HED3	25:B:801:BCR:H401	1.96	0.46
2:B:66:LEU:HD11	25:B:845:BCR:H271	1.97	0.46
2:B:549:PRO:HD2	3:C:62:PHE:CZ	2.51	0.46
17:5:78:ALA:HB1	17:5:190:GLY:HA3	1.97	0.46
22:5:610:CLA:CBB	30:5:620:LUT:H32	2.45	0.46
22:6:601:CLA:HBB1	24:6:619:LHG:H261	1.97	0.46
22:A:842:CLA:H102	22:A:842:CLA:H61	1.56	0.46
13:3:177:PHE:CE2	29:3:608:CHL:HBB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:611:CLA:HHC	22:7:611:CLA:HBB1	1.96	0.46
16:4:215:GLU:HB2	22:4:610:CLA:C1B	2.46	0.46
22:4:604:CLA:C1C	25:4:621:BCR:H393	2.45	0.46
18:6:100:ALA:O	18:6:104:VAL:HB	2.16	0.46
22:A:854:CLA:HBB1	2:B:526:LEU:HD21	1.97	0.46
22:B:814:CLA:HMA2	25:B:845:BCR:H282	1.97	0.46
25:B:846:BCR:H15C	25:B:846:BCR:H351	1.84	0.46
16:4:204:SER:OG	22:4:610:CLA:HAA1	2.15	0.46
16:4:232:GLN:NE2	30:4:619:LUT:H42	2.30	0.46
20:9:62:ARG:HD2	20:9:66:TYR:CZ	2.50	0.46
17:5:247:ILE:HD11	25:5:625:BCR:H15C	1.98	0.46
18:6:256:TRP:HB3	22:6:622:CLA:HED1	1.98	0.46
29:6:606:CHL:HAA1	25:6:623:BCR:H21C	1.97	0.46
2:B:177:ASN:HD22	2:B:294:THR:HG23	1.81	0.46
22:B:805:CLA:C1C	22:B:829:CLA:HMB3	2.44	0.46
12:1:217:ASN:HD21	15:8:121:SER:HB2	1.80	0.46
16:4:81:PHE:CE1	22:4:601:CLA:HAB	2.51	0.46
17:5:86:ALA:HB2	30:5:620:LUT:H401	1.97	0.46
17:5:89:LEU:HD22	22:5:612:CLA:HBB2	1.98	0.46
1:A:216:HIS:C	1:A:216:HIS:CD2	2.94	0.46
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.98	0.46
2:B:545:SER:HA	6:F:224:VAL:CG1	2.44	0.46
14:7:146:ALA:HB1	14:7:155:GLU:H	1.81	0.46
15:8:153:PHE:HB2	15:8:157:GLU:HB3	1.97	0.46
16:4:61:TRP:O	22:4:601:CLA:ND	2.49	0.46
16:4:255:THR:H	16:4:258:GLN:HB2	1.79	0.46
17:5:142:ASN:ND2	18:6:35:GLY:O	2.48	0.46
25:5:625:BCR:H351	25:5:625:BCR:H15C	1.66	0.46
25:G:205:BCR:H20C	25:G:205:BCR:H361	1.82	0.46
16:4:106:PHE:CE2	29:4:608:CHL:HED2	2.51	0.46
29:4:618:CHL:CAB	25:4:621:BCR:C10	2.85	0.46
2:B:276:HIS:HE1	22:B:816:CLA:NA	2.12	0.46
13:3:159:GLU:OE2	13:3:162:ARG:CZ	2.64	0.46
12:Z:153:TYR:HB3	22:Z:610:CLA:HED2	1.97	0.46
19:2:218:PRO:CG	22:2:601:CLA:HMA3	2.45	0.46
22:A:841:CLA:HHC	22:A:841:CLA:HBB1	1.98	0.46
2:B:204:ARG:NH2	2:B:252:GLY:O	2.49	0.46
13:3:92:VAL:HG21	13:3:191:ALA:HB1	1.98	0.46
15:8:55:ASP:OD1	30:8:618:LUT:O23	2.33	0.46
12:Z:142:GLU:HG3	22:Z:609:CLA:C4B	2.46	0.46
22:A:804:CLA:HHC	22:A:804:CLA:HBB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:LEU:O	4:D:77:LYS:NZ	2.46	0.45
22:Z:602:CLA:H41	22:Z:602:CLA:H61	1.60	0.45
22:Z:608:CLA:HBB1	22:Z:608:CLA:H151	1.98	0.45
17:5:172:PHE:HD2	30:5:620:LUT:H222	1.81	0.45
18:6:256:TRP:HB3	22:6:622:CLA:CED	2.47	0.45
22:A:816:CLA:H41	22:A:816:CLA:H62	1.76	0.45
22:A:829:CLA:HBA2	22:A:829:CLA:H3A	1.70	0.45
22:B:812:CLA:H143	22:B:812:CLA:H111	1.84	0.45
16:4:232:GLN:NE2	30:4:619:LUT:O3	2.45	0.45
18:6:69:GLU:HG2	18:6:132:LEU:HD12	1.97	0.45
18:6:223:VAL:HB	22:6:616:CLA:C1C	2.46	0.45
22:A:815:CLA:HBD	22:A:815:CLA:HAA1	1.98	0.45
22:6:614:CLA:HED1	24:6:619:LHG:H221	1.97	0.45
22:9:602:CLA:CBB	30:9:617:LUT:H32	2.46	0.45
22:A:841:CLA:HED2	2:B:421:SER:HB3	1.97	0.45
12:1:50:PRO:O	12:1:56:ASN:ND2	2.50	0.45
25:7:623:BCR:H342	22:8:614:CLA:H62	1.99	0.45
16:4:111:VAL:HG22	16:4:229:PHE:HE2	1.81	0.45
20:9:116:PHE:HD1	22:9:609:CLA:HBB2	1.82	0.45
1:A:219:HIS:HE1	22:A:816:CLA:C4D	2.30	0.45
1:A:277:THR:HA	22:A:818:CLA:HED1	1.98	0.45
2:B:426:VAL:HG21	2:B:529:HIS:CD2	2.51	0.45
2:B:588:ILE:HA	2:B:591:VAL:HG22	1.97	0.45
22:B:816:CLA:CHD	22:B:817:CLA:HBB2	2.47	0.45
12:1:209:HIS:CD2	22:1:614:CLA:NC	2.84	0.45
22:3:607:CLA:H142	22:3:617:CLA:HBB2	1.98	0.45
18:6:205:LEU:HD22	30:6:621:LUT:H163	1.98	0.45
29:7:607:CHL:H61	29:7:607:CHL:H41	1.78	0.45
16:4:208:ILE:HD11	22:4:610:CLA:C2A	2.46	0.45
1:A:356:ASN:O	1:A:360:PHE:HB2	2.17	0.45
22:A:802:CLA:HAA2	22:A:802:CLA:CBD	2.46	0.45
22:A:816:CLA:H111	13:3:232:GLY:HA3	1.99	0.45
15:8:132:PHE:CE2	25:8:619:BCR:H10C	2.52	0.45
15:8:143:LYS:HB2	15:8:146:SER:HB2	1.99	0.45
15:8:190:LEU:HA	15:8:193:VAL:HG12	1.99	0.45
22:8:610:CLA:H91	22:8:610:CLA:H111	1.83	0.45
16:4:163:ARG:HE	16:4:174:ALA:HB1	1.82	0.45
17:5:133:GLU:HG3	22:5:609:CLA:C1B	2.47	0.45
1:A:226:LYS:HD3	1:A:253:LEU:HD23	1.98	0.45
22:A:806:CLA:HBA1	22:A:806:CLA:H3A	1.78	0.45
22:A:829:CLA:H52	22:A:829:CLA:H8	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ARG:HB2	22:B:813:CLA:HBC2	1.99	0.45
5:E:55:GLN:HE21	6:F:222:ILE:HB	1.82	0.45
15:8:155:GLY:HA3	12:Z:74:PHE:CZ	2.52	0.45
20:9:171:GLY:O	20:9:175:GLN:HB3	2.17	0.45
1:A:54:ALA:HB2	24:A:846:LHG:HC82	1.99	0.45
22:B:820:CLA:H3A	22:B:820:CLA:CGA	2.47	0.45
25:B:844:BCR:H351	25:B:844:BCR:H15C	1.76	0.45
22:8:606:CLA:HHC	22:8:606:CLA:HBB1	1.99	0.45
22:A:842:CLA:H41	22:A:842:CLA:H62	1.62	0.45
2:B:173:GLU:HG3	2:B:302:MET:HE3	1.99	0.45
25:3:717:BCR:H341	25:3:717:BCR:H11C	1.71	0.45
22:8:602:CLA:H52	30:8:618:LUT:H28	1.99	0.45
16:4:244:LEU:HD22	30:4:619:LUT:H163	1.98	0.45
25:6:625:BCR:H11C	25:6:625:BCR:H341	1.73	0.45
25:A:856:BCR:H391	9:J:12:PRO:HB2	1.98	0.44
2:B:194:HIS:HE1	22:B:814:CLA:C1A	2.30	0.44
22:5:609:CLA:HBA1	22:5:621:CLA:HMD1	1.99	0.44
30:5:620:LUT:H15	30:5:620:LUT:H201	1.84	0.44
18:6:178:LYS:NZ	22:6:611:CLA:O1D	2.41	0.44
15:8:175:PRO:HD2	30:8:617:LUT:H23	1.99	0.44
30:4:619:LUT:H401	30:4:619:LUT:H35	1.77	0.44
22:6:604:CLA:H41	22:6:604:CLA:H62	1.79	0.44
29:9:607:CHL:HBB1	28:9:620:LMG:H121	1.99	0.44
22:A:841:CLA:H121	22:F:303:CLA:HAC1	1.99	0.44
22:7:620:CLA:O2A	18:6:250:CYS:O	2.34	0.44
30:8:617:LUT:H401	30:8:617:LUT:H35	1.83	0.44
29:4:606:CHL:H51	29:4:608:CHL:HHB	1.99	0.44
17:5:122:LEU:HD11	22:6:616:CLA:HBA2	1.99	0.44
19:2:38:PRO:HG2	19:2:52:ASP:HB3	1.98	0.44
1:A:425:ASN:OD1	1:A:426:LEU:N	2.48	0.44
22:A:834:CLA:HBB2	11:L:103:LEU:HD12	2.00	0.44
13:3:78:SER:OG	13:3:82:ILE:O	2.34	0.44
13:3:184:PHE:CZ	29:3:608:CHL:HBB1	2.53	0.44
22:3:610:CLA:H141	22:3:610:CLA:H162	1.86	0.44
25:7:623:BCR:H15C	25:7:623:BCR:H351	1.81	0.44
22:5:606:CLA:HBA2	25:5:622:BCR:H19C	1.99	0.44
22:5:617:CLA:CED	24:6:619:LHG:H142	2.47	0.44
22:A:802:CLA:O2A	22:A:802:CLA:HMA2	2.18	0.44
22:A:813:CLA:H41	22:A:813:CLA:H62	1.83	0.44
25:A:848:BCR:H11C	25:A:848:BCR:H341	1.87	0.44
3:C:19:ARG:HG2	4:D:159:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:3:718:BCR:H20C	25:3:718:BCR:H361	1.85	0.44
22:8:612:CLA:H41	22:8:612:CLA:H61	1.62	0.44
29:4:606:CHL:H3A	25:4:621:BCR:C21	2.48	0.44
29:4:608:CHL:HMA1	25:4:621:BCR:H361	2.00	0.44
22:A:809:CLA:HAB	25:J:3003:BCR:H352	2.00	0.44
22:A:825:CLA:H2	25:A:850:BCR:H363	2.00	0.44
22:B:807:CLA:O1A	8:I:83:THR:OG1	2.32	0.44
22:7:601:CLA:H62	22:7:601:CLA:H41	1.76	0.44
1:A:150:ALA:HB2	1:A:378:PRO:HD2	2.00	0.44
25:A:850:BCR:H24C	25:A:850:BCR:H371	1.81	0.44
22:B:814:CLA:HHB	25:B:845:BCR:H23C	2.00	0.44
22:5:612:CLA:H41	22:5:612:CLA:H62	1.71	0.44
18:6:125:GLU:HG3	22:6:609:CLA:NB	2.32	0.44
1:A:711:PRO:HA	6:F:171:LEU:HD11	2.00	0.44
22:A:834:CLA:H61	22:A:834:CLA:H41	1.76	0.44
22:B:819:CLA:H102	22:B:823:CLA:H43	1.99	0.44
22:B:820:CLA:CGA	22:B:820:CLA:C3A	2.96	0.44
7:G:89:THR:HG21	7:G:96:ASN:HA	2.00	0.44
22:Z:613:CLA:H2	22:Z:614:CLA:OBD	2.17	0.44
16:4:208:ILE:HG12	16:4:212:LYS:HG3	2.00	0.44
17:5:109:LEU:HB2	17:5:114:THR:HA	2.00	0.44
1:A:121:ILE:HG12	1:A:122:VAL:HG13	2.00	0.44
1:A:683:LEU:HB2	22:A:802:CLA:HMC2	2.00	0.44
22:A:802:CLA:HMD2	2:B:534:ILE:HG12	2.00	0.44
22:B:818:CLA:H3A	22:B:818:CLA:HBA2	1.68	0.44
22:6:604:CLA:H61	25:6:623:BCR:H402	1.99	0.44
22:6:616:CLA:HBB2	22:6:622:CLA:HMD2	1.99	0.44
19:2:174:GLN:OE1	22:2:613:CLA:ND	2.51	0.44
1:A:685:PHE:HA	23:A:844:PQN:H9	2.00	0.43
22:A:815:CLA:H102	22:A:817:CLA:C4B	2.47	0.43
25:A:851:BCR:H15C	25:A:851:BCR:H351	1.84	0.43
22:B:813:CLA:H203	22:B:828:CLA:H2	2.00	0.43
22:1:610:CLA:H93	22:1:610:CLA:H61	1.91	0.43
20:9:123:GLU:HG3	22:9:609:CLA:NB	2.32	0.43
22:A:822:CLA:H111	22:A:822:CLA:H152	1.74	0.43
22:A:823:CLA:H11	25:K:4001:BCR:H271	2.00	0.43
22:A:831:CLA:H142	22:A:831:CLA:H111	1.84	0.43
22:B:806:CLA:H72	22:B:806:CLA:H111	1.66	0.43
22:1:602:CLA:H92	22:1:602:CLA:H61	1.89	0.43
22:1:604:CLA:H62	22:1:604:CLA:H41	1.73	0.43
22:4:612:CLA:HMA1	22:4:612:CLA:H2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:610:CLA:H92	22:2:610:CLA:H62	1.86	0.43
30:2:617:LUT:H11	30:2:617:LUT:H191	1.91	0.43
30:2:617:LUT:H31	30:2:617:LUT:H391	1.91	0.43
1:A:296:HIS:HB3	22:A:819:CLA:HMB1	2.00	0.43
22:A:815:CLA:H122	22:3:607:CLA:CMC	2.48	0.43
22:A:841:CLA:HBB1	22:A:841:CLA:H111	2.00	0.43
7:G:91:ASP:OD2	7:G:92:PRO:HD2	2.18	0.43
15:8:54:PHE:HB3	22:8:602:CLA:C3D	2.48	0.43
30:5:620:LUT:C8	30:5:620:LUT:H181	2.48	0.43
20:9:62:ARG:CD	20:9:66:TYR:CE2	2.96	0.43
1:A:458:HIS:CE1	22:A:835:CLA:CHA	3.00	0.43
1:A:707:LEU:HD11	22:B:831:CLA:HMB1	2.00	0.43
22:B:805:CLA:HBC2	22:B:829:CLA:HMA1	1.99	0.43
22:B:833:CLA:HBA1	9:J:36:PRO:HG2	2.00	0.43
25:G:205:BCR:H11C	25:G:205:BCR:H341	1.90	0.43
13:3:73:LEU:HG	22:3:602:CLA:HAA2	2.00	0.43
13:3:97:TRP:CE2	29:3:608:CHL:HED2	2.53	0.43
14:7:130:TRP:CZ2	25:7:623:BCR:HC8	2.53	0.43
22:7:620:CLA:CBA	18:6:250:CYS:O	2.65	0.43
15:8:122:LEU:HD11	22:8:606:CLA:C2D	2.49	0.43
12:Z:182:ARG:HA	12:Z:185:MET:HE3	2.00	0.43
21:A:801:CL0:H15	21:A:801:CL0:H2	1.99	0.43
17:5:159:ASN:HB3	17:5:165:PRO:HA	2.01	0.43
17:5:171:PRO:HD2	30:5:620:LUT:C23	2.41	0.43
30:2:617:LUT:H35	30:2:617:LUT:H401	1.64	0.43
1:A:329:HIS:HA	22:A:845:CLA:HBC2	2.01	0.43
22:A:839:CLA:H62	22:A:839:CLA:H41	1.79	0.43
2:B:43:LEU:HD22	4:D:186:PHE:CZ	2.54	0.43
27:B:850:DGD:HA62	27:B:850:DGD:HA92	1.78	0.43
3:C:41:SER:HB2	4:D:168:ALA:H	1.83	0.43
25:F:305:BCR:HC8	25:F:305:BCR:C33	2.48	0.43
11:L:54:MET:HE3	11:L:54:MET:HB3	1.71	0.43
15:8:48:LEU:HD21	15:8:70:GLN:HG3	1.99	0.43
15:8:132:PHE:CD2	25:8:619:BCR:H12C	2.53	0.43
17:5:110:PRO:HG3	22:5:604:CLA:HBD	2.01	0.43
1:A:29:TRP:CZ3	22:A:805:CLA:H92	2.54	0.43
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.84	0.43
22:A:823:CLA:HBA2	22:A:823:CLA:H3A	1.60	0.43
22:B:823:CLA:HMD3	22:B:824:CLA:HHC	2.01	0.43
13:3:249:HIS:CD2	22:3:614:CLA:NC	2.87	0.43
22:3:603:CLA:H2	22:3:603:CLA:H61	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:240:LEU:HD12	15:8:242:PHE:CZ	2.54	0.43
22:4:602:CLA:CBB	30:4:620:LUT:H32	2.48	0.43
17:5:60:LEU:HD13	22:5:602:CLA:H42	2.00	0.43
1:A:112:LYS:HA	1:A:113:PRO:HD3	1.91	0.43
1:A:472:PHE:CZ	22:A:835:CLA:HMA2	2.54	0.43
22:A:825:CLA:H12	25:A:850:BCR:H14C	2.01	0.43
25:A:849:BCR:H371	25:A:849:BCR:H24C	1.86	0.43
7:G:45:PHE:HA	7:G:48:ILE:HG22	2.01	0.43
11:L:57:THR:HG22	11:L:58:PRO:CD	2.48	0.43
15:8:242:PHE:CE2	15:8:243:LEU:CG	2.85	0.43
22:6:601:CLA:HBB1	24:6:619:LHG:C26	2.48	0.43
19:2:215:CYS:C	19:2:218:PRO:HD2	2.44	0.43
20:9:97:TRP:CD1	20:9:98:GLU:HG3	2.53	0.43
22:9:610:CLA:CBB	30:9:616:LUT:H32	2.49	0.43
6:F:139:LEU:HD13	22:F:304:CLA:HED3	2.00	0.43
25:7:624:BCR:H15C	25:7:624:BCR:H351	1.82	0.43
6:F:137:PRO:HG3	25:F:305:BCR:H281	1.99	0.43
6:F:158:TYR:HA	6:F:202:TRP:HZ2	1.84	0.43
12:1:55:GLY:H	12:1:175:LEU:HD23	1.83	0.43
24:1:620:LHG:H132	24:1:620:LHG:H101	1.85	0.43
16:4:111:VAL:CG1	30:4:619:LUT:H12	2.39	0.43
17:5:228:LEU:HG	22:5:614:CLA:HED1	2.01	0.43
20:9:163:ARG:HA	20:9:166:MET:HE3	2.01	0.43
1:A:433:HIS:HB3	11:L:55:LEU:HD11	2.01	0.42
1:A:480:GLN:HA	1:A:481:PRO:HD3	1.91	0.42
1:A:740:TRP:HB2	22:A:829:CLA:HBB1	2.00	0.42
22:A:805:CLA:H42	22:A:812:CLA:CBB	2.28	0.42
22:A:811:CLA:HAA1	13:3:82:ILE:HD12	2.01	0.42
11:L:80:ALA:HB3	11:L:83:LEU:HD23	2.00	0.42
30:7:622:LUT:H35	30:7:622:LUT:H401	1.88	0.42
22:8:610:CLA:HBB1	22:8:610:CLA:H51	2.01	0.42
12:Z:188:PHE:CD2	30:Z:618:LUT:H12	2.54	0.42
25:4:621:BCR:H15C	25:4:621:BCR:H351	1.75	0.42
18:6:163:PRO:HD2	30:6:621:LUT:H23	2.01	0.42
18:6:255:LEU:HB2	22:6:622:CLA:HMA1	2.01	0.42
22:B:841:CLA:HMB3	22:1:603:CLA:H92	2.01	0.42
22:8:610:CLA:H92	22:8:610:CLA:H61	1.83	0.42
30:Z:619:LUT:H15	30:Z:619:LUT:H201	1.78	0.42
22:6:610:CLA:CBB	30:6:621:LUT:H32	2.49	0.42
1:A:426:LEU:HB3	22:A:825:CLA:HMC2	2.01	0.42
1:A:540:ALA:HB1	22:A:839:CLA:HMB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:805:CLA:CBB	22:A:812:CLA:C14	2.96	0.42
22:A:831:CLA:H41	22:A:831:CLA:H61	1.68	0.42
25:A:849:BCR:H15C	25:A:849:BCR:H351	1.83	0.42
25:A:851:BCR:H20C	25:A:851:BCR:H361	1.90	0.42
25:A:856:BCR:H361	25:A:856:BCR:H20C	1.83	0.42
12:1:139:ALA:HA	22:1:609:CLA:HAB	2.00	0.42
14:7:82:GLY:O	14:7:86:ILE:HG12	2.19	0.42
22:8:610:CLA:CBB	30:8:617:LUT:H32	2.49	0.42
25:4:621:BCR:C33	25:4:621:BCR:HC8	2.50	0.42
18:6:242:LYS:HB2	25:6:625:BCR:H343	2.01	0.42
22:A:833:CLA:H143	22:A:833:CLA:H111	1.88	0.42
4:D:172:MET:HE3	5:E:68:ARG:HH12	1.84	0.42
22:1:602:CLA:H61	22:1:602:CLA:H41	1.57	0.42
22:7:612:CLA:H41	22:7:612:CLA:H62	1.85	0.42
15:8:83:GLY:O	15:8:87:ILE:HG12	2.19	0.42
22:4:610:CLA:CBB	30:4:619:LUT:H32	2.49	0.42
17:5:218:HIS:CD2	22:5:614:CLA:NC	2.86	0.42
22:5:602:CLA:CBB	30:5:624:LUT:H32	2.49	0.42
20:9:169:PHE:CZ	30:9:617:LUT:H10	2.54	0.42
1:A:465:LEU:HD13	2:B:96:HIS:O	2.20	0.42
25:B:801:BCR:H11C	25:B:801:BCR:H341	1.81	0.42
22:B:805:CLA:H162	22:B:805:CLA:H193	1.82	0.42
22:3:603:CLA:H141	22:3:603:CLA:H162	1.83	0.42
22:Z:604:CLA:H62	22:Z:604:CLA:H41	1.71	0.42
24:4:622:LHG:HC91	25:6:623:BCR:HC41	2.01	0.42
17:5:172:PHE:CD2	30:5:620:LUT:H222	2.54	0.42
22:6:609:CLA:HBA1	22:6:609:CLA:H3A	1.85	0.42
19:2:159:LYS:HB3	22:2:611:CLA:HMD1	2.01	0.42
20:9:52:ASP:OD1	30:9:617:LUT:O23	2.35	0.42
1:A:220:VAL:HG13	1:A:240:PRO:HB3	2.01	0.42
1:A:397:ILE:HG21	22:A:830:CLA:HHC	2.01	0.42
1:A:429:ARG:HG2	1:A:432:ARG:HH22	1.85	0.42
22:A:818:CLA:H62	22:A:818:CLA:H41	1.59	0.42
22:A:842:CLA:C4D	22:A:842:CLA:H12	2.49	0.42
2:B:610:PHE:O	2:B:614:SER:HB3	2.19	0.42
2:B:722:TYR:HB2	22:B:802:CLA:HED2	2.01	0.42
30:3:621:LUT:H35	30:3:621:LUT:H401	1.91	0.42
30:8:618:LUT:H201	30:8:618:LUT:H15	1.79	0.42
1:A:646:LEU:HD13	2:B:652:LEU:HD21	2.02	0.42
22:A:835:CLA:HBC3	22:B:803:CLA:H143	2.01	0.42
2:B:118:THR:OG1	22:B:827:CLA:O1A	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:825:CLA:H193	22:B:825:CLA:H161	1.91	0.42
22:B:829:CLA:H92	22:B:829:CLA:H61	1.91	0.42
12:Z:78:GLU:HG2	12:Z:178:ILE:HD11	2.00	0.42
30:Z:618:LUT:H15	30:Z:618:LUT:H201	1.87	0.42
30:4:620:LUT:H35	30:4:620:LUT:H401	1.82	0.42
25:4:621:BCR:C23	25:4:621:BCR:H383	2.49	0.42
25:5:625:BCR:H11C	25:5:625:BCR:H341	1.73	0.42
1:A:60:ASP:OD2	1:A:350:HIS:NE2	2.51	0.42
22:A:808:CLA:HMB2	22:A:809:CLA:H3A	2.00	0.42
2:B:71:TRP:CE2	8:I:71:PRO:HG2	2.55	0.42
2:B:416:LYS:HZ1	6:F:226:PRO:HG3	1.42	0.42
2:B:518:PHE:CE1	2:B:522:HIS:CE1	3.07	0.42
22:B:832:CLA:H61	25:F:305:BCR:H312	2.02	0.42
25:B:848:BCR:H15C	25:B:848:BCR:H351	1.85	0.42
6:F:182:ASP:HA	6:F:185:ILE:HG22	2.01	0.42
30:1:617:LUT:H35	30:1:617:LUT:H401	1.88	0.42
22:Z:602:CLA:H72	22:Z:602:CLA:H111	1.89	0.42
1:A:197:MET:HE2	22:A:814:CLA:HHD	2.02	0.42
1:A:426:LEU:HD13	22:A:825:CLA:C1C	2.49	0.42
2:B:375:HIS:HB2	22:B:827:CLA:C1B	2.50	0.42
12:1:158:PHE:HZ	22:1:608:CLA:NC	2.17	0.42
22:4:612:CLA:H52	22:4:612:CLA:H11	1.77	0.42
30:5:620:LUT:H11	30:5:620:LUT:H191	1.96	0.42
1:A:349:TRP:HB3	22:A:806:CLA:HAC1	2.00	0.42
22:B:830:CLA:CBB	22:B:841:CLA:H142	2.50	0.42
25:B:843:BCR:H15C	25:B:843:BCR:H351	1.86	0.42
25:L:205:BCR:H11C	25:L:205:BCR:H341	1.90	0.42
16:4:149:LEU:HD21	29:4:606:CHL:HMD2	2.02	0.42
22:A:815:CLA:H62	22:A:815:CLA:H41	1.88	0.41
22:B:815:CLA:H11	22:B:815:CLA:H51	1.80	0.41
22:B:825:CLA:HMA1	25:B:847:BCR:H14C	2.01	0.41
22:3:604:CLA:H11	22:5:616:CLA:HED2	2.01	0.41
22:3:610:CLA:H142	22:3:610:CLA:H111	1.86	0.41
22:5:609:CLA:H3A	22:5:609:CLA:HBA2	1.65	0.41
1:A:166:GLY:HA2	25:A:848:BCR:HC22	2.02	0.41
22:A:827:CLA:H52	22:A:836:CLA:HBB2	2.01	0.41
2:B:86:ARG:HA	2:B:87:PRO:HD3	1.88	0.41
2:B:194:HIS:HB2	22:B:814:CLA:CHC	2.50	0.41
2:B:300:HIS:HB3	2:B:305:ILE:HD11	2.02	0.41
2:B:463:TRP:NE1	22:F:304:CLA:HAA2	2.35	0.41
2:B:610:PHE:O	2:B:614:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:846:BCR:H24C	25:B:846:BCR:H371	1.83	0.41
25:K:4004:BCR:H351	25:K:4004:BCR:H15C	1.78	0.41
22:3:604:CLA:HBA1	22:3:606:CLA:C1D	2.50	0.41
15:8:88:LEU:O	15:8:92:LEU:N	2.43	0.41
15:8:174:ASP:OD1	30:8:617:LUT:O23	2.29	0.41
22:4:611:CLA:H61	22:4:611:CLA:H41	1.60	0.41
22:6:612:CLA:H41	22:6:612:CLA:H62	1.82	0.41
1:A:576:ASP:CG	3:C:53:ARG:HH21	2.29	0.41
22:A:832:CLA:CED	11:L:55:LEU:HD11	2.47	0.41
13:3:216:LYS:HD3	22:3:612:CLA:HAA2	2.01	0.41
22:7:610:CLA:CBB	30:7:621:LUT:H32	2.48	0.41
22:Z:611:CLA:H203	22:Z:611:CLA:H161	1.92	0.41
16:4:220:ARG:HA	16:4:223:MET:HE3	2.03	0.41
19:2:219:MET:O	19:2:219:MET:SD	2.79	0.41
1:A:536:HIS:CG	22:A:839:CLA:HED2	2.55	0.41
22:A:840:CLA:H161	22:A:840:CLA:H121	1.69	0.41
2:B:176:LEU:HD23	2:B:176:LEU:HA	1.92	0.41
13:3:68:ASP:OD1	30:3:622:LUT:O23	2.38	0.41
13:3:246:LEU:HD21	30:3:621:LUT:H163	2.02	0.41
1:A:256:SER:OG	1:A:271:GLU:O	2.32	0.41
1:A:413:MET:HE1	1:A:431:ILE:HD11	2.03	0.41
22:A:820:CLA:HBA2	22:A:820:CLA:H3A	1.91	0.41
25:J:3003:BCR:H15C	25:J:3003:BCR:H351	1.84	0.41
30:3:621:LUT:H15	30:3:621:LUT:H201	1.90	0.41
15:8:212:ALA:HB2	22:8:616:CLA:HED2	2.01	0.41
12:Z:173:LEU:HD23	12:Z:176:LYS:HD2	2.02	0.41
22:Z:613:CLA:H141	25:4:621:BCR:H322	2.01	0.41
16:4:232:GLN:HE22	30:4:619:LUT:C4	2.33	0.41
22:4:601:CLA:H112	22:4:601:CLA:H72	1.74	0.41
30:4:620:LUT:H15	30:4:620:LUT:H201	1.89	0.41
1:A:408:HIS:HE1	22:A:831:CLA:NA	2.19	0.41
22:A:816:CLA:H92	22:A:816:CLA:H61	1.84	0.41
22:A:841:CLA:H62	22:A:841:CLA:H102	1.89	0.41
22:A:843:CLA:H13	22:A:843:CLA:H101	1.89	0.41
2:B:316:LEU:HD22	22:B:830:CLA:HMD3	2.02	0.41
22:B:840:CLA:HHD	22:B:840:CLA:HAC1	1.91	0.41
25:I:172:BCR:H15C	25:I:172:BCR:H351	1.87	0.41
22:1:610:CLA:CBB	30:1:617:LUT:H32	2.51	0.41
25:3:719:BCR:H20C	25:3:719:BCR:H361	1.90	0.41
15:8:88:LEU:HD11	30:8:617:LUT:H10	2.03	0.41
22:6:610:CLA:H92	22:6:610:CLA:H61	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HG23	1:A:122:VAL:HG22	2.03	0.41
1:A:474:ASP:O	1:A:478:GLN:NE2	2.54	0.41
22:1:614:CLA:H91	22:1:614:CLA:H112	1.86	0.41
22:8:602:CLA:HBB1	22:8:602:CLA:H51	2.02	0.41
30:Z:619:LUT:H391	30:Z:619:LUT:H31	1.76	0.41
16:4:208:ILE:CG1	22:4:610:CLA:HMA1	2.51	0.41
1:A:162:THR:HG23	22:A:815:CLA:O1A	2.20	0.41
22:A:835:CLA:C5	22:A:835:CLA:H92	2.50	0.41
2:B:685:LYS:HE3	11:L:54:MET:SD	2.61	0.41
22:B:841:CLA:H161	22:B:841:CLA:H192	1.73	0.41
25:K:4001:BCR:H361	25:K:4001:BCR:H20C	1.81	0.41
22:3:603:CLA:H92	22:3:603:CLA:H62	1.89	0.41
25:8:619:BCR:H15C	25:8:619:BCR:H351	1.81	0.41
18:6:181:ARG:HA	18:6:184:MET:HE3	2.03	0.41
22:6:612:CLA:HMA2	22:6:612:CLA:H2	2.03	0.41
1:A:692:TYR:CE2	22:A:802:CLA:HMD1	2.56	0.41
21:A:801:CL0:H41	21:A:801:CL0:H49	1.95	0.41
22:A:824:CLA:H3A	22:A:824:CLA:HBA2	1.77	0.41
22:A:834:CLA:H52	22:A:834:CLA:H11	1.85	0.41
25:A:851:BCR:H11C	25:A:851:BCR:H341	1.85	0.41
2:B:181:SER:HB3	2:B:289:GLY:HA3	2.03	0.41
22:B:815:CLA:H91	25:B:843:BCR:H23C	2.03	0.41
22:B:835:CLA:H3A	22:B:835:CLA:HBA2	1.71	0.41
22:B:840:CLA:H193	22:B:840:CLA:H161	1.96	0.41
25:B:843:BCR:H362	25:G:205:BCR:H312	2.03	0.41
6:F:223:THR:HB	6:F:227:ARG:HH21	1.86	0.41
12:1:64:LEU:HD13	22:1:602:CLA:H42	2.03	0.41
12:1:67:GLU:HA	12:1:68:PRO:HD3	1.85	0.41
12:1:84:TRP:CE2	22:1:608:CLA:HED2	2.56	0.41
12:1:189:LEU:HD21	22:1:602:CLA:H18	2.02	0.41
29:1:601:CHL:HMD1	25:8:619:BCR:HC21	2.01	0.41
25:3:718:BCR:H15C	25:3:718:BCR:H351	1.83	0.41
25:3:718:BCR:H322	22:5:601:CLA:H101	2.02	0.41
22:7:602:CLA:H121	22:7:602:CLA:H161	1.85	0.41
22:7:613:CLA:HHD	22:7:616:CLA:OBD	2.21	0.41
12:Z:161:LEU:HD12	30:Z:617:LUT:H222	2.02	0.41
29:6:607:CHL:H41	29:6:607:CHL:H62	1.76	0.41
20:9:157:LYS:O	20:9:161:ASN:HB2	2.21	0.41
22:A:802:CLA:H152	22:A:842:CLA:CBB	2.51	0.41
25:A:849:BCR:H272	25:3:719:BCR:H352	2.03	0.41
22:B:802:CLA:H142	22:B:802:CLA:H111	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:834:CLA:H161	22:B:834:CLA:H122	1.76	0.41
27:B:850:DGD:HE2	3:C:70:GLY:C	2.46	0.41
14:7:77:ARG:NE	14:7:190:GLU:OE2	2.50	0.41
14:7:231:PHE:O	14:7:237:SER:OG	2.38	0.41
22:Z:614:CLA:H142	22:Z:614:CLA:H112	1.86	0.41
22:4:604:CLA:HMB2	30:4:620:LUT:H7	2.03	0.41
18:6:127:ARG:NH2	29:6:618:CHL:HMC	2.36	0.41
25:6:623:BCR:H24C	25:6:623:BCR:H371	1.90	0.41
22:A:841:CLA:H2	22:A:841:CLA:H61	1.86	0.40
2:B:152:PHE:CZ	19:2:220:ILE:HD13	2.56	0.40
2:B:320:HIS:CD2	22:B:823:CLA:ND	2.89	0.40
22:B:808:CLA:H102	22:B:808:CLA:H62	1.84	0.40
22:B:809:CLA:H91	22:B:809:CLA:H111	1.94	0.40
4:D:74:LEU:HD22	4:D:78:ALA:HB2	2.03	0.40
22:1:608:CLA:HBB1	22:1:608:CLA:H121	2.02	0.40
30:3:622:LUT:H15	30:3:622:LUT:H201	1.88	0.40
22:8:601:CLA:H122	22:8:614:CLA:HBA2	2.04	0.40
22:8:609:CLA:H3A	22:8:609:CLA:HBA1	1.83	0.40
18:6:149:LEU:HA	18:6:150:PRO:HD3	1.90	0.40
22:6:601:CLA:H151	22:6:601:CLA:H112	1.78	0.40
25:6:623:BCR:H15C	25:6:623:BCR:H351	1.89	0.40
1:A:316:TRP:CD1	10:K:87:VAL:HG21	2.56	0.40
1:A:677:PHE:CD2	25:A:852:BCR:H363	2.57	0.40
25:A:848:BCR:H402	25:3:719:BCR:HC7	2.03	0.40
2:B:16:ASP:HB3	2:B:21:ARG:HB2	2.03	0.40
25:B:846:BCR:H20C	25:B:846:BCR:H361	1.97	0.40
25:3:719:BCR:H11C	25:3:719:BCR:H341	1.96	0.40
30:7:621:LUT:H15	30:7:621:LUT:H201	1.96	0.40
22:A:802:CLA:H42	22:A:802:CLA:HHB	2.02	0.40
25:A:850:BCR:H20C	25:A:850:BCR:H361	1.84	0.40
25:A:856:BCR:H11C	25:A:856:BCR:H341	1.88	0.40
2:B:194:HIS:HE1	22:B:814:CLA:NA	2.16	0.40
5:E:62:VAL:HG22	5:E:71:VAL:HG22	2.04	0.40
25:7:623:BCR:H11C	25:7:623:BCR:H341	1.92	0.40
22:Z:610:CLA:CBB	30:Z:617:LUT:H32	2.52	0.40
22:Z:611:CLA:H72	22:Z:611:CLA:H111	1.93	0.40
16:4:156:LEU:CD1	25:4:621:BCR:C35	2.99	0.40
22:5:606:CLA:HBB1	29:5:607:CHL:CMC	2.51	0.40
30:6:624:LUT:H201	30:6:624:LUT:H15	1.84	0.40
30:2:616:LUT:H401	30:2:616:LUT:H35	1.76	0.40
22:9:603:CLA:HBB1	22:9:603:CLA:HHC	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:TRP:NE1	22:A:831:CLA:HMD3	2.37	0.40
25:A:850:BCR:H11C	25:A:850:BCR:H341	1.84	0.40
2:B:157:HIS:HE1	22:B:811:CLA:C1A	2.34	0.40
2:B:390:HIS:HA	2:B:393:ILE:HD12	2.03	0.40
2:B:601:THR:HG21	2:B:610:PHE:HB2	2.03	0.40
4:D:66:ILE:HB	4:D:105:ILE:HB	2.03	0.40
25:3:717:BCR:H15C	25:3:717:BCR:H351	1.87	0.40
14:7:198:MET:SD	22:7:602:CLA:HBB1	2.62	0.40
22:Z:602:CLA:H52	30:Z:618:LUT:H28	2.02	0.40
22:Z:612:CLA:H11	22:Z:612:CLA:H51	1.81	0.40
16:4:160:VAL:HG13	29:4:608:CHL:NB	2.37	0.40
22:4:601:CLA:H111	22:4:601:CLA:H142	1.78	0.40
22:5:617:CLA:CMB	22:6:622:CLA:CBC	3.00	0.40
30:2:616:LUT:H11	30:2:616:LUT:H191	1.97	0.40
1:A:428:ASP:O	1:A:432:ARG:HB2	2.21	0.40
22:A:843:CLA:H62	22:A:843:CLA:H41	1.68	0.40
2:B:157:HIS:HE1	22:B:811:CLA:NA	2.18	0.40
25:F:305:BCR:H11C	25:F:305:BCR:H341	1.76	0.40
7:G:32:LEU:HB3	7:G:33:ASP:H	1.60	0.40
7:G:91:ASP:OD2	7:G:92:PRO:N	2.55	0.40
12:1:42:GLY:HA3	15:8:146:SER:OG	2.21	0.40
12:1:138:MET:O	12:1:142:GLU:HG2	2.22	0.40
13:3:156:GLN:O	13:3:160:LEU:CB	2.61	0.40
22:3:603:CLA:HHC	22:3:603:CLA:HBB1	2.02	0.40
22:7:613:CLA:H122	22:7:613:CLA:H162	1.81	0.40
16:4:247:HIS:CD2	22:4:614:CLA:C1C	3.04	0.40
18:6:164:PHE:O	30:6:621:LUT:O23	2.32	0.40
18:6:192:MET:HG3	22:6:613:CLA:HAC2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	734/751 (98%)	713 (97%)	20 (3%)	1 (0%)	48 77
2	B	730/755 (97%)	708 (97%)	22 (3%)	0	100 100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100 100
4	D	142/161 (88%)	135 (95%)	7 (5%)	0	100 100
5	E	59/73 (81%)	55 (93%)	4 (7%)	0	100 100
6	F	163/165 (99%)	155 (95%)	8 (5%)	0	100 100
7	G	64/94 (68%)	64 (100%)	0	0	100 100
8	I	35/106 (33%)	34 (97%)	1 (3%)	0	100 100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100 100
10	K	41/87 (47%)	41 (100%)	0	0	100 100
11	L	114/156 (73%)	108 (95%)	5 (4%)	1 (1%)	14 41
12	1	192/194 (99%)	186 (97%)	6 (3%)	0	100 100
12	Z	188/194 (97%)	181 (96%)	7 (4%)	0	100 100
13	3	200/268 (75%)	191 (96%)	9 (4%)	0	100 100
14	7	210/215 (98%)	200 (95%)	10 (5%)	0	100 100
15	8	215/217 (99%)	206 (96%)	9 (4%)	0	100 100
16	4	199/236 (84%)	187 (94%)	11 (6%)	1 (0%)	24 54
17	5	219/229 (96%)	201 (92%)	18 (8%)	0	100 100
18	6	227/232 (98%)	216 (95%)	11 (5%)	0	100 100
19	2	107/221 (48%)	107 (100%)	0	0	100 100
20	9	144/189 (76%)	136 (94%)	8 (6%)	0	100 100
All	All	4098/4665 (88%)	3933 (96%)	162 (4%)	3 (0%)	49 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	L	187	VAL
16	4	208	ILE
1	A	122	VAL

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	599/610 (98%)	592 (99%)	7 (1%)	63 86
2	B	596/617 (97%)	595 (100%)	1 (0%)	87 96
3	C	69/70 (99%)	69 (100%)	0	100 100
4	D	121/129 (94%)	120 (99%)	1 (1%)	73 90
5	E	52/62 (84%)	52 (100%)	0	100 100
6	F	127/127 (100%)	127 (100%)	0	100 100
7	G	48/69 (70%)	48 (100%)	0	100 100
8	I	31/76 (41%)	31 (100%)	0	100 100
9	J	35/37 (95%)	35 (100%)	0	100 100
10	K	30/60 (50%)	30 (100%)	0	100 100
11	L	85/119 (71%)	84 (99%)	1 (1%)	63 86
12	1	137/137 (100%)	137 (100%)	0	100 100
12	Z	137/137 (100%)	137 (100%)	0	100 100
13	3	155/209 (74%)	154 (99%)	1 (1%)	78 93
14	7	164/164 (100%)	164 (100%)	0	100 100
15	8	163/163 (100%)	163 (100%)	0	100 100
16	4	159/185 (86%)	158 (99%)	1 (1%)	78 93
17	5	181/184 (98%)	180 (99%)	1 (1%)	78 93
18	6	183/185 (99%)	183 (100%)	0	100 100
19	2	70/178 (39%)	69 (99%)	1 (1%)	59 85
20	9	118/143 (82%)	118 (100%)	0	100 100
All	All	3260/3661 (89%)	3246 (100%)	14 (0%)	81 94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	205	LEU
1	A	206	LEU
1	A	286	THR
1	A	372	TYR
1	A	584	CYS
1	A	657	VAL

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Mol	Chain	Res	Type
2	B	479	LEU
4	D	139	TYR
11	L	54	MET
13	3	160	LEU
16	4	208	ILE
17	5	202	LEU
19	2	219	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	489	ASN
1	A	722	GLN
2	B	84	HIS
2	B	159	GLN
2	B	253	GLN
2	B	276	HIS
4	D	127	GLN
5	E	55	GLN
5	E	78	GLN
7	G	118	ASN
11	L	108	ASN
12	1	56	ASN
13	3	88	GLN
13	3	234	GLN
13	3	245	ASN
13	3	257	ASN
13	3	261	ASN
14	7	184	GLN
14	7	207	GLN
15	8	147	GLN
12	Z	221	ASN
16	4	72	ASN
16	4	153	GLN
16	4	166	GLN
16	4	175	ASN
17	5	203	GLN
18	6	60	ASN
18	6	88	GLN
18	6	130	GLN
18	6	227	GLN
20	9	87	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

313 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	9	604	20	54,58,73	2.35	20 (37%)	65,95,113	3.13	29 (44%)
22	CLA	B	836	2	64,68,73	2.09	20 (31%)	77,107,113	3.00	32 (41%)
22	CLA	3	617	13	50,54,73	2.38	20 (40%)	60,90,113	3.22	27 (45%)
22	CLA	1	602	12	69,73,73	2.02	19 (27%)	83,113,113	2.77	32 (38%)
30	LUT	9	616	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
22	CLA	8	603	15	49,53,73	2.38	20 (40%)	59,89,113	3.24	26 (44%)
22	CLA	B	839	-	69,73,73	2.04	21 (30%)	83,113,113	2.77	28 (33%)
22	CLA	A	808	1	69,73,73	2.02	21 (30%)	83,113,113	2.90	31 (37%)
22	CLA	1	606	-	56,60,73	2.28	19 (33%)	67,97,113	3.08	31 (46%)
22	CLA	4	602	16	64,68,73	2.10	19 (29%)	77,107,113	2.87	29 (37%)
22	CLA	9	610	20	64,68,73	2.14	20 (31%)	77,107,113	2.93	29 (37%)
24	LHG	A	855	-	29,29,48	1.20	2 (6%)	32,35,54	1.17	3 (9%)
22	CLA	B	802	2	69,73,73	1.94	19 (27%)	83,113,113	2.95	31 (37%)
22	CLA	8	608	-	54,58,73	2.23	19 (35%)	65,95,113	3.20	28 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	806	2	69,73,73	2.01	20 (28%)	83,113,113	2.84	32 (38%)
22	CLA	9	602	20	64,68,73	2.12	19 (29%)	77,107,113	2.95	31 (40%)
22	CLA	5	617	17	50,54,73	2.32	21 (42%)	60,90,113	4.37	27 (45%)
22	CLA	7	609	14	54,58,73	2.30	20 (37%)	65,95,113	3.27	30 (46%)
22	CLA	1	616	12	50,54,73	2.38	20 (40%)	60,90,113	3.07	28 (46%)
22	CLA	3	610	13	69,73,73	2.00	18 (26%)	83,113,113	2.89	33 (39%)
22	CLA	B	824	-	69,73,73	2.00	19 (27%)	83,113,113	2.78	30 (36%)
29	CHL	3	608	-	70,74,74	1.92	19 (27%)	80,114,114	2.91	25 (31%)
22	CLA	2	614	-	49,53,73	2.46	20 (40%)	59,89,113	3.27	26 (44%)
22	CLA	7	602	14	69,73,73	2.03	19 (27%)	83,113,113	2.90	31 (37%)
22	CLA	7	616	14	50,54,73	2.42	21 (42%)	60,90,113	3.31	26 (43%)
22	CLA	5	614	17	49,53,73	2.42	20 (40%)	59,89,113	3.39	28 (47%)
22	CLA	A	814	1	69,73,73	2.00	20 (28%)	83,113,113	2.91	29 (34%)
26	SF4	C	102	3	0,12,12	-	-	-		
22	CLA	A	840	1	69,73,73	1.99	21 (30%)	83,113,113	2.93	30 (36%)
22	CLA	5	612	17	56,60,73	2.24	20 (35%)	67,97,113	3.10	29 (43%)
22	CLA	2	610	19	64,68,73	2.16	20 (31%)	77,107,113	2.93	29 (37%)
22	CLA	4	601	16	65,69,73	2.06	20 (30%)	78,108,113	2.91	30 (38%)
22	CLA	B	809	2	69,73,73	1.97	18 (26%)	83,113,113	2.75	30 (36%)
22	CLA	Z	609	12	69,73,73	2.05	20 (28%)	83,113,113	2.80	30 (36%)
29	CHL	9	606	-	46,50,74	2.35	20 (43%)	51,85,114	3.63	25 (49%)
29	CHL	8	607	-	60,64,74	2.11	20 (33%)	68,102,114	3.13	27 (39%)
22	CLA	8	604	-	50,54,73	2.36	19 (38%)	60,90,113	3.12	28 (46%)
22	CLA	B	803	-	69,73,73	1.94	20 (28%)	83,113,113	2.71	28 (33%)
22	CLA	8	606	-	46,50,73	2.44	20 (43%)	55,85,113	3.31	25 (45%)
25	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.76	15 (26%)
22	CLA	A	822	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	28 (33%)
22	CLA	3	620	-	60,64,73	2.19	20 (33%)	72,102,113	2.94	29 (40%)
29	CHL	6	608	-	55,59,74	2.20	19 (34%)	62,96,114	3.43	30 (48%)
22	CLA	Z	602	12	69,73,73	2.02	21 (30%)	83,113,113	2.83	32 (38%)
30	LUT	1	618	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
30	LUT	Z	617	-	42,43,43	0.77	0	51,60,60	1.69	15 (29%)
22	CLA	5	606	-	59,63,73	2.23	20 (33%)	71,101,113	3.02	30 (42%)
24	LHG	B	851	22	22,22,48	1.15	2 (9%)	25,28,54	1.24	2 (8%)
22	CLA	6	622	18	49,53,73	2.39	20 (40%)	59,89,113	3.25	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CHL	4	618	16	47,51,74	2.33	20 (42%)	52,86,114	3.58	24 (46%)
22	CLA	A	804	1	69,73,73	1.97	18 (26%)	83,113,113	2.93	34 (40%)
22	CLA	9	609	-	54,58,73	2.30	20 (37%)	65,95,113	3.18	30 (46%)
22	CLA	B	822	2	63,67,73	2.12	19 (30%)	75,105,113	2.94	30 (40%)
24	LHG	7	625	22	36,36,48	1.02	2 (5%)	39,42,54	1.13	3 (7%)
22	CLA	L	203	11	69,73,73	1.99	20 (28%)	83,113,113	2.84	29 (34%)
22	CLA	B	841	24	69,73,73	2.07	21 (30%)	83,113,113	2.85	30 (36%)
22	CLA	2	607	-	54,58,73	2.36	20 (37%)	65,95,113	3.15	29 (44%)
24	LHG	A	847	22	37,37,48	1.06	2 (5%)	40,43,54	1.26	4 (10%)
25	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.75	11 (19%)
22	CLA	6	617	18	50,54,73	2.37	20 (40%)	60,90,113	3.23	27 (45%)
22	CLA	A	843	-	69,73,73	2.01	21 (30%)	83,113,113	2.68	30 (36%)
22	CLA	B	811	2	58,62,73	2.21	19 (32%)	73,100,113	3.17	35 (47%)
22	CLA	F	301	-	69,73,73	2.02	19 (27%)	83,113,113	2.87	32 (38%)
22	CLA	3	609	13	54,58,73	2.29	21 (38%)	65,95,113	3.15	29 (44%)
22	CLA	A	842	1	69,73,73	2.00	19 (27%)	83,113,113	2.87	30 (36%)
22	CLA	3	613	13	59,63,73	2.17	19 (32%)	71,101,113	2.86	27 (38%)
22	CLA	B	831	2	53,57,73	2.30	18 (33%)	62,93,113	3.22	25 (40%)
25	BCR	L	205	-	41,41,41	0.71	0	56,56,56	1.60	12 (21%)
22	CLA	3	607	13	64,68,73	2.12	22 (34%)	77,107,113	2.97	31 (40%)
25	BCR	3	717	-	41,41,41	0.75	0	56,56,56	1.87	16 (28%)
22	CLA	B	825	-	69,73,73	2.01	20 (28%)	83,113,113	2.76	31 (37%)
22	CLA	B	820	2	60,64,73	2.21	20 (33%)	72,102,113	2.99	29 (40%)
22	CLA	1	613	-	69,73,73	2.00	19 (27%)	83,113,113	2.70	28 (33%)
22	CLA	5	609	17	54,58,73	2.29	22 (40%)	65,95,113	3.22	30 (46%)
24	LHG	8	620	22	36,36,48	1.02	2 (5%)	39,42,54	1.14	5 (12%)
22	CLA	6	610	-	64,68,73	2.13	21 (32%)	77,107,113	2.93	32 (41%)
22	CLA	6	611	24	59,63,73	2.23	21 (35%)	71,101,113	2.92	29 (40%)
25	BCR	A	852	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
22	CLA	2	611	-	59,63,73	2.24	20 (33%)	71,101,113	2.99	30 (42%)
22	CLA	2	612	19	56,60,73	2.28	20 (35%)	67,97,113	3.09	28 (41%)
24	LHG	5	623	22	36,36,48	1.07	2 (5%)	39,42,54	1.10	3 (7%)
22	CLA	A	812	1,22	69,73,73	1.99	22 (31%)	83,113,113	2.95	27 (32%)
22	CLA	A	817	-	61,65,73	2.16	20 (32%)	73,103,113	2.96	29 (39%)
22	CLA	1	609	12	69,73,73	2.04	21 (30%)	83,113,113	2.84	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	6	609	18	54,58,73	2.30	22 (40%)	65,95,113	3.15	29 (44%)
24	LHG	1	620	22	42,42,48	0.99	2 (4%)	45,48,54	1.10	3 (6%)
22	CLA	A	831	1	69,73,73	1.98	18 (26%)	83,113,113	2.78	30 (36%)
24	LHG	Z	620	22	42,42,48	0.99	2 (4%)	45,48,54	1.06	2 (4%)
22	CLA	6	613	-	60,64,73	2.21	20 (33%)	72,102,113	2.91	29 (40%)
22	CLA	6	603	18	50,54,73	2.34	20 (40%)	60,90,113	3.27	28 (46%)
30	LUT	3	621	-	42,43,43	0.77	0	51,60,60	1.52	13 (25%)
22	CLA	A	818	1	69,73,73	1.97	19 (27%)	83,113,113	2.96	30 (36%)
22	CLA	B	816	2	59,63,73	2.14	19 (32%)	71,101,113	3.13	29 (40%)
22	CLA	8	601	15	69,73,73	2.03	21 (30%)	83,113,113	2.79	31 (37%)
22	CLA	1	610	12	64,68,73	2.11	19 (29%)	77,107,113	3.01	34 (44%)
25	BCR	6	623	-	41,41,41	0.65	0	56,56,56	1.98	18 (32%)
22	CLA	Z	610	12	64,68,73	2.09	21 (32%)	77,107,113	3.01	31 (40%)
30	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.67	11 (21%)
30	LUT	Z	618	-	42,43,43	0.71	0	51,60,60	1.58	12 (23%)
22	CLA	A	837	1	49,53,73	2.46	20 (40%)	59,89,113	3.12	28 (47%)
29	CHL	7	607	-	58,62,74	2.18	20 (34%)	65,99,114	3.11	26 (40%)
22	CLA	8	613	15	69,73,73	2.01	20 (28%)	83,113,113	2.69	28 (33%)
22	CLA	A	835	1	69,73,73	2.07	21 (30%)	83,113,113	2.82	28 (33%)
22	CLA	B	804	2	49,53,73	2.36	21 (42%)	59,89,113	3.41	31 (52%)
29	CHL	Z	601	12	57,61,74	2.23	22 (38%)	64,98,114	3.30	23 (35%)
25	BCR	A	849	-	41,41,41	0.78	0	56,56,56	1.80	17 (30%)
22	CLA	2	602	19	49,53,73	2.44	20 (40%)	59,89,113	3.26	26 (44%)
22	CLA	7	613	14	69,73,73	1.98	19 (27%)	83,113,113	2.75	26 (31%)
22	CLA	A	826	-	69,73,73	2.02	19 (27%)	83,113,113	2.81	28 (33%)
22	CLA	F	304	6	69,73,73	2.06	21 (30%)	83,113,113	2.83	28 (33%)
22	CLA	3	612	13	50,54,73	2.37	21 (42%)	60,90,113	3.36	28 (46%)
25	BCR	K	4004	-	41,41,41	0.70	0	56,56,56	1.74	14 (25%)
22	CLA	7	612	14	56,60,73	2.24	19 (33%)	67,97,113	3.15	30 (44%)
22	CLA	6	612	18	56,60,73	2.24	20 (35%)	67,97,113	3.08	27 (40%)
27	DGD	B	850	-	67,67,67	0.80	2 (2%)	81,81,81	1.03	4 (4%)
23	PQN	A	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.04	2 (4%)
29	CHL	5	608	-	55,59,74	2.19	20 (36%)	62,96,114	3.21	26 (41%)
22	CLA	3	602	13	64,68,73	2.11	22 (34%)	77,107,113	2.94	33 (42%)
22	CLA	4	611	24	59,63,73	2.22	21 (35%)	71,101,113	2.93	31 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	7	604	-	60,64,73	2.16	20 (33%)	72,102,113	3.02	29 (40%)
22	CLA	5	611	24	59,63,73	2.22	21 (35%)	71,101,113	3.01	29 (40%)
22	CLA	4	614	16	49,53,73	2.41	20 (40%)	59,89,113	3.20	27 (45%)
25	BCR	F	305	-	41,41,41	0.69	0	56,56,56	1.88	13 (23%)
22	CLA	5	601	17	69,73,73	2.05	20 (28%)	83,113,113	2.82	31 (37%)
22	CLA	B	829	2	69,73,73	2.05	20 (28%)	83,113,113	3.06	33 (39%)
22	CLA	B	805	2	69,73,73	2.00	19 (27%)	83,113,113	2.88	29 (34%)
22	CLA	B	823	2	64,68,73	2.11	20 (31%)	77,107,113	2.82	32 (41%)
22	CLA	1	614	12	69,73,73	2.05	20 (28%)	83,113,113	2.89	27 (32%)
22	CLA	B	818	2	64,68,73	2.08	19 (29%)	77,107,113	2.87	34 (44%)
30	LUT	7	621	-	42,43,43	0.73	0	51,60,60	1.53	10 (19%)
22	CLA	5	613	17	60,64,73	2.17	20 (33%)	72,102,113	2.94	28 (38%)
22	CLA	A	805	1,22	59,63,73	2.21	21 (35%)	71,101,113	3.02	28 (39%)
22	CLA	1	612	12	56,60,73	2.24	20 (35%)	67,97,113	3.11	32 (47%)
22	CLA	B	832	2	69,73,73	1.99	19 (27%)	83,113,113	2.85	31 (37%)
22	CLA	Z	612	12	56,60,73	2.24	20 (35%)	67,97,113	3.15	28 (41%)
22	CLA	A	836	1	54,58,73	2.30	21 (38%)	65,95,113	3.10	32 (49%)
22	CLA	A	815	1	64,68,73	2.16	21 (32%)	77,107,113	2.94	29 (37%)
22	CLA	9	614	20	49,53,73	2.45	20 (40%)	59,89,113	3.32	30 (50%)
22	CLA	B	812	2	69,73,73	2.03	21 (30%)	83,113,113	2.81	30 (36%)
22	CLA	B	817	2	63,67,73	2.09	19 (30%)	75,105,113	2.95	30 (40%)
22	CLA	9	612	-	56,60,73	2.29	20 (35%)	67,97,113	3.08	30 (44%)
22	CLA	A	813	1	58,62,73	2.22	21 (36%)	69,99,113	3.04	30 (43%)
22	CLA	5	604	17	54,58,73	2.32	19 (35%)	65,95,113	3.07	30 (46%)
30	LUT	Z	619	-	42,43,43	0.71	0	51,60,60	1.76	12 (23%)
29	CHL	4	607	-	55,59,74	2.24	20 (36%)	62,96,114	3.34	27 (43%)
29	CHL	9	607	-	55,59,74	2.27	21 (38%)	62,96,114	3.24	26 (41%)
22	CLA	A	834	1	69,73,73	2.02	20 (28%)	83,113,113	2.92	32 (38%)
22	CLA	A	827	-	69,73,73	2.03	20 (28%)	83,113,113	2.81	30 (36%)
22	CLA	7	614	14	47,51,73	2.39	21 (44%)	56,86,113	3.44	29 (51%)
25	BCR	B	847	-	41,41,41	0.76	0	56,56,56	1.71	14 (25%)
30	LUT	5	620	-	42,43,43	0.78	0	51,60,60	1.72	14 (27%)
22	CLA	8	602	15	66,70,73	2.02	19 (28%)	79,109,113	2.95	31 (39%)
25	BCR	B	843	-	41,41,41	0.72	0	56,56,56	1.56	8 (14%)
25	BCR	I	172	-	41,41,41	0.67	0	56,56,56	1.97	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	4	603	16	50,54,73	2.36	18 (36%)	60,90,113	3.27	27 (45%)
22	CLA	5	603	17	50,54,73	2.34	20 (40%)	60,90,113	3.22	27 (45%)
23	PQN	B	842	-	34,34,34	1.56	2 (5%)	42,45,45	0.94	2 (4%)
29	CHL	6	606	-	60,64,74	2.17	21 (35%)	68,102,114	3.21	28 (41%)
22	CLA	B	835	-	49,53,73	2.41	20 (40%)	59,89,113	3.12	27 (45%)
22	CLA	A	854	-	69,73,73	2.02	20 (28%)	83,113,113	2.92	31 (37%)
30	LUT	8	617	-	42,43,43	0.77	0	51,60,60	1.70	13 (25%)
22	CLA	A	809	1	69,73,73	2.02	21 (30%)	83,113,113	2.92	32 (38%)
22	CLA	B	828	2	69,73,73	2.00	20 (28%)	83,113,113	2.69	31 (37%)
22	CLA	4	616	16	45,49,73	2.49	19 (42%)	54,84,113	3.47	28 (51%)
24	LHG	4	623	-	31,31,48	1.14	2 (6%)	34,37,54	1.14	3 (8%)
22	CLA	B	808	2	69,73,73	2.02	21 (30%)	83,113,113	2.83	29 (34%)
22	CLA	7	601	14	69,73,73	2.01	20 (28%)	83,113,113	2.88	29 (34%)
25	BCR	B	846	-	41,41,41	0.76	0	56,56,56	2.01	15 (26%)
22	CLA	A	828	1	69,73,73	1.99	20 (28%)	83,113,113	2.91	27 (32%)
22	CLA	B	826	2	69,73,73	1.99	19 (27%)	83,113,113	2.83	32 (38%)
28	LMG	9	620	-	44,44,55	0.85	2 (4%)	52,52,63	1.23	2 (3%)
25	BCR	3	719	-	41,41,41	0.69	0	56,56,56	1.64	13 (23%)
22	CLA	7	608	-	54,58,73	2.27	18 (33%)	65,95,113	3.16	27 (41%)
22	CLA	3	604	-	69,73,73	2.02	18 (26%)	83,113,113	2.73	27 (32%)
22	CLA	L	204	-	54,58,73	2.33	20 (37%)	65,95,113	3.17	27 (41%)
22	CLA	A	845	24	56,60,73	2.27	20 (35%)	67,97,113	3.17	26 (38%)
25	BCR	7	623	-	41,41,41	0.78	1 (2%)	56,56,56	1.93	15 (26%)
22	CLA	Z	614	12	69,73,73	2.06	20 (28%)	83,113,113	2.83	30 (36%)
22	CLA	B	821	2	50,54,73	2.37	21 (42%)	60,90,113	3.20	25 (41%)
22	CLA	A	807	1	69,73,73	2.02	20 (28%)	83,113,113	2.84	28 (33%)
25	BCR	B	848	-	41,41,41	0.73	0	56,56,56	1.53	10 (17%)
22	CLA	1	604	-	61,65,73	2.18	19 (31%)	73,103,113	2.94	31 (42%)
22	CLA	B	838	2	51,55,73	2.34	20 (39%)	61,91,113	3.24	29 (47%)
22	CLA	B	814	2	64,68,73	2.09	19 (29%)	77,107,113	2.91	32 (41%)
22	CLA	A	825	1	59,63,73	2.16	18 (30%)	71,101,113	2.99	30 (42%)
26	SF4	C	101	3	0,12,12	-	-	-		
22	CLA	2	601	19	50,54,73	2.41	20 (40%)	60,90,113	3.24	28 (46%)
22	CLA	2	606	-	45,49,73	2.52	20 (44%)	54,84,113	3.39	28 (51%)
22	CLA	5	602	17	69,73,73	2.01	19 (27%)	83,113,113	2.87	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	8	610	15	64,68,73	2.10	21 (32%)	77,107,113	2.94	33 (42%)
24	LHG	6	619	22	48,48,48	0.94	2 (4%)	51,54,54	0.98	2 (3%)
22	CLA	J	3002	9	46,50,73	2.42	19 (41%)	55,85,113	3.38	26 (47%)
22	CLA	3	611	-	45,49,73	2.50	20 (44%)	54,84,113	3.38	28 (51%)
22	CLA	A	832	1	54,58,73	2.25	19 (35%)	65,95,113	3.08	29 (44%)
22	CLA	7	611	24	45,49,73	2.47	22 (48%)	54,84,113	3.45	30 (55%)
22	CLA	9	613	-	54,58,73	2.32	21 (38%)	65,95,113	3.10	30 (46%)
30	LUT	4	620	-	42,43,43	0.73	0	51,60,60	1.50	10 (19%)
22	CLA	B	810	2	69,73,73	2.04	21 (30%)	83,113,113	2.86	28 (33%)
22	CLA	Z	608	-	69,73,73	2.04	20 (28%)	83,113,113	2.78	28 (33%)
22	CLA	G	203	7	54,58,73	2.30	21 (38%)	65,95,113	3.26	31 (47%)
22	CLA	A	811	1	69,73,73	2.00	19 (27%)	83,113,113	2.85	31 (37%)
29	CHL	5	618	17	47,51,74	2.35	20 (42%)	52,86,114	3.62	23 (44%)
25	BCR	7	624	-	41,41,41	0.67	0	56,56,56	1.75	12 (21%)
22	CLA	B	813	2	69,73,73	2.00	18 (26%)	83,113,113	2.82	33 (39%)
22	CLA	3	614	13	49,53,73	2.44	20 (40%)	59,89,113	3.31	26 (44%)
25	BCR	4	621	-	41,41,41	0.70	0	56,56,56	2.00	18 (32%)
22	CLA	A	833	1	69,73,73	2.04	20 (28%)	83,113,113	2.75	30 (36%)
29	CHL	1	601	12	57,61,74	2.19	21 (36%)	64,98,114	3.39	29 (45%)
22	CLA	2	613	19	54,58,73	2.35	20 (37%)	65,95,113	3.20	32 (49%)
25	BCR	5	625	-	41,41,41	0.71	0	56,56,56	2.25	15 (26%)
22	CLA	B	834	2	69,73,73	2.06	21 (30%)	83,113,113	2.83	33 (39%)
22	CLA	B	827	2	69,73,73	2.01	20 (28%)	83,113,113	2.84	31 (37%)
22	CLA	A	820	1	69,73,73	2.01	21 (30%)	83,113,113	2.85	30 (36%)
25	BCR	G	205	-	41,41,41	0.72	0	56,56,56	1.50	7 (12%)
30	LUT	8	618	-	42,43,43	0.79	0	51,60,60	1.56	11 (21%)
22	CLA	7	603	14	50,54,73	2.37	21 (42%)	60,90,113	3.33	26 (43%)
22	CLA	Z	616	12	50,54,73	2.41	20 (40%)	60,90,113	3.16	26 (43%)
25	BCR	B	801	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
30	LUT	9	617	-	42,43,43	0.75	0	51,60,60	1.60	13 (25%)
24	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
22	CLA	7	606	-	46,50,73	2.38	19 (41%)	55,85,113	3.51	27 (49%)
30	LUT	6	621	-	42,43,43	0.73	0	51,60,60	1.62	11 (21%)
26	SF4	A	853	1,2	0,12,12	-	-	-		
22	CLA	7	620	-	64,68,73	2.14	20 (31%)	77,107,113	2.88	30 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CHL	Z	607	-	52,56,74	2.30	21 (40%)	58,92,114	3.25	26 (44%)
22	CLA	B	852	-	69,73,73	2.06	20 (28%)	83,113,113	2.69	29 (34%)
22	CLA	Z	606	-	56,60,73	2.30	21 (37%)	67,97,113	3.13	32 (47%)
22	CLA	K	4003	10	50,54,73	2.39	19 (38%)	60,90,113	3.23	25 (41%)
22	CLA	B	819	-	69,73,73	2.04	19 (27%)	83,113,113	2.68	31 (37%)
22	CLA	3	603	13	69,73,73	1.99	19 (27%)	83,113,113	2.76	30 (36%)
29	CHL	4	608	-	55,59,74	2.16	19 (34%)	62,96,114	3.29	25 (40%)
22	CLA	A	803	-	69,73,73	2.01	20 (28%)	83,113,113	2.97	31 (37%)
22	CLA	A	830	1	69,73,73	1.96	19 (27%)	83,113,113	2.76	30 (36%)
22	CLA	4	610	16	64,68,73	2.12	19 (29%)	77,107,113	2.88	32 (41%)
22	CLA	2	603	19	50,54,73	2.39	21 (42%)	60,90,113	3.35	28 (46%)
30	LUT	5	624	-	42,43,43	0.77	0	51,60,60	1.54	11 (21%)
22	CLA	A	821	1	49,53,73	2.37	19 (38%)	59,89,113	3.14	27 (45%)
22	CLA	A	819	1	69,73,73	2.02	20 (28%)	83,113,113	2.84	31 (37%)
22	CLA	A	816	1	69,73,73	2.07	21 (30%)	83,113,113	2.77	28 (33%)
25	BCR	J	3003	-	41,41,41	0.74	0	56,56,56	1.74	13 (23%)
25	BCR	K	4001	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
30	LUT	3	622	-	42,43,43	0.80	0	51,60,60	1.67	10 (19%)
22	CLA	6	614	18	49,53,73	2.41	20 (40%)	59,89,113	3.38	28 (47%)
22	CLA	B	807	2	69,73,73	2.03	19 (27%)	83,113,113	2.84	29 (34%)
22	CLA	1	611	24	69,73,73	2.06	22 (31%)	83,113,113	2.77	28 (33%)
30	LUT	2	616	-	42,43,43	0.75	0	51,60,60	1.72	15 (29%)
22	CLA	1	608	-	69,73,73	2.01	20 (28%)	83,113,113	2.79	29 (34%)
22	CLA	4	613	16	60,64,73	2.18	19 (31%)	72,102,113	3.00	30 (41%)
28	LMG	J	3001	-	35,35,55	0.94	2 (5%)	43,43,63	1.23	5 (11%)
22	CLA	8	609	15	50,54,73	2.38	21 (42%)	60,90,113	3.20	30 (50%)
22	CLA	6	602	18	69,73,73	2.02	19 (27%)	83,113,113	2.84	29 (34%)
22	CLA	A	839	1	69,73,73	2.00	21 (30%)	83,113,113	2.89	30 (36%)
22	CLA	A	802	-	69,73,73	2.09	21 (30%)	83,113,113	2.80	31 (37%)
22	CLA	8	612	15	56,60,73	2.24	20 (35%)	67,97,113	3.10	32 (47%)
22	CLA	G	204	7	50,54,73	2.42	20 (40%)	60,90,113	3.22	26 (43%)
22	CLA	A	806	1	69,73,73	1.99	19 (27%)	83,113,113	2.83	26 (31%)
22	CLA	4	604	-	54,58,73	2.32	20 (37%)	65,95,113	3.10	30 (46%)
29	CHL	5	607	-	55,59,74	2.24	22 (40%)	62,96,114	3.36	27 (43%)
25	BCR	L	201	-	41,41,41	0.72	0	56,56,56	1.73	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LUT	7	622	-	42,43,43	0.75	0	51,60,60	1.49	10 (19%)
21	CL0	A	801	1	69,73,73	1.95	18 (26%)	83,113,113	2.88	32 (38%)
22	CLA	1	603	12	69,73,73	2.02	19 (27%)	83,113,113	2.86	31 (37%)
29	CHL	6	618	18	47,51,74	2.32	20 (42%)	52,86,114	3.54	24 (46%)
30	LUT	2	617	-	42,43,43	0.72	0	51,60,60	1.79	12 (23%)
30	LUT	1	619	-	42,43,43	0.76	0	51,60,60	1.83	14 (27%)
25	BCR	6	625	-	41,41,41	0.67	0	56,56,56	2.05	16 (28%)
22	CLA	K	4002	-	49,53,73	2.45	21 (42%)	59,89,113	3.26	28 (47%)
22	CLA	7	610	14	64,68,73	2.13	18 (28%)	77,107,113	3.03	32 (41%)
22	CLA	9	603	20	50,54,73	2.39	20 (40%)	60,90,113	3.36	29 (48%)
22	CLA	3	606	-	46,50,73	2.44	17 (36%)	55,85,113	3.35	27 (49%)
30	LUT	6	624	-	42,43,43	0.72	0	51,60,60	1.44	8 (15%)
22	CLA	9	611	-	59,63,73	2.24	20 (33%)	71,101,113	2.97	29 (40%)
22	CLA	A	829	1	69,73,73	1.96	19 (27%)	83,113,113	2.89	31 (37%)
22	CLA	B	840	2	69,73,73	2.05	19 (27%)	83,113,113	2.89	28 (33%)
25	BCR	B	845	-	41,41,41	0.73	0	56,56,56	1.84	15 (26%)
22	CLA	B	837	2	69,73,73	2.00	19 (27%)	83,113,113	2.94	31 (37%)
22	CLA	B	833	2	62,66,73	2.14	20 (32%)	74,104,113	3.08	31 (41%)
25	BCR	8	619	-	41,41,41	0.71	0	56,56,56	1.83	15 (26%)
22	CLA	2	609	19	54,58,73	2.36	21 (38%)	65,95,113	3.16	32 (49%)
22	CLA	A	823	1	53,57,73	2.31	20 (37%)	62,93,113	3.20	25 (40%)
22	CLA	8	616	15	50,54,73	2.36	20 (40%)	60,90,113	3.08	27 (45%)
25	BCR	5	622	-	41,41,41	0.66	0	56,56,56	1.87	15 (26%)
29	CHL	4	606	-	60,64,74	2.13	19 (31%)	68,102,114	3.07	26 (38%)
25	BCR	3	718	-	41,41,41	0.74	0	56,56,56	1.90	17 (30%)
25	BCR	A	851	-	41,41,41	0.81	2 (4%)	56,56,56	1.83	12 (21%)
22	CLA	A	824	1	55,59,73	2.26	21 (38%)	66,96,113	3.16	28 (42%)
29	CHL	6	607	-	60,64,74	2.13	23 (38%)	68,102,114	3.20	31 (45%)
22	CLA	A	810	1	69,73,73	1.99	19 (27%)	83,113,113	2.81	33 (39%)
22	CLA	A	838	1	55,59,73	2.27	19 (34%)	66,96,113	3.22	33 (50%)
22	CLA	6	604	-	69,73,73	2.05	20 (28%)	83,113,113	2.72	29 (34%)
24	LHG	4	622	22	48,48,48	0.96	2 (4%)	51,54,54	1.09	3 (5%)
22	CLA	F	303	-	49,53,73	2.40	20 (40%)	59,89,113	3.27	26 (44%)
22	CLA	5	610	17	64,68,73	2.10	21 (32%)	77,107,113	2.95	32 (41%)
22	CLA	8	611	24	50,54,73	2.38	20 (40%)	60,90,113	3.20	28 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	815	2	61,65,73	2.13	19 (31%)	73,103,113	3.04	30 (41%)
29	CHL	1	607	-	52,56,74	2.30	21 (40%)	58,92,114	3.20	23 (39%)
22	CLA	6	601	18	69,73,73	2.02	20 (28%)	83,113,113	2.85	30 (36%)
25	BCR	A	850	-	41,41,41	0.70	0	56,56,56	1.90	12 (21%)
22	CLA	8	614	15	59,63,73	2.20	20 (33%)	71,101,113	2.96	31 (43%)
22	CLA	Z	613	-	69,73,73	2.03	19 (27%)	83,113,113	2.72	29 (34%)
22	CLA	Z	603	12	61,65,73	2.18	19 (31%)	73,103,113	3.03	34 (46%)
22	CLA	B	830	2	54,58,73	2.27	20 (37%)	65,95,113	3.23	30 (46%)
22	CLA	Z	611	24	69,73,73	2.06	20 (28%)	83,113,113	2.77	28 (33%)
22	CLA	4	612	16	56,60,73	2.24	21 (37%)	67,97,113	3.16	31 (46%)
22	CLA	6	616	18	50,54,73	2.39	20 (40%)	60,90,113	3.22	30 (50%)
22	CLA	5	616	17	50,54,73	2.36	22 (44%)	60,90,113	3.16	28 (46%)
22	CLA	9	601	20	50,54,73	2.43	20 (40%)	60,90,113	3.22	27 (45%)
30	LUT	1	617	-	42,43,43	0.75	0	51,60,60	1.69	13 (25%)
22	CLA	A	841	1	69,73,73	2.03	20 (28%)	83,113,113	2.93	32 (38%)
22	CLA	5	621	-	50,54,73	2.38	21 (42%)	60,90,113	3.04	26 (43%)
22	CLA	Z	604	-	61,65,73	2.17	19 (31%)	73,103,113	2.91	29 (39%)
25	BCR	A	856	-	41,41,41	0.74	0	56,56,56	1.77	13 (23%)
22	CLA	4	609	16	54,58,73	2.30	20 (37%)	65,95,113	3.19	31 (47%)

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	9	604	20	-	8/21/97/115	-
22	CLA	B	836	2	-	5/33/109/115	-
22	CLA	3	617	13	-	5/17/93/115	-
22	CLA	1	602	12	-	13/39/115/115	-
30	LUT	9	616	-	-	2/29/67/67	0/2/2/2
22	CLA	8	603	15	-	4/15/91/115	-
22	CLA	B	839	-	-	9/39/115/115	-
22	CLA	A	808	1	-	10/39/115/115	-
22	CLA	1	606	-	-	5/24/100/115	-
22	CLA	4	602	16	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	610	20	-	6/33/109/115	-
24	LHG	A	855	-	-	10/34/34/53	-
22	CLA	B	802	2	-	11/39/115/115	-
22	CLA	8	608	-	-	3/21/97/115	-
22	CLA	B	806	2	-	15/39/115/115	-
22	CLA	9	602	20	-	11/33/109/115	-
22	CLA	5	617	17	-	6/17/93/115	-
22	CLA	7	609	14	-	7/21/97/115	-
22	CLA	1	616	12	-	5/17/93/115	-
22	CLA	3	610	13	-	14/39/115/115	-
22	CLA	B	824	-	-	11/39/115/115	-
29	CHL	3	608	-	-	22/41/117/117	-
22	CLA	2	614	-	-	4/15/91/115	-
22	CLA	7	602	14	-	12/39/115/115	-
22	CLA	7	616	14	-	7/17/93/115	-
22	CLA	5	614	17	-	3/15/91/115	-
22	CLA	A	814	1	-	17/39/115/115	-
26	SF4	C	102	3	-	-	0/6/5/5
22	CLA	A	840	1	-	8/39/115/115	-
22	CLA	5	612	17	-	4/24/100/115	-
22	CLA	2	610	19	-	13/33/109/115	-
22	CLA	4	601	16	-	13/35/111/115	-
22	CLA	B	809	2	-	14/39/115/115	-
22	CLA	Z	609	12	-	6/39/115/115	-
29	CHL	9	606	-	-	6/12/88/117	-
29	CHL	8	607	-	-	11/29/105/117	-
22	CLA	8	604	-	-	5/17/93/115	-
22	CLA	B	803	-	-	6/39/115/115	-
22	CLA	8	606	-	-	4/12/88/115	-
25	BCR	A	848	-	-	4/29/63/63	0/2/2/2
22	CLA	A	822	-	-	15/39/115/115	-
22	CLA	3	620	-	-	8/29/105/115	-
29	CHL	6	608	-	-	6/23/99/117	-
22	CLA	Z	602	12	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LUT	1	618	-	-	3/29/67/67	0/2/2/2
30	LUT	Z	617	-	-	4/29/67/67	0/2/2/2
22	CLA	5	606	-	-	5/27/103/115	-
24	LHG	B	851	22	-	12/26/26/53	-
22	CLA	6	622	18	-	5/15/91/115	-
29	CHL	4	618	16	-	6/14/90/117	-
22	CLA	A	804	1	-	12/39/115/115	-
22	CLA	9	609	-	-	2/21/97/115	-
22	CLA	B	822	2	-	10/32/108/115	-
24	LHG	7	625	22	-	10/41/41/53	-
22	CLA	L	203	11	-	10/39/115/115	-
22	CLA	B	841	24	-	5/39/115/115	-
22	CLA	2	607	-	-	7/21/97/115	-
24	LHG	A	847	22	-	14/42/42/53	-
25	BCR	B	844	-	-	7/29/63/63	0/2/2/2
22	CLA	6	617	18	-	5/17/93/115	-
22	CLA	A	843	-	-	19/39/115/115	-
22	CLA	B	811	2	-	5/25/101/115	-
22	CLA	F	301	-	-	10/39/115/115	-
22	CLA	3	609	13	-	7/21/97/115	-
22	CLA	A	842	1	-	16/39/115/115	-
22	CLA	3	613	13	-	16/27/103/115	-
22	CLA	B	831	2	-	5/20/96/115	-
25	BCR	L	205	-	-	9/29/63/63	0/2/2/2
22	CLA	3	607	13	-	17/33/109/115	-
25	BCR	3	717	-	-	5/29/63/63	0/2/2/2
22	CLA	B	825	-	-	9/39/115/115	-
22	CLA	B	820	2	-	7/29/105/115	-
22	CLA	1	613	-	-	9/39/115/115	-
22	CLA	5	609	17	-	6/21/97/115	-
24	LHG	8	620	22	-	14/41/41/53	-
22	CLA	6	610	-	-	11/33/109/115	-
22	CLA	6	611	24	-	9/27/103/115	-
25	BCR	A	852	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	611	-	-	9/27/103/115	-
22	CLA	2	612	19	-	7/24/100/115	-
24	LHG	5	623	22	-	10/41/41/53	-
22	CLA	A	812	1,22	-	15/39/115/115	-
22	CLA	A	817	-	-	6/30/106/115	-
22	CLA	1	609	12	-	9/39/115/115	-
22	CLA	6	609	18	-	6/21/97/115	-
24	LHG	1	620	22	-	14/47/47/53	-
22	CLA	A	831	1	-	16/39/115/115	-
24	LHG	Z	620	22	-	15/47/47/53	-
22	CLA	6	613	-	-	4/29/105/115	-
22	CLA	6	603	18	-	3/17/93/115	-
30	LUT	3	621	-	-	5/29/67/67	0/2/2/2
22	CLA	A	818	1	-	14/39/115/115	-
22	CLA	B	816	2	-	10/27/103/115	-
22	CLA	8	601	15	-	15/39/115/115	-
22	CLA	1	610	12	-	14/33/109/115	-
25	BCR	6	623	-	-	9/29/63/63	0/2/2/2
22	CLA	Z	610	12	-	16/33/109/115	-
30	LUT	4	619	-	-	2/29/67/67	0/2/2/2
30	LUT	Z	618	-	-	4/29/67/67	0/2/2/2
22	CLA	A	837	1	-	11/15/91/115	-
29	CHL	7	607	-	-	11/27/103/117	-
22	CLA	8	613	15	-	14/39/115/115	-
22	CLA	A	835	1	-	4/39/115/115	-
22	CLA	B	804	2	-	4/15/91/115	-
29	CHL	Z	601	12	-	13/26/102/117	-
25	BCR	A	849	-	-	3/29/63/63	0/2/2/2
22	CLA	2	602	19	-	6/15/91/115	-
22	CLA	7	613	14	-	10/39/115/115	-
22	CLA	A	826	-	-	16/39/115/115	-
22	CLA	F	304	6	-	11/39/115/115	-
22	CLA	3	612	13	-	3/17/93/115	-
25	BCR	K	4004	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	612	14	-	7/24/100/115	-
22	CLA	6	612	18	-	5/24/100/115	-
27	DGD	B	850	-	-	17/55/95/95	0/2/2/2
23	PQN	A	844	-	-	12/23/43/43	0/2/2/2
29	CHL	5	608	-	-	10/23/99/117	-
22	CLA	3	602	13	-	8/33/109/115	-
22	CLA	4	611	24	-	10/27/103/115	-
22	CLA	7	604	-	-	11/29/105/115	-
22	CLA	5	611	24	-	9/27/103/115	-
22	CLA	4	614	16	-	4/15/91/115	-
25	BCR	F	305	-	-	2/29/63/63	0/2/2/2
22	CLA	5	601	17	-	11/39/115/115	-
22	CLA	B	829	2	-	11/39/115/115	-
22	CLA	B	805	2	-	14/39/115/115	-
22	CLA	B	823	2	-	10/33/109/115	-
22	CLA	1	614	12	-	15/39/115/115	-
22	CLA	B	818	2	-	14/33/109/115	-
30	LUT	7	621	-	-	3/29/67/67	0/2/2/2
22	CLA	5	613	17	-	8/29/105/115	-
22	CLA	A	805	1,22	-	8/27/103/115	-
22	CLA	1	612	12	-	8/24/100/115	-
22	CLA	B	832	2	-	9/39/115/115	-
22	CLA	Z	612	12	-	8/24/100/115	-
22	CLA	A	836	1	-	2/21/97/115	-
22	CLA	A	815	1	-	11/33/109/115	-
22	CLA	9	614	20	-	6/15/91/115	-
22	CLA	B	812	2	-	14/39/115/115	-
22	CLA	B	817	2	-	14/32/108/115	-
22	CLA	9	612	-	-	6/24/100/115	-
22	CLA	A	813	1	-	7/26/102/115	-
22	CLA	5	604	17	-	7/21/97/115	-
30	LUT	Z	619	-	-	4/29/67/67	0/2/2/2
29	CHL	4	607	-	-	9/23/99/117	-
29	CHL	9	607	-	-	9/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	834	1	-	12/39/115/115	-
22	CLA	A	827	-	-	8/39/115/115	-
22	CLA	7	614	14	-	4/13/89/115	-
25	BCR	B	847	-	-	7/29/63/63	0/2/2/2
30	LUT	5	620	-	-	0/29/67/67	0/2/2/2
22	CLA	8	602	15	-	12/36/112/115	-
25	BCR	B	843	-	-	10/29/63/63	0/2/2/2
25	BCR	I	172	-	-	6/29/63/63	0/2/2/2
22	CLA	4	603	16	-	3/17/93/115	-
22	CLA	5	603	17	-	1/17/93/115	-
23	PQN	B	842	-	-	4/23/43/43	0/2/2/2
29	CHL	6	606	-	-	8/29/105/117	-
22	CLA	B	835	-	-	7/15/91/115	-
22	CLA	A	854	-	-	14/39/115/115	-
30	LUT	8	617	-	-	2/29/67/67	0/2/2/2
22	CLA	A	809	1	-	17/39/115/115	-
22	CLA	B	828	2	-	9/39/115/115	-
22	CLA	4	616	16	-	2/10/86/115	-
24	LHG	4	623	-	-	9/36/36/53	-
22	CLA	B	808	2	-	12/39/115/115	-
22	CLA	7	601	14	-	18/39/115/115	-
25	BCR	B	846	-	-	5/29/63/63	0/2/2/2
22	CLA	A	828	1	-	11/39/115/115	-
22	CLA	B	826	2	-	9/39/115/115	-
28	LMG	9	620	-	-	16/39/59/70	0/1/1/1
25	BCR	3	719	-	-	4/29/63/63	0/2/2/2
22	CLA	7	608	-	-	3/21/97/115	-
22	CLA	3	604	-	-	11/39/115/115	-
22	CLA	L	204	-	-	7/21/97/115	-
22	CLA	A	845	24	-	15/24/100/115	-
25	BCR	7	623	-	-	7/29/63/63	0/2/2/2
22	CLA	Z	614	12	-	11/39/115/115	-
22	CLA	B	821	2	-	6/17/93/115	-
22	CLA	A	807	1	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	848	-	-	3/29/63/63	0/2/2/2
22	CLA	1	604	-	-	10/30/106/115	-
22	CLA	B	838	2	-	4/18/94/115	-
22	CLA	B	814	2	-	13/33/109/115	-
22	CLA	A	825	1	-	9/27/103/115	-
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	2	601	19	-	9/17/93/115	-
22	CLA	2	606	-	-	3/10/86/115	-
22	CLA	5	602	17	-	12/39/115/115	-
22	CLA	8	610	15	-	14/33/109/115	-
24	LHG	6	619	22	-	11/53/53/53	-
22	CLA	J	3002	9	-	4/12/88/115	-
22	CLA	3	611	-	-	4/10/86/115	-
22	CLA	A	832	1	-	4/21/97/115	-
22	CLA	7	611	24	-	2/10/86/115	-
22	CLA	9	613	-	-	10/21/97/115	-
30	LUT	4	620	-	-	3/29/67/67	0/2/2/2
22	CLA	B	810	2	-	13/39/115/115	-
22	CLA	Z	608	-	-	19/39/115/115	-
22	CLA	G	203	7	-	5/21/97/115	-
22	CLA	A	811	1	-	10/39/115/115	-
29	CHL	5	618	17	-	6/14/90/117	-
25	BCR	7	624	-	-	4/29/63/63	0/2/2/2
22	CLA	B	813	2	-	15/39/115/115	-
22	CLA	3	614	13	-	4/15/91/115	-
25	BCR	4	621	-	-	3/29/63/63	0/2/2/2
22	CLA	A	833	1	-	10/39/115/115	-
29	CHL	1	601	12	-	13/26/102/117	-
22	CLA	2	613	19	-	5/21/97/115	-
25	BCR	5	625	-	-	7/29/63/63	0/2/2/2
22	CLA	B	834	2	-	13/39/115/115	-
22	CLA	B	827	2	-	18/39/115/115	-
22	CLA	A	820	1	-	14/39/115/115	-
25	BCR	G	205	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LUT	8	618	-	-	4/29/67/67	0/2/2/2
22	CLA	7	603	14	-	4/17/93/115	-
22	CLA	Z	616	12	-	6/17/93/115	-
25	BCR	B	801	-	-	9/29/63/63	0/2/2/2
30	LUT	9	617	-	-	2/29/67/67	0/2/2/2
24	LHG	A	846	-	-	16/53/53/53	-
22	CLA	7	606	-	-	7/12/88/115	-
30	LUT	6	621	-	-	2/29/67/67	0/2/2/2
26	SF4	A	853	1,2	-	-	0/6/5/5
22	CLA	7	620	-	-	10/33/109/115	-
29	CHL	Z	607	-	-	6/20/96/117	-
22	CLA	B	852	-	-	7/39/115/115	-
22	CLA	Z	606	-	-	4/24/100/115	-
22	CLA	K	4003	10	-	3/17/93/115	-
22	CLA	B	819	-	-	11/39/115/115	-
22	CLA	3	603	13	-	7/39/115/115	-
29	CHL	4	608	-	-	8/23/99/117	-
22	CLA	A	803	-	-	4/39/115/115	-
22	CLA	A	830	1	-	8/39/115/115	-
22	CLA	4	610	16	-	11/33/109/115	-
22	CLA	2	603	19	-	8/17/93/115	-
30	LUT	5	624	-	-	3/29/67/67	0/2/2/2
22	CLA	A	821	1	-	2/15/91/115	-
22	CLA	A	819	1	-	14/39/115/115	-
22	CLA	A	816	1	-	10/39/115/115	-
25	BCR	J	3003	-	-	8/29/63/63	0/2/2/2
25	BCR	K	4001	-	-	5/29/63/63	0/2/2/2
30	LUT	3	622	-	-	2/29/67/67	0/2/2/2
22	CLA	6	614	18	-	6/15/91/115	-
22	CLA	B	807	2	-	13/39/115/115	-
22	CLA	1	611	24	-	11/39/115/115	-
30	LUT	2	616	-	-	0/29/67/67	0/2/2/2
22	CLA	1	608	-	-	13/39/115/115	-
22	CLA	4	613	16	-	12/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	J	3001	-	-	12/30/50/70	0/1/1/1
22	CLA	8	609	15	-	5/17/93/115	-
22	CLA	6	602	18	-	13/39/115/115	-
22	CLA	A	839	1	-	13/39/115/115	-
22	CLA	A	802	-	-	5/39/115/115	-
22	CLA	8	612	15	-	6/24/100/115	-
22	CLA	G	204	7	-	6/17/93/115	-
22	CLA	A	806	1	-	16/39/115/115	-
22	CLA	4	604	-	-	6/21/97/115	-
29	CHL	5	607	-	-	12/23/99/117	-
25	BCR	L	201	-	-	8/29/63/63	0/2/2/2
30	LUT	7	622	-	-	3/29/67/67	0/2/2/2
21	CL0	A	801	1	-	6/39/115/115	-
22	CLA	1	603	12	-	10/39/115/115	-
29	CHL	6	618	18	-	8/14/90/117	-
30	LUT	2	617	-	-	3/29/67/67	0/2/2/2
30	LUT	1	619	-	-	2/29/67/67	0/2/2/2
25	BCR	6	625	-	-	9/29/63/63	0/2/2/2
22	CLA	K	4002	-	-	8/15/91/115	-
22	CLA	7	610	14	-	8/33/109/115	-
22	CLA	9	603	20	-	1/17/93/115	-
22	CLA	3	606	-	-	0/12/88/115	-
30	LUT	6	624	-	-	3/29/67/67	0/2/2/2
22	CLA	9	611	-	-	12/27/103/115	-
22	CLA	A	829	1	-	21/39/115/115	-
22	CLA	B	840	2	-	8/39/115/115	-
25	BCR	B	845	-	-	10/29/63/63	0/2/2/2
22	CLA	B	837	2	-	12/39/115/115	-
22	CLA	B	833	2	-	10/31/107/115	-
25	BCR	8	619	-	-	6/29/63/63	0/2/2/2
22	CLA	2	609	19	-	6/21/97/115	-
22	CLA	A	823	1	-	12/20/96/115	-
22	CLA	8	616	15	-	4/17/93/115	-
25	BCR	5	622	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	4	606	-	-	3/29/105/117	-
25	BCR	3	718	-	-	4/29/63/63	0/2/2/2
25	BCR	A	851	-	-	4/29/63/63	0/2/2/2
22	CLA	A	824	1	-	8/23/99/115	-
29	CHL	6	607	-	-	14/29/105/117	-
22	CLA	A	810	1	-	12/39/115/115	-
22	CLA	A	838	1	-	6/23/99/115	-
22	CLA	6	604	-	-	13/39/115/115	-
24	LHG	4	622	22	-	19/53/53/53	-
22	CLA	F	303	-	-	4/15/91/115	-
22	CLA	5	610	17	-	9/33/109/115	-
22	CLA	8	611	24	-	5/17/93/115	-
22	CLA	B	815	2	-	8/30/106/115	-
29	CHL	1	607	-	-	7/20/96/117	-
22	CLA	6	601	18	-	16/39/115/115	-
25	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	8	614	15	-	8/27/103/115	-
22	CLA	Z	613	-	-	13/39/115/115	-
22	CLA	Z	603	12	-	11/30/106/115	-
22	CLA	B	830	2	-	5/21/97/115	-
22	CLA	Z	611	24	-	18/39/115/115	-
22	CLA	4	612	16	-	3/24/100/115	-
22	CLA	6	616	18	-	4/17/93/115	-
22	CLA	5	616	17	-	8/17/93/115	-
22	CLA	9	601	20	-	8/17/93/115	-
30	LUT	1	617	-	-	2/29/67/67	0/2/2/2
22	CLA	A	841	1	-	9/39/115/115	-
22	CLA	5	621	-	-	5/17/93/115	-
22	CLA	Z	604	-	-	11/30/106/115	-
25	BCR	A	856	-	-	7/29/63/63	0/2/2/2
22	CLA	4	609	16	-	7/21/97/115	-

All (4805) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	842	PQN	C3-C2	7.50	1.48	1.35
23	A	844	PQN	C3-C2	7.35	1.48	1.35
22	B	840	CLA	C3C-C2C	6.11	1.49	1.36
22	A	817	CLA	C1D-ND	5.56	1.44	1.37
22	L	204	CLA	C3C-C2C	5.48	1.48	1.36
22	2	609	CLA	C1D-ND	5.48	1.44	1.37
22	7	609	CLA	C3C-C2C	5.47	1.48	1.36
22	A	816	CLA	C3C-C2C	5.47	1.48	1.36
22	A	802	CLA	C3C-C2C	5.45	1.48	1.36
22	Z	611	CLA	C3C-C2C	5.44	1.48	1.36
22	Z	606	CLA	C1D-ND	5.43	1.44	1.37
22	Z	614	CLA	C3C-C2C	5.43	1.48	1.36
22	2	606	CLA	C3C-C2C	5.43	1.48	1.36
22	3	607	CLA	C3C-C2C	5.42	1.48	1.36
22	6	614	CLA	C3C-C2C	5.42	1.48	1.36
22	6	609	CLA	C3C-C2C	5.42	1.48	1.36
22	A	835	CLA	C3C-C2C	5.41	1.48	1.36
22	A	845	CLA	C3C-C2C	5.41	1.48	1.36
22	9	609	CLA	C3C-C2C	5.41	1.48	1.36
22	B	827	CLA	C3C-C2C	5.41	1.48	1.36
22	1	614	CLA	C3C-C2C	5.40	1.48	1.36
22	1	611	CLA	C3C-C2C	5.40	1.48	1.36
22	4	616	CLA	C1D-ND	5.40	1.44	1.37
22	2	606	CLA	C1D-ND	5.40	1.44	1.37
22	B	825	CLA	C3C-C2C	5.40	1.48	1.36
22	8	614	CLA	C3C-C2C	5.39	1.48	1.36
22	A	822	CLA	C3C-C2C	5.38	1.48	1.36
22	2	607	CLA	C3C-C2C	5.38	1.48	1.36
22	9	604	CLA	C1D-ND	5.37	1.44	1.37
22	7	601	CLA	C3C-C2C	5.37	1.48	1.36
22	4	610	CLA	C3C-C2C	5.36	1.48	1.36
22	3	614	CLA	C1D-ND	5.36	1.44	1.37
22	2	611	CLA	C3C-C2C	5.36	1.48	1.36
22	7	610	CLA	CHC-C1C	5.35	1.49	1.38
22	2	611	CLA	C1D-ND	5.35	1.44	1.37
22	2	609	CLA	C3C-C2C	5.35	1.48	1.36
22	7	616	CLA	C1D-ND	5.35	1.44	1.37
22	B	835	CLA	C3C-C2C	5.34	1.48	1.36
22	K	4002	CLA	C3C-C2C	5.34	1.48	1.36
22	9	603	CLA	C1D-ND	5.34	1.44	1.37
22	5	611	CLA	C3C-C2C	5.34	1.48	1.36
22	A	823	CLA	C3C-C2C	5.34	1.48	1.36
22	2	601	CLA	C1D-ND	5.34	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	601	CLA	C3C-C2C	5.34	1.48	1.36
22	2	602	CLA	C1D-ND	5.33	1.44	1.37
22	9	601	CLA	C3C-C2C	5.33	1.48	1.36
22	B	841	CLA	C3C-C2C	5.33	1.48	1.36
22	5	606	CLA	C3C-C2C	5.33	1.48	1.36
22	A	828	CLA	C3C-C2C	5.33	1.48	1.36
22	9	604	CLA	C3C-C2C	5.33	1.48	1.36
22	J	3002	CLA	C3C-C2C	5.33	1.48	1.36
22	A	805	CLA	C3C-C2C	5.32	1.48	1.36
22	B	852	CLA	C3C-C2C	5.32	1.48	1.36
22	2	607	CLA	C1D-ND	5.32	1.44	1.37
22	B	821	CLA	C3C-C2C	5.32	1.48	1.36
29	Z	601	CHL	C2C-C3C	5.32	1.48	1.36
22	A	815	CLA	C3C-C2C	5.32	1.48	1.36
22	B	820	CLA	C3C-C2C	5.32	1.48	1.36
22	A	845	CLA	C1D-ND	5.32	1.44	1.37
22	9	614	CLA	C3C-C2C	5.31	1.48	1.36
22	7	620	CLA	C3C-C2C	5.31	1.48	1.36
22	9	611	CLA	C3C-C2C	5.31	1.48	1.36
29	1	601	CHL	C2C-C3C	5.31	1.48	1.36
22	A	834	CLA	C3C-C2C	5.31	1.48	1.36
22	2	603	CLA	C1D-ND	5.31	1.44	1.37
22	8	611	CLA	C1D-ND	5.31	1.44	1.37
22	B	830	CLA	C3C-C2C	5.31	1.48	1.36
22	2	610	CLA	C3C-C2C	5.31	1.48	1.36
22	B	838	CLA	C3C-C2C	5.31	1.48	1.36
22	K	4003	CLA	C3C-C2C	5.30	1.48	1.36
22	7	602	CLA	C3C-C2C	5.30	1.48	1.36
22	2	614	CLA	C3C-C2C	5.30	1.48	1.36
22	5	611	CLA	C1D-ND	5.30	1.44	1.37
29	7	607	CHL	C2C-C3C	5.30	1.48	1.36
29	9	607	CHL	C2C-C3C	5.30	1.48	1.36
22	7	620	CLA	C1D-ND	5.30	1.44	1.37
22	4	601	CLA	C3C-C2C	5.30	1.48	1.36
22	A	827	CLA	C3C-C2C	5.30	1.48	1.36
22	8	606	CLA	C3C-C2C	5.29	1.48	1.36
22	6	604	CLA	C3C-C2C	5.29	1.48	1.36
22	2	610	CLA	C1D-ND	5.29	1.44	1.37
22	A	841	CLA	C3C-C2C	5.29	1.48	1.36
22	9	601	CLA	C1D-ND	5.29	1.44	1.37
22	A	820	CLA	C3C-C2C	5.29	1.48	1.36
22	G	204	CLA	C3C-C2C	5.29	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	612	CLA	C3C-C2C	5.29	1.48	1.36
22	2	602	CLA	C3C-C2C	5.29	1.48	1.36
22	1	609	CLA	C1D-ND	5.28	1.44	1.37
22	G	203	CLA	C3C-C2C	5.28	1.48	1.36
22	Z	609	CLA	C1D-ND	5.28	1.44	1.37
22	5	604	CLA	C1D-ND	5.28	1.44	1.37
22	B	810	CLA	C3C-C2C	5.28	1.47	1.36
22	4	611	CLA	C3C-C2C	5.28	1.47	1.36
22	A	819	CLA	C3C-C2C	5.28	1.47	1.36
22	5	617	CLA	C3C-C2C	5.27	1.47	1.36
22	B	811	CLA	C3C-C2C	5.27	1.47	1.36
22	A	813	CLA	C3C-C2C	5.27	1.47	1.36
29	5	618	CHL	C2C-C3C	5.27	1.48	1.36
22	Z	611	CLA	C1D-ND	5.27	1.44	1.37
22	2	613	CLA	C1D-ND	5.27	1.44	1.37
22	B	819	CLA	C3C-C2C	5.27	1.47	1.36
22	9	612	CLA	C1D-ND	5.27	1.44	1.37
22	A	838	CLA	C3C-C2C	5.27	1.47	1.36
22	7	604	CLA	C1D-ND	5.26	1.44	1.37
22	A	809	CLA	C3C-C2C	5.26	1.47	1.36
22	A	839	CLA	C3C-C2C	5.26	1.47	1.36
22	5	609	CLA	C3C-C2C	5.26	1.47	1.36
22	L	203	CLA	C3C-C2C	5.26	1.47	1.36
22	8	609	CLA	C3C-C2C	5.26	1.47	1.36
22	1	604	CLA	C3C-C2C	5.26	1.47	1.36
22	9	612	CLA	C3C-C2C	5.26	1.47	1.36
22	B	834	CLA	C1D-ND	5.26	1.44	1.37
22	A	854	CLA	C3C-C2C	5.25	1.47	1.36
22	3	611	CLA	C3C-C2C	5.25	1.47	1.36
22	2	601	CLA	O2D-CGD	5.25	1.46	1.33
22	2	609	CLA	O2D-CGD	5.25	1.46	1.33
22	A	824	CLA	C3C-C2C	5.25	1.47	1.36
22	Z	603	CLA	C3C-C2C	5.25	1.47	1.36
22	4	603	CLA	C3C-C2C	5.25	1.47	1.36
22	2	614	CLA	C1D-ND	5.24	1.44	1.37
22	A	816	CLA	C1D-ND	5.24	1.44	1.37
22	2	607	CLA	O2D-CGD	5.24	1.46	1.33
22	4	614	CLA	C3C-C2C	5.24	1.47	1.36
22	4	616	CLA	C3C-C2C	5.24	1.47	1.36
22	2	613	CLA	C3C-C2C	5.24	1.47	1.36
22	Z	612	CLA	C3C-C2C	5.24	1.47	1.36
22	2	601	CLA	C3C-C2C	5.24	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	608	CLA	C3C-C2C	5.24	1.47	1.36
22	7	614	CLA	C3C-C2C	5.24	1.47	1.36
22	B	834	CLA	C3C-C2C	5.24	1.47	1.36
22	3	606	CLA	C3C-C2C	5.23	1.47	1.36
22	3	612	CLA	C3C-C2C	5.23	1.47	1.36
22	Z	608	CLA	C3C-C2C	5.23	1.47	1.36
22	F	304	CLA	C1D-ND	5.23	1.44	1.37
22	B	822	CLA	C3C-C2C	5.23	1.47	1.36
22	Z	616	CLA	C3C-C2C	5.23	1.47	1.36
22	K	4002	CLA	C1D-ND	5.23	1.44	1.37
29	6	607	CHL	C2C-C3C	5.23	1.47	1.36
22	5	621	CLA	C3C-C2C	5.23	1.47	1.36
22	3	604	CLA	C3C-C2C	5.23	1.47	1.36
22	Z	604	CLA	C3C-C2C	5.23	1.47	1.36
22	B	832	CLA	C3C-C2C	5.23	1.47	1.36
22	5	614	CLA	C3C-C2C	5.23	1.47	1.36
22	6	601	CLA	C3C-C2C	5.23	1.47	1.36
22	9	611	CLA	O2D-CGD	5.22	1.45	1.33
22	9	614	CLA	C1D-ND	5.22	1.44	1.37
22	A	807	CLA	C3C-C2C	5.22	1.47	1.36
22	2	603	CLA	C3C-C2C	5.22	1.47	1.36
22	B	826	CLA	C3C-C2C	5.22	1.47	1.36
22	B	831	CLA	C3C-C2C	5.22	1.47	1.36
22	B	839	CLA	C3C-C2C	5.22	1.47	1.36
22	7	614	CLA	C1D-ND	5.22	1.44	1.37
22	5	616	CLA	C1D-ND	5.22	1.44	1.37
22	8	616	CLA	C3C-C2C	5.22	1.47	1.36
22	Z	606	CLA	C3C-C2C	5.22	1.47	1.36
22	B	807	CLA	C3C-C2C	5.21	1.47	1.36
22	F	304	CLA	C3C-C2C	5.21	1.47	1.36
22	1	608	CLA	C3C-C2C	5.21	1.47	1.36
22	9	603	CLA	C3C-C2C	5.21	1.47	1.36
22	6	613	CLA	C3C-C2C	5.21	1.47	1.36
22	B	829	CLA	C3C-C2C	5.21	1.47	1.36
22	A	831	CLA	C3C-C2C	5.21	1.47	1.36
22	4	604	CLA	C3C-C2C	5.21	1.47	1.36
22	A	837	CLA	C3C-C2C	5.21	1.47	1.36
22	F	301	CLA	C3C-C2C	5.21	1.47	1.36
22	5	603	CLA	C3C-C2C	5.21	1.47	1.36
22	4	602	CLA	C3C-C2C	5.21	1.47	1.36
22	2	614	CLA	O2D-CGD	5.21	1.45	1.33
29	6	607	CHL	O2D-CGD	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	616	CLA	C3C-C2C	5.21	1.47	1.36
22	A	836	CLA	C3C-C2C	5.20	1.47	1.36
22	6	611	CLA	C3C-C2C	5.20	1.47	1.36
22	6	617	CLA	C3C-C2C	5.20	1.47	1.36
22	4	611	CLA	C1D-ND	5.20	1.44	1.37
22	9	602	CLA	C1D-ND	5.20	1.44	1.37
22	3	614	CLA	C3C-C2C	5.20	1.47	1.36
22	9	611	CLA	C1D-ND	5.20	1.44	1.37
22	1	612	CLA	C3C-C2C	5.20	1.47	1.36
22	8	604	CLA	C3C-C2C	5.20	1.47	1.36
22	6	602	CLA	C3C-C2C	5.20	1.47	1.36
22	A	821	CLA	C3C-C2C	5.20	1.47	1.36
22	1	606	CLA	C3C-C2C	5.20	1.47	1.36
22	Z	609	CLA	C3C-C2C	5.20	1.47	1.36
22	1	603	CLA	C1D-ND	5.20	1.44	1.37
22	1	603	CLA	C3C-C2C	5.19	1.47	1.36
22	8	603	CLA	C3C-C2C	5.19	1.47	1.36
22	A	826	CLA	C1D-ND	5.19	1.44	1.37
22	9	609	CLA	C1D-ND	5.19	1.44	1.37
22	9	610	CLA	C1D-ND	5.19	1.44	1.37
22	A	804	CLA	C3C-C2C	5.19	1.47	1.36
22	2	612	CLA	O2D-CGD	5.19	1.45	1.33
22	7	606	CLA	C1D-ND	5.19	1.44	1.37
22	7	603	CLA	C3C-C2C	5.19	1.47	1.36
22	Z	608	CLA	C1D-ND	5.19	1.44	1.37
22	7	606	CLA	C3C-C2C	5.19	1.47	1.36
22	3	611	CLA	C1D-ND	5.19	1.44	1.37
22	9	610	CLA	C3C-C2C	5.19	1.47	1.36
22	6	603	CLA	C3C-C2C	5.18	1.47	1.36
22	4	612	CLA	C3C-C2C	5.18	1.47	1.36
22	5	612	CLA	C3C-C2C	5.18	1.47	1.36
22	8	601	CLA	C3C-C2C	5.18	1.47	1.36
22	G	204	CLA	C1D-ND	5.18	1.44	1.37
22	9	613	CLA	C3C-C2C	5.18	1.47	1.36
22	3	606	CLA	O2D-CGD	5.18	1.45	1.33
22	Z	614	CLA	O2D-CGD	5.18	1.45	1.33
22	A	833	CLA	C3C-C2C	5.18	1.47	1.36
22	Z	616	CLA	C1D-ND	5.17	1.44	1.37
22	7	609	CLA	O2D-CGD	5.17	1.45	1.33
22	3	609	CLA	C3C-C2C	5.17	1.47	1.36
22	F	303	CLA	C1D-ND	5.17	1.44	1.37
22	8	606	CLA	C1D-ND	5.17	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	603	CLA	C1D-ND	5.17	1.44	1.37
22	A	842	CLA	C3C-C2C	5.17	1.47	1.36
22	A	826	CLA	C3C-C2C	5.17	1.47	1.36
22	6	622	CLA	C3C-C2C	5.17	1.47	1.36
22	B	852	CLA	O2D-CGD	5.17	1.45	1.33
22	5	616	CLA	C3C-C2C	5.17	1.47	1.36
22	2	612	CLA	C1D-ND	5.17	1.44	1.37
22	F	303	CLA	O2D-CGD	5.17	1.45	1.33
22	3	620	CLA	C3C-C2C	5.17	1.47	1.36
22	B	837	CLA	C3C-C2C	5.17	1.47	1.36
22	A	810	CLA	C3C-C2C	5.17	1.47	1.36
22	4	613	CLA	C1D-ND	5.17	1.44	1.37
22	B	808	CLA	C3C-C2C	5.17	1.47	1.36
22	3	620	CLA	C1D-ND	5.17	1.44	1.37
22	2	602	CLA	O2D-CGD	5.16	1.45	1.33
22	B	805	CLA	C3C-C2C	5.16	1.47	1.36
22	B	806	CLA	C3C-C2C	5.16	1.47	1.36
22	2	606	CLA	O2D-CGD	5.16	1.45	1.33
22	Z	604	CLA	O2D-CGD	5.16	1.45	1.33
22	4	609	CLA	O2D-CGD	5.16	1.45	1.33
22	B	815	CLA	C3C-C2C	5.16	1.47	1.36
22	6	610	CLA	C3C-C2C	5.16	1.47	1.36
22	A	828	CLA	C1D-ND	5.16	1.44	1.37
22	8	610	CLA	C3C-C2C	5.16	1.47	1.36
22	9	610	CLA	O2D-CGD	5.16	1.45	1.33
22	7	611	CLA	C1D-ND	5.16	1.44	1.37
22	J	3002	CLA	C1D-ND	5.16	1.44	1.37
22	9	612	CLA	O2D-CGD	5.16	1.45	1.33
22	A	817	CLA	C3C-C2C	5.15	1.47	1.36
22	4	616	CLA	O2D-CGD	5.15	1.45	1.33
22	B	810	CLA	C1D-ND	5.15	1.44	1.37
22	B	829	CLA	C1D-ND	5.15	1.44	1.37
22	A	854	CLA	CHC-C1C	5.15	1.49	1.38
22	Z	614	CLA	C1D-ND	5.15	1.44	1.37
22	A	818	CLA	C3C-C2C	5.15	1.47	1.36
22	7	603	CLA	C1D-ND	5.15	1.44	1.37
22	1	602	CLA	C3C-C2C	5.15	1.47	1.36
22	B	833	CLA	C3C-C2C	5.15	1.47	1.36
22	2	603	CLA	O2D-CGD	5.15	1.45	1.33
22	6	611	CLA	C1D-ND	5.15	1.44	1.37
22	B	828	CLA	C3C-C2C	5.15	1.47	1.36
29	9	606	CHL	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	610	CLA	CHC-C1C	5.14	1.49	1.38
22	9	603	CLA	O2D-CGD	5.14	1.45	1.33
22	Z	613	CLA	C3C-C2C	5.14	1.47	1.36
22	G	203	CLA	C1D-ND	5.14	1.44	1.37
22	B	823	CLA	O2D-CGD	5.14	1.45	1.33
22	B	827	CLA	O2D-CGD	5.14	1.45	1.33
22	5	604	CLA	O2D-CGD	5.14	1.45	1.33
22	3	617	CLA	C3C-C2C	5.14	1.47	1.36
22	5	604	CLA	C3C-C2C	5.14	1.47	1.36
22	A	835	CLA	C1D-ND	5.14	1.44	1.37
29	6	618	CHL	O2D-CGD	5.14	1.45	1.33
22	G	204	CLA	O2D-CGD	5.14	1.45	1.33
22	8	608	CLA	C1D-ND	5.14	1.44	1.37
29	Z	607	CHL	C2C-C3C	5.14	1.47	1.36
22	B	823	CLA	C3C-C2C	5.14	1.47	1.36
22	2	610	CLA	O2D-CGD	5.13	1.45	1.33
22	2	611	CLA	O2D-CGD	5.13	1.45	1.33
22	7	616	CLA	C3C-C2C	5.13	1.47	1.36
22	6	614	CLA	C1D-ND	5.13	1.44	1.37
22	B	814	CLA	C3C-C2C	5.13	1.47	1.36
22	8	613	CLA	C1D-ND	5.13	1.44	1.37
22	4	604	CLA	O2D-CGD	5.13	1.45	1.33
22	3	606	CLA	C1D-ND	5.12	1.44	1.37
22	5	606	CLA	C1D-ND	5.12	1.44	1.37
22	5	610	CLA	C3C-C2C	5.12	1.47	1.36
22	A	812	CLA	C3C-C2C	5.12	1.47	1.36
22	7	616	CLA	O2D-CGD	5.12	1.45	1.33
22	A	845	CLA	O2D-CGD	5.12	1.45	1.33
22	L	204	CLA	O2D-CGD	5.12	1.45	1.33
29	9	607	CHL	O2D-CGD	5.12	1.45	1.33
22	K	4003	CLA	O2D-CGD	5.12	1.45	1.33
22	9	601	CLA	O2D-CGD	5.12	1.45	1.33
22	6	613	CLA	C1D-ND	5.12	1.44	1.37
22	6	612	CLA	C3C-C2C	5.12	1.47	1.36
22	A	836	CLA	O2D-CGD	5.12	1.45	1.33
22	A	808	CLA	C3C-C2C	5.12	1.47	1.36
29	5	607	CHL	C2C-C3C	5.12	1.47	1.36
22	6	603	CLA	O2D-CGD	5.12	1.45	1.33
22	5	612	CLA	O2D-CGD	5.12	1.45	1.33
29	4	606	CHL	O2D-CGD	5.11	1.45	1.33
22	1	604	CLA	O2D-CGD	5.11	1.45	1.33
22	7	611	CLA	C3C-C2C	5.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	602	CLA	C3C-C2C	5.11	1.47	1.36
22	4	604	CLA	C1D-ND	5.11	1.44	1.37
22	Z	606	CLA	O2D-CGD	5.11	1.45	1.33
22	Z	612	CLA	O2D-CGD	5.11	1.45	1.33
22	Z	613	CLA	O2D-CGD	5.11	1.45	1.33
22	4	603	CLA	O2D-CGD	5.11	1.45	1.33
22	A	819	CLA	O2D-CGD	5.11	1.45	1.33
22	A	802	CLA	O2D-CGD	5.11	1.45	1.33
22	1	608	CLA	C1D-ND	5.11	1.44	1.37
22	8	603	CLA	C1D-ND	5.11	1.44	1.37
22	4	609	CLA	C1D-ND	5.11	1.44	1.37
22	B	804	CLA	C3C-C2C	5.11	1.47	1.36
22	6	610	CLA	C1D-ND	5.11	1.44	1.37
22	F	304	CLA	O2D-CGD	5.11	1.45	1.33
22	B	816	CLA	C1D-ND	5.10	1.44	1.37
22	K	4003	CLA	C1D-ND	5.10	1.44	1.37
22	7	610	CLA	C1D-ND	5.10	1.44	1.37
22	9	614	CLA	O2D-CGD	5.10	1.45	1.33
22	3	613	CLA	C3C-C2C	5.10	1.47	1.36
22	5	603	CLA	O2D-CGD	5.10	1.45	1.33
22	1	609	CLA	C3C-C2C	5.10	1.47	1.36
22	7	612	CLA	C3C-C2C	5.10	1.47	1.36
22	4	603	CLA	C1D-ND	5.10	1.44	1.37
22	A	843	CLA	O2D-CGD	5.10	1.45	1.33
22	7	604	CLA	O2D-CGD	5.10	1.45	1.33
22	A	832	CLA	C3C-C2C	5.10	1.47	1.36
22	A	841	CLA	O2D-CGD	5.09	1.45	1.33
22	9	609	CLA	O2D-CGD	5.09	1.45	1.33
22	3	613	CLA	O2D-CGD	5.09	1.45	1.33
22	1	606	CLA	O2D-CGD	5.09	1.45	1.33
22	1	606	CLA	C1D-ND	5.09	1.44	1.37
22	1	613	CLA	C3C-C2C	5.09	1.47	1.36
22	B	812	CLA	C3C-C2C	5.09	1.47	1.36
22	9	602	CLA	C3C-C2C	5.09	1.47	1.36
22	4	602	CLA	O2D-CGD	5.09	1.45	1.33
22	2	613	CLA	O2D-CGD	5.09	1.45	1.33
22	B	807	CLA	C1D-ND	5.09	1.44	1.37
22	L	203	CLA	O2D-CGD	5.09	1.45	1.33
22	9	613	CLA	C1D-ND	5.09	1.44	1.37
29	Z	607	CHL	O2D-CGD	5.09	1.45	1.33
22	5	609	CLA	C1D-ND	5.08	1.44	1.37
22	B	818	CLA	C3C-C2C	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	604	CLA	C1D-ND	5.08	1.44	1.37
22	6	616	CLA	C1D-ND	5.08	1.44	1.37
22	Z	611	CLA	O2D-CGD	5.08	1.45	1.33
29	4	607	CHL	O2D-CGD	5.08	1.45	1.33
22	B	806	CLA	O2D-CGD	5.08	1.45	1.33
22	6	613	CLA	O2D-CGD	5.08	1.45	1.33
21	A	801	CL0	C3C-C2C	5.08	1.47	1.36
29	1	607	CHL	C2C-C3C	5.08	1.47	1.36
22	1	612	CLA	O2D-CGD	5.08	1.45	1.33
22	B	819	CLA	O2D-CGD	5.08	1.45	1.33
22	A	833	CLA	C1D-ND	5.08	1.44	1.37
22	7	613	CLA	O2D-CGD	5.08	1.45	1.33
22	7	610	CLA	C3C-C2C	5.08	1.47	1.36
22	5	621	CLA	O2D-CGD	5.08	1.45	1.33
22	B	807	CLA	O2D-CGD	5.07	1.45	1.33
29	7	607	CHL	O2D-CGD	5.07	1.45	1.33
22	8	612	CLA	O2D-CGD	5.07	1.45	1.33
22	B	839	CLA	C1D-ND	5.07	1.44	1.37
22	3	612	CLA	C1D-ND	5.07	1.44	1.37
22	G	203	CLA	O2D-CGD	5.07	1.45	1.33
22	4	614	CLA	O2D-CGD	5.07	1.45	1.33
22	F	301	CLA	C1D-ND	5.07	1.44	1.37
22	5	613	CLA	O2D-CGD	5.07	1.45	1.33
22	9	604	CLA	O2D-CGD	5.07	1.45	1.33
22	A	840	CLA	C3C-C2C	5.07	1.47	1.36
29	6	606	CHL	O2D-CGD	5.07	1.45	1.33
29	5	618	CHL	O2D-CGD	5.07	1.45	1.33
29	4	618	CHL	C2C-C3C	5.06	1.47	1.36
22	8	613	CLA	O2D-CGD	5.06	1.45	1.33
22	A	815	CLA	C1D-ND	5.06	1.44	1.37
22	3	614	CLA	O2D-CGD	5.06	1.45	1.33
22	3	612	CLA	O2D-CGD	5.06	1.45	1.33
22	6	612	CLA	O2D-CGD	5.06	1.45	1.33
22	1	614	CLA	C1D-ND	5.06	1.44	1.37
22	3	609	CLA	C1D-ND	5.06	1.44	1.37
22	A	803	CLA	C3C-C2C	5.06	1.47	1.36
22	4	613	CLA	C3C-C2C	5.06	1.47	1.36
22	5	606	CLA	O2D-CGD	5.06	1.45	1.33
29	6	618	CHL	C2C-C3C	5.06	1.47	1.36
29	8	607	CHL	C2C-C3C	5.05	1.47	1.36
22	B	817	CLA	C3C-C2C	5.05	1.47	1.36
22	5	611	CLA	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	C1D-ND	5.05	1.44	1.37
22	3	602	CLA	C1D-ND	5.05	1.44	1.37
22	B	820	CLA	O2D-CGD	5.05	1.45	1.33
22	3	611	CLA	O2D-CGD	5.05	1.45	1.33
22	Z	603	CLA	C1D-ND	5.05	1.44	1.37
22	A	815	CLA	O2D-CGD	5.05	1.45	1.33
22	B	822	CLA	O2D-CGD	5.05	1.45	1.33
22	Z	602	CLA	C3C-C2C	5.05	1.47	1.36
22	B	813	CLA	C1D-ND	5.05	1.44	1.37
22	8	604	CLA	O2D-CGD	5.05	1.45	1.33
22	4	609	CLA	C3C-C2C	5.05	1.47	1.36
22	A	825	CLA	C3C-C2C	5.05	1.47	1.36
22	A	817	CLA	O2D-CGD	5.05	1.45	1.33
22	6	616	CLA	C3C-C2C	5.04	1.47	1.36
22	A	838	CLA	C1D-ND	5.04	1.44	1.37
22	Z	604	CLA	C1D-ND	5.04	1.44	1.37
22	1	610	CLA	O2D-CGD	5.04	1.45	1.33
22	B	821	CLA	C1D-ND	5.04	1.44	1.37
22	8	616	CLA	O2D-CGD	5.04	1.45	1.33
22	A	811	CLA	C3C-C2C	5.04	1.47	1.36
22	B	805	CLA	O2D-CGD	5.04	1.45	1.33
22	7	611	CLA	O2D-CGD	5.04	1.45	1.33
22	8	606	CLA	O2D-CGD	5.03	1.45	1.33
22	4	612	CLA	O2D-CGD	5.03	1.45	1.33
22	3	607	CLA	O2D-CGD	5.03	1.45	1.33
22	B	833	CLA	C1D-ND	5.03	1.44	1.37
22	1	616	CLA	C1D-ND	5.03	1.44	1.37
22	8	611	CLA	C3C-C2C	5.03	1.47	1.36
22	3	617	CLA	O2D-CGD	5.03	1.45	1.33
22	6	603	CLA	C1D-ND	5.03	1.44	1.37
22	A	823	CLA	O2D-CGD	5.03	1.45	1.33
29	1	607	CHL	O2D-CGD	5.03	1.45	1.33
22	1	611	CLA	O2D-CGD	5.03	1.45	1.33
29	6	606	CHL	C2C-C3C	5.03	1.47	1.36
22	3	617	CLA	C1D-ND	5.03	1.44	1.37
22	B	839	CLA	O2D-CGD	5.03	1.45	1.33
29	4	608	CHL	O2D-CGD	5.03	1.45	1.33
22	J	3002	CLA	O2D-CGD	5.03	1.45	1.33
22	1	611	CLA	C1D-ND	5.03	1.44	1.37
22	A	824	CLA	O2D-CGD	5.02	1.45	1.33
22	A	830	CLA	C3C-C2C	5.02	1.47	1.36
22	8	612	CLA	C3C-C2C	5.02	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	618	CHL	O2D-CGD	5.02	1.45	1.33
22	Z	610	CLA	CHC-C1C	5.02	1.48	1.38
22	8	611	CLA	O2D-CGD	5.02	1.45	1.33
22	7	612	CLA	O2D-CGD	5.02	1.45	1.33
22	7	620	CLA	O2D-CGD	5.02	1.45	1.33
22	5	601	CLA	O2D-CGD	5.02	1.45	1.33
22	3	620	CLA	O2D-CGD	5.02	1.45	1.33
22	7	602	CLA	C1D-ND	5.02	1.44	1.37
22	3	603	CLA	O2D-CGD	5.02	1.45	1.33
22	6	617	CLA	O2D-CGD	5.02	1.45	1.33
22	1	614	CLA	O2D-CGD	5.02	1.45	1.33
22	6	611	CLA	O2D-CGD	5.02	1.45	1.33
22	B	811	CLA	O2D-CGD	5.02	1.45	1.33
22	B	836	CLA	C3C-C2C	5.02	1.47	1.36
22	6	609	CLA	C1D-ND	5.02	1.44	1.37
22	1	616	CLA	O2D-CGD	5.02	1.45	1.33
22	9	602	CLA	O2D-CGD	5.02	1.45	1.33
22	B	835	CLA	O2D-CGD	5.01	1.45	1.33
29	8	607	CHL	O2D-CGD	5.01	1.45	1.33
22	9	613	CLA	O2D-CGD	5.01	1.45	1.33
22	B	821	CLA	O2D-CGD	5.01	1.45	1.33
22	6	616	CLA	O2D-CGD	5.01	1.45	1.33
22	7	613	CLA	C3C-C2C	5.01	1.47	1.36
22	5	613	CLA	C1D-ND	5.01	1.43	1.37
22	A	826	CLA	O2D-CGD	5.01	1.45	1.33
22	3	603	CLA	C3C-C2C	5.01	1.47	1.36
22	A	807	CLA	O2D-CGD	5.01	1.45	1.33
22	8	601	CLA	C1D-ND	5.01	1.43	1.37
29	4	607	CHL	C2C-C3C	5.01	1.47	1.36
22	F	303	CLA	C3C-C2C	5.01	1.47	1.36
22	B	841	CLA	O2D-CGD	5.01	1.45	1.33
22	1	613	CLA	O2D-CGD	5.01	1.45	1.33
22	B	822	CLA	C1D-ND	5.00	1.43	1.37
22	6	604	CLA	O2D-CGD	5.00	1.45	1.33
22	A	816	CLA	O2D-CGD	5.00	1.45	1.33
22	B	840	CLA	O2D-CGD	5.00	1.45	1.33
22	Z	603	CLA	O2D-CGD	5.00	1.45	1.33
29	6	608	CHL	O2D-CGD	5.00	1.45	1.33
22	B	809	CLA	C3C-C2C	5.00	1.47	1.36
22	B	824	CLA	C3C-C2C	5.00	1.47	1.36
22	A	836	CLA	C1D-ND	5.00	1.43	1.37
22	8	610	CLA	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	821	CLA	O2D-CGD	4.99	1.45	1.33
22	7	602	CLA	O2D-CGD	4.99	1.45	1.33
22	Z	616	CLA	O2D-CGD	4.99	1.45	1.33
22	Z	609	CLA	O2D-CGD	4.99	1.45	1.33
22	5	614	CLA	C1D-ND	4.99	1.43	1.37
22	A	820	CLA	O2D-CGD	4.99	1.45	1.33
22	A	825	CLA	O2D-CGD	4.99	1.45	1.33
22	A	814	CLA	C3C-C2C	4.99	1.47	1.36
22	B	838	CLA	O2D-CGD	4.99	1.45	1.33
22	K	4002	CLA	O2D-CGD	4.99	1.45	1.33
22	8	608	CLA	O2D-CGD	4.99	1.45	1.33
22	5	614	CLA	O2D-CGD	4.99	1.45	1.33
22	4	611	CLA	O2D-CGD	4.99	1.45	1.33
22	A	808	CLA	C1D-ND	4.99	1.43	1.37
22	B	811	CLA	C1D-ND	4.99	1.43	1.37
22	3	610	CLA	CHC-C1C	4.98	1.48	1.38
22	5	613	CLA	C3C-C2C	4.98	1.47	1.36
22	B	840	CLA	C1D-ND	4.98	1.43	1.37
22	Z	602	CLA	C1D-ND	4.98	1.43	1.37
22	A	830	CLA	O2D-CGD	4.98	1.45	1.33
22	B	812	CLA	C1D-ND	4.98	1.43	1.37
22	3	603	CLA	C1D-ND	4.98	1.43	1.37
22	B	817	CLA	O2D-CGD	4.98	1.45	1.33
22	6	609	CLA	O2D-CGD	4.98	1.45	1.33
22	A	839	CLA	C1D-ND	4.98	1.43	1.37
22	4	610	CLA	O2D-CGD	4.98	1.45	1.33
22	B	828	CLA	O2D-CGD	4.98	1.45	1.33
22	1	608	CLA	O2D-CGD	4.98	1.45	1.33
22	8	614	CLA	O2D-CGD	4.98	1.45	1.33
22	6	610	CLA	O2D-CGD	4.98	1.45	1.33
22	B	817	CLA	C1D-ND	4.98	1.43	1.37
22	8	603	CLA	O2D-CGD	4.98	1.45	1.33
22	7	612	CLA	C1D-ND	4.97	1.43	1.37
22	B	812	CLA	O2D-CGD	4.97	1.45	1.33
22	B	810	CLA	O2D-CGD	4.97	1.45	1.33
22	3	602	CLA	C3C-C2C	4.97	1.47	1.36
22	A	825	CLA	C1D-ND	4.97	1.43	1.37
22	B	818	CLA	C1D-ND	4.97	1.43	1.37
22	3	604	CLA	O2D-CGD	4.97	1.45	1.33
22	7	603	CLA	O2D-CGD	4.97	1.45	1.33
22	Z	608	CLA	O2D-CGD	4.97	1.45	1.33
22	A	835	CLA	O2D-CGD	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	840	CLA	C1D-ND	4.97	1.43	1.37
22	A	812	CLA	O2D-CGD	4.97	1.45	1.33
22	4	613	CLA	O2D-CGD	4.96	1.45	1.33
22	A	823	CLA	C1D-ND	4.96	1.43	1.37
22	Z	610	CLA	O2D-CGD	4.96	1.45	1.33
22	Z	602	CLA	O2D-CGD	4.96	1.45	1.33
22	A	834	CLA	C1D-ND	4.96	1.43	1.37
22	B	815	CLA	C1D-ND	4.96	1.43	1.37
22	6	617	CLA	C1D-ND	4.96	1.43	1.37
22	7	608	CLA	O2D-CGD	4.96	1.45	1.33
22	7	610	CLA	O2D-CGD	4.96	1.45	1.33
22	A	829	CLA	O2D-CGD	4.96	1.45	1.33
22	5	601	CLA	C1D-ND	4.96	1.43	1.37
22	5	602	CLA	C3C-C2C	4.96	1.47	1.36
22	B	820	CLA	C1D-ND	4.95	1.43	1.37
22	7	602	CLA	CHC-C1C	4.95	1.48	1.38
22	5	612	CLA	C1D-ND	4.95	1.43	1.37
22	7	604	CLA	C3C-C2C	4.95	1.47	1.36
22	A	811	CLA	O2D-CGD	4.95	1.45	1.33
22	5	602	CLA	O2D-CGD	4.95	1.45	1.33
22	B	837	CLA	C1D-ND	4.95	1.43	1.37
22	6	622	CLA	O2D-CGD	4.95	1.45	1.33
22	3	602	CLA	O2D-CGD	4.94	1.45	1.33
22	B	831	CLA	CHC-C1C	4.94	1.48	1.38
22	4	612	CLA	C1D-ND	4.94	1.43	1.37
22	B	841	CLA	C1D-ND	4.94	1.43	1.37
29	Z	601	CHL	O2D-CGD	4.94	1.45	1.33
22	B	831	CLA	O2D-CGD	4.94	1.45	1.33
22	A	843	CLA	C3C-C2C	4.94	1.47	1.36
22	B	818	CLA	O2D-CGD	4.94	1.45	1.33
22	B	834	CLA	O2D-CGD	4.94	1.45	1.33
22	A	832	CLA	O2D-CGD	4.94	1.45	1.33
22	A	837	CLA	O2D-CGD	4.94	1.45	1.33
22	5	610	CLA	O2D-CGD	4.93	1.45	1.33
22	5	617	CLA	O2D-CGD	4.93	1.45	1.33
22	L	204	CLA	C1D-ND	4.93	1.43	1.37
22	A	802	CLA	C1D-ND	4.93	1.43	1.37
22	8	613	CLA	C3C-C2C	4.93	1.47	1.36
22	1	612	CLA	C1D-ND	4.92	1.43	1.37
22	8	601	CLA	O2D-CGD	4.92	1.45	1.33
22	B	816	CLA	O2D-CGD	4.92	1.45	1.33
22	1	602	CLA	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	612	CLA	C1D-ND	4.92	1.43	1.37
22	6	602	CLA	C1D-ND	4.92	1.43	1.37
22	6	602	CLA	O2D-CGD	4.92	1.45	1.33
22	1	604	CLA	C1D-ND	4.92	1.43	1.37
22	3	610	CLA	C3C-C2C	4.92	1.47	1.36
22	A	806	CLA	O2D-CGD	4.92	1.45	1.33
29	3	608	CHL	C2C-C3C	4.92	1.47	1.36
22	B	833	CLA	O2D-CGD	4.92	1.45	1.33
22	B	852	CLA	C1D-ND	4.91	1.43	1.37
22	B	808	CLA	O2D-CGD	4.91	1.45	1.33
22	3	610	CLA	O2D-CGD	4.91	1.45	1.33
22	6	601	CLA	C1D-ND	4.91	1.43	1.37
22	B	825	CLA	CHC-C1C	4.91	1.48	1.38
22	8	609	CLA	O2D-CGD	4.91	1.45	1.33
22	B	806	CLA	C1D-ND	4.91	1.43	1.37
22	A	833	CLA	O2D-CGD	4.91	1.45	1.33
22	A	805	CLA	O2D-CGD	4.91	1.45	1.33
22	A	827	CLA	O2D-CGD	4.91	1.45	1.33
22	1	609	CLA	O2D-CGD	4.91	1.45	1.33
22	A	822	CLA	O2D-CGD	4.90	1.45	1.33
22	8	602	CLA	C1D-ND	4.90	1.43	1.37
22	A	834	CLA	O2D-CGD	4.89	1.45	1.33
22	A	829	CLA	C3C-C2C	4.89	1.47	1.36
22	A	808	CLA	O2D-CGD	4.89	1.45	1.33
22	7	606	CLA	O2D-CGD	4.89	1.45	1.33
22	8	604	CLA	C1D-ND	4.89	1.43	1.37
22	A	827	CLA	CHC-C1C	4.89	1.48	1.38
22	A	818	CLA	O2D-CGD	4.89	1.45	1.33
22	4	614	CLA	C1D-ND	4.89	1.43	1.37
22	A	841	CLA	C1D-ND	4.88	1.43	1.37
22	6	601	CLA	O2D-CGD	4.88	1.45	1.33
22	A	803	CLA	C1D-ND	4.88	1.43	1.37
22	A	842	CLA	C1D-ND	4.88	1.43	1.37
21	A	801	CL0	O2D-CGD	4.88	1.45	1.33
22	8	602	CLA	O2D-CGD	4.88	1.45	1.33
22	B	809	CLA	O2D-CGD	4.88	1.45	1.33
22	3	607	CLA	C1D-ND	4.88	1.43	1.37
22	A	815	CLA	CHC-C1C	4.88	1.48	1.38
22	1	613	CLA	C1D-ND	4.87	1.43	1.37
22	B	826	CLA	O2D-CGD	4.87	1.45	1.33
29	1	601	CHL	O2D-CGD	4.87	1.45	1.33
22	B	835	CLA	C1D-ND	4.87	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	836	CLA	C1D-ND	4.87	1.43	1.37
22	4	601	CLA	C1D-ND	4.87	1.43	1.37
22	8	609	CLA	C1D-ND	4.87	1.43	1.37
22	A	809	CLA	O2D-CGD	4.87	1.45	1.33
29	4	606	CHL	C2C-C3C	4.87	1.47	1.36
29	3	608	CHL	O2D-CGD	4.87	1.45	1.33
22	A	810	CLA	O2D-CGD	4.87	1.45	1.33
22	3	604	CLA	C1D-ND	4.86	1.43	1.37
22	Z	613	CLA	C1D-ND	4.86	1.43	1.37
22	B	836	CLA	O2D-CGD	4.86	1.45	1.33
22	B	823	CLA	C1D-ND	4.86	1.43	1.37
22	1	610	CLA	C3C-C2C	4.86	1.47	1.36
22	1	602	CLA	C1D-ND	4.86	1.43	1.37
22	B	802	CLA	C3C-C2C	4.86	1.47	1.36
22	A	814	CLA	C1D-ND	4.85	1.43	1.37
22	B	829	CLA	O2D-CGD	4.85	1.45	1.33
29	6	608	CHL	C2C-C3C	4.84	1.47	1.36
22	7	614	CLA	O2D-CGD	4.84	1.45	1.33
22	7	609	CLA	C1D-ND	4.84	1.43	1.37
22	5	609	CLA	O2D-CGD	4.84	1.45	1.33
22	A	818	CLA	C1D-ND	4.84	1.43	1.37
22	A	843	CLA	C1D-ND	4.84	1.43	1.37
22	B	803	CLA	C3C-C2C	4.83	1.47	1.36
22	8	612	CLA	C1D-ND	4.83	1.43	1.37
22	1	603	CLA	O2D-CGD	4.83	1.45	1.33
22	6	612	CLA	C1D-ND	4.83	1.43	1.37
22	B	830	CLA	O2D-CGD	4.82	1.45	1.33
22	B	838	CLA	CHC-C1C	4.82	1.48	1.38
22	7	601	CLA	C1D-ND	4.82	1.43	1.37
29	5	608	CHL	O2D-CGD	4.82	1.45	1.33
22	A	842	CLA	O2D-CGD	4.82	1.45	1.33
22	5	616	CLA	O2D-CGD	4.82	1.45	1.33
22	7	601	CLA	O2D-CGD	4.82	1.45	1.33
22	A	831	CLA	O2D-CGD	4.82	1.45	1.33
22	B	814	CLA	O2D-CGD	4.81	1.44	1.33
22	4	602	CLA	C1D-ND	4.81	1.43	1.37
22	F	301	CLA	O2D-CGD	4.81	1.44	1.33
22	A	812	CLA	C1D-ND	4.81	1.43	1.37
22	5	602	CLA	CHC-C1C	4.80	1.48	1.38
22	B	813	CLA	C3C-C2C	4.80	1.46	1.36
22	B	814	CLA	C1D-ND	4.80	1.43	1.37
22	B	816	CLA	C3C-C2C	4.80	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	824	CLA	O2D-CGD	4.80	1.44	1.33
22	6	602	CLA	CHC-C1C	4.80	1.48	1.38
22	A	838	CLA	O2D-CGD	4.80	1.44	1.33
22	Z	610	CLA	C3C-C2C	4.80	1.46	1.36
22	A	811	CLA	C1D-ND	4.79	1.43	1.37
22	A	819	CLA	C1D-ND	4.79	1.43	1.37
22	3	613	CLA	C1D-ND	4.79	1.43	1.37
22	A	824	CLA	C1D-ND	4.79	1.43	1.37
22	B	802	CLA	O2D-CGD	4.79	1.44	1.33
29	9	606	CHL	C2C-C3C	4.79	1.47	1.36
22	7	613	CLA	C1D-ND	4.79	1.43	1.37
22	4	613	CLA	O2A-CGA	4.78	1.47	1.33
22	A	806	CLA	C3C-C2C	4.78	1.46	1.36
22	A	840	CLA	O2D-CGD	4.78	1.44	1.33
22	A	813	CLA	O2D-CGD	4.77	1.44	1.33
29	4	608	CHL	C2C-C3C	4.77	1.47	1.36
22	A	827	CLA	C1D-ND	4.77	1.43	1.37
22	8	610	CLA	C1D-ND	4.77	1.43	1.37
22	A	809	CLA	C1D-ND	4.77	1.43	1.37
22	8	614	CLA	C1D-ND	4.77	1.43	1.37
22	A	816	CLA	CHC-C1C	4.77	1.48	1.38
22	B	830	CLA	CHC-C1C	4.77	1.48	1.38
29	5	607	CHL	O2D-CGD	4.77	1.44	1.33
22	B	832	CLA	C1D-ND	4.77	1.43	1.37
22	4	601	CLA	O2D-CGD	4.76	1.44	1.33
22	A	805	CLA	CHC-C1C	4.76	1.48	1.38
22	6	622	CLA	C1D-ND	4.76	1.43	1.37
29	4	608	CHL	CHC-C1C	4.75	1.48	1.38
22	A	813	CLA	C1D-ND	4.75	1.43	1.37
22	A	807	CLA	C1D-ND	4.75	1.43	1.37
22	A	829	CLA	C1D-ND	4.75	1.43	1.37
22	B	815	CLA	O2D-CGD	4.75	1.44	1.33
22	5	610	CLA	CHC-C1C	4.74	1.48	1.38
22	1	602	CLA	CHC-C1C	4.74	1.48	1.38
22	5	610	CLA	C1D-ND	4.74	1.43	1.37
22	A	809	CLA	CHC-C1C	4.74	1.48	1.38
22	B	841	CLA	CHC-C1C	4.74	1.48	1.38
22	Z	610	CLA	C1D-ND	4.74	1.43	1.37
22	B	804	CLA	O2D-CGD	4.73	1.44	1.33
22	5	602	CLA	C1D-ND	4.73	1.43	1.37
22	A	839	CLA	O2D-CGD	4.73	1.44	1.33
22	A	804	CLA	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	805	CLA	C1D-ND	4.72	1.43	1.37
22	9	610	CLA	CHC-C1C	4.72	1.48	1.38
22	A	828	CLA	O2D-CGD	4.72	1.44	1.33
22	4	610	CLA	C1D-ND	4.72	1.43	1.37
29	6	606	CHL	CHC-C1C	4.72	1.48	1.38
22	A	802	CLA	CHC-C1C	4.71	1.48	1.38
22	B	831	CLA	C1D-ND	4.71	1.43	1.37
22	A	821	CLA	C1D-ND	4.71	1.43	1.37
22	B	819	CLA	C1D-ND	4.71	1.43	1.37
29	5	608	CHL	C2C-C3C	4.71	1.46	1.36
22	B	805	CLA	CHC-C1C	4.71	1.48	1.38
22	B	838	CLA	C1D-ND	4.70	1.43	1.37
22	2	614	CLA	CHC-C1C	4.70	1.48	1.38
22	B	829	CLA	CHC-C1C	4.70	1.48	1.38
22	9	602	CLA	CHC-C1C	4.70	1.48	1.38
22	A	835	CLA	CHC-C1C	4.70	1.48	1.38
22	7	608	CLA	CHC-C1C	4.70	1.48	1.38
22	1	606	CLA	CHC-C1C	4.70	1.48	1.38
22	A	837	CLA	CHC-C1C	4.68	1.48	1.38
22	B	803	CLA	O2D-CGD	4.68	1.44	1.33
22	B	816	CLA	CHC-C1C	4.67	1.48	1.38
22	6	614	CLA	CHC-C1C	4.67	1.48	1.38
22	A	820	CLA	C1D-ND	4.67	1.43	1.37
22	B	820	CLA	CHC-C1C	4.67	1.48	1.38
22	B	837	CLA	O2D-CGD	4.66	1.44	1.33
21	A	801	CL0	C1D-ND	4.66	1.43	1.37
22	A	828	CLA	CHC-C1C	4.66	1.48	1.38
22	B	832	CLA	O2D-CGD	4.66	1.44	1.33
22	F	301	CLA	CHC-C1C	4.66	1.48	1.38
22	8	614	CLA	CHC-C1C	4.66	1.48	1.38
29	5	608	CHL	CHC-C1C	4.66	1.48	1.38
22	2	607	CLA	CHC-C1C	4.66	1.48	1.38
22	A	833	CLA	CHC-C1C	4.66	1.48	1.38
22	5	606	CLA	CHC-C1C	4.66	1.48	1.38
22	A	829	CLA	CHC-C1C	4.65	1.48	1.38
22	A	803	CLA	O2D-CGD	4.65	1.44	1.33
22	2	610	CLA	CHC-C1C	4.65	1.48	1.38
22	Z	602	CLA	CHC-C1C	4.64	1.48	1.38
22	K	4002	CLA	CHC-C1C	4.64	1.47	1.38
22	8	608	CLA	C3C-C2C	4.64	1.46	1.36
22	4	614	CLA	CHC-C1C	4.64	1.47	1.38
22	B	804	CLA	C1D-ND	4.64	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	831	CLA	C1B-NB	-4.64	1.32	1.37
22	7	608	CLA	C1D-ND	4.64	1.43	1.37
22	F	304	CLA	O2A-CGA	4.63	1.46	1.33
22	8	602	CLA	CHC-C1C	4.63	1.47	1.38
22	6	610	CLA	CHC-C1C	4.63	1.47	1.38
22	A	806	CLA	C1D-ND	4.63	1.43	1.37
22	9	611	CLA	CHC-C1C	4.63	1.47	1.38
22	Z	613	CLA	CHC-C1C	4.63	1.47	1.38
22	B	830	CLA	C1D-ND	4.63	1.43	1.37
22	A	810	CLA	C1D-ND	4.63	1.43	1.37
22	A	813	CLA	CHC-C1C	4.62	1.47	1.38
22	4	610	CLA	CHC-C1C	4.62	1.47	1.38
22	B	826	CLA	C1D-ND	4.62	1.43	1.37
22	1	610	CLA	C1D-ND	4.62	1.43	1.37
22	A	822	CLA	CHC-C1C	4.62	1.47	1.38
22	A	814	CLA	O2D-CGD	4.62	1.44	1.33
22	B	819	CLA	CHC-C1C	4.61	1.47	1.38
22	8	610	CLA	CHC-C1C	4.61	1.47	1.38
23	B	842	PQN	C10-C5	4.61	1.48	1.40
22	5	613	CLA	O2A-CGA	4.61	1.46	1.33
22	1	614	CLA	CHC-C1C	4.61	1.47	1.38
22	B	837	CLA	CHC-C1C	4.61	1.47	1.38
22	B	841	CLA	CHD-C1D	4.61	1.47	1.38
22	A	831	CLA	C1D-ND	4.61	1.43	1.37
22	B	813	CLA	O2D-CGD	4.61	1.44	1.33
22	Z	614	CLA	CHC-C1C	4.61	1.47	1.38
22	7	609	CLA	CHC-C1C	4.60	1.47	1.38
22	A	854	CLA	O2D-CGD	4.60	1.44	1.33
22	A	811	CLA	CHC-C1C	4.60	1.47	1.38
22	1	604	CLA	CHC-C1C	4.60	1.47	1.38
22	9	614	CLA	CHC-C1C	4.60	1.47	1.38
22	8	616	CLA	C1D-ND	4.60	1.43	1.37
22	A	819	CLA	CHC-C1C	4.60	1.47	1.38
22	B	814	CLA	CHC-C1C	4.59	1.47	1.38
22	B	824	CLA	C1D-ND	4.59	1.43	1.37
29	5	607	CHL	O2A-CGA	4.59	1.46	1.33
22	B	804	CLA	CHC-C1C	4.59	1.47	1.38
22	1	604	CLA	CHD-C1D	4.59	1.47	1.38
22	L	204	CLA	CHC-C1C	4.59	1.47	1.38
22	Z	616	CLA	CHC-C1C	4.59	1.47	1.38
22	2	606	CLA	CHC-C1C	4.58	1.47	1.38
22	4	604	CLA	CHC-C1C	4.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	852	CLA	CHC-C1C	4.58	1.47	1.38
22	A	832	CLA	CHC-C1C	4.58	1.47	1.38
22	5	621	CLA	C1D-ND	4.58	1.43	1.37
22	B	827	CLA	CHC-C1C	4.58	1.47	1.38
29	Z	601	CHL	CHC-C1C	4.58	1.47	1.38
22	A	854	CLA	C1D-ND	4.58	1.43	1.37
22	Z	606	CLA	CHC-C1C	4.57	1.47	1.38
29	4	607	CHL	CHC-C1C	4.57	1.47	1.38
22	6	604	CLA	CHC-C1C	4.56	1.47	1.38
22	B	824	CLA	CHC-C1C	4.56	1.47	1.38
22	Z	611	CLA	CHC-C1C	4.56	1.47	1.38
22	B	806	CLA	CHC-C1C	4.56	1.47	1.38
22	3	609	CLA	O2D-CGD	4.56	1.44	1.33
22	9	604	CLA	CHD-C1D	4.56	1.47	1.38
22	B	835	CLA	CHC-C1C	4.55	1.47	1.38
22	6	614	CLA	O2D-CGD	4.55	1.44	1.33
22	5	617	CLA	C1D-ND	4.55	1.43	1.37
22	4	602	CLA	CHC-C1C	4.55	1.47	1.38
22	6	613	CLA	CHC-C1C	4.55	1.47	1.38
29	9	607	CHL	CHC-C1C	4.55	1.47	1.38
22	5	604	CLA	CHD-C1D	4.55	1.47	1.38
22	B	821	CLA	CHC-C1C	4.54	1.47	1.38
22	1	609	CLA	O2A-CGA	4.54	1.46	1.33
29	9	606	CHL	CHC-C1C	4.54	1.47	1.38
22	B	834	CLA	CHD-C1D	4.54	1.47	1.38
22	K	4002	CLA	CHD-C1D	4.54	1.47	1.38
29	1	607	CHL	CHC-C1C	4.54	1.47	1.38
22	B	813	CLA	CHC-C1C	4.54	1.47	1.38
22	6	622	CLA	CHC-C1C	4.54	1.47	1.38
22	L	203	CLA	C1D-ND	4.53	1.43	1.37
22	2	602	CLA	CHC-C1C	4.53	1.47	1.38
22	3	610	CLA	C1D-ND	4.53	1.43	1.37
22	B	832	CLA	CHC-C1C	4.53	1.47	1.38
22	G	204	CLA	CHC-C1C	4.53	1.47	1.38
29	6	606	CHL	O2A-CGA	4.53	1.46	1.33
22	8	616	CLA	CHC-C1C	4.53	1.47	1.38
22	7	620	CLA	CHC-C1C	4.53	1.47	1.38
22	Z	603	CLA	CHD-C1D	4.52	1.47	1.38
22	7	614	CLA	CHC-C1C	4.52	1.47	1.38
22	Z	603	CLA	O2A-CGA	4.52	1.46	1.33
22	B	808	CLA	C1D-ND	4.52	1.43	1.37
22	B	827	CLA	C1D-ND	4.51	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	604	CLA	CHD-C1D	4.51	1.47	1.38
22	A	802	CLA	CHD-C1D	4.51	1.47	1.38
22	7	616	CLA	CHC-C1C	4.51	1.47	1.38
22	9	601	CLA	CHC-C1C	4.51	1.47	1.38
22	B	825	CLA	C1D-ND	4.51	1.43	1.37
22	Z	609	CLA	CHD-C1D	4.51	1.47	1.38
22	4	613	CLA	CHC-C1C	4.51	1.47	1.38
22	5	614	CLA	O2A-CGA	4.50	1.45	1.30
22	3	614	CLA	O2A-CGA	4.50	1.45	1.30
22	3	614	CLA	CHC-C1C	4.50	1.47	1.38
23	A	844	PQN	C10-C5	4.50	1.48	1.40
22	3	611	CLA	CHC-C1C	4.50	1.47	1.38
22	A	804	CLA	C1D-ND	4.50	1.43	1.37
22	5	601	CLA	CHC-C1C	4.50	1.47	1.38
22	7	616	CLA	CHD-C1D	4.50	1.47	1.38
22	Z	608	CLA	CHC-C1C	4.50	1.47	1.38
22	A	821	CLA	O2A-CGA	4.50	1.45	1.30
22	4	603	CLA	CHD-C1D	4.50	1.47	1.38
22	B	822	CLA	CHC-C1C	4.50	1.47	1.38
29	3	608	CHL	C1B-NB	-4.50	1.32	1.37
22	5	621	CLA	CHC-C1C	4.50	1.47	1.38
22	A	822	CLA	C1D-ND	4.50	1.43	1.37
22	3	602	CLA	CHC-C1C	4.50	1.47	1.38
22	B	809	CLA	C1D-ND	4.50	1.43	1.37
22	2	614	CLA	O2A-CGA	4.49	1.45	1.30
22	2	602	CLA	O2A-CGA	4.49	1.45	1.30
22	B	825	CLA	O2D-CGD	4.49	1.44	1.33
22	8	601	CLA	CHC-C1C	4.49	1.47	1.38
22	9	604	CLA	CHC-C1C	4.49	1.47	1.38
22	B	834	CLA	CHC-C1C	4.49	1.47	1.38
22	2	611	CLA	CHC-C1C	4.49	1.47	1.38
22	9	614	CLA	CHD-C1D	4.49	1.47	1.38
22	9	614	CLA	O2A-CGA	4.49	1.45	1.30
22	6	611	CLA	CHC-C1C	4.49	1.47	1.38
22	1	603	CLA	O2A-CGA	4.49	1.46	1.33
22	K	4002	CLA	O2A-CGA	4.49	1.45	1.30
22	B	820	CLA	CHD-C1D	4.48	1.47	1.38
22	5	614	CLA	CHC-C1C	4.48	1.47	1.38
22	9	613	CLA	O2A-CGA	4.48	1.46	1.33
22	B	812	CLA	O2A-CGA	4.48	1.46	1.33
29	4	618	CHL	CHC-C1C	4.48	1.47	1.38
22	A	815	CLA	CHD-C1D	4.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	609	CLA	CHD-C1D	4.47	1.47	1.38
22	8	609	CLA	CHC-C1C	4.47	1.47	1.38
22	B	833	CLA	CHC-C1C	4.47	1.47	1.38
22	B	823	CLA	CHC-C1C	4.47	1.47	1.38
22	6	622	CLA	O2A-CGA	4.47	1.45	1.30
22	2	609	CLA	CHC-C1C	4.47	1.47	1.38
22	8	608	CLA	CHC-C1C	4.47	1.47	1.38
22	5	617	CLA	CHC-C1C	4.47	1.47	1.38
22	K	4003	CLA	CHC-C1C	4.47	1.47	1.38
29	1	601	CHL	CHC-C1C	4.47	1.47	1.38
22	8	603	CLA	O2A-CGA	4.47	1.45	1.30
22	1	616	CLA	CHC-C1C	4.46	1.47	1.38
22	B	828	CLA	O2A-CGA	4.46	1.46	1.33
22	6	612	CLA	CHC-C1C	4.46	1.47	1.38
22	A	835	CLA	CHD-C1D	4.46	1.47	1.38
22	B	811	CLA	CHC-C1C	4.46	1.47	1.38
22	2	606	CLA	CHD-C1D	4.46	1.47	1.38
22	7	613	CLA	O2A-CGA	4.46	1.46	1.33
22	A	837	CLA	CHD-C1D	4.45	1.47	1.38
22	4	611	CLA	CHD-C1D	4.45	1.47	1.38
22	A	839	CLA	CHC-C1C	4.45	1.47	1.38
22	1	611	CLA	O2A-CGA	4.45	1.46	1.33
22	A	826	CLA	CHD-C1D	4.45	1.47	1.38
22	3	606	CLA	CHD-C1D	4.45	1.47	1.38
22	2	612	CLA	CHD-C1D	4.45	1.47	1.38
22	5	611	CLA	CHC-C1C	4.45	1.47	1.38
29	5	607	CHL	CHC-C1C	4.45	1.47	1.38
22	B	814	CLA	O2A-CGA	4.45	1.46	1.33
29	7	607	CHL	CHC-C1C	4.44	1.47	1.38
22	A	837	CLA	O2A-CGA	4.44	1.45	1.30
22	7	603	CLA	CHC-C1C	4.44	1.47	1.38
22	A	818	CLA	CHC-C1C	4.44	1.47	1.38
22	A	823	CLA	CHC-C1C	4.44	1.47	1.38
22	2	613	CLA	CHC-C1C	4.44	1.47	1.38
22	4	616	CLA	CHD-C1D	4.44	1.47	1.38
22	J	3002	CLA	CHD-C1D	4.44	1.47	1.38
22	2	601	CLA	CHC-C1C	4.43	1.47	1.38
22	9	612	CLA	CHD-C1D	4.43	1.47	1.38
22	5	604	CLA	CHC-C1C	4.43	1.47	1.38
22	2	601	CLA	CHD-C1D	4.43	1.47	1.38
22	A	806	CLA	CHC-C1C	4.43	1.47	1.38
22	B	810	CLA	CHC-C1C	4.43	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	839	CLA	CHC-C1C	4.43	1.47	1.38
22	2	607	CLA	CHD-C1D	4.43	1.47	1.38
22	A	841	CLA	CHC-C1C	4.43	1.47	1.38
22	6	617	CLA	CHC-C1C	4.43	1.47	1.38
29	6	608	CHL	CHC-C1C	4.43	1.47	1.38
29	4	606	CHL	CHC-C1C	4.43	1.47	1.38
22	B	835	CLA	O2A-CGA	4.43	1.45	1.30
22	3	609	CLA	CHC-C1C	4.42	1.47	1.38
29	6	607	CHL	CHC-C1C	4.42	1.47	1.38
22	3	606	CLA	CHC-C1C	4.42	1.47	1.38
22	G	204	CLA	CHD-C1D	4.42	1.47	1.38
29	6	618	CHL	CHC-C1C	4.42	1.47	1.38
29	4	606	CHL	O2A-CGA	4.42	1.46	1.33
22	8	606	CLA	CHC-C1C	4.42	1.47	1.38
22	B	815	CLA	CHC-C1C	4.42	1.47	1.38
22	9	610	CLA	O2A-CGA	4.42	1.46	1.33
22	8	613	CLA	CHC-C1C	4.41	1.47	1.38
22	J	3002	CLA	CHC-C1C	4.41	1.47	1.38
22	3	617	CLA	CHC-C1C	4.41	1.47	1.38
24	4	622	LHG	O7-C7	4.41	1.46	1.34
22	2	613	CLA	CHD-C1D	4.41	1.47	1.38
22	F	303	CLA	O2A-CGA	4.41	1.45	1.30
22	3	620	CLA	CHC-C1C	4.41	1.47	1.38
22	1	603	CLA	CHD-C1D	4.41	1.47	1.38
22	3	611	CLA	CHD-C1D	4.41	1.46	1.38
22	G	203	CLA	CHC-C1C	4.41	1.47	1.38
22	4	612	CLA	CHC-C1C	4.40	1.47	1.38
22	6	616	CLA	CHD-C1D	4.40	1.46	1.38
22	B	802	CLA	C1D-ND	4.40	1.43	1.37
22	L	203	CLA	CHC-C1C	4.40	1.47	1.38
22	6	613	CLA	O2A-CGA	4.40	1.46	1.33
22	9	601	CLA	CHD-C1D	4.40	1.46	1.38
22	6	616	CLA	CHC-C1C	4.40	1.47	1.38
22	Z	612	CLA	O2A-CGA	4.40	1.46	1.33
22	9	613	CLA	CHD-C1D	4.40	1.46	1.38
22	3	604	CLA	CHC-C1C	4.40	1.47	1.38
22	B	826	CLA	CHC-C1C	4.40	1.47	1.38
22	A	818	CLA	O2A-CGA	4.40	1.46	1.33
22	A	836	CLA	O2A-CGA	4.40	1.46	1.33
22	B	812	CLA	CHC-C1C	4.40	1.47	1.38
22	5	609	CLA	CHC-C1C	4.40	1.47	1.38
22	3	609	CLA	O2A-CGA	4.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	613	CLA	O2A-CGA	4.40	1.46	1.33
22	4	601	CLA	CHC-C1C	4.40	1.47	1.38
22	Z	604	CLA	CHC-C1C	4.40	1.47	1.38
22	8	611	CLA	CHD-C1D	4.40	1.46	1.38
22	B	819	CLA	CHD-C1D	4.40	1.46	1.38
22	2	603	CLA	CHD-C1D	4.40	1.46	1.38
22	F	303	CLA	CHC-C1C	4.40	1.47	1.38
22	9	612	CLA	CHC-C1C	4.40	1.47	1.38
22	K	4003	CLA	CHD-C1D	4.39	1.46	1.38
22	A	810	CLA	CHC-C1C	4.39	1.47	1.38
29	Z	607	CHL	CHC-C1C	4.39	1.47	1.38
22	8	612	CLA	CHC-C1C	4.39	1.47	1.38
22	Z	613	CLA	O2A-CGA	4.39	1.46	1.33
22	3	614	CLA	CHD-C1D	4.39	1.46	1.38
22	6	610	CLA	CHD-C1D	4.39	1.46	1.38
22	5	611	CLA	CHD-C1D	4.39	1.46	1.38
22	9	609	CLA	CHC-C1C	4.38	1.47	1.38
22	8	609	CLA	CHD-C1D	4.38	1.46	1.38
29	8	607	CHL	CHC-C1C	4.38	1.47	1.38
22	B	828	CLA	C1B-NB	-4.38	1.32	1.37
22	B	818	CLA	CHD-C1D	4.38	1.46	1.38
22	2	602	CLA	CHD-C1D	4.38	1.46	1.38
22	8	611	CLA	CHC-C1C	4.38	1.47	1.38
22	A	804	CLA	CHC-C1C	4.38	1.47	1.38
22	A	854	CLA	O2A-CGA	4.37	1.46	1.33
22	A	830	CLA	CHC-C1C	4.37	1.47	1.38
22	3	617	CLA	CHD-C1D	4.37	1.46	1.38
22	A	808	CLA	CHC-C1C	4.37	1.47	1.38
22	6	613	CLA	CHD-C1D	4.37	1.46	1.38
22	Z	612	CLA	CHC-C1C	4.37	1.47	1.38
22	2	611	CLA	CHD-C1D	4.37	1.46	1.38
22	B	815	CLA	O2A-CGA	4.37	1.46	1.33
22	5	601	CLA	O2A-CGA	4.37	1.46	1.33
22	2	607	CLA	O2A-CGA	4.37	1.46	1.33
22	2	610	CLA	CHD-C1D	4.37	1.46	1.38
22	1	613	CLA	O2A-CGA	4.37	1.46	1.33
22	B	836	CLA	CHC-C1C	4.36	1.47	1.38
22	B	805	CLA	C1D-ND	4.36	1.43	1.37
22	A	838	CLA	CHD-C1D	4.36	1.46	1.38
22	9	603	CLA	CHD-C1D	4.36	1.46	1.38
22	7	614	CLA	CHD-C1D	4.36	1.46	1.38
22	A	810	CLA	O2A-CGA	4.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	613	CLA	CHC-C1C	4.36	1.47	1.38
22	Z	604	CLA	CHD-C1D	4.36	1.46	1.38
22	7	611	CLA	CHD-C1D	4.36	1.46	1.38
22	4	614	CLA	O2A-CGA	4.35	1.45	1.30
22	Z	609	CLA	O2A-CGA	4.35	1.46	1.33
22	6	611	CLA	CHD-C1D	4.35	1.46	1.38
22	6	611	CLA	O2A-CGA	4.35	1.46	1.33
22	8	612	CLA	O2A-CGA	4.35	1.46	1.33
22	6	612	CLA	O2A-CGA	4.35	1.46	1.33
22	B	836	CLA	O2A-CGA	4.35	1.46	1.33
22	A	823	CLA	O2A-CGA	4.35	1.46	1.33
22	2	612	CLA	O2A-CGA	4.35	1.46	1.33
22	A	803	CLA	CHC-C1C	4.35	1.47	1.38
22	8	613	CLA	O2A-CGA	4.34	1.46	1.33
22	F	304	CLA	CHC-C1C	4.34	1.47	1.38
22	1	611	CLA	CHD-C1D	4.34	1.46	1.38
22	3	602	CLA	CHD-C1D	4.34	1.46	1.38
22	8	606	CLA	CHD-C1D	4.34	1.46	1.38
29	7	607	CHL	CHD-C1D	4.34	1.46	1.38
22	A	820	CLA	CHC-C1C	4.34	1.47	1.38
22	1	611	CLA	CHC-C1C	4.34	1.47	1.38
22	7	601	CLA	CHC-C1C	4.34	1.47	1.38
22	2	612	CLA	CHC-C1C	4.34	1.47	1.38
22	B	817	CLA	CHD-C1D	4.34	1.46	1.38
22	6	604	CLA	CHD-C1D	4.34	1.46	1.38
22	A	840	CLA	O2A-CGA	4.34	1.46	1.33
22	A	845	CLA	CHC-C1C	4.34	1.47	1.38
22	A	838	CLA	O2A-CGA	4.34	1.46	1.33
22	A	825	CLA	O2A-CGA	4.34	1.46	1.33
22	5	614	CLA	CHD-C1D	4.34	1.46	1.38
22	7	608	CLA	O2A-CGA	4.34	1.46	1.33
22	B	803	CLA	CHC-C1C	4.34	1.47	1.38
29	5	618	CHL	CHC-C1C	4.34	1.47	1.38
22	6	601	CLA	CHC-C1C	4.34	1.47	1.38
22	Z	611	CLA	CHD-C1D	4.34	1.46	1.38
22	B	807	CLA	O2A-CGA	4.34	1.46	1.33
22	3	604	CLA	CHD-C1D	4.33	1.46	1.38
22	A	822	CLA	O2A-CGA	4.33	1.46	1.33
22	B	822	CLA	O2A-CGA	4.33	1.46	1.33
22	Z	608	CLA	CHD-C1D	4.33	1.46	1.38
22	9	602	CLA	CHD-C1D	4.33	1.46	1.38
22	A	817	CLA	CHD-C1D	4.33	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	614	CLA	CHD-C1D	4.33	1.46	1.38
22	5	610	CLA	O2A-CGA	4.33	1.46	1.33
22	4	611	CLA	CHC-C1C	4.33	1.47	1.38
22	9	612	CLA	O2A-CGA	4.33	1.46	1.33
22	A	824	CLA	CHC-C1C	4.32	1.47	1.38
22	7	606	CLA	CHC-C1C	4.32	1.47	1.38
22	A	803	CLA	C1B-NB	-4.32	1.32	1.37
22	4	602	CLA	CHD-C1D	4.32	1.46	1.38
22	A	814	CLA	CHC-C1C	4.32	1.47	1.38
22	9	610	CLA	CHD-C1D	4.32	1.46	1.38
22	6	614	CLA	O2A-CGA	4.32	1.45	1.30
22	2	614	CLA	CHD-C1D	4.32	1.46	1.38
22	A	805	CLA	CHD-C1D	4.32	1.46	1.38
22	3	607	CLA	CHD-C1D	4.32	1.46	1.38
22	B	839	CLA	O2A-CGA	4.32	1.46	1.33
29	1	607	CHL	O2A-CGA	4.32	1.46	1.33
22	B	824	CLA	O2A-CGA	4.31	1.45	1.33
22	B	833	CLA	O2A-CGA	4.31	1.45	1.33
22	B	811	CLA	CHD-C1D	4.31	1.46	1.38
22	3	612	CLA	CHD-C1D	4.31	1.46	1.38
22	6	614	CLA	CHD-C1D	4.31	1.46	1.38
22	A	843	CLA	CHD-C1D	4.31	1.46	1.38
22	7	612	CLA	O2A-CGA	4.31	1.45	1.33
22	7	603	CLA	CHD-C1D	4.31	1.46	1.38
22	4	609	CLA	O2A-CGA	4.31	1.45	1.33
22	Z	614	CLA	CHD-C1D	4.31	1.46	1.38
22	Z	606	CLA	CHD-C1D	4.31	1.46	1.38
22	3	607	CLA	O2A-CGA	4.31	1.45	1.33
22	B	811	CLA	O2A-CGA	4.31	1.45	1.33
22	5	612	CLA	O2A-CGA	4.31	1.45	1.33
22	6	601	CLA	CHD-C1D	4.31	1.46	1.38
22	A	834	CLA	CHC-C1C	4.31	1.47	1.38
22	Z	606	CLA	O2A-CGA	4.31	1.45	1.33
22	A	812	CLA	CHC-C1C	4.31	1.47	1.38
22	1	612	CLA	CHC-C1C	4.31	1.47	1.38
22	G	203	CLA	O2A-CGA	4.31	1.45	1.33
29	7	607	CHL	O2A-CGA	4.31	1.45	1.33
22	5	601	CLA	CHD-C1D	4.30	1.46	1.38
22	A	845	CLA	O2A-CGA	4.30	1.45	1.33
24	A	855	LHG	O8-C23	4.30	1.45	1.33
29	1	601	CHL	O2A-CGA	4.30	1.45	1.33
22	6	603	CLA	CHD-C1D	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	609	CLA	CHD-C1D	4.30	1.46	1.38
29	4	606	CHL	CHD-C1D	4.30	1.46	1.38
22	5	603	CLA	CHC-C1C	4.30	1.47	1.38
22	A	833	CLA	CHD-C1D	4.30	1.46	1.38
22	A	807	CLA	O2A-CGA	4.30	1.45	1.33
22	L	203	CLA	O2A-CGA	4.30	1.45	1.33
22	1	609	CLA	CHC-C1C	4.30	1.47	1.38
29	Z	607	CHL	O2A-CGA	4.30	1.45	1.33
22	Z	616	CLA	CHD-C1D	4.30	1.46	1.38
22	Z	608	CLA	O2A-CGA	4.30	1.45	1.33
22	A	825	CLA	CHD-C1D	4.30	1.46	1.38
22	1	613	CLA	CHC-C1C	4.29	1.47	1.38
22	B	840	CLA	O2A-CGA	4.29	1.45	1.33
22	B	826	CLA	C1B-NB	-4.29	1.32	1.37
22	B	816	CLA	O2A-CGA	4.29	1.45	1.33
22	B	833	CLA	CHD-C1D	4.29	1.46	1.38
22	2	611	CLA	O2A-CGA	4.29	1.45	1.33
22	4	604	CLA	O2A-CGA	4.29	1.45	1.33
22	A	832	CLA	O2A-CGA	4.29	1.45	1.33
22	1	614	CLA	O2A-CGA	4.29	1.45	1.33
22	A	832	CLA	C1D-ND	4.29	1.43	1.37
29	9	606	CHL	CHD-C1D	4.29	1.46	1.38
22	A	808	CLA	CHD-C1D	4.29	1.46	1.38
22	1	604	CLA	O2A-CGA	4.29	1.45	1.33
22	6	610	CLA	O2A-CGA	4.29	1.45	1.33
22	5	604	CLA	O2A-CGA	4.28	1.45	1.33
22	1	608	CLA	CHC-C1C	4.28	1.47	1.38
22	A	813	CLA	O2A-CGA	4.28	1.45	1.33
22	5	611	CLA	O2A-CGA	4.28	1.45	1.33
22	5	606	CLA	O2A-CGA	4.28	1.45	1.33
22	B	807	CLA	CHD-C1D	4.28	1.46	1.38
22	9	604	CLA	O2A-CGA	4.28	1.45	1.33
22	F	304	CLA	CHD-C1D	4.28	1.46	1.38
22	5	609	CLA	CHD-C1D	4.28	1.46	1.38
22	A	830	CLA	C1D-ND	4.28	1.43	1.37
22	B	814	CLA	CHD-C1D	4.28	1.46	1.38
22	1	612	CLA	CHD-C1D	4.28	1.46	1.38
22	B	809	CLA	C1B-NB	-4.28	1.32	1.37
29	5	608	CHL	CHD-C1D	4.28	1.46	1.38
22	A	843	CLA	CHC-C1C	4.28	1.47	1.38
22	B	852	CLA	CHD-C1D	4.28	1.46	1.38
22	9	609	CLA	CHD-C1D	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	816	CLA	CHD-C1D	4.28	1.46	1.38
22	6	617	CLA	CHD-C1D	4.28	1.46	1.38
29	Z	601	CHL	O2A-CGA	4.28	1.45	1.33
22	7	620	CLA	CHD-C1D	4.28	1.46	1.38
22	2	613	CLA	O2A-CGA	4.28	1.45	1.33
22	A	817	CLA	O2A-CGA	4.28	1.45	1.33
22	A	835	CLA	O2A-CGA	4.28	1.45	1.33
22	Z	613	CLA	CHD-C1D	4.28	1.46	1.38
22	5	621	CLA	CHD-C1D	4.28	1.46	1.38
22	7	612	CLA	CHC-C1C	4.28	1.47	1.38
22	6	604	CLA	O2A-CGA	4.28	1.45	1.33
29	4	607	CHL	O2A-CGA	4.28	1.45	1.33
22	B	804	CLA	O2A-CGA	4.28	1.45	1.30
22	B	828	CLA	C1D-ND	4.28	1.43	1.37
22	8	603	CLA	CHD-C1D	4.27	1.46	1.38
22	6	609	CLA	CHC-C1C	4.27	1.47	1.38
22	B	820	CLA	O2A-CGA	4.27	1.45	1.33
22	5	613	CLA	CHD-C1D	4.27	1.46	1.38
22	4	613	CLA	CHD-C1D	4.27	1.46	1.38
22	L	204	CLA	O2A-CGA	4.27	1.45	1.33
22	3	602	CLA	O2A-CGA	4.27	1.45	1.33
22	A	824	CLA	O2A-CGA	4.27	1.45	1.33
22	1	606	CLA	O2A-CGA	4.27	1.45	1.33
22	A	842	CLA	CHC-C1C	4.27	1.47	1.38
22	3	620	CLA	O2A-CGA	4.26	1.45	1.33
22	2	610	CLA	O2A-CGA	4.26	1.45	1.33
22	B	839	CLA	CHD-C1D	4.26	1.46	1.38
22	3	607	CLA	CHC-C1C	4.26	1.47	1.38
22	8	604	CLA	CHD-C1D	4.26	1.46	1.38
22	A	840	CLA	CHC-C1C	4.26	1.47	1.38
22	B	840	CLA	CHD-C1D	4.26	1.46	1.38
22	5	616	CLA	CHD-C1D	4.26	1.46	1.38
22	7	602	CLA	O2A-CGA	4.26	1.45	1.33
29	9	607	CHL	O2A-CGA	4.26	1.45	1.33
22	A	806	CLA	C1B-NB	-4.26	1.32	1.37
22	8	604	CLA	CHC-C1C	4.26	1.47	1.38
22	4	612	CLA	O2A-CGA	4.26	1.45	1.33
22	1	610	CLA	O2A-CGA	4.25	1.45	1.33
22	B	830	CLA	O2A-CGA	4.25	1.45	1.33
24	6	619	LHG	O8-C23	4.25	1.45	1.33
22	1	608	CLA	O2A-CGA	4.25	1.45	1.33
22	A	807	CLA	CHC-C1C	4.25	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	612	CLA	O2A-CGA	4.25	1.45	1.33
22	3	609	CLA	CHD-C1D	4.25	1.46	1.38
22	8	602	CLA	O2A-CGA	4.25	1.45	1.33
22	3	613	CLA	CHC-C1C	4.25	1.47	1.38
29	9	607	CHL	CHD-C1D	4.25	1.46	1.38
22	B	852	CLA	O2A-CGA	4.25	1.45	1.33
22	5	602	CLA	O2A-CGA	4.25	1.45	1.33
22	B	823	CLA	CHD-C1D	4.25	1.46	1.38
22	A	837	CLA	C1B-NB	-4.25	1.32	1.37
22	B	819	CLA	O2A-CGA	4.24	1.45	1.33
22	B	817	CLA	O2A-CGA	4.24	1.45	1.33
22	8	608	CLA	O2A-CGA	4.24	1.45	1.33
22	B	836	CLA	CHD-C1D	4.24	1.46	1.38
22	A	845	CLA	CHD-C1D	4.24	1.46	1.38
22	7	620	CLA	O2A-CGA	4.24	1.45	1.33
22	9	611	CLA	CHD-C1D	4.24	1.46	1.38
22	Z	614	CLA	O2A-CGA	4.24	1.45	1.33
22	1	616	CLA	CHD-C1D	4.24	1.46	1.38
22	A	839	CLA	CHD-C1D	4.23	1.46	1.38
22	6	603	CLA	CHC-C1C	4.23	1.47	1.38
22	B	810	CLA	CHD-C1D	4.23	1.46	1.38
22	B	808	CLA	CHC-C1C	4.23	1.47	1.38
22	A	808	CLA	O2A-CGA	4.23	1.45	1.33
22	B	815	CLA	CHD-C1D	4.23	1.46	1.38
22	4	611	CLA	O2A-CGA	4.23	1.45	1.33
22	9	603	CLA	CHC-C1C	4.23	1.47	1.38
22	4	610	CLA	O2A-CGA	4.23	1.45	1.33
22	2	603	CLA	CHC-C1C	4.23	1.47	1.38
22	2	609	CLA	O2A-CGA	4.23	1.45	1.33
22	4	601	CLA	CHD-C1D	4.22	1.46	1.38
22	A	820	CLA	C1B-NB	-4.22	1.32	1.37
22	5	606	CLA	CHD-C1D	4.22	1.46	1.38
22	B	827	CLA	O2A-CGA	4.22	1.45	1.33
22	A	815	CLA	O2A-CGA	4.22	1.45	1.33
29	3	608	CHL	CHC-C1C	4.22	1.47	1.38
22	4	616	CLA	CHC-C1C	4.22	1.47	1.38
22	Z	603	CLA	CHC-C1C	4.22	1.47	1.38
22	1	606	CLA	CHD-C1D	4.22	1.46	1.38
22	B	813	CLA	CHD-C1D	4.22	1.46	1.38
22	6	609	CLA	CHD-C1D	4.22	1.46	1.38
22	B	806	CLA	O2A-CGA	4.22	1.45	1.33
22	B	841	CLA	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	606	CHL	CHD-C1D	4.22	1.46	1.38
22	L	204	CLA	CHD-C1D	4.22	1.46	1.38
24	1	620	LHG	O8-C23	4.22	1.45	1.33
22	A	821	CLA	CHD-C1D	4.21	1.46	1.38
22	5	613	CLA	CHC-C1C	4.21	1.47	1.38
22	8	610	CLA	O2A-CGA	4.21	1.45	1.33
22	7	611	CLA	CHC-C1C	4.21	1.47	1.38
22	B	835	CLA	CHD-C1D	4.21	1.46	1.38
22	9	611	CLA	O2A-CGA	4.21	1.45	1.33
29	5	618	CHL	CHD-C1D	4.21	1.46	1.38
22	A	816	CLA	O2A-CGA	4.21	1.45	1.33
29	6	608	CHL	CHD-C1D	4.21	1.46	1.38
22	A	821	CLA	CHC-C1C	4.21	1.47	1.38
22	B	831	CLA	O2A-CGA	4.20	1.45	1.33
22	3	620	CLA	CHD-C1D	4.20	1.46	1.38
22	B	802	CLA	CHC-C1C	4.20	1.47	1.38
22	B	810	CLA	O2A-CGA	4.20	1.45	1.33
22	6	612	CLA	CHD-C1D	4.20	1.46	1.38
22	8	601	CLA	O2A-CGA	4.20	1.45	1.33
22	A	826	CLA	CHC-C1C	4.20	1.47	1.38
22	B	841	CLA	CHD-C4C	4.20	1.48	1.39
22	A	807	CLA	CHD-C1D	4.20	1.46	1.38
22	8	614	CLA	CHD-C1D	4.20	1.46	1.38
22	B	831	CLA	C1B-NB	-4.19	1.32	1.37
22	5	612	CLA	CHD-C1D	4.19	1.46	1.38
22	5	612	CLA	CHC-C1C	4.19	1.47	1.38
22	6	609	CLA	O2A-CGA	4.19	1.45	1.33
24	4	622	LHG	O8-C23	4.19	1.45	1.33
22	Z	609	CLA	CHC-C1C	4.19	1.47	1.38
22	B	821	CLA	CHD-C1D	4.19	1.46	1.38
22	7	612	CLA	CHD-C1D	4.19	1.46	1.38
22	8	614	CLA	O2A-CGA	4.19	1.45	1.33
22	4	612	CLA	CHD-C1D	4.19	1.46	1.38
22	8	603	CLA	CHC-C1C	4.19	1.47	1.38
22	7	601	CLA	O2A-CGA	4.19	1.45	1.33
22	B	837	CLA	CHD-C1D	4.19	1.46	1.38
22	7	608	CLA	CHD-C1D	4.18	1.46	1.38
22	Z	611	CLA	O2A-CGA	4.18	1.45	1.33
22	5	609	CLA	O2A-CGA	4.18	1.45	1.33
22	3	617	CLA	O2A-CGA	4.18	1.46	1.33
24	6	619	LHG	O7-C7	4.18	1.46	1.34
22	Z	604	CLA	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	815	CLA	CHD-C4C	4.18	1.48	1.39
22	A	836	CLA	CHC-C1C	4.18	1.47	1.38
22	F	301	CLA	O2A-CGA	4.18	1.45	1.33
22	B	803	CLA	C1B-NB	-4.18	1.32	1.37
29	6	607	CHL	CHD-C1D	4.18	1.46	1.38
22	1	602	CLA	O2A-CGA	4.18	1.45	1.33
22	A	802	CLA	CHD-C4C	4.18	1.48	1.39
29	4	608	CHL	O2A-CGA	4.18	1.45	1.33
29	4	607	CHL	CHD-C1D	4.18	1.46	1.38
29	5	608	CHL	O2A-CGA	4.18	1.45	1.33
22	6	601	CLA	O2A-CGA	4.17	1.45	1.33
22	A	836	CLA	CHD-C1D	4.17	1.46	1.38
22	A	814	CLA	O2A-CGA	4.17	1.45	1.33
22	A	820	CLA	O2A-CGA	4.17	1.45	1.33
22	A	838	CLA	CHC-C1C	4.17	1.47	1.38
22	A	824	CLA	CHD-C1D	4.17	1.46	1.38
24	5	623	LHG	O8-C23	4.17	1.45	1.33
22	7	604	CLA	O2A-CGA	4.17	1.45	1.33
22	B	807	CLA	CHC-C1C	4.17	1.47	1.38
22	Z	610	CLA	O2A-CGA	4.17	1.45	1.33
22	A	802	CLA	O2A-CGA	4.16	1.45	1.33
22	6	614	CLA	CHD-C4C	4.16	1.48	1.39
29	6	608	CHL	O2A-CGA	4.16	1.45	1.33
22	3	603	CLA	O2A-CGA	4.16	1.45	1.33
22	B	838	CLA	O2A-CGA	4.16	1.45	1.33
22	A	822	CLA	CHD-C1D	4.16	1.46	1.38
22	6	602	CLA	O2A-CGA	4.16	1.45	1.33
22	9	614	CLA	CHD-C4C	4.16	1.48	1.39
22	9	602	CLA	O2A-CGA	4.16	1.45	1.33
22	B	829	CLA	O2A-CGA	4.16	1.45	1.33
22	B	826	CLA	O2A-CGA	4.16	1.45	1.33
29	6	607	CHL	O2A-CGA	4.16	1.45	1.33
29	Z	607	CHL	CHD-C1D	4.16	1.46	1.38
22	B	809	CLA	CHD-C1D	4.16	1.46	1.38
22	1	608	CLA	CHD-C1D	4.16	1.46	1.38
22	4	609	CLA	CHD-C1D	4.16	1.46	1.38
22	5	616	CLA	CHC-C1C	4.16	1.47	1.38
22	B	834	CLA	O2A-CGA	4.15	1.45	1.33
22	4	602	CLA	O2A-CGA	4.15	1.45	1.33
22	8	616	CLA	CHD-C1D	4.15	1.46	1.38
22	9	609	CLA	O2A-CGA	4.15	1.45	1.33
22	B	822	CLA	CHD-C1D	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	614	CLA	CHD-C1D	4.15	1.46	1.38
22	7	613	CLA	CHC-C1C	4.15	1.46	1.38
22	7	613	CLA	CHD-C1D	4.15	1.46	1.38
22	7	609	CLA	O2A-CGA	4.15	1.45	1.33
22	B	818	CLA	O2A-CGA	4.15	1.45	1.33
22	A	806	CLA	CHD-C1D	4.15	1.46	1.38
22	A	805	CLA	O2A-CGA	4.15	1.45	1.33
22	8	612	CLA	C1B-NB	-4.15	1.32	1.37
22	B	806	CLA	CHD-C1D	4.14	1.46	1.38
29	3	608	CHL	O2A-CGA	4.14	1.45	1.33
22	B	812	CLA	CHD-C1D	4.14	1.46	1.38
22	A	813	CLA	CHD-C1D	4.14	1.46	1.38
22	3	610	CLA	O2A-CGA	4.14	1.45	1.33
22	A	832	CLA	CHD-C1D	4.14	1.46	1.38
22	A	820	CLA	CHD-C1D	4.14	1.46	1.38
22	A	834	CLA	CHD-C1D	4.14	1.46	1.38
29	4	618	CHL	CHD-C1D	4.14	1.46	1.38
22	B	805	CLA	O2A-CGA	4.14	1.45	1.33
22	B	802	CLA	O2A-CGA	4.14	1.45	1.33
22	A	842	CLA	O2A-CGA	4.14	1.45	1.33
22	8	613	CLA	CHD-C1D	4.14	1.46	1.38
22	B	805	CLA	C1B-NB	-4.14	1.32	1.37
22	B	808	CLA	CHD-C1D	4.14	1.46	1.38
22	7	604	CLA	CHD-C1D	4.14	1.46	1.38
22	A	833	CLA	C1B-NB	-4.13	1.32	1.37
22	9	604	CLA	CHD-C4C	4.13	1.48	1.39
22	B	809	CLA	O2A-CGA	4.13	1.45	1.33
22	8	601	CLA	CHD-C1D	4.13	1.46	1.38
22	A	817	CLA	CHD-C4C	4.13	1.48	1.39
22	4	609	CLA	CHC-C1C	4.13	1.46	1.38
24	Z	620	LHG	O7-C7	4.13	1.46	1.34
22	A	829	CLA	O2A-CGA	4.13	1.45	1.33
22	Z	602	CLA	O2A-CGA	4.13	1.45	1.33
22	4	601	CLA	O2A-CGA	4.13	1.45	1.33
22	A	822	CLA	C1B-NB	-4.13	1.32	1.37
22	A	821	CLA	C1B-NB	-4.13	1.32	1.37
22	3	603	CLA	CHC-C1C	4.13	1.46	1.38
22	3	604	CLA	O2A-CGA	4.13	1.45	1.33
29	5	607	CHL	CHD-C1D	4.13	1.46	1.38
22	A	835	CLA	CHD-C4C	4.13	1.48	1.39
22	8	612	CLA	CHD-C1D	4.13	1.46	1.38
22	7	610	CLA	O2A-CGA	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	833	CLA	O2A-CGA	4.12	1.45	1.33
22	B	824	CLA	CHD-C1D	4.12	1.46	1.38
22	5	602	CLA	CHD-C1D	4.12	1.46	1.38
22	7	606	CLA	C1B-NB	-4.12	1.32	1.37
24	A	847	LHG	O7-C7	4.12	1.45	1.34
22	5	610	CLA	CHD-C1D	4.12	1.46	1.38
22	7	616	CLA	C3D-C2D	4.12	1.50	1.39
22	8	610	CLA	CHD-C1D	4.12	1.46	1.38
22	G	203	CLA	CHD-C1D	4.12	1.46	1.38
24	A	847	LHG	O8-C23	4.12	1.45	1.33
22	A	831	CLA	O2A-CGA	4.12	1.45	1.33
22	B	820	CLA	CHD-C4C	4.12	1.48	1.39
22	A	817	CLA	CHC-C1C	4.12	1.46	1.38
29	4	608	CHL	CHD-C1D	4.11	1.46	1.38
22	A	826	CLA	O2A-CGA	4.11	1.45	1.33
22	1	603	CLA	CHC-C1C	4.11	1.46	1.38
29	8	607	CHL	O2A-CGA	4.11	1.45	1.33
22	7	616	CLA	CHD-C4C	4.11	1.48	1.39
22	A	839	CLA	O2A-CGA	4.11	1.45	1.33
22	9	612	CLA	CHD-C4C	4.11	1.48	1.39
22	F	301	CLA	CHD-C1D	4.10	1.46	1.38
22	A	841	CLA	O2A-CGA	4.10	1.45	1.33
22	B	825	CLA	O2A-CGA	4.10	1.45	1.33
22	B	830	CLA	CHD-C1D	4.10	1.46	1.38
22	B	808	CLA	O2A-CGA	4.10	1.45	1.33
22	A	811	CLA	O2A-CGA	4.10	1.45	1.33
24	Z	620	LHG	O8-C23	4.10	1.45	1.33
22	A	831	CLA	CHC-C1C	4.10	1.46	1.38
22	A	819	CLA	O2A-CGA	4.10	1.45	1.33
24	1	620	LHG	O7-C7	4.10	1.45	1.34
22	B	832	CLA	O2A-CGA	4.10	1.45	1.33
24	A	855	LHG	O7-C7	4.10	1.45	1.34
22	4	610	CLA	CHD-C1D	4.10	1.46	1.38
22	6	617	CLA	O2A-CGA	4.10	1.46	1.33
22	B	818	CLA	C1B-NB	-4.09	1.32	1.37
22	A	825	CLA	CHC-C1C	4.09	1.46	1.38
22	1	613	CLA	CHD-C1D	4.09	1.46	1.38
22	B	823	CLA	O2A-CGA	4.09	1.45	1.33
22	5	604	CLA	CHD-C4C	4.09	1.48	1.39
22	7	610	CLA	CHC-C4B	4.09	1.48	1.39
22	A	843	CLA	O2A-CGA	4.09	1.45	1.33
24	4	623	LHG	O8-C23	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	842	CLA	CHD-C1D	4.09	1.46	1.38
22	1	604	CLA	CHD-C4C	4.09	1.48	1.39
22	4	604	CLA	CHD-C4C	4.09	1.48	1.39
22	2	606	CLA	CHD-C4C	4.09	1.48	1.39
22	6	603	CLA	O2A-CGA	4.09	1.46	1.33
22	A	830	CLA	C1B-NB	-4.08	1.32	1.37
22	B	819	CLA	CHD-C4C	4.08	1.48	1.39
22	A	813	CLA	C1B-NB	-4.08	1.32	1.37
22	A	833	CLA	CHD-C4C	4.08	1.48	1.39
22	A	837	CLA	CHD-C4C	4.08	1.48	1.39
22	3	614	CLA	CHD-C4C	4.08	1.48	1.39
24	B	851	LHG	O7-C7	4.08	1.45	1.34
22	B	828	CLA	CHD-C1D	4.08	1.46	1.38
22	A	814	CLA	CHD-C1D	4.08	1.46	1.38
22	A	828	CLA	O2A-CGA	4.08	1.45	1.33
22	5	614	CLA	CHD-C4C	4.08	1.48	1.39
22	B	803	CLA	C1D-ND	4.08	1.42	1.37
22	9	601	CLA	O2A-CGA	4.08	1.46	1.33
22	6	601	CLA	CHD-C4C	4.08	1.48	1.39
22	3	603	CLA	CHD-C1D	4.07	1.46	1.38
22	7	604	CLA	CHC-C1C	4.07	1.46	1.38
22	Z	612	CLA	CHD-C1D	4.07	1.46	1.38
22	G	204	CLA	O2A-CGA	4.07	1.46	1.33
22	A	854	CLA	CHD-C1D	4.07	1.46	1.38
22	A	819	CLA	CHD-C1D	4.06	1.46	1.38
22	B	834	CLA	CHD-C4C	4.06	1.48	1.39
22	B	829	CLA	CHD-C1D	4.06	1.46	1.38
22	2	603	CLA	CHD-C4C	4.06	1.48	1.39
22	4	603	CLA	CHC-C1C	4.06	1.46	1.38
22	4	610	CLA	C1B-NB	-4.06	1.32	1.37
22	B	809	CLA	CHC-C1C	4.06	1.46	1.38
22	2	609	CLA	CHD-C4C	4.06	1.48	1.39
22	7	610	CLA	CHD-C1D	4.06	1.46	1.38
24	A	846	LHG	O7-C7	4.06	1.45	1.34
22	A	803	CLA	CHD-C1D	4.06	1.46	1.38
22	4	602	CLA	CHD-C4C	4.05	1.48	1.39
22	A	827	CLA	CHD-C1D	4.05	1.46	1.38
22	3	611	CLA	CHD-C4C	4.05	1.48	1.39
22	7	616	CLA	O2A-CGA	4.05	1.45	1.33
22	2	610	CLA	CHD-C4C	4.05	1.48	1.39
21	A	801	CL0	O2A-CGA	4.05	1.45	1.33
22	B	808	CLA	C1B-NB	-4.05	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	814	CLA	CHD-C4C	4.05	1.48	1.39
22	2	602	CLA	CHD-C4C	4.05	1.48	1.39
22	A	806	CLA	O2A-CGA	4.05	1.45	1.33
24	4	623	LHG	O7-C7	4.05	1.45	1.34
22	A	854	CLA	C1B-NB	-4.05	1.32	1.37
22	A	854	CLA	C3D-C2D	4.05	1.50	1.39
22	A	805	CLA	CHD-C4C	4.05	1.48	1.39
22	5	617	CLA	O2A-CGA	4.05	1.45	1.33
22	B	828	CLA	CHC-C1C	4.04	1.46	1.38
22	6	602	CLA	CHD-C1D	4.04	1.46	1.38
24	5	623	LHG	O7-C7	4.04	1.45	1.34
22	4	601	CLA	CHD-C4C	4.04	1.48	1.39
22	Z	616	CLA	O2A-CGA	4.04	1.45	1.33
22	Z	603	CLA	CHD-C4C	4.04	1.48	1.39
22	7	609	CLA	CHD-C1D	4.04	1.46	1.38
27	B	850	DGD	O1G-C1A	4.04	1.45	1.33
22	7	603	CLA	O2A-CGA	4.04	1.45	1.33
22	2	613	CLA	CHD-C4C	4.04	1.48	1.39
22	5	616	CLA	O2A-CGA	4.04	1.45	1.33
22	B	810	CLA	CHD-C4C	4.04	1.48	1.39
22	2	601	CLA	O2A-CGA	4.04	1.45	1.33
22	B	818	CLA	CHC-C1C	4.04	1.46	1.38
22	6	616	CLA	CHD-C4C	4.03	1.48	1.39
22	B	817	CLA	C4B-NB	-4.03	1.32	1.37
22	B	803	CLA	O2A-CGA	4.03	1.45	1.33
22	3	613	CLA	CHD-C1D	4.03	1.46	1.38
22	K	4002	CLA	CHD-C4C	4.03	1.48	1.39
22	7	602	CLA	CHD-C1D	4.03	1.46	1.38
29	1	601	CHL	CHD-C1D	4.03	1.46	1.38
22	2	611	CLA	CHD-C4C	4.03	1.48	1.39
22	K	4003	CLA	O2A-CGA	4.03	1.45	1.33
22	2	614	CLA	CHD-C4C	4.02	1.48	1.39
22	A	834	CLA	O2A-CGA	4.02	1.45	1.33
22	8	611	CLA	O2A-CGA	4.02	1.45	1.33
22	Z	609	CLA	CHD-C4C	4.02	1.48	1.39
22	B	827	CLA	C1B-NB	-4.02	1.32	1.37
22	5	603	CLA	CHD-C1D	4.02	1.46	1.38
22	6	622	CLA	CHD-C4C	4.02	1.48	1.39
22	B	821	CLA	O2A-CGA	4.02	1.45	1.33
29	1	607	CHL	OBD-CAD	4.02	1.29	1.22
22	2	601	CLA	CHD-C4C	4.02	1.48	1.39
22	G	204	CLA	CHD-C4C	4.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	204	CLA	CHD-C4C	4.02	1.48	1.39
22	1	609	CLA	CHD-C4C	4.02	1.48	1.39
22	A	804	CLA	CHD-C1D	4.02	1.46	1.38
22	8	616	CLA	O2A-CGA	4.01	1.45	1.33
22	Z	614	CLA	CHD-C4C	4.01	1.48	1.39
22	B	813	CLA	C1B-NB	-4.01	1.32	1.37
22	B	838	CLA	CHC-C4B	4.01	1.48	1.39
22	5	621	CLA	O2A-CGA	4.01	1.45	1.33
29	6	618	CHL	CHD-C1D	4.01	1.46	1.38
22	3	606	CLA	CHD-C4C	4.01	1.48	1.39
22	A	831	CLA	CHD-C1D	4.01	1.46	1.38
22	Z	606	CLA	CHD-C4C	4.01	1.48	1.39
22	B	839	CLA	CHD-C4C	4.01	1.48	1.39
22	Z	616	CLA	CHD-C4C	4.01	1.48	1.39
22	6	616	CLA	C1B-NB	-4.01	1.32	1.37
22	9	601	CLA	CHD-C4C	4.01	1.48	1.39
22	5	603	CLA	O2A-CGA	4.00	1.45	1.33
22	7	606	CLA	CHD-C1D	4.00	1.46	1.38
22	9	613	CLA	CHD-C4C	4.00	1.48	1.39
22	9	610	CLA	CHD-C4C	4.00	1.48	1.39
22	Z	602	CLA	CHD-C1D	4.00	1.46	1.38
22	3	612	CLA	CHC-C1C	4.00	1.46	1.38
22	B	832	CLA	CHD-C1D	4.00	1.46	1.38
22	A	823	CLA	CHD-C1D	4.00	1.46	1.38
22	8	604	CLA	O2A-CGA	3.99	1.45	1.33
22	5	606	CLA	CHD-C4C	3.99	1.48	1.39
22	1	614	CLA	CHD-C4C	3.99	1.48	1.39
22	A	809	CLA	CHD-C1D	3.99	1.46	1.38
22	Z	608	CLA	CHD-C4C	3.99	1.48	1.39
22	6	610	CLA	CHD-C4C	3.99	1.48	1.39
29	Z	601	CHL	CHD-C1D	3.99	1.46	1.38
22	6	616	CLA	O2A-CGA	3.99	1.45	1.33
22	6	617	CLA	CHD-C4C	3.99	1.48	1.39
22	2	603	CLA	O2A-CGA	3.99	1.45	1.33
22	7	602	CLA	CHC-C4B	3.98	1.48	1.39
22	8	609	CLA	O2A-CGA	3.98	1.45	1.33
22	5	610	CLA	CHD-C4C	3.98	1.48	1.39
22	1	616	CLA	O2A-CGA	3.98	1.45	1.33
22	9	603	CLA	O2A-CGA	3.98	1.45	1.33
22	8	606	CLA	CHD-C4C	3.98	1.48	1.39
24	7	625	LHG	O8-C23	3.98	1.45	1.33
22	7	620	CLA	CHD-C4C	3.98	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	616	CLA	CHD-C4C	3.98	1.48	1.39
22	2	607	CLA	CHD-C4C	3.98	1.48	1.39
22	3	620	CLA	CHD-C4C	3.97	1.48	1.39
21	A	801	CL0	C1B-NB	-3.97	1.32	1.37
22	3	604	CLA	C1B-NB	-3.97	1.32	1.37
22	1	602	CLA	CHD-C1D	3.97	1.46	1.38
24	A	846	LHG	O8-C23	3.97	1.44	1.33
22	A	802	CLA	C3D-C2D	3.97	1.50	1.39
22	B	836	CLA	C1B-NB	-3.97	1.32	1.37
22	2	612	CLA	CHD-C4C	3.97	1.48	1.39
22	4	603	CLA	CHD-C4C	3.97	1.48	1.39
22	Z	604	CLA	CHD-C4C	3.97	1.48	1.39
29	8	607	CHL	CHD-C1D	3.96	1.46	1.38
22	A	811	CLA	CHD-C1D	3.96	1.46	1.38
22	J	3002	CLA	CHD-C4C	3.96	1.48	1.39
22	6	604	CLA	CHD-C4C	3.96	1.48	1.39
22	7	609	CLA	CHD-C4C	3.96	1.48	1.39
29	1	607	CHL	CHD-C1D	3.96	1.46	1.38
22	B	837	CLA	O2A-CGA	3.96	1.44	1.33
22	B	825	CLA	C1B-NB	-3.96	1.32	1.37
29	Z	601	CHL	C1D-ND	-3.96	1.32	1.37
22	A	838	CLA	CHD-C4C	3.96	1.48	1.39
22	7	614	CLA	CHD-C4C	3.95	1.48	1.39
22	3	612	CLA	O2A-CGA	3.95	1.45	1.33
22	A	812	CLA	CHD-C1D	3.95	1.46	1.38
22	B	827	CLA	CHD-C1D	3.95	1.46	1.38
22	B	813	CLA	O2A-CGA	3.95	1.44	1.33
22	B	805	CLA	CHC-C4B	3.95	1.48	1.39
22	B	819	CLA	C1B-NB	-3.95	1.32	1.37
22	6	611	CLA	CHD-C4C	3.95	1.48	1.39
22	1	610	CLA	CHC-C4B	3.95	1.48	1.39
22	B	852	CLA	C3D-C2D	3.95	1.49	1.39
22	1	611	CLA	CHD-C4C	3.95	1.48	1.39
22	9	603	CLA	CHD-C4C	3.95	1.48	1.39
22	6	613	CLA	CHD-C4C	3.95	1.48	1.39
22	A	804	CLA	O2A-CGA	3.95	1.44	1.33
22	A	812	CLA	O2A-CGA	3.95	1.44	1.33
22	A	841	CLA	CHD-C1D	3.95	1.46	1.38
22	A	825	CLA	CHD-C4C	3.94	1.48	1.39
22	5	611	CLA	CHD-C4C	3.94	1.48	1.39
22	A	809	CLA	O2A-CGA	3.94	1.44	1.33
22	A	803	CLA	O2A-CGA	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	607	CHL	OBD-CAD	3.94	1.29	1.22
22	5	609	CLA	CHD-C4C	3.94	1.48	1.39
22	9	602	CLA	CHD-C4C	3.94	1.48	1.39
22	B	826	CLA	CHD-C1D	3.94	1.46	1.38
22	8	604	CLA	CHD-C4C	3.94	1.48	1.39
21	A	801	CL0	CHD-C1D	3.94	1.46	1.38
22	B	832	CLA	C1B-NB	-3.94	1.32	1.37
22	B	835	CLA	C1B-NB	-3.94	1.32	1.37
22	1	603	CLA	CHD-C4C	3.94	1.48	1.39
22	B	841	CLA	C3D-C2D	3.94	1.49	1.39
22	3	610	CLA	CHC-C4B	3.94	1.48	1.39
22	9	611	CLA	CHD-C4C	3.94	1.48	1.39
22	B	804	CLA	C1B-NB	-3.94	1.32	1.37
22	1	602	CLA	CHC-C4B	3.94	1.48	1.39
21	A	801	CL0	CHC-C1C	3.93	1.46	1.38
22	3	612	CLA	C1B-NB	-3.93	1.32	1.37
22	B	831	CLA	CHC-C4B	3.93	1.48	1.39
22	B	824	CLA	C1B-NB	-3.93	1.32	1.37
22	7	612	CLA	C1B-NB	-3.93	1.33	1.37
22	G	204	CLA	OBD-CAD	3.93	1.29	1.22
22	F	301	CLA	CHD-C4C	3.93	1.48	1.39
22	A	841	CLA	C1B-NB	-3.93	1.33	1.37
22	K	4003	CLA	CHD-C4C	3.93	1.48	1.39
22	8	609	CLA	CHD-C4C	3.92	1.48	1.39
22	5	601	CLA	CHD-C4C	3.92	1.48	1.39
22	6	602	CLA	CHC-C4B	3.92	1.48	1.39
22	3	610	CLA	CHD-C1D	3.92	1.46	1.38
22	4	610	CLA	CHD-C4C	3.92	1.48	1.39
22	8	611	CLA	CHD-C4C	3.92	1.48	1.39
22	B	802	CLA	C1B-NB	-3.92	1.33	1.37
22	B	817	CLA	CHC-C1C	3.92	1.46	1.38
22	6	622	CLA	CHD-C1D	3.92	1.46	1.38
22	3	602	CLA	CHD-C4C	3.92	1.48	1.39
22	G	203	CLA	CHD-C4C	3.92	1.48	1.39
22	8	601	CLA	CHD-C4C	3.92	1.48	1.39
22	B	823	CLA	C3D-C2D	3.92	1.49	1.39
22	7	603	CLA	CHD-C4C	3.92	1.48	1.39
22	Z	610	CLA	CHC-C4B	3.91	1.48	1.39
22	4	611	CLA	CHD-C4C	3.91	1.48	1.39
22	Z	611	CLA	CHD-C4C	3.91	1.48	1.39
22	A	822	CLA	CHD-C4C	3.91	1.48	1.39
22	3	607	CLA	CHD-C4C	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	603	CLA	CHD-C4C	3.91	1.48	1.39
22	B	836	CLA	CHD-C4C	3.91	1.48	1.39
22	A	830	CLA	O2A-CGA	3.91	1.44	1.33
22	3	604	CLA	CHD-C4C	3.91	1.48	1.39
22	A	827	CLA	O2A-CGA	3.91	1.44	1.33
22	A	826	CLA	CHD-C4C	3.91	1.48	1.39
22	5	617	CLA	CHD-C4C	3.91	1.48	1.39
22	4	603	CLA	O2A-CGA	3.91	1.45	1.33
22	F	303	CLA	CHD-C1D	3.90	1.46	1.38
22	A	840	CLA	C1B-NB	-3.90	1.33	1.37
22	A	816	CLA	CHD-C4C	3.90	1.48	1.39
22	B	823	CLA	CHD-C4C	3.90	1.48	1.39
22	B	838	CLA	CHD-C4C	3.90	1.48	1.39
22	4	613	CLA	CHD-C4C	3.90	1.48	1.39
22	8	614	CLA	C3D-C2D	3.90	1.49	1.39
22	A	839	CLA	CHD-C4C	3.90	1.48	1.39
22	A	841	CLA	CHC-C4B	3.89	1.48	1.39
22	B	807	CLA	CHD-C4C	3.89	1.48	1.39
22	B	818	CLA	CHD-C4C	3.89	1.48	1.39
22	A	806	CLA	CHD-C4C	3.89	1.48	1.39
22	B	833	CLA	CHD-C4C	3.89	1.48	1.39
22	3	610	CLA	CHD-C4C	3.89	1.48	1.39
22	5	603	CLA	C1B-NB	-3.89	1.33	1.37
22	9	609	CLA	CHD-C4C	3.89	1.48	1.39
24	8	620	LHG	O7-C7	3.88	1.45	1.34
22	A	835	CLA	C3D-C2D	3.88	1.49	1.39
22	6	609	CLA	CHD-C4C	3.88	1.48	1.39
22	3	603	CLA	C1B-NB	-3.88	1.33	1.37
22	3	617	CLA	CHD-C4C	3.88	1.48	1.39
24	8	620	LHG	O8-C23	3.88	1.44	1.33
22	A	813	CLA	CHD-C4C	3.88	1.48	1.39
22	1	612	CLA	C1B-NB	-3.88	1.33	1.37
22	5	621	CLA	C1B-NB	-3.88	1.33	1.37
29	3	608	CHL	CHD-C1D	3.88	1.45	1.38
29	1	601	CHL	C1B-NB	-3.88	1.33	1.37
22	1	608	CLA	CHD-C4C	3.88	1.48	1.39
22	5	602	CLA	CHC-C4B	3.88	1.48	1.39
22	3	607	CLA	C3D-C2D	3.88	1.49	1.39
22	B	817	CLA	CHD-C4C	3.88	1.48	1.39
22	A	810	CLA	CHD-C1D	3.87	1.45	1.38
22	7	611	CLA	C1B-NB	-3.87	1.33	1.37
22	B	820	CLA	C3D-C2D	3.87	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	809	CLA	CHD-C4C	3.87	1.48	1.39
22	B	852	CLA	CHD-C4C	3.87	1.48	1.39
27	B	850	DGD	O2G-C1B	3.87	1.45	1.34
22	7	601	CLA	CHD-C1D	3.87	1.45	1.38
22	3	609	CLA	CHD-C4C	3.87	1.48	1.39
22	A	815	CLA	C3D-C2D	3.87	1.49	1.39
22	7	611	CLA	CHD-C4C	3.87	1.48	1.39
22	B	811	CLA	CHD-C4C	3.87	1.48	1.39
22	B	840	CLA	CHD-C4C	3.87	1.48	1.39
22	B	840	CLA	C1B-NB	-3.87	1.33	1.37
22	2	612	CLA	C3D-C2D	3.86	1.49	1.39
22	B	840	CLA	CHC-C1C	3.86	1.46	1.38
22	5	602	CLA	CHD-C4C	3.86	1.48	1.39
22	B	812	CLA	CHD-C4C	3.86	1.48	1.39
22	5	603	CLA	CHD-C4C	3.86	1.48	1.39
22	5	616	CLA	CHD-C4C	3.86	1.48	1.39
22	B	804	CLA	CHD-C1D	3.86	1.45	1.38
22	Z	612	CLA	CHD-C4C	3.86	1.48	1.39
22	1	602	CLA	CHD-C4C	3.86	1.48	1.39
22	1	606	CLA	CHC-C4B	3.86	1.48	1.39
22	A	807	CLA	CHD-C4C	3.86	1.48	1.39
22	A	841	CLA	C3D-C2D	3.85	1.49	1.39
22	A	843	CLA	C3D-C2D	3.85	1.49	1.39
22	2	611	CLA	C3D-C2D	3.85	1.49	1.39
22	Z	610	CLA	CHD-C1D	3.85	1.45	1.38
22	A	854	CLA	CHC-C4B	3.85	1.48	1.39
22	A	823	CLA	CHD-C4C	3.85	1.48	1.39
22	8	603	CLA	CHD-C4C	3.85	1.48	1.39
22	B	839	CLA	C1B-NB	-3.85	1.33	1.37
22	F	301	CLA	CHC-C4B	3.84	1.48	1.39
22	4	609	CLA	CHD-C4C	3.84	1.48	1.39
29	5	618	CHL	CHD-C4C	3.84	1.48	1.39
22	1	606	CLA	C1B-NB	-3.84	1.33	1.37
22	2	610	CLA	C3D-C2D	3.84	1.49	1.39
22	3	612	CLA	CHD-C4C	3.84	1.48	1.39
22	8	614	CLA	CHD-C4C	3.84	1.48	1.39
22	1	616	CLA	CHD-C4C	3.83	1.48	1.39
22	B	803	CLA	C3D-C2D	3.83	1.49	1.39
22	8	609	CLA	C1B-NB	-3.83	1.33	1.37
22	7	602	CLA	CHD-C4C	3.83	1.48	1.39
22	A	808	CLA	C1B-NB	-3.83	1.33	1.37
22	6	611	CLA	C3D-C2D	3.83	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	304	CLA	CHD-C4C	3.83	1.48	1.39
22	B	821	CLA	CHD-C4C	3.83	1.48	1.39
22	4	614	CLA	CHD-C4C	3.82	1.48	1.39
22	A	820	CLA	CHD-C4C	3.82	1.48	1.39
22	B	837	CLA	CHD-C4C	3.82	1.48	1.39
22	8	608	CLA	CHD-C1D	3.82	1.45	1.38
22	6	612	CLA	CHD-C4C	3.82	1.48	1.39
22	4	609	CLA	C3D-C2D	3.82	1.49	1.39
22	1	610	CLA	CHD-C1D	3.82	1.45	1.38
22	A	829	CLA	CHD-C1D	3.82	1.45	1.38
22	A	827	CLA	CHD-C4C	3.82	1.47	1.39
22	7	601	CLA	C1B-NB	-3.82	1.33	1.37
22	B	809	CLA	C3D-C2D	3.82	1.49	1.39
22	2	613	CLA	C3D-C2D	3.82	1.49	1.39
22	8	609	CLA	C3D-C2D	3.82	1.49	1.39
22	8	613	CLA	CHD-C4C	3.82	1.47	1.39
22	Z	602	CLA	CHC-C4B	3.82	1.48	1.39
22	7	608	CLA	C1B-NB	-3.82	1.33	1.37
22	A	840	CLA	CHD-C1D	3.82	1.45	1.38
22	1	606	CLA	CHD-C4C	3.82	1.47	1.39
22	7	613	CLA	C1B-NB	-3.82	1.33	1.37
22	2	607	CLA	C3D-C2D	3.82	1.49	1.39
22	A	804	CLA	C1B-NB	-3.81	1.33	1.37
22	5	613	CLA	CHD-C4C	3.81	1.47	1.39
22	A	805	CLA	C3D-C2D	3.81	1.49	1.39
22	2	609	CLA	C3D-C2D	3.81	1.49	1.39
22	7	608	CLA	CHC-C4B	3.81	1.47	1.39
22	6	604	CLA	C1B-NB	-3.81	1.33	1.37
22	B	812	CLA	CHC-C4B	3.81	1.47	1.39
22	A	836	CLA	C1B-NB	-3.81	1.33	1.37
22	8	601	CLA	C1B-NB	-3.81	1.33	1.37
22	5	613	CLA	C1B-NB	-3.81	1.33	1.37
24	7	625	LHG	O7-C7	3.80	1.45	1.34
22	5	601	CLA	C3D-C2D	3.80	1.49	1.39
22	5	609	CLA	C3D-C2D	3.80	1.49	1.39
22	9	604	CLA	C3D-C2D	3.80	1.49	1.39
22	9	614	CLA	C3D-C2D	3.80	1.49	1.39
22	A	836	CLA	C3D-C2D	3.80	1.49	1.39
22	A	836	CLA	CHD-C4C	3.80	1.47	1.39
22	B	822	CLA	CHD-C4C	3.80	1.47	1.39
22	A	840	CLA	CHD-C4C	3.80	1.47	1.39
22	A	834	CLA	CHD-C4C	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	832	CLA	CHD-C4C	3.80	1.47	1.39
22	Z	604	CLA	C1B-NB	-3.80	1.33	1.37
22	4	611	CLA	C3D-C2D	3.80	1.49	1.39
22	6	602	CLA	CHD-C4C	3.80	1.47	1.39
22	B	832	CLA	CHD-C4C	3.80	1.47	1.39
22	1	610	CLA	CHD-C4C	3.79	1.47	1.39
22	5	604	CLA	C3D-C2D	3.79	1.49	1.39
22	B	835	CLA	CHD-C4C	3.79	1.47	1.39
22	2	606	CLA	C3D-C2D	3.79	1.49	1.39
22	8	610	CLA	CHD-C4C	3.79	1.47	1.39
22	B	831	CLA	CHD-C1D	3.79	1.45	1.38
22	A	816	CLA	C3D-C2D	3.79	1.49	1.39
22	B	830	CLA	CHD-C4C	3.79	1.47	1.39
22	7	601	CLA	CHD-C4C	3.79	1.47	1.39
22	1	614	CLA	C3D-C2D	3.79	1.49	1.39
22	4	612	CLA	C1B-NB	-3.79	1.33	1.37
22	B	806	CLA	CHD-C4C	3.79	1.47	1.39
22	7	612	CLA	CHD-C4C	3.79	1.47	1.39
22	A	810	CLA	C1B-NB	-3.79	1.33	1.37
22	9	612	CLA	C3D-C2D	3.79	1.49	1.39
29	7	607	CHL	C1B-NB	-3.79	1.33	1.37
22	L	203	CLA	CHD-C4C	3.78	1.47	1.39
22	A	803	CLA	C4B-NB	-3.78	1.33	1.37
22	L	203	CLA	C3D-C2D	3.78	1.49	1.39
22	2	614	CLA	C3D-C2D	3.78	1.49	1.39
22	A	814	CLA	CHD-C4C	3.78	1.47	1.39
22	A	807	CLA	C1B-NB	-3.78	1.33	1.37
22	F	303	CLA	C1B-NB	-3.78	1.33	1.37
22	A	819	CLA	CHD-C4C	3.78	1.47	1.39
22	A	816	CLA	CHC-C4B	3.78	1.47	1.39
22	9	609	CLA	C3D-C2D	3.78	1.49	1.39
22	A	803	CLA	CHD-C4C	3.78	1.47	1.39
22	A	821	CLA	CHD-C4C	3.78	1.47	1.39
29	8	607	CHL	C1B-NB	-3.78	1.33	1.37
22	B	816	CLA	CHD-C1D	3.78	1.45	1.38
22	5	621	CLA	CHD-C4C	3.78	1.47	1.39
22	A	825	CLA	C3D-C2D	3.78	1.49	1.39
22	4	610	CLA	C3D-C2D	3.78	1.49	1.39
22	B	829	CLA	CHD-C4C	3.78	1.47	1.39
22	5	614	CLA	C3D-C2D	3.78	1.49	1.39
22	B	807	CLA	C3D-C2D	3.77	1.49	1.39
22	8	613	CLA	C3D-C2D	3.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	818	CLA	CHD-C1D	3.77	1.45	1.38
22	B	811	CLA	C1B-NB	-3.77	1.33	1.37
22	9	601	CLA	C3D-C2D	3.77	1.49	1.39
22	8	606	CLA	C1B-NB	-3.77	1.33	1.37
22	A	804	CLA	CHD-C4C	3.77	1.47	1.39
22	9	610	CLA	C3D-C2D	3.77	1.49	1.39
22	A	827	CLA	C1B-NB	-3.77	1.33	1.37
22	B	838	CLA	CHD-C1D	3.77	1.45	1.38
22	1	611	CLA	C3D-C2D	3.77	1.49	1.39
22	A	842	CLA	CHD-C4C	3.77	1.47	1.39
22	7	610	CLA	C3B-C4B	3.76	1.51	1.42
22	9	604	CLA	OBD-CAD	3.76	1.29	1.22
22	B	815	CLA	CHD-C4C	3.76	1.47	1.39
22	A	845	CLA	C1B-NB	-3.76	1.33	1.37
22	4	609	CLA	C1B-NB	-3.76	1.33	1.37
22	6	610	CLA	C3D-C2D	3.76	1.49	1.39
22	8	606	CLA	C3D-C2D	3.76	1.49	1.39
29	1	607	CHL	C1B-NB	-3.76	1.33	1.37
22	4	604	CLA	C3D-C2D	3.76	1.49	1.39
29	4	606	CHL	C1B-NB	-3.76	1.33	1.37
22	3	611	CLA	C3D-C2D	3.76	1.49	1.39
22	Z	602	CLA	CHD-C4C	3.76	1.47	1.39
22	7	614	CLA	C1B-NB	-3.76	1.33	1.37
29	9	607	CHL	CHD-C4C	3.76	1.47	1.39
22	A	829	CLA	C4B-NB	-3.76	1.33	1.37
22	A	845	CLA	CHD-C4C	3.76	1.47	1.39
22	2	610	CLA	CHC-C4B	3.76	1.47	1.39
22	A	814	CLA	C1B-NB	-3.76	1.33	1.37
22	B	806	CLA	C1B-NB	-3.76	1.33	1.37
22	2	602	CLA	C3D-C2D	3.76	1.49	1.39
22	6	601	CLA	OBD-CAD	3.76	1.29	1.22
22	A	839	CLA	C1B-NB	-3.76	1.33	1.37
22	5	601	CLA	C1B-NB	-3.75	1.33	1.37
22	L	204	CLA	OBD-CAD	3.75	1.28	1.22
22	Z	609	CLA	C3D-C2D	3.75	1.49	1.39
22	A	843	CLA	CHD-C4C	3.75	1.47	1.39
22	1	602	CLA	C3D-C2D	3.75	1.49	1.39
22	A	809	CLA	C1B-NB	-3.75	1.33	1.37
29	6	606	CHL	CHD-C4C	3.75	1.47	1.39
22	1	613	CLA	CHD-C4C	3.75	1.47	1.39
22	A	812	CLA	CHD-C4C	3.75	1.47	1.39
22	8	608	CLA	CHD-C4C	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	604	CLA	C1B-NB	-3.75	1.33	1.37
22	7	604	CLA	CHB-C1B	3.75	1.47	1.39
22	B	809	CLA	CHD-C4C	3.75	1.47	1.39
22	B	821	CLA	C3D-C2D	3.75	1.49	1.39
29	6	608	CHL	C1D-ND	-3.75	1.33	1.37
22	7	610	CLA	CHD-C4C	3.75	1.47	1.39
22	4	612	CLA	C3D-C2D	3.75	1.49	1.39
29	4	618	CHL	CHD-C4C	3.75	1.47	1.39
22	A	826	CLA	C1B-NB	-3.75	1.33	1.37
22	2	601	CLA	C3D-C2D	3.75	1.49	1.39
22	B	827	CLA	CHD-C4C	3.75	1.47	1.39
22	Z	614	CLA	C3D-C2D	3.75	1.49	1.39
22	B	835	CLA	C3D-C2D	3.74	1.49	1.39
22	3	603	CLA	CHD-C4C	3.74	1.47	1.39
22	B	813	CLA	CHD-C4C	3.74	1.47	1.39
29	6	606	CHL	CHC-C4B	3.74	1.47	1.39
22	A	815	CLA	CHC-C4B	3.74	1.47	1.39
22	A	827	CLA	CHC-C4B	3.74	1.47	1.39
22	7	609	CLA	C3D-C2D	3.74	1.49	1.39
22	1	610	CLA	C3D-C2D	3.74	1.49	1.39
22	G	204	CLA	C3D-C2D	3.74	1.49	1.39
22	1	616	CLA	C3D-C2D	3.74	1.49	1.39
22	7	614	CLA	C3D-C2D	3.74	1.49	1.39
22	A	832	CLA	C1B-NB	-3.74	1.33	1.37
22	3	613	CLA	CHD-C4C	3.74	1.47	1.39
22	7	604	CLA	CHD-C4C	3.74	1.47	1.39
22	K	4002	CLA	C3D-C2D	3.74	1.49	1.39
22	1	612	CLA	CHD-C4C	3.74	1.47	1.39
22	Z	610	CLA	CHD-C4C	3.73	1.47	1.39
22	A	828	CLA	CHC-C4B	3.73	1.47	1.39
22	8	606	CLA	CHC-C4B	3.73	1.47	1.39
22	K	4003	CLA	C3D-C2D	3.73	1.49	1.39
22	1	612	CLA	C3D-C2D	3.73	1.49	1.39
22	9	610	CLA	OBD-CAD	3.73	1.28	1.22
22	3	612	CLA	C3D-C2D	3.73	1.49	1.39
22	7	606	CLA	CHD-C4C	3.73	1.47	1.39
22	A	837	CLA	C3D-C2D	3.73	1.49	1.39
22	5	606	CLA	C1B-NB	-3.73	1.33	1.37
22	F	303	CLA	CHD-C4C	3.73	1.47	1.39
22	Z	606	CLA	C3D-C2D	3.73	1.49	1.39
22	8	602	CLA	CHD-C1D	3.73	1.45	1.38
29	9	607	CHL	OBD-CAD	3.73	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	OBD-CAD	3.73	1.28	1.22
22	9	601	CLA	OBD-CAD	3.73	1.28	1.22
22	A	811	CLA	C1B-NB	-3.73	1.33	1.37
22	Z	603	CLA	C1B-NB	-3.73	1.33	1.37
22	2	610	CLA	OBD-CAD	3.73	1.28	1.22
29	Z	601	CHL	OBD-CAD	3.73	1.28	1.22
22	B	803	CLA	CHD-C1D	3.73	1.45	1.38
22	3	617	CLA	C1B-NB	-3.72	1.33	1.37
22	6	609	CLA	C3D-C2D	3.72	1.49	1.39
22	9	613	CLA	C3D-C2D	3.72	1.49	1.39
22	6	616	CLA	C3D-C2D	3.72	1.49	1.39
22	Z	611	CLA	C3D-C2D	3.72	1.49	1.39
22	5	606	CLA	OBD-CAD	3.72	1.28	1.22
22	B	815	CLA	C3D-C2D	3.72	1.49	1.39
22	9	611	CLA	CHC-C4B	3.72	1.47	1.39
22	2	611	CLA	OBD-CAD	3.72	1.28	1.22
22	A	824	CLA	C1B-NB	-3.72	1.33	1.37
29	6	608	CHL	C1B-NB	-3.72	1.33	1.37
22	Z	609	CLA	C1B-NB	-3.72	1.33	1.37
22	8	611	CLA	C3D-C2D	3.72	1.49	1.39
22	A	823	CLA	C3D-C2D	3.72	1.49	1.39
22	A	828	CLA	C1B-NB	-3.72	1.33	1.37
22	B	837	CLA	CHC-C4B	3.72	1.47	1.39
22	9	611	CLA	C3D-C2D	3.72	1.49	1.39
22	2	606	CLA	OBD-CAD	3.71	1.28	1.22
22	8	602	CLA	CHC-C4B	3.71	1.47	1.39
22	2	607	CLA	CHC-C4B	3.71	1.47	1.39
22	B	811	CLA	C3D-C2D	3.71	1.49	1.39
22	A	830	CLA	C3D-C2D	3.71	1.49	1.39
22	6	601	CLA	C3D-C2D	3.71	1.49	1.39
22	5	610	CLA	C1B-NB	-3.71	1.33	1.37
22	3	617	CLA	C3D-C2D	3.71	1.49	1.39
22	G	203	CLA	C3D-C2D	3.71	1.49	1.39
22	A	841	CLA	CHD-C4C	3.71	1.47	1.39
22	8	616	CLA	CHD-C4C	3.71	1.47	1.39
22	6	612	CLA	C1B-NB	-3.71	1.33	1.37
22	3	612	CLA	OBD-CAD	3.71	1.28	1.22
22	5	611	CLA	C3D-C2D	3.71	1.49	1.39
22	Z	616	CLA	C3D-C2D	3.71	1.49	1.39
22	1	609	CLA	C1B-NB	-3.71	1.33	1.37
22	8	616	CLA	C1B-NB	-3.71	1.33	1.37
22	2	613	CLA	OBD-CAD	3.71	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	606	CLA	CHC-C4B	3.71	1.47	1.39
22	4	612	CLA	CHD-C4C	3.71	1.47	1.39
22	Z	602	CLA	C1B-NB	-3.71	1.33	1.37
22	2	614	CLA	OBD-CAD	3.71	1.28	1.22
22	A	809	CLA	CHC-C4B	3.71	1.47	1.39
22	A	819	CLA	CHC-C4B	3.71	1.47	1.39
22	A	830	CLA	CHD-C1D	3.71	1.45	1.38
22	A	839	CLA	C3D-C2D	3.71	1.49	1.39
22	3	613	CLA	C3D-C2D	3.71	1.49	1.39
22	8	608	CLA	CHC-C4B	3.71	1.47	1.39
22	A	824	CLA	CHD-C4C	3.70	1.47	1.39
22	5	612	CLA	CHD-C4C	3.70	1.47	1.39
22	A	822	CLA	C3D-C2D	3.70	1.49	1.39
22	B	852	CLA	CHC-C4B	3.70	1.47	1.39
22	B	818	CLA	C3D-C2D	3.70	1.49	1.39
22	3	611	CLA	CHC-C4B	3.70	1.47	1.39
22	5	612	CLA	C3D-C2D	3.70	1.49	1.39
22	9	602	CLA	C3D-C2D	3.70	1.49	1.39
22	B	852	CLA	OBD-CAD	3.70	1.28	1.22
22	1	613	CLA	C1B-NB	-3.70	1.33	1.37
22	9	604	CLA	C1B-NB	-3.70	1.33	1.37
22	A	808	CLA	CHD-C4C	3.70	1.47	1.39
22	A	803	CLA	C3D-C2D	3.70	1.49	1.39
22	B	829	CLA	CHB-C1B	3.70	1.47	1.39
22	A	831	CLA	CHD-C4C	3.70	1.47	1.39
22	Z	606	CLA	CHC-C4B	3.70	1.47	1.39
22	F	301	CLA	C1B-NB	-3.70	1.33	1.37
22	B	825	CLA	CHD-C4C	3.70	1.47	1.39
22	2	603	CLA	C3D-C2D	3.70	1.49	1.39
22	Z	616	CLA	C1B-NB	-3.70	1.33	1.37
22	Z	606	CLA	C1B-NB	-3.70	1.33	1.37
22	5	617	CLA	C1B-NB	-3.70	1.33	1.37
22	B	805	CLA	CHD-C1D	3.70	1.45	1.38
22	2	606	CLA	CHC-C4B	3.70	1.47	1.39
22	3	606	CLA	C3D-C2D	3.70	1.49	1.39
22	9	611	CLA	OBD-CAD	3.69	1.28	1.22
22	B	834	CLA	C3D-C2D	3.69	1.49	1.39
29	5	618	CHL	C1B-NB	-3.69	1.33	1.37
22	B	838	CLA	CHB-C1B	3.69	1.47	1.39
22	Z	613	CLA	CHD-C4C	3.69	1.47	1.39
22	B	829	CLA	CHC-C4B	3.69	1.47	1.39
22	A	811	CLA	C3D-C2D	3.69	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	808	CLA	CHD-C4C	3.69	1.47	1.39
22	4	603	CLA	C1B-NB	-3.69	1.33	1.37
22	5	606	CLA	C3D-C2D	3.69	1.49	1.39
22	B	807	CLA	C1B-NB	-3.69	1.33	1.37
22	3	604	CLA	C3D-C2D	3.69	1.49	1.39
22	7	620	CLA	C3D-C2D	3.69	1.49	1.39
29	6	607	CHL	OBD-CAD	3.69	1.28	1.22
22	5	613	CLA	C3D-C2D	3.69	1.49	1.39
22	B	816	CLA	CHC-C4B	3.69	1.47	1.39
22	B	833	CLA	C3D-C2D	3.69	1.49	1.39
22	4	613	CLA	C3D-C2D	3.69	1.49	1.39
22	8	604	CLA	OBD-CAD	3.69	1.28	1.22
29	4	618	CHL	OBD-CAD	3.69	1.28	1.22
22	8	614	CLA	CHC-C4B	3.69	1.47	1.39
22	B	812	CLA	C1B-NB	-3.69	1.33	1.37
22	B	825	CLA	CHC-C4B	3.69	1.47	1.39
22	A	805	CLA	CHC-C4B	3.68	1.47	1.39
29	9	606	CHL	OBD-CAD	3.68	1.28	1.22
22	3	603	CLA	C3D-C2D	3.68	1.49	1.39
22	2	614	CLA	CHC-C4B	3.68	1.47	1.39
22	B	805	CLA	CHD-C4C	3.68	1.47	1.39
22	3	607	CLA	C1B-NB	-3.68	1.33	1.37
22	8	610	CLA	C4B-NB	-3.68	1.33	1.37
22	9	603	CLA	C1B-NB	-3.68	1.33	1.37
22	5	621	CLA	CHC-C4B	3.68	1.47	1.39
22	8	611	CLA	C1B-NB	-3.68	1.33	1.37
22	Z	604	CLA	OBD-CAD	3.68	1.28	1.22
22	B	810	CLA	C3D-C2D	3.68	1.49	1.39
22	Z	614	CLA	CHC-C4B	3.68	1.47	1.39
29	5	608	CHL	C1B-NB	-3.68	1.33	1.37
22	9	603	CLA	C3D-C2D	3.68	1.49	1.39
22	6	614	CLA	OBD-CAD	3.68	1.28	1.22
22	1	604	CLA	C1B-NB	-3.68	1.33	1.37
29	4	606	CHL	OBD-CAD	3.68	1.28	1.22
29	9	606	CHL	CHD-C4C	3.68	1.47	1.39
22	A	834	CLA	C1B-NB	-3.67	1.33	1.37
22	B	835	CLA	OBD-CAD	3.67	1.28	1.22
22	7	601	CLA	CHC-C4B	3.67	1.47	1.39
22	A	808	CLA	C3D-C2D	3.67	1.49	1.39
22	A	809	CLA	C3D-C2D	3.67	1.49	1.39
29	5	608	CHL	CHD-C4C	3.67	1.47	1.39
22	2	607	CLA	OBD-CAD	3.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	612	CLA	C3D-C2D	3.67	1.49	1.39
29	5	607	CHL	CHD-C4C	3.67	1.47	1.39
22	5	606	CLA	CHC-C4B	3.67	1.47	1.39
22	A	808	CLA	OBD-CAD	3.67	1.28	1.22
22	B	803	CLA	CHD-C4C	3.67	1.47	1.39
22	2	602	CLA	OBD-CAD	3.67	1.28	1.22
22	A	818	CLA	C1B-NB	-3.67	1.33	1.37
22	L	204	CLA	C3D-C2D	3.67	1.49	1.39
22	4	609	CLA	CHC-C4B	3.67	1.47	1.39
22	9	602	CLA	CHC-C4B	3.67	1.47	1.39
22	B	819	CLA	C3D-C2D	3.66	1.49	1.39
22	6	617	CLA	C3D-C2D	3.66	1.49	1.39
22	3	609	CLA	C1B-NB	-3.66	1.33	1.37
22	B	841	CLA	CHC-C4B	3.66	1.47	1.39
22	4	616	CLA	C3D-C2D	3.66	1.49	1.39
22	A	825	CLA	C1B-NB	-3.66	1.33	1.37
22	1	604	CLA	OBD-CAD	3.66	1.28	1.22
22	7	613	CLA	C3D-C2D	3.66	1.49	1.39
22	4	601	CLA	OBD-CAD	3.66	1.28	1.22
22	Z	603	CLA	C3D-C2D	3.66	1.49	1.39
22	B	829	CLA	C1B-C2B	3.66	1.51	1.43
22	6	611	CLA	C1B-NB	-3.66	1.33	1.37
22	3	606	CLA	C1B-NB	-3.66	1.33	1.37
22	Z	610	CLA	C3D-C2D	3.66	1.49	1.39
22	6	604	CLA	OBD-CAD	3.66	1.28	1.22
22	A	831	CLA	C3D-C2D	3.66	1.49	1.39
22	A	812	CLA	C1B-NB	-3.66	1.33	1.37
22	A	843	CLA	C1B-NB	-3.66	1.33	1.37
22	A	838	CLA	C1B-NB	-3.66	1.33	1.37
22	8	614	CLA	C1B-NB	-3.66	1.33	1.37
29	7	607	CHL	CHD-C4C	3.66	1.47	1.39
22	4	604	CLA	OBD-CAD	3.66	1.28	1.22
22	A	810	CLA	CHD-C4C	3.65	1.47	1.39
22	A	835	CLA	CHC-C4B	3.65	1.47	1.39
22	Z	604	CLA	C3D-C2D	3.65	1.49	1.39
22	6	613	CLA	OBD-CAD	3.65	1.28	1.22
22	B	825	CLA	CHD-C1D	3.65	1.45	1.38
22	B	822	CLA	C1B-NB	-3.65	1.33	1.37
22	3	613	CLA	C1B-NB	-3.65	1.33	1.37
22	B	822	CLA	C3D-C2D	3.65	1.49	1.39
22	9	601	CLA	CHC-C4B	3.65	1.47	1.39
22	4	614	CLA	CHC-C4B	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	604	CLA	C3D-C2D	3.65	1.49	1.39
22	4	614	CLA	C3D-C2D	3.65	1.49	1.39
22	B	813	CLA	C3D-C2D	3.65	1.49	1.39
22	6	609	CLA	C1B-NB	-3.65	1.33	1.37
22	7	604	CLA	OBD-CAD	3.65	1.28	1.22
22	8	616	CLA	C3D-C2D	3.65	1.49	1.39
22	Z	602	CLA	C3D-C2D	3.65	1.49	1.39
29	5	618	CHL	OBD-CAD	3.65	1.28	1.22
22	Z	612	CLA	C1B-NB	-3.65	1.33	1.37
22	B	830	CLA	CHC-C4B	3.65	1.47	1.39
22	K	4002	CLA	CHC-C4B	3.65	1.47	1.39
22	4	616	CLA	OBD-CAD	3.65	1.28	1.22
29	6	606	CHL	OBD-CAD	3.65	1.28	1.22
22	A	833	CLA	CHC-C4B	3.64	1.47	1.39
22	3	614	CLA	C3D-C2D	3.64	1.49	1.39
22	A	841	CLA	C3B-C4B	3.64	1.51	1.42
22	3	613	CLA	OBD-CAD	3.64	1.28	1.22
22	8	603	CLA	C3D-C2D	3.64	1.49	1.39
22	6	602	CLA	C3D-C2D	3.64	1.49	1.39
22	K	4003	CLA	OBD-CAD	3.64	1.28	1.22
22	2	601	CLA	OBD-CAD	3.64	1.28	1.22
22	B	822	CLA	CHC-C4B	3.64	1.47	1.39
21	A	801	CL0	C3D-C2D	3.64	1.49	1.39
22	7	608	CLA	CHD-C4C	3.64	1.47	1.39
22	B	837	CLA	C1B-NB	-3.64	1.33	1.37
22	6	616	CLA	OBD-CAD	3.64	1.28	1.22
22	Z	612	CLA	OBD-CAD	3.64	1.28	1.22
22	3	610	CLA	C1B-NB	-3.64	1.33	1.37
22	7	620	CLA	CHC-C4B	3.64	1.47	1.39
22	1	609	CLA	C3D-C2D	3.64	1.49	1.39
22	5	604	CLA	OBD-CAD	3.64	1.28	1.22
29	6	618	CHL	OBD-CAD	3.64	1.28	1.22
22	5	602	CLA	C1B-NB	-3.64	1.33	1.37
22	9	609	CLA	OBD-CAD	3.64	1.28	1.22
22	A	813	CLA	CHC-C4B	3.64	1.47	1.39
22	A	811	CLA	CHD-C4C	3.64	1.47	1.39
22	B	839	CLA	C3D-C2D	3.63	1.49	1.39
22	B	820	CLA	OBD-CAD	3.63	1.28	1.22
22	Z	612	CLA	C3D-C2D	3.63	1.49	1.39
22	3	620	CLA	CHC-C4B	3.63	1.47	1.39
22	Z	616	CLA	CHC-C4B	3.63	1.47	1.39
22	1	610	CLA	C1B-NB	-3.63	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	830	CLA	CHC-C4B	3.63	1.47	1.39
22	B	820	CLA	CHB-C1B	3.63	1.47	1.39
22	7	611	CLA	C3D-C2D	3.63	1.49	1.39
22	6	604	CLA	C3D-C2D	3.63	1.49	1.39
22	A	802	CLA	CHC-C4B	3.63	1.47	1.39
22	Z	611	CLA	CHC-C4B	3.63	1.47	1.39
22	B	804	CLA	C3D-C2D	3.63	1.49	1.39
22	8	601	CLA	CHC-C4B	3.63	1.47	1.39
22	A	807	CLA	C3D-C2D	3.63	1.49	1.39
29	4	607	CHL	CHD-C4C	3.63	1.47	1.39
22	B	826	CLA	CHC-C4B	3.63	1.47	1.39
22	F	303	CLA	CHC-C4B	3.63	1.47	1.39
22	1	606	CLA	C3D-C2D	3.63	1.49	1.39
22	7	612	CLA	C3D-C2D	3.63	1.49	1.39
22	Z	613	CLA	C3D-C2D	3.63	1.49	1.39
22	7	614	CLA	OBD-CAD	3.63	1.28	1.22
22	F	303	CLA	C3D-C2D	3.63	1.49	1.39
22	A	832	CLA	C3D-C2D	3.63	1.49	1.39
22	B	804	CLA	CHD-C4C	3.63	1.47	1.39
22	6	614	CLA	C1B-NB	-3.63	1.33	1.37
22	A	817	CLA	OBD-CAD	3.63	1.28	1.22
22	3	604	CLA	OBD-CAD	3.63	1.28	1.22
22	2	609	CLA	OBD-CAD	3.63	1.28	1.22
22	A	812	CLA	C3D-C2D	3.63	1.49	1.39
22	8	613	CLA	OBD-CAD	3.62	1.28	1.22
22	9	613	CLA	OBD-CAD	3.62	1.28	1.22
29	4	607	CHL	OBD-CAD	3.62	1.28	1.22
22	B	815	CLA	C1B-NB	-3.62	1.33	1.37
22	B	830	CLA	C1B-NB	-3.62	1.33	1.37
29	Z	601	CHL	CHC-C4B	3.62	1.47	1.39
22	B	823	CLA	OBD-CAD	3.62	1.28	1.22
22	8	612	CLA	C3D-C2D	3.62	1.49	1.39
22	5	609	CLA	C1B-NB	-3.62	1.33	1.37
29	8	607	CHL	C1D-ND	-3.62	1.33	1.37
22	2	603	CLA	OBD-CAD	3.62	1.28	1.22
22	B	831	CLA	CHD-C4C	3.62	1.47	1.39
29	6	618	CHL	CHD-C4C	3.62	1.47	1.39
22	3	620	CLA	OBD-CAD	3.62	1.28	1.22
22	A	823	CLA	OBD-CAD	3.62	1.28	1.22
22	A	823	CLA	C1B-NB	-3.62	1.33	1.37
22	A	829	CLA	C3D-C2D	3.62	1.49	1.39
22	7	603	CLA	C3D-C2D	3.62	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	204	CLA	C1B-NB	-3.62	1.33	1.37
22	A	811	CLA	CHC-C4B	3.62	1.47	1.39
22	Z	608	CLA	CHC-C4B	3.62	1.47	1.39
22	A	802	CLA	OBD-CAD	3.62	1.28	1.22
22	1	616	CLA	C1B-NB	-3.62	1.33	1.37
22	9	612	CLA	CHC-C4B	3.62	1.47	1.39
22	L	203	CLA	OBD-CAD	3.61	1.28	1.22
22	5	612	CLA	C1B-NB	-3.61	1.33	1.37
22	B	834	CLA	OBD-CAD	3.61	1.28	1.22
22	Z	611	CLA	OBD-CAD	3.61	1.28	1.22
29	5	607	CHL	OBD-CAD	3.61	1.28	1.22
22	L	203	CLA	CHC-C4B	3.61	1.47	1.39
22	B	828	CLA	OBD-CAD	3.61	1.28	1.22
29	6	606	CHL	C3B-C4B	3.61	1.51	1.42
22	A	843	CLA	OBD-CAD	3.61	1.28	1.22
22	3	606	CLA	CHC-C4B	3.61	1.47	1.39
22	4	604	CLA	C1B-NB	-3.61	1.33	1.37
22	3	609	CLA	C3D-C2D	3.61	1.49	1.39
22	B	824	CLA	CHD-C4C	3.61	1.47	1.39
22	3	602	CLA	C1B-NB	-3.61	1.33	1.37
22	Z	613	CLA	OBD-CAD	3.61	1.28	1.22
22	5	602	CLA	OBD-CAD	3.61	1.28	1.22
22	B	816	CLA	C1B-NB	-3.61	1.33	1.37
22	B	824	CLA	OBD-CAD	3.61	1.28	1.22
22	F	304	CLA	C1B-NB	-3.61	1.33	1.37
22	F	304	CLA	C3D-C2D	3.61	1.49	1.39
22	2	612	CLA	OBD-CAD	3.61	1.28	1.22
29	7	607	CHL	OBD-CAD	3.61	1.28	1.22
22	8	612	CLA	CHD-C4C	3.61	1.47	1.39
22	A	828	CLA	CHD-C1D	3.61	1.45	1.38
22	B	832	CLA	CHC-C4B	3.61	1.47	1.39
22	3	611	CLA	OBD-CAD	3.61	1.28	1.22
22	6	617	CLA	C1B-NB	-3.60	1.33	1.37
29	Z	607	CHL	C1B-NB	-3.60	1.33	1.37
22	5	610	CLA	C3D-C2D	3.60	1.49	1.39
22	6	622	CLA	CHC-C4B	3.60	1.47	1.39
22	6	603	CLA	C3D-C2D	3.60	1.49	1.39
22	8	602	CLA	CHD-C4C	3.60	1.47	1.39
22	B	808	CLA	C3D-C2D	3.60	1.49	1.39
22	4	614	CLA	C1B-NB	-3.60	1.33	1.37
22	6	613	CLA	CHC-C4B	3.60	1.47	1.39
22	4	612	CLA	CHC-C4B	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	819	CLA	C4B-NB	-3.60	1.33	1.37
22	6	613	CLA	C1B-NB	-3.60	1.33	1.37
22	A	836	CLA	CHC-C4B	3.60	1.47	1.39
22	1	603	CLA	C3D-C2D	3.60	1.49	1.39
22	1	604	CLA	C3D-C2D	3.60	1.49	1.39
22	A	826	CLA	C3D-C2D	3.60	1.49	1.39
22	8	610	CLA	C3D-C2D	3.60	1.49	1.39
22	Z	609	CLA	OBD-CAD	3.60	1.28	1.22
22	A	833	CLA	C3D-C2D	3.60	1.49	1.39
22	5	616	CLA	C3D-C2D	3.60	1.49	1.39
22	5	610	CLA	CHC-C4B	3.60	1.47	1.39
22	8	616	CLA	CHC-C4B	3.60	1.47	1.39
29	4	608	CHL	CHC-C4B	3.60	1.47	1.39
22	1	614	CLA	C1B-NB	-3.60	1.33	1.37
22	8	610	CLA	CHC-C4B	3.60	1.47	1.39
22	Z	611	CLA	C1B-NB	-3.60	1.33	1.37
22	A	837	CLA	CHC-C4B	3.60	1.47	1.39
22	J	3002	CLA	C3D-C2D	3.60	1.48	1.39
22	A	810	CLA	CHC-C4B	3.60	1.47	1.39
22	3	620	CLA	C3D-C2D	3.60	1.48	1.39
22	5	612	CLA	OBD-CAD	3.60	1.28	1.22
22	3	614	CLA	OBD-CAD	3.60	1.28	1.22
22	B	837	CLA	C3D-C2D	3.60	1.48	1.39
29	6	618	CHL	C3D-C2D	3.59	1.48	1.39
22	B	838	CLA	C1B-NB	-3.59	1.33	1.37
22	6	622	CLA	C1B-NB	-3.59	1.33	1.37
22	A	854	CLA	CHD-C4C	3.59	1.47	1.39
22	2	609	CLA	CHC-C4B	3.59	1.47	1.39
22	8	603	CLA	C1B-NB	-3.59	1.33	1.37
22	Z	613	CLA	CHC-C4B	3.59	1.47	1.39
22	B	810	CLA	CHC-C4B	3.59	1.47	1.39
22	A	815	CLA	OBD-CAD	3.59	1.28	1.22
22	B	824	CLA	C3D-C2D	3.59	1.48	1.39
22	A	835	CLA	OBD-CAD	3.59	1.28	1.22
22	B	804	CLA	OBD-CAD	3.59	1.28	1.22
22	6	622	CLA	C3D-C2D	3.59	1.48	1.39
22	A	816	CLA	C1B-NB	-3.59	1.33	1.37
22	3	620	CLA	C1B-NB	-3.59	1.33	1.37
22	6	610	CLA	C1B-NB	-3.59	1.33	1.37
22	A	845	CLA	C3D-C2D	3.59	1.48	1.39
22	B	839	CLA	CHC-C4B	3.59	1.47	1.39
22	3	602	CLA	C4B-NB	-3.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	610	CLA	CHC-C4B	3.59	1.47	1.39
22	1	602	CLA	C1B-NB	-3.58	1.33	1.37
22	3	602	CLA	C3D-C2D	3.58	1.48	1.39
22	5	601	CLA	OBD-CAD	3.58	1.28	1.22
29	6	608	CHL	OBD-CAD	3.58	1.28	1.22
22	5	617	CLA	CHD-C1D	3.58	1.45	1.38
22	B	832	CLA	C3D-C2D	3.58	1.48	1.39
22	6	604	CLA	CHC-C4B	3.58	1.47	1.39
22	B	817	CLA	C1B-NB	-3.58	1.33	1.37
22	1	611	CLA	C1B-NB	-3.58	1.33	1.37
22	5	611	CLA	CHC-C4B	3.58	1.47	1.39
22	7	620	CLA	OBD-CAD	3.58	1.28	1.22
22	6	622	CLA	OBD-CAD	3.58	1.28	1.22
22	7	603	CLA	CHC-C4B	3.58	1.47	1.39
22	1	612	CLA	OBD-CAD	3.58	1.28	1.22
22	A	820	CLA	C3D-C2D	3.58	1.48	1.39
22	B	805	CLA	C3D-C2D	3.58	1.48	1.39
22	5	614	CLA	CHC-C4B	3.58	1.47	1.39
22	A	819	CLA	C3D-C2D	3.58	1.48	1.39
22	B	827	CLA	C3D-C2D	3.58	1.48	1.39
22	B	817	CLA	C3D-C2D	3.58	1.48	1.39
22	5	617	CLA	C3D-C2D	3.58	1.48	1.39
22	B	806	CLA	CHC-C4B	3.58	1.47	1.39
22	8	606	CLA	OBD-CAD	3.58	1.28	1.22
22	4	603	CLA	C3D-C2D	3.58	1.48	1.39
22	A	829	CLA	CHC-C4B	3.58	1.47	1.39
22	B	825	CLA	OBD-CAD	3.58	1.28	1.22
22	B	824	CLA	CHC-C4B	3.57	1.47	1.39
22	L	204	CLA	CHC-C4B	3.57	1.47	1.39
22	4	602	CLA	C1B-NB	-3.57	1.33	1.37
22	1	609	CLA	OBD-CAD	3.57	1.28	1.22
29	4	608	CHL	CHD-C4C	3.57	1.47	1.39
22	B	814	CLA	CHC-C4B	3.57	1.47	1.39
22	A	807	CLA	OBD-CAD	3.57	1.28	1.22
22	B	821	CLA	CHC-C4B	3.57	1.47	1.39
22	J	3002	CLA	OBD-CAD	3.57	1.28	1.22
22	L	203	CLA	C1B-NB	-3.57	1.33	1.37
22	B	816	CLA	CHD-C4C	3.57	1.47	1.39
22	9	602	CLA	OBD-CAD	3.57	1.28	1.22
22	8	608	CLA	C1B-NB	-3.57	1.33	1.37
29	4	618	CHL	C1B-NB	-3.57	1.33	1.37
22	B	828	CLA	C3D-C2D	3.57	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	828	CLA	CHD-C4C	3.57	1.47	1.39
22	4	611	CLA	C1B-NB	-3.57	1.33	1.37
22	B	836	CLA	C4B-NB	-3.56	1.33	1.37
22	7	602	CLA	C1B-NB	-3.56	1.33	1.37
22	A	834	CLA	OBD-CAD	3.56	1.28	1.22
22	A	845	CLA	OBD-CAD	3.56	1.28	1.22
22	B	833	CLA	OBD-CAD	3.56	1.28	1.22
22	9	610	CLA	CHC-C4B	3.56	1.47	1.39
29	5	607	CHL	C4B-NB	-3.56	1.33	1.37
22	A	818	CLA	CHC-C4B	3.56	1.47	1.39
22	5	601	CLA	CHC-C4B	3.56	1.47	1.39
22	1	606	CLA	OBD-CAD	3.56	1.28	1.22
22	6	611	CLA	OBD-CAD	3.56	1.28	1.22
22	A	805	CLA	OBD-CAD	3.56	1.28	1.22
22	1	614	CLA	CHC-C4B	3.56	1.47	1.39
22	B	817	CLA	OBD-CAD	3.56	1.28	1.22
22	A	845	CLA	CHC-C4B	3.56	1.47	1.39
22	2	611	CLA	CHC-C4B	3.56	1.47	1.39
22	5	621	CLA	OBD-CAD	3.56	1.28	1.22
22	6	613	CLA	C3D-C2D	3.56	1.48	1.39
22	6	609	CLA	OBD-CAD	3.56	1.28	1.22
22	B	829	CLA	C4B-NB	-3.56	1.33	1.37
22	K	4002	CLA	OBD-CAD	3.56	1.28	1.22
22	3	602	CLA	CHC-C4B	3.56	1.47	1.39
22	A	818	CLA	C3D-C2D	3.56	1.48	1.39
29	1	601	CHL	CHC-C4B	3.56	1.47	1.39
22	B	808	CLA	OBD-CAD	3.56	1.28	1.22
22	B	812	CLA	C3D-C2D	3.56	1.48	1.39
22	A	818	CLA	CHD-C4C	3.56	1.47	1.39
22	B	852	CLA	C1B-NB	-3.56	1.33	1.37
22	7	612	CLA	OBD-CAD	3.55	1.28	1.22
22	A	842	CLA	C3D-C2D	3.55	1.48	1.39
22	A	823	CLA	CHC-C4B	3.55	1.47	1.39
22	A	842	CLA	CHC-C4B	3.55	1.47	1.39
22	2	613	CLA	C1B-NB	-3.55	1.33	1.37
22	5	613	CLA	C3B-C4B	3.55	1.51	1.42
22	1	613	CLA	C3D-C2D	3.55	1.48	1.39
22	A	824	CLA	OBD-CAD	3.55	1.28	1.22
22	F	304	CLA	OBD-CAD	3.55	1.28	1.22
22	1	608	CLA	CHC-C4B	3.55	1.47	1.39
22	B	841	CLA	OBD-CAD	3.55	1.28	1.22
22	3	617	CLA	OBD-CAD	3.55	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	204	CLA	CHC-C4B	3.55	1.47	1.39
22	B	830	CLA	C3D-C2D	3.55	1.48	1.39
22	9	604	CLA	CHC-C4B	3.55	1.47	1.39
22	Z	608	CLA	C1B-NB	-3.55	1.33	1.37
29	6	607	CHL	C1B-NB	-3.55	1.33	1.37
22	B	804	CLA	CHC-C4B	3.55	1.47	1.39
22	B	814	CLA	C1B-NB	-3.55	1.33	1.37
22	7	616	CLA	C1B-NB	-3.55	1.33	1.37
22	L	203	CLA	CHD-C1D	3.55	1.45	1.38
22	9	614	CLA	CHC-C4B	3.55	1.47	1.39
22	7	613	CLA	CHD-C4C	3.55	1.47	1.39
22	1	616	CLA	CHC-C4B	3.55	1.47	1.39
22	9	612	CLA	OBD-CAD	3.55	1.28	1.22
22	B	806	CLA	C3D-C2D	3.55	1.48	1.39
22	J	3002	CLA	CHC-C4B	3.55	1.47	1.39
22	7	616	CLA	CHC-C4B	3.55	1.47	1.39
22	A	834	CLA	C4B-NB	-3.55	1.33	1.37
22	4	611	CLA	CHC-C4B	3.55	1.47	1.39
22	3	606	CLA	OBD-CAD	3.55	1.28	1.22
22	Z	613	CLA	C1B-NB	-3.55	1.33	1.37
29	5	608	CHL	CHC-C4B	3.55	1.47	1.39
22	B	814	CLA	OBD-CAD	3.55	1.28	1.22
22	4	613	CLA	OBD-CAD	3.54	1.28	1.22
22	5	603	CLA	C3D-C2D	3.54	1.48	1.39
29	Z	601	CHL	CHD-C4C	3.54	1.47	1.39
29	6	607	CHL	CHD-C4C	3.54	1.47	1.39
22	A	821	CLA	C3D-C2D	3.54	1.48	1.39
22	B	836	CLA	C3D-C2D	3.54	1.48	1.39
22	A	842	CLA	C1B-NB	-3.54	1.33	1.37
22	A	813	CLA	C3D-C2D	3.54	1.48	1.39
22	B	813	CLA	OBD-CAD	3.54	1.28	1.22
22	6	602	CLA	C1B-NB	-3.54	1.33	1.37
22	6	611	CLA	CHC-C4B	3.54	1.47	1.39
22	6	612	CLA	CHC-C4B	3.54	1.47	1.39
22	4	602	CLA	CHC-C4B	3.54	1.47	1.39
29	5	618	CHL	C4B-NB	-3.54	1.33	1.37
22	7	609	CLA	OBD-CAD	3.54	1.28	1.22
22	B	840	CLA	C3D-C2D	3.54	1.48	1.39
22	B	841	CLA	CHB-C1B	3.54	1.47	1.39
22	3	614	CLA	CHC-C4B	3.54	1.47	1.39
22	B	823	CLA	C1B-NB	-3.54	1.33	1.37
22	8	602	CLA	C3D-C2D	3.54	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	603	CLA	C1B-NB	-3.54	1.33	1.37
22	A	826	CLA	OBD-CAD	3.54	1.28	1.22
22	Z	602	CLA	OBD-CAD	3.54	1.28	1.22
22	A	805	CLA	C1B-NB	-3.54	1.33	1.37
22	A	817	CLA	CHB-C1B	3.54	1.47	1.39
22	B	802	CLA	CHC-C4B	3.54	1.47	1.39
22	9	603	CLA	CHC-C4B	3.54	1.47	1.39
22	A	818	CLA	OBD-CAD	3.54	1.28	1.22
22	7	602	CLA	C3D-C2D	3.54	1.48	1.39
29	3	608	CHL	C1D-ND	-3.54	1.33	1.37
22	1	608	CLA	C1B-NB	-3.53	1.33	1.37
22	7	601	CLA	OBD-CAD	3.53	1.28	1.22
22	4	601	CLA	C3D-C2D	3.53	1.48	1.39
22	B	834	CLA	C1B-NB	-3.53	1.33	1.37
22	B	831	CLA	C3D-C2D	3.53	1.48	1.39
22	A	838	CLA	C3D-C2D	3.53	1.48	1.39
22	B	820	CLA	CHC-C4B	3.53	1.47	1.39
22	6	602	CLA	OBD-CAD	3.53	1.28	1.22
29	1	601	CHL	C1D-ND	-3.53	1.33	1.37
29	8	607	CHL	OBD-CAD	3.53	1.28	1.22
29	5	618	CHL	C1D-ND	-3.53	1.33	1.37
22	7	610	CLA	C1B-NB	-3.53	1.33	1.37
29	6	608	CHL	CHD-C4C	3.53	1.47	1.39
22	B	826	CLA	CHD-C4C	3.53	1.47	1.39
22	3	602	CLA	OBD-CAD	3.53	1.28	1.22
22	A	802	CLA	CHB-C1B	3.53	1.47	1.39
29	1	607	CHL	CHD-C4C	3.53	1.47	1.39
22	7	603	CLA	C1B-NB	-3.53	1.33	1.37
22	1	603	CLA	C1B-NB	-3.53	1.33	1.37
22	B	835	CLA	CHC-C4B	3.52	1.47	1.39
29	4	607	CHL	C1B-NB	-3.52	1.33	1.37
22	7	614	CLA	CHC-C4B	3.52	1.47	1.39
22	B	810	CLA	C1B-NB	-3.52	1.33	1.37
22	G	203	CLA	C1B-NB	-3.52	1.33	1.37
21	A	801	CL0	CHD-C4C	3.52	1.47	1.39
22	4	610	CLA	OBD-CAD	3.52	1.28	1.22
22	5	611	CLA	C1B-NB	-3.52	1.33	1.37
22	A	822	CLA	CHC-C4B	3.52	1.47	1.39
22	A	830	CLA	OBD-CAD	3.52	1.28	1.22
22	8	613	CLA	C1B-NB	-3.52	1.33	1.37
22	1	604	CLA	CHC-C4B	3.52	1.47	1.39
22	A	840	CLA	C3D-C2D	3.52	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	601	CHL	C3D-C2D	3.52	1.48	1.39
22	7	606	CLA	OBD-CAD	3.52	1.28	1.22
22	A	829	CLA	C1B-NB	-3.52	1.33	1.37
22	1	616	CLA	OBD-CAD	3.52	1.28	1.22
22	9	602	CLA	C1B-NB	-3.52	1.33	1.37
29	1	601	CHL	CHD-C4C	3.52	1.47	1.39
22	1	609	CLA	CHC-C4B	3.51	1.47	1.39
22	9	603	CLA	OBD-CAD	3.51	1.28	1.22
22	9	609	CLA	CHC-C4B	3.51	1.47	1.39
22	3	611	CLA	C1B-NB	-3.51	1.33	1.37
22	A	830	CLA	CHD-C4C	3.51	1.47	1.39
22	2	601	CLA	CHC-C4B	3.51	1.47	1.39
22	B	812	CLA	OBD-CAD	3.51	1.28	1.22
22	9	614	CLA	OBD-CAD	3.51	1.28	1.22
22	B	834	CLA	CHC-C4B	3.51	1.47	1.39
22	2	614	CLA	CHB-C1B	3.51	1.47	1.39
22	A	829	CLA	CHD-C4C	3.51	1.47	1.39
22	1	611	CLA	C4B-NB	-3.51	1.33	1.37
22	4	613	CLA	C1B-NB	-3.51	1.33	1.37
22	8	608	CLA	CHB-C1B	3.51	1.47	1.39
22	A	813	CLA	OBD-CAD	3.51	1.28	1.22
22	7	610	CLA	C3D-C2D	3.51	1.48	1.39
22	Z	608	CLA	C3D-C2D	3.51	1.48	1.39
22	A	810	CLA	OBD-CAD	3.51	1.28	1.22
22	5	616	CLA	OBD-CAD	3.51	1.28	1.22
29	Z	601	CHL	C1B-NB	-3.51	1.33	1.37
22	4	602	CLA	C3D-C2D	3.51	1.48	1.39
29	4	618	CHL	C1D-ND	-3.51	1.33	1.37
22	1	603	CLA	CHB-C1B	3.51	1.47	1.39
22	5	617	CLA	CHC-C4B	3.51	1.47	1.39
22	3	617	CLA	CHC-C4B	3.51	1.47	1.39
22	5	611	CLA	OBD-CAD	3.51	1.28	1.22
22	6	617	CLA	CHC-C4B	3.51	1.47	1.39
22	J	3002	CLA	C1B-NB	-3.51	1.33	1.37
22	7	601	CLA	C3D-C2D	3.51	1.48	1.39
22	B	833	CLA	CHB-C1B	3.50	1.47	1.39
22	1	612	CLA	CHC-C4B	3.50	1.47	1.39
22	A	811	CLA	OBD-CAD	3.50	1.28	1.22
22	B	802	CLA	CHD-C1D	3.50	1.45	1.38
29	Z	607	CHL	CHD-C4C	3.50	1.47	1.39
22	Z	606	CLA	OBD-CAD	3.50	1.28	1.22
22	4	614	CLA	OBD-CAD	3.50	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	835	CLA	CHB-C1B	3.50	1.47	1.39
22	K	4003	CLA	C1B-NB	-3.50	1.33	1.37
22	2	602	CLA	CHC-C4B	3.50	1.47	1.39
29	9	607	CHL	CHC-C4B	3.50	1.47	1.39
22	5	616	CLA	C1B-NB	-3.50	1.33	1.37
22	7	606	CLA	C3B-C4B	3.50	1.50	1.42
22	Z	610	CLA	C1B-NB	-3.50	1.33	1.37
22	B	802	CLA	OBD-CAD	3.50	1.28	1.22
29	3	608	CHL	CHD-C4C	3.50	1.47	1.39
22	F	304	CLA	CHC-C4B	3.50	1.47	1.39
29	4	618	CHL	C3D-C2D	3.50	1.48	1.39
22	9	613	CLA	C1B-NB	-3.50	1.33	1.37
22	B	811	CLA	OBD-CAD	3.49	1.28	1.22
22	2	613	CLA	CHC-C4B	3.49	1.47	1.39
22	A	824	CLA	C3D-C2D	3.49	1.48	1.39
22	A	834	CLA	C3D-C2D	3.49	1.48	1.39
22	A	832	CLA	CHC-C4B	3.49	1.47	1.39
22	B	810	CLA	OBD-CAD	3.49	1.28	1.22
22	1	611	CLA	CHC-C4B	3.49	1.47	1.39
22	5	616	CLA	CHC-C4B	3.49	1.47	1.39
22	8	612	CLA	OBD-CAD	3.49	1.28	1.22
22	5	609	CLA	OBD-CAD	3.49	1.28	1.22
29	5	618	CHL	C3D-C2D	3.49	1.48	1.39
22	8	616	CLA	OBD-CAD	3.49	1.28	1.22
22	6	617	CLA	OBD-CAD	3.49	1.28	1.22
22	A	806	CLA	C3D-C2D	3.49	1.48	1.39
22	B	829	CLA	OBD-CAD	3.49	1.28	1.22
22	B	823	CLA	CHC-C4B	3.49	1.47	1.39
29	4	606	CHL	CHC-C4B	3.49	1.47	1.39
22	A	814	CLA	C4B-NB	-3.48	1.33	1.37
22	B	815	CLA	CHC-C4B	3.48	1.47	1.39
22	3	611	CLA	CHB-C1B	3.48	1.47	1.39
29	4	618	CHL	CHC-C4B	3.48	1.47	1.39
22	4	604	CLA	CHC-C4B	3.48	1.47	1.39
22	B	803	CLA	C4B-NB	-3.48	1.33	1.37
22	7	604	CLA	C3D-C2D	3.48	1.48	1.39
22	3	607	CLA	OBD-CAD	3.48	1.28	1.22
22	6	610	CLA	C4B-NB	-3.48	1.33	1.37
22	A	814	CLA	C3D-C2D	3.48	1.48	1.39
22	7	602	CLA	C3B-C4B	3.48	1.50	1.42
22	B	808	CLA	C4B-NB	-3.48	1.33	1.37
22	B	819	CLA	OBD-CAD	3.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	616	CLA	CHB-C1B	3.48	1.47	1.39
22	A	819	CLA	C1B-NB	-3.48	1.33	1.37
22	B	825	CLA	C4B-NB	-3.48	1.33	1.37
22	B	809	CLA	OBD-CAD	3.48	1.28	1.22
22	3	612	CLA	C3B-C4B	3.48	1.50	1.42
22	8	616	CLA	CHB-C1B	3.48	1.47	1.39
22	B	815	CLA	OBD-CAD	3.48	1.28	1.22
22	4	602	CLA	OBD-CAD	3.48	1.28	1.22
29	6	618	CHL	C1D-ND	-3.48	1.33	1.37
22	G	203	CLA	CHC-C4B	3.48	1.47	1.39
22	6	614	CLA	CHC-C4B	3.48	1.47	1.39
29	4	606	CHL	CHD-C4C	3.48	1.47	1.39
22	5	617	CLA	OBD-CAD	3.48	1.28	1.22
22	3	609	CLA	CHC-C4B	3.48	1.47	1.39
22	A	833	CLA	OBD-CAD	3.48	1.28	1.22
22	B	827	CLA	OBD-CAD	3.48	1.28	1.22
22	L	204	CLA	CHB-C1B	3.48	1.47	1.39
22	A	812	CLA	CHC-C4B	3.47	1.47	1.39
22	1	616	CLA	CHB-C1B	3.47	1.47	1.39
22	1	610	CLA	OBD-CAD	3.47	1.28	1.22
22	1	613	CLA	OBD-CAD	3.47	1.28	1.22
22	3	607	CLA	C4B-NB	-3.47	1.33	1.37
22	7	608	CLA	C3D-C2D	3.47	1.48	1.39
22	A	828	CLA	C3D-C2D	3.47	1.48	1.39
22	B	818	CLA	OBD-CAD	3.47	1.28	1.22
22	A	817	CLA	C3D-C2D	3.47	1.48	1.39
22	5	614	CLA	OBD-CAD	3.47	1.28	1.22
22	A	809	CLA	OBD-CAD	3.47	1.28	1.22
22	1	611	CLA	OBD-CAD	3.47	1.28	1.22
22	9	612	CLA	CHB-C1B	3.47	1.47	1.39
22	B	840	CLA	C4B-NB	-3.47	1.33	1.37
22	9	614	CLA	C1B-NB	-3.47	1.33	1.37
22	A	814	CLA	OBD-CAD	3.46	1.28	1.22
22	9	611	CLA	CHB-C1B	3.46	1.47	1.39
22	F	303	CLA	C3B-C4B	3.46	1.50	1.42
22	G	203	CLA	OBD-CAD	3.46	1.28	1.22
22	6	612	CLA	OBD-CAD	3.46	1.28	1.22
22	B	816	CLA	C3D-C2D	3.46	1.48	1.39
22	A	804	CLA	CHC-C4B	3.46	1.47	1.39
22	8	606	CLA	C3B-C4B	3.46	1.50	1.42
22	5	609	CLA	CHC-C4B	3.46	1.47	1.39
22	3	609	CLA	OBD-CAD	3.46	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	604	CLA	CHC-C4B	3.46	1.47	1.39
22	Z	612	CLA	CHC-C4B	3.46	1.47	1.39
22	7	620	CLA	C1B-NB	-3.46	1.33	1.37
29	4	618	CHL	C4B-NB	-3.46	1.33	1.37
29	9	607	CHL	C1B-NB	-3.46	1.33	1.37
22	7	613	CLA	OBD-CAD	3.46	1.28	1.22
22	9	613	CLA	CHC-C4B	3.46	1.47	1.39
29	6	618	CHL	C1B-NB	-3.46	1.33	1.37
22	B	821	CLA	CHB-C1B	3.46	1.47	1.39
22	A	832	CLA	OBD-CAD	3.46	1.28	1.22
29	8	607	CHL	CHD-C4C	3.46	1.47	1.39
29	Z	607	CHL	C1D-ND	-3.46	1.33	1.37
29	9	607	CHL	C1D-ND	-3.46	1.33	1.37
29	Z	607	CHL	C4B-NB	-3.46	1.33	1.37
22	A	827	CLA	C3D-C2D	3.45	1.48	1.39
22	3	612	CLA	CHC-C4B	3.45	1.47	1.39
22	4	616	CLA	CHB-C1B	3.45	1.47	1.39
22	9	601	CLA	C1B-NB	-3.45	1.33	1.37
22	8	608	CLA	C3D-C2D	3.45	1.48	1.39
22	B	819	CLA	CHC-C4B	3.45	1.47	1.39
29	9	606	CHL	CHC-C4B	3.45	1.47	1.39
22	A	817	CLA	CHC-C4B	3.45	1.47	1.39
22	8	603	CLA	CHC-C4B	3.45	1.47	1.39
22	3	607	CLA	CHC-C4B	3.45	1.47	1.39
22	4	616	CLA	CHC-C4B	3.45	1.47	1.39
22	Z	616	CLA	OBD-CAD	3.45	1.28	1.22
22	8	609	CLA	C4B-NB	-3.45	1.33	1.37
22	B	838	CLA	C3D-C2D	3.45	1.48	1.39
22	8	609	CLA	CHC-C4B	3.45	1.47	1.39
22	B	840	CLA	OBD-CAD	3.45	1.28	1.22
22	4	601	CLA	C1B-NB	-3.45	1.33	1.37
22	A	815	CLA	CHB-C1B	3.45	1.47	1.39
22	7	609	CLA	CHC-C4B	3.45	1.47	1.39
22	B	807	CLA	C4B-NB	-3.45	1.33	1.37
22	5	603	CLA	C4B-NB	-3.45	1.33	1.37
22	3	606	CLA	C3B-C4B	3.45	1.50	1.42
22	A	834	CLA	CHC-C4B	3.45	1.47	1.39
22	B	832	CLA	OBD-CAD	3.45	1.28	1.22
22	7	606	CLA	C3D-C2D	3.45	1.48	1.39
22	A	836	CLA	OBD-CAD	3.45	1.28	1.22
22	B	821	CLA	OBD-CAD	3.45	1.28	1.22
22	K	4003	CLA	CHC-C4B	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	802	CLA	CHD-C4C	3.44	1.47	1.39
29	1	607	CHL	C1D-ND	-3.44	1.33	1.37
22	7	611	CLA	C3A-C2A	-3.44	1.51	1.54
22	8	611	CLA	CHC-C4B	3.44	1.47	1.39
22	2	610	CLA	C1B-NB	-3.44	1.33	1.37
22	B	822	CLA	OBD-CAD	3.44	1.28	1.22
22	B	827	CLA	CHC-C4B	3.44	1.47	1.39
22	8	603	CLA	CHB-C1B	3.44	1.47	1.39
22	A	842	CLA	OBD-CAD	3.44	1.28	1.22
22	A	804	CLA	OBD-CAD	3.44	1.28	1.22
22	B	821	CLA	C1B-NB	-3.44	1.33	1.37
22	A	810	CLA	C3D-C2D	3.44	1.48	1.39
22	8	601	CLA	C3D-C2D	3.44	1.48	1.39
29	5	608	CHL	OBD-CAD	3.44	1.28	1.22
22	8	610	CLA	C1B-NB	-3.44	1.33	1.37
22	9	611	CLA	C1B-NB	-3.44	1.33	1.37
22	1	608	CLA	C3D-C2D	3.44	1.48	1.39
22	8	612	CLA	CHC-C4B	3.44	1.47	1.39
29	6	618	CHL	CHC-C4B	3.44	1.47	1.39
22	7	611	CLA	CHC-C4B	3.44	1.47	1.39
22	Z	604	CLA	CHC-C4B	3.44	1.47	1.39
22	4	601	CLA	CHB-C1B	3.43	1.47	1.39
22	5	612	CLA	CHC-C4B	3.43	1.47	1.39
29	4	608	CHL	C1B-NB	-3.43	1.33	1.37
22	A	824	CLA	CHC-C4B	3.43	1.47	1.39
22	2	607	CLA	CHB-C1B	3.43	1.47	1.39
29	5	608	CHL	C1D-ND	-3.43	1.33	1.37
22	5	613	CLA	OBD-CAD	3.43	1.28	1.22
22	3	604	CLA	CHC-C4B	3.43	1.47	1.39
22	5	613	CLA	CHC-C4B	3.43	1.47	1.39
22	A	807	CLA	CHC-C4B	3.43	1.47	1.39
22	5	603	CLA	CHC-C4B	3.43	1.47	1.39
22	6	601	CLA	CHC-C4B	3.43	1.47	1.39
22	A	816	CLA	OBD-CAD	3.43	1.28	1.22
22	2	612	CLA	CHC-C4B	3.43	1.47	1.39
22	A	840	CLA	CHC-C4B	3.43	1.47	1.39
22	4	610	CLA	CHC-C4B	3.42	1.47	1.39
22	2	612	CLA	CHB-C1B	3.42	1.47	1.39
22	7	609	CLA	C4B-NB	-3.42	1.33	1.37
22	Z	614	CLA	C1B-NB	-3.42	1.33	1.37
29	9	607	CHL	C3D-C2D	3.42	1.48	1.39
22	L	203	CLA	CHB-C1B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	607	CHL	CHC-C4B	3.42	1.47	1.39
22	8	602	CLA	C1B-NB	-3.42	1.33	1.37
22	5	604	CLA	C1B-NB	-3.42	1.33	1.37
22	6	609	CLA	CHC-C4B	3.42	1.47	1.39
22	2	603	CLA	C1B-NB	-3.42	1.33	1.37
22	8	613	CLA	CHC-C4B	3.42	1.47	1.39
22	1	608	CLA	CHB-C1B	3.42	1.47	1.39
22	A	839	CLA	CHC-C4B	3.42	1.47	1.39
21	A	801	CL0	OBD-CAD	3.42	1.28	1.22
29	4	607	CHL	C1D-ND	-3.41	1.33	1.37
29	4	606	CHL	C1D-ND	-3.41	1.33	1.37
22	8	611	CLA	OBD-CAD	3.41	1.28	1.22
22	2	606	CLA	C1B-NB	-3.41	1.33	1.37
22	A	806	CLA	OBD-CAD	3.41	1.28	1.22
22	B	831	CLA	OBD-CAD	3.41	1.28	1.22
22	F	303	CLA	OBD-CAD	3.41	1.28	1.22
22	4	616	CLA	C1B-NB	-3.41	1.33	1.37
22	5	602	CLA	C3D-C2D	3.41	1.48	1.39
22	K	4003	CLA	CHB-C1B	3.41	1.47	1.39
22	3	620	CLA	CHB-C1B	3.41	1.47	1.39
22	5	610	CLA	OBD-CAD	3.41	1.28	1.22
22	A	805	CLA	CHB-C1B	3.41	1.47	1.39
22	A	804	CLA	C3B-C4B	3.41	1.50	1.42
29	Z	607	CHL	CHC-C4B	3.41	1.47	1.39
22	A	821	CLA	OBD-CAD	3.41	1.28	1.22
29	8	607	CHL	CHC-C4B	3.41	1.47	1.39
22	B	814	CLA	C3D-C2D	3.41	1.48	1.39
22	2	601	CLA	CHB-C1B	3.40	1.47	1.39
22	B	804	CLA	C4B-NB	-3.40	1.33	1.37
22	A	838	CLA	OBD-CAD	3.40	1.28	1.22
22	A	823	CLA	CHB-C1B	3.40	1.47	1.39
22	B	831	CLA	C3B-C4B	3.40	1.50	1.42
22	9	609	CLA	C1B-NB	-3.40	1.33	1.37
29	6	606	CHL	C1B-NB	-3.40	1.33	1.37
22	A	838	CLA	CHC-C4B	3.40	1.47	1.39
22	3	603	CLA	CHB-C1B	3.40	1.47	1.39
22	4	613	CLA	CHC-C4B	3.40	1.47	1.39
22	A	843	CLA	CHC-C4B	3.40	1.47	1.39
22	8	604	CLA	CHB-C1B	3.40	1.47	1.39
22	7	612	CLA	CHC-C4B	3.40	1.47	1.39
22	A	828	CLA	C3B-C4B	3.40	1.50	1.42
22	7	616	CLA	CHB-C1B	3.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	613	CLA	CHB-C1B	3.39	1.47	1.39
29	Z	607	CHL	CHB-C1B	3.39	1.47	1.39
22	9	601	CLA	CHB-C1B	3.39	1.47	1.39
22	Z	614	CLA	OBD-CAD	3.39	1.28	1.22
22	2	609	CLA	C1B-NB	-3.39	1.33	1.37
22	2	611	CLA	CHB-C1B	3.39	1.47	1.39
22	3	614	CLA	C1B-NB	-3.39	1.33	1.37
29	1	607	CHL	C3D-C2D	3.39	1.48	1.39
22	A	821	CLA	CHC-C4B	3.39	1.47	1.39
29	6	608	CHL	C3D-C2D	3.39	1.48	1.39
29	4	607	CHL	CHC-C4B	3.39	1.47	1.39
22	A	820	CLA	OBD-CAD	3.39	1.28	1.22
22	B	811	CLA	CHC-C4B	3.39	1.47	1.39
29	4	607	CHL	C3D-C2D	3.39	1.48	1.39
22	2	612	CLA	C1B-NB	-3.38	1.33	1.37
22	1	613	CLA	CHB-C1B	3.38	1.47	1.39
22	Z	608	CLA	CHB-C1B	3.38	1.47	1.39
29	9	607	CHL	CHB-C1B	3.38	1.47	1.39
22	B	839	CLA	OBD-CAD	3.38	1.28	1.22
22	8	614	CLA	OBD-CAD	3.38	1.28	1.22
22	B	813	CLA	CHC-C4B	3.38	1.47	1.39
22	1	606	CLA	C3B-C4B	3.38	1.50	1.42
22	2	603	CLA	CHC-C4B	3.38	1.47	1.39
22	1	613	CLA	CHC-C4B	3.38	1.47	1.39
22	8	601	CLA	OBD-CAD	3.38	1.28	1.22
29	6	618	CHL	C4B-NB	-3.38	1.33	1.37
22	8	602	CLA	OBD-CAD	3.38	1.28	1.22
22	4	611	CLA	OBD-CAD	3.38	1.28	1.22
29	9	606	CHL	C3D-C2D	3.38	1.48	1.39
22	6	604	CLA	CHB-C1B	3.37	1.47	1.39
22	B	810	CLA	CHB-C1B	3.37	1.47	1.39
22	B	830	CLA	OBD-CAD	3.37	1.28	1.22
22	K	4002	CLA	C1B-NB	-3.37	1.33	1.37
29	8	607	CHL	CHB-C1B	3.37	1.47	1.39
29	6	607	CHL	C3D-C2D	3.37	1.48	1.39
22	B	820	CLA	C1B-NB	-3.37	1.33	1.37
22	B	833	CLA	C1B-NB	-3.37	1.33	1.37
22	A	841	CLA	OBD-CAD	3.37	1.28	1.22
22	A	827	CLA	C4B-NB	-3.37	1.33	1.37
22	Z	606	CLA	C3B-C4B	3.37	1.50	1.42
22	A	827	CLA	OBD-CAD	3.37	1.28	1.22
22	A	843	CLA	CHB-C1B	3.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	606	CLA	C3B-C4B	3.37	1.50	1.42
22	A	824	CLA	CHB-C1B	3.37	1.47	1.39
22	B	808	CLA	CHC-C4B	3.37	1.47	1.39
22	A	802	CLA	C4B-NB	-3.37	1.33	1.37
22	9	612	CLA	C1B-NB	-3.37	1.33	1.37
22	B	805	CLA	OBD-CAD	3.36	1.28	1.22
22	5	604	CLA	CHC-C4B	3.36	1.47	1.39
22	7	610	CLA	OBD-CAD	3.36	1.28	1.22
22	8	602	CLA	CHB-C1B	3.36	1.47	1.39
22	8	601	CLA	CHB-C1B	3.36	1.47	1.39
22	6	601	CLA	C1B-NB	-3.36	1.33	1.37
22	K	4002	CLA	CHB-C1B	3.36	1.46	1.39
22	9	613	CLA	CHB-C1B	3.36	1.46	1.39
22	7	611	CLA	C3B-C4B	3.36	1.50	1.42
22	B	836	CLA	CHC-C4B	3.36	1.46	1.39
22	1	602	CLA	OBD-CAD	3.36	1.28	1.22
22	3	603	CLA	CHC-C4B	3.36	1.46	1.39
22	7	604	CLA	C1B-NB	-3.36	1.33	1.37
22	Z	603	CLA	OBD-CAD	3.36	1.28	1.22
22	G	204	CLA	CHB-C1B	3.36	1.46	1.39
22	Z	608	CLA	OBD-CAD	3.36	1.28	1.22
29	Z	601	CHL	C4B-NB	-3.36	1.33	1.37
22	B	833	CLA	CHC-C4B	3.36	1.46	1.39
22	7	601	CLA	CHB-C1B	3.36	1.46	1.39
22	A	802	CLA	C1B-NB	-3.36	1.33	1.37
22	5	621	CLA	C3D-C2D	3.36	1.48	1.39
22	A	806	CLA	C4B-NB	-3.36	1.33	1.37
22	B	807	CLA	OBD-CAD	3.36	1.28	1.22
22	B	802	CLA	C3D-C2D	3.36	1.48	1.39
29	4	607	CHL	CHB-C1B	3.35	1.46	1.39
22	B	824	CLA	C4B-NB	-3.35	1.33	1.37
22	2	606	CLA	CHB-C1B	3.35	1.46	1.39
22	4	609	CLA	C4B-NB	-3.35	1.33	1.37
22	B	812	CLA	C3B-C4B	3.35	1.50	1.42
22	7	620	CLA	CHB-C1B	3.35	1.46	1.39
22	A	803	CLA	CHC-C4B	3.35	1.46	1.39
22	6	603	CLA	CHC-C4B	3.35	1.46	1.39
29	6	607	CHL	CHC-C4B	3.35	1.46	1.39
22	1	602	CLA	C3B-C4B	3.35	1.50	1.42
29	9	606	CHL	C1B-NB	-3.35	1.33	1.37
22	A	812	CLA	OBD-CAD	3.35	1.28	1.22
22	B	805	CLA	CHB-C1B	3.35	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	604	CLA	CHC-C4B	3.35	1.46	1.39
29	9	606	CHL	CHB-C1B	3.35	1.46	1.39
29	7	607	CHL	C4B-NB	-3.35	1.33	1.37
22	2	611	CLA	C1B-NB	-3.35	1.33	1.37
22	F	301	CLA	C3D-C2D	3.35	1.48	1.39
22	A	828	CLA	CHD-C4C	3.35	1.46	1.39
22	B	809	CLA	C4B-NB	-3.34	1.33	1.37
29	5	607	CHL	C3D-C2D	3.34	1.48	1.39
22	6	622	CLA	CHB-C1B	3.34	1.46	1.39
22	5	611	CLA	CHB-C1B	3.34	1.46	1.39
22	B	805	CLA	C3B-C4B	3.34	1.50	1.42
22	7	603	CLA	OBD-CAD	3.34	1.28	1.22
22	Z	610	CLA	OBD-CAD	3.34	1.28	1.22
22	A	820	CLA	C4B-NB	-3.34	1.33	1.37
29	5	607	CHL	C1B-NB	-3.34	1.33	1.37
22	3	613	CLA	CHC-C4B	3.34	1.46	1.39
22	A	809	CLA	C3B-C4B	3.34	1.50	1.42
22	A	842	CLA	CHB-C1B	3.34	1.46	1.39
22	7	608	CLA	OBD-CAD	3.34	1.28	1.22
22	8	612	CLA	C3B-C4B	3.34	1.50	1.42
22	Z	609	CLA	CHC-C4B	3.34	1.46	1.39
22	3	610	CLA	C3B-C4B	3.34	1.50	1.42
29	4	606	CHL	CHB-C1B	3.33	1.46	1.39
22	G	203	CLA	CHB-C1B	3.33	1.46	1.39
22	2	609	CLA	CHB-C1B	3.33	1.46	1.39
22	5	601	CLA	CHB-C1B	3.33	1.46	1.39
22	B	802	CLA	CHB-C1B	3.33	1.46	1.39
22	4	609	CLA	OBD-CAD	3.33	1.28	1.22
22	A	812	CLA	C4B-NB	-3.33	1.33	1.37
22	Z	611	CLA	CHB-C1B	3.33	1.46	1.39
22	A	840	CLA	OBD-CAD	3.33	1.28	1.22
22	2	614	CLA	C1B-NB	-3.33	1.33	1.37
22	7	611	CLA	CHB-C1B	3.33	1.46	1.39
22	Z	606	CLA	CHB-C1B	3.33	1.46	1.39
22	5	614	CLA	CHB-C1B	3.33	1.46	1.39
22	6	616	CLA	CHC-C4B	3.33	1.46	1.39
22	A	835	CLA	C1B-NB	-3.32	1.33	1.37
22	A	826	CLA	CHC-C4B	3.32	1.46	1.39
29	5	607	CHL	CHC-C4B	3.32	1.46	1.39
22	A	826	CLA	CHB-C1B	3.32	1.46	1.39
22	5	616	CLA	C4B-NB	-3.32	1.33	1.37
22	B	827	CLA	C4B-NB	-3.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	204	CLA	C1B-NB	-3.32	1.33	1.37
22	Z	603	CLA	CHC-C4B	3.32	1.46	1.39
22	6	616	CLA	CHB-C1B	3.32	1.46	1.39
22	7	608	CLA	CHB-C1B	3.32	1.46	1.39
22	B	826	CLA	C3D-C2D	3.32	1.48	1.39
22	A	825	CLA	OBD-CAD	3.32	1.28	1.22
22	A	813	CLA	C3B-C4B	3.32	1.50	1.42
22	A	835	CLA	C4B-NB	-3.32	1.33	1.37
22	B	807	CLA	CHC-C4B	3.31	1.46	1.39
22	A	825	CLA	CHB-C1B	3.31	1.46	1.39
22	6	612	CLA	CHB-C1B	3.31	1.46	1.39
22	3	610	CLA	C3D-C2D	3.31	1.48	1.39
22	1	603	CLA	CHC-C4B	3.31	1.46	1.39
29	1	607	CHL	CHB-C1B	3.31	1.46	1.39
22	4	601	CLA	CHC-C4B	3.31	1.46	1.39
22	A	814	CLA	CHB-C1B	3.31	1.46	1.39
22	A	820	CLA	CHC-C4B	3.31	1.46	1.39
29	3	608	CHL	CHC-C4B	3.31	1.46	1.39
22	4	612	CLA	CHB-C1B	3.31	1.46	1.39
22	8	611	CLA	C4B-NB	-3.31	1.33	1.37
22	A	836	CLA	CHB-C1B	3.31	1.46	1.39
22	9	610	CLA	C1B-NB	-3.30	1.33	1.37
22	6	601	CLA	CHB-C1B	3.30	1.46	1.39
22	A	810	CLA	CHB-C1B	3.30	1.46	1.39
22	B	822	CLA	CHB-C1B	3.30	1.46	1.39
22	4	612	CLA	OBD-CAD	3.30	1.28	1.22
22	B	852	CLA	CHB-C1B	3.30	1.46	1.39
29	9	607	CHL	C4B-NB	-3.30	1.33	1.37
29	Z	607	CHL	C3D-C2D	3.30	1.48	1.39
22	Z	604	CLA	CHB-C1B	3.30	1.46	1.39
21	A	801	CL0	CHC-C4B	3.30	1.46	1.39
29	5	618	CHL	CHC-C4B	3.30	1.46	1.39
22	2	610	CLA	CHB-C1B	3.30	1.46	1.39
22	2	607	CLA	C1B-NB	-3.30	1.33	1.37
22	A	807	CLA	C4B-NB	-3.30	1.33	1.37
22	9	604	CLA	CHB-C1B	3.30	1.46	1.39
29	6	607	CHL	C4B-NB	-3.30	1.33	1.37
22	A	828	CLA	CHB-C1B	3.29	1.46	1.39
22	A	818	CLA	C3B-C4B	3.29	1.50	1.42
22	J	3002	CLA	CHB-C1B	3.29	1.46	1.39
22	1	610	CLA	C3B-C4B	3.29	1.50	1.42
22	A	808	CLA	C3B-C4B	3.29	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	614	CLA	C1B-NB	-3.29	1.33	1.37
22	Z	603	CLA	CHB-C1B	3.29	1.46	1.39
22	A	819	CLA	OBD-CAD	3.29	1.28	1.22
22	5	603	CLA	CHB-C1B	3.29	1.46	1.39
22	B	819	CLA	C4B-NB	-3.29	1.33	1.37
22	B	838	CLA	C3B-C4B	3.29	1.50	1.42
29	4	606	CHL	C3D-C2D	3.29	1.48	1.39
22	A	815	CLA	C1B-NB	-3.29	1.33	1.37
29	8	607	CHL	C3D-C2D	3.28	1.48	1.39
29	9	606	CHL	C1D-ND	-3.28	1.33	1.37
22	Z	613	CLA	CHB-C1B	3.28	1.46	1.39
22	6	614	CLA	C3D-C2D	3.28	1.48	1.39
22	A	831	CLA	OBD-CAD	3.28	1.28	1.22
22	4	614	CLA	CHB-C1B	3.28	1.46	1.39
29	6	606	CHL	C3D-C2D	3.28	1.48	1.39
22	3	613	CLA	CHB-C1B	3.28	1.46	1.39
29	1	607	CHL	C4B-NB	-3.28	1.33	1.37
22	9	603	CLA	C3B-C4B	3.28	1.50	1.42
29	6	607	CHL	C1D-ND	-3.28	1.33	1.37
22	2	602	CLA	CHB-C1B	3.28	1.46	1.39
22	B	825	CLA	C3D-C2D	3.27	1.48	1.39
22	3	614	CLA	CHB-C1B	3.27	1.46	1.39
22	A	838	CLA	C4B-NB	-3.27	1.33	1.37
29	6	608	CHL	CHB-C1B	3.27	1.46	1.39
22	A	814	CLA	CHC-C4B	3.27	1.46	1.39
22	B	803	CLA	OBD-CAD	3.27	1.28	1.22
22	B	838	CLA	OBD-CAD	3.27	1.28	1.22
22	B	828	CLA	CHC-C4B	3.27	1.46	1.39
22	A	833	CLA	C3B-C4B	3.27	1.50	1.42
22	7	604	CLA	C4B-NB	-3.27	1.33	1.37
29	6	606	CHL	C1D-ND	-3.27	1.33	1.37
22	B	818	CLA	CHC-C4B	3.27	1.46	1.39
29	6	606	CHL	CHB-C1B	3.27	1.46	1.39
22	6	603	CLA	CHB-C1B	3.27	1.46	1.39
22	A	821	CLA	CHB-C1B	3.26	1.46	1.39
22	4	603	CLA	CHC-C4B	3.26	1.46	1.39
22	5	621	CLA	CHB-C1B	3.26	1.46	1.39
22	8	606	CLA	CHB-C1B	3.26	1.46	1.39
22	B	841	CLA	C1B-NB	-3.26	1.33	1.37
22	F	304	CLA	CHB-C1B	3.26	1.46	1.39
22	F	303	CLA	CHB-C1B	3.26	1.46	1.39
29	4	608	CHL	CHB-C1B	3.26	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	610	CLA	C4B-NB	-3.26	1.33	1.37
29	6	608	CHL	CHC-C4B	3.26	1.46	1.39
29	6	608	CHL	C4B-NB	-3.26	1.33	1.37
22	Z	602	CLA	C3B-C4B	3.26	1.50	1.42
22	9	614	CLA	CHB-C1B	3.25	1.46	1.39
22	6	602	CLA	C3B-C4B	3.25	1.50	1.42
29	5	607	CHL	C1D-ND	-3.25	1.33	1.37
22	B	839	CLA	CHB-C1B	3.25	1.46	1.39
22	3	606	CLA	CHB-C1B	3.25	1.46	1.39
22	6	617	CLA	CHB-C1B	3.25	1.46	1.39
22	B	840	CLA	CHB-C1B	3.25	1.46	1.39
22	A	817	CLA	C1B-NB	-3.25	1.33	1.37
22	A	806	CLA	CHC-C4B	3.25	1.46	1.39
29	1	601	CHL	CHB-C1B	3.25	1.46	1.39
22	6	613	CLA	C3B-C4B	3.25	1.50	1.42
22	B	832	CLA	C3B-C4B	3.25	1.50	1.42
22	1	608	CLA	OBD-CAD	3.24	1.28	1.22
22	8	613	CLA	CHB-C1B	3.24	1.46	1.39
22	5	621	CLA	C4B-NB	-3.24	1.33	1.37
22	B	803	CLA	CHC-C4B	3.24	1.46	1.39
22	7	603	CLA	CHB-C1B	3.24	1.46	1.39
29	Z	601	CHL	CHB-C1B	3.24	1.46	1.39
22	4	611	CLA	CHB-C1B	3.24	1.46	1.39
22	A	816	CLA	C3B-C4B	3.24	1.50	1.42
22	A	808	CLA	CHC-C4B	3.24	1.46	1.39
22	8	614	CLA	CHB-C1B	3.24	1.46	1.39
29	7	607	CHL	CHC-C4B	3.24	1.46	1.39
22	6	617	CLA	C4B-NB	-3.24	1.33	1.37
22	B	811	CLA	CHB-C1B	3.24	1.46	1.39
22	Z	614	CLA	CHB-C1B	3.24	1.46	1.39
22	9	609	CLA	C4B-NB	-3.24	1.33	1.37
22	8	608	CLA	OBD-CAD	3.24	1.28	1.22
22	5	616	CLA	CHB-C1B	3.24	1.46	1.39
22	4	604	CLA	C4B-NB	-3.23	1.33	1.37
22	B	807	CLA	CHB-C1B	3.23	1.46	1.39
22	B	811	CLA	C4B-NB	-3.23	1.33	1.37
22	2	601	CLA	C1B-NB	-3.23	1.33	1.37
22	2	602	CLA	C1B-NB	-3.23	1.33	1.37
22	8	604	CLA	C4B-NB	-3.23	1.33	1.37
22	1	612	CLA	C3B-C4B	3.23	1.50	1.42
29	5	608	CHL	C3D-C2D	3.23	1.47	1.39
22	Z	612	CLA	CHB-C1B	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	830	CLA	C3B-C4B	3.23	1.50	1.42
22	A	807	CLA	CHB-C1B	3.23	1.46	1.39
22	F	301	CLA	C3B-C4B	3.23	1.50	1.42
22	7	613	CLA	CHC-C4B	3.23	1.46	1.39
22	1	606	CLA	CHB-C1B	3.22	1.46	1.39
22	6	611	CLA	CHB-C1B	3.22	1.46	1.39
22	9	603	CLA	CHB-C1B	3.22	1.46	1.39
22	5	606	CLA	CHB-C1B	3.22	1.46	1.39
29	4	607	CHL	C4B-NB	-3.22	1.33	1.37
22	A	822	CLA	C4B-NB	-3.22	1.33	1.37
29	5	607	CHL	MG-NA	-3.22	1.98	2.06
22	7	612	CLA	C3B-C4B	3.21	1.50	1.42
29	5	618	CHL	CHB-C1B	3.21	1.46	1.39
22	B	834	CLA	C3B-C4B	3.21	1.50	1.42
22	B	824	CLA	CHB-C1B	3.21	1.46	1.39
22	6	610	CLA	OBD-CAD	3.21	1.28	1.22
22	4	602	CLA	CHB-C1B	3.21	1.46	1.39
29	4	618	CHL	CHB-C1B	3.21	1.46	1.39
22	8	611	CLA	CHB-C1B	3.21	1.46	1.39
22	5	612	CLA	CHB-C1B	3.21	1.46	1.39
22	A	831	CLA	CHB-C1B	3.20	1.46	1.39
22	B	826	CLA	C3B-C4B	3.20	1.50	1.42
29	4	606	CHL	C3B-C4B	3.20	1.50	1.42
22	3	609	CLA	C4B-NB	-3.20	1.33	1.37
22	1	604	CLA	CHB-C1B	3.20	1.46	1.39
22	A	831	CLA	C4B-NB	-3.20	1.33	1.37
22	1	604	CLA	C4B-NB	-3.20	1.33	1.37
22	B	826	CLA	OBD-CAD	3.20	1.28	1.22
22	7	611	CLA	OBD-CAD	3.20	1.28	1.22
22	8	609	CLA	OBD-CAD	3.20	1.28	1.22
22	B	841	CLA	C4B-NB	-3.19	1.33	1.37
22	F	301	CLA	OBD-CAD	3.19	1.28	1.22
22	Z	602	CLA	CHB-C1B	3.19	1.46	1.39
29	7	607	CHL	CHB-C1B	3.19	1.46	1.39
22	4	603	CLA	CHB-C1B	3.19	1.46	1.39
22	B	814	CLA	C4B-NB	-3.19	1.33	1.37
22	Z	604	CLA	C4B-NB	-3.19	1.33	1.37
22	4	612	CLA	C3B-C4B	3.19	1.50	1.42
22	B	812	CLA	CHB-C1B	3.19	1.46	1.39
22	9	610	CLA	CHB-C1B	3.19	1.46	1.39
29	4	608	CHL	C1D-ND	-3.19	1.33	1.37
22	1	614	CLA	CHB-C1B	3.19	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	607	CHL	C3D-C2D	3.18	1.47	1.39
22	1	614	CLA	C4B-NB	-3.18	1.33	1.37
22	2	613	CLA	CHB-C1B	3.18	1.46	1.39
22	1	609	CLA	CHB-C1B	3.18	1.46	1.39
29	7	607	CHL	C1D-ND	-3.18	1.33	1.37
22	A	828	CLA	OBD-CAD	3.18	1.28	1.22
22	B	817	CLA	CHC-C4B	3.18	1.46	1.39
22	2	603	CLA	CHB-C1B	3.18	1.46	1.39
29	1	601	CHL	OBD-CAD	3.18	1.28	1.22
29	6	618	CHL	CHB-C1B	3.18	1.46	1.39
22	6	602	CLA	CHB-C1B	3.18	1.46	1.39
22	A	843	CLA	C4B-NB	-3.18	1.33	1.37
22	A	816	CLA	CHB-C1B	3.18	1.46	1.39
22	A	834	CLA	CHB-C1B	3.18	1.46	1.39
22	8	603	CLA	OBD-CAD	3.18	1.28	1.22
22	2	602	CLA	C4B-NB	-3.18	1.33	1.37
22	7	613	CLA	CHB-C1B	3.18	1.46	1.39
22	5	617	CLA	CHB-C1B	3.18	1.46	1.39
22	B	836	CLA	CHB-C1B	3.18	1.46	1.39
22	B	830	CLA	C4B-NB	-3.17	1.33	1.37
22	A	845	CLA	CHB-C1B	3.17	1.46	1.39
22	B	802	CLA	C4B-NB	-3.17	1.33	1.37
22	A	822	CLA	OBD-CAD	3.17	1.27	1.22
22	A	832	CLA	C4B-NB	-3.17	1.33	1.37
22	B	818	CLA	C4B-NB	-3.17	1.33	1.37
22	1	616	CLA	C4B-NB	-3.17	1.33	1.37
22	3	604	CLA	C4B-NB	-3.17	1.33	1.37
22	A	811	CLA	CHB-C1B	3.17	1.46	1.39
22	B	829	CLA	C3D-C2D	3.17	1.47	1.39
22	A	808	CLA	CHB-C1B	3.17	1.46	1.39
22	6	609	CLA	C4B-NB	-3.17	1.33	1.37
22	Z	610	CLA	C3B-C4B	3.17	1.50	1.42
22	A	829	CLA	OBD-CAD	3.17	1.27	1.22
22	3	610	CLA	OBD-CAD	3.17	1.27	1.22
22	7	609	CLA	C1B-NB	-3.16	1.33	1.37
22	A	805	CLA	C4B-NB	-3.16	1.33	1.37
22	7	616	CLA	OBD-CAD	3.16	1.27	1.22
22	3	617	CLA	C4B-NB	-3.16	1.33	1.37
22	L	203	CLA	C3B-C4B	3.16	1.50	1.42
22	B	830	CLA	CHB-C1B	3.16	1.46	1.39
22	A	820	CLA	CHB-C1B	3.16	1.46	1.39
22	3	617	CLA	CHB-C1B	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	825	CLA	CHC-C4B	3.16	1.46	1.39
22	B	820	CLA	C4B-NB	-3.16	1.33	1.37
22	7	612	CLA	CHB-C1B	3.15	1.46	1.39
22	8	612	CLA	CHB-C1B	3.15	1.46	1.39
29	5	608	CHL	C4B-NB	-3.15	1.33	1.37
22	A	845	CLA	C3B-C4B	3.15	1.50	1.42
22	A	836	CLA	C3B-C4B	3.15	1.50	1.42
29	1	601	CHL	C3D-C2D	3.15	1.47	1.39
22	2	613	CLA	C4B-NB	-3.15	1.33	1.37
22	Z	610	CLA	CHB-C1B	3.14	1.46	1.39
22	A	842	CLA	C3B-C4B	3.14	1.50	1.42
22	3	603	CLA	C3B-C4B	3.14	1.50	1.42
22	B	823	CLA	C4B-NB	-3.14	1.33	1.37
22	3	604	CLA	CHB-C1B	3.14	1.46	1.39
22	5	604	CLA	CHB-C1B	3.14	1.46	1.39
22	3	620	CLA	C3B-C4B	3.14	1.50	1.42
22	1	613	CLA	C4B-NB	-3.14	1.33	1.37
22	8	601	CLA	C4B-NB	-3.14	1.33	1.37
22	B	835	CLA	CHB-C1B	3.14	1.46	1.39
22	A	815	CLA	C4B-NB	-3.14	1.33	1.37
22	4	602	CLA	C4B-NB	-3.14	1.33	1.37
22	1	614	CLA	OBD-CAD	3.14	1.27	1.22
22	B	817	CLA	CHB-C1B	3.14	1.46	1.39
22	9	609	CLA	CHB-C1B	3.14	1.46	1.39
29	4	608	CHL	C3D-C2D	3.13	1.47	1.39
22	B	833	CLA	C4B-NB	-3.13	1.33	1.37
22	7	608	CLA	C3B-C4B	3.13	1.50	1.42
22	7	602	CLA	OBD-CAD	3.13	1.27	1.22
22	6	604	CLA	C4B-NB	-3.13	1.33	1.37
22	6	611	CLA	C4B-NB	-3.13	1.33	1.37
22	B	808	CLA	CHB-C1B	3.13	1.46	1.39
22	B	834	CLA	CHB-C1B	3.12	1.46	1.39
22	A	840	CLA	C3B-C4B	3.12	1.50	1.42
22	B	823	CLA	CHB-C1B	3.12	1.46	1.39
29	8	607	CHL	C4B-NB	-3.12	1.33	1.37
22	5	602	CLA	CHB-C1B	3.12	1.46	1.39
22	3	607	CLA	CHB-C1B	3.12	1.46	1.39
22	B	806	CLA	CHB-C1B	3.12	1.46	1.39
22	F	301	CLA	CHB-C1B	3.12	1.46	1.39
22	5	611	CLA	C4B-NB	-3.12	1.33	1.37
22	B	809	CLA	CHB-C1B	3.12	1.46	1.39
22	9	602	CLA	C4B-NB	-3.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	813	CLA	CHB-C1B	3.11	1.46	1.39
22	A	804	CLA	CHB-C1B	3.11	1.46	1.39
22	B	852	CLA	C4B-NB	-3.11	1.34	1.37
22	2	607	CLA	C4B-NB	-3.11	1.34	1.37
22	4	604	CLA	CHB-C1B	3.11	1.46	1.39
22	Z	609	CLA	CHB-C1B	3.11	1.46	1.39
29	3	608	CHL	C3D-C2D	3.11	1.47	1.39
22	4	613	CLA	CHB-C1B	3.11	1.46	1.39
22	A	806	CLA	CHB-C1B	3.11	1.46	1.39
22	4	603	CLA	OBD-CAD	3.10	1.27	1.22
22	8	614	CLA	C4B-NB	-3.10	1.34	1.37
22	6	614	CLA	CHB-C1B	3.10	1.46	1.39
22	A	837	CLA	C3B-C4B	3.10	1.50	1.42
22	B	816	CLA	C4B-NB	-3.10	1.34	1.37
22	7	614	CLA	CHB-C1B	3.10	1.46	1.39
22	A	803	CLA	CHB-C1B	3.10	1.46	1.39
22	7	602	CLA	CHB-C1B	3.10	1.46	1.39
22	B	816	CLA	CHB-C1B	3.10	1.46	1.39
22	B	839	CLA	C4B-NB	-3.10	1.34	1.37
22	Z	613	CLA	C4B-NB	-3.10	1.34	1.37
22	G	204	CLA	C3B-C4B	3.10	1.50	1.42
22	A	854	CLA	C4B-NB	-3.10	1.34	1.37
29	5	607	CHL	CHB-C1B	3.10	1.46	1.39
22	3	603	CLA	OBD-CAD	3.10	1.27	1.22
22	K	4003	CLA	C3B-C4B	3.09	1.50	1.42
22	B	826	CLA	CHB-C1B	3.09	1.46	1.39
29	5	608	CHL	CHB-C1B	3.09	1.46	1.39
22	4	611	CLA	C4B-NB	-3.09	1.34	1.37
22	B	837	CLA	C3B-C4B	3.09	1.50	1.42
22	A	839	CLA	OBD-CAD	3.09	1.27	1.22
22	B	814	CLA	CHB-C1B	3.09	1.46	1.39
22	5	609	CLA	C4B-NB	-3.09	1.34	1.37
21	A	801	CL0	CHB-C1B	3.09	1.46	1.39
22	6	612	CLA	C3B-C4B	3.09	1.50	1.42
29	1	601	CHL	C4B-NB	-3.09	1.34	1.37
29	9	606	CHL	C4B-NB	-3.09	1.34	1.37
22	7	620	CLA	C4B-NB	-3.08	1.34	1.37
22	A	811	CLA	C3B-C4B	3.08	1.50	1.42
22	9	602	CLA	CHB-C1B	3.08	1.46	1.39
22	A	821	CLA	C4B-NB	-3.08	1.34	1.37
22	5	610	CLA	CHB-C1B	3.08	1.46	1.39
22	2	607	CLA	C3B-C4B	3.07	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	610	CLA	CHB-C1B	3.07	1.46	1.39
22	A	803	CLA	OBD-CAD	3.07	1.27	1.22
22	6	614	CLA	C4B-NB	-3.07	1.34	1.37
29	1	607	CHL	C3B-C4B	3.07	1.49	1.42
22	Z	611	CLA	C4B-NB	-3.07	1.34	1.37
22	A	819	CLA	CHB-C1B	3.07	1.46	1.39
22	9	612	CLA	C3B-C4B	3.07	1.49	1.42
22	B	813	CLA	C4B-NB	-3.07	1.34	1.37
22	7	601	CLA	C4B-NB	-3.07	1.34	1.37
29	4	606	CHL	C4B-NB	-3.06	1.34	1.37
22	1	602	CLA	CHB-C1B	3.06	1.46	1.39
22	6	609	CLA	CHB-C1B	3.06	1.46	1.39
22	A	837	CLA	C4B-NB	-3.06	1.34	1.37
22	6	603	CLA	OBD-CAD	3.06	1.27	1.22
22	A	854	CLA	OBD-CAD	3.06	1.27	1.22
22	7	606	CLA	CHB-C1B	3.06	1.46	1.39
22	Z	614	CLA	C3B-C4B	3.06	1.49	1.42
22	3	602	CLA	CHB-C1B	3.06	1.46	1.39
22	2	601	CLA	C4B-NB	-3.06	1.34	1.37
22	2	611	CLA	C4B-NB	-3.06	1.34	1.37
22	J	3002	CLA	C3B-C4B	3.05	1.49	1.42
22	3	609	CLA	CHB-C1B	3.05	1.46	1.39
22	F	304	CLA	C3B-C4B	3.05	1.49	1.42
22	3	610	CLA	CHB-C1B	3.05	1.46	1.39
22	B	831	CLA	C4B-NB	-3.05	1.34	1.37
22	5	610	CLA	C4B-NB	-3.05	1.34	1.37
22	B	826	CLA	C4B-NB	-3.05	1.34	1.37
22	A	831	CLA	CHC-C4B	3.05	1.46	1.39
22	A	825	CLA	C4B-NB	-3.05	1.34	1.37
22	K	4002	CLA	C4B-NB	-3.04	1.34	1.37
29	3	608	CHL	C3B-C4B	3.04	1.49	1.42
22	5	602	CLA	C3B-C4B	3.04	1.49	1.42
22	7	609	CLA	CHB-C1B	3.04	1.46	1.39
22	B	828	CLA	C3B-C4B	3.04	1.49	1.42
22	A	827	CLA	CHB-C1B	3.04	1.46	1.39
22	4	609	CLA	C3B-C4B	3.04	1.49	1.42
22	A	832	CLA	CHB-C1B	3.04	1.46	1.39
22	A	826	CLA	C4B-NB	-3.04	1.34	1.37
22	A	812	CLA	CHB-C1B	3.04	1.46	1.39
22	Z	612	CLA	C3B-C4B	3.04	1.49	1.42
29	6	607	CHL	C3B-C4B	3.03	1.49	1.42
22	8	616	CLA	C4B-NB	-3.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	810	CLA	C4B-NB	-3.03	1.34	1.37
22	L	204	CLA	C4B-NB	-3.03	1.34	1.37
22	B	835	CLA	C3B-C4B	3.03	1.49	1.42
22	B	806	CLA	C3B-C4B	3.03	1.49	1.42
22	5	601	CLA	C4B-NB	-3.03	1.34	1.37
22	4	610	CLA	CHB-C1B	3.03	1.46	1.39
22	6	611	CLA	C3B-C4B	3.03	1.49	1.42
29	9	606	CHL	C3B-C4B	3.03	1.49	1.42
22	Z	609	CLA	C4B-NB	-3.03	1.34	1.37
22	B	815	CLA	CHB-C1B	3.03	1.46	1.39
22	B	828	CLA	CHB-C1B	3.03	1.46	1.39
22	4	610	CLA	C4B-NB	-3.03	1.34	1.37
22	2	610	CLA	C3B-C4B	3.03	1.49	1.42
22	4	613	CLA	C3B-C4B	3.02	1.49	1.42
22	Z	603	CLA	C4B-NB	-3.02	1.34	1.37
22	7	620	CLA	C3B-C4B	3.02	1.49	1.42
22	B	810	CLA	C4B-NB	-3.02	1.34	1.37
22	3	612	CLA	CHB-C1B	3.02	1.46	1.39
22	3	614	CLA	C4B-NB	-3.02	1.34	1.37
22	9	604	CLA	C3B-C4B	3.02	1.49	1.42
29	4	608	CHL	OBD-CAD	3.02	1.27	1.22
22	5	617	CLA	C4B-NB	-3.02	1.34	1.37
22	6	610	CLA	CHB-C1B	3.02	1.46	1.39
22	2	614	CLA	C3B-C4B	3.02	1.49	1.42
22	A	838	CLA	CHB-C1B	3.02	1.46	1.39
22	9	614	CLA	C3B-C4B	3.02	1.49	1.42
22	5	614	CLA	C4B-NB	-3.02	1.34	1.37
22	B	806	CLA	C4B-NB	-3.02	1.34	1.37
22	7	603	CLA	C4B-NB	-3.02	1.34	1.37
22	2	614	CLA	C4B-NB	-3.02	1.34	1.37
22	B	825	CLA	CHB-C1B	3.02	1.46	1.39
22	6	601	CLA	C4B-NB	-3.02	1.34	1.37
22	1	611	CLA	CHB-C1B	3.02	1.46	1.39
22	B	827	CLA	CHB-C1B	3.01	1.46	1.39
22	1	610	CLA	C4B-NB	-3.01	1.34	1.37
22	F	304	CLA	C4B-NB	-3.01	1.34	1.37
22	A	823	CLA	C4B-NB	-3.01	1.34	1.37
22	A	837	CLA	CHB-C1B	3.01	1.46	1.39
22	A	838	CLA	C3B-C4B	3.01	1.49	1.42
22	Z	616	CLA	C3B-C4B	3.01	1.49	1.42
29	1	607	CHL	MG-NA	-3.01	1.99	2.06
22	K	4003	CLA	C4B-NB	-3.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	603	CLA	OBD-CAD	3.00	1.27	1.22
22	8	608	CLA	C4B-NB	-3.00	1.34	1.37
29	4	608	CHL	C4B-NB	-3.00	1.34	1.37
22	Z	608	CLA	C3B-C4B	3.00	1.49	1.42
22	9	611	CLA	C3B-C4B	3.00	1.49	1.42
22	Z	608	CLA	C4B-NB	-3.00	1.34	1.37
22	4	603	CLA	C4B-NB	-3.00	1.34	1.37
22	4	616	CLA	C3A-C2A	-3.00	1.51	1.54
22	B	815	CLA	C4B-NB	-3.00	1.34	1.37
22	Z	610	CLA	C4B-NB	-3.00	1.34	1.37
22	6	603	CLA	C4B-NB	-3.00	1.34	1.37
22	4	616	CLA	C3B-C4B	2.99	1.49	1.42
22	A	840	CLA	CHB-C1B	2.99	1.46	1.39
22	B	839	CLA	C3B-C4B	2.99	1.49	1.42
22	Z	606	CLA	C4B-NB	-2.99	1.34	1.37
22	4	614	CLA	C3B-C4B	2.99	1.49	1.42
22	B	837	CLA	C4B-NB	-2.99	1.34	1.37
22	9	601	CLA	C3B-C4B	2.99	1.49	1.42
22	6	616	CLA	C3B-C4B	2.99	1.49	1.42
22	Z	611	CLA	C3B-C4B	2.99	1.49	1.42
22	8	603	CLA	C4B-NB	-2.99	1.34	1.37
22	5	612	CLA	C4B-NB	-2.99	1.34	1.37
22	B	837	CLA	CHB-C1B	2.99	1.46	1.39
22	A	818	CLA	CHB-C1B	2.99	1.46	1.39
22	Z	616	CLA	C4B-NB	-2.98	1.34	1.37
22	3	606	CLA	C4B-NB	-2.98	1.34	1.37
29	1	601	CHL	C3B-C4B	2.98	1.49	1.42
22	B	822	CLA	C3B-C4B	2.98	1.49	1.42
22	2	613	CLA	C3B-C4B	2.98	1.49	1.42
22	5	601	CLA	C3B-C4B	2.98	1.49	1.42
22	9	601	CLA	C4B-NB	-2.97	1.34	1.37
22	4	610	CLA	C3B-C4B	2.97	1.49	1.42
22	B	810	CLA	C3B-C4B	2.97	1.49	1.42
29	3	608	CHL	C4B-NB	-2.97	1.34	1.37
22	Z	614	CLA	C4B-NB	-2.97	1.34	1.37
21	A	801	CL0	C3B-C4B	2.97	1.49	1.42
22	K	4002	CLA	C3B-C4B	2.97	1.49	1.42
22	B	835	CLA	C4B-NB	-2.97	1.34	1.37
22	B	852	CLA	C3B-C4B	2.97	1.49	1.42
22	4	616	CLA	C4B-NB	-2.97	1.34	1.37
22	A	824	CLA	C3B-C4B	2.97	1.49	1.42
22	2	601	CLA	C3B-C4B	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	609	CLA	CHB-C1B	2.97	1.46	1.39
22	B	821	CLA	C4B-NB	-2.96	1.34	1.37
22	5	613	CLA	CHB-C1B	2.96	1.46	1.39
22	A	813	CLA	CHB-C1B	2.96	1.46	1.39
22	3	614	CLA	C3B-C4B	2.96	1.49	1.42
22	9	613	CLA	C4B-NB	-2.96	1.34	1.37
22	2	611	CLA	C3B-C4B	2.96	1.49	1.42
22	B	816	CLA	C3B-C4B	2.95	1.49	1.42
22	2	606	CLA	C3B-C4B	2.95	1.49	1.42
29	8	607	CHL	C3B-C4B	2.95	1.49	1.42
22	2	606	CLA	C4B-NB	-2.95	1.34	1.37
22	A	845	CLA	C4B-NB	-2.95	1.34	1.37
22	1	614	CLA	C3B-C4B	2.95	1.49	1.42
22	4	601	CLA	C4B-NB	-2.95	1.34	1.37
22	8	614	CLA	C3B-C4B	2.95	1.49	1.42
22	A	817	CLA	C3B-C4B	2.94	1.49	1.42
22	A	826	CLA	C3B-C4B	2.94	1.49	1.42
22	3	611	CLA	C3B-C4B	2.94	1.49	1.42
22	J	3002	CLA	C4B-NB	-2.94	1.34	1.37
22	1	608	CLA	C4B-NB	-2.94	1.34	1.37
29	9	607	CHL	C3B-C4B	2.94	1.49	1.42
22	5	614	CLA	C3B-C4B	2.94	1.49	1.42
22	2	612	CLA	C3B-C4B	2.94	1.49	1.42
22	2	603	CLA	C3B-C4B	2.94	1.49	1.42
22	2	609	CLA	C3B-C4B	2.94	1.49	1.42
22	A	839	CLA	C4B-NB	-2.94	1.34	1.37
22	7	616	CLA	C3B-C4B	2.94	1.49	1.42
29	3	608	CHL	CHB-C1B	2.94	1.46	1.39
22	B	821	CLA	C3B-C4B	2.94	1.49	1.42
22	B	828	CLA	C4B-NB	-2.93	1.34	1.37
22	8	602	CLA	C4B-NB	-2.93	1.34	1.37
22	4	603	CLA	C3B-C4B	2.93	1.49	1.42
22	A	828	CLA	C4B-NB	-2.93	1.34	1.37
22	A	804	CLA	C3D-C2D	2.93	1.47	1.39
22	9	611	CLA	C4B-NB	-2.93	1.34	1.37
22	5	617	CLA	C3B-C4B	2.93	1.49	1.42
22	A	809	CLA	C4B-NB	-2.93	1.34	1.37
22	A	824	CLA	C4B-NB	-2.93	1.34	1.37
29	4	607	CHL	MG-NA	-2.93	1.99	2.06
22	B	806	CLA	OBD-CAD	2.93	1.27	1.22
22	A	821	CLA	C3B-C4B	2.93	1.49	1.42
22	9	612	CLA	C4B-NB	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	802	CLA	C3B-C4B	2.92	1.49	1.42
22	6	622	CLA	C4B-NB	-2.92	1.34	1.37
22	A	830	CLA	CHB-C1B	2.92	1.46	1.39
22	9	613	CLA	C3B-C4B	2.92	1.49	1.42
22	B	809	CLA	CHC-C4B	2.92	1.46	1.39
22	B	827	CLA	C3B-C4B	2.92	1.49	1.42
22	4	614	CLA	C4B-NB	-2.92	1.34	1.37
22	A	839	CLA	CHB-C1B	2.92	1.46	1.39
22	B	819	CLA	CHB-C1B	2.92	1.46	1.39
22	1	612	CLA	CHB-C1B	2.92	1.46	1.39
22	A	813	CLA	C4B-NB	-2.92	1.34	1.37
29	3	608	CHL	OBD-CAD	2.92	1.27	1.22
22	4	611	CLA	C3B-C4B	2.92	1.49	1.42
22	1	603	CLA	C4B-NB	-2.91	1.34	1.37
22	A	830	CLA	C4B-NB	-2.91	1.34	1.37
22	A	836	CLA	C4B-NB	-2.91	1.34	1.37
22	7	614	CLA	C4B-NB	-2.91	1.34	1.37
22	5	602	CLA	C4B-NB	-2.91	1.34	1.37
22	B	837	CLA	OBD-CAD	2.91	1.27	1.22
22	1	611	CLA	C3B-C4B	2.91	1.49	1.42
22	3	611	CLA	C4B-NB	-2.91	1.34	1.37
22	B	832	CLA	CHB-C1B	2.91	1.45	1.39
22	1	609	CLA	C4B-NB	-2.91	1.34	1.37
22	7	612	CLA	C4B-NB	-2.91	1.34	1.37
22	5	610	CLA	C3B-C4B	2.91	1.49	1.42
22	6	622	CLA	C3B-C4B	2.91	1.49	1.42
22	B	840	CLA	CHC-C4B	2.91	1.45	1.39
22	7	614	CLA	C3B-C4B	2.91	1.49	1.42
22	9	602	CLA	C3B-C4B	2.91	1.49	1.42
22	A	804	CLA	C4B-NB	-2.91	1.34	1.37
22	1	608	CLA	C3B-C4B	2.91	1.49	1.42
22	A	833	CLA	CHB-C1B	2.90	1.45	1.39
22	3	611	CLA	C3A-C2A	-2.90	1.51	1.54
22	A	809	CLA	CHB-C1B	2.90	1.45	1.39
22	8	611	CLA	C3B-C4B	2.90	1.49	1.42
29	4	607	CHL	C3B-C4B	2.90	1.49	1.42
22	5	611	CLA	C3B-C4B	2.90	1.49	1.42
22	3	613	CLA	C3B-C4B	2.90	1.49	1.42
22	8	609	CLA	CHB-C1B	2.89	1.45	1.39
22	5	612	CLA	C3B-C4B	2.89	1.49	1.42
22	8	601	CLA	C3B-C4B	2.89	1.49	1.42
22	A	808	CLA	C4B-NB	-2.89	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	613	CLA	C4B-NB	-2.89	1.34	1.37
22	B	816	CLA	OBD-CAD	2.89	1.27	1.22
22	F	301	CLA	C4B-NB	-2.89	1.34	1.37
22	Z	613	CLA	C3B-C4B	2.89	1.49	1.42
22	2	603	CLA	C4B-NB	-2.88	1.34	1.37
22	7	616	CLA	C4B-NB	-2.88	1.34	1.37
22	A	854	CLA	CHB-C1B	2.88	1.45	1.39
22	8	616	CLA	C3B-C4B	2.88	1.49	1.42
29	6	607	CHL	CHB-C1B	2.88	1.45	1.39
22	8	610	CLA	C3B-C4B	2.88	1.49	1.42
22	B	818	CLA	CHB-C1B	2.87	1.45	1.39
22	5	604	CLA	C4B-NB	-2.87	1.34	1.37
22	B	825	CLA	C3B-C4B	2.87	1.49	1.42
29	8	607	CHL	MG-NA	-2.87	1.99	2.06
29	4	618	CHL	MG-NA	-2.87	1.99	2.06
22	1	616	CLA	C3B-C4B	2.87	1.49	1.42
22	7	603	CLA	C3B-C4B	2.87	1.49	1.42
29	6	618	CHL	C3B-C4B	2.87	1.49	1.42
22	A	823	CLA	C3B-C4B	2.87	1.49	1.42
22	1	610	CLA	CHB-C1B	2.87	1.45	1.39
22	G	203	CLA	C3B-C4B	2.87	1.49	1.42
22	6	610	CLA	C3B-C4B	2.87	1.49	1.42
22	G	204	CLA	C4B-NB	-2.87	1.34	1.37
22	B	804	CLA	CHB-C1B	2.87	1.45	1.39
22	G	203	CLA	C4B-NB	-2.87	1.34	1.37
22	A	827	CLA	C3B-C4B	2.87	1.49	1.42
22	2	612	CLA	C4B-NB	-2.86	1.34	1.37
22	8	610	CLA	OBD-CAD	2.86	1.27	1.22
22	8	602	CLA	C3B-C4B	2.86	1.49	1.42
22	A	822	CLA	CHB-C1B	2.86	1.45	1.39
22	6	609	CLA	C3B-C4B	2.86	1.49	1.42
22	5	604	CLA	C3B-C4B	2.86	1.49	1.42
29	Z	607	CHL	MG-NA	-2.86	1.99	2.06
22	L	204	CLA	C3B-C4B	2.86	1.49	1.42
22	A	804	CLA	C3D-C4D	-2.85	1.37	1.44
22	5	621	CLA	C3B-C4B	2.85	1.49	1.42
22	1	609	CLA	C3B-C4B	2.85	1.49	1.42
22	7	610	CLA	C4B-NB	-2.85	1.34	1.37
29	1	601	CHL	C3D-C4D	-2.85	1.37	1.44
22	B	834	CLA	C4B-NB	-2.85	1.34	1.37
22	5	609	CLA	C3B-C4B	2.85	1.49	1.42
22	A	810	CLA	C3B-C4B	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	831	CLA	CHB-C1B	2.84	1.45	1.39
29	Z	601	CHL	C3B-C4B	2.84	1.49	1.42
29	5	608	CHL	C3B-C4B	2.84	1.49	1.42
22	A	815	CLA	C3B-C4B	2.84	1.49	1.42
22	6	614	CLA	C3B-C4B	2.84	1.49	1.42
29	7	607	CHL	C3B-C4B	2.84	1.49	1.42
22	A	805	CLA	C3B-C4B	2.84	1.49	1.42
22	5	616	CLA	C3B-C4B	2.84	1.49	1.42
22	A	812	CLA	C3B-C4B	2.83	1.49	1.42
22	7	601	CLA	C3B-C4B	2.83	1.49	1.42
29	5	607	CHL	C3B-C4B	2.83	1.49	1.42
22	B	823	CLA	C3B-C4B	2.83	1.49	1.42
22	6	617	CLA	C3B-C4B	2.83	1.49	1.42
22	L	203	CLA	C4B-NB	-2.83	1.34	1.37
22	2	609	CLA	C4B-NB	-2.83	1.34	1.37
22	3	617	CLA	C3B-C4B	2.83	1.49	1.42
22	2	610	CLA	C4B-NB	-2.83	1.34	1.37
22	F	303	CLA	C4B-NB	-2.82	1.34	1.37
22	1	603	CLA	C3B-C4B	2.82	1.49	1.42
22	A	816	CLA	C4B-NB	-2.82	1.34	1.37
22	A	854	CLA	C3B-C4B	2.82	1.49	1.42
22	4	613	CLA	C4B-NB	-2.82	1.34	1.37
22	7	611	CLA	C4B-NB	-2.82	1.34	1.37
22	8	613	CLA	C3B-C4B	2.82	1.49	1.42
22	A	841	CLA	CHB-C1B	2.82	1.45	1.39
22	B	815	CLA	C3B-C4B	2.81	1.49	1.42
22	A	840	CLA	C4B-NB	-2.81	1.34	1.37
22	9	604	CLA	C4B-NB	-2.81	1.34	1.37
22	Z	602	CLA	C4B-NB	-2.81	1.34	1.37
29	4	606	CHL	MG-NA	-2.81	1.99	2.06
22	7	608	CLA	C4B-NB	-2.81	1.34	1.37
29	4	608	CHL	C3B-C4B	2.81	1.49	1.42
29	9	607	CHL	MG-NA	-2.81	1.99	2.06
22	9	614	CLA	C4B-NB	-2.81	1.34	1.37
22	6	601	CLA	C3B-C4B	2.81	1.49	1.42
22	7	613	CLA	C3B-C4B	2.80	1.49	1.42
22	3	620	CLA	C4B-NB	-2.80	1.34	1.37
29	4	618	CHL	C3B-C4B	2.79	1.49	1.42
22	1	606	CLA	C4B-NB	-2.79	1.34	1.37
22	A	811	CLA	C4B-NB	-2.79	1.34	1.37
22	6	616	CLA	C4B-NB	-2.79	1.34	1.37
22	A	842	CLA	C4B-NB	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	608	CLA	C3B-C4B	2.79	1.49	1.42
22	A	839	CLA	C3B-C4B	2.79	1.49	1.42
22	Z	603	CLA	C3B-C4B	2.79	1.49	1.42
22	A	832	CLA	C3B-C4B	2.78	1.49	1.42
22	Z	610	CLA	C1C-C2C	2.78	1.50	1.44
22	8	606	CLA	C4B-NB	-2.78	1.34	1.37
22	A	829	CLA	CHB-C1B	2.78	1.45	1.39
29	Z	607	CHL	C3B-C4B	2.77	1.49	1.42
22	6	603	CLA	C3B-C4B	2.77	1.49	1.42
22	B	803	CLA	C3B-C4B	2.77	1.49	1.42
22	1	613	CLA	C3B-C4B	2.76	1.49	1.42
22	5	603	CLA	C4D-CHA	2.76	1.48	1.38
22	3	610	CLA	C4B-NB	-2.76	1.34	1.37
22	3	613	CLA	C4B-NB	-2.76	1.34	1.37
22	6	613	CLA	C4B-NB	-2.76	1.34	1.37
29	6	607	CHL	MG-NA	-2.76	1.99	2.06
29	5	608	CHL	MG-NA	-2.76	1.99	2.06
22	Z	612	CLA	C4B-NB	-2.76	1.34	1.37
22	B	803	CLA	CHB-C1B	2.75	1.45	1.39
22	B	812	CLA	C4B-NB	-2.75	1.34	1.37
22	1	610	CLA	C1C-C2C	2.75	1.49	1.44
22	3	602	CLA	C3B-C4B	2.75	1.49	1.42
22	5	606	CLA	C4B-NB	-2.75	1.34	1.37
22	9	604	CLA	C4C-C3C	2.75	1.49	1.45
22	B	840	CLA	C1C-NC	-2.75	1.33	1.37
22	6	602	CLA	C4B-NB	-2.75	1.34	1.37
22	4	611	CLA	C4D-CHA	2.75	1.48	1.38
22	2	609	CLA	C4D-CHA	2.75	1.48	1.38
22	A	837	CLA	C4D-CHA	2.75	1.48	1.38
22	L	204	CLA	C4C-C3C	2.75	1.49	1.45
22	8	611	CLA	C4D-CHA	2.74	1.48	1.38
29	6	608	CHL	MG-NA	-2.74	1.99	2.06
22	B	841	CLA	C3B-C4B	2.74	1.49	1.42
22	A	814	CLA	C3B-C4B	2.74	1.49	1.42
22	3	604	CLA	C3B-C4B	2.74	1.49	1.42
22	B	836	CLA	OBD-CAD	2.74	1.27	1.22
22	3	609	CLA	C3B-C4B	2.74	1.49	1.42
22	A	802	CLA	C3B-C4B	2.73	1.49	1.42
22	A	833	CLA	C4B-NB	-2.73	1.34	1.37
22	A	807	CLA	C3B-C4B	2.73	1.49	1.42
22	A	822	CLA	C3B-C4B	2.73	1.49	1.42
29	3	608	CHL	C3D-C4D	-2.73	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	835	CLA	C3B-C4B	2.73	1.49	1.42
22	9	601	CLA	C4D-CHA	2.73	1.48	1.38
22	1	612	CLA	C4B-NB	-2.73	1.34	1.37
29	5	618	CHL	MG-NA	-2.73	1.99	2.06
29	9	606	CHL	MG-NA	-2.72	1.99	2.06
22	7	610	CLA	CHB-C1B	2.72	1.45	1.39
22	8	601	CLA	C4D-CHA	2.72	1.48	1.38
22	6	612	CLA	C4B-NB	-2.72	1.34	1.37
22	B	822	CLA	C4B-NB	-2.72	1.34	1.37
22	B	813	CLA	C3B-C4B	2.72	1.49	1.42
22	Z	609	CLA	C4D-CHA	2.72	1.48	1.38
22	K	4002	CLA	C4D-CHA	2.72	1.48	1.38
22	8	609	CLA	C3B-C4B	2.72	1.49	1.42
22	7	609	CLA	C3B-C4B	2.72	1.49	1.42
22	B	808	CLA	C3B-C4B	2.71	1.49	1.42
22	B	830	CLA	C3B-C4B	2.71	1.49	1.42
22	9	611	CLA	C4D-CHA	2.71	1.48	1.38
22	4	609	CLA	C4D-CHA	2.71	1.48	1.38
22	7	611	CLA	C4D-CHA	2.71	1.48	1.38
22	3	603	CLA	C4D-CHA	2.71	1.48	1.38
22	Z	609	CLA	C3B-C4B	2.71	1.49	1.42
22	B	804	CLA	C3B-C4B	2.70	1.49	1.42
29	8	607	CHL	C3D-C4D	-2.70	1.38	1.44
22	B	829	CLA	C3B-C4B	2.70	1.49	1.42
22	7	614	CLA	C4D-CHA	2.70	1.48	1.38
22	5	604	CLA	C4C-C3C	2.70	1.49	1.45
22	F	303	CLA	C4D-CHA	2.70	1.48	1.38
22	5	616	CLA	C4D-CHA	2.70	1.48	1.38
22	4	609	CLA	CHB-C1B	2.69	1.45	1.39
22	B	840	CLA	C3B-C4B	2.69	1.49	1.42
22	B	819	CLA	C3B-C4B	2.69	1.49	1.42
22	5	606	CLA	C4D-CHA	2.69	1.48	1.38
22	4	602	CLA	C3B-C4B	2.69	1.49	1.42
22	B	807	CLA	C4D-CHA	2.69	1.48	1.38
22	A	834	CLA	C3B-C4B	2.69	1.49	1.42
22	8	603	CLA	C3B-C4B	2.69	1.49	1.42
22	6	609	CLA	C4D-CHA	2.69	1.47	1.38
29	6	606	CHL	C4B-NB	-2.69	1.34	1.37
22	7	606	CLA	C4B-NB	-2.69	1.34	1.37
22	A	817	CLA	C4B-NB	-2.68	1.34	1.37
22	3	620	CLA	C4D-CHA	2.68	1.47	1.38
22	6	604	CLA	C4D-CHA	2.68	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	603	CLA	C4D-CHA	2.68	1.47	1.38
22	B	814	CLA	C3B-C4B	2.68	1.49	1.42
22	3	607	CLA	C3B-C4B	2.68	1.49	1.42
22	5	604	CLA	C4D-CHA	2.68	1.47	1.38
22	4	604	CLA	C3B-C4B	2.68	1.49	1.42
22	9	603	CLA	C4B-NB	-2.68	1.34	1.37
22	3	611	CLA	C4D-CHA	2.67	1.47	1.38
22	B	833	CLA	C3B-C4B	2.67	1.49	1.42
22	B	807	CLA	C3B-C4B	2.67	1.49	1.42
22	B	818	CLA	C3B-C4B	2.67	1.49	1.42
22	5	611	CLA	C4D-CHA	2.67	1.47	1.38
22	B	835	CLA	C4D-CHA	2.67	1.47	1.38
22	B	836	CLA	C4D-CHA	2.67	1.47	1.38
22	8	612	CLA	C4B-NB	-2.67	1.34	1.37
22	A	843	CLA	C4D-CHA	2.67	1.47	1.38
22	Z	616	CLA	C4D-CHA	2.67	1.47	1.38
22	F	304	CLA	C4D-CHA	2.67	1.47	1.38
22	5	603	CLA	C3D-C4D	-2.67	1.38	1.44
22	B	820	CLA	C3B-C4B	2.67	1.49	1.42
22	6	603	CLA	C4D-CHA	2.67	1.47	1.38
22	7	616	CLA	C4D-CHA	2.66	1.47	1.38
22	9	610	CLA	C3B-C4B	2.66	1.49	1.42
29	5	618	CHL	C3B-C4B	2.66	1.49	1.42
22	1	604	CLA	C3B-C4B	2.66	1.49	1.42
22	1	616	CLA	C4D-CHA	2.66	1.47	1.38
22	G	204	CLA	C4D-CHA	2.66	1.47	1.38
22	3	604	CLA	C4D-CHA	2.66	1.47	1.38
22	8	604	CLA	C3B-C4B	2.66	1.49	1.42
29	7	607	CHL	MG-NA	-2.66	1.99	2.06
22	A	816	CLA	C4D-CHA	2.66	1.47	1.38
22	B	834	CLA	C4D-CHA	2.66	1.47	1.38
22	2	606	CLA	C4D-CHA	2.66	1.47	1.38
22	8	609	CLA	C4D-CHA	2.66	1.47	1.38
22	B	805	CLA	C4D-CHA	2.66	1.47	1.38
22	A	836	CLA	C4D-CHA	2.66	1.47	1.38
22	1	603	CLA	C4D-CHA	2.65	1.47	1.38
22	B	852	CLA	C4D-CHA	2.65	1.47	1.38
22	7	620	CLA	C4D-CHA	2.65	1.47	1.38
22	B	833	CLA	C1B-C2B	2.65	1.49	1.43
22	5	601	CLA	C4D-CHA	2.65	1.47	1.38
22	A	839	CLA	C4D-CHA	2.65	1.47	1.38
22	9	613	CLA	C4D-CHA	2.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	613	CLA	C4D-CHA	2.65	1.47	1.38
29	3	608	CHL	MG-NA	-2.65	2.00	2.06
22	9	609	CLA	C3B-C4B	2.65	1.49	1.42
22	B	836	CLA	C3D-C4D	-2.65	1.38	1.44
22	1	609	CLA	C4D-CHA	2.65	1.47	1.38
22	B	811	CLA	C4D-CHA	2.65	1.47	1.38
22	8	616	CLA	C4D-CHA	2.65	1.47	1.38
22	9	614	CLA	C4D-CHA	2.65	1.47	1.38
22	8	613	CLA	C4B-NB	-2.65	1.34	1.37
22	B	809	CLA	C4D-CHA	2.65	1.47	1.38
22	3	606	CLA	C4D-CHA	2.65	1.47	1.38
22	B	806	CLA	C3D-C4D	-2.65	1.38	1.44
22	6	604	CLA	C3B-C4B	2.65	1.49	1.42
22	B	823	CLA	C4D-CHA	2.64	1.47	1.38
29	4	607	CHL	C3D-C4D	-2.64	1.38	1.44
22	A	819	CLA	C3B-C4B	2.64	1.48	1.42
22	5	614	CLA	C4D-CHA	2.64	1.47	1.38
29	6	606	CHL	C3D-C4D	-2.64	1.38	1.44
22	B	824	CLA	C3B-C4B	2.64	1.48	1.42
22	2	613	CLA	C4D-CHA	2.64	1.47	1.38
22	5	609	CLA	C4D-CHA	2.64	1.47	1.38
22	Z	604	CLA	C3B-C4B	2.64	1.48	1.42
22	G	203	CLA	C4D-CHA	2.64	1.47	1.38
22	B	806	CLA	C4D-CHA	2.64	1.47	1.38
22	9	602	CLA	C4D-CHA	2.64	1.47	1.38
22	3	610	CLA	C1C-C2C	2.64	1.49	1.44
22	Z	613	CLA	C4D-CHA	2.64	1.47	1.38
21	A	801	CL0	C4B-NB	-2.64	1.34	1.37
22	5	612	CLA	C4D-CHA	2.64	1.47	1.38
22	6	616	CLA	C4D-CHA	2.63	1.47	1.38
22	9	609	CLA	C4D-CHA	2.63	1.47	1.38
22	B	818	CLA	C4D-CHA	2.63	1.47	1.38
22	B	815	CLA	C4D-CHA	2.63	1.47	1.38
22	6	611	CLA	C4D-CHA	2.63	1.47	1.38
22	A	840	CLA	C4D-CHA	2.63	1.47	1.38
29	6	618	CHL	MG-NA	-2.63	2.00	2.06
22	9	612	CLA	C4D-CHA	2.63	1.47	1.38
22	Z	604	CLA	C4D-CHA	2.63	1.47	1.38
22	2	601	CLA	C4D-CHA	2.63	1.47	1.38
22	2	603	CLA	C4D-CHA	2.63	1.47	1.38
22	A	845	CLA	C4D-CHA	2.63	1.47	1.38
22	B	833	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	614	CLA	C4D-CHA	2.63	1.47	1.38
22	A	841	CLA	C4B-NB	-2.63	1.34	1.37
22	A	831	CLA	C4D-CHA	2.62	1.47	1.38
22	3	607	CLA	C4D-CHA	2.62	1.47	1.38
22	B	836	CLA	C3B-C4B	2.62	1.48	1.42
21	A	801	CL0	C4D-CHA	2.62	1.47	1.38
29	6	606	CHL	MG-NA	-2.62	2.00	2.06
29	6	606	CHL	C2C-C1C	2.62	1.50	1.44
22	A	826	CLA	C4D-CHA	2.62	1.47	1.38
22	A	834	CLA	C1B-C2B	2.62	1.49	1.43
22	8	614	CLA	C4D-CHA	2.61	1.47	1.38
22	Z	608	CLA	C4D-CHA	2.61	1.47	1.38
22	B	814	CLA	C3D-C4D	-2.61	1.38	1.44
22	J	3002	CLA	C4D-CHA	2.61	1.47	1.38
22	6	610	CLA	C4D-CHA	2.61	1.47	1.38
22	A	830	CLA	C4D-CHA	2.61	1.47	1.38
22	A	822	CLA	C4D-CHA	2.61	1.47	1.38
22	A	818	CLA	C4B-NB	-2.61	1.34	1.37
22	B	817	CLA	C4D-CHA	2.61	1.47	1.38
22	A	833	CLA	C4D-CHA	2.61	1.47	1.38
22	7	603	CLA	C3D-C4D	-2.61	1.38	1.44
22	Z	614	CLA	C4D-CHA	2.60	1.47	1.38
22	A	828	CLA	C4D-CHA	2.60	1.47	1.38
29	6	608	CHL	C3D-C4D	-2.60	1.38	1.44
22	B	826	CLA	C4D-CHA	2.60	1.47	1.38
22	4	603	CLA	C4D-CHA	2.60	1.47	1.38
22	A	813	CLA	C4D-CHA	2.60	1.47	1.38
22	A	832	CLA	C4D-CHA	2.60	1.47	1.38
22	A	838	CLA	C4D-CHA	2.60	1.47	1.38
22	Z	606	CLA	C4D-CHA	2.60	1.47	1.38
22	5	621	CLA	C4C-C3C	2.60	1.49	1.45
29	Z	601	CHL	MG-NA	-2.60	2.00	2.06
22	4	616	CLA	C4D-CHA	2.60	1.47	1.38
22	F	301	CLA	C3D-C4D	-2.60	1.38	1.44
22	B	839	CLA	C4D-CHA	2.60	1.47	1.38
22	3	609	CLA	C4D-CHA	2.60	1.47	1.38
22	5	621	CLA	C4D-CHA	2.60	1.47	1.38
22	A	809	CLA	C4D-CHA	2.60	1.47	1.38
22	6	622	CLA	C4D-CHA	2.60	1.47	1.38
22	A	829	CLA	C3B-C4B	2.60	1.48	1.42
22	B	813	CLA	C4D-CHA	2.60	1.47	1.38
22	8	610	CLA	C4D-CHA	2.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	612	CLA	C4D-CHA	2.59	1.47	1.38
22	1	603	CLA	C1B-C2B	2.59	1.49	1.43
29	7	607	CHL	C3D-C4D	-2.59	1.38	1.44
22	A	842	CLA	C4D-CHA	2.59	1.47	1.38
22	2	607	CLA	C4D-CHA	2.59	1.47	1.38
22	A	808	CLA	C4D-CHA	2.59	1.47	1.38
22	1	608	CLA	C4D-CHA	2.59	1.47	1.38
22	A	819	CLA	C4D-CHA	2.59	1.47	1.38
22	B	802	CLA	C1B-C2B	2.59	1.49	1.43
22	B	840	CLA	C4D-CHA	2.58	1.47	1.38
22	A	841	CLA	C4D-CHA	2.58	1.47	1.38
22	3	612	CLA	C4B-NB	-2.58	1.34	1.37
22	A	842	CLA	C3D-C4D	-2.58	1.38	1.44
22	B	824	CLA	C4D-CHA	2.58	1.47	1.38
29	4	606	CHL	C3D-C4D	-2.58	1.38	1.44
22	B	819	CLA	C4D-CHA	2.58	1.47	1.38
22	B	828	CLA	C4D-CHA	2.58	1.47	1.38
22	8	603	CLA	C3D-C4D	-2.58	1.38	1.44
22	1	602	CLA	C4B-NB	-2.58	1.34	1.37
22	A	823	CLA	C4D-CHA	2.58	1.47	1.38
22	4	612	CLA	C4B-NB	-2.58	1.34	1.37
29	5	618	CHL	C3D-C4D	-2.58	1.38	1.44
22	F	301	CLA	C4D-CHA	2.58	1.47	1.38
22	4	610	CLA	C4D-CHA	2.58	1.47	1.38
29	Z	601	CHL	C3D-C4D	-2.58	1.38	1.44
22	7	602	CLA	C4B-NB	-2.58	1.34	1.37
22	A	825	CLA	C4D-CHA	2.57	1.47	1.38
22	2	602	CLA	C4D-CHA	2.57	1.47	1.38
22	4	604	CLA	C4D-CHA	2.57	1.47	1.38
22	B	823	CLA	C4C-C3C	2.57	1.49	1.45
22	3	613	CLA	C4D-CHA	2.57	1.47	1.38
22	1	606	CLA	C4D-CHA	2.57	1.47	1.38
22	7	609	CLA	C4D-CHA	2.57	1.47	1.38
22	5	610	CLA	C4D-CHA	2.57	1.47	1.38
22	A	821	CLA	C4D-CHA	2.57	1.47	1.38
22	2	612	CLA	C4C-C3C	2.57	1.49	1.45
22	6	612	CLA	C4D-CHA	2.57	1.47	1.38
22	4	601	CLA	C4D-CHA	2.57	1.47	1.38
29	4	608	CHL	C2C-C1C	2.57	1.50	1.44
22	B	804	CLA	C4D-CHA	2.57	1.47	1.38
22	Z	611	CLA	C4D-CHA	2.57	1.47	1.38
22	A	807	CLA	C4D-CHA	2.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	837	CLA	C4D-CHA	2.56	1.47	1.38
22	A	806	CLA	C3B-C4B	2.56	1.48	1.42
22	4	612	CLA	C4D-CHA	2.56	1.47	1.38
22	2	602	CLA	C3B-C4B	2.56	1.48	1.42
22	B	832	CLA	C4B-NB	-2.56	1.34	1.37
22	8	606	CLA	C4D-CHA	2.56	1.47	1.38
22	A	825	CLA	C3B-C4B	2.56	1.48	1.42
22	9	603	CLA	C4D-CHA	2.56	1.47	1.38
22	7	612	CLA	C4D-CHA	2.56	1.47	1.38
22	8	612	CLA	C4D-CHA	2.56	1.47	1.38
22	A	824	CLA	C1B-C2B	2.56	1.49	1.43
22	4	601	CLA	C1B-C2B	2.56	1.49	1.43
22	2	606	CLA	C3A-C2A	-2.56	1.52	1.54
22	A	834	CLA	C4D-CHA	2.56	1.47	1.38
22	8	602	CLA	C4D-CHA	2.56	1.47	1.38
22	9	604	CLA	C4D-CHA	2.56	1.47	1.38
22	3	617	CLA	C4D-CHA	2.56	1.47	1.38
22	A	809	CLA	C1C-C2C	2.56	1.49	1.44
22	7	604	CLA	C4D-CHA	2.55	1.47	1.38
22	L	204	CLA	C4D-CHA	2.55	1.47	1.38
22	B	829	CLA	C3D-C4D	-2.55	1.38	1.44
22	6	617	CLA	C4D-CHA	2.55	1.47	1.38
22	A	843	CLA	C3B-C4B	2.55	1.48	1.42
22	B	830	CLA	C4D-CHA	2.55	1.47	1.38
22	7	610	CLA	C4D-CHA	2.55	1.47	1.38
22	7	613	CLA	C4D-CHA	2.55	1.47	1.38
22	Z	612	CLA	C4D-CHA	2.55	1.47	1.38
22	4	614	CLA	C4D-CHA	2.55	1.47	1.38
22	K	4003	CLA	C4D-CHA	2.55	1.47	1.38
22	B	820	CLA	C3D-C4D	-2.55	1.38	1.44
22	1	604	CLA	C4D-CHA	2.55	1.47	1.38
22	B	840	CLA	C3D-C4D	-2.55	1.38	1.44
22	1	611	CLA	C4D-CHA	2.55	1.47	1.38
22	1	602	CLA	C4D-CHA	2.55	1.47	1.38
22	2	601	CLA	C1B-C2B	2.55	1.49	1.43
29	4	618	CHL	C3D-C4D	-2.54	1.38	1.44
22	Z	616	CLA	C1B-C2B	2.54	1.49	1.43
22	5	613	CLA	C4D-CHA	2.54	1.47	1.38
22	A	824	CLA	C4D-CHA	2.54	1.47	1.38
22	3	613	CLA	C4C-C3C	2.54	1.49	1.45
22	4	601	CLA	C3B-C4B	2.54	1.48	1.42
22	Z	610	CLA	C4D-CHA	2.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	204	CLA	C1B-C2B	2.54	1.49	1.43
22	2	611	CLA	C4D-CHA	2.54	1.47	1.38
22	8	613	CLA	C4D-CHA	2.54	1.47	1.38
22	B	826	CLA	C3D-C4D	-2.54	1.38	1.44
22	2	612	CLA	C1B-C2B	2.54	1.49	1.43
22	2	614	CLA	C4D-CHA	2.54	1.47	1.38
22	B	838	CLA	C4D-CHA	2.54	1.47	1.38
22	7	603	CLA	C4D-CHA	2.54	1.47	1.38
22	8	603	CLA	C4D-CHA	2.54	1.47	1.38
22	5	621	CLA	C3D-C4D	-2.54	1.38	1.44
29	9	607	CHL	C1B-C2B	2.53	1.49	1.43
22	7	608	CLA	C4D-CHA	2.53	1.47	1.38
22	7	610	CLA	C1C-C2C	2.53	1.49	1.44
22	4	602	CLA	C4C-C3C	2.53	1.49	1.45
22	B	839	CLA	C3D-C4D	-2.53	1.38	1.44
22	2	610	CLA	C4D-CHA	2.53	1.47	1.38
22	B	829	CLA	C1C-C2C	2.53	1.49	1.44
22	B	812	CLA	C4D-CHA	2.53	1.47	1.38
22	B	817	CLA	C3D-C4D	-2.53	1.38	1.44
22	6	601	CLA	C4D-CHA	2.53	1.47	1.38
22	B	821	CLA	C4D-CHA	2.53	1.47	1.38
22	4	603	CLA	C3D-C4D	-2.53	1.38	1.44
22	A	803	CLA	C4D-CHA	2.53	1.47	1.38
22	8	601	CLA	C4C-C3C	2.53	1.49	1.45
22	B	803	CLA	C4D-CHA	2.53	1.47	1.38
22	B	820	CLA	C1B-C2B	2.53	1.49	1.43
22	Z	602	CLA	C4D-CHA	2.53	1.47	1.38
29	5	608	CHL	C3D-C4D	-2.53	1.38	1.44
22	6	602	CLA	C4D-CHA	2.52	1.47	1.38
22	4	613	CLA	C4D-CHA	2.52	1.47	1.38
29	6	608	CHL	C2C-C1C	2.52	1.49	1.44
22	9	610	CLA	C4D-CHA	2.52	1.47	1.38
22	2	603	CLA	C4C-C3C	2.52	1.49	1.45
22	A	828	CLA	C3D-C4D	-2.52	1.38	1.44
22	2	613	CLA	C4C-C3C	2.52	1.49	1.45
22	B	822	CLA	C4D-CHA	2.52	1.47	1.38
22	3	603	CLA	C4B-NB	-2.52	1.34	1.37
22	2	603	CLA	C1B-C2B	2.52	1.49	1.43
22	B	803	CLA	C1C-NC	-2.52	1.34	1.37
29	4	607	CHL	C1B-C2B	2.52	1.49	1.43
29	9	607	CHL	C3D-C4D	-2.52	1.38	1.44
22	A	814	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	612	CLA	C4D-CHA	2.52	1.47	1.38
22	B	816	CLA	C4D-CHA	2.52	1.47	1.38
22	9	612	CLA	C1B-C2B	2.52	1.49	1.43
22	A	819	CLA	C3D-C4D	-2.52	1.38	1.44
22	B	816	CLA	C3D-C4D	-2.52	1.38	1.44
22	K	4003	CLA	C1B-C2B	2.52	1.49	1.43
22	B	841	CLA	C1B-C2B	2.52	1.49	1.43
22	3	612	CLA	C4D-CHA	2.52	1.47	1.38
22	6	601	CLA	C1B-C2B	2.52	1.49	1.43
22	A	825	CLA	C1B-C2B	2.51	1.49	1.43
29	9	607	CHL	C4C-C3C	2.51	1.49	1.45
22	A	817	CLA	C4D-CHA	2.51	1.47	1.38
22	6	622	CLA	C1B-C2B	2.51	1.49	1.43
22	8	604	CLA	C4D-CHA	2.51	1.47	1.38
22	B	827	CLA	C4D-CHA	2.51	1.47	1.38
22	A	805	CLA	C3D-C4D	-2.51	1.38	1.44
22	B	831	CLA	C4D-CHA	2.51	1.47	1.38
22	6	613	CLA	C4D-CHA	2.51	1.47	1.38
29	5	607	CHL	C3D-C4D	-2.51	1.38	1.44
22	A	818	CLA	C4D-CHA	2.51	1.47	1.38
22	9	614	CLA	C4C-C3C	2.51	1.49	1.45
22	1	610	CLA	C4D-CHA	2.51	1.47	1.38
22	3	610	CLA	C4D-CHA	2.51	1.47	1.38
22	7	606	CLA	C4D-CHA	2.51	1.47	1.38
22	1	614	CLA	C4D-CHA	2.51	1.47	1.38
22	Z	609	CLA	C4C-C3C	2.50	1.49	1.45
22	B	852	CLA	C1B-C2B	2.50	1.49	1.43
22	B	830	CLA	C3D-C4D	-2.50	1.38	1.44
22	7	601	CLA	C4D-CHA	2.50	1.47	1.38
22	8	610	CLA	C1C-C2C	2.50	1.49	1.44
29	4	608	CHL	C3D-C4D	-2.50	1.38	1.44
22	4	616	CLA	C1B-C2B	2.50	1.49	1.43
22	7	608	CLA	C3D-C4D	-2.50	1.38	1.44
22	9	613	CLA	C1B-C2B	2.50	1.49	1.43
22	2	611	CLA	C1B-C2B	2.50	1.49	1.43
29	9	606	CHL	C3D-C4D	-2.50	1.38	1.44
22	A	814	CLA	C1B-C2B	2.50	1.49	1.43
22	1	616	CLA	C1B-C2B	2.50	1.49	1.43
22	A	810	CLA	C4D-CHA	2.50	1.47	1.38
22	A	829	CLA	C4D-CHA	2.50	1.47	1.38
22	G	203	CLA	C1B-C2B	2.50	1.49	1.43
22	4	611	CLA	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	608	CLA	C4D-CHA	2.50	1.47	1.38
22	B	810	CLA	C4D-CHA	2.49	1.47	1.38
22	A	806	CLA	C3D-C4D	-2.49	1.38	1.44
29	Z	607	CHL	C3D-C4D	-2.49	1.38	1.44
22	9	601	CLA	C4C-C3C	2.49	1.49	1.45
22	A	820	CLA	C4D-CHA	2.49	1.47	1.38
22	2	609	CLA	C4C-C3C	2.49	1.49	1.45
29	1	601	CHL	MG-NA	-2.49	2.00	2.06
22	9	603	CLA	C4C-C3C	2.49	1.49	1.45
22	B	811	CLA	C1B-C2B	2.49	1.49	1.43
22	A	838	CLA	C3D-C4D	-2.49	1.38	1.44
22	4	602	CLA	C4D-CHA	2.49	1.47	1.38
22	2	614	CLA	C1B-C2B	2.49	1.49	1.43
22	A	816	CLA	C4C-C3C	2.49	1.49	1.45
22	3	602	CLA	C4D-CHA	2.49	1.47	1.38
22	9	601	CLA	C1B-C2B	2.49	1.49	1.43
22	4	614	CLA	C1C-C2C	2.49	1.49	1.44
22	5	617	CLA	C4D-CHA	2.48	1.47	1.38
22	A	829	CLA	C1C-C2C	2.48	1.49	1.44
22	B	808	CLA	C4D-CHA	2.48	1.47	1.38
22	6	603	CLA	C3D-C4D	-2.48	1.38	1.44
22	3	611	CLA	C4C-C3C	2.48	1.49	1.45
22	4	616	CLA	C4C-C3C	2.48	1.49	1.45
22	A	806	CLA	C4D-CHA	2.48	1.47	1.38
29	Z	601	CHL	C2C-C1C	2.48	1.49	1.44
29	6	618	CHL	C3D-C4D	-2.48	1.38	1.44
29	6	607	CHL	C3D-C4D	-2.48	1.38	1.44
22	A	835	CLA	C1B-C2B	2.48	1.49	1.43
22	A	815	CLA	C3D-C4D	-2.47	1.38	1.44
22	B	811	CLA	C4B-C3B	2.47	1.49	1.43
29	8	607	CHL	C1B-C2B	2.47	1.49	1.43
22	4	602	CLA	C3D-C4D	-2.47	1.38	1.44
22	A	822	CLA	C3D-C4D	-2.47	1.38	1.44
22	A	854	CLA	C1C-C2C	2.47	1.49	1.44
29	Z	607	CHL	C1B-C2B	2.47	1.49	1.43
29	6	608	CHL	C3B-C4B	2.47	1.48	1.42
22	A	835	CLA	C3D-C4D	-2.47	1.38	1.44
22	B	841	CLA	C3D-C4D	-2.47	1.38	1.44
22	B	832	CLA	C4D-CHA	2.47	1.47	1.38
22	5	602	CLA	C3D-C4D	-2.47	1.38	1.44
22	2	607	CLA	C4C-C3C	2.47	1.49	1.45
22	A	802	CLA	C3D-C4D	-2.47	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	827	CLA	C3D-C4D	-2.47	1.38	1.44
22	B	807	CLA	C3D-C4D	-2.47	1.38	1.44
22	B	807	CLA	C1B-C2B	2.46	1.49	1.43
22	Z	603	CLA	C1B-C2B	2.46	1.49	1.43
22	3	611	CLA	C1B-C2B	2.46	1.49	1.43
22	Z	613	CLA	C1C-C2C	2.46	1.49	1.44
22	6	609	CLA	C4C-C3C	2.46	1.49	1.45
22	7	620	CLA	C1B-C2B	2.46	1.49	1.43
22	A	820	CLA	C3B-C4B	2.46	1.48	1.42
22	F	304	CLA	C1B-C2B	2.46	1.49	1.43
22	8	610	CLA	C3D-C4D	-2.46	1.38	1.44
22	B	814	CLA	C4D-CHA	2.46	1.47	1.38
22	2	614	CLA	C4C-C3C	2.46	1.49	1.45
22	A	802	CLA	C1B-C2B	2.46	1.49	1.43
22	2	613	CLA	C1B-C2B	2.46	1.49	1.43
22	B	810	CLA	C1B-C2B	2.46	1.49	1.43
22	Z	612	CLA	C1B-C2B	2.45	1.49	1.43
22	G	204	CLA	C4C-C3C	2.45	1.49	1.45
22	2	606	CLA	C4C-C3C	2.45	1.49	1.45
22	B	825	CLA	C3D-C4D	-2.45	1.38	1.44
22	A	854	CLA	C4D-CHA	2.45	1.47	1.38
22	A	807	CLA	C3D-C4D	-2.45	1.38	1.44
22	7	602	CLA	C4D-CHA	2.45	1.47	1.38
22	2	609	CLA	C1B-C2B	2.45	1.49	1.43
22	B	838	CLA	C3D-C4D	-2.45	1.38	1.44
22	B	852	CLA	C4C-C3C	2.45	1.49	1.45
29	6	618	CHL	C2C-C1C	2.45	1.49	1.44
22	B	805	CLA	C4B-NB	-2.45	1.34	1.37
22	A	832	CLA	C3D-C4D	-2.44	1.38	1.44
22	A	811	CLA	C4D-CHA	2.44	1.47	1.38
22	B	829	CLA	C4D-CHA	2.44	1.47	1.38
22	3	614	CLA	C4C-C3C	2.44	1.49	1.45
22	A	835	CLA	C4D-CHA	2.44	1.47	1.38
24	B	851	LHG	O8-C23	2.44	1.45	1.33
22	B	816	CLA	C1C-C2C	2.44	1.49	1.44
22	B	828	CLA	C3D-C4D	-2.44	1.38	1.44
22	A	840	CLA	C3D-C4D	-2.44	1.38	1.44
29	4	606	CHL	C2C-C1C	2.44	1.49	1.44
22	6	614	CLA	C4D-CHA	2.44	1.47	1.38
22	A	815	CLA	C1B-C2B	2.44	1.49	1.43
22	7	609	CLA	C4C-C3C	2.44	1.49	1.45
22	6	602	CLA	C1C-C2C	2.44	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	614	CLA	C1B-C2B	2.44	1.49	1.43
22	5	613	CLA	C4C-C3C	2.44	1.49	1.45
22	7	614	CLA	C4C-C3C	2.44	1.49	1.45
22	A	825	CLA	C3D-C4D	-2.44	1.38	1.44
22	A	808	CLA	C1C-C2C	2.43	1.49	1.44
22	Z	603	CLA	C4C-C3C	2.43	1.49	1.45
22	3	613	CLA	C1B-C2B	2.43	1.49	1.43
22	A	826	CLA	C3D-C4D	-2.43	1.38	1.44
22	4	613	CLA	C1B-C2B	2.43	1.49	1.43
29	6	618	CHL	C1B-C2B	2.43	1.49	1.43
22	B	806	CLA	C1C-C2C	2.43	1.49	1.44
22	6	614	CLA	C3D-C4D	-2.43	1.38	1.44
22	7	601	CLA	C1B-C2B	2.43	1.49	1.43
22	9	604	CLA	C1B-C2B	2.43	1.49	1.43
22	9	611	CLA	C1B-C2B	2.43	1.49	1.43
22	5	603	CLA	OBD-CAD	2.43	1.26	1.22
22	A	820	CLA	C3D-C4D	-2.43	1.38	1.44
22	5	602	CLA	C4D-CHA	2.43	1.47	1.38
21	A	801	CL0	C3D-C4D	-2.43	1.38	1.44
22	7	604	CLA	C1B-C2B	2.43	1.49	1.43
22	8	601	CLA	C1B-C2B	2.43	1.49	1.43
22	Z	604	CLA	C4C-C3C	2.43	1.49	1.45
22	B	820	CLA	C4D-CHA	2.43	1.47	1.38
22	2	602	CLA	C1B-C2B	2.43	1.49	1.43
22	9	613	CLA	C4C-C3C	2.43	1.49	1.45
29	4	608	CHL	MG-NA	-2.43	2.00	2.06
22	A	814	CLA	C3D-C4D	-2.43	1.38	1.44
22	5	612	CLA	C1B-C2B	2.43	1.49	1.43
22	1	613	CLA	C1B-C2B	2.42	1.49	1.43
22	7	616	CLA	C4C-C3C	2.42	1.49	1.45
22	5	614	CLA	C4C-C3C	2.42	1.49	1.45
22	7	613	CLA	C1B-C2B	2.42	1.49	1.43
22	Z	616	CLA	C4C-C3C	2.42	1.49	1.45
22	A	817	CLA	C3D-C4D	-2.42	1.38	1.44
22	A	810	CLA	C3D-C4D	-2.42	1.38	1.44
22	8	606	CLA	C3D-C4D	-2.42	1.38	1.44
22	L	203	CLA	C4D-CHA	2.42	1.47	1.38
22	G	204	CLA	C1B-C2B	2.42	1.48	1.43
22	1	616	CLA	C4C-C3C	2.42	1.49	1.45
22	2	611	CLA	C4C-C3C	2.42	1.49	1.45
22	7	610	CLA	CHB-C4A	-2.42	1.31	1.37
22	B	811	CLA	C3D-C4D	-2.41	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	603	CLA	C3D-C4D	-2.41	1.38	1.44
22	Z	611	CLA	C1B-C2B	2.41	1.48	1.43
22	B	834	CLA	C4C-C3C	2.41	1.49	1.45
22	2	607	CLA	C1B-C2B	2.41	1.48	1.43
29	5	607	CHL	C1B-C2B	2.41	1.48	1.43
22	B	808	CLA	C1B-C2B	2.41	1.48	1.43
22	7	608	CLA	C1C-C2C	2.41	1.49	1.44
22	A	816	CLA	C3D-C4D	-2.41	1.38	1.44
22	6	611	CLA	C4C-C3C	2.41	1.49	1.45
22	6	622	CLA	C4C-C3C	2.41	1.49	1.45
22	3	614	CLA	C1B-C2B	2.41	1.48	1.43
22	F	301	CLA	C1C-C2C	2.41	1.49	1.44
22	A	821	CLA	C3D-C4D	-2.41	1.38	1.44
22	B	822	CLA	C3D-C4D	-2.41	1.38	1.44
22	9	611	CLA	C1C-C2C	2.41	1.49	1.44
29	7	607	CHL	C1B-C2B	2.41	1.48	1.43
22	B	838	CLA	C4B-NB	-2.41	1.34	1.37
22	B	824	CLA	C3D-C4D	-2.41	1.38	1.44
22	A	807	CLA	C1B-C2B	2.41	1.48	1.43
22	1	608	CLA	C3D-C4D	-2.41	1.38	1.44
22	7	601	CLA	C3D-C4D	-2.40	1.38	1.44
22	2	610	CLA	C4C-C3C	2.40	1.49	1.45
22	B	834	CLA	C3D-C4D	-2.40	1.38	1.44
29	5	608	CHL	C4D-CHA	2.40	1.46	1.38
22	B	819	CLA	C3D-C4D	-2.40	1.38	1.44
22	3	609	CLA	C4C-C3C	2.40	1.49	1.45
22	6	617	CLA	C1B-C2B	2.40	1.48	1.43
22	B	802	CLA	C4D-CHA	2.40	1.46	1.38
22	7	616	CLA	C1D-C2D	2.40	1.50	1.45
22	7	616	CLA	C1B-C2B	2.40	1.48	1.43
22	B	821	CLA	C1B-C2B	2.40	1.48	1.43
22	A	813	CLA	C3D-C4D	-2.40	1.38	1.44
29	9	606	CHL	C2C-C1C	2.40	1.49	1.44
22	9	603	CLA	C3D-C4D	-2.40	1.38	1.44
22	B	841	CLA	C4D-CHA	2.40	1.46	1.38
22	3	617	CLA	C3D-C4D	-2.40	1.38	1.44
22	2	602	CLA	C4C-C3C	2.40	1.49	1.45
29	1	607	CHL	C1B-C2B	2.40	1.48	1.43
22	1	612	CLA	C3D-C4D	-2.40	1.38	1.44
22	4	611	CLA	C1B-C2B	2.40	1.48	1.43
22	5	617	CLA	C1B-C2B	2.40	1.48	1.43
22	A	827	CLA	C4D-CHA	2.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	603	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	812	CLA	C4D-CHA	2.39	1.46	1.38
22	B	804	CLA	C1C-C2C	2.39	1.49	1.44
22	A	802	CLA	C4D-CHA	2.39	1.46	1.38
22	A	824	CLA	C3D-C4D	-2.39	1.38	1.44
22	8	609	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	838	CLA	C4C-C3C	2.39	1.49	1.45
22	A	815	CLA	C4D-CHA	2.39	1.46	1.38
22	6	613	CLA	C4C-C3C	2.39	1.49	1.45
22	4	614	CLA	C1B-C2B	2.39	1.48	1.43
22	B	813	CLA	C4C-C3C	2.39	1.49	1.45
22	1	603	CLA	C4C-C3C	2.39	1.49	1.45
22	5	602	CLA	C1C-C2C	2.39	1.49	1.44
22	1	611	CLA	C3D-C4D	-2.39	1.38	1.44
22	B	828	CLA	C4C-C3C	2.39	1.49	1.45
22	8	608	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	837	CLA	C4C-C3C	2.38	1.49	1.45
22	J	3002	CLA	C4C-C3C	2.38	1.49	1.45
22	4	601	CLA	C4C-C3C	2.38	1.49	1.45
22	B	840	CLA	C1B-C2B	2.38	1.48	1.43
22	9	612	CLA	C4C-C3C	2.38	1.49	1.45
22	5	601	CLA	C1B-C2B	2.38	1.48	1.43
29	1	607	CHL	C4D-CHA	2.38	1.46	1.38
22	2	606	CLA	C1B-C2B	2.38	1.48	1.43
22	1	606	CLA	C3D-C4D	-2.38	1.38	1.44
22	A	812	CLA	C1B-C2B	2.38	1.48	1.43
22	F	303	CLA	C1C-NC	-2.38	1.34	1.37
22	B	836	CLA	C3B-C2B	2.38	1.49	1.41
22	8	603	CLA	C1B-C2B	2.38	1.48	1.43
22	A	831	CLA	C3B-C4B	2.38	1.48	1.42
29	Z	601	CHL	C4C-C3C	2.38	1.49	1.45
22	A	825	CLA	C4C-C3C	2.38	1.49	1.45
22	B	808	CLA	C4C-C3C	2.38	1.49	1.45
22	1	609	CLA	C1B-C2B	2.38	1.48	1.43
22	A	808	CLA	C3D-C4D	-2.38	1.38	1.44
22	8	601	CLA	C1C-C2C	2.38	1.49	1.44
22	7	610	CLA	C3D-C4D	-2.37	1.38	1.44
22	Z	613	CLA	C1B-C2B	2.37	1.48	1.43
22	4	613	CLA	C4C-C3C	2.37	1.49	1.45
22	B	809	CLA	C3D-C4D	-2.37	1.38	1.44
22	B	824	CLA	C1B-C2B	2.37	1.48	1.43
22	A	836	CLA	C4C-C3C	2.37	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	610	CLA	C3D-C4D	-2.37	1.38	1.44
22	8	616	CLA	C1B-C2B	2.37	1.48	1.43
22	5	603	CLA	C3B-C4B	2.37	1.48	1.42
22	5	611	CLA	C1B-C2B	2.37	1.48	1.43
22	7	602	CLA	C3D-C4D	-2.37	1.38	1.44
22	8	602	CLA	C1B-C2B	2.37	1.48	1.43
22	7	612	CLA	C3D-C4D	-2.37	1.38	1.44
29	9	606	CHL	C3A-C2A	-2.36	1.52	1.54
22	B	818	CLA	C3D-C4D	-2.36	1.38	1.44
22	A	813	CLA	C1C-C2C	2.36	1.49	1.44
22	6	604	CLA	C1C-C2C	2.36	1.49	1.44
22	B	832	CLA	C3D-C4D	-2.36	1.38	1.44
22	B	817	CLA	C4C-C3C	2.36	1.49	1.45
22	1	604	CLA	C4C-C3C	2.36	1.49	1.45
22	4	603	CLA	C4C-C3C	2.36	1.49	1.45
22	1	614	CLA	C4C-C3C	2.36	1.49	1.45
22	5	616	CLA	C4C-C3C	2.36	1.49	1.45
22	5	616	CLA	C1B-C2B	2.36	1.48	1.43
22	3	613	CLA	C3D-C4D	-2.36	1.38	1.44
22	A	843	CLA	C1B-C2B	2.36	1.48	1.43
22	5	604	CLA	C1B-C2B	2.36	1.48	1.43
22	A	810	CLA	C1B-C2B	2.36	1.48	1.43
22	8	611	CLA	C4C-C3C	2.36	1.49	1.45
22	A	804	CLA	C1C-NC	-2.36	1.34	1.37
29	4	608	CHL	C4D-CHA	2.36	1.46	1.38
22	6	612	CLA	C1B-C2B	2.36	1.48	1.43
29	9	606	CHL	C1B-C2B	2.36	1.48	1.43
29	5	608	CHL	C2C-C1C	2.36	1.49	1.44
29	6	608	CHL	C1B-C2B	2.36	1.48	1.43
22	K	4002	CLA	C4C-C3C	2.36	1.49	1.45
22	2	606	CLA	C1C-C2C	2.36	1.49	1.44
22	A	839	CLA	C4C-C3C	2.36	1.49	1.45
22	7	620	CLA	C4C-C3C	2.36	1.49	1.45
22	A	833	CLA	C3D-C4D	-2.36	1.38	1.44
22	3	602	CLA	C3D-C4D	-2.36	1.38	1.44
22	9	610	CLA	C1B-C2B	2.36	1.48	1.43
22	6	613	CLA	C3D-C4D	-2.36	1.38	1.44
22	2	601	CLA	C4C-C3C	2.35	1.49	1.45
22	A	803	CLA	C3B-C4B	2.35	1.48	1.42
22	B	828	CLA	C1C-NC	-2.35	1.34	1.37
22	1	610	CLA	CHB-C4A	-2.35	1.32	1.37
22	3	609	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	825	CLA	C4D-CHA	2.35	1.46	1.38
29	5	618	CHL	C1B-C2B	2.35	1.48	1.43
22	7	611	CLA	C4C-C3C	2.35	1.49	1.45
22	5	614	CLA	C1B-C2B	2.35	1.48	1.43
22	B	819	CLA	C4C-C3C	2.35	1.49	1.45
22	B	808	CLA	C3D-C4D	-2.35	1.38	1.44
22	6	610	CLA	C3D-C4D	-2.35	1.38	1.44
22	6	613	CLA	C1B-C2B	2.35	1.48	1.43
22	A	808	CLA	C1B-C2B	2.35	1.48	1.43
22	A	812	CLA	C3D-C4D	-2.35	1.38	1.44
22	5	609	CLA	C4C-C3C	2.35	1.49	1.45
22	7	606	CLA	C3D-C4D	-2.35	1.38	1.44
22	4	603	CLA	C1B-C2B	2.35	1.48	1.43
22	8	613	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	803	CLA	C3D-C4D	-2.35	1.38	1.44
22	B	811	CLA	C4C-C3C	2.35	1.49	1.45
22	A	805	CLA	C1C-C2C	2.35	1.49	1.44
22	1	611	CLA	C4C-C3C	2.35	1.49	1.45
22	8	604	CLA	C4C-C3C	2.35	1.49	1.45
22	7	604	CLA	C3B-C4B	2.35	1.48	1.42
22	Z	614	CLA	C1B-C2B	2.35	1.48	1.43
29	5	618	CHL	C4C-C3C	2.35	1.49	1.45
22	7	609	CLA	C3D-C4D	-2.35	1.38	1.44
22	A	815	CLA	C4C-C3C	2.35	1.49	1.45
22	3	612	CLA	C4C-C3C	2.35	1.49	1.45
22	1	602	CLA	C3D-C4D	-2.34	1.38	1.44
22	3	603	CLA	C3D-C4D	-2.34	1.38	1.44
22	Z	602	CLA	C3D-C4D	-2.34	1.38	1.44
22	8	616	CLA	C3D-C4D	-2.34	1.38	1.44
22	2	610	CLA	C1C-C2C	2.34	1.49	1.44
22	A	842	CLA	C1B-C2B	2.34	1.48	1.43
22	B	838	CLA	C1B-C2B	2.34	1.48	1.43
22	8	608	CLA	C1B-C2B	2.34	1.48	1.43
22	3	602	CLA	C3B-C2B	2.34	1.49	1.41
22	2	610	CLA	C3D-C4D	-2.34	1.38	1.44
22	A	817	CLA	C4C-C3C	2.34	1.49	1.45
22	A	838	CLA	C1C-NC	-2.34	1.34	1.37
22	B	807	CLA	C4C-C3C	2.34	1.49	1.45
22	B	810	CLA	C4C-C3C	2.34	1.49	1.45
22	4	604	CLA	C3D-C4D	-2.34	1.38	1.44
22	7	613	CLA	C4C-C3C	2.34	1.49	1.45
22	3	606	CLA	C3D-C4D	-2.34	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	612	CLA	C1B-C2B	2.34	1.48	1.43
22	B	826	CLA	C1C-NC	-2.34	1.34	1.37
22	B	810	CLA	C3D-C4D	-2.34	1.38	1.44
22	1	604	CLA	C3D-C4D	-2.34	1.38	1.44
22	B	821	CLA	C3D-C4D	-2.34	1.38	1.44
22	8	602	CLA	C3D-C4D	-2.34	1.38	1.44
22	A	805	CLA	C4D-CHA	2.34	1.46	1.38
29	9	607	CHL	C2C-C1C	2.34	1.49	1.44
22	8	601	CLA	C3D-C4D	-2.33	1.38	1.44
22	J	3002	CLA	C3D-C4D	-2.33	1.38	1.44
22	7	614	CLA	C1B-C2B	2.33	1.48	1.43
29	4	606	CHL	C4D-CHA	2.33	1.46	1.38
22	9	609	CLA	C4C-C3C	2.33	1.49	1.45
29	6	607	CHL	C1B-C2B	2.33	1.48	1.43
22	B	827	CLA	C3D-C4D	-2.33	1.38	1.44
22	A	819	CLA	C4C-C3C	2.33	1.49	1.45
22	A	835	CLA	C4C-C3C	2.33	1.49	1.45
22	B	820	CLA	C4C-C3C	2.33	1.49	1.45
29	3	608	CHL	C4D-CHA	2.33	1.46	1.38
22	A	802	CLA	C4C-C3C	2.33	1.49	1.45
22	5	606	CLA	C3D-C4D	-2.33	1.38	1.44
22	9	610	CLA	C1C-C2C	2.33	1.49	1.44
22	8	611	CLA	C1B-C2B	2.33	1.48	1.43
22	K	4003	CLA	C4C-C3C	2.33	1.49	1.45
22	5	611	CLA	C4C-C3C	2.33	1.49	1.45
22	G	203	CLA	C3D-C4D	-2.33	1.38	1.44
22	5	617	CLA	C4C-C3C	2.33	1.49	1.45
22	4	612	CLA	C1B-C2B	2.32	1.48	1.43
22	5	601	CLA	C3D-C4D	-2.32	1.38	1.44
22	5	617	CLA	C3D-C4D	-2.32	1.38	1.44
22	A	815	CLA	C1C-C2C	2.32	1.49	1.44
22	B	837	CLA	C3D-C4D	-2.32	1.38	1.44
22	6	612	CLA	C3D-C4D	-2.32	1.38	1.44
22	2	601	CLA	C3D-C4D	-2.32	1.38	1.44
22	7	609	CLA	C1B-C2B	2.32	1.48	1.43
22	A	841	CLA	C1C-C2C	2.32	1.49	1.44
29	1	601	CHL	C2C-C1C	2.32	1.49	1.44
22	A	827	CLA	C1C-C2C	2.32	1.49	1.44
22	1	608	CLA	C1B-C2B	2.32	1.48	1.43
22	6	614	CLA	C4C-C3C	2.32	1.49	1.45
22	9	610	CLA	C3D-C4D	-2.32	1.38	1.44
22	Z	604	CLA	C1B-C2B	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	606	CLA	C4C-C3C	2.31	1.49	1.45
22	Z	604	CLA	C3D-C4D	-2.31	1.39	1.44
22	K	4002	CLA	C1B-C2B	2.31	1.48	1.43
22	Z	616	CLA	C3D-C4D	-2.31	1.39	1.44
22	9	609	CLA	C1B-C2B	2.31	1.48	1.43
29	Z	607	CHL	C4D-CHA	2.31	1.46	1.38
22	6	603	CLA	C4C-C3C	2.31	1.49	1.45
22	L	203	CLA	C1B-C2B	2.31	1.48	1.43
29	4	618	CHL	C1B-C2B	2.31	1.48	1.43
29	6	607	CHL	C4D-CHA	2.31	1.46	1.38
22	2	603	CLA	C3D-C4D	-2.31	1.39	1.44
22	8	612	CLA	C3D-C4D	-2.31	1.39	1.44
22	A	823	CLA	C1B-C2B	2.31	1.48	1.43
22	A	817	CLA	C1B-C2B	2.31	1.48	1.43
22	A	845	CLA	C3D-C4D	-2.31	1.39	1.44
22	8	613	CLA	C1B-C2B	2.31	1.48	1.43
22	A	834	CLA	C3D-C4D	-2.31	1.39	1.44
22	B	840	CLA	C4C-C3C	2.31	1.49	1.45
22	B	841	CLA	C1C-C2C	2.31	1.49	1.44
22	5	613	CLA	C4B-NB	-2.31	1.34	1.37
22	B	841	CLA	C4C-C3C	2.30	1.49	1.45
22	J	3002	CLA	C1B-C2B	2.30	1.48	1.43
22	B	830	CLA	C1C-C2C	2.30	1.49	1.44
22	3	609	CLA	C3D-C4D	-2.30	1.39	1.44
22	6	602	CLA	C3D-C4D	-2.30	1.39	1.44
29	3	608	CHL	CHB-C4A	-2.30	1.32	1.37
22	3	611	CLA	C1C-C2C	2.30	1.49	1.44
22	2	607	CLA	C1C-C2C	2.30	1.49	1.44
22	6	603	CLA	C1B-C2B	2.30	1.48	1.43
22	1	602	CLA	C1C-C2C	2.30	1.49	1.44
22	B	831	CLA	CHB-C4A	-2.30	1.32	1.37
29	1	601	CHL	C1B-C2B	2.30	1.48	1.43
22	B	822	CLA	C1B-C2B	2.30	1.48	1.43
29	6	606	CHL	C4D-CHA	2.30	1.46	1.38
22	4	604	CLA	C4C-C3C	2.30	1.49	1.45
22	A	811	CLA	C3D-C4D	-2.30	1.39	1.44
22	Z	609	CLA	C3D-C4D	-2.30	1.39	1.44
22	6	611	CLA	C1B-C2B	2.30	1.48	1.43
22	9	611	CLA	C4C-C3C	2.30	1.49	1.45
22	1	606	CLA	C1C-C2C	2.30	1.49	1.44
22	B	831	CLA	C3D-C4D	-2.30	1.39	1.44
22	7	613	CLA	C3D-C4D	-2.30	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	829	CLA	C1B-NB	-2.30	1.35	1.37
22	Z	614	CLA	C4C-C3C	2.30	1.49	1.45
22	B	823	CLA	C1B-C2B	2.30	1.48	1.43
22	F	304	CLA	C4C-C3C	2.30	1.49	1.45
22	K	4003	CLA	C3D-C4D	-2.30	1.39	1.44
22	A	836	CLA	C3D-C4D	-2.30	1.39	1.44
22	A	818	CLA	C3D-C4D	-2.30	1.39	1.44
22	B	833	CLA	C3D-C4D	-2.30	1.39	1.44
22	F	304	CLA	C3D-C4D	-2.30	1.39	1.44
22	8	616	CLA	C1C-C2C	2.29	1.49	1.44
22	A	841	CLA	C3D-C4D	-2.29	1.39	1.44
22	3	614	CLA	C3D-C4D	-2.29	1.39	1.44
29	7	607	CHL	C4D-CHA	2.29	1.46	1.38
22	8	604	CLA	C1B-C2B	2.29	1.48	1.43
22	5	621	CLA	C3B-C2B	2.29	1.49	1.41
22	1	613	CLA	C4C-C3C	2.29	1.49	1.45
22	A	837	CLA	C3D-C4D	-2.29	1.39	1.44
22	Z	614	CLA	C1C-C2C	2.29	1.49	1.44
22	6	612	CLA	C1C-C2C	2.29	1.49	1.44
22	B	839	CLA	C4C-C3C	2.29	1.49	1.45
22	B	817	CLA	C1C-NC	-2.29	1.34	1.37
22	B	837	CLA	C1C-C2C	2.29	1.49	1.44
22	3	620	CLA	C1B-C2B	2.29	1.48	1.43
22	B	836	CLA	C1B-C2B	2.29	1.48	1.43
22	A	829	CLA	C3D-C4D	-2.29	1.39	1.44
22	5	612	CLA	C4C-C3C	2.29	1.49	1.45
22	5	612	CLA	C3D-C4D	-2.29	1.39	1.44
22	8	604	CLA	C3D-C4D	-2.29	1.39	1.44
21	A	801	CL0	C1B-C2B	2.29	1.48	1.43
22	6	604	CLA	C4C-C3C	2.29	1.49	1.45
22	Z	608	CLA	C1B-C2B	2.29	1.48	1.43
22	1	614	CLA	C1B-C2B	2.29	1.48	1.43
22	A	831	CLA	C3D-C4D	-2.29	1.39	1.44
22	4	616	CLA	C3D-C4D	-2.29	1.39	1.44
22	9	601	CLA	C1C-C2C	2.29	1.49	1.44
22	A	832	CLA	C1C-C2C	2.28	1.49	1.44
22	B	831	CLA	C1C-C2C	2.28	1.49	1.44
22	8	613	CLA	C1C-C2C	2.28	1.49	1.44
22	3	620	CLA	C3D-C4D	-2.28	1.39	1.44
29	1	601	CHL	C4D-CHA	2.28	1.46	1.38
22	B	805	CLA	C3D-C4D	-2.28	1.39	1.44
22	Z	606	CLA	C3D-C4D	-2.28	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	822	CLA	C1C-C2C	2.28	1.49	1.44
22	A	822	CLA	CHB-C4A	-2.28	1.32	1.37
22	A	832	CLA	C4C-C3C	2.28	1.49	1.45
22	6	601	CLA	C3D-C4D	-2.28	1.39	1.44
22	3	603	CLA	C1B-C2B	2.28	1.48	1.43
22	5	604	CLA	C3D-C4D	-2.28	1.39	1.44
29	5	607	CHL	C4D-CHA	2.28	1.46	1.38
22	Z	609	CLA	C1B-C2B	2.28	1.48	1.43
22	5	613	CLA	C3D-C4D	-2.28	1.39	1.44
22	B	808	CLA	C1C-NC	-2.28	1.34	1.37
22	B	829	CLA	C3B-C2B	2.28	1.48	1.41
22	5	614	CLA	C3D-C4D	-2.28	1.39	1.44
22	6	622	CLA	C3D-C4D	-2.28	1.39	1.44
22	6	614	CLA	C1B-C2B	2.28	1.48	1.43
29	7	607	CHL	C4C-C3C	2.28	1.49	1.45
22	6	609	CLA	C3D-C4D	-2.28	1.39	1.44
22	9	603	CLA	C1B-C2B	2.28	1.48	1.43
22	2	614	CLA	C1C-C2C	2.28	1.49	1.44
22	G	203	CLA	C4C-C3C	2.28	1.49	1.45
22	3	617	CLA	C4C-C3C	2.28	1.49	1.45
22	Z	611	CLA	C3D-C4D	-2.28	1.39	1.44
22	3	602	CLA	C1B-C2B	2.28	1.48	1.43
22	A	828	CLA	C1C-C2C	2.28	1.49	1.44
22	A	823	CLA	C3D-C4D	-2.28	1.39	1.44
22	4	614	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	814	CLA	C4C-C3C	2.27	1.49	1.45
22	3	612	CLA	C3D-C4D	-2.27	1.39	1.44
22	9	602	CLA	C1B-C2B	2.27	1.48	1.43
22	4	601	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	845	CLA	C1C-NC	-2.27	1.34	1.37
22	6	617	CLA	C3D-C4D	-2.27	1.39	1.44
22	A	803	CLA	C4C-C3C	2.27	1.49	1.45
29	6	606	CHL	C1B-C2B	2.27	1.48	1.43
22	7	604	CLA	C1C-C2C	2.27	1.49	1.44
22	A	805	CLA	C1B-C2B	2.27	1.48	1.43
22	A	823	CLA	C4C-C3C	2.27	1.48	1.45
22	6	616	CLA	C4C-C3C	2.27	1.48	1.45
22	8	602	CLA	C1C-C2C	2.27	1.49	1.44
22	B	817	CLA	C1B-C2B	2.27	1.48	1.43
22	A	814	CLA	C1C-NC	-2.27	1.34	1.37
22	5	610	CLA	C3D-C4D	-2.27	1.39	1.44
22	2	602	CLA	C1C-C2C	2.26	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	609	CLA	C4C-C3C	2.26	1.48	1.45
22	B	837	CLA	C1B-C2B	2.26	1.48	1.43
22	3	607	CLA	C3D-C4D	-2.26	1.39	1.44
22	8	616	CLA	C3B-C2B	2.26	1.48	1.41
22	4	610	CLA	C3D-C4D	-2.26	1.39	1.44
22	A	843	CLA	C4C-C3C	2.26	1.48	1.45
22	9	610	CLA	C4C-C3C	2.26	1.48	1.45
22	4	612	CLA	C3D-C4D	-2.26	1.39	1.44
22	7	611	CLA	C1B-C2B	2.26	1.48	1.43
22	A	826	CLA	C4C-C3C	2.26	1.48	1.45
22	6	614	CLA	C1C-C2C	2.26	1.48	1.44
22	A	833	CLA	CHB-C4A	-2.26	1.32	1.37
22	9	602	CLA	C4C-C3C	2.26	1.48	1.45
22	2	613	CLA	C3D-C4D	-2.26	1.39	1.44
22	B	816	CLA	C1B-C2B	2.26	1.48	1.43
22	2	610	CLA	C1B-C2B	2.26	1.48	1.43
22	A	839	CLA	C3D-C4D	-2.26	1.39	1.44
22	8	609	CLA	C4C-C3C	2.26	1.48	1.45
22	A	816	CLA	C1C-C2C	2.26	1.48	1.44
22	B	813	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	845	CLA	C4C-C3C	2.25	1.48	1.45
29	5	607	CHL	C1C-NC	-2.25	1.34	1.37
22	Z	606	CLA	C4C-C3C	2.25	1.48	1.45
22	A	845	CLA	C1B-C2B	2.25	1.48	1.43
29	4	618	CHL	C4D-CHA	2.25	1.46	1.38
22	A	806	CLA	C4C-C3C	2.25	1.48	1.45
22	B	812	CLA	C3D-C4D	-2.25	1.39	1.44
22	9	602	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	843	CLA	C3D-C4D	-2.25	1.39	1.44
22	6	611	CLA	C3D-C4D	-2.25	1.39	1.44
22	A	828	CLA	C1C-NC	-2.25	1.34	1.37
22	8	603	CLA	C4C-C3C	2.25	1.48	1.45
29	3	608	CHL	C2C-C1C	2.25	1.49	1.44
22	B	852	CLA	C1C-C2C	2.25	1.48	1.44
29	8	607	CHL	C1C-NC	-2.25	1.34	1.37
22	7	604	CLA	C3D-C4D	-2.25	1.39	1.44
22	4	609	CLA	C3D-C4D	-2.25	1.39	1.44
22	B	814	CLA	C1B-C2B	2.25	1.48	1.43
22	B	815	CLA	C3D-C4D	-2.25	1.39	1.44
22	8	614	CLA	C1B-C2B	2.25	1.48	1.43
29	4	608	CHL	C1B-C2B	2.25	1.48	1.43
22	L	203	CLA	C1C-C2C	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	612	CLA	C3D-C4D	-2.25	1.39	1.44
29	9	607	CHL	C4D-CHA	2.25	1.46	1.38
22	3	612	CLA	C1B-C2B	2.24	1.48	1.43
22	1	616	CLA	C3D-C4D	-2.24	1.39	1.44
22	2	613	CLA	C1C-C2C	2.24	1.48	1.44
29	9	606	CHL	C4D-CHA	2.24	1.46	1.38
22	B	821	CLA	C4C-C3C	2.24	1.48	1.45
22	A	811	CLA	C1C-C2C	2.24	1.48	1.44
22	Z	610	CLA	C3D-C4D	-2.24	1.39	1.44
29	Z	601	CHL	C1B-C2B	2.24	1.48	1.43
22	8	608	CLA	C1C-C2C	2.24	1.48	1.44
22	Z	612	CLA	C3D-C4D	-2.24	1.39	1.44
22	B	818	CLA	CHB-C4A	-2.24	1.32	1.37
22	5	610	CLA	C1C-C2C	2.24	1.48	1.44
22	2	607	CLA	C3D-C4D	-2.24	1.39	1.44
22	B	835	CLA	C3D-C4D	-2.24	1.39	1.44
22	A	830	CLA	CHB-C4A	-2.24	1.32	1.37
22	A	809	CLA	C3D-C4D	-2.24	1.39	1.44
22	B	822	CLA	C4C-C3C	2.23	1.48	1.45
22	A	824	CLA	C4C-C3C	2.23	1.48	1.45
22	B	813	CLA	C1C-NC	-2.23	1.34	1.37
22	3	614	CLA	C1C-C2C	2.23	1.48	1.44
22	4	610	CLA	C4C-C3C	2.23	1.48	1.45
22	1	610	CLA	C3D-C4D	-2.23	1.39	1.44
22	A	813	CLA	C4C-C3C	2.23	1.48	1.45
22	3	620	CLA	C4C-C3C	2.23	1.48	1.45
22	5	606	CLA	C4C-C3C	2.23	1.48	1.45
22	2	614	CLA	C3D-C4D	-2.23	1.39	1.44
22	8	612	CLA	C1C-C2C	2.23	1.48	1.44
29	1	607	CHL	C3D-C4D	-2.23	1.39	1.44
22	4	614	CLA	C4C-C3C	2.23	1.48	1.45
22	6	617	CLA	C4C-C3C	2.23	1.48	1.45
22	A	812	CLA	C1C-NC	-2.23	1.34	1.37
22	4	616	CLA	C3B-C2B	2.23	1.48	1.41
22	4	611	CLA	C3D-C4D	-2.23	1.39	1.44
22	6	610	CLA	C1C-C2C	2.23	1.48	1.44
22	Z	612	CLA	C1C-C2C	2.23	1.48	1.44
22	2	614	CLA	C3B-C2B	2.23	1.48	1.41
29	4	618	CHL	C2C-C1C	2.23	1.49	1.44
22	K	4002	CLA	C3D-C4D	-2.23	1.39	1.44
22	9	609	CLA	C3D-C4D	-2.23	1.39	1.44
22	7	612	CLA	C1B-C2B	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	838	CLA	C1C-C2C	2.23	1.48	1.44
22	5	617	CLA	C1C-C2C	2.23	1.48	1.44
22	Z	608	CLA	C3D-C4D	-2.22	1.39	1.44
22	B	832	CLA	C1C-C2C	2.22	1.48	1.44
22	5	603	CLA	C1B-C2B	2.22	1.48	1.43
22	6	609	CLA	C1B-C2B	2.22	1.48	1.43
22	9	611	CLA	C3D-C4D	-2.22	1.39	1.44
22	9	611	CLA	C3B-C2B	2.22	1.48	1.41
22	B	833	CLA	C4C-C3C	2.22	1.48	1.45
22	B	841	CLA	C3B-C2B	2.22	1.48	1.41
22	A	818	CLA	C1B-C2B	2.22	1.48	1.43
22	B	827	CLA	C1C-C2C	2.22	1.48	1.44
22	K	4002	CLA	C1C-C2C	2.22	1.48	1.44
22	A	826	CLA	C1B-C2B	2.22	1.48	1.43
22	3	604	CLA	C3D-C4D	-2.22	1.39	1.44
22	Z	614	CLA	C3D-C4D	-2.22	1.39	1.44
22	5	601	CLA	C4C-C3C	2.22	1.48	1.45
22	B	832	CLA	C1B-C2B	2.22	1.48	1.43
22	9	613	CLA	C1C-C2C	2.22	1.48	1.44
29	Z	601	CHL	C3B-C2B	2.22	1.48	1.41
22	A	828	CLA	C1B-C2B	2.22	1.48	1.43
22	5	613	CLA	C1B-C2B	2.22	1.48	1.43
22	A	831	CLA	C4C-C3C	2.22	1.48	1.45
22	1	609	CLA	C3D-C4D	-2.22	1.39	1.44
22	3	617	CLA	C1B-C2B	2.22	1.48	1.43
22	B	820	CLA	C1C-C2C	2.22	1.48	1.44
29	Z	607	CHL	C4C-C3C	2.22	1.48	1.45
22	5	606	CLA	C1C-C2C	2.21	1.48	1.44
22	4	602	CLA	C1C-C2C	2.21	1.48	1.44
22	1	613	CLA	C3D-C4D	-2.21	1.39	1.44
22	5	609	CLA	C3D-C4D	-2.21	1.39	1.44
22	A	804	CLA	C4D-CHA	2.21	1.46	1.38
22	2	610	CLA	C3B-C2B	2.21	1.48	1.41
22	A	835	CLA	C1C-C2C	2.21	1.48	1.44
22	B	821	CLA	C1C-C2C	2.21	1.48	1.44
22	8	614	CLA	C1C-C2C	2.21	1.48	1.44
22	7	620	CLA	C1C-C2C	2.21	1.48	1.44
22	9	614	CLA	C1C-C2C	2.21	1.48	1.44
22	7	604	CLA	C4C-C3C	2.21	1.48	1.45
22	6	616	CLA	C3B-C2B	2.21	1.48	1.41
22	5	621	CLA	C1C-C2C	2.21	1.48	1.44
22	A	841	CLA	C1C-NC	-2.21	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	841	CLA	CHB-C4A	-2.21	1.32	1.37
22	3	617	CLA	C1C-C2C	2.21	1.48	1.44
22	Z	606	CLA	C1B-C2B	2.21	1.48	1.43
22	B	814	CLA	C1C-C2C	2.21	1.48	1.44
22	8	614	CLA	C4C-C3C	2.21	1.48	1.45
22	L	203	CLA	C3D-C4D	-2.21	1.39	1.44
22	A	833	CLA	C1C-C2C	2.21	1.48	1.44
22	2	609	CLA	C1C-C2C	2.21	1.48	1.44
22	2	602	CLA	C3D-C4D	-2.21	1.39	1.44
22	3	612	CLA	C1C-NC	-2.21	1.34	1.37
22	9	602	CLA	C1C-C2C	2.21	1.48	1.44
29	1	607	CHL	C3B-C2B	2.21	1.48	1.41
22	3	602	CLA	C1C-C2C	2.21	1.48	1.44
22	B	836	CLA	C4C-C3C	2.21	1.48	1.45
22	7	601	CLA	C3B-C2B	2.21	1.48	1.41
22	7	602	CLA	C1C-C2C	2.20	1.48	1.44
22	Z	616	CLA	C1C-C2C	2.20	1.48	1.44
22	3	613	CLA	C1C-C2C	2.20	1.48	1.44
22	6	622	CLA	C1C-C2C	2.20	1.48	1.44
22	7	603	CLA	C1B-C2B	2.20	1.48	1.43
22	L	204	CLA	C3D-C4D	-2.20	1.39	1.44
22	9	601	CLA	C3B-C2B	2.20	1.48	1.41
22	3	607	CLA	C4C-C3C	2.20	1.48	1.45
22	2	606	CLA	C3B-C2B	2.20	1.48	1.41
22	A	840	CLA	C4C-C3C	2.20	1.48	1.45
22	4	609	CLA	C1C-NC	-2.20	1.34	1.37
22	B	852	CLA	C3B-C2B	2.20	1.48	1.41
22	A	806	CLA	C1B-C2B	2.20	1.48	1.43
22	9	612	CLA	C3D-C4D	-2.20	1.39	1.44
22	3	607	CLA	C1B-C2B	2.20	1.48	1.43
22	8	606	CLA	C1B-C2B	2.20	1.48	1.43
22	2	613	CLA	C3B-C2B	2.20	1.48	1.41
22	5	614	CLA	C1C-C2C	2.20	1.48	1.44
22	A	803	CLA	C1B-C2B	2.20	1.48	1.43
22	6	612	CLA	C4C-C3C	2.20	1.48	1.45
22	2	609	CLA	C3B-C2B	2.20	1.48	1.41
22	7	609	CLA	C1C-C2C	2.20	1.48	1.44
22	5	602	CLA	C1B-C2B	2.20	1.48	1.43
22	A	840	CLA	C1B-C2B	2.19	1.48	1.43
22	9	604	CLA	C3D-C4D	-2.19	1.39	1.44
22	B	834	CLA	C1C-C2C	2.19	1.48	1.44
22	5	601	CLA	C1C-C2C	2.19	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	807	CLA	C1C-NC	-2.19	1.34	1.37
22	7	612	CLA	C4C-C3C	2.19	1.48	1.45
22	1	612	CLA	C1B-C2B	2.19	1.48	1.43
29	5	618	CHL	C4D-CHA	2.19	1.46	1.38
22	6	604	CLA	C1B-C2B	2.19	1.48	1.43
22	9	604	CLA	C1C-C2C	2.19	1.48	1.44
22	9	612	CLA	C1C-C2C	2.19	1.48	1.44
22	5	616	CLA	C3D-C4D	-2.19	1.39	1.44
22	8	614	CLA	C3B-C2B	2.19	1.48	1.41
22	1	606	CLA	C1B-C2B	2.19	1.48	1.43
22	L	203	CLA	C4C-C3C	2.19	1.48	1.45
22	5	621	CLA	C1B-C2B	2.19	1.48	1.43
22	A	839	CLA	C1C-C2C	2.19	1.48	1.44
22	B	815	CLA	C1B-C2B	2.19	1.48	1.43
22	A	837	CLA	C1C-C2C	2.19	1.48	1.44
22	B	812	CLA	C4C-C3C	2.19	1.48	1.45
22	6	616	CLA	C3D-C4D	-2.19	1.39	1.44
22	A	815	CLA	C3B-C2B	2.18	1.48	1.41
29	4	618	CHL	C3B-C2B	2.18	1.48	1.41
22	A	830	CLA	C1C-NC	-2.18	1.34	1.37
29	6	607	CHL	C4C-C3C	2.18	1.48	1.45
22	2	607	CLA	C3B-C2B	2.18	1.48	1.41
22	8	610	CLA	CHB-C4A	-2.18	1.32	1.37
22	8	606	CLA	C4C-C3C	2.18	1.48	1.45
22	A	820	CLA	CHB-C4A	-2.18	1.32	1.37
22	2	611	CLA	C1C-C2C	2.18	1.48	1.44
22	A	806	CLA	C3B-C2B	2.18	1.48	1.41
22	6	604	CLA	C3D-C4D	-2.18	1.39	1.44
22	3	604	CLA	C4C-C3C	2.18	1.48	1.45
22	A	830	CLA	C3D-C4D	-2.18	1.39	1.44
22	8	612	CLA	C1C-NC	-2.18	1.34	1.37
22	Z	611	CLA	C1C-C2C	2.18	1.48	1.44
22	Z	602	CLA	C1C-C2C	2.18	1.48	1.44
22	7	620	CLA	C3B-C2B	2.18	1.48	1.41
22	G	204	CLA	C3D-C4D	-2.18	1.39	1.44
22	3	603	CLA	C4C-C3C	2.18	1.48	1.45
22	G	203	CLA	C3B-C2B	2.18	1.48	1.41
22	B	803	CLA	C1B-C2B	2.18	1.48	1.43
22	B	804	CLA	C3D-C4D	-2.18	1.39	1.44
22	4	611	CLA	C3B-C2B	2.18	1.48	1.41
22	A	829	CLA	CHB-C4A	-2.18	1.32	1.37
22	Z	616	CLA	C3B-C2B	2.17	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	611	CLA	C3D-C4D	-2.17	1.39	1.44
22	8	611	CLA	C3D-C4D	-2.17	1.39	1.44
22	8	614	CLA	C3D-C4D	-2.17	1.39	1.44
22	4	610	CLA	CHB-C4A	-2.17	1.32	1.37
22	1	614	CLA	C3D-C4D	-2.17	1.39	1.44
22	1	612	CLA	C4C-C3C	2.17	1.48	1.45
29	6	618	CHL	C4D-CHA	2.17	1.46	1.38
21	A	801	CL0	C1C-NC	-2.17	1.34	1.37
22	A	805	CLA	C4C-C3C	2.17	1.48	1.45
22	B	820	CLA	C3B-C2B	2.17	1.48	1.41
22	B	830	CLA	C4C-C3C	2.17	1.48	1.45
22	7	611	CLA	C3D-C4D	-2.17	1.39	1.44
22	Z	613	CLA	C3B-C2B	2.17	1.48	1.41
22	3	607	CLA	C1C-C2C	2.17	1.48	1.44
22	9	613	CLA	C3D-C4D	-2.17	1.39	1.44
22	1	608	CLA	C1C-C2C	2.17	1.48	1.44
22	A	854	CLA	C3D-C4D	-2.17	1.39	1.44
22	6	616	CLA	C1C-NC	-2.17	1.34	1.37
22	Z	608	CLA	C4C-C3C	2.17	1.48	1.45
22	Z	611	CLA	C4C-C3C	2.17	1.48	1.45
22	Z	612	CLA	C4C-C3C	2.17	1.48	1.45
22	B	823	CLA	C3D-C4D	-2.17	1.39	1.44
22	A	815	CLA	C1D-C2D	2.17	1.49	1.45
22	2	601	CLA	C3B-C2B	2.17	1.48	1.41
22	F	303	CLA	C3D-C4D	-2.17	1.39	1.44
22	4	609	CLA	CHB-C4A	-2.17	1.32	1.37
22	8	606	CLA	C1C-NC	-2.17	1.34	1.37
22	4	601	CLA	C1C-NC	-2.17	1.34	1.37
29	7	607	CHL	C3B-C2B	2.17	1.48	1.41
22	A	827	CLA	C1B-C2B	2.17	1.48	1.43
29	8	607	CHL	C4D-CHA	2.17	1.46	1.38
22	5	612	CLA	C1C-NC	-2.16	1.34	1.37
29	Z	607	CHL	C3B-C2B	2.16	1.48	1.41
22	2	606	CLA	C3D-C4D	-2.16	1.39	1.44
22	8	613	CLA	C4C-C3C	2.16	1.48	1.45
22	B	841	CLA	C1D-C2D	2.16	1.49	1.45
22	Z	608	CLA	C1C-C2C	2.16	1.48	1.44
22	3	602	CLA	C4C-C3C	2.16	1.48	1.45
22	B	825	CLA	C1C-C2C	2.16	1.48	1.44
22	2	611	CLA	C3D-C4D	-2.16	1.39	1.44
22	6	601	CLA	C4C-C3C	2.16	1.48	1.45
22	B	804	CLA	C3B-C2B	2.16	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	612	CLA	C3B-C2B	2.16	1.48	1.41
22	A	812	CLA	C1A-CHA	2.16	1.52	1.43
22	A	840	CLA	C1C-C2C	2.16	1.48	1.44
22	2	612	CLA	C1C-C2C	2.16	1.48	1.44
22	3	611	CLA	C3B-C2B	2.16	1.48	1.41
22	A	854	CLA	C1B-C2B	2.16	1.48	1.43
25	A	851	BCR	C21-C22	-2.16	1.32	1.35
22	7	616	CLA	C3D-C4D	-2.16	1.39	1.44
22	7	603	CLA	C4C-C3C	2.16	1.48	1.45
22	7	606	CLA	C1C-NC	-2.16	1.34	1.37
22	1	616	CLA	C3B-C2B	2.16	1.48	1.41
22	1	616	CLA	C1C-C2C	2.16	1.48	1.44
22	6	610	CLA	C4C-C3C	2.16	1.48	1.45
29	4	607	CHL	C4D-CHA	2.16	1.46	1.38
29	5	608	CHL	CHB-C4A	-2.16	1.32	1.37
22	4	613	CLA	C3D-C4D	-2.16	1.39	1.44
29	4	607	CHL	C2C-C1C	2.15	1.49	1.44
29	1	607	CHL	C2C-C1C	2.15	1.49	1.44
29	6	618	CHL	C3B-C2B	2.15	1.48	1.41
22	6	616	CLA	C1B-C2B	2.15	1.48	1.43
22	7	608	CLA	C1B-C2B	2.15	1.48	1.43
29	5	618	CHL	C3B-C2B	2.15	1.48	1.41
22	1	602	CLA	CHB-C4A	-2.15	1.32	1.37
22	B	852	CLA	C3D-C4D	-2.15	1.39	1.44
22	A	833	CLA	C4C-C3C	2.15	1.48	1.45
22	B	803	CLA	C4C-C3C	2.15	1.48	1.45
22	9	614	CLA	C3D-C4D	-2.15	1.39	1.44
22	3	620	CLA	C1C-C2C	2.15	1.48	1.44
22	B	837	CLA	C4C-C3C	2.15	1.48	1.45
22	A	823	CLA	C1C-C2C	2.15	1.48	1.44
22	B	825	CLA	C3B-C2B	2.15	1.48	1.41
22	B	802	CLA	C1C-C2C	2.15	1.48	1.44
22	K	4003	CLA	C3B-C2B	2.15	1.48	1.41
22	A	809	CLA	C1B-C2B	2.15	1.48	1.43
22	9	609	CLA	C1C-C2C	2.15	1.48	1.44
22	A	835	CLA	C3B-C2B	2.15	1.48	1.41
29	1	601	CHL	C3B-C2B	2.15	1.48	1.41
22	5	610	CLA	C1B-C2B	2.15	1.48	1.43
22	B	803	CLA	C3D-C4D	-2.15	1.39	1.44
22	7	620	CLA	C3D-C4D	-2.15	1.39	1.44
29	6	618	CHL	C4C-C3C	2.15	1.48	1.45
22	Z	604	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	825	CLA	C1B-C2B	2.15	1.48	1.43
22	B	819	CLA	CHB-C4A	-2.15	1.32	1.37
29	1	601	CHL	C4C-C3C	2.15	1.48	1.45
22	5	603	CLA	C3B-C2B	2.14	1.48	1.41
22	B	830	CLA	C1B-C2B	2.14	1.48	1.43
22	B	821	CLA	C3B-C2B	2.14	1.48	1.41
22	2	611	CLA	C3B-C2B	2.14	1.48	1.41
22	4	604	CLA	C1B-C2B	2.14	1.48	1.43
22	A	802	CLA	C1C-C2C	2.14	1.48	1.44
22	8	606	CLA	C1C-C2C	2.14	1.48	1.44
22	6	617	CLA	C1C-C2C	2.14	1.48	1.44
22	A	810	CLA	C4C-C3C	2.14	1.48	1.45
29	6	608	CHL	C4D-CHA	2.14	1.46	1.38
22	8	616	CLA	C4C-C3C	2.14	1.48	1.45
22	B	806	CLA	C1B-C2B	2.14	1.48	1.43
22	Z	613	CLA	C3D-C4D	-2.14	1.39	1.44
22	2	603	CLA	C1C-C2C	2.14	1.48	1.44
22	B	834	CLA	C3B-C2B	2.14	1.48	1.41
22	A	803	CLA	C3B-C2B	2.14	1.48	1.41
22	B	839	CLA	C3B-C2B	2.14	1.48	1.41
22	B	827	CLA	C4C-C3C	2.13	1.48	1.45
22	6	613	CLA	C1C-C2C	2.13	1.48	1.44
28	9	620	LMG	O4-C4	-2.13	1.37	1.43
22	A	807	CLA	C4C-C3C	2.13	1.48	1.45
22	G	204	CLA	C3B-C2B	2.13	1.48	1.41
22	A	811	CLA	C1B-C2B	2.13	1.48	1.43
22	J	3002	CLA	C3B-C2B	2.13	1.48	1.41
22	5	611	CLA	C3D-C4D	-2.13	1.39	1.44
22	B	811	CLA	C1C-C2C	2.13	1.48	1.44
29	4	618	CHL	C4C-C3C	2.13	1.48	1.45
22	1	608	CLA	C4C-C3C	2.13	1.48	1.45
22	4	610	CLA	C1C-NC	-2.13	1.34	1.37
22	A	821	CLA	C1B-C2B	2.13	1.48	1.43
22	B	839	CLA	C1C-NC	-2.13	1.34	1.37
22	A	813	CLA	CHB-C4A	-2.13	1.32	1.37
22	6	603	CLA	C1C-C2C	2.13	1.48	1.44
22	G	203	CLA	C1C-C2C	2.13	1.48	1.44
22	Z	602	CLA	C1C-NC	-2.13	1.34	1.37
22	A	802	CLA	C3B-C2B	2.13	1.48	1.41
22	K	4002	CLA	C3B-C2B	2.13	1.48	1.41
29	4	607	CHL	C3B-C2B	2.13	1.48	1.41
22	2	609	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	812	CLA	C1C-C2C	2.13	1.48	1.44
22	3	614	CLA	C3B-C2B	2.13	1.48	1.41
22	6	617	CLA	C3B-C2B	2.13	1.48	1.41
22	B	815	CLA	C4C-C3C	2.13	1.48	1.45
22	4	614	CLA	C3B-C2B	2.13	1.48	1.41
29	9	607	CHL	C3B-C2B	2.13	1.48	1.41
22	B	812	CLA	C1B-C2B	2.13	1.48	1.43
22	B	810	CLA	C3B-C2B	2.13	1.48	1.41
22	A	836	CLA	C1C-NC	-2.13	1.34	1.37
22	B	835	CLA	C1C-C2C	2.13	1.48	1.44
22	G	204	CLA	C1C-C2C	2.13	1.48	1.44
22	2	602	CLA	C3B-C2B	2.12	1.48	1.41
22	L	204	CLA	C1C-C2C	2.12	1.48	1.44
22	J	3002	CLA	C1C-C2C	2.12	1.48	1.44
22	1	611	CLA	C1C-C2C	2.12	1.48	1.44
22	Z	608	CLA	C3B-C2B	2.12	1.48	1.41
22	Z	610	CLA	C1B-C2B	2.12	1.48	1.43
22	A	808	CLA	C4C-C3C	2.12	1.48	1.45
22	B	833	CLA	C1C-NC	-2.12	1.34	1.37
22	5	616	CLA	C1C-C2C	2.12	1.48	1.44
22	5	609	CLA	C1A-CHA	2.12	1.51	1.43
22	A	824	CLA	C1C-C2C	2.12	1.48	1.44
22	B	827	CLA	CHB-C4A	-2.12	1.32	1.37
22	B	835	CLA	C4C-C3C	2.12	1.48	1.45
29	Z	601	CHL	C4D-CHA	2.12	1.45	1.38
22	3	607	CLA	C1C-NC	-2.12	1.34	1.37
22	6	622	CLA	C3B-C2B	2.12	1.48	1.41
22	A	837	CLA	CHB-C4A	-2.12	1.32	1.37
22	B	805	CLA	C1C-C2C	2.12	1.48	1.44
22	7	603	CLA	C1C-C2C	2.12	1.48	1.44
22	B	826	CLA	C1B-C2B	2.12	1.48	1.43
22	3	606	CLA	C1B-C2B	2.12	1.48	1.43
22	5	617	CLA	C3B-C2B	2.12	1.48	1.41
22	Z	614	CLA	C3B-C2B	2.12	1.48	1.41
22	8	609	CLA	C1B-C2B	2.12	1.48	1.43
22	A	822	CLA	C4C-C3C	2.12	1.48	1.45
22	Z	611	CLA	C3B-C2B	2.12	1.48	1.41
22	4	604	CLA	C1C-C2C	2.12	1.48	1.44
22	8	601	CLA	C3B-C2B	2.12	1.48	1.41
22	5	609	CLA	C1B-C2B	2.12	1.48	1.43
22	1	614	CLA	C3B-C2B	2.12	1.48	1.41
22	B	839	CLA	C1C-C2C	2.12	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	822	CLA	C1C-C2C	2.11	1.48	1.44
22	4	609	CLA	C1B-C2B	2.11	1.48	1.43
22	B	839	CLA	C1B-C2B	2.11	1.48	1.43
29	5	618	CHL	C2C-C1C	2.11	1.49	1.44
22	A	824	CLA	C1C-NC	-2.11	1.34	1.37
22	7	612	CLA	C1C-NC	-2.11	1.34	1.37
22	8	609	CLA	C1C-C2C	2.11	1.48	1.44
22	4	612	CLA	C1C-NC	-2.11	1.34	1.37
22	5	617	CLA	C1C-NC	-2.11	1.34	1.37
22	A	816	CLA	C3B-C2B	2.11	1.48	1.41
22	2	603	CLA	C3B-C2B	2.11	1.48	1.41
22	5	616	CLA	C3B-C2B	2.11	1.48	1.41
22	9	613	CLA	C3B-C2B	2.11	1.48	1.41
22	Z	602	CLA	C1B-C2B	2.11	1.48	1.43
22	8	611	CLA	C3B-C2B	2.11	1.48	1.41
22	1	611	CLA	C1B-C2B	2.11	1.48	1.43
22	A	818	CLA	C1C-NC	-2.11	1.34	1.37
29	Z	607	CHL	C2C-C1C	2.11	1.49	1.44
22	4	601	CLA	C3B-C2B	2.11	1.48	1.41
22	3	610	CLA	CHB-C4A	-2.11	1.32	1.37
22	A	810	CLA	C1C-C2C	2.11	1.48	1.44
22	6	611	CLA	C1C-C2C	2.10	1.48	1.44
22	A	819	CLA	CHB-C4A	-2.10	1.32	1.37
22	7	614	CLA	C1C-C2C	2.10	1.48	1.44
22	A	834	CLA	C1C-C2C	2.10	1.48	1.44
22	5	601	CLA	C3B-C2B	2.10	1.48	1.41
22	F	303	CLA	C4C-C3C	2.10	1.48	1.45
22	3	604	CLA	C1B-C2B	2.10	1.48	1.43
22	9	614	CLA	C3B-C2B	2.10	1.48	1.41
22	B	838	CLA	C4C-C3C	2.10	1.48	1.45
22	5	611	CLA	C1C-C2C	2.10	1.48	1.44
22	7	616	CLA	C3B-C2B	2.10	1.48	1.41
22	A	803	CLA	C1C-C2C	2.10	1.48	1.44
22	3	609	CLA	C1C-C2C	2.10	1.48	1.44
22	A	836	CLA	C3B-C2B	2.10	1.48	1.41
22	7	606	CLA	C1C-C2C	2.10	1.48	1.44
22	9	604	CLA	C3B-C2B	2.10	1.48	1.41
22	8	608	CLA	C3B-C2B	2.10	1.48	1.41
22	5	603	CLA	C1C-C2C	2.10	1.48	1.44
22	A	820	CLA	C1A-CHA	2.10	1.51	1.43
22	L	204	CLA	C3B-C2B	2.10	1.48	1.41
22	6	613	CLA	C3B-C2B	2.10	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	303	CLA	C3B-C2B	2.10	1.48	1.41
29	8	607	CHL	C3B-C2B	2.10	1.48	1.41
22	A	843	CLA	C1C-NC	-2.10	1.34	1.37
22	B	836	CLA	C1C-NC	-2.10	1.34	1.37
22	B	810	CLA	C1C-C2C	2.10	1.48	1.44
22	5	606	CLA	C1B-C2B	2.10	1.48	1.43
22	2	601	CLA	C1C-C2C	2.10	1.48	1.44
25	A	851	BCR	C10-C9	-2.10	1.33	1.35
22	5	614	CLA	C3B-C2B	2.10	1.48	1.41
22	A	835	CLA	C1D-C2D	2.10	1.49	1.45
22	7	603	CLA	C1C-NC	-2.10	1.34	1.37
22	7	614	CLA	C1A-CHA	2.10	1.51	1.43
22	A	833	CLA	C3B-C2B	2.10	1.48	1.41
22	B	828	CLA	CHB-C4A	-2.10	1.32	1.37
22	Z	610	CLA	CHB-C4A	-2.09	1.32	1.37
22	5	609	CLA	CHB-C4A	-2.09	1.32	1.37
22	5	611	CLA	C3B-C2B	2.09	1.48	1.41
22	8	612	CLA	C3B-C2B	2.09	1.48	1.41
22	A	817	CLA	C1C-NC	-2.09	1.34	1.37
22	4	612	CLA	C3B-C2B	2.09	1.48	1.41
22	5	612	CLA	C3B-C2B	2.09	1.48	1.41
22	A	839	CLA	CHB-C4A	-2.09	1.32	1.37
22	5	602	CLA	CHB-C4A	-2.09	1.32	1.37
22	A	841	CLA	C4C-C3C	2.09	1.48	1.45
22	B	818	CLA	C4C-C3C	2.09	1.48	1.45
22	B	809	CLA	C1B-C2B	2.09	1.48	1.43
22	2	603	CLA	C1D-C2D	2.09	1.49	1.45
29	9	606	CHL	C3B-C2B	2.09	1.48	1.41
22	A	820	CLA	C1B-C2B	2.09	1.48	1.43
22	1	604	CLA	C1B-C2B	2.09	1.48	1.43
22	A	834	CLA	C4C-C3C	2.09	1.48	1.45
22	B	812	CLA	C1C-NC	-2.09	1.34	1.37
22	Z	612	CLA	C3B-C2B	2.09	1.48	1.41
22	8	610	CLA	C1C-NC	-2.09	1.34	1.37
22	A	820	CLA	C4C-C3C	2.09	1.48	1.45
22	4	612	CLA	C1C-C2C	2.09	1.48	1.44
29	5	608	CHL	C1B-C2B	2.09	1.48	1.43
22	A	805	CLA	C3B-C2B	2.09	1.48	1.41
22	4	609	CLA	C4C-C3C	2.09	1.48	1.45
22	4	602	CLA	C1B-C2B	2.09	1.48	1.43
22	B	808	CLA	C3B-C2B	2.08	1.48	1.41
22	B	818	CLA	C1A-CHA	2.08	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	819	CLA	C1C-C2C	2.08	1.48	1.44
22	B	817	CLA	C3B-C4B	2.08	1.47	1.42
22	A	807	CLA	C3B-C2B	2.08	1.48	1.41
22	Z	609	CLA	C1A-CHA	2.08	1.51	1.43
22	7	611	CLA	C1C-NC	-2.08	1.34	1.37
22	A	824	CLA	C3B-C2B	2.08	1.48	1.41
22	A	802	CLA	C1D-C2D	2.08	1.49	1.45
22	5	613	CLA	C1C-C2C	2.08	1.48	1.44
22	1	611	CLA	CHB-C4A	-2.08	1.32	1.37
22	5	610	CLA	C4C-C3C	2.08	1.48	1.45
22	1	613	CLA	C1C-C2C	2.08	1.48	1.44
22	1	608	CLA	C3B-C2B	2.08	1.48	1.41
22	7	606	CLA	C3B-C2B	2.08	1.48	1.41
22	B	802	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	827	CLA	CHB-C4A	-2.08	1.32	1.37
22	6	611	CLA	C3B-C2B	2.08	1.48	1.41
22	1	611	CLA	C1C-NC	-2.08	1.34	1.37
22	7	614	CLA	C3B-C2B	2.08	1.48	1.41
22	Z	609	CLA	C3B-C2B	2.08	1.48	1.41
22	5	610	CLA	C3B-C2B	2.08	1.48	1.41
22	5	609	CLA	C1C-C2C	2.07	1.48	1.44
22	B	814	CLA	C4C-C3C	2.07	1.48	1.45
22	A	831	CLA	C1C-NC	-2.07	1.34	1.37
22	7	602	CLA	CHB-C4A	-2.07	1.32	1.37
22	8	613	CLA	C3B-C2B	2.07	1.48	1.41
22	B	803	CLA	C1A-CHA	2.07	1.51	1.43
22	7	601	CLA	C1C-C2C	2.07	1.48	1.44
22	B	835	CLA	C3B-C2B	2.07	1.48	1.41
22	9	601	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	836	CLA	C1B-C2B	2.07	1.48	1.43
22	8	610	CLA	C1B-C2B	2.07	1.48	1.43
22	F	301	CLA	C3B-C2B	2.07	1.48	1.41
22	1	609	CLA	C1A-CHA	2.07	1.51	1.43
22	A	842	CLA	C4C-C3C	2.07	1.48	1.45
22	8	603	CLA	C1C-C2C	2.07	1.48	1.44
22	Z	603	CLA	C3B-C2B	2.07	1.48	1.41
22	A	842	CLA	C1C-C2C	2.07	1.48	1.44
29	6	606	CHL	C3B-C2B	2.07	1.48	1.41
22	7	601	CLA	C1C-NC	-2.07	1.34	1.37
22	6	609	CLA	C1A-CHA	2.07	1.51	1.43
22	A	812	CLA	C4C-C3C	2.07	1.48	1.45
22	6	610	CLA	CHB-C4A	-2.07	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	609	CLA	C1A-CHA	2.07	1.51	1.43
22	A	838	CLA	C1B-C2B	2.07	1.48	1.43
22	Z	606	CLA	C1C-C2C	2.07	1.48	1.44
22	B	806	CLA	CHB-C4A	-2.07	1.32	1.37
22	B	833	CLA	C3B-C2B	2.06	1.48	1.41
22	1	614	CLA	C1C-C2C	2.06	1.48	1.44
22	7	614	CLA	CHB-C4A	-2.06	1.32	1.37
22	6	612	CLA	C3B-C2B	2.06	1.48	1.41
22	B	816	CLA	C3B-C2B	2.06	1.48	1.41
22	A	816	CLA	C1B-C2B	2.06	1.48	1.43
22	A	840	CLA	C1C-NC	-2.06	1.34	1.37
22	3	602	CLA	CHB-C4A	-2.06	1.32	1.37
29	5	607	CHL	C4C-C3C	2.06	1.48	1.45
22	A	854	CLA	CHB-C4A	-2.06	1.32	1.37
22	B	832	CLA	CHB-C4A	-2.06	1.32	1.37
22	4	604	CLA	CHB-C4A	-2.06	1.32	1.37
22	B	834	CLA	C1B-C2B	2.06	1.48	1.43
22	9	610	CLA	C3B-C2B	2.06	1.48	1.41
22	F	304	CLA	C1C-C2C	2.06	1.48	1.44
22	6	610	CLA	C3B-C2B	2.06	1.48	1.41
22	B	827	CLA	C1A-CHA	2.06	1.51	1.43
22	1	611	CLA	C3B-C2B	2.06	1.48	1.41
22	8	609	CLA	C3B-C2B	2.06	1.48	1.41
22	3	602	CLA	C1C-NC	-2.06	1.34	1.37
22	A	809	CLA	C3B-C2B	2.06	1.48	1.41
22	A	814	CLA	C3B-C2B	2.06	1.48	1.41
22	B	823	CLA	C1C-C2C	2.06	1.48	1.44
22	A	813	CLA	C3B-C2B	2.06	1.48	1.41
22	A	834	CLA	C3B-C2B	2.06	1.48	1.41
22	1	604	CLA	C1C-C2C	2.05	1.48	1.44
29	4	606	CHL	C1B-C2B	2.05	1.48	1.43
22	6	602	CLA	C3B-C2B	2.05	1.48	1.41
22	3	609	CLA	C1C-NC	-2.05	1.34	1.37
22	A	827	CLA	C3B-C2B	2.05	1.48	1.41
25	7	623	BCR	C38-C26	2.05	1.54	1.50
22	B	804	CLA	C1B-C2B	2.05	1.48	1.43
29	6	606	CHL	C4C-C3C	2.05	1.48	1.45
22	B	824	CLA	C1C-C2C	2.05	1.48	1.44
22	2	612	CLA	C3B-C2B	2.05	1.48	1.41
22	8	609	CLA	CHB-C4A	-2.05	1.32	1.37
22	7	616	CLA	C1C-C2C	2.05	1.48	1.44
22	A	832	CLA	C1B-C2B	2.05	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	808	CLA	C1C-NC	-2.05	1.34	1.37
22	A	839	CLA	C1B-C2B	2.05	1.48	1.43
22	B	838	CLA	C3B-C2B	2.05	1.48	1.41
22	5	616	CLA	C1C-NC	-2.05	1.34	1.37
29	6	607	CHL	CHB-C4A	-2.05	1.32	1.37
22	F	304	CLA	C3B-C2B	2.05	1.48	1.41
22	1	606	CLA	C4C-C3C	2.05	1.48	1.45
22	7	611	CLA	C3B-C2B	2.05	1.48	1.41
22	Z	610	CLA	C3B-C2B	2.05	1.48	1.41
28	J	3001	LMG	O7-C8	-2.05	1.41	1.46
22	1	609	CLA	C3B-C2B	2.04	1.48	1.41
22	B	805	CLA	C1B-C2B	2.04	1.48	1.43
22	5	611	CLA	C1A-CHA	2.04	1.51	1.43
22	9	603	CLA	C3B-C2B	2.04	1.48	1.41
22	8	604	CLA	C1C-NC	-2.04	1.34	1.37
22	B	828	CLA	C1B-C2B	2.04	1.48	1.43
22	4	613	CLA	C1C-C2C	2.04	1.48	1.44
22	3	609	CLA	C3B-C2B	2.04	1.48	1.41
22	A	826	CLA	C1C-NC	-2.04	1.34	1.37
22	9	613	CLA	C1A-CHA	2.04	1.51	1.43
22	5	613	CLA	CHB-C4A	-2.04	1.32	1.37
22	3	603	CLA	C1C-NC	-2.04	1.34	1.37
22	B	834	CLA	CHB-C4A	-2.04	1.32	1.37
22	8	601	CLA	C1A-CHA	2.04	1.51	1.43
22	8	610	CLA	C3B-C2B	2.04	1.48	1.41
22	A	805	CLA	C1D-C2D	2.04	1.49	1.45
22	B	807	CLA	C3B-C2B	2.04	1.48	1.41
22	6	609	CLA	C3B-C2B	2.04	1.48	1.41
22	7	611	CLA	C1A-CHA	2.04	1.51	1.43
22	A	818	CLA	CHB-C4A	-2.04	1.32	1.37
22	5	606	CLA	C3B-C2B	2.04	1.48	1.41
22	A	829	CLA	C1C-NC	-2.04	1.34	1.37
22	B	821	CLA	C1C-NC	-2.04	1.34	1.37
22	B	812	CLA	C3B-C2B	2.04	1.48	1.41
22	6	603	CLA	C3B-C2B	2.04	1.48	1.41
22	A	809	CLA	C4C-C3C	2.04	1.48	1.45
22	9	603	CLA	C1C-C2C	2.03	1.48	1.44
22	Z	606	CLA	C1C-NC	-2.03	1.34	1.37
22	6	609	CLA	C1C-C2C	2.03	1.48	1.44
22	3	607	CLA	C3B-C2B	2.03	1.48	1.41
22	3	612	CLA	C3B-C2B	2.03	1.48	1.41
22	4	611	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	607	CHL	C4C-C3C	2.03	1.48	1.45
22	B	802	CLA	C1C-NC	-2.03	1.34	1.37
22	A	845	CLA	C3B-C2B	2.03	1.48	1.41
22	4	612	CLA	C4C-C3C	2.03	1.48	1.45
22	4	611	CLA	C1C-C2C	2.03	1.48	1.44
22	2	609	CLA	C1A-CHA	2.03	1.51	1.43
29	6	607	CHL	C2C-C1C	2.03	1.48	1.44
22	F	304	CLA	C1A-CHA	2.03	1.51	1.43
22	7	603	CLA	C3B-C2B	2.03	1.48	1.41
22	B	830	CLA	CHB-C4A	-2.03	1.32	1.37
22	B	829	CLA	C4C-C3C	2.03	1.48	1.45
29	6	607	CHL	C1C-NC	-2.03	1.34	1.37
22	A	836	CLA	C1C-C2C	2.03	1.48	1.44
22	B	805	CLA	C3B-C2B	2.03	1.48	1.41
22	A	843	CLA	C1C-C2C	2.03	1.48	1.44
22	A	809	CLA	C1C-NC	-2.03	1.34	1.37
22	B	823	CLA	C1C-NC	-2.03	1.34	1.37
22	A	811	CLA	C3B-C2B	2.03	1.48	1.41
22	8	611	CLA	C1A-CHA	2.03	1.51	1.43
22	A	804	CLA	C1C-C2C	2.03	1.48	1.44
29	5	607	CHL	CHB-C4A	-2.03	1.32	1.37
22	3	620	CLA	C3B-C2B	2.03	1.48	1.41
29	6	607	CHL	C3B-C2B	2.02	1.48	1.41
22	Z	602	CLA	CHB-C4A	-2.02	1.32	1.37
22	A	821	CLA	C3B-C2B	2.02	1.48	1.41
22	A	808	CLA	C3B-C2B	2.02	1.48	1.41
22	A	819	CLA	C3B-C2B	2.02	1.48	1.41
22	F	303	CLA	C1B-C2B	2.02	1.48	1.43
22	A	812	CLA	C3B-C2B	2.02	1.48	1.41
28	9	620	LMG	C4-C5	2.02	1.57	1.53
22	B	819	CLA	C1C-C2C	2.02	1.48	1.44
22	7	604	CLA	C1C-NC	-2.02	1.34	1.37
22	A	837	CLA	C1A-CHA	2.02	1.51	1.43
22	8	603	CLA	C1C-NC	-2.02	1.34	1.37
22	Z	606	CLA	C3B-C2B	2.02	1.48	1.41
22	7	606	CLA	CHB-C4A	-2.02	1.32	1.37
22	5	603	CLA	C4C-C3C	2.02	1.48	1.45
22	G	203	CLA	C1C-NC	-2.02	1.34	1.37
22	3	612	CLA	C1C-C2C	2.02	1.48	1.44
22	5	610	CLA	CHB-C4A	-2.02	1.32	1.37
22	3	617	CLA	C3B-C2B	2.02	1.48	1.41
22	6	601	CLA	C3B-C2B	2.02	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	603	CLA	C1C-NC	-2.02	1.34	1.37
22	1	612	CLA	C1C-C2C	2.02	1.48	1.44
22	B	826	CLA	C3B-C2B	2.02	1.48	1.41
22	6	611	CLA	C1A-CHA	2.02	1.51	1.43
22	1	609	CLA	C1C-C2C	2.02	1.48	1.44
22	A	830	CLA	C1A-CHA	2.02	1.51	1.43
22	A	823	CLA	C3B-C2B	2.02	1.48	1.41
22	B	810	CLA	C1C-NC	-2.02	1.34	1.37
22	B	809	CLA	C4C-C3C	2.02	1.48	1.45
22	7	611	CLA	C1C-C2C	2.02	1.48	1.44
22	8	606	CLA	C3B-C2B	2.02	1.48	1.41
22	B	809	CLA	CHB-C4A	-2.02	1.32	1.37
22	B	825	CLA	C4C-C3C	2.02	1.48	1.45
22	1	612	CLA	C3B-C2B	2.01	1.48	1.41
22	B	804	CLA	CHB-C4A	-2.01	1.32	1.37
29	5	607	CHL	C3B-C2B	2.01	1.48	1.41
22	1	602	CLA	C1B-C2B	2.01	1.48	1.43
22	Z	602	CLA	C4C-C3C	2.01	1.48	1.45
22	A	828	CLA	C3B-C2B	2.01	1.48	1.41
22	A	839	CLA	C3B-C2B	2.01	1.48	1.41
22	7	602	CLA	C4C-C3C	2.01	1.48	1.45
22	A	817	CLA	C1D-C2D	2.01	1.49	1.45
22	A	843	CLA	C3B-C2B	2.01	1.48	1.41
22	6	602	CLA	C1B-C2B	2.01	1.48	1.43
22	A	854	CLA	C3B-C2B	2.01	1.48	1.41
22	A	820	CLA	C1C-C2C	2.01	1.48	1.44
22	8	602	CLA	C3B-C2B	2.01	1.48	1.41
22	B	806	CLA	C3B-C2B	2.01	1.48	1.41
22	7	609	CLA	C1A-CHA	2.01	1.51	1.43
22	A	812	CLA	C1C-C2C	2.01	1.48	1.44
22	5	621	CLA	C1A-CHA	2.01	1.51	1.43
22	5	604	CLA	C1C-C2C	2.01	1.48	1.44
22	K	4002	CLA	C1A-CHA	2.01	1.51	1.43
22	6	601	CLA	C1C-C2C	2.01	1.48	1.44
22	7	614	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	824	CLA	C3B-C2B	2.01	1.48	1.41
22	B	835	CLA	C1A-CHA	2.01	1.51	1.43
22	7	613	CLA	C1C-NC	-2.01	1.34	1.37
29	Z	601	CHL	CHB-C4A	-2.01	1.32	1.37
22	Z	610	CLA	C1A-CHA	2.01	1.51	1.43
22	A	813	CLA	C1B-C2B	2.01	1.48	1.43
22	L	203	CLA	C1C-NC	-2.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	815	CLA	C3B-C2B	2.01	1.48	1.41
22	6	609	CLA	CHB-C4A	-2.01	1.32	1.37
22	F	301	CLA	C4C-C3C	2.01	1.48	1.45
22	A	840	CLA	C1A-CHA	2.01	1.51	1.43
22	5	609	CLA	C3B-C2B	2.00	1.48	1.41
22	B	804	CLA	C1C-NC	-2.00	1.34	1.37
22	B	808	CLA	C1C-C2C	2.00	1.48	1.44
22	1	610	CLA	C3B-C2B	2.00	1.48	1.41
22	3	607	CLA	C1A-CHA	2.00	1.51	1.43
22	6	604	CLA	C1A-CHA	2.00	1.51	1.43
22	5	616	CLA	C1A-CHA	2.00	1.51	1.43
28	J	3001	LMG	C4-C5	2.00	1.57	1.53
22	6	610	CLA	C1B-C2B	2.00	1.48	1.43
22	A	816	CLA	C1A-CHA	2.00	1.51	1.43
22	A	821	CLA	C4C-C3C	2.00	1.48	1.45
22	6	614	CLA	C3B-C2B	2.00	1.48	1.41

All (7711) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	617	CLA	O2A-CGA-O1A	-13.94	79.44	123.14
22	5	617	CLA	O2A-CGA-CBA	12.13	160.18	112.23
29	6	608	CHL	C4A-NA-C1A	-11.78	101.41	106.71
22	5	617	CLA	O1A-CGA-CBA	-11.02	80.75	123.73
29	Z	601	CHL	C4A-NA-C1A	-10.94	101.79	106.71
29	1	601	CHL	C4A-NA-C1A	-10.61	101.94	106.71
22	L	203	CLA	C1D-ND-C4D	-10.34	98.99	106.33
29	9	606	CHL	C4A-NA-C1A	-10.31	102.07	106.71
29	4	608	CHL	C2D-C1D-ND	10.26	117.67	110.10
29	1	607	CHL	C2D-C1D-ND	10.25	117.66	110.10
22	B	829	CLA	C1D-ND-C4D	-10.16	99.11	106.33
29	6	618	CHL	C2D-C1D-ND	10.15	117.59	110.10
22	A	818	CLA	C1D-ND-C4D	-10.12	99.15	106.33
29	4	618	CHL	C4A-NA-C1A	-10.01	102.21	106.71
29	5	618	CHL	C4A-NA-C1A	-10.00	102.21	106.71
22	7	602	CLA	C1D-ND-C4D	-10.00	99.23	106.33
29	3	608	CHL	C2D-C1D-ND	9.97	117.45	110.10
22	7	604	CLA	C1D-ND-C4D	-9.96	99.26	106.33
22	B	838	CLA	C1D-ND-C4D	-9.95	99.27	106.33
22	B	802	CLA	C1D-ND-C4D	-9.93	99.28	106.33
22	A	823	CLA	C1D-ND-C4D	-9.88	99.31	106.33
22	5	617	CLA	C1D-ND-C4D	-9.88	99.32	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	812	CLA	C1D-ND-C4D	-9.88	99.32	106.33
29	6	607	CHL	C2D-C1D-ND	9.87	117.38	110.10
22	8	602	CLA	C1D-ND-C4D	-9.87	99.32	106.33
22	7	608	CLA	C1D-ND-C4D	-9.85	99.33	106.33
29	Z	607	CHL	C2D-C1D-ND	9.82	117.34	110.10
22	A	854	CLA	C1D-ND-C4D	-9.80	99.37	106.33
29	8	607	CHL	C2D-C1D-ND	9.80	117.33	110.10
22	7	606	CLA	C1D-ND-C4D	-9.79	99.38	106.33
22	5	602	CLA	C1D-ND-C4D	-9.78	99.39	106.33
29	Z	601	CHL	C2D-C1D-ND	9.77	117.30	110.10
29	5	607	CHL	C2D-C1D-ND	9.77	117.30	110.10
29	6	606	CHL	C4A-NA-C1A	-9.74	102.33	106.71
29	6	606	CHL	C2D-C1D-ND	9.72	117.27	110.10
22	A	803	CLA	C1D-ND-C4D	-9.71	99.43	106.33
29	4	607	CHL	C4A-NA-C1A	-9.71	102.34	106.71
22	7	610	CLA	C2B-C1B-NB	9.69	116.73	110.23
29	4	607	CHL	C2D-C1D-ND	9.68	117.24	110.10
22	6	602	CLA	C1D-ND-C4D	-9.67	99.47	106.33
22	L	204	CLA	C1D-ND-C4D	-9.63	99.49	106.33
29	9	606	CHL	C2D-C1D-ND	9.63	117.20	110.10
29	5	618	CHL	C2D-C1D-ND	9.59	117.17	110.10
29	4	606	CHL	C2D-C1D-ND	9.58	117.16	110.10
22	B	821	CLA	C1D-ND-C4D	-9.58	99.53	106.33
29	9	607	CHL	C2D-C1D-ND	9.55	117.14	110.10
22	B	837	CLA	C1D-ND-C4D	-9.55	99.55	106.33
22	1	614	CLA	C1D-ND-C4D	-9.55	99.55	106.33
22	B	804	CLA	C2B-C1B-NB	9.53	116.62	110.23
22	5	617	CLA	C2D-C1D-ND	9.51	117.11	110.10
29	4	618	CHL	C2D-C1D-ND	9.50	117.10	110.10
29	5	608	CHL	C2D-C1D-ND	9.49	117.10	110.10
22	A	816	CLA	C1D-ND-C4D	-9.48	99.60	106.33
22	A	841	CLA	C1D-ND-C4D	-9.47	99.61	106.33
22	2	614	CLA	C1D-ND-C4D	-9.47	99.61	106.33
22	5	614	CLA	C1D-ND-C4D	-9.46	99.62	106.33
22	A	845	CLA	C1D-ND-C4D	-9.45	99.62	106.33
22	2	610	CLA	C1D-ND-C4D	-9.45	99.62	106.33
22	9	604	CLA	C1D-ND-C4D	-9.44	99.63	106.33
22	A	808	CLA	C1D-ND-C4D	-9.43	99.63	106.33
29	6	608	CHL	C2D-C1D-ND	9.43	117.05	110.10
22	A	828	CLA	C1D-ND-C4D	-9.43	99.64	106.33
22	7	609	CLA	C2B-C1B-NB	9.43	116.55	110.23
22	B	816	CLA	C1D-ND-C4D	-9.42	99.64	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	822	CLA	C1D-ND-C4D	-9.42	99.64	106.33
22	B	812	CLA	C1D-ND-C4D	-9.42	99.64	106.33
22	A	842	CLA	C1D-ND-C4D	-9.41	99.65	106.33
22	L	203	CLA	C2D-C1D-ND	9.41	117.04	110.10
22	A	827	CLA	C1D-ND-C4D	-9.40	99.66	106.33
22	B	831	CLA	C1D-ND-C4D	-9.39	99.67	106.33
22	B	841	CLA	C1D-ND-C4D	-9.39	99.67	106.33
22	Z	602	CLA	C1D-ND-C4D	-9.39	99.67	106.33
22	A	804	CLA	C1D-ND-C4D	-9.38	99.67	106.33
22	4	616	CLA	C1D-ND-C4D	-9.38	99.67	106.33
22	A	841	CLA	C2B-C1B-NB	9.36	116.51	110.23
22	7	601	CLA	C1D-ND-C4D	-9.36	99.69	106.33
22	6	614	CLA	C1D-ND-C4D	-9.36	99.69	106.33
22	2	607	CLA	C1D-ND-C4D	-9.35	99.69	106.33
22	Z	610	CLA	C1D-ND-C4D	-9.35	99.69	106.33
22	A	809	CLA	C1D-ND-C4D	-9.34	99.70	106.33
22	A	806	CLA	C1D-ND-C4D	-9.33	99.70	106.33
29	1	601	CHL	C2D-C1D-ND	9.33	116.98	110.10
22	4	609	CLA	C2B-C1B-NB	9.32	116.48	110.23
22	B	805	CLA	C1D-ND-C4D	-9.32	99.72	106.33
22	A	811	CLA	C1D-ND-C4D	-9.32	99.72	106.33
22	A	836	CLA	C1D-ND-C4D	-9.29	99.73	106.33
22	8	609	CLA	C2B-C1B-NB	9.29	116.46	110.23
22	1	610	CLA	C1D-ND-C4D	-9.28	99.74	106.33
22	3	614	CLA	C1D-ND-C4D	-9.28	99.74	106.33
22	A	814	CLA	C1D-ND-C4D	-9.28	99.74	106.33
22	B	833	CLA	C1D-ND-C4D	-9.28	99.74	106.33
22	4	614	CLA	C1D-ND-C4D	-9.28	99.74	106.33
29	6	618	CHL	C4A-NA-C1A	-9.27	102.54	106.71
22	3	610	CLA	C1D-ND-C4D	-9.26	99.75	106.33
22	6	613	CLA	C1D-ND-C4D	-9.24	99.77	106.33
22	2	602	CLA	C1D-ND-C4D	-9.24	99.77	106.33
22	5	613	CLA	C2B-C1B-NB	9.23	116.42	110.23
22	8	608	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	B	804	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	B	825	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	2	611	CLA	C1D-ND-C4D	-9.21	99.79	106.33
22	A	805	CLA	C1D-ND-C4D	-9.21	99.79	106.33
22	7	609	CLA	C1D-ND-C4D	-9.21	99.80	106.33
22	4	602	CLA	C1D-ND-C4D	-9.21	99.80	106.33
22	4	601	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	A	829	CLA	C2B-C1B-NB	9.20	116.40	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	827	CLA	C2B-C1B-NB	9.19	116.39	110.23
22	A	802	CLA	C1D-ND-C4D	-9.19	99.81	106.33
22	6	622	CLA	C1D-ND-C4D	-9.19	99.81	106.33
22	A	815	CLA	C1D-ND-C4D	-9.16	99.83	106.33
22	A	810	CLA	C1D-ND-C4D	-9.16	99.83	106.33
22	5	609	CLA	C2B-C1B-NB	9.15	116.37	110.23
22	7	612	CLA	C1D-ND-C4D	-9.15	99.83	106.33
22	6	601	CLA	C1D-ND-C4D	-9.14	99.84	106.33
22	3	602	CLA	C1D-ND-C4D	-9.14	99.84	106.33
22	G	203	CLA	C1D-ND-C4D	-9.14	99.84	106.33
22	A	834	CLA	C1D-ND-C4D	-9.13	99.85	106.33
22	4	612	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	B	820	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	Z	614	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	1	602	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	3	612	CLA	C2B-C1B-NB	9.11	116.34	110.23
22	7	613	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	A	824	CLA	C1D-ND-C4D	-9.10	99.87	106.33
29	7	607	CHL	C2D-C1D-ND	9.09	116.80	110.10
22	9	610	CLA	C1D-ND-C4D	-9.09	99.88	106.33
22	B	836	CLA	C2B-C1B-NB	9.08	116.32	110.23
22	Z	611	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	2	613	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	9	614	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	7	620	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	3	612	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	3	620	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	8	614	CLA	C1D-ND-C4D	-9.06	99.90	106.33
22	1	608	CLA	C1D-ND-C4D	-9.06	99.90	106.33
22	A	817	CLA	C1D-ND-C4D	-9.06	99.90	106.33
22	B	811	CLA	C1D-ND-C4D	-9.05	99.90	106.33
22	B	832	CLA	C1D-ND-C4D	-9.03	99.92	106.33
22	K	4002	CLA	C1D-ND-C4D	-9.03	99.92	106.33
29	8	607	CHL	C4A-NA-C1A	-9.03	102.65	106.71
22	4	613	CLA	C1D-ND-C4D	-9.03	99.92	106.33
22	A	830	CLA	C1D-ND-C4D	-9.03	99.92	106.33
22	4	604	CLA	C1D-ND-C4D	-9.02	99.92	106.33
22	8	606	CLA	C1D-ND-C4D	-9.02	99.93	106.33
22	A	835	CLA	C1D-ND-C4D	-9.02	99.93	106.33
22	A	840	CLA	C1D-ND-C4D	-9.02	99.93	106.33
22	F	304	CLA	C1D-ND-C4D	-9.02	99.93	106.33
22	A	818	CLA	C2D-C1D-ND	9.01	116.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	854	CLA	C2D-C1D-ND	9.01	116.74	110.10
22	9	602	CLA	C1D-ND-C4D	-9.01	99.94	106.33
22	5	610	CLA	C1D-ND-C4D	-9.01	99.94	106.33
22	3	607	CLA	C2B-C1B-NB	9.00	116.27	110.23
22	A	813	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	A	825	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	8	604	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	B	802	CLA	C2D-C1D-ND	8.99	116.73	110.10
22	Z	613	CLA	C1D-ND-C4D	-8.99	99.95	106.33
22	F	303	CLA	C1D-ND-C4D	-8.99	99.95	106.33
22	B	805	CLA	C2D-C1D-ND	8.99	116.73	110.10
22	B	840	CLA	C1D-ND-C4D	-8.98	99.95	106.33
22	B	826	CLA	C1D-ND-C4D	-8.98	99.95	106.33
22	Z	612	CLA	C1D-ND-C4D	-8.98	99.96	106.33
22	Z	608	CLA	C1D-ND-C4D	-8.98	99.96	106.33
22	B	830	CLA	C1D-ND-C4D	-8.98	99.96	106.33
22	B	815	CLA	C1D-ND-C4D	-8.97	99.96	106.33
22	3	607	CLA	C1D-ND-C4D	-8.97	99.96	106.33
22	G	204	CLA	C1D-ND-C4D	-8.97	99.96	106.33
22	7	610	CLA	C1D-ND-C4D	-8.97	99.96	106.33
22	3	604	CLA	C1D-ND-C4D	-8.97	99.96	106.33
22	2	606	CLA	C1D-ND-C4D	-8.97	99.97	106.33
22	7	616	CLA	C1D-ND-C4D	-8.96	99.97	106.33
22	1	613	CLA	C1D-ND-C4D	-8.96	99.97	106.33
22	1	610	CLA	C2B-C1B-NB	8.95	116.23	110.23
22	1	606	CLA	C1D-ND-C4D	-8.94	99.98	106.33
22	J	3002	CLA	C1D-ND-C4D	-8.93	99.99	106.33
22	B	810	CLA	C1D-ND-C4D	-8.92	100.00	106.33
22	9	603	CLA	C1D-ND-C4D	-8.92	100.00	106.33
22	A	828	CLA	C2D-C1D-ND	8.91	116.67	110.10
22	2	603	CLA	C2B-C1B-NB	8.91	116.20	110.23
22	Z	606	CLA	C1D-ND-C4D	-8.90	100.01	106.33
29	6	607	CHL	C2B-C1B-NB	8.89	116.19	110.23
22	1	603	CLA	C1D-ND-C4D	-8.89	100.02	106.33
22	4	609	CLA	C1D-ND-C4D	-8.88	100.03	106.33
22	1	609	CLA	C1D-ND-C4D	-8.87	100.03	106.33
22	B	831	CLA	C2B-C1B-NB	8.87	116.18	110.23
22	9	613	CLA	C1D-ND-C4D	-8.87	100.04	106.33
22	A	804	CLA	C2B-C1B-NB	8.86	116.17	110.23
22	A	807	CLA	C1D-ND-C4D	-8.85	100.05	106.33
22	5	606	CLA	C1D-ND-C4D	-8.85	100.05	106.33
22	A	829	CLA	C1D-ND-C4D	-8.84	100.05	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	612	CLA	C1D-ND-C4D	-8.84	100.05	106.33
22	2	603	CLA	C1D-ND-C4D	-8.84	100.06	106.33
22	A	830	CLA	C2B-C1B-NB	8.84	116.16	110.23
22	A	811	CLA	C2B-C1B-NB	8.83	116.15	110.23
22	B	808	CLA	C1D-ND-C4D	-8.83	100.06	106.33
22	B	827	CLA	C1D-ND-C4D	-8.83	100.06	106.33
22	6	612	CLA	C1D-ND-C4D	-8.83	100.06	106.33
22	2	601	CLA	C1D-ND-C4D	-8.82	100.07	106.33
22	3	617	CLA	C1D-ND-C4D	-8.81	100.08	106.33
22	A	820	CLA	C1D-ND-C4D	-8.81	100.08	106.33
22	A	841	CLA	C2D-C1D-ND	8.81	116.59	110.10
22	3	603	CLA	C1D-ND-C4D	-8.81	100.08	106.33
22	9	612	CLA	C1D-ND-C4D	-8.81	100.08	106.33
22	1	612	CLA	C1D-ND-C4D	-8.80	100.08	106.33
22	A	809	CLA	C2B-C1B-NB	8.80	116.13	110.23
22	1	612	CLA	C2B-C1B-NB	8.79	116.13	110.23
22	B	839	CLA	C1D-ND-C4D	-8.79	100.09	106.33
22	7	614	CLA	C1D-ND-C4D	-8.79	100.09	106.33
22	6	609	CLA	C2B-C1B-NB	8.78	116.12	110.23
22	6	603	CLA	C1D-ND-C4D	-8.77	100.10	106.33
21	A	801	CL0	C1D-ND-C4D	-8.77	100.11	106.33
22	A	819	CLA	C1D-ND-C4D	-8.77	100.11	106.33
22	6	610	CLA	C2B-C1B-NB	8.77	116.11	110.23
22	K	4003	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	6	616	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	3	609	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	7	603	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	6	604	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	7	614	CLA	C2B-C1B-NB	8.76	116.10	110.23
22	1	611	CLA	C1D-ND-C4D	-8.76	100.11	106.33
22	A	803	CLA	C2B-C1B-NB	8.75	116.10	110.23
22	B	852	CLA	C1D-ND-C4D	-8.75	100.12	106.33
22	5	612	CLA	C1D-ND-C4D	-8.75	100.12	106.33
22	B	814	CLA	C1D-ND-C4D	-8.74	100.13	106.33
22	9	601	CLA	C1D-ND-C4D	-8.74	100.13	106.33
22	2	609	CLA	C2B-C1B-NB	8.74	116.09	110.23
22	B	815	CLA	C2B-C1B-NB	8.74	116.09	110.23
22	Z	616	CLA	C1D-ND-C4D	-8.73	100.13	106.33
22	A	839	CLA	C1D-ND-C4D	-8.72	100.14	106.33
22	9	614	CLA	C2B-C1B-NB	8.72	116.08	110.23
29	5	607	CHL	C4A-NA-C1A	-8.71	102.79	106.71
22	B	834	CLA	C1D-ND-C4D	-8.71	100.15	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	606	CLA	C1D-ND-C4D	-8.70	100.15	106.33
22	A	839	CLA	C2B-C1B-NB	8.70	116.06	110.23
22	A	818	CLA	C2B-C1B-NB	8.68	116.05	110.23
22	B	806	CLA	C1D-ND-C4D	-8.66	100.18	106.33
22	B	824	CLA	C1D-ND-C4D	-8.66	100.18	106.33
22	9	609	CLA	C2B-C1B-NB	8.66	116.04	110.23
22	A	854	CLA	C2B-C1B-NB	8.66	116.04	110.23
22	A	823	CLA	C2D-C1D-ND	8.65	116.48	110.10
22	A	819	CLA	C2B-C1B-NB	8.65	116.03	110.23
22	Z	604	CLA	C1D-ND-C4D	-8.65	100.19	106.33
22	A	833	CLA	C1D-ND-C4D	-8.65	100.19	106.33
22	5	601	CLA	C1D-ND-C4D	-8.65	100.19	106.33
22	A	821	CLA	C1D-ND-C4D	-8.65	100.19	106.33
22	B	813	CLA	C1D-ND-C4D	-8.65	100.19	106.33
22	B	816	CLA	C2D-C1D-ND	8.65	116.47	110.10
22	A	834	CLA	C2B-C1B-NB	8.64	116.03	110.23
22	7	602	CLA	C2D-C1D-ND	8.64	116.47	110.10
22	A	838	CLA	C1D-ND-C4D	-8.64	100.20	106.33
22	1	604	CLA	C1D-ND-C4D	-8.64	100.20	106.33
22	B	814	CLA	C2B-C1B-NB	8.64	116.02	110.23
22	9	611	CLA	C1D-ND-C4D	-8.63	100.20	106.33
22	5	614	CLA	C2B-C1B-NB	8.63	116.02	110.23
22	5	609	CLA	C1D-ND-C4D	-8.63	100.20	106.33
22	6	609	CLA	C1D-ND-C4D	-8.63	100.20	106.33
22	B	804	CLA	C2D-C1D-ND	8.63	116.46	110.10
22	A	840	CLA	C2B-C1B-NB	8.62	116.01	110.23
22	1	614	CLA	C2B-C1B-NB	8.62	116.01	110.23
22	3	609	CLA	C2B-C1B-NB	8.62	116.01	110.23
22	A	829	CLA	C2D-C1D-ND	8.62	116.46	110.10
22	Z	609	CLA	C2B-C1B-NB	8.62	116.01	110.23
22	4	613	CLA	C2B-C1B-NB	8.62	116.01	110.23
22	B	831	CLA	C2D-C1D-ND	8.61	116.45	110.10
22	A	813	CLA	C2B-C1B-NB	8.61	116.00	110.23
22	6	614	CLA	C2B-C1B-NB	8.60	116.00	110.23
22	A	812	CLA	C2D-C1D-ND	8.60	116.44	110.10
22	9	602	CLA	C2B-C1B-NB	8.60	116.00	110.23
22	A	806	CLA	C2B-C1B-NB	8.60	116.00	110.23
22	B	807	CLA	C1D-ND-C4D	-8.60	100.23	106.33
22	2	612	CLA	C1D-ND-C4D	-8.59	100.23	106.33
22	6	617	CLA	C1D-ND-C4D	-8.59	100.23	106.33
22	5	611	CLA	C1D-ND-C4D	-8.59	100.23	106.33
22	8	613	CLA	C1D-ND-C4D	-8.59	100.24	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	610	CLA	C1D-ND-C4D	-8.58	100.24	106.33
22	8	602	CLA	C2D-C1D-ND	8.58	116.42	110.10
22	2	613	CLA	C2B-C1B-NB	8.58	115.98	110.23
22	B	835	CLA	C1D-ND-C4D	-8.57	100.25	106.33
22	9	603	CLA	C2B-C1B-NB	8.57	115.98	110.23
22	5	613	CLA	C1D-ND-C4D	-8.57	100.25	106.33
22	A	838	CLA	C2B-C1B-NB	8.57	115.97	110.23
22	B	834	CLA	C2B-C1B-NB	8.56	115.97	110.23
22	8	603	CLA	C1D-ND-C4D	-8.56	100.25	106.33
22	B	837	CLA	C2B-C1B-NB	8.56	115.97	110.23
22	B	828	CLA	C1D-ND-C4D	-8.56	100.25	106.33
22	B	830	CLA	C2B-C1B-NB	8.56	115.97	110.23
22	A	814	CLA	C2B-C1B-NB	8.56	115.97	110.23
29	5	607	CHL	C2B-C1B-NB	8.55	115.97	110.23
22	A	831	CLA	C1D-ND-C4D	-8.55	100.26	106.33
22	Z	614	CLA	C2B-C1B-NB	8.55	115.96	110.23
22	1	616	CLA	C1D-ND-C4D	-8.54	100.27	106.33
22	Z	603	CLA	C1D-ND-C4D	-8.54	100.27	106.33
22	5	610	CLA	C2B-C1B-NB	8.54	115.96	110.23
22	F	301	CLA	C1D-ND-C4D	-8.53	100.27	106.33
29	5	608	CHL	C4A-NA-C1A	-8.53	102.87	106.71
22	6	611	CLA	C1D-ND-C4D	-8.53	100.28	106.33
22	7	608	CLA	C2D-C1D-ND	8.51	116.38	110.10
22	6	610	CLA	C1D-ND-C4D	-8.51	100.29	106.33
22	8	611	CLA	C1D-ND-C4D	-8.51	100.29	106.33
22	B	803	CLA	C2D-C1D-ND	8.50	116.37	110.10
22	1	604	CLA	C2B-C1B-NB	8.50	115.93	110.23
22	7	602	CLA	C2B-C1B-NB	8.50	115.93	110.23
29	4	608	CHL	C4A-NA-C1A	-8.50	102.89	106.71
22	3	613	CLA	C1D-ND-C4D	-8.50	100.30	106.33
22	A	845	CLA	C2B-C1B-NB	8.50	115.93	110.23
22	B	803	CLA	C1D-ND-C4D	-8.50	100.30	106.33
22	7	611	CLA	C1D-ND-C4D	-8.50	100.30	106.33
22	B	839	CLA	C2B-C1B-NB	8.50	115.93	110.23
22	B	806	CLA	C2B-C1B-NB	8.49	115.92	110.23
22	A	803	CLA	C2D-C1D-ND	8.49	116.36	110.10
22	A	830	CLA	C2D-C1D-ND	8.48	116.36	110.10
22	3	602	CLA	C2B-C1B-NB	8.48	115.92	110.23
22	7	612	CLA	C2B-C1B-NB	8.48	115.92	110.23
22	7	606	CLA	C2B-C1B-NB	8.48	115.92	110.23
22	4	603	CLA	C2B-C1B-NB	8.48	115.91	110.23
22	2	609	CLA	C1D-ND-C4D	-8.48	100.31	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	610	CLA	C1D-ND-C4D	-8.47	100.32	106.33
22	8	616	CLA	C1D-ND-C4D	-8.47	100.32	106.33
22	1	611	CLA	C2B-C1B-NB	8.47	115.91	110.23
22	6	602	CLA	C2B-C1B-NB	8.46	115.91	110.23
22	5	616	CLA	C1D-ND-C4D	-8.45	100.33	106.33
22	1	609	CLA	C2B-C1B-NB	8.44	115.89	110.23
22	B	819	CLA	C1D-ND-C4D	-8.44	100.34	106.33
22	7	604	CLA	C2D-C1D-ND	8.43	116.31	110.10
22	B	829	CLA	C2B-C1B-NB	8.42	115.88	110.23
22	3	611	CLA	C1D-ND-C4D	-8.42	100.35	106.33
22	8	612	CLA	C2B-C1B-NB	8.42	115.88	110.23
22	F	304	CLA	C2B-C1B-NB	8.42	115.88	110.23
22	2	601	CLA	C2B-C1B-NB	8.41	115.87	110.23
22	6	617	CLA	C2B-C1B-NB	8.41	115.87	110.23
22	9	609	CLA	C1D-ND-C4D	-8.40	100.36	106.33
22	F	301	CLA	C2B-C1B-NB	8.40	115.86	110.23
22	G	204	CLA	C2B-C1B-NB	8.40	115.86	110.23
22	Z	610	CLA	C2B-C1B-NB	8.40	115.86	110.23
22	A	812	CLA	C2B-C1B-NB	8.40	115.86	110.23
22	A	809	CLA	C2D-C1D-ND	8.40	116.29	110.10
22	3	606	CLA	C2B-C1B-NB	8.38	115.85	110.23
22	B	833	CLA	C2B-C1B-NB	8.38	115.85	110.23
22	A	833	CLA	C2B-C1B-NB	8.38	115.85	110.23
22	3	611	CLA	C2B-C1B-NB	8.38	115.85	110.23
22	8	608	CLA	C2D-C1D-ND	8.38	116.28	110.10
22	B	809	CLA	C1D-ND-C4D	-8.37	100.39	106.33
22	5	617	CLA	C2B-C1B-NB	8.37	115.84	110.23
22	4	611	CLA	C1D-ND-C4D	-8.37	100.39	106.33
22	B	810	CLA	C2B-C1B-NB	8.37	115.84	110.23
22	B	825	CLA	C2B-C1B-NB	8.37	115.84	110.23
22	8	601	CLA	C1D-ND-C4D	-8.36	100.39	106.33
22	7	611	CLA	C2B-C1B-NB	8.36	115.84	110.23
22	4	603	CLA	C1D-ND-C4D	-8.36	100.40	106.33
22	Z	609	CLA	C1D-ND-C4D	-8.35	100.40	106.33
22	A	832	CLA	C1D-ND-C4D	-8.34	100.41	106.33
22	5	602	CLA	C2B-C1B-NB	8.34	115.83	110.23
22	5	606	CLA	C2B-C1B-NB	8.34	115.83	110.23
22	2	611	CLA	C2B-C1B-NB	8.34	115.83	110.23
22	B	811	CLA	C2B-C1B-NB	8.34	115.82	110.23
22	B	824	CLA	C2B-C1B-NB	8.34	115.82	110.23
22	7	616	CLA	C2D-C1D-ND	8.33	116.25	110.10
29	4	606	CHL	C4A-NA-C1A	-8.33	102.96	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	602	CLA	C2D-C1D-ND	8.33	116.24	110.10
22	Z	612	CLA	C2B-C1B-NB	8.32	115.81	110.23
22	5	604	CLA	C1D-ND-C4D	-8.32	100.42	106.33
22	Z	611	CLA	C2B-C1B-NB	8.32	115.81	110.23
22	1	610	CLA	C2D-C1D-ND	8.32	116.24	110.10
22	A	826	CLA	C1D-ND-C4D	-8.32	100.42	106.33
22	7	609	CLA	C2D-C1D-ND	8.32	116.23	110.10
22	A	827	CLA	C2B-C1B-NB	8.32	115.81	110.23
22	7	606	CLA	C2D-C1D-ND	8.31	116.23	110.10
22	A	840	CLA	C2D-C1D-ND	8.31	116.23	110.10
22	1	606	CLA	C2B-C1B-NB	8.31	115.80	110.23
22	F	303	CLA	C2D-C1D-ND	8.31	116.23	110.10
22	J	3002	CLA	C2B-C1B-NB	8.31	115.80	110.23
22	4	611	CLA	C2B-C1B-NB	8.29	115.79	110.23
22	A	808	CLA	C2B-C1B-NB	8.29	115.79	110.23
22	Z	610	CLA	C2D-C1D-ND	8.28	116.21	110.10
22	6	614	CLA	CMD-C2D-C1D	8.28	139.30	124.71
22	7	601	CLA	C2B-C1B-NB	8.27	115.77	110.23
22	L	204	CLA	C2D-C1D-ND	8.26	116.19	110.10
22	B	838	CLA	C2D-C1D-ND	8.26	116.19	110.10
22	B	818	CLA	C2B-C1B-NB	8.26	115.77	110.23
22	5	611	CLA	C2B-C1B-NB	8.26	115.77	110.23
22	B	808	CLA	C2B-C1B-NB	8.26	115.77	110.23
22	B	821	CLA	C2D-C1D-ND	8.25	116.18	110.10
22	B	802	CLA	C2B-C1B-NB	8.25	115.76	110.23
22	B	817	CLA	C1D-ND-C4D	-8.24	100.48	106.33
22	Z	606	CLA	C2B-C1B-NB	8.24	115.76	110.23
22	9	611	CLA	C2B-C1B-NB	8.24	115.76	110.23
22	6	622	CLA	C2D-C1D-ND	8.24	116.18	110.10
22	B	823	CLA	C2B-C1B-NB	8.23	115.75	110.23
22	B	838	CLA	C2B-C1B-NB	8.23	115.75	110.23
22	K	4002	CLA	C2B-C1B-NB	8.22	115.74	110.23
22	7	616	CLA	C2B-C1B-NB	8.22	115.74	110.23
22	6	611	CLA	C2B-C1B-NB	8.22	115.74	110.23
22	B	823	CLA	C1D-ND-C4D	-8.22	100.50	106.33
22	B	813	CLA	C2B-C1B-NB	8.21	115.74	110.23
22	A	822	CLA	C1D-ND-C4D	-8.21	100.50	106.33
22	B	803	CLA	C2B-C1B-NB	8.21	115.73	110.23
22	A	811	CLA	C2D-C1D-ND	8.20	116.15	110.10
22	8	609	CLA	C1D-ND-C4D	-8.20	100.51	106.33
22	3	610	CLA	C2B-C1B-NB	8.20	115.73	110.23
22	G	203	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	9	613	CLA	C2B-C1B-NB	8.19	115.72	110.23
22	A	845	CLA	C2D-C1D-ND	8.19	116.14	110.10
22	G	203	CLA	C2B-C1B-NB	8.18	115.72	110.23
22	3	614	CLA	C2B-C1B-NB	8.18	115.72	110.23
22	Z	602	CLA	C2B-C1B-NB	8.18	115.72	110.23
22	Z	602	CLA	C2D-C1D-ND	8.18	116.13	110.10
29	4	618	CHL	C2B-C1B-NB	8.18	115.72	110.23
22	9	601	CLA	C2B-C1B-NB	8.18	115.71	110.23
22	8	610	CLA	C2B-C1B-NB	8.17	115.71	110.23
22	5	616	CLA	C2B-C1B-NB	8.17	115.71	110.23
22	3	617	CLA	C2B-C1B-NB	8.17	115.71	110.23
22	B	827	CLA	C2D-C1D-ND	8.17	116.12	110.10
29	3	608	CHL	C4A-NA-C1A	-8.17	103.03	106.71
22	B	807	CLA	C2B-C1B-NB	8.16	115.70	110.23
22	B	812	CLA	C2D-C1D-ND	8.16	116.12	110.10
22	B	805	CLA	C2B-C1B-NB	8.15	115.69	110.23
22	5	601	CLA	C2B-C1B-NB	8.15	115.69	110.23
22	5	612	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	B	812	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	K	4003	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	A	843	CLA	C1D-ND-C4D	-8.14	100.55	106.33
22	1	602	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	2	607	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	4	610	CLA	C2B-C1B-NB	8.13	115.68	110.23
22	6	612	CLA	C2B-C1B-NB	8.12	115.68	110.23
22	B	832	CLA	C2B-C1B-NB	8.12	115.68	110.23
22	B	836	CLA	C1D-ND-C4D	-8.12	100.57	106.33
22	7	601	CLA	C2D-C1D-ND	8.11	116.08	110.10
22	7	613	CLA	C2D-C1D-ND	8.10	116.08	110.10
22	7	620	CLA	C2B-C1B-NB	8.10	115.66	110.23
22	8	614	CLA	C2B-C1B-NB	8.10	115.66	110.23
22	A	837	CLA	C2B-C1B-NB	8.09	115.66	110.23
29	6	606	CHL	C2B-C1B-NB	8.09	115.66	110.23
22	5	604	CLA	C2B-C1B-NB	8.08	115.65	110.23
22	5	603	CLA	C1D-ND-C4D	-8.08	100.59	106.33
29	5	608	CHL	C2B-C1B-NB	8.08	115.65	110.23
22	1	602	CLA	C2D-C1D-ND	8.06	116.05	110.10
22	1	614	CLA	C2D-C1D-ND	8.06	116.05	110.10
22	B	828	CLA	C2B-C1B-NB	8.06	115.64	110.23
22	A	842	CLA	C2D-C1D-ND	8.06	116.05	110.10
22	A	824	CLA	C2B-C1B-NB	8.06	115.64	110.23
22	B	837	CLA	C2D-C1D-ND	8.06	116.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	606	CLA	C2B-C1B-NB	8.06	115.64	110.23
29	5	618	CHL	C2B-C1B-NB	8.05	115.63	110.23
22	A	837	CLA	C1D-ND-C4D	-8.04	100.62	106.33
22	L	204	CLA	C2B-C1B-NB	8.04	115.62	110.23
22	F	303	CLA	C2B-C1B-NB	8.04	115.62	110.23
29	6	618	CHL	C2B-C1B-NB	8.04	115.62	110.23
22	5	621	CLA	C2B-C1B-NB	8.03	115.62	110.23
29	7	607	CHL	C2B-C1B-NB	8.03	115.61	110.23
22	2	610	CLA	C2B-C1B-NB	8.02	115.61	110.23
22	A	832	CLA	C2B-C1B-NB	8.02	115.61	110.23
22	8	614	CLA	C2D-C1D-ND	8.02	116.01	110.10
22	4	612	CLA	C2B-C1B-NB	8.02	115.61	110.23
21	A	801	CL0	C2D-C1D-ND	8.02	116.01	110.10
22	2	602	CLA	C2B-C1B-NB	8.01	115.60	110.23
22	B	815	CLA	C2D-C1D-ND	8.01	116.01	110.10
22	A	836	CLA	C2D-C1D-ND	8.01	116.00	110.10
22	5	602	CLA	C2D-C1D-ND	8.00	116.00	110.10
22	8	611	CLA	C2B-C1B-NB	7.99	115.59	110.23
22	9	612	CLA	C2B-C1B-NB	7.99	115.59	110.23
22	A	808	CLA	C2D-C1D-ND	7.99	115.99	110.10
22	Z	603	CLA	C2B-C1B-NB	7.99	115.59	110.23
22	B	816	CLA	C2B-C1B-NB	7.99	115.59	110.23
22	B	835	CLA	C2B-C1B-NB	7.98	115.58	110.23
22	9	604	CLA	C2B-C1B-NB	7.98	115.58	110.23
22	2	614	CLA	C2D-C1D-ND	7.98	115.99	110.10
22	5	614	CLA	C2D-C1D-ND	7.98	115.98	110.10
22	A	817	CLA	CMD-C2D-C1D	7.98	138.77	124.71
22	A	820	CLA	C2B-C1B-NB	7.97	115.58	110.23
22	4	612	CLA	C2D-C1D-ND	7.97	115.98	110.10
22	A	814	CLA	C2D-C1D-ND	7.97	115.98	110.10
22	B	829	CLA	C2D-C1D-ND	7.97	115.98	110.10
22	B	822	CLA	C2B-C1B-NB	7.97	115.57	110.23
22	A	831	CLA	C2D-C1D-ND	7.94	115.96	110.10
22	A	816	CLA	C2B-C1B-NB	7.94	115.56	110.23
29	9	607	CHL	C2B-C1B-NB	7.94	115.55	110.23
22	5	610	CLA	C2D-C1D-ND	7.94	115.95	110.10
22	2	612	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	8	601	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	8	608	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	A	816	CLA	C2D-C1D-ND	7.93	115.95	110.10
22	6	616	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	4	614	CLA	C2B-C1B-NB	7.93	115.55	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	603	CLA	C2B-C1B-NB	7.92	115.54	110.23
22	4	613	CLA	C2D-C1D-ND	7.91	115.94	110.10
29	1	601	CHL	C2B-C1B-NB	7.91	115.54	110.23
22	B	817	CLA	C2B-C1B-NB	7.91	115.53	110.23
22	4	604	CLA	C2B-C1B-NB	7.91	115.53	110.23
22	A	807	CLA	C2B-C1B-NB	7.90	115.53	110.23
22	2	607	CLA	C2D-C1D-ND	7.90	115.92	110.10
22	A	819	CLA	C2D-C1D-ND	7.89	115.92	110.10
22	Z	608	CLA	C2B-C1B-NB	7.89	115.52	110.23
22	4	614	CLA	C2D-C1D-ND	7.89	115.92	110.10
22	6	601	CLA	C2B-C1B-NB	7.89	115.52	110.23
22	7	614	CLA	C2D-C1D-ND	7.89	115.92	110.10
22	9	610	CLA	C2B-C1B-NB	7.88	115.52	110.23
22	B	826	CLA	C2D-C1D-ND	7.87	115.91	110.10
22	3	607	CLA	C2D-C1D-ND	7.87	115.91	110.10
29	Z	601	CHL	C2B-C1B-NB	7.87	115.51	110.23
22	B	818	CLA	C1D-ND-C4D	-7.86	100.75	106.33
22	3	604	CLA	C2D-C1D-ND	7.86	115.90	110.10
29	1	607	CHL	C2B-C1B-NB	7.86	115.50	110.23
22	A	820	CLA	C2D-C1D-ND	7.86	115.90	110.10
22	7	612	CLA	C2D-C1D-ND	7.86	115.90	110.10
22	2	610	CLA	C2D-C1D-ND	7.86	115.89	110.10
22	B	829	CLA	CMD-C2D-C1D	7.86	138.56	124.71
22	5	609	CLA	C2D-C1D-ND	7.85	115.89	110.10
22	2	614	CLA	C2B-C1B-NB	7.85	115.50	110.23
22	B	826	CLA	C2B-C1B-NB	7.85	115.50	110.23
22	Z	613	CLA	C2D-C1D-ND	7.85	115.89	110.10
22	4	601	CLA	C2B-C1B-NB	7.84	115.49	110.23
22	F	301	CLA	CMD-C2D-C1D	7.84	138.53	124.71
22	4	609	CLA	C2D-C1D-ND	7.82	115.87	110.10
22	A	805	CLA	C2B-C1B-NB	7.82	115.48	110.23
22	9	604	CLA	C2D-C1D-ND	7.82	115.87	110.10
22	2	606	CLA	C2B-C1B-NB	7.82	115.47	110.23
22	B	835	CLA	C2D-C1D-ND	7.81	115.86	110.10
22	Z	616	CLA	C2B-C1B-NB	7.81	115.47	110.23
22	B	819	CLA	C2B-C1B-NB	7.81	115.47	110.23
22	Z	608	CLA	C2D-C1D-ND	7.80	115.85	110.10
25	I	172	BCR	C24-C23-C22	-7.80	114.45	126.23
22	Z	614	CLA	C2D-C1D-ND	7.80	115.85	110.10
22	8	602	CLA	C2B-C1B-NB	7.80	115.46	110.23
22	1	613	CLA	C2D-C1D-ND	7.79	115.85	110.10
22	6	603	CLA	C2D-C1D-ND	7.79	115.84	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	834	CLA	C2D-C1D-ND	7.79	115.84	110.10
22	9	610	CLA	C2D-C1D-ND	7.78	115.84	110.10
22	B	813	CLA	C2D-C1D-ND	7.78	115.84	110.10
22	B	852	CLA	C2D-C1D-ND	7.78	115.83	110.10
22	4	602	CLA	C2B-C1B-NB	7.77	115.44	110.23
22	3	603	CLA	C2D-C1D-ND	7.77	115.83	110.10
22	A	828	CLA	C2B-C1B-NB	7.76	115.44	110.23
22	7	613	CLA	C2B-C1B-NB	7.76	115.44	110.23
22	4	616	CLA	C2B-C1B-NB	7.76	115.44	110.23
22	B	811	CLA	C2D-C1D-ND	7.76	115.82	110.10
22	A	823	CLA	C2B-C1B-NB	7.76	115.43	110.23
22	3	613	CLA	C2B-C1B-NB	7.76	115.43	110.23
22	7	620	CLA	C2D-C1D-ND	7.76	115.82	110.10
22	4	601	CLA	C2D-C1D-ND	7.76	115.82	110.10
22	A	807	CLA	C2D-C1D-ND	7.75	115.82	110.10
22	A	824	CLA	C2D-C1D-ND	7.75	115.81	110.10
22	5	606	CLA	C2D-C1D-ND	7.75	115.81	110.10
22	2	611	CLA	C2D-C1D-ND	7.75	115.81	110.10
22	7	611	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	A	822	CLA	C2B-C1B-NB	7.74	115.42	110.23
22	6	601	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	9	614	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	2	613	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	3	610	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	8	613	CLA	C2B-C1B-NB	7.74	115.42	110.23
22	1	608	CLA	C2D-C1D-ND	7.74	115.81	110.10
22	3	620	CLA	C2D-C1D-ND	7.73	115.80	110.10
29	3	608	CHL	C2B-C1B-NB	7.73	115.41	110.23
22	1	603	CLA	C2B-C1B-NB	7.72	115.41	110.23
22	A	825	CLA	C2D-C1D-ND	7.72	115.80	110.10
22	A	810	CLA	C2D-C1D-ND	7.72	115.79	110.10
22	5	611	CLA	C2D-C1D-ND	7.71	115.79	110.10
29	9	607	CHL	C4A-NA-C1A	-7.71	103.24	106.71
22	B	833	CLA	C2D-C1D-ND	7.71	115.79	110.10
22	B	832	CLA	C2D-C1D-ND	7.71	115.79	110.10
22	9	602	CLA	C2D-C1D-ND	7.71	115.79	110.10
22	Z	604	CLA	C2B-C1B-NB	7.71	115.40	110.23
22	Z	612	CLA	C2D-C1D-ND	7.71	115.78	110.10
22	7	608	CLA	C2B-C1B-NB	7.71	115.40	110.23
22	4	610	CLA	C2D-C1D-ND	7.70	115.78	110.10
22	5	621	CLA	C1D-ND-C4D	-7.70	100.86	106.33
22	B	821	CLA	C2B-C1B-NB	7.70	115.39	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	616	CLA	C2D-C1D-ND	7.70	115.78	110.10
22	Z	613	CLA	C2B-C1B-NB	7.70	115.39	110.23
22	B	806	CLA	C2D-C1D-ND	7.69	115.77	110.10
22	B	822	CLA	C2D-C1D-ND	7.69	115.77	110.10
22	6	622	CLA	C2B-C1B-NB	7.69	115.39	110.23
22	2	602	CLA	C2D-C1D-ND	7.69	115.77	110.10
22	A	806	CLA	C2D-C1D-ND	7.69	115.77	110.10
22	1	603	CLA	C2D-C1D-ND	7.68	115.76	110.10
22	A	826	CLA	C2B-C1B-NB	7.67	115.38	110.23
22	1	606	CLA	C2D-C1D-ND	7.67	115.76	110.10
22	6	603	CLA	C2B-C1B-NB	7.67	115.38	110.23
22	8	606	CLA	C2D-C1D-ND	7.67	115.76	110.10
22	B	809	CLA	C2D-C1D-ND	7.67	115.75	110.10
22	A	825	CLA	C2B-C1B-NB	7.67	115.37	110.23
22	A	813	CLA	C2D-C1D-ND	7.66	115.75	110.10
22	5	612	CLA	C2D-C1D-ND	7.66	115.75	110.10
22	6	613	CLA	C2B-C1B-NB	7.66	115.37	110.23
22	6	609	CLA	C2D-C1D-ND	7.66	115.75	110.10
22	3	612	CLA	C2D-C1D-ND	7.66	115.75	110.10
22	Z	611	CLA	C2D-C1D-ND	7.66	115.75	110.10
22	3	614	CLA	C2D-C1D-ND	7.65	115.74	110.10
22	4	616	CLA	C2D-C1D-ND	7.65	115.74	110.10
22	Z	606	CLA	C2D-C1D-ND	7.64	115.73	110.10
22	A	836	CLA	C2B-C1B-NB	7.63	115.35	110.23
22	8	610	CLA	C2D-C1D-ND	7.63	115.73	110.10
22	F	304	CLA	C2D-C1D-ND	7.63	115.73	110.10
22	K	4002	CLA	C2D-C1D-ND	7.62	115.72	110.10
29	3	608	CHL	CMD-C2D-C1D	7.62	138.15	124.71
22	4	602	CLA	C2D-C1D-ND	7.62	115.72	110.10
22	5	603	CLA	C2B-C1B-NB	7.62	115.34	110.23
22	8	611	CLA	C2D-C1D-ND	7.61	115.71	110.10
29	4	608	CHL	CMD-C2D-C1D	7.61	138.13	124.71
22	B	807	CLA	C2D-C1D-ND	7.61	115.71	110.10
29	4	608	CHL	C2B-C1B-NB	7.61	115.33	110.23
22	B	852	CLA	C2B-C1B-NB	7.61	115.33	110.23
29	Z	607	CHL	C2B-C1B-NB	7.61	115.33	110.23
22	G	204	CLA	C2D-C1D-ND	7.61	115.71	110.10
22	1	609	CLA	C2D-C1D-ND	7.61	115.71	110.10
22	A	804	CLA	CMD-C2D-C1D	7.61	138.12	124.71
22	3	602	CLA	C2D-C1D-ND	7.60	115.70	110.10
22	B	830	CLA	C2D-C1D-ND	7.60	115.70	110.10
22	1	608	CLA	C2B-C1B-NB	7.59	115.32	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	617	CLA	C2D-C1D-ND	7.58	115.69	110.10
22	K	4003	CLA	C2D-C1D-ND	7.58	115.69	110.10
22	5	603	CLA	C2D-C1D-ND	7.57	115.69	110.10
22	Z	616	CLA	C2D-C1D-ND	7.57	115.68	110.10
22	A	839	CLA	C2D-C1D-ND	7.56	115.68	110.10
22	B	810	CLA	C2D-C1D-ND	7.56	115.68	110.10
22	A	802	CLA	C2B-C1B-NB	7.56	115.30	110.23
22	9	601	CLA	C2D-C1D-ND	7.56	115.67	110.10
22	6	616	CLA	C2D-C1D-ND	7.55	115.67	110.10
29	6	607	CHL	C4A-NA-C1A	-7.55	103.31	106.71
22	2	606	CLA	C2D-C1D-ND	7.55	115.67	110.10
22	8	601	CLA	C2D-C1D-ND	7.55	115.67	110.10
22	9	609	CLA	C2D-C1D-ND	7.54	115.66	110.10
22	A	842	CLA	C2B-C1B-NB	7.54	115.29	110.23
22	5	601	CLA	C2D-C1D-ND	7.54	115.66	110.10
22	7	616	CLA	CHD-C1D-ND	-7.53	117.54	124.45
22	B	840	CLA	C2D-C1D-ND	7.52	115.65	110.10
22	A	827	CLA	C2D-C1D-ND	7.52	115.65	110.10
22	8	616	CLA	C2B-C1B-NB	7.52	115.27	110.23
22	B	840	CLA	C2B-C1B-NB	7.51	115.26	110.23
22	A	835	CLA	C2B-C1B-NB	7.50	115.26	110.23
22	B	808	CLA	C2D-C1D-ND	7.50	115.63	110.10
22	4	604	CLA	C2D-C1D-ND	7.50	115.63	110.10
22	L	203	CLA	C2B-C1B-NB	7.49	115.26	110.23
22	9	612	CLA	C2D-C1D-ND	7.49	115.63	110.10
22	B	841	CLA	C2B-C1B-NB	7.49	115.25	110.23
22	3	603	CLA	C2B-C1B-NB	7.49	115.25	110.23
22	A	822	CLA	C2D-C1D-ND	7.48	115.62	110.10
22	3	609	CLA	C2D-C1D-ND	7.48	115.62	110.10
22	2	601	CLA	C2D-C1D-ND	7.48	115.62	110.10
22	8	603	CLA	C2B-C1B-NB	7.47	115.24	110.23
22	A	815	CLA	C2B-C1B-NB	7.47	115.24	110.23
22	6	617	CLA	C2D-C1D-ND	7.47	115.61	110.10
22	B	823	CLA	C2D-C1D-ND	7.47	115.61	110.10
22	J	3002	CLA	C2D-C1D-ND	7.46	115.60	110.10
22	9	611	CLA	C2D-C1D-ND	7.46	115.60	110.10
22	5	613	CLA	C2D-C1D-ND	7.45	115.60	110.10
22	B	820	CLA	C2B-C1B-NB	7.45	115.23	110.23
22	8	604	CLA	C2D-C1D-ND	7.45	115.59	110.10
22	9	613	CLA	C2D-C1D-ND	7.44	115.59	110.10
22	6	612	CLA	C2D-C1D-ND	7.44	115.59	110.10
22	A	821	CLA	C2D-C1D-ND	7.43	115.58	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	609	CLA	C2D-C1D-ND	7.43	115.58	110.10
22	A	843	CLA	C2D-C1D-ND	7.43	115.58	110.10
22	6	604	CLA	C2D-C1D-ND	7.42	115.58	110.10
22	7	610	CLA	C2D-C1D-ND	7.42	115.57	110.10
29	7	607	CHL	CMD-C2D-C1D	7.42	137.79	124.71
22	1	612	CLA	C2D-C1D-ND	7.42	115.57	110.10
22	8	612	CLA	C2D-C1D-ND	7.41	115.57	110.10
22	B	841	CLA	C2D-C1D-ND	7.41	115.56	110.10
22	Z	604	CLA	C2D-C1D-ND	7.41	115.56	110.10
22	1	611	CLA	C2D-C1D-ND	7.41	115.56	110.10
22	A	833	CLA	C2D-C1D-ND	7.40	115.56	110.10
22	6	611	CLA	C2D-C1D-ND	7.40	115.56	110.10
22	6	604	CLA	C2B-C1B-NB	7.40	115.19	110.23
21	A	801	CL0	C2B-C1B-NB	7.39	115.19	110.23
22	3	620	CLA	C2B-C1B-NB	7.39	115.19	110.23
22	3	611	CLA	C2D-C1D-ND	7.38	115.55	110.10
22	8	613	CLA	C2D-C1D-ND	7.38	115.54	110.10
22	A	802	CLA	C2D-C1D-ND	7.37	115.53	110.10
22	4	611	CLA	C2D-C1D-ND	7.36	115.53	110.10
22	B	824	CLA	C2D-C1D-ND	7.36	115.53	110.10
22	6	613	CLA	C2D-C1D-ND	7.36	115.53	110.10
22	2	609	CLA	C2D-C1D-ND	7.36	115.53	110.10
22	1	613	CLA	C2B-C1B-NB	7.35	115.16	110.23
29	4	607	CHL	C2B-C1B-NB	7.34	115.15	110.23
29	9	606	CHL	C2B-C1B-NB	7.34	115.15	110.23
22	7	603	CLA	C2D-C1D-ND	7.34	115.51	110.10
22	9	603	CLA	C2D-C1D-ND	7.33	115.51	110.10
22	A	805	CLA	C2D-C1D-ND	7.32	115.50	110.10
22	3	606	CLA	C2D-C1D-ND	7.32	115.50	110.10
22	B	825	CLA	C2D-C1D-ND	7.30	115.48	110.10
22	B	809	CLA	C2B-C1B-NB	7.30	115.12	110.23
22	1	616	CLA	C2D-C1D-ND	7.28	115.47	110.10
22	A	810	CLA	C2B-C1B-NB	7.28	115.11	110.23
29	7	607	CHL	C4A-NA-C1A	-7.27	103.44	106.71
22	2	612	CLA	C2D-C1D-ND	7.27	115.46	110.10
22	A	832	CLA	C2D-C1D-ND	7.27	115.46	110.10
29	6	606	CHL	CMD-C2D-C1D	7.26	137.51	124.71
22	A	828	CLA	CHD-C4C-C3C	-7.26	114.16	124.84
22	8	603	CLA	C2D-C1D-ND	7.26	115.46	110.10
22	6	610	CLA	C2D-C1D-ND	7.26	115.46	110.10
22	2	603	CLA	C2D-C1D-ND	7.26	115.45	110.10
22	B	839	CLA	C2D-C1D-ND	7.23	115.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	614	CLA	C2D-C1D-ND	7.23	115.43	110.10
22	1	616	CLA	C2B-C1B-NB	7.23	115.08	110.23
22	8	601	CLA	CMD-C2D-C1D	7.21	137.41	124.71
22	A	821	CLA	C2B-C1B-NB	7.20	115.06	110.23
22	B	836	CLA	C2D-C1D-ND	7.19	115.40	110.10
22	8	608	CLA	CMD-C2D-C1D	7.18	137.37	124.71
29	5	608	CHL	CMD-C2D-C1D	7.18	137.37	124.71
22	B	820	CLA	C2D-C1D-ND	7.17	115.39	110.10
22	B	834	CLA	CMD-C2D-C1D	7.17	137.34	124.71
22	B	828	CLA	C2D-C1D-ND	7.17	115.39	110.10
22	F	301	CLA	C2D-C1D-ND	7.15	115.38	110.10
29	9	607	CHL	CMD-C2D-C1D	7.15	137.32	124.71
22	7	603	CLA	CMD-C2D-C1D	7.15	137.32	124.71
22	3	613	CLA	C2D-C1D-ND	7.15	115.37	110.10
22	A	815	CLA	C2D-C1D-ND	7.14	115.37	110.10
22	A	835	CLA	C2D-C1D-ND	7.14	115.37	110.10
29	6	608	CHL	C2B-C1B-NB	7.14	115.02	110.23
22	B	819	CLA	C2D-C1D-ND	7.13	115.36	110.10
22	3	614	CLA	CMD-C2D-C1D	7.13	137.29	124.71
22	B	834	CLA	C2D-C1D-ND	7.13	115.36	110.10
29	8	607	CHL	C2B-C1B-NB	7.12	115.01	110.23
25	B	801	BCR	C16-C15-C14	-7.12	108.88	123.47
22	7	601	CLA	CMD-C2D-C1D	7.11	137.25	124.71
22	A	831	CLA	C2B-C1B-NB	7.11	115.00	110.23
22	3	604	CLA	C2B-C1B-NB	7.10	114.99	110.23
22	5	604	CLA	C2D-C1D-ND	7.10	115.34	110.10
22	A	838	CLA	CMD-C2D-C1D	7.10	137.22	124.71
22	5	602	CLA	CMD-C2D-C1D	7.10	137.22	124.71
22	B	817	CLA	C2D-C1D-ND	7.09	115.33	110.10
22	A	840	CLA	CMD-C2D-C1D	7.09	137.20	124.71
22	B	840	CLA	C2C-C1C-NC	7.08	116.60	109.97
29	4	606	CHL	C2B-C1B-NB	7.08	114.98	110.23
22	A	826	CLA	CMD-C2D-C1D	7.07	137.18	124.71
22	Z	603	CLA	C2D-C1D-ND	7.07	115.32	110.10
22	A	838	CLA	C2D-C1D-ND	7.06	115.31	110.10
22	8	616	CLA	C2D-C1D-ND	7.06	115.31	110.10
22	1	608	CLA	CMD-C2D-C1D	7.06	137.16	124.71
22	B	826	CLA	CMD-C2D-C1D	7.06	137.15	124.71
22	6	613	CLA	CMD-C2D-C1D	7.06	137.15	124.71
22	Z	608	CLA	CMD-C2D-C1D	7.06	137.15	124.71
22	J	3002	CLA	CMD-C2D-C1D	7.05	137.15	124.71
22	9	603	CLA	C4A-NA-C1A	-7.05	103.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	834	CLA	CMD-C2D-C1D	7.05	137.13	124.71
22	A	837	CLA	C2D-C1D-ND	7.04	115.29	110.10
22	B	814	CLA	CMD-C2D-C1D	7.04	137.12	124.71
22	A	826	CLA	C2D-C1D-ND	7.03	115.28	110.10
22	Z	609	CLA	C2D-C1D-ND	7.03	115.28	110.10
22	Z	606	CLA	CMD-C2D-C1D	7.03	137.10	124.71
29	4	606	CHL	CMD-C2D-C1D	7.03	137.09	124.71
22	7	614	CLA	O2D-CGD-CBD	7.02	123.75	111.27
29	4	607	CHL	CMD-C2D-C1D	7.02	137.08	124.71
22	1	604	CLA	CMD-C2D-C1D	7.02	137.08	124.71
22	B	816	CLA	CMD-C2D-C1D	7.01	137.08	124.71
22	A	827	CLA	CMD-C2D-C1D	7.01	137.07	124.71
29	1	601	CHL	CMD-C2D-C1D	7.01	137.07	124.71
22	A	814	CLA	CMD-C2D-C1D	6.99	137.03	124.71
29	5	607	CHL	CMD-C2D-C1D	6.99	137.03	124.71
22	B	802	CLA	CHD-C4C-C3C	-6.99	114.57	124.84
22	B	812	CLA	CMD-C2D-C1D	6.98	137.02	124.71
22	A	817	CLA	C2D-C1D-ND	6.98	115.25	110.10
22	9	603	CLA	CMD-C2D-C1D	6.95	136.97	124.71
22	B	818	CLA	C2D-C1D-ND	6.95	115.23	110.10
22	B	836	CLA	CMD-C2D-C1D	6.95	136.96	124.71
22	A	802	CLA	CHD-C1D-ND	-6.95	118.07	124.45
22	B	840	CLA	CMD-C2D-C1D	6.94	136.95	124.71
22	B	810	CLA	CMD-C2D-C1D	6.94	136.94	124.71
22	8	604	CLA	C2B-C1B-NB	6.94	114.88	110.23
22	B	817	CLA	CMD-C2D-C1D	6.93	136.92	124.71
22	7	606	CLA	CMD-C2D-C1D	6.93	136.92	124.71
29	6	608	CHL	CMD-C2D-C1D	6.92	136.90	124.71
22	1	609	CLA	CMD-C2D-C1D	6.91	136.89	124.71
22	4	603	CLA	CMD-C2D-C1D	6.90	136.88	124.71
22	5	603	CLA	CMD-C2D-C1D	6.90	136.88	124.71
29	3	608	CHL	C1C-C2C-C3C	-6.90	101.64	107.11
22	4	603	CLA	C2D-C1D-ND	6.89	115.18	110.10
22	7	604	CLA	CMD-C2D-C1D	6.89	136.86	124.71
22	7	616	CLA	CMD-C2D-C1D	6.89	136.86	124.71
29	5	618	CHL	CMD-C2D-C1D	6.89	136.86	124.71
22	2	609	CLA	CMD-C2D-C1D	6.89	136.86	124.71
22	2	603	CLA	CMD-C2D-C1D	6.89	136.86	124.71
22	B	816	CLA	CHD-C4C-C3C	-6.89	114.72	124.84
22	1	604	CLA	C2D-C1D-ND	6.88	115.17	110.10
22	3	606	CLA	CMD-C2D-C1D	6.88	136.84	124.71
22	2	614	CLA	CMD-C2D-C1D	6.88	136.83	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	602	CLA	CHD-C4C-C3C	-6.88	114.73	124.84
22	Z	603	CLA	CMD-C2D-C1D	6.88	136.83	124.71
22	3	620	CLA	CMD-C2D-C1D	6.87	136.83	124.71
29	9	606	CHL	CMD-C2D-C1D	6.87	136.81	124.71
22	2	601	CLA	CMD-C2D-C1D	6.86	136.81	124.71
22	5	606	CLA	CMD-C2D-C1D	6.86	136.80	124.71
22	6	602	CLA	CMD-C2D-C1D	6.85	136.79	124.71
22	A	819	CLA	CMD-C2D-C1D	6.85	136.79	124.71
22	B	832	CLA	CMD-C2D-C1D	6.85	136.78	124.71
22	K	4002	CLA	CMD-C2D-C1D	6.85	136.78	124.71
22	B	806	CLA	CMD-C2D-C1D	6.84	136.77	124.71
22	L	204	CLA	CMD-C2D-C1D	6.84	136.77	124.71
22	A	824	CLA	CMD-C2D-C1D	6.84	136.76	124.71
22	A	815	CLA	CHD-C1D-ND	-6.84	118.17	124.45
29	Z	607	CHL	C4A-NA-C1A	-6.84	103.63	106.71
22	A	843	CLA	C2B-C1B-NB	6.83	114.81	110.23
22	6	603	CLA	CMD-C2D-C1D	6.82	136.74	124.71
22	A	828	CLA	CMD-C2D-C1D	6.82	136.73	124.71
22	B	833	CLA	CMD-C2D-C1D	6.81	136.72	124.71
22	Z	604	CLA	CMD-C2D-C1D	6.81	136.72	124.71
22	4	604	CLA	CMD-C2D-C1D	6.81	136.71	124.71
22	A	808	CLA	CMD-C2D-C1D	6.80	136.71	124.71
22	3	602	CLA	CMD-C2D-C1D	6.80	136.69	124.71
22	B	831	CLA	CMD-C2D-C1D	6.79	136.69	124.71
22	7	614	CLA	CMD-C2D-C1D	6.79	136.68	124.71
22	2	610	CLA	CMD-C2D-C1D	6.79	136.68	124.71
22	6	614	CLA	CHD-C1D-ND	-6.79	118.22	124.45
22	3	610	CLA	CMD-C2D-C1D	6.79	136.67	124.71
22	B	839	CLA	CMD-C2D-C1D	6.78	136.67	124.71
29	4	618	CHL	CMD-C2D-C1D	6.76	136.63	124.71
22	K	4003	CLA	CMD-C2D-C1D	6.76	136.63	124.71
29	6	607	CHL	CMD-C2D-C1D	6.76	136.63	124.71
22	A	833	CLA	CMD-C2D-C1D	6.76	136.62	124.71
22	9	610	CLA	CMD-C2D-C1D	6.75	136.61	124.71
22	G	204	CLA	CMD-C2D-C1D	6.75	136.61	124.71
22	6	601	CLA	CMD-C2D-C1D	6.74	136.60	124.71
22	3	612	CLA	C4A-NA-C1A	-6.73	103.68	106.71
22	8	611	CLA	CMD-C2D-C1D	6.73	136.57	124.71
22	B	837	CLA	CMD-C2D-C1D	6.72	136.56	124.71
22	9	601	CLA	CMD-C2D-C1D	6.72	136.56	124.71
22	2	602	CLA	CMD-C2D-C1D	6.72	136.55	124.71
22	6	616	CLA	CMD-C2D-C1D	6.71	136.55	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	835	CLA	CMD-C2D-C1D	6.71	136.54	124.71
22	1	603	CLA	CMD-C2D-C1D	6.71	136.54	124.71
22	7	610	CLA	CMD-C2D-C1D	6.70	136.53	124.71
22	4	616	CLA	CMD-C2D-C1D	6.70	136.53	124.71
22	2	607	CLA	CMD-C2D-C1D	6.70	136.53	124.71
22	B	807	CLA	CMD-C2D-C1D	6.70	136.52	124.71
29	8	607	CHL	C1D-ND-C4D	-6.70	101.58	106.33
22	A	837	CLA	CMD-C2D-C1D	6.69	136.51	124.71
22	A	820	CLA	CMD-C2D-C1D	6.69	136.51	124.71
22	9	614	CLA	CMD-C2D-C1D	6.69	136.51	124.71
22	A	842	CLA	CMD-C2D-C1D	6.69	136.50	124.71
22	9	604	CLA	CMD-C2D-C1D	6.69	136.50	124.71
22	Z	609	CLA	CMD-C2D-C1D	6.69	136.50	124.71
22	A	815	CLA	CMD-C2D-C1D	6.68	136.49	124.71
22	B	814	CLA	C2D-C1D-ND	6.68	115.03	110.10
22	6	622	CLA	CMD-C2D-C1D	6.68	136.49	124.71
22	Z	614	CLA	CMD-C2D-C1D	6.68	136.48	124.71
22	4	602	CLA	CMD-C2D-C1D	6.68	136.48	124.71
22	B	819	CLA	CMD-C2D-C1D	6.68	136.48	124.71
29	4	607	CHL	C1D-ND-C4D	-6.67	101.60	106.33
22	8	602	CLA	CMD-C2D-C1D	6.67	136.47	124.71
22	3	609	CLA	CMD-C2D-C1D	6.67	136.46	124.71
22	1	614	CLA	CMD-C2D-C1D	6.66	136.46	124.71
22	6	610	CLA	CMD-C2D-C1D	6.66	136.46	124.71
22	7	608	CLA	CMD-C2D-C1D	6.66	136.45	124.71
22	4	601	CLA	CMD-C2D-C1D	6.66	136.45	124.71
22	6	604	CLA	CMD-C2D-C1D	6.66	136.45	124.71
22	F	304	CLA	CMD-C2D-C1D	6.66	136.44	124.71
22	A	835	CLA	CHD-C1D-ND	-6.66	118.34	124.45
22	2	606	CLA	CMD-C2D-C1D	6.65	136.44	124.71
22	G	203	CLA	CMD-C2D-C1D	6.65	136.44	124.71
22	F	303	CLA	CMD-C2D-C1D	6.65	136.43	124.71
22	5	604	CLA	CMD-C2D-C1D	6.64	136.41	124.71
22	B	815	CLA	CMD-C2D-C1D	6.64	136.41	124.71
22	7	620	CLA	CMD-C2D-C1D	6.63	136.41	124.71
22	B	811	CLA	CMD-C2D-C1D	6.63	136.39	124.71
22	8	604	CLA	CMD-C2D-C1D	6.62	136.38	124.71
22	3	604	CLA	CMD-C2D-C1D	6.61	136.37	124.71
22	A	809	CLA	CMD-C2D-C1D	6.61	136.37	124.71
22	5	616	CLA	CMD-C2D-C1D	6.61	136.37	124.71
22	A	813	CLA	CMD-C2D-C1D	6.61	136.36	124.71
22	9	602	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	5	617	CLA	CMD-C2D-C1D	6.60	136.35	124.71
22	8	603	CLA	CMD-C2D-C1D	6.60	136.35	124.71
22	1	606	CLA	CMD-C2D-C1D	6.60	136.35	124.71
22	Z	602	CLA	CMD-C2D-C1D	6.59	136.34	124.71
29	8	607	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
22	A	845	CLA	CMD-C2D-C1D	6.59	136.32	124.71
22	9	612	CLA	CMD-C2D-C1D	6.58	136.31	124.71
22	5	610	CLA	CMD-C2D-C1D	6.58	136.31	124.71
22	B	841	CLA	CHD-C1D-ND	-6.57	118.41	124.45
22	9	613	CLA	CMD-C2D-C1D	6.57	136.30	124.71
22	A	805	CLA	CHD-C1D-ND	-6.57	118.42	124.45
22	A	839	CLA	CMD-C2D-C1D	6.56	136.27	124.71
22	B	825	CLA	CMD-C2D-C1D	6.56	136.27	124.71
22	Z	611	CLA	CMD-C2D-C1D	6.56	136.27	124.71
22	7	602	CLA	CMD-C2D-C1D	6.55	136.26	124.71
22	B	830	CLA	CMD-C2D-C1D	6.55	136.26	124.71
22	B	820	CLA	CMD-C2D-C1D	6.55	136.25	124.71
22	5	617	CLA	CHD-C1D-ND	-6.55	118.44	124.45
22	1	614	CLA	CHD-C1D-ND	-6.54	118.44	124.45
22	8	612	CLA	CMD-C2D-C1D	6.53	136.23	124.71
22	B	818	CLA	CMD-C2D-C1D	6.53	136.23	124.71
22	B	837	CLA	O2D-CGD-CBD	6.53	122.88	111.27
22	7	604	CLA	C2C-C1C-NC	6.53	116.09	109.97
22	B	841	CLA	CMD-C2D-C1D	6.53	136.22	124.71
22	A	806	CLA	CMD-C2D-C1D	6.53	136.22	124.71
25	5	625	BCR	C11-C10-C9	-6.53	117.99	127.31
22	2	613	CLA	CMD-C2D-C1D	6.53	136.22	124.71
22	2	603	CLA	C4A-NA-C1A	-6.52	103.77	106.71
29	6	618	CHL	C1D-ND-C4D	-6.52	101.70	106.33
22	B	836	CLA	C4A-NA-C1A	-6.51	103.78	106.71
22	B	822	CLA	CMD-C2D-C1D	6.50	136.16	124.71
22	A	803	CLA	CMD-C2D-C1D	6.50	136.16	124.71
22	A	802	CLA	CMD-C2D-C1D	6.49	136.16	124.71
22	B	805	CLA	CMD-C2D-C1D	6.49	136.15	124.71
22	7	612	CLA	CMD-C2D-C1D	6.49	136.15	124.71
22	B	805	CLA	O2D-CGD-CBD	6.49	122.79	111.27
22	B	829	CLA	C3B-C2B-C1B	-6.48	99.33	107.16
22	2	610	CLA	CHD-C1D-ND	-6.48	118.50	124.45
22	8	606	CLA	CMD-C2D-C1D	6.48	136.13	124.71
22	9	611	CLA	CMD-C2D-C1D	6.48	136.13	124.71
22	F	301	CLA	C4A-NA-C1A	-6.47	103.80	106.71
22	B	830	CLA	O2D-CGD-CBD	6.47	122.77	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z	607	CHL	CMD-C2D-C1D	6.47	136.11	124.71
29	Z	607	CHL	C1D-ND-C4D	-6.46	101.74	106.33
22	A	805	CLA	CMD-C2D-C1D	6.46	136.10	124.71
22	5	611	CLA	CMD-C2D-C1D	6.46	136.10	124.71
22	3	617	CLA	CMD-C2D-C1D	6.46	136.10	124.71
22	A	817	CLA	CHD-C1D-ND	-6.46	118.52	124.45
22	A	829	CLA	CHD-C4C-C3C	-6.46	115.35	124.84
22	Z	616	CLA	CMD-C2D-C1D	6.45	136.09	124.71
22	B	838	CLA	CMD-C2D-C1D	6.45	136.09	124.71
22	9	609	CLA	CMD-C2D-C1D	6.45	136.09	124.71
22	B	837	CLA	CHD-C1D-ND	-6.45	118.53	124.45
22	A	803	CLA	CHD-C1D-ND	-6.45	118.53	124.45
22	A	816	CLA	CMD-C2D-C1D	6.44	136.06	124.71
22	2	612	CLA	CMD-C2D-C1D	6.43	136.05	124.71
22	B	813	CLA	CMD-C2D-C1D	6.43	136.04	124.71
22	1	611	CLA	CMD-C2D-C1D	6.43	136.04	124.71
22	5	609	CLA	CMD-C2D-C1D	6.43	136.04	124.71
22	7	610	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
22	A	812	CLA	CMD-C2D-C1D	6.42	136.03	124.71
22	A	818	CLA	CMD-C2D-C1D	6.42	136.03	124.71
22	B	824	CLA	O2D-CGD-CBD	6.42	122.67	111.27
22	B	804	CLA	O2D-CGD-CBD	6.41	122.66	111.27
22	Z	612	CLA	CMD-C2D-C1D	6.40	136.00	124.71
22	B	832	CLA	CHD-C1D-ND	-6.40	118.57	124.45
22	A	809	CLA	O2D-CGD-CBD	6.39	122.63	111.27
22	A	807	CLA	CMD-C2D-C1D	6.39	135.97	124.71
22	3	612	CLA	CMD-C2D-C1D	6.39	135.97	124.71
22	5	614	CLA	O2D-CGD-CBD	6.38	122.61	111.27
29	Z	601	CHL	C1D-ND-C4D	-6.38	101.80	106.33
29	8	607	CHL	CMD-C2D-C1D	6.38	135.95	124.71
22	8	608	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
29	9	606	CHL	C1D-ND-C4D	-6.37	101.81	106.33
22	B	805	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
22	B	834	CLA	CHD-C1D-ND	-6.36	118.61	124.45
22	B	820	CLA	CHD-C1D-ND	-6.35	118.62	124.45
22	2	614	CLA	CHD-C1D-ND	-6.35	118.62	124.45
22	4	612	CLA	CMD-C2D-C1D	6.34	135.90	124.71
22	A	808	CLA	CHD-C1D-ND	-6.34	118.62	124.45
22	A	812	CLA	CHD-C1D-ND	-6.34	118.63	124.45
29	6	606	CHL	C1D-ND-C4D	-6.33	101.84	106.33
22	8	603	CLA	C4A-NA-C1A	-6.33	103.86	106.71
22	A	825	CLA	CMD-C2D-C1D	6.33	135.87	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	609	CLA	CMD-C2D-C1D	6.33	135.86	124.71
22	A	822	CLA	CMD-C2D-C1D	6.32	135.85	124.71
29	6	607	CHL	C2C-C3C-C4C	-6.32	101.98	106.49
22	A	854	CLA	O2D-CGD-CBD	6.32	122.50	111.27
22	3	603	CLA	CMD-C2D-C1D	6.32	135.84	124.71
22	5	613	CLA	CMD-C2D-C1D	6.31	135.84	124.71
22	7	608	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
22	4	604	CLA	CHD-C1D-ND	-6.31	118.66	124.45
22	7	609	CLA	CHD-C1D-ND	-6.31	118.66	124.45
22	5	614	CLA	CMD-C2D-C1D	6.31	135.83	124.71
22	A	804	CLA	C2D-C1D-ND	6.30	114.75	110.10
22	A	838	CLA	C2C-C1C-NC	6.30	115.88	109.97
22	A	831	CLA	O2D-CGD-CBD	6.30	122.46	111.27
29	4	608	CHL	C1D-ND-C4D	-6.30	101.86	106.33
22	B	804	CLA	CMD-C2D-C1D	6.30	135.81	124.71
22	Z	610	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
22	A	814	CLA	CHD-C1D-ND	-6.29	118.67	124.45
29	3	608	CHL	CHD-C4C-C3C	-6.29	115.59	124.84
22	B	806	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
22	L	204	CLA	CHD-C1D-ND	-6.29	118.68	124.45
22	A	839	CLA	O2D-CGD-CBD	6.29	122.44	111.27
29	1	607	CHL	CMD-C2D-C1D	6.28	135.79	124.71
22	2	602	CLA	CHD-C1D-ND	-6.28	118.68	124.45
22	6	601	CLA	CHD-C1D-ND	-6.28	118.68	124.45
22	2	611	CLA	CMD-C2D-C1D	6.28	135.78	124.71
22	A	826	CLA	C2C-C1C-NC	6.27	115.85	109.97
22	A	809	CLA	CHD-C1D-ND	-6.27	118.69	124.45
22	F	301	CLA	CHD-C1D-ND	-6.27	118.69	124.45
22	3	613	CLA	C2C-C1C-NC	6.27	115.84	109.97
22	1	610	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
22	1	603	CLA	C2C-C1C-NC	6.26	115.83	109.97
22	B	810	CLA	CHD-C1D-ND	-6.25	118.71	124.45
22	K	4003	CLA	CHD-C1D-ND	-6.25	118.71	124.45
22	7	611	CLA	CMD-C2D-C1D	6.25	135.73	124.71
29	5	618	CHL	C1D-ND-C4D	-6.25	101.90	106.33
21	A	801	CL0	CHD-C4C-C3C	-6.25	115.66	124.84
22	B	827	CLA	CMD-C2D-C1D	6.24	135.72	124.71
22	B	815	CLA	CHD-C1D-ND	-6.24	118.72	124.45
22	B	821	CLA	CMD-C2D-C1D	6.24	135.71	124.71
22	A	840	CLA	O2D-CGD-CBD	6.24	122.35	111.27
29	6	607	CHL	C1D-ND-C4D	-6.23	101.91	106.33
22	7	603	CLA	CHD-C1D-ND	-6.23	118.73	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	610	CLA	CMD-C2D-C1D	6.23	135.69	124.71
22	7	614	CLA	CHD-C1D-ND	-6.23	118.73	124.45
29	6	608	CHL	C1C-C2C-C3C	-6.23	102.17	107.11
22	1	609	CLA	CHD-C1D-ND	-6.23	118.73	124.45
22	4	603	CLA	C2C-C1C-NC	6.23	115.81	109.97
22	3	614	CLA	CHD-C1D-ND	-6.22	118.73	124.45
22	6	617	CLA	CMD-C2D-C1D	6.22	135.68	124.71
25	5	625	BCR	C7-C8-C9	-6.22	116.84	126.23
22	4	603	CLA	C4A-NA-C1A	-6.22	103.91	106.71
22	B	832	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
22	A	828	CLA	O2D-CGD-CBD	6.21	122.30	111.27
22	A	818	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
22	4	611	CLA	CMD-C2D-C1D	6.21	135.66	124.71
22	7	602	CLA	CHD-C1D-ND	-6.21	118.75	124.45
22	1	613	CLA	CMD-C2D-C1D	6.21	135.66	124.71
22	B	807	CLA	C2C-C1C-NC	6.21	115.79	109.97
22	B	818	CLA	C2C-C1C-NC	6.21	115.79	109.97
22	5	612	CLA	CMD-C2D-C1D	6.21	135.65	124.71
22	B	831	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
22	3	612	CLA	C2C-C1C-NC	6.20	115.78	109.97
22	3	611	CLA	CMD-C2D-C1D	6.20	135.64	124.71
22	5	601	CLA	CMD-C2D-C1D	6.20	135.64	124.71
29	1	607	CHL	C1D-ND-C4D	-6.20	101.93	106.33
22	5	604	CLA	C2C-C1C-NC	6.20	115.78	109.97
22	9	603	CLA	C2C-C1C-NC	6.20	115.78	109.97
22	1	604	CLA	CHD-C1D-ND	-6.19	118.76	124.45
29	3	608	CHL	C1D-ND-C4D	-6.19	101.94	106.33
22	4	610	CLA	CMD-C2D-C1D	6.19	135.62	124.71
22	4	613	CLA	CMD-C2D-C1D	6.19	135.61	124.71
22	6	609	CLA	CMD-C2D-C1D	6.19	135.61	124.71
22	6	612	CLA	CMD-C2D-C1D	6.18	135.61	124.71
22	6	611	CLA	CMD-C2D-C1D	6.18	135.61	124.71
22	7	604	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
22	A	817	CLA	C2C-C1C-NC	6.17	115.76	109.97
22	1	612	CLA	CMD-C2D-C1D	6.17	135.59	124.71
22	1	616	CLA	CMD-C2D-C1D	6.17	135.59	124.71
22	8	609	CLA	CMD-C2D-C1D	6.17	135.59	124.71
22	A	827	CLA	CHD-C1D-ND	-6.17	118.78	124.45
22	Z	614	CLA	CHD-C1D-ND	-6.17	118.78	124.45
21	A	801	CL0	C2C-C1C-NC	6.17	115.75	109.97
29	1	607	CHL	C4A-NA-C1A	-6.16	103.94	106.71
22	5	602	CLA	CHD-C1D-ND	-6.16	118.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	617	LUT	C35-C34-C33	-6.16	118.52	127.31
22	6	602	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
22	5	621	CLA	C2D-C1D-ND	6.16	114.64	110.10
22	A	818	CLA	O2D-CGD-CBD	6.16	122.21	111.27
22	4	616	CLA	C2C-C1C-NC	6.16	115.74	109.97
22	A	817	CLA	C2B-C1B-NB	6.15	114.36	110.23
22	A	823	CLA	CMD-C2D-C1D	6.15	135.56	124.71
22	6	601	CLA	O2D-CGD-CBD	6.15	122.20	111.27
22	7	606	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
22	5	602	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
22	9	614	CLA	CHD-C1D-ND	-6.14	118.81	124.45
22	3	604	CLA	CHD-C1D-ND	-6.13	118.82	124.45
22	6	609	CLA	C2C-C1C-NC	6.12	115.71	109.97
22	B	841	CLA	C4A-NA-C1A	-6.12	103.95	106.71
22	7	603	CLA	C4A-NA-C1A	-6.12	103.95	106.71
22	9	604	CLA	CHD-C1D-ND	-6.12	118.83	124.45
22	7	608	CLA	CHD-C1D-ND	-6.12	118.83	124.45
22	B	833	CLA	CHD-C1D-ND	-6.12	118.83	124.45
22	2	607	CLA	CHD-C1D-ND	-6.11	118.84	124.45
22	Z	613	CLA	CMD-C2D-C1D	6.11	135.48	124.71
22	5	621	CLA	CMD-C2D-C1D	6.10	135.47	124.71
22	A	822	CLA	CHD-C1D-ND	-6.10	118.85	124.45
22	B	829	CLA	CHD-C1D-ND	-6.10	118.85	124.45
22	5	609	CLA	CHD-C1D-ND	-6.09	118.86	124.45
29	5	607	CHL	C1D-ND-C4D	-6.09	102.01	106.33
22	B	826	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
22	A	811	CLA	CMD-C2D-C1D	6.09	135.44	124.71
22	A	821	CLA	C2C-C1C-NC	6.09	115.67	109.97
22	A	823	CLA	CHD-C1D-ND	-6.09	118.86	124.45
22	4	601	CLA	CHD-C1D-ND	-6.08	118.86	124.45
22	B	829	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
22	1	602	CLA	CMD-C2D-C1D	6.08	135.43	124.71
22	5	614	CLA	CHD-C1D-ND	-6.08	118.87	124.45
22	6	613	CLA	CHD-C1D-ND	-6.08	118.87	124.45
22	A	826	CLA	CHD-C1D-ND	-6.08	118.87	124.45
22	A	810	CLA	CMD-C2D-C1D	6.07	135.42	124.71
22	B	831	CLA	CHD-C1D-ND	-6.07	118.87	124.45
22	A	839	CLA	CHD-C1D-ND	-6.07	118.87	124.45
22	2	609	CLA	CHD-C1D-ND	-6.07	118.88	124.45
22	8	601	CLA	O2D-CGD-CBD	6.07	122.05	111.27
22	9	603	CLA	CHD-C1D-ND	-6.07	118.88	124.45
22	B	806	CLA	CHD-C1D-ND	-6.07	118.88	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	811	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
22	8	612	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
22	A	812	CLA	C2C-C1C-NC	6.07	115.66	109.97
22	7	610	CLA	C4A-NA-C1A	-6.07	103.98	106.71
29	4	606	CHL	C1D-ND-C4D	-6.06	102.03	106.33
22	B	808	CLA	C2C-C1C-NC	6.06	115.65	109.97
22	1	602	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
22	B	809	CLA	C2C-C1C-NC	6.06	115.65	109.97
22	3	609	CLA	CHD-C1D-ND	-6.06	118.89	124.45
22	B	835	CLA	CMD-C2D-C1D	6.06	135.39	124.71
22	A	825	CLA	CHD-C1D-ND	-6.05	118.89	124.45
22	B	811	CLA	C1B-C2B-C3B	-6.05	101.28	107.03
22	B	803	CLA	CHD-C1D-ND	-6.05	118.89	124.45
22	8	613	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
22	A	836	CLA	C2C-C1C-NC	6.05	115.64	109.97
22	2	603	CLA	C2C-C1C-NC	6.05	115.64	109.97
22	B	809	CLA	CMD-C2D-C1D	6.04	135.36	124.71
25	5	625	BCR	C15-C14-C13	-6.04	118.69	127.31
22	2	606	CLA	CHD-C1D-ND	-6.04	118.90	124.45
22	A	838	CLA	C4A-NA-C1A	-6.04	103.99	106.71
22	8	608	CLA	CHD-C1D-ND	-6.04	118.90	124.45
22	Z	609	CLA	C2C-C1C-NC	6.04	115.63	109.97
22	7	611	CLA	CAA-C2A-C3A	-6.04	102.01	116.10
22	7	610	CLA	CHD-C1D-ND	-6.04	118.91	124.45
22	2	613	CLA	CHD-C1D-ND	-6.04	118.91	124.45
22	8	613	CLA	CMD-C2D-C1D	6.04	135.35	124.71
22	B	808	CLA	CMD-C2D-C1D	6.04	135.35	124.71
22	6	616	CLA	CHD-C1D-ND	-6.03	118.91	124.45
22	A	804	CLA	C4A-NA-C1A	-6.03	103.99	106.71
22	B	828	CLA	C2C-C1C-NC	6.03	115.62	109.97
22	Z	606	CLA	CHD-C1D-ND	-6.03	118.91	124.45
22	B	840	CLA	CHD-C1D-ND	-6.03	118.91	124.45
22	9	610	CLA	CHD-C1D-ND	-6.03	118.91	124.45
22	7	602	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
22	1	606	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
22	4	614	CLA	CMD-C2D-C1D	6.02	135.33	124.71
22	5	612	CLA	C2C-C1C-NC	6.02	115.61	109.97
22	8	610	CLA	C4A-NA-C1A	-6.02	104.00	106.71
22	3	603	CLA	C2C-C1C-NC	6.02	115.61	109.97
22	3	610	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
22	5	610	CLA	CHD-C1D-ND	-6.02	118.93	124.45
22	A	815	CLA	O2D-CGD-CBD	6.01	121.95	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	833	CLA	O2D-CGD-CBD	6.01	121.95	111.27
29	Z	601	CHL	C2C-C3C-C4C	-6.01	102.20	106.49
29	1	601	CHL	C1D-ND-C4D	-6.01	102.06	106.33
22	8	611	CLA	CHD-C1D-ND	-6.01	118.93	124.45
29	5	607	CHL	C2C-C3C-C4C	-6.01	102.21	106.49
22	B	826	CLA	O2D-CGD-CBD	6.00	121.94	111.27
22	9	602	CLA	CHD-C1D-ND	-6.00	118.94	124.45
22	9	609	CLA	CHD-C1D-ND	-6.00	118.94	124.45
22	A	840	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
22	B	838	CLA	CHD-C1D-ND	-6.00	118.94	124.45
22	B	817	CLA	C2C-C1C-NC	6.00	115.59	109.97
22	4	612	CLA	CHD-C1D-ND	-6.00	118.94	124.45
22	8	604	CLA	CHD-C1D-ND	-6.00	118.94	124.45
22	A	806	CLA	O2D-CGD-CBD	6.00	121.93	111.27
22	2	612	CLA	C4A-NA-C1A	-6.00	104.01	106.71
22	3	620	CLA	CHD-C1D-ND	-6.00	118.94	124.45
22	4	612	CLA	C4A-NA-C1A	-6.00	104.01	106.71
22	A	806	CLA	CHD-C1D-ND	-5.99	118.94	124.45
22	A	815	CLA	C4A-NA-C1A	-5.99	104.01	106.71
22	Z	603	CLA	C2C-C1C-NC	5.99	115.59	109.97
29	6	608	CHL	C1D-ND-C4D	-5.99	102.08	106.33
22	8	602	CLA	CHD-C1D-ND	-5.99	118.95	124.45
22	Z	609	CLA	CHD-C1D-ND	-5.99	118.95	124.45
22	9	612	CLA	C2C-C1C-NC	5.98	115.58	109.97
29	4	618	CHL	C1D-ND-C4D	-5.98	102.09	106.33
22	A	831	CLA	CMD-C2D-C1D	5.97	135.24	124.71
22	6	614	CLA	C4A-NA-C1A	-5.97	104.02	106.71
22	Z	611	CLA	CHD-C1D-ND	-5.97	118.97	124.45
22	K	4002	CLA	CHD-C1D-ND	-5.97	118.97	124.45
22	7	601	CLA	CHD-C1D-ND	-5.97	118.97	124.45
22	7	601	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
22	B	825	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
22	5	603	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
22	7	620	CLA	CHD-C1D-ND	-5.96	118.98	124.45
25	6	625	BCR	C15-C14-C13	-5.96	118.81	127.31
22	Z	610	CLA	CMD-C2D-C1D	5.96	135.21	124.71
22	B	819	CLA	CHD-C1D-ND	-5.96	118.98	124.45
22	B	824	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
22	B	822	CLA	CHD-C1D-ND	-5.95	118.98	124.45
22	6	602	CLA	CHD-C1D-ND	-5.95	118.98	124.45
22	Z	613	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
22	5	616	CLA	C2C-C1C-NC	5.95	115.55	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	603	CLA	C2C-C1C-NC	5.95	115.55	109.97
22	Z	612	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
22	1	608	CLA	CHD-C1D-ND	-5.95	118.99	124.45
22	B	812	CLA	CHD-C1D-ND	-5.94	118.99	124.45
22	3	612	CLA	CHD-C1D-ND	-5.94	118.99	124.45
22	B	836	CLA	O2D-CGD-CBD	5.94	121.83	111.27
22	F	301	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
22	B	839	CLA	CHD-C1D-ND	-5.94	119.00	124.45
22	Z	602	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
22	9	612	CLA	CHD-C1D-ND	-5.94	119.00	124.45
22	A	834	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
22	1	611	CLA	CHD-C1D-ND	-5.93	119.00	124.45
22	5	621	CLA	C2C-C1C-NC	5.93	115.52	109.97
22	8	616	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
22	A	818	CLA	CHD-C1D-ND	-5.92	119.01	124.45
29	6	608	CHL	CHD-C4C-C3C	-5.92	116.14	124.84
22	4	614	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
22	K	4003	CLA	C2C-C1C-NC	5.91	115.51	109.97
22	A	833	CLA	CHD-C1D-ND	-5.91	119.02	124.45
22	J	3002	CLA	CHD-C1D-ND	-5.91	119.02	124.45
22	7	613	CLA	CMD-C2D-C1D	5.91	135.13	124.71
29	4	608	CHL	CHD-C4C-C3C	-5.91	116.15	124.84
22	A	842	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
22	B	838	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
22	Z	608	CLA	CHD-C1D-ND	-5.91	119.03	124.45
22	8	601	CLA	C2C-C1C-NC	5.91	115.50	109.97
22	A	814	CLA	O2D-CGD-CBD	5.90	121.76	111.27
22	A	816	CLA	CHD-C1D-ND	-5.90	119.03	124.45
22	A	838	CLA	CHD-C1D-ND	-5.90	119.03	124.45
22	4	609	CLA	C2C-C1C-NC	5.90	115.50	109.97
22	K	4002	CLA	O2D-CGD-CBD	5.89	121.74	111.27
29	9	607	CHL	C1D-ND-C4D	-5.89	102.15	106.33
22	A	830	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	1	608	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	A	804	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	9	611	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
22	A	829	CLA	CMD-C2D-C1D	5.89	135.09	124.71
22	4	602	CLA	CHD-C1D-ND	-5.89	119.04	124.45
22	7	611	CLA	C2C-C1C-NC	5.88	115.48	109.97
22	8	610	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
22	8	604	CLA	C2C-C1C-NC	5.88	115.48	109.97
22	A	831	CLA	C2C-C1C-NC	5.88	115.48	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	601	CLA	CHD-C1D-ND	-5.88	119.05	124.45
22	5	614	CLA	C4A-NA-C1A	-5.88	104.06	106.71
22	G	204	CLA	CHD-C1D-ND	-5.88	119.05	124.45
22	A	821	CLA	CMD-C2D-C1D	5.88	135.07	124.71
22	G	203	CLA	C4A-NA-C1A	-5.88	104.06	106.71
22	B	821	CLA	CHD-C1D-ND	-5.88	119.05	124.45
22	6	610	CLA	CHD-C1D-ND	-5.87	119.06	124.45
22	6	612	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
25	A	852	BCR	C20-C21-C22	-5.87	118.93	127.31
22	B	841	CLA	O2D-CGD-CBD	5.87	121.70	111.27
22	2	612	CLA	CHD-C1D-ND	-5.87	119.06	124.45
22	A	834	CLA	CHD-C1D-ND	-5.86	119.06	124.45
22	6	609	CLA	CHD-C1D-ND	-5.86	119.06	124.45
22	B	806	CLA	C4A-NA-C1A	-5.86	104.07	106.71
22	6	622	CLA	CHD-C1D-ND	-5.86	119.07	124.45
22	G	203	CLA	CHD-C1D-ND	-5.86	119.07	124.45
22	7	613	CLA	C2C-C1C-NC	5.86	115.46	109.97
22	A	837	CLA	CHD-C1D-ND	-5.86	119.07	124.45
22	B	813	CLA	O2D-CGD-CBD	5.86	121.67	111.27
22	5	601	CLA	O2D-CGD-CBD	5.85	121.67	111.27
22	2	601	CLA	CHD-C1D-ND	-5.85	119.08	124.45
22	A	841	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
22	B	824	CLA	CMD-C2D-C1D	5.85	135.02	124.71
22	A	843	CLA	C2C-C1C-NC	5.85	115.45	109.97
22	B	807	CLA	CHD-C1D-ND	-5.85	119.08	124.45
22	7	603	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
22	2	611	CLA	CHD-C1D-ND	-5.84	119.08	124.45
22	B	804	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
22	A	812	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
22	3	606	CLA	CHD-C1D-ND	-5.84	119.09	124.45
22	A	804	CLA	CHD-C1D-ND	-5.84	119.09	124.45
22	4	616	CLA	CHD-C1D-ND	-5.83	119.09	124.45
22	A	836	CLA	CMD-C2D-C1D	5.83	134.99	124.71
22	A	826	CLA	C4A-NA-C1A	-5.83	104.08	106.71
22	8	603	CLA	C2C-C1C-NC	5.83	115.43	109.97
22	9	609	CLA	C2C-C1C-NC	5.83	115.43	109.97
22	A	824	CLA	C2C-C1C-NC	5.83	115.43	109.97
22	A	809	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
22	L	203	CLA	CHD-C1D-ND	-5.82	119.10	124.45
22	2	613	CLA	C2C-C1C-NC	5.82	115.43	109.97
22	F	303	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
22	4	611	CLA	C2C-C1C-NC	5.82	115.42	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	811	CLA	C2C-C1C-NC	5.81	115.42	109.97
22	6	603	CLA	C4A-NA-C1A	-5.81	104.09	106.71
22	B	805	CLA	CHD-C1D-ND	-5.81	119.11	124.45
22	A	843	CLA	CMD-C2D-C1D	5.81	134.95	124.71
22	3	602	CLA	CHD-C1D-ND	-5.81	119.12	124.45
22	9	613	CLA	CHD-C1D-ND	-5.81	119.12	124.45
29	5	608	CHL	C1D-ND-C4D	-5.81	102.21	106.33
22	B	818	CLA	O2D-CGD-CBD	5.81	121.58	111.27
22	F	304	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
22	B	813	CLA	CHD-C1D-ND	-5.80	119.12	124.45
22	A	835	CLA	O2D-CGD-CBD	5.80	121.58	111.27
22	B	830	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
22	9	602	CLA	O2D-CGD-CBD	5.80	121.57	111.27
22	A	808	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
22	B	811	CLA	CHD-C1D-ND	-5.79	119.13	124.45
22	F	303	CLA	CHD-C1D-ND	-5.79	119.13	124.45
22	B	829	CLA	CMB-C2B-C1B	5.79	134.19	125.37
22	4	603	CLA	CHD-C1D-ND	-5.79	119.13	124.45
22	B	837	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
22	4	601	CLA	O2D-CGD-CBD	5.79	121.55	111.27
22	5	613	CLA	C2C-C1C-NC	5.79	115.39	109.97
22	4	612	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
22	A	842	CLA	CHD-C1D-ND	-5.79	119.14	124.45
22	B	811	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
22	4	609	CLA	CMD-C2D-C1D	5.78	134.90	124.71
22	7	609	CLA	C3B-C2B-C1B	-5.78	100.19	107.16
29	5	618	CHL	O2D-CGD-CBD	5.78	121.54	111.27
22	6	603	CLA	CHD-C1D-ND	-5.78	119.14	124.45
22	Z	612	CLA	CHD-C1D-ND	-5.78	119.14	124.45
29	6	618	CHL	C1C-C2C-C3C	-5.78	102.53	107.11
22	5	601	CLA	CHD-C1D-ND	-5.77	119.15	124.45
25	6	625	BCR	C7-C8-C9	-5.77	117.51	126.23
22	Z	603	CLA	CHD-C1D-ND	-5.77	119.15	124.45
22	B	827	CLA	CHD-C4C-C3C	-5.77	116.37	124.84
22	A	813	CLA	CHD-C1D-ND	-5.76	119.16	124.45
22	A	819	CLA	CHD-C1D-ND	-5.76	119.16	124.45
22	A	807	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
22	Z	608	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
22	2	603	CLA	CHD-C1D-ND	-5.76	119.16	124.45
22	Z	604	CLA	CHD-C1D-ND	-5.76	119.16	124.45
22	A	832	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	B	835	CLA	CHD-C4C-C3C	-5.75	116.38	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	816	CLA	CHD-C1D-ND	-5.75	119.17	124.45
22	5	601	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	5	611	CLA	CHD-C1D-ND	-5.75	119.17	124.45
22	2	609	CLA	C2C-C1C-NC	5.75	115.36	109.97
22	Z	611	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
22	7	612	CLA	CHD-C1D-ND	-5.74	119.17	124.45
22	5	609	CLA	C2C-C1C-NC	5.74	115.35	109.97
29	1	607	CHL	C2C-C3C-C4C	-5.74	102.40	106.49
22	7	613	CLA	CHD-C1D-ND	-5.74	119.18	124.45
22	G	203	CLA	C2C-C1C-NC	5.74	115.35	109.97
22	A	832	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
29	6	618	CHL	CMD-C2D-C1D	5.73	134.82	124.71
22	B	822	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
22	B	811	CLA	C3B-C4B-NB	5.73	114.07	110.23
29	4	607	CHL	C1C-C2C-C3C	-5.73	102.56	107.11
29	1	601	CHL	O2D-CGD-CBD	5.73	121.45	111.27
22	9	610	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
22	A	825	CLA	C2C-C1C-NC	5.73	115.34	109.97
22	8	614	CLA	CHD-C1D-ND	-5.73	119.19	124.45
22	A	845	CLA	CHD-C4C-C3C	-5.72	116.42	124.84
22	1	611	CLA	C2C-C1C-NC	5.72	115.33	109.97
22	B	840	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
22	1	614	CLA	C2C-C1C-NC	5.72	115.33	109.97
29	7	607	CHL	C1D-ND-C4D	-5.72	102.27	106.33
29	1	601	CHL	C2C-C3C-C4C	-5.72	102.41	106.49
22	Z	612	CLA	C2C-C1C-NC	5.72	115.33	109.97
22	8	606	CLA	CHD-C1D-ND	-5.72	119.20	124.45
22	B	813	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
22	6	604	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
22	3	620	CLA	C2C-C1C-NC	5.71	115.32	109.97
29	4	608	CHL	C3D-C2D-C1D	-5.71	98.04	105.83
22	A	827	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
29	9	607	CHL	C2C-C3C-C4C	-5.71	102.42	106.49
22	A	841	CLA	CHD-C1D-ND	-5.71	119.21	124.45
22	3	604	CLA	C2C-C1C-NC	5.71	115.32	109.97
22	5	606	CLA	CHD-C1D-ND	-5.71	119.21	124.45
22	3	610	CLA	CHD-C1D-ND	-5.70	119.21	124.45
22	A	810	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
22	L	203	CLA	CMD-C2D-C1D	5.70	134.76	124.71
22	7	612	CLA	C2C-C1C-NC	5.70	115.31	109.97
22	5	611	CLA	C2C-C1C-NC	5.70	115.31	109.97
22	9	604	CLA	C2C-C1C-NC	5.70	115.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	845	CLA	CHD-C1D-ND	-5.70	119.22	124.45
22	B	836	CLA	CHD-C1D-ND	-5.70	119.22	124.45
22	9	601	CLA	C2C-C1C-NC	5.70	115.31	109.97
22	9	602	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
22	B	830	CLA	CHD-C1D-ND	-5.70	119.22	124.45
22	6	610	CLA	C4A-NA-C1A	-5.70	104.14	106.71
22	A	845	CLA	C2C-C1C-NC	5.70	115.31	109.97
22	1	603	CLA	CHD-C1D-ND	-5.70	119.22	124.45
22	A	820	CLA	C4A-NA-C1A	-5.69	104.15	106.71
22	A	824	CLA	CHD-C1D-ND	-5.69	119.22	124.45
22	B	817	CLA	CHD-C1D-ND	-5.69	119.22	124.45
22	2	612	CLA	C2C-C1C-NC	5.69	115.30	109.97
22	4	613	CLA	CHD-C1D-ND	-5.69	119.23	124.45
22	A	841	CLA	CMD-C2D-C1D	5.69	134.74	124.71
22	B	814	CLA	CHD-C1D-ND	-5.68	119.23	124.45
22	A	803	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
22	8	616	CLA	CMD-C2D-C1D	5.68	134.73	124.71
22	A	842	CLA	C2C-C1C-NC	5.68	115.30	109.97
22	B	804	CLA	CHD-C1D-ND	-5.68	119.24	124.45
22	8	614	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
22	3	607	CLA	C2C-C1C-NC	5.68	115.29	109.97
22	5	603	CLA	C2C-C1C-NC	5.67	115.29	109.97
29	4	608	CHL	C1C-C2C-C3C	-5.67	102.61	107.11
22	6	617	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
22	A	854	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
22	A	838	CLA	O2D-CGD-CBD	5.66	121.33	111.27
22	1	612	CLA	C2C-C1C-NC	5.66	115.28	109.97
22	1	606	CLA	CHD-C1D-ND	-5.66	119.25	124.45
22	A	820	CLA	CHD-C4C-C3C	-5.66	116.53	124.84
22	B	802	CLA	CMD-C2D-C1D	5.66	134.68	124.71
22	9	613	CLA	C2C-C1C-NC	5.66	115.27	109.97
22	B	820	CLA	O2D-CGD-CBD	5.65	121.32	111.27
22	8	611	CLA	O2D-CGD-CBD	5.65	121.32	111.27
22	9	614	CLA	C2C-C1C-NC	5.65	115.27	109.97
29	8	607	CHL	CHD-C4C-C3C	-5.65	116.53	124.84
22	2	601	CLA	C2C-C1C-NC	5.65	115.26	109.97
22	B	809	CLA	CHD-C1D-ND	-5.65	119.26	124.45
22	B	810	CLA	C4A-NA-C1A	-5.65	104.17	106.71
22	B	814	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
22	3	610	CLA	C4A-NA-C1A	-5.65	104.17	106.71
22	A	829	CLA	C3B-C2B-C1B	-5.64	100.35	107.16
22	A	816	CLA	O2D-CGD-CBD	5.64	121.30	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	610	CLA	CHD-C1D-ND	-5.64	119.27	124.45
22	6	612	CLA	C4A-NA-C1A	-5.64	104.17	106.71
22	A	820	CLA	C2C-C1C-NC	5.64	115.26	109.97
22	3	617	CLA	CHD-C1D-ND	-5.64	119.27	124.45
22	6	604	CLA	CHD-C1D-ND	-5.64	119.27	124.45
22	3	603	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	3	607	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	5	604	CLA	CHD-C1D-ND	-5.63	119.28	124.45
22	7	616	CLA	C2C-C1C-NC	5.63	115.25	109.97
22	A	821	CLA	O2D-CGD-CBD	5.63	121.28	111.27
22	3	607	CLA	CMD-C2D-C1D	5.63	134.64	124.71
22	A	832	CLA	O2D-CGD-CBD	5.63	121.28	111.27
22	A	805	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
22	5	610	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
22	B	815	CLA	O2D-CGD-CBD	5.63	121.27	111.27
22	3	613	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
22	5	601	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
22	B	823	CLA	CMD-C2D-C1D	5.62	134.62	124.71
22	7	611	CLA	O2D-CGD-CBD	5.62	121.26	111.27
22	A	816	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
22	8	603	CLA	CHD-C1D-ND	-5.62	119.29	124.45
29	5	618	CHL	C1C-C2C-C3C	-5.62	102.65	107.11
22	5	611	CLA	O2D-CGD-CBD	5.62	121.25	111.27
22	B	852	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
22	7	603	CLA	O2D-CGD-CBD	5.61	121.25	111.27
29	3	608	CHL	C3D-C2D-C1D	-5.61	98.17	105.83
29	4	606	CHL	CHD-C4C-C3C	-5.61	116.59	124.84
22	8	611	CLA	C2C-C1C-NC	5.61	115.23	109.97
22	9	611	CLA	C2C-C1C-NC	5.61	115.23	109.97
22	A	836	CLA	CHD-C1D-ND	-5.61	119.30	124.45
22	B	818	CLA	CHD-C1D-ND	-5.61	119.30	124.45
22	5	603	CLA	CHD-C1D-ND	-5.61	119.30	124.45
22	5	612	CLA	CHD-C1D-ND	-5.61	119.30	124.45
29	Z	601	CHL	CMD-C2D-C1D	5.61	134.60	124.71
22	5	603	CLA	C4A-NA-C1A	-5.61	104.19	106.71
22	7	606	CLA	CHD-C1D-ND	-5.61	119.30	124.45
29	Z	607	CHL	C2C-C3C-C4C	-5.61	102.49	106.49
22	A	832	CLA	CMD-C2D-C1D	5.61	134.59	124.71
22	A	805	CLA	C4A-NA-C1A	-5.61	104.19	106.71
22	A	813	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
22	Z	606	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
22	1	616	CLA	C2C-C1C-NC	5.60	115.22	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	608	CLA	C2C-C1C-NC	5.60	115.22	109.97
22	A	820	CLA	CHD-C1D-ND	-5.60	119.31	124.45
22	B	818	CLA	C4A-NA-C1A	-5.60	104.19	106.71
22	A	834	CLA	C2C-C1C-NC	5.60	115.21	109.97
22	4	613	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
22	3	617	CLA	C2C-C1C-NC	5.59	115.21	109.97
22	9	601	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
22	4	601	CLA	C2C-C1C-NC	5.59	115.21	109.97
22	A	841	CLA	C2C-C1C-NC	5.59	115.21	109.97
22	8	616	CLA	C2C-C1C-NC	5.59	115.21	109.97
22	5	606	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
22	A	807	CLA	CHD-C1D-ND	-5.59	119.32	124.45
22	4	609	CLA	CHD-C1D-ND	-5.58	119.32	124.45
22	3	611	CLA	C2C-C1C-NC	5.58	115.20	109.97
22	A	824	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
22	B	803	CLA	CMD-C2D-C1D	5.58	134.54	124.71
22	4	609	CLA	C4A-NA-C1A	-5.58	104.20	106.71
22	Z	616	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
21	A	801	CL0	CMD-C2D-C1D	5.57	134.53	124.71
22	F	304	CLA	CHD-C1D-ND	-5.57	119.33	124.45
22	A	833	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
22	A	810	CLA	C2C-C1C-NC	5.57	115.19	109.97
22	A	840	CLA	C2C-C1C-NC	5.56	115.19	109.97
22	6	612	CLA	C2C-C1C-NC	5.56	115.18	109.97
22	8	613	CLA	C2C-C1C-NC	5.56	115.18	109.97
22	B	852	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	8	603	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
22	Z	616	CLA	CHD-C1D-ND	-5.56	119.34	124.45
22	B	808	CLA	O2D-CGD-CBD	5.56	121.14	111.27
22	B	812	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
22	1	602	CLA	CHD-C1D-ND	-5.56	119.35	124.45
22	A	819	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
22	Z	604	CLA	C2C-C1C-NC	5.55	115.17	109.97
22	7	620	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
22	3	603	CLA	CHD-C1D-ND	-5.55	119.35	124.45
22	7	613	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
22	6	603	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
22	Z	603	CLA	O2D-CGD-CBD	5.54	121.12	111.27
22	Z	610	CLA	CHD-C1D-ND	-5.54	119.36	124.45
22	5	611	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
22	1	612	CLA	CHD-C1D-ND	-5.54	119.36	124.45
22	9	611	CLA	CHD-C1D-ND	-5.54	119.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	606	CHL	C1C-C2C-C3C	-5.54	102.71	107.11
22	4	609	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
22	A	854	CLA	CHD-C1D-ND	-5.54	119.36	124.45
22	1	609	CLA	C2C-C1C-NC	5.54	115.16	109.97
22	Z	616	CLA	C2C-C1C-NC	5.53	115.16	109.97
22	7	606	CLA	O2D-CGD-CBD	5.53	121.10	111.27
22	J	3002	CLA	C2C-C1C-NC	5.53	115.16	109.97
22	7	603	CLA	C2C-C1C-NC	5.53	115.16	109.97
22	8	609	CLA	CHD-C1D-ND	-5.53	119.37	124.45
22	A	823	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
22	3	607	CLA	CHD-C1D-ND	-5.53	119.37	124.45
22	2	606	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
22	A	839	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
22	1	612	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
22	1	616	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
22	8	612	CLA	CHD-C1D-ND	-5.52	119.38	124.45
22	6	601	CLA	C2C-C1C-NC	5.52	115.15	109.97
22	7	614	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
22	3	611	CLA	CAA-C2A-C3A	-5.52	103.22	116.10
29	7	607	CHL	C2C-C3C-C4C	-5.52	102.55	106.49
22	2	601	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
22	7	604	CLA	C2B-C1B-NB	5.52	113.93	110.23
22	B	821	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
22	B	808	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	4	612	CLA	C2C-C1C-NC	5.51	115.14	109.97
22	A	819	CLA	C3B-C2B-C1B	-5.51	100.51	107.16
29	9	606	CHL	C1C-C2C-C3C	-5.51	102.74	107.11
22	7	612	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	A	808	CLA	O2D-CGD-CBD	5.51	121.06	111.27
22	5	612	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	4	613	CLA	C2C-C1C-NC	5.51	115.13	109.97
22	8	609	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	4	614	CLA	CHD-C1D-ND	-5.50	119.40	124.45
22	5	616	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
22	B	832	CLA	C2C-C1C-NC	5.50	115.13	109.97
22	7	604	CLA	CHD-C1D-ND	-5.50	119.40	124.45
22	9	612	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
22	1	603	CLA	O2D-CGD-CBD	5.50	121.04	111.27
22	B	839	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
22	6	611	CLA	CHD-C1D-ND	-5.50	119.40	124.45
22	7	609	CLA	C2C-C1C-NC	5.50	115.12	109.97
22	3	602	CLA	CHD-C4C-C3C	-5.50	116.76	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	613	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
22	G	203	CLA	O2D-CGD-CBD	5.50	121.03	111.27
22	3	606	CLA	C2C-C1C-NC	5.50	115.12	109.97
22	6	617	CLA	C2C-C1C-NC	5.50	115.12	109.97
22	4	611	CLA	CHD-C1D-ND	-5.49	119.41	124.45
22	Z	614	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
22	6	614	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
22	2	610	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
22	A	854	CLA	C4A-NA-C1A	-5.49	104.24	106.71
22	F	304	CLA	C2C-C1C-NC	5.49	115.11	109.97
22	B	817	CLA	C3B-C2B-C1B	-5.49	100.54	107.16
22	3	607	CLA	C3B-C2B-C1B	-5.48	100.54	107.16
22	3	609	CLA	C2C-C1C-NC	5.48	115.11	109.97
22	Z	602	CLA	CHD-C1D-ND	-5.48	119.42	124.45
22	6	604	CLA	C2C-C1C-NC	5.48	115.11	109.97
22	B	807	CLA	O2D-CGD-CBD	5.48	121.00	111.27
22	B	827	CLA	O2D-CGD-CBD	5.48	121.00	111.27
22	1	610	CLA	CMD-C2D-C1D	5.47	134.36	124.71
22	6	617	CLA	CHD-C1D-ND	-5.47	119.42	124.45
22	7	606	CLA	C2C-C1C-NC	5.47	115.10	109.97
22	5	606	CLA	C2C-C1C-NC	5.47	115.10	109.97
22	3	603	CLA	C4A-NA-C1A	-5.47	104.25	106.71
22	3	602	CLA	O2D-CGD-CBD	5.47	120.99	111.27
22	B	804	CLA	C3B-C2B-C1B	-5.47	100.56	107.16
22	3	617	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
22	B	836	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
29	1	601	CHL	CHD-C4C-C3C	-5.47	116.81	124.84
22	A	840	CLA	CHD-C1D-ND	-5.46	119.43	124.45
22	1	610	CLA	CHD-C1D-ND	-5.46	119.44	124.45
22	6	611	CLA	C2C-C1C-NC	5.46	115.08	109.97
22	K	4003	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
29	9	606	CHL	CHD-C4C-C3C	-5.46	116.82	124.84
22	B	815	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
22	J	3002	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
22	A	807	CLA	C2C-C1C-NC	5.46	115.08	109.97
22	F	303	CLA	C2C-C1C-NC	5.46	115.08	109.97
22	2	611	CLA	C2C-C1C-NC	5.45	115.08	109.97
22	G	203	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
22	3	611	CLA	CHD-C1D-ND	-5.45	119.44	124.45
22	A	839	CLA	C2C-C1C-NC	5.45	115.08	109.97
29	4	607	CHL	CHD-C4C-C3C	-5.45	116.83	124.84
22	8	606	CLA	C2C-C1C-NC	5.45	115.08	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	616	CLA	C2C-C1C-NC	5.45	115.08	109.97
22	A	815	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
22	A	811	CLA	CHD-C1D-ND	-5.44	119.45	124.45
22	9	614	CLA	C4A-NA-C1A	-5.44	104.26	106.71
22	L	204	CLA	C2C-C1C-NC	5.44	115.07	109.97
22	2	614	CLA	C2C-C1C-NC	5.44	115.07	109.97
22	A	822	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
22	A	829	CLA	C4A-NA-C1A	-5.44	104.26	106.71
29	5	607	CHL	C3D-C2D-C1D	-5.44	98.41	105.83
22	A	835	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
22	7	602	CLA	O2D-CGD-CBD	5.44	120.93	111.27
22	8	606	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
22	G	204	CLA	C2C-C1C-NC	5.43	115.06	109.97
22	A	843	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
22	1	613	CLA	C2C-C1C-NC	5.42	115.05	109.97
22	A	821	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
22	2	614	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
22	7	606	CLA	C4A-NA-C1A	-5.42	104.27	106.71
22	A	808	CLA	C2C-C1C-NC	5.41	115.04	109.97
22	2	603	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
22	7	614	CLA	C2C-C1C-NC	5.41	115.04	109.97
22	F	303	CLA	C4A-NA-C1A	-5.41	104.27	106.71
22	B	810	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	L	203	CLA	C2C-C1C-NC	5.41	115.04	109.97
22	L	203	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	A	804	CLA	O2D-CGD-CBD	5.41	120.88	111.27
29	6	606	CHL	C3D-C2D-C1D	-5.41	98.45	105.83
22	3	614	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
29	9	607	CHL	O2D-CGD-CBD	5.41	120.88	111.27
22	B	828	CLA	C4A-NA-C1A	-5.41	104.28	106.71
22	B	839	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	K	4002	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
29	4	618	CHL	C1C-C2C-C3C	-5.40	102.83	107.11
29	1	607	CHL	CHD-C4C-C3C	-5.40	116.90	124.84
22	A	831	CLA	CHD-C1D-ND	-5.40	119.49	124.45
22	4	609	CLA	C3B-C2B-C1B	-5.40	100.64	107.16
22	A	814	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
22	6	610	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
22	1	613	CLA	CHD-C1D-ND	-5.40	119.49	124.45
29	6	607	CHL	CHD-C4C-C3C	-5.40	116.91	124.84
22	A	837	CLA	O2D-CGD-CBD	5.40	120.86	111.27
22	B	841	CLA	CHD-C4C-C3C	-5.39	116.91	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	607	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
22	Z	606	CLA	C2C-C1C-NC	5.39	115.02	109.97
22	7	620	CLA	C2C-C1C-NC	5.39	115.02	109.97
22	8	610	CLA	CHD-C1D-ND	-5.39	119.50	124.45
22	A	829	CLA	CHD-C1D-ND	-5.38	119.51	124.45
22	5	617	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
22	5	614	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
22	B	852	CLA	C2C-C1C-NC	5.38	115.01	109.97
22	A	803	CLA	O2D-CGD-CBD	5.38	120.83	111.27
22	2	606	CLA	C2C-C1C-NC	5.38	115.01	109.97
22	6	622	CLA	C2C-C1C-NC	5.37	115.01	109.97
22	B	835	CLA	CHD-C1D-ND	-5.37	119.52	124.45
22	3	617	CLA	O2D-CGD-CBD	5.37	120.82	111.27
22	A	802	CLA	C4A-NA-C1A	-5.37	104.29	106.71
25	B	846	BCR	C39-C30-C25	-5.37	101.59	110.30
22	9	614	CLA	O2D-CGD-CBD	5.37	120.81	111.27
22	5	609	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
22	8	601	CLA	CHD-C1D-ND	-5.37	119.52	124.45
22	2	612	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
22	B	835	CLA	C2C-C1C-NC	5.37	115.00	109.97
22	3	614	CLA	C2C-C1C-NC	5.37	115.00	109.97
22	8	601	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
29	6	607	CHL	C3D-C2D-C1D	-5.37	98.51	105.83
22	A	819	CLA	C4A-NA-C1A	-5.37	104.29	106.71
22	Z	613	CLA	CHD-C1D-ND	-5.36	119.52	124.45
22	B	807	CLA	CHD-C4C-C3C	-5.36	116.95	124.84
22	5	613	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
22	3	604	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
22	4	603	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
22	6	616	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
22	A	828	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
22	2	611	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
22	B	827	CLA	CHD-C1D-ND	-5.36	119.53	124.45
22	B	821	CLA	C2C-C1C-NC	5.36	114.99	109.97
22	8	609	CLA	C3B-C2B-C1B	-5.36	100.70	107.16
22	9	603	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
22	4	602	CLA	C2C-C1C-NC	5.36	114.99	109.97
22	4	604	CLA	C2C-C1C-NC	5.35	114.99	109.97
22	A	820	CLA	O2D-CGD-CBD	5.35	120.78	111.27
22	7	601	CLA	O2D-CGD-CBD	5.35	120.78	111.27
29	6	606	CHL	CHD-C4C-C3C	-5.35	116.98	124.84
22	B	814	CLA	C3B-C2B-C1B	-5.35	100.70	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	815	CLA	C2C-C1C-NC	5.35	114.98	109.97
22	B	809	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
22	Z	603	CLA	C4A-NA-C1A	-5.35	104.30	106.71
22	8	614	CLA	CMD-C2D-C1D	5.35	134.13	124.71
22	A	826	CLA	O2D-CGD-CBD	5.35	120.77	111.27
22	B	810	CLA	C2C-C1C-NC	5.34	114.98	109.97
22	A	831	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
29	6	606	CHL	O2D-CGD-CBD	5.34	120.76	111.27
29	5	608	CHL	C1C-C2C-C3C	-5.34	102.87	107.11
22	B	833	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
22	A	835	CLA	C4A-NA-C1A	-5.34	104.31	106.71
22	1	602	CLA	C4A-NA-C1A	-5.34	104.31	106.71
22	1	611	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
22	6	613	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
22	Z	608	CLA	C2C-C1C-NC	5.33	114.97	109.97
22	7	612	CLA	C4A-NA-C1A	-5.33	104.31	106.71
22	A	834	CLA	C3B-C2B-C1B	-5.33	100.73	107.16
22	K	4002	CLA	C2C-C1C-NC	5.33	114.97	109.97
22	6	601	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
22	5	614	CLA	C2C-C1C-NC	5.33	114.96	109.97
22	B	820	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
22	A	837	CLA	C2C-C1C-NC	5.33	114.96	109.97
22	5	617	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
22	A	824	CLA	O2D-CGD-CBD	5.32	120.73	111.27
22	3	606	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
22	7	609	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
22	A	813	CLA	C4A-NA-C1A	-5.32	104.31	106.71
22	B	830	CLA	C4A-NA-C1A	-5.32	104.31	106.71
22	3	614	CLA	C4A-NA-C1A	-5.32	104.31	106.71
22	B	812	CLA	C2C-C1C-NC	5.32	114.95	109.97
22	4	616	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
22	2	602	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
22	B	836	CLA	C2C-C1C-NC	5.31	114.95	109.97
22	5	613	CLA	CHD-C1D-ND	-5.31	119.57	124.45
22	3	609	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
22	A	807	CLA	O2D-CGD-CBD	5.31	120.70	111.27
22	1	603	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
29	1	607	CHL	C3D-C2D-C1D	-5.30	98.60	105.83
22	9	614	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
22	B	818	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
22	5	612	CLA	C4A-NA-C1A	-5.30	104.33	106.71
22	B	811	CLA	O2D-CGD-CBD	5.29	120.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	803	CLA	C3B-C2B-C1B	-5.29	100.77	107.16
22	B	816	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
22	7	616	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
22	6	609	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
22	A	827	CLA	C4A-NA-C1A	-5.29	104.33	106.71
22	9	613	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
22	Z	614	CLA	C2C-C1C-NC	5.29	114.92	109.97
22	G	204	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
22	A	828	CLA	CHD-C1D-ND	-5.29	119.60	124.45
22	4	610	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
22	B	823	CLA	CHD-C1D-ND	-5.28	119.60	124.45
29	9	607	CHL	C3D-C2D-C1D	-5.28	98.62	105.83
22	B	852	CLA	CHD-C1D-ND	-5.28	119.60	124.45
22	5	616	CLA	CHD-C1D-ND	-5.28	119.60	124.45
22	Z	610	CLA	O2D-CGD-CBD	5.28	120.65	111.27
22	B	822	CLA	C2C-C1C-NC	5.28	114.92	109.97
22	7	611	CLA	CHD-C1D-ND	-5.27	119.61	124.45
22	8	612	CLA	C4A-NA-C1A	-5.27	104.33	106.71
22	5	621	CLA	O2D-CGD-CBD	5.27	120.64	111.27
22	5	621	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
22	9	609	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
22	6	612	CLA	CHD-C1D-ND	-5.27	119.61	124.45
22	B	832	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	B	831	CLA	O2D-CGD-CBD	5.27	120.63	111.27
22	A	837	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
22	B	836	CLA	C3B-C2B-C1B	-5.26	100.81	107.16
22	A	802	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
22	3	620	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
29	4	606	CHL	C3D-C2D-C1D	-5.26	98.66	105.83
22	3	612	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
22	6	617	CLA	C4A-NA-C1A	-5.26	104.34	106.71
25	L	201	BCR	C7-C8-C9	-5.25	118.30	126.23
22	B	820	CLA	C4A-NA-C1A	-5.25	104.35	106.71
22	B	826	CLA	C4A-NA-C1A	-5.25	104.35	106.71
29	6	606	CHL	C1C-C2C-C3C	-5.25	102.95	107.11
29	6	618	CHL	C3D-C2D-C1D	-5.25	98.67	105.83
29	9	606	CHL	C3D-C2D-C1D	-5.25	98.67	105.83
22	4	610	CLA	O2D-CGD-CBD	5.24	120.59	111.27
22	7	611	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
22	4	616	CLA	CAA-C2A-C3A	-5.24	103.86	116.10
22	A	838	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	8	609	CLA	C4A-NA-C1A	-5.24	104.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	622	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	A	826	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	1	609	CLA	C4A-NA-C1A	-5.24	104.35	106.71
29	5	608	CHL	C3D-C2D-C1D	-5.24	98.68	105.83
22	2	607	CLA	C2C-C1C-NC	5.24	114.88	109.97
22	B	826	CLA	CHD-C1D-ND	-5.23	119.65	124.45
22	B	811	CLA	C4A-NA-C1A	-5.23	104.36	106.71
22	Z	610	CLA	C4A-NA-C1A	-5.23	104.36	106.71
22	2	602	CLA	C2C-C1C-NC	5.23	114.87	109.97
29	5	618	CHL	C3D-C2D-C1D	-5.22	98.70	105.83
22	1	614	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
22	8	602	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	Z	606	CLA	O2D-CGD-CBD	5.22	120.54	111.27
29	6	608	CHL	CHD-C1D-ND	-5.22	119.66	124.45
22	2	613	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
29	1	601	CHL	C1C-C2C-C3C	-5.22	102.97	107.11
22	Z	603	CLA	CHD-C4C-C3C	-5.21	117.17	124.84
22	6	611	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
22	A	823	CLA	C2C-C1C-NC	5.21	114.86	109.97
22	A	813	CLA	O2D-CGD-CBD	5.21	120.53	111.27
22	3	611	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
22	2	610	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	A	817	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
22	8	612	CLA	C2C-C1C-NC	5.20	114.84	109.97
22	Z	611	CLA	C2C-C1C-NC	5.20	114.84	109.97
22	B	813	CLA	C4A-NA-C1A	-5.20	104.37	106.71
22	B	834	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
22	4	602	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
22	4	604	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
22	1	616	CLA	CHD-C1D-ND	-5.20	119.67	124.45
22	B	820	CLA	C2C-C1C-NC	5.20	114.84	109.97
22	B	822	CLA	O2D-CGD-CBD	5.20	120.50	111.27
22	B	824	CLA	C3B-C2B-C1B	-5.20	100.89	107.16
22	5	606	CLA	C4A-NA-C1A	-5.20	104.37	106.71
22	1	604	CLA	C2C-C1C-NC	5.19	114.84	109.97
29	4	618	CHL	C3D-C2D-C1D	-5.19	98.75	105.83
22	9	609	CLA	C3B-C2B-C1B	-5.18	100.91	107.16
22	1	609	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
22	B	834	CLA	C2C-C1C-NC	5.18	114.83	109.97
22	A	817	CLA	O2D-CGD-CBD	5.18	120.48	111.27
29	6	618	CHL	CHD-C4C-C3C	-5.18	117.22	124.84
22	3	611	CLA	O2D-CGD-CBD	5.18	120.47	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	608	CHL	CHD-C4C-C3C	-5.18	117.22	124.84
29	Z	607	CHL	C1C-C2C-C3C	-5.18	103.00	107.11
22	B	825	CLA	CHD-C1D-ND	-5.18	119.69	124.45
22	1	610	CLA	C4A-NA-C1A	-5.18	104.38	106.71
22	5	617	CLA	C4A-NA-C1A	-5.18	104.38	106.71
22	8	609	CLA	C2C-C1C-NC	5.17	114.82	109.97
22	3	604	CLA	C4A-NA-C1A	-5.17	104.38	106.71
22	A	803	CLA	C2C-C1C-NC	5.17	114.82	109.97
22	4	610	CLA	C4A-NA-C1A	-5.17	104.38	106.71
22	2	602	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
29	7	607	CHL	C1C-C2C-C3C	-5.17	103.01	107.11
29	4	607	CHL	C3D-C2D-C1D	-5.16	98.78	105.83
25	A	852	BCR	C7-C8-C9	-5.16	118.43	126.23
22	1	606	CLA	C4A-NA-C1A	-5.16	104.39	106.71
22	4	612	CLA	O2D-CGD-CBD	5.16	120.44	111.27
29	6	608	CHL	C3D-C2D-C1D	-5.16	98.79	105.83
29	5	618	CHL	C2C-C3C-C4C	-5.16	102.81	106.49
22	A	827	CLA	C3B-C2B-C1B	-5.16	100.93	107.16
29	1	601	CHL	C3D-C2D-C1D	-5.16	98.79	105.83
22	B	817	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
22	7	601	CLA	C2C-C1C-NC	5.15	114.80	109.97
22	8	614	CLA	C2C-C1C-NC	5.15	114.80	109.97
22	7	610	CLA	C3B-C2B-C1B	-5.15	100.95	107.16
22	B	824	CLA	CHD-C1D-ND	-5.15	119.72	124.45
29	4	618	CHL	O2D-CGD-CBD	5.15	120.41	111.27
22	B	829	CLA	C2C-C1C-NC	5.15	114.79	109.97
22	3	617	CLA	C4A-NA-C1A	-5.14	104.39	106.71
29	4	618	CHL	C3B-C2B-C1B	-5.14	100.95	107.16
22	8	613	CLA	CHD-C1D-ND	-5.14	119.73	124.45
22	Z	604	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
22	B	834	CLA	C4A-NA-C1A	-5.14	104.39	106.71
22	A	833	CLA	C2C-C1C-NC	5.14	114.79	109.97
22	B	806	CLA	C2C-C1C-NC	5.14	114.79	109.97
22	B	838	CLA	C2C-C1C-NC	5.14	114.79	109.97
29	3	608	CHL	CHD-C1D-ND	-5.14	119.73	124.45
29	7	607	CHL	C3D-C2D-C1D	-5.14	98.82	105.83
22	6	610	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
22	A	830	CLA	C4A-NA-C1A	-5.13	104.40	106.71
22	6	613	CLA	C2C-C1C-NC	5.13	114.78	109.97
29	6	607	CHL	O2D-CGD-CBD	5.13	120.39	111.27
22	5	603	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	6	622	CLA	O2D-CGD-CBD	5.12	120.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	828	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
22	8	606	CLA	C4A-NA-C1A	-5.12	104.40	106.71
22	9	610	CLA	C3B-C2B-C1B	-5.12	100.98	107.16
22	A	813	CLA	C2C-C1C-NC	5.12	114.77	109.97
22	B	819	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
22	B	817	CLA	O2D-CGD-CBD	5.12	120.37	111.27
22	8	604	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
22	A	814	CLA	C2C-C1C-NC	5.11	114.76	109.97
22	3	614	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	A	825	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
22	5	603	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
22	A	836	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
22	5	602	CLA	C4A-NA-C1A	-5.11	104.41	106.71
22	2	609	CLA	CHD-C4C-C3C	-5.11	117.34	124.84
22	B	827	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
25	A	850	BCR	C16-C17-C18	-5.10	120.03	127.31
22	Z	612	CLA	O2D-CGD-CBD	5.10	120.33	111.27
22	B	823	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
29	Z	601	CHL	CHD-C4C-C3C	-5.10	117.35	124.84
22	6	601	CLA	C4A-NA-C1A	-5.10	104.41	106.71
22	B	830	CLA	C3B-C2B-C1B	-5.10	101.01	107.16
22	L	204	CLA	CHD-C4C-C3C	-5.10	117.35	124.84
22	5	617	CLA	C2C-C1C-NC	5.09	114.75	109.97
29	Z	607	CHL	CHD-C4C-C3C	-5.09	117.36	124.84
22	2	610	CLA	C2C-C1C-NC	5.09	114.74	109.97
22	6	614	CLA	C2C-C1C-NC	5.09	114.74	109.97
29	Z	607	CHL	C3D-C2D-C1D	-5.09	98.89	105.83
22	1	610	CLA	O2D-CGD-CBD	5.09	120.31	111.27
25	6	623	BCR	C7-C8-C9	-5.09	118.55	126.23
22	A	818	CLA	C2C-C1C-NC	5.09	114.74	109.97
22	2	603	CLA	O2D-CGD-CBD	5.08	120.30	111.27
22	B	830	CLA	C2C-C1C-NC	5.08	114.73	109.97
22	9	602	CLA	C3B-C2B-C1B	-5.08	101.03	107.16
22	9	603	CLA	O2D-CGD-CBD	5.08	120.30	111.27
22	8	603	CLA	O2D-CGD-CBD	5.08	120.30	111.27
22	9	610	CLA	C2C-C1C-NC	5.08	114.73	109.97
29	Z	601	CHL	C1C-C2C-C3C	-5.08	103.08	107.11
29	8	607	CHL	C3D-C2D-C1D	-5.07	98.91	105.83
29	4	618	CHL	CHD-C1D-ND	-5.07	119.79	124.45
22	3	606	CLA	C4A-NA-C1A	-5.07	104.42	106.71
22	3	602	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
22	3	612	CLA	O2D-CGD-CBD	5.07	120.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	854	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
22	6	610	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	2	607	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	8	608	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
22	B	833	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
22	A	833	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	5	604	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
22	A	833	CLA	C4A-NA-C1A	-5.07	104.43	106.71
22	A	829	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
22	1	612	CLA	C4A-NA-C1A	-5.06	104.43	106.71
22	B	819	CLA	C2C-C1C-NC	5.06	114.72	109.97
22	3	609	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
22	A	823	CLA	O2D-CGD-CBD	5.06	120.26	111.27
22	8	610	CLA	O2D-CGD-CBD	5.06	120.26	111.27
22	7	616	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
22	6	617	CLA	O2D-CGD-CBD	5.06	120.25	111.27
22	8	611	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
22	7	610	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	A	806	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
22	6	617	CLA	C3B-C2B-C1B	-5.05	101.06	107.16
29	5	607	CHL	C3B-C2B-C1B	-5.05	101.06	107.16
22	A	830	CLA	C2C-C1C-NC	5.05	114.70	109.97
22	A	832	CLA	C4A-NA-C1A	-5.05	104.44	106.71
22	A	841	CLA	C4A-NA-C1A	-5.05	104.44	106.71
22	B	823	CLA	C2C-C1C-NC	5.05	114.70	109.97
22	A	814	CLA	C3B-C2B-C1B	-5.05	101.07	107.16
25	4	621	BCR	C15-C14-C13	-5.04	120.11	127.31
22	1	611	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
22	A	843	CLA	CHD-C1D-ND	-5.04	119.82	124.45
22	6	609	CLA	C4A-NA-C1A	-5.04	104.44	106.71
29	6	606	CHL	C2C-C3C-C4C	-5.04	102.90	106.49
22	A	840	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
22	G	204	CLA	O2D-CGD-CBD	5.03	120.21	111.27
22	3	613	CLA	CMD-C2D-C1D	5.03	133.57	124.71
22	6	603	CLA	O2D-CGD-CBD	5.03	120.20	111.27
22	A	816	CLA	C2C-C1C-NC	5.02	114.68	109.97
22	B	805	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
22	F	303	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
29	9	607	CHL	CHD-C1D-ND	-5.02	119.84	124.45
22	A	819	CLA	O2D-CGD-CBD	5.01	120.17	111.27
22	B	805	CLA	C2C-C1C-NC	5.01	114.67	109.97
22	B	824	CLA	C2C-C1C-NC	5.00	114.66	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	812	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	3	606	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	B	816	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	B	823	CLA	C3B-C2B-C1B	-5.00	101.12	107.16
22	J	3002	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	1	614	CLA	C4A-NA-C1A	-5.00	104.46	106.71
22	6	614	CLA	C3B-C2B-C1B	-5.00	101.13	107.16
29	Z	601	CHL	C3B-C2B-C1B	-5.00	101.13	107.16
22	B	803	CLA	C3B-C2B-C1B	-5.00	101.13	107.16
22	B	823	CLA	C4A-NA-C1A	-5.00	104.46	106.71
22	1	603	CLA	C4A-NA-C1A	-5.00	104.46	106.71
22	4	611	CLA	CHD-C4C-C3C	-5.00	117.50	124.84
22	J	3002	CLA	C4A-NA-C1A	-5.00	104.46	106.71
22	B	814	CLA	C2C-C1C-NC	4.99	114.65	109.97
22	B	821	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	A	815	CLA	C2C-C1C-NC	4.99	114.64	109.97
22	B	825	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
22	Z	602	CLA	C4A-NA-C1A	-4.99	104.46	106.71
25	J	3003	BCR	C24-C23-C22	-4.99	118.70	126.23
22	F	304	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	5	610	CLA	O2D-CGD-CBD	4.98	120.11	111.27
29	5	618	CHL	C3B-C2B-C1B	-4.98	101.15	107.16
22	7	614	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
22	6	610	CLA	C2C-C1C-NC	4.97	114.63	109.97
29	6	618	CHL	C2C-C3C-C4C	-4.97	102.94	106.49
22	2	606	CLA	CAA-C2A-C3A	-4.97	104.50	116.10
29	5	618	CHL	CHD-C1D-ND	-4.97	119.89	124.45
22	G	204	CLA	C4A-NA-C1A	-4.97	104.47	106.71
22	B	803	CLA	CAC-C3C-C4C	4.97	131.26	124.81
22	A	845	CLA	O2D-CGD-CBD	4.97	120.10	111.27
22	1	604	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
22	1	610	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
22	8	610	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
22	Z	610	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
22	2	601	CLA	C3B-C2B-C1B	-4.97	101.17	107.16
22	Z	616	CLA	O2D-CGD-CBD	4.96	120.09	111.27
22	9	604	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
22	9	609	CLA	O2D-CGD-CBD	4.96	120.08	111.27
22	F	301	CLA	C2C-C1C-NC	4.96	114.62	109.97
22	L	203	CLA	O2D-CGD-CBD	4.96	120.08	111.27
22	2	613	CLA	C3B-C2B-C1B	-4.96	101.18	107.16
22	B	831	CLA	C3D-C2D-C1D	-4.96	99.07	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	802	CLA	CHD-C1D-ND	-4.96	119.90	124.45
22	A	835	CLA	C2C-C1C-NC	4.96	114.61	109.97
22	A	810	CLA	CHD-C1D-ND	-4.95	119.90	124.45
22	A	839	CLA	C4A-NA-C1A	-4.95	104.48	106.71
22	Z	614	CLA	C4A-NA-C1A	-4.95	104.48	106.71
29	6	618	CHL	O2D-CGD-CBD	4.95	120.07	111.27
22	5	616	CLA	C3B-C2B-C1B	-4.95	101.18	107.16
21	A	801	CL0	O2D-CGD-CBD	4.95	120.07	111.27
22	A	835	CLA	C3B-C2B-C1B	-4.95	101.18	107.16
22	5	609	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
22	B	807	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
29	5	607	CHL	CHD-C4C-C3C	-4.95	117.57	124.84
22	5	617	CLA	O2D-CGD-CBD	4.95	120.06	111.27
22	2	611	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
22	2	609	CLA	C3B-C2B-C1B	-4.94	101.19	107.16
22	Z	614	CLA	C3B-C2B-C1B	-4.94	101.19	107.16
25	A	852	BCR	C16-C17-C18	-4.94	120.26	127.31
25	B	801	BCR	C20-C21-C22	-4.94	120.26	127.31
22	B	833	CLA	C2C-C1C-NC	4.94	114.60	109.97
22	5	617	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
22	5	609	CLA	O2D-CGD-CBD	4.94	120.04	111.27
22	3	617	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
21	A	801	CL0	C4A-NA-C1A	-4.94	104.49	106.71
22	B	841	CLA	C2C-C1C-NC	4.93	114.59	109.97
25	B	848	BCR	C16-C17-C18	-4.93	120.27	127.31
22	B	839	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	3	602	CLA	C2C-C1C-NC	4.93	114.59	109.97
22	B	841	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
22	A	821	CLA	CHD-C1D-ND	-4.93	119.92	124.45
22	A	812	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
22	L	204	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
29	6	607	CHL	C3B-C2B-C1B	-4.93	101.21	107.16
22	A	806	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
22	A	802	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
22	B	802	CLA	C3C-C4C-NC	4.92	116.09	110.57
22	B	816	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
22	A	841	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
22	9	602	CLA	C4A-NA-C1A	-4.92	104.49	106.71
22	5	610	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
22	B	837	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
29	5	607	CHL	CHD-C1D-ND	-4.92	119.93	124.45
22	7	620	CLA	C3B-C2B-C1B	-4.92	101.22	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	845	BCR	C24-C23-C22	-4.92	118.81	126.23
22	7	620	CLA	O2D-CGD-CBD	4.92	120.00	111.27
22	9	609	CLA	C4A-NA-C1A	-4.91	104.50	106.71
22	B	815	CLA	C3B-C2B-C1B	-4.91	101.24	107.16
22	A	807	CLA	C4A-NA-C1A	-4.91	104.50	106.71
29	4	618	CHL	CHD-C4C-C3C	-4.91	117.63	124.84
22	6	609	CLA	C3B-C2B-C1B	-4.91	101.24	107.16
22	B	832	CLA	C4A-NA-C1A	-4.90	104.50	106.71
22	1	614	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
22	G	203	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
22	Z	611	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
29	6	618	CHL	C3B-C2B-C1B	-4.90	101.25	107.16
22	B	827	CLA	C2C-C1C-NC	4.90	114.56	109.97
22	K	4002	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	9	611	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	A	824	CLA	C4A-NA-C1A	-4.90	104.50	106.71
22	B	816	CLA	C4A-NA-C1A	-4.90	104.50	106.71
22	1	611	CLA	C4A-NA-C1A	-4.90	104.50	106.71
22	3	607	CLA	C4A-NA-C1A	-4.90	104.50	106.71
22	B	802	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	3	611	CLA	C3B-C2B-C1B	-4.89	101.25	107.16
22	B	828	CLA	CMD-C2D-C1D	4.89	133.34	124.71
22	3	607	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	9	607	CHL	C3B-C2B-C1B	-4.89	101.26	107.16
22	A	818	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
22	5	602	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
22	B	814	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	B	805	CLA	C3C-C4C-NC	4.89	116.05	110.57
22	8	608	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
22	7	609	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
22	9	614	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
29	9	607	CHL	C1C-C2C-C3C	-4.88	103.24	107.11
22	A	839	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
22	5	610	CLA	C4A-NA-C1A	-4.88	104.51	106.71
22	L	203	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
22	A	805	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
22	B	808	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
29	Z	601	CHL	O2D-CGD-CBD	4.87	119.93	111.27
22	1	604	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
22	Z	613	CLA	C2C-C1C-NC	4.87	114.54	109.97
22	4	614	CLA	C2C-C1C-NC	4.87	114.54	109.97
22	2	614	CLA	C3B-C2B-C1B	-4.87	101.28	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	602	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
22	B	820	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
29	5	608	CHL	C3B-C2B-C1B	-4.87	101.28	107.16
22	5	614	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
22	A	840	CLA	C4A-NA-C1A	-4.86	104.52	106.71
22	Z	612	CLA	C4A-NA-C1A	-4.86	104.52	106.71
22	6	603	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
22	A	806	CLA	C2C-C1C-NC	4.86	114.53	109.97
22	A	822	CLA	C2C-C1C-NC	4.86	114.53	109.97
22	9	602	CLA	C2C-C1C-NC	4.86	114.53	109.97
25	3	718	BCR	C16-C17-C18	-4.86	120.38	127.31
22	4	611	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
22	B	827	CLA	C4A-NA-C1A	-4.86	104.52	106.71
22	Z	609	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
22	B	810	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
22	4	614	CLA	C4A-NA-C1A	-4.86	104.52	106.71
22	L	204	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	A	832	CLA	CHD-C1D-ND	-4.85	119.99	124.45
22	2	610	CLA	C4A-NA-C1A	-4.85	104.53	106.71
22	B	804	CLA	C2C-C1C-NC	4.85	114.51	109.97
22	2	603	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
22	9	601	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
22	8	614	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
25	5	622	BCR	C15-C14-C13	-4.84	120.40	127.31
22	B	814	CLA	C4A-NA-C1A	-4.84	104.53	106.71
29	7	607	CHL	CHD-C4C-C3C	-4.84	117.72	124.84
22	5	621	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
22	8	602	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
22	6	601	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
22	B	841	CLA	C3D-C4D-ND	4.84	118.06	110.24
29	Z	601	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
22	B	806	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
21	A	801	CL0	CAA-C2A-C3A	-4.83	99.54	112.78
22	8	616	CLA	O2D-CGD-CBD	4.83	119.86	111.27
22	5	611	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
22	6	611	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
22	A	831	CLA	C4A-NA-C1A	-4.83	104.53	106.71
21	A	801	CL0	CHD-C1D-ND	-4.83	120.01	124.45
22	5	603	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
22	2	607	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
22	8	608	CLA	O2D-CGD-CBD	4.83	119.85	111.27
22	8	601	CLA	C3B-C2B-C1B	-4.83	101.33	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	815	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
29	7	607	CHL	C3B-C2B-C1B	-4.83	101.33	107.16
22	A	838	CLA	C3B-C2B-C1B	-4.83	101.34	107.16
22	5	601	CLA	C3B-C2B-C1B	-4.83	101.34	107.16
22	B	806	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
22	A	809	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
22	Z	604	CLA	O2D-CGD-CBD	4.82	119.83	111.27
22	B	808	CLA	CHD-C1D-ND	-4.82	120.03	124.45
22	4	603	CLA	O2D-CGD-CBD	4.81	119.82	111.27
22	A	802	CLA	C2C-C1C-NC	4.81	114.48	109.97
22	5	610	CLA	C2C-C1C-NC	4.81	114.48	109.97
22	A	809	CLA	C2C-C1C-NC	4.81	114.48	109.97
22	Z	609	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
29	4	618	CHL	C2C-C3C-C4C	-4.80	103.06	106.49
22	2	602	CLA	O2D-CGD-CBD	4.80	119.81	111.27
22	2	614	CLA	O2D-CGD-CBD	4.80	119.80	111.27
22	6	602	CLA	C2C-C1C-NC	4.80	114.47	109.97
22	A	854	CLA	CMD-C2D-C1D	4.80	133.16	124.71
22	B	804	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
22	9	612	CLA	C4A-NA-C1A	-4.79	104.55	106.71
22	4	610	CLA	C2C-C1C-NC	4.79	114.46	109.97
22	7	608	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
22	3	614	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
22	2	606	CLA	O2D-CGD-CBD	4.79	119.77	111.27
29	Z	607	CHL	O2D-CGD-CBD	4.78	119.77	111.27
22	G	203	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
22	4	602	CLA	C4A-NA-C1A	-4.78	104.56	106.71
22	F	301	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
29	4	607	CHL	CHD-C1D-ND	-4.78	120.06	124.45
22	A	830	CLA	CMD-C2D-C1D	4.78	133.13	124.71
22	A	803	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
22	8	608	CLA	C2C-C1C-NC	4.77	114.44	109.97
22	A	842	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	A	823	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
22	Z	613	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
22	A	805	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	7	604	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
22	9	610	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	B	803	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
22	A	819	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	B	838	CLA	O2D-CGD-CBD	4.76	119.73	111.27
22	Z	602	CLA	C2C-C1C-NC	4.76	114.43	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	606	CLA	O2D-CGD-CBD	4.76	119.73	111.27
22	A	802	CLA	C3D-C4D-ND	4.76	117.93	110.24
29	9	606	CHL	O2D-CGD-CBD	4.76	119.72	111.27
22	2	609	CLA	C4A-NA-C1A	-4.76	104.57	106.71
22	A	805	CLA	C2C-C1C-NC	4.75	114.43	109.97
22	B	813	CLA	C2C-C1C-NC	4.75	114.42	109.97
25	A	848	BCR	C16-C17-C18	-4.75	120.53	127.31
22	7	601	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
25	F	305	BCR	C11-C10-C9	-4.75	120.53	127.31
22	A	845	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
29	4	608	CHL	C3B-C2B-C1B	-4.75	101.43	107.16
22	A	814	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
22	2	613	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	A	811	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	B	807	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
22	A	815	CLA	C3D-C4D-ND	4.75	117.92	110.24
22	5	606	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
22	7	616	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
30	4	619	LUT	C35-C34-C33	-4.75	120.54	127.31
22	A	805	CLA	C3D-C4D-ND	4.75	117.92	110.24
29	1	601	CHL	C3B-C2B-C1B	-4.74	101.43	107.16
22	A	812	CLA	C4A-NA-C1A	-4.74	104.57	106.71
22	2	606	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
29	6	608	CHL	C3B-C2B-C1B	-4.74	101.44	107.16
22	B	831	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
22	4	604	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
22	9	601	CLA	O2D-CGD-CBD	4.74	119.69	111.27
22	6	602	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
29	4	606	CHL	C2C-C3C-C4C	-4.74	103.11	106.49
22	5	616	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
22	B	815	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
22	8	602	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
22	9	604	CLA	O2D-CGD-CBD	4.73	119.68	111.27
22	7	603	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
22	A	807	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
22	6	602	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
22	8	610	CLA	C2C-C1C-NC	4.73	114.40	109.97
22	B	852	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
22	A	809	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
22	B	837	CLA	C2C-C1C-NC	4.73	114.40	109.97
25	3	717	BCR	C11-C10-C9	-4.73	120.56	127.31
22	9	610	CLA	C4A-NA-C1A	-4.73	104.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	204	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
22	J	3002	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
22	Z	616	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
22	B	812	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
22	4	611	CLA	O2D-CGD-CBD	4.72	119.66	111.27
22	B	840	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
22	A	811	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
22	9	609	CLA	C1D-CHD-C4C	-4.72	115.87	126.06
22	6	622	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
22	4	601	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
22	6	622	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
22	4	601	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
22	1	608	CLA	C4A-NA-C1A	-4.72	104.58	106.71
22	1	614	CLA	O2D-CGD-CBD	4.72	119.65	111.27
29	4	606	CHL	O2D-CGD-CBD	4.72	119.65	111.27
22	7	608	CLA	C2C-C1C-NC	4.72	114.39	109.97
22	4	614	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
22	B	836	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
22	A	820	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
22	K	4003	CLA	O2D-CGD-CBD	4.71	119.65	111.27
22	1	609	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
22	1	608	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
29	Z	607	CHL	C3B-C2B-C1B	-4.71	101.47	107.16
30	2	616	LUT	C35-C34-C33	-4.71	120.58	127.31
22	Z	602	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
22	3	613	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	B	820	CLA	C3D-C4D-ND	4.71	117.86	110.24
22	6	611	CLA	O2D-CGD-CBD	4.71	119.63	111.27
22	8	603	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
29	9	606	CHL	CHD-C1D-ND	-4.71	120.13	124.45
29	1	607	CHL	C1C-C2C-C3C	-4.70	103.38	107.11
22	Z	608	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
22	8	611	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
22	B	821	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
30	6	621	LUT	C35-C34-C33	-4.70	120.60	127.31
22	6	612	CLA	O2D-CGD-CBD	4.70	119.62	111.27
29	5	618	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
22	2	606	CLA	C4A-NA-C1A	-4.70	104.59	106.71
22	A	834	CLA	C4A-NA-C1A	-4.70	104.59	106.71
22	A	812	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
30	Z	619	LUT	C31-C30-C29	-4.69	120.61	127.31
22	B	813	CLA	C3D-C2D-C1D	-4.69	99.43	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	602	CLA	O2D-CGD-CBD	4.69	119.61	111.27
22	9	613	CLA	O2D-CGD-CBD	4.69	119.60	111.27
22	1	602	CLA	C2C-C1C-NC	4.69	114.37	109.97
22	Z	609	CLA	C4A-NA-C1A	-4.69	104.60	106.71
29	1	607	CHL	C3B-C2B-C1B	-4.69	101.50	107.16
22	7	606	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
22	9	612	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
22	8	614	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	4	613	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
22	7	601	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
22	2	614	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
22	B	839	CLA	C3B-C2B-C1B	-4.68	101.52	107.16
22	A	842	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
22	Z	606	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
22	8	616	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
22	L	204	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
22	B	827	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
22	B	802	CLA	C2C-C1C-NC	4.67	114.35	109.97
22	9	611	CLA	O2D-CGD-CBD	4.67	119.56	111.27
22	K	4003	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
22	A	806	CLA	C4A-NA-C1A	-4.66	104.61	106.71
22	5	609	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	A	828	CLA	C3C-C4C-NC	4.66	115.80	110.57
22	4	602	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
22	2	610	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
29	4	607	CHL	C3B-C2B-C1B	-4.66	101.53	107.16
22	2	601	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
29	6	607	CHL	C1C-C2C-C3C	-4.66	103.42	107.11
22	7	611	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	1	603	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	9	610	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	B	826	CLA	C2C-C1C-NC	4.66	114.34	109.97
22	B	828	CLA	O2D-CGD-CBD	4.66	119.54	111.27
29	4	607	CHL	O2D-CGD-CBD	4.66	119.54	111.27
29	9	607	CHL	CHD-C4C-C3C	-4.66	118.00	124.84
22	9	609	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
22	2	602	CLA	C4A-NA-C1A	-4.65	104.61	106.71
22	A	804	CLA	C2C-C1C-NC	4.65	114.33	109.97
22	A	819	CLA	C2C-C1C-NC	4.65	114.33	109.97
22	5	612	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	9	613	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	7	614	CLA	C3D-C2D-C1D	-4.65	99.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	609	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
22	F	304	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	A	804	CLA	C3D-C4D-ND	4.65	117.75	110.24
29	4	608	CHL	CHD-C1D-ND	-4.64	120.19	124.45
22	A	824	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
22	A	828	CLA	C4A-NA-C1A	-4.64	104.62	106.71
22	1	602	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	1	612	CLA	O2D-CGD-CBD	4.64	119.51	111.27
22	Z	610	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	B	825	CLA	C4A-NA-C1A	-4.64	104.62	106.71
22	B	852	CLA	C4A-NA-C1A	-4.64	104.62	106.71
22	B	826	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	2	613	CLA	C4A-NA-C1A	-4.64	104.62	106.71
22	8	601	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	8	616	CLA	CHD-C1D-ND	-4.63	120.19	124.45
25	B	843	BCR	C15-C14-C13	-4.63	120.70	127.31
22	2	607	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	B	852	CLA	O2D-CGD-CBD	4.63	119.50	111.27
29	6	606	CHL	CHD-C1D-ND	-4.63	120.20	124.45
29	7	607	CHL	O2D-CGD-CBD	4.63	119.50	111.27
22	7	611	CLA	C4A-NA-C1A	-4.63	104.62	106.71
22	2	610	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
22	7	612	CLA	O2D-CGD-CBD	4.63	119.49	111.27
22	B	813	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
22	Z	614	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
22	A	845	CLA	C4A-NA-C1A	-4.62	104.63	106.71
22	A	854	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
22	2	612	CLA	O2D-CGD-CBD	4.62	119.48	111.27
22	B	832	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
22	A	811	CLA	C4A-NA-C1A	-4.62	104.63	106.71
22	3	620	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	A	822	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	Z	612	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
22	7	612	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	A	834	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	B	817	CLA	C4A-NA-C1A	-4.62	104.63	106.71
22	A	831	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	5	610	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
22	K	4003	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	Z	608	CLA	C4A-NA-C1A	-4.61	104.63	106.71
22	3	620	CLA	C4A-NA-C1A	-4.61	104.63	106.71
22	8	602	CLA	C2C-C1C-NC	4.61	114.29	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	301	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	A	816	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	8	611	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	2	613	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
29	Z	601	CHL	C3C-C4C-NC	4.61	115.74	110.57
25	6	623	BCR	C28-C27-C26	-4.60	105.86	114.08
22	6	604	CLA	C3B-C2B-C1B	-4.60	101.60	107.16
22	5	611	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
22	A	835	CLA	C3D-C4D-ND	4.60	117.69	110.24
22	1	606	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
22	9	602	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
22	3	603	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
22	4	603	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
22	1	616	CLA	O2D-CGD-CBD	4.60	119.43	111.27
22	8	606	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
22	B	829	CLA	CHB-C1B-NB	-4.59	119.39	124.26
22	7	602	CLA	C4A-NA-C1A	-4.59	104.64	106.71
22	A	841	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
22	8	610	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
22	5	601	CLA	C4A-NA-C1A	-4.59	104.64	106.71
22	3	610	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
22	B	810	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
22	7	620	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
22	4	612	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
22	B	818	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
22	Z	606	CLA	C4A-NA-C1A	-4.58	104.64	106.71
22	A	808	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	F	304	CLA	C4A-NA-C1A	-4.58	104.65	106.71
22	A	803	CLA	CAA-C2A-C3A	-4.58	100.23	112.78
22	A	813	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	A	818	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	A	826	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	B	837	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	7	603	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	A	832	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	7	602	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	A	823	CLA	C3B-C2B-C1B	-4.58	101.64	107.16
22	1	606	CLA	C2C-C1C-NC	4.58	114.26	109.97
22	5	612	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	1	609	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	B	834	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
22	A	807	CLA	C3D-C2D-C1D	-4.57	99.59	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	606	CLA	O2D-CGD-CBD	4.57	119.39	111.27
22	Z	611	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	5	604	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
22	3	604	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	2	612	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
22	Z	603	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
22	B	811	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
22	B	837	CLA	C4A-NA-C1A	-4.57	104.65	106.71
22	6	616	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
25	5	625	BCR	C16-C17-C18	-4.56	120.80	127.31
22	1	614	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
22	5	612	CLA	O2D-CGD-CBD	4.56	119.38	111.27
22	A	845	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	1	612	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	Z	604	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	A	808	CLA	C4A-NA-C1A	-4.56	104.66	106.71
22	9	614	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	A	816	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	1	608	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	A	825	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	4	616	CLA	O2D-CGD-CBD	4.56	119.36	111.27
22	4	614	CLA	O2D-CGD-CBD	4.56	119.36	111.27
25	K	4004	BCR	C16-C17-C18	-4.56	120.81	127.31
22	B	821	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
22	B	831	CLA	C4A-NA-C1A	-4.56	104.66	106.71
22	3	602	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	A	833	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	L	203	CLA	C3D-C4D-ND	4.55	117.60	110.24
22	Z	608	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
22	B	825	CLA	CAA-C2A-C3A	-4.55	100.31	112.78
22	3	613	CLA	C3C-C4C-NC	4.55	115.67	110.57
22	B	835	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	3	614	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	B	840	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	7	613	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	F	301	CLA	O2D-CGD-CBD	4.55	119.35	111.27
22	A	829	CLA	C3C-C4C-NC	4.55	115.67	110.57
22	Z	613	CLA	O2D-CGD-CBD	4.55	119.35	111.27
22	1	606	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
22	5	604	CLA	O2D-CGD-CBD	4.55	119.35	111.27
25	F	305	BCR	C15-C14-C13	-4.55	120.82	127.31
22	4	613	CLA	C3D-C2D-C1D	-4.55	99.63	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	822	CLA	C4A-NA-C1A	-4.54	104.66	106.71
22	6	601	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
30	1	619	LUT	C15-C14-C13	-4.54	120.83	127.31
22	9	604	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
22	B	802	CLA	C1D-CHD-C4C	-4.54	116.26	126.06
22	B	817	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
22	9	601	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
22	2	609	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
22	1	604	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	F	304	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
22	B	818	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
22	5	613	CLA	O2D-CGD-CBD	4.54	119.33	111.27
29	8	607	CHL	C3C-C4C-NC	4.54	115.66	110.57
22	A	830	CLA	CHD-C1D-ND	-4.53	120.29	124.45
22	6	602	CLA	O2D-CGD-CBD	4.53	119.32	111.27
22	8	604	CLA	O2D-CGD-CBD	4.53	119.32	111.27
29	4	607	CHL	C2C-C3C-C4C	-4.53	103.26	106.49
22	4	604	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	2	603	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	5	601	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	9	603	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	4	602	CLA	O2D-CGD-CBD	4.52	119.30	111.27
22	1	616	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
22	6	609	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	6	610	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
22	4	604	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
25	K	4001	BCR	C11-C10-C9	-4.52	120.86	127.31
22	1	614	CLA	C3D-C4D-ND	4.52	117.54	110.24
22	B	809	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
25	K	4001	BCR	C28-C27-C26	-4.51	106.02	114.08
24	4	622	LHG	O7-C7-C8	4.51	121.23	111.50
22	7	614	CLA	C4A-NA-C1A	-4.51	104.68	106.71
22	3	609	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
25	A	850	BCR	C3-C4-C5	-4.51	106.02	114.08
22	3	617	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
25	B	843	BCR	C16-C15-C14	-4.51	114.24	123.47
22	B	803	CLA	C2C-C1C-NC	4.51	114.20	109.97
22	8	603	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
22	9	612	CLA	O2D-CGD-CBD	4.51	119.28	111.27
25	B	844	BCR	C15-C14-C13	-4.50	120.88	127.31
22	Z	602	CLA	C3B-C2B-C1B	-4.50	101.72	107.16
22	A	830	CLA	C3B-C2B-C1B	-4.50	101.72	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	610	CLA	O2D-CGD-CBD	4.50	119.27	111.27
22	K	4002	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	3	612	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	4	602	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	B	838	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	A	811	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
29	5	608	CHL	CHD-C1D-ND	-4.50	120.32	124.45
22	6	609	CLA	O2D-CGD-CBD	4.50	119.26	111.27
22	A	827	CLA	C3D-C4D-ND	4.50	117.52	110.24
22	A	813	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	J	3002	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	B	812	CLA	O2D-CGD-CBD	4.50	119.26	111.27
22	2	611	CLA	O2D-CGD-CBD	4.50	119.26	111.27
22	B	838	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
22	5	606	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
22	A	811	CLA	O2D-CGD-CBD	4.50	119.26	111.27
22	B	818	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
25	4	621	BCR	C11-C10-C9	-4.49	120.90	127.31
22	A	829	CLA	C2C-C1C-NC	4.49	114.18	109.97
22	B	802	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
22	Z	616	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
22	6	604	CLA	C4A-NA-C1A	-4.49	104.69	106.71
22	5	602	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
22	5	602	CLA	C3D-C4D-ND	4.49	117.50	110.24
22	9	612	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
22	5	614	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
22	Z	602	CLA	O2D-CGD-CBD	4.49	119.24	111.27
22	4	616	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
22	5	604	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
22	4	609	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
22	3	607	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
25	I	172	BCR	C20-C21-C22	-4.49	120.91	127.31
22	B	829	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	B	809	CLA	C4A-NA-C1A	-4.48	104.69	106.71
22	3	612	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
22	6	602	CLA	C4A-NA-C1A	-4.48	104.69	106.71
22	Z	612	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	A	832	CLA	C3C-C4C-NC	4.48	115.60	110.57
22	7	608	CLA	O2D-CGD-CBD	4.48	119.23	111.27
22	Z	604	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
21	A	801	CL0	C3D-C2D-C1D	-4.48	99.72	105.83
22	B	838	CLA	C3D-C4D-ND	4.48	117.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	601	CLA	C4A-NA-C1A	-4.48	104.69	106.71
30	5	620	LUT	C35-C34-C33	-4.47	120.93	127.31
22	5	602	CLA	C2C-C1C-NC	4.47	114.16	109.97
22	G	204	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
22	B	829	CLA	C3C-C4C-NC	4.47	115.58	110.57
22	9	604	CLA	C3D-C4D-ND	4.47	117.47	110.24
22	Z	606	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
22	6	617	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
22	B	810	CLA	CAA-C2A-C3A	-4.47	100.54	112.78
22	2	602	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
22	B	835	CLA	C4A-NA-C1A	-4.47	104.70	106.71
22	9	604	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
22	4	610	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
22	2	606	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
29	1	601	CHL	C3C-C4C-NC	4.46	115.58	110.57
22	4	601	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	4	611	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	A	820	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
25	A	849	BCR	C16-C17-C18	-4.46	120.94	127.31
30	Z	619	LUT	C15-C14-C13	-4.46	120.94	127.31
22	Z	609	CLA	O2D-CGD-CBD	4.46	119.19	111.27
22	9	611	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
22	3	606	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
22	2	610	CLA	C3D-C4D-ND	4.46	117.45	110.24
22	6	604	CLA	O2D-CGD-CBD	4.46	119.19	111.27
29	5	608	CHL	O2D-CGD-CBD	4.46	119.19	111.27
22	B	839	CLA	C4A-NA-C1A	-4.46	104.70	106.71
22	6	611	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
22	7	613	CLA	O2D-CGD-CBD	4.45	119.18	111.27
22	6	614	CLA	O2D-CGD-CBD	4.45	119.18	111.27
22	Z	609	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
22	B	833	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
22	1	613	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
27	B	850	DGD	O2G-C1B-C2B	4.45	121.09	111.50
29	9	606	CHL	C2C-C3C-C4C	-4.45	103.32	106.49
22	5	609	CLA	C4A-NA-C1A	-4.44	104.71	106.71
22	A	841	CLA	C3C-C4C-NC	4.44	115.56	110.57
22	1	610	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	A	837	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
29	6	607	CHL	C3C-C4C-NC	4.44	115.55	110.57
22	1	613	CLA	O2D-CGD-CBD	4.44	119.16	111.27
29	8	607	CHL	O2D-CGD-CBD	4.44	119.16	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	826	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
22	5	614	CLA	C3D-C4D-ND	4.44	117.42	110.24
22	B	834	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	A	810	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
22	7	610	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	B	803	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
22	Z	610	CLA	CMC-C2C-C1C	4.44	131.80	125.04
22	A	828	CLA	C1D-CHD-C4C	-4.44	116.49	126.06
22	2	611	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
22	7	616	CLA	O2D-CGD-CBD	4.44	119.15	111.27
22	A	836	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
22	A	843	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
22	1	611	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
22	B	816	CLA	C3C-C4C-NC	4.43	115.54	110.57
22	2	614	CLA	C3D-C4D-ND	4.43	117.41	110.24
22	3	611	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
22	A	802	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
22	5	621	CLA	C4A-NA-C1A	-4.43	104.72	106.71
22	6	604	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
22	1	602	CLA	C3B-C2B-C1B	-4.43	101.82	107.16
22	1	613	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
22	4	616	CLA	C3B-C2B-C1B	-4.43	101.82	107.16
22	B	819	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
22	A	810	CLA	C4A-NA-C1A	-4.42	104.72	106.71
22	7	608	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
22	B	822	CLA	C3D-C4D-ND	4.42	117.39	110.24
25	7	623	BCR	C16-C17-C18	-4.42	121.00	127.31
22	A	839	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
29	9	606	CHL	C3B-C2B-C1B	-4.42	101.83	107.16
22	A	854	CLA	C3C-C4C-NC	4.42	115.53	110.57
22	A	840	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
22	Z	603	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
22	B	833	CLA	C4A-NA-C1A	-4.42	104.72	106.71
22	A	836	CLA	O2D-CGD-CBD	4.42	119.11	111.27
22	B	829	CLA	C3D-C4D-ND	4.42	117.38	110.24
22	A	812	CLA	C3C-C4C-NC	4.42	115.52	110.57
22	A	823	CLA	C3D-C4D-ND	4.41	117.38	110.24
22	8	613	CLA	C3C-C4C-NC	4.41	115.52	110.57
22	A	811	CLA	C1D-CHD-C4C	-4.41	116.54	126.06
22	1	603	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
22	B	816	CLA	C1D-CHD-C4C	-4.41	116.55	126.06
29	6	608	CHL	O2D-CGD-CBD	4.41	119.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	611	CLA	C4A-NA-C1A	-4.41	104.72	106.71
22	A	825	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
22	A	806	CLA	CAC-C3C-C4C	4.41	130.53	124.81
22	8	613	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
25	G	205	BCR	C16-C17-C18	-4.41	121.02	127.31
22	5	613	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
22	6	614	CLA	C3D-C4D-ND	4.40	117.36	110.24
22	B	809	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
22	6	613	CLA	C3D-C4D-ND	4.40	117.36	110.24
22	B	822	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
22	7	602	CLA	C3D-C4D-ND	4.40	117.36	110.24
22	A	824	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	3	606	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
22	L	204	CLA	C3D-C4D-ND	4.40	117.35	110.24
22	2	612	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	4	601	CLA	C4A-NA-C1A	-4.40	104.73	106.71
29	7	607	CHL	CHD-C1D-ND	-4.40	120.42	124.45
25	B	844	BCR	C7-C8-C9	-4.39	119.59	126.23
22	A	803	CLA	C3D-C4D-ND	4.39	117.34	110.24
22	A	843	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
22	B	809	CLA	O2D-CGD-CBD	4.39	119.07	111.27
25	6	623	BCR	C15-C14-C13	-4.39	121.05	127.31
22	B	802	CLA	O2D-CGD-CBD	4.39	119.07	111.27
22	9	603	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
22	A	804	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
22	A	812	CLA	C3D-C4D-ND	4.38	117.33	110.24
22	4	603	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	4	614	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	B	852	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	A	835	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	A	854	CLA	CAA-C2A-C3A	-4.38	100.78	112.78
22	A	854	CLA	C3D-C4D-ND	4.38	117.32	110.24
22	B	821	CLA	C3D-C4D-ND	4.38	117.32	110.24
29	4	606	CHL	CHD-C1D-ND	-4.38	120.43	124.45
22	8	610	CLA	C1D-CHD-C4C	-4.38	116.61	126.06
22	6	603	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
22	B	841	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
22	Z	611	CLA	O2D-CGD-CBD	4.38	119.05	111.27
22	A	805	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
29	6	606	CHL	C3B-C2B-C1B	-4.37	101.88	107.16
22	2	609	CLA	O2D-CGD-CBD	4.37	119.04	111.27
22	B	825	CLA	C3D-C4D-ND	4.37	117.31	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	827	CLA	C2C-C1C-NC	4.37	114.07	109.97
22	2	607	CLA	C3D-C4D-ND	4.37	117.31	110.24
22	7	616	CLA	C4A-NA-C1A	-4.37	104.74	106.71
22	4	616	CLA	C3D-C4D-ND	4.37	117.30	110.24
22	6	602	CLA	C3D-C4D-ND	4.37	117.30	110.24
22	B	830	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
22	6	614	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	A	815	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	B	812	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
22	B	833	CLA	C3D-C4D-ND	4.36	117.29	110.24
22	8	602	CLA	C3D-C4D-ND	4.36	117.29	110.24
22	Z	613	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	3	612	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
22	A	817	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
22	A	830	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
22	B	839	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
22	B	840	CLA	O2D-CGD-CBD	4.35	119.00	111.27
22	5	612	CLA	C1D-CHD-C4C	-4.35	116.67	126.06
22	B	828	CLA	CHD-C1D-ND	-4.35	120.45	124.45
22	K	4002	CLA	C4A-NA-C1A	-4.35	104.75	106.71
22	A	821	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
22	1	610	CLA	C1D-CHD-C4C	-4.35	116.67	126.06
22	A	838	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
22	3	602	CLA	C3D-C4D-ND	4.35	117.27	110.24
22	7	608	CLA	C3D-C4D-ND	4.35	117.27	110.24
22	A	810	CLA	O2D-CGD-CBD	4.35	118.99	111.27
22	B	837	CLA	C3D-C4D-ND	4.35	117.27	110.24
22	A	830	CLA	C3C-C4C-NC	4.35	115.44	110.57
22	3	620	CLA	O2D-CGD-CBD	4.34	118.99	111.27
21	A	801	CL0	C3C-C4C-NC	4.34	115.44	110.57
22	B	823	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
22	3	613	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	6	612	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	5	609	CLA	C1D-CHD-C4C	-4.34	116.69	126.06
22	B	827	CLA	C3C-C4C-NC	4.34	115.44	110.57
22	A	843	CLA	O2D-CGD-CBD	4.34	118.98	111.27
22	B	819	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
22	7	604	CLA	C3D-C4D-ND	4.34	117.26	110.24
22	B	805	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
29	5	607	CHL	O2D-CGD-CBD	4.34	118.98	111.27
22	9	613	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
22	8	614	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	5	616	CLA	C4A-NA-C1A	-4.34	104.76	106.71
22	4	604	CLA	C3D-C4D-ND	4.34	117.25	110.24
22	5	621	CLA	C3C-C4C-NC	4.34	115.43	110.57
22	B	822	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
22	7	602	CLA	C2C-C1C-NC	4.33	114.03	109.97
25	A	856	BCR	C20-C21-C22	-4.33	121.13	127.31
30	2	617	LUT	C35-C15-C14	-4.33	114.60	123.47
22	6	612	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
22	2	602	CLA	C3D-C4D-ND	4.33	117.24	110.24
22	5	621	CLA	CHD-C1D-ND	-4.33	120.48	124.45
22	A	808	CLA	C3D-C4D-ND	4.33	117.24	110.24
22	B	820	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
22	A	822	CLA	C4A-NA-C1A	-4.32	104.76	106.71
22	1	612	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
22	7	612	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
22	A	809	CLA	C4A-NA-C1A	-4.32	104.76	106.71
22	8	612	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
25	A	851	BCR	C16-C17-C18	-4.32	121.15	127.31
22	A	817	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
22	A	818	CLA	C3D-C4D-ND	4.32	117.22	110.24
22	8	604	CLA	C3D-C4D-ND	4.32	117.22	110.24
22	3	612	CLA	C3D-C4D-ND	4.32	117.22	110.24
22	7	613	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
22	2	611	CLA	C3D-C4D-ND	4.32	117.22	110.24
22	B	840	CLA	C3C-C4C-NC	4.32	115.41	110.57
22	7	604	CLA	C3C-C4C-NC	4.32	115.41	110.57
22	4	609	CLA	C1D-CHD-C4C	-4.31	116.75	126.06
22	4	613	CLA	O2D-CGD-CBD	4.31	118.94	111.27
29	5	607	CHL	C1D-CHD-C4C	-4.31	116.75	126.06
22	A	806	CLA	C3D-C4D-ND	4.31	117.22	110.24
24	A	847	LHG	O7-C7-C8	4.31	120.80	111.50
29	8	607	CHL	C1C-C2C-C3C	-4.31	103.69	107.11
25	6	625	BCR	C3-C4-C5	-4.31	106.38	114.08
25	K	4001	BCR	C15-C16-C17	-4.31	114.65	123.47
22	6	613	CLA	O2D-CGD-CBD	4.31	118.92	111.27
22	8	613	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
22	8	606	CLA	CAA-C2A-C3A	-4.31	103.50	114.26
30	2	616	LUT	C7-C8-C9	-4.30	119.73	126.23
22	A	843	CLA	C4A-NA-C1A	-4.30	104.77	106.71
22	A	816	CLA	C3D-C4D-ND	4.30	117.19	110.24
22	B	829	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	3	614	CLA	C3D-C4D-ND	4.30	117.19	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	606	CLA	C3B-C2B-C1B	-4.30	101.98	107.16
22	8	604	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
22	6	613	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
22	B	832	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
22	B	835	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
29	4	608	CHL	O2D-CGD-CBD	4.29	118.89	111.27
22	A	828	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
25	A	850	BCR	C15-C14-C13	-4.29	121.19	127.31
22	1	602	CLA	O2D-CGD-CBD	4.28	118.88	111.27
22	6	601	CLA	C3D-C4D-ND	4.28	117.17	110.24
22	A	830	CLA	O2D-CGD-CBD	4.28	118.87	111.27
22	A	827	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
22	A	836	CLA	C3D-C4D-ND	4.28	117.16	110.24
22	3	607	CLA	C3D-C4D-ND	4.28	117.16	110.24
22	9	603	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
22	9	614	CLA	C3D-C4D-ND	4.28	117.16	110.24
22	4	610	CLA	C3B-C2B-C1B	-4.27	102.00	107.16
29	8	607	CHL	C3B-C2B-C1B	-4.27	102.00	107.16
22	A	806	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
25	I	172	BCR	C3-C4-C5	-4.27	106.45	114.08
29	1	607	CHL	CHD-C1D-ND	-4.27	120.53	124.45
22	B	816	CLA	C2C-C1C-NC	4.27	113.97	109.97
22	4	602	CLA	C3D-C4D-ND	4.27	117.14	110.24
22	7	604	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
22	A	817	CLA	C3D-C4D-ND	4.27	117.14	110.24
22	F	303	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
22	7	608	CLA	C4A-NA-C1A	-4.27	104.79	106.71
25	K	4001	BCR	C16-C17-C18	-4.27	121.22	127.31
22	8	612	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
22	B	829	CLA	C1D-CHD-C4C	-4.26	116.86	126.06
22	8	613	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	B	840	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
22	8	604	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
22	8	616	CLA	C3C-C4C-NC	4.26	115.35	110.57
22	4	604	CLA	C4A-NA-C1A	-4.26	104.79	106.71
22	2	614	CLA	C4A-NA-C1A	-4.26	104.79	106.71
22	6	613	CLA	C3B-C2B-C1B	-4.26	102.03	107.16
22	A	808	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
29	5	607	CHL	C1C-C2C-C3C	-4.25	103.74	107.11
25	6	625	BCR	C11-C10-C9	-4.25	121.24	127.31
22	B	825	CLA	C2C-C1C-NC	4.25	113.95	109.97
22	4	614	CLA	C3D-C4D-ND	4.25	117.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	604	CLA	C3D-C4D-ND	4.25	117.11	110.24
22	4	612	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
21	A	801	CL0	C1D-CHD-C4C	-4.24	116.90	126.06
22	B	835	CLA	O2D-CGD-CBD	4.24	118.81	111.27
22	B	814	CLA	C3D-C4D-ND	4.24	117.10	110.24
22	B	819	CLA	C4A-NA-C1A	-4.24	104.80	106.71
22	3	610	CLA	CMC-C2C-C1C	4.24	131.50	125.04
22	B	810	CLA	O2D-CGD-CBD	4.24	118.80	111.27
22	A	825	CLA	C3B-C4B-NB	4.24	114.45	110.52
22	1	616	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
22	Z	614	CLA	C3D-C4D-ND	4.24	117.09	110.24
22	A	822	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
22	9	610	CLA	C3D-C4D-ND	4.24	117.09	110.24
21	A	801	CL0	CMB-C2B-C1B	4.24	131.82	125.37
22	3	613	CLA	CHD-C1D-ND	-4.24	120.56	124.45
22	Z	611	CLA	C3D-C4D-ND	4.24	117.09	110.24
22	2	613	CLA	C3D-C4D-ND	4.23	117.09	110.24
22	1	610	CLA	CMC-C2C-C1C	4.23	131.49	125.04
22	B	812	CLA	C3D-C4D-ND	4.23	117.08	110.24
22	B	809	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
22	9	603	CLA	C3D-C4D-ND	4.23	117.08	110.24
22	A	814	CLA	C3C-C4C-NC	4.23	115.31	110.57
22	8	614	CLA	C3D-C4D-ND	4.23	117.08	110.24
22	Z	602	CLA	C3D-C4D-ND	4.23	117.08	110.24
22	L	203	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
22	3	610	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
22	B	826	CLA	C3C-C4C-NC	4.23	115.31	110.57
22	K	4003	CLA	C4A-NA-C1A	-4.23	104.81	106.71
29	8	607	CHL	C1D-CHD-C4C	-4.22	116.94	126.06
22	A	825	CLA	C3D-C4D-ND	4.22	117.07	110.24
22	2	603	CLA	C3D-C4D-ND	4.22	117.07	110.24
22	A	841	CLA	O2D-CGD-CBD	4.22	118.77	111.27
22	B	840	CLA	C3B-C4B-NB	4.22	114.43	110.52
22	A	821	CLA	C4A-NA-C1A	-4.22	104.81	106.71
22	3	611	CLA	C4A-NA-C1A	-4.22	104.81	106.71
22	A	836	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
22	6	612	CLA	C3D-C4D-ND	4.22	117.07	110.24
22	4	616	CLA	C4A-NA-C1A	-4.22	104.81	106.71
22	3	604	CLA	O2D-CGD-CBD	4.22	118.76	111.27
22	F	303	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
22	7	606	CLA	C3D-C4D-ND	4.22	117.06	110.24
22	7	612	CLA	C3D-C4D-ND	4.22	117.06	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	612	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
22	4	612	CLA	C3D-C4D-ND	4.22	117.06	110.24
22	B	815	CLA	C4A-NA-C1A	-4.21	104.81	106.71
22	9	613	CLA	C3D-C4D-ND	4.21	117.05	110.24
22	8	606	CLA	C3D-C4D-ND	4.21	117.05	110.24
22	7	612	CLA	C1D-CHD-C4C	-4.21	116.97	126.06
25	6	623	BCR	C11-C10-C9	-4.21	121.30	127.31
25	5	625	BCR	C11-C12-C13	-4.21	114.59	126.42
22	1	604	CLA	C4A-NA-C1A	-4.21	104.81	106.71
22	4	601	CLA	C3D-C4D-ND	4.21	117.04	110.24
22	Z	610	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
22	A	802	CLA	O2D-CGD-CBD	4.21	118.74	111.27
22	Z	612	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
22	A	833	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
22	A	842	CLA	O2A-C1-C2	4.21	119.69	108.64
24	1	620	LHG	O7-C7-C8	4.20	120.56	111.50
22	8	612	CLA	C3D-C4D-ND	4.20	117.04	110.24
22	A	810	CLA	C3D-C2D-C1D	-4.20	100.09	105.83
22	2	606	CLA	C3D-C4D-ND	4.20	117.04	110.24
22	A	829	CLA	C1D-CHD-C4C	-4.20	116.99	126.06
22	1	603	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
29	6	618	CHL	C3C-C4C-NC	4.20	115.28	110.57
22	5	613	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	A	842	CLA	C1-C2-C3	-4.20	118.79	126.04
25	7	623	BCR	C21-C20-C19	-4.20	110.12	123.22
22	G	204	CLA	C3D-C4D-ND	4.20	117.03	110.24
22	A	845	CLA	C3C-C4C-NC	4.20	115.28	110.57
22	1	612	CLA	C3D-C4D-ND	4.19	117.02	110.24
22	B	813	CLA	C3C-C4C-NC	4.19	115.27	110.57
22	B	809	CLA	C3B-C4B-NB	4.19	114.40	110.52
22	6	609	CLA	C1D-CHD-C4C	-4.19	117.02	126.06
25	A	849	BCR	C11-C10-C9	-4.19	121.33	127.31
25	4	621	BCR	C33-C5-C6	-4.19	119.82	124.53
22	B	840	CLA	CAC-C3C-C2C	4.19	134.70	127.53
22	A	842	CLA	C3D-C4D-ND	4.19	117.02	110.24
22	3	604	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
25	3	718	BCR	C15-C14-C13	-4.19	121.33	127.31
22	8	602	CLA	C3C-C4C-NC	4.19	115.27	110.57
22	2	612	CLA	C3D-C4D-ND	4.19	117.01	110.24
22	A	812	CLA	C1D-CHD-C4C	-4.19	117.03	126.06
22	B	830	CLA	C3D-C4D-ND	4.19	117.01	110.24
22	A	821	CLA	C3D-C2D-C1D	-4.18	100.12	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	842	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
22	B	808	CLA	C3C-C4C-NC	4.18	115.26	110.57
22	K	4002	CLA	C3D-C4D-ND	4.18	117.00	110.24
22	Z	612	CLA	C3D-C4D-ND	4.18	117.00	110.24
22	Z	610	CLA	C3D-C4D-ND	4.18	117.00	110.24
22	A	818	CLA	C1D-CHD-C4C	-4.18	117.04	126.06
22	5	616	CLA	C1D-CHD-C4C	-4.18	117.04	126.06
29	4	606	CHL	C3C-C4C-NC	4.18	115.26	110.57
22	B	828	CLA	C3D-C4D-ND	4.18	117.00	110.24
25	A	856	BCR	C16-C17-C18	-4.18	121.35	127.31
22	A	831	CLA	C3B-C4B-NB	4.18	114.39	110.52
22	6	616	CLA	O2D-CGD-CBD	4.18	118.69	111.27
22	6	613	CLA	C4A-NA-C1A	-4.18	104.83	106.71
22	B	812	CLA	C4A-NA-C1A	-4.17	104.83	106.71
22	A	813	CLA	C3D-C4D-ND	4.17	116.99	110.24
22	Z	608	CLA	O2D-CGD-CBD	4.17	118.68	111.27
29	1	607	CHL	C1D-CHD-C4C	-4.17	117.06	126.06
22	2	601	CLA	C4A-NA-C1A	-4.17	104.83	106.71
22	1	611	CLA	C3D-C4D-ND	4.17	116.98	110.24
22	B	824	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
22	B	802	CLA	C4A-NA-C1A	-4.17	104.83	106.71
22	B	810	CLA	C3D-C4D-ND	4.17	116.98	110.24
22	7	601	CLA	C3D-C4D-ND	4.17	116.98	110.24
22	Z	609	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
22	8	616	CLA	C4A-NA-C1A	-4.16	104.83	106.71
22	Z	614	CLA	O2D-CGD-CBD	4.16	118.67	111.27
22	A	811	CLA	C3D-C4D-ND	4.16	116.97	110.24
22	B	804	CLA	C3C-C4C-NC	4.16	115.24	110.57
22	4	603	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
29	Z	607	CHL	C1D-CHD-C4C	-4.16	117.08	126.06
22	A	810	CLA	C3D-C4D-ND	4.16	116.97	110.24
22	B	834	CLA	C3D-C4D-ND	4.16	116.97	110.24
22	7	611	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
22	B	832	CLA	C3D-C4D-ND	4.16	116.97	110.24
25	A	856	BCR	C15-C16-C17	-4.16	114.95	123.47
22	7	620	CLA	C3D-C4D-ND	4.16	116.96	110.24
30	8	617	LUT	C35-C34-C33	-4.16	121.38	127.31
22	B	806	CLA	C3C-C4C-NC	4.16	115.23	110.57
22	1	602	CLA	C3D-C4D-ND	4.16	116.96	110.24
22	B	815	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
22	A	811	CLA	C3C-C4C-NC	4.16	115.23	110.57
25	3	719	BCR	C16-C17-C18	-4.16	121.38	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	608	CLA	O2D-CGD-CBD	4.16	118.65	111.27
22	A	810	CLA	C3C-C4C-NC	4.15	115.23	110.57
22	A	809	CLA	C3D-C4D-ND	4.15	116.96	110.24
29	6	607	CHL	CHD-C1D-ND	-4.15	120.64	124.45
22	1	604	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
22	9	602	CLA	C3D-C4D-ND	4.15	116.95	110.24
25	K	4004	BCR	C15-C14-C13	-4.15	121.39	127.31
22	B	808	CLA	C3D-C4D-ND	4.15	116.95	110.24
22	9	612	CLA	C3D-C4D-ND	4.15	116.95	110.24
25	B	846	BCR	C40-C30-C25	4.15	117.03	110.30
22	A	838	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
22	A	834	CLA	C3D-C4D-ND	4.15	116.95	110.24
22	A	840	CLA	C3C-C4C-NC	4.15	115.22	110.57
22	B	852	CLA	C3D-C4D-ND	4.15	116.94	110.24
22	A	814	CLA	C3D-C4D-ND	4.14	116.94	110.24
22	F	301	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
22	7	610	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
29	Z	607	CHL	C3C-C4C-NC	4.14	115.22	110.57
22	2	607	CLA	C4A-NA-C1A	-4.14	104.84	106.71
22	B	834	CLA	O2D-CGD-CBD	4.14	118.63	111.27
22	Z	610	CLA	C3C-C4C-NC	4.14	115.22	110.57
29	1	607	CHL	C3C-C4C-NC	4.14	115.22	110.57
29	3	608	CHL	C1D-CHD-C4C	-4.14	117.13	126.06
22	J	3002	CLA	CAA-C2A-C3A	-4.14	103.92	114.26
22	7	616	CLA	C3D-C4D-ND	4.14	116.93	110.24
22	B	826	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
22	A	826	CLA	CMB-C2B-C1B	4.14	131.67	125.37
22	A	837	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
22	A	810	CLA	O2A-CGA-CBA	4.14	124.89	111.91
22	A	821	CLA	C1D-CHD-C4C	-4.14	117.14	126.06
22	B	811	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	4	613	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	A	845	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	B	840	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	2	601	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	6	616	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	B	832	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
22	9	609	CLA	C3C-C4C-NC	4.13	115.20	110.57
22	B	839	CLA	C3D-C4D-ND	4.13	116.91	110.24
22	8	612	CLA	C3C-C4C-NC	4.13	115.20	110.57
22	B	838	CLA	C3C-C4C-NC	4.13	115.20	110.57
22	7	613	CLA	C3D-C4D-ND	4.13	116.91	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	612	CLA	C1D-CHD-C4C	-4.13	117.16	126.06
22	3	604	CLA	C3D-C4D-ND	4.12	116.91	110.24
25	L	205	BCR	C24-C23-C22	4.12	132.47	126.23
22	1	610	CLA	C3D-C4D-ND	4.12	116.91	110.24
22	2	611	CLA	C4A-NA-C1A	-4.12	104.85	106.71
22	Z	603	CLA	C3D-C4D-ND	4.12	116.91	110.24
25	L	201	BCR	C15-C14-C13	-4.12	121.43	127.31
22	8	616	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
22	Z	603	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
22	7	610	CLA	C3D-C4D-ND	4.12	116.91	110.24
22	A	824	CLA	C3D-C4D-ND	4.12	116.91	110.24
22	7	609	CLA	CMA-C3A-C4A	-4.12	100.70	111.77
22	7	609	CLA	C3D-C4D-ND	4.12	116.90	110.24
29	7	607	CHL	C1D-CHD-C4C	-4.12	117.17	126.06
22	B	830	CLA	C3C-C4C-NC	4.12	115.19	110.57
22	8	612	CLA	C1D-CHD-C4C	-4.11	117.18	126.06
22	B	813	CLA	CAC-C3C-C4C	4.11	130.15	124.81
25	A	851	BCR	C15-C14-C13	-4.11	121.44	127.31
22	3	620	CLA	C3D-C4D-ND	4.11	116.89	110.24
25	B	844	BCR	C16-C17-C18	-4.11	121.44	127.31
22	A	836	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
22	A	831	CLA	C3C-C4C-NC	4.11	115.18	110.57
22	3	610	CLA	C3D-C4D-ND	4.11	116.88	110.24
22	Z	602	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
22	3	617	CLA	C3D-C4D-ND	4.11	116.88	110.24
22	2	603	CLA	C3B-C4B-NB	4.10	114.32	110.52
22	1	612	CLA	C1D-CHD-C4C	-4.10	117.20	126.06
22	1	611	CLA	O2D-CGD-CBD	4.10	118.56	111.27
22	7	603	CLA	C3D-C4D-ND	4.10	116.88	110.24
22	A	842	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
22	B	808	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
22	3	606	CLA	C3D-C4D-ND	4.10	116.87	110.24
22	B	840	CLA	C4A-NA-C1A	-4.10	104.86	106.71
22	3	620	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
22	Z	609	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
29	5	608	CHL	C2C-C3C-C4C	-4.10	103.57	106.49
22	8	603	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
29	6	606	CHL	C3C-C4C-NC	4.10	115.17	110.57
22	2	609	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
22	J	3002	CLA	C3D-C4D-ND	4.10	116.86	110.24
22	A	821	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
22	B	802	CLA	C3D-C4D-ND	4.09	116.86	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	4003	CLA	C3D-C4D-ND	4.09	116.86	110.24
22	B	825	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
22	3	613	CLA	C3D-C4D-ND	4.09	116.86	110.24
22	B	807	CLA	C3C-C4C-NC	4.09	115.16	110.57
22	6	609	CLA	C3C-C4C-NC	4.09	115.16	110.57
22	Z	606	CLA	C3D-C4D-ND	4.09	116.86	110.24
25	5	622	BCR	C3-C4-C5	-4.09	106.77	114.08
22	1	613	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
22	5	601	CLA	C3D-C4D-ND	4.09	116.86	110.24
22	6	604	CLA	C3D-C4D-ND	4.09	116.86	110.24
22	A	826	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
22	A	829	CLA	O2D-CGD-CBD	4.09	118.53	111.27
22	3	612	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
22	B	804	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
22	F	304	CLA	C3D-C4D-ND	4.09	116.85	110.24
22	A	832	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
22	A	803	CLA	C4A-NA-C1A	-4.09	104.87	106.71
22	B	831	CLA	C3C-C4C-NC	4.09	115.16	110.57
22	8	614	CLA	C3C-C4C-NC	4.09	115.16	110.57
22	A	837	CLA	C4A-NA-C1A	-4.09	104.87	106.71
22	A	838	CLA	C3D-C4D-ND	4.09	116.85	110.24
22	A	841	CLA	C3D-C4D-ND	4.09	116.85	110.24
25	3	718	BCR	C3-C4-C5	-4.09	106.78	114.08
29	4	608	CHL	C2C-C3C-C4C	-4.09	103.58	106.49
22	B	811	CLA	C3C-C4C-NC	4.08	115.15	110.57
22	Z	612	CLA	C3C-C4C-NC	4.08	115.15	110.57
22	5	617	CLA	C3C-C4C-NC	4.08	115.15	110.57
22	A	818	CLA	C3C-C4C-NC	4.08	115.15	110.57
25	7	624	BCR	C3-C4-C5	-4.08	106.79	114.08
22	3	610	CLA	O2A-CGA-CBA	4.08	124.71	111.91
22	8	614	CLA	C4A-NA-C1A	-4.08	104.87	106.71
22	4	609	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
22	A	839	CLA	C3D-C4D-ND	4.08	116.83	110.24
22	B	819	CLA	C3D-C4D-ND	4.08	116.83	110.24
22	5	610	CLA	C3D-C4D-ND	4.08	116.83	110.24
22	1	610	CLA	O2A-CGA-CBA	4.07	124.69	111.91
22	A	843	CLA	C3C-C4C-NC	4.07	115.14	110.57
22	8	608	CLA	C4A-NA-C1A	-4.07	104.88	106.71
22	1	602	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
25	6	623	BCR	C3-C4-C5	-4.07	106.81	114.08
22	6	610	CLA	C3D-C4D-ND	4.07	116.82	110.24
22	7	606	CLA	C1D-CHD-C4C	-4.07	117.28	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	817	CLA	C4A-NA-C1A	-4.07	104.88	106.71
25	8	619	BCR	C15-C14-C13	-4.07	121.50	127.31
22	B	802	CLA	CAA-C2A-C3A	-4.07	101.64	112.78
22	A	807	CLA	C3D-C4D-ND	4.07	116.81	110.24
22	7	608	CLA	C3C-C4C-NC	4.06	115.13	110.57
22	A	845	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
22	8	613	CLA	C3D-C4D-ND	4.06	116.81	110.24
22	5	612	CLA	C3D-C4D-ND	4.06	116.81	110.24
22	A	825	CLA	O2D-CGD-CBD	4.06	118.48	111.27
22	7	613	CLA	C3C-C4C-NC	4.06	115.12	110.57
22	B	831	CLA	C3D-C4D-ND	4.06	116.80	110.24
22	6	616	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
22	8	616	CLA	C3D-C4D-ND	4.06	116.80	110.24
22	9	601	CLA	C3D-C4D-ND	4.06	116.80	110.24
22	2	612	CLA	C1D-CHD-C4C	-4.06	117.31	126.06
22	G	203	CLA	C3D-C4D-ND	4.06	116.80	110.24
22	3	609	CLA	C3D-C4D-ND	4.06	116.80	110.24
22	A	824	CLA	C3C-C4C-NC	4.05	115.12	110.57
22	B	824	CLA	C3D-C4D-ND	4.05	116.80	110.24
25	B	845	BCR	C7-C8-C9	-4.05	120.11	126.23
22	L	204	CLA	C4A-NA-C1A	-4.05	104.88	106.71
22	5	606	CLA	C3D-C4D-ND	4.05	116.79	110.24
25	F	305	BCR	C7-C8-C9	-4.05	120.11	126.23
21	A	801	CL0	C1C-C2C-C3C	-4.05	102.70	106.96
22	8	602	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
22	2	614	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
22	5	604	CLA	C3D-C4D-ND	4.05	116.79	110.24
22	1	613	CLA	C3D-C4D-ND	4.05	116.79	110.24
22	A	841	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
29	3	608	CHL	C3C-C4C-NC	4.05	115.11	110.57
22	7	604	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
22	7	616	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
22	A	828	CLA	C2C-C1C-NC	4.05	113.76	109.97
22	Z	613	CLA	C3D-C4D-ND	4.05	116.78	110.24
22	6	602	CLA	C3C-C4C-NC	4.05	115.11	110.57
22	4	609	CLA	C3D-C4D-ND	4.05	116.78	110.24
22	5	617	CLA	C3D-C4D-ND	4.04	116.78	110.24
22	A	816	CLA	C3C-C4C-NC	4.04	115.11	110.57
29	6	618	CHL	CHD-C1D-ND	-4.04	120.74	124.45
22	B	810	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
22	B	824	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
22	A	838	CLA	C1C-C2C-C3C	-4.04	102.71	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	601	CLA	C4A-NA-C1A	-4.04	104.89	106.71
22	9	611	CLA	C3C-C4C-NC	4.04	115.10	110.57
22	K	4003	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
22	3	606	CLA	CAA-C2A-C3A	-4.04	104.17	114.26
22	6	616	CLA	C4A-NA-C1A	-4.04	104.89	106.71
22	B	815	CLA	C3D-C4D-ND	4.04	116.77	110.24
22	1	616	CLA	C3D-C4D-ND	4.04	116.77	110.24
29	6	607	CHL	C1D-CHD-C4C	-4.04	117.35	126.06
22	8	608	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
22	7	606	CLA	C3C-C4C-NC	4.04	115.10	110.57
22	3	613	CLA	CAC-C3C-C4C	4.04	130.05	124.81
22	A	834	CLA	O2D-CGD-CBD	4.03	118.44	111.27
22	A	833	CLA	C3D-C4D-ND	4.03	116.77	110.24
22	B	823	CLA	CAC-C3C-C4C	4.03	130.04	124.81
22	A	826	CLA	C3C-C4C-NC	4.03	115.09	110.57
25	K	4001	BCR	C7-C8-C9	-4.03	120.14	126.23
22	2	609	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
22	B	819	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	A	803	CLA	C3C-C4C-NC	4.03	115.09	110.57
22	3	613	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
22	1	606	CLA	C3D-C4D-ND	4.03	116.75	110.24
22	8	603	CLA	C3D-C4D-ND	4.03	116.75	110.24
22	5	604	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
22	Z	613	CLA	C4A-NA-C1A	-4.03	104.90	106.71
22	4	616	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
22	3	603	CLA	C3D-C4D-ND	4.03	116.75	110.24
22	A	831	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
22	5	612	CLA	C3C-C4C-NC	4.02	115.08	110.57
22	A	808	CLA	C3C-C4C-NC	4.02	115.08	110.57
29	1	601	CHL	CHD-C1D-ND	-4.02	120.76	124.45
22	B	828	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
22	B	808	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
22	A	834	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
22	B	817	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
22	A	840	CLA	C1D-CHD-C4C	-4.02	117.40	126.06
22	A	818	CLA	C4A-NA-C1A	-4.01	104.90	106.71
22	B	826	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
22	A	820	CLA	C3D-C4D-ND	4.01	116.73	110.24
22	B	814	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
22	1	608	CLA	C3D-C4D-ND	4.01	116.72	110.24
25	7	623	BCR	C15-C14-C13	-4.01	121.59	127.31
22	6	616	CLA	CAA-C2A-C3A	-4.01	101.80	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	803	CLA	O2D-CGD-CBD	4.01	118.39	111.27
22	Z	604	CLA	C3D-C4D-ND	4.01	116.72	110.24
22	6	617	CLA	C3C-C4C-NC	4.01	115.06	110.57
22	A	813	CLA	C3C-C4C-NC	4.01	115.06	110.57
22	3	620	CLA	C1C-C2C-C3C	-4.01	102.75	106.96
22	7	606	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
22	9	603	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
29	4	608	CHL	C3C-C4C-NC	4.00	115.06	110.57
29	9	607	CHL	C3C-C4C-NC	4.00	115.06	110.57
25	B	843	BCR	C20-C21-C22	-4.00	121.60	127.31
22	6	617	CLA	C3D-C4D-ND	4.00	116.71	110.24
30	8	618	LUT	C15-C14-C13	-4.00	121.60	127.31
22	5	616	CLA	C3C-C4C-NC	4.00	115.06	110.57
22	5	613	CLA	C3D-C4D-ND	4.00	116.71	110.24
22	A	819	CLA	C3C-C4C-NC	4.00	115.06	110.57
25	A	852	BCR	C20-C19-C18	-4.00	115.18	126.42
22	6	612	CLA	C3C-C4C-NC	4.00	115.06	110.57
22	2	603	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
22	6	622	CLA	C3D-C4D-ND	4.00	116.70	110.24
22	7	620	CLA	C4A-NA-C1A	-4.00	104.91	106.71
22	A	842	CLA	C3C-C4C-NC	4.00	115.05	110.57
22	Z	613	CLA	C3C-C4C-NC	4.00	115.05	110.57
22	A	822	CLA	O2D-CGD-CBD	4.00	118.37	111.27
22	A	807	CLA	CAA-C2A-C3A	-3.99	101.84	112.78
25	4	621	BCR	C38-C26-C25	-3.99	120.04	124.53
22	B	803	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
22	A	825	CLA	C4A-NA-C1A	-3.99	104.91	106.71
22	Z	616	CLA	C4A-NA-C1A	-3.99	104.91	106.71
22	1	609	CLA	C3D-C4D-ND	3.99	116.69	110.24
22	B	832	CLA	C3C-C4C-NC	3.99	115.05	110.57
29	3	608	CHL	O2D-CGD-CBD	3.99	118.36	111.27
29	6	608	CHL	C3C-C4C-NC	3.99	115.05	110.57
25	5	622	BCR	C28-C27-C26	-3.99	106.95	114.08
22	Z	608	CLA	C3D-C4D-ND	3.99	116.69	110.24
29	6	606	CHL	C1D-CHD-C4C	-3.99	117.46	126.06
22	8	604	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
22	6	611	CLA	C3D-C4D-ND	3.98	116.68	110.24
22	A	809	CLA	C3C-C4C-NC	3.98	115.04	110.57
22	B	852	CLA	C3C-C4C-NC	3.98	115.04	110.57
22	3	604	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
29	4	606	CHL	C3B-C2B-C1B	-3.98	102.35	107.16
22	1	610	CLA	CAA-C2A-C3A	-3.98	101.87	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	601	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
22	B	836	CLA	C3B-C4B-NB	3.98	114.21	110.52
22	1	609	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
22	3	609	CLA	C4A-NA-C1A	-3.98	104.92	106.71
22	A	804	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
22	8	601	CLA	C1C-C2C-C3C	-3.98	102.78	106.96
22	A	832	CLA	C3D-C4D-ND	3.97	116.67	110.24
29	1	607	CHL	O2D-CGD-CBD	3.97	118.33	111.27
25	3	717	BCR	C28-C27-C26	-3.97	106.98	114.08
22	7	609	CLA	C3C-C4C-NC	3.97	115.03	110.57
22	1	606	CLA	C3C-C4C-NC	3.97	115.02	110.57
22	4	611	CLA	C4A-NA-C1A	-3.97	104.92	106.71
22	B	825	CLA	C3D-C2D-C1D	-3.97	100.42	105.83
22	A	830	CLA	C3D-C4D-ND	3.97	116.66	110.24
25	7	624	BCR	C16-C17-C18	-3.97	121.65	127.31
30	9	616	LUT	C35-C34-C33	-3.97	121.65	127.31
22	A	817	CLA	CMB-C2B-C1B	3.97	131.41	125.37
22	5	603	CLA	C3C-C4C-NC	3.97	115.02	110.57
22	7	604	CLA	C4A-NA-C1A	-3.97	104.92	106.71
22	F	304	CLA	C1D-CHD-C4C	-3.96	117.50	126.06
22	6	603	CLA	C1D-CHD-C4C	-3.96	117.50	126.06
22	7	601	CLA	O2A-CGA-CBA	3.96	124.35	111.91
22	1	603	CLA	C3D-C4D-ND	3.96	116.65	110.24
22	6	609	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
22	6	601	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
22	4	603	CLA	C3D-C4D-ND	3.96	116.65	110.24
22	3	610	CLA	C2C-C1C-NC	3.96	113.68	109.97
22	Z	613	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
22	7	611	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
22	7	601	CLA	C3C-C4C-NC	3.96	115.01	110.57
22	2	601	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
22	Z	612	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
22	B	814	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	5	603	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
25	4	621	BCR	C7-C8-C9	-3.95	120.26	126.23
22	A	820	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
22	5	611	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
22	5	613	CLA	C3C-C4C-NC	3.95	115.00	110.57
22	8	613	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
22	A	834	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
22	B	807	CLA	C3D-C4D-ND	3.95	116.63	110.24
22	9	612	CLA	C1C-C2C-C3C	-3.95	102.80	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	610	CLA	C3C-C4C-NC	3.95	115.00	110.57
22	3	613	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	1	610	CLA	C3C-C4C-NC	3.95	115.00	110.57
22	A	821	CLA	C3D-C4D-ND	3.95	116.63	110.24
22	4	611	CLA	C1D-CHD-C4C	-3.95	117.55	126.06
25	8	619	BCR	C16-C17-C18	-3.94	121.68	127.31
22	3	603	CLA	C3C-C4C-NC	3.94	114.99	110.57
22	6	603	CLA	C3C-C4C-NC	3.94	114.99	110.57
22	A	827	CLA	CAA-C2A-C3A	-3.94	101.98	112.78
22	Z	609	CLA	C3D-C4D-ND	3.94	116.61	110.24
22	Z	616	CLA	C3D-C4D-ND	3.94	116.61	110.24
22	1	609	CLA	CAA-C2A-C3A	-3.94	101.99	112.78
22	L	203	CLA	C3C-C4C-NC	3.94	114.99	110.57
25	B	845	BCR	C3-C4-C5	-3.94	107.04	114.08
22	5	609	CLA	C3C-C4C-NC	3.94	114.99	110.57
22	9	611	CLA	C3D-C4D-ND	3.94	116.61	110.24
22	F	301	CLA	C3C-C4C-NC	3.93	114.98	110.57
22	4	613	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
22	8	610	CLA	C3C-C4C-NC	3.93	114.98	110.57
22	A	834	CLA	CAA-C2A-C3A	-3.93	102.01	112.78
22	3	602	CLA	C4A-NA-C1A	-3.93	104.94	106.71
22	4	610	CLA	C3D-C4D-ND	3.93	116.60	110.24
22	7	614	CLA	C3D-C4D-ND	3.93	116.60	110.24
22	9	614	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
22	1	603	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
22	1	614	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
22	5	606	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
22	6	603	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
22	4	612	CLA	C3C-C4C-NC	3.93	114.98	110.57
29	9	607	CHL	C1D-CHD-C4C	-3.93	117.58	126.06
22	8	608	CLA	CMC-C2C-C1C	3.93	131.02	125.04
22	8	603	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
22	F	304	CLA	C3C-C4C-NC	3.93	114.97	110.57
22	1	603	CLA	C3B-C4B-NB	3.93	114.16	110.52
22	G	203	CLA	C3C-C4C-NC	3.93	114.97	110.57
22	K	4003	CLA	C3C-C4C-NC	3.93	114.97	110.57
29	6	618	CHL	C1D-CHD-C4C	-3.92	117.59	126.06
22	Z	616	CLA	C3C-C4C-NC	3.92	114.97	110.57
22	1	608	CLA	C3C-C4C-NC	3.92	114.97	110.57
22	6	610	CLA	C1D-CHD-C4C	-3.92	117.59	126.06
22	4	603	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
22	3	603	CLA	C1C-C2C-C3C	-3.92	102.83	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	603	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
22	Z	611	CLA	C4A-NA-C1A	-3.92	104.94	106.71
22	B	824	CLA	C4A-NA-C1A	-3.92	104.94	106.71
22	5	604	CLA	C4A-NA-C1A	-3.92	104.94	106.71
22	A	838	CLA	C3C-C4C-NC	3.92	114.96	110.57
22	8	601	CLA	C3C-C4C-NC	3.92	114.96	110.57
22	A	826	CLA	C3D-C4D-ND	3.92	116.57	110.24
29	5	618	CHL	C3C-C4C-NC	3.92	114.96	110.57
25	7	623	BCR	C27-C26-C25	-3.91	117.05	122.73
22	A	803	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
22	F	303	CLA	C3D-C4D-ND	3.91	116.56	110.24
25	A	850	BCR	C28-C27-C26	-3.91	107.09	114.08
22	7	602	CLA	C3C-C4C-NC	3.91	114.95	110.57
22	B	804	CLA	C3D-C4D-ND	3.91	116.56	110.24
25	J	3003	BCR	C20-C21-C22	-3.91	121.73	127.31
22	L	203	CLA	C4A-NA-C1A	-3.91	104.95	106.71
22	B	809	CLA	C3D-C4D-ND	3.91	116.56	110.24
22	6	603	CLA	C3D-C4D-ND	3.91	116.56	110.24
22	A	804	CLA	CAA-C2A-C3A	-3.91	102.08	112.78
22	7	603	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
29	4	608	CHL	C1D-CHD-C4C	-3.91	117.63	126.06
22	5	621	CLA	CAC-C3C-C4C	3.91	129.88	124.81
22	A	823	CLA	C4A-NA-C1A	-3.90	104.95	106.71
22	4	601	CLA	C3B-C4B-NB	3.90	114.14	110.52
22	5	602	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
22	A	842	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
22	A	810	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
30	1	619	LUT	C35-C34-C33	-3.90	121.74	127.31
22	B	828	CLA	C3C-C4C-NC	3.90	114.95	110.57
22	7	609	CLA	C4A-NA-C1A	-3.90	104.95	106.71
22	3	609	CLA	O2D-CGD-CBD	3.90	118.20	111.27
22	B	813	CLA	C3D-C4D-ND	3.90	116.55	110.24
22	1	611	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
22	B	816	CLA	C3D-C4D-ND	3.90	116.54	110.24
22	6	604	CLA	C3C-C4C-NC	3.90	114.94	110.57
22	3	607	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
22	A	820	CLA	C3B-C4B-NB	3.90	114.13	110.52
22	9	612	CLA	C3C-C4C-NC	3.90	114.94	110.57
25	A	849	BCR	C15-C14-C13	-3.90	121.75	127.31
22	B	828	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
22	B	807	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
22	7	611	CLA	C1C-C2C-C3C	-3.90	102.86	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	603	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
22	B	826	CLA	C3D-C4D-ND	3.89	116.54	110.24
29	4	606	CHL	C1D-CHD-C4C	-3.89	117.66	126.06
22	B	811	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
22	1	616	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
22	B	823	CLA	C3D-C4D-ND	3.89	116.53	110.24
22	3	611	CLA	C3D-C4D-ND	3.89	116.53	110.24
22	1	608	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
22	3	611	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
22	B	802	CLA	CMB-C2B-C1B	3.89	131.29	125.37
22	A	817	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
29	3	608	CHL	C3B-C2B-C1B	-3.89	102.47	107.16
22	1	609	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	7	604	CLA	C3B-C2B-C1B	-3.89	102.47	107.16
22	5	613	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	B	835	CLA	C3C-C4C-NC	3.89	114.93	110.57
22	3	607	CLA	C3C-C4C-NC	3.89	114.93	110.57
22	B	817	CLA	C3D-C4D-ND	3.88	116.52	110.24
25	B	846	BCR	C3-C4-C5	-3.88	107.14	114.08
22	7	610	CLA	O2A-CGA-CBA	3.88	124.09	111.91
22	1	612	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
25	8	619	BCR	C28-C27-C26	-3.88	107.14	114.08
22	6	612	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
22	A	819	CLA	C3D-C4D-ND	3.88	116.52	110.24
22	2	609	CLA	C3D-C4D-ND	3.88	116.51	110.24
22	B	852	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
22	A	839	CLA	C3C-C4C-NC	3.88	114.92	110.57
22	6	616	CLA	C3B-C4B-NB	3.88	114.11	110.52
22	4	616	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
22	B	823	CLA	C3C-C4C-NC	3.88	114.92	110.57
22	G	203	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
22	4	610	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
22	A	839	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
22	Z	602	CLA	C3C-C4C-NC	3.88	114.92	110.57
22	B	806	CLA	C3D-C4D-ND	3.87	116.50	110.24
22	4	611	CLA	C1C-C2C-C3C	-3.87	102.88	106.96
29	9	606	CHL	C3C-C4C-NC	3.87	114.92	110.57
22	3	606	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
22	A	830	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
29	7	607	CHL	C3C-C4C-NC	3.87	114.91	110.57
22	4	614	CLA	C3C-C4C-NC	3.87	114.91	110.57
22	A	836	CLA	C1D-CHD-C4C	-3.87	117.71	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	611	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
22	3	607	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
22	5	609	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
25	K	4004	BCR	C20-C21-C22	-3.87	121.79	127.31
22	8	616	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
25	3	719	BCR	C3-C4-C5	-3.87	107.17	114.08
22	Z	608	CLA	C3C-C4C-NC	3.87	114.91	110.57
22	9	601	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
25	B	844	BCR	C24-C23-C22	-3.87	120.39	126.23
22	B	824	CLA	C3C-C4C-NC	3.86	114.91	110.57
22	Z	611	CLA	C3C-C4C-NC	3.86	114.91	110.57
22	5	601	CLA	C3C-C4C-NC	3.86	114.91	110.57
22	B	836	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
22	1	606	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
22	A	807	CLA	C3C-C4C-NC	3.86	114.90	110.57
22	B	834	CLA	CMA-C3A-C4A	-3.86	101.39	111.77
22	B	822	CLA	C3C-C4C-NC	3.86	114.90	110.57
24	Z	620	LHG	O7-C7-C8	3.86	119.82	111.50
25	6	625	BCR	C28-C27-C26	-3.86	107.18	114.08
29	4	618	CHL	C1D-CHD-C4C	-3.86	117.73	126.06
22	5	609	CLA	C1-C2-C3	-3.86	120.51	126.75
22	7	606	CLA	CAA-C2A-C3A	-3.86	104.62	114.26
22	5	616	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
22	B	831	CLA	C2C-C1C-NC	3.86	113.59	109.97
22	1	611	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
22	8	610	CLA	CAA-C2A-C3A	-3.86	102.22	112.78
22	A	822	CLA	C3D-C4D-ND	3.86	116.47	110.24
29	4	607	CHL	C1D-CHD-C4C	-3.85	117.74	126.06
22	8	608	CLA	C3D-C4D-ND	3.85	116.47	110.24
22	A	808	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
30	4	620	LUT	C35-C34-C33	-3.85	121.81	127.31
22	5	610	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
29	5	607	CHL	C2A-C3A-C4A	-3.85	95.65	101.87
22	Z	604	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
22	Z	614	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
22	6	617	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
22	4	611	CLA	C3D-C4D-ND	3.85	116.47	110.24
22	9	603	CLA	C3C-C4C-NC	3.85	114.89	110.57
22	4	604	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
22	B	835	CLA	C3D-C4D-ND	3.85	116.46	110.24
22	2	613	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
29	9	606	CHL	C1D-CHD-C4C	-3.85	117.76	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	610	CLA	C1D-CHD-C4C	-3.84	117.76	126.06
22	B	803	CLA	C3C-C4C-NC	3.84	114.88	110.57
22	6	602	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
22	B	828	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
22	B	821	CLA	C4A-NA-C1A	-3.84	104.98	106.71
22	9	611	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	J	3002	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	6	616	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	A	812	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	3	610	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	A	825	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	7	613	CLA	C3B-C4B-NB	3.84	114.07	110.52
22	5	614	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	Z	610	CLA	O2A-CGA-CBA	3.84	123.94	111.91
22	B	827	CLA	C3D-C4D-ND	3.84	116.44	110.24
22	6	609	CLA	C3D-C4D-ND	3.84	116.44	110.24
22	1	604	CLA	C1C-C2C-C3C	-3.83	102.92	106.96
24	6	619	LHG	O7-C7-C8	3.83	119.76	111.50
22	6	604	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
22	7	602	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
22	B	836	CLA	C3C-C4C-NC	3.83	114.87	110.57
22	B	837	CLA	C3C-C4C-NC	3.83	114.87	110.57
22	B	805	CLA	C3D-C4D-ND	3.83	116.43	110.24
22	2	613	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
22	F	303	CLA	O2D-CGD-CBD	3.83	118.07	111.27
22	8	613	CLA	C4A-NA-C1A	-3.83	104.98	106.71
22	7	603	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
22	4	616	CLA	C3B-C4B-NB	3.83	114.07	110.52
22	Z	611	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
22	B	808	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
22	3	602	CLA	C1D-CHD-C4C	-3.83	117.81	126.06
22	A	814	CLA	C3B-C4B-NB	3.83	114.06	110.52
22	A	831	CLA	C3D-C4D-ND	3.82	116.42	110.24
22	A	824	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
22	L	203	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
29	4	607	CHL	CBC-CAC-C3C	-3.82	101.89	112.43
22	4	602	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
22	A	820	CLA	C3C-C4C-NC	3.82	114.86	110.57
22	B	818	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
22	5	604	CLA	CAC-C3C-C4C	3.82	129.77	124.81
22	7	601	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
22	1	613	CLA	C3C-C4C-NC	3.82	114.86	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	613	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
22	1	609	CLA	O2D-CGD-CBD	3.82	118.05	111.27
22	A	843	CLA	C3D-C4D-ND	3.82	116.41	110.24
22	B	833	CLA	C3B-C4B-NB	3.81	114.05	110.52
22	3	612	CLA	C3C-C4C-NC	3.81	114.85	110.57
22	Z	606	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
22	9	613	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
22	A	820	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
22	1	611	CLA	C3C-C4C-NC	3.81	114.85	110.57
22	3	617	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
29	Z	607	CHL	CHD-C1D-ND	-3.81	120.95	124.45
22	9	601	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
29	6	608	CHL	C1D-CHD-C4C	-3.81	117.84	126.06
22	2	614	CLA	C3C-C4C-NC	3.81	114.84	110.57
22	4	613	CLA	C4A-NA-C1A	-3.81	104.99	106.71
29	6	608	CHL	C2C-C3C-C4C	-3.81	103.78	106.49
22	Z	608	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
22	8	606	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
29	8	607	CHL	CHD-C1D-ND	-3.81	120.96	124.45
22	B	833	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
22	A	843	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
22	Z	603	CLA	C3B-C4B-NB	3.81	114.05	110.52
22	B	811	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
22	2	606	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
22	J	3002	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
22	A	839	CLA	C1-C2-C3	-3.80	119.46	126.04
22	7	612	CLA	C3C-C4C-NC	3.80	114.84	110.57
22	B	835	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
22	7	608	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
22	9	609	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
22	B	839	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
22	5	604	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
22	Z	610	CLA	C2C-C1C-NC	3.79	113.53	109.97
22	B	812	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
29	Z	601	CHL	CHD-C1D-ND	-3.79	120.97	124.45
22	2	613	CLA	C3C-C4C-NC	3.79	114.83	110.57
22	F	301	CLA	C3D-C4D-ND	3.79	116.37	110.24
22	4	614	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
22	A	833	CLA	C3C-C4C-NC	3.79	114.83	110.57
22	7	608	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
22	A	837	CLA	C3D-C4D-ND	3.79	116.37	110.24
22	B	832	CLA	C1D-CHD-C4C	-3.79	117.88	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	601	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
22	7	606	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
22	3	617	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
22	8	609	CLA	C3D-C4D-ND	3.79	116.37	110.24
22	6	611	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
22	9	601	CLA	C3C-C4C-NC	3.79	114.82	110.57
22	B	821	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
22	7	610	CLA	CAA-C2A-C3A	-3.79	102.41	112.78
22	9	609	CLA	C3D-C4D-ND	3.79	116.36	110.24
22	A	834	CLA	C3C-C4C-NC	3.79	114.82	110.57
22	A	843	CLA	CAC-C3C-C4C	3.79	129.72	124.81
22	A	807	CLA	C1D-CHD-C4C	-3.78	117.89	126.06
22	B	821	CLA	C3C-C4C-NC	3.78	114.81	110.57
22	3	617	CLA	C3C-C4C-NC	3.78	114.81	110.57
25	5	622	BCR	C16-C17-C18	-3.78	121.91	127.31
21	A	801	CL0	C3D-C4D-ND	3.78	116.36	110.24
22	5	613	CLA	C3B-C4B-NB	3.78	114.02	110.52
22	9	612	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	A	827	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	5	621	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
22	4	602	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
22	Z	609	CLA	C3B-C4B-NB	3.78	114.02	110.52
22	A	826	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
22	5	611	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
22	1	616	CLA	C3C-C4C-NC	3.78	114.81	110.57
22	5	602	CLA	C3C-C4C-NC	3.78	114.81	110.57
30	Z	619	LUT	C35-C34-C33	-3.78	121.92	127.31
22	A	832	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
22	2	612	CLA	C3C-C4C-NC	3.77	114.80	110.57
22	8	611	CLA	CAC-C3C-C4C	3.77	129.70	124.81
25	7	624	BCR	C15-C14-C13	-3.77	121.93	127.31
22	A	840	CLA	C3D-C4D-ND	3.77	116.34	110.24
22	8	609	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
22	A	804	CLA	C3C-C4C-NC	3.77	114.80	110.57
22	B	815	CLA	C3C-C4C-NC	3.77	114.80	110.57
22	G	203	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
22	1	614	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
22	2	611	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
22	3	603	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	7	625	LHG	O7-C7-C8	3.77	119.62	111.50
22	Z	616	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
22	5	606	CLA	C1D-CHD-C4C	-3.77	117.93	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	604	CLA	C4A-NA-C1A	-3.77	105.01	106.71
22	8	606	CLA	C3C-C4C-NC	3.77	114.79	110.57
22	F	303	CLA	C3C-C4C-NC	3.76	114.79	110.57
22	B	806	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
22	7	612	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
22	5	609	CLA	C3D-C4D-ND	3.76	116.33	110.24
22	3	603	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
22	7	601	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
22	A	823	CLA	C3C-C4C-NC	3.76	114.79	110.57
22	9	613	CLA	C3C-C4C-NC	3.76	114.79	110.57
22	B	807	CLA	C4A-NA-C1A	-3.76	105.02	106.71
22	7	613	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
22	5	612	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
25	B	844	BCR	C28-C27-C26	-3.76	107.37	114.08
21	A	801	CL0	C3B-C2B-C1B	-3.76	102.63	107.16
24	4	623	LHG	O7-C7-C8	3.76	119.60	111.50
22	B	809	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
22	9	602	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
22	3	611	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
22	1	608	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
22	A	836	CLA	C4A-NA-C1A	-3.75	105.02	106.71
22	8	608	CLA	C3C-C4C-NC	3.75	114.78	110.57
22	B	803	CLA	C3D-C4D-ND	3.75	116.31	110.24
22	5	601	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
21	A	801	CL0	C3B-C4B-NB	3.75	114.00	110.52
22	4	603	CLA	C3B-C4B-NB	3.75	114.00	110.52
25	K	4004	BCR	C24-C23-C22	-3.75	120.57	126.23
22	9	613	CLA	C3B-C4B-NB	3.75	114.00	110.52
29	4	607	CHL	C3C-C4C-NC	3.75	114.78	110.57
22	3	614	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
22	4	610	CLA	O2A-CGA-CBA	3.75	123.67	111.91
22	8	609	CLA	C3C-C4C-NC	3.75	114.77	110.57
22	9	610	CLA	C3C-C4C-NC	3.75	114.77	110.57
22	3	609	CLA	C1D-CHD-C4C	-3.75	117.98	126.06
22	8	610	CLA	C3D-C4D-ND	3.75	116.30	110.24
22	5	611	CLA	C3D-C4D-ND	3.75	116.30	110.24
22	B	821	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
22	A	842	CLA	C4A-NA-C1A	-3.74	105.02	106.71
29	1	601	CHL	C1D-CHD-C4C	-3.74	117.98	126.06
29	5	607	CHL	C3C-C4C-NC	3.74	114.77	110.57
22	3	609	CLA	CAA-C2A-C3A	-3.74	102.53	112.78
22	B	807	CLA	C1D-CHD-C4C	-3.74	117.99	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	806	CLA	C3B-C4B-NB	3.74	113.98	110.52
22	1	616	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
22	A	854	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	2	607	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	1	602	CLA	C3C-C4C-NC	3.74	114.76	110.57
22	A	803	CLA	C3B-C4B-NB	3.74	113.98	110.52
22	Z	603	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
22	2	610	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
22	K	4002	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
22	B	803	CLA	C4C-C3C-C2C	-3.73	101.46	106.90
22	B	806	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
22	7	620	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
22	4	612	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
22	9	604	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
22	B	817	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
22	3	614	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
22	4	601	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
30	5	620	LUT	C18-C5-C6	-3.73	120.34	124.53
22	7	603	CLA	C3C-C4C-NC	3.73	114.75	110.57
22	B	802	CLA	CMA-C3A-C4A	-3.73	101.75	111.77
22	7	604	CLA	CMB-C2B-C1B	3.73	131.04	125.37
22	B	836	CLA	C3D-C4D-ND	3.73	116.27	110.24
22	A	836	CLA	C3C-C4C-NC	3.73	114.75	110.57
22	A	814	CLA	CAC-C3C-C4C	3.72	129.64	124.81
22	8	611	CLA	C3D-C4D-ND	3.72	116.26	110.24
22	B	835	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
25	B	847	BCR	C15-C16-C17	-3.72	115.85	123.47
22	4	604	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
22	8	606	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
22	B	818	CLA	C3D-C4D-ND	3.72	116.25	110.24
22	4	613	CLA	C3C-C4C-NC	3.72	114.74	110.57
22	6	622	CLA	C4A-NA-C1A	-3.72	105.03	106.71
22	9	611	CLA	C4A-NA-C1A	-3.72	105.03	106.71
22	9	613	CLA	C4A-NA-C1A	-3.72	105.03	106.71
29	4	618	CHL	C3C-C4C-NC	3.72	114.74	110.57
22	B	825	CLA	C3C-C4C-NC	3.72	114.74	110.57
22	7	620	CLA	C3C-C4C-NC	3.72	114.74	110.57
22	B	830	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
22	A	841	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
22	1	612	CLA	C3C-C4C-NC	3.72	114.74	110.57
22	A	819	CLA	CAC-C3C-C4C	3.72	129.63	124.81
22	B	828	CLA	C1C-C2C-C3C	-3.72	103.05	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	622	CLA	C3C-C4C-NC	3.72	114.74	110.57
24	A	855	LHG	O7-C7-C8	3.71	119.51	111.50
25	A	851	BCR	C11-C10-C9	-3.71	122.01	127.31
22	2	606	CLA	C3C-C4C-NC	3.71	114.74	110.57
22	2	612	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
22	B	839	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
22	8	616	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
22	5	611	CLA	C4A-NA-C1A	-3.71	105.04	106.71
22	5	611	CLA	C3C-C4C-NC	3.71	114.73	110.57
22	6	613	CLA	C3C-C4C-NC	3.71	114.73	110.57
25	7	623	BCR	C29-C30-C25	3.71	116.19	110.48
22	4	609	CLA	C3C-C4C-NC	3.71	114.73	110.57
22	2	611	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
22	B	808	CLA	C4A-NA-C1A	-3.71	105.04	106.71
22	B	811	CLA	C4B-C3B-C2B	-3.71	103.51	107.03
22	3	609	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
22	B	813	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
22	B	834	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
22	6	622	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
22	5	621	CLA	C3D-C4D-ND	3.71	116.24	110.24
22	F	301	CLA	CAA-C2A-C3A	-3.71	102.63	112.78
22	B	806	CLA	O2D-CGD-CBD	3.71	117.86	111.27
22	B	808	CLA	C3B-C4B-NB	3.71	113.95	110.52
25	7	623	BCR	C3-C4-C5	-3.71	107.46	114.08
30	8	617	LUT	C7-C8-C9	-3.71	120.64	126.23
22	B	812	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
22	4	616	CLA	CAC-C3C-C4C	3.70	129.62	124.81
22	8	606	CLA	O2D-CGD-CBD	3.70	117.85	111.27
25	B	801	BCR	C3-C4-C5	-3.70	107.47	114.08
22	A	837	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
22	A	808	CLA	C3B-C4B-NB	3.70	113.95	110.52
22	A	828	CLA	CHD-C4C-NC	3.70	130.03	124.20
22	A	828	CLA	C3D-C4D-ND	3.70	116.22	110.24
25	B	843	BCR	C11-C10-C9	-3.70	122.03	127.31
22	3	620	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
22	5	616	CLA	C3D-C4D-ND	3.70	116.22	110.24
22	B	814	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
22	5	614	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
22	F	304	CLA	C3B-C4B-NB	3.70	113.94	110.52
24	B	851	LHG	O7-C7-C8	3.69	119.46	111.50
22	B	822	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
22	A	814	CLA	C4A-NA-C1A	-3.69	105.05	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	813	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
22	5	613	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
22	5	621	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
22	A	806	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
22	7	611	CLA	C3B-C4B-NB	3.69	113.94	110.52
22	B	820	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
22	A	821	CLA	C3C-C4C-NC	3.69	114.71	110.57
22	B	840	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
22	A	839	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
22	B	810	CLA	C3C-C4C-NC	3.69	114.71	110.57
22	L	204	CLA	C3C-C4C-NC	3.69	114.71	110.57
22	G	204	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
22	6	611	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
22	B	823	CLA	CMB-C2B-C1B	3.68	130.98	125.37
22	A	810	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
25	8	619	BCR	C21-C20-C19	-3.68	111.73	123.22
22	2	606	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
22	3	610	CLA	C3C-C4C-NC	3.68	114.70	110.57
22	A	805	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
22	8	602	CLA	CHD-C4C-NC	3.68	130.00	124.20
22	A	809	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
22	8	603	CLA	C3C-C4C-NC	3.68	114.70	110.57
22	7	601	CLA	C3B-C4B-NB	3.68	113.93	110.52
22	A	837	CLA	C3C-C4C-NC	3.68	114.69	110.57
22	4	603	CLA	C3C-C4C-NC	3.68	114.69	110.57
22	A	843	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
22	A	807	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
22	1	616	CLA	C4A-NA-C1A	-3.67	105.05	106.71
29	5	607	CHL	C3B-C4B-NB	3.67	113.92	110.52
22	3	607	CLA	CAA-C2A-C3A	-3.67	102.72	112.78
30	7	621	LUT	C7-C8-C9	-3.67	120.69	126.23
30	4	619	LUT	C7-C8-C9	-3.67	120.69	126.23
22	A	833	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
22	6	614	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
22	B	839	CLA	C3C-C4C-NC	3.67	114.69	110.57
22	7	620	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
30	3	622	LUT	C7-C8-C9	-3.67	120.69	126.23
22	8	608	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
22	B	817	CLA	CMB-C2B-C1B	3.67	130.96	125.37
22	A	822	CLA	C3C-C4C-NC	3.67	114.69	110.57
22	1	614	CLA	C3C-C4C-NC	3.67	114.69	110.57
22	Z	616	CLA	C1C-C2C-C3C	-3.67	103.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	617	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
22	B	813	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
22	4	610	CLA	C3C-C4C-NC	3.67	114.68	110.57
22	4	613	CLA	C3B-C4B-NB	3.67	113.92	110.52
22	A	811	CLA	C1-C2-C3	-3.67	119.70	126.04
22	Z	604	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
22	B	805	CLA	C1D-CHD-C4C	-3.66	118.15	126.06
22	K	4003	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
22	B	817	CLA	C3C-C4C-NC	3.66	114.68	110.57
22	8	611	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
22	K	4002	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
22	Z	614	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
22	7	613	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
22	Z	610	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
25	3	718	BCR	C28-C27-C26	-3.66	107.54	114.08
22	9	602	CLA	C3C-C4C-NC	3.66	114.67	110.57
22	A	823	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
22	8	601	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
22	7	611	CLA	C3D-C4D-ND	3.65	116.15	110.24
22	A	802	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
22	A	835	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
22	L	203	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
29	5	608	CHL	CAC-C3C-C4C	3.65	129.55	124.81
22	9	604	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
22	7	614	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
22	4	616	CLA	C3C-C4C-NC	3.65	114.67	110.57
22	3	613	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
22	A	827	CLA	C3C-C4C-NC	3.65	114.66	110.57
22	2	601	CLA	C3C-C4C-NC	3.65	114.66	110.57
22	2	602	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
30	5	620	LUT	C15-C14-C13	-3.64	122.11	127.31
22	A	825	CLA	CAC-C3C-C4C	3.64	129.54	124.81
22	Z	604	CLA	C4A-NA-C1A	-3.64	105.07	106.71
22	3	602	CLA	C3C-C4C-NC	3.64	114.66	110.57
25	K	4001	BCR	C2-C3-C4	-3.64	103.24	111.38
29	5	608	CHL	C1D-CHD-C4C	-3.64	118.20	126.06
22	A	834	CLA	C3B-C4B-NB	3.64	113.89	110.52
25	B	801	BCR	C21-C20-C19	-3.64	111.86	123.22
22	7	609	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
22	B	828	CLA	C3B-C4B-NB	3.64	113.89	110.52
22	5	617	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
22	2	607	CLA	C1C-C2C-C3C	-3.64	103.13	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	604	CLA	O2D-CGD-CBD	3.64	117.73	111.27
22	B	841	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
22	B	822	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
29	9	607	CHL	CAC-C3C-C4C	3.64	129.53	124.81
22	A	808	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
22	B	841	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
22	3	606	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
22	Z	606	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
22	A	837	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
22	A	823	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
22	3	611	CLA	C3C-C4C-NC	3.63	114.64	110.57
22	F	301	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
22	3	604	CLA	C3C-C4C-NC	3.63	114.64	110.57
22	8	611	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
22	A	821	CLA	CBC-CAC-C3C	-3.63	102.43	112.43
22	B	827	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
22	1	609	CLA	C3B-C4B-NB	3.62	113.88	110.52
25	F	305	BCR	C38-C26-C25	-3.62	120.46	124.53
29	5	618	CHL	C1D-CHD-C4C	-3.62	118.24	126.06
22	A	831	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	B	833	CLA	C3C-C4C-NC	3.62	114.63	110.57
22	A	820	CLA	CBA-CAA-C2A	3.62	124.56	113.86
22	B	809	CLA	C3C-C4C-NC	3.62	114.63	110.57
22	6	603	CLA	C3B-C4B-NB	3.62	113.88	110.52
22	8	612	CLA	O2D-CGD-CBD	3.62	117.70	111.27
22	6	611	CLA	C3C-C4C-NC	3.62	114.63	110.57
24	8	620	LHG	O7-C7-C8	3.62	119.30	111.50
22	A	824	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
22	3	606	CLA	C3C-C4C-NC	3.62	114.63	110.57
22	B	807	CLA	C3B-C4B-NB	3.62	113.87	110.52
22	K	4002	CLA	C3C-C4C-NC	3.62	114.63	110.57
22	8	611	CLA	C3C-C4C-NC	3.62	114.63	110.57
25	B	846	BCR	C21-C20-C19	-3.62	111.93	123.22
22	6	614	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	3	602	CLA	C3B-C4B-NB	3.62	113.87	110.52
22	A	819	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
22	9	614	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
22	Z	614	CLA	C3C-C4C-NC	3.61	114.62	110.57
22	B	819	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
22	B	823	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
22	6	622	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
22	3	620	CLA	C3C-C4C-NC	3.61	114.62	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Z	606	CLA	C3C-C4C-NC	3.61	114.62	110.57
22	2	603	CLA	C3C-C4C-NC	3.61	114.62	110.57
30	Z	617	LUT	C35-C15-C14	-3.61	116.07	123.47
22	B	820	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
22	7	614	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
22	3	603	CLA	C3B-C4B-NB	3.61	113.87	110.52
22	7	612	CLA	C3B-C4B-NB	3.61	113.86	110.52
22	2	602	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
22	6	616	CLA	C3C-C4C-NC	3.61	114.62	110.57
22	F	303	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
25	B	845	BCR	C16-C17-C18	-3.61	122.16	127.31
22	6	604	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
22	2	612	CLA	C3B-C4B-NB	3.61	113.86	110.52
29	6	607	CHL	C3B-C4B-NB	3.61	113.86	110.52
22	A	832	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
22	Z	608	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
22	Z	610	CLA	CAC-C3C-C4C	3.61	129.49	124.81
22	4	613	CLA	O2A-CGA-CBA	3.60	123.22	111.91
22	B	838	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
25	J	3003	BCR	C15-C14-C13	-3.60	122.17	127.31
22	B	840	CLA	CHC-C1C-C2C	-3.60	116.72	126.73
22	J	3002	CLA	C3C-C4C-NC	3.60	114.61	110.57
22	7	609	CLA	CHB-C4A-NA	3.60	129.49	124.51
22	4	613	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
22	7	614	CLA	C3C-C4C-NC	3.60	114.61	110.57
22	A	805	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
22	5	606	CLA	C3C-C4C-NC	3.60	114.61	110.57
22	B	834	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
22	2	607	CLA	C3C-C4C-NC	3.60	114.61	110.57
22	8	602	CLA	C4A-NA-C1A	-3.60	105.09	106.71
22	A	825	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
22	9	604	CLA	C3C-C4C-NC	3.60	114.60	110.57
24	5	623	LHG	O7-C7-C8	3.60	119.25	111.50
22	B	817	CLA	CAA-C2A-C3A	-3.60	102.93	112.78
22	8	610	CLA	O2A-CGA-CBA	3.59	123.19	111.91
22	6	614	CLA	C3C-C4C-NC	3.59	114.60	110.57
22	2	611	CLA	C3C-C4C-NC	3.59	114.60	110.57
22	B	812	CLA	C3C-C4C-NC	3.59	114.60	110.57
22	A	829	CLA	C3D-C4D-ND	3.59	116.05	110.24
22	G	204	CLA	C3C-C4C-NC	3.59	114.60	110.57
22	3	614	CLA	C3C-C4C-NC	3.59	114.60	110.57
25	B	846	BCR	C15-C14-C13	-3.59	122.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	612	CLA	C3B-C4B-NB	3.59	113.84	110.52
22	B	816	CLA	CMC-C2C-C1C	3.59	130.50	125.04
22	Z	611	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
22	6	613	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	2	602	CLA	C3C-C4C-NC	3.58	114.59	110.57
25	K	4004	BCR	C3-C4-C5	-3.58	107.68	114.08
22	5	610	CLA	C3C-C4C-NC	3.58	114.59	110.57
22	3	613	CLA	C3B-C4B-NB	3.58	113.84	110.52
22	B	819	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	1	603	CLA	C3C-C4C-NC	3.58	114.59	110.57
22	3	609	CLA	C3C-C4C-NC	3.58	114.58	110.57
22	7	611	CLA	C3C-C4C-NC	3.58	114.58	110.57
22	B	831	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
22	5	612	CLA	C3B-C4B-NB	3.58	113.83	110.52
22	A	828	CLA	C4C-C3C-C2C	-3.58	101.69	106.90
22	A	825	CLA	C3C-C4C-NC	3.57	114.58	110.57
30	Z	617	LUT	C35-C34-C33	-3.57	122.21	127.31
25	3	717	BCR	C21-C20-C19	-3.57	112.06	123.22
22	2	614	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
22	A	815	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
22	2	609	CLA	C3B-C4B-NB	3.57	113.83	110.52
22	G	204	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
22	A	815	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
29	9	606	CHL	C2A-C3A-C4A	-3.57	97.23	101.78
25	5	625	BCR	C3-C4-C5	-3.57	107.70	114.08
25	7	624	BCR	C11-C10-C9	-3.57	122.22	127.31
22	6	614	CLA	CAA-C2A-C3A	-3.57	103.00	112.78
22	B	815	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
22	6	616	CLA	CHC-C1C-C2C	-3.57	116.82	126.73
22	4	610	CLA	CAA-C2A-C3A	-3.57	103.01	112.78
22	5	614	CLA	C3C-C4C-NC	3.57	114.57	110.57
22	6	617	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
25	B	848	BCR	C15-C14-C13	-3.56	122.22	127.31
22	8	601	CLA	C3D-C4D-ND	3.56	116.00	110.24
22	8	613	CLA	C3B-C4B-NB	3.56	113.82	110.52
22	A	833	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
22	8	612	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
22	1	613	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
22	8	604	CLA	C3C-C4C-NC	3.56	114.56	110.57
29	3	608	CHL	C2C-C3C-C4C	-3.56	103.95	106.49
22	5	614	CLA	C3B-C4B-NB	3.56	113.82	110.52
30	8	617	LUT	C15-C14-C13	-3.56	122.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	614	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
25	B	846	BCR	C16-C17-C18	-3.56	122.24	127.31
22	A	854	CLA	C4C-C3C-C2C	-3.55	101.72	106.90
22	A	831	CLA	C3B-C2B-C1B	-3.55	102.87	107.16
22	2	610	CLA	C3C-C4C-NC	3.55	114.56	110.57
22	B	810	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
29	9	606	CHL	CAC-C3C-C4C	3.55	129.42	124.81
22	8	602	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
25	A	850	BCR	C11-C10-C9	-3.55	122.24	127.31
30	1	618	LUT	C35-C34-C33	-3.55	122.24	127.31
22	6	616	CLA	CAC-C3C-C4C	3.55	129.42	124.81
22	A	817	CLA	C3B-C4B-NB	3.55	113.81	110.52
22	B	805	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
22	3	602	CLA	O2A-CGA-CBA	3.55	123.04	111.91
30	4	619	LUT	C35-C15-C14	-3.55	116.21	123.47
22	B	837	CLA	C4-C3-C5	3.55	121.24	115.27
22	A	840	CLA	C3B-C4B-NB	3.55	113.80	110.52
22	5	609	CLA	C3B-C4B-NB	3.55	113.80	110.52
25	7	624	BCR	C7-C8-C9	-3.55	120.88	126.23
22	8	604	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
22	A	854	CLA	C2C-C1C-NC	3.54	113.29	109.97
22	Z	604	CLA	C3C-C4C-NC	3.54	114.55	110.57
22	A	810	CLA	C11-C10-C8	-3.54	104.47	115.92
29	1	601	CHL	O2D-CGD-O1D	-3.54	116.91	123.84
22	2	613	CLA	CAC-C3C-C4C	3.54	129.40	124.81
22	A	824	CLA	C3B-C4B-NB	3.54	113.80	110.52
22	A	835	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
22	8	614	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
22	A	816	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
22	5	610	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
22	B	804	CLA	C4A-NA-C1A	-3.54	105.12	106.71
22	A	802	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
22	2	610	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
22	F	304	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
22	4	614	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
22	B	837	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
22	A	814	CLA	C1-O2A-CGA	3.53	125.71	116.44
22	A	822	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
22	8	604	CLA	C4A-NA-C1A	-3.53	105.12	106.71
22	6	610	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
29	4	607	CHL	C3D-C4D-ND	3.53	115.94	110.24
22	B	838	CLA	C1D-CHD-C4C	-3.53	118.45	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	609	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
25	B	846	BCR	C24-C23-C22	-3.52	120.91	126.23
22	8	613	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
29	5	608	CHL	C3C-C4C-NC	3.52	114.52	110.57
22	B	826	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
22	8	608	CLA	CHD-C4C-NC	3.52	129.75	124.20
22	4	611	CLA	CAC-C3C-C4C	3.52	129.38	124.81
22	2	613	CLA	C3B-C4B-NB	3.52	113.78	110.52
22	6	610	CLA	C3C-C4C-NC	3.52	114.52	110.57
30	6	624	LUT	C15-C14-C13	-3.52	122.29	127.31
22	B	803	CLA	CAA-C2A-C3A	-3.51	103.15	112.78
22	A	854	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
22	B	816	CLA	CHD-C4C-NC	3.51	129.74	124.20
22	A	829	CLA	CMC-C2C-C1C	3.51	130.39	125.04
25	K	4001	BCR	C3-C4-C5	-3.51	107.80	114.08
22	1	604	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
22	B	805	CLA	O2A-CGA-CBA	3.51	122.93	111.91
22	A	814	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
30	Z	617	LUT	C10-C11-C12	-3.51	112.27	123.22
22	Z	603	CLA	C3C-C4C-NC	3.51	114.50	110.57
22	3	604	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
22	A	813	CLA	C1-O2A-CGA	3.51	125.64	116.44
24	A	846	LHG	O7-C7-C8	3.51	119.06	111.50
22	9	603	CLA	C3B-C4B-NB	3.51	113.77	110.52
29	Z	607	CHL	C3B-C4B-NB	3.50	113.77	110.52
22	B	802	CLA	C4C-C3C-C2C	-3.50	101.79	106.90
22	A	822	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
22	A	840	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
22	A	807	CLA	C3B-C4B-NB	3.50	113.77	110.52
30	1	617	LUT	C35-C34-C33	-3.50	122.31	127.31
22	A	813	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
22	6	601	CLA	C3C-C4C-NC	3.50	114.50	110.57
22	B	814	CLA	C3C-C4C-NC	3.50	114.50	110.57
22	5	621	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
25	A	848	BCR	C28-C27-C26	-3.50	107.83	114.08
22	6	601	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
25	A	849	BCR	C20-C21-C22	-3.50	122.32	127.31
30	1	617	LUT	C10-C11-C12	-3.50	112.30	123.22
22	B	823	CLA	O2D-CGD-CBD	3.50	117.48	111.27
22	2	609	CLA	C3C-C4C-NC	3.50	114.49	110.57
22	4	611	CLA	C3C-C4C-NC	3.50	114.49	110.57
22	Z	612	CLA	C3B-C4B-NB	3.49	113.76	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	602	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
22	9	614	CLA	C3C-C4C-NC	3.49	114.49	110.57
22	2	601	CLA	O2D-CGD-CBD	3.49	117.47	111.27
22	6	617	CLA	CAA-C2A-C3A	-3.49	103.22	112.78
30	6	621	LUT	C35-C15-C14	-3.49	116.32	123.47
22	A	803	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
22	B	841	CLA	C1-C2-C3	-3.49	120.01	126.04
22	9	610	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
22	5	614	CLA	CAC-C3C-C4C	3.49	129.34	124.81
22	2	601	CLA	C3B-C4B-NB	3.49	113.75	110.52
22	A	805	CLA	C3C-C4C-NC	3.49	114.48	110.57
22	G	203	CLA	C3B-C4B-NB	3.49	113.75	110.52
22	Z	613	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
22	A	804	CLA	C3D-C2D-C1D	-3.48	101.08	105.83
22	6	610	CLA	CAA-C2A-C3A	-3.48	103.24	112.78
22	9	602	CLA	CAC-C3C-C4C	3.48	129.33	124.81
22	Z	609	CLA	CAA-C2A-C3A	-3.48	103.24	112.78
22	A	841	CLA	O2A-CGA-CBA	3.48	122.84	111.91
22	K	4003	CLA	C3B-C4B-NB	3.48	113.75	110.52
29	Z	601	CHL	C3D-C4D-ND	3.48	115.87	110.24
22	6	609	CLA	C3B-C4B-NB	3.48	113.74	110.52
22	A	815	CLA	C3C-C4C-NC	3.48	114.47	110.57
22	7	609	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
29	8	607	CHL	C3D-C4D-ND	3.48	115.86	110.24
25	B	845	BCR	C34-C9-C10	-3.48	118.05	122.92
29	Z	601	CHL	C1D-CHD-C4C	-3.48	118.56	126.06
22	B	837	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
22	B	816	CLA	CAC-C3C-C4C	3.47	129.32	124.81
22	B	824	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
25	B	846	BCR	C11-C10-C9	-3.47	122.36	127.31
29	3	608	CHL	CBC-CAC-C3C	-3.47	102.86	112.43
22	A	845	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
22	A	827	CLA	O2D-CGD-CBD	3.47	117.44	111.27
22	2	609	CLA	CAA-C2A-C3A	-3.47	103.27	112.78
22	5	604	CLA	C3C-C4C-NC	3.47	114.46	110.57
22	Z	604	CLA	C3B-C4B-NB	3.47	113.73	110.52
22	1	610	CLA	C2C-C1C-NC	3.47	113.22	109.97
22	L	204	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
25	5	625	BCR	C23-C22-C21	-3.46	113.62	118.94
22	L	203	CLA	CMB-C2B-C1B	3.46	130.65	125.37
22	9	604	CLA	C3B-C4B-NB	3.46	113.73	110.52
22	B	809	CLA	CAA-C2A-C3A	-3.46	103.30	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	610	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
30	1	619	LUT	C31-C30-C29	-3.46	122.37	127.31
22	L	204	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
22	B	832	CLA	O2A-CGA-CBA	3.46	122.75	111.91
22	B	836	CLA	CAC-C3C-C4C	3.46	129.29	124.81
22	K	4003	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
22	B	820	CLA	C3C-C4C-NC	3.46	114.45	110.57
22	B	852	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
22	3	602	CLA	CAC-C3C-C4C	3.45	129.29	124.81
22	B	829	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
22	Z	609	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
22	9	604	CLA	CAC-C3C-C4C	3.45	129.28	124.81
21	A	801	CL0	O2A-CGA-CBA	3.45	122.73	111.91
22	A	832	CLA	CAC-C3C-C4C	3.45	129.28	124.81
25	3	717	BCR	C16-C17-C18	-3.45	122.39	127.31
22	6	613	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
30	9	617	LUT	C35-C15-C14	-3.44	116.42	123.47
22	5	616	CLA	O2D-CGD-CBD	3.44	117.38	111.27
22	A	817	CLA	CHC-C1C-C2C	-3.44	117.18	126.73
22	5	604	CLA	C3B-C4B-NB	3.44	113.71	110.52
25	A	856	BCR	C38-C26-C25	-3.44	120.67	124.53
25	F	305	BCR	C33-C5-C6	-3.44	120.67	124.53
29	Z	601	CHL	CAC-C3C-C4C	3.44	129.27	124.81
25	B	801	BCR	C11-C10-C9	-3.43	122.41	127.31
22	A	830	CLA	C1-C2-C3	-3.43	120.10	126.04
22	9	614	CLA	C3B-C4B-NB	3.43	113.70	110.52
22	B	833	CLA	CAA-C2A-C3A	-3.43	103.37	112.78
22	7	610	CLA	CMC-C2C-C1C	3.43	130.26	125.04
25	B	847	BCR	C21-C20-C19	-3.43	112.51	123.22
22	A	812	CLA	C3B-C4B-NB	3.43	113.70	110.52
22	9	601	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
22	7	610	CLA	CHD-C4C-NC	3.43	129.60	124.20
22	A	830	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
22	5	603	CLA	C3D-C4D-ND	3.43	115.78	110.24
22	A	802	CLA	C1-C2-C3	-3.43	120.12	126.04
22	A	818	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
25	K	4001	BCR	C32-C1-C6	-3.42	104.75	110.30
22	F	303	CLA	CAC-C3C-C4C	3.42	129.25	124.81
22	1	606	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
22	A	809	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
27	B	850	DGD	C2G-O2G-C1B	-3.42	109.37	117.79
22	A	814	CLA	C1D-CHD-C4C	-3.42	118.68	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	840	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
22	B	830	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
22	A	835	CLA	C3C-C4C-NC	3.41	114.40	110.57
30	Z	618	LUT	C10-C11-C12	-3.41	112.57	123.22
22	4	601	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
22	B	818	CLA	C3C-C4C-NC	3.41	114.39	110.57
22	F	303	CLA	CAA-C2A-C3A	-3.41	103.45	112.78
22	B	802	CLA	CMA-C3A-C2A	-3.40	100.10	113.83
22	A	825	CLA	O2A-CGA-CBA	3.40	122.59	111.91
22	B	828	CLA	CHC-C1C-C2C	-3.40	117.28	126.73
22	B	827	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
22	3	610	CLA	CAC-C3C-C4C	3.40	129.22	124.81
30	5	620	LUT	C8-C7-C6	-3.40	117.67	127.20
22	5	604	CLA	CHC-C1C-C2C	-3.40	117.30	126.73
25	A	856	BCR	C15-C14-C13	-3.39	122.47	127.31
25	J	3003	BCR	C16-C17-C18	-3.39	122.47	127.31
25	B	848	BCR	C10-C11-C12	-3.39	112.63	123.22
25	B	846	BCR	C7-C8-C9	-3.39	121.11	126.23
25	A	856	BCR	C33-C5-C6	-3.39	120.72	124.53
22	3	609	CLA	C3B-C4B-NB	3.39	113.66	110.52
22	B	817	CLA	CAC-C3C-C4C	3.39	129.21	124.81
29	5	618	CHL	C3D-C4D-ND	3.39	115.72	110.24
22	A	819	CLA	C1-C2-C3	-3.39	120.18	126.04
22	A	817	CLA	C3B-C2B-C1B	-3.39	103.07	107.16
22	A	817	CLA	CBC-CAC-C3C	-3.38	103.10	112.43
22	9	614	CLA	CAC-C3C-C4C	3.38	129.20	124.81
30	3	622	LUT	C2-C3-C4	3.38	114.94	110.30
22	8	612	CLA	C3B-C4B-NB	3.38	113.65	110.52
22	8	612	CLA	C4-C3-C5	3.38	120.96	115.27
29	5	618	CHL	C3B-C4B-NB	3.38	113.65	110.52
22	A	831	CLA	CHC-C1C-C2C	-3.38	117.35	126.73
22	A	845	CLA	C4C-C3C-C2C	-3.38	101.98	106.90
22	A	803	CLA	CAC-C3C-C4C	3.37	129.19	124.81
22	A	838	CLA	C4-C3-C5	3.37	119.84	115.98
22	A	810	CLA	CMB-C2B-C1B	3.37	130.50	125.37
29	7	607	CHL	C3B-C4B-NB	3.37	113.64	110.52
22	1	602	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
22	1	603	CLA	CMB-C2B-C1B	3.37	130.50	125.37
22	6	622	CLA	CAC-C3C-C4C	3.37	129.18	124.81
22	B	810	CLA	C3B-C4B-NB	3.37	113.64	110.52
22	1	614	CLA	C3B-C4B-NB	3.37	113.64	110.52
22	7	604	CLA	CAC-C3C-C4C	3.36	129.17	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	718	BCR	C7-C8-C9	-3.36	121.15	126.23
29	6	608	CHL	CMB-C2B-C1B	3.36	130.49	125.37
22	7	609	CLA	C1-C2-C3	-3.36	121.32	126.75
25	3	719	BCR	C15-C14-C13	-3.36	122.52	127.31
22	A	828	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
22	A	841	CLA	CMA-C3A-C4A	-3.36	102.75	111.77
25	A	848	BCR	C7-C8-C9	-3.36	121.17	126.23
22	A	834	CLA	C4-C3-C5	3.36	120.92	115.27
22	1	613	CLA	C3B-C4B-NB	3.35	113.63	110.52
22	3	612	CLA	C3B-C4B-NB	3.35	113.63	110.52
22	7	611	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
29	6	618	CHL	C3D-C4D-ND	3.35	115.66	110.24
22	8	611	CLA	C3B-C4B-NB	3.35	113.63	110.52
22	5	613	CLA	CAC-C3C-C4C	3.35	129.16	124.81
22	2	603	CLA	CAC-C3C-C4C	3.35	129.16	124.81
22	7	603	CLA	CAA-C2A-C3A	-3.35	103.60	112.78
22	A	825	CLA	CHC-C1C-C2C	-3.35	117.42	126.73
22	A	827	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
22	4	611	CLA	C3B-C4B-NB	3.35	113.62	110.52
22	A	805	CLA	C1-C2-C3	-3.35	120.26	126.04
25	B	847	BCR	C24-C23-C22	-3.35	121.18	126.23
22	4	612	CLA	C3B-C4B-NB	3.34	113.62	110.52
22	1	609	CLA	O2A-CGA-CBA	3.34	122.39	111.91
22	A	845	CLA	C3B-C4B-NB	3.34	113.61	110.52
29	4	618	CHL	C2A-C3A-C4A	-3.34	96.48	101.87
22	Z	603	CLA	CHC-C1C-C2C	-3.34	117.46	126.73
22	5	613	CLA	CHC-C1C-C2C	-3.34	117.46	126.73
22	A	806	CLA	C3C-C4C-NC	3.34	114.31	110.57
22	A	819	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
22	5	602	CLA	CMC-C2C-C1C	3.34	130.12	125.04
22	Z	602	CLA	CAC-C3C-C4C	3.33	129.14	124.81
22	B	823	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
22	2	611	CLA	C3B-C4B-NB	3.33	113.61	110.52
22	7	616	CLA	C3C-C4C-NC	3.33	114.31	110.57
22	B	817	CLA	CHC-C1C-C2C	-3.33	117.48	126.73
30	Z	617	LUT	C30-C31-C32	-3.33	112.82	123.22
22	B	804	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
22	B	837	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
22	Z	609	CLA	C3C-C4C-NC	3.33	114.30	110.57
22	3	612	CLA	CHC-C1C-C2C	-3.33	117.48	126.73
22	6	609	CLA	CHC-C1C-C2C	-3.33	117.49	126.73
29	6	618	CHL	C3B-C4B-NB	3.33	113.60	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	608	CHL	C2A-C3A-C4A	-3.33	96.49	101.87
22	8	613	CLA	CAC-C3C-C4C	3.32	129.12	124.81
25	B	844	BCR	C11-C10-C9	-3.32	122.57	127.31
22	B	818	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
29	8	607	CHL	C3B-C4B-NB	3.32	113.60	110.52
22	Z	604	CLA	CAC-C3C-C4C	3.32	129.12	124.81
22	A	831	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	7	604	CLA	C3B-C4B-NB	3.32	113.59	110.52
22	A	831	CLA	C4-C3-C5	3.32	120.85	115.27
22	1	609	CLA	C3C-C4C-NC	3.31	114.29	110.57
22	3	607	CLA	O2A-CGA-CBA	3.31	122.31	111.91
22	5	602	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
30	8	618	LUT	C35-C34-C33	-3.31	122.58	127.31
22	5	603	CLA	C3B-C4B-NB	3.31	113.59	110.52
29	5	607	CHL	CAC-C3C-C4C	3.31	129.10	124.81
22	9	612	CLA	C3B-C4B-NB	3.31	113.58	110.52
22	A	839	CLA	C4-C3-C5	3.31	120.84	115.27
22	B	809	CLA	CHC-C1C-C2C	-3.31	117.54	126.73
29	9	606	CHL	C3D-C4D-ND	3.31	115.59	110.24
22	5	606	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
22	A	804	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
22	5	611	CLA	C3B-C4B-NB	3.30	113.58	110.52
29	6	608	CHL	C3D-C4D-ND	3.30	115.58	110.24
22	3	603	CLA	CAA-C2A-C3A	-3.30	103.73	112.78
22	A	802	CLA	C3C-C4C-NC	3.30	114.28	110.57
22	A	838	CLA	CHC-C1C-C2C	-3.30	117.56	126.73
22	3	602	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
22	4	616	CLA	CHC-C1C-C2C	-3.30	117.56	126.73
22	F	304	CLA	CAA-C2A-C3A	-3.30	103.73	112.78
22	B	802	CLA	C3B-C4B-NB	3.30	113.58	110.52
22	B	838	CLA	C4A-NA-C1A	-3.30	105.22	106.71
22	6	613	CLA	CAC-C3C-C4C	3.30	129.09	124.81
22	9	613	CLA	CAC-C3C-C4C	3.30	129.09	124.81
22	A	821	CLA	CHC-C1C-C2C	-3.30	117.57	126.73
22	9	602	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
22	B	831	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
22	4	602	CLA	C3C-C4C-NC	3.30	114.27	110.57
22	A	825	CLA	CMB-C2B-C1B	3.30	130.39	125.37
22	3	614	CLA	C3B-C4B-NB	3.30	113.57	110.52
22	B	833	CLA	CMB-C2B-C1B	3.30	130.39	125.37
22	A	834	CLA	C1-C2-C3	-3.29	120.35	126.04
25	8	619	BCR	C11-C10-C9	-3.29	122.61	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	819	CLA	CAC-C3C-C4C	3.29	129.08	124.81
22	8	603	CLA	C3B-C4B-NB	3.29	113.57	110.52
22	5	612	CLA	CHC-C1C-C2C	-3.29	117.59	126.73
22	5	602	CLA	CHD-C4C-NC	3.29	129.39	124.20
22	B	819	CLA	C3C-C4C-NC	3.29	114.26	110.57
22	5	617	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
30	1	619	LUT	C10-C11-C12	-3.29	112.96	123.22
22	3	611	CLA	C3B-C4B-NB	3.29	113.56	110.52
22	G	204	CLA	C3B-C4B-NB	3.29	113.56	110.52
22	B	829	CLA	CMA-C3A-C2A	-3.29	100.57	113.83
22	1	613	CLA	C4A-NA-C1A	-3.29	105.23	106.71
22	5	617	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
22	B	815	CLA	C3B-C4B-NB	3.28	113.56	110.52
22	5	611	CLA	CAA-C2A-C3A	-3.28	103.79	112.78
22	4	610	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
22	7	610	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
22	4	610	CLA	CHC-C1C-C2C	-3.28	117.62	126.73
22	Z	602	CLA	C4-C3-C5	3.28	120.79	115.27
22	B	841	CLA	C3C-C4C-NC	3.28	114.25	110.57
22	3	613	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
22	B	803	CLA	CHC-C1C-C2C	-3.28	117.62	126.73
22	B	828	CLA	CAC-C3C-C4C	3.28	129.06	124.81
22	7	613	CLA	CAC-C3C-C4C	3.28	129.06	124.81
22	4	601	CLA	CHC-C1C-C2C	-3.28	117.63	126.73
22	Z	610	CLA	C1-C2-C3	-3.28	120.38	126.04
22	A	840	CLA	CAC-C3C-C4C	3.28	129.06	124.81
22	4	603	CLA	CHC-C1C-C2C	-3.28	117.63	126.73
25	A	851	BCR	C20-C21-C22	-3.28	122.64	127.31
25	B	845	BCR	C15-C14-C13	-3.27	122.64	127.31
22	1	610	CLA	CAC-C3C-C4C	3.27	129.06	124.81
22	1	610	CLA	CHD-C4C-NC	3.27	129.36	124.20
21	A	801	CL0	C1-C2-C3	-3.27	120.38	126.04
25	L	201	BCR	C16-C17-C18	-3.27	122.64	127.31
22	4	604	CLA	C3C-C4C-NC	3.27	114.24	110.57
30	3	622	LUT	C18-C5-C6	-3.27	120.85	124.53
25	F	305	BCR	C15-C16-C17	-3.27	116.77	123.47
25	L	201	BCR	C34-C9-C10	-3.27	118.34	122.92
22	9	603	CLA	CAC-C3C-C4C	3.27	129.05	124.81
22	3	610	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
22	5	601	CLA	O2A-CGA-CBA	3.27	122.16	111.91
22	A	816	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
22	G	203	CLA	CAC-C3C-C4C	3.26	129.05	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	616	CLA	CAC-C3C-C4C	3.26	129.05	124.81
22	6	616	CLA	C1C-C2C-C3C	-3.26	103.52	106.96
22	A	822	CLA	C1-O2A-CGA	3.26	125.01	116.44
22	B	840	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
22	A	842	CLA	CMB-C2B-C1B	3.26	130.34	125.37
22	L	204	CLA	CAC-C3C-C4C	3.26	129.04	124.81
22	A	809	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	A	830	CLA	CAC-C3C-C4C	3.26	129.04	124.81
22	B	802	CLA	CHD-C4C-NC	3.26	129.34	124.20
22	B	822	CLA	C3B-C4B-NB	3.26	113.54	110.52
22	5	621	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
29	Z	601	CHL	C2A-C1A-CHA	-3.26	118.16	123.86
22	3	614	CLA	CAC-C3C-C4C	3.26	129.04	124.81
22	7	616	CLA	C3B-C4B-NB	3.26	113.54	110.52
22	7	611	CLA	CHC-C1C-C2C	-3.26	117.69	126.73
22	A	826	CLA	CHC-C1C-C2C	-3.26	117.69	126.73
22	7	602	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
22	5	616	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
30	7	621	LUT	C35-C15-C14	-3.25	116.81	123.47
29	4	606	CHL	CAC-C3C-C4C	3.25	129.03	124.81
22	B	804	CLA	CHB-C4A-NA	3.25	129.01	124.51
30	8	618	LUT	C10-C11-C12	-3.25	113.07	123.22
22	B	834	CLA	C3C-C4C-NC	3.25	114.22	110.57
22	A	811	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
22	A	808	CLA	CMC-C2C-C1C	3.25	129.98	125.04
22	5	609	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
25	G	205	BCR	C11-C10-C9	-3.25	122.68	127.31
22	8	604	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
25	6	625	BCR	C16-C17-C18	-3.25	122.68	127.31
22	B	829	CLA	C4A-NA-C1A	-3.25	105.25	106.71
22	7	610	CLA	C2C-C1C-NC	3.25	113.01	109.97
22	B	834	CLA	CAC-C3C-C4C	3.24	129.02	124.81
29	4	618	CHL	C3D-C4D-ND	3.24	115.48	110.24
22	A	831	CLA	CAC-C3C-C4C	3.24	129.02	124.81
22	B	821	CLA	C3B-C4B-NB	3.24	113.52	110.52
22	B	814	CLA	CMB-C2B-C1B	3.24	130.31	125.37
22	8	616	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
22	7	608	CLA	CHD-C4C-NC	3.24	129.31	124.20
22	5	617	CLA	CAC-C3C-C4C	3.24	129.01	124.81
22	8	611	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
22	7	601	CLA	CHB-C1B-NB	-3.24	120.83	124.26
22	1	602	CLA	CHD-C4C-NC	3.24	129.30	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	610	CLA	CHD-C4C-NC	3.24	129.30	124.20
22	A	837	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
22	B	836	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
22	3	609	CLA	CHB-C4A-NA	3.24	128.99	124.51
22	1	612	CLA	C3B-C4B-NB	3.23	113.52	110.52
22	8	604	CLA	C3B-C4B-NB	3.23	113.52	110.52
22	B	816	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
22	3	613	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
22	7	616	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
22	9	601	CLA	C3B-C4B-NB	3.23	113.51	110.52
22	B	839	CLA	C3B-C4B-NB	3.23	113.51	110.52
22	A	841	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
22	A	817	CLA	C3C-C4C-NC	3.23	114.19	110.57
22	6	617	CLA	C3B-C4B-NB	3.23	113.51	110.52
29	9	607	CHL	C3B-C4B-NB	3.23	113.51	110.52
25	6	623	BCR	C16-C17-C18	-3.23	122.71	127.31
22	4	602	CLA	CAC-C3C-C4C	3.22	128.99	124.81
22	6	611	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
22	A	835	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
29	3	608	CHL	CHD-C4C-NC	3.22	129.28	124.20
25	4	621	BCR	C15-C16-C17	-3.22	116.88	123.47
22	2	602	CLA	CAC-C3C-C4C	3.22	128.99	124.81
22	7	604	CLA	CMC-C2C-C1C	3.22	129.94	125.04
22	4	604	CLA	C1-C2-C3	-3.22	121.55	126.75
22	7	616	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
22	1	609	CLA	CHC-C1C-C2C	-3.22	117.80	126.73
22	3	609	CLA	CAC-C3C-C4C	3.22	128.98	124.81
22	2	612	CLA	CHC-C1C-C2C	-3.22	117.80	126.73
22	3	610	CLA	CMA-C3A-C2A	-3.21	100.86	113.83
30	1	617	LUT	C30-C31-C32	-3.21	113.19	123.22
22	B	830	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
22	Z	606	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
29	Z	607	CHL	C3D-C4D-ND	3.21	115.43	110.24
22	L	204	CLA	C3B-C4B-NB	3.21	113.49	110.52
22	5	610	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
22	8	609	CLA	C3B-C4B-NB	3.21	113.49	110.52
22	9	609	CLA	C3B-C4B-NB	3.21	113.49	110.52
25	A	848	BCR	C16-C15-C14	-3.21	116.90	123.47
30	2	617	LUT	C7-C8-C9	-3.21	121.39	126.23
25	I	172	BCR	C20-C19-C18	-3.21	117.41	126.42
22	7	614	CLA	C3B-C4B-NB	3.21	113.49	110.52
22	2	609	CLA	CHC-C1C-C2C	-3.21	117.83	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	J	3003	BCR	C3-C4-C5	-3.21	108.35	114.08
22	4	611	CLA	CHC-C1C-C2C	-3.20	117.83	126.73
22	A	804	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
22	B	818	CLA	C4-C3-C5	3.20	120.66	115.27
22	A	842	CLA	C3B-C4B-NB	3.20	113.49	110.52
22	9	613	CLA	CHC-C1C-C2C	-3.20	117.83	126.73
22	B	820	CLA	C1-C2-C3	-3.20	120.50	126.04
22	A	816	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
22	1	609	CLA	CAC-C3C-C4C	3.20	128.97	124.81
25	J	3003	BCR	C38-C26-C25	-3.20	120.93	124.53
22	B	829	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	3	611	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	Z	616	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	A	807	CLA	O2A-CGA-CBA	3.20	121.95	111.91
22	B	832	CLA	CHD-C4C-NC	3.20	129.24	124.20
22	A	829	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	B	837	CLA	CMB-C2B-C1B	3.20	130.24	125.37
29	8	607	CHL	CAC-C3C-C4C	3.20	128.96	124.81
22	4	601	CLA	C3C-C4C-NC	3.20	114.16	110.57
22	A	836	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
22	8	603	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
22	A	826	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	4	609	CLA	CHC-C1C-C2C	-3.20	117.86	126.73
22	9	604	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
22	3	603	CLA	O2D-CGD-CBD	3.19	116.94	111.27
22	1	611	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
22	F	304	CLA	CAC-C3C-C4C	3.19	128.95	124.81
22	5	614	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
22	B	824	CLA	CAC-C3C-C4C	3.19	128.95	124.81
22	7	609	CLA	O2D-CGD-CBD	3.19	116.94	111.27
21	A	801	CL0	CBC-CAC-C3C	-3.19	103.63	112.43
22	9	603	CLA	CHC-C1C-C2C	-3.19	117.87	126.73
25	B	847	BCR	C15-C14-C13	-3.19	122.76	127.31
22	1	604	CLA	CAC-C3C-C4C	3.19	128.94	124.81
22	6	601	CLA	C3B-C4B-NB	3.19	113.47	110.52
29	1	601	CHL	O2A-C1-C2	3.19	117.01	108.64
25	B	847	BCR	C16-C17-C18	-3.19	122.76	127.31
22	5	616	CLA	C3B-C4B-NB	3.19	113.47	110.52
22	A	831	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
22	6	603	CLA	CHC-C1C-C2C	-3.18	117.88	126.73
22	3	603	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	1	616	CLA	C3B-C4B-NB	3.18	113.47	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	807	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	A	839	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
22	1	603	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	1	616	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
22	A	837	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	1	606	CLA	C4-C3-C5	3.18	120.62	115.27
22	A	804	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
22	B	829	CLA	C3B-C4B-NB	3.18	113.47	110.52
22	A	802	CLA	C2A-C1A-CHA	-3.18	118.30	123.86
22	G	204	CLA	CAC-C3C-C4C	3.18	128.93	124.81
22	2	611	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
22	A	809	CLA	C1-C2-C3	-3.18	120.55	126.04
30	Z	618	LUT	C15-C14-C13	-3.17	122.78	127.31
22	9	611	CLA	C4-C3-C5	3.17	120.61	115.27
22	B	833	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
22	5	611	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
22	1	612	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
22	9	610	CLA	CAC-C3C-C4C	3.17	128.92	124.81
22	7	613	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
22	Z	610	CLA	CHD-C4C-NC	3.17	129.20	124.20
22	3	606	CLA	CHC-C1C-C2C	-3.17	117.93	126.73
30	6	621	LUT	C7-C8-C9	-3.17	121.45	126.23
22	A	845	CLA	CHC-C1C-C2C	-3.17	117.93	126.73
22	B	810	CLA	CHC-C1C-C2C	-3.17	117.94	126.73
22	1	604	CLA	C3B-C4B-NB	3.17	113.45	110.52
22	G	203	CLA	C1-C2-C3	-3.17	121.63	126.75
21	A	801	CL0	CHC-C1C-C2C	-3.17	117.94	126.73
25	I	172	BCR	C16-C17-C18	-3.17	122.79	127.31
30	1	617	LUT	C35-C15-C14	-3.16	116.99	123.47
29	6	608	CHL	C2A-C1A-CHA	-3.16	118.33	123.86
22	7	612	CLA	CHC-C1C-C2C	-3.16	117.94	126.73
22	A	835	CLA	C1-C2-C3	-3.16	120.57	126.04
22	3	620	CLA	C3B-C4B-NB	3.16	113.45	110.52
25	L	205	BCR	C28-C27-C26	-3.16	108.43	114.08
25	6	623	BCR	C11-C12-C13	-3.16	117.53	126.42
22	3	604	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
22	A	812	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
22	B	808	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
22	5	611	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	B	826	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
22	B	832	CLA	CMB-C2B-C1B	3.16	130.18	125.37
22	A	811	CLA	CAC-C3C-C4C	3.16	128.91	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	620	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
25	A	850	BCR	C24-C23-C22	-3.16	121.46	126.23
22	B	825	CLA	CHD-C4C-NC	3.16	129.18	124.20
22	A	816	CLA	CAC-C3C-C4C	3.16	128.91	124.81
22	B	826	CLA	C3B-C4B-NB	3.16	113.44	110.52
25	L	205	BCR	C29-C30-C25	3.16	115.34	110.48
22	Z	603	CLA	CAC-C3C-C4C	3.16	128.91	124.81
22	B	808	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
22	B	807	CLA	CHC-C1C-C2C	-3.16	117.96	126.73
22	1	603	CLA	CHC-C1C-C2C	-3.16	117.96	126.73
22	9	610	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
22	A	806	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
22	5	616	CLA	CHC-C1C-C2C	-3.15	117.97	126.73
22	B	810	CLA	CAC-C3C-C4C	3.15	128.90	124.81
22	B	807	CLA	O2A-CGA-CBA	3.15	121.80	111.91
22	4	613	CLA	CAC-C3C-C4C	3.15	128.90	124.81
22	1	604	CLA	C3C-C4C-NC	3.15	114.10	110.57
22	B	830	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	B	819	CLA	CAA-C2A-C3A	-3.15	104.15	112.78
22	Z	606	CLA	C4-C3-C5	3.15	120.57	115.27
22	2	601	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
29	4	618	CHL	CAC-C3C-C4C	3.15	128.89	124.81
22	B	806	CLA	CHD-C4C-NC	3.15	129.16	124.20
22	A	843	CLA	C3B-C4B-NB	3.15	113.44	110.52
22	1	613	CLA	CAC-C3C-C4C	3.15	128.89	124.81
22	A	811	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	A	832	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	B	833	CLA	CAC-C3C-C4C	3.15	128.89	124.81
22	2	613	CLA	O2A-CGA-CBA	3.15	121.78	111.91
22	B	839	CLA	CAC-C3C-C4C	3.15	128.89	124.81
22	Z	604	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
22	Z	609	CLA	CAC-C3C-C4C	3.14	128.89	124.81
22	8	610	CLA	CMC-C2C-C1C	3.14	129.83	125.04
22	L	204	CLA	C4C-C3C-C2C	-3.14	102.31	106.90
22	Z	616	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
22	3	609	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
22	A	811	CLA	C1C-C2C-C3C	-3.14	103.65	106.96
22	A	815	CLA	C1-C2-C3	-3.14	120.61	126.04
22	2	613	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
22	J	3002	CLA	C3B-C4B-NB	3.14	113.43	110.52
29	5	618	CHL	CAC-C3C-C4C	3.14	128.88	124.81
22	A	839	CLA	CHC-C1C-C2C	-3.14	118.01	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	611	CLA	CAA-C2A-C3A	-3.14	104.18	112.78
22	4	613	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
22	1	616	CLA	CAC-C3C-C4C	3.14	128.88	124.81
22	A	843	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
22	1	606	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
25	A	851	BCR	C21-C20-C19	-3.14	113.43	123.22
22	Z	608	CLA	C3B-C4B-NB	3.14	113.42	110.52
22	8	609	CLA	CHC-C1C-C2C	-3.14	118.02	126.73
22	B	804	CLA	C3B-C4B-NB	3.14	113.42	110.52
25	7	624	BCR	C28-C27-C26	-3.14	108.48	114.08
22	2	601	CLA	CAC-C3C-C4C	3.14	128.88	124.81
22	G	203	CLA	CHC-C1C-C2C	-3.14	118.02	126.73
22	A	841	CLA	CHC-C4B-NB	-3.13	120.94	124.26
22	4	601	CLA	CAC-C3C-C4C	3.13	128.88	124.81
22	9	601	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
22	Z	602	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
22	5	601	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
22	B	828	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
22	B	825	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
22	4	609	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	6	610	CLA	O2A-CGA-CBA	3.13	121.73	111.91
22	A	818	CLA	CHD-C4C-NC	3.13	129.14	124.20
29	1	601	CHL	C1-C2-C3	3.13	131.46	126.04
29	6	607	CHL	C4-C3-C5	3.13	120.53	115.27
22	B	819	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
22	A	816	CLA	C4A-NA-C1A	-3.13	105.30	106.71
22	A	806	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
22	B	824	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
22	7	609	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
22	A	826	CLA	C4-C3-C5	3.13	120.53	115.27
22	6	603	CLA	CAC-C3C-C4C	3.13	128.87	124.81
22	L	204	CLA	CMB-C2B-C1B	3.13	130.13	125.37
22	F	303	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
22	B	831	CLA	CHD-C4C-NC	3.12	129.13	124.20
22	A	829	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
22	7	614	CLA	CAC-C3C-C4C	3.12	128.86	124.81
22	1	613	CLA	CMB-C2B-C1B	3.12	130.12	125.37
22	5	621	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
22	9	612	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
22	A	833	CLA	C4-C3-C5	3.12	120.52	115.27
22	9	609	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
22	B	836	CLA	C4C-C3C-C2C	-3.12	102.35	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	717	BCR	C15-C14-C13	-3.12	122.86	127.31
22	A	829	CLA	CMB-C2B-C1B	3.12	130.12	125.37
22	B	804	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
22	A	811	CLA	C3B-C4B-NB	3.12	113.41	110.52
22	3	610	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
22	B	823	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
22	6	611	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
22	Z	604	CLA	C4-C3-C5	3.12	120.52	115.27
22	1	606	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
22	Z	602	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
22	2	607	CLA	CAC-C3C-C4C	3.12	128.85	124.81
30	2	616	LUT	C15-C14-C13	-3.12	122.86	127.31
22	A	804	CLA	C3B-C4B-NB	3.12	113.41	110.52
30	5	624	LUT	C10-C11-C12	-3.11	113.50	123.22
22	7	611	CLA	CAC-C3C-C4C	3.11	128.85	124.81
22	7	612	CLA	O2A-CGA-CBA	3.11	121.67	111.91
22	A	840	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
29	6	606	CHL	C3D-C4D-ND	3.11	115.27	110.24
22	6	602	CLA	CHD-C4C-NC	3.11	129.10	124.20
22	B	827	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
22	6	613	CLA	C3B-C4B-NB	3.11	113.40	110.52
22	7	606	CLA	CHD-C4C-NC	3.11	129.10	124.20
25	7	623	BCR	C38-C26-C27	3.11	119.58	113.62
22	7	614	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
22	A	805	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
29	1	607	CHL	C3B-C4B-NB	3.11	113.40	110.52
22	8	610	CLA	C1-C2-C3	-3.11	120.67	126.04
22	7	606	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
29	6	606	CHL	CAC-C3C-C4C	3.11	128.84	124.81
22	B	852	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
22	B	808	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
22	6	622	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
22	8	611	CLA	C4A-NA-C1A	-3.10	105.31	106.71
22	B	808	CLA	CBA-CAA-C2A	3.10	123.02	113.86
22	7	603	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	Z	611	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	6	602	CLA	CMC-C2C-C1C	3.10	129.76	125.04
22	7	609	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
22	6	614	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	1	604	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
22	Z	612	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
22	A	804	CLA	C1-C2-C3	-3.10	120.68	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	842	CLA	C4-C3-C5	3.10	120.48	115.27
22	B	813	CLA	O2A-CGA-CBA	3.10	121.63	111.91
22	8	601	CLA	CAC-C3C-C4C	3.10	128.83	124.81
22	2	607	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	A	836	CLA	CAC-C3C-C4C	3.10	128.83	124.81
22	B	808	CLA	CAC-C3C-C4C	3.10	128.83	124.81
29	6	606	CHL	C4-C3-C5	3.10	120.48	115.27
22	7	614	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	8	609	CLA	CHB-C4A-NA	3.10	128.79	124.51
22	1	614	CLA	CHC-C1C-C2C	-3.09	118.13	126.73
30	9	616	LUT	C10-C11-C12	-3.09	113.56	123.22
22	Z	616	CLA	C3B-C4B-NB	3.09	113.39	110.52
22	A	817	CLA	CAC-C3C-C4C	3.09	128.82	124.81
30	1	617	LUT	C15-C14-C13	-3.09	122.90	127.31
22	6	616	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
22	G	203	CLA	O2A-CGA-CBA	3.09	121.61	111.91
22	A	803	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
22	A	839	CLA	CAC-C3C-C4C	3.09	128.82	124.81
25	B	801	BCR	C15-C16-C17	3.09	129.80	123.47
25	6	625	BCR	C15-C16-C17	-3.09	117.15	123.47
22	A	814	CLA	CHC-C1C-C2C	-3.09	118.16	126.73
22	A	818	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
22	3	617	CLA	CAA-C2A-C3A	-3.09	104.33	112.78
30	9	617	LUT	C10-C11-C12	-3.09	113.59	123.22
22	A	834	CLA	CHD-C4C-NC	3.09	129.06	124.20
22	B	804	CLA	CMA-C3A-C4A	-3.08	103.48	111.77
22	B	811	CLA	CHC-C1C-C2C	-3.08	118.16	126.73
22	3	603	CLA	CHC-C1C-C2C	-3.08	118.16	126.73
22	3	610	CLA	C1-C2-C3	-3.08	120.71	126.04
22	7	602	CLA	CHD-C4C-NC	3.08	129.06	124.20
25	3	719	BCR	C20-C21-C22	-3.08	122.91	127.31
22	6	611	CLA	CAC-C3C-C4C	3.08	128.81	124.81
22	4	604	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
22	8	613	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	2	614	CLA	CAC-C3C-C4C	3.08	128.81	124.81
22	4	612	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
22	A	841	CLA	CHB-C4A-NA	3.08	128.77	124.51
22	F	301	CLA	O2A-CGA-CBA	3.08	121.57	111.91
22	8	614	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
29	6	618	CHL	CAC-C3C-C4C	3.08	128.81	124.81
22	5	617	CLA	C3B-C4B-NB	3.08	113.37	110.52
22	B	824	CLA	O2A-CGA-CBA	3.08	121.57	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	612	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	A	834	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
22	A	813	CLA	CAC-C3C-C4C	3.08	128.80	124.81
22	A	832	CLA	C3B-C4B-NB	3.08	113.37	110.52
25	A	850	BCR	C20-C21-C22	-3.08	122.92	127.31
22	2	603	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
29	5	608	CHL	C2A-C3A-C4A	-3.07	96.90	101.87
22	B	820	CLA	C3B-C4B-NB	3.07	113.37	110.52
22	1	611	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
22	Z	611	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
22	9	611	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
22	A	814	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	K	4003	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
22	A	823	CLA	C3B-C4B-NB	3.07	113.36	110.52
25	A	856	BCR	C11-C10-C9	-3.07	122.93	127.31
22	9	611	CLA	C3B-C4B-NB	3.07	113.36	110.52
22	Z	610	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
29	4	606	CHL	CMB-C2B-C1B	3.07	130.04	125.37
22	B	836	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	A	830	CLA	C3B-C4B-NB	3.07	113.36	110.52
22	B	852	CLA	CAC-C3C-C4C	3.07	128.79	124.81
22	A	810	CLA	CAC-C3C-C4C	3.07	128.79	124.81
22	J	3002	CLA	CHC-C1C-C2C	-3.06	118.22	126.73
22	8	612	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
22	2	601	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
22	A	842	CLA	CHC-C1C-C2C	-3.06	118.22	126.73
22	7	616	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
22	B	814	CLA	CMA-C3A-C4A	-3.06	103.54	111.77
22	5	603	CLA	CHC-C1C-C2C	-3.06	118.22	126.73
22	4	602	CLA	CHC-C1C-C2C	-3.06	118.22	126.73
30	1	619	LUT	C19-C9-C8	3.06	122.90	118.08
22	2	612	CLA	C4-C3-C5	3.06	120.42	115.27
29	6	607	CHL	C3D-C4D-ND	3.06	115.19	110.24
22	8	606	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
22	B	833	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
22	B	825	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
22	2	612	CLA	CAC-C3C-C4C	3.06	128.78	124.81
22	6	601	CLA	CMB-C2B-C1B	3.06	130.03	125.37
22	A	808	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	A	848	BCR	C11-C10-C9	-3.06	122.94	127.31
22	6	609	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
22	8	614	CLA	O2A-CGA-CBA	3.06	121.51	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	815	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	7	601	CLA	O2A-CGA-O1A	-3.06	115.88	123.59
22	B	836	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
22	A	813	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
22	G	204	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
22	A	810	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
25	3	717	BCR	C24-C23-C22	-3.05	121.62	126.23
22	6	617	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
22	A	804	CLA	CHD-C4C-NC	3.05	129.01	124.20
22	A	812	CLA	C1-C2-C3	-3.05	120.76	126.04
30	4	619	LUT	C30-C31-C32	-3.05	113.69	123.22
22	F	304	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
22	B	827	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
22	B	824	CLA	CHD-C4C-NC	3.05	129.01	124.20
22	B	840	CLA	CMC-C2C-C3C	3.05	134.40	126.12
25	5	625	BCR	C37-C22-C23	3.05	122.88	118.08
22	7	609	CLA	CMB-C2B-C1B	3.05	130.01	125.37
29	5	607	CHL	C3D-C4D-ND	3.05	115.17	110.24
30	8	617	LUT	C39-C29-C28	3.05	122.88	118.08
22	B	815	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
29	9	606	CHL	CBC-CAC-C3C	-3.05	104.03	112.43
22	F	304	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
22	6	617	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
22	8	604	CLA	CAA-C2A-C3A	-3.05	104.43	112.78
29	9	607	CHL	C3D-C4D-ND	3.05	115.17	110.24
22	4	610	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	6	617	CLA	CAC-C3C-C4C	3.05	128.76	124.81
22	A	803	CLA	O2A-CGA-CBA	3.05	121.47	111.91
22	3	611	CLA	CHC-C1C-C2C	-3.04	118.27	126.73
22	1	610	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
22	B	835	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
22	7	603	CLA	CHD-C4C-NC	3.04	129.00	124.20
22	1	613	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
22	A	812	CLA	CAC-C3C-C4C	3.04	128.76	124.81
22	1	606	CLA	CHD-C4C-NC	3.04	129.00	124.20
22	B	813	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
22	B	841	CLA	O2A-CGA-CBA	3.04	121.45	111.91
22	B	823	CLA	CMA-C3A-C2A	-3.04	101.57	113.83
22	4	603	CLA	CAC-C3C-C4C	3.04	128.75	124.81
22	7	620	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
29	3	608	CHL	C3B-C4B-NB	3.04	113.33	110.52
22	Z	608	CLA	CHC-C1C-C2C	-3.04	118.29	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	801	CL0	CMA-C3A-C4A	-3.04	103.61	111.77
22	A	803	CLA	CMC-C2C-C1C	3.04	129.66	125.04
29	4	606	CHL	C3D-C4D-ND	3.04	115.15	110.24
22	8	602	CLA	CMB-C2B-C1B	3.03	129.99	125.37
29	1	601	CHL	O2A-CGA-CBA	3.03	121.43	111.91
22	9	610	CLA	C1-C2-C3	-3.03	120.80	126.04
22	9	609	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
22	B	833	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
22	A	843	CLA	C4-C3-C5	3.03	120.37	115.27
22	7	620	CLA	O2A-CGA-CBA	3.03	121.42	111.91
22	A	807	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
22	5	611	CLA	C4-C3-C5	3.03	120.37	115.27
22	6	601	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
22	7	603	CLA	CHC-C1C-C2C	-3.03	118.31	126.73
22	5	610	CLA	O2A-CGA-CBA	3.03	121.42	111.91
22	A	829	CLA	CHD-C4C-NC	3.03	128.98	124.20
25	A	851	BCR	C24-C23-C22	-3.03	121.66	126.23
22	7	610	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	5	609	CLA	O2A-CGA-CBA	3.03	121.42	111.91
22	B	830	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	4	621	BCR	C23-C24-C25	-3.03	118.70	127.20
22	3	606	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	A	821	CLA	C3B-C4B-NB	3.03	113.32	110.52
22	3	617	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
22	Z	602	CLA	CHD-C4C-NC	3.03	128.97	124.20
22	B	833	CLA	CHB-C1B-NB	-3.03	121.05	124.26
22	B	839	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
22	Z	603	CLA	C4-C3-C2	-3.03	115.92	123.68
22	8	616	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
22	B	821	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	B	830	CLA	C1-C2-C3	-3.02	121.86	126.75
22	5	602	CLA	CMB-C2B-C1B	3.02	129.97	125.37
22	2	602	CLA	C3B-C4B-NB	3.02	113.32	110.52
22	8	609	CLA	CMA-C3A-C4A	-3.02	103.65	111.77
22	Z	616	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
22	Z	606	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
30	4	620	LUT	C15-C14-C13	-3.02	123.00	127.31
22	B	814	CLA	CHD-C4C-NC	3.02	128.96	124.20
22	A	811	CLA	CMC-C2C-C1C	3.02	129.64	125.04
22	A	843	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	A	830	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
22	1	610	CLA	O2A-CGA-O1A	-3.02	115.97	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	824	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	A	808	CLA	CAC-C3C-C4C	3.02	128.73	124.81
22	B	811	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	B	805	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
22	2	606	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
22	7	613	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	B	824	CLA	CMC-C2C-C1C	3.02	129.63	125.04
30	Z	618	LUT	C7-C8-C9	-3.02	121.68	126.23
22	3	607	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
29	1	601	CHL	C3D-C4D-ND	3.02	115.12	110.24
22	B	808	CLA	C4-C3-C5	3.02	120.35	115.27
22	Z	612	CLA	O2A-CGA-CBA	3.02	121.37	111.91
29	4	607	CHL	C3B-C4B-NB	3.02	113.31	110.52
22	A	834	CLA	CMB-C2B-C1B	3.02	129.96	125.37
22	A	805	CLA	CHD-C4C-NC	3.01	128.95	124.20
22	2	614	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
22	B	813	CLA	C3B-C4B-NB	3.01	113.31	110.52
22	A	820	CLA	C1-C2-C3	-3.01	120.83	126.04
22	A	813	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	Z	614	CLA	C3B-C4B-NB	3.01	113.31	110.52
22	A	833	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
22	6	601	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
22	1	608	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
22	6	601	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	B	838	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
25	L	205	BCR	C23-C24-C25	-3.01	118.75	127.20
25	6	625	BCR	C11-C12-C13	-3.01	117.96	126.42
22	B	832	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
22	B	807	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
22	8	609	CLA	CAC-C3C-C4C	3.01	128.71	124.81
30	5	624	LUT	C38-C25-C24	-3.01	117.12	123.56
22	4	614	CLA	CHD-C4C-NC	3.01	128.94	124.20
22	B	834	CLA	C3B-C4B-NB	3.01	113.31	110.52
22	1	603	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
22	A	812	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
29	4	618	CHL	CBC-CAC-C3C	-3.01	104.14	112.43
22	B	837	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
22	A	839	CLA	C3B-C4B-NB	3.01	113.30	110.52
22	B	818	CLA	C3B-C4B-NB	3.01	113.30	110.52
22	A	806	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
22	B	833	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	B	847	BCR	C11-C10-C9	-3.00	123.02	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	613	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
29	9	607	CHL	CMB-C2B-C1B	3.00	129.94	125.37
22	6	610	CLA	CAC-C3C-C4C	3.00	128.70	124.81
22	A	807	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
22	B	816	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
22	7	606	CLA	CHC-C4B-NB	-3.00	121.08	124.26
22	B	803	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	A	835	CLA	C2A-C1A-CHA	-3.00	118.62	123.86
22	1	614	CLA	C4-C3-C5	3.00	120.31	115.27
22	7	606	CLA	C3B-C4B-NB	3.00	113.30	110.52
29	7	607	CHL	C4-C3-C5	3.00	120.31	115.27
22	2	609	CLA	CAC-C3C-C4C	3.00	128.70	124.81
22	A	836	CLA	CMA-C3A-C4A	-2.99	103.72	111.77
22	7	601	CLA	CHD-C4C-NC	2.99	128.92	124.20
22	B	821	CLA	CHC-C1C-C2C	-2.99	118.41	126.73
22	B	812	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
22	6	622	CLA	C3B-C4B-NB	2.99	113.29	110.52
29	9	606	CHL	C3B-C4B-NB	2.99	113.29	110.52
22	B	804	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	8	616	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
22	B	841	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	5	604	CLA	CMB-C2B-C1B	2.99	129.93	125.37
22	F	303	CLA	CHD-C4C-NC	2.99	128.92	124.20
22	B	852	CLA	C3B-C4B-NB	2.99	113.29	110.52
22	8	601	CLA	C3B-C4B-NB	2.99	113.29	110.52
29	Z	607	CHL	CAC-C3C-C4C	2.99	128.69	124.81
22	A	820	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
22	B	834	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
22	B	832	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
22	1	608	CLA	O2A-CGA-CBA	2.99	121.29	111.91
22	A	814	CLA	C4-C3-C5	2.99	120.30	115.27
22	3	614	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
22	8	601	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
22	B	807	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	A	838	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
22	7	606	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	4	609	CLA	C1-C2-C3	-2.99	121.92	126.75
22	F	301	CLA	CHD-C4C-NC	2.99	128.91	124.20
22	5	603	CLA	CHD-C4C-NC	2.99	128.91	124.20
22	A	823	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	7	609	CLA	CAC-C3C-C4C	2.98	128.68	124.81
21	A	801	CL0	C4C-C3C-C2C	-2.98	102.55	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	602	CLA	C4-C3-C5	2.98	120.29	115.27
22	Z	611	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
22	B	805	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
22	6	612	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
22	A	802	CLA	C3B-C4B-NB	2.98	113.28	110.52
22	1	604	CLA	C4-C3-C5	2.98	120.29	115.27
22	B	827	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	B	808	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
22	7	603	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	4	613	CLA	CMB-C2B-C1B	2.98	129.91	125.37
22	5	613	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	A	815	CLA	C2A-C1A-CHA	-2.98	118.65	123.86
30	9	616	LUT	C7-C8-C9	-2.98	121.73	126.23
22	A	829	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	B	810	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
22	B	813	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
22	B	813	CLA	C1-C2-C3	-2.98	120.89	126.04
21	A	801	CL0	CHD-C4C-NC	2.98	128.90	124.20
22	8	604	CLA	CAC-C3C-C4C	2.98	128.67	124.81
30	5	624	LUT	C15-C14-C13	-2.98	123.06	127.31
22	B	820	CLA	C2A-C1A-CHA	-2.98	118.65	123.86
22	5	616	CLA	CAC-C3C-C4C	2.98	128.67	124.81
22	B	808	CLA	O2A-CGA-CBA	2.98	121.25	111.91
22	B	852	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
22	B	817	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
22	Z	603	CLA	C4-C3-C5	2.98	120.28	115.27
22	3	613	CLA	C4A-NA-C1A	-2.98	105.37	106.71
22	7	602	CLA	O2A-CGA-CBA	2.98	121.25	111.91
22	F	303	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
22	2	602	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
25	3	717	BCR	C38-C26-C25	-2.97	121.19	124.53
22	8	610	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
22	A	827	CLA	CHD-C4C-NC	2.97	128.89	124.20
22	A	836	CLA	C1-C2-C3	-2.97	121.94	126.75
22	2	610	CLA	CAC-C3C-C4C	2.97	128.67	124.81
22	G	203	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	8	611	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	B	817	CLA	O2A-CGA-CBA	2.97	121.22	111.91
22	B	826	CLA	O2A-CGA-CBA	2.97	121.22	111.91
22	5	616	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	B	834	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	A	840	CLA	CHC-C1C-C2C	-2.97	118.49	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	612	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
22	2	612	CLA	CMB-C2B-C1B	2.97	129.89	125.37
22	K	4002	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
22	A	823	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	3	620	CLA	CAC-C3C-C4C	2.97	128.66	124.81
22	8	609	CLA	C4C-C3C-C2C	-2.97	102.58	106.90
30	7	622	LUT	C15-C14-C13	-2.96	123.08	127.31
22	9	604	CLA	C1-C2-C3	-2.96	121.96	126.75
22	A	827	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	B	812	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	8	603	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	7	602	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
22	A	838	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	8	612	CLA	CHD-C4C-NC	2.96	128.87	124.20
22	Z	611	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
22	7	614	CLA	O1D-CGD-CBD	-2.96	118.42	124.48
22	B	823	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
22	3	607	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	9	602	CLA	CHD-C4C-NC	2.96	128.87	124.20
22	A	804	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
22	1	613	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	A	823	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
22	3	620	CLA	CBC-CAC-C3C	-2.96	104.28	112.43
22	Z	603	CLA	C1-O2A-CGA	2.96	124.20	116.44
22	B	840	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
22	B	838	CLA	O2A-CGA-CBA	2.96	121.19	111.91
22	1	611	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
22	A	804	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
22	B	826	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	Z	616	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
22	8	613	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
22	B	835	CLA	C3B-C4B-NB	2.96	113.26	110.52
22	B	836	CLA	C4-C3-C5	2.96	120.24	115.27
22	B	815	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
22	2	611	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
29	4	607	CHL	O2A-CGA-CBA	2.95	121.18	111.91
22	6	614	CLA	CMD-C2D-C3D	-2.95	120.82	127.61
22	5	602	CLA	O2A-CGA-CBA	2.95	121.17	111.91
22	7	606	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
22	7	604	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
22	A	812	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
22	A	828	CLA	CMB-C2B-C1B	2.95	129.86	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	814	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
22	9	610	CLA	O2A-CGA-CBA	2.95	121.17	111.91
22	5	609	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
22	B	809	CLA	CAC-C3C-C4C	2.95	128.64	124.81
29	3	608	CHL	C3D-C4D-ND	2.95	115.01	110.24
22	5	601	CLA	C3B-C4B-NB	2.95	113.25	110.52
22	B	805	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
30	9	617	LUT	C30-C31-C32	-2.95	114.02	123.22
22	A	809	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
22	A	840	CLA	O2A-CGA-CBA	2.95	121.16	111.91
30	8	617	LUT	C35-C15-C14	-2.95	117.44	123.47
22	3	602	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
22	4	616	CLA	CMA-C3A-C2A	-2.95	109.22	116.10
22	5	613	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
29	1	601	CHL	CAC-C3C-C4C	2.95	128.63	124.81
29	6	607	CHL	CAC-C3C-C4C	2.95	128.63	124.81
22	B	841	CLA	C2A-C1A-CHA	-2.95	118.71	123.86
25	4	621	BCR	C20-C21-C22	-2.95	123.11	127.31
22	A	824	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
22	1	608	CLA	CHD-C4C-NC	2.95	128.85	124.20
22	6	611	CLA	C4-C3-C5	2.95	120.23	115.27
25	6	625	BCR	C21-C20-C19	-2.95	114.03	123.22
22	5	610	CLA	CHD-C4C-NC	2.95	128.84	124.20
22	8	606	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	4	612	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	B	824	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
25	I	172	BCR	C15-C14-C13	-2.94	123.11	127.31
22	B	812	CLA	C1-O2A-CGA	2.94	124.17	116.44
22	Z	613	CLA	CHD-C4C-NC	2.94	128.84	124.20
22	A	818	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	A	810	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
22	2	612	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	B	838	CLA	CMB-C2B-C1B	2.94	129.85	125.37
22	7	620	CLA	C3B-C4B-NB	2.94	113.25	110.52
22	4	610	CLA	CAC-C3C-C4C	2.94	128.63	124.81
22	B	841	CLA	C3B-C4B-NB	2.94	113.24	110.52
22	B	841	CLA	CHD-C4C-NC	2.94	128.84	124.20
25	B	845	BCR	C16-C15-C14	-2.94	117.45	123.47
22	J	3002	CLA	CAC-C3C-C4C	2.94	128.63	124.81
22	3	603	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
22	7	606	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	4	610	CLA	C3B-C4B-NB	2.94	113.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	304	CLA	C1-O2A-CGA	2.94	124.16	116.44
22	B	820	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
22	L	204	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
22	B	824	CLA	CMB-C2B-C1B	2.94	129.84	125.37
22	7	613	CLA	CMB-C2B-C1B	2.94	129.84	125.37
22	A	811	CLA	CHD-C4C-NC	2.94	128.83	124.20
22	Z	608	CLA	CAC-C3C-C4C	2.94	128.62	124.81
22	7	601	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
29	1	607	CHL	C3D-C4D-ND	2.94	114.99	110.24
22	B	806	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
22	Z	614	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
22	B	837	CLA	CAC-C3C-C4C	2.94	128.62	124.81
22	5	606	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
22	2	607	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
22	7	604	CLA	CHD-C4C-NC	2.93	128.83	124.20
22	L	203	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
22	B	814	CLA	CMC-C2C-C1C	2.93	129.51	125.04
22	A	843	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
22	A	816	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
22	A	837	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	3	614	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
22	Z	608	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
22	2	614	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
22	5	621	CLA	C3B-C4B-NB	2.93	113.23	110.52
22	A	839	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
22	Z	608	CLA	O2A-CGA-CBA	2.93	121.11	111.91
22	3	604	CLA	C3B-C4B-NB	2.93	113.23	110.52
22	A	818	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
22	B	833	CLA	C4-C3-C5	2.93	120.20	115.27
22	2	610	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
22	8	610	CLA	CHD-C4C-NC	2.93	128.82	124.20
22	B	824	CLA	C3B-C4B-NB	2.93	113.23	110.52
22	7	620	CLA	CAC-C3C-C4C	2.93	128.61	124.81
22	A	822	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
22	B	821	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
22	9	602	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
22	5	612	CLA	C4-C3-C5	2.93	120.19	115.27
22	1	614	CLA	CAA-C2A-C3A	-2.93	104.76	112.78
22	7	612	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
29	6	608	CHL	CHD-C4C-NC	2.93	128.81	124.20
22	B	829	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	2	606	CLA	C3B-C4B-NB	2.93	113.23	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	822	CLA	CAA-C2A-C3A	-2.93	104.77	112.78
22	5	610	CLA	CAC-C3C-C4C	2.92	128.60	124.81
22	1	612	CLA	O2A-CGA-CBA	2.92	121.08	111.91
22	3	602	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
22	F	301	CLA	CMC-C2C-C1C	2.92	129.49	125.04
22	4	611	CLA	CAA-C2A-C3A	-2.92	104.77	112.78
22	6	609	CLA	C1-C2-C3	-2.92	122.02	126.75
22	9	610	CLA	CHD-C4C-NC	2.92	128.81	124.20
29	5	618	CHL	C2A-C3A-C4A	-2.92	97.15	101.87
29	6	607	CHL	CHB-C4A-NA	2.92	128.55	124.51
22	3	610	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	A	851	BCR	C15-C16-C17	-2.92	117.49	123.47
22	A	832	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
22	3	603	CLA	CMB-C2B-C1B	2.92	129.82	125.37
30	7	621	LUT	C30-C31-C32	-2.92	114.11	123.22
30	7	622	LUT	C38-C25-C24	-2.92	117.31	123.56
25	G	205	BCR	C16-C15-C14	-2.92	117.50	123.47
22	7	602	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
22	B	837	CLA	CHD-C4C-NC	2.92	128.80	124.20
22	A	822	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
22	2	611	CLA	C4-C3-C5	2.92	120.18	115.27
22	5	604	CLA	C1-C2-C3	-2.92	122.03	126.75
22	9	614	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
22	A	809	CLA	CMC-C2C-C1C	2.92	129.48	125.04
22	7	610	CLA	CHC-C4B-NB	-2.92	121.17	124.26
22	6	604	CLA	CMB-C2B-C1B	2.92	129.81	125.37
22	B	826	CLA	CHD-C4C-NC	2.92	128.80	124.20
22	A	823	CLA	O2A-CGA-CBA	2.91	121.06	111.91
24	4	622	LHG	C6-C5-C4	-2.91	104.89	111.79
22	3	606	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
22	1	603	CLA	CBC-CAC-C3C	-2.91	104.40	112.43
22	4	604	CLA	CAC-C3C-C4C	2.91	128.59	124.81
22	Z	613	CLA	CMC-C2C-C1C	2.91	129.48	125.04
22	B	835	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
22	B	839	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
22	A	814	CLA	CHB-C1B-NB	-2.91	121.17	124.26
22	B	802	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
22	G	203	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
22	2	610	CLA	C3B-C4B-NB	2.91	113.22	110.52
22	6	604	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
22	A	804	CLA	CHC-C4B-NB	-2.91	121.18	124.26
22	4	614	CLA	C3B-C4B-NB	2.91	113.21	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	810	CLA	C11-C12-C13	-2.91	106.52	115.92
22	A	828	CLA	CAC-C3C-C2C	2.91	132.50	127.53
22	B	823	CLA	O2A-CGA-CBA	2.91	121.03	111.91
22	B	817	CLA	C3B-C4B-NB	2.91	113.21	110.52
22	A	842	CLA	CHD-C4C-NC	2.91	128.79	124.20
30	3	621	LUT	C30-C31-C32	-2.91	114.14	123.22
29	4	608	CHL	CHD-C4C-NC	2.91	128.78	124.20
22	4	604	CLA	C3B-C4B-NB	2.91	113.21	110.52
22	A	815	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	6	603	CLA	CAA-C2A-C3A	-2.90	104.82	112.78
22	A	838	CLA	C3B-C4B-NB	2.90	113.21	110.52
22	7	601	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
22	6	613	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
22	K	4002	CLA	C3B-C4B-NB	2.90	113.21	110.52
22	B	802	CLA	C1-C2-C3	-2.90	121.02	126.04
22	1	608	CLA	C3B-C4B-NB	2.90	113.21	110.52
22	7	612	CLA	CAC-C3C-C4C	2.90	128.57	124.81
22	A	827	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	4	614	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	B	825	CLA	C3B-C4B-NB	2.90	113.21	110.52
22	A	854	CLA	CAC-C3C-C4C	2.90	128.57	124.81
22	B	830	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
22	A	824	CLA	CMB-C2B-C1B	2.90	129.78	125.37
22	6	602	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
25	F	305	BCR	C23-C24-C25	-2.90	119.06	127.20
25	A	851	BCR	C16-C15-C14	-2.90	117.54	123.47
22	Z	606	CLA	CHD-C4C-NC	2.90	128.77	124.20
25	L	205	BCR	C20-C21-C22	-2.90	123.18	127.31
22	5	602	CLA	CAC-C3C-C4C	2.90	128.57	124.81
22	8	604	CLA	CMB-C2B-C1B	2.90	129.78	125.37
25	A	851	BCR	C10-C11-C12	-2.90	114.18	123.22
22	5	606	CLA	CHD-C4C-NC	2.89	128.76	124.20
22	B	814	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	A	812	CLA	CMB-C2B-C1B	2.89	129.78	125.37
22	5	617	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
22	4	611	CLA	C4-C3-C5	2.89	120.14	115.27
22	Z	613	CLA	CAC-C3C-C4C	2.89	128.56	124.81
22	A	814	CLA	O2A-CGA-CBA	2.89	120.99	111.91
22	A	814	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	A	840	CLA	CHD-C4C-NC	2.89	128.76	124.20
22	B	829	CLA	O2A-CGA-CBA	2.89	120.98	111.91
30	2	616	LUT	C35-C15-C14	-2.89	117.55	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	809	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	Z	614	CLA	C4-C3-C5	2.89	120.13	115.27
22	7	601	CLA	C4-C3-C5	2.89	120.13	115.27
22	B	822	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
22	Z	612	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
22	Z	613	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
22	B	827	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
22	4	603	CLA	CBC-CAC-C3C	-2.89	104.47	112.43
22	A	833	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
22	A	819	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
22	9	602	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
29	7	607	CHL	C3D-C4D-ND	2.89	114.91	110.24
22	A	842	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	B	825	CLA	O2D-CGD-CBD	2.89	116.40	111.27
22	7	601	CLA	C4A-NA-C1A	-2.89	105.41	106.71
22	A	843	CLA	CMB-C2B-C1B	2.89	129.77	125.37
22	5	601	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	A	803	CLA	C4-C3-C5	2.89	120.13	115.27
22	A	826	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
22	B	819	CLA	CMB-C2B-C1B	2.89	129.76	125.37
22	A	835	CLA	CHD-C4C-NC	2.89	128.75	124.20
22	Z	612	CLA	CHD-C4C-NC	2.88	128.75	124.20
22	6	603	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
30	7	622	LUT	C35-C34-C33	-2.88	123.19	127.31
22	A	841	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
22	B	826	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
22	A	808	CLA	C1-C2-C3	-2.88	121.06	126.04
22	A	818	CLA	C3B-C4B-NB	2.88	113.19	110.52
22	5	610	CLA	CMC-C2C-C1C	2.88	129.43	125.04
22	A	845	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
22	9	609	CLA	C1-C2-C3	-2.88	122.09	126.75
22	Z	606	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
22	B	814	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	A	849	BCR	C34-C9-C8	2.88	122.61	118.08
22	1	608	CLA	CAC-C3C-C4C	2.88	128.55	124.81
22	4	601	CLA	CMB-C2B-C1B	2.88	129.75	125.37
22	B	815	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
22	L	203	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
30	8	617	LUT	C20-C13-C12	2.88	122.61	118.08
22	B	836	CLA	O2A-CGA-CBA	2.88	120.94	111.91
22	A	824	CLA	C1-C2-C3	-2.88	121.07	126.04
22	1	611	CLA	CAC-C3C-C4C	2.88	128.54	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	808	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
22	1	602	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
22	B	827	CLA	O2A-CGA-CBA	2.88	120.93	111.91
22	4	603	CLA	CAA-C2A-C3A	-2.88	104.91	112.78
22	7	620	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
22	Z	606	CLA	C3B-C4B-NB	2.87	113.18	110.52
22	5	609	CLA	CHB-C4A-NA	2.87	128.49	124.51
22	4	612	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	A	842	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
22	8	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
30	4	619	LUT	C20-C13-C12	2.87	122.61	118.08
22	7	609	CLA	C3B-C4B-NB	2.87	113.18	110.52
22	B	825	CLA	O2A-CGA-CBA	2.87	120.92	111.91
22	9	613	CLA	CMB-C2B-C1B	2.87	129.74	125.37
22	1	616	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
30	7	622	LUT	C10-C11-C12	-2.87	114.25	123.22
29	5	607	CHL	C1-O2A-CGA	2.87	123.98	116.44
22	7	610	CLA	CHB-C1B-C2B	-2.87	119.13	127.24
22	A	810	CLA	C3B-C4B-NB	2.87	113.18	110.52
22	B	812	CLA	CHD-C4C-NC	2.87	128.73	124.20
22	6	612	CLA	CHD-C4C-NC	2.87	128.73	124.20
22	A	835	CLA	C3B-C4B-NB	2.87	113.18	110.52
22	6	611	CLA	C3B-C4B-NB	2.87	113.18	110.52
22	9	603	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
22	A	807	CLA	CHD-C4C-NC	2.87	128.72	124.20
22	2	607	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
22	A	837	CLA	C3B-C4B-NB	2.87	113.17	110.52
22	9	611	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
22	3	613	CLA	CMB-C2B-C1B	2.87	129.74	125.37
22	5	610	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
22	B	817	CLA	C1-C2-C3	-2.87	121.09	126.04
22	B	833	CLA	O2A-CGA-CBA	2.87	120.90	111.91
22	A	802	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
22	8	602	CLA	C3B-C4B-NB	2.87	113.17	110.52
22	8	616	CLA	C3B-C4B-NB	2.87	113.17	110.52
22	5	610	CLA	C3B-C4B-NB	2.87	113.17	110.52
25	A	848	BCR	C15-C14-C13	-2.87	123.22	127.31
22	B	826	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	A	807	CLA	CMB-C2B-C1B	2.86	129.73	125.37
25	7	623	BCR	C2-C1-C6	2.86	114.89	110.48
22	6	614	CLA	CAC-C3C-C4C	2.86	128.53	124.81
22	Z	608	CLA	CHD-C4C-NC	2.86	128.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	814	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
22	B	829	CLA	C4-C3-C5	2.86	120.09	115.27
22	F	304	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	Z	606	CLA	CAC-C3C-C4C	2.86	128.52	124.81
22	3	609	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
22	9	610	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
29	1	601	CHL	C2A-C1A-CHA	-2.86	118.86	123.86
22	2	610	CLA	C4-C3-C5	2.86	120.08	115.27
22	B	816	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
22	9	611	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	L	203	CLA	C3B-C4B-NB	2.86	113.17	110.52
25	3	717	BCR	C16-C15-C14	-2.86	117.62	123.47
29	1	607	CHL	CAC-C3C-C4C	2.86	128.52	124.81
22	4	613	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
25	4	621	BCR	C24-C23-C22	-2.86	121.92	126.23
22	1	602	CLA	CMB-C2B-C1B	2.86	129.72	125.37
22	Z	613	CLA	C3B-C4B-NB	2.86	113.17	110.52
22	B	822	CLA	CAC-C3C-C4C	2.86	128.52	124.81
22	3	612	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
22	4	602	CLA	C3B-C4B-NB	2.86	113.17	110.52
29	4	618	CHL	C3B-C4B-NB	2.86	113.17	110.52
22	6	604	CLA	CAC-C3C-C4C	2.86	128.52	124.81
22	9	602	CLA	CMB-C2B-C1B	2.86	129.72	125.37
30	3	622	LUT	C20-C13-C12	2.86	122.58	118.08
22	F	301	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
22	2	614	CLA	C3B-C4B-NB	2.85	113.16	110.52
29	4	608	CHL	CAC-C3C-C4C	2.85	128.51	124.81
22	Z	611	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	A	847	LHG	O8-C23-C24	2.85	120.86	111.91
22	2	613	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
22	A	843	CLA	O2A-CGA-CBA	2.85	120.86	111.91
25	A	852	BCR	C15-C14-C13	-2.85	123.24	127.31
22	7	601	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	B	806	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
25	5	625	BCR	C40-C30-C25	2.85	114.92	110.30
22	A	818	CLA	CMB-C2B-C1B	2.85	129.71	125.37
22	B	840	CLA	CMB-C2B-C1B	2.85	129.71	125.37
25	K	4001	BCR	C2-C1-C6	2.85	114.87	110.48
22	3	606	CLA	C3B-C4B-NB	2.85	113.16	110.52
22	8	602	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
22	1	602	CLA	CMC-C2C-C1C	2.85	129.38	125.04
22	7	614	CLA	C4C-C3C-C2C	-2.85	102.75	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	609	CLA	C1-C2-C3	-2.85	122.14	126.75
30	9	617	LUT	C18-C5-C6	-2.85	121.33	124.53
22	9	604	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
22	B	822	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
22	A	815	CLA	CHD-C4C-NC	2.85	128.69	124.20
22	A	804	CLA	CAC-C3C-C4C	2.85	128.50	124.81
22	F	301	CLA	C1-C2-C3	-2.85	121.12	126.04
29	4	606	CHL	O2A-CGA-CBA	2.85	120.84	111.91
30	3	621	LUT	C35-C34-C33	-2.85	123.25	127.31
22	3	603	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
22	B	835	CLA	CHD-C4C-NC	2.84	128.69	124.20
22	8	616	CLA	CAC-C3C-C4C	2.84	128.50	124.81
22	4	612	CLA	CHD-C4C-NC	2.84	128.68	124.20
22	A	805	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
22	A	809	CLA	CHD-C4C-NC	2.84	128.68	124.20
22	A	835	CLA	CAC-C3C-C4C	2.84	128.50	124.81
22	4	609	CLA	CED-O2D-CGD	2.84	122.36	115.94
22	B	822	CLA	CHD-C4C-NC	2.84	128.68	124.20
22	3	610	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	A	841	CLA	C1-C2-C3	-2.84	121.13	126.04
29	5	608	CHL	C3D-C4D-ND	2.84	114.83	110.24
22	B	832	CLA	C3B-C4B-NB	2.84	113.15	110.52
22	3	607	CLA	C3B-C4B-NB	2.84	113.15	110.52
22	G	204	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	A	802	CLA	CMB-C2B-C1B	2.84	129.69	125.37
22	3	604	CLA	CAC-C3C-C4C	2.84	128.49	124.81
22	2	606	CLA	CAC-C3C-C4C	2.84	128.49	124.81
22	B	806	CLA	C1-C2-C3	-2.84	121.14	126.04
22	3	611	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	B	813	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	A	832	CLA	C1-C2-C3	-2.84	122.16	126.75
22	6	611	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	1	611	CLA	O2A-CGA-CBA	2.84	120.81	111.91
22	B	805	CLA	C4-C3-C5	2.84	120.04	115.27
22	A	816	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
22	2	610	CLA	CHD-C4C-NC	2.84	128.67	124.20
22	A	806	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
22	7	603	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
22	7	614	CLA	CHD-C4C-NC	2.83	128.67	124.20
22	J	3002	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
22	3	602	CLA	CMC-C2C-C1C	2.83	129.35	125.04
22	K	4002	CLA	CAC-C3C-C4C	2.83	128.49	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	611	CLA	CAC-C3C-C4C	2.83	128.49	124.81
22	7	611	CLA	CMA-C3A-C2A	-2.83	109.49	116.10
22	A	832	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	B	803	CLA	O2A-CGA-CBA	2.83	120.80	111.91
22	8	613	CLA	CMC-C2C-C1C	2.83	129.35	125.04
22	4	612	CLA	CAC-C3C-C4C	2.83	128.48	124.81
30	7	622	LUT	C7-C8-C9	-2.83	121.96	126.23
22	A	830	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
22	9	601	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
22	A	817	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	B	837	CLA	CHB-C4A-NA	2.83	128.43	124.51
22	B	822	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
22	A	835	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
22	3	617	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
22	A	836	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	9	610	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
22	B	808	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	B	810	CLA	O2A-CGA-CBA	2.83	120.78	111.91
22	B	841	CLA	CAC-C3C-C4C	2.83	128.48	124.81
22	9	613	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
22	2	609	CLA	C1-C2-C3	-2.83	122.18	126.75
22	7	602	CLA	CAC-C3C-C4C	2.83	128.48	124.81
22	B	818	CLA	CBA-CAA-C2A	2.83	122.20	113.86
22	4	613	CLA	O2A-C1-C2	2.83	116.06	108.64
22	4	601	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	6	614	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
22	4	601	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
22	5	609	CLA	CAC-C3C-C4C	2.82	128.47	124.81
30	1	618	LUT	C38-C25-C24	-2.82	117.52	123.56
22	8	612	CLA	O2A-CGA-CBA	2.82	120.77	111.91
22	A	815	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
22	8	611	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
22	A	835	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
22	B	818	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	B	834	CLA	CMA-C3A-C2A	-2.82	102.45	113.83
22	A	802	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
30	1	617	LUT	C21-C26-C27	-2.82	109.14	112.70
22	A	818	CLA	C4-C3-C5	2.82	120.02	115.27
22	9	612	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
22	9	602	CLA	C3B-C4B-NB	2.82	113.13	110.52
24	7	625	LHG	O8-C23-C24	2.82	120.76	111.91
22	2	602	CLA	C4C-C3C-C2C	-2.82	102.79	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	838	CLA	CHD-C4C-NC	2.82	128.65	124.20
22	9	612	CLA	CAC-C3C-C4C	2.82	128.47	124.81
22	A	842	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
22	8	609	CLA	CED-O2D-CGD	2.82	122.31	115.94
22	8	608	CLA	C3B-C4B-NB	2.82	113.13	110.52
22	1	608	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
22	2	601	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
22	1	616	CLA	CMB-C2B-C1B	2.82	129.66	125.37
22	6	614	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
22	6	612	CLA	CAC-C3C-C4C	2.82	128.46	124.81
22	A	833	CLA	CAC-C3C-C4C	2.82	128.46	124.81
22	2	606	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
25	4	621	BCR	C33-C5-C4	2.82	119.02	113.62
22	A	813	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
22	6	612	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
22	4	613	CLA	CHD-C4C-NC	2.81	128.64	124.20
21	A	801	CL0	O2D-CGD-O1D	-2.81	118.34	123.84
22	8	616	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	A	836	CLA	C3B-C4B-NB	2.81	113.12	110.52
22	1	611	CLA	C3B-C4B-NB	2.81	113.12	110.52
22	B	824	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
22	8	603	CLA	CHD-C4C-NC	2.81	128.64	124.20
22	4	613	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	8	612	CLA	CAC-C3C-C4C	2.81	128.46	124.81
30	Z	618	LUT	C38-C25-C24	-2.81	117.54	123.56
22	K	4002	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	3	612	CLA	CAC-C3C-C4C	2.81	128.46	124.81
30	7	621	LUT	C20-C13-C12	2.81	122.50	118.08
22	Z	603	CLA	CMB-C2B-C1B	2.81	129.65	125.37
30	1	618	LUT	C10-C11-C12	-2.81	114.45	123.22
25	J	3003	BCR	C10-C11-C12	-2.81	114.45	123.22
22	Z	610	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
29	5	607	CHL	CMB-C2B-C1B	2.81	129.65	125.37
22	6	610	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
22	B	806	CLA	CMC-C2C-C1C	2.81	129.32	125.04
22	1	614	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	B	851	LHG	C5-O7-C7	-2.81	110.88	117.79
30	3	622	LUT	C10-C11-C12	-2.81	114.46	123.22
22	6	614	CLA	CHD-C4C-NC	2.81	128.63	124.20
29	3	608	CHL	O2A-CGA-CBA	2.81	120.72	111.91
22	7	604	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
22	2	611	CLA	C4C-C3C-C2C	-2.81	102.81	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	610	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
25	B	845	BCR	C37-C22-C21	-2.81	118.99	122.92
22	4	601	CLA	CHB-C1B-NB	-2.81	121.29	124.26
22	B	823	CLA	C4-C3-C5	2.81	119.99	115.27
22	A	815	CLA	O2A-CGA-CBA	2.81	120.71	111.91
22	8	611	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	6	622	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
25	B	801	BCR	C2-C1-C6	2.80	114.80	110.48
30	2	617	LUT	C11-C10-C9	-2.80	123.31	127.31
22	5	603	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
22	1	612	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
22	8	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	3	607	CLA	CMB-C2B-C1B	2.80	129.64	125.37
22	B	812	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
22	8	608	CLA	C1-C2-C3	-2.80	122.22	126.75
22	A	805	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
22	8	603	CLA	CMB-C2B-C1B	2.80	129.64	125.37
22	A	812	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	8	614	CLA	C3B-C4B-NB	2.80	113.11	110.52
25	8	619	BCR	C37-C22-C23	2.80	122.49	118.08
25	L	201	BCR	C11-C10-C9	-2.80	123.31	127.31
22	A	802	CLA	CHD-C4C-NC	2.80	128.62	124.20
22	6	604	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
22	5	612	CLA	CAC-C3C-C4C	2.80	128.44	124.81
25	B	801	BCR	C15-C14-C13	-2.80	123.31	127.31
25	L	205	BCR	C16-C17-C18	-2.80	123.31	127.31
25	4	621	BCR	C3-C4-C5	-2.80	109.08	114.08
22	6	604	CLA	CHD-C4C-NC	2.80	128.61	124.20
22	A	836	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
22	B	830	CLA	CAC-C3C-C4C	2.80	128.44	124.81
22	A	820	CLA	CHD-C4C-NC	2.80	128.61	124.20
22	9	610	CLA	CMB-C2B-C1B	2.80	129.63	125.37
30	4	619	LUT	C12-C13-C14	-2.80	114.65	118.94
22	5	601	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
22	1	613	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
22	2	601	CLA	CHD-C4C-NC	2.80	128.61	124.20
25	3	718	BCR	C16-C15-C14	-2.80	117.74	123.47
25	3	718	BCR	C21-C20-C19	-2.80	114.49	123.22
22	B	829	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	9	613	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	B	822	CLA	CMB-C2B-C1B	2.80	129.63	125.37
22	7	608	CLA	C4C-C3C-C2C	-2.80	102.82	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	607	CLA	C1-C2-C3	-2.80	122.23	126.75
22	A	806	CLA	CAA-CBA-CGA	-2.79	105.09	113.25
22	A	826	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	9	602	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	A	817	CLA	CHD-C4C-NC	2.79	128.61	124.20
22	B	820	CLA	C4-C3-C5	2.79	119.97	115.27
22	Z	602	CLA	CMC-C2C-C1C	2.79	129.29	125.04
22	Z	614	CLA	CHD-C4C-NC	2.79	128.60	124.20
22	5	610	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
22	5	611	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
22	K	4003	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
22	8	608	CLA	O2A-CGA-CBA	2.79	120.67	111.91
22	A	816	CLA	C4-C3-C5	2.79	119.97	115.27
22	6	609	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	8	610	CLA	C3B-C4B-NB	2.79	113.11	110.52
22	Z	602	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
22	A	820	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
22	K	4002	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
25	B	844	BCR	C20-C21-C22	-2.79	123.33	127.31
22	A	827	CLA	CMC-C2C-C1C	2.79	129.29	125.04
22	4	604	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	3	617	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	4	616	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
22	B	805	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	7	613	CLA	O2A-CGA-CBA	2.79	120.65	111.91
22	A	834	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
22	3	614	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
22	1	606	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	3	609	CLA	CMB-C2B-C1B	2.78	129.61	125.37
22	B	837	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
29	7	607	CHL	CAC-C3C-C4C	2.78	128.42	124.81
22	A	808	CLA	CHD-C4C-NC	2.78	128.59	124.20
22	B	834	CLA	CHD-C4C-NC	2.78	128.59	124.20
22	B	841	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	8	601	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
22	1	602	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
22	A	815	CLA	C3B-C4B-NB	2.78	113.09	110.52
22	B	820	CLA	CAC-C3C-C4C	2.78	128.42	124.81
22	B	807	CLA	CMB-C2B-C1B	2.78	129.60	125.37
22	Z	604	CLA	CMB-C2B-C1B	2.78	129.60	125.37
22	6	610	CLA	C3B-C4B-NB	2.78	113.09	110.52
22	3	602	CLA	CHD-C4C-NC	2.78	128.58	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	621	CLA	CAA-C2A-C1A	2.78	121.08	111.97
22	8	614	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
22	7	609	CLA	CED-O2D-CGD	2.78	122.22	115.94
22	A	854	CLA	C3B-C4B-NB	2.78	113.09	110.52
22	Z	614	CLA	O2A-CGA-CBA	2.78	120.62	111.91
22	7	620	CLA	CHD-C4C-NC	2.78	128.58	124.20
22	3	610	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
22	A	833	CLA	C3B-C4B-NB	2.78	113.09	110.52
22	3	612	CLA	CHC-C4B-NB	-2.78	121.32	124.26
22	4	611	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
22	3	620	CLA	CMB-C2B-C1B	2.78	129.60	125.37
22	9	609	CLA	CMB-C2B-C1B	2.78	129.60	125.37
30	3	621	LUT	C15-C14-C13	-2.78	123.35	127.31
22	5	602	CLA	CAA-C2A-C3A	-2.78	105.18	112.78
22	6	610	CLA	CHD-C4C-NC	2.77	128.58	124.20
22	5	614	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
22	5	611	CLA	CHD-C4C-NC	2.77	128.57	124.20
22	2	601	CLA	CMB-C2B-C1B	2.77	129.59	125.37
22	L	203	CLA	CAC-C3C-C4C	2.77	128.41	124.81
22	4	603	CLA	CMB-C2B-C1B	2.77	129.59	125.37
22	7	602	CLA	CHB-C4A-NA	2.77	128.35	124.51
22	B	807	CLA	CHB-C4A-NA	2.77	128.35	124.51
25	A	849	BCR	C32-C1-C6	2.77	114.80	110.30
22	9	612	CLA	O2A-CGA-CBA	2.77	120.61	111.91
22	1	610	CLA	C1-C2-C3	-2.77	121.25	126.04
22	4	609	CLA	CMB-C2B-C1B	2.77	129.59	125.37
22	4	610	CLA	C1-C2-C3	-2.77	121.25	126.04
22	4	609	CLA	CHD-C4C-NC	2.77	128.57	124.20
22	5	603	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
22	J	3002	CLA	CHD-C4C-NC	2.77	128.57	124.20
22	B	837	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
29	6	608	CHL	O2A-CGA-CBA	2.77	120.60	111.91
22	A	815	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	4	623	LHG	O8-C23-C24	2.77	120.60	111.91
30	Z	617	LUT	C15-C14-C13	-2.77	123.36	127.31
22	B	838	CLA	C3B-C4B-NB	2.77	113.08	110.52
25	K	4001	BCR	C35-C13-C12	2.77	122.44	118.08
22	9	601	CLA	CHD-C4C-NC	2.77	128.56	124.20
22	8	603	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
30	4	620	LUT	C10-C11-C12	-2.77	114.58	123.22
22	4	604	CLA	CHD-C4C-NC	2.77	128.56	124.20
22	1	606	CLA	CAC-C3C-C4C	2.77	128.40	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	808	CLA	C4-C3-C5	2.77	119.92	115.27
30	8	618	LUT	C38-C25-C24	-2.77	117.64	123.56
22	B	802	CLA	CMC-C2C-C1C	2.77	129.25	125.04
27	B	850	DGD	O1G-C1A-C2A	2.77	120.58	111.91
22	B	803	CLA	C3B-C4B-NB	2.76	113.08	110.52
22	B	819	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
22	8	604	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
22	1	612	CLA	CAC-C3C-C4C	2.76	128.40	124.81
22	7	611	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
22	A	828	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
22	6	612	CLA	C4-C3-C5	2.76	119.92	115.27
22	B	818	CLA	CHD-C4C-NC	2.76	128.55	124.20
22	B	839	CLA	CHD-C4C-NC	2.76	128.55	124.20
22	2	610	CLA	C1-C2-C3	-2.76	121.27	126.04
30	6	624	LUT	C16-C1-C6	-2.76	105.82	110.30
25	7	623	BCR	C15-C16-C17	-2.76	117.82	123.47
22	2	606	CLA	CHD-C4C-NC	2.76	128.55	124.20
22	Z	606	CLA	O2A-CGA-CBA	2.76	120.57	111.91
30	1	618	LUT	C3-C4-C5	-2.76	106.36	111.85
22	Z	603	CLA	C6-C5-C3	-2.76	106.22	113.45
22	B	826	CLA	C1-C2-C3	-2.76	121.27	126.04
30	3	622	LUT	C15-C35-C34	-2.76	117.83	123.47
22	A	802	CLA	CAC-C3C-C4C	2.76	128.39	124.81
22	1	603	CLA	CHB-C1B-NB	-2.76	121.34	124.26
22	A	805	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
22	A	837	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
22	A	824	CLA	CAC-C3C-C4C	2.76	128.39	124.81
23	A	844	PQN	C11-C12-C13	-2.76	122.20	126.79
25	3	718	BCR	C11-C12-C13	-2.76	118.67	126.42
22	5	602	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
22	B	805	CLA	CAC-C3C-C4C	2.76	128.39	124.81
22	B	834	CLA	O2A-CGA-CBA	2.76	120.56	111.91
22	5	611	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	B	820	CLA	CHD-C4C-NC	2.75	128.54	124.20
22	8	606	CLA	CAC-C3C-C4C	2.75	128.38	124.81
22	B	815	CLA	C4-C3-C5	2.75	119.90	115.27
22	6	610	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
22	B	808	CLA	CMB-C2B-C1B	2.75	129.56	125.37
22	A	818	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	B	815	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	B	820	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	F	303	CLA	CHC-C4B-NB	-2.75	121.34	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	849	BCR	C24-C23-C22	-2.75	122.08	126.23
22	1	612	CLA	CHD-C4C-NC	2.75	128.54	124.20
29	1	601	CHL	C3B-C4B-NB	2.75	113.07	110.52
22	4	602	CLA	CHD-C4C-NC	2.75	128.53	124.20
22	A	829	CLA	C1-C2-C3	-2.75	121.29	126.04
30	6	621	LUT	C18-C5-C6	-2.75	121.44	124.53
29	6	606	CHL	CHC-C4B-NB	-2.75	121.35	124.26
22	A	808	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
22	B	816	CLA	O2A-CGA-CBA	2.75	120.53	111.91
25	B	846	BCR	C29-C30-C25	2.75	114.71	110.48
22	7	602	CLA	CHC-C1C-C2C	-2.75	119.11	126.73
22	A	805	CLA	O2A-CGA-CBA	2.74	120.52	111.91
22	Z	603	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
22	4	614	CLA	CMC-C2C-C1C	2.74	129.22	125.04
22	A	825	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
22	7	608	CLA	O2A-CGA-CBA	2.74	120.52	111.91
25	A	848	BCR	C20-C21-C22	-2.74	123.40	127.31
22	A	823	CLA	CMB-C2B-C1B	2.74	129.54	125.37
22	B	814	CLA	O2A-CGA-CBA	2.74	120.51	111.91
22	B	806	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
22	4	612	CLA	O2A-CGA-CBA	2.74	120.51	111.91
22	A	816	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
30	2	616	LUT	C18-C5-C4	2.74	119.43	114.36
22	Z	614	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
22	2	611	CLA	CMB-C2B-C1B	2.74	129.54	125.37
22	A	854	CLA	O2A-CGA-CBA	2.74	120.51	111.91
22	B	820	CLA	O2A-CGA-CBA	2.74	120.51	111.91
22	9	610	CLA	CMC-C2C-C1C	2.74	129.21	125.04
22	8	616	CLA	CHD-C4C-NC	2.74	128.52	124.20
22	5	601	CLA	CHD-C4C-NC	2.74	128.52	124.20
22	5	606	CLA	O2A-CGA-CBA	2.74	120.50	111.91
22	A	833	CLA	CHD-C4C-NC	2.74	128.52	124.20
22	A	806	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	Z	604	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
22	8	610	CLA	C4-C3-C5	2.74	119.88	115.27
25	A	850	BCR	C16-C15-C14	-2.74	117.87	123.47
22	3	607	CLA	CHD-C4C-NC	2.74	128.52	124.20
30	5	624	LUT	C18-C5-C6	-2.74	121.45	124.53
22	8	613	CLA	CHD-C4C-NC	2.74	128.51	124.20
22	A	825	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
22	A	828	CLA	CAA-C2A-C3A	-2.74	105.29	112.78
22	2	613	CLA	CHB-C4A-NA	2.74	128.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	603	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
25	F	305	BCR	C21-C20-C19	-2.74	114.68	123.22
22	A	815	CLA	C4-C3-C5	2.74	119.87	115.27
29	4	608	CHL	C3D-C4D-ND	2.74	114.66	110.24
22	3	607	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
29	4	607	CHL	CMB-C2B-C1B	2.73	129.53	125.37
22	F	304	CLA	CMB-C2B-C1B	2.73	129.53	125.37
22	1	602	CLA	O2A-CGA-CBA	2.73	120.49	111.91
25	6	623	BCR	C16-C15-C14	-2.73	117.87	123.47
22	3	614	CLA	CHD-C4C-NC	2.73	128.51	124.20
22	A	839	CLA	CMB-C2B-C1B	2.73	129.53	125.37
22	A	807	CLA	CAC-C3C-C4C	2.73	128.36	124.81
22	A	814	CLA	CMB-C2B-C1B	2.73	129.53	125.37
22	B	812	CLA	C3B-C4B-NB	2.73	113.05	110.52
22	B	831	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
22	3	611	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
22	8	601	CLA	C4-C3-C5	2.73	119.87	115.27
25	A	852	BCR	C29-C30-C25	2.73	114.69	110.48
22	B	806	CLA	C3B-C4B-NB	2.73	113.05	110.52
22	A	816	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	5	623	LHG	O8-C23-C24	2.73	120.48	111.91
22	B	811	CLA	CHD-C4C-NC	2.73	128.51	124.20
30	6	621	LUT	C30-C31-C32	-2.73	114.69	123.22
22	5	606	CLA	CAC-C3C-C4C	2.73	128.35	124.81
22	A	811	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
29	6	606	CHL	C2A-C3A-C4A	-2.73	97.46	101.87
22	B	838	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	A	823	CLA	CHD-C4C-NC	2.73	128.50	124.20
22	B	820	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
22	B	830	CLA	C3B-C4B-NB	2.73	113.05	110.52
22	B	804	CLA	CHD-C4C-NC	2.73	128.50	124.20
30	Z	617	LUT	C17-C1-C6	2.73	114.72	110.30
22	B	829	CLA	CHD-C4C-NC	2.73	128.50	124.20
30	6	621	LUT	C20-C13-C12	2.73	122.38	118.08
25	B	845	BCR	C2-C1-C6	2.73	114.68	110.48
30	7	622	LUT	C35-C15-C14	-2.73	117.89	123.47
22	A	828	CLA	O2A-CGA-CBA	2.73	120.47	111.91
22	4	614	CLA	CHC-C1C-C2C	-2.73	119.16	126.73
22	A	817	CLA	CMD-C2D-C3D	-2.73	121.34	127.61
22	1	610	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
22	A	840	CLA	CMB-C2B-C1B	2.73	129.52	125.37
22	Z	616	CLA	O2D-CGD-O1D	-2.73	118.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	718	BCR	C2-C1-C6	2.73	114.68	110.48
22	A	829	CLA	C4-C3-C5	2.72	119.86	115.27
22	1	614	CLA	O2A-CGA-CBA	2.72	120.46	111.91
25	B	843	BCR	C11-C12-C13	-2.72	118.76	126.42
22	5	614	CLA	CMC-C2C-C1C	2.72	129.19	125.04
22	5	614	CLA	CHD-C4C-NC	2.72	128.50	124.20
22	6	601	CLA	CHD-C4C-NC	2.72	128.50	124.20
22	B	804	CLA	CMC-C2C-C1C	2.72	129.19	125.04
22	A	820	CLA	C2A-C3A-C4A	-2.72	97.47	101.87
22	B	840	CLA	O2A-CGA-CBA	2.72	120.45	111.91
22	8	601	CLA	CMB-C2B-C1B	2.72	129.51	125.37
22	B	830	CLA	CHD-C4C-NC	2.72	128.49	124.20
22	2	603	CLA	CHD-C4C-NC	2.72	128.49	124.20
30	4	619	LUT	C39-C29-C28	2.72	122.37	118.08
30	1	618	LUT	C35-C15-C14	-2.72	117.90	123.47
30	6	624	LUT	C10-C11-C12	-2.72	114.72	123.22
22	4	609	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
22	5	601	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
22	Z	613	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
29	9	607	CHL	CHB-C1B-NB	-2.72	121.38	124.26
22	6	610	CLA	C1-C2-C3	-2.72	121.34	126.04
22	2	603	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
25	5	622	BCR	C2-C1-C6	2.72	114.67	110.48
22	1	609	CLA	CHD-C4C-NC	2.72	128.49	124.20
22	A	809	CLA	CBA-CAA-C2A	2.72	121.89	113.86
22	7	614	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
22	B	810	CLA	CMB-C2B-C1B	2.72	129.51	125.37
30	Z	618	LUT	C35-C34-C33	-2.72	123.43	127.31
22	A	803	CLA	CHB-C1B-C2B	-2.72	119.56	127.24
22	8	609	CLA	CHD-C4C-NC	2.71	128.48	124.20
30	1	619	LUT	C15-C35-C34	-2.71	117.91	123.47
22	B	852	CLA	O2A-CGA-CBA	2.71	120.42	111.91
22	9	602	CLA	CMC-C2C-C1C	2.71	129.17	125.04
25	4	621	BCR	C16-C17-C18	-2.71	123.44	127.31
22	A	819	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
22	K	4003	CLA	CAC-C3C-C4C	2.71	128.33	124.81
22	2	607	CLA	CHD-C4C-NC	2.71	128.48	124.20
29	6	608	CHL	C3B-C4B-NB	2.71	113.03	110.52
22	6	602	CLA	CAC-C3C-C4C	2.71	128.33	124.81
29	5	618	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
22	A	815	CLA	CAC-C3C-C4C	2.71	128.33	124.81
22	B	822	CLA	O2A-CGA-CBA	2.71	120.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	616	CLA	CHD-C4C-NC	2.71	128.47	124.20
22	6	604	CLA	C3B-C4B-NB	2.71	113.03	110.52
22	L	204	CLA	C1-C2-C3	-2.71	122.37	126.75
25	A	851	BCR	C34-C9-C8	2.71	122.35	118.08
25	A	849	BCR	C16-C15-C14	-2.71	117.92	123.47
22	A	810	CLA	C4-C3-C5	2.71	119.83	115.27
22	K	4002	CLA	CHD-C4C-NC	2.71	128.47	124.20
22	8	606	CLA	C3B-C4B-NB	2.71	113.03	110.52
29	Z	607	CHL	O2A-CGA-CBA	2.71	120.41	111.91
22	4	609	CLA	CAC-C3C-C4C	2.71	128.32	124.81
22	9	603	CLA	CMB-C2B-C1B	2.71	129.49	125.37
22	A	845	CLA	O2A-CGA-CBA	2.71	120.40	111.91
22	B	827	CLA	C3B-C4B-NB	2.71	113.03	110.52
22	A	822	CLA	CHD-C4C-NC	2.71	128.47	124.20
22	1	604	CLA	CMA-C3A-C4A	-2.70	104.50	111.77
22	A	829	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	A	803	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
22	Z	609	CLA	O2A-CGA-CBA	2.70	120.39	111.91
22	Z	610	CLA	C4-C3-C5	2.70	119.82	115.27
22	4	602	CLA	O2A-CGA-CBA	2.70	120.39	111.91
22	B	805	CLA	CHD-C4C-NC	2.70	128.46	124.20
22	9	614	CLA	CHD-C4C-NC	2.70	128.46	124.20
22	9	609	CLA	CHA-C1A-NA	-2.70	120.21	126.40
30	9	617	LUT	C35-C34-C33	-2.70	123.46	127.31
22	A	838	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	3	603	CLA	CHD-C4C-NC	2.70	128.46	124.20
22	B	814	CLA	CAC-C3C-C4C	2.70	128.31	124.81
22	A	854	CLA	CHA-C1A-NA	-2.70	120.22	126.40
23	B	842	PQN	C11-C12-C13	-2.70	122.30	126.79
22	A	806	CLA	CMC-C2C-C1C	2.70	129.15	125.04
22	B	830	CLA	CMB-C2B-C1B	2.70	129.48	125.37
25	5	625	BCR	C21-C20-C19	-2.70	114.80	123.22
22	5	606	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
22	F	301	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
22	B	819	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	3	621	LUT	C35-C15-C14	-2.70	117.95	123.47
22	B	821	CLA	CHD-C4C-NC	2.70	128.45	124.20
22	2	603	CLA	CMB-C2B-C1B	2.70	129.47	125.37
22	7	608	CLA	C1-C2-C3	-2.69	122.39	126.75
22	B	820	CLA	CMB-C2B-C1B	2.69	129.47	125.37
25	B	844	BCR	C29-C30-C25	2.69	114.63	110.48
22	5	606	CLA	CMB-C2B-C1B	2.69	129.47	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Z	608	CLA	C4-C3-C5	2.69	119.80	115.27
22	9	612	CLA	CMB-C2B-C1B	2.69	129.47	125.37
24	A	847	LHG	C5-O7-C7	-2.69	111.16	117.79
22	B	838	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
22	B	832	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
25	A	848	BCR	C29-C30-C25	2.69	114.62	110.48
22	5	601	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
22	3	602	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
22	9	602	CLA	O2A-CGA-CBA	2.69	120.34	111.91
22	B	828	CLA	O2A-CGA-CBA	2.69	120.34	111.91
22	5	614	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
30	5	624	LUT	C15-C35-C34	-2.69	117.97	123.47
22	2	611	CLA	CHD-C4C-NC	2.69	128.44	124.20
22	3	617	CLA	C3B-C4B-NB	2.69	113.01	110.52
22	6	617	CLA	CHD-C4C-NC	2.68	128.43	124.20
22	Z	610	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
22	Z	614	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	1	613	CLA	C1-O2A-CGA	2.68	123.48	116.44
22	B	808	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	A	818	CLA	O2A-CGA-CBA	2.68	120.33	111.91
22	Z	613	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
22	5	611	CLA	CAC-C3C-C4C	2.68	128.29	124.81
29	5	608	CHL	O2A-CGA-CBA	2.68	120.32	111.91
22	B	819	CLA	CHD-C4C-NC	2.68	128.43	124.20
22	2	601	CLA	CED-O2D-CGD	2.68	122.00	115.94
29	Z	607	CHL	CMB-C2B-C1B	2.68	129.45	125.37
22	A	835	CLA	C4-C3-C5	2.68	119.78	115.27
22	A	803	CLA	CHA-C1A-NA	-2.68	120.26	126.40
21	A	801	CL0	CHB-C4A-NA	2.68	128.22	124.51
25	8	619	BCR	C23-C24-C25	-2.68	119.68	127.20
22	6	602	CLA	O2A-CGA-CBA	2.68	120.31	111.91
22	A	803	CLA	CHD-C4C-NC	2.68	128.42	124.20
29	7	607	CHL	O2A-CGA-CBA	2.68	120.31	111.91
22	6	612	CLA	CMC-C2C-C1C	2.68	129.12	125.04
22	A	843	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
22	B	812	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
22	B	815	CLA	CAC-C3C-C4C	2.68	128.28	124.81
22	9	610	CLA	C3B-C4B-NB	2.68	113.00	110.52
22	7	612	CLA	CHD-C4C-NC	2.67	128.42	124.20
22	1	602	CLA	CHC-C1C-C2C	-2.67	119.30	126.73
22	4	614	CLA	CAC-C3C-C4C	2.67	128.28	124.81
22	7	613	CLA	C4A-NA-C1A	-2.67	105.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	827	CLA	C1-C2-C3	-2.67	121.42	126.04
29	1	601	CHL	C4-C3-C2	-2.67	116.82	123.68
25	B	846	BCR	C28-C27-C26	-2.67	109.31	114.08
22	9	609	CLA	O2A-CGA-CBA	2.67	120.29	111.91
22	A	828	CLA	C3B-C4B-NB	2.67	112.99	110.52
24	1	620	LHG	O8-C23-C24	2.67	120.29	111.91
22	Z	614	CLA	CMB-C2B-C1B	2.67	129.44	125.37
22	A	808	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
22	A	821	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	A	826	CLA	C3B-C4B-NB	2.67	112.99	110.52
22	4	609	CLA	O2A-CGA-CBA	2.67	120.29	111.91
22	6	616	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	8	614	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
30	2	616	LUT	C3-C4-C5	-2.67	106.53	111.85
22	Z	603	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
22	A	810	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
29	6	606	CHL	CMB-C2B-C1B	2.67	129.44	125.37
22	B	834	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
22	5	604	CLA	O2A-CGA-CBA	2.67	120.28	111.91
22	2	614	CLA	CMB-C2B-C1B	2.67	129.43	125.37
22	6	602	CLA	C1-C2-C3	-2.67	121.43	126.04
22	8	604	CLA	CMA-C3A-C2A	-2.67	103.07	113.83
22	1	604	CLA	CMB-C2B-C1B	2.67	129.43	125.37
22	B	810	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	B	805	CLA	CMB-C2B-C1B	2.67	129.43	125.37
22	A	819	CLA	C1-O2A-CGA	2.67	123.44	116.44
22	F	301	CLA	CAC-C3C-C4C	2.67	128.27	124.81
22	B	823	CLA	C3B-C4B-NB	2.67	112.99	110.52
30	2	617	LUT	C18-C5-C6	-2.67	121.53	124.53
22	2	602	CLA	CMB-C2B-C1B	2.67	129.43	125.37
22	3	604	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
22	A	835	CLA	CMB-C2B-C1B	2.66	129.43	125.37
22	5	616	CLA	CMB-C2B-C1B	2.66	129.43	125.37
22	Z	611	CLA	C1-C2-C3	-2.66	121.44	126.04
22	A	803	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
22	3	604	CLA	CHD-C4C-NC	2.66	128.40	124.20
29	8	607	CHL	CMB-C2B-C1B	2.66	129.43	125.37
25	3	718	BCR	C29-C30-C25	2.66	114.58	110.48
30	3	622	LUT	C15-C14-C13	-2.66	123.51	127.31
25	8	619	BCR	C32-C1-C6	2.66	114.62	110.30
22	5	603	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
22	A	827	CLA	C1-C2-C3	-2.66	121.44	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	617	CLA	CMB-C2B-C1B	2.66	129.42	125.37
25	G	205	BCR	C10-C11-C12	-2.66	114.91	123.22
22	B	825	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	8	614	CLA	CAC-C3C-C4C	2.66	128.26	124.81
29	4	607	CHL	CHD-C4C-NC	2.66	128.39	124.20
22	1	604	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	G	203	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	7	608	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
30	3	622	LUT	C30-C31-C32	-2.66	114.92	123.22
22	6	602	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
22	3	620	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
22	Z	614	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
22	1	603	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
25	A	848	BCR	C31-C1-C6	-2.65	105.99	110.30
25	8	619	BCR	C3-C4-C5	-2.65	109.34	114.08
22	9	614	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
22	B	821	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	B	824	CLA	O2A-CGA-O1A	-2.65	116.89	123.59
22	3	613	CLA	O2A-CGA-CBA	2.65	120.23	111.91
22	B	827	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	A	819	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	B	811	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
30	7	621	LUT	C38-C25-C24	-2.65	117.88	123.56
22	3	617	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	3	603	CLA	O2A-CGA-CBA	2.65	120.23	111.91
25	7	623	BCR	C20-C21-C22	-2.65	123.53	127.31
25	A	852	BCR	C34-C9-C10	-2.65	119.21	122.92
22	A	840	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	B	847	BCR	C20-C21-C22	-2.65	123.53	127.31
22	1	612	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	A	845	CLA	CHC-C4B-NB	-2.65	121.45	124.26
22	B	809	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	3	609	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	Z	616	CLA	CHD-C4C-NC	2.65	128.38	124.20
25	5	622	BCR	C21-C20-C19	-2.65	114.95	123.22
22	A	845	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	2	602	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	3	617	CLA	CMB-C2B-C1B	2.65	129.40	125.37
22	B	852	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	7	610	CLA	CMB-C2B-C1B	2.65	129.40	125.37
22	B	815	CLA	CHD-C4C-NC	2.65	128.38	124.20
22	7	616	CLA	CMB-C2B-C1B	2.65	129.40	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	606	CLA	CMB-C2B-C1B	2.65	129.40	125.37
22	4	610	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
22	B	833	CLA	CHD-C4C-NC	2.65	128.37	124.20
22	Z	606	CLA	CMB-C2B-C1B	2.65	129.40	125.37
22	6	622	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	4	602	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
22	5	604	CLA	CAA-C2A-C3A	-2.64	105.53	112.78
22	1	603	CLA	CHD-C4C-NC	2.64	128.37	124.20
22	2	609	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
22	2	609	CLA	C4C-C3C-C2C	-2.64	103.04	106.90
22	9	601	CLA	CAC-C3C-C4C	2.64	128.24	124.81
22	A	830	CLA	CHD-C4C-NC	2.64	128.37	124.20
22	2	601	CLA	CGD-CBD-CAD	-2.64	102.17	110.73
22	B	804	CLA	CHC-C1C-C2C	-2.64	119.39	126.73
25	5	622	BCR	C37-C22-C23	2.64	122.24	118.08
22	B	817	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	B	841	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
22	7	611	CLA	CHC-C4B-NB	-2.64	121.46	124.26
22	B	803	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	A	846	LHG	O8-C23-C24	2.64	120.20	111.91
22	4	614	CLA	CMB-C2B-C1B	2.64	129.39	125.37
29	4	607	CHL	C1-C2-C3	-2.64	122.48	126.75
30	9	617	LUT	C21-C26-C27	-2.64	109.36	112.70
22	1	613	CLA	CHD-C4C-NC	2.64	128.37	124.20
22	A	804	CLA	CMA-C3A-C4A	-2.64	104.68	111.77
22	B	811	CLA	O2A-CGA-CBA	2.64	120.19	111.91
22	B	802	CLA	O2A-CGA-CBA	2.64	120.19	111.91
22	K	4002	CLA	CMB-C2B-C1B	2.64	129.39	125.37
22	A	839	CLA	CHD-C4C-NC	2.64	128.36	124.20
22	A	805	CLA	C4-C3-C5	2.64	119.71	115.27
22	Z	609	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	A	836	CLA	O2A-CGA-CBA	2.64	120.19	111.91
22	8	608	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
22	B	832	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	A	829	CLA	C1-O2A-CGA	2.64	123.36	116.44
22	A	832	CLA	CMC-C2C-C1C	2.64	129.06	125.04
22	B	825	CLA	C4-C3-C5	2.64	119.71	115.27
22	5	604	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
29	1	607	CHL	O2A-CGA-CBA	2.64	120.18	111.91
22	1	604	CLA	CHD-C4C-NC	2.64	128.36	124.20
22	8	602	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
22	A	825	CLA	C1-C2-C3	-2.64	121.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	838	CLA	CBA-CAA-C2A	-2.64	106.08	113.86
22	5	610	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
22	A	827	CLA	CMB-C2B-C1B	2.63	129.38	125.37
22	B	815	CLA	CMB-C2B-C1B	2.63	129.38	125.37
22	3	606	CLA	CHD-C4C-NC	2.63	128.35	124.20
22	8	606	CLA	CHD-C4C-NC	2.63	128.35	124.20
22	8	614	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
22	B	827	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	K	4004	BCR	C2-C1-C6	2.63	114.53	110.48
22	B	814	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
22	8	614	CLA	CHD-C4C-NC	2.63	128.35	124.20
25	3	717	BCR	C7-C8-C9	-2.63	122.26	126.23
29	9	606	CHL	CMB-C2B-C1B	2.63	129.38	125.37
25	I	172	BCR	C10-C11-C12	-2.63	115.01	123.22
25	A	856	BCR	C31-C1-C6	-2.63	106.03	110.30
22	6	614	CLA	CMB-C2B-C1B	2.63	129.37	125.37
22	8	604	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	7	604	CLA	C1-C2-C3	-2.63	121.50	126.04
25	3	717	BCR	C32-C1-C6	2.63	114.56	110.30
22	B	819	CLA	C4-C3-C5	2.63	119.69	115.27
29	8	607	CHL	C2A-C1A-CHA	-2.63	119.26	123.86
22	B	807	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
30	1	619	LUT	C8-C9-C10	-2.63	114.91	118.94
22	A	821	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	7	610	CLA	O2A-CGA-O1A	-2.63	116.97	123.59
22	6	622	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	B	827	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
22	4	603	CLA	CHD-C4C-NC	2.62	128.34	124.20
22	5	610	CLA	CMA-C3A-C2A	-2.62	103.24	113.83
22	2	613	CLA	CMB-C2B-C1B	2.62	129.37	125.37
22	7	603	CLA	CMB-C2B-C1B	2.62	129.36	125.37
30	5	620	LUT	C31-C30-C29	-2.62	123.57	127.31
22	A	805	CLA	C3B-C4B-NB	2.62	112.95	110.52
30	3	622	LUT	C38-C25-C24	-2.62	117.95	123.56
22	B	811	CLA	CAC-C3C-C4C	2.62	128.21	124.81
22	B	802	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
30	7	621	LUT	C35-C34-C33	-2.62	123.57	127.31
22	A	854	CLA	CHB-C1B-C2B	-2.62	119.84	127.24
22	G	204	CLA	CHD-C4C-NC	2.62	128.33	124.20
30	5	620	LUT	C7-C8-C9	-2.62	122.28	126.23
29	4	608	CHL	C1-C2-C3	-2.62	122.52	126.75
22	8	602	CLA	CHB-C4A-NA	2.62	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	621	BCR	C11-C12-C13	-2.62	119.06	126.42
22	7	614	CLA	CMB-C2B-C1B	2.62	129.35	125.37
22	3	609	CLA	O2A-CGA-CBA	2.62	120.12	111.91
22	8	614	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	6	604	CLA	C4-C3-C5	2.62	119.67	115.27
22	J	3002	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	B	837	CLA	C3B-C4B-NB	2.62	112.94	110.52
22	5	606	CLA	C1-C2-C3	-2.62	121.52	126.04
22	4	601	CLA	O2A-CGA-CBA	2.62	120.12	111.91
22	8	606	CLA	CHC-C4B-NB	-2.62	121.49	124.26
22	B	805	CLA	O1D-CGD-CBD	-2.62	119.13	124.48
30	Z	617	LUT	C20-C13-C12	2.61	122.20	118.08
21	A	801	CL0	CMA-C3A-C2A	-2.61	103.28	113.83
22	B	836	CLA	CHD-C4C-NC	2.61	128.32	124.20
22	B	811	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	6	604	CLA	O2A-CGA-CBA	2.61	120.11	111.91
30	1	618	LUT	C7-C8-C9	-2.61	122.29	126.23
22	5	601	CLA	CAC-C3C-C4C	2.61	128.20	124.81
22	B	811	CLA	CMB-C2B-C1B	2.61	129.35	125.37
22	8	602	CLA	O2A-CGA-CBA	2.61	120.10	111.91
22	Z	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	5	603	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	7	604	CLA	O2A-CGA-CBA	2.61	120.10	111.91
22	8	610	CLA	CAC-C3C-C4C	2.61	128.20	124.81
22	A	829	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
30	1	617	LUT	C20-C13-C12	2.61	122.19	118.08
22	3	620	CLA	O2A-CGA-CBA	2.61	120.10	111.91
22	2	613	CLA	C1-C2-C3	-2.61	122.53	126.75
22	A	815	CLA	CMB-C2B-C1B	2.61	129.34	125.37
22	6	603	CLA	CHD-C4C-NC	2.61	128.31	124.20
30	Z	617	LUT	C21-C26-C27	-2.61	109.40	112.70
22	3	620	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
22	A	816	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	Z	603	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	A	809	CLA	C3B-C4B-NB	2.61	112.94	110.52
22	A	813	CLA	CHD-C4C-NC	2.61	128.31	124.20
25	6	625	BCR	C37-C22-C23	2.61	122.18	118.08
25	L	201	BCR	C33-C5-C6	-2.61	121.60	124.53
22	1	610	CLA	C4-C3-C5	2.61	119.66	115.27
22	A	810	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	6	603	CLA	CMB-C2B-C1B	2.61	129.34	125.37
22	Z	610	CLA	O1D-CGD-CBD	-2.61	119.15	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	604	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	3	621	LUT	C10-C11-C12	-2.61	115.09	123.22
25	K	4001	BCR	C29-C30-C25	2.60	114.49	110.48
28	J	3001	LMG	O6-C1-O1	-2.60	103.81	109.97
30	1	618	LUT	C15-C14-C13	-2.60	123.59	127.31
22	8	603	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
22	B	825	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
30	Z	617	LUT	C39-C29-C28	2.60	122.18	118.08
22	5	601	CLA	CMB-C2B-C1B	2.60	129.33	125.37
22	2	610	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	4	616	CLA	CHD-C4C-NC	2.60	128.31	124.20
22	9	612	CLA	CHD-C4C-NC	2.60	128.30	124.20
22	7	609	CLA	O2A-CGA-CBA	2.60	120.07	111.91
29	5	607	CHL	O2A-CGA-CBA	2.60	120.07	111.91
22	G	203	CLA	CMB-C2B-C1B	2.60	129.33	125.37
22	5	612	CLA	O2A-CGA-CBA	2.60	120.07	111.91
22	A	821	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
30	9	617	LUT	C15-C14-C13	-2.60	123.60	127.31
22	4	604	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
22	6	622	CLA	CMB-C2B-C1B	2.60	129.33	125.37
25	B	848	BCR	C21-C20-C19	-2.60	115.11	123.22
22	B	803	CLA	CHC-C1C-NC	2.60	128.14	124.20
22	3	604	CLA	CMB-C2B-C1B	2.60	129.32	125.37
22	A	845	CLA	CHD-C4C-NC	2.60	128.30	124.20
25	5	625	BCR	C23-C24-C25	-2.60	119.91	127.20
22	3	602	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	A	824	CLA	O2A-CGA-CBA	2.60	120.06	111.91
22	5	610	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	6	604	CLA	CMC-C2C-C1C	2.59	128.99	125.04
22	6	616	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
22	B	831	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	4	611	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	5	617	CLA	CMB-C2B-C1B	2.59	129.32	125.37
22	A	804	CLA	O2A-CGA-CBA	2.59	120.04	111.91
30	5	620	LUT	C11-C10-C9	-2.59	123.61	127.31
22	1	602	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	B	841	CLA	CMB-C2B-C1B	2.59	129.31	125.37
22	7	616	CLA	CHD-C4C-NC	2.59	128.29	124.20
22	9	613	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
22	A	833	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	2	614	CLA	CHD-C4C-NC	2.59	128.28	124.20
25	B	847	BCR	C32-C1-C6	2.59	114.50	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z	601	CHL	C3B-C4B-NB	2.59	112.92	110.52
22	B	813	CLA	CHD-C4C-NC	2.59	128.28	124.20
22	A	830	CLA	O2A-CGA-CBA	2.59	120.03	111.91
22	1	610	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	6	601	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
22	1	606	CLA	CMB-C2B-C1B	2.59	129.31	125.37
22	5	613	CLA	O2A-CGA-CBA	2.59	120.03	111.91
22	7	603	CLA	CAC-C3C-C4C	2.59	128.16	124.81
22	B	802	CLA	CHC-C1C-C2C	-2.59	119.55	126.73
22	7	611	CLA	CHD-C4C-NC	2.59	128.28	124.20
25	J	3003	BCR	C11-C10-C9	-2.58	123.62	127.31
22	5	612	CLA	CMB-C2B-C1B	2.58	129.31	125.37
22	9	611	CLA	CAC-C3C-C4C	2.58	128.16	124.81
22	A	819	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	8	611	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
22	7	601	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
25	B	846	BCR	C20-C21-C22	-2.58	123.62	127.31
29	4	608	CHL	CMB-C2B-C1B	2.58	129.30	125.37
22	A	806	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	A	813	CLA	C3B-C4B-NB	2.58	112.91	110.52
22	2	610	CLA	O2A-CGA-CBA	2.58	120.01	111.91
22	A	827	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
22	2	603	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
25	3	718	BCR	C37-C22-C23	2.58	122.14	118.08
24	A	855	LHG	O8-C23-C24	2.58	120.01	111.91
22	A	812	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	2	610	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
22	B	852	CLA	C4-C3-C5	2.58	119.61	115.27
22	B	839	CLA	C1-C2-C3	-2.58	121.58	126.04
22	3	603	CLA	C1-C2-C3	-2.58	121.58	126.04
29	7	607	CHL	CMB-C2B-C1B	2.58	129.30	125.37
22	A	805	CLA	CAC-C3C-C4C	2.58	128.16	124.81
29	9	606	CHL	CHD-C4C-NC	2.58	128.27	124.20
22	A	821	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
30	8	617	LUT	C38-C25-C24	-2.58	118.04	123.56
25	6	623	BCR	C21-C20-C19	-2.58	115.17	123.22
22	A	819	CLA	CHD-C4C-NC	2.58	128.26	124.20
22	5	614	CLA	CMB-C2B-C1B	2.58	129.29	125.37
22	A	845	CLA	C4-C3-C5	2.58	119.60	115.27
22	1	603	CLA	C4-C3-C5	2.58	119.60	115.27
22	1	608	CLA	C4-C3-C5	2.58	119.60	115.27
22	5	602	CLA	CBC-CAC-C3C	-2.58	105.33	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	619	LUT	C8-C7-C6	-2.58	119.97	127.20
22	3	620	CLA	CHD-C4C-NC	2.58	128.26	124.20
22	6	613	CLA	CHD-C4C-NC	2.58	128.26	124.20
22	B	831	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	1	616	CLA	CAA-C2A-C3A	-2.58	105.73	112.78
29	4	607	CHL	C2A-C3A-C4A	-2.58	97.71	101.87
25	B	848	BCR	C16-C15-C14	-2.57	118.20	123.47
22	8	610	CLA	CMB-C2B-C1B	2.57	129.29	125.37
22	B	824	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	B	809	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
22	7	612	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	B	829	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
22	A	832	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	5	613	CLA	CHC-C4B-NB	-2.57	121.53	124.26
22	7	602	CLA	CMB-C2B-C1B	2.57	129.29	125.37
22	A	834	CLA	O2A-CGA-CBA	2.57	119.98	111.91
29	6	607	CHL	CMB-C2B-C1B	2.57	129.28	125.37
25	4	621	BCR	C8-C7-C6	-2.57	119.98	127.20
22	B	804	CLA	CAC-C3C-C4C	2.57	128.15	124.81
22	Z	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
29	5	618	CHL	CBC-CAC-C3C	-2.57	105.35	112.43
29	5	608	CHL	CHD-C4C-NC	2.57	128.25	124.20
29	4	606	CHL	C2A-C3A-C4A	-2.57	97.72	101.87
22	Z	609	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
22	B	814	CLA	C3B-C4B-NB	2.57	112.90	110.52
22	K	4003	CLA	CMB-C2B-C1B	2.57	129.28	125.37
24	6	619	LHG	O8-C23-C24	2.57	119.97	111.91
22	1	604	CLA	O2A-CGA-CBA	2.57	119.97	111.91
22	B	840	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	5	613	CLA	C1-O2A-CGA	2.57	123.18	116.44
22	2	602	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	A	824	CLA	CHD-C4C-NC	2.57	128.25	124.20
22	Z	612	CLA	CMB-C2B-C1B	2.57	129.28	125.37
30	6	621	LUT	C1-C2-C3	2.57	119.44	113.64
22	7	612	CLA	C4-C3-C5	2.57	119.59	115.27
28	9	620	LMG	O6-C1-O1	-2.57	103.90	109.97
22	9	613	CLA	C1-O2A-CGA	2.57	123.17	116.44
22	A	808	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	7	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
29	4	606	CHL	C3B-C4B-NB	2.56	112.89	110.52
25	5	622	BCR	C29-C30-C25	2.56	114.43	110.48
22	5	616	CLA	CHB-C4A-NA	2.56	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	602	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
22	A	832	CLA	O2A-CGA-CBA	2.56	119.95	111.91
22	4	610	CLA	CHD-C4C-NC	2.56	128.24	124.20
22	2	612	CLA	CHD-C4C-NC	2.56	128.24	124.20
22	G	204	CLA	CMB-C2B-C1B	2.56	129.27	125.37
29	6	618	CHL	C2A-C1A-CHA	-2.56	119.38	123.86
22	A	803	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	B	823	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	A	809	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
22	A	804	CLA	CMB-C2B-C1B	2.56	129.27	125.37
22	G	204	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
22	Z	612	CLA	C1-C2-C3	-2.56	121.61	126.04
22	Z	604	CLA	O2A-CGA-CBA	2.56	119.94	111.91
25	F	305	BCR	C11-C12-C13	-2.56	119.22	126.42
22	B	833	CLA	CAA-C2A-C1A	-2.56	103.59	111.97
22	B	836	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
22	4	609	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	9	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	4	619	LUT	C10-C11-C12	-2.56	115.23	123.22
25	5	625	BCR	C20-C19-C18	-2.56	119.23	126.42
22	L	204	CLA	O2A-CGA-CBA	2.56	119.93	111.91
22	B	829	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
22	A	842	CLA	CAC-C3C-C4C	2.56	128.13	124.81
22	A	827	CLA	O2A-CGA-CBA	2.56	119.93	111.91
22	A	807	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	3	718	BCR	C11-C10-C9	-2.56	123.66	127.31
22	6	612	CLA	O2A-CGA-CBA	2.56	119.93	111.91
29	6	606	CHL	C3B-C4B-NB	2.56	112.89	110.52
22	B	816	CLA	CMB-C2B-C1B	2.56	129.26	125.37
22	1	604	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
22	3	612	CLA	CMB-C2B-C1B	2.55	129.26	125.37
22	3	611	CLA	CMB-C2B-C1B	2.55	129.26	125.37
29	6	618	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
22	B	823	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
22	A	829	CLA	C3B-C4B-NB	2.55	112.88	110.52
22	A	836	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
22	6	612	CLA	CMB-C2B-C1B	2.55	129.26	125.37
22	B	840	CLA	C1-C2-C3	-2.55	121.63	126.04
22	1	603	CLA	O2A-CGA-CBA	2.55	119.91	111.91
22	3	611	CLA	CHB-C1B-NB	-2.55	121.56	124.26
22	9	609	CLA	CAC-C3C-C4C	2.55	128.12	124.81
22	B	830	CLA	O2A-CGA-CBA	2.55	119.91	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	620	LUT	C35-C15-C14	-2.55	118.25	123.47
22	8	614	CLA	C4-C3-C5	2.55	119.56	115.27
29	Z	601	CHL	C4-C3-C5	2.55	119.56	115.27
22	5	621	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	Z	611	CLA	O2A-CGA-CBA	2.55	119.90	111.91
25	A	851	BCR	C23-C24-C25	-2.55	120.05	127.20
22	A	854	CLA	CMC-C2C-C1C	2.55	128.92	125.04
22	6	613	CLA	C1-C2-C3	-2.55	121.64	126.04
22	A	820	CLA	CAC-C3C-C4C	2.55	128.11	124.81
30	Z	619	LUT	C10-C11-C12	-2.55	115.27	123.22
22	5	609	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	A	823	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
22	3	611	CLA	CMA-C3A-C2A	-2.54	110.16	116.10
22	6	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	A	809	CLA	CMB-C2B-C1B	2.54	129.24	125.37
22	A	812	CLA	CHD-C4C-NC	2.54	128.21	124.20
22	1	608	CLA	CMB-C2B-C1B	2.54	129.24	125.37
29	4	606	CHL	CBC-CAC-C3C	-2.54	105.43	112.43
30	7	622	LUT	C30-C31-C32	-2.54	115.29	123.22
25	B	846	BCR	C2-C1-C6	2.54	114.39	110.48
22	7	613	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	1	619	LUT	C38-C25-C24	-2.54	118.12	123.56
22	Z	602	CLA	CMB-C2B-C1B	2.54	129.24	125.37
22	5	606	CLA	C3B-C4B-NB	2.54	112.87	110.52
22	7	602	CLA	C4-C3-C5	2.54	119.54	115.27
22	K	4003	CLA	CHD-C4C-NC	2.54	128.21	124.20
22	A	804	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
22	5	613	CLA	CMB-C2B-C1B	2.54	129.24	125.37
30	Z	618	LUT	C30-C31-C32	-2.54	115.29	123.22
22	A	837	CLA	CHD-C4C-NC	2.54	128.20	124.20
22	8	608	CLA	CAC-C3C-C4C	2.54	128.10	124.81
22	4	602	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
22	B	838	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
22	G	203	CLA	CHD-C4C-NC	2.54	128.20	124.20
22	4	614	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
22	7	608	CLA	CMB-C2B-C1B	2.54	129.23	125.37
22	9	614	CLA	CMB-C2B-C1B	2.54	129.23	125.37
22	8	613	CLA	C1-O2A-CGA	2.54	123.10	116.44
22	A	841	CLA	CHD-C4C-NC	2.54	128.20	124.20
25	F	305	BCR	C35-C13-C14	-2.54	119.37	122.92
22	6	609	CLA	CAC-C3C-C4C	2.54	128.10	124.81
22	B	807	CLA	C1-C2-C3	-2.54	121.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	614	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
22	B	822	CLA	CMC-C2C-C1C	2.54	128.90	125.04
22	F	303	CLA	C3B-C4B-NB	2.54	112.87	110.52
22	6	601	CLA	O2A-CGA-CBA	2.53	119.86	111.91
22	Z	602	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
25	L	201	BCR	C20-C21-C22	-2.53	123.69	127.31
22	8	602	CLA	C4-C3-C5	2.53	119.53	115.27
22	1	602	CLA	CAC-C3C-C4C	2.53	128.10	124.81
22	2	611	CLA	CHB-C4A-NA	2.53	128.02	124.51
25	F	305	BCR	C24-C23-C22	-2.53	122.41	126.23
22	B	809	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	7	609	CLA	CMA-C3A-C2A	-2.53	103.61	113.83
22	B	829	CLA	CMC-C2C-C1C	2.53	128.90	125.04
22	5	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	9	614	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	6	616	CLA	CHC-C1C-NC	2.53	128.04	124.20
22	B	812	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
22	9	611	CLA	O2A-CGA-CBA	2.53	119.85	111.91
22	5	616	CLA	CHD-C4C-NC	2.53	128.19	124.20
22	6	611	CLA	CHD-C4C-NC	2.53	128.19	124.20
22	5	603	CLA	CAC-C3C-C4C	2.53	128.09	124.81
22	B	827	CLA	CHD-C4C-NC	2.53	128.19	124.20
22	B	803	CLA	CMB-C2B-C1B	2.53	129.22	125.37
22	1	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B	806	CLA	O2A-CGA-CBA	2.53	119.85	111.91
30	Z	619	LUT	C15-C35-C34	-2.53	118.29	123.47
22	9	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B	830	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
22	B	803	CLA	C4-C3-C5	2.53	119.52	115.27
30	1	617	LUT	C39-C29-C28	2.53	122.06	118.08
22	B	812	CLA	CHC-C4B-NB	-2.53	121.58	124.26
25	7	623	BCR	C11-C10-C9	-2.53	123.70	127.31
22	7	613	CLA	CHD-C4C-NC	2.53	128.19	124.20
22	3	606	CLA	CHC-C4B-NB	-2.53	121.58	124.26
22	4	601	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
30	9	616	LUT	C35-C15-C14	-2.53	118.30	123.47
22	5	611	CLA	O2A-CGA-CBA	2.53	119.84	111.91
22	6	614	CLA	CHB-C4A-NA	2.53	128.00	124.51
22	3	606	CLA	CMB-C2B-C1B	2.53	129.22	125.37
22	A	812	CLA	O2A-CGA-CBA	2.53	119.83	111.91
22	1	614	CLA	CAC-C3C-C4C	2.52	128.09	124.81
22	1	614	CLA	O2D-CGD-O1D	-2.52	118.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	614	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	1	608	CLA	CAA-CBA-CGA	-2.52	105.88	113.25
22	B	809	CLA	CMB-C2B-C1B	2.52	129.21	125.37
22	1	614	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	5	617	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	A	822	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	1	614	CLA	CMB-C2B-C1B	2.52	129.21	125.37
22	3	611	CLA	CHD-C4C-NC	2.52	128.17	124.20
22	6	610	CLA	CMC-C2C-C1C	2.52	128.88	125.04
29	4	607	CHL	CAC-C3C-C4C	2.52	128.08	124.81
22	L	203	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
22	9	614	CLA	CMC-C2C-C1C	2.52	128.87	125.04
29	6	606	CHL	O2D-CGD-O1D	-2.52	118.92	123.84
22	3	607	CLA	C1-O2A-CGA	2.52	123.05	116.44
22	A	842	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	Z	604	CLA	CHD-C4C-NC	2.52	128.17	124.20
30	9	616	LUT	C3-C4-C5	-2.52	106.84	111.85
25	3	719	BCR	C10-C11-C12	-2.52	115.36	123.22
22	5	613	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
22	B	806	CLA	CMB-C2B-C1B	2.52	129.20	125.37
22	7	616	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
22	5	612	CLA	CHD-C4C-NC	2.51	128.17	124.20
30	2	617	LUT	C31-C30-C29	-2.51	123.72	127.31
22	2	609	CLA	CHD-C4C-NC	2.51	128.16	124.20
22	B	835	CLA	CAC-C3C-C4C	2.51	128.07	124.81
22	Z	614	CLA	CAC-C3C-C4C	2.51	128.07	124.81
22	4	601	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
29	4	608	CHL	C3B-C4B-NB	2.51	112.85	110.52
22	7	616	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	8	609	CLA	CMB-C2B-C1B	2.51	129.19	125.37
22	3	611	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	1	613	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	I	172	BCR	C28-C27-C26	-2.51	109.59	114.08
25	B	847	BCR	C34-C9-C8	2.51	122.03	118.08
22	B	804	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
22	A	834	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	B	811	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	J	3001	LMG	C1-C2-C3	-2.51	104.77	110.00
30	Z	619	LUT	C38-C25-C24	-2.51	118.19	123.56
22	B	840	CLA	CHD-C4C-NC	2.51	128.16	124.20
22	A	816	CLA	CMB-C2B-C1B	2.51	129.19	125.37
30	3	621	LUT	C18-C5-C6	-2.51	121.71	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	601	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	B	813	CLA	C4-C3-C5	2.51	119.49	115.27
22	9	611	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
22	B	817	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	Z	618	LUT	C3-C4-C5	-2.51	106.86	111.85
22	B	826	CLA	C4-C3-C5	2.51	119.49	115.27
22	B	831	CLA	CAC-C3C-C4C	2.51	128.06	124.81
22	A	843	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	A	837	CLA	CHB-C1B-C2B	-2.51	120.16	127.24
22	A	840	CLA	C4-C3-C5	2.51	119.48	115.27
29	4	606	CHL	CHD-C4C-NC	2.50	128.15	124.20
22	A	802	CLA	C4-C3-C5	2.50	119.48	115.27
22	A	854	CLA	CMA-C3A-C4A	-2.50	105.04	111.77
22	5	611	CLA	CMB-C2B-C1B	2.50	129.18	125.37
22	A	813	CLA	CMC-C2C-C1C	2.50	128.85	125.04
22	6	611	CLA	CMB-C2B-C1B	2.50	129.18	125.37
22	7	610	CLA	C1-C2-C3	-2.50	121.71	126.04
22	9	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	A	852	BCR	C10-C11-C12	-2.50	115.41	123.22
22	1	611	CLA	CHD-C4C-NC	2.50	128.15	124.20
22	B	802	CLA	CAC-C3C-C4C	2.50	128.06	124.81
22	2	601	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
22	5	613	CLA	C4A-NA-C1A	-2.50	105.58	106.71
22	1	609	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
22	7	612	CLA	CMB-C2B-C1B	2.50	129.18	125.37
22	B	824	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
22	8	601	CLA	CMC-C2C-C1C	2.50	128.85	125.04
22	A	817	CLA	O2A-CGA-CBA	2.50	119.76	111.91
22	5	604	CLA	CHD-C4C-NC	2.50	128.15	124.20
22	3	604	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
22	1	614	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	9	613	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	2	611	CLA	O2A-CGA-CBA	2.50	119.75	111.91
22	B	831	CLA	CHB-C1B-C2B	-2.50	120.17	127.24
22	B	807	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
22	9	603	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	Z	611	CLA	CMB-C2B-C1B	2.50	129.18	125.37
22	9	612	CLA	C4-C3-C5	2.50	119.47	115.27
22	5	602	CLA	CHC-C1C-C2C	-2.50	119.79	126.73
22	Z	603	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
22	B	812	CLA	CMC-C2C-C1C	2.50	128.84	125.04
22	A	807	CLA	C1-C2-C3	-2.50	121.72	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	616	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
22	B	802	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	6	625	BCR	C29-C30-C25	2.50	114.33	110.48
30	1	619	LUT	C18-C5-C6	-2.50	121.72	124.53
22	9	614	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
29	4	618	CHL	O2D-CGD-O1D	-2.50	118.96	123.84
22	A	821	CLA	CAC-C3C-C4C	2.50	128.05	124.81
22	1	613	CLA	CHB-C4A-NA	2.50	127.96	124.51
22	7	620	CLA	CHB-C4A-NA	2.50	127.96	124.51
25	A	848	BCR	C32-C1-C6	2.50	114.35	110.30
22	1	603	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
22	3	602	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
22	5	610	CLA	C1-C2-C3	-2.50	121.73	126.04
22	7	616	CLA	CMC-C2C-C1C	2.50	128.84	125.04
22	J	3002	CLA	CMB-C2B-C1B	2.50	129.17	125.37
22	2	609	CLA	CMB-C2B-C1B	2.50	129.17	125.37
22	Z	609	CLA	C1-C2-C3	-2.49	121.73	126.04
22	6	622	CLA	CMC-C2C-C1C	2.49	128.84	125.04
22	B	825	CLA	CAC-C3C-C4C	2.49	128.05	124.81
25	4	621	BCR	C38-C26-C27	2.49	118.41	113.62
22	A	806	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
22	9	612	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
22	Z	606	CLA	C1-C2-C3	-2.49	121.73	126.04
22	8	608	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
22	B	841	CLA	C4-C3-C5	2.49	119.46	115.27
22	B	838	CLA	CHC-C4B-NB	-2.49	121.62	124.26
25	B	845	BCR	C11-C10-C9	-2.49	123.75	127.31
22	3	603	CLA	CMC-C2C-C1C	2.49	128.83	125.04
22	8	608	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	3	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	A	838	CLA	O2A-CGA-CBA	2.49	119.72	111.91
22	A	822	CLA	CAC-C3C-C4C	2.49	128.04	124.81
25	5	622	BCR	C11-C12-C13	-2.49	119.42	126.42
22	3	607	CLA	CAC-C3C-C4C	2.49	128.04	124.81
22	Z	602	CLA	O2A-CGA-CBA	2.49	119.72	111.91
25	3	719	BCR	C2-C1-C6	2.49	114.31	110.48
22	B	816	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	6	622	CLA	CHD-C4C-NC	2.49	128.12	124.20
30	6	624	LUT	C38-C25-C24	-2.49	118.24	123.56
22	7	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	L	203	CLA	CHD-C4C-NC	2.49	128.12	124.20
22	2	607	CLA	CMB-C2B-C1B	2.49	129.16	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	601	CLA	CAC-C3C-C4C	2.49	128.03	124.81
22	1	608	CLA	CMC-C2C-C1C	2.49	128.82	125.04
25	B	801	BCR	C16-C17-C18	-2.49	123.76	127.31
22	B	838	CLA	CHB-C1B-NB	-2.49	121.63	124.26
22	1	608	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
22	B	829	CLA	CAC-C3C-C4C	2.48	128.03	124.81
22	6	604	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
25	8	619	BCR	C31-C1-C6	-2.48	106.27	110.30
22	8	604	CLA	CHD-C4C-NC	2.48	128.12	124.20
22	A	841	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	8	616	CLA	CMB-C2B-C1B	2.48	129.15	125.37
22	6	602	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
22	B	817	CLA	CHB-C1B-NB	-2.48	121.63	124.26
22	4	602	CLA	C1-C2-C3	-2.48	121.75	126.04
25	B	845	BCR	C21-C20-C19	-2.48	115.47	123.22
22	B	828	CLA	CMB-C2B-C1B	2.48	129.15	125.37
22	8	612	CLA	CMB-C2B-C1B	2.48	129.15	125.37
22	9	602	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
29	1	607	CHL	CMB-C2B-C1B	2.48	129.15	125.37
22	7	610	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
30	8	618	LUT	C7-C8-C9	-2.48	122.49	126.23
22	6	622	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
22	Z	613	CLA	CMB-C2B-C1B	2.48	129.14	125.37
22	Z	614	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
29	6	618	CHL	CBC-CAC-C3C	-2.48	105.60	112.43
22	A	839	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
22	8	609	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
22	2	607	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
22	7	614	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	F	301	CLA	CMD-C2D-C3D	-2.48	121.92	127.61
22	8	612	CLA	CHC-C4B-NB	-2.48	121.64	124.26
22	6	603	CLA	CBC-CAC-C3C	-2.48	105.61	112.43
30	2	616	LUT	C21-C26-C27	-2.48	109.57	112.70
29	4	607	CHL	C2A-C1A-CHA	-2.48	119.53	123.86
29	4	608	CHL	O2A-CGA-CBA	2.47	119.67	111.91
22	4	601	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	A	808	CLA	CHC-C4B-NB	-2.47	121.64	124.26
22	6	616	CLA	CAA-CBA-CGA	-2.47	106.03	113.25
22	1	604	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
22	A	817	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
22	7	604	CLA	CED-O2D-CGD	2.47	121.53	115.94
22	7	613	CLA	CAA-C2A-C3A	-2.47	106.01	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	601	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
22	7	602	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	A	836	CLA	CMB-C2B-C1B	2.47	129.13	125.37
22	B	821	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	Z	602	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
22	B	812	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	A	825	CLA	CHD-C4C-NC	2.47	128.09	124.20
22	A	805	CLA	CMB-C2B-C1B	2.47	129.12	125.37
22	Z	611	CLA	CAC-C3C-C4C	2.47	128.01	124.81
22	Z	616	CLA	CMB-C2B-C1B	2.47	129.12	125.37
22	A	822	CLA	C1-C2-C3	-2.47	121.78	126.04
22	2	613	CLA	CAA-C2A-C1A	2.47	120.05	111.97
22	3	604	CLA	C4-C3-C5	2.47	119.42	115.27
22	B	852	CLA	CMB-C2B-C1B	2.46	129.12	125.37
30	4	620	LUT	C19-C9-C8	2.46	121.96	118.08
22	B	816	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	8	601	CLA	CHD-C4C-NC	2.46	128.09	124.20
30	4	619	LUT	C28-C29-C30	-2.46	115.16	118.94
22	2	609	CLA	O2A-CGA-CBA	2.46	119.64	111.91
25	B	801	BCR	C34-C9-C10	-2.46	119.47	122.92
22	A	802	CLA	C1-O2A-CGA	2.46	122.90	116.44
22	B	836	CLA	CMB-C2B-C3B	2.46	132.55	126.59
29	1	607	CHL	CHB-C1B-NB	-2.46	121.65	124.26
22	A	826	CLA	CHA-C1A-NA	-2.46	120.76	126.40
22	3	614	CLA	CMB-C2B-C1B	2.46	129.12	125.37
22	Z	602	CLA	C3B-C4B-NB	2.46	112.80	110.52
22	3	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	837	CLA	O2A-CGA-CBA	2.46	119.62	111.91
22	A	836	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
25	I	172	BCR	C29-C30-C25	2.46	114.26	110.48
22	1	609	CLA	CMC-C2C-C1C	2.46	128.78	125.04
22	A	819	CLA	O2A-CGA-CBA	2.46	119.62	111.91
29	Z	601	CHL	O2A-CGA-CBA	2.46	119.62	111.91
22	7	608	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
25	7	624	BCR	C2-C1-C6	2.46	114.26	110.48
22	A	828	CLA	CHC-C1C-C2C	-2.46	119.91	126.73
22	B	834	CLA	CMC-C2C-C1C	2.46	128.78	125.04
22	F	304	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
30	9	616	LUT	C18-C5-C6	-2.46	121.77	124.53
22	6	613	CLA	CMB-C2B-C1B	2.46	129.11	125.37
22	6	601	CLA	C1-C2-C3	-2.46	121.80	126.04
22	3	612	CLA	O2D-CGD-O1D	-2.46	119.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	841	CLA	CHB-C1B-C2B	-2.46	120.30	127.24
25	L	205	BCR	C11-C10-C9	-2.46	123.81	127.31
22	1	609	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	Z	612	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
22	1	616	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	1	606	CLA	CHC-C4B-NB	-2.45	121.66	124.26
25	A	848	BCR	C3-C4-C5	-2.45	109.70	114.08
22	B	819	CLA	C3B-C4B-NB	2.45	112.79	110.52
25	A	850	BCR	C7-C8-C9	-2.45	122.53	126.23
22	A	845	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	4	610	CLA	CHC-C1C-NC	2.45	127.92	124.20
22	L	203	CLA	C4-C3-C5	2.45	119.39	115.27
22	L	203	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	Z	613	CLA	C1-O2A-CGA	2.45	122.88	116.44
22	9	613	CLA	O2A-CGA-CBA	2.45	119.59	111.91
22	9	610	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
22	A	833	CLA	CHB-C1B-C2B	-2.45	120.32	127.24
22	7	620	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
22	7	602	CLA	CHC-C4B-NB	-2.45	121.67	124.26
22	7	608	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	A	807	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	A	801	CL0	CAC-C3C-C4C	2.45	127.99	124.81
22	2	607	CLA	O2A-CGA-CBA	2.45	119.59	111.91
22	6	601	CLA	CHB-C1B-NB	-2.45	121.67	124.26
22	9	603	CLA	CHC-C4B-NB	-2.45	121.67	124.26
25	5	622	BCR	C8-C7-C6	-2.45	120.33	127.20
22	B	830	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	4	612	CLA	C4-C3-C5	2.45	119.39	115.27
22	B	817	CLA	CHD-C4C-NC	2.45	128.06	124.20
22	3	607	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	4	609	CLA	C3B-C4B-NB	2.45	112.78	110.52
22	B	809	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
30	2	617	LUT	C15-C14-C13	-2.44	123.82	127.31
29	8	607	CHL	O2A-CGA-CBA	2.44	119.58	111.91
22	A	804	CLA	C4-C3-C5	2.44	119.38	115.27
22	A	820	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
29	5	608	CHL	C3B-C4B-NB	2.44	112.78	110.52
22	4	604	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	8	613	CLA	CMB-C2B-C1B	2.44	129.09	125.37
22	2	603	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
22	5	609	CLA	CHD-C4C-NC	2.44	128.05	124.20
22	7	614	CLA	CBC-CAC-C3C	-2.44	105.70	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	620	LUT	C10-C11-C12	-2.44	115.60	123.22
22	5	603	CLA	CMC-C2C-C1C	2.44	128.76	125.04
22	A	838	CLA	CMB-C2B-C1B	2.44	129.09	125.37
22	7	620	CLA	CMB-C2B-C1B	2.44	129.09	125.37
29	9	607	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
22	B	805	CLA	C4A-NA-C1A	-2.44	105.61	106.71
22	B	816	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
22	3	606	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
30	1	618	LUT	C30-C31-C32	-2.44	115.61	123.22
22	3	612	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
22	6	609	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	A	840	CLA	CMC-C2C-C1C	2.44	128.75	125.04
22	A	821	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	9	609	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	L	204	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
29	5	618	CHL	CMB-C2B-C1B	2.44	129.08	125.37
22	B	839	CLA	O2A-CGA-CBA	2.44	119.56	111.91
29	6	607	CHL	C1-C2-C3	-2.44	121.83	126.04
22	8	616	CLA	CMC-C2C-C1C	2.44	128.75	125.04
22	B	814	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
22	A	824	CLA	C4-C3-C5	2.44	118.77	115.98
22	8	611	CLA	CMB-C2B-C1B	2.44	129.08	125.37
22	B	828	CLA	C1-C2-C3	-2.44	121.83	126.04
22	3	617	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
22	K	4002	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	Z	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	B	835	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
22	B	818	CLA	CHB-C1B-C2B	-2.43	120.36	127.24
22	B	809	CLA	C4-C3-C5	2.43	119.36	115.27
22	B	819	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
22	4	616	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	8	608	CLA	CMB-C2B-C1B	2.43	129.07	125.37
22	9	612	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	A	833	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	B	841	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	7	603	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	1	612	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	A	818	CLA	CHC-C4B-NB	-2.43	121.68	124.26
22	4	616	CLA	CHB-C1B-NB	-2.43	121.68	124.26
22	6	609	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
22	B	810	CLA	C4-C3-C5	2.43	119.36	115.27
29	9	606	CHL	C2A-C1A-CHA	-2.43	119.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	611	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	4	604	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
22	3	604	CLA	C1-C2-C3	-2.43	121.84	126.04
25	4	621	BCR	C28-C27-C26	-2.43	109.74	114.08
30	7	621	LUT	C10-C11-C12	-2.43	115.63	123.22
22	5	613	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	7	608	CLA	C3B-C4B-NB	2.43	112.77	110.52
22	3	612	CLA	CHD-C4C-NC	2.43	128.03	124.20
30	8	617	LUT	C10-C11-C12	-2.43	115.64	123.22
22	K	4003	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	A	830	CLA	CHC-C4B-NB	-2.43	121.69	124.26
22	5	601	CLA	C1-C2-C3	-2.43	121.84	126.04
25	5	622	BCR	C34-C9-C8	2.43	121.90	118.08
25	I	172	BCR	C7-C8-C9	-2.43	122.57	126.23
22	3	614	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	9	611	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	8	610	CLA	CMA-C3A-C2A	-2.42	104.05	113.83
22	B	816	CLA	C3B-C4B-NB	2.42	112.76	110.52
22	1	612	CLA	C4-C3-C5	2.42	119.35	115.27
22	7	609	CLA	CHB-C1B-NB	-2.42	121.69	124.26
22	2	613	CLA	CHA-C1A-NA	-2.42	120.85	126.40
29	6	608	CHL	CAA-CBA-CGA	-2.42	106.17	113.25
22	6	610	CLA	CMA-C3A-C2A	-2.42	104.06	113.83
22	1	616	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
22	B	811	CLA	CAB-C3B-C2B	2.42	129.86	123.59
22	4	602	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
22	A	834	CLA	CAC-C3C-C4C	2.42	127.95	124.81
29	6	618	CHL	CMB-C2B-C1B	2.42	129.05	125.37
22	B	832	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	Z	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	Z	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	6	611	CLA	O2A-CGA-CBA	2.42	119.50	111.91
22	4	612	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
22	5	616	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
22	2	610	CLA	CMC-C2C-C1C	2.42	128.72	125.04
22	A	833	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
22	Z	612	CLA	CAC-C3C-C4C	2.42	127.94	124.81
22	4	611	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	2	613	CLA	CMC-C2C-C1C	2.42	128.72	125.04
22	9	601	CLA	CMB-C2B-C1B	2.42	129.05	125.37
22	4	611	CLA	CHD-C4C-NC	2.42	128.01	124.20
22	B	835	CLA	CHB-C4A-NA	2.42	127.85	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	602	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	5	602	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	A	824	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
22	4	612	CLA	CMB-C2B-C1B	2.41	129.05	125.37
22	6	610	CLA	C4-C3-C5	2.41	119.33	115.27
22	1	606	CLA	O2A-CGA-CBA	2.41	119.48	111.91
30	1	618	LUT	C20-C13-C12	2.41	121.88	118.08
22	A	811	CLA	CMB-C2B-C1B	2.41	129.04	125.37
22	L	203	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	1	602	CLA	C4-C3-C5	2.41	119.33	115.27
25	B	844	BCR	C33-C5-C6	-2.41	121.82	124.53
22	A	819	CLA	CMC-C2C-C1C	2.41	128.71	125.04
22	6	604	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	B	852	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
22	2	602	CLA	CMC-C2C-C1C	2.41	128.71	125.04
22	Z	609	CLA	CMB-C2B-C1B	2.41	129.04	125.37
22	9	611	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
25	G	205	BCR	C7-C8-C9	-2.41	122.59	126.23
22	B	809	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	B	833	CLA	C1-C2-C3	-2.41	121.87	126.04
25	B	848	BCR	C33-C5-C6	-2.41	121.82	124.53
25	J	3003	BCR	C15-C16-C17	-2.41	118.54	123.47
22	9	604	CLA	O2A-CGA-CBA	2.41	119.47	111.91
22	2	613	CLA	CHD-C4C-NC	2.41	128.00	124.20
22	5	606	CLA	CMC-C2C-C1C	2.41	128.71	125.04
25	B	843	BCR	C16-C17-C18	-2.41	123.87	127.31
22	A	830	CLA	CHB-C1B-C2B	-2.41	120.44	127.24
22	B	808	CLA	CHD-C4C-NC	2.41	128.00	124.20
22	8	601	CLA	O2A-CGA-CBA	2.41	119.46	111.91
28	9	620	LMG	O3-C3-C2	-2.41	104.78	110.35
22	8	616	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	A	829	CLA	CHC-C1C-C2C	-2.41	120.04	126.73
24	Z	620	LHG	O8-C23-C24	2.41	119.46	111.91
22	B	805	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
22	B	823	CLA	C1-C2-C3	-2.41	121.88	126.04
23	B	842	PQN	C14-C13-C15	2.41	119.32	115.27
22	A	832	CLA	CHD-C4C-NC	2.41	127.99	124.20
22	A	843	CLA	CHD-C4C-NC	2.40	127.99	124.20
22	B	812	CLA	CHB-C4A-NA	2.40	127.84	124.51
29	4	618	CHL	CMB-C2B-C1B	2.40	129.03	125.37
22	B	819	CLA	C1-C2-C3	-2.40	121.89	126.04
22	A	842	CLA	O2A-CGA-CBA	2.40	119.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	845	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	B	834	CLA	CED-O2D-CGD	2.40	121.37	115.94
22	A	811	CLA	CMA-C3A-C2A	-2.40	104.14	113.83
25	A	849	BCR	C15-C16-C17	-2.40	118.56	123.47
22	8	602	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
22	A	827	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	6	601	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	Z	601	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
22	B	813	CLA	CMC-C2C-C1C	2.40	128.69	125.04
22	3	620	CLA	C1-C2-C3	-2.40	121.89	126.04
22	A	841	CLA	C3B-C4B-NB	2.40	112.74	110.52
22	5	602	CLA	C4-C3-C5	2.40	119.31	115.27
22	Z	609	CLA	CHD-C4C-NC	2.40	127.98	124.20
22	B	831	CLA	CHC-C1C-C2C	-2.40	120.06	126.73
22	4	613	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
22	5	602	CLA	C3B-C4B-NB	2.40	112.74	110.52
22	4	609	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
22	3	602	CLA	CMB-C2B-C3B	2.40	132.40	126.59
22	2	603	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	A	814	CLA	C1-C2-C3	-2.40	121.90	126.04
22	8	602	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	A	818	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
22	2	612	CLA	O2A-CGA-CBA	2.40	119.43	111.91
22	A	809	CLA	CAC-C3C-C4C	2.40	127.92	124.81
22	A	835	CLA	O2A-CGA-CBA	2.40	119.43	111.91
30	9	616	LUT	C30-C31-C32	-2.40	115.74	123.22
22	L	203	CLA	CHB-C4A-NA	2.40	127.82	124.51
29	Z	607	CHL	CHB-C4A-NA	2.40	127.82	124.51
22	8	602	CLA	CMC-C2C-C1C	2.39	128.69	125.04
22	9	604	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
29	6	618	CHL	C2A-C3A-C4A	-2.39	98.00	101.87
30	3	621	LUT	C38-C25-C24	-2.39	118.44	123.56
22	8	612	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
22	B	827	CLA	CHB-C1B-C2B	-2.39	120.48	127.24
30	2	616	LUT	C18-C5-C6	-2.39	121.84	124.53
22	B	838	CLA	CAC-C3C-C4C	2.39	127.91	124.81
22	A	854	CLA	CHD-C4C-NC	2.39	127.97	124.20
22	A	808	CLA	CMB-C2B-C1B	2.39	129.01	125.37
22	1	610	CLA	CMA-C3A-C2A	-2.39	104.18	113.83
22	B	822	CLA	C4-C3-C5	2.39	119.29	115.27
22	B	824	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
22	A	854	CLA	C1C-C2C-C3C	-2.39	104.45	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	614	CLA	CMB-C2B-C1B	2.39	129.00	125.37
22	2	612	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
25	K	4001	BCR	C7-C6-C5	2.39	127.24	121.46
22	2	607	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	B	824	CLA	C1-C2-C3	-2.39	121.92	126.04
22	6	614	CLA	CHB-C1B-C2B	-2.39	120.50	127.24
22	1	609	CLA	CMB-C2B-C1B	2.39	129.00	125.37
22	8	611	CLA	CHD-C4C-NC	2.39	127.96	124.20
30	8	618	LUT	C15-C35-C34	-2.38	118.59	123.47
22	A	838	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
22	F	304	CLA	C1-C2-C3	-2.38	121.92	126.04
22	3	617	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	7	620	CLA	C4-C3-C5	2.38	119.28	115.27
22	9	611	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	9	610	CLA	CHB-C4A-NA	2.38	127.81	124.51
25	7	624	BCR	C29-C30-C25	2.38	114.15	110.48
22	9	603	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	A	841	CLA	CMB-C2B-C1B	2.38	129.00	125.37
22	Z	612	CLA	C4-C3-C5	2.38	119.28	115.27
22	6	622	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
22	Z	602	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	7	609	CLA	CHD-C4C-NC	2.38	127.95	124.20
25	6	623	BCR	C24-C23-C22	-2.38	122.64	126.23
22	B	822	CLA	C1-C2-C3	-2.38	121.93	126.04
22	B	806	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	2	609	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	1	612	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	7	610	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
29	5	618	CHL	C2A-C1A-CHA	-2.38	119.70	123.86
22	A	832	CLA	CMB-C2B-C1B	2.38	128.99	125.37
22	4	602	CLA	CMB-C2B-C1B	2.38	128.99	125.37
22	B	813	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
23	A	844	PQN	C14-C13-C15	2.38	119.27	115.27
22	B	809	CLA	CMC-C2C-C1C	2.38	128.66	125.04
22	2	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
22	B	817	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
22	8	603	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
22	3	602	CLA	C1-C2-C3	-2.38	121.93	126.04
22	1	613	CLA	CMC-C2C-C1C	2.38	128.66	125.04
22	6	602	CLA	CMB-C2B-C1B	2.38	128.99	125.37
22	4	604	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
22	3	620	CLA	CMC-C2C-C1C	2.38	128.66	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	819	CLA	CBA-CAA-C2A	2.38	120.88	113.86
25	L	201	BCR	C24-C23-C22	-2.38	122.65	126.23
25	8	619	BCR	C29-C30-C25	2.37	114.14	110.48
29	6	608	CHL	CHB-C1B-NB	-2.37	121.74	124.26
25	J	3003	BCR	C16-C15-C14	-2.37	118.61	123.47
22	4	601	CLA	CHD-C4C-NC	2.37	127.94	124.20
25	3	719	BCR	C24-C23-C22	-2.37	122.65	126.23
22	L	204	CLA	CHD-C4C-NC	2.37	127.94	124.20
25	7	623	BCR	C31-C1-C6	-2.37	106.45	110.30
22	A	854	CLA	O2A-C1-C2	2.37	114.87	108.64
22	6	602	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
22	Z	606	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	A	811	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	1	613	CLA	O2A-CGA-CBA	2.37	119.35	111.91
22	A	827	CLA	C3B-C4B-NB	2.37	112.71	110.52
22	3	617	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	B	823	CLA	CED-O2D-CGD	2.37	121.30	115.94
22	A	831	CLA	O2A-CGA-CBA	2.37	119.34	111.91
22	Z	609	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
25	L	205	BCR	C38-C26-C25	-2.37	121.87	124.53
25	B	847	BCR	C36-C18-C19	2.37	121.81	118.08
22	7	602	CLA	CMC-C2C-C1C	2.37	128.65	125.04
30	Z	619	LUT	C11-C10-C9	-2.37	123.93	127.31
22	8	612	CLA	CMC-C2C-C1C	2.37	128.64	125.04
22	A	837	CLA	CHB-C4A-NA	2.37	127.78	124.51
30	Z	619	LUT	C19-C9-C8	2.37	121.81	118.08
25	K	4001	BCR	C20-C21-C22	-2.37	123.93	127.31
29	6	606	CHL	CBC-CAC-C3C	-2.37	105.91	112.43
22	A	811	CLA	CHB-C1B-NB	-2.37	121.75	124.26
22	B	819	CLA	O2A-CGA-CBA	2.37	119.33	111.91
22	1	612	CLA	CBC-CAC-C3C	-2.36	105.91	112.43
22	B	818	CLA	CHB-C4A-NA	2.36	127.78	124.51
29	6	606	CHL	O2A-CGA-CBA	2.36	119.32	111.91
29	9	607	CHL	O2A-CGA-CBA	2.36	119.32	111.91
22	Z	606	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
22	9	609	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	A	837	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
22	7	614	CLA	CMC-C2C-C1C	2.36	128.63	125.04
22	B	803	CLA	C11-C12-C13	-2.36	108.29	115.92
22	J	3002	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	B	839	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
25	J	3003	BCR	C2-C1-C6	2.36	114.11	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z	607	CHL	CHB-C1B-NB	-2.36	121.76	124.26
22	5	613	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
22	3	614	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	B	814	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
22	Z	608	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
30	9	617	LUT	C19-C9-C8	2.36	121.80	118.08
22	8	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	A	810	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
22	4	609	CLA	CMC-C2C-C1C	2.36	128.63	125.04
25	F	305	BCR	C16-C17-C18	-2.36	123.94	127.31
22	B	809	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	5	622	BCR	C31-C1-C6	-2.36	106.47	110.30
22	4	611	CLA	O2A-CGA-CBA	2.36	119.31	111.91
22	2	601	CLA	CHB-C4A-NA	2.36	127.77	124.51
29	6	607	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
22	2	602	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
25	6	623	BCR	C38-C26-C25	-2.36	121.88	124.53
22	A	833	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
22	6	613	CLA	O2A-CGA-CBA	2.36	119.31	111.91
22	3	607	CLA	C4-C3-C5	2.36	119.24	115.27
22	5	621	CLA	CHA-C1A-NA	-2.36	121.00	126.40
22	A	809	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
22	4	610	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	G	204	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	7	612	CLA	CHC-C4B-NB	-2.36	121.76	124.26
22	7	616	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	A	836	CLA	CHD-C4C-NC	2.36	127.92	124.20
25	K	4004	BCR	C38-C26-C25	-2.36	121.88	124.53
29	7	607	CHL	CHB-C1B-NB	-2.36	121.76	124.26
22	7	620	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	8	616	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
22	7	604	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
25	7	623	BCR	C37-C22-C23	2.35	121.79	118.08
30	6	621	LUT	C10-C11-C12	-2.35	115.87	123.22
29	3	608	CHL	CMB-C2B-C1B	2.35	128.96	125.37
22	1	606	CLA	C3B-C4B-NB	2.35	112.70	110.52
22	4	616	CLA	CMC-C2C-C1C	2.35	128.62	125.04
22	4	613	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
30	1	619	LUT	C2-C3-C4	2.35	113.53	110.30
22	8	612	CLA	CHB-C4A-NA	2.35	127.77	124.51
29	7	607	CHL	CHB-C4A-NA	2.35	127.77	124.51
22	2	603	CLA	CMC-C2C-C1C	2.35	128.62	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	621	LUT	C39-C29-C28	2.35	121.78	118.08
22	Z	608	CLA	CMB-C2B-C1B	2.35	128.95	125.37
22	B	803	CLA	C4A-NA-C1A	-2.35	105.65	106.71
22	A	815	CLA	CMC-C2C-C1C	2.35	128.62	125.04
22	6	610	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
22	B	818	CLA	CAC-C3C-C4C	2.35	127.86	124.81
22	B	840	CLA	C4-C3-C5	2.35	119.22	115.27
22	A	838	CLA	CHB-C4A-NA	2.35	127.76	124.51
30	1	619	LUT	C22-C23-C24	-2.35	109.07	111.74
25	G	205	BCR	C37-C22-C23	2.35	121.78	118.08
22	B	841	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
22	4	603	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	3	611	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
22	3	609	CLA	CMC-C2C-C1C	2.35	128.61	125.04
22	8	612	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
22	Z	606	CLA	CMC-C2C-C1C	2.35	128.61	125.04
29	5	608	CHL	CHA-C1A-NA	-2.35	121.03	126.40
22	A	841	CLA	CMA-C3A-C2A	-2.35	104.37	113.83
22	4	613	CLA	CMC-C2C-C1C	2.35	128.61	125.04
22	8	610	CLA	CHC-C1C-C2C	-2.35	120.22	126.73
22	1	613	CLA	C6-C7-C8	-2.35	108.34	115.92
30	5	624	LUT	C20-C13-C12	2.34	121.77	118.08
30	4	620	LUT	C35-C15-C14	-2.34	118.67	123.47
22	3	613	CLA	C1-C2-C3	-2.34	121.99	126.04
22	A	805	CLA	CMC-C2C-C1C	2.34	128.61	125.04
22	5	617	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	839	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	5	622	BCR	C16-C15-C14	-2.34	118.68	123.47
30	4	619	LUT	C38-C25-C24	-2.34	118.55	123.56
22	F	304	CLA	C4-C3-C5	2.34	119.21	115.27
22	A	838	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	8	610	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
22	2	607	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	2	601	CLA	CHB-C1B-NB	-2.34	121.78	124.26
22	5	610	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
25	B	848	BCR	C34-C9-C8	2.34	121.77	118.08
22	A	818	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
22	8	604	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	6	625	BCR	C23-C22-C21	-2.34	115.35	118.94
22	6	617	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
29	4	618	CHL	CHB-C1B-NB	-2.34	121.78	124.26
22	Z	610	CLA	CMB-C2B-C1B	2.34	128.93	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	852	BCR	C16-C15-C14	-2.34	118.69	123.47
22	6	610	CLA	CHB-C4A-NA	2.34	127.74	124.51
29	6	608	CHL	CHB-C4A-NA	2.34	127.74	124.51
22	2	607	CLA	CMC-C2C-C1C	2.34	128.59	125.04
29	4	608	CHL	C2A-C3A-C4A	-2.33	98.10	101.87
22	B	807	CLA	CHD-C4C-NC	2.33	127.88	124.20
22	7	608	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
29	Z	607	CHL	O2D-CGD-O1D	-2.33	119.27	123.84
22	B	812	CLA	CMB-C2B-C1B	2.33	128.92	125.37
29	1	607	CHL	CHD-C4C-NC	2.33	127.88	124.20
22	4	604	CLA	CMC-C2C-C1C	2.33	128.59	125.04
30	2	616	LUT	C38-C25-C24	-2.33	118.57	123.56
22	A	830	CLA	CMB-C2B-C1B	2.33	128.92	125.37
22	F	304	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	A	805	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
30	4	620	LUT	C3-C4-C5	-2.33	107.21	111.85
22	7	601	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	8	601	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	8	601	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
22	3	610	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
22	A	802	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
22	6	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	5	610	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
22	B	838	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	9	601	CLA	CHB-C4A-NA	2.33	127.73	124.51
29	6	607	CHL	O2A-CGA-CBA	2.33	119.22	111.91
22	B	819	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	A	829	CLA	CHA-C1A-NA	-2.33	121.06	126.40
22	8	602	CLA	C1-C2-C3	-2.33	122.01	126.04
22	B	832	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
22	B	839	CLA	CMC-C2C-C1C	2.33	128.59	125.04
22	3	612	CLA	CHB-C1B-C2B	-2.33	120.66	127.24
22	6	603	CLA	CMC-C2C-C1C	2.33	128.59	125.04
22	L	203	CLA	O2A-CGA-CBA	2.33	119.21	111.91
22	A	842	CLA	CMC-C2C-C1C	2.33	128.58	125.04
22	Z	606	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
22	3	602	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
25	L	205	BCR	C33-C5-C6	-2.33	121.92	124.53
22	B	818	CLA	C4C-C3C-C2C	-2.33	103.51	106.90
22	6	609	CLA	O2A-CGA-CBA	2.33	119.21	111.91
22	A	815	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
22	A	822	CLA	C3B-C4B-NB	2.33	112.67	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	620	LUT	C38-C25-C24	-2.33	118.58	123.56
22	9	602	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
22	8	613	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	L	204	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
29	6	607	CHL	CED-O2D-CGD	2.33	121.20	115.94
22	B	831	CLA	CMB-C2B-C1B	2.33	128.91	125.37
22	B	834	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
22	Z	602	CLA	CHC-C4B-NB	-2.32	121.80	124.26
25	A	849	BCR	C31-C1-C6	-2.32	106.53	110.30
22	3	611	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	J	3001	LMG	O1-C7-C8	-2.32	105.29	110.90
29	Z	607	CHL	CBC-CAC-C3C	-2.32	106.03	112.43
22	B	837	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
30	Z	617	LUT	C19-C9-C8	2.32	121.74	118.08
22	1	610	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
22	B	806	CLA	CAC-C3C-C4C	2.32	127.82	124.81
22	1	608	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	B	822	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	Z	614	CLA	CED-O2D-CGD	2.32	121.19	115.94
29	5	607	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
22	8	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	9	607	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
22	3	609	CLA	CHB-C1B-NB	-2.32	121.80	124.26
22	5	606	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
22	7	604	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
22	4	612	CLA	C1-C2-C3	-2.32	122.03	126.04
29	5	607	CHL	CHB-C4A-NA	2.32	127.72	124.51
22	A	804	CLA	CMA-C3A-C2A	-2.32	104.48	113.83
25	5	625	BCR	C35-C13-C14	-2.32	119.68	122.92
22	K	4003	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	L	204	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	820	CLA	C11-C10-C8	-2.32	108.43	115.92
22	A	834	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
22	B	811	CLA	CMA-C3A-C2A	-2.32	104.49	113.83
29	6	606	CHL	CHD-C4C-NC	2.32	127.85	124.20
22	B	840	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
22	A	835	CLA	CMC-C2C-C1C	2.31	128.56	125.04
22	1	604	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
22	6	602	CLA	CHB-C4A-NA	2.31	127.71	124.51
30	8	617	LUT	C30-C31-C32	-2.31	116.00	123.22
30	7	621	LUT	C16-C1-C6	-2.31	106.55	110.30
22	B	832	CLA	CHA-C1A-NA	-2.31	121.10	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	604	CLA	CHD-C4C-NC	2.31	127.85	124.20
22	6	616	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	5	603	CLA	OBD-CAD-C3D	-2.31	122.95	128.52
22	B	837	CLA	CMC-C2C-C1C	2.31	128.56	125.04
22	7	603	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
22	A	825	CLA	CHB-C1B-NB	-2.31	121.81	124.26
22	A	830	CLA	CED-O2D-CGD	2.31	121.17	115.94
22	1	610	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	Z	604	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	A	810	CLA	CMC-C2C-C1C	2.31	128.56	125.04
22	A	826	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
22	9	610	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	A	835	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
22	6	612	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	B	826	CLA	CMB-C2B-C1B	2.31	128.89	125.37
22	8	602	CLA	CAC-C3C-C2C	2.31	131.48	127.53
22	A	811	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	B	818	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
30	8	617	LUT	C18-C5-C6	-2.31	121.94	124.53
22	F	301	CLA	CHB-C1B-C2B	-2.31	120.72	127.24
22	B	806	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
22	B	805	CLA	CHC-C4B-NB	-2.31	121.81	124.26
22	F	301	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
22	Z	613	CLA	O2A-CGA-CBA	2.31	119.15	111.91
22	B	822	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
22	4	611	CLA	C1-C2-C3	-2.31	122.06	126.04
22	5	617	CLA	CHD-C4C-NC	2.31	127.84	124.20
29	5	608	CHL	CBC-CAC-C3C	-2.31	106.08	112.43
22	Z	610	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	B	816	CLA	C4-C3-C5	2.31	119.15	115.27
22	1	609	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
29	4	606	CHL	C1-C2-C3	-2.30	122.06	126.04
29	5	608	CHL	C1-C2-C3	-2.30	123.02	126.75
22	A	825	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	5	606	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	A	822	CLA	CHB-C1B-C2B	-2.30	120.73	127.24
22	A	854	CLA	CMB-C2B-C1B	2.30	128.88	125.37
25	3	717	BCR	C34-C9-C10	-2.30	119.70	122.92
22	2	606	CLA	CMC-C2C-C1C	2.30	128.54	125.04
22	B	829	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
22	B	832	CLA	C4-C3-C5	2.30	119.14	115.27
29	4	606	CHL	C4-C3-C5	2.30	119.14	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	616	LUT	C38-C25-C24	-2.30	118.64	123.56
22	A	803	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	1	612	CLA	CHB-C1B-C2B	-2.30	120.74	127.24
22	5	601	CLA	O2A-C1-C2	2.30	114.68	108.64
22	B	811	CLA	C4-C3-C5	2.30	119.14	115.27
22	8	604	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
22	3	613	CLA	CMC-C2C-C1C	2.30	128.54	125.04
22	A	843	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	824	CLA	C4-C3-C5	2.30	119.14	115.27
22	8	608	CLA	C5-C3-C4	2.30	119.68	114.60
22	B	813	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
22	A	831	CLA	CHD-C4C-NC	2.30	127.82	124.20
22	Z	616	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	3	608	CHL	CHB-C4A-NA	2.30	127.69	124.51
22	B	832	CLA	C6-C7-C8	-2.30	108.50	115.92
24	4	622	LHG	O8-C23-C24	2.30	119.11	111.91
22	7	608	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	4	610	CLA	CHB-C1B-C2B	-2.30	120.75	127.24
22	9	611	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
22	A	825	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
22	5	603	CLA	CHA-C1A-NA	-2.30	121.14	126.40
22	A	832	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
25	7	624	BCR	C39-C30-C25	-2.29	106.58	110.30
22	A	820	CLA	CHB-C1B-C2B	-2.29	120.76	127.24
22	B	803	CLA	CHB-C1B-C2B	-2.29	120.76	127.24
22	5	610	CLA	C4-C3-C5	2.29	119.13	115.27
22	A	807	CLA	CHB-C1B-NB	-2.29	121.83	124.26
30	6	621	LUT	C38-C25-C24	-2.29	118.65	123.56
22	7	613	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
22	G	204	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	4	607	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
25	I	172	BCR	C11-C10-C9	-2.29	124.04	127.31
22	5	614	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
29	8	607	CHL	CHD-C4C-NC	2.29	127.81	124.20
22	7	601	CLA	CMB-C2B-C1B	2.29	128.85	125.37
22	4	614	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	2	609	CLA	CHB-C1B-NB	-2.29	121.83	124.26
22	A	810	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
22	5	609	CLA	CHA-C1A-NA	-2.29	121.16	126.40
22	6	617	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	A	834	CLA	CHB-C1B-NB	-2.29	121.83	124.26
22	2	610	CLA	CBC-CAC-C3C	-2.29	106.12	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	L	201	BCR	C38-C26-C25	-2.29	121.96	124.53
25	3	717	BCR	C36-C18-C19	2.29	121.68	118.08
22	A	831	CLA	C1-C2-C3	-2.29	122.09	126.04
25	K	4004	BCR	C16-C15-C14	-2.29	118.79	123.47
25	8	619	BCR	C16-C15-C14	-2.29	118.79	123.47
22	B	818	CLA	C2A-C3A-C4A	-2.29	98.18	101.87
22	9	609	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
22	6	604	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	Z	609	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	2	602	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
22	1	606	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	B	826	CLA	CHB-C4A-NA	2.28	127.67	124.51
22	2	606	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	A	813	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
25	A	856	BCR	C20-C19-C18	-2.28	120.00	126.42
22	B	816	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
22	B	839	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
30	Z	619	LUT	C18-C5-C6	-2.28	121.96	124.53
22	7	611	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
22	9	609	CLA	CAA-C2A-C1A	2.28	119.46	111.97
29	6	608	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
22	1	602	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
22	K	4002	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	6	612	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
27	B	850	DGD	O2G-C1B-O1B	-2.28	118.19	123.70
22	2	609	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	7	612	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
25	K	4004	BCR	C10-C11-C12	-2.28	116.10	123.22
22	B	818	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	B	818	CLA	CMB-C2B-C1B	2.28	128.84	125.37
22	1	616	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	3	614	CLA	CHB-C4A-NA	2.28	127.67	124.51
22	B	836	CLA	C1-C2-C3	-2.28	122.10	126.04
30	Z	619	LUT	C31-C32-C33	-2.28	120.01	126.42
22	5	621	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	9	612	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
22	9	613	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	A	819	CLA	CMB-C2B-C1B	2.28	128.84	125.37
29	5	608	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
22	1	610	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
29	6	607	CHL	O1D-CGD-CBD	-2.28	119.83	124.48
25	A	848	BCR	C35-C13-C12	2.28	121.66	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	624	BCR	C20-C21-C22	-2.28	124.06	127.31
22	6	610	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
30	3	621	LUT	C16-C1-C6	-2.28	106.61	110.30
30	3	621	LUT	C39-C29-C28	2.28	121.66	118.08
22	A	807	CLA	CMC-C2C-C1C	2.28	128.50	125.04
22	6	601	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
25	3	719	BCR	C11-C10-C9	-2.27	124.06	127.31
22	8	610	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
22	5	612	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
22	B	815	CLA	CHB-C1B-NB	-2.27	121.85	124.26
22	A	818	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
22	6	613	CLA	CMC-C2C-C1C	2.27	128.50	125.04
22	8	609	CLA	O2A-CGA-CBA	2.27	121.21	112.23
22	1	602	CLA	C1-C2-C3	-2.27	122.11	126.04
22	B	838	CLA	CMC-C2C-C1C	2.27	128.50	125.04
22	2	602	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	B	815	CLA	CMA-C3A-C4A	-2.27	105.67	111.77
22	Z	604	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
30	7	621	LUT	C31-C30-C29	-2.27	124.07	127.31
22	Z	614	CLA	CMC-C2C-C1C	2.27	128.50	125.04
22	3	603	CLA	CED-O2D-CGD	2.27	121.07	115.94
22	3	610	CLA	C4-C3-C5	2.27	119.09	115.27
22	9	604	CLA	C5-C3-C4	2.27	119.62	114.60
22	B	828	CLA	CHC-C4B-NB	-2.27	121.85	124.26
22	K	4002	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
22	A	814	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	7	611	CLA	CMB-C2B-C1B	2.27	128.82	125.37
22	3	610	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
25	6	623	BCR	C33-C5-C6	-2.27	121.98	124.53
22	B	814	CLA	CHB-C1B-NB	-2.27	121.86	124.26
25	A	850	BCR	C1-C6-C7	2.27	122.20	115.78
30	9	617	LUT	C16-C1-C6	-2.27	106.62	110.30
22	A	831	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
22	4	610	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	B	826	CLA	CAA-CBA-CGA	-2.27	106.63	113.25
25	3	719	BCR	C29-C30-C25	2.27	113.97	110.48
22	1	612	CLA	C1-C2-C3	-2.27	122.12	126.04
22	4	601	CLA	C1-C2-C3	-2.27	122.12	126.04
30	8	617	LUT	C28-C29-C30	-2.27	115.46	118.94
22	L	203	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
22	7	612	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
25	K	4004	BCR	C7-C8-C9	-2.27	122.81	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	624	LUT	C39-C29-C28	2.27	121.65	118.08
22	1	612	CLA	CBA-CAA-C2A	-2.27	107.17	113.86
22	5	621	CLA	CHB-C4A-NA	2.27	127.64	124.51
22	5	611	CLA	C1-C2-C3	-2.27	122.12	126.04
22	4	616	CLA	CMB-C2B-C1B	2.27	128.82	125.37
29	1	601	CHL	CMB-C2B-C1B	2.27	128.82	125.37
22	B	837	CLA	CBA-CAA-C2A	2.26	120.55	113.86
25	5	625	BCR	C28-C27-C26	-2.26	110.03	114.08
21	A	801	CL0	CGD-CBD-CAD	-2.26	103.40	110.73
22	B	818	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	A	809	CLA	C6-C5-C3	-2.26	107.52	113.45
22	1	606	CLA	CMC-C2C-C1C	2.26	128.48	125.04
22	5	601	CLA	CMC-C2C-C1C	2.26	128.48	125.04
22	6	609	CLA	CHD-C4C-NC	2.26	127.77	124.20
22	7	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	5	612	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	A	816	CLA	C3B-C4B-NB	2.26	112.61	110.52
29	8	607	CHL	C4-C3-C5	2.26	119.07	115.27
30	1	619	LUT	C1-C2-C3	2.26	118.75	113.64
22	A	826	CLA	CHD-C4C-NC	2.26	127.76	124.20
22	6	601	CLA	C4-C3-C5	2.26	119.07	115.27
22	Z	602	CLA	C1-C2-C3	-2.26	122.14	126.04
30	2	616	LUT	C20-C13-C12	2.26	121.63	118.08
22	B	808	CLA	C1-C2-C3	-2.26	122.14	126.04
30	5	620	LUT	C21-C26-C27	-2.26	109.85	112.70
22	8	602	CLA	CHB-C1B-NB	-2.26	121.87	124.26
22	A	826	CLA	C1-O2A-CGA	2.26	122.36	116.44
22	B	821	CLA	CHB-C4A-NA	2.26	127.63	124.51
22	7	616	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
22	4	611	CLA	CMB-C2B-C1B	2.25	128.80	125.37
22	2	606	CLA	CMB-C2B-C1B	2.25	128.80	125.37
25	B	844	BCR	C29-C28-C27	-2.25	106.34	111.38
22	1	606	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
22	A	820	CLA	CMC-C2C-C1C	2.25	128.47	125.04
25	A	856	BCR	C11-C12-C13	-2.25	120.08	126.42
22	A	854	CLA	C1-C2-C3	-2.25	122.15	126.04
30	Z	617	LUT	C38-C25-C24	-2.25	118.74	123.56
22	B	828	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
29	6	608	CHL	CBC-CAC-C3C	-2.25	106.22	112.43
22	3	613	CLA	CHD-C4C-NC	2.25	127.75	124.20
22	7	602	CLA	CHB-C1B-C2B	-2.25	120.88	127.24
22	1	616	CLA	CMC-C2C-C1C	2.25	128.47	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	617	LUT	C20-C13-C12	2.25	121.62	118.08
22	6	610	CLA	CED-O2D-CGD	2.25	121.03	115.94
22	7	606	CLA	CHB-C4A-NA	2.25	127.62	124.51
30	7	622	LUT	C39-C29-C28	2.25	121.62	118.08
22	2	609	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	B	814	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
22	A	810	CLA	C16-C15-C13	-2.25	108.65	115.92
25	3	717	BCR	C37-C22-C23	2.25	121.62	118.08
25	3	717	BCR	C38-C26-C27	2.25	117.93	113.62
25	B	845	BCR	C36-C18-C19	2.25	121.62	118.08
22	Z	606	CLA	CHC-C4B-NB	-2.25	121.88	124.26
22	A	815	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
22	3	604	CLA	CMC-C2C-C1C	2.25	128.46	125.04
22	F	303	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	1	601	CHL	C4-C3-C5	2.25	119.05	115.27
22	Z	603	CLA	CMA-C3A-C4A	-2.25	105.74	111.77
24	5	623	LHG	C6-C5-C4	-2.25	106.48	111.79
22	B	828	CLA	CHD-C4C-NC	2.25	127.74	124.20
22	A	833	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	4	602	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
22	A	823	CLA	CMC-C2C-C1C	2.25	128.46	125.04
22	Z	608	CLA	CMC-C2C-C1C	2.25	128.46	125.04
22	A	813	CLA	CHB-C4A-NA	2.24	127.62	124.51
22	4	602	CLA	C4-C3-C5	2.24	119.05	115.27
22	A	822	CLA	CED-O2D-CGD	2.24	121.01	115.94
22	A	832	CLA	C5-C3-C4	2.24	119.56	114.60
22	5	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	9	614	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	6	613	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
22	1	604	CLA	CMC-C2C-C1C	2.24	128.45	125.04
22	6	617	CLA	CMC-C2C-C1C	2.24	128.45	125.04
22	B	804	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
22	2	606	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
22	1	611	CLA	CMB-C2B-C1B	2.24	128.78	125.37
22	A	809	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
22	5	602	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	Z	609	CLA	CHB-C1B-NB	-2.24	121.89	124.26
22	3	612	CLA	CHA-C1A-NA	-2.24	121.27	126.40
22	B	821	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
22	A	827	CLA	C4-C3-C5	2.24	119.04	115.27
22	B	823	CLA	CHD-C4C-NC	2.24	127.73	124.20
22	A	818	CLA	CAC-C3C-C4C	2.24	127.72	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	4001	BCR	C1-C6-C5	-2.24	119.46	122.61
25	B	847	BCR	C11-C12-C13	-2.24	120.13	126.42
22	6	616	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	B	805	CLA	C3B-C4B-NB	2.24	112.59	110.52
22	9	603	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
22	B	820	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
22	Z	603	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
25	B	801	BCR	C29-C30-C25	2.24	113.92	110.48
25	K	4004	BCR	C11-C10-C9	-2.24	124.12	127.31
22	A	816	CLA	C1-C2-C3	-2.24	122.17	126.04
30	Z	619	LUT	C8-C7-C6	-2.24	120.92	127.20
22	B	823	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
22	5	616	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
29	4	618	CHL	C2A-C1A-CHA	-2.24	119.95	123.86
22	5	613	CLA	CMC-C2C-C1C	2.24	128.44	125.04
22	3	603	CLA	CHC-C4B-NB	-2.24	121.89	124.26
22	6	616	CLA	CAA-C2A-C1A	-2.24	104.65	111.97
22	4	612	CLA	CMC-C2C-C1C	2.24	128.44	125.04
22	A	828	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	6	610	CLA	CHB-C1B-C2B	-2.23	120.93	127.24
22	1	614	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
21	A	801	CL0	CMC-C2C-C1C	2.23	128.44	125.04
29	1	607	CHL	CHB-C4A-NA	2.23	127.60	124.51
22	A	836	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
29	4	608	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
22	B	811	CLA	CMB-C2B-C3B	2.23	129.37	123.59
22	B	828	CLA	CHB-C4A-NA	2.23	127.60	124.51
30	5	620	LUT	C20-C13-C12	2.23	121.59	118.08
30	6	624	LUT	C3-C4-C5	-2.23	107.41	111.85
22	A	836	CLA	CMA-C3A-C2A	-2.23	104.83	113.83
30	Z	617	LUT	C16-C1-C6	-2.23	106.68	110.30
30	4	620	LUT	C20-C13-C12	2.23	121.59	118.08
22	3	610	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	A	809	CLA	C1-O2A-CGA	2.23	122.30	116.44
29	5	618	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
22	3	604	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	Z	602	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	5	612	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
22	5	604	CLA	CMC-C2C-C1C	2.23	128.43	125.04
29	9	606	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
22	B	836	CLA	CHA-C1A-NA	-2.23	121.30	126.40
22	A	854	CLA	CHB-C4A-NA	2.23	127.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	606	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	Z	612	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	A	848	BCR	C24-C23-C22	-2.23	122.87	126.23
22	4	610	CLA	CMA-C3A-C2A	-2.23	104.85	113.83
25	A	849	BCR	C35-C13-C12	2.23	121.58	118.08
30	3	621	LUT	C1-C2-C3	2.22	118.67	113.64
22	7	620	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
24	A	855	LHG	C5-O7-C7	-2.22	112.32	117.79
22	A	822	CLA	CAA-CBA-CGA	2.22	119.75	113.25
22	A	811	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
22	Z	616	CLA	CMC-C2C-C1C	2.22	128.42	125.04
22	7	610	CLA	C4-C3-C5	2.22	119.01	115.27
22	8	613	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
25	A	856	BCR	C23-C24-C25	-2.22	120.96	127.20
25	8	619	BCR	C7-C8-C9	-2.22	122.88	126.23
22	Z	604	CLA	CMC-C2C-C1C	2.22	128.42	125.04
22	B	825	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
22	3	602	CLA	C4-C3-C5	2.22	119.00	115.27
22	B	832	CLA	CMC-C2C-C1C	2.22	128.42	125.04
22	3	607	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
29	1	607	CHL	CBC-CAC-C3C	-2.22	106.31	112.43
22	2	613	CLA	C5-C3-C4	2.22	119.50	114.60
25	B	845	BCR	C10-C11-C12	-2.22	116.29	123.22
22	Z	612	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
22	5	612	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
22	A	839	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
22	8	601	CLA	C6-C7-C8	-2.22	108.75	115.92
22	5	611	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
29	5	607	CHL	CHB-C1B-NB	-2.22	121.91	124.26
22	7	610	CLA	C2A-C3A-C4A	-2.22	98.29	101.87
25	3	719	BCR	C34-C9-C8	2.22	121.57	118.08
25	A	849	BCR	C21-C20-C19	-2.21	116.31	123.22
22	8	612	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
22	8	608	CLA	CHB-C1B-NB	-2.21	121.91	124.26
22	3	613	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	A	802	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
22	6	610	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
30	3	621	LUT	C20-C13-C12	2.21	121.56	118.08
22	B	818	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	4	602	CLA	CMC-C2C-C1C	2.21	128.41	125.04
30	8	618	LUT	C16-C1-C6	-2.21	106.71	110.30
30	2	617	LUT	C3-C4-C5	-2.21	107.45	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	852	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
22	5	606	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
22	B	815	CLA	C1-C2-C3	-2.21	122.22	126.04
22	K	4002	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	Z	603	CLA	O2A-CGA-CBA	2.21	118.84	111.91
22	A	802	CLA	CED-O2D-CGD	2.21	120.94	115.94
22	9	609	CLA	CHD-C4C-NC	2.21	127.69	124.20
22	B	836	CLA	CMC-C2C-C1C	2.21	128.40	125.04
22	3	620	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	4	613	CLA	CHB-C1B-C2B	-2.21	121.00	127.24
22	A	802	CLA	O2A-CGA-CBA	2.21	118.83	111.91
30	Z	617	LUT	C28-C29-C30	-2.21	115.55	118.94
22	5	602	CLA	CHB-C1B-C2B	-2.21	121.00	127.24
22	7	620	CLA	CMC-C2C-C1C	2.21	128.40	125.04
22	9	604	CLA	CMB-C2B-C1B	2.21	128.73	125.37
22	B	825	CLA	CAA-C2A-C1A	-2.21	104.74	111.97
22	2	609	CLA	C5-C3-C4	2.21	119.47	114.60
22	8	606	CLA	CHB-C4A-NA	2.21	127.56	124.51
29	5	608	CHL	CMB-C2B-C1B	2.21	128.73	125.37
22	A	830	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	B	810	CLA	CHB-C1B-NB	-2.20	121.92	124.26
22	A	854	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
25	K	4004	BCR	C35-C13-C12	2.20	121.55	118.08
25	5	625	BCR	C2-C1-C6	2.20	113.87	110.48
22	A	834	CLA	C11-C10-C8	-2.20	108.80	115.92
22	A	808	CLA	O2A-CGA-CBA	2.20	118.82	111.91
22	B	852	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	1	606	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	Z	604	CLA	C1-C2-C3	-2.20	122.23	126.04
22	4	609	CLA	CHB-C1B-C2B	-2.20	121.02	127.24
22	B	827	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	B	821	CLA	CMC-C2C-C1C	2.20	128.39	125.04
21	A	801	CL0	O2A-CGA-O1A	-2.20	118.04	123.59
22	B	830	CLA	C5-C3-C4	2.20	119.46	114.60
25	4	621	BCR	C21-C20-C19	-2.20	116.35	123.22
22	6	602	CLA	C3B-C4B-NB	2.20	112.56	110.52
22	A	834	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
25	3	718	BCR	C23-C22-C21	-2.20	115.57	118.94
29	5	607	CHL	CBC-CAC-C3C	-2.20	106.37	112.43
22	7	609	CLA	CBA-CAA-C2A	2.20	120.35	113.86
22	A	826	CLA	C1-C2-C3	-2.20	122.24	126.04
22	A	831	CLA	CMA-C3A-C2A	-2.20	104.96	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Z	603	CLA	CHB-C1B-NB	-2.20	121.93	124.26
22	B	805	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	B	826	CLA	CAC-C3C-C4C	2.20	127.66	124.81
22	1	603	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
29	5	607	CHL	CHD-C4C-NC	2.20	127.67	124.20
22	G	204	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
22	2	612	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
22	J	3002	CLA	CMC-C2C-C1C	2.20	128.38	125.04
29	1	601	CHL	C2A-C3A-C4A	-2.20	98.32	101.87
22	A	819	CLA	C3B-C4B-NB	2.20	112.55	110.52
22	B	819	CLA	CHB-C1B-C2B	-2.20	121.04	127.24
29	Z	601	CHL	C2A-C3A-C4A	-2.20	98.32	101.87
22	8	614	CLA	C1-C2-C3	-2.19	122.25	126.04
30	8	617	LUT	C16-C1-C6	-2.19	106.74	110.30
22	B	810	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
22	B	831	CLA	CHC-C4B-NB	-2.19	121.93	124.26
29	6	608	CHL	C1-C2-C3	-2.19	123.20	126.75
22	B	813	CLA	CHB-C4A-NA	2.19	127.55	124.51
22	B	831	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
22	7	609	CLA	C5-C3-C4	2.19	119.44	114.60
22	9	609	CLA	C5-C3-C4	2.19	119.44	114.60
22	7	606	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
30	8	618	LUT	C30-C31-C32	-2.19	116.38	123.22
22	7	601	CLA	C4-C3-C2	-2.19	118.06	123.68
22	2	606	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	L	201	BCR	C21-C20-C19	-2.19	116.38	123.22
22	B	826	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
22	3	602	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
22	B	825	CLA	CMC-C2C-C1C	2.19	128.37	125.04
25	I	172	BCR	C2-C1-C6	2.19	113.85	110.48
22	3	612	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	1	602	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
22	9	603	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
25	B	848	BCR	C8-C9-C10	-2.19	115.58	118.94
22	B	834	CLA	C4-C3-C5	2.19	118.95	115.27
25	B	847	BCR	C31-C1-C6	-2.19	106.75	110.30
22	3	602	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
22	2	611	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
22	F	301	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	A	839	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
22	B	812	CLA	O2A-CGA-CBA	2.19	118.77	111.91
29	4	608	CHL	C5-C3-C4	2.18	119.43	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	603	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	9	613	CLA	CHB-C1B-NB	-2.18	121.94	124.26
30	2	616	LUT	C16-C1-C6	-2.18	106.76	110.30
25	A	849	BCR	C3-C4-C5	-2.18	110.18	114.08
22	7	604	CLA	C4-C3-C5	2.18	118.94	115.27
22	B	813	CLA	CHB-C1B-C2B	-2.18	121.07	127.24
22	Z	612	CLA	CMC-C2C-C1C	2.18	128.36	125.04
30	1	618	LUT	C39-C29-C28	2.18	121.52	118.08
22	A	821	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
30	8	618	LUT	C19-C9-C8	2.18	121.52	118.08
29	8	607	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
25	6	623	BCR	C1-C6-C7	2.18	121.95	115.78
22	B	828	CLA	CMA-C3A-C2A	-2.18	105.03	113.83
25	3	717	BCR	C29-C28-C27	-2.18	106.50	111.38
22	9	614	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
30	Z	618	LUT	C20-C13-C12	2.18	121.51	118.08
22	A	802	CLA	CMC-C2C-C1C	2.18	128.36	125.04
22	G	203	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	4	601	CLA	C4-C3-C5	2.18	118.94	115.27
22	A	809	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
22	5	616	CLA	O2A-CGA-CBA	2.18	120.84	112.23
25	J	3003	BCR	C34-C9-C8	2.18	121.51	118.08
28	J	3001	LMG	O3-C3-C2	-2.18	105.31	110.35
25	I	172	BCR	C16-C15-C14	-2.18	119.01	123.47
22	Z	608	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	B	813	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
30	5	624	LUT	C1-C2-C3	2.18	118.56	113.64
22	B	807	CLA	CMC-C2C-C1C	2.18	128.35	125.04
29	6	607	CHL	CMA-C3A-C4A	-2.18	105.92	111.77
30	6	624	LUT	C39-C29-C28	2.18	121.51	118.08
25	8	619	BCR	C2-C1-C6	2.18	113.83	110.48
22	6	612	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	B	802	CLA	CHB-C1B-NB	-2.18	121.95	124.26
22	9	604	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
22	9	612	CLA	CMC-C2C-C1C	2.17	128.35	125.04
22	A	804	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
22	A	813	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
25	3	717	BCR	C11-C12-C13	-2.17	120.31	126.42
22	7	606	CLA	CMC-C2C-C1C	2.17	128.35	125.04
29	6	608	CHL	C5-C3-C4	2.17	119.41	114.60
29	9	606	CHL	CAA-C2A-C3A	-2.17	111.03	116.10
29	4	618	CHL	CHD-C4C-NC	2.17	127.63	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	623	BCR	C2-C1-C6	2.17	113.83	110.48
30	5	620	LUT	C39-C29-C28	2.17	121.50	118.08
22	6	613	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	B	804	CLA	CMB-C2B-C3B	2.17	131.85	126.59
22	A	817	CLA	CHB-C4A-NA	2.17	127.52	124.51
29	8	607	CHL	CHB-C4A-NA	2.17	127.52	124.51
22	A	831	CLA	CMA-C3A-C4A	-2.17	105.94	111.77
30	8	618	LUT	C20-C13-C12	2.17	121.50	118.08
22	9	603	CLA	CMC-C2C-C1C	2.17	128.35	125.04
22	A	825	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
22	7	602	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
22	9	602	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
22	B	832	CLA	C1-C2-C3	-2.17	122.29	126.04
22	5	612	CLA	C1-C2-C3	-2.17	122.29	126.04
22	A	816	CLA	O2A-CGA-CBA	2.17	118.72	111.91
22	2	614	CLA	CMC-C2C-C1C	2.17	128.34	125.04
22	7	610	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
22	B	802	CLA	C4-C3-C5	2.17	118.92	115.27
22	4	609	CLA	CBA-CAA-C2A	2.17	120.27	113.86
22	5	621	CLA	O2A-CGA-CBA	2.17	120.80	112.23
22	7	611	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
22	A	840	CLA	C1-O2A-CGA	2.17	122.13	116.44
22	J	3002	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
22	8	603	CLA	CMC-C2C-C1C	2.17	128.34	125.04
22	Z	610	CLA	CHC-C1C-C2C	-2.17	120.71	126.73
22	5	610	CLA	CMB-C2B-C1B	2.17	128.67	125.37
25	A	849	BCR	C8-C7-C6	-2.17	121.11	127.20
25	3	719	BCR	C16-C15-C14	-2.17	119.03	123.47
30	2	617	LUT	C18-C5-C4	2.17	118.37	114.36
22	6	614	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
22	B	820	CLA	CMC-C2C-C1C	2.17	128.34	125.04
22	A	830	CLA	CMC-C2C-C1C	2.17	128.34	125.04
29	7	607	CHL	CHC-C1C-C2C	-2.17	118.25	126.11
24	8	620	LHG	O8-C23-C24	2.17	118.71	111.91
22	2	607	CLA	C5-C3-C4	2.17	119.39	114.60
29	9	607	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
22	A	824	CLA	CHB-C4A-NA	2.17	127.51	124.51
30	5	620	LUT	C30-C31-C32	-2.17	116.46	123.22
22	F	303	CLA	CHB-C1B-C2B	-2.17	121.12	127.24
25	F	305	BCR	C36-C18-C19	2.16	121.49	118.08
24	A	846	LHG	C6-C5-C4	-2.16	106.67	111.79
22	A	808	CLA	C1-O2A-CGA	2.16	122.12	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	609	CLA	C4-C3-C5	2.16	118.91	115.27
30	1	617	LUT	C38-C25-C24	-2.16	118.93	123.56
24	8	620	LHG	C6-C5-C4	-2.16	106.67	111.79
22	6	611	CLA	CMC-C2C-C1C	2.16	128.33	125.04
29	1	601	CHL	CHD-C4C-NC	2.16	127.61	124.20
22	A	814	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
25	5	622	BCR	C23-C24-C25	-2.16	121.13	127.20
25	6	625	BCR	C23-C24-C25	-2.16	121.13	127.20
25	G	205	BCR	C15-C14-C13	-2.16	124.22	127.31
22	G	203	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	6	602	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
22	7	601	CLA	C1-C2-C3	-2.16	122.30	126.04
22	A	803	CLA	CMB-C2B-C3B	2.16	131.82	126.59
22	A	819	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	A	833	CLA	C1-C2-C3	-2.16	122.31	126.04
22	Z	616	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
22	B	832	CLA	CHB-C1B-C2B	-2.16	121.13	127.24
22	1	606	CLA	CHB-C1B-C2B	-2.16	121.13	127.24
25	A	848	BCR	C10-C11-C12	-2.16	116.47	123.22
25	K	4004	BCR	C20-C19-C18	-2.16	120.35	126.42
22	2	607	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
22	B	837	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
22	2	603	CLA	CHB-C1B-NB	-2.16	121.97	124.26
22	A	840	CLA	CHA-C1A-NA	-2.16	121.45	126.40
30	Z	618	LUT	C35-C15-C14	-2.16	119.05	123.47
25	A	850	BCR	C32-C1-C6	2.16	113.80	110.30
22	5	611	CLA	CMC-C2C-C1C	2.16	128.33	125.04
22	5	606	CLA	CHB-C1B-C2B	-2.16	121.14	127.24
22	B	826	CLA	CHC-C4B-NB	-2.16	121.97	124.26
22	8	613	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
22	B	812	CLA	CHB-C1B-C2B	-2.16	121.14	127.24
22	2	609	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
22	B	822	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
29	6	607	CHL	CHB-C1B-NB	-2.16	121.97	124.26
22	B	833	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
22	6	604	CLA	C1-C2-C3	-2.16	122.31	126.04
22	B	828	CLA	O2D-CGD-O1D	-2.15	119.62	123.84
22	6	609	CLA	C5-C3-C4	2.15	119.36	114.60
22	A	818	CLA	C4-C3-C2	-2.15	118.15	123.68
25	L	201	BCR	C15-C16-C17	-2.15	119.06	123.47
25	7	624	BCR	C37-C22-C23	2.15	121.47	118.08
22	B	833	CLA	O1D-CGD-CBD	-2.15	120.08	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	604	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
22	L	204	CLA	C5-C3-C4	2.15	119.36	114.60
22	8	611	CLA	CMC-C2C-C1C	2.15	128.32	125.04
22	A	824	CLA	CHB-C1B-NB	-2.15	121.98	124.26
22	8	614	CLA	CMC-C2C-C1C	2.15	128.32	125.04
22	B	813	CLA	CMB-C2B-C1B	2.15	128.65	125.37
22	A	828	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
22	9	602	CLA	C1-C2-C3	-2.15	122.32	126.04
22	B	839	CLA	CHB-C4A-NA	2.15	127.49	124.51
22	2	601	CLA	CMC-C2C-C1C	2.15	128.31	125.04
25	3	718	BCR	C4-C5-C6	-2.15	119.61	122.73
22	3	617	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
22	F	303	CLA	CMB-C2B-C1B	2.15	128.64	125.37
29	3	608	CHL	C2A-C3A-C4A	-2.15	98.40	101.87
29	9	607	CHL	C5-C3-C4	2.15	119.35	114.60
22	Z	613	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
22	1	609	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	9	604	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
22	B	852	CLA	C1-C2-C3	-2.15	122.33	126.04
22	B	811	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
22	8	614	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	B	818	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
22	A	811	CLA	C1-O2A-CGA	2.15	122.08	116.44
22	Z	603	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	9	607	CHL	C1-C2-C3	-2.15	123.28	126.75
30	9	616	LUT	C21-C26-C27	-2.15	109.99	112.70
25	6	625	BCR	C2-C1-C6	2.15	113.79	110.48
22	B	852	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	A	823	CLA	CHB-C4A-NA	2.15	127.48	124.51
22	9	603	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	Z	603	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
30	Z	618	LUT	C40-C33-C32	2.15	121.46	118.08
22	B	804	CLA	CHB-C1B-C2B	-2.15	121.18	127.24
22	B	834	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
22	8	611	CLA	CED-O2D-CGD	2.14	120.79	115.94
29	6	606	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
22	2	614	CLA	CHB-C4A-NA	2.14	127.48	124.51
22	Z	610	CLA	CHB-C1B-C2B	-2.14	121.18	127.24
22	5	614	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
22	B	823	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
25	6	625	BCR	C33-C5-C6	-2.14	122.12	124.53
29	6	618	CHL	CHB-C4A-NA	2.14	127.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	613	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
22	9	610	CLA	C6-C7-C8	-2.14	108.99	115.92
22	F	303	CLA	CMC-C2C-C1C	2.14	128.30	125.04
22	B	803	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
22	B	810	CLA	C1-C2-C3	-2.14	122.34	126.04
22	A	838	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
22	3	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	835	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
22	A	837	CLA	CMC-C2C-C1C	2.14	128.30	125.04
24	8	620	LHG	C5-O7-C7	-2.14	112.52	117.79
22	Z	611	CLA	C4-C3-C5	2.14	118.87	115.27
22	6	609	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	1	611	CLA	C1-C2-C3	-2.14	122.34	126.04
22	B	830	CLA	CMC-C2C-C1C	2.14	128.30	125.04
30	9	617	LUT	C38-C25-C24	-2.14	118.98	123.56
22	G	203	CLA	C5-C3-C4	2.14	119.33	114.60
22	A	817	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
22	6	616	CLA	O2A-CGA-CBA	2.14	120.68	112.23
22	A	834	CLA	CMC-C2C-C1C	2.14	128.29	125.04
25	B	848	BCR	C37-C22-C23	2.14	121.44	118.08
22	4	611	CLA	CMC-C2C-C1C	2.14	128.29	125.04
22	3	614	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
22	Z	610	CLA	C3B-C4B-NB	2.14	112.50	110.52
22	A	817	CLA	C1-C2-C3	-2.14	122.35	126.04
28	J	3001	LMG	O2-C2-C1	-2.14	104.86	110.05
22	4	601	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
25	L	201	BCR	C37-C22-C23	2.13	121.44	118.08
22	6	604	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
24	8	620	LHG	C25-C24-C23	-2.13	105.86	113.62
22	7	608	CLA	C5-C3-C4	2.13	119.31	114.60
22	2	613	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
22	B	838	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	5	604	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
22	9	601	CLA	CMC-C2C-C1C	2.13	128.29	125.04
25	6	623	BCR	C29-C30-C25	2.13	113.76	110.48
22	A	810	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
22	4	610	CLA	C4-C3-C5	2.13	118.86	115.27
22	Z	608	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
22	B	839	CLA	C1-O2A-CGA	2.13	122.03	116.44
22	B	834	CLA	CMB-C2B-C1B	2.13	128.61	125.37
22	3	612	CLA	O2A-CGA-CBA	2.13	120.65	112.23
22	8	609	CLA	CHB-C1B-NB	-2.13	122.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	609	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
30	6	624	LUT	C19-C9-C8	2.13	121.43	118.08
22	8	601	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	B	827	CLA	C6-C7-C8	-2.13	109.03	115.92
25	J	3003	BCR	C31-C1-C6	-2.13	106.84	110.30
22	4	610	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
30	4	619	LUT	C21-C26-C27	-2.13	110.01	112.70
30	1	617	LUT	C19-C9-C8	2.13	121.43	118.08
30	7	622	LUT	C20-C13-C12	2.13	121.43	118.08
22	A	838	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
22	B	809	CLA	C1-C2-C3	-2.13	122.36	126.04
22	A	817	CLA	C4-C3-C5	2.13	118.85	115.27
22	5	601	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
22	A	838	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
22	B	818	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	A	804	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
22	A	840	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
22	A	824	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
22	9	603	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	B	829	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
22	4	612	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	K	4002	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
24	1	620	LHG	C5-O7-C7	-2.12	112.56	117.79
25	A	850	BCR	C21-C20-C19	-2.12	116.59	123.22
22	7	612	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
29	8	607	CHL	C1-C2-C3	-2.12	122.37	126.04
22	5	614	CLA	CHA-C1A-NA	-2.12	121.54	126.40
22	A	820	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
22	A	808	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
22	A	827	CLA	CGD-CBD-CAD	-2.12	103.86	110.73
22	7	611	CLA	C2A-C3A-C4A	-2.12	99.08	101.78
22	Z	614	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
25	A	856	BCR	C34-C9-C8	2.12	121.42	118.08
22	L	203	CLA	C1-C2-C3	-2.12	122.38	126.04
22	5	614	CLA	CGD-CBD-CAD	-2.12	103.87	110.73
29	Z	607	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
22	2	603	CLA	O2A-CGA-CBA	2.12	120.61	112.23
25	L	205	BCR	C35-C13-C12	2.12	121.42	118.08
22	2	612	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
22	1	602	CLA	C3B-C4B-NB	2.12	112.48	110.52
22	6	603	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	6	622	CLA	CHB-C1B-NB	-2.12	122.01	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	813	CLA	CHA-C1A-NA	-2.12	121.55	126.40
25	8	619	BCR	C23-C22-C21	-2.12	115.69	118.94
30	1	617	LUT	C18-C5-C6	-2.12	122.15	124.53
22	2	614	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
30	5	624	LUT	C7-C8-C9	-2.12	123.03	126.23
22	7	602	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
22	A	830	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	A	829	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
22	1	603	CLA	C1-C2-C3	-2.12	122.38	126.04
30	4	620	LUT	C21-C26-C27	-2.12	110.03	112.70
25	7	624	BCR	C21-C20-C19	-2.12	116.61	123.22
22	B	825	CLA	C1-C2-C3	-2.12	122.38	126.04
25	B	843	BCR	C36-C18-C19	2.12	121.41	118.08
22	Z	610	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
22	B	819	CLA	CMC-C2C-C1C	2.12	128.26	125.04
22	4	604	CLA	C5-C3-C4	2.12	119.28	114.60
22	7	611	CLA	CMC-C2C-C1C	2.12	128.26	125.04
22	3	620	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
22	Z	606	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
29	6	607	CHL	CHD-C4C-NC	2.11	127.53	124.20
22	3	609	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
22	6	613	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
22	9	611	CLA	C1-C2-C3	-2.11	122.39	126.04
22	6	614	CLA	CMC-C2C-C1C	2.11	128.26	125.04
30	8	617	LUT	C1-C2-C3	2.11	118.41	113.64
22	1	608	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	B	825	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
22	1	608	CLA	C1-C2-C3	-2.11	122.39	126.04
22	1	604	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
30	2	617	LUT	C16-C1-C6	-2.11	106.88	110.30
29	Z	601	CHL	CMB-C2B-C1B	2.11	128.58	125.37
25	B	845	BCR	C23-C22-C21	2.11	122.18	118.94
22	A	819	CLA	CBB-CAB-C3B	-2.11	117.13	127.62
22	B	804	CLA	O2A-CGA-CBA	2.11	120.81	114.03
22	A	829	CLA	CHB-C1B-C2B	-2.11	121.28	127.24
22	Z	604	CLA	CHB-C1B-NB	-2.11	122.03	124.26
29	8	607	CHL	CHC-C4B-NB	-2.11	122.03	124.26
22	B	836	CLA	CHB-C1B-C2B	-2.11	121.28	127.24
30	2	616	LUT	C10-C11-C12	-2.11	116.64	123.22
29	4	606	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
22	A	831	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
22	B	829	CLA	CMA-C3A-C4A	-2.11	106.11	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	832	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
22	B	833	CLA	CHB-C4A-NA	2.11	127.42	124.51
22	2	610	CLA	CHB-C1B-C2B	-2.11	121.29	127.24
22	B	835	CLA	CMC-C2C-C1C	2.11	128.25	125.04
22	B	841	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
25	B	847	BCR	C8-C9-C10	-2.10	115.71	118.94
22	3	606	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
22	A	841	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
22	7	613	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	A	851	BCR	C7-C8-C9	-2.10	123.06	126.23
22	B	814	CLA	C4-C3-C5	2.10	118.81	115.27
22	5	609	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
22	7	610	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	6	617	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	6	614	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
22	B	822	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
22	A	825	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
22	9	613	CLA	C5-C3-C4	2.10	119.25	114.60
22	4	604	CLA	CED-O2D-CGD	2.10	120.69	115.94
22	A	829	CLA	O2A-CGA-CBA	2.10	118.50	111.91
22	B	806	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
22	B	815	CLA	C1-O2A-CGA	2.10	121.96	116.44
22	9	604	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	A	852	BCR	C37-C22-C23	2.10	121.39	118.08
22	B	825	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
22	6	617	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
30	5	620	LUT	C18-C5-C4	2.10	118.24	114.36
22	B	837	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
30	Z	617	LUT	C8-C9-C10	-2.10	115.72	118.94
22	A	819	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
30	7	622	LUT	C16-C1-C6	-2.10	106.90	110.30
22	6	616	CLA	C2A-C3A-C4A	-2.10	98.48	101.87
22	A	836	CLA	CHC-C4B-NB	-2.10	122.04	124.26
22	1	602	CLA	CHC-C4B-NB	-2.10	122.04	124.26
29	9	606	CHL	CHB-C4A-NA	2.10	127.41	124.51
22	9	614	CLA	O2A-CGA-CBA	2.10	120.76	114.03
22	A	827	CLA	CHB-C1B-C2B	-2.10	121.32	127.24
22	4	604	CLA	O2A-CGA-CBA	2.09	118.48	111.91
29	5	608	CHL	C5-C3-C4	2.09	119.23	114.60
22	8	603	CLA	CHA-C1A-NA	-2.09	121.60	126.40
25	3	718	BCR	C15-C16-C17	-2.09	119.19	123.47
29	4	607	CHL	C5-C3-C4	2.09	119.22	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	606	CLA	C2A-C3A-C4A	-2.09	99.11	101.78
29	4	608	CHL	CBC-CAC-C3C	-2.09	106.66	112.43
22	9	601	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
22	Z	614	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
22	2	610	CLA	CHB-C4A-NA	2.09	127.40	124.51
25	K	4001	BCR	C4-C5-C6	-2.09	119.69	122.73
25	A	849	BCR	C11-C12-C13	-2.09	120.54	126.42
30	2	617	LUT	C1-C2-C3	2.09	118.36	113.64
25	B	846	BCR	C16-C15-C14	-2.09	119.19	123.47
22	1	616	CLA	CHB-C1B-NB	-2.09	122.05	124.26
22	4	614	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
29	3	608	CHL	C1-C2-C3	-2.09	122.43	126.04
22	A	822	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
29	6	618	CHL	CHD-C4C-NC	2.09	127.49	124.20
22	F	301	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	B	827	CLA	C4-C3-C5	2.09	118.78	115.27
22	7	603	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
22	2	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
30	9	617	LUT	C3-C4-C5	-2.09	107.70	111.85
22	9	603	CLA	O2A-CGA-CBA	2.09	120.47	112.23
22	1	611	CLA	CHB-C1B-C2B	-2.09	121.35	127.24
22	F	301	CLA	CMB-C2B-C1B	2.09	128.54	125.37
25	3	718	BCR	C20-C21-C22	-2.09	124.33	127.31
25	B	844	BCR	C11-C12-C13	-2.08	120.56	126.42
22	A	826	CLA	CMC-C2C-C1C	2.08	128.21	125.04
22	A	816	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
22	1	610	CLA	CHC-C4B-NB	-2.08	122.05	124.26
29	6	608	CHL	CBB-CAB-C3B	-2.08	117.25	127.62
22	8	609	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	6	624	LUT	C20-C13-C12	2.08	121.36	118.08
30	Z	619	LUT	C1-C2-C3	2.08	118.35	113.64
22	3	610	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
25	A	848	BCR	C21-C20-C19	-2.08	116.72	123.22
22	G	204	CLA	CMC-C2C-C1C	2.08	128.21	125.04
22	8	609	CLA	CMA-C3A-C2A	-2.08	105.43	113.83
22	B	820	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
22	B	834	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
22	B	811	CLA	C1-C2-C3	-2.08	122.44	126.04
29	6	608	CHL	CAA-C2A-C1A	-2.08	105.16	111.97
30	Z	617	LUT	C12-C13-C14	-2.08	115.75	118.94
22	5	606	CLA	CHC-C4B-NB	-2.08	122.06	124.26
22	A	841	CLA	C11-C10-C8	-2.08	109.20	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	836	CLA	C5-C3-C4	2.08	119.20	114.60
22	1	612	CLA	C1-O2A-CGA	2.08	121.90	116.44
22	A	813	CLA	CHC-C4B-NB	-2.08	122.06	124.26
22	8	601	CLA	CHB-C1B-NB	-2.08	122.06	124.26
22	2	614	CLA	CHA-C1A-NA	-2.08	121.64	126.40
25	K	4004	BCR	C35-C13-C14	-2.08	120.01	122.92
22	A	843	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
22	A	843	CLA	CED-O2D-CGD	2.08	120.64	115.94
22	3	607	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
22	9	614	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
22	4	616	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
29	9	607	CHL	CHB-C4A-NA	2.08	127.39	124.51
22	A	836	CLA	CMC-C2C-C1C	2.08	128.20	125.04
22	5	621	CLA	CHD-C4C-NC	2.08	127.48	124.20
22	8	616	CLA	CHB-C1B-NB	-2.08	122.06	124.26
25	A	849	BCR	C20-C19-C18	-2.08	120.58	126.42
30	4	620	LUT	C30-C31-C32	-2.08	116.74	123.22
22	8	612	CLA	C4-C3-C2	-2.08	118.35	123.68
22	1	604	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
30	1	618	LUT	C11-C10-C9	-2.08	124.35	127.31
25	7	623	BCR	C10-C11-C12	-2.08	116.74	123.22
22	3	613	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
22	6	603	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	8	601	CLA	C16-C15-C13	-2.07	109.21	115.92
22	B	811	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	1	616	CLA	O2A-CGA-CBA	2.07	120.43	112.23
22	8	612	CLA	CED-O2D-CGD	2.07	120.63	115.94
22	A	812	CLA	CMC-C2C-C1C	2.07	128.20	125.04
22	8	610	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
22	3	610	CLA	CMB-C2B-C1B	2.07	128.53	125.37
29	6	607	CHL	O2D-CGD-O1D	-2.07	119.78	123.84
24	A	847	LHG	C6-C5-C4	-2.07	106.88	111.79
22	2	612	CLA	CHB-C4A-NA	2.07	127.38	124.51
22	5	609	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
22	K	4003	CLA	CHC-C1C-NC	2.07	127.35	124.20
22	Z	609	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	6	609	CLA	CMB-C2B-C1B	2.07	128.53	125.37
22	B	835	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
22	3	603	CLA	CHB-C4A-NA	2.07	127.38	124.51
22	B	823	CLA	CHB-C1B-NB	-2.07	122.06	124.26
22	2	606	CLA	CMA-C3A-C2A	-2.07	111.27	116.10
22	6	602	CLA	CHB-C1B-C2B	-2.07	121.39	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	5	609	CLA	CHB-C1B-NB	-2.07	122.06	124.26
25	5	622	BCR	C11-C10-C9	-2.07	124.36	127.31
29	3	608	CHL	C2A-C1A-CHA	-2.07	120.24	123.86
22	B	839	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	1	604	CLA	C1-C2-C3	-2.07	122.46	126.04
25	I	172	BCR	C15-C16-C17	-2.07	119.23	123.47
22	1	602	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
22	Z	602	CLA	CMA-C3A-C2A	-2.07	105.48	113.83
22	1	611	CLA	CED-O2D-CGD	2.07	120.62	115.94
22	7	610	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
22	4	611	CLA	C1-O2A-CGA	2.07	121.87	116.44
22	A	831	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	7	607	CHL	C2A-C1A-CHA	-2.07	120.24	123.86
22	9	614	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
22	B	809	CLA	CHA-C1A-NA	-2.07	121.66	126.40
25	6	623	BCR	C34-C9-C10	-2.07	120.03	122.92
22	B	804	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
22	3	610	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
30	1	618	LUT	C16-C1-C6	-2.07	106.95	110.30
22	3	607	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	A	833	CLA	CHC-C4B-NB	-2.07	122.07	124.26
22	B	818	CLA	C1-C2-C3	-2.06	122.47	126.04
22	B	825	CLA	CMB-C2B-C1B	2.06	128.51	125.37
22	2	614	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
29	3	608	CHL	C4-C3-C5	2.06	118.74	115.27
22	A	809	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
22	5	616	CLA	CHA-C1A-NA	-2.06	121.67	126.40
25	6	625	BCR	C34-C9-C10	-2.06	120.03	122.92
22	6	609	CLA	CHB-C1B-NB	-2.06	122.07	124.26
22	3	610	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
22	8	614	CLA	CHA-C1A-NA	-2.06	121.68	126.40
30	1	619	LUT	C30-C31-C32	-2.06	116.78	123.22
22	8	613	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
22	G	203	CLA	CHB-C1B-NB	-2.06	122.08	124.26
30	Z	618	LUT	C15-C35-C34	-2.06	119.25	123.47
22	B	835	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	1	610	CLA	CMB-C2B-C1B	2.06	128.51	125.37
25	L	205	BCR	C21-C20-C19	-2.06	116.79	123.22
30	Z	618	LUT	C16-C1-C6	-2.06	106.96	110.30
22	A	802	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	4	603	CLA	CHA-C1A-NA	-2.06	121.68	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	838	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
22	6	613	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
22	3	617	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
22	Z	609	CLA	C11-C10-C8	-2.06	109.27	115.92
25	6	623	BCR	C37-C22-C23	2.06	121.32	118.08
22	8	602	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
22	A	813	CLA	CMB-C2B-C1B	2.06	128.50	125.37
22	A	821	CLA	CMB-C2B-C1B	2.06	128.50	125.37
25	B	848	BCR	C23-C24-C25	-2.06	121.42	127.20
22	2	611	CLA	CED-O2D-CGD	2.06	120.59	115.94
25	B	801	BCR	C10-C11-C12	-2.06	116.80	123.22
22	B	834	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
22	B	807	CLA	C4-C3-C5	2.06	118.73	115.27
30	5	624	LUT	C30-C31-C32	-2.06	116.80	123.22
22	4	611	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
25	B	845	BCR	C8-C9-C10	2.06	122.10	118.94
30	1	617	LUT	C31-C30-C29	-2.06	124.38	127.31
30	2	616	LUT	C11-C10-C9	-2.06	124.38	127.31
22	8	613	CLA	O2A-CGA-CBA	2.06	118.36	111.91
22	A	821	CLA	CMC-C2C-C1C	2.06	128.17	125.04
22	Z	611	CLA	CMC-C2C-C1C	2.06	128.17	125.04
22	B	836	CLA	CHB-C4A-NA	2.06	127.35	124.51
22	B	828	CLA	CHB-C1B-C2B	-2.05	121.43	127.24
22	2	611	CLA	C1-C2-C3	-2.05	122.49	126.04
22	2	609	CLA	CED-O2D-CGD	2.05	120.58	115.94
25	I	172	BCR	C29-C28-C27	-2.05	106.79	111.38
22	A	813	CLA	C4-C3-C5	2.05	118.73	115.27
25	B	801	BCR	C34-C9-C8	2.05	121.31	118.08
30	5	624	LUT	C19-C9-C8	2.05	121.31	118.08
29	6	607	CHL	CHC-C1C-C2C	-2.05	118.66	126.11
25	A	852	BCR	C40-C30-C25	-2.05	106.97	110.30
22	2	612	CLA	CHA-C1A-NA	-2.05	121.69	126.40
22	A	840	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
22	B	830	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
22	2	611	CLA	CMC-C2C-C1C	2.05	128.16	125.04
30	9	617	LUT	C39-C29-C28	2.05	121.31	118.08
22	B	813	CLA	CHA-C1A-NA	-2.05	121.70	126.40
25	3	719	BCR	C29-C28-C27	-2.05	106.79	111.38
22	B	816	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
24	7	625	LHG	O8-C23-O10	-2.05	118.41	123.59
22	7	620	CLA	C1-C2-C3	-2.05	122.49	126.04
29	6	606	CHL	CHB-C1B-C2B	-2.05	121.44	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	621	LUT	C28-C29-C30	-2.05	115.79	118.94
22	A	837	CLA	CHA-C1A-NA	-2.05	121.70	126.40
22	3	602	CLA	CBA-CAA-C2A	2.05	119.92	113.86
22	B	811	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
22	4	609	CLA	CHA-C1A-NA	-2.05	121.70	126.40
22	1	610	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
22	8	604	CLA	CMC-C2C-C1C	2.05	128.16	125.04
22	Z	611	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
30	9	616	LUT	C8-C7-C6	-2.05	121.44	127.20
22	5	610	CLA	C11-C10-C8	-2.05	109.29	115.92
30	9	616	LUT	C39-C29-C28	2.05	121.31	118.08
22	B	829	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	A	825	CLA	CMC-C2C-C1C	2.05	128.16	125.04
29	1	601	CHL	OBD-CAD-C3D	-2.05	123.59	128.52
22	B	806	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	B	836	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	5	601	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	814	CLA	C1-C2-C3	-2.05	122.50	126.04
22	4	614	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
25	4	621	BCR	C36-C18-C19	2.05	121.30	118.08
29	Z	607	CHL	CHD-C4C-NC	2.05	127.43	124.20
30	3	621	LUT	C19-C9-C8	2.05	121.30	118.08
22	9	613	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
22	A	811	CLA	C4-C3-C5	2.05	118.71	115.27
22	5	616	CLA	CMC-C2C-C1C	2.05	128.16	125.04
22	8	604	CLA	CHB-C1B-NB	-2.05	122.09	124.26
22	B	826	CLA	OBD-CAD-C3D	-2.05	123.60	128.52
22	4	610	CLA	CMA-C3A-C4A	-2.05	106.28	111.77
25	6	623	BCR	C7-C6-C5	-2.05	116.51	121.46
22	5	609	CLA	C5-C3-C4	2.04	119.12	114.60
22	7	602	CLA	CMA-C3A-C2A	-2.04	105.58	113.83
22	A	828	CLA	CHC-C4B-NB	-2.04	122.09	124.26
22	7	606	CLA	CAC-C3C-C4C	2.04	127.46	124.81
25	B	843	BCR	C23-C24-C25	-2.04	121.46	127.20
22	8	606	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
22	4	612	CLA	CHC-C4B-NB	-2.04	122.10	124.26
30	3	621	LUT	C40-C33-C32	2.04	121.29	118.08
22	4	604	CLA	CHB-C1B-C2B	-2.04	121.47	127.24
22	5	604	CLA	CHB-C1B-C2B	-2.04	121.47	127.24
22	A	804	CLA	CHB-C4A-NA	2.04	127.33	124.51
22	7	620	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	1	612	CLA	CHC-C4B-NB	-2.04	122.10	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	603	CLA	CMC-C2C-C1C	2.04	128.15	125.04
25	A	856	BCR	C32-C1-C6	2.04	113.61	110.30
30	2	616	LUT	C30-C31-C32	-2.04	116.85	123.22
22	9	614	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	A	837	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	1	606	CLA	C1-C2-C3	-2.04	122.52	126.04
22	5	614	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
29	6	607	CHL	C2A-C3A-C4A	-2.04	98.58	101.87
22	A	820	CLA	CED-O2D-CGD	2.04	120.55	115.94
22	B	815	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
22	B	810	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	B	834	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	B	841	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
22	A	831	CLA	CHB-C4A-NA	2.04	127.33	124.51
22	7	614	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
22	7	614	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	F	301	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
22	A	838	CLA	CHA-C1A-NA	-2.04	121.73	126.40
30	2	616	LUT	C39-C29-C28	2.04	121.29	118.08
22	Z	602	CLA	CHB-C1B-C2B	-2.04	121.49	127.24
22	B	813	CLA	CHC-C1C-NC	2.04	127.29	124.20
30	7	621	LUT	C39-C29-C28	2.04	121.28	118.08
22	7	612	CLA	CHB-C1B-C2B	-2.04	121.49	127.24
22	A	827	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
30	3	622	LUT	C40-C33-C32	2.03	121.28	118.08
30	2	617	LUT	C20-C13-C12	2.03	121.28	118.08
22	1	610	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
29	6	606	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
22	1	603	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	7	607	CHL	C1-C2-C3	-2.03	122.53	126.04
22	B	823	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
29	4	606	CHL	CBA-CAA-C2A	-2.03	107.86	113.86
22	A	841	CLA	CMC-C2C-C1C	2.03	128.14	125.04
22	B	836	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
22	5	604	CLA	C5-C3-C4	2.03	119.09	114.60
22	4	603	CLA	CMC-C2C-C1C	2.03	128.13	125.04
25	B	847	BCR	C3-C4-C5	-2.03	110.45	114.08
29	8	607	CHL	CHC-C1C-C2C	-2.03	118.74	126.11
22	Z	606	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
22	A	842	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
25	B	801	BCR	C7-C8-C9	-2.03	123.16	126.23
22	4	612	CLA	CHB-C1B-C2B	-2.03	121.50	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	852	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	G	203	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
29	4	607	CHL	CHB-C4A-NA	2.03	127.32	124.51
22	4	613	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	1	611	CLA	C4-C3-C5	2.03	118.69	115.27
29	1	601	CHL	CHB-C4A-NA	2.03	127.32	124.51
22	F	301	CLA	CGD-CBD-CAD	-2.03	104.16	110.73
22	F	301	CLA	C3B-C4B-NB	2.03	112.40	110.52
25	3	719	BCR	C35-C13-C12	2.03	121.28	118.08
22	4	609	CLA	C5-C3-C4	2.03	119.09	114.60
22	B	804	CLA	CHB-C1B-NB	-2.03	122.11	124.26
22	2	613	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	810	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	9	609	CLA	CHB-C1B-NB	-2.03	122.11	124.26
22	B	828	CLA	CBA-CAA-C2A	2.03	119.84	113.86
22	Z	613	CLA	C4-C3-C5	2.03	118.68	115.27
22	B	817	CLA	CHA-C1A-NA	-2.03	121.76	126.40
22	A	803	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
22	A	843	CLA	C1-C2-C3	-2.03	122.54	126.04
22	3	602	CLA	C2A-C3A-C4A	-2.03	98.60	101.87
22	B	806	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
22	3	607	CLA	C1-C2-C3	-2.03	122.54	126.04
22	A	841	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
22	6	611	CLA	C1-C2-C3	-2.02	122.54	126.04
22	A	839	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
22	B	827	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
22	G	203	CLA	CMC-C2C-C1C	2.02	128.12	125.04
30	8	618	LUT	C39-C29-C28	2.02	121.26	118.08
29	5	607	CHL	CGD-CBD-CAD	-2.02	104.19	110.73
22	3	606	CLA	CED-O2D-CGD	2.02	120.51	115.94
22	8	610	CLA	CED-O2D-CGD	2.02	120.51	115.94
29	Z	607	CHL	CHC-C1C-C2C	-2.02	118.79	126.11
22	3	620	CLA	CED-O2D-CGD	2.02	120.50	115.94
22	8	609	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
22	A	830	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
29	7	607	CHL	CED-O2D-CGD	2.02	120.50	115.94
22	A	837	CLA	C2A-C3A-C4A	-2.02	98.61	101.87
22	B	828	CLA	CED-O2D-CGD	2.02	120.50	115.94
22	8	609	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
25	A	849	BCR	C28-C27-C26	-2.02	110.48	114.08
22	6	613	CLA	C1-O2A-CGA	2.02	121.73	116.44
25	3	718	BCR	C35-C13-C12	2.02	121.25	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	817	CLA	CBB-CAB-C3B	-2.02	117.59	127.62
22	5	612	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	5	609	CLA	CHB-C1B-C2B	-2.02	121.55	127.24
25	B	846	BCR	C15-C16-C17	-2.02	119.35	123.47
25	L	205	BCR	C10-C11-C12	-2.01	116.93	123.22
22	B	826	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	A	852	BCR	C11-C10-C9	-2.01	124.44	127.31
22	9	612	CLA	CHB-C1B-NB	-2.01	122.13	124.26
22	4	613	CLA	C4-C3-C5	2.01	118.66	115.27
22	4	603	CLA	CHB-C4A-NA	2.01	127.30	124.51
22	6	616	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
22	1	610	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
22	A	839	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	B	835	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
25	7	623	BCR	C34-C9-C8	2.01	121.24	118.08
22	9	602	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
22	1	602	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
22	K	4002	CLA	O2A-CGA-CBA	2.01	120.48	114.03
24	4	623	LHG	O8-C23-O10	-2.01	118.52	123.59
22	6	611	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
22	B	806	CLA	C4-C3-C5	2.01	118.65	115.27
30	1	617	LUT	C8-C7-C6	-2.01	121.56	127.20
22	F	304	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
22	9	612	CLA	CHB-C4A-NA	2.01	127.29	124.51
22	1	612	CLA	CMC-C2C-C1C	2.01	128.09	125.04
22	8	611	CLA	O2A-CGA-CBA	2.01	120.16	112.23
22	2	613	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
22	B	811	CLA	CMC-C2C-C1C	2.01	128.09	125.04
22	8	612	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
22	A	833	CLA	CHA-C1A-NA	-2.01	121.81	126.40
25	A	852	BCR	C28-C27-C26	-2.01	110.50	114.08
22	A	834	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
22	B	806	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
22	6	603	CLA	O2A-CGA-CBA	2.00	120.15	112.23
22	B	819	CLA	CHC-C1C-NC	2.00	127.24	124.20
22	A	820	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
22	6	622	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	A	838	CLA	C1-C2-C3	-2.00	122.58	126.04
22	A	806	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
22	9	612	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	A	810	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	4	611	CLA	CHB-C1B-NB	-2.00	122.14	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	601	CLA	CHB-C1B-NB	-2.00	122.14	124.26
22	Z	608	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	8	610	CLA	CHB-C1B-C2B	-2.00	121.59	127.24

There are no chirality outliers.

All (2615) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	804	CLA	CAD-CBD-CGD-O1D
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	814	CLA	C2B-C3B-CAB-CBB
22	A	814	CLA	C4B-C3B-CAB-CBB
22	A	814	CLA	C2-C3-C5-C6
22	A	814	CLA	C4-C3-C5-C6
22	A	815	CLA	C2-C3-C5-C6
22	A	815	CLA	C4-C3-C5-C6
22	A	816	CLA	C2-C3-C5-C6
22	A	816	CLA	C4-C3-C5-C6
22	A	818	CLA	CHA-CBD-CGD-O1D
22	A	818	CLA	CHA-CBD-CGD-O2D
22	A	818	CLA	C2-C3-C5-C6
22	A	818	CLA	C4-C3-C5-C6
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	819	CLA	C4B-C3B-CAB-CBB
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	822	CLA	C4B-C3B-CAB-CBB
22	A	823	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C3A-C2A-CAA-CBA
22	A	829	CLA	C2B-C3B-CAB-CBB
22	A	829	CLA	C4B-C3B-CAB-CBB
22	A	829	CLA	CBD-CGD-O2D-CED
22	A	831	CLA	CHA-CBD-CGD-O1D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	A	831	CLA	C4-C3-C5-C6
22	A	834	CLA	C2-C3-C5-C6
22	A	834	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	835	CLA	C4-C3-C5-C6
22	A	837	CLA	C1A-C2A-CAA-CBA
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	A	843	CLA	C4-C3-C5-C6
22	B	802	CLA	CHA-CBD-CGD-O1D
22	B	802	CLA	CHA-CBD-CGD-O2D
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	809	CLA	C2B-C3B-CAB-CBB
22	B	809	CLA	C4B-C3B-CAB-CBB
22	B	810	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C3A-C2A-CAA-CBA
22	B	813	CLA	C2B-C3B-CAB-CBB
22	B	813	CLA	C4B-C3B-CAB-CBB
22	B	817	CLA	C2B-C3B-CAB-CBB
22	B	817	CLA	C4B-C3B-CAB-CBB
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	818	CLA	C2-C3-C5-C6
22	B	818	CLA	C4-C3-C5-C6
22	B	819	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C4B-C3B-CAB-CBB
22	B	823	CLA	C2B-C3B-CAB-CBB
22	B	823	CLA	C4B-C3B-CAB-CBB
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	C2-C3-C5-C6
22	B	823	CLA	C4-C3-C5-C6
22	B	824	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	C4-C3-C5-C6
22	B	830	CLA	C2B-C3B-CAB-CBB
22	B	830	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O2D
22	B	836	CLA	C2-C3-C5-C6
22	B	836	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	837	CLA	C2-C3-C5-C6
22	B	837	CLA	C4-C3-C5-C6
22	F	301	CLA	CHA-CBD-CGD-O1D
22	F	304	CLA	CHA-CBD-CGD-O1D
22	F	304	CLA	CHA-CBD-CGD-O2D
22	G	203	CLA	CHA-CBD-CGD-O1D
22	G	203	CLA	CHA-CBD-CGD-O2D
22	J	3002	CLA	CHA-CBD-CGD-O2D
22	L	204	CLA	CHA-CBD-CGD-O1D
22	L	204	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	C2-C3-C5-C6
22	1	603	CLA	C4-C3-C5-C6
22	1	604	CLA	C2B-C3B-CAB-CBB
22	1	604	CLA	C4B-C3B-CAB-CBB
22	1	604	CLA	C2-C3-C5-C6
22	1	604	CLA	C4-C3-C5-C6
22	1	610	CLA	C2-C3-C5-C6
22	1	610	CLA	C4-C3-C5-C6
22	1	613	CLA	CHA-CBD-CGD-O1D
22	1	613	CLA	CHA-CBD-CGD-O2D
22	3	607	CLA	C1A-C2A-CAA-CBA
22	3	607	CLA	C2-C1-O2A-CGA
22	3	607	CLA	C11-C10-C8-C9
22	3	611	CLA	CHA-CBD-CGD-O1D
22	3	611	CLA	CHA-CBD-CGD-O2D
22	7	601	CLA	C2A-CAA-CBA-CGA
22	7	601	CLA	C2-C3-C5-C6
22	7	601	CLA	C4-C3-C5-C6
22	7	603	CLA	CHA-CBD-CGD-O1D
22	7	603	CLA	CHA-CBD-CGD-O2D
22	7	604	CLA	C2B-C3B-CAB-CBB
22	7	604	CLA	C4B-C3B-CAB-CBB
22	7	606	CLA	C1A-C2A-CAA-CBA
22	7	606	CLA	C3A-C2A-CAA-CBA
22	7	606	CLA	CHA-CBD-CGD-O1D
22	7	606	CLA	CHA-CBD-CGD-O2D
22	7	609	CLA	C1A-C2A-CAA-CBA
22	7	609	CLA	C3A-C2A-CAA-CBA
22	7	609	CLA	C2B-C3B-CAB-CBB
22	7	609	CLA	C4B-C3B-CAB-CBB
22	8	602	CLA	C2B-C3B-CAB-CBB
22	8	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	8	606	CLA	CBD-CGD-O2D-CED
22	8	609	CLA	C4B-C3B-CAB-CBB
22	8	610	CLA	C2B-C3B-CAB-CBB
22	8	610	CLA	C4B-C3B-CAB-CBB
22	Z	602	CLA	CBD-CGD-O2D-CED
22	Z	608	CLA	CBD-CGD-O2D-CED
22	Z	610	CLA	C4B-C3B-CAB-CBB
22	Z	610	CLA	C2-C3-C5-C6
22	Z	610	CLA	C4-C3-C5-C6
22	Z	613	CLA	CHA-CBD-CGD-O1D
22	Z	613	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	C2B-C3B-CAB-CBB
22	4	602	CLA	C4B-C3B-CAB-CBB
22	4	609	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C3A-C2A-CAA-CBA
22	5	609	CLA	C1A-C2A-CAA-CBA
22	5	609	CLA	C3A-C2A-CAA-CBA
22	5	609	CLA	C2A-CAA-CBA-CGA
22	5	610	CLA	C2B-C3B-CAB-CBB
22	5	610	CLA	C4B-C3B-CAB-CBB
22	5	611	CLA	C2-C3-C5-C6
22	5	611	CLA	C4-C3-C5-C6
22	5	612	CLA	C2-C3-C5-C6
22	5	612	CLA	C4-C3-C5-C6
22	5	617	CLA	C2A-CAA-CBA-CGA
22	5	617	CLA	CHA-CBD-CGD-O1D
22	5	617	CLA	CHA-CBD-CGD-O2D
22	5	621	CLA	CHA-CBD-CGD-O1D
22	6	604	CLA	C4B-C3B-CAB-CBB
22	6	611	CLA	C2-C3-C5-C6
22	6	611	CLA	C4-C3-C5-C6
22	6	614	CLA	C2B-C3B-CAB-CBB
22	6	614	CLA	C4B-C3B-CAB-CBB
22	6	614	CLA	CBD-CGD-O2D-CED
22	6	616	CLA	C2B-C3B-CAB-CBB
22	6	616	CLA	C4B-C3B-CAB-CBB
22	2	610	CLA	C2-C3-C5-C6
22	2	610	CLA	C4-C3-C5-C6
22	2	611	CLA	C2-C3-C5-C6
22	2	611	CLA	C4-C3-C5-C6
22	2	612	CLA	C2-C3-C5-C6
22	2	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	2	613	CLA	C1A-C2A-CAA-CBA
22	9	602	CLA	C2-C3-C5-C6
22	9	602	CLA	C4-C3-C5-C6
22	9	610	CLA	C2B-C3B-CAB-CBB
22	9	610	CLA	C4B-C3B-CAB-CBB
22	9	611	CLA	C4-C3-C5-C6
22	9	612	CLA	C3-C5-C6-C7
24	A	846	LHG	C3-O3-P-O5
24	A	847	LHG	C4-O6-P-O4
24	A	855	LHG	C4-O6-P-O4
24	B	851	LHG	C3-O3-P-O5
24	B	851	LHG	C4-O6-P-O5
24	B	851	LHG	O9-C7-O7-C5
24	1	620	LHG	O2-C2-C3-O3
24	1	620	LHG	C24-C23-O8-C6
24	Z	620	LHG	O2-C2-C3-O3
24	Z	620	LHG	C4-O6-P-O5
24	4	622	LHG	C3-O3-P-O4
24	5	623	LHG	C4-O6-P-O5
24	6	619	LHG	C3-O3-P-O6
25	A	848	BCR	C1-C6-C7-C8
25	A	850	BCR	C1-C6-C7-C8
25	A	850	BCR	C23-C24-C25-C30
25	B	801	BCR	C21-C22-C23-C24
25	B	801	BCR	C37-C22-C23-C24
25	B	843	BCR	C7-C8-C9-C10
25	B	843	BCR	C7-C8-C9-C34
25	B	843	BCR	C21-C22-C23-C24
25	B	843	BCR	C37-C22-C23-C24
25	B	844	BCR	C1-C6-C7-C8
25	B	844	BCR	C7-C8-C9-C10
25	B	844	BCR	C7-C8-C9-C34
25	B	845	BCR	C7-C8-C9-C10
25	B	845	BCR	C7-C8-C9-C34
25	B	845	BCR	C37-C22-C23-C24
25	B	846	BCR	C1-C6-C7-C8
25	B	846	BCR	C23-C24-C25-C30
25	G	205	BCR	C1-C6-C7-C8
25	I	172	BCR	C1-C6-C7-C8
25	I	172	BCR	C17-C18-C19-C20
25	I	172	BCR	C36-C18-C19-C20
25	I	172	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	I	172	BCR	C37-C22-C23-C24
25	J	3003	BCR	C7-C8-C9-C34
25	J	3003	BCR	C17-C18-C19-C20
25	J	3003	BCR	C36-C18-C19-C20
25	K	4001	BCR	C21-C22-C23-C24
25	K	4001	BCR	C37-C22-C23-C24
25	K	4004	BCR	C1-C6-C7-C8
25	K	4004	BCR	C23-C24-C25-C30
25	3	717	BCR	C1-C6-C7-C8
25	3	718	BCR	C11-C12-C13-C14
25	3	719	BCR	C1-C6-C7-C8
25	3	719	BCR	C7-C8-C9-C34
25	7	623	BCR	C1-C6-C7-C8
25	7	623	BCR	C17-C18-C19-C20
25	7	623	BCR	C23-C24-C25-C26
25	7	624	BCR	C1-C6-C7-C8
25	7	624	BCR	C23-C24-C25-C30
25	8	619	BCR	C1-C6-C7-C8
25	8	619	BCR	C36-C18-C19-C20
25	5	622	BCR	C11-C12-C13-C14
25	5	622	BCR	C11-C12-C13-C35
25	5	625	BCR	C1-C6-C7-C8
25	5	625	BCR	C7-C8-C9-C10
25	5	625	BCR	C7-C8-C9-C34
25	6	623	BCR	C5-C6-C7-C8
25	6	623	BCR	C7-C8-C9-C10
25	6	623	BCR	C7-C8-C9-C34
25	6	623	BCR	C11-C12-C13-C14
25	6	623	BCR	C11-C12-C13-C35
25	6	625	BCR	C7-C8-C9-C10
25	6	625	BCR	C7-C8-C9-C34
27	B	850	DGD	O2G-C2G-C3G-O3G
27	B	850	DGD	O6D-C1D-O3G-C3G
29	1	601	CHL	C1C-C2C-CMC-OMC
29	1	601	CHL	C3C-C2C-CMC-OMC
29	1	601	CHL	CHA-CBD-CGD-O1D
29	1	601	CHL	CHA-CBD-CGD-O2D
29	1	601	CHL	CAD-CBD-CGD-O1D
29	1	601	CHL	CAD-CBD-CGD-O2D
29	1	601	CHL	O2A-C1-C2-C3
29	1	601	CHL	C2-C3-C5-C6
29	1	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	1	607	CHL	C3C-C2C-CMC-OMC
29	3	608	CHL	C14-C13-C15-C16
29	7	607	CHL	C1C-C2C-CMC-OMC
29	7	607	CHL	C3C-C2C-CMC-OMC
29	8	607	CHL	C1A-C2A-CAA-CBA
29	8	607	CHL	C2A-CAA-CBA-CGA
29	8	607	CHL	C1C-C2C-CMC-OMC
29	8	607	CHL	C3C-C2C-CMC-OMC
29	Z	601	CHL	C1C-C2C-CMC-OMC
29	Z	601	CHL	C3C-C2C-CMC-OMC
29	Z	601	CHL	CHA-CBD-CGD-O1D
29	Z	601	CHL	CHA-CBD-CGD-O2D
29	Z	607	CHL	C1C-C2C-CMC-OMC
29	Z	607	CHL	C3C-C2C-CMC-OMC
29	4	607	CHL	C1C-C2C-CMC-OMC
29	4	607	CHL	C3C-C2C-CMC-OMC
29	4	608	CHL	C2B-C3B-CAB-CBB
29	4	608	CHL	C4B-C3B-CAB-CBB
29	4	608	CHL	CBD-CGD-O2D-CED
29	4	618	CHL	C3C-C2C-CMC-OMC
29	5	607	CHL	C1A-C2A-CAA-CBA
29	5	607	CHL	C1C-C2C-CMC-OMC
29	5	607	CHL	C3C-C2C-CMC-OMC
29	5	607	CHL	CBD-CGD-O2D-CED
29	5	608	CHL	C1A-C2A-CAA-CBA
29	5	608	CHL	C3A-C2A-CAA-CBA
29	5	608	CHL	C2B-C3B-CAB-CBB
29	5	608	CHL	C4B-C3B-CAB-CBB
29	5	608	CHL	C1C-C2C-CMC-OMC
29	5	608	CHL	C3C-C2C-CMC-OMC
29	5	608	CHL	CBD-CGD-O2D-CED
29	5	618	CHL	C3C-C2C-CMC-OMC
29	6	607	CHL	C1A-C2A-CAA-CBA
29	6	607	CHL	C1C-C2C-CMC-OMC
29	6	607	CHL	C3C-C2C-CMC-OMC
29	6	608	CHL	C1A-C2A-CAA-CBA
29	6	608	CHL	C2B-C3B-CAB-CBB
29	6	608	CHL	C4B-C3B-CAB-CBB
29	6	618	CHL	C1A-C2A-CAA-CBA
29	6	618	CHL	C3A-C2A-CAA-CBA
29	9	607	CHL	C3C-C2C-CMC-OMC
29	9	607	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	9	607	CHL	CHA-CBD-CGD-O2D
30	1	619	LUT	C1-C6-C7-C8
30	8	617	LUT	C1-C6-C7-C8
30	4	620	LUT	C1-C6-C7-C8
30	9	616	LUT	C1-C6-C7-C8
22	Z	611	CLA	O1D-CGD-O2D-CED
29	1	607	CHL	O1D-CGD-O2D-CED
22	1	611	CLA	O1D-CGD-O2D-CED
22	5	616	CLA	O1D-CGD-O2D-CED
29	5	607	CHL	O1D-CGD-O2D-CED
22	A	825	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
22	B	803	CLA	CBD-CGD-O2D-CED
22	1	602	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	CBD-CGD-O2D-CED
22	7	608	CLA	CBD-CGD-O2D-CED
22	Z	611	CLA	CBD-CGD-O2D-CED
22	5	606	CLA	CBD-CGD-O2D-CED
22	5	616	CLA	CBD-CGD-O2D-CED
22	6	602	CLA	CBD-CGD-O2D-CED
22	2	601	CLA	CBD-CGD-O2D-CED
29	1	607	CHL	CBD-CGD-O2D-CED
29	3	608	CHL	CBD-CGD-O2D-CED
29	6	608	CHL	CBD-CGD-O2D-CED
24	1	620	LHG	O10-C23-O8-C6
24	Z	620	LHG	O10-C23-O8-C6
22	7	608	CLA	O1D-CGD-O2D-CED
29	6	608	CHL	O1D-CGD-O2D-CED
22	B	840	CLA	C4C-C3C-CAC-CBC
22	B	803	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	8	606	CLA	O1D-CGD-O2D-CED
22	6	614	CLA	O1D-CGD-O2D-CED
29	3	608	CHL	O1D-CGD-O2D-CED
29	5	608	CHL	O1D-CGD-O2D-CED
24	Z	620	LHG	C24-C23-O8-C6
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	824	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	CBD-CGD-O2D-CED
22	B	835	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	F	301	CLA	CBD-CGD-O2D-CED
22	K	4002	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CBD-CGD-O2D-CED
22	3	613	CLA	CBD-CGD-O2D-CED
22	7	604	CLA	CBD-CGD-O2D-CED
22	Z	613	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	CBD-CGD-O2D-CED
22	4	611	CLA	CBD-CGD-O2D-CED
22	6	616	CLA	CBD-CGD-O2D-CED
29	4	607	CHL	CBD-CGD-O2D-CED
22	B	840	CLA	C2C-C3C-CAC-CBC
22	A	806	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	O1A-CGA-O2A-C1
22	B	822	CLA	O1A-CGA-O2A-C1
22	1	611	CLA	O1A-CGA-O2A-C1
22	A	829	CLA	O1D-CGD-O2D-CED
29	4	608	CHL	O1D-CGD-O2D-CED
22	3	620	CLA	CBD-CGD-O2D-CED
22	Z	603	CLA	CBD-CGD-O2D-CED
29	6	618	CHL	CBD-CGD-O2D-CED
22	Z	602	CLA	O1D-CGD-O2D-CED
22	Z	608	CLA	O1D-CGD-O2D-CED
22	5	617	CLA	O1A-CGA-O2A-C1
22	A	802	CLA	C3-C5-C6-C7
22	A	806	CLA	C3-C5-C6-C7
22	A	808	CLA	C3-C5-C6-C7
22	A	816	CLA	C3-C5-C6-C7
22	A	817	CLA	C3-C5-C6-C7
22	A	818	CLA	C3-C5-C6-C7
22	A	819	CLA	C3-C5-C6-C7
22	A	825	CLA	C3-C5-C6-C7
22	A	826	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	A	840	CLA	C3-C5-C6-C7
22	A	843	CLA	C3-C5-C6-C7
22	A	854	CLA	C3-C5-C6-C7
22	B	807	CLA	C3-C5-C6-C7
22	B	808	CLA	C3-C5-C6-C7
22	B	809	CLA	C3-C5-C6-C7
22	B	818	CLA	C3-C5-C6-C7
22	B	822	CLA	C3-C5-C6-C7
22	B	824	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	827	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	B	841	CLA	C3-C5-C6-C7
22	F	301	CLA	C3-C5-C6-C7
22	1	608	CLA	C3-C5-C6-C7
22	1	611	CLA	C3-C5-C6-C7
22	3	607	CLA	C3-C5-C6-C7
22	3	620	CLA	C3-C5-C6-C7
22	7	604	CLA	C3-C5-C6-C7
22	7	620	CLA	C3-C5-C6-C7
22	8	614	CLA	C3-C5-C6-C7
22	4	611	CLA	C3-C5-C6-C7
22	5	613	CLA	C3-C5-C6-C7
22	2	610	CLA	C3-C5-C6-C7
22	2	611	CLA	C3-C5-C6-C7
22	9	610	CLA	C3-C5-C6-C7
22	9	611	CLA	C3-C5-C6-C7
29	8	607	CHL	C3-C5-C6-C7
22	A	845	CLA	CBA-CGA-O2A-C1
22	B	822	CLA	CBA-CGA-O2A-C1
22	1	611	CLA	CBA-CGA-O2A-C1
22	Z	602	CLA	CBA-CGA-O2A-C1
22	5	601	CLA	CBA-CGA-O2A-C1
24	B	851	LHG	C8-C7-O7-C5
22	B	810	CLA	CBD-CGD-O2D-CED
22	7	606	CLA	CBD-CGD-O2D-CED
29	9	606	CHL	CBD-CGD-O2D-CED
22	B	834	CLA	O1A-CGA-O2A-C1
22	A	845	CLA	C3-C5-C6-C7
22	7	612	CLA	C3-C5-C6-C7
22	8	612	CLA	C3-C5-C6-C7
22	5	612	CLA	C3-C5-C6-C7
22	6	612	CLA	C3-C5-C6-C7
22	2	612	CLA	C3-C5-C6-C7
22	6	604	CLA	C4-C3-C5-C6
22	6	610	CLA	C4-C3-C5-C6
22	A	831	CLA	C2-C3-C5-C6
22	A	835	CLA	C2-C3-C5-C6
22	B	829	CLA	C2-C3-C5-C6
22	9	611	CLA	C2-C3-C5-C6
22	F	303	CLA	CBD-CGD-O2D-CED
22	2	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	825	CLA	C2A-CAA-CBA-CGA
22	A	837	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C2A-CAA-CBA-CGA
22	B	824	CLA	C2A-CAA-CBA-CGA
22	B	839	CLA	C2A-CAA-CBA-CGA
22	3	607	CLA	C2A-CAA-CBA-CGA
22	Z	609	CLA	C2A-CAA-CBA-CGA
22	5	601	CLA	C2A-CAA-CBA-CGA
22	5	614	CLA	C2A-CAA-CBA-CGA
22	5	621	CLA	C2A-CAA-CBA-CGA
22	2	602	CLA	C2A-CAA-CBA-CGA
22	9	601	CLA	C2A-CAA-CBA-CGA
22	9	614	CLA	C2A-CAA-CBA-CGA
29	1	607	CHL	C2A-CAA-CBA-CGA
29	4	608	CHL	C2A-CAA-CBA-CGA
29	5	608	CHL	C2A-CAA-CBA-CGA
22	A	804	CLA	C3-C5-C6-C7
22	A	807	CLA	C3-C5-C6-C7
22	B	802	CLA	C3-C5-C6-C7
22	B	806	CLA	C3-C5-C6-C7
22	B	820	CLA	C3-C5-C6-C7
22	1	602	CLA	C3-C5-C6-C7
22	3	610	CLA	C3-C5-C6-C7
22	Z	608	CLA	C3-C5-C6-C7
22	Z	611	CLA	C3-C5-C6-C7
22	4	613	CLA	C3-C5-C6-C7
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	815	CLA	CBA-CGA-O2A-C1
22	A	824	CLA	CBA-CGA-O2A-C1
22	A	829	CLA	CBA-CGA-O2A-C1
22	A	842	CLA	CBA-CGA-O2A-C1
22	B	818	CLA	CBA-CGA-O2A-C1
22	B	825	CLA	CBA-CGA-O2A-C1
22	3	607	CLA	CBA-CGA-O2A-C1
22	5	602	CLA	CBA-CGA-O2A-C1
22	6	611	CLA	CBA-CGA-O2A-C1
22	9	611	CLA	CBA-CGA-O2A-C1
22	1	602	CLA	O1D-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1A-CGA-O2A-C1
22	A	845	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	833	CLA	O1A-CGA-O2A-C1
22	Z	611	CLA	O1A-CGA-O2A-C1
22	5	601	CLA	O1A-CGA-O2A-C1
22	2	601	CLA	O1D-CGD-O2D-CED
22	A	818	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	CBD-CGD-O2D-CED
22	8	604	CLA	CBD-CGD-O2D-CED
22	5	602	CLA	CBD-CGD-O2D-CED
29	4	618	CHL	CBD-CGD-O2D-CED
29	5	618	CHL	CBD-CGD-O2D-CED
22	5	606	CLA	O1D-CGD-O2D-CED
22	A	809	CLA	C3-C5-C6-C7
22	A	831	CLA	C3-C5-C6-C7
22	A	839	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	852	CLA	C3-C5-C6-C7
22	6	602	CLA	C3-C5-C6-C7
29	3	608	CHL	C3-C5-C6-C7
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	820	CLA	CBA-CGA-O2A-C1
22	B	833	CLA	CBA-CGA-O2A-C1
22	7	620	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CBA-CGA-O2A-C1
22	9	602	CLA	CBA-CGA-O2A-C1
29	6	607	CHL	CBA-CGA-O2A-C1
22	A	812	CLA	O1A-CGA-O2A-C1
22	A	815	CLA	O1A-CGA-O2A-C1
22	A	829	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1A-CGA-O2A-C1
22	3	607	CLA	O1A-CGA-O2A-C1
22	Z	602	CLA	O1A-CGA-O2A-C1
22	A	809	CLA	CBD-CGD-O2D-CED
22	G	204	CLA	CBD-CGD-O2D-CED
22	8	609	CLA	CBD-CGD-O2D-CED
22	Z	610	CLA	CBD-CGD-O2D-CED
22	6	610	CLA	CBD-CGD-O2D-CED
22	6	611	CLA	O1A-CGA-O2A-C1
22	A	805	CLA	C3-C5-C6-C7
22	B	812	CLA	C3-C5-C6-C7
22	B	815	CLA	C3-C5-C6-C7
22	3	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	834	CLA	CBA-CGA-O2A-C1
22	Z	611	CLA	CBA-CGA-O2A-C1
22	6	602	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	O1A-CGA-O2A-C1
22	7	620	CLA	O1A-CGA-O2A-C1
22	4	602	CLA	O1A-CGA-O2A-C1
22	5	602	CLA	O1A-CGA-O2A-C1
22	9	602	CLA	O1A-CGA-O2A-C1
22	9	611	CLA	O1A-CGA-O2A-C1
22	1	606	CLA	C3-C5-C6-C7
22	Z	606	CLA	C3-C5-C6-C7
22	A	808	CLA	C4-C3-C5-C6
22	A	833	CLA	C4-C3-C5-C6
22	A	839	CLA	C4-C3-C5-C6
22	A	842	CLA	C4-C3-C5-C6
22	1	602	CLA	C4-C3-C5-C6
22	1	606	CLA	C4-C3-C5-C6
22	8	610	CLA	C4-C3-C5-C6
22	8	612	CLA	C4-C3-C5-C6
22	Z	602	CLA	C4-C3-C5-C6
22	Z	604	CLA	C4-C3-C5-C6
22	Z	606	CLA	C4-C3-C5-C6
22	4	611	CLA	C4-C3-C5-C6
22	A	808	CLA	C2-C3-C5-C6
22	A	833	CLA	C2-C3-C5-C6
22	A	839	CLA	C2-C3-C5-C6
22	A	842	CLA	C2-C3-C5-C6
22	A	843	CLA	C2-C3-C5-C6
22	1	602	CLA	C2-C3-C5-C6
22	1	606	CLA	C2-C3-C5-C6
22	8	610	CLA	C2-C3-C5-C6
22	8	612	CLA	C2-C3-C5-C6
22	Z	602	CLA	C2-C3-C5-C6
22	Z	604	CLA	C2-C3-C5-C6
22	Z	606	CLA	C2-C3-C5-C6
22	4	611	CLA	C2-C3-C5-C6
22	A	854	CLA	C2A-CAA-CBA-CGA
22	B	827	CLA	C2A-CAA-CBA-CGA
22	B	852	CLA	C2A-CAA-CBA-CGA
29	Z	607	CHL	C2A-CAA-CBA-CGA
22	A	824	CLA	O1A-CGA-O2A-C1
29	6	607	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	4	611	CLA	CBA-CGA-O2A-C1
22	5	611	CLA	CBA-CGA-O2A-C1
22	8	614	CLA	CBD-CGD-O2D-CED
22	9	613	CLA	CBD-CGD-O2D-CED
22	A	810	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	O1A-CGA-O2A-C1
22	6	602	CLA	O1D-CGD-O2D-CED
22	B	808	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	O1D-CGD-O2D-CED
24	1	620	LHG	C1-C2-C3-O3
24	Z	620	LHG	C1-C2-C3-O3
28	9	620	LMG	O9-C10-O7-C8
22	5	611	CLA	O1A-CGA-O2A-C1
22	6	602	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	C3-C5-C6-C7
22	7	604	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	809	CLA	CBA-CGA-O2A-C1
22	A	843	CLA	CBA-CGA-O2A-C1
22	B	810	CLA	CBA-CGA-O2A-C1
22	B	814	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	B	831	CLA	CBA-CGA-O2A-C1
22	1	602	CLA	CBA-CGA-O2A-C1
22	3	602	CLA	CBA-CGA-O2A-C1
22	3	620	CLA	CBA-CGA-O2A-C1
22	7	604	CLA	CBA-CGA-O2A-C1
22	8	602	CLA	CBA-CGA-O2A-C1
22	8	612	CLA	CBA-CGA-O2A-C1
22	Z	604	CLA	CBA-CGA-O2A-C1
22	6	609	CLA	CBA-CGA-O2A-C1
22	6	612	CLA	CBA-CGA-O2A-C1
22	9	613	CLA	CBA-CGA-O2A-C1
22	5	604	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	CBD-CGD-O2D-CED
22	9	614	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	C10-C11-C12-C13
22	1	610	CLA	C5-C6-C7-C8
22	Z	611	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	5	610	CLA	C10-C11-C12-C13
22	6	601	CLA	C10-C11-C12-C13
22	4	612	CLA	C3-C5-C6-C7
29	Z	601	CHL	C3-C5-C6-C7
28	9	620	LMG	O1-C7-C8-O7
22	7	612	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	O1A-CGA-O2A-C1
22	B	810	CLA	O1A-CGA-O2A-C1
22	7	604	CLA	O1A-CGA-O2A-C1
22	8	602	CLA	O1A-CGA-O2A-C1
22	6	612	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	C4-C3-C5-C6
22	3	610	CLA	C4-C3-C5-C6
22	6	604	CLA	C2-C3-C5-C6
22	A	827	CLA	C6-C7-C8-C9
22	A	828	CLA	C14-C13-C15-C16
22	A	839	CLA	C14-C13-C15-C16
22	B	805	CLA	C6-C7-C8-C9
22	B	818	CLA	C6-C7-C8-C9
22	1	610	CLA	C6-C7-C8-C9
22	7	601	CLA	C11-C12-C13-C14
22	Z	610	CLA	C6-C7-C8-C9
23	A	844	PQN	C24-C23-C25-C26
22	3	603	CLA	O1D-CGD-O2D-CED
22	4	613	CLA	CBD-CGD-O2D-CED
22	7	620	CLA	C5-C6-C7-C8
22	A	815	CLA	C2A-CAA-CBA-CGA
25	A	852	BCR	C7-C8-C9-C34
25	A	856	BCR	C37-C22-C23-C24
25	B	844	BCR	C37-C22-C23-C24
25	L	205	BCR	C7-C8-C9-C34
25	L	205	BCR	C37-C22-C23-C24
25	3	718	BCR	C11-C12-C13-C35
25	7	623	BCR	C36-C18-C19-C20
25	4	621	BCR	C7-C8-C9-C34
25	6	625	BCR	C11-C12-C13-C35
25	A	856	BCR	C21-C22-C23-C24
25	B	844	BCR	C21-C22-C23-C24
25	L	205	BCR	C21-C22-C23-C24
25	4	621	BCR	C7-C8-C9-C10
25	6	625	BCR	C11-C12-C13-C14
28	9	620	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	A	843	CLA	O1A-CGA-O2A-C1
22	B	831	CLA	O1A-CGA-O2A-C1
22	3	620	CLA	O1A-CGA-O2A-C1
22	8	612	CLA	O1A-CGA-O2A-C1
22	Z	604	CLA	O1A-CGA-O2A-C1
22	6	609	CLA	O1A-CGA-O2A-C1
22	B	812	CLA	C10-C11-C12-C13
22	B	818	CLA	C8-C10-C11-C12
22	B	839	CLA	C15-C16-C17-C18
22	6	601	CLA	C8-C10-C11-C12
23	B	842	PQN	C20-C21-C22-C23
22	1	603	CLA	C3-C5-C6-C7
22	Z	602	CLA	C3-C5-C6-C7
22	A	817	CLA	C8-C10-C11-C12
22	A	814	CLA	CBA-CGA-O2A-C1
22	A	826	CLA	C10-C11-C12-C13
22	A	830	CLA	C13-C15-C16-C17
22	B	805	CLA	C15-C16-C17-C18
22	B	812	CLA	C5-C6-C7-C8
22	B	834	CLA	C10-C11-C12-C13
22	B	837	CLA	C8-C10-C11-C12
22	B	837	CLA	C15-C16-C17-C18
22	1	611	CLA	C8-C10-C11-C12
22	3	610	CLA	C13-C15-C16-C17
22	8	613	CLA	C5-C6-C7-C8
22	Z	608	CLA	C5-C6-C7-C8
22	K	4002	CLA	O1D-CGD-O2D-CED
22	A	845	CLA	CBD-CGD-O2D-CED
22	B	809	CLA	CBD-CGD-O2D-CED
22	A	808	CLA	C10-C11-C12-C13
22	A	814	CLA	C8-C10-C11-C12
22	B	802	CLA	C10-C11-C12-C13
22	B	825	CLA	C13-C15-C16-C17
22	B	834	CLA	C5-C6-C7-C8
22	8	601	CLA	C13-C15-C16-C17
22	8	613	CLA	C15-C16-C17-C18
22	Z	608	CLA	C8-C10-C11-C12
22	Z	608	CLA	C15-C16-C17-C18
22	Z	611	CLA	C5-C6-C7-C8
24	A	847	LHG	C7-C8-C9-C10
28	J	3001	LMG	C28-C29-C30-C31
28	9	620	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	4	607	CHL	O1D-CGD-O2D-CED
22	A	826	CLA	C13-C15-C16-C17
22	B	810	CLA	C5-C6-C7-C8
22	B	837	CLA	C13-C15-C16-C17
22	3	613	CLA	O1D-CGD-O2D-CED
22	A	806	CLA	C2-C1-O2A-CGA
22	B	810	CLA	C10-C11-C12-C13
22	B	829	CLA	C10-C11-C12-C13
24	1	620	LHG	C7-C8-C9-C10
22	A	838	CLA	CBD-CGD-O2D-CED
22	B	832	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	CBD-CGD-O2D-CED
22	8	602	CLA	C13-C15-C16-C17
22	A	814	CLA	C10-C11-C12-C13
22	A	809	CLA	C12-C13-C15-C16
22	A	842	CLA	C6-C7-C8-C10
22	A	822	CLA	C3-C5-C6-C7
22	Z	613	CLA	C3-C5-C6-C7
22	A	814	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	7	612	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C2A-CAA-CBA-CGA
22	G	203	CLA	C2A-CAA-CBA-CGA
22	1	602	CLA	C2A-CAA-CBA-CGA
22	Z	602	CLA	C2A-CAA-CBA-CGA
22	5	602	CLA	C2A-CAA-CBA-CGA
22	B	835	CLA	O1D-CGD-O2D-CED
22	F	301	CLA	O1D-CGD-O2D-CED
22	3	620	CLA	O1D-CGD-O2D-CED
22	4	611	CLA	O1D-CGD-O2D-CED
22	6	616	CLA	O1D-CGD-O2D-CED
22	A	834	CLA	C5-C6-C7-C8
22	B	827	CLA	C10-C11-C12-C13
22	B	821	CLA	CBA-CGA-O2A-C1
22	1	602	CLA	O1A-CGA-O2A-C1
22	3	609	CLA	CBD-CGD-O2D-CED
22	8	602	CLA	CBD-CGD-O2D-CED
22	A	831	CLA	C8-C10-C11-C12
22	A	839	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	4	602	CLA	C10-C11-C12-C13
22	A	824	CLA	O1D-CGD-O2D-CED
29	6	618	CHL	O1D-CGD-O2D-CED
24	Z	620	LHG	C7-C8-C9-C10
22	B	808	CLA	C15-C16-C17-C18
22	1	604	CLA	C5-C6-C7-C8
22	A	809	CLA	O1A-CGA-O2A-C1
22	B	829	CLA	O1A-CGA-O2A-C1
22	4	611	CLA	O1A-CGA-O2A-C1
22	9	613	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	C15-C16-C17-C18
22	7	601	CLA	C8-C10-C11-C12
29	3	608	CHL	C8-C10-C11-C12
22	B	817	CLA	C5-C6-C7-C8
22	3	604	CLA	C10-C11-C12-C13
22	4	601	CLA	C10-C11-C12-C13
22	6	610	CLA	C5-C6-C7-C8
29	3	608	CHL	C10-C11-C12-C13
24	A	855	LHG	C4-O6-P-O3
24	B	851	LHG	C3-O3-P-O6
24	7	625	LHG	C4-O6-P-O3
24	8	620	LHG	C3-O3-P-O6
24	8	620	LHG	C4-O6-P-O3
24	4	622	LHG	C3-O3-P-O6
24	5	623	LHG	C4-O6-P-O3
22	A	835	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	8	613	CLA	C3-C5-C6-C7
22	B	811	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	F	304	CLA	CBA-CGA-O2A-C1
22	1	604	CLA	CBA-CGA-O2A-C1
22	7	602	CLA	CBA-CGA-O2A-C1
24	4	622	LHG	C24-C23-O8-C6
29	7	607	CHL	CBA-CGA-O2A-C1
22	B	823	CLA	O1D-CGD-O2D-CED
22	Z	613	CLA	O1D-CGD-O2D-CED
22	6	601	CLA	C5-C6-C7-C8
22	A	811	CLA	O1D-CGD-O2D-CED
29	9	606	CHL	O1D-CGD-O2D-CED
22	6	612	CLA	C4-C3-C5-C6
29	7	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	7	610	CLA	C10-C11-C12-C13
22	6	602	CLA	C10-C11-C12-C13
22	A	803	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C2A-CAA-CBA-CGA
22	A	834	CLA	C2A-CAA-CBA-CGA
22	4	602	CLA	C2A-CAA-CBA-CGA
22	6	602	CLA	C2A-CAA-CBA-CGA
22	2	610	CLA	C2A-CAA-CBA-CGA
22	9	602	CLA	C2A-CAA-CBA-CGA
22	B	816	CLA	C3-C5-C6-C7
22	3	613	CLA	C3-C5-C6-C7
22	9	602	CLA	C3-C5-C6-C7
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	CBA-CGA-O2A-C1
22	1	612	CLA	CBA-CGA-O2A-C1
22	B	832	CLA	C13-C15-C16-C17
22	1	611	CLA	C5-C6-C7-C8
22	3	602	CLA	CBD-CGD-O2D-CED
25	7	623	BCR	C19-C20-C21-C22
22	6	601	CLA	C3-C5-C6-C7
28	J	3001	LMG	C12-C13-C14-C15
28	9	620	LMG	C11-C12-C13-C14
28	9	620	LMG	C29-C30-C31-C32
22	B	810	CLA	O1D-CGD-O2D-CED
22	Z	603	CLA	O1D-CGD-O2D-CED
22	3	613	CLA	C6-C7-C8-C10
22	2	611	CLA	CBA-CGA-O2A-C1
22	F	303	CLA	O1D-CGD-O2D-CED
22	B	827	CLA	C8-C10-C11-C12
22	G	204	CLA	CBA-CGA-O2A-C1
22	B	822	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	CBA-CGA-O2A-C1
27	B	850	DGD	C3B-C4B-C5B-C6B
22	A	831	CLA	C10-C11-C12-C13
22	B	826	CLA	C10-C11-C12-C13
22	9	602	CLA	C5-C6-C7-C8
22	A	825	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	O1A-CGA-O2A-C1
22	1	604	CLA	O1A-CGA-O2A-C1
22	1	612	CLA	O1A-CGA-O2A-C1
22	A	814	CLA	C16-C17-C18-C20
22	3	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	7	602	CLA	C16-C17-C18-C20
22	2	602	CLA	O1D-CGD-O2D-CED
22	3	607	CLA	C4-C3-C5-C6
22	3	613	CLA	C4-C3-C5-C6
22	6	610	CLA	C2-C3-C5-C6
22	A	808	CLA	C11-C12-C13-C14
22	A	809	CLA	C14-C13-C15-C16
22	A	819	CLA	C11-C10-C8-C9
22	A	822	CLA	C11-C10-C8-C9
22	B	805	CLA	C11-C10-C8-C9
22	B	809	CLA	C11-C12-C13-C14
22	B	812	CLA	C11-C10-C8-C9
22	B	832	CLA	C6-C7-C8-C9
22	1	610	CLA	C11-C10-C8-C9
22	3	607	CLA	C6-C7-C8-C9
22	Z	613	CLA	C6-C7-C8-C9
22	6	602	CLA	C6-C7-C8-C9
24	Z	620	LHG	C23-C24-C25-C26
22	A	842	CLA	C5-C6-C7-C8
22	Z	613	CLA	C10-C11-C12-C13
22	A	830	CLA	C2A-CAA-CBA-CGA
22	2	613	CLA	C2A-CAA-CBA-CGA
29	3	608	CHL	C2A-CAA-CBA-CGA
22	A	818	CLA	O1A-CGA-O2A-C1
22	3	602	CLA	O1A-CGA-O2A-C1
24	A	847	LHG	O1-C1-C2-C3
25	B	845	BCR	C21-C22-C23-C24
25	8	619	BCR	C17-C18-C19-C20
22	A	807	CLA	C5-C6-C7-C8
22	A	841	CLA	C8-C10-C11-C12
24	5	623	LHG	C23-C24-C25-C26
27	B	850	DGD	C3A-C4A-C5A-C6A
27	B	850	DGD	C7B-C8B-C9B-CAB
22	A	827	CLA	C4B-C3B-CAB-CBB
22	A	832	CLA	C4B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	B	807	CLA	C4B-C3B-CAB-CBB
22	B	814	CLA	C4B-C3B-CAB-CBB
22	B	824	CLA	C4B-C3B-CAB-CBB
22	B	829	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	3	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	3	607	CLA	C4B-C3B-CAB-CBB
22	8	604	CLA	C4B-C3B-CAB-CBB
22	Z	604	CLA	C4B-C3B-CAB-CBB
22	4	604	CLA	C4B-C3B-CAB-CBB
22	6	610	CLA	C4B-C3B-CAB-CBB
22	2	602	CLA	C4B-C3B-CAB-CBB
22	9	602	CLA	C4B-C3B-CAB-CBB
22	9	609	CLA	C4B-C3B-CAB-CBB
29	6	606	CHL	C6-C7-C8-C9
29	6	606	CHL	C6-C7-C8-C10
28	9	620	LMG	O6-C1-O1-C7
22	B	806	CLA	C8-C10-C11-C12
22	B	812	CLA	C15-C16-C17-C18
24	7	625	LHG	C25-C26-C27-C28
28	9	620	LMG	C30-C31-C32-C33
22	Z	616	CLA	CBA-CGA-O2A-C1
22	7	606	CLA	O1D-CGD-O2D-CED
24	7	625	LHG	C10-C11-C12-C13
24	1	620	LHG	C23-C24-C25-C26
22	B	810	CLA	C3-C5-C6-C7
22	A	819	CLA	CBA-CGA-O2A-C1
29	4	618	CHL	O1D-CGD-O2D-CED
22	A	803	CLA	C3A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	807	CLA	C3A-C2A-CAA-CBA
22	A	834	CLA	C3A-C2A-CAA-CBA
22	A	837	CLA	C3A-C2A-CAA-CBA
22	B	824	CLA	C3A-C2A-CAA-CBA
22	B	826	CLA	C3A-C2A-CAA-CBA
22	1	612	CLA	C3A-C2A-CAA-CBA
22	3	617	CLA	C3A-C2A-CAA-CBA
22	Z	612	CLA	C3A-C2A-CAA-CBA
22	5	601	CLA	C3A-C2A-CAA-CBA
29	Z	601	CHL	C3A-C2A-CAA-CBA
22	A	820	CLA	C13-C15-C16-C17
22	A	837	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1A-CGA-O2A-C1
22	B	811	CLA	O1A-CGA-O2A-C1
24	4	622	LHG	O10-C23-O8-C6
29	7	607	CHL	O1A-CGA-O2A-C1
29	3	608	CHL	C16-C17-C18-C19
29	3	608	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	4	623	LHG	C9-C10-C11-C12
22	A	834	CLA	C3-C5-C6-C7
22	F	304	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	C10-C11-C12-C13
22	8	601	CLA	C8-C10-C11-C12
22	6	602	CLA	C8-C10-C11-C12
22	B	806	CLA	C4-C3-C5-C6
22	B	816	CLA	C4-C3-C5-C6
29	6	607	CHL	C4-C3-C5-C6
22	A	822	CLA	CBA-CGA-O2A-C1
22	B	828	CLA	CBA-CGA-O2A-C1
22	1	614	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	C2-C3-C5-C6
22	B	819	CLA	C2-C3-C5-C6
22	3	610	CLA	C2-C3-C5-C6
22	3	613	CLA	C2-C3-C5-C6
22	4	613	CLA	C2-C3-C5-C6
22	4	603	CLA	CBA-CGA-O2A-C1
24	A	847	LHG	C15-C16-C17-C18
22	B	820	CLA	O1A-CGA-O2A-C1
22	7	602	CLA	O1A-CGA-O2A-C1
22	7	602	CLA	C16-C17-C18-C19
22	A	819	CLA	C2B-C3B-CAB-CBB
22	A	822	CLA	C2B-C3B-CAB-CBB
22	A	825	CLA	C2B-C3B-CAB-CBB
22	A	827	CLA	C2B-C3B-CAB-CBB
22	A	832	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C2B-C3B-CAB-CBB
22	A	843	CLA	C2B-C3B-CAB-CBB
22	B	807	CLA	C2B-C3B-CAB-CBB
22	B	814	CLA	C2B-C3B-CAB-CBB
22	B	824	CLA	C2B-C3B-CAB-CBB
22	B	829	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C2B-C3B-CAB-CBB
22	L	204	CLA	C2B-C3B-CAB-CBB
22	3	604	CLA	C2B-C3B-CAB-CBB
22	3	607	CLA	C2B-C3B-CAB-CBB
22	3	609	CLA	C2B-C3B-CAB-CBB
22	8	604	CLA	C2B-C3B-CAB-CBB
22	8	609	CLA	C2B-C3B-CAB-CBB
22	Z	604	CLA	C2B-C3B-CAB-CBB
22	Z	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	Z	613	CLA	C2B-C3B-CAB-CBB
22	4	604	CLA	C2B-C3B-CAB-CBB
22	6	604	CLA	C2B-C3B-CAB-CBB
22	6	610	CLA	C2B-C3B-CAB-CBB
22	2	602	CLA	C2B-C3B-CAB-CBB
22	9	602	CLA	C2B-C3B-CAB-CBB
22	9	609	CLA	C2B-C3B-CAB-CBB
29	5	607	CHL	C2B-C3B-CAB-CBB
22	A	816	CLA	C5-C6-C7-C8
22	B	802	CLA	C15-C16-C17-C18
22	A	814	CLA	C3-C5-C6-C7
22	B	817	CLA	C3-C5-C6-C7
22	2	609	CLA	CBA-CGA-O2A-C1
22	A	829	CLA	C2-C1-O2A-CGA
22	B	834	CLA	C2-C1-O2A-CGA
22	1	608	CLA	C2-C1-O2A-CGA
22	1	614	CLA	C2-C1-O2A-CGA
22	Z	614	CLA	C2-C1-O2A-CGA
28	J	3001	LMG	C30-C31-C32-C33
22	3	604	CLA	C13-C15-C16-C17
24	A	846	LHG	C23-C24-C25-C26
22	B	805	CLA	C3-C5-C6-C7
25	A	848	BCR	C5-C6-C7-C8
25	A	850	BCR	C5-C6-C7-C8
25	A	850	BCR	C23-C24-C25-C26
25	A	856	BCR	C1-C6-C7-C8
25	A	856	BCR	C5-C6-C7-C8
25	A	856	BCR	C23-C24-C25-C26
25	A	856	BCR	C23-C24-C25-C30
25	B	844	BCR	C5-C6-C7-C8
25	B	846	BCR	C5-C6-C7-C8
25	B	846	BCR	C23-C24-C25-C26
25	B	848	BCR	C1-C6-C7-C8
25	B	848	BCR	C5-C6-C7-C8
25	G	205	BCR	C5-C6-C7-C8
25	I	172	BCR	C5-C6-C7-C8
25	J	3003	BCR	C23-C24-C25-C26
25	J	3003	BCR	C23-C24-C25-C30
25	K	4004	BCR	C5-C6-C7-C8
25	K	4004	BCR	C23-C24-C25-C26
25	L	201	BCR	C1-C6-C7-C8
25	L	201	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	L	201	BCR	C23-C24-C25-C26
25	L	201	BCR	C23-C24-C25-C30
25	L	205	BCR	C23-C24-C25-C26
25	L	205	BCR	C23-C24-C25-C30
25	3	717	BCR	C5-C6-C7-C8
25	3	717	BCR	C23-C24-C25-C26
25	3	717	BCR	C23-C24-C25-C30
25	3	719	BCR	C5-C6-C7-C8
25	7	623	BCR	C5-C6-C7-C8
25	7	623	BCR	C23-C24-C25-C30
25	7	624	BCR	C5-C6-C7-C8
25	7	624	BCR	C23-C24-C25-C26
25	8	619	BCR	C5-C6-C7-C8
25	8	619	BCR	C23-C24-C25-C26
25	8	619	BCR	C23-C24-C25-C30
25	5	622	BCR	C1-C6-C7-C8
25	5	622	BCR	C5-C6-C7-C8
25	5	622	BCR	C23-C24-C25-C26
25	5	622	BCR	C23-C24-C25-C30
25	5	625	BCR	C5-C6-C7-C8
25	5	625	BCR	C23-C24-C25-C26
25	5	625	BCR	C23-C24-C25-C30
25	6	623	BCR	C1-C6-C7-C8
25	6	623	BCR	C23-C24-C25-C26
25	6	623	BCR	C23-C24-C25-C30
25	6	625	BCR	C1-C6-C7-C8
25	6	625	BCR	C5-C6-C7-C8
30	1	617	LUT	C1-C6-C7-C8
30	1	617	LUT	C5-C6-C7-C8
30	1	619	LUT	C5-C6-C7-C8
30	3	622	LUT	C1-C6-C7-C8
30	3	622	LUT	C5-C6-C7-C8
30	8	617	LUT	C5-C6-C7-C8
30	Z	617	LUT	C5-C6-C7-C8
30	Z	619	LUT	C1-C6-C7-C8
30	Z	619	LUT	C5-C6-C7-C8
30	4	620	LUT	C5-C6-C7-C8
30	6	621	LUT	C1-C6-C7-C8
30	6	621	LUT	C5-C6-C7-C8
30	9	616	LUT	C5-C6-C7-C8
30	9	617	LUT	C1-C6-C7-C8
30	9	617	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	J	3001	LMG	O6-C5-C6-O5
24	4	622	LHG	C15-C16-C17-C18
22	A	832	CLA	CBA-CGA-O2A-C1
22	5	610	CLA	CBA-CGA-O2A-C1
29	8	607	CHL	CBA-CGA-O2A-C1
22	A	833	CLA	C10-C11-C12-C13
22	B	813	CLA	C10-C11-C12-C13
29	6	606	CHL	C5-C6-C7-C8
22	8	604	CLA	O1D-CGD-O2D-CED
22	2	611	CLA	O1A-CGA-O2A-C1
28	9	620	LMG	O6-C5-C6-O5
22	B	823	CLA	C10-C11-C12-C13
22	B	812	CLA	C4-C3-C5-C6
22	4	613	CLA	C4-C3-C5-C6
29	5	618	CHL	O1D-CGD-O2D-CED
22	A	806	CLA	C11-C12-C13-C15
22	A	808	CLA	C11-C12-C13-C15
22	A	808	CLA	C12-C13-C15-C16
22	A	829	CLA	C2-C3-C5-C6
22	A	841	CLA	C11-C10-C8-C7
22	B	806	CLA	C11-C12-C13-C15
22	B	809	CLA	C11-C12-C13-C15
22	B	812	CLA	C2-C3-C5-C6
22	B	812	CLA	C11-C10-C8-C7
22	B	813	CLA	C11-C10-C8-C7
22	B	815	CLA	C11-C10-C8-C7
22	B	816	CLA	C2-C3-C5-C6
22	B	839	CLA	C6-C7-C8-C10
22	1	608	CLA	C2-C3-C5-C6
22	Z	610	CLA	C11-C10-C8-C7
22	Z	613	CLA	C6-C7-C8-C10
22	6	602	CLA	C6-C7-C8-C10
23	A	844	PQN	C22-C23-C25-C26
29	3	608	CHL	C11-C10-C8-C7
22	8	601	CLA	C3-C5-C6-C7
22	A	819	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	O1A-CGA-O2A-C1
22	1	614	CLA	O1A-CGA-O2A-C1
22	7	620	CLA	C10-C11-C12-C13
25	B	801	BCR	C15-C16-C17-C18
27	B	850	DGD	C1B-C2B-C3B-C4B
22	A	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	819	CLA	CBA-CGA-O2A-C1
22	B	827	CLA	CBA-CGA-O2A-C1
22	L	203	CLA	CBA-CGA-O2A-C1
22	Z	614	CLA	CBA-CGA-O2A-C1
22	4	604	CLA	CBA-CGA-O2A-C1
22	6	604	CLA	CBA-CGA-O2A-C1
22	6	610	CLA	CBA-CGA-O2A-C1
29	1	601	CHL	CBA-CGA-O2A-C1
29	5	607	CHL	CBA-CGA-O2A-C1
22	F	303	CLA	C2A-CAA-CBA-CGA
22	7	602	CLA	C2A-CAA-CBA-CGA
22	8	602	CLA	C2A-CAA-CBA-CGA
22	4	609	CLA	C2A-CAA-CBA-CGA
22	5	610	CLA	C2A-CAA-CBA-CGA
22	9	604	CLA	C2A-CAA-CBA-CGA
22	A	818	CLA	C10-C11-C12-C13
22	7	601	CLA	C5-C6-C7-C8
22	7	601	CLA	C15-C16-C17-C18
29	3	608	CHL	C5-C6-C7-C8
22	A	822	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	O1D-CGD-O2D-CED
22	A	840	CLA	C10-C11-C12-C13
22	A	841	CLA	C15-C16-C17-C18
22	B	809	CLA	C15-C16-C17-C18
22	B	840	CLA	C3-C5-C6-C7
22	A	819	CLA	CBD-CGD-O2D-CED
22	4	609	CLA	CBD-CGD-O2D-CED
22	B	805	CLA	CBA-CGA-O2A-C1
22	B	812	CLA	CBA-CGA-O2A-C1
22	4	612	CLA	CBA-CGA-O2A-C1
24	7	625	LHG	C11-C10-C9-C8
24	A	847	LHG	C8-C7-O7-C5
24	8	620	LHG	C8-C7-O7-C5
27	B	850	DGD	C2B-C1B-O2G-C2G
22	A	806	CLA	C8-C10-C11-C12
22	8	613	CLA	C10-C11-C12-C13
28	9	620	LMG	C2-C1-O1-C7
22	4	610	CLA	C5-C6-C7-C8
24	A	846	LHG	O7-C5-C6-O8
22	2	609	CLA	O1A-CGA-O2A-C1
22	A	843	CLA	C13-C15-C16-C17
22	A	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	1	608	CLA	C4-C3-C5-C6
22	A	822	CLA	C2-C3-C5-C6
22	3	607	CLA	C2-C3-C5-C6
29	7	607	CHL	C2-C3-C5-C6
29	6	607	CHL	C2-C3-C5-C6
22	A	808	CLA	C14-C13-C15-C16
22	A	812	CLA	C14-C13-C15-C16
22	A	818	CLA	C6-C7-C8-C9
22	A	841	CLA	C11-C10-C8-C9
22	B	806	CLA	C11-C12-C13-C14
22	B	813	CLA	C11-C10-C8-C9
22	B	815	CLA	C11-C10-C8-C9
22	7	602	CLA	C11-C10-C8-C9
22	Z	610	CLA	C11-C10-C8-C9
22	6	604	CLA	C6-C7-C8-C9
29	3	608	CHL	C11-C10-C8-C9
22	B	828	CLA	C3-C5-C6-C7
22	6	611	CLA	C3-C5-C6-C7
29	6	606	CHL	C3-C5-C6-C7
22	G	204	CLA	O1D-CGD-O2D-CED
22	5	602	CLA	O1D-CGD-O2D-CED
22	A	819	CLA	C2A-CAA-CBA-CGA
22	B	828	CLA	C2A-CAA-CBA-CGA
22	3	602	CLA	C2A-CAA-CBA-CGA
22	6	610	CLA	C2A-CAA-CBA-CGA
30	3	621	LUT	C27-C28-C29-C39
22	1	602	CLA	C5-C6-C7-C8
22	1	608	CLA	C13-C15-C16-C17
25	3	719	BCR	C7-C8-C9-C10
22	A	832	CLA	O1A-CGA-O2A-C1
22	B	812	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	Z	614	CLA	O1A-CGA-O2A-C1
22	6	604	CLA	O1A-CGA-O2A-C1
29	1	601	CHL	O1A-CGA-O2A-C1
29	5	607	CHL	O1A-CGA-O2A-C1
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	807	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	821	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	824	CLA	C1A-C2A-CAA-CBA
22	A	825	CLA	C1A-C2A-CAA-CBA
22	A	829	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	832	CLA	C1A-C2A-CAA-CBA
22	B	835	CLA	C1A-C2A-CAA-CBA
22	B	852	CLA	C1A-C2A-CAA-CBA
22	F	304	CLA	C1A-C2A-CAA-CBA
22	1	602	CLA	C1A-C2A-CAA-CBA
22	1	610	CLA	C1A-C2A-CAA-CBA
22	1	611	CLA	C1A-C2A-CAA-CBA
22	1	612	CLA	C1A-C2A-CAA-CBA
22	1	614	CLA	C1A-C2A-CAA-CBA
22	3	602	CLA	C1A-C2A-CAA-CBA
22	3	610	CLA	C1A-C2A-CAA-CBA
22	3	617	CLA	C1A-C2A-CAA-CBA
22	7	602	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	C1A-C2A-CAA-CBA
22	7	614	CLA	C1A-C2A-CAA-CBA
22	8	604	CLA	C1A-C2A-CAA-CBA
22	8	610	CLA	C1A-C2A-CAA-CBA
22	8	614	CLA	C1A-C2A-CAA-CBA
22	Z	610	CLA	C1A-C2A-CAA-CBA
22	Z	611	CLA	C1A-C2A-CAA-CBA
22	Z	612	CLA	C1A-C2A-CAA-CBA
22	4	610	CLA	C1A-C2A-CAA-CBA
22	4	611	CLA	C1A-C2A-CAA-CBA
22	5	601	CLA	C1A-C2A-CAA-CBA
22	5	610	CLA	C1A-C2A-CAA-CBA
22	5	611	CLA	C1A-C2A-CAA-CBA
22	5	616	CLA	C1A-C2A-CAA-CBA
22	6	602	CLA	C1A-C2A-CAA-CBA
22	6	610	CLA	C1A-C2A-CAA-CBA
22	6	611	CLA	C1A-C2A-CAA-CBA
22	6	614	CLA	C1A-C2A-CAA-CBA
22	2	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	2	611	CLA	C1A-C2A-CAA-CBA
22	9	610	CLA	C1A-C2A-CAA-CBA
27	B	850	DGD	O6E-C5E-C6E-O5E
29	7	607	CHL	C1A-C2A-CAA-CBA
29	Z	607	CHL	C1A-C2A-CAA-CBA
22	A	814	CLA	C16-C17-C18-C19
27	B	850	DGD	O1B-C1B-O2G-C2G
24	4	623	LHG	C8-C7-O7-C5
22	B	821	CLA	O1A-CGA-O2A-C1
22	A	830	CLA	C5-C6-C7-C8
22	A	833	CLA	C8-C10-C11-C12
22	7	613	CLA	C15-C16-C17-C18
24	A	847	LHG	C4-O6-P-O3
24	4	622	LHG	C23-C24-C25-C26
22	B	829	CLA	CBD-CGD-O2D-CED
22	5	613	CLA	CBD-CGD-O2D-CED
29	8	607	CHL	O1A-CGA-O2A-C1
22	2	610	CLA	C8-C10-C11-C12
22	9	610	CLA	C10-C11-C12-C13
23	A	844	PQN	C15-C16-C17-C18
22	1	608	CLA	CBA-CGA-O2A-C1
22	Z	603	CLA	C5-C6-C7-C8
24	8	620	LHG	O9-C7-O7-C5
22	A	822	CLA	C4-C3-C5-C6
21	A	801	CL0	C15-C16-C17-C18
22	A	802	CLA	C15-C16-C17-C18
22	B	832	CLA	C10-C11-C12-C13
22	L	203	CLA	O1A-CGA-O2A-C1
22	4	612	CLA	O1A-CGA-O2A-C1
22	5	610	CLA	O1A-CGA-O2A-C1
22	9	610	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	C3-C5-C6-C7
22	B	817	CLA	C11-C12-C13-C14
24	5	623	LHG	C4-C5-C6-O8
27	B	850	DGD	C2B-C3B-C4B-C5B
28	J	3001	LMG	O1-C7-C8-C9
28	J	3001	LMG	C7-C8-C9-O8
28	9	620	LMG	C31-C32-C33-C34
22	A	809	CLA	C13-C15-C16-C17
29	3	608	CHL	C15-C16-C17-C18
22	A	817	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	6	610	CLA	O1A-CGA-O2A-C1
22	3	610	CLA	C10-C11-C12-C13
22	Z	610	CLA	C5-C6-C7-C8
22	B	805	CLA	O1A-CGA-O2A-C1
22	K	4003	CLA	CBA-CGA-O2A-C1
27	B	850	DGD	C7A-C8A-C9A-CAA
24	6	619	LHG	C24-C23-O8-C6
22	8	610	CLA	C8-C10-C11-C12
22	1	608	CLA	O1A-CGA-O2A-C1
22	4	604	CLA	O1A-CGA-O2A-C1
22	A	843	CLA	C15-C16-C17-C18
22	B	813	CLA	C8-C10-C11-C12
22	A	826	CLA	C4-C3-C5-C6
22	1	614	CLA	C4-C3-C5-C6
22	8	601	CLA	C4-C3-C5-C6
22	Z	611	CLA	C4-C3-C5-C6
22	6	613	CLA	C4-C3-C5-C6
24	8	620	LHG	C12-C13-C14-C15
22	6	612	CLA	C2-C3-C5-C6
22	9	612	CLA	CBA-CGA-O2A-C1
24	4	623	LHG	C13-C14-C15-C16
22	8	611	CLA	CBD-CGD-O2D-CED
29	Z	601	CHL	CBD-CGD-O2D-CED
22	3	613	CLA	C5-C6-C7-C8
22	Z	608	CLA	C13-C15-C16-C17
23	A	844	PQN	C23-C25-C26-C27
22	A	810	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C2A-CAA-CBA-CGA
22	F	304	CLA	C2A-CAA-CBA-CGA
22	7	609	CLA	C2A-CAA-CBA-CGA
22	B	841	CLA	C15-C16-C17-C18
22	A	840	CLA	C2-C1-O2A-CGA
22	A	845	CLA	C2-C1-O2A-CGA
22	B	831	CLA	C2-C1-O2A-CGA
22	B	836	CLA	C2-C1-O2A-CGA
22	Z	608	CLA	C2-C1-O2A-CGA
22	5	601	CLA	C2-C1-O2A-CGA
22	2	610	CLA	C2-C1-O2A-CGA
22	B	808	CLA	O1D-CGD-O2D-CED
22	4	613	CLA	O1D-CGD-O2D-CED
22	8	609	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	9	620	LMG	C17-C18-C19-C20
22	A	839	CLA	CBA-CGA-O2A-C1
22	B	852	CLA	CBA-CGA-O2A-C1
22	8	601	CLA	CBA-CGA-O2A-C1
22	B	832	CLA	O1D-CGD-O2D-CED
22	Z	612	CLA	C3-C5-C6-C7
22	B	830	CLA	CAA-CBA-CGA-O2A
24	A	847	LHG	O9-C7-O7-C5
22	A	822	CLA	C10-C11-C12-C13
22	8	610	CLA	C10-C11-C12-C13
22	9	612	CLA	O1A-CGA-O2A-C1
22	A	845	CLA	C4-C3-C5-C6
22	B	824	CLA	C4-C3-C5-C6
22	5	613	CLA	C4-C3-C5-C6
22	A	807	CLA	C11-C12-C13-C15
22	A	812	CLA	C6-C7-C8-C10
22	A	815	CLA	C6-C7-C8-C10
22	A	818	CLA	C6-C7-C8-C10
22	A	820	CLA	C11-C12-C13-C15
22	A	827	CLA	C6-C7-C8-C10
22	A	829	CLA	C6-C7-C8-C10
22	A	829	CLA	C12-C13-C15-C16
22	A	831	CLA	C11-C10-C8-C7
22	A	842	CLA	C11-C10-C8-C7
22	A	843	CLA	C6-C7-C8-C10
22	B	826	CLA	C11-C10-C8-C7
22	B	832	CLA	C6-C7-C8-C10
22	B	837	CLA	C11-C10-C8-C7
22	1	610	CLA	C6-C7-C8-C10
22	1	614	CLA	C2-C3-C5-C6
22	1	614	CLA	C12-C13-C15-C16
22	3	607	CLA	C6-C7-C8-C10
22	7	602	CLA	C11-C10-C8-C7
22	7	604	CLA	C6-C7-C8-C10
22	Z	611	CLA	C2-C3-C5-C6
22	5	602	CLA	C11-C10-C8-C7
22	5	602	CLA	C12-C13-C15-C16
22	5	613	CLA	C2-C3-C5-C6
22	6	604	CLA	C6-C7-C8-C10
22	6	613	CLA	C2-C3-C5-C6
22	A	812	CLA	C3-C5-C6-C7
22	Z	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	1	620	LHG	C24-C25-C26-C27
22	A	807	CLA	C11-C12-C13-C14
22	A	812	CLA	C6-C7-C8-C9
22	A	815	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C12-C13-C14
22	A	829	CLA	C6-C7-C8-C9
22	A	829	CLA	C14-C13-C15-C16
22	A	842	CLA	C6-C7-C8-C9
22	B	826	CLA	C11-C10-C8-C9
22	B	826	CLA	C11-C12-C13-C14
22	B	834	CLA	C11-C10-C8-C9
22	B	839	CLA	C6-C7-C8-C9
22	3	610	CLA	C14-C13-C15-C16
22	7	604	CLA	C6-C7-C8-C9
22	Z	608	CLA	C11-C10-C8-C9
22	5	601	CLA	C11-C10-C8-C9
22	5	602	CLA	C11-C10-C8-C9
22	6	601	CLA	C11-C10-C8-C9
22	6	602	CLA	C11-C10-C8-C9
23	A	844	PQN	C19-C18-C20-C21
22	8	614	CLA	CBA-CGA-O2A-C1
22	5	604	CLA	CBA-CGA-O2A-C1
22	7	610	CLA	C5-C6-C7-C8
22	B	833	CLA	O1D-CGD-O2D-CED
22	7	616	CLA	C2A-CAA-CBA-CGA
22	2	614	CLA	C2A-CAA-CBA-CGA
22	6	610	CLA	O1D-CGD-O2D-CED
25	B	847	BCR	C7-C8-C9-C34
25	J	3003	BCR	C7-C8-C9-C10
22	5	604	CLA	O1D-CGD-O2D-CED
24	4	623	LHG	O9-C7-O7-C5
22	A	826	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	CBA-CGA-O2A-C1
22	7	601	CLA	CBA-CGA-O2A-C1
22	8	610	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	C10-C11-C12-C13
22	B	816	CLA	C5-C6-C7-C8
22	7	602	CLA	C8-C10-C11-C12
22	7	602	CLA	C15-C16-C17-C18
22	Z	610	CLA	C8-C10-C11-C12
22	3	609	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
22	G	204	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	C4B-C3B-CAB-CBB
22	A	825	CLA	C4B-C3B-CAB-CBB
22	A	843	CLA	C4B-C3B-CAB-CBB
22	A	854	CLA	C4B-C3B-CAB-CBB
22	B	816	CLA	C4B-C3B-CAB-CBB
22	B	822	CLA	C4B-C3B-CAB-CBB
22	L	204	CLA	C4B-C3B-CAB-CBB
22	3	609	CLA	C4B-C3B-CAB-CBB
22	Z	609	CLA	C4B-C3B-CAB-CBB
22	Z	613	CLA	C4B-C3B-CAB-CBB
22	4	601	CLA	C4B-C3B-CAB-CBB
22	5	604	CLA	C4B-C3B-CAB-CBB
22	5	609	CLA	C4B-C3B-CAB-CBB
22	6	617	CLA	C4B-C3B-CAB-CBB
29	5	607	CHL	C4B-C3B-CAB-CBB
22	A	809	CLA	C5-C6-C7-C8
24	B	851	LHG	O6-C4-C5-C6
21	A	801	CL0	C3-C5-C6-C7
22	1	614	CLA	C3-C5-C6-C7
22	7	601	CLA	CBD-CGD-O2D-CED
22	B	806	CLA	C10-C11-C12-C13
22	B	818	CLA	C5-C6-C7-C8
22	A	810	CLA	C4-C3-C5-C6
22	8	602	CLA	C4-C3-C5-C6
22	Z	614	CLA	C4-C3-C5-C6
22	A	826	CLA	C2-C3-C5-C6
22	A	845	CLA	C2-C3-C5-C6
22	B	824	CLA	C2-C3-C5-C6
22	4	610	CLA	C8-C10-C11-C12
22	9	613	CLA	O1D-CGD-O2D-CED
22	4	601	CLA	C2A-CAA-CBA-CGA
22	A	823	CLA	CBA-CGA-O2A-C1
22	B	807	CLA	CBA-CGA-O2A-C1
22	B	822	CLA	C10-C11-C12-C13
22	A	824	CLA	C3A-C2A-CAA-CBA
22	A	829	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	C3A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	835	CLA	C3A-C2A-CAA-CBA
22	3	604	CLA	C3A-C2A-CAA-CBA
22	6	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	6	608	CHL	C3A-C2A-CAA-CBA
30	Z	618	LUT	C29-C30-C31-C32
22	6	604	CLA	C3-C5-C6-C7
22	A	830	CLA	CBA-CGA-O2A-C1
22	B	807	CLA	C13-C15-C16-C17
22	B	818	CLA	C10-C11-C12-C13
24	A	846	LHG	C4-C5-C6-O8
27	B	850	DGD	C1G-C2G-C3G-O3G
28	9	620	LMG	O1-C7-C8-C9
22	B	814	CLA	CBD-CGD-O2D-CED
28	J	3001	LMG	C31-C32-C33-C34
22	Z	610	CLA	O1D-CGD-O2D-CED
22	A	829	CLA	C5-C6-C7-C8
22	A	838	CLA	O1D-CGD-O2D-CED
22	B	827	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	C5-C6-C7-C8
22	7	612	CLA	C4-C3-C5-C6
22	A	810	CLA	C2-C3-C5-C6
22	Z	614	CLA	C2-C3-C5-C6
27	B	850	DGD	C4B-C5B-C6B-C7B
22	7	616	CLA	CBA-CGA-O2A-C1
24	A	855	LHG	C3-O3-P-O6
29	4	606	CHL	C3C-C2C-CMC-OMC
29	6	618	CHL	C3C-C2C-CMC-OMC
29	9	606	CHL	C3C-C2C-CMC-OMC
24	8	620	LHG	C23-C24-C25-C26
24	6	619	LHG	O10-C23-O8-C6
22	B	840	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	C2A-CAA-CBA-CGA
29	4	607	CHL	C2A-CAA-CBA-CGA
24	A	847	LHG	O1-C1-C2-O2
22	8	614	CLA	O1A-CGA-O2A-C1
22	A	802	CLA	C5-C6-C7-C8
22	B	817	CLA	CAA-CBA-CGA-O2A
22	A	812	CLA	C2B-C3B-CAB-CBB
22	A	854	CLA	C2B-C3B-CAB-CBB
22	B	816	CLA	C2B-C3B-CAB-CBB
22	Z	609	CLA	C2B-C3B-CAB-CBB
22	4	601	CLA	C2B-C3B-CAB-CBB
22	5	604	CLA	C2B-C3B-CAB-CBB
22	5	609	CLA	C2B-C3B-CAB-CBB
22	6	601	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	6	617	CLA	C2B-C3B-CAB-CBB
24	7	625	LHG	C26-C27-C28-C29
22	B	852	CLA	O1A-CGA-O2A-C1
22	8	601	CLA	O1A-CGA-O2A-C1
22	5	604	CLA	O1A-CGA-O2A-C1
22	1	613	CLA	C3-C5-C6-C7
24	4	622	LHG	O7-C5-C6-O8
28	J	3001	LMG	O7-C8-C9-O8
22	3	610	CLA	C8-C10-C11-C12
22	A	810	CLA	C2-C1-O2A-CGA
22	A	833	CLA	C2-C1-O2A-CGA
22	B	802	CLA	C2-C1-O2A-CGA
22	B	817	CLA	C2-C1-O2A-CGA
22	3	609	CLA	C2-C1-O2A-CGA
22	3	613	CLA	C2-C1-O2A-CGA
22	8	613	CLA	C2-C1-O2A-CGA
22	Z	602	CLA	C2-C1-O2A-CGA
22	Z	612	CLA	C2-C1-O2A-CGA
22	4	613	CLA	C2-C1-O2A-CGA
22	5	613	CLA	C2-C1-O2A-CGA
22	1	614	CLA	O1D-CGD-O2D-CED
22	6	604	CLA	O1D-CGD-O2D-CED
22	2	601	CLA	CAA-CBA-CGA-O2A
22	A	816	CLA	C14-C13-C15-C16
22	A	843	CLA	C14-C13-C15-C16
22	B	817	CLA	C11-C10-C8-C9
22	B	825	CLA	C6-C7-C8-C9
22	B	837	CLA	C11-C10-C8-C9
22	B	839	CLA	C14-C13-C15-C16
22	B	840	CLA	C14-C13-C15-C16
22	4	602	CLA	C11-C10-C8-C9
22	5	602	CLA	C14-C13-C15-C16
22	1	603	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	C13-C15-C16-C17
22	B	808	CLA	C13-C15-C16-C17
22	3	607	CLA	C8-C10-C11-C12
22	A	826	CLA	O1A-CGA-O2A-C1
22	7	601	CLA	O1A-CGA-O2A-C1
22	3	620	CLA	C2A-CAA-CBA-CGA
22	A	843	CLA	C16-C17-C18-C20
25	A	848	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	A	848	BCR	C23-C24-C25-C30
25	A	851	BCR	C1-C6-C7-C8
25	A	851	BCR	C5-C6-C7-C8
25	A	851	BCR	C23-C24-C25-C30
25	B	801	BCR	C1-C6-C7-C8
25	B	801	BCR	C5-C6-C7-C8
25	B	843	BCR	C23-C24-C25-C26
25	B	843	BCR	C23-C24-C25-C30
25	B	845	BCR	C23-C24-C25-C26
25	B	845	BCR	C23-C24-C25-C30
25	B	847	BCR	C5-C6-C7-C8
25	B	847	BCR	C23-C24-C25-C26
25	B	847	BCR	C23-C24-C25-C30
25	J	3003	BCR	C5-C6-C7-C8
25	L	205	BCR	C1-C6-C7-C8
25	L	205	BCR	C5-C6-C7-C8
25	3	718	BCR	C23-C24-C25-C26
25	3	718	BCR	C23-C24-C25-C30
25	6	625	BCR	C23-C24-C25-C26
25	6	625	BCR	C23-C24-C25-C30
30	3	621	LUT	C1-C6-C7-C8
30	3	621	LUT	C5-C6-C7-C8
30	7	621	LUT	C1-C6-C7-C8
30	7	621	LUT	C5-C6-C7-C8
30	8	618	LUT	C5-C6-C7-C8
30	Z	617	LUT	C1-C6-C7-C8
30	4	619	LUT	C1-C6-C7-C8
30	4	619	LUT	C5-C6-C7-C8
30	5	624	LUT	C1-C6-C7-C8
30	5	624	LUT	C5-C6-C7-C8
30	6	624	LUT	C1-C6-C7-C8
30	6	624	LUT	C5-C6-C7-C8
30	2	617	LUT	C1-C6-C7-C8
22	1	614	CLA	C8-C10-C11-C12
22	Z	611	CLA	C15-C16-C17-C18
22	9	614	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	C13-C15-C16-C17
22	1	608	CLA	C15-C16-C17-C18
22	1	613	CLA	C10-C11-C12-C13
22	A	845	CLA	O1D-CGD-O2D-CED
24	A	855	LHG	C8-C7-O7-C5
24	A	846	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
22	9	611	CLA	C6-C7-C8-C9
22	4	609	CLA	O1D-CGD-O2D-CED
22	8	614	CLA	O1D-CGD-O2D-CED
22	A	814	CLA	C11-C12-C13-C15
22	A	818	CLA	C11-C12-C13-C15
22	B	817	CLA	C11-C10-C8-C7
22	B	825	CLA	C6-C7-C8-C10
22	B	826	CLA	C11-C12-C13-C15
22	B	834	CLA	C11-C10-C8-C7
22	B	839	CLA	C12-C13-C15-C16
22	B	840	CLA	C12-C13-C15-C16
22	L	203	CLA	C11-C12-C13-C15
22	1	609	CLA	C11-C10-C8-C7
22	1	610	CLA	C11-C10-C8-C7
22	8	601	CLA	C11-C12-C13-C15
22	Z	608	CLA	C2-C3-C5-C6
22	Z	608	CLA	C11-C10-C8-C7
22	4	602	CLA	C11-C10-C8-C7
22	6	601	CLA	C11-C10-C8-C7
22	6	602	CLA	C11-C10-C8-C7
23	A	844	PQN	C17-C18-C20-C21
29	3	608	CHL	C12-C13-C15-C16
27	B	850	DGD	CDB-CEB-CFB-CGB
25	B	801	BCR	C19-C20-C21-C22
25	B	843	BCR	C15-C16-C17-C18
25	K	4001	BCR	C13-C14-C15-C16
30	1	618	LUT	C29-C30-C31-C32
22	A	842	CLA	C3-C5-C6-C7
22	B	832	CLA	C3-C5-C6-C7
22	2	603	CLA	CBD-CGD-O2D-CED
22	A	815	CLA	C10-C11-C12-C13
22	B	805	CLA	C10-C11-C12-C13
23	B	842	PQN	C15-C16-C17-C18
22	3	613	CLA	CBA-CGA-O2A-C1
22	4	610	CLA	CBA-CGA-O2A-C1
22	2	607	CLA	CBA-CGA-O2A-C1
24	8	620	LHG	C24-C23-O8-C6
22	A	804	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	812	CLA	CAD-CBD-CGD-O2D
22	A	817	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	842	CLA	CAD-CBD-CGD-O2D
22	B	825	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	F	303	CLA	CAD-CBD-CGD-O2D
22	1	610	CLA	CAD-CBD-CGD-O2D
22	3	607	CLA	CAD-CBD-CGD-O2D
22	8	608	CLA	CAD-CBD-CGD-O2D
22	Z	602	CLA	CAD-CBD-CGD-O2D
22	4	602	CLA	CAD-CBD-CGD-O2D
22	4	610	CLA	CAD-CBD-CGD-O2D
22	4	614	CLA	CAD-CBD-CGD-O2D
22	6	604	CLA	CAD-CBD-CGD-O2D
22	6	614	CLA	CAD-CBD-CGD-O2D
22	2	602	CLA	CAD-CBD-CGD-O2D
22	2	603	CLA	CAD-CBD-CGD-O2D
22	2	606	CLA	CAD-CBD-CGD-O2D
22	2	612	CLA	CAD-CBD-CGD-O2D
22	9	602	CLA	CAD-CBD-CGD-O2D
29	4	608	CHL	CAD-CBD-CGD-O2D
22	A	806	CLA	C15-C16-C17-C18
22	8	610	CLA	C5-C6-C7-C8
22	A	805	CLA	C4-C3-C5-C6
22	Z	608	CLA	C4-C3-C5-C6
23	B	842	PQN	C14-C13-C15-C16
21	A	801	CL0	C16-C17-C18-C20
22	A	842	CLA	C16-C17-C18-C19
22	B	834	CLA	C8-C10-C11-C12
22	A	805	CLA	C2-C3-C5-C6
28	9	620	LMG	C7-C8-C9-O8
24	B	851	LHG	O6-C4-C5-O7
24	7	625	LHG	O6-C4-C5-O7
22	B	809	CLA	O1D-CGD-O2D-CED
24	6	619	LHG	C16-C17-C18-C19
22	1	609	CLA	C2A-CAA-CBA-CGA
22	6	601	CLA	C2A-CAA-CBA-CGA
22	2	611	CLA	C2A-CAA-CBA-CGA
22	3	613	CLA	O1A-CGA-O2A-C1
22	8	610	CLA	C11-C12-C13-C15
24	A	855	LHG	O9-C7-O7-C5
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	807	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	814	CLA	CHA-CBD-CGD-O1D
22	A	815	CLA	CHA-CBD-CGD-O1D
22	A	826	CLA	CHA-CBD-CGD-O1D
22	A	826	CLA	CHA-CBD-CGD-O2D
22	A	839	CLA	CHA-CBD-CGD-O1D
22	A	839	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	CHA-CBD-CGD-O1D
22	A	840	CLA	CHA-CBD-CGD-O2D
22	A	845	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O2D
22	A	854	CLA	CHA-CBD-CGD-O1D
22	A	854	CLA	CHA-CBD-CGD-O2D
22	B	815	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	837	CLA	CHA-CBD-CGD-O1D
22	B	837	CLA	CHA-CBD-CGD-O2D
22	F	301	CLA	CHA-CBD-CGD-O2D
22	J	3002	CLA	CHA-CBD-CGD-O1D
22	7	601	CLA	CHA-CBD-CGD-O1D
22	7	601	CLA	CHA-CBD-CGD-O2D
22	7	602	CLA	CHA-CBD-CGD-O2D
22	7	611	CLA	CHA-CBD-CGD-O1D
22	7	611	CLA	CHA-CBD-CGD-O2D
22	8	601	CLA	CHA-CBD-CGD-O1D
22	8	601	CLA	CHA-CBD-CGD-O2D
22	8	602	CLA	CHA-CBD-CGD-O1D
22	8	602	CLA	CHA-CBD-CGD-O2D
22	8	611	CLA	CHA-CBD-CGD-O1D
22	8	611	CLA	CHA-CBD-CGD-O2D
22	4	601	CLA	CHA-CBD-CGD-O1D
22	4	601	CLA	CHA-CBD-CGD-O2D
22	5	611	CLA	CHA-CBD-CGD-O1D
22	5	611	CLA	CHA-CBD-CGD-O2D
22	5	621	CLA	CHA-CBD-CGD-O2D
22	6	601	CLA	CHA-CBD-CGD-O1D
22	6	601	CLA	CHA-CBD-CGD-O2D
22	2	601	CLA	CHA-CBD-CGD-O1D
22	9	601	CLA	CHA-CBD-CGD-O1D
22	9	601	CLA	CHA-CBD-CGD-O2D
22	9	604	CLA	CHA-CBD-CGD-O1D
22	9	604	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	4	603	CLA	O1A-CGA-O2A-C1
22	Z	603	CLA	C3-C5-C6-C7
22	A	830	CLA	O1A-CGA-O2A-C1
22	A	833	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1D-CGD-O2D-CED
24	5	623	LHG	O7-C5-C6-O8
28	9	620	LMG	O7-C8-C9-O8
22	A	823	CLA	O1A-CGA-O2A-C1
22	A	842	CLA	C16-C17-C18-C20
22	B	829	CLA	O1D-CGD-O2D-CED
24	1	620	LHG	C25-C26-C27-C28
22	B	807	CLA	C4-C3-C5-C6
22	3	604	CLA	C4-C3-C5-C6
22	B	807	CLA	O1A-CGA-O2A-C1
22	1	603	CLA	O1A-CGA-O2A-C1
22	3	604	CLA	C2-C3-C5-C6
23	B	842	PQN	C12-C13-C15-C16
22	8	602	CLA	O1D-CGD-O2D-CED
22	Z	610	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	C5-C6-C7-C8
22	A	814	CLA	C11-C12-C13-C14
22	A	818	CLA	C11-C12-C13-C14
22	A	854	CLA	C14-C13-C15-C16
22	B	812	CLA	C11-C12-C13-C14
22	B	841	CLA	C6-C7-C8-C9
22	2	610	CLA	C11-C10-C8-C9
29	Z	601	CHL	O1D-CGD-O2D-CED
22	A	819	CLA	CAA-CBA-CGA-O2A
24	A	846	LHG	C10-C11-C12-C13
22	A	839	CLA	O1A-CGA-O2A-C1
22	L	204	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	C8-C10-C11-C12
22	Z	616	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	816	CLA	C1A-C2A-CAA-CBA
22	A	845	CLA	C1A-C2A-CAA-CBA
22	B	826	CLA	C1A-C2A-CAA-CBA
22	K	4002	CLA	C1A-C2A-CAA-CBA
22	L	203	CLA	C1A-C2A-CAA-CBA
22	7	604	CLA	C1A-C2A-CAA-CBA
22	Z	614	CLA	C1A-C2A-CAA-CBA
22	4	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	6	604	CLA	C1A-C2A-CAA-CBA
22	2	607	CLA	C1A-C2A-CAA-CBA
22	7	612	CLA	C2-C1-O2A-CGA
22	7	601	CLA	O1D-CGD-O2D-CED
22	A	808	CLA	C13-C15-C16-C17
22	7	613	CLA	C10-C11-C12-C13
24	A	846	LHG	C3-O3-P-O6
24	4	622	LHG	C4-O6-P-O3
24	6	619	LHG	C4-O6-P-O3
24	6	619	LHG	C11-C10-C9-C8
22	B	828	CLA	C4-C3-C5-C6
22	B	832	CLA	CAA-CBA-CGA-O2A
22	L	203	CLA	C3-C5-C6-C7
22	1	609	CLA	C3-C5-C6-C7
22	8	602	CLA	C2-C3-C5-C6
22	2	607	CLA	O1A-CGA-O2A-C1
22	A	807	CLA	C4B-C3B-CAB-CBB
22	A	811	CLA	C4B-C3B-CAB-CBB
22	A	823	CLA	C4B-C3B-CAB-CBB
22	A	837	CLA	C4B-C3B-CAB-CBB
22	A	839	CLA	C4B-C3B-CAB-CBB
22	B	802	CLA	C4B-C3B-CAB-CBB
22	B	806	CLA	C4B-C3B-CAB-CBB
22	B	808	CLA	C4B-C3B-CAB-CBB
22	B	810	CLA	C4B-C3B-CAB-CBB
22	B	815	CLA	C4B-C3B-CAB-CBB
22	B	818	CLA	C4B-C3B-CAB-CBB
22	B	827	CLA	C4B-C3B-CAB-CBB
22	B	835	CLA	C4B-C3B-CAB-CBB
22	B	852	CLA	C4B-C3B-CAB-CBB
22	G	203	CLA	C4B-C3B-CAB-CBB
22	K	4002	CLA	C4B-C3B-CAB-CBB
22	1	603	CLA	C4B-C3B-CAB-CBB
22	1	608	CLA	C4B-C3B-CAB-CBB
22	1	609	CLA	C4B-C3B-CAB-CBB
22	1	610	CLA	C4B-C3B-CAB-CBB
22	1	613	CLA	C4B-C3B-CAB-CBB
22	1	614	CLA	C4B-C3B-CAB-CBB
22	1	616	CLA	C4B-C3B-CAB-CBB
22	3	611	CLA	C4B-C3B-CAB-CBB
22	3	614	CLA	C4B-C3B-CAB-CBB
22	3	617	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	7	601	CLA	C4B-C3B-CAB-CBB
22	7	603	CLA	C4B-C3B-CAB-CBB
22	7	614	CLA	C4B-C3B-CAB-CBB
22	7	616	CLA	C4B-C3B-CAB-CBB
22	7	620	CLA	C4B-C3B-CAB-CBB
22	8	601	CLA	C4B-C3B-CAB-CBB
22	8	603	CLA	C4B-C3B-CAB-CBB
22	8	608	CLA	C4B-C3B-CAB-CBB
22	8	611	CLA	C4B-C3B-CAB-CBB
22	8	613	CLA	C4B-C3B-CAB-CBB
22	8	614	CLA	C4B-C3B-CAB-CBB
22	8	616	CLA	C4B-C3B-CAB-CBB
22	Z	603	CLA	C4B-C3B-CAB-CBB
22	Z	608	CLA	C4B-C3B-CAB-CBB
22	Z	611	CLA	C4B-C3B-CAB-CBB
22	Z	614	CLA	C4B-C3B-CAB-CBB
22	Z	616	CLA	C4B-C3B-CAB-CBB
22	4	610	CLA	C4B-C3B-CAB-CBB
22	4	611	CLA	C4B-C3B-CAB-CBB
22	4	613	CLA	C4B-C3B-CAB-CBB
22	4	614	CLA	C4B-C3B-CAB-CBB
22	5	601	CLA	C4B-C3B-CAB-CBB
22	5	602	CLA	C4B-C3B-CAB-CBB
22	5	611	CLA	C4B-C3B-CAB-CBB
22	5	614	CLA	C4B-C3B-CAB-CBB
22	5	617	CLA	C4B-C3B-CAB-CBB
22	5	621	CLA	C4B-C3B-CAB-CBB
22	6	601	CLA	C4B-C3B-CAB-CBB
22	6	603	CLA	C4B-C3B-CAB-CBB
22	6	609	CLA	C4B-C3B-CAB-CBB
22	6	611	CLA	C4B-C3B-CAB-CBB
22	6	622	CLA	C4B-C3B-CAB-CBB
22	2	601	CLA	C4B-C3B-CAB-CBB
22	2	603	CLA	C4B-C3B-CAB-CBB
22	2	606	CLA	C4B-C3B-CAB-CBB
22	2	607	CLA	C4B-C3B-CAB-CBB
22	2	609	CLA	C4B-C3B-CAB-CBB
22	2	610	CLA	C4B-C3B-CAB-CBB
22	2	611	CLA	C4B-C3B-CAB-CBB
22	2	612	CLA	C4B-C3B-CAB-CBB
22	2	613	CLA	C4B-C3B-CAB-CBB
22	2	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	9	601	CLA	C4B-C3B-CAB-CBB
22	9	604	CLA	C4B-C3B-CAB-CBB
22	9	611	CLA	C4B-C3B-CAB-CBB
22	9	612	CLA	C4B-C3B-CAB-CBB
22	9	613	CLA	C4B-C3B-CAB-CBB
22	9	614	CLA	C4B-C3B-CAB-CBB
24	A	847	LHG	C4-O6-P-O5
24	B	851	LHG	C3-O3-P-O4
24	7	625	LHG	C4-O6-P-O4
24	8	620	LHG	C3-O3-P-O5
24	8	620	LHG	C4-O6-P-O5
24	5	623	LHG	C4-O6-P-O4
24	6	619	LHG	C3-O3-P-O4
29	1	601	CHL	C4B-C3B-CAB-CBB
29	7	607	CHL	C4B-C3B-CAB-CBB
29	Z	601	CHL	C4B-C3B-CAB-CBB
29	Z	607	CHL	C4B-C3B-CAB-CBB
29	4	607	CHL	C4B-C3B-CAB-CBB
29	4	618	CHL	C4B-C3B-CAB-CBB
29	5	618	CHL	C4B-C3B-CAB-CBB
29	6	607	CHL	C4B-C3B-CAB-CBB
29	6	618	CHL	C4B-C3B-CAB-CBB
29	9	606	CHL	C4B-C3B-CAB-CBB
29	9	607	CHL	C4B-C3B-CAB-CBB
22	B	809	CLA	C16-C17-C18-C20
22	L	203	CLA	C16-C17-C18-C20
22	7	601	CLA	C10-C11-C12-C13
22	A	834	CLA	CBA-CGA-O2A-C1
24	7	625	LHG	O6-C4-C5-C6
22	8	610	CLA	C2A-CAA-CBA-CGA
22	1	612	CLA	C3-C5-C6-C7
22	B	816	CLA	C6-C7-C8-C10
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	A	815	CLA	CAD-CBD-CGD-O1D
22	A	816	CLA	CAD-CBD-CGD-O1D
22	A	826	CLA	CAD-CBD-CGD-O1D
22	A	839	CLA	CAD-CBD-CGD-O1D
22	A	845	CLA	CAD-CBD-CGD-O1D
22	A	854	CLA	CAD-CBD-CGD-O1D
22	B	837	CLA	CAD-CBD-CGD-O1D
22	B	841	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	J	3002	CLA	CAD-CBD-CGD-O1D
22	7	601	CLA	CAD-CBD-CGD-O1D
22	7	606	CLA	CAD-CBD-CGD-O1D
22	7	620	CLA	CAD-CBD-CGD-O1D
22	8	601	CLA	CAD-CBD-CGD-O1D
22	4	601	CLA	CAD-CBD-CGD-O1D
22	6	601	CLA	CAD-CBD-CGD-O1D
22	2	601	CLA	CAD-CBD-CGD-O1D
22	9	601	CLA	CAD-CBD-CGD-O1D
22	9	604	CLA	CAD-CBD-CGD-O1D
29	Z	601	CHL	CAD-CBD-CGD-O1D
24	A	846	LHG	C9-C10-C11-C12
22	A	804	CLA	C13-C15-C16-C17
22	A	854	CLA	C13-C15-C16-C17
22	7	610	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	C12-C13-C15-C16
22	A	816	CLA	C12-C13-C15-C16
22	A	819	CLA	C6-C7-C8-C10
22	A	833	CLA	C11-C10-C8-C7
22	A	839	CLA	C12-C13-C15-C16
22	A	854	CLA	C12-C13-C15-C16
22	B	819	CLA	C12-C13-C15-C16
22	B	827	CLA	C6-C7-C8-C10
22	2	610	CLA	C11-C10-C8-C7
23	A	844	PQN	C21-C22-C23-C25
29	5	607	CHL	C3A-C2A-CAA-CBA
25	L	205	BCR	C13-C14-C15-C16
22	A	804	CLA	C8-C10-C11-C12
24	4	622	LHG	C13-C14-C15-C16
22	A	834	CLA	O1A-CGA-O2A-C1
22	L	204	CLA	O1A-CGA-O2A-C1
22	8	610	CLA	O1A-CGA-O2A-C1
22	5	616	CLA	C2A-CAA-CBA-CGA
24	7	625	LHG	C23-C24-C25-C26
29	1	607	CHL	C1C-C2C-CMC-OMC
29	3	608	CHL	C1C-C2C-CMC-OMC
29	4	606	CHL	C1C-C2C-CMC-OMC
29	4	618	CHL	C1C-C2C-CMC-OMC
29	5	618	CHL	C1C-C2C-CMC-OMC
29	6	618	CHL	C1C-C2C-CMC-OMC
29	9	606	CHL	C1C-C2C-CMC-OMC
29	9	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	A	855	LHG	O7-C5-C6-O8
22	4	601	CLA	C8-C10-C11-C12
29	4	607	CHL	CAA-CBA-CGA-O2A
22	9	611	CLA	C6-C7-C8-C10
22	Z	614	CLA	C3-C5-C6-C7
22	A	836	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	C4-C3-C5-C6
22	B	827	CLA	C4-C3-C5-C6
22	8	601	CLA	C2-C3-C5-C6
22	A	819	CLA	C6-C7-C8-C9
22	A	831	CLA	C11-C10-C8-C9
22	B	827	CLA	C11-C10-C8-C9
22	L	203	CLA	C11-C12-C13-C14
22	1	602	CLA	C6-C7-C8-C9
22	1	609	CLA	C11-C10-C8-C9
22	8	613	CLA	C6-C7-C8-C9
22	A	831	CLA	O1A-CGA-O2A-C1
22	A	827	CLA	C3-C5-C6-C7
24	4	622	LHG	C27-C28-C29-C30
22	4	601	CLA	O1A-CGA-O2A-C1
24	8	620	LHG	O10-C23-O8-C6
22	Z	614	CLA	C2A-CAA-CBA-CGA
25	B	801	BCR	C13-C14-C15-C16
22	A	828	CLA	C10-C11-C12-C13
22	3	602	CLA	O1D-CGD-O2D-CED
25	L	205	BCR	C7-C8-C9-C10
30	3	621	LUT	C27-C28-C29-C30
22	A	823	CLA	C2B-C3B-CAB-CBB
22	A	837	CLA	C2B-C3B-CAB-CBB
22	A	839	CLA	C2B-C3B-CAB-CBB
22	B	815	CLA	C2B-C3B-CAB-CBB
22	B	818	CLA	C2B-C3B-CAB-CBB
22	B	821	CLA	C2B-C3B-CAB-CBB
22	B	822	CLA	C2B-C3B-CAB-CBB
22	B	825	CLA	C2B-C3B-CAB-CBB
22	B	852	CLA	C2B-C3B-CAB-CBB
22	K	4002	CLA	C2B-C3B-CAB-CBB
22	1	610	CLA	C2B-C3B-CAB-CBB
22	1	614	CLA	C2B-C3B-CAB-CBB
22	1	616	CLA	C2B-C3B-CAB-CBB
22	3	611	CLA	C2B-C3B-CAB-CBB
22	3	617	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	7	601	CLA	C2B-C3B-CAB-CBB
22	7	614	CLA	C2B-C3B-CAB-CBB
22	7	616	CLA	C2B-C3B-CAB-CBB
22	8	608	CLA	C2B-C3B-CAB-CBB
22	8	611	CLA	C2B-C3B-CAB-CBB
22	8	614	CLA	C2B-C3B-CAB-CBB
22	8	616	CLA	C2B-C3B-CAB-CBB
22	Z	611	CLA	C2B-C3B-CAB-CBB
22	Z	614	CLA	C2B-C3B-CAB-CBB
22	4	610	CLA	C2B-C3B-CAB-CBB
22	4	611	CLA	C2B-C3B-CAB-CBB
22	4	614	CLA	C2B-C3B-CAB-CBB
22	4	616	CLA	C2B-C3B-CAB-CBB
22	5	611	CLA	C2B-C3B-CAB-CBB
22	5	614	CLA	C2B-C3B-CAB-CBB
22	5	617	CLA	C2B-C3B-CAB-CBB
22	5	621	CLA	C2B-C3B-CAB-CBB
22	6	603	CLA	C2B-C3B-CAB-CBB
22	6	609	CLA	C2B-C3B-CAB-CBB
22	6	622	CLA	C2B-C3B-CAB-CBB
22	2	601	CLA	C2B-C3B-CAB-CBB
22	2	603	CLA	C2B-C3B-CAB-CBB
22	2	606	CLA	C2B-C3B-CAB-CBB
22	2	607	CLA	C2B-C3B-CAB-CBB
22	2	609	CLA	C2B-C3B-CAB-CBB
22	2	611	CLA	C2B-C3B-CAB-CBB
22	2	612	CLA	C2B-C3B-CAB-CBB
22	2	614	CLA	C2B-C3B-CAB-CBB
22	9	611	CLA	C2B-C3B-CAB-CBB
22	9	614	CLA	C2B-C3B-CAB-CBB
29	7	607	CHL	C2B-C3B-CAB-CBB
29	Z	601	CHL	C2B-C3B-CAB-CBB
29	Z	607	CHL	C2B-C3B-CAB-CBB
29	4	618	CHL	C2B-C3B-CAB-CBB
29	5	618	CHL	C2B-C3B-CAB-CBB
29	6	618	CHL	C2B-C3B-CAB-CBB
27	B	850	DGD	CAB-CBB-CCB-CDB
22	B	807	CLA	C2-C3-C5-C6
22	F	304	CLA	C15-C16-C17-C18
22	7	613	CLA	C13-C15-C16-C17
22	B	816	CLA	C6-C7-C8-C9
24	A	847	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
24	A	846	LHG	C14-C15-C16-C17
22	A	823	CLA	C1-C2-C3-C4
22	B	831	CLA	C1-C2-C3-C4
22	Z	608	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	C2A-CAA-CBA-CGA
29	Z	601	CHL	C2A-CAA-CBA-CGA
22	4	601	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	C2-C1-O2A-CGA
22	A	831	CLA	C2-C1-O2A-CGA
22	A	834	CLA	C2-C1-O2A-CGA
22	A	854	CLA	C2-C1-O2A-CGA
22	1	604	CLA	C2-C1-O2A-CGA
22	1	609	CLA	C2-C1-O2A-CGA
22	8	612	CLA	C2-C1-O2A-CGA
22	5	609	CLA	C2-C1-O2A-CGA
29	3	608	CHL	C2-C1-O2A-CGA
29	6	607	CHL	C2-C1-O2A-CGA
22	3	609	CLA	CAA-CBA-CGA-O2A
22	Z	609	CLA	C3-C5-C6-C7
22	K	4003	CLA	O1A-CGA-O2A-C1
22	A	831	CLA	CBA-CGA-O2A-C1
24	8	620	LHG	O6-C4-C5-O7
22	B	807	CLA	C5-C6-C7-C8
25	A	849	BCR	C1-C6-C7-C8
25	A	851	BCR	C23-C24-C25-C26
25	B	847	BCR	C1-C6-C7-C8
25	J	3003	BCR	C1-C6-C7-C8
30	Z	618	LUT	C5-C6-C7-C8
30	2	617	LUT	C5-C6-C7-C8
24	A	847	LHG	C10-C11-C12-C13
24	4	623	LHG	C11-C10-C9-C8
22	A	805	CLA	C6-C7-C8-C9
22	A	843	CLA	C16-C17-C18-C19
22	A	843	CLA	C8-C10-C11-C12
28	J	3001	LMG	O1-C7-C8-O7
24	A	846	LHG	C4-O6-P-O3
24	A	847	LHG	C3-O3-P-O6
24	1	620	LHG	C3-O3-P-O6
24	1	620	LHG	C4-O6-P-O3
24	7	625	LHG	C3-O3-P-O6
24	Z	620	LHG	C3-O3-P-O6
24	Z	620	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
24	4	623	LHG	C3-O3-P-O6
24	4	623	LHG	C4-O6-P-O3
24	5	623	LHG	C3-O3-P-O6
22	A	812	CLA	C10-C11-C12-C13
22	B	808	CLA	C4-C3-C5-C6
22	A	810	CLA	C12-C13-C15-C16
22	B	805	CLA	C11-C10-C8-C7
22	B	818	CLA	C6-C7-C8-C10
22	A	807	CLA	C14-C13-C15-C16
22	A	842	CLA	C11-C10-C8-C9
22	A	843	CLA	C6-C7-C8-C9
22	1	614	CLA	C14-C13-C15-C16
25	B	846	BCR	C19-C20-C21-C22
30	8	618	LUT	C29-C30-C31-C32
30	Z	617	LUT	C7-C8-C9-C19
30	Z	619	LUT	C27-C28-C29-C39
22	Z	608	CLA	CBA-CGA-O2A-C1
29	6	606	CHL	CBA-CGA-O2A-C1
22	9	611	CLA	C5-C6-C7-C8
24	4	622	LHG	C12-C13-C14-C15
22	A	826	CLA	C15-C16-C17-C18
22	A	822	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	CBA-CGA-O2A-C1
24	4	622	LHG	C11-C12-C13-C14
22	A	831	CLA	C4B-C3B-CAB-CBB
22	B	821	CLA	C4B-C3B-CAB-CBB
22	B	825	CLA	C4B-C3B-CAB-CBB
22	B	839	CLA	C4B-C3B-CAB-CBB
22	B	840	CLA	C4B-C3B-CAB-CBB
22	A	813	CLA	C2A-CAA-CBA-CGA
22	7	610	CLA	C2A-CAA-CBA-CGA
25	4	621	BCR	C9-C10-C11-C12
25	5	622	BCR	C13-C14-C15-C16
25	6	625	BCR	C13-C14-C15-C16
30	5	624	LUT	C29-C30-C31-C32
30	6	624	LUT	C29-C30-C31-C32
24	8	620	LHG	O6-C4-C5-C6
22	A	822	CLA	O1D-CGD-O2D-CED
24	A	846	LHG	O6-C4-C5-O7
24	A	847	LHG	O6-C4-C5-O7
22	4	610	CLA	O1A-CGA-O2A-C1
22	B	837	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	7	613	CLA	C2-C3-C5-C6
22	A	828	CLA	C5-C6-C7-C8
22	6	611	CLA	C5-C6-C7-C8
24	4	623	LHG	O2-C2-C3-O3
22	A	813	CLA	C6-C7-C8-C9
22	B	834	CLA	CBD-CGD-O2D-CED
21	A	801	CL0	C2-C1-O2A-CGA
22	A	805	CLA	C2-C1-O2A-CGA
22	A	822	CLA	C2-C1-O2A-CGA
22	A	830	CLA	C2-C1-O2A-CGA
22	A	842	CLA	C2-C1-O2A-CGA
22	B	827	CLA	C2-C1-O2A-CGA
22	B	833	CLA	C2-C1-O2A-CGA
22	1	612	CLA	C2-C1-O2A-CGA
22	Z	604	CLA	C2-C1-O2A-CGA
22	Z	611	CLA	C2-C1-O2A-CGA
29	8	607	CHL	C2-C1-O2A-CGA
24	Z	620	LHG	C28-C29-C30-C31
29	6	606	CHL	O1A-CGA-O2A-C1
22	A	843	CLA	C2A-CAA-CBA-CGA
22	B	807	CLA	C2A-CAA-CBA-CGA
22	3	613	CLA	C2A-CAA-CBA-CGA
22	Z	604	CLA	C2A-CAA-CBA-CGA
22	2	603	CLA	C2A-CAA-CBA-CGA
22	9	613	CLA	C2A-CAA-CBA-CGA
24	6	619	LHG	O7-C5-C6-O8
22	4	613	CLA	C3A-C2A-CAA-CBA
29	6	606	CHL	C3A-C2A-CAA-CBA
24	6	619	LHG	C11-C12-C13-C14
22	B	827	CLA	C2-C3-C5-C6
22	B	828	CLA	C2-C3-C5-C6
22	A	804	CLA	C6-C7-C8-C9
22	A	826	CLA	C6-C7-C8-C9
22	B	808	CLA	C14-C13-C15-C16
22	B	809	CLA	C6-C7-C8-C9
22	8	610	CLA	C11-C10-C8-C9
22	4	601	CLA	C11-C12-C13-C14
29	3	608	CHL	C6-C7-C8-C9
22	A	820	CLA	C16-C17-C18-C19
22	A	843	CLA	C10-C11-C12-C13
24	A	855	LHG	C4-C5-C6-O8
25	A	852	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
25	A	852	BCR	C16-C17-C18-C36
25	B	845	BCR	C11-C10-C9-C34
25	B	845	BCR	C20-C21-C22-C37
25	F	305	BCR	C35-C13-C14-C15
25	L	201	BCR	C11-C10-C9-C34
22	3	604	CLA	C2A-CAA-CBA-CGA
22	2	609	CLA	C2A-CAA-CBA-CGA
22	F	301	CLA	C8-C10-C11-C12
22	B	834	CLA	O1D-CGD-O2D-CED
22	A	826	CLA	C16-C17-C18-C19
22	B	809	CLA	C16-C17-C18-C19
22	L	203	CLA	C16-C17-C18-C19
22	A	806	CLA	O2A-C1-C2-C3
29	5	607	CHL	O2A-C1-C2-C3
25	A	852	BCR	C37-C22-C23-C24
25	B	801	BCR	C7-C8-C9-C34
25	L	201	BCR	C37-C22-C23-C24
24	4	622	LHG	C10-C11-C12-C13
22	4	610	CLA	C10-C11-C12-C13
22	A	840	CLA	C4-C3-C5-C6
22	B	810	CLA	C4-C3-C5-C6
22	L	203	CLA	C4-C3-C5-C6
22	A	808	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	L	204	CLA	C1A-C2A-CAA-CBA
22	3	604	CLA	C1A-C2A-CAA-CBA
22	7	608	CLA	C1A-C2A-CAA-CBA
22	4	602	CLA	C1A-C2A-CAA-CBA
22	9	602	CLA	C1A-C2A-CAA-CBA
29	Z	601	CHL	C1A-C2A-CAA-CBA
29	6	606	CHL	C1A-C2A-CAA-CBA
22	A	822	CLA	C11-C12-C13-C15
22	A	831	CLA	C12-C13-C15-C16
22	B	841	CLA	C6-C7-C8-C10
22	7	601	CLA	C11-C12-C13-C15
22	8	613	CLA	C6-C7-C8-C10
22	Z	610	CLA	C6-C7-C8-C10
22	Z	611	CLA	C12-C13-C15-C16
22	A	829	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	851	LHG	C4-O6-P-O3
29	3	608	CHL	C3C-C2C-CMC-OMC
24	A	846	LHG	C12-C13-C14-C15
22	B	827	CLA	CAA-CBA-CGA-O2A
23	A	844	PQN	C20-C21-C22-C23
22	1	610	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C8-C10-C11-C12
22	B	830	CLA	CAA-CBA-CGA-O1A
22	Z	613	CLA	C8-C10-C11-C12
29	7	607	CHL	C5-C6-C7-C8
22	B	826	CLA	C3-C5-C6-C7
22	A	806	CLA	C4-C3-C5-C6
22	A	830	CLA	C4-C3-C5-C6
22	B	820	CLA	C4-C3-C5-C6
22	1	609	CLA	C4-C3-C5-C6
22	A	807	CLA	C2B-C3B-CAB-CBB
22	A	811	CLA	C2B-C3B-CAB-CBB
22	A	831	CLA	C2B-C3B-CAB-CBB
22	B	802	CLA	C2B-C3B-CAB-CBB
22	B	806	CLA	C2B-C3B-CAB-CBB
22	B	808	CLA	C2B-C3B-CAB-CBB
22	B	810	CLA	C2B-C3B-CAB-CBB
22	B	827	CLA	C2B-C3B-CAB-CBB
22	B	835	CLA	C2B-C3B-CAB-CBB
22	B	839	CLA	C2B-C3B-CAB-CBB
22	B	840	CLA	C2B-C3B-CAB-CBB
22	G	203	CLA	C2B-C3B-CAB-CBB
22	1	603	CLA	C2B-C3B-CAB-CBB
22	1	608	CLA	C2B-C3B-CAB-CBB
22	1	609	CLA	C2B-C3B-CAB-CBB
22	1	613	CLA	C2B-C3B-CAB-CBB
22	3	613	CLA	C2B-C3B-CAB-CBB
22	3	614	CLA	C2B-C3B-CAB-CBB
22	7	603	CLA	C2B-C3B-CAB-CBB
22	7	610	CLA	C2B-C3B-CAB-CBB
22	7	620	CLA	C2B-C3B-CAB-CBB
22	8	601	CLA	C2B-C3B-CAB-CBB
22	8	603	CLA	C2B-C3B-CAB-CBB
22	8	613	CLA	C2B-C3B-CAB-CBB
22	Z	603	CLA	C2B-C3B-CAB-CBB
22	Z	608	CLA	C2B-C3B-CAB-CBB
22	Z	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	Z	616	CLA	C2B-C3B-CAB-CBB
22	4	613	CLA	C2B-C3B-CAB-CBB
22	5	601	CLA	C2B-C3B-CAB-CBB
22	5	602	CLA	C2B-C3B-CAB-CBB
22	6	611	CLA	C2B-C3B-CAB-CBB
22	2	610	CLA	C2B-C3B-CAB-CBB
22	2	613	CLA	C2B-C3B-CAB-CBB
22	9	601	CLA	C2B-C3B-CAB-CBB
22	9	604	CLA	C2B-C3B-CAB-CBB
22	9	612	CLA	C2B-C3B-CAB-CBB
22	9	613	CLA	C2B-C3B-CAB-CBB
29	1	601	CHL	C2B-C3B-CAB-CBB
29	4	607	CHL	C2B-C3B-CAB-CBB
29	6	607	CHL	C2B-C3B-CAB-CBB
29	9	606	CHL	C2B-C3B-CAB-CBB
29	9	607	CHL	C2B-C3B-CAB-CBB
22	A	827	CLA	O1A-CGA-O2A-C1
22	1	616	CLA	CBD-CGD-O2D-CED
25	A	852	BCR	C11-C10-C9-C8
25	A	852	BCR	C16-C17-C18-C19
25	B	845	BCR	C11-C10-C9-C8
25	B	845	BCR	C20-C21-C22-C23
25	F	305	BCR	C12-C13-C14-C15
25	L	201	BCR	C11-C10-C9-C8
22	A	826	CLA	C8-C10-C11-C12
22	1	614	CLA	C2A-CAA-CBA-CGA
25	A	856	BCR	C15-C16-C17-C18
25	K	4001	BCR	C15-C16-C17-C18
22	7	616	CLA	O1A-CGA-O2A-C1
24	5	623	LHG	C1-C2-C3-O3
29	7	607	CHL	O1D-CGD-O2D-CED
22	A	813	CLA	C4-C3-C5-C6
22	B	822	CLA	C4-C3-C5-C6
22	F	301	CLA	C4-C3-C5-C6
22	7	604	CLA	C2-C1-O2A-CGA
22	Z	606	CLA	C2-C1-O2A-CGA
22	Z	609	CLA	C2-C1-O2A-CGA
22	5	606	CLA	C2-C1-O2A-CGA
22	9	613	CLA	C2-C1-O2A-CGA
29	4	607	CHL	C2-C1-O2A-CGA
22	B	814	CLA	O1D-CGD-O2D-CED
22	2	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	810	CLA	C2-C3-C5-C6
22	L	203	CLA	C2-C3-C5-C6
22	B	802	CLA	C8-C10-C11-C12
21	A	801	CL0	CAA-CBA-CGA-O2A
22	A	807	CLA	C11-C10-C8-C9
22	A	840	CLA	C11-C12-C13-C14
22	A	813	CLA	O1A-CGA-O2A-C1
22	A	841	CLA	C2A-CAA-CBA-CGA
22	Z	610	CLA	C2A-CAA-CBA-CGA
22	A	805	CLA	C6-C7-C8-C10
22	3	610	CLA	CBA-CGA-O2A-C1
22	Z	610	CLA	O1A-CGA-O2A-C1
25	A	849	BCR	C5-C6-C7-C8
25	A	849	BCR	C23-C24-C25-C30
25	B	843	BCR	C1-C6-C7-C8
25	B	844	BCR	C23-C24-C25-C30
25	K	4001	BCR	C23-C24-C25-C30
30	1	618	LUT	C1-C6-C7-C8
30	7	622	LUT	C1-C6-C7-C8
30	8	618	LUT	C1-C6-C7-C8
30	Z	618	LUT	C1-C6-C7-C8
22	A	829	CLA	CAA-CBA-CGA-O2A
24	B	851	LHG	C4-C5-C6-O8
25	3	717	BCR	C15-C16-C17-C18
22	B	802	CLA	C4-C3-C5-C6
22	B	814	CLA	C4-C3-C5-C6
22	7	613	CLA	C4-C3-C5-C6
23	A	844	PQN	C14-C13-C15-C16
25	B	847	BCR	C7-C8-C9-C10
22	Z	614	CLA	C10-C11-C12-C13
22	A	806	CLA	C2-C3-C5-C6
22	A	820	CLA	C2-C3-C5-C6
22	B	808	CLA	C2-C3-C5-C6
22	3	614	CLA	CAA-CBA-CGA-O2A
22	Z	611	CLA	C2A-CAA-CBA-CGA
23	A	844	PQN	C18-C20-C21-C22
27	B	850	DGD	CEA-CFA-CGA-CHA
22	2	609	CLA	CAA-CBA-CGA-O2A
24	6	619	LHG	C10-C11-C12-C13
29	6	607	CHL	C3-C5-C6-C7
22	3	614	CLA	CAA-CBA-CGA-O1A
22	4	616	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	8	613	CLA	C13-C15-C16-C17
22	5	602	CLA	C8-C10-C11-C12
28	J	3001	LMG	C10-C11-C12-C13
22	B	817	CLA	C4-C3-C5-C6
22	8	613	CLA	C4-C3-C5-C6
22	A	807	CLA	C11-C10-C8-C7
22	A	812	CLA	C12-C13-C15-C16
22	A	828	CLA	C2-C3-C5-C6
22	A	828	CLA	C12-C13-C15-C16
22	B	827	CLA	C11-C10-C8-C7
22	4	613	CLA	C6-C7-C8-C10
29	3	608	CHL	CBA-CGA-O2A-C1
22	B	819	CLA	C10-C11-C12-C13
25	6	623	BCR	C13-C14-C15-C16
30	4	620	LUT	C9-C10-C11-C12
22	1	616	CLA	CAA-CBA-CGA-O2A
22	4	613	CLA	CAA-CBA-CGA-O2A
24	1	620	LHG	O7-C7-C8-C9
24	4	622	LHG	O7-C7-C8-C9
22	1	606	CLA	O1A-CGA-O2A-C1
22	A	809	CLA	C4-C3-C5-C6
22	B	809	CLA	C4-C3-C5-C6
22	A	840	CLA	C2-C3-C5-C6
22	F	301	CLA	C2-C3-C5-C6
22	7	612	CLA	C2-C3-C5-C6
22	7	613	CLA	CBD-CGD-O2D-CED
24	A	846	LHG	C16-C17-C18-C19
22	B	807	CLA	CAA-CBA-CGA-O2A
22	B	824	CLA	CAA-CBA-CGA-O2A
22	3	612	CLA	CAA-CBA-CGA-O2A
22	Z	612	CLA	CAA-CBA-CGA-O2A
24	4	622	LHG	C14-C15-C16-C17
22	A	812	CLA	C11-C10-C8-C9
22	A	826	CLA	C14-C13-C15-C16
22	A	828	CLA	C11-C10-C8-C9
22	A	833	CLA	C11-C10-C8-C9
22	B	819	CLA	C14-C13-C15-C16
22	B	827	CLA	C6-C7-C8-C9
22	3	604	CLA	C11-C12-C13-C14
22	8	601	CLA	C11-C12-C13-C14
22	Z	611	CLA	C14-C13-C15-C16
22	A	854	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	834	CLA	C3A-C2A-CAA-CBA
22	2	603	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	C3A-C2A-CAA-CBA
29	8	607	CHL	C3A-C2A-CAA-CBA
24	5	623	LHG	O2-C2-C3-O3
24	Z	620	LHG	C24-C25-C26-C27
22	K	4002	CLA	CAA-CBA-CGA-O2A
22	A	821	CLA	CAD-CBD-CGD-O2D
22	A	838	CLA	CAD-CBD-CGD-O2D
22	B	803	CLA	CAD-CBD-CGD-O2D
22	B	805	CLA	CAD-CBD-CGD-O2D
22	B	814	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	824	CLA	CAD-CBD-CGD-O2D
22	B	830	CLA	CAD-CBD-CGD-O2D
22	B	836	CLA	CAD-CBD-CGD-O2D
22	B	838	CLA	CAD-CBD-CGD-O2D
22	K	4002	CLA	CAD-CBD-CGD-O2D
22	1	603	CLA	CAD-CBD-CGD-O2D
22	1	604	CLA	CAD-CBD-CGD-O2D
22	1	608	CLA	CAD-CBD-CGD-O2D
22	3	609	CLA	CAD-CBD-CGD-O2D
22	3	610	CLA	CAD-CBD-CGD-O2D
22	7	612	CLA	CAD-CBD-CGD-O2D
22	7	614	CLA	CAD-CBD-CGD-O2D
22	Z	603	CLA	CAD-CBD-CGD-O2D
22	Z	604	CLA	CAD-CBD-CGD-O2D
22	5	603	CLA	CAD-CBD-CGD-O2D
22	5	610	CLA	CAD-CBD-CGD-O2D
22	9	611	CLA	CAD-CBD-CGD-O2D
22	9	612	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	C2A-CAA-CBA-CGA
22	4	610	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C4C-C3C-CAC-CBC
22	B	813	CLA	CAA-CBA-CGA-O2A
22	7	616	CLA	CAA-CBA-CGA-O2A
21	A	801	CL0	O1A-CGA-O2A-C1
22	A	803	CLA	C4-C3-C5-C6
22	A	807	CLA	C4-C3-C5-C6
22	A	811	CLA	C4-C3-C5-C6
22	B	836	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	805	CLA	C13-C15-C16-C17
22	A	807	CLA	C2-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	B	814	CLA	C2-C3-C5-C6
22	B	820	CLA	C2-C3-C5-C6
22	1	609	CLA	C2-C3-C5-C6
23	A	844	PQN	C12-C13-C15-C16
22	B	838	CLA	CAA-CBA-CGA-O2A
22	1	612	CLA	CAA-CBA-CGA-O2A
22	1	613	CLA	CAA-CBA-CGA-O2A
22	6	613	CLA	CAA-CBA-CGA-O2A
22	9	604	CLA	CAA-CBA-CGA-O2A
29	3	608	CHL	CAA-CBA-CGA-O2A
29	8	607	CHL	CAA-CBA-CGA-O2A
22	2	610	CLA	O1A-CGA-O2A-C1
25	A	852	BCR	C7-C8-C9-C10
25	B	801	BCR	C7-C8-C9-C10
25	B	847	BCR	C21-C22-C23-C24
30	7	621	LUT	C11-C12-C13-C14
24	4	622	LHG	C4-C5-C6-O8
22	1	606	CLA	CBA-CGA-O2A-C1
22	A	802	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	CAA-CBA-CGA-O2A
22	7	613	CLA	CAA-CBA-CGA-O2A
24	A	855	LHG	O8-C23-C24-C25
24	A	846	LHG	C25-C26-C27-C28
29	5	608	CHL	O2A-C1-C2-C3
22	A	806	CLA	CAA-CBA-CGA-O2A
22	B	817	CLA	CAA-CBA-CGA-O1A
22	A	837	CLA	CAA-CBA-CGA-O1A
22	A	837	CLA	CAA-CBA-CGA-O2A
22	6	622	CLA	CAA-CBA-CGA-O2A
22	1	610	CLA	CBD-CGD-O2D-CED
22	A	814	CLA	CHA-CBD-CGD-O2D
22	A	815	CLA	CHA-CBD-CGD-O2D
22	A	816	CLA	CHA-CBD-CGD-O1D
22	A	820	CLA	CHA-CBD-CGD-O2D
22	A	822	CLA	CHA-CBD-CGD-O1D
22	A	822	CLA	CHA-CBD-CGD-O2D
22	A	823	CLA	CHA-CBD-CGD-O2D
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	829	CLA	CHA-CBD-CGD-O2D
22	B	804	CLA	CHA-CBD-CGD-O1D
22	B	813	CLA	CHA-CBD-CGD-O1D
22	B	815	CLA	CHA-CBD-CGD-O1D
22	B	821	CLA	CHA-CBD-CGD-O1D
22	G	204	CLA	CHA-CBD-CGD-O2D
22	1	602	CLA	CHA-CBD-CGD-O2D
22	3	602	CLA	CHA-CBD-CGD-O1D
22	3	602	CLA	CHA-CBD-CGD-O2D
22	7	602	CLA	CHA-CBD-CGD-O1D
22	7	613	CLA	CHA-CBD-CGD-O2D
22	7	620	CLA	CHA-CBD-CGD-O1D
22	7	620	CLA	CHA-CBD-CGD-O2D
22	8	606	CLA	CHA-CBD-CGD-O1D
22	8	606	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	CHA-CBD-CGD-O2D
22	4	604	CLA	CHA-CBD-CGD-O1D
22	4	604	CLA	CHA-CBD-CGD-O2D
22	5	616	CLA	CHA-CBD-CGD-O1D
22	5	616	CLA	CHA-CBD-CGD-O2D
22	6	603	CLA	CHA-CBD-CGD-O2D
22	2	601	CLA	CHA-CBD-CGD-O2D
22	3	620	CLA	CAA-CBA-CGA-O2A
22	9	601	CLA	CAA-CBA-CGA-O2A
22	B	817	CLA	C2-C3-C5-C6
24	5	623	LHG	O6-C4-C5-C6
22	8	603	CLA	CAA-CBA-CGA-O2A
24	4	622	LHG	C11-C10-C9-C8
24	6	619	LHG	C13-C14-C15-C16
22	Z	604	CLA	C5-C6-C7-C8
22	A	843	CLA	CAA-CBA-CGA-O2A
22	B	809	CLA	CAA-CBA-CGA-O2A
22	B	812	CLA	CAA-CBA-CGA-O2A
22	8	613	CLA	CAA-CBA-CGA-O2A
22	4	601	CLA	CAA-CBA-CGA-O2A
29	1	607	CHL	CAA-CBA-CGA-O2A
28	9	620	LMG	C23-C24-C25-C26
22	A	813	CLA	CAA-CBA-CGA-O2A
22	A	828	CLA	CAA-CBA-CGA-O2A
22	1	603	CLA	CAA-CBA-CGA-O2A
22	8	616	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	5	606	CLA	CAA-CBA-CGA-O2A
22	6	601	CLA	CAA-CBA-CGA-O2A
22	9	613	CLA	CAA-CBA-CGA-O2A
22	A	823	CLA	C2A-CAA-CBA-CGA
22	6	617	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	C4C-C3C-CAC-CBC
22	2	610	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	CAA-CBA-CGA-O2A
22	5	613	CLA	CAA-CBA-CGA-O2A
22	3	610	CLA	CBD-CGD-O2D-CED
22	K	4002	CLA	CAA-CBA-CGA-O1A
22	5	613	CLA	O1D-CGD-O2D-CED
22	5	601	CLA	C13-C15-C16-C17
22	A	811	CLA	C2-C3-C5-C6
22	B	805	CLA	C6-C7-C8-C10
22	B	812	CLA	C11-C12-C13-C15
22	F	304	CLA	C12-C13-C15-C16
22	Z	609	CLA	C11-C10-C8-C7
22	6	601	CLA	C6-C7-C8-C10
22	8	610	CLA	C11-C12-C13-C14
22	B	816	CLA	CAA-CBA-CGA-O2A
22	8	609	CLA	CAA-CBA-CGA-O2A
22	Z	613	CLA	CAA-CBA-CGA-O2A
22	2	607	CLA	CAA-CBA-CGA-O2A
22	A	810	CLA	C14-C13-C15-C16
22	3	610	CLA	C6-C7-C8-C9
22	B	807	CLA	CAA-CBA-CGA-O1A
24	1	620	LHG	O9-C7-C8-C9
25	B	843	BCR	C13-C14-C15-C16
25	5	625	BCR	C9-C10-C11-C12
30	7	622	LUT	C29-C30-C31-C32
22	8	601	CLA	C10-C11-C12-C13
22	F	304	CLA	C2B-C3B-CAB-CBB
22	A	813	CLA	CBA-CGA-O2A-C1
22	A	823	CLA	CAA-CBA-CGA-O2A
22	7	616	CLA	CAA-CBA-CGA-O1A
29	6	607	CHL	C2A-CAA-CBA-CGA
22	7	613	CLA	CAA-CBA-CGA-O1A
22	Z	616	CLA	CAA-CBA-CGA-O2A
24	8	620	LHG	O7-C7-C8-C9
22	4	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	8	607	CHL	CAA-CBA-CGA-O1A
22	A	820	CLA	C16-C17-C18-C20
22	3	603	CLA	C2-C3-C5-C6
22	8	613	CLA	C2-C3-C5-C6
25	L	201	BCR	C21-C22-C23-C24
30	Z	619	LUT	C27-C28-C29-C30
22	A	828	CLA	CBA-CGA-O2A-C1
22	Z	603	CLA	CBA-CGA-O2A-C1
24	A	846	LHG	C29-C30-C31-C32
22	A	817	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C1A-C2A-CAA-CBA
22	A	854	CLA	C1A-C2A-CAA-CBA
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	834	CLA	C1A-C2A-CAA-CBA
22	5	604	CLA	C1A-C2A-CAA-CBA
22	6	609	CLA	C1A-C2A-CAA-CBA
22	2	603	CLA	C1A-C2A-CAA-CBA
22	9	614	CLA	C1A-C2A-CAA-CBA
29	4	606	CHL	C1A-C2A-CAA-CBA
29	4	608	CHL	C1A-C2A-CAA-CBA
22	A	802	CLA	CAA-CBA-CGA-O1A
22	3	612	CLA	CAA-CBA-CGA-O1A
22	3	613	CLA	CAA-CBA-CGA-O1A
22	A	823	CLA	C2-C1-O2A-CGA
22	B	814	CLA	C2-C1-O2A-CGA
22	1	602	CLA	C2-C1-O2A-CGA
22	Z	608	CLA	C10-C11-C12-C13
22	B	813	CLA	CAA-CBA-CGA-O1A
22	B	824	CLA	CAA-CBA-CGA-O1A
22	Z	616	CLA	CAA-CBA-CGA-O1A
22	2	601	CLA	CAA-CBA-CGA-O1A
24	1	620	LHG	C4-C5-C6-O8
22	B	805	CLA	CAA-CBA-CGA-O2A
24	Z	620	LHG	C13-C14-C15-C16
22	A	842	CLA	C2A-CAA-CBA-CGA
22	3	610	CLA	C2A-CAA-CBA-CGA
29	5	607	CHL	C2A-CAA-CBA-CGA
22	A	845	CLA	C2C-C3C-CAC-CBC
29	6	607	CHL	C2C-C3C-CAC-CBC
22	A	812	CLA	C16-C17-C18-C19
22	1	613	CLA	CAA-CBA-CGA-O1A
22	9	601	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	4	622	LHG	O9-C7-C8-C9
22	A	842	CLA	C13-C15-C16-C17
24	4	622	LHG	C32-C33-C34-C35
22	B	804	CLA	CAA-CBA-CGA-O2A
22	8	603	CLA	CAA-CBA-CGA-O1A
24	Z	620	LHG	O7-C7-C8-C9
22	B	809	CLA	CAA-CBA-CGA-O1A
22	B	838	CLA	CAA-CBA-CGA-O1A
22	Z	612	CLA	CAA-CBA-CGA-O1A
22	Z	613	CLA	CAA-CBA-CGA-O1A
22	9	604	CLA	CAA-CBA-CGA-O1A
22	9	613	CLA	CAA-CBA-CGA-O1A
24	8	620	LHG	O9-C7-C8-C9
29	3	608	CHL	O1A-CGA-O2A-C1
22	6	622	CLA	CAA-CBA-CGA-O1A
22	A	810	CLA	C4B-C3B-CAB-CBB
22	A	838	CLA	C4B-C3B-CAB-CBB
22	B	820	CLA	C4B-C3B-CAB-CBB
22	B	837	CLA	C4B-C3B-CAB-CBB
22	F	304	CLA	C4B-C3B-CAB-CBB
22	G	204	CLA	C4B-C3B-CAB-CBB
22	J	3002	CLA	C4B-C3B-CAB-CBB
22	1	611	CLA	C4B-C3B-CAB-CBB
22	3	612	CLA	C4B-C3B-CAB-CBB
22	3	613	CLA	C4B-C3B-CAB-CBB
22	7	610	CLA	C4B-C3B-CAB-CBB
22	Z	612	CLA	C4B-C3B-CAB-CBB
22	4	603	CLA	C4B-C3B-CAB-CBB
22	5	612	CLA	C4B-C3B-CAB-CBB
22	5	616	CLA	C4B-C3B-CAB-CBB
24	A	855	LHG	C3-O3-P-O4
24	Z	620	LHG	C3-O3-P-O5
24	4	623	LHG	C4-O6-P-O5
24	1	620	LHG	O7-C5-C6-O8
22	A	806	CLA	CAA-CBA-CGA-O1A
22	A	843	CLA	CAA-CBA-CGA-O1A
22	1	603	CLA	CAA-CBA-CGA-O1A
22	1	612	CLA	CAA-CBA-CGA-O1A
22	1	616	CLA	CAA-CBA-CGA-O1A
22	3	620	CLA	CAA-CBA-CGA-O1A
24	A	855	LHG	O10-C23-C24-C25
22	Z	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	843	BCR	C5-C6-C7-C8
25	B	848	BCR	C23-C24-C25-C30
30	1	618	LUT	C5-C6-C7-C8
30	7	622	LUT	C5-C6-C7-C8
22	Z	611	CLA	C8-C10-C11-C12
22	6	613	CLA	CAA-CBA-CGA-O1A
28	J	3001	LMG	O10-C28-C29-C30
22	7	610	CLA	O1A-CGA-O2A-C1
29	4	608	CHL	CAA-CBA-CGA-O2A
22	F	301	CLA	C16-C17-C18-C20
29	1	607	CHL	CAA-CBA-CGA-O1A
22	A	826	CLA	CAA-CBA-CGA-O2A
22	Z	603	CLA	CAA-CBA-CGA-O2A
22	B	839	CLA	C13-C15-C16-C17
22	B	806	CLA	CAA-CBA-CGA-O1A
22	8	613	CLA	CAA-CBA-CGA-O1A
29	3	608	CHL	CAA-CBA-CGA-O1A
22	A	838	CLA	CAD-CBD-CGD-O1D
22	B	813	CLA	CAD-CBD-CGD-O1D
22	B	826	CLA	CAD-CBD-CGD-O1D
22	6	622	CLA	CAD-CBD-CGD-O1D
22	2	614	CLA	CAD-CBD-CGD-O1D
22	A	828	CLA	O1A-CGA-O2A-C1
29	9	607	CHL	O1A-CGA-O2A-C1
22	A	828	CLA	CAA-CBA-CGA-O1A
22	4	601	CLA	CAA-CBA-CGA-O1A
22	2	607	CLA	CAA-CBA-CGA-O1A
22	5	610	CLA	C5-C6-C7-C8
22	A	810	CLA	C6-C7-C8-C9
22	B	813	CLA	C14-C13-C15-C16
22	F	304	CLA	C14-C13-C15-C16
22	1	611	CLA	C14-C13-C15-C16
22	Z	608	CLA	C14-C13-C15-C16
22	6	601	CLA	C6-C7-C8-C9
23	A	844	PQN	C21-C22-C23-C24
22	A	829	CLA	C10-C11-C12-C13
22	A	841	CLA	CAA-CBA-CGA-O2A
22	B	828	CLA	CAA-CBA-CGA-O2A
22	4	609	CLA	CAA-CBA-CGA-O2A
22	6	617	CLA	CAA-CBA-CGA-O2A
24	A	847	LHG	O7-C7-C8-C9
24	B	851	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	9	607	CHL	CAA-CBA-CGA-O2A
22	A	835	CLA	C5-C6-C7-C8
22	B	816	CLA	CAA-CBA-CGA-O1A
22	7	613	CLA	O1D-CGD-O2D-CED
22	B	831	CLA	CAA-CBA-CGA-O2A
22	7	609	CLA	CAA-CBA-CGA-O2A
22	A	820	CLA	C3-C5-C6-C7
22	A	828	CLA	C4-C3-C5-C6
22	4	610	CLA	C4-C3-C5-C6
22	A	809	CLA	C6-C7-C8-C10
22	B	806	CLA	C11-C10-C8-C7
22	B	807	CLA	C11-C10-C8-C7
22	B	812	CLA	C6-C7-C8-C10
22	B	814	CLA	C6-C7-C8-C10
22	1	611	CLA	C12-C13-C15-C16
22	3	607	CLA	C3A-C2A-CAA-CBA
22	3	607	CLA	C11-C10-C8-C7
22	3	610	CLA	C6-C7-C8-C10
22	Z	608	CLA	C12-C13-C15-C16
29	6	607	CHL	C3A-C2A-CAA-CBA
22	A	813	CLA	CAA-CBA-CGA-O1A
22	8	616	CLA	CAA-CBA-CGA-O1A
22	A	810	CLA	CAA-CBA-CGA-O2A
22	3	617	CLA	CAA-CBA-CGA-O2A
22	5	616	CLA	CAA-CBA-CGA-O2A
22	9	611	CLA	CAA-CBA-CGA-O2A
24	A	846	LHG	O8-C23-C24-C25
22	1	610	CLA	C8-C10-C11-C12
25	K	4004	BCR	C21-C22-C23-C24
30	3	621	LUT	C11-C12-C13-C14
30	8	618	LUT	C7-C8-C9-C10
30	Z	617	LUT	C7-C8-C9-C10
30	Z	618	LUT	C7-C8-C9-C10
30	2	617	LUT	C11-C12-C13-C14
22	B	811	CLA	CAA-CBA-CGA-O1A
22	7	609	CLA	CAA-CBA-CGA-O1A
22	4	609	CLA	CAA-CBA-CGA-O1A
22	5	606	CLA	CAA-CBA-CGA-O1A
22	5	613	CLA	CAA-CBA-CGA-O1A
22	6	601	CLA	CAA-CBA-CGA-O1A
28	J	3001	LMG	O8-C28-C29-C30
22	B	817	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	820	CLA	C8-C10-C11-C12
22	4	602	CLA	C5-C6-C7-C8
22	5	601	CLA	C10-C11-C12-C13
22	Z	603	CLA	CAA-CBA-CGA-O1A
24	B	851	LHG	O9-C7-C8-C9
24	Z	620	LHG	O9-C7-C8-C9
29	9	607	CHL	CBA-CGA-O2A-C1
22	B	806	CLA	C5-C6-C7-C8
22	1	613	CLA	C13-C15-C16-C17
22	A	811	CLA	CAA-CBA-CGA-O2A
22	K	4003	CLA	CAA-CBA-CGA-O2A
22	2	612	CLA	CAA-CBA-CGA-O2A
22	9	603	CLA	CAA-CBA-CGA-O2A
22	A	823	CLA	CAA-CBA-CGA-O1A
22	A	854	CLA	C8-C10-C11-C12
22	6	617	CLA	CAA-CBA-CGA-O1A
22	3	603	CLA	C4-C3-C5-C6
22	A	804	CLA	CAA-CBA-CGA-O2A
22	F	301	CLA	C13-C15-C16-C17

There are no ring outliers.

264 monomers are involved in 801 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	836	CLA	2	0
22	3	617	CLA	3	0
22	1	602	CLA	8	0
30	9	616	LUT	4	0
22	B	839	CLA	4	0
22	A	808	CLA	2	0
22	1	606	CLA	2	0
22	4	602	CLA	1	0
22	9	610	CLA	1	0
22	B	802	CLA	2	0
22	B	806	CLA	2	0
22	9	602	CLA	2	0
22	5	617	CLA	4	0
22	7	609	CLA	3	0
22	1	616	CLA	1	0
22	3	610	CLA	3	0
22	B	824	CLA	1	0
29	3	608	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	602	CLA	2	0
22	7	616	CLA	1	0
22	5	614	CLA	3	0
22	A	814	CLA	1	0
22	A	840	CLA	2	0
22	5	612	CLA	2	0
22	2	610	CLA	2	0
22	4	601	CLA	6	0
22	B	809	CLA	1	0
22	Z	609	CLA	1	0
22	8	604	CLA	1	0
22	B	803	CLA	4	0
22	8	606	CLA	2	0
25	A	848	BCR	5	0
22	A	822	CLA	1	0
22	Z	602	CLA	3	0
30	1	618	LUT	5	0
30	Z	617	LUT	5	0
22	5	606	CLA	2	0
22	6	622	CLA	10	0
29	4	618	CHL	7	0
22	A	804	CLA	2	0
22	9	609	CLA	10	0
22	B	822	CLA	1	0
22	B	841	CLA	12	0
24	A	847	LHG	3	0
25	B	844	BCR	2	0
22	A	843	CLA	6	0
22	B	811	CLA	3	0
22	F	301	CLA	1	0
22	3	609	CLA	1	0
22	A	842	CLA	10	0
22	3	613	CLA	1	0
22	B	831	CLA	5	0
25	L	205	BCR	2	0
22	3	607	CLA	5	0
25	3	717	BCR	3	0
22	B	825	CLA	5	0
22	B	820	CLA	15	0
22	1	613	CLA	2	0
22	5	609	CLA	6	0
24	8	620	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	610	CLA	5	0
22	6	611	CLA	2	0
25	A	852	BCR	3	0
22	2	611	CLA	2	0
22	2	612	CLA	1	0
22	A	812	CLA	12	0
22	A	817	CLA	4	0
22	1	609	CLA	2	0
22	6	609	CLA	2	0
24	1	620	LHG	2	0
22	A	831	CLA	8	0
24	Z	620	LHG	1	0
22	6	613	CLA	2	0
30	3	621	LUT	4	0
22	A	818	CLA	3	0
22	B	816	CLA	5	0
22	8	601	CLA	1	0
22	1	610	CLA	5	0
25	6	623	BCR	7	0
22	Z	610	CLA	3	0
30	4	619	LUT	12	0
30	Z	618	LUT	4	0
22	A	837	CLA	1	0
29	7	607	CHL	1	0
22	8	613	CLA	1	0
22	A	835	CLA	23	0
29	Z	601	CHL	1	0
25	A	849	BCR	5	0
22	2	602	CLA	1	0
22	7	613	CLA	3	0
22	F	304	CLA	2	0
22	3	612	CLA	2	0
25	K	4004	BCR	1	0
22	7	612	CLA	1	0
22	6	612	CLA	2	0
27	B	850	DGD	2	0
23	A	844	PQN	4	0
29	5	608	CHL	2	0
22	3	602	CLA	1	0
22	4	611	CLA	6	0
22	7	604	CLA	1	0
22	4	614	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	305	BCR	15	0
22	5	601	CLA	1	0
22	B	829	CLA	5	0
22	B	805	CLA	4	0
22	B	823	CLA	4	0
22	1	614	CLA	3	0
22	B	818	CLA	4	0
30	7	621	LUT	6	0
22	5	613	CLA	2	0
22	A	805	CLA	20	0
22	B	832	CLA	5	0
22	Z	612	CLA	1	0
22	A	836	CLA	2	0
22	A	815	CLA	20	0
22	B	812	CLA	8	0
22	B	817	CLA	4	0
22	9	612	CLA	1	0
22	A	813	CLA	2	0
22	5	604	CLA	1	0
30	Z	619	LUT	2	0
29	4	607	CHL	1	0
29	9	607	CHL	1	0
22	A	834	CLA	3	0
22	A	827	CLA	1	0
25	B	847	BCR	3	0
30	5	620	LUT	16	0
22	8	602	CLA	3	0
25	B	843	BCR	5	0
25	I	172	BCR	1	0
23	B	842	PQN	1	0
29	6	606	CHL	2	0
22	B	835	CLA	1	0
22	A	854	CLA	5	0
30	8	617	LUT	7	0
22	A	809	CLA	4	0
22	B	828	CLA	2	0
22	4	616	CLA	6	0
22	B	808	CLA	1	0
22	7	601	CLA	4	0
25	B	846	BCR	6	0
22	A	828	CLA	1	0
22	B	826	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	9	620	LMG	1	0
25	3	719	BCR	6	0
22	7	608	CLA	1	0
22	3	604	CLA	2	0
22	A	845	CLA	1	0
25	7	623	BCR	5	0
22	Z	614	CLA	2	0
22	B	821	CLA	1	0
22	A	807	CLA	8	0
25	B	848	BCR	3	0
22	1	604	CLA	1	0
22	B	838	CLA	2	0
22	B	814	CLA	5	0
22	A	825	CLA	4	0
22	2	601	CLA	4	0
22	5	602	CLA	3	0
22	8	610	CLA	5	0
24	6	619	LHG	19	0
22	A	832	CLA	5	0
22	7	611	CLA	1	0
30	4	620	LUT	5	0
22	Z	608	CLA	4	0
22	A	811	CLA	3	0
25	7	624	BCR	1	0
22	B	813	CLA	3	0
22	3	614	CLA	1	0
25	4	621	BCR	39	0
22	A	833	CLA	3	0
29	1	601	CHL	1	0
22	2	613	CLA	9	0
25	5	625	BCR	7	0
22	B	834	CLA	1	0
22	B	827	CLA	4	0
22	A	820	CLA	3	0
25	G	205	BCR	3	0
30	8	618	LUT	5	0
25	B	801	BCR	5	0
30	9	617	LUT	4	0
24	A	846	LHG	2	0
22	7	606	CLA	1	0
30	6	621	LUT	5	0
22	7	620	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Z	606	CLA	2	0
22	K	4003	CLA	3	0
22	B	819	CLA	1	0
22	3	603	CLA	4	0
29	4	608	CHL	8	0
22	A	803	CLA	1	0
22	A	830	CLA	3	0
22	4	610	CLA	9	0
30	5	624	LUT	4	0
22	A	821	CLA	1	0
22	A	819	CLA	4	0
22	A	816	CLA	7	0
25	J	3003	BCR	2	0
25	K	4001	BCR	4	0
30	3	622	LUT	3	0
22	6	614	CLA	2	0
22	B	807	CLA	2	0
22	1	611	CLA	1	0
30	2	616	LUT	3	0
22	1	608	CLA	4	0
22	4	613	CLA	2	0
22	8	609	CLA	2	0
22	6	602	CLA	1	0
22	A	839	CLA	3	0
22	A	802	CLA	28	0
22	8	612	CLA	1	0
22	A	806	CLA	4	0
22	4	604	CLA	7	0
29	5	607	CHL	3	0
25	L	201	BCR	7	0
30	7	622	LUT	2	0
21	A	801	CL0	3	0
22	1	603	CLA	3	0
29	6	618	CHL	2	0
30	2	617	LUT	3	0
30	1	619	LUT	1	0
25	6	625	BCR	3	0
22	7	610	CLA	2	0
22	9	603	CLA	1	0
22	3	606	CLA	3	0
30	6	624	LUT	3	0
22	A	829	CLA	5	0

Continued on next page...

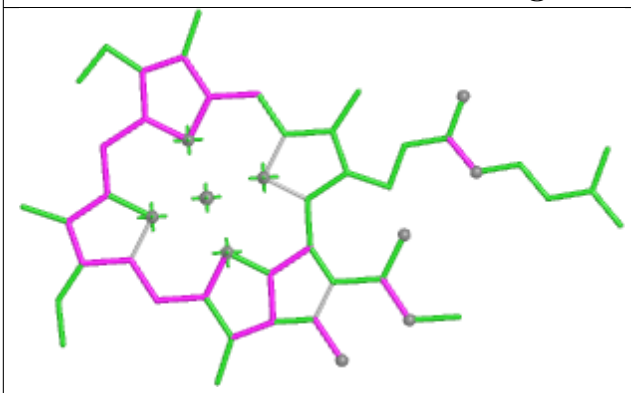
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	840	CLA	4	0
25	B	845	BCR	4	0
22	B	837	CLA	3	0
22	B	833	CLA	2	0
25	8	619	BCR	6	0
22	A	823	CLA	2	0
22	8	616	CLA	1	0
25	5	622	BCR	4	0
29	4	606	CHL	9	0
25	3	718	BCR	3	0
25	A	851	BCR	3	0
22	A	824	CLA	1	0
29	6	607	CHL	5	0
22	A	838	CLA	1	0
22	6	604	CLA	4	0
24	4	622	LHG	3	0
22	F	303	CLA	2	0
22	5	610	CLA	1	0
22	8	611	CLA	1	0
22	B	815	CLA	4	0
29	1	607	CHL	4	0
22	6	601	CLA	6	0
25	A	850	BCR	5	0
22	8	614	CLA	3	0
22	Z	613	CLA	3	0
22	Z	603	CLA	1	0
22	B	830	CLA	2	0
22	Z	611	CLA	2	0
22	4	612	CLA	2	0
22	6	616	CLA	6	0
22	5	616	CLA	1	0
30	1	617	LUT	7	0
22	A	841	CLA	12	0
22	5	621	CLA	1	0
22	Z	604	CLA	1	0
25	A	856	BCR	4	0

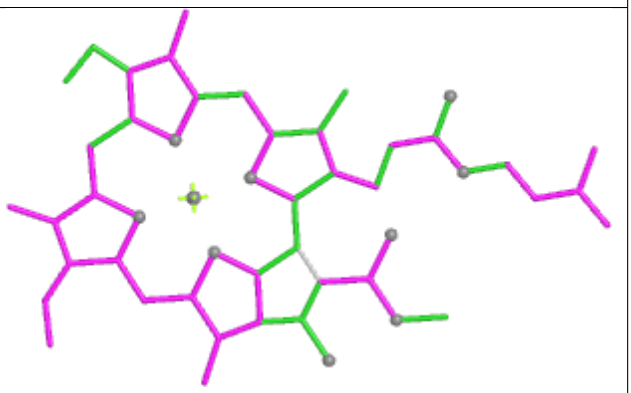
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

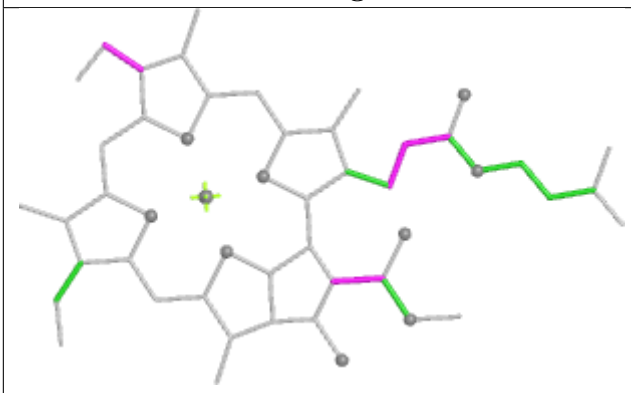
Ligand CLA 9 604



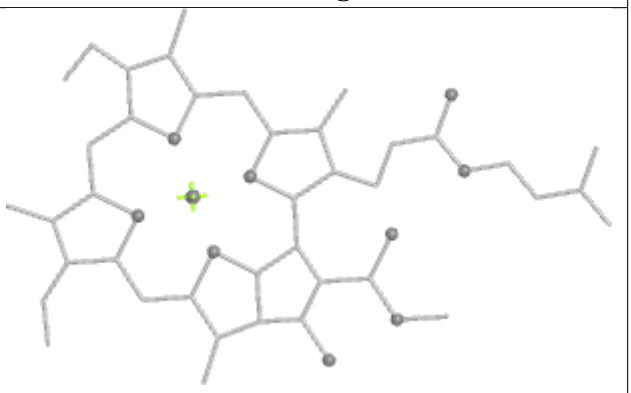
Bond lengths



Bond angles

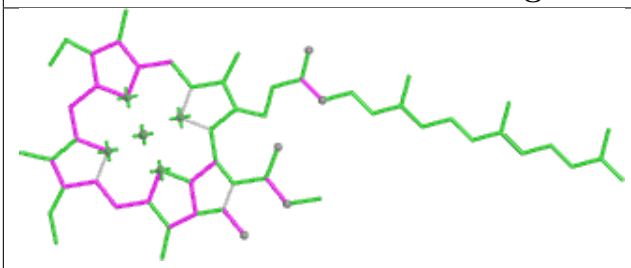


Torsions

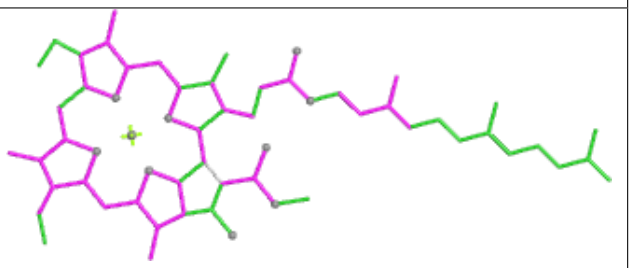


Rings

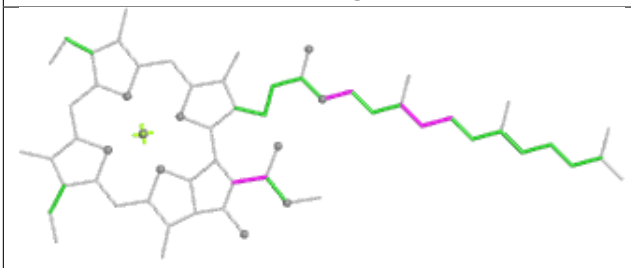
Ligand CLA B 836



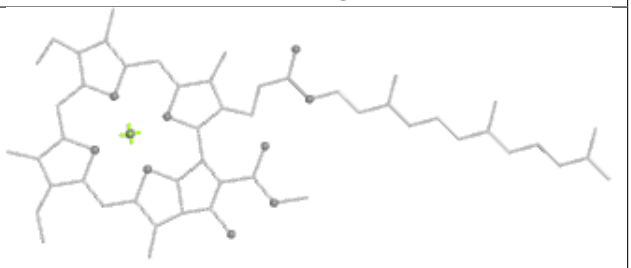
Bond lengths



Bond angles

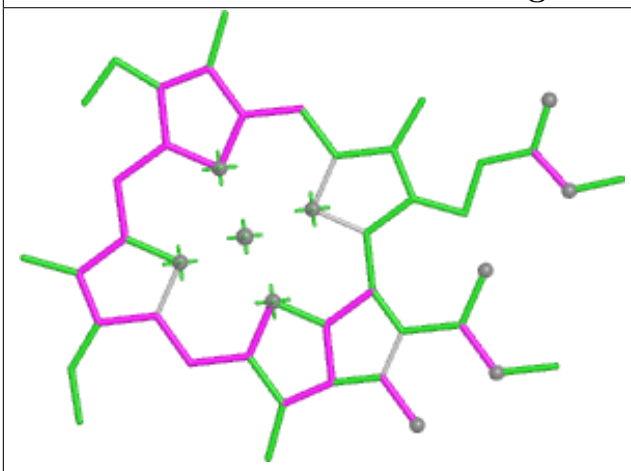


Torsions

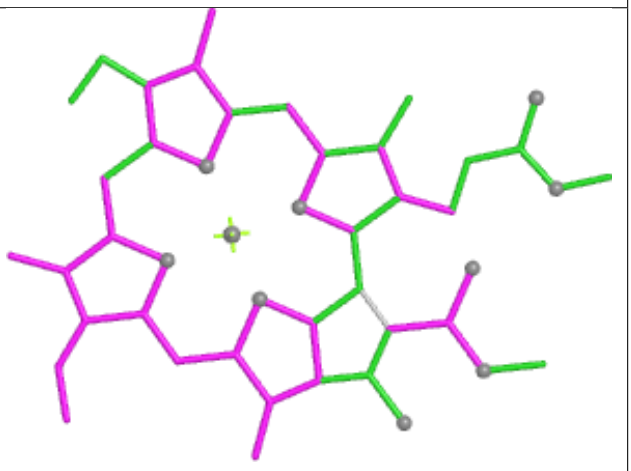


Rings

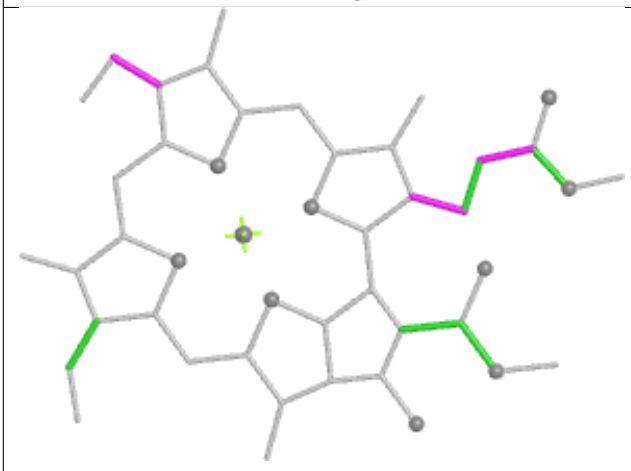
Ligand CLA 3 617



Bond lengths



Bond angles

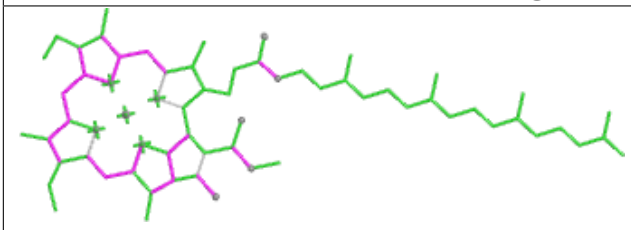


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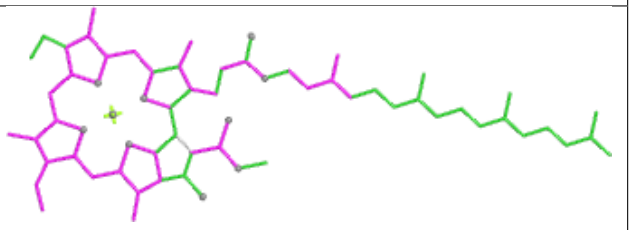


Rings

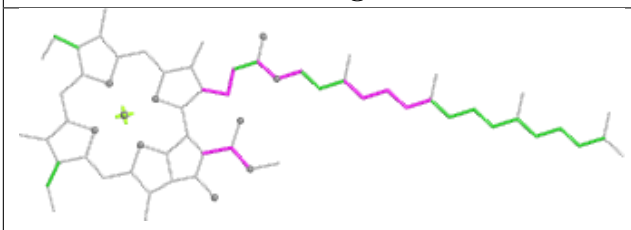
Ligand CLA 1 602



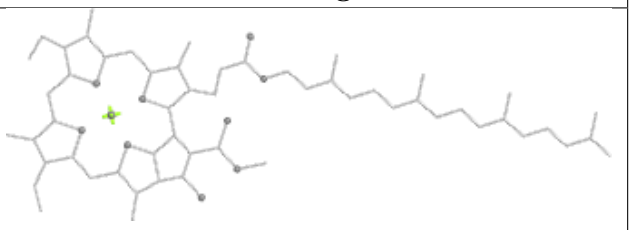
Bond lengths



Bond angles



Torsions

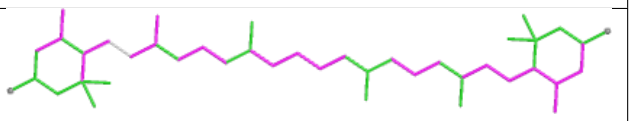


Rings

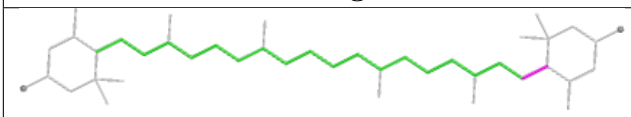
Ligand LUT 9 616



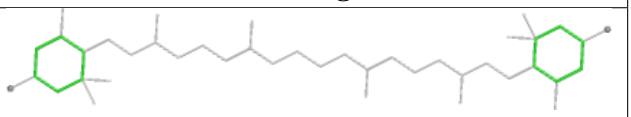
Bond lengths



Bond angles

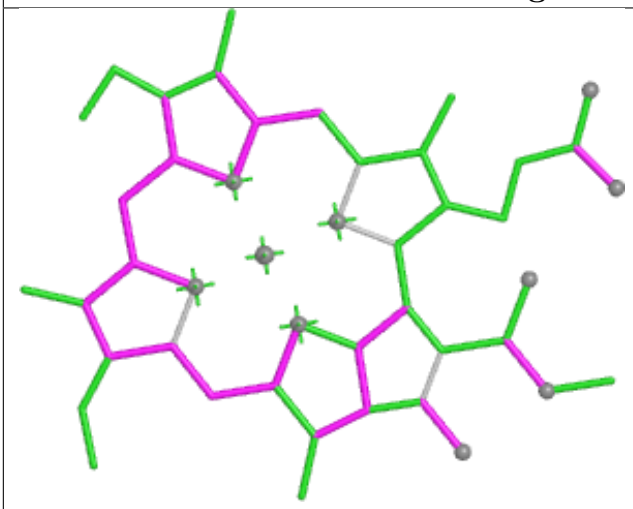


Torsions

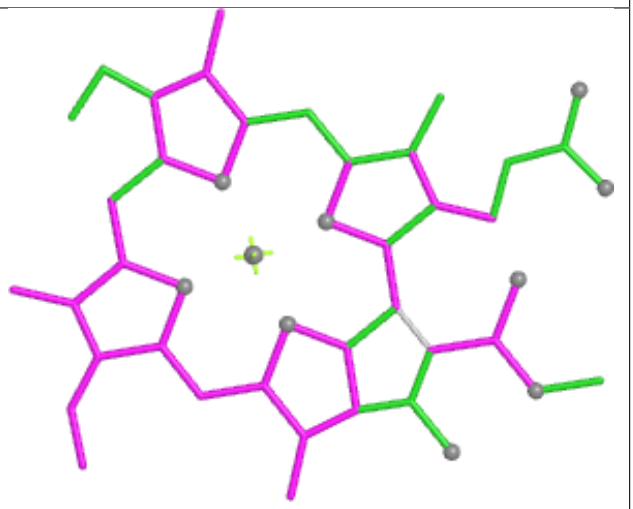


Rings

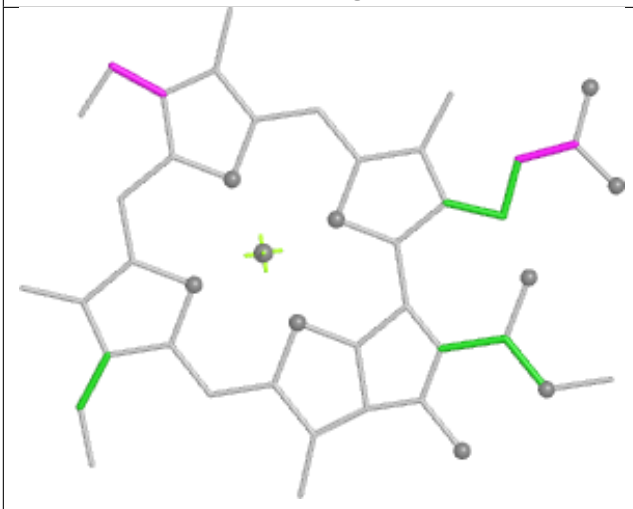
Ligand CLA 8 603



Bond lengths



Bond angles

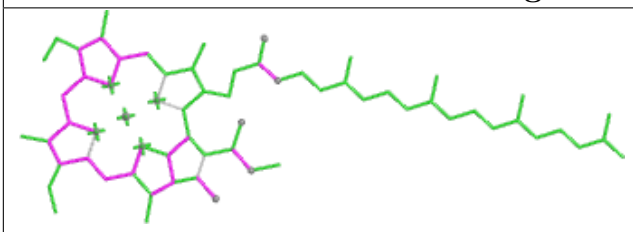


Torsions

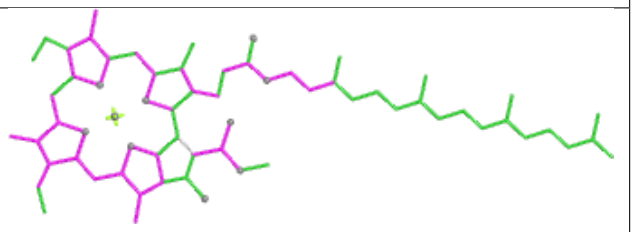


Rings

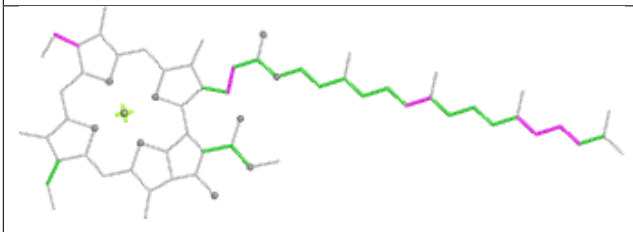
Ligand CLA B 839



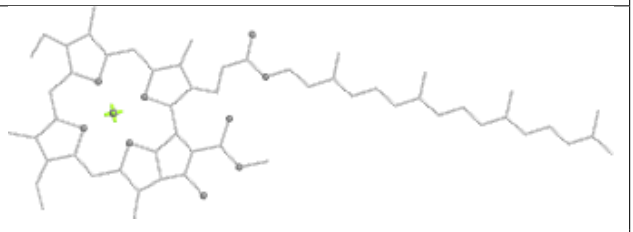
Bond lengths



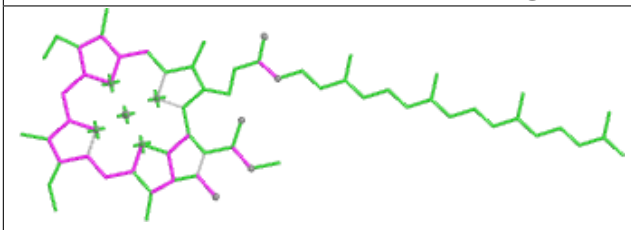
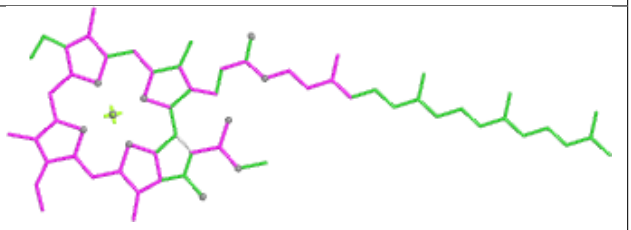
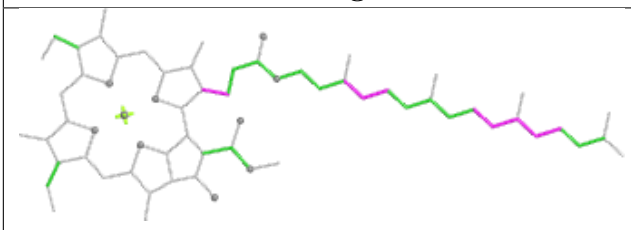
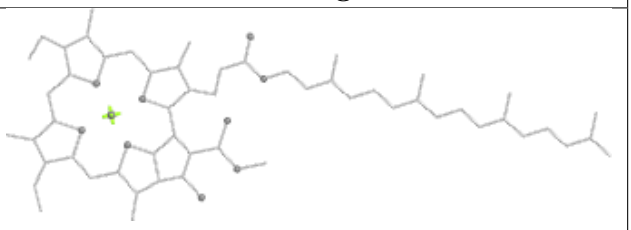
Bond angles

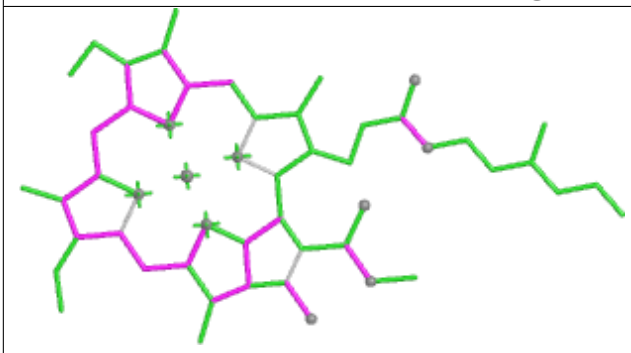
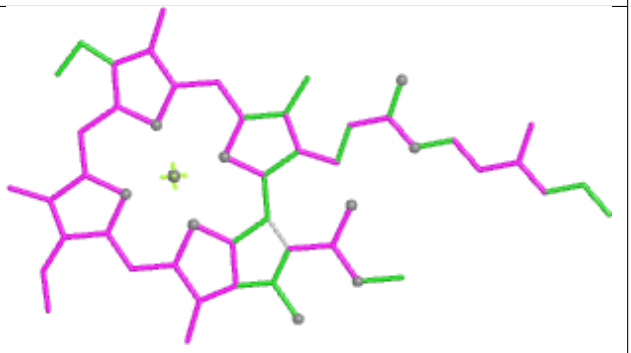
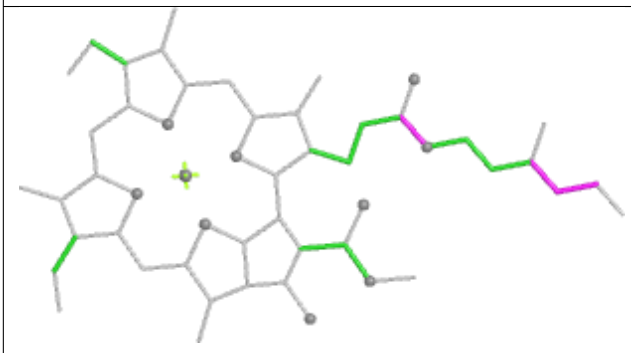
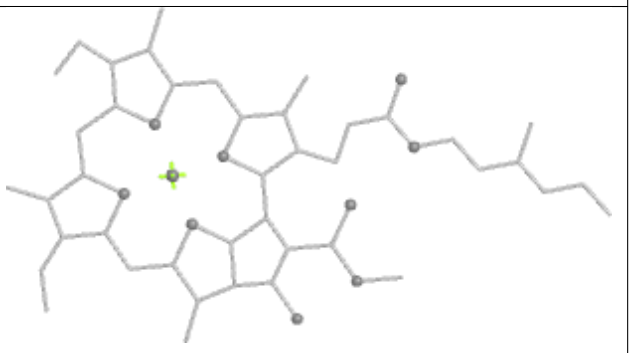


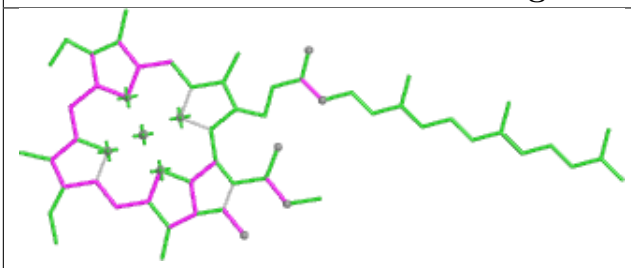
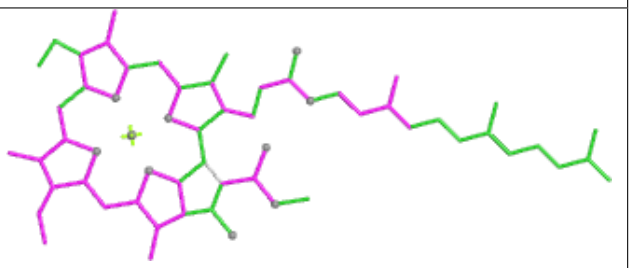
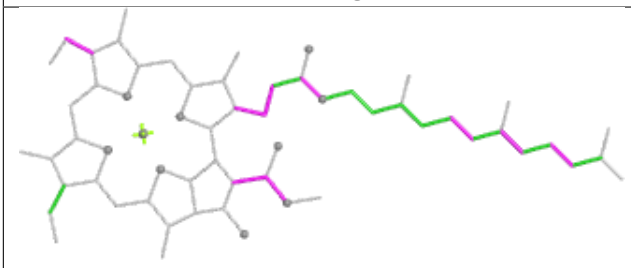
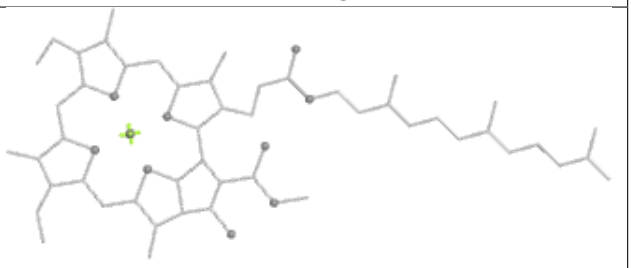
Torsions

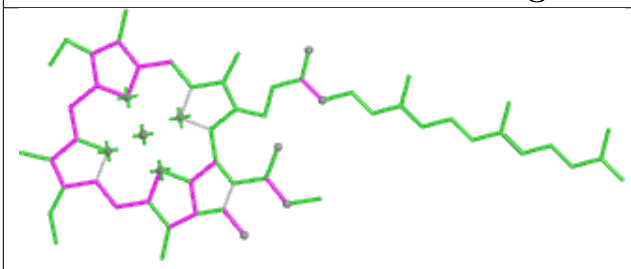
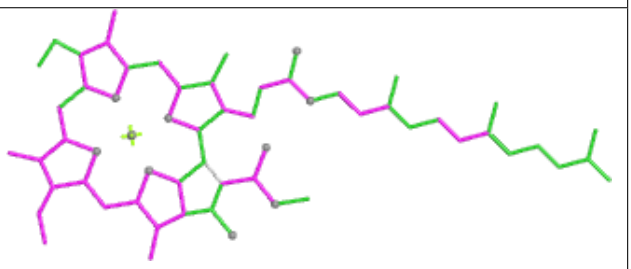
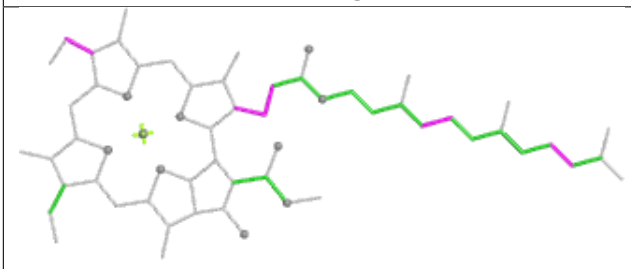
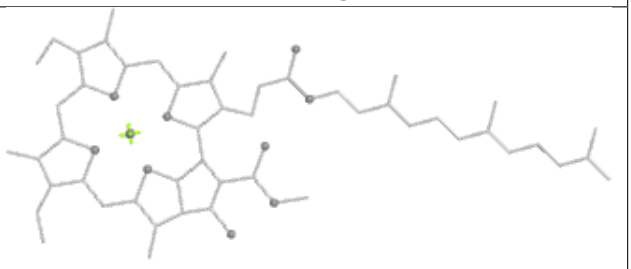


Rings

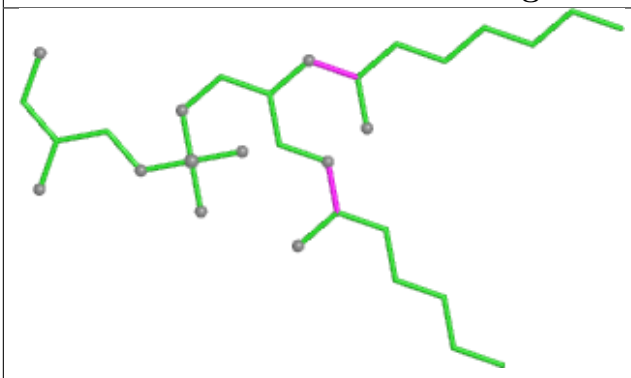
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

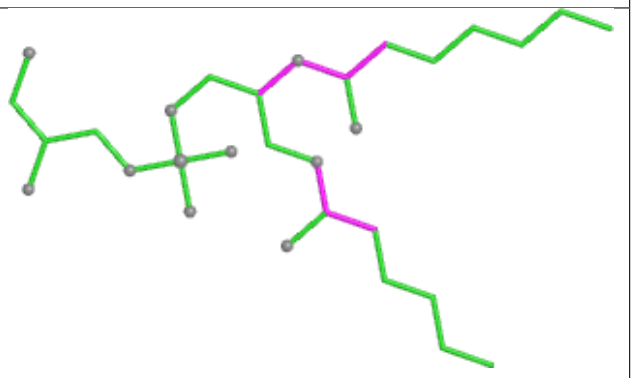
Ligand CLA 4 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

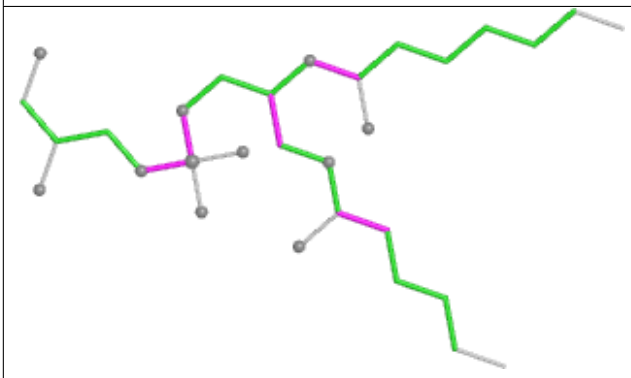
Ligand LHG A 855



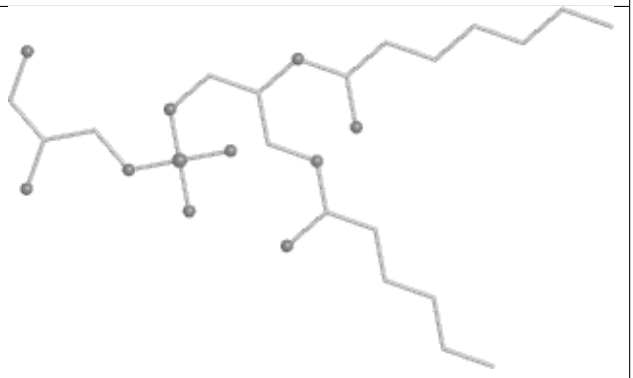
Bond lengths



Bond angles

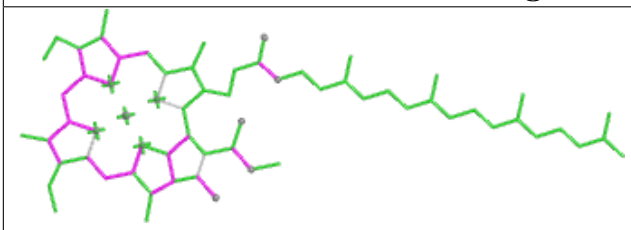


Torsions

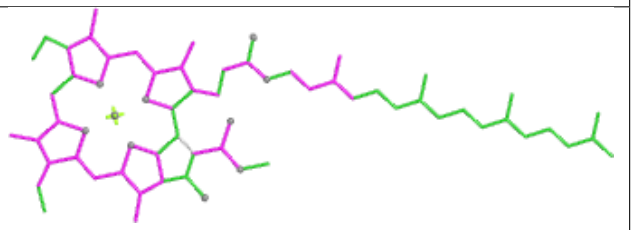


Rings

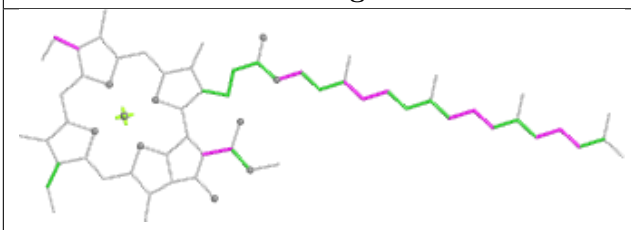
Ligand CLA B 802



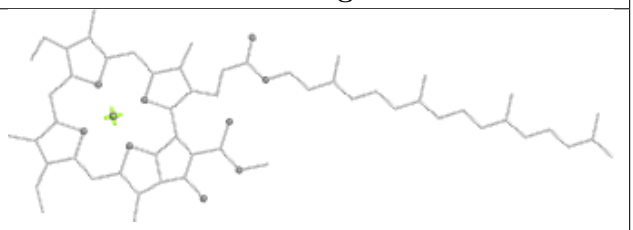
Bond lengths



Bond angles

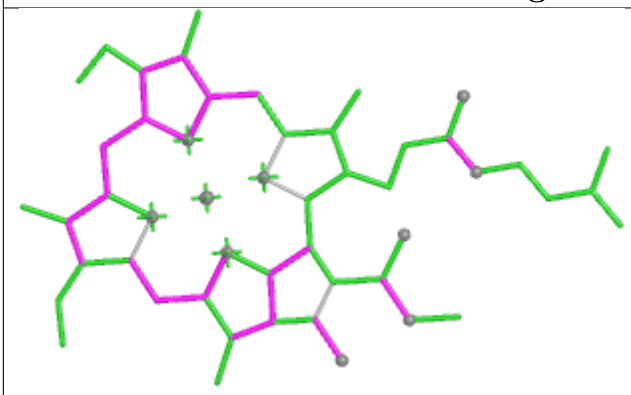


Torsions

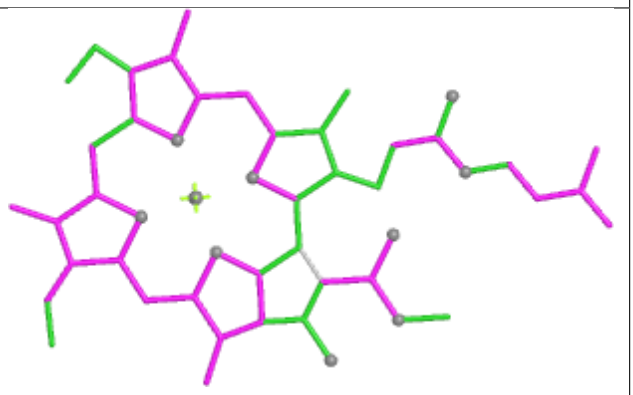


Rings

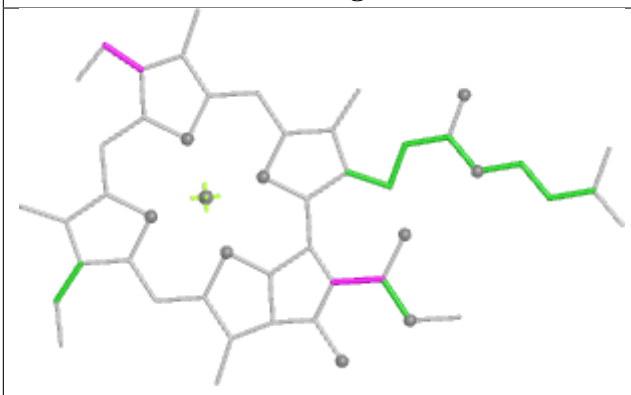
Ligand CLA 8 608



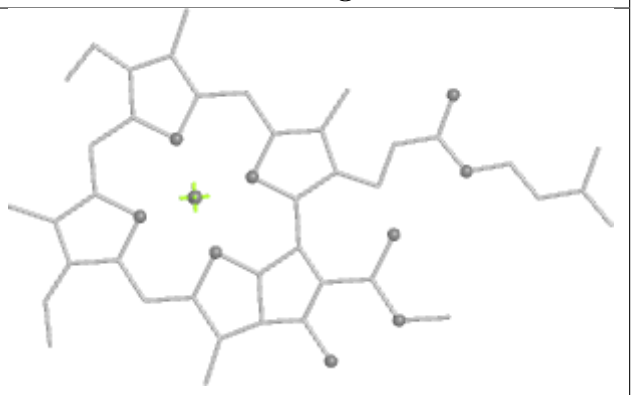
Bond lengths



Bond angles

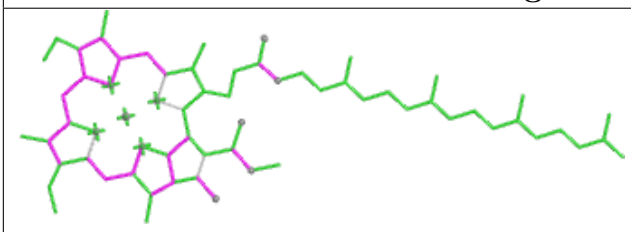


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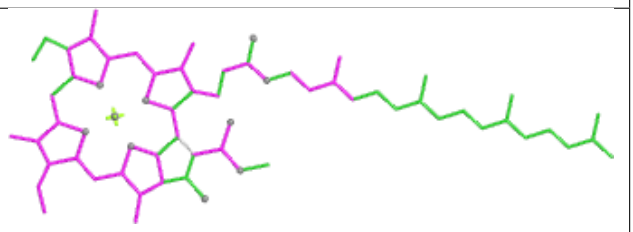


Rings

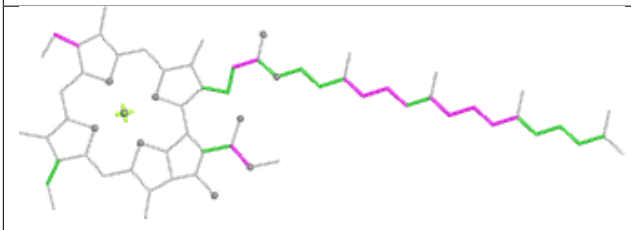
Ligand CLA B 806



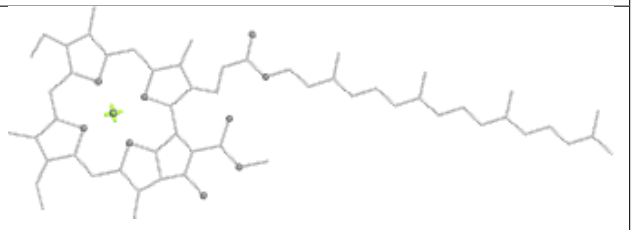
Bond lengths



Bond angles

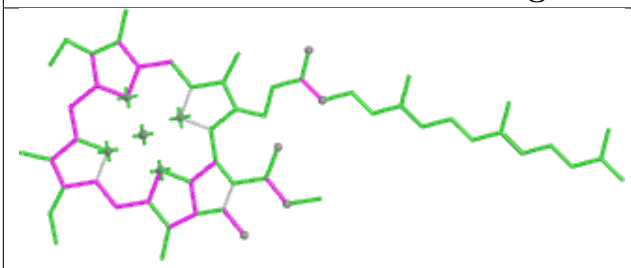


Torsions

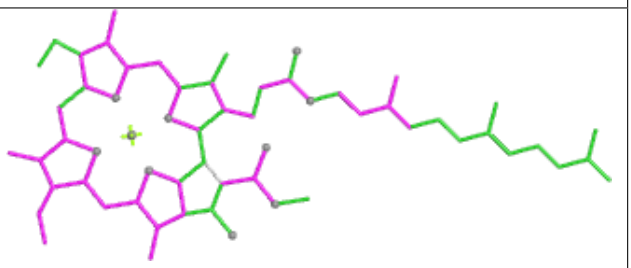


Rings

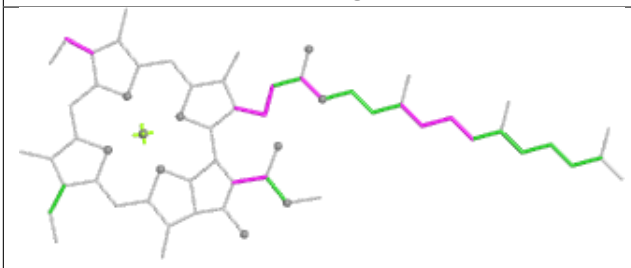
Ligand CLA 9 602



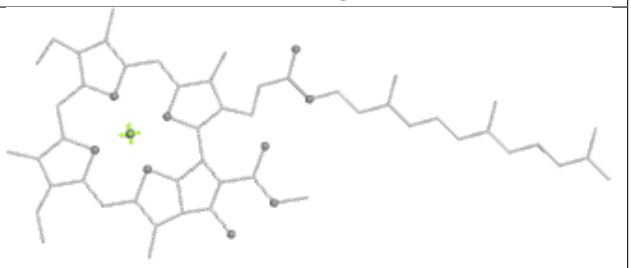
Bond lengths



Bond angles

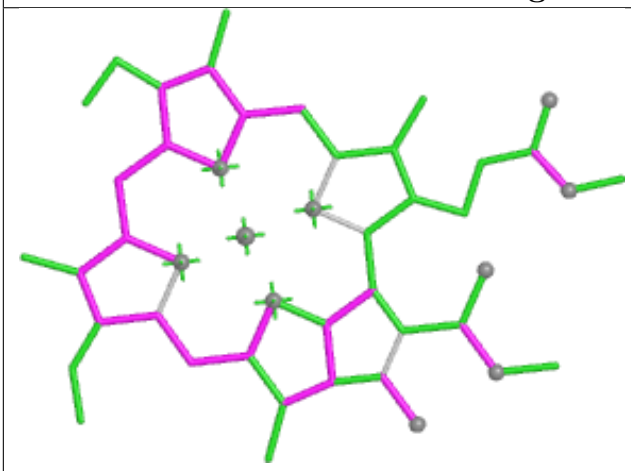


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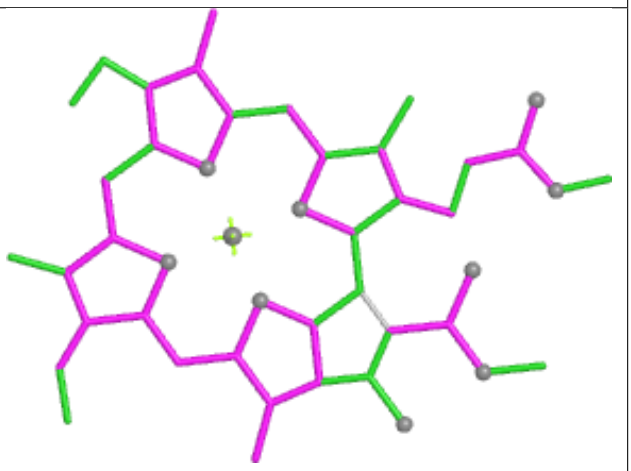


Rings

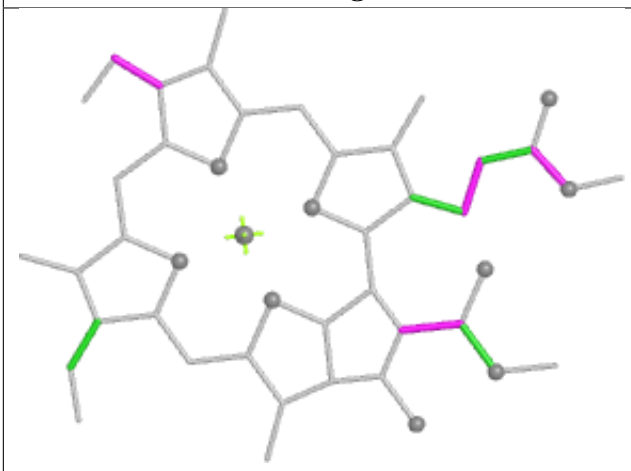
Ligand CLA 5 617



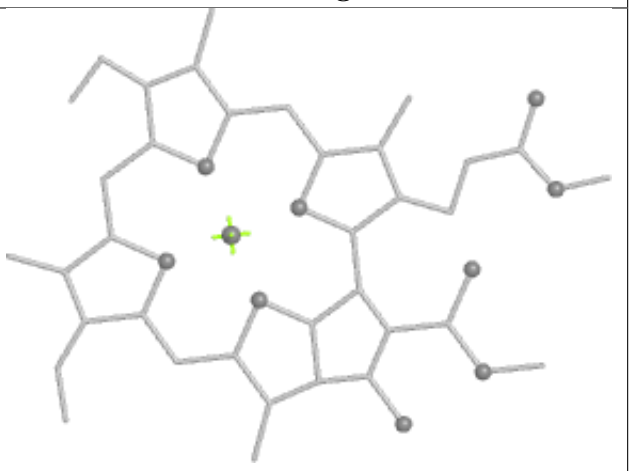
Bond lengths



Bond angles

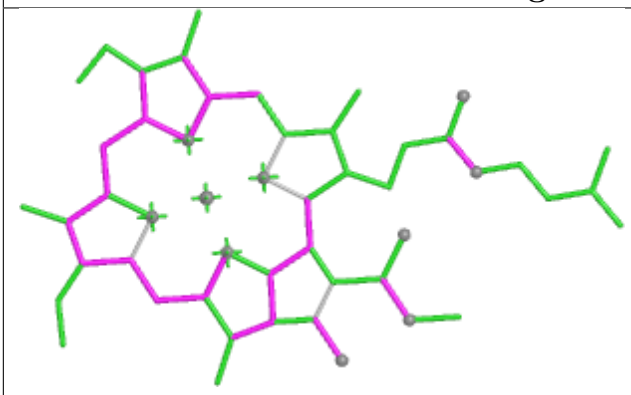


Torsions

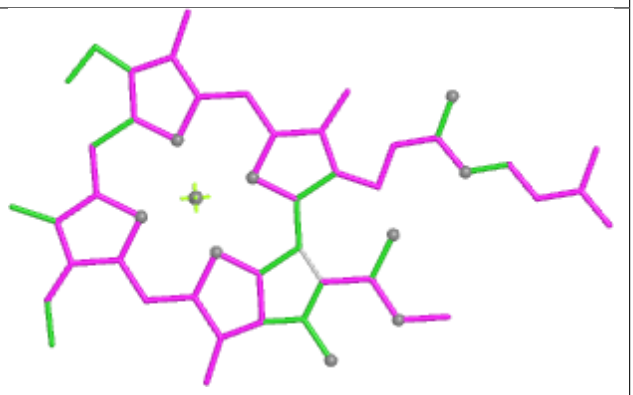


Rings

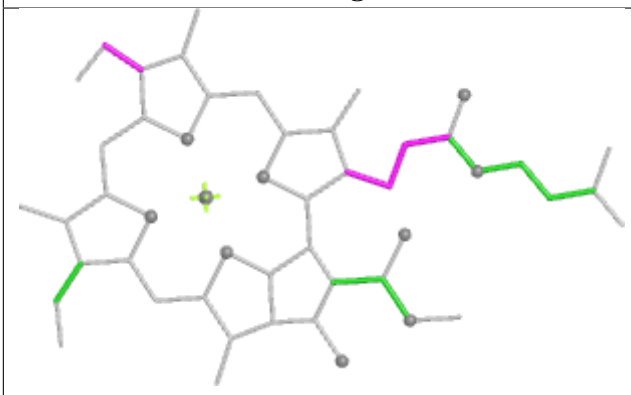
Ligand CLA 7 609



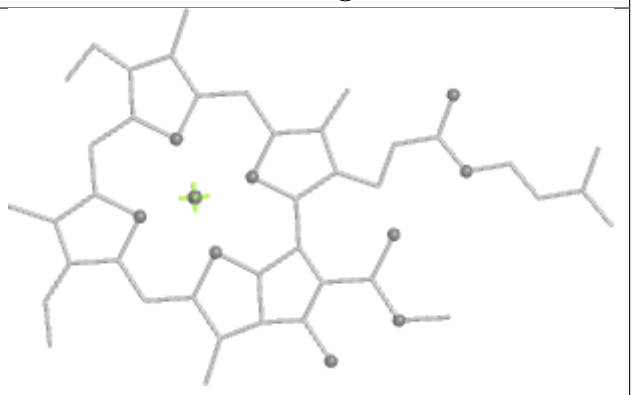
Bond lengths



Bond angles

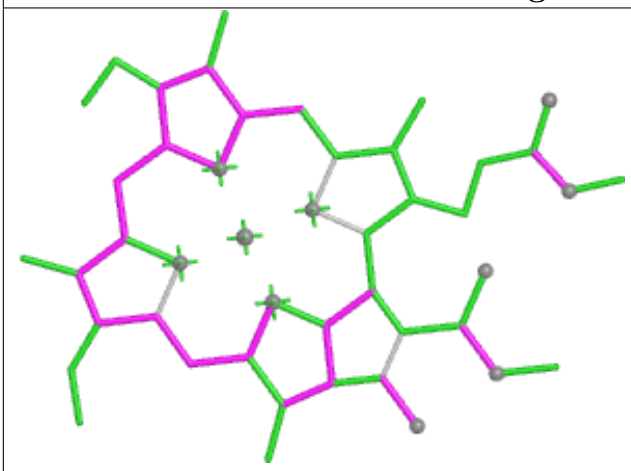


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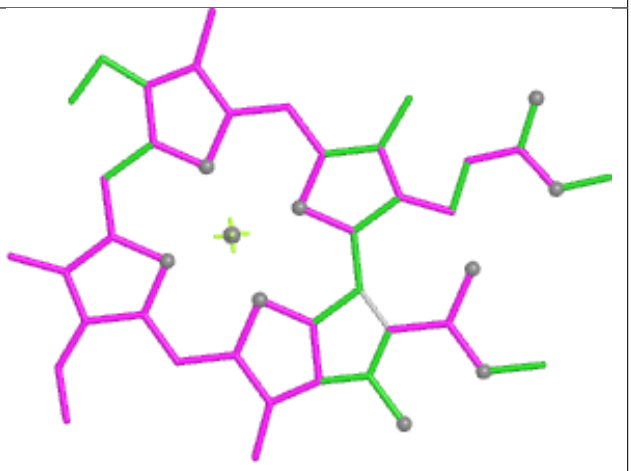


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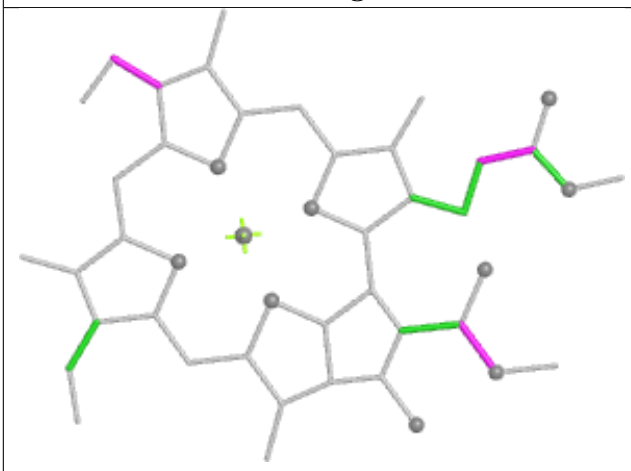
Ligand CLA 1 616



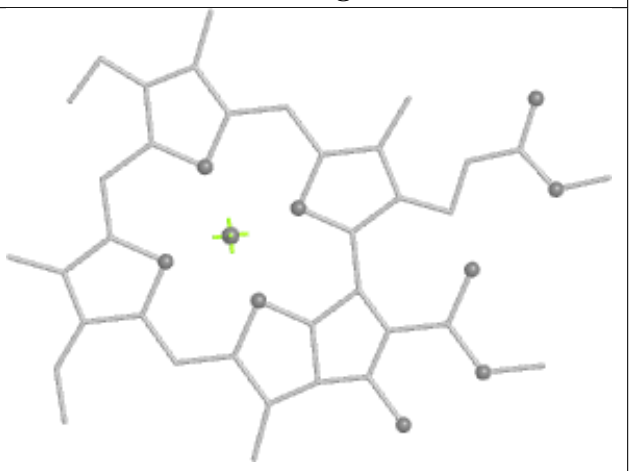
Bond lengths



Bond angles

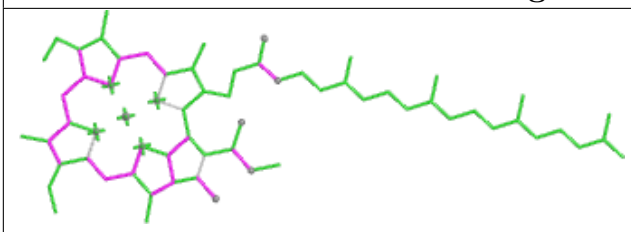


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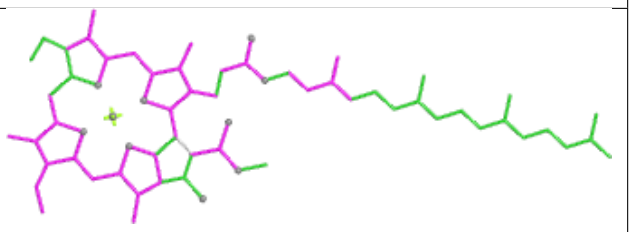


Rings

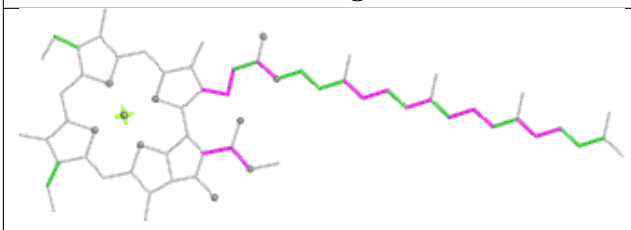
Ligand CLA 3 610



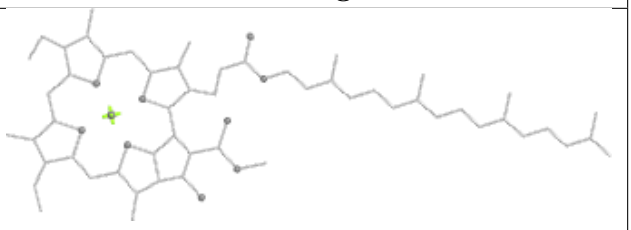
Bond lengths



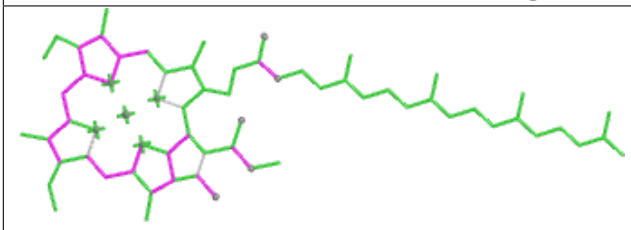
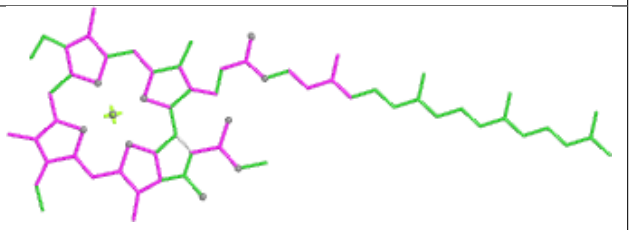
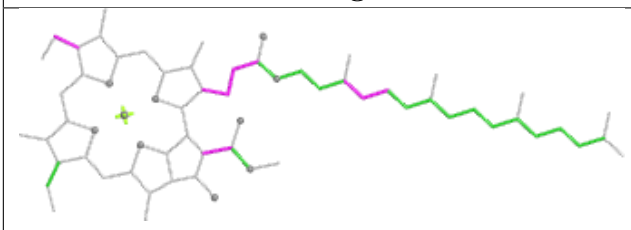
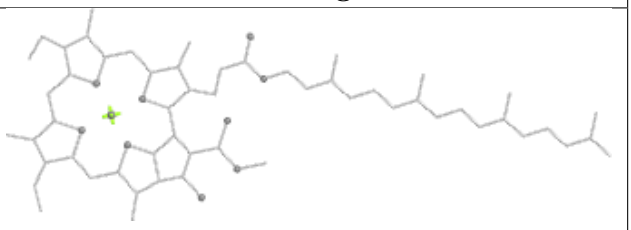
Bond angles

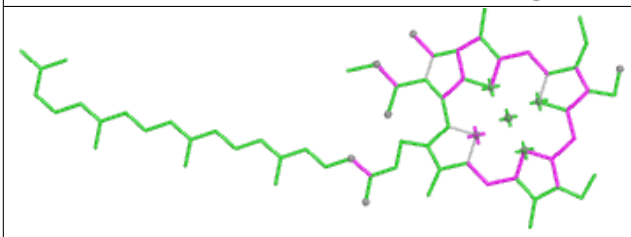
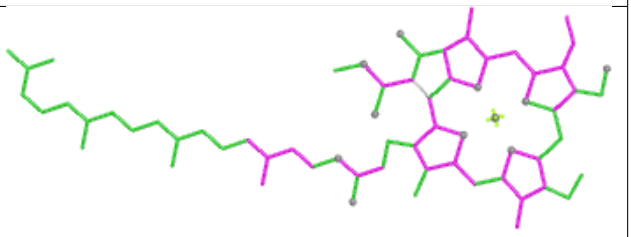
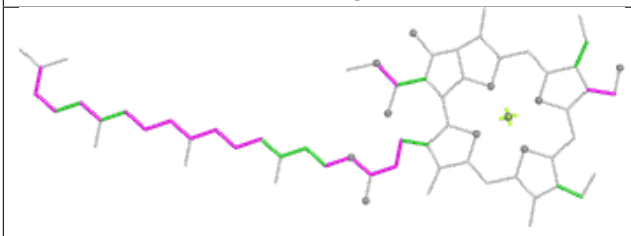
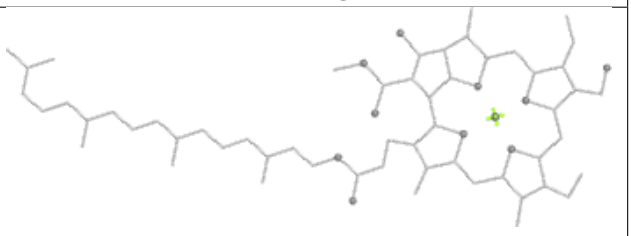


Torsions

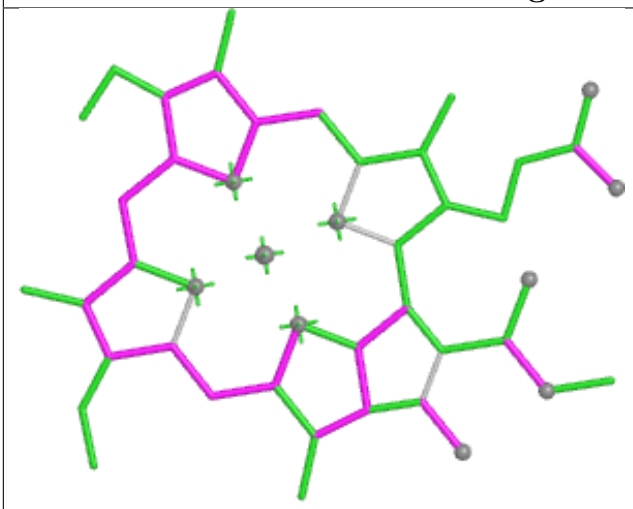


Rings

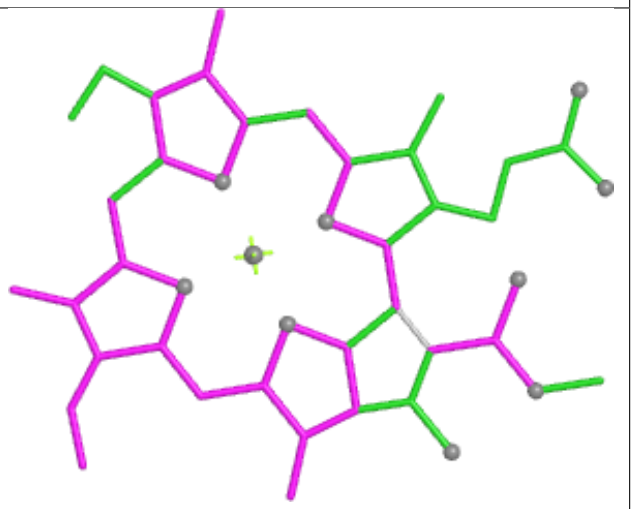
Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 3 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

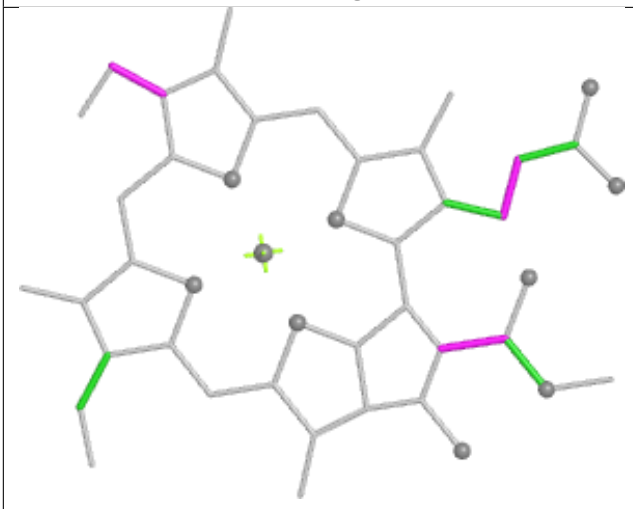
Ligand CLA 2 614



Bond lengths



Bond angles

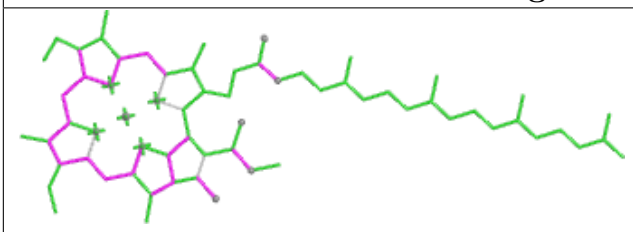


Torsions

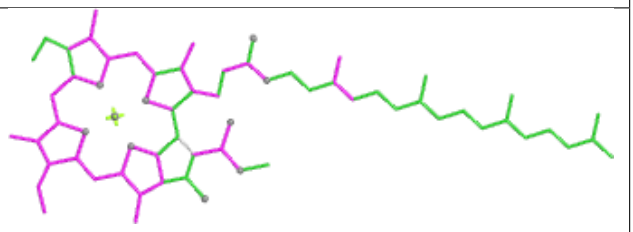


Rings

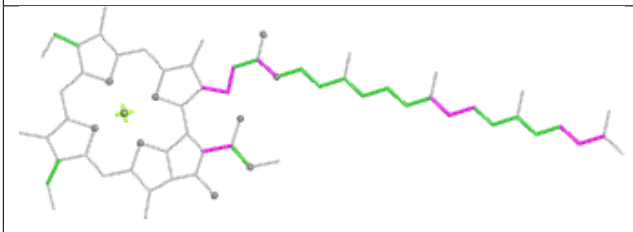
Ligand CLA 7 602



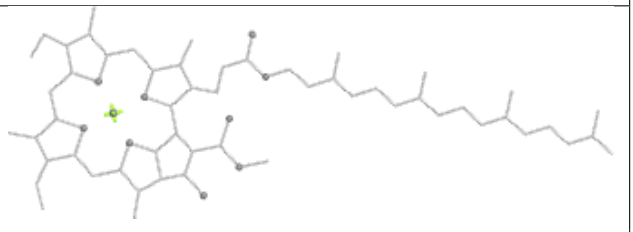
Bond lengths



Bond angles

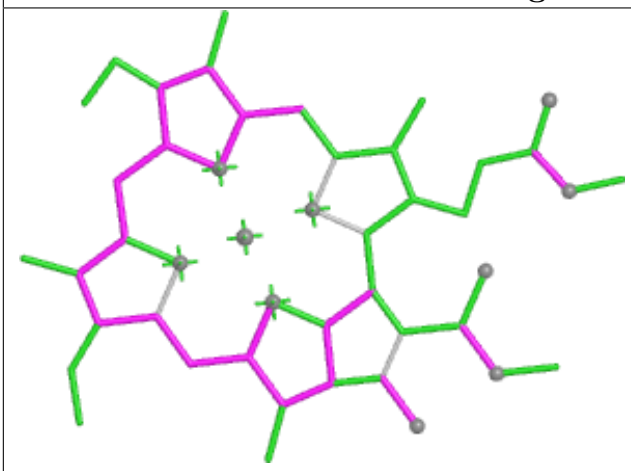


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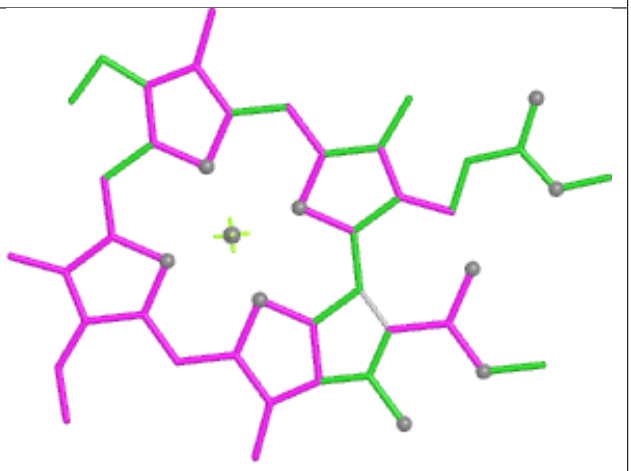


Rings

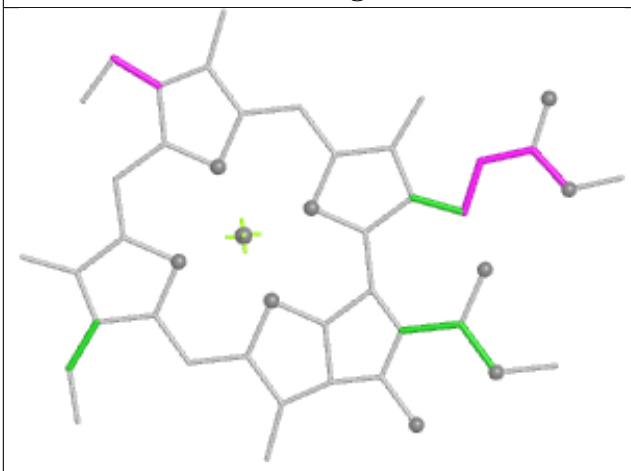
Ligand CLA 7 616



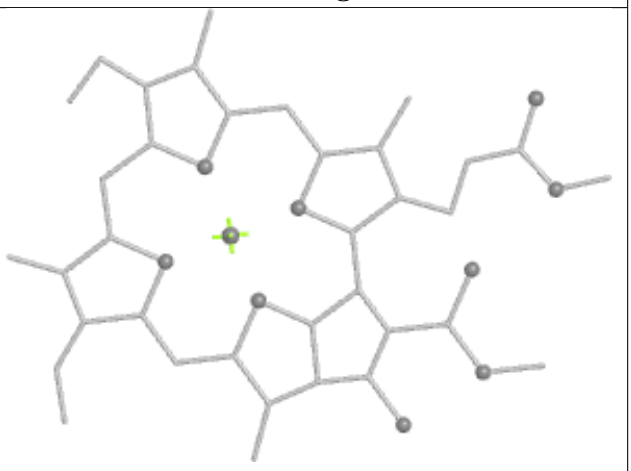
Bond lengths



Bond angles

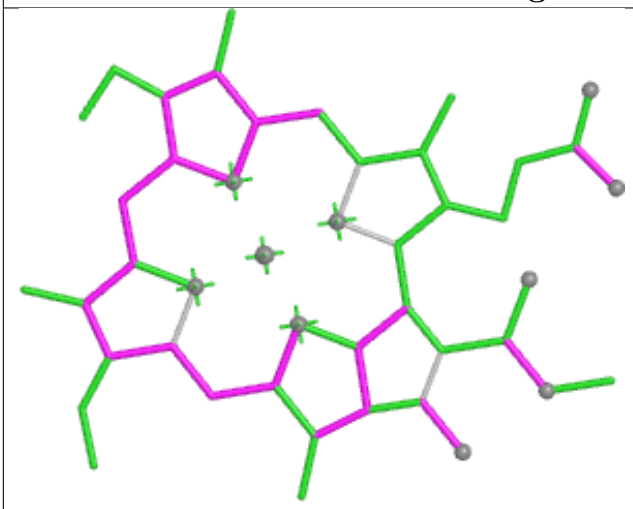


Torsions

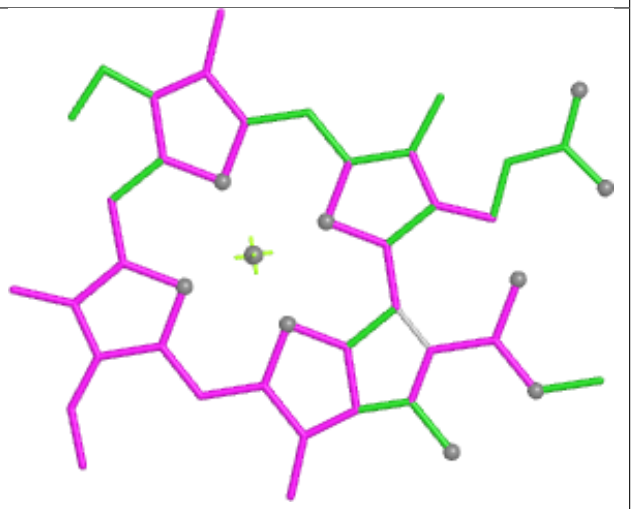


Rings

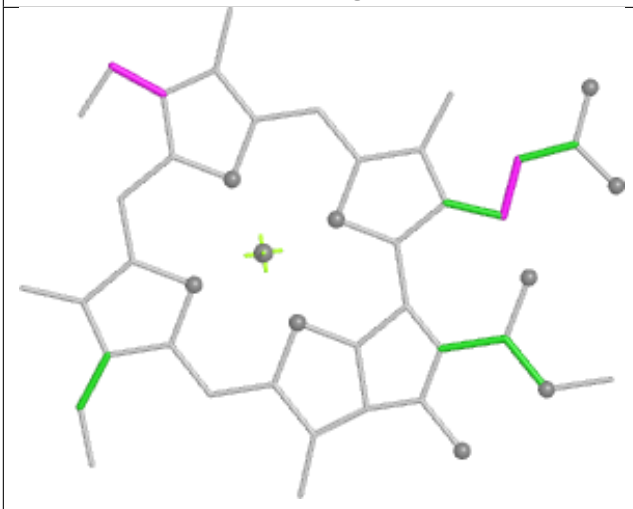
Ligand CLA 5 614



Bond lengths



Bond angles

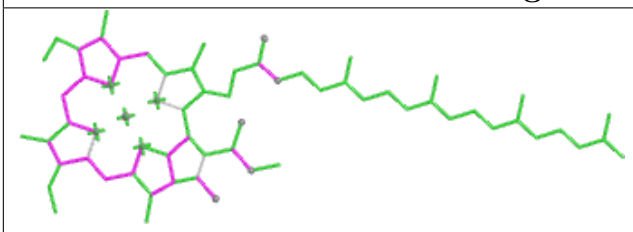


Torsions

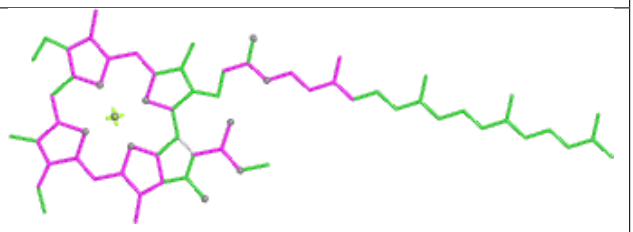


Rings

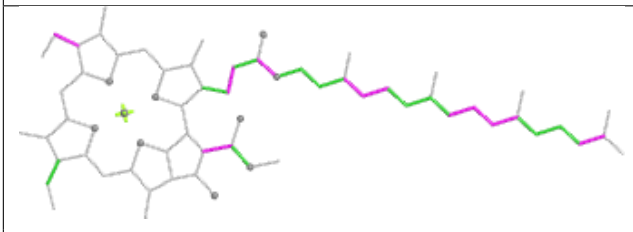
Ligand CLA A 814



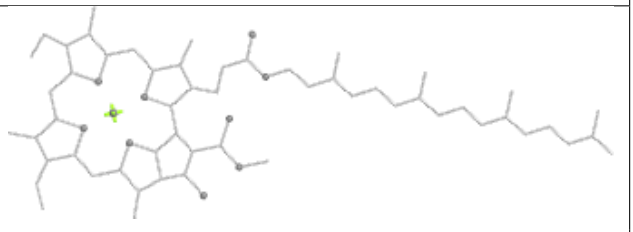
Bond lengths



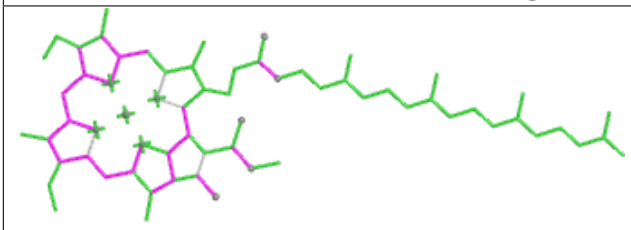
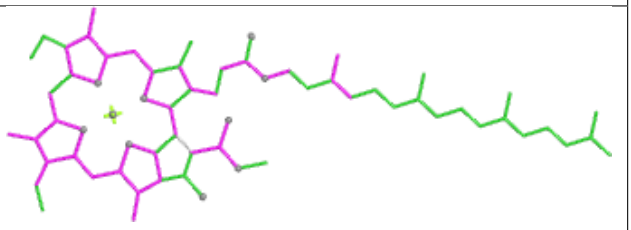
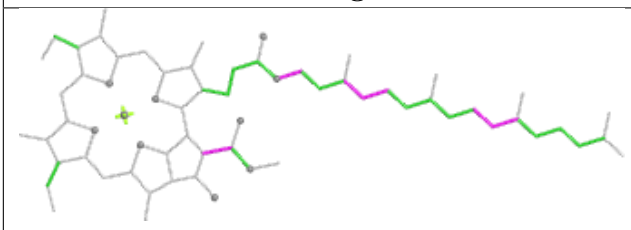
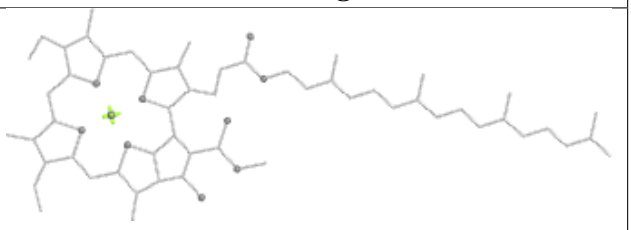
Bond angles

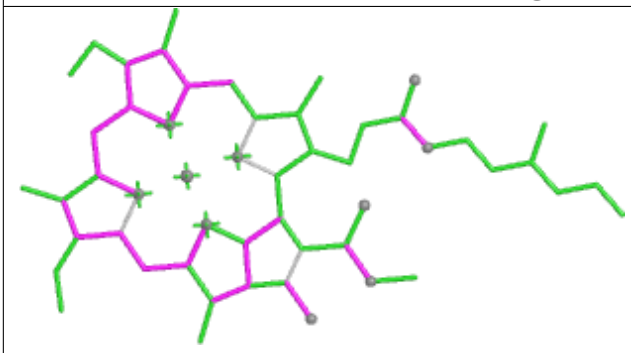
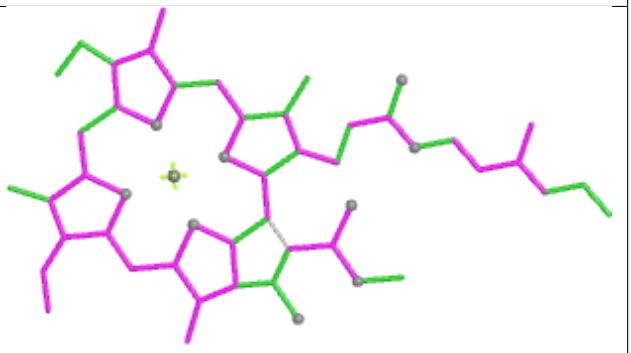
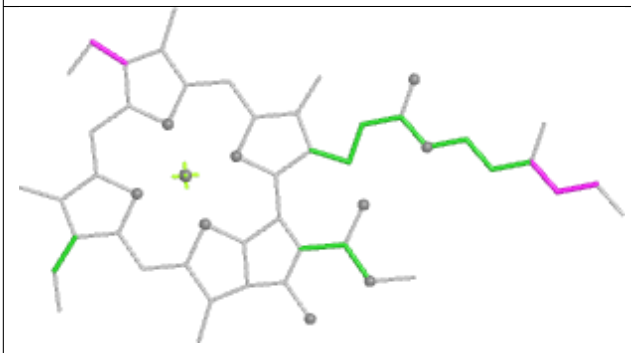
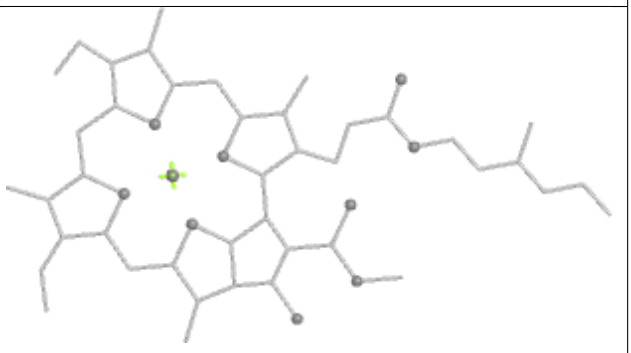


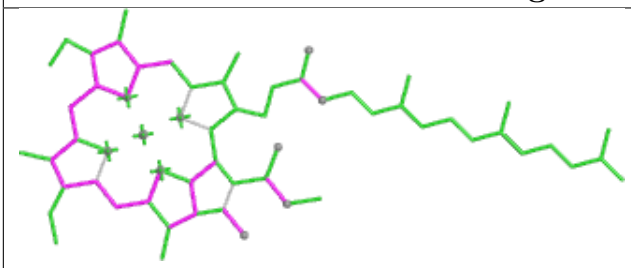
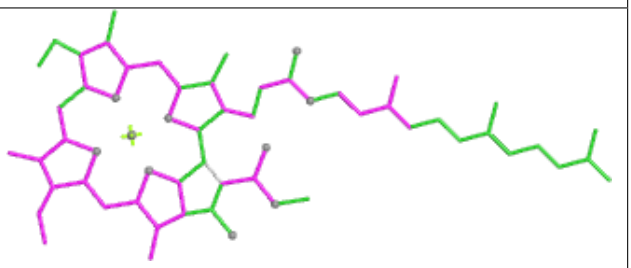
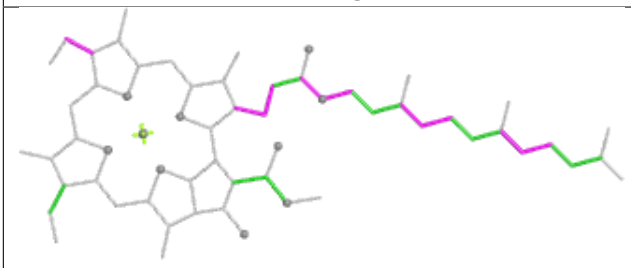
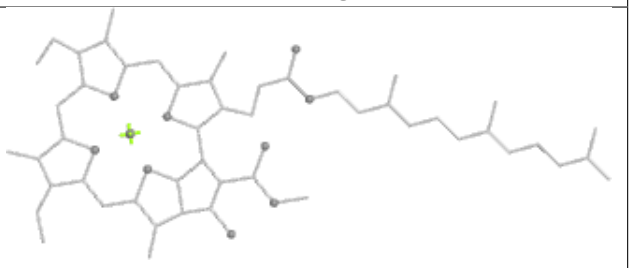
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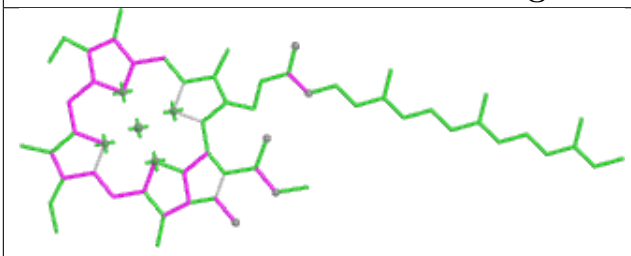
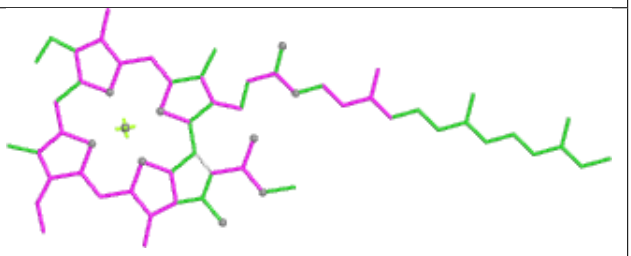
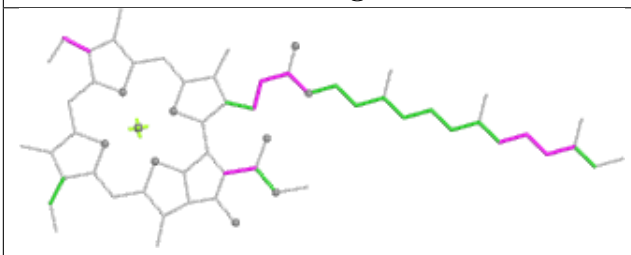
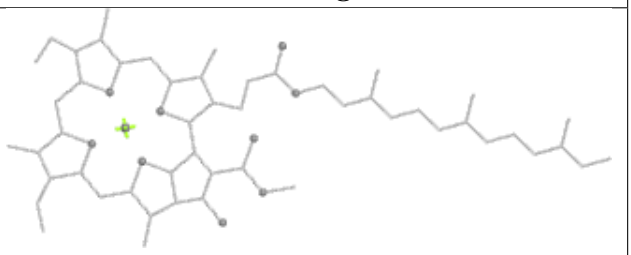


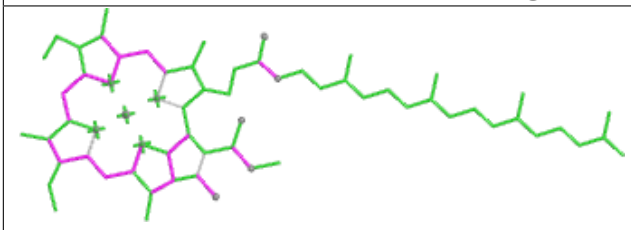
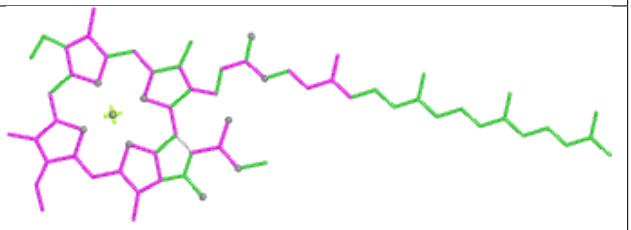
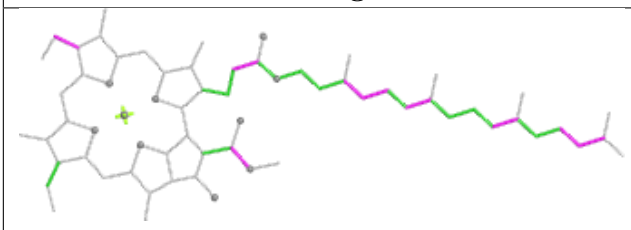
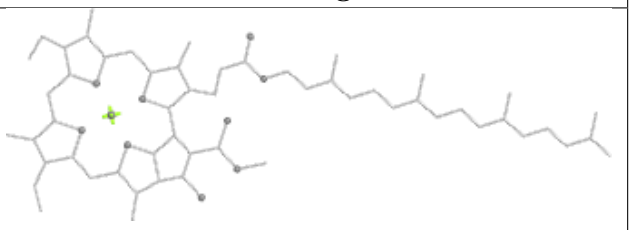
Rings

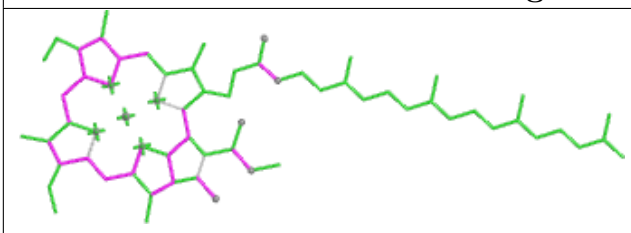
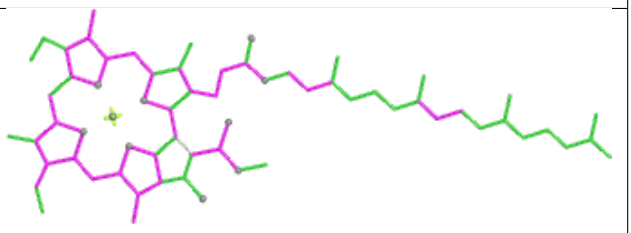
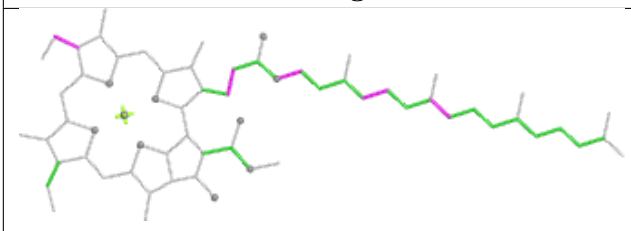
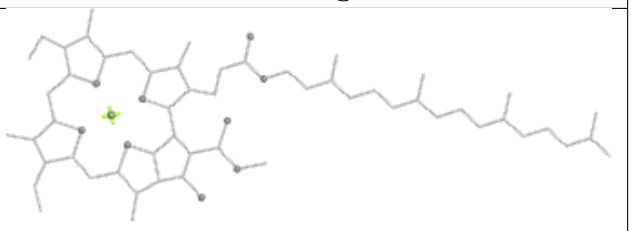
Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

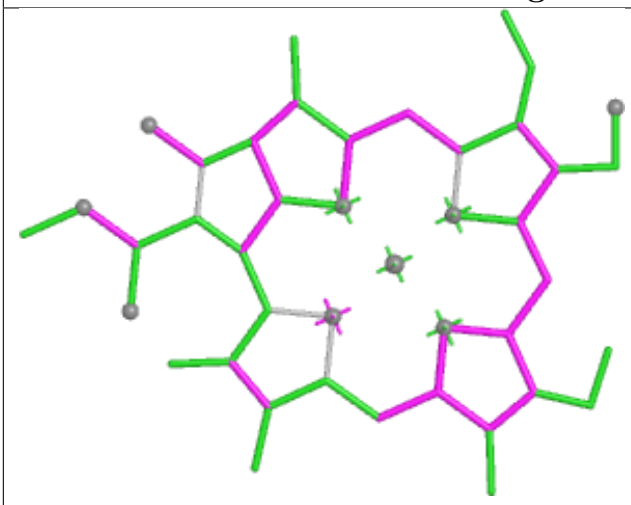
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

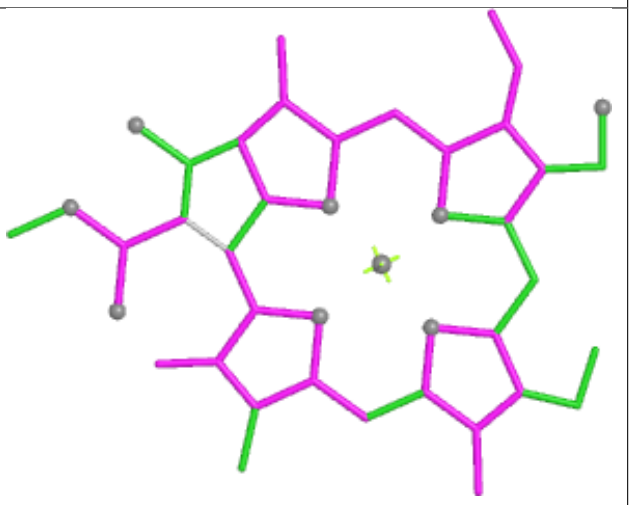
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Z 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

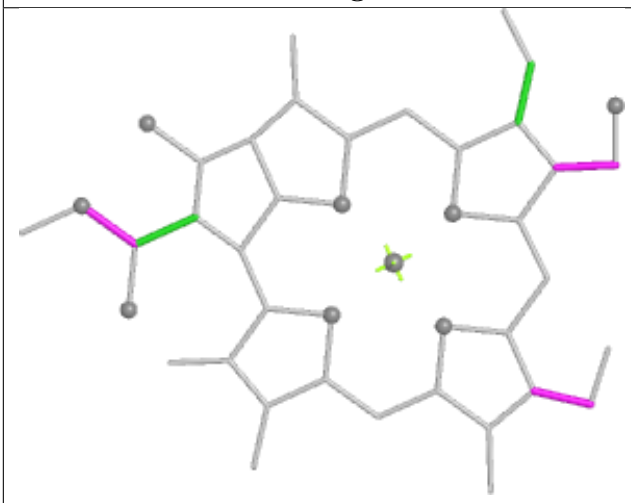
Ligand CHL 9 606



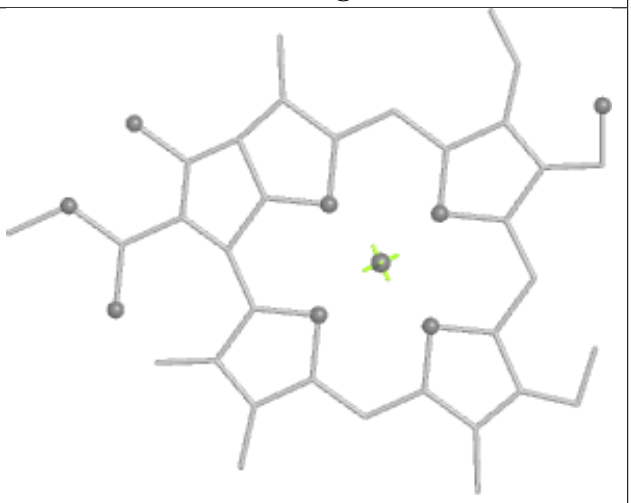
Bond lengths



Bond angles

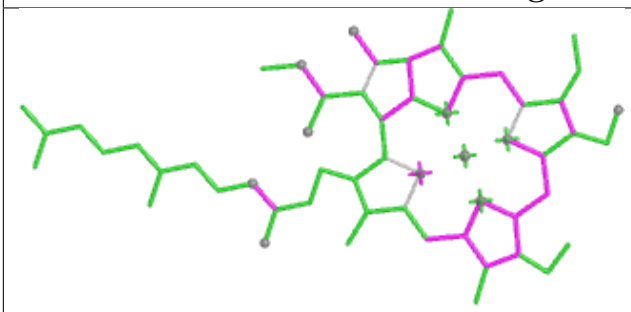


Torsions

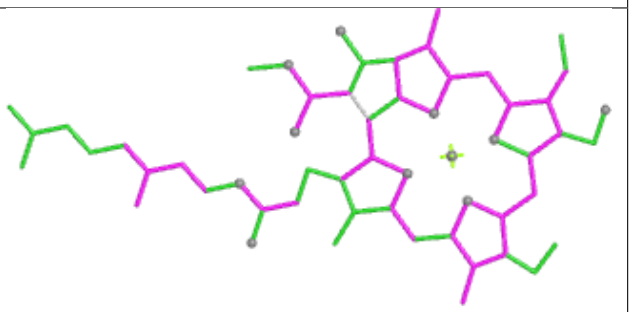


Rings

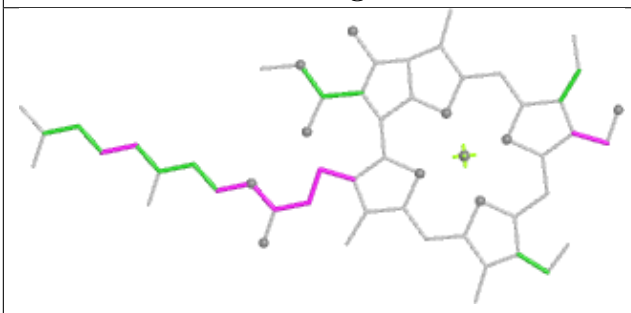
Ligand CHL 8 607



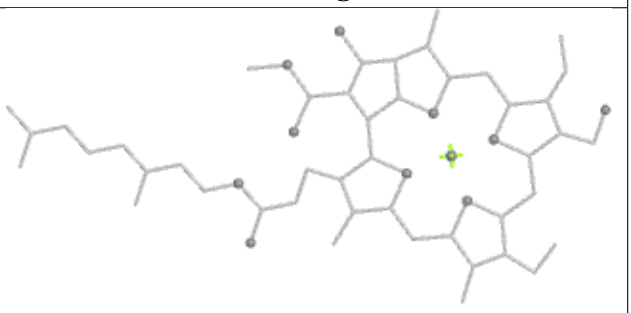
Bond lengths



Bond angles

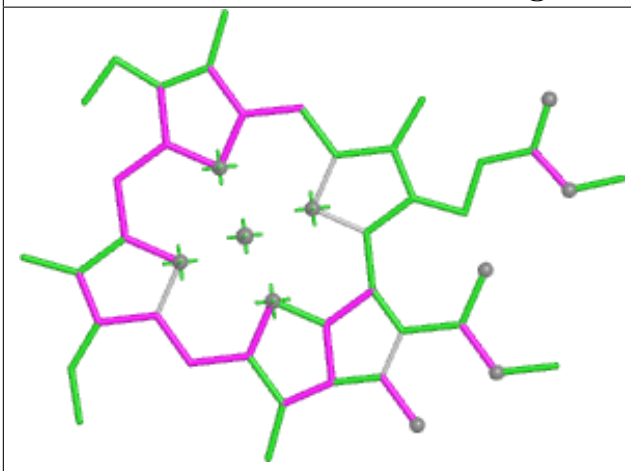


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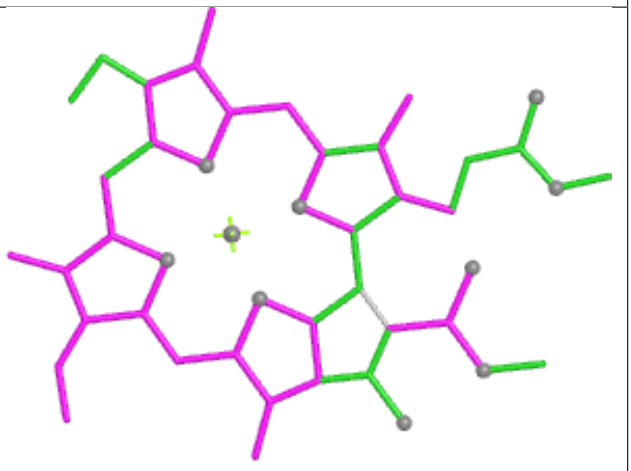


Rings

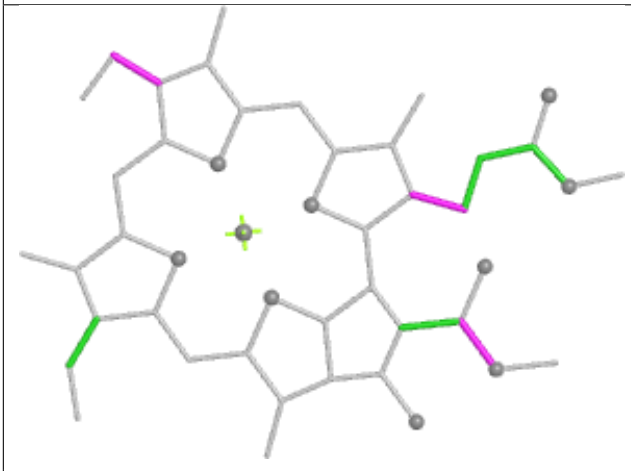
Ligand CLA 8 604



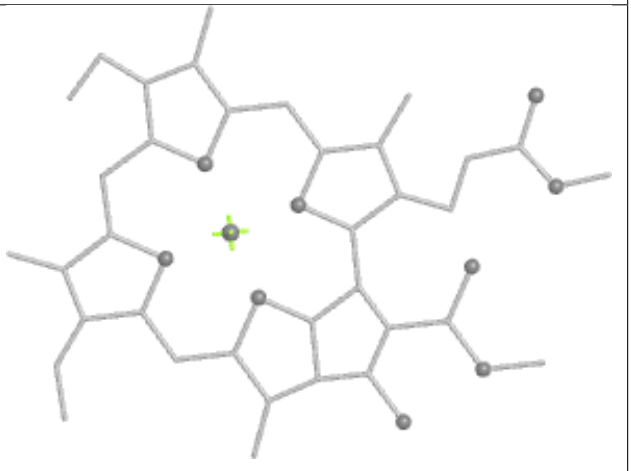
Bond lengths



Bond angles

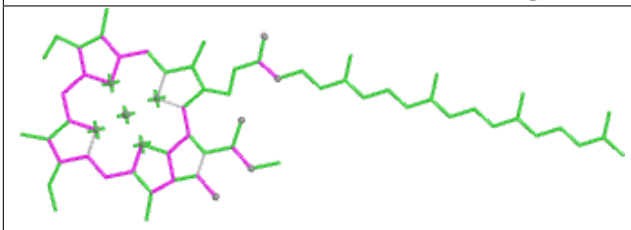


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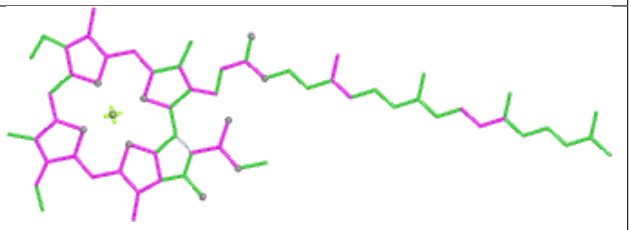


Rings

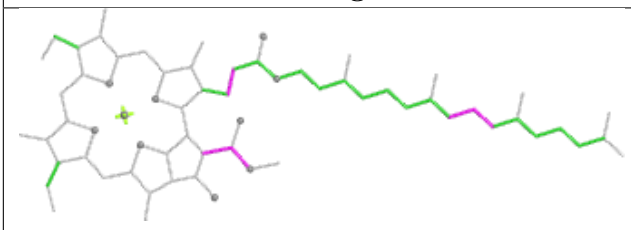
Ligand CLA B 803



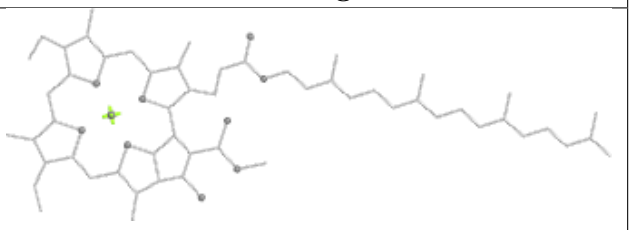
Bond lengths



Bond angles

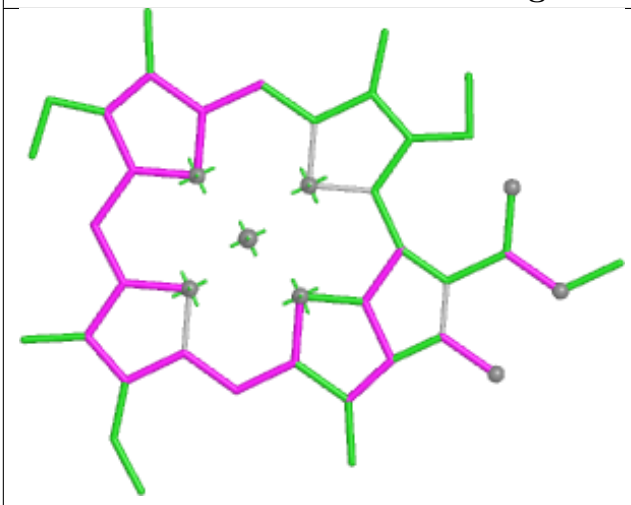


Torsions



Rings

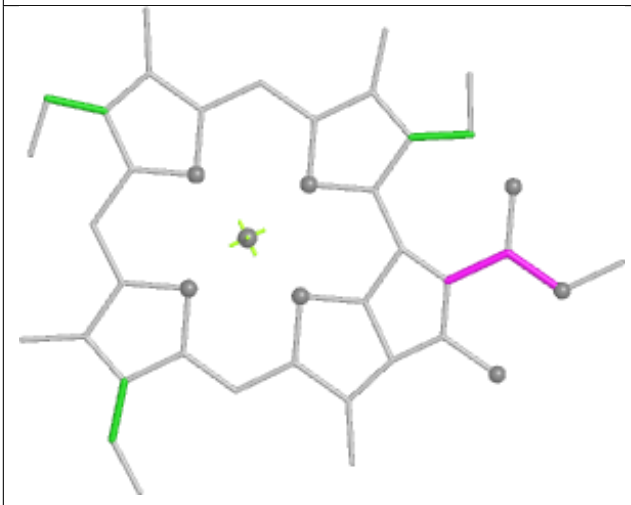
Ligand CLA 8 606



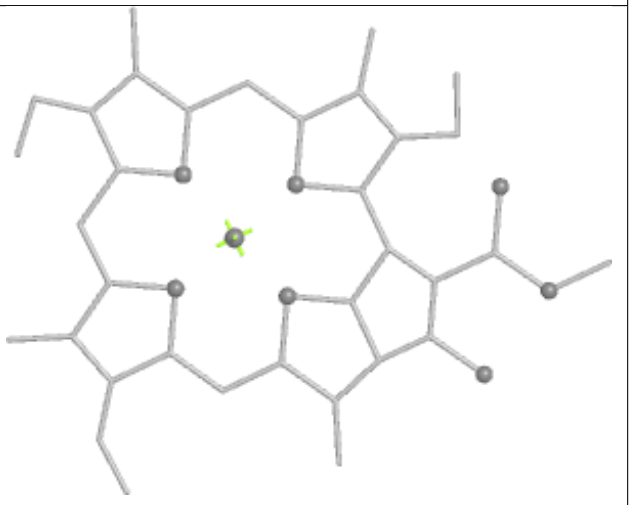
Bond lengths



Bond angles

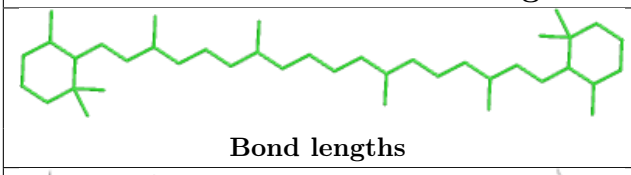


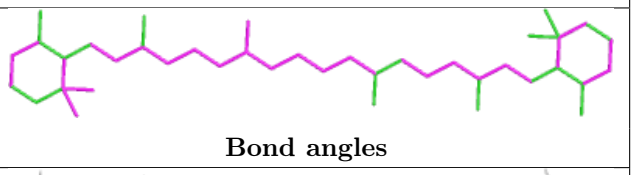
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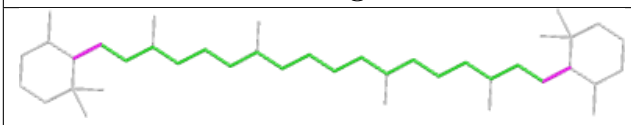


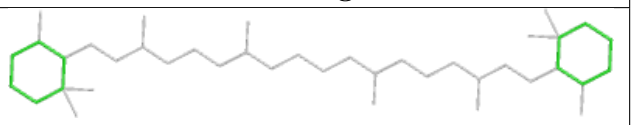
Rings

Ligand BCR A 848

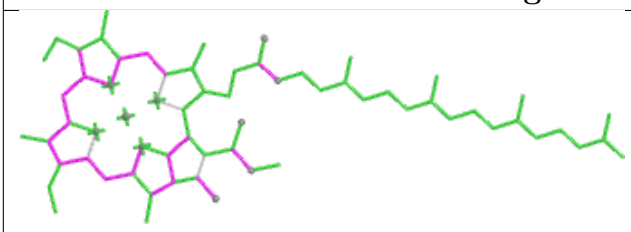

Bond lengths

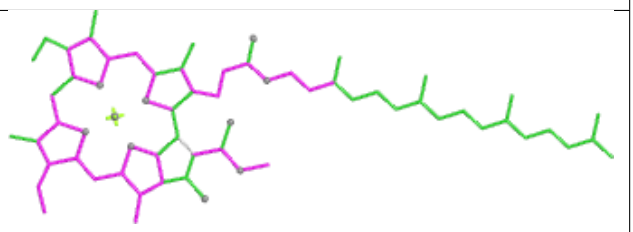

Bond angles

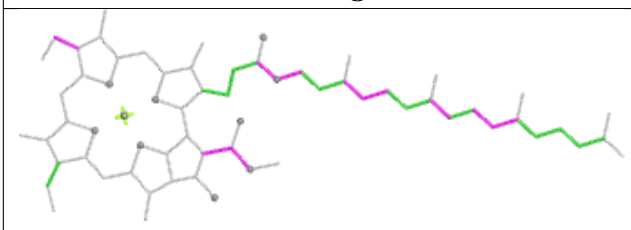

Torsions

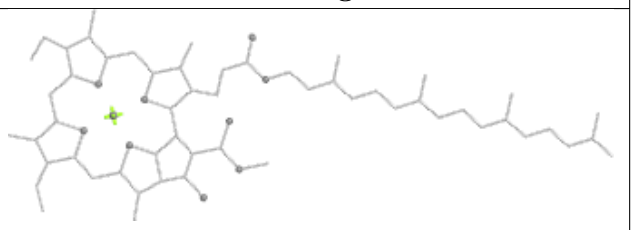

Rings

Ligand CLA A 822

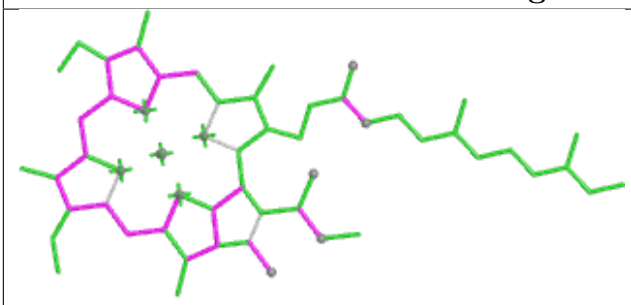

Bond lengths

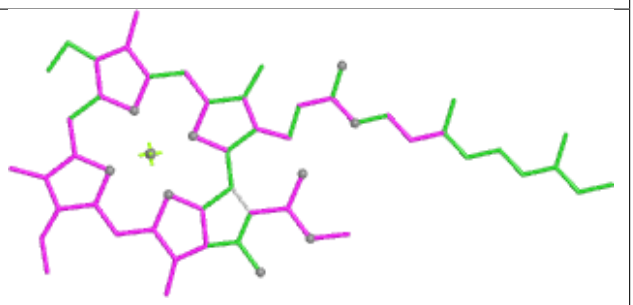

Bond angles

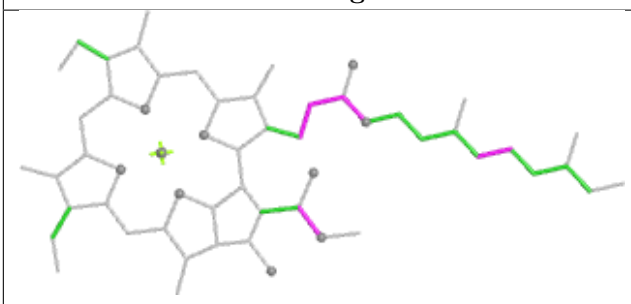

Torsions

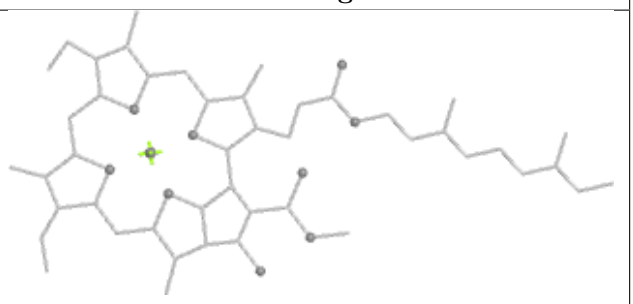

Rings

Ligand CLA 3 620

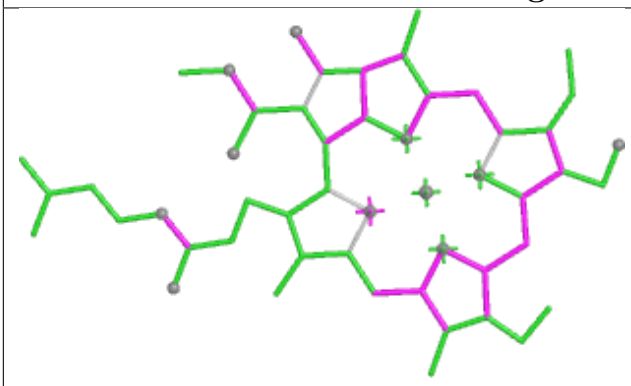

Bond lengths


Bond angles

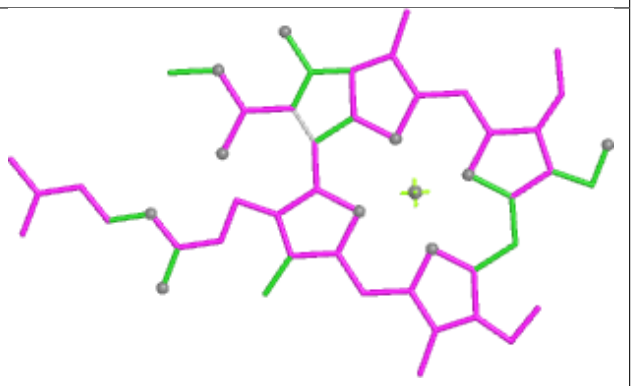

Torsions


Rings

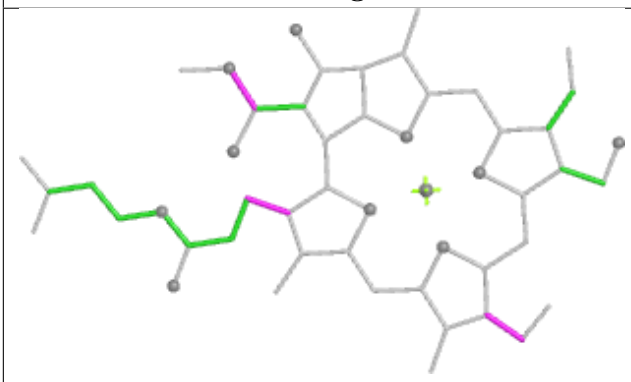
Ligand CHL 6 608



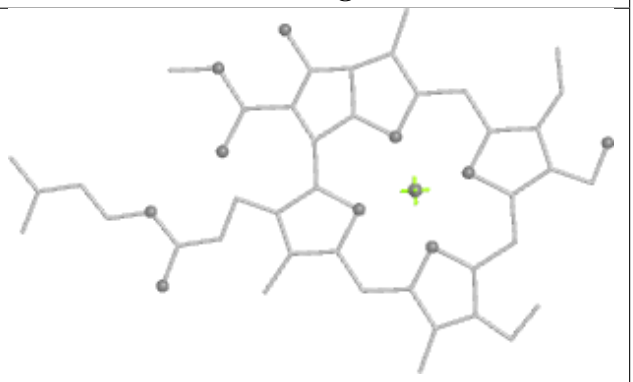
Bond lengths



Bond angles

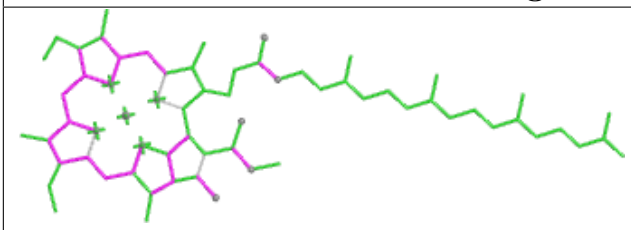


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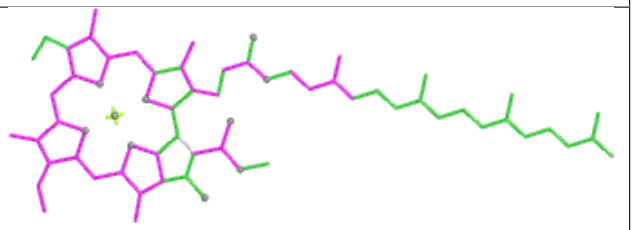


Rings

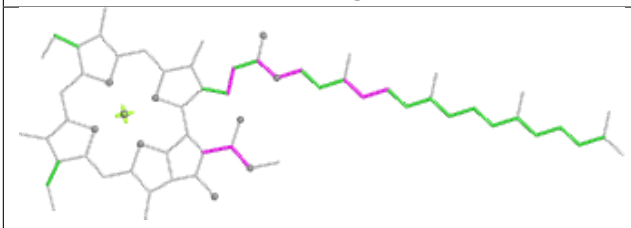
Ligand CLA Z 602



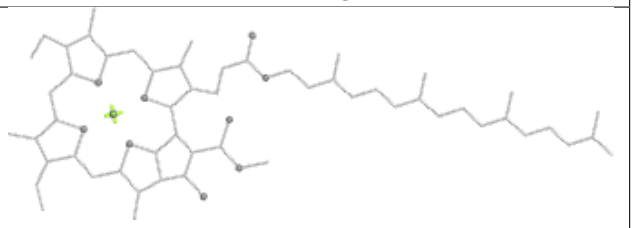
Bond lengths



Bond angles

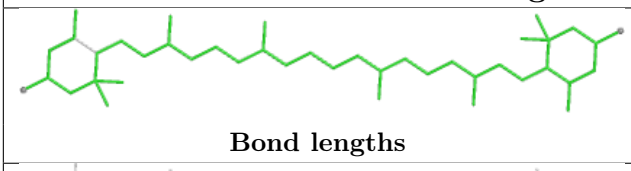


Torsions

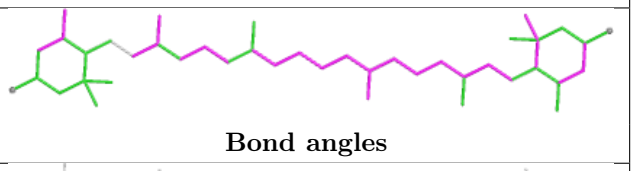


Rings

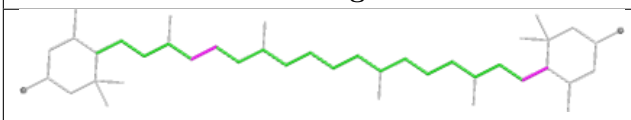
Ligand LUT 1 618



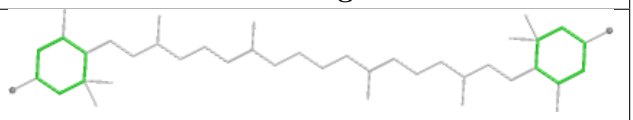
Bond lengths



Bond angles



Torsions

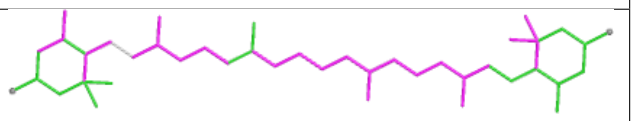


Rings

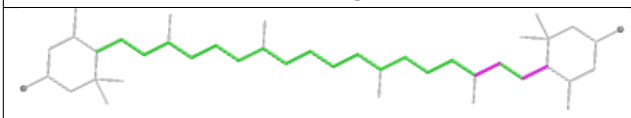
Ligand LUT Z 617



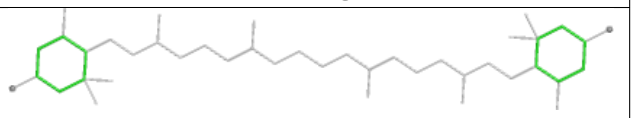
Bond lengths



Bond angles

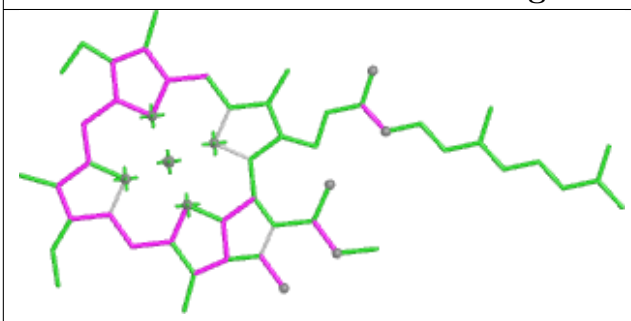


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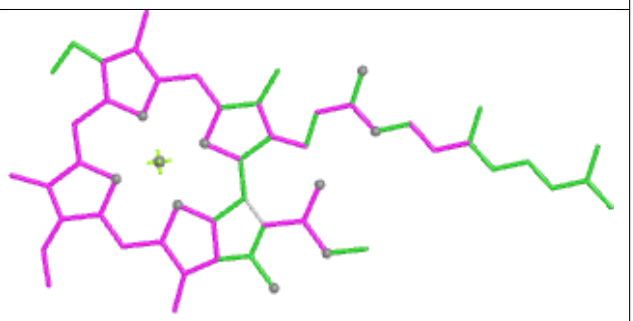


Rings

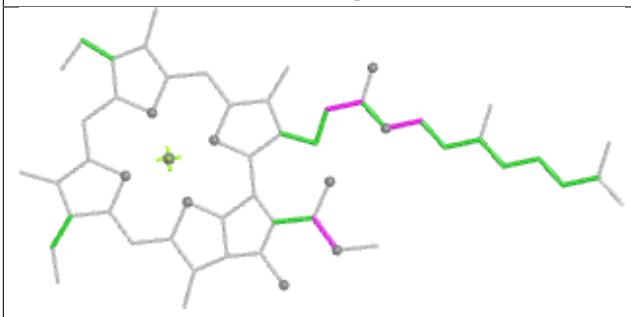
Ligand CLA 5 606



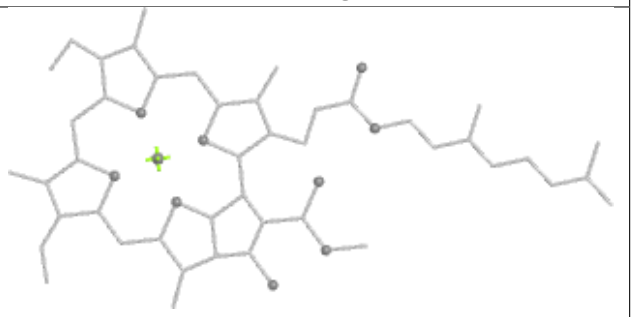
Bond lengths



Bond angles

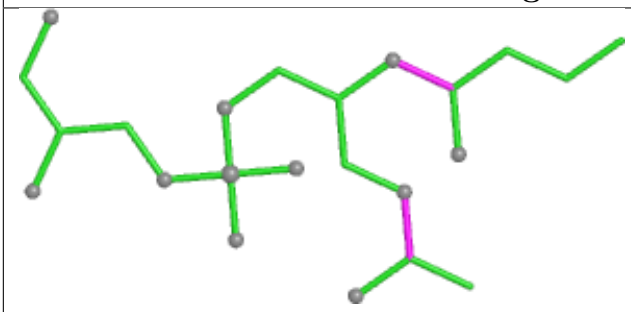


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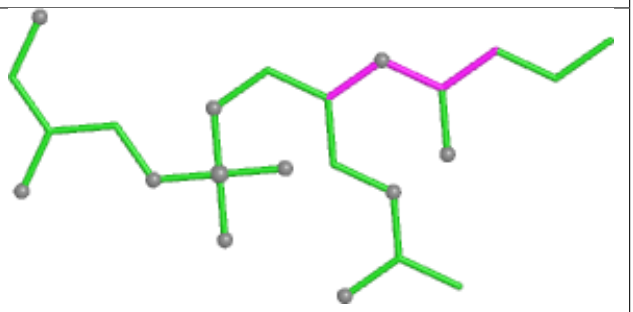


Rings

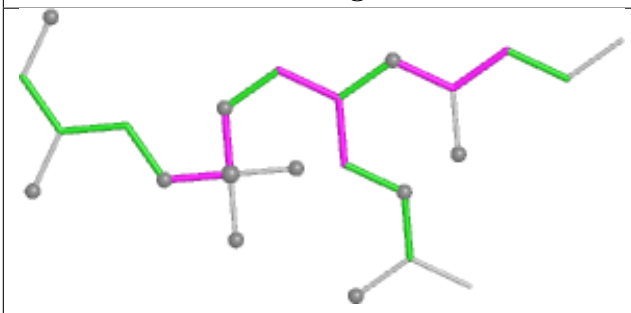
Ligand LHG B 851



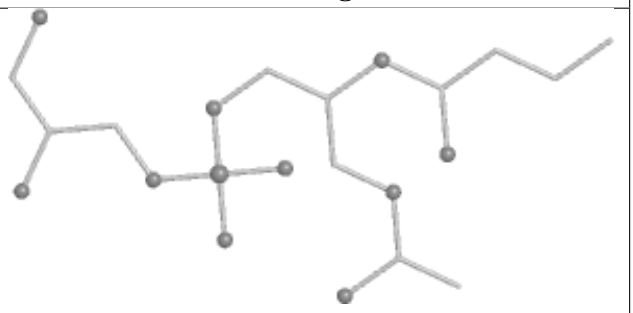
Bond lengths



Bond angles

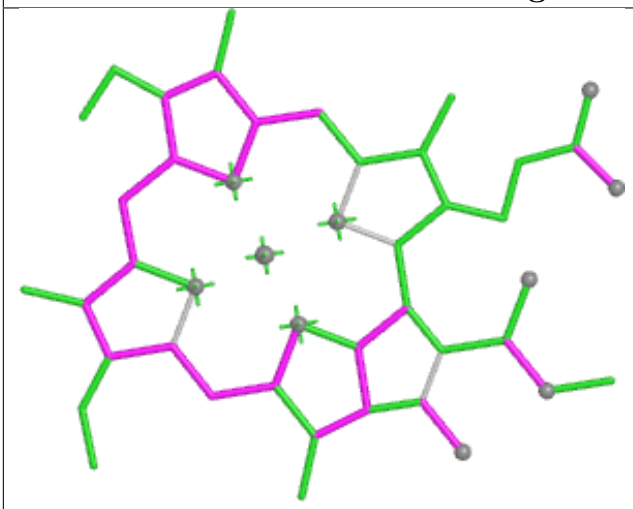


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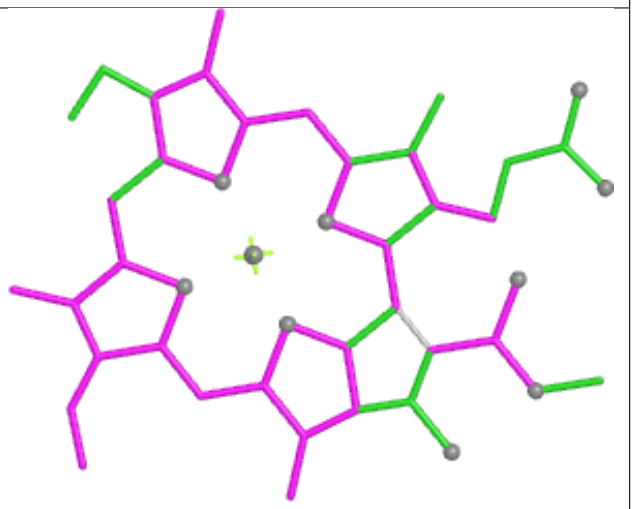


Rings

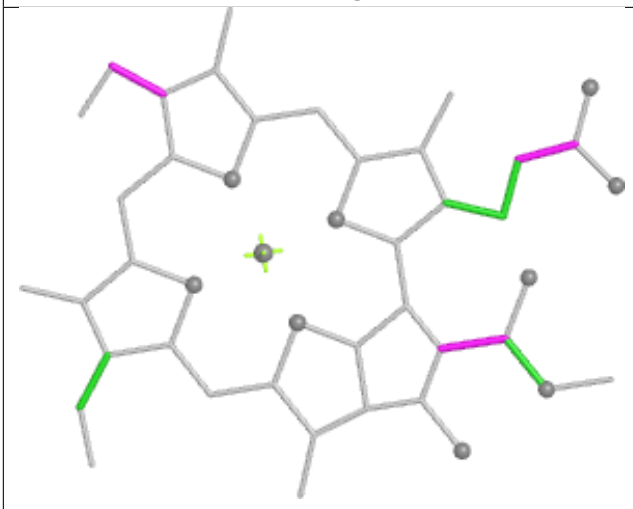
Ligand CLA 6 622



Bond lengths



Bond angles

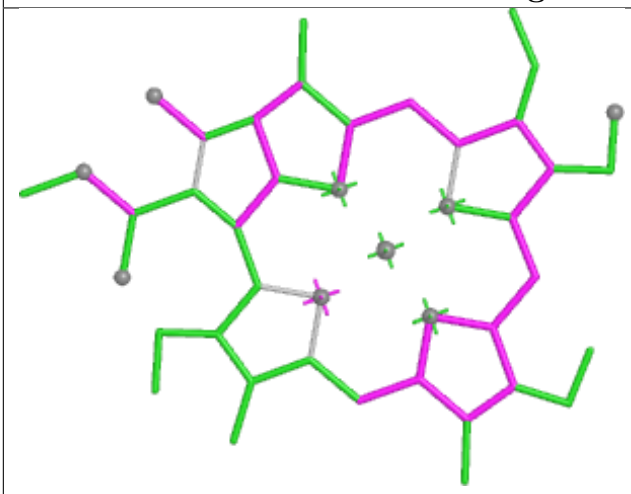


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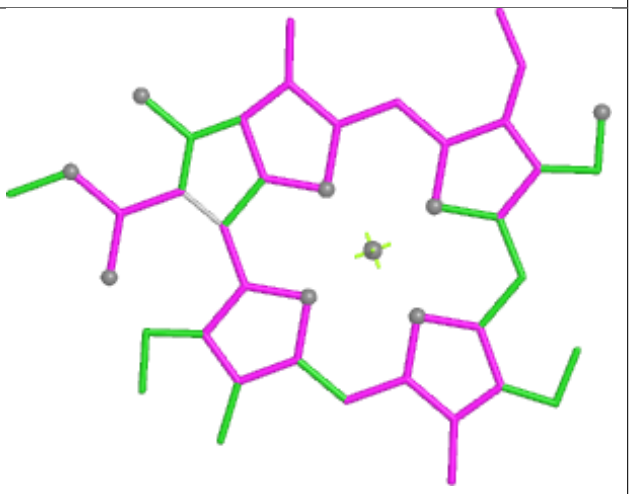


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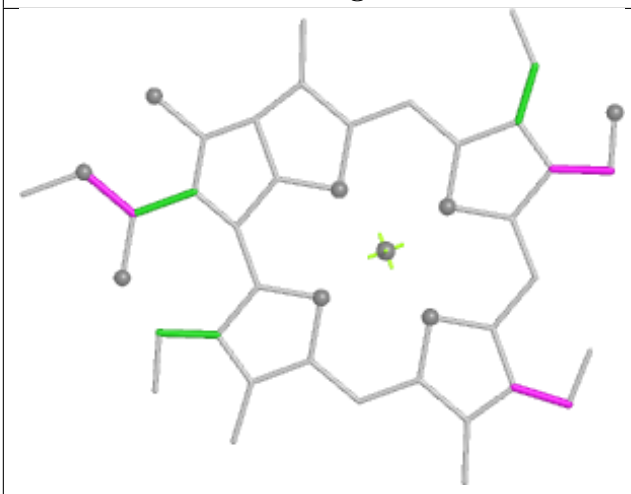
Ligand CHL 4 618



Bond lengths



Bond angles

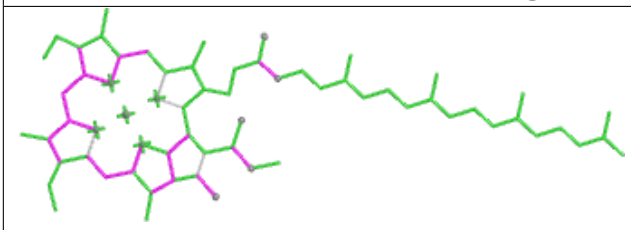


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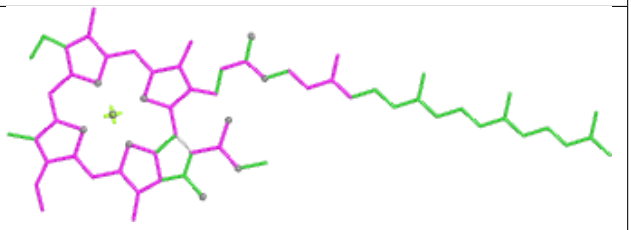


Rings

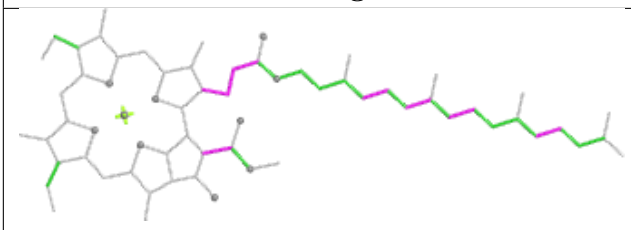
Ligand CLA A 804



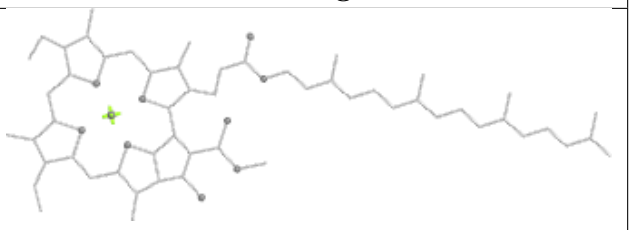
Bond lengths



Bond angles

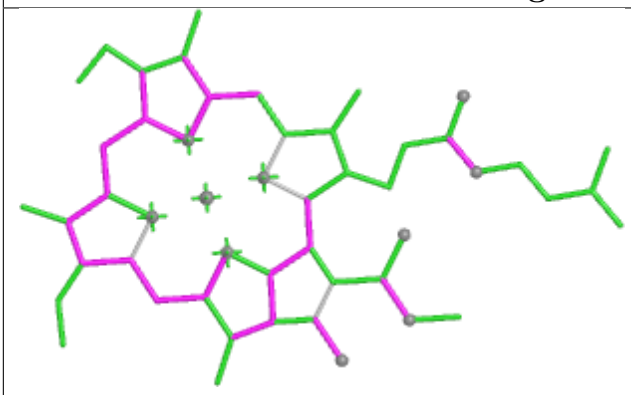


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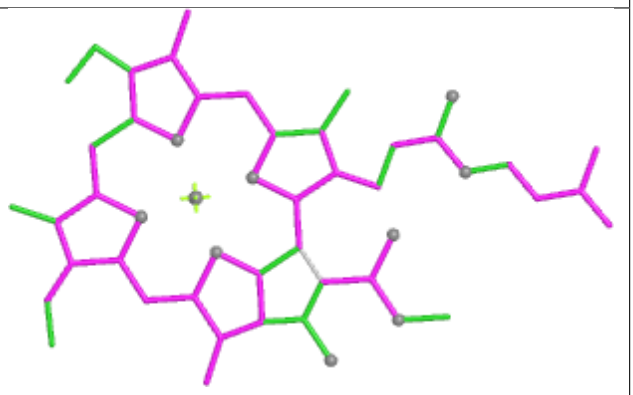


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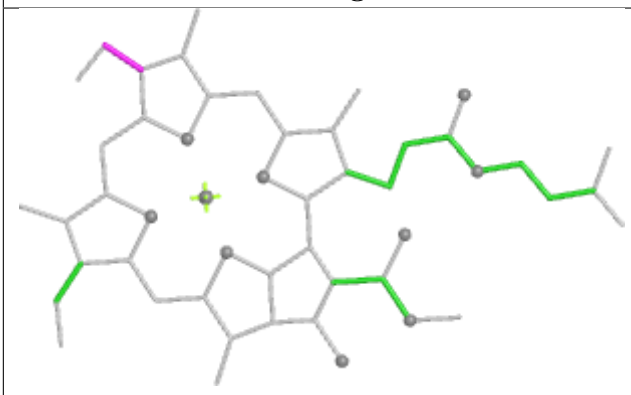
Ligand CLA 9 609



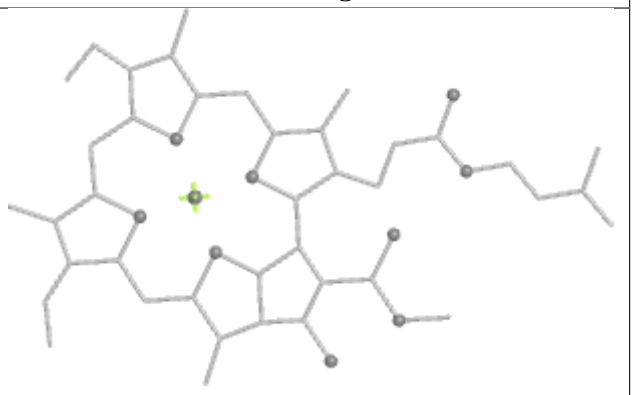
Bond lengths



Bond angles

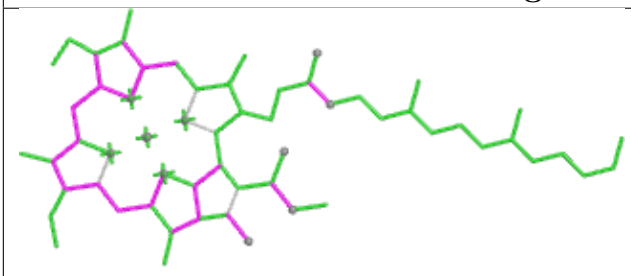


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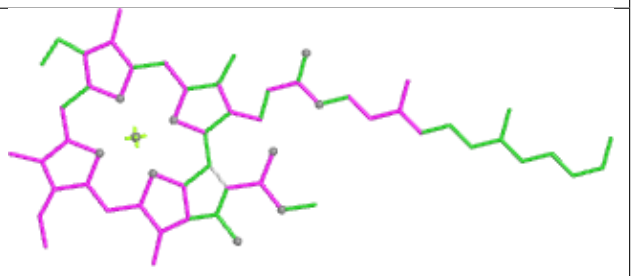


Rings

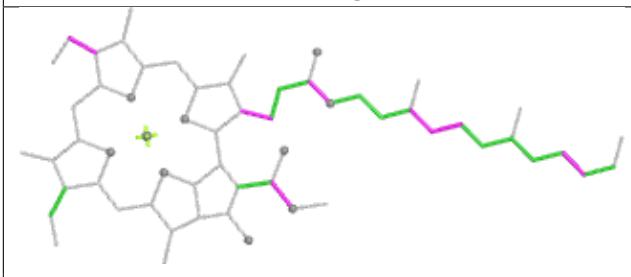
Ligand CLA B 822



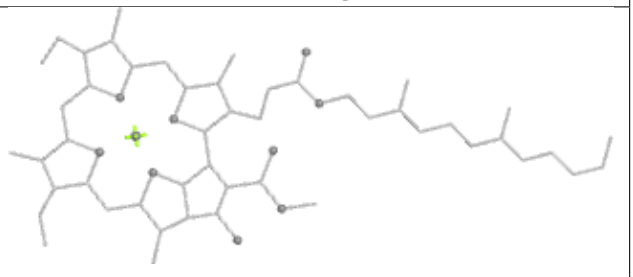
Bond lengths



Bond angles

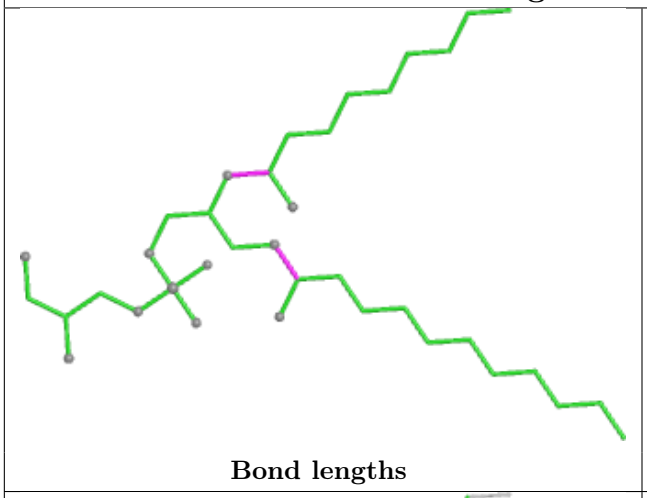


Torsions

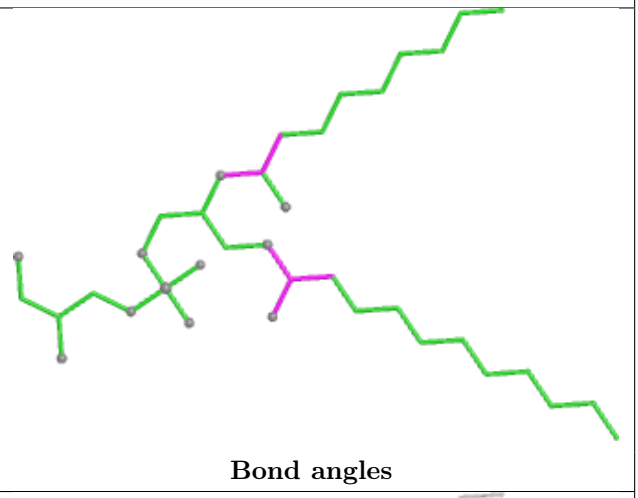


Rings

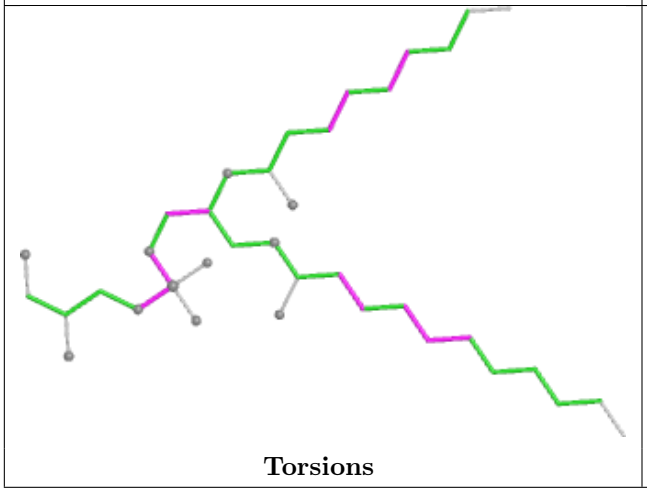
Ligand LHG 7 625



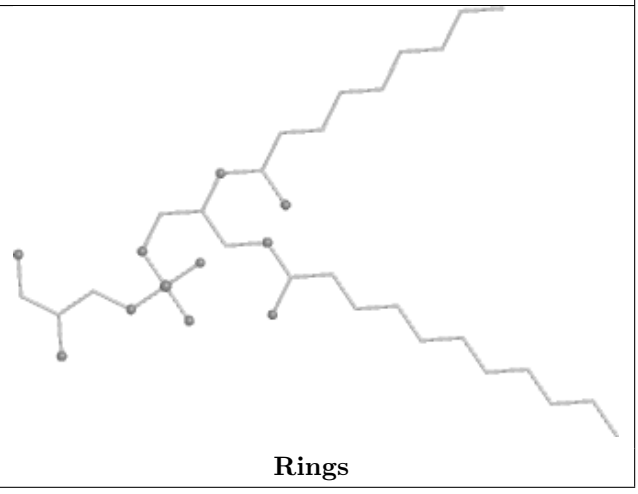
Bond lengths



Bond angles

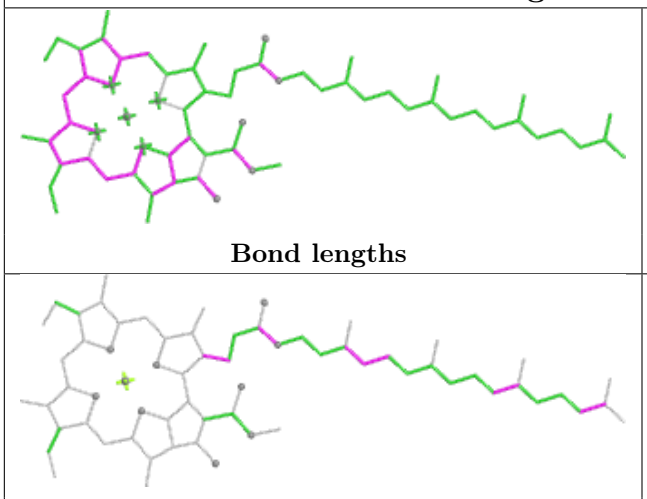


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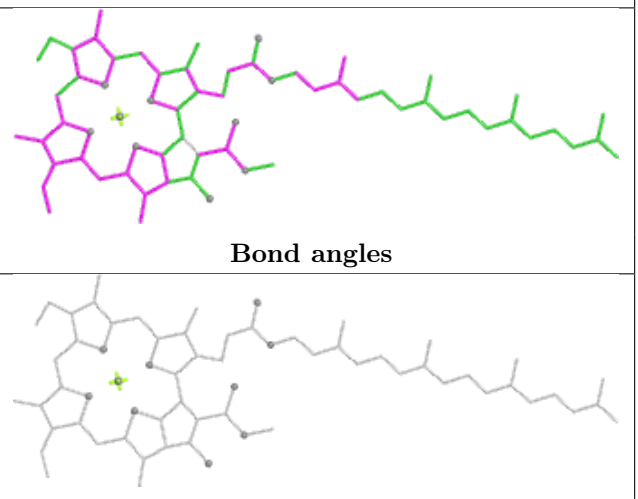


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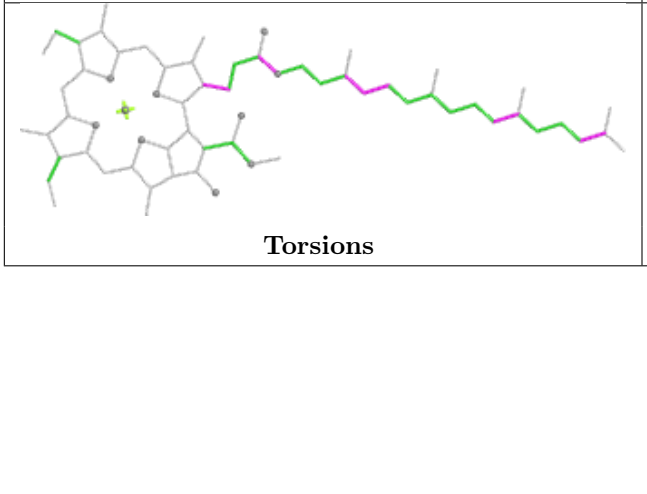
Ligand CLA L 203



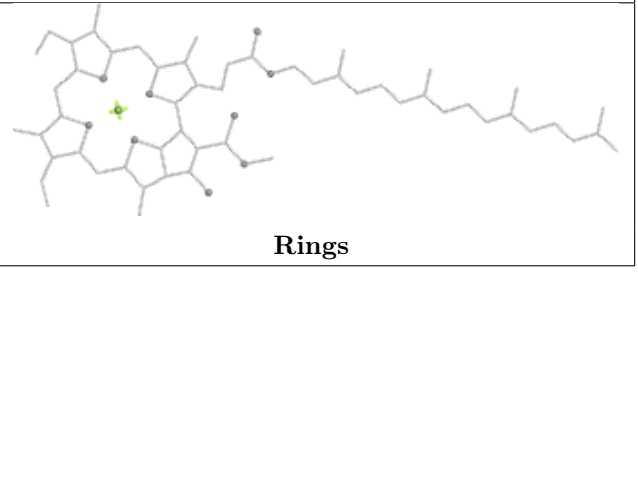
Bond lengths



Bond angles

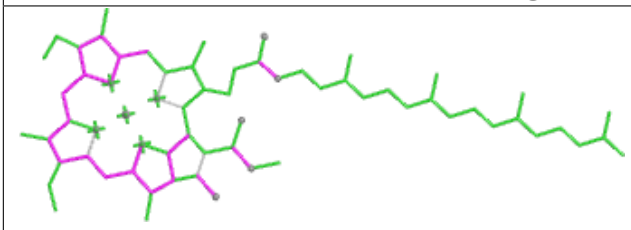


Torsions

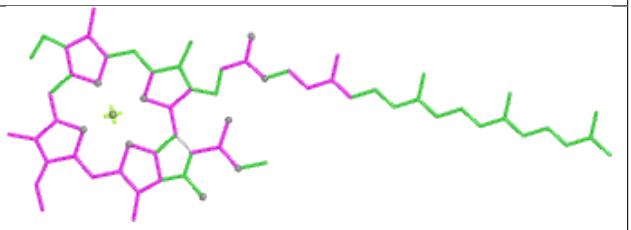


Rings

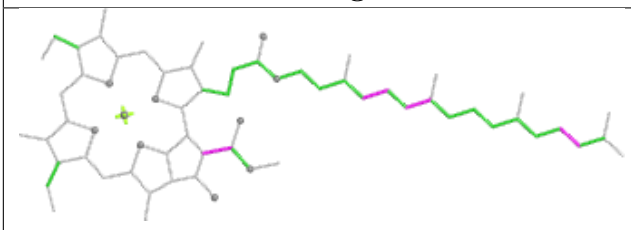
Ligand CLA B 841



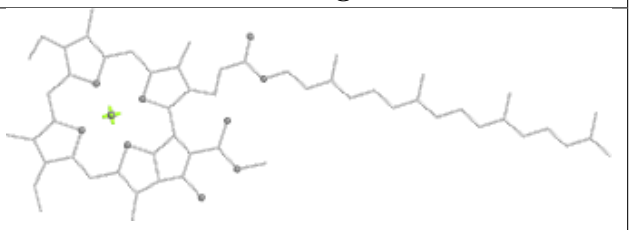
Bond lengths



Bond angles

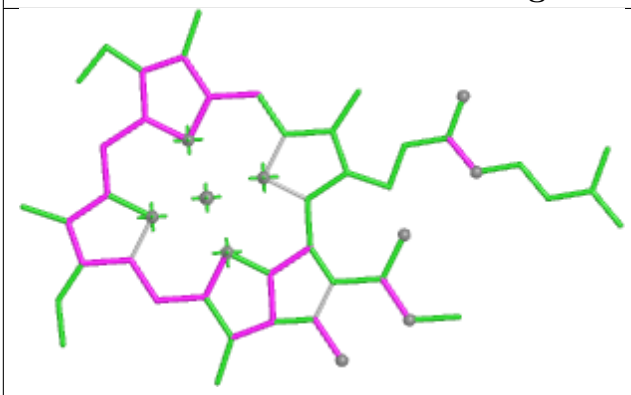


Torsions

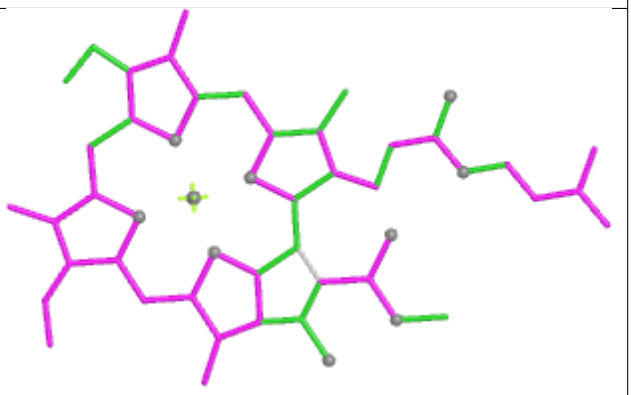


Rings

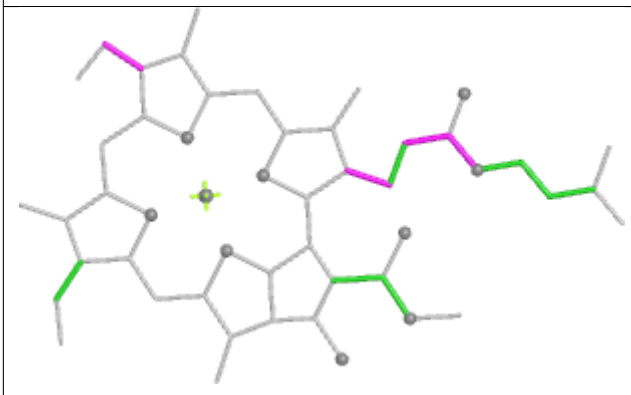
Ligand CLA 2 607



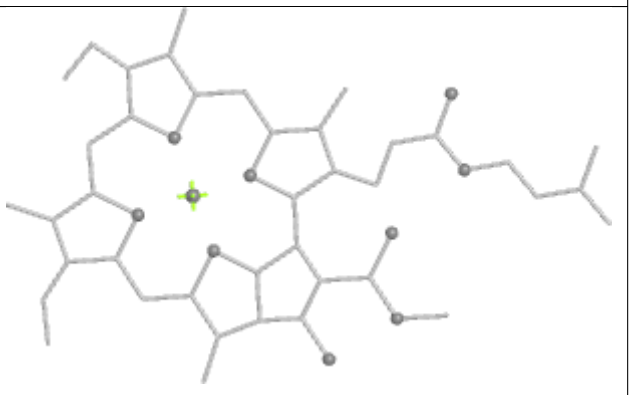
Bond lengths



Bond angles

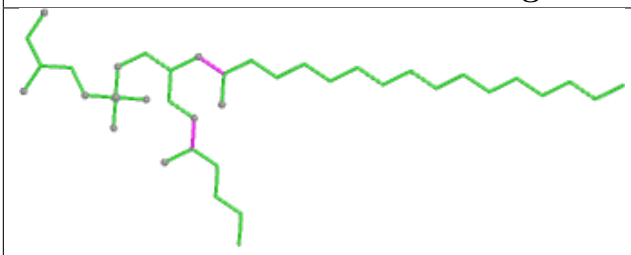


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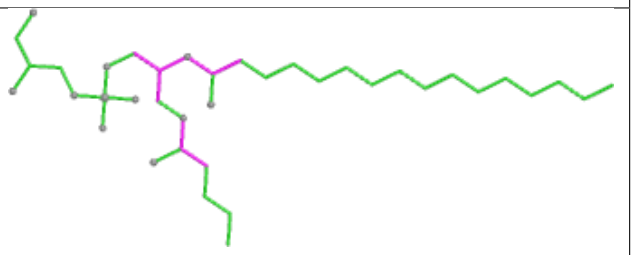


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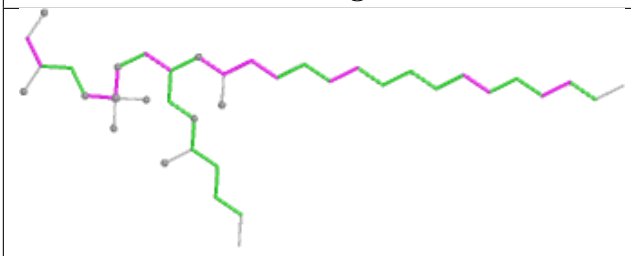
Ligand LHG A 847



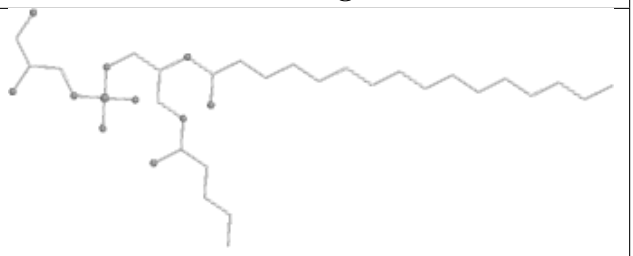
Bond lengths



Bond angles



Torsions

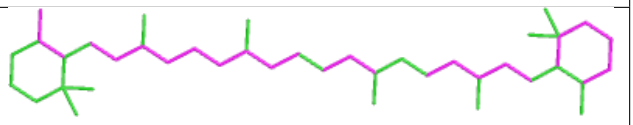


Rings

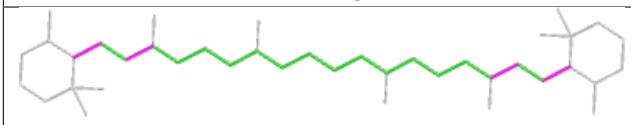
Ligand BCR B 844



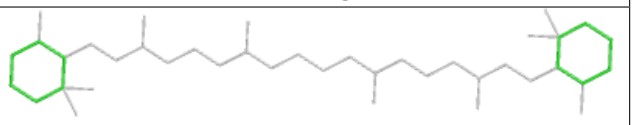
Bond lengths



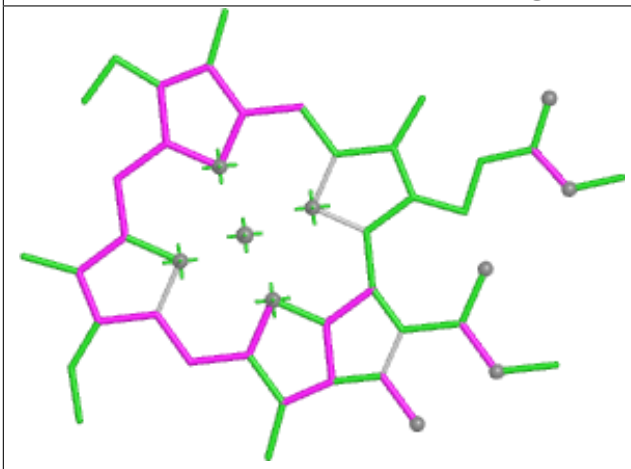
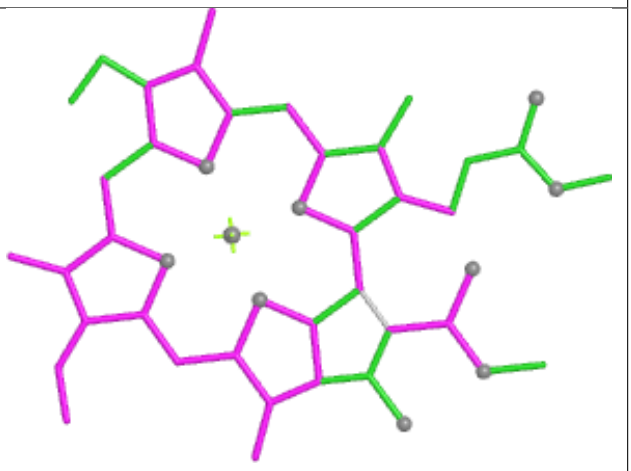
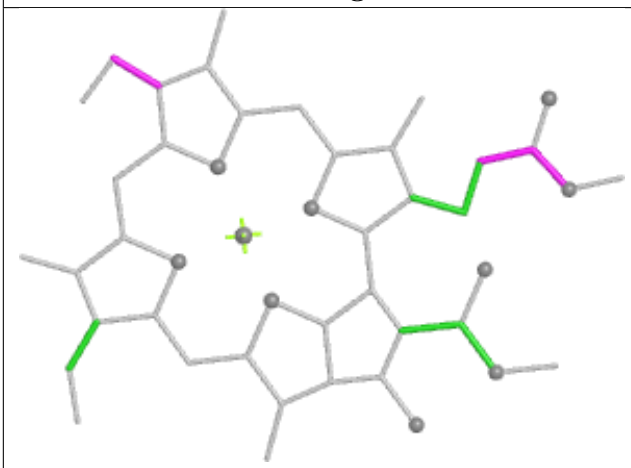
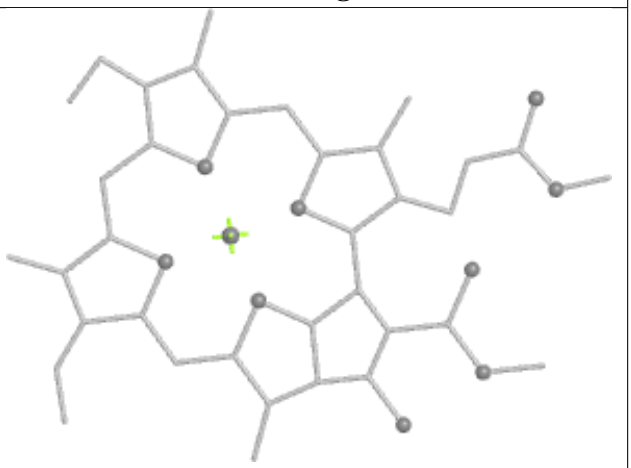
Bond angles

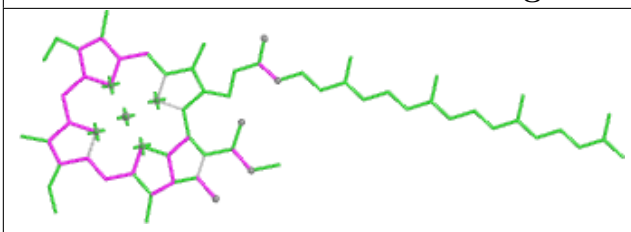
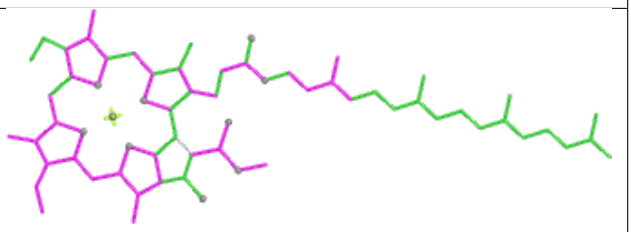
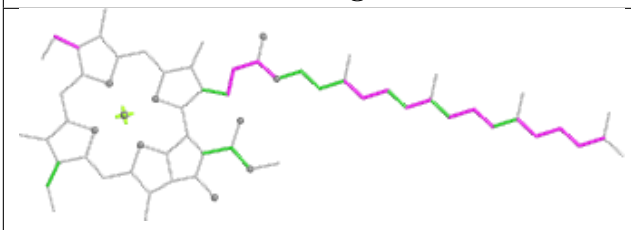
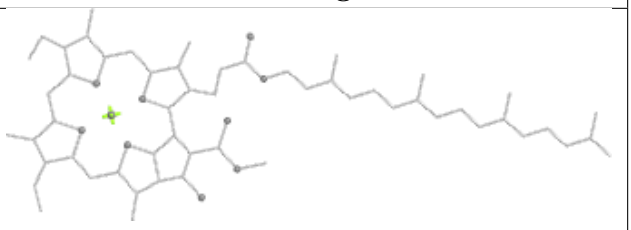


Torsions

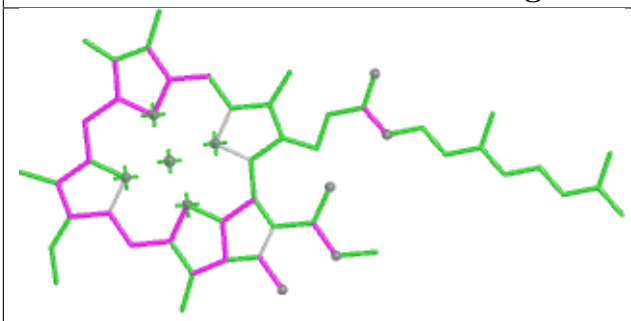


Rings

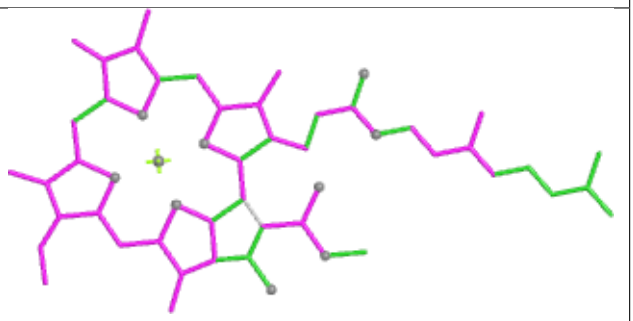
Ligand CLA 6 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

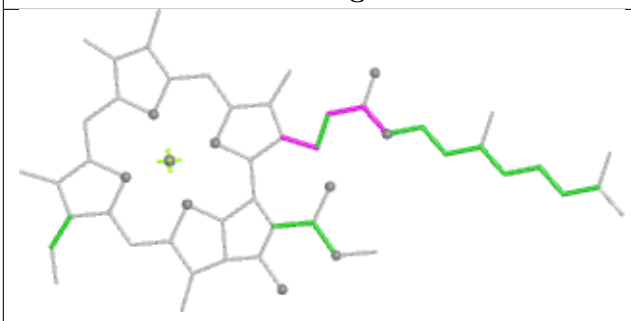
Ligand CLA B 811



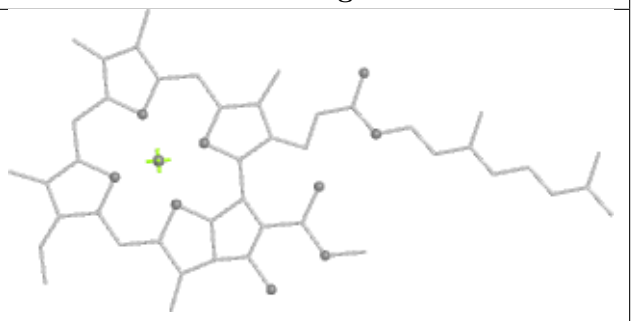
Bond lengths



Bond angles

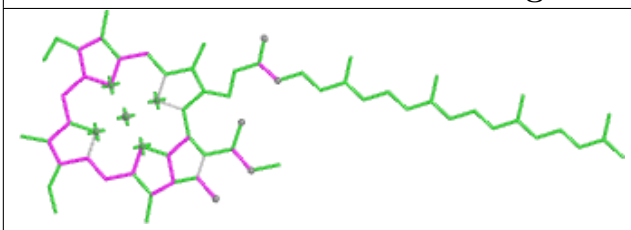


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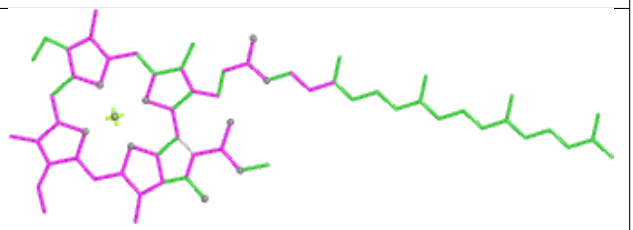


Rings

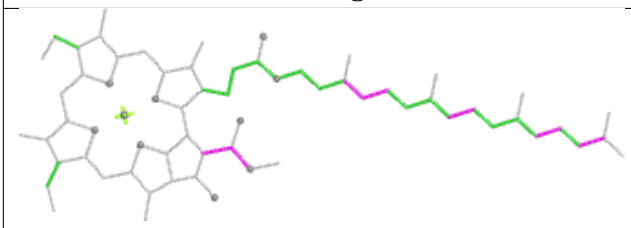
Ligand CLA F 301



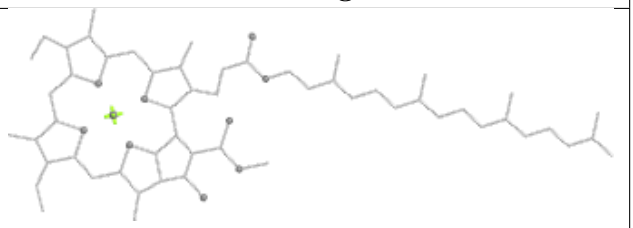
Bond lengths



Bond angles

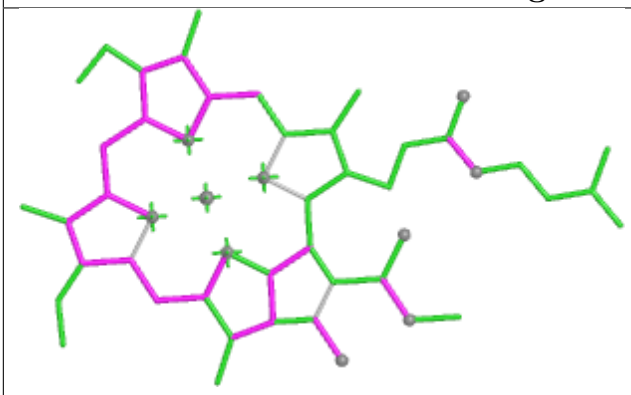


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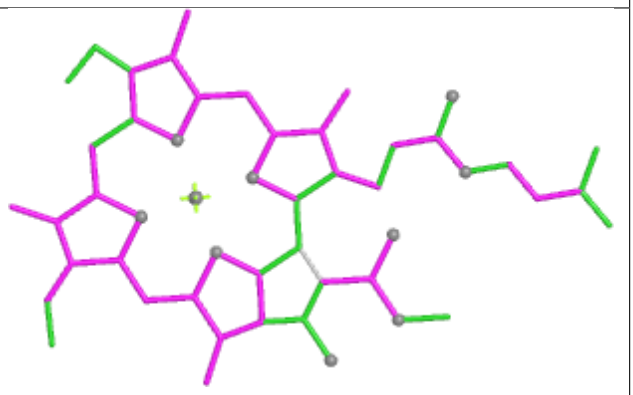


Rings

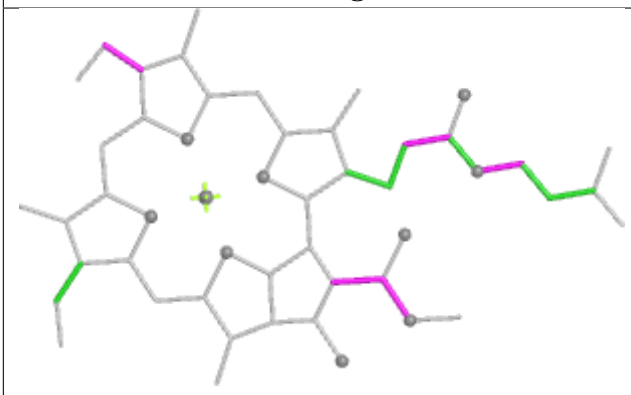
Ligand CLA 3 609



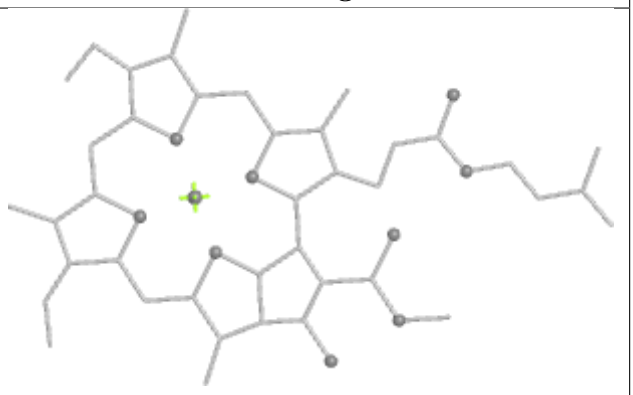
Bond lengths



Bond angles

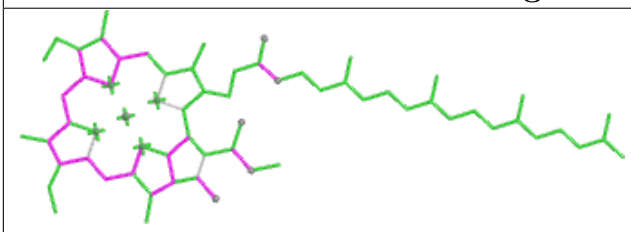


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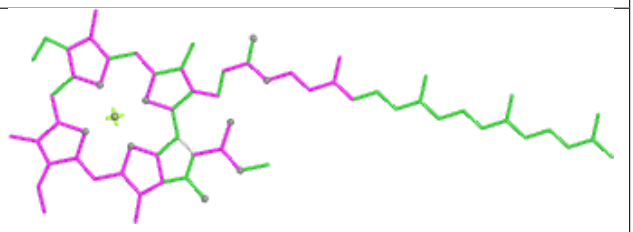


Rings

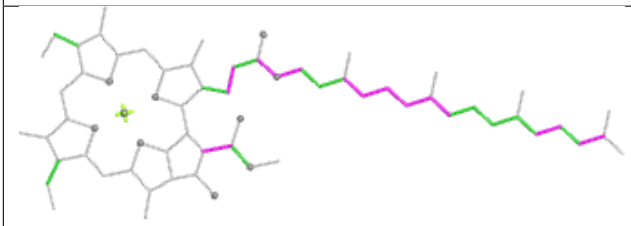
Ligand CLA A 842



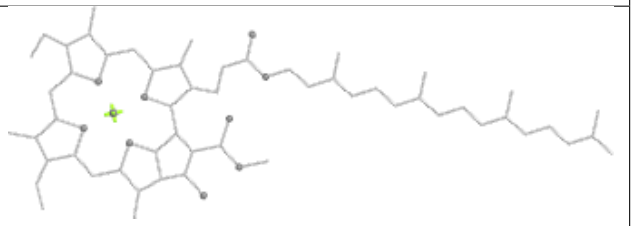
Bond lengths



Bond angles

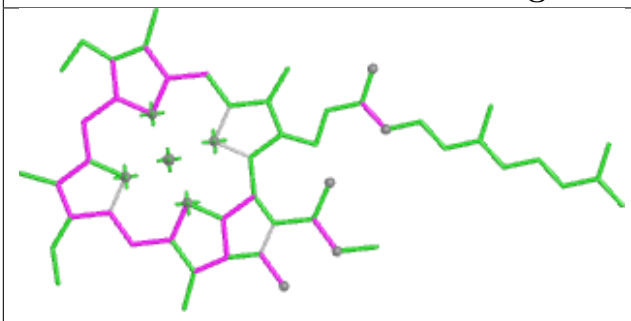


Torsions

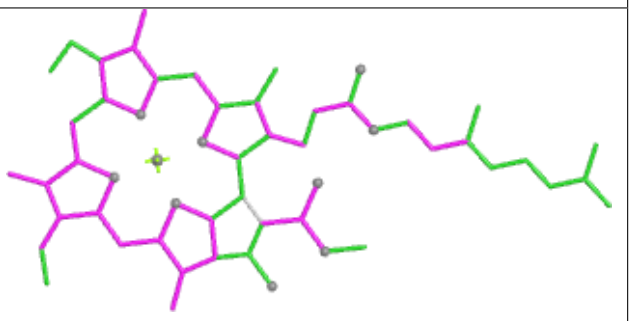


Rings

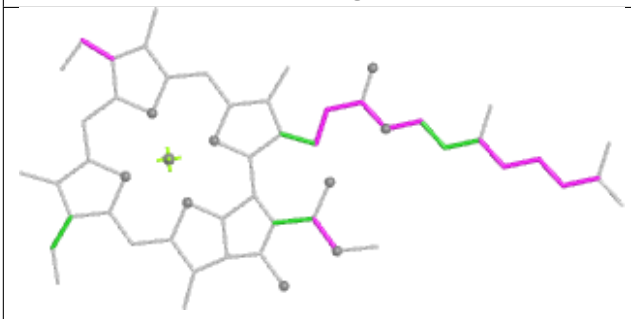
Ligand CLA 3 613



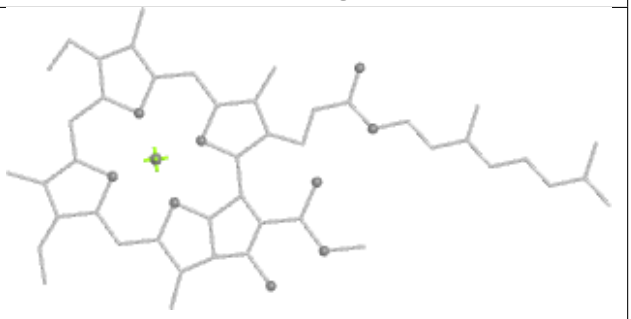
Bond lengths



Bond angles

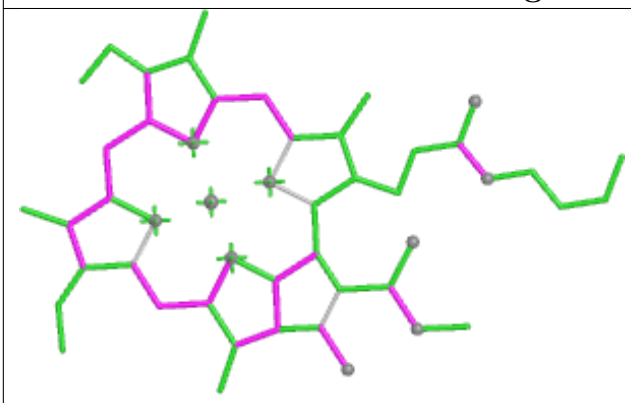


Torsions

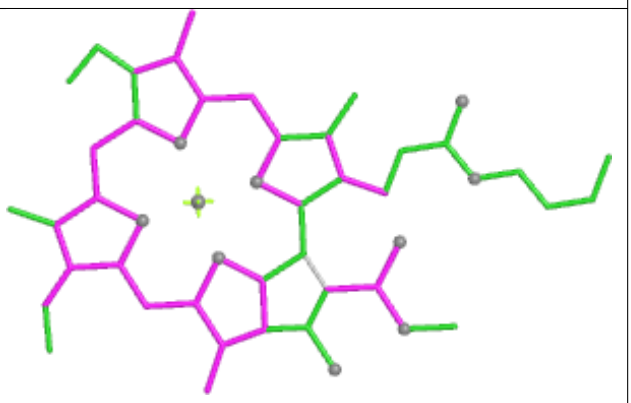


Rings

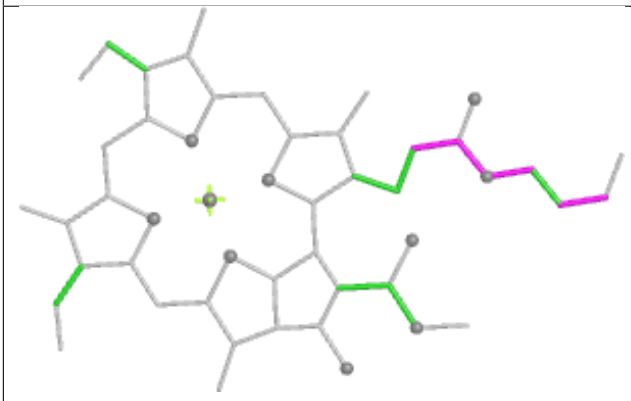
Ligand CLA B 831



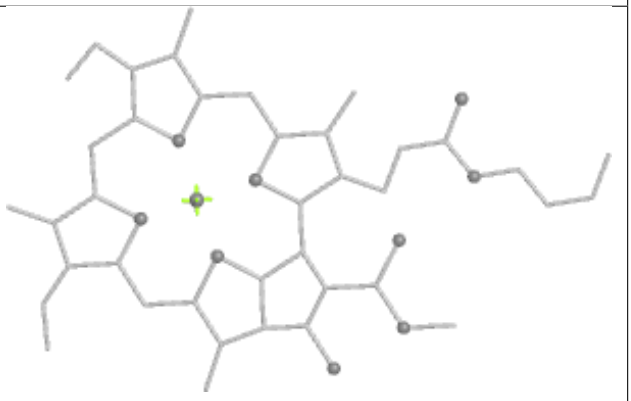
Bond lengths



Bond angles

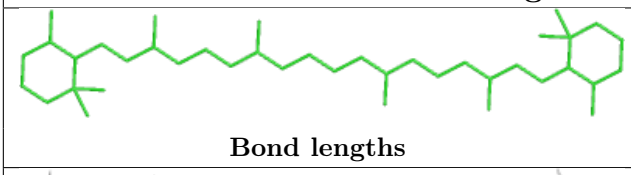


Torsions

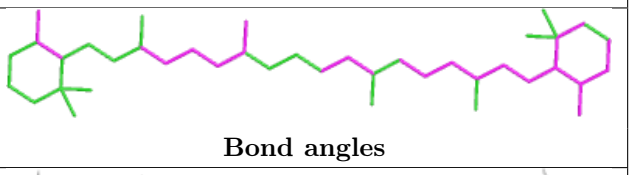


Rings

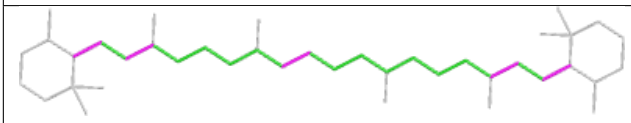
Ligand BCR L 205



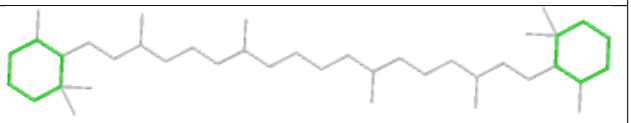
Bond lengths



Bond angles

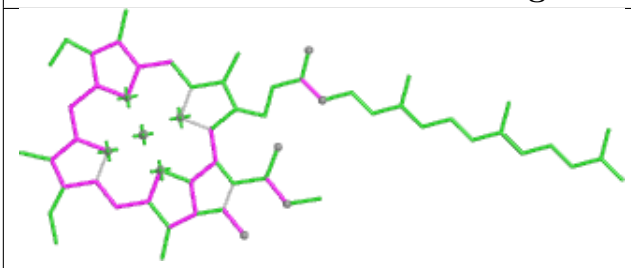


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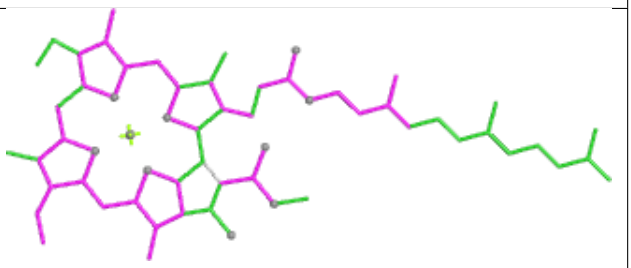


Rings

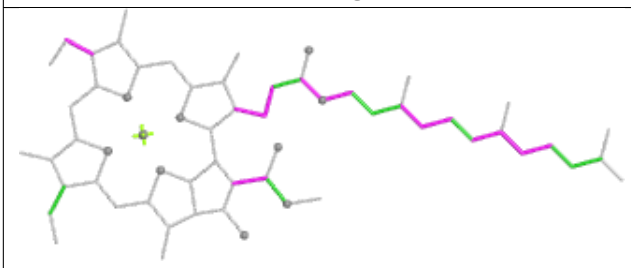
Ligand CLA 3 607



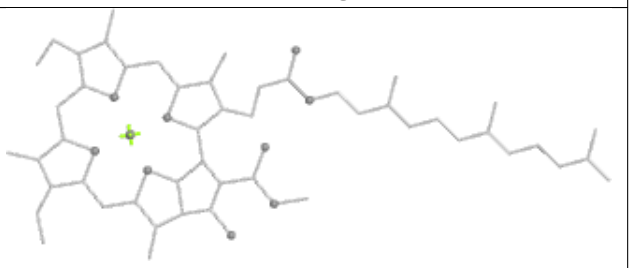
Bond lengths



Bond angles



Torsions

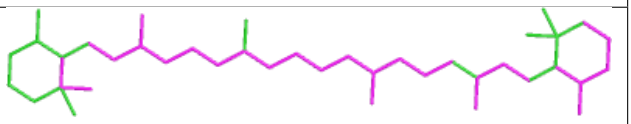


Rings

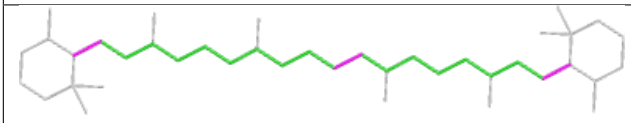
Ligand BCR 3 717



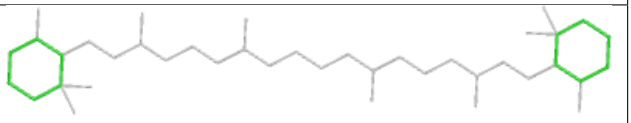
Bond lengths



Bond angles

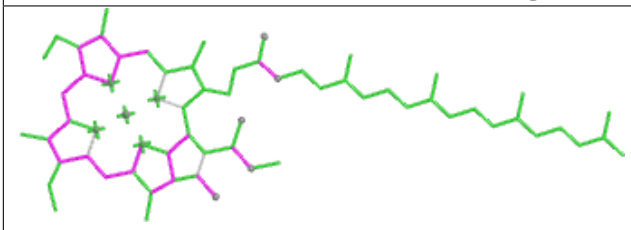


Torsions

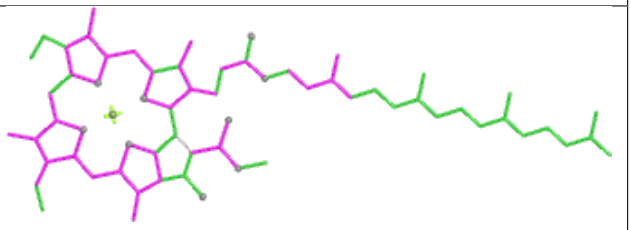


Rings

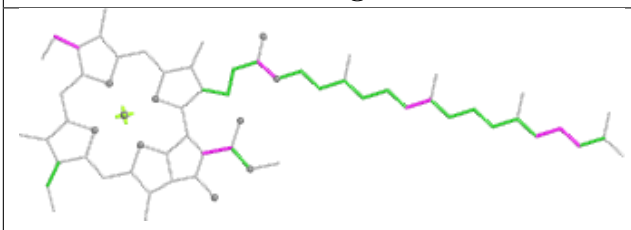
Ligand CLA B 825



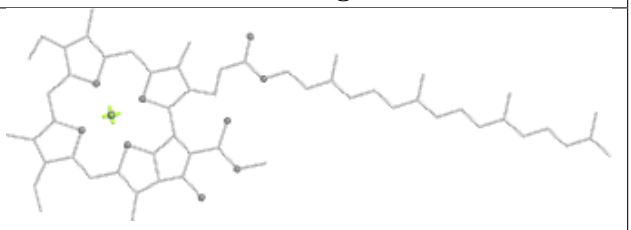
Bond lengths



Bond angles

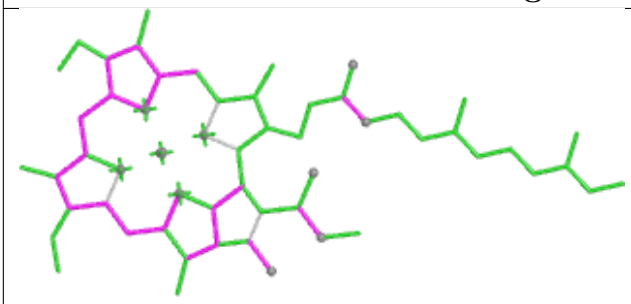


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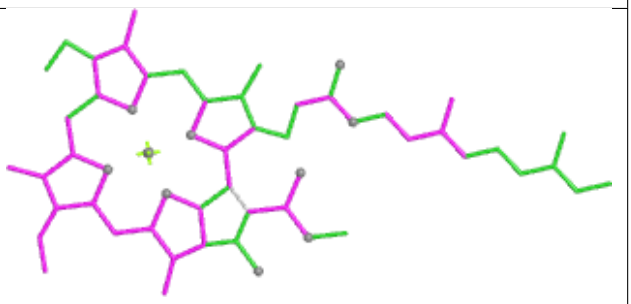


Rings

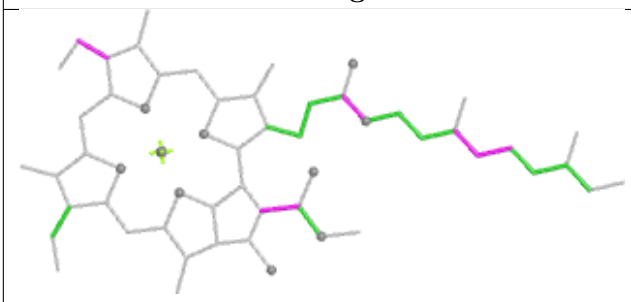
Ligand CLA B 820



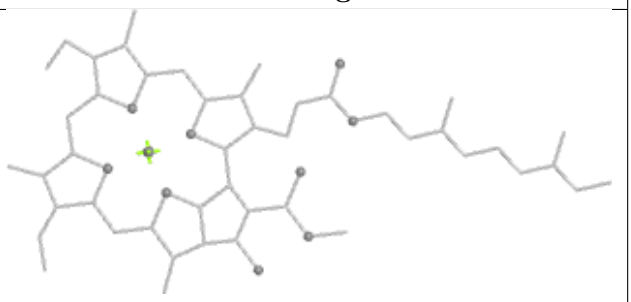
Bond lengths



Bond angles

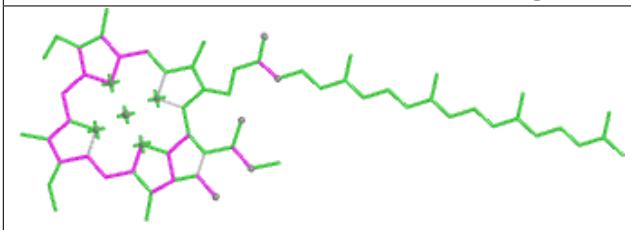


Torsions

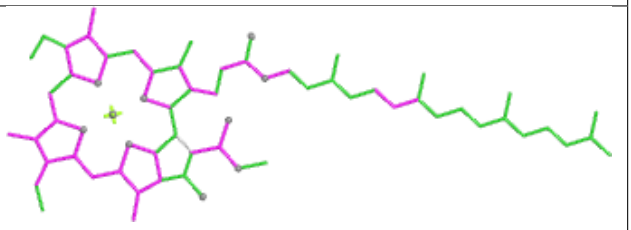


Rings

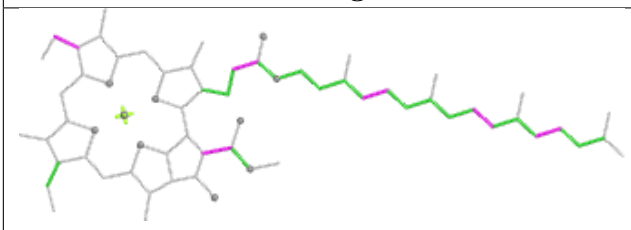
Ligand CLA 1 613



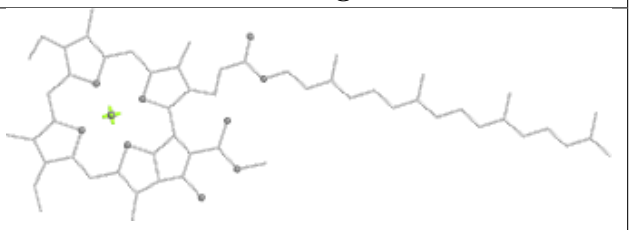
Bond lengths



Bond angles

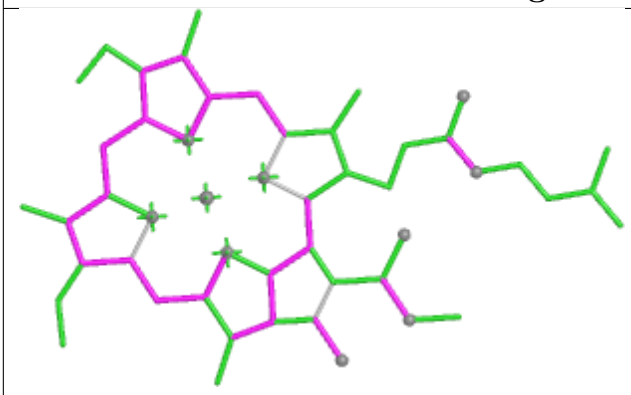


Torsions

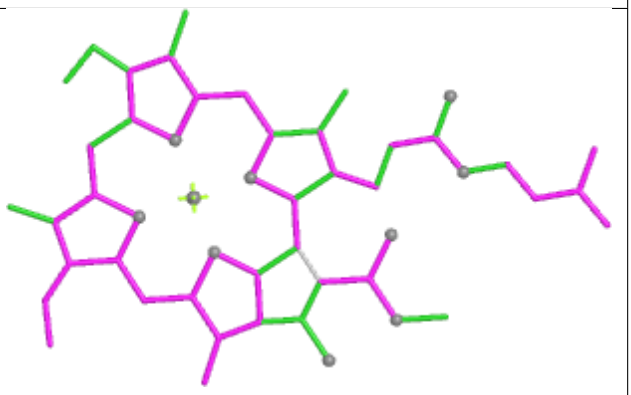


Rings

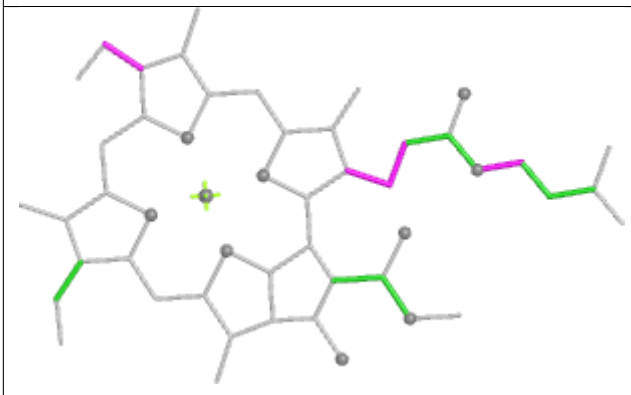
Ligand CLA 5 609



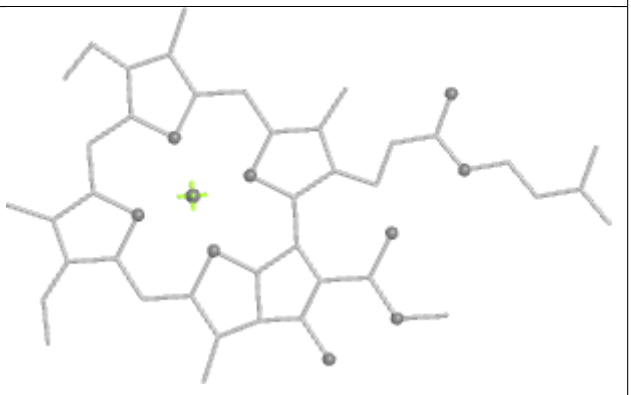
Bond lengths



Bond angles

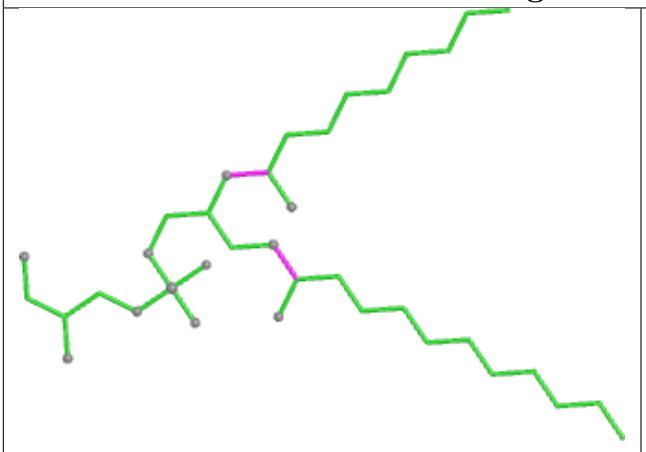


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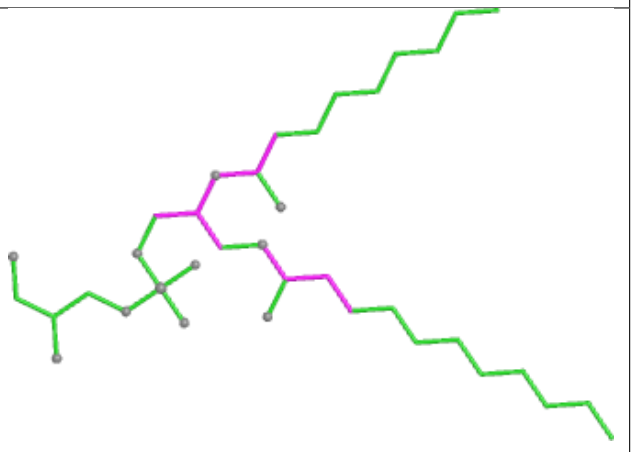


Rings

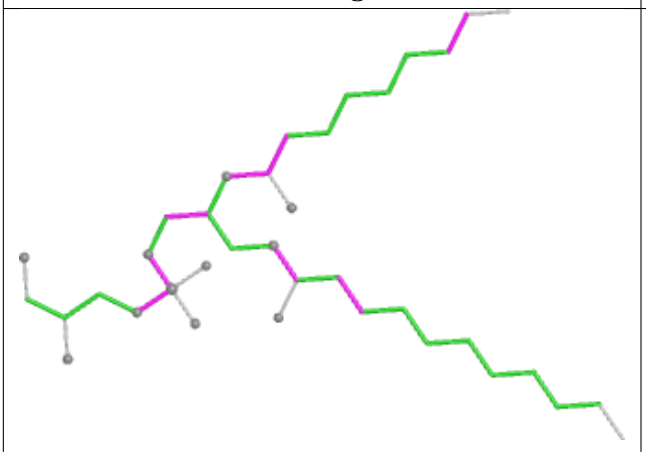
Ligand LHG 8 620



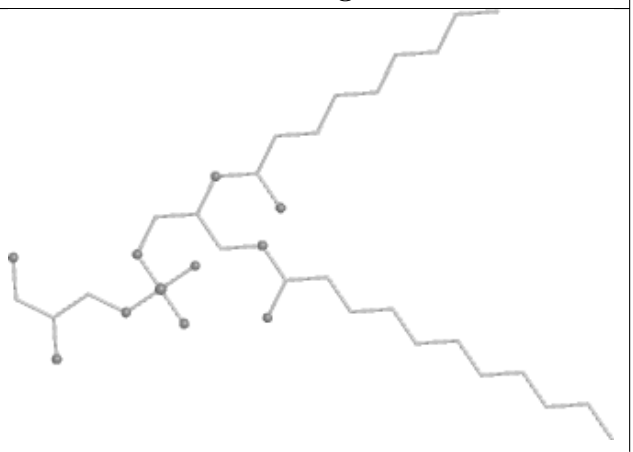
Bond lengths



Bond angles

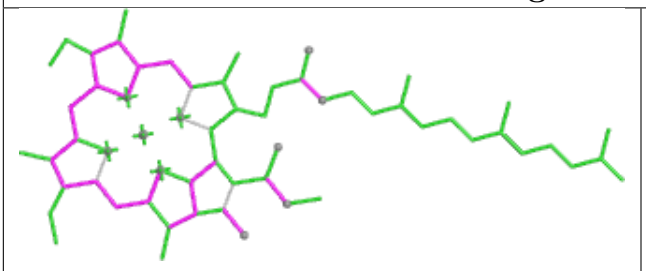


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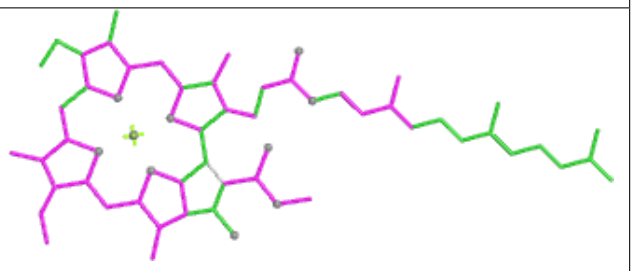


Rings

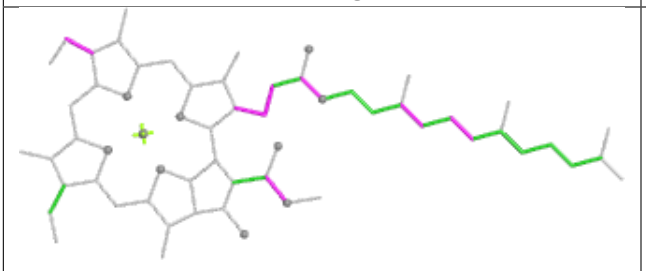
Ligand CLA 6 610



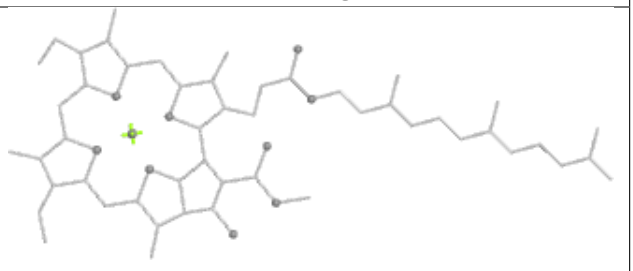
Bond lengths



Bond angles

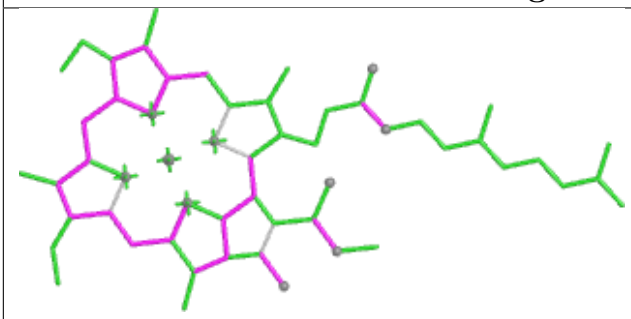


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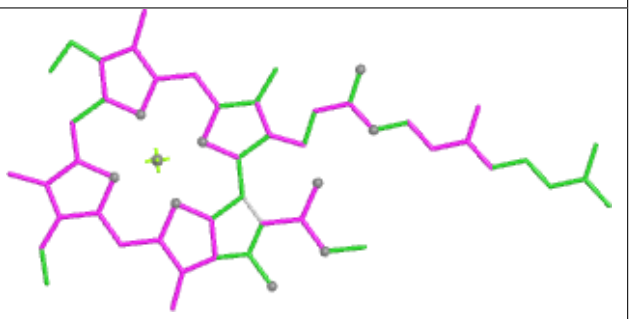


Rings

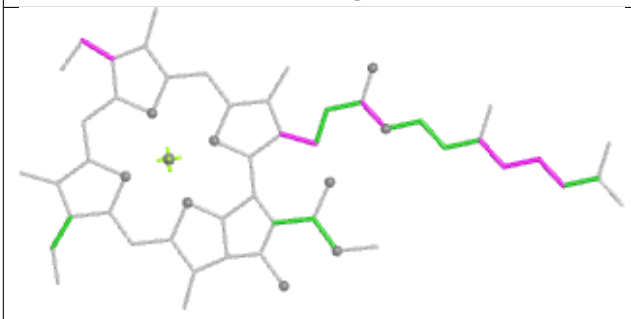
Ligand CLA 6 611



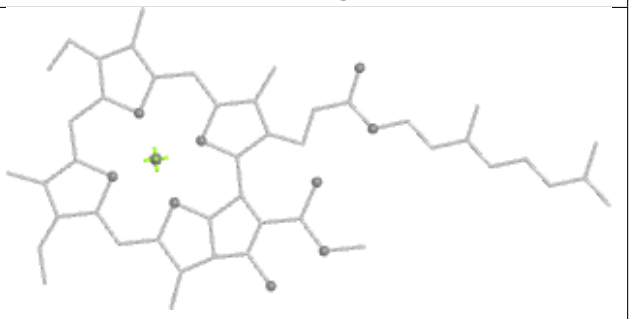
Bond lengths



Bond angles

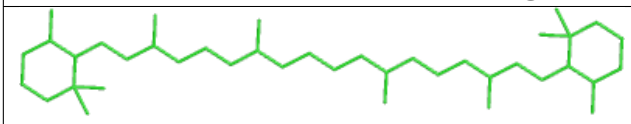


Torsions

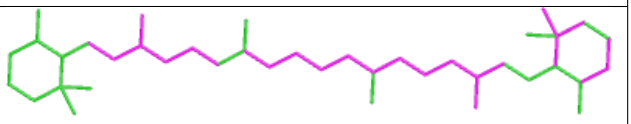


Rings

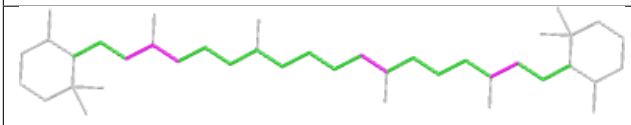
Ligand BCR A 852



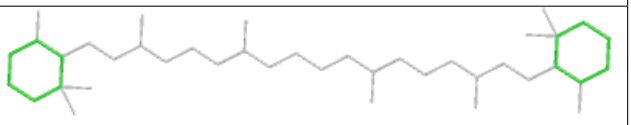
Bond lengths



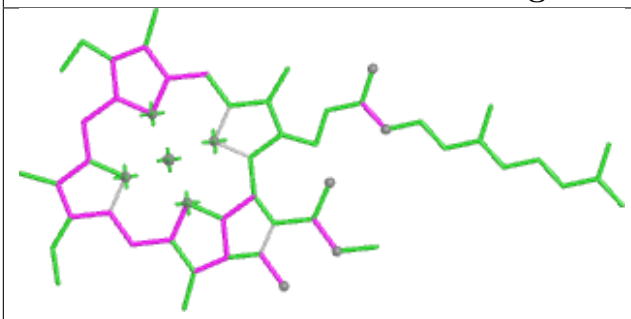
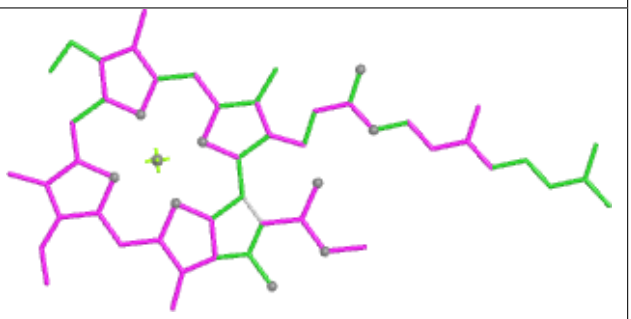
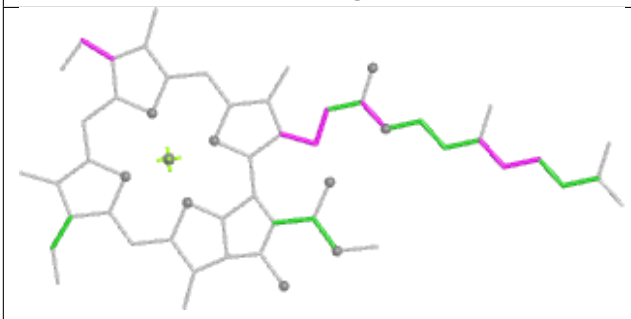
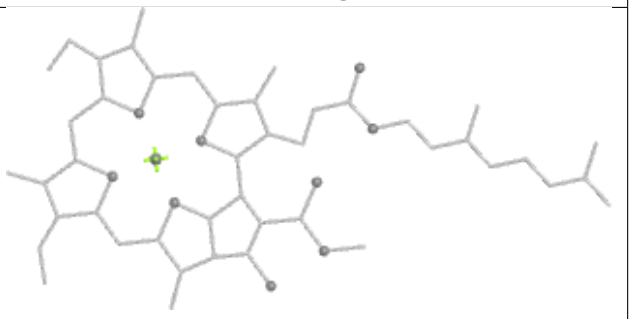
Bond angles

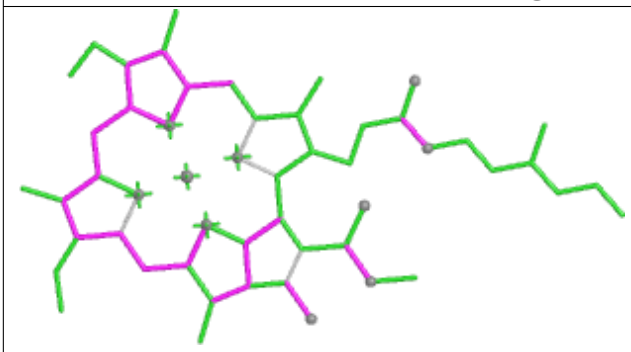
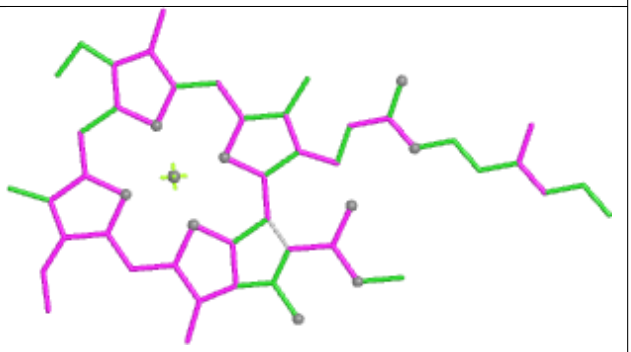
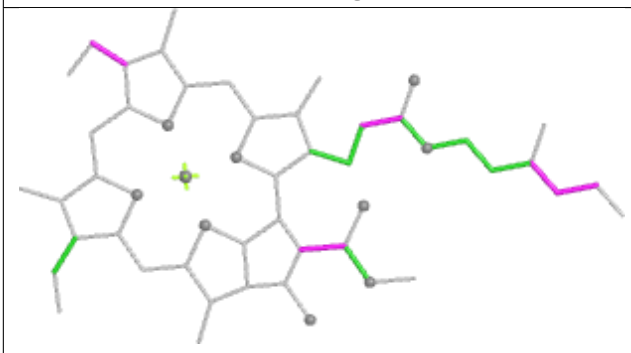
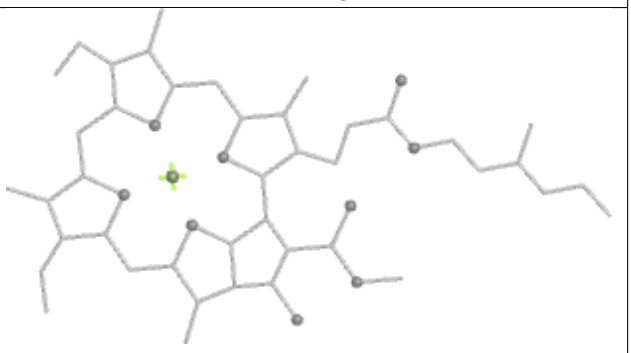


Torsions

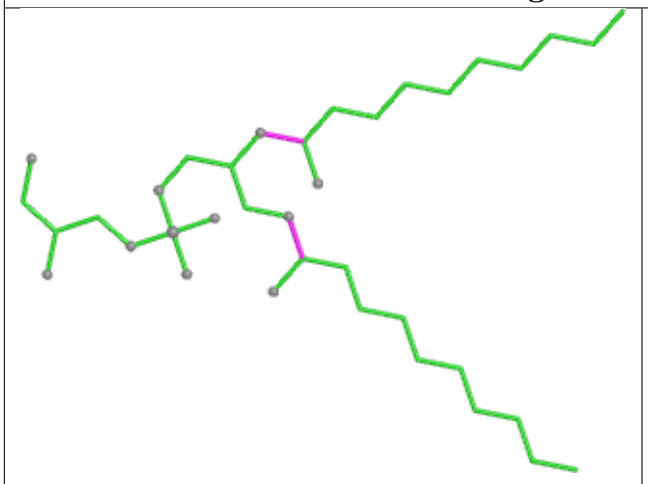


Rings

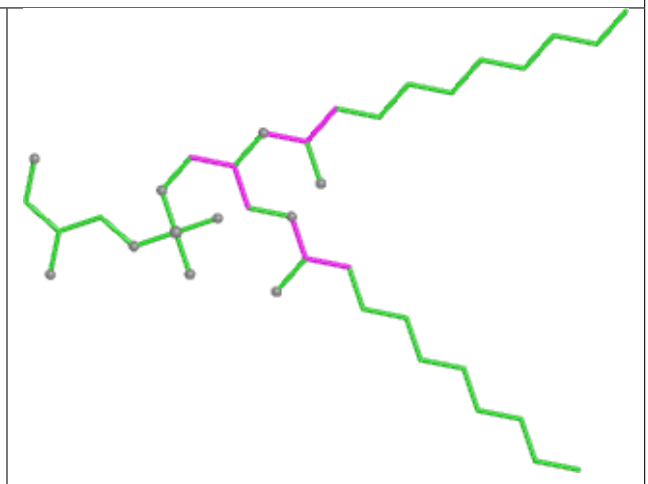
Ligand CLA 2 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

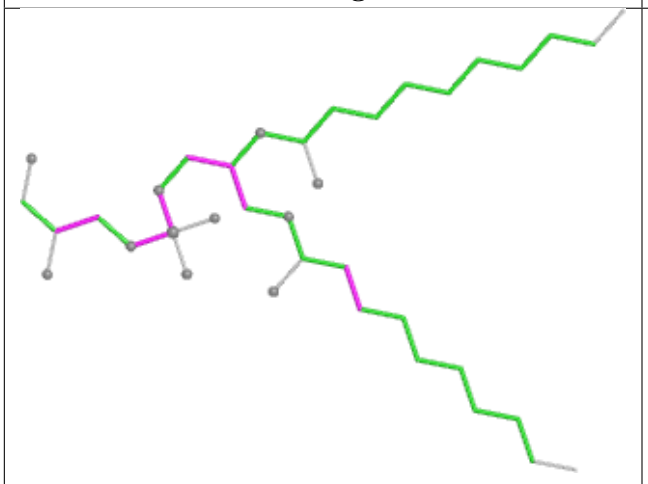
Ligand LHG 5 623



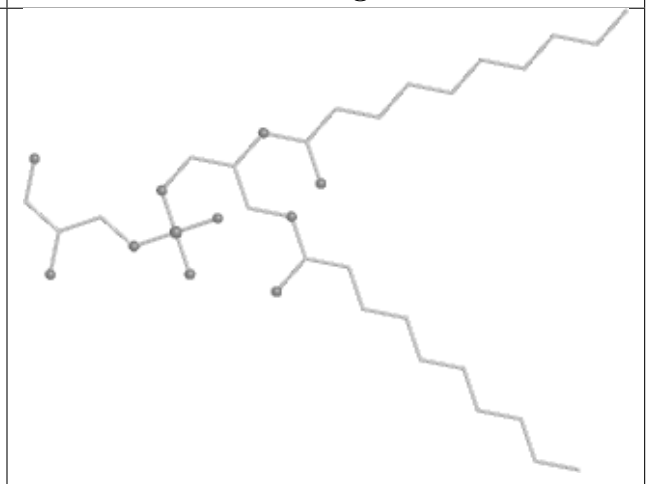
Bond lengths



Bond angles

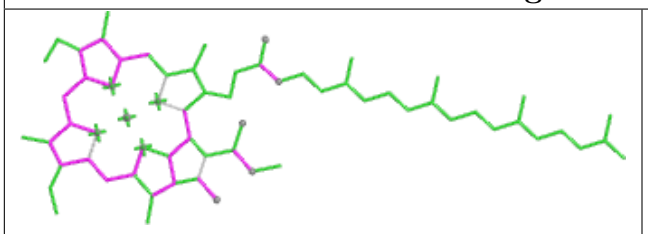


Torsions

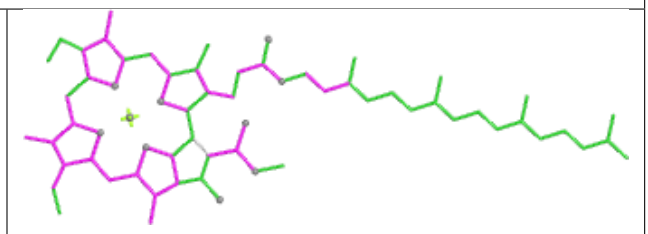


Rings

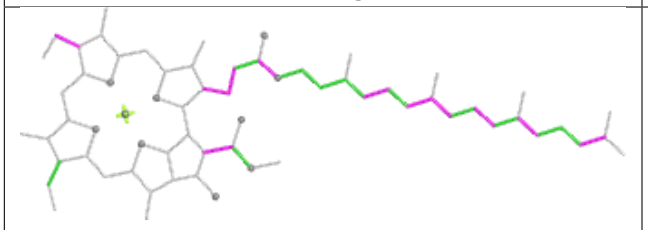
Ligand CLA A 812



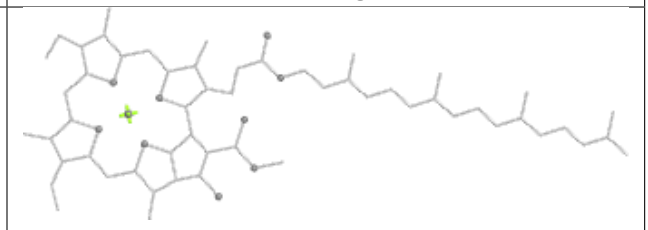
Bond lengths



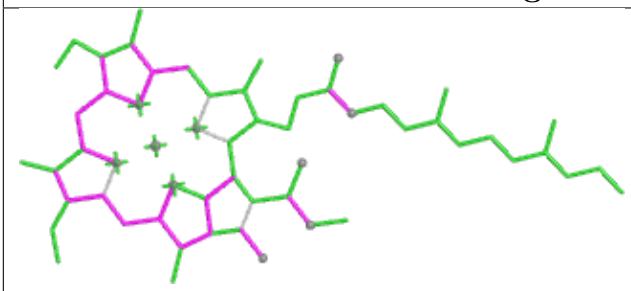
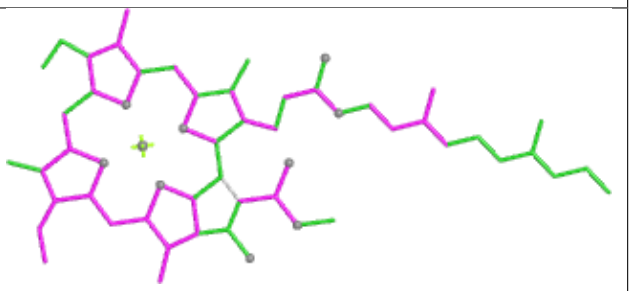
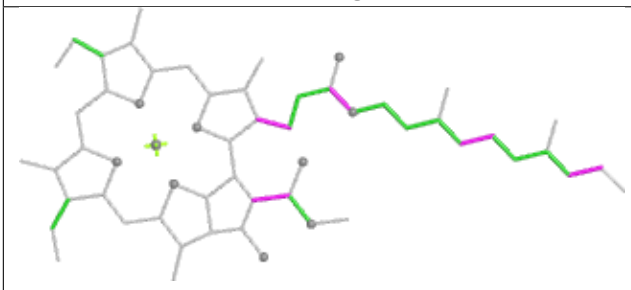
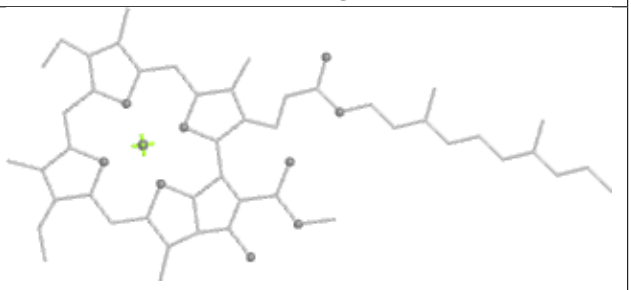
Bond angles

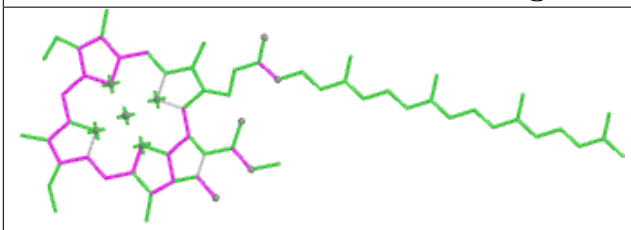
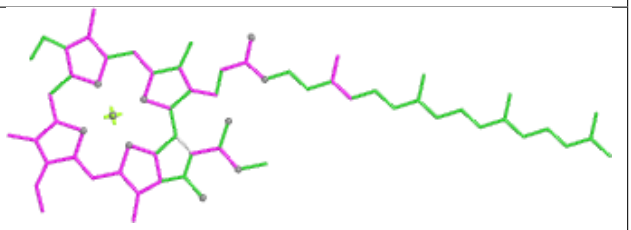
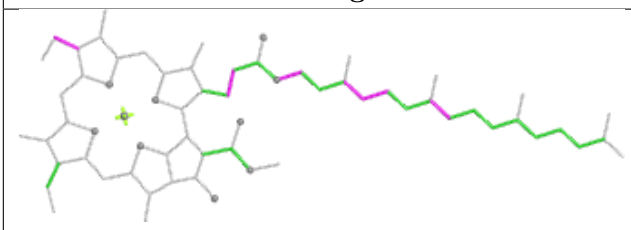
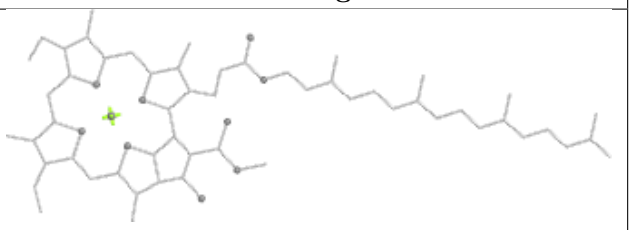


Torsions

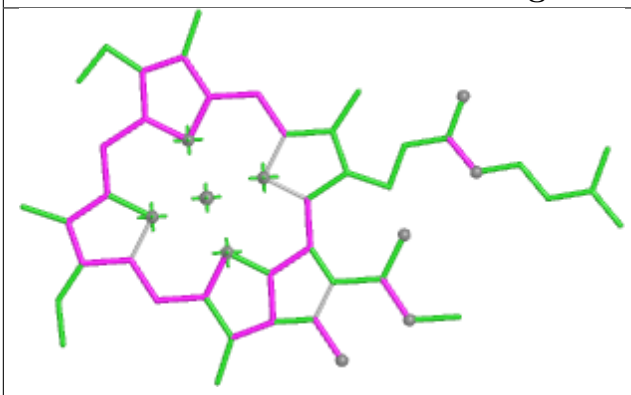


Rings

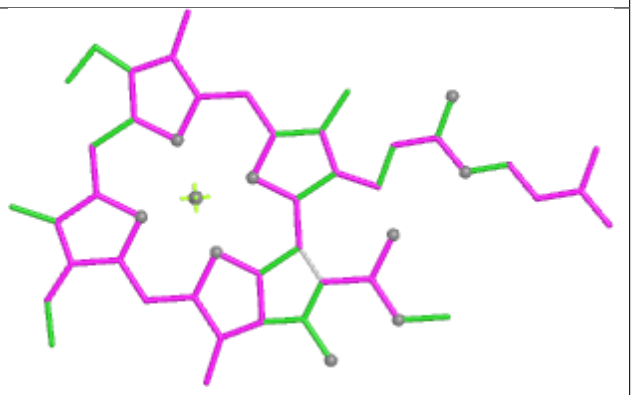
Ligand CLA A 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

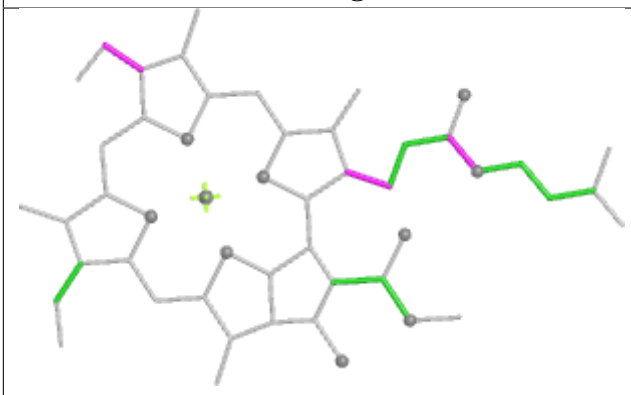
Ligand CLA 6 609



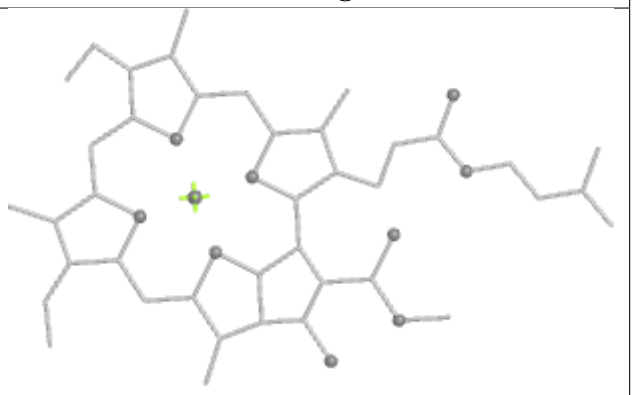
Bond lengths



Bond angles

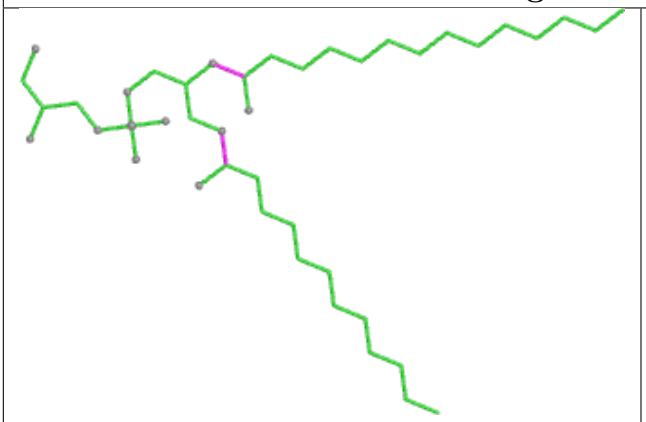


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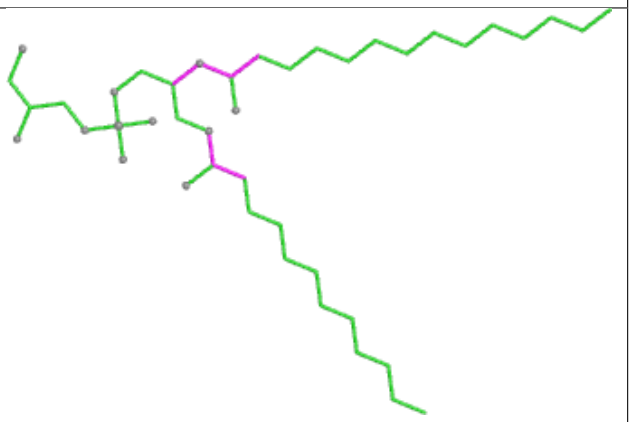


Rings

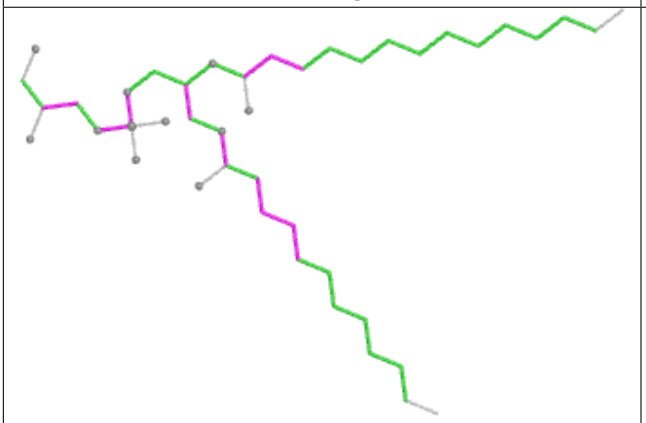
Ligand LHG 1 620



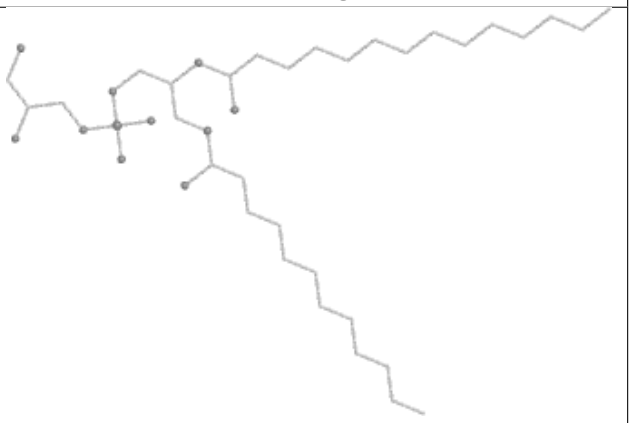
Bond lengths



Bond angles

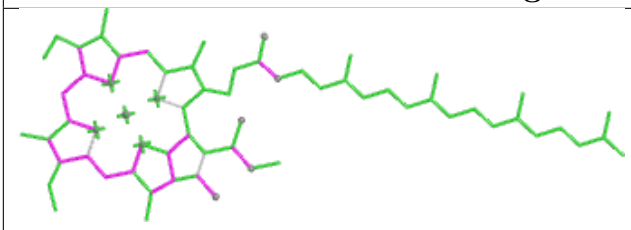


Torsions

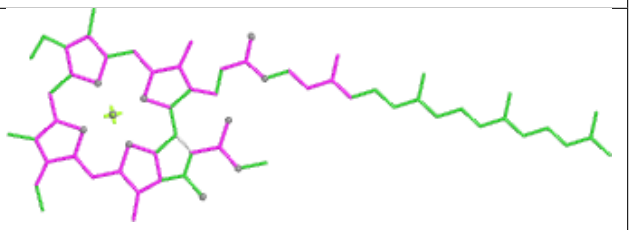


Rings

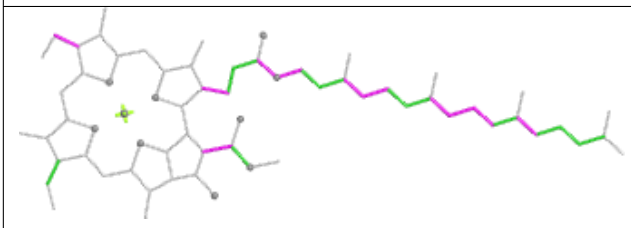
Ligand CLA A 831



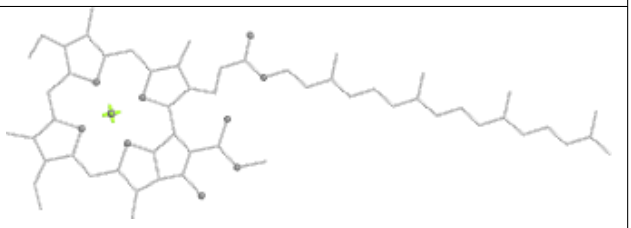
Bond lengths



Bond angles

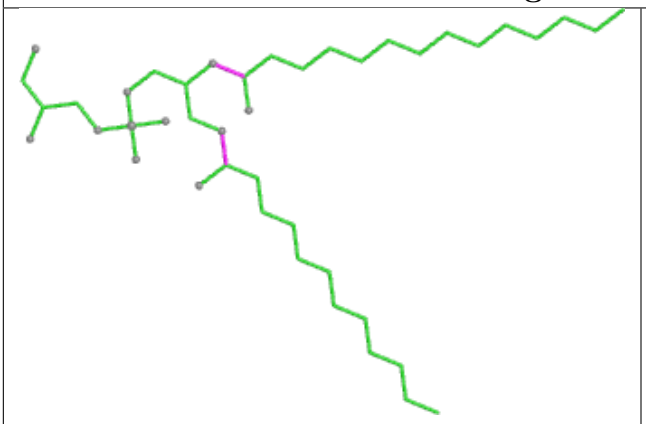


Torsions

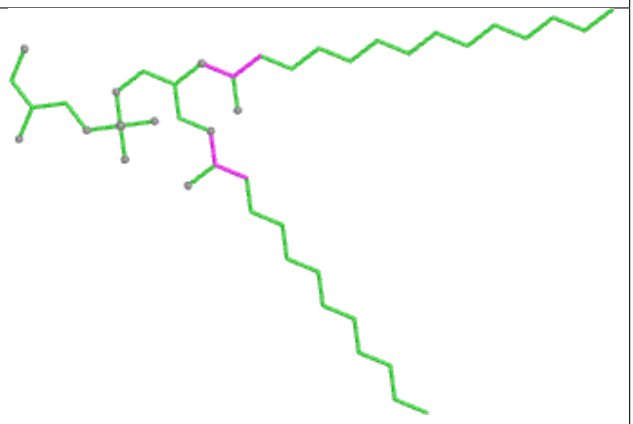


Rings

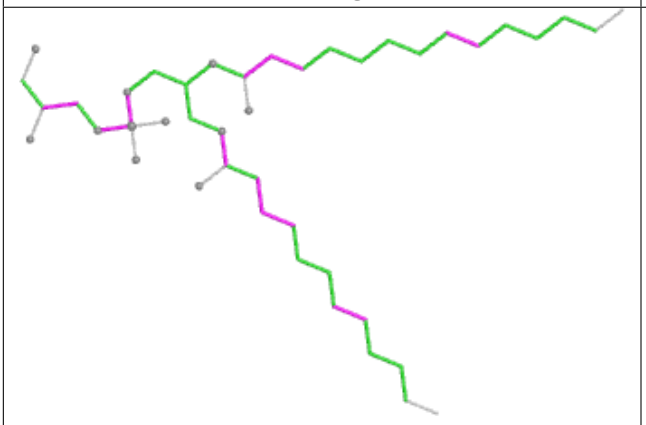
Ligand LHG Z 620



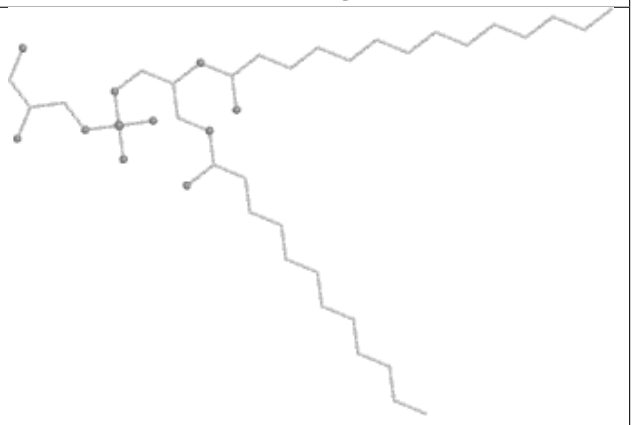
Bond lengths



Bond angles

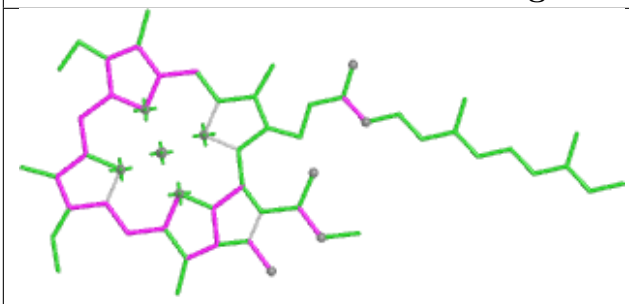


Torsions

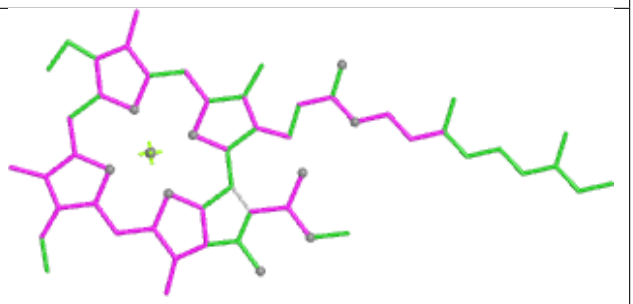


Rings

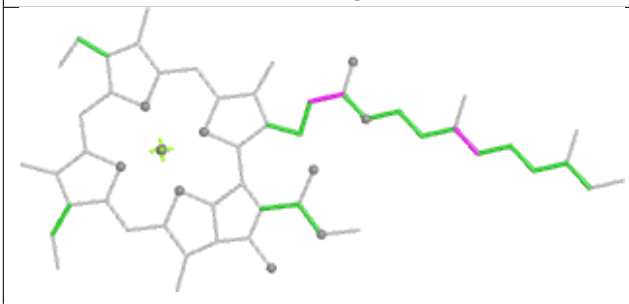
Ligand CLA 6 613



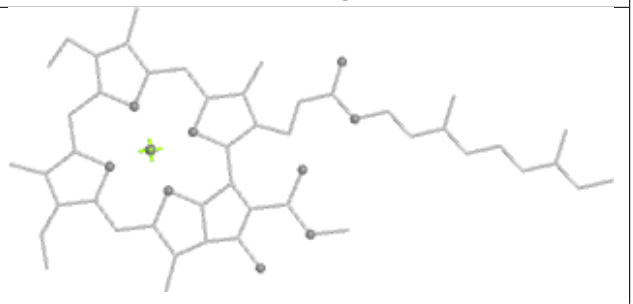
Bond lengths



Bond angles

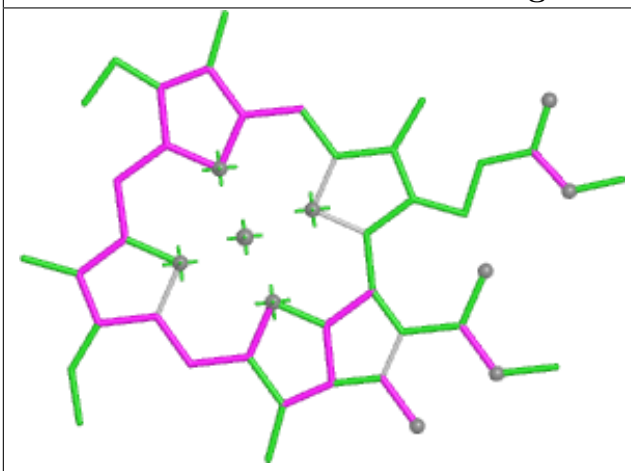


Torsions

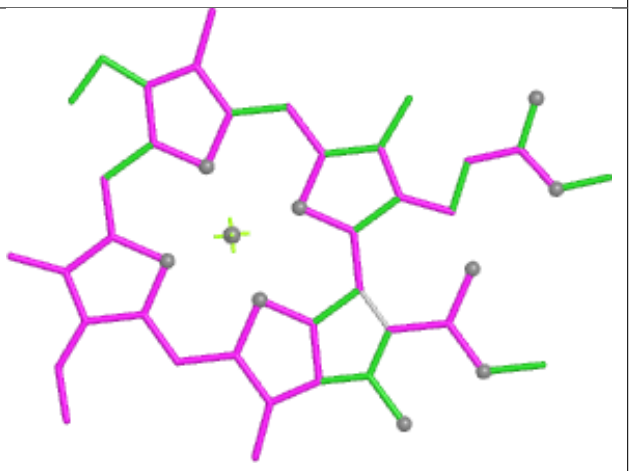


Rings

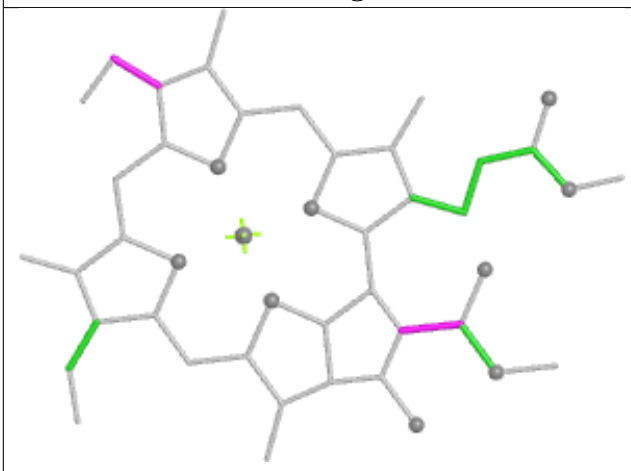
Ligand CLA 6 603



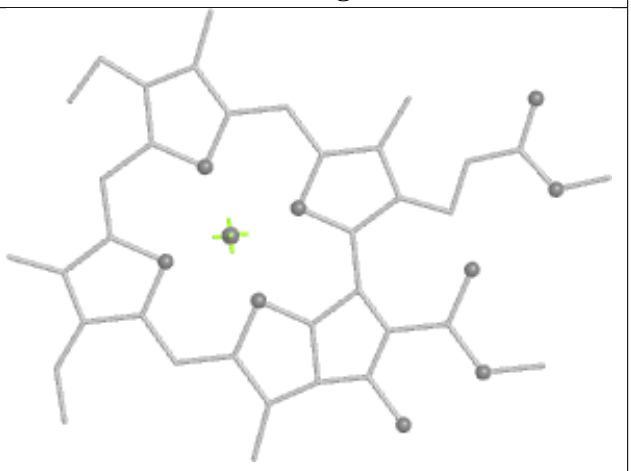
Bond lengths



Bond angles



Torsions



Rings

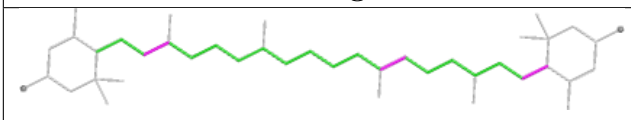
Ligand LUT 3 621



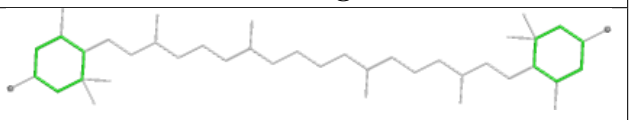
Bond lengths



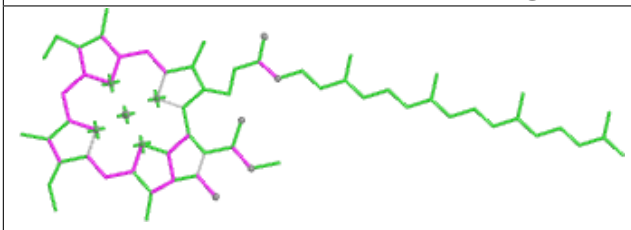
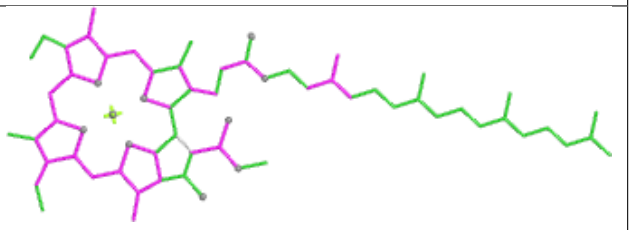
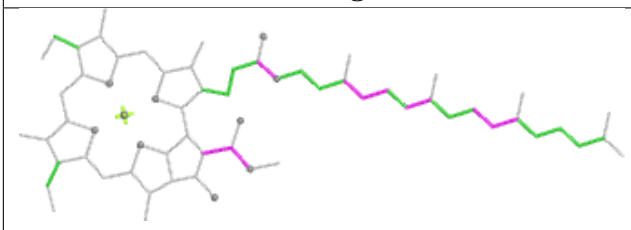
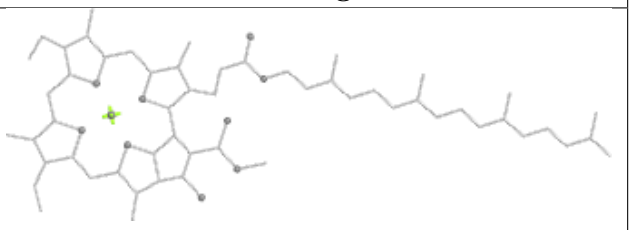
Bond angles

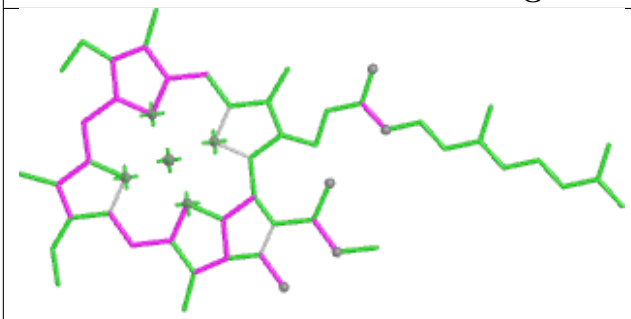
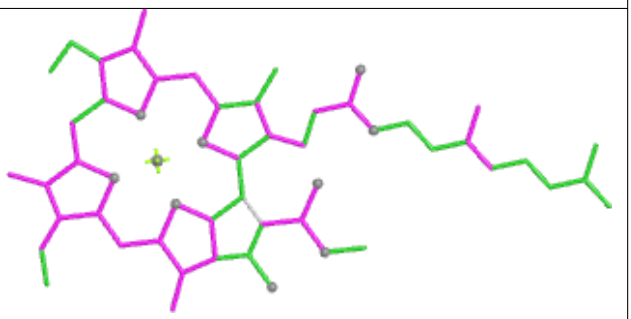
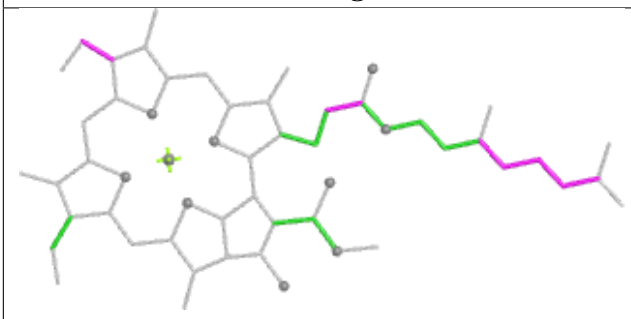
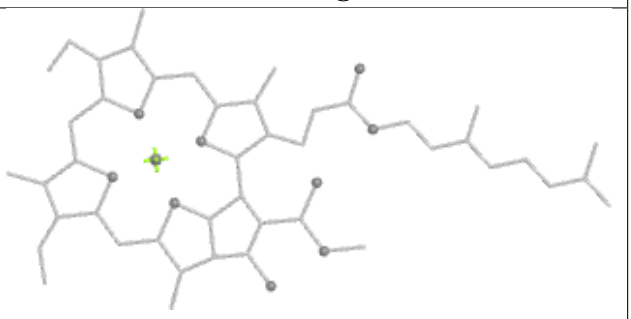


Torsions

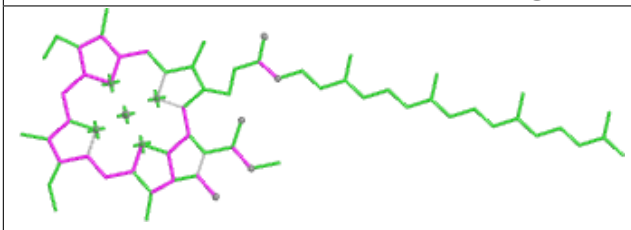


Rings

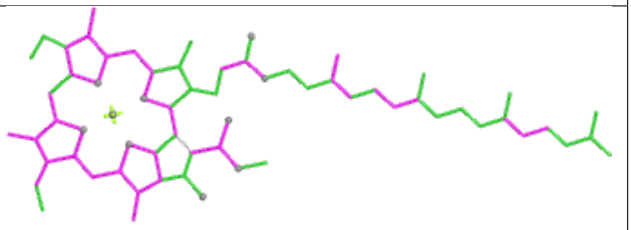
Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

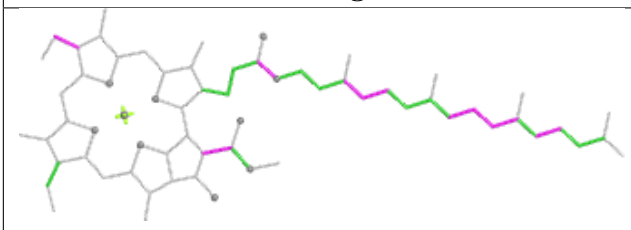
Ligand CLA 8 601



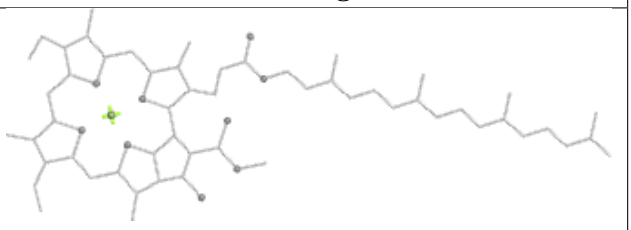
Bond lengths



Bond angles

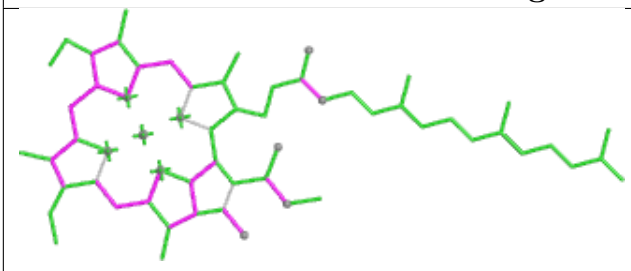


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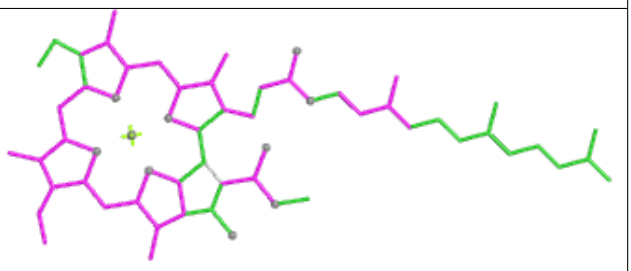


Rings

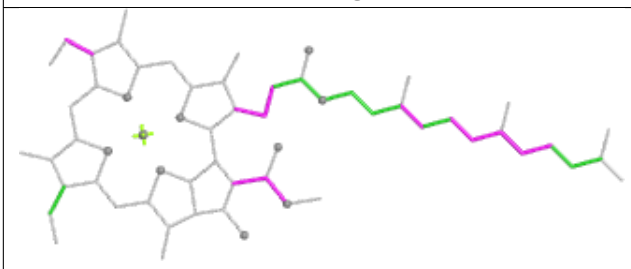
Ligand CLA 1 610



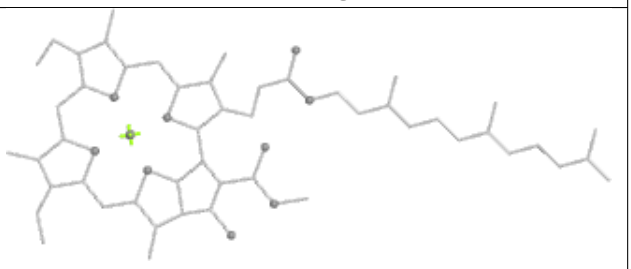
Bond lengths



Bond angles



Torsions

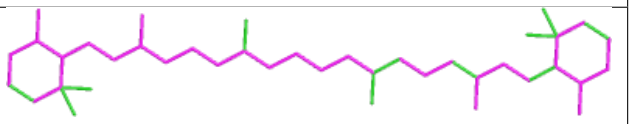


Rings

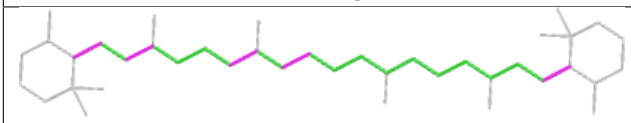
Ligand BCR 6 623



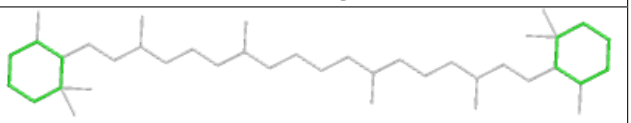
Bond lengths



Bond angles

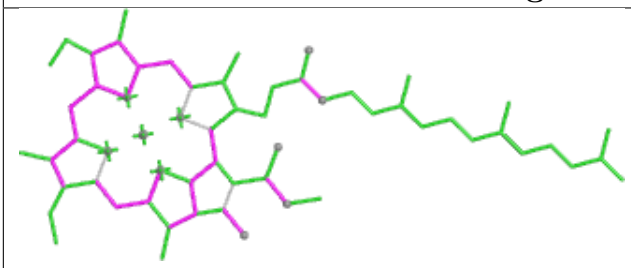


Torsions

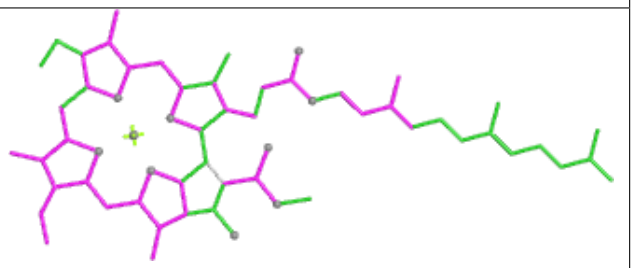


Rings

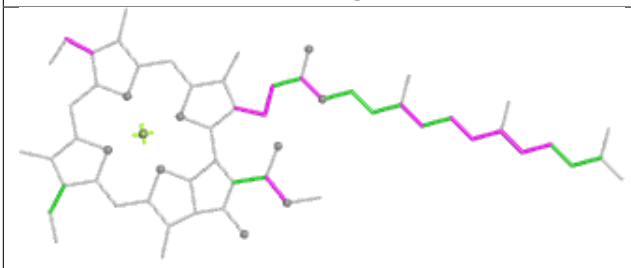
Ligand CLA Z 610



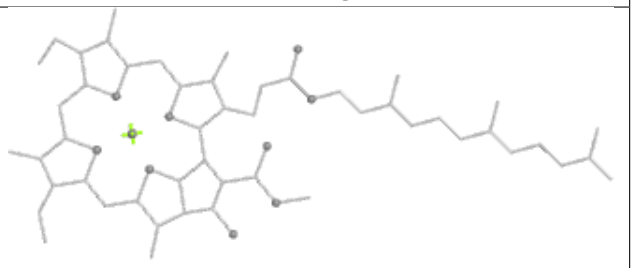
Bond lengths



Bond angles

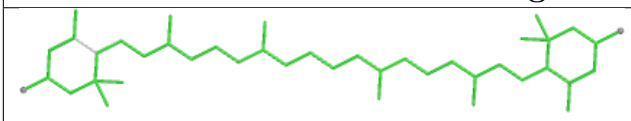


Torsions

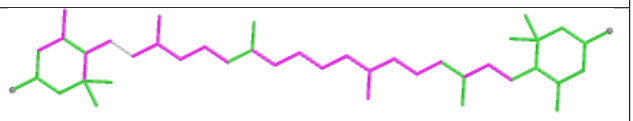


Rings

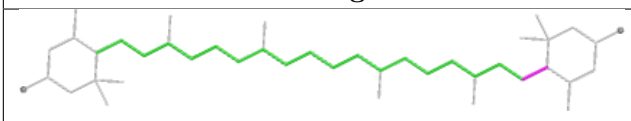
Ligand LUT 4 619



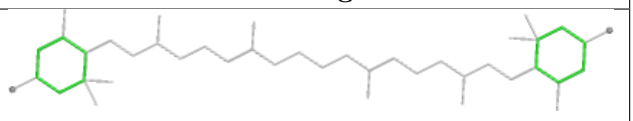
Bond lengths



Bond angles



Torsions

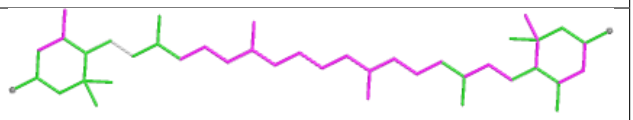


Rings

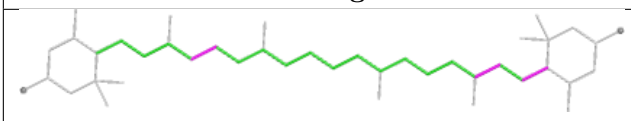
Ligand LUT Z 618



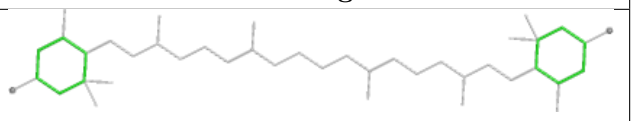
Bond lengths



Bond angles

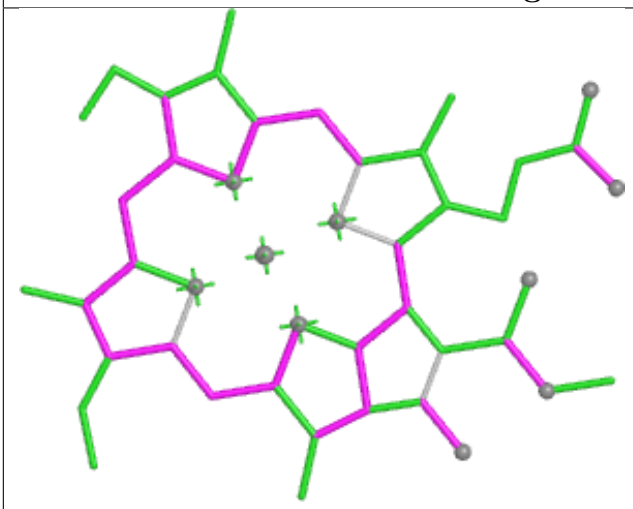


Torsions

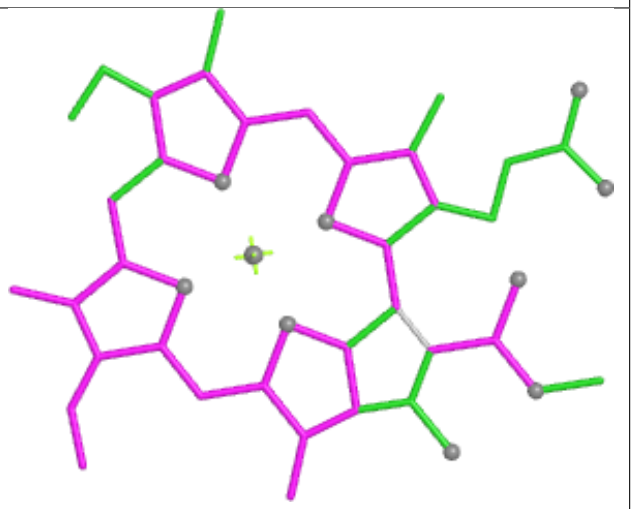


Rings

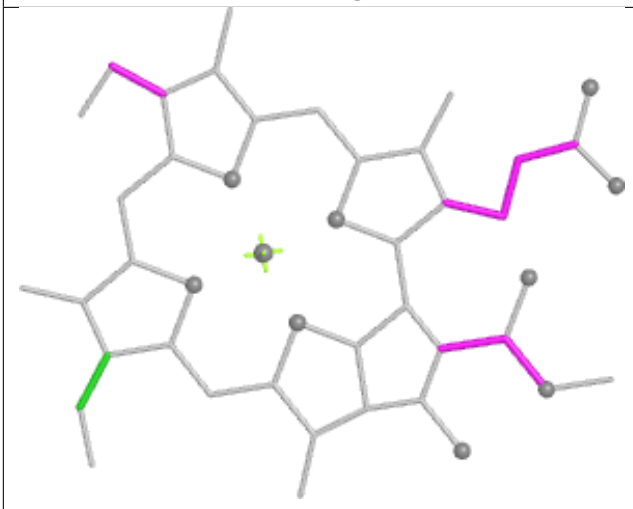
Ligand CLA A 837



Bond lengths



Bond angles

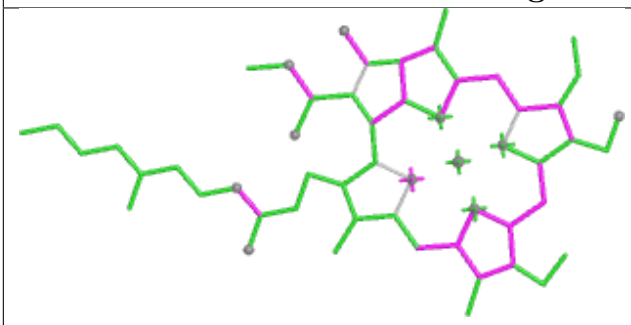


Torsions

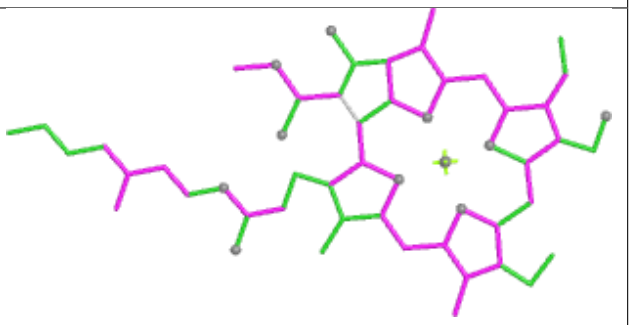


Rings

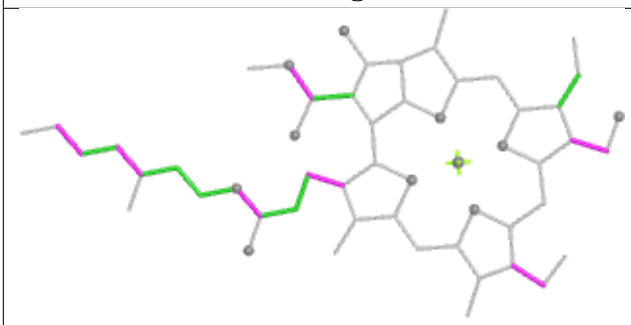
Ligand CHL 7 607



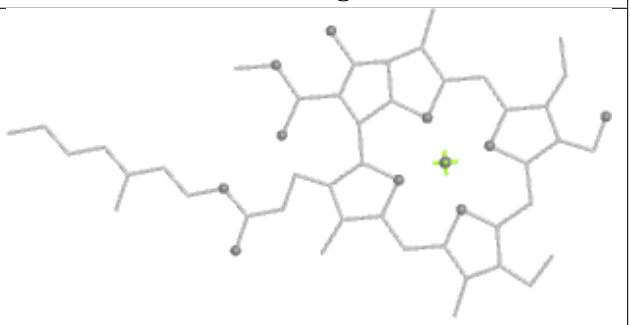
Bond lengths



Bond angles

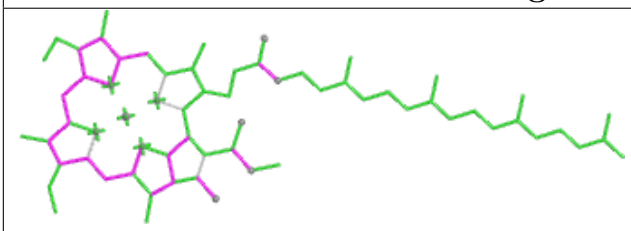


Torsions

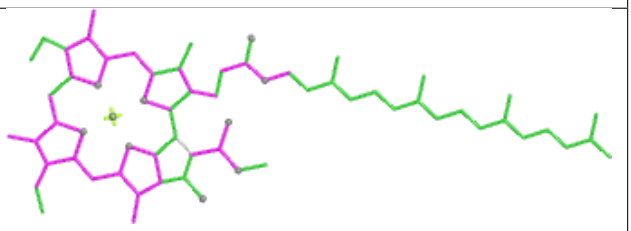


Rings

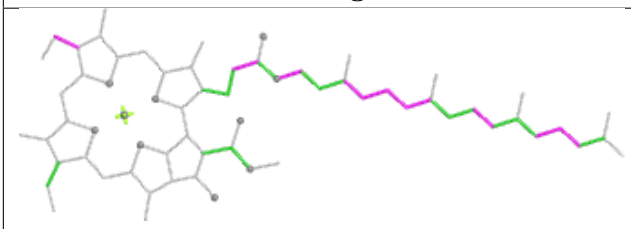
Ligand CLA 8 613



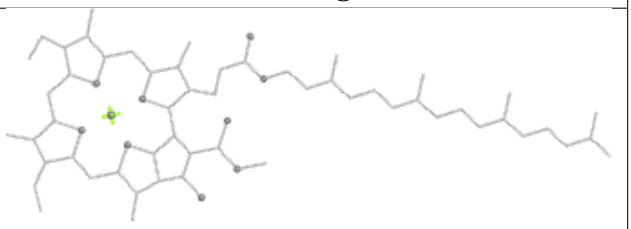
Bond lengths



Bond angles

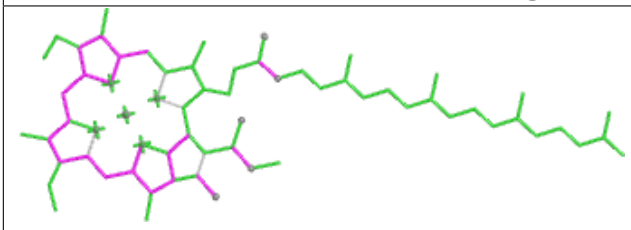


Torsions

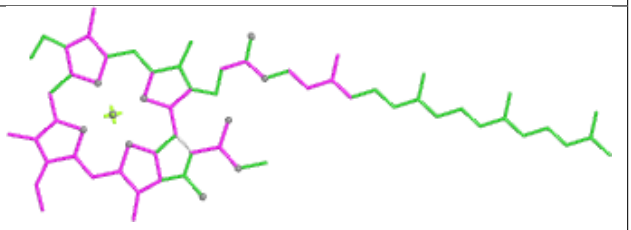


Rings

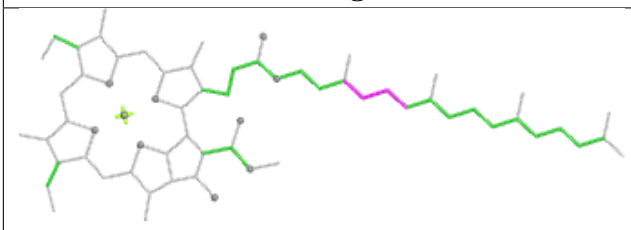
Ligand CLA A 835



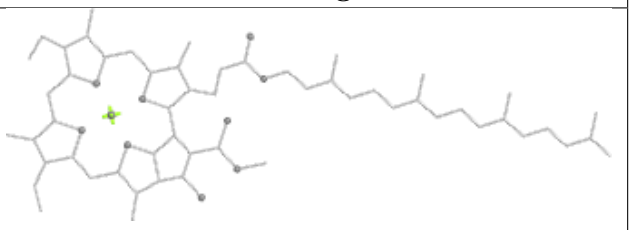
Bond lengths



Bond angles

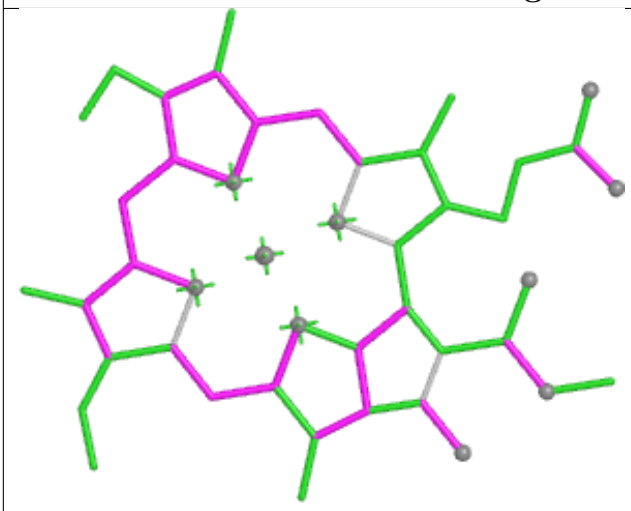


Torsions

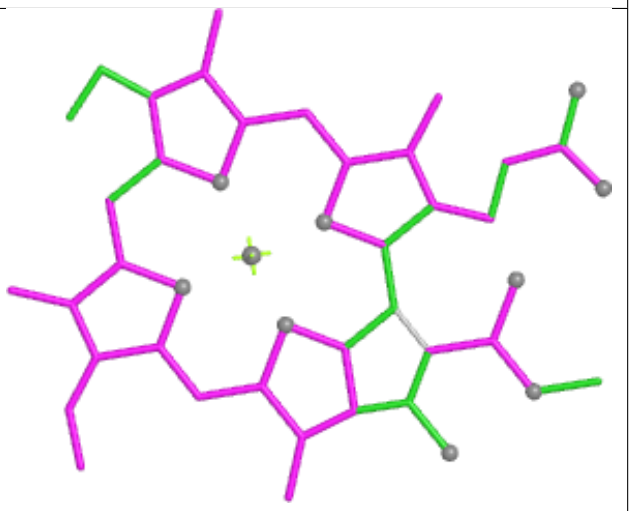


Rings

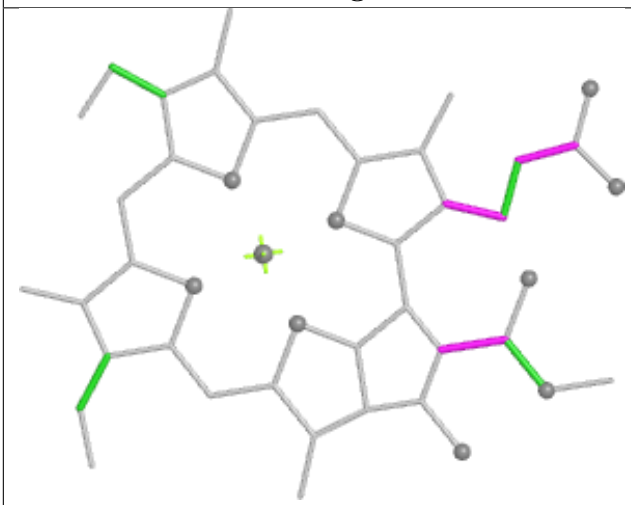
Ligand CLA B 804



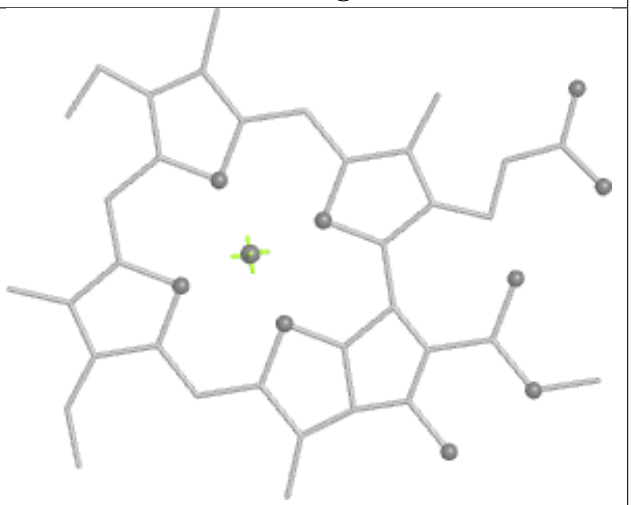
Bond lengths



Bond angles

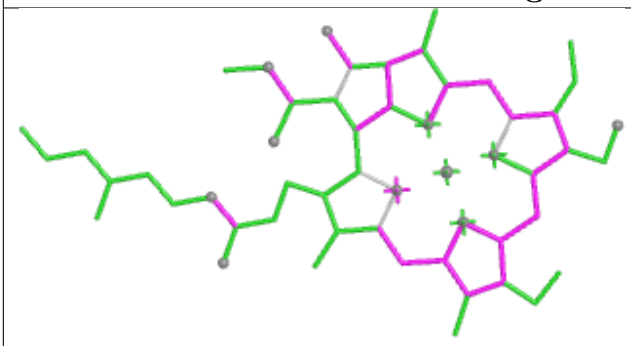


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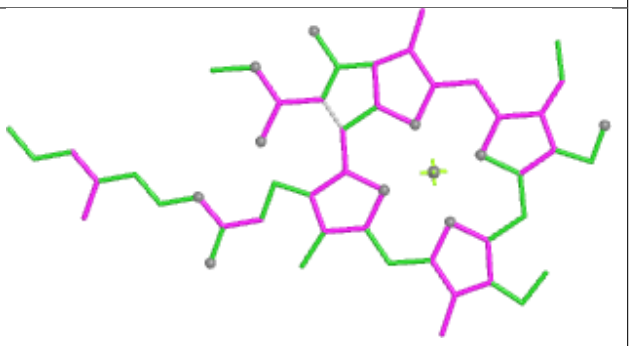


Rings

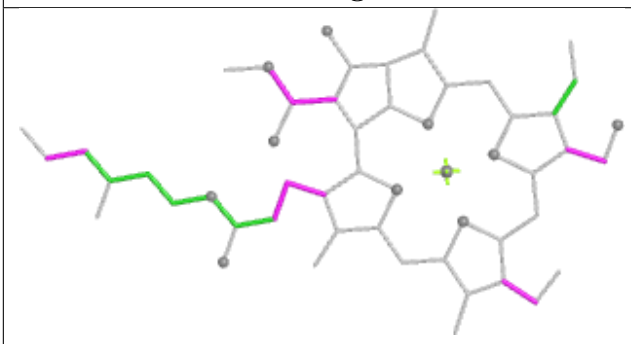
Ligand CHL Z 601



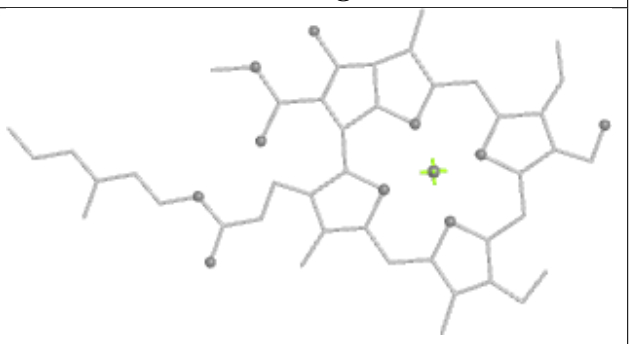
Bond lengths



Bond angles

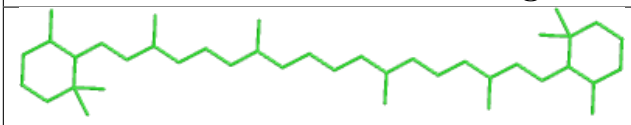


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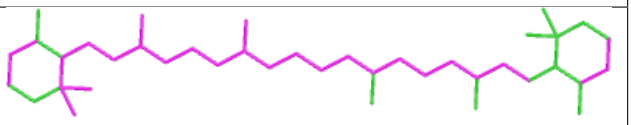


Rings

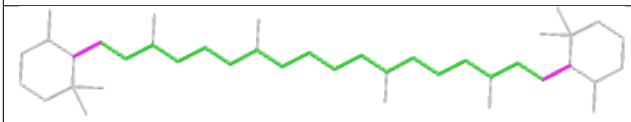
Ligand BCR A 849



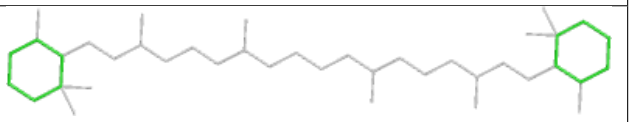
Bond lengths



Bond angles

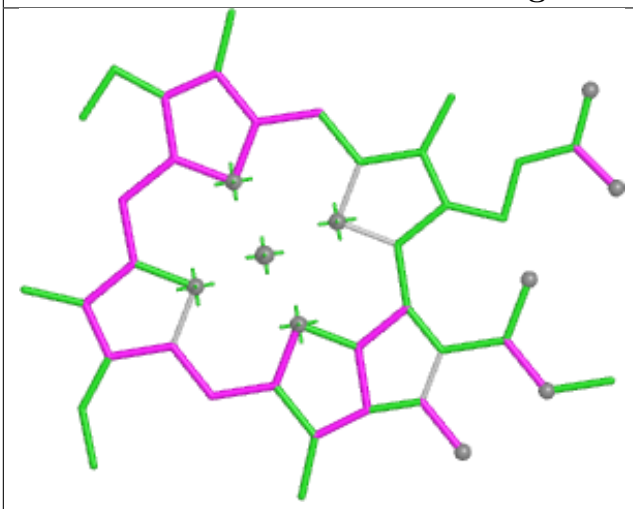


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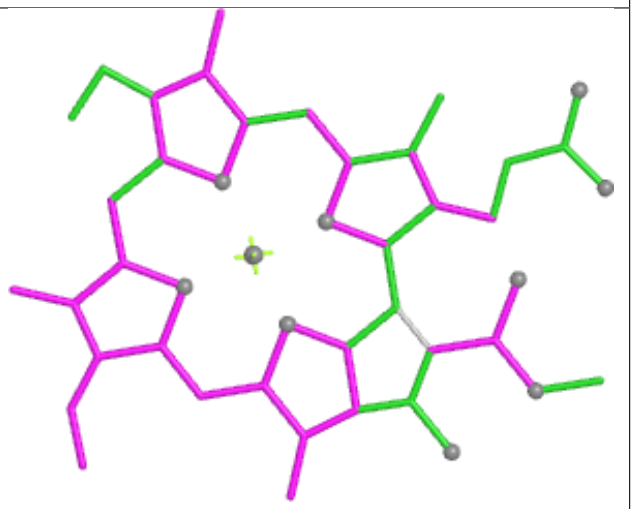


Rings

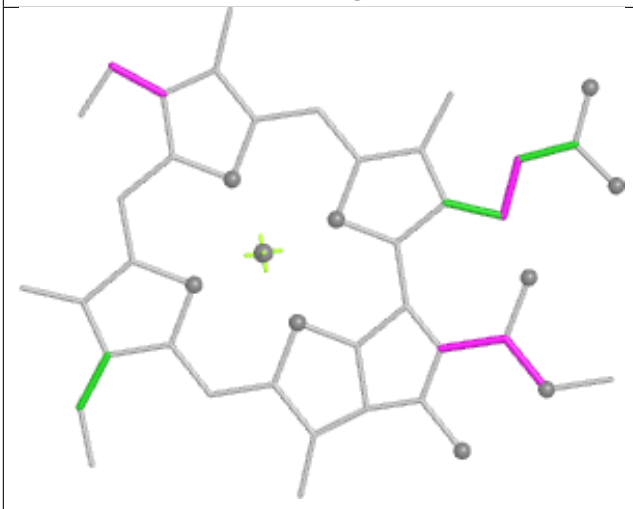
Ligand CLA 2 602



Bond lengths



Bond angles

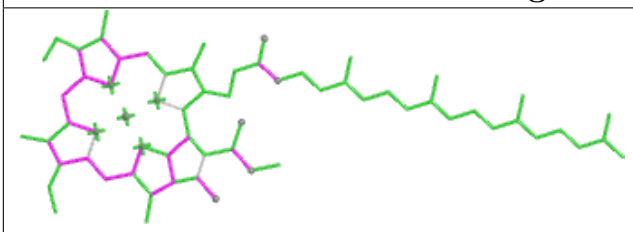


Torsions

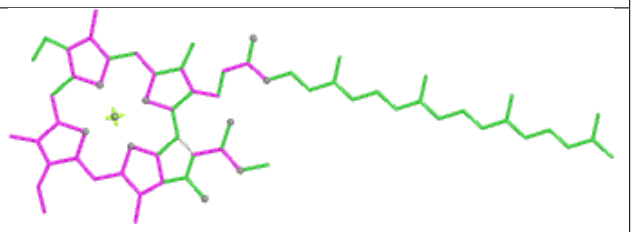


Rings

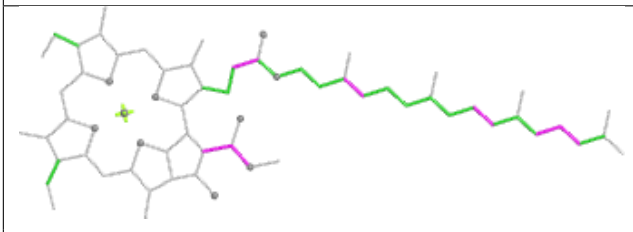
Ligand CLA 7 613



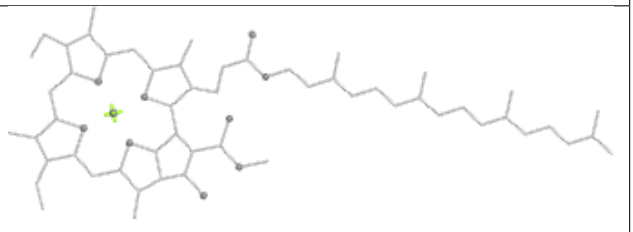
Bond lengths



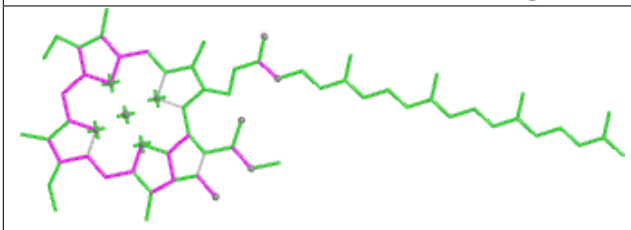
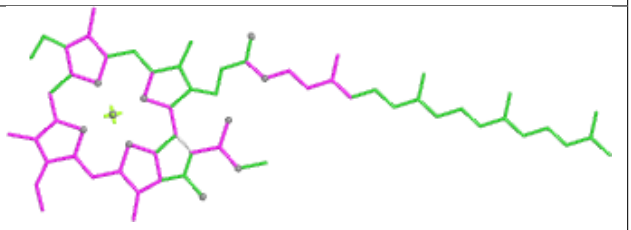
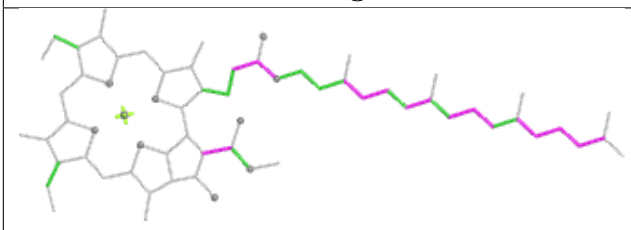
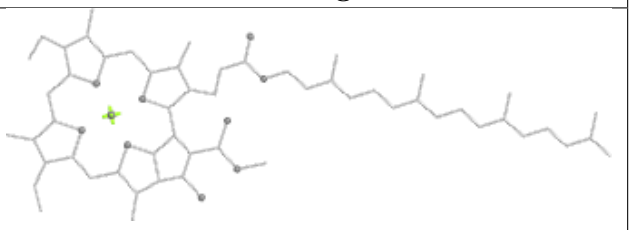
Bond angles

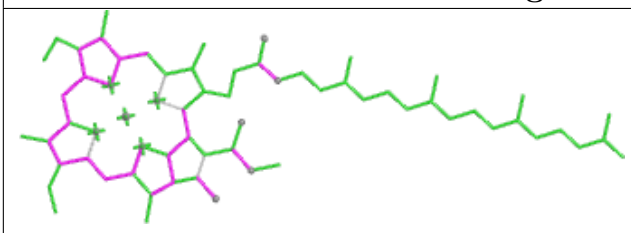
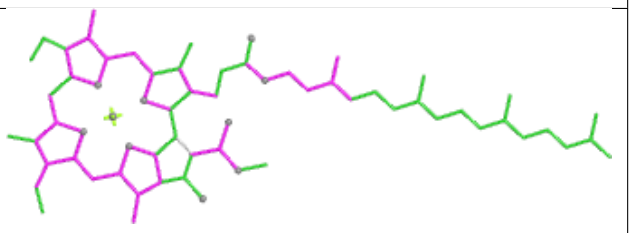
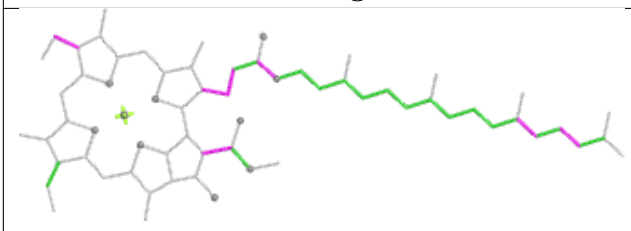
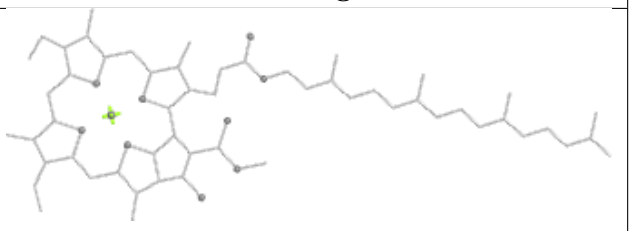


Torsions

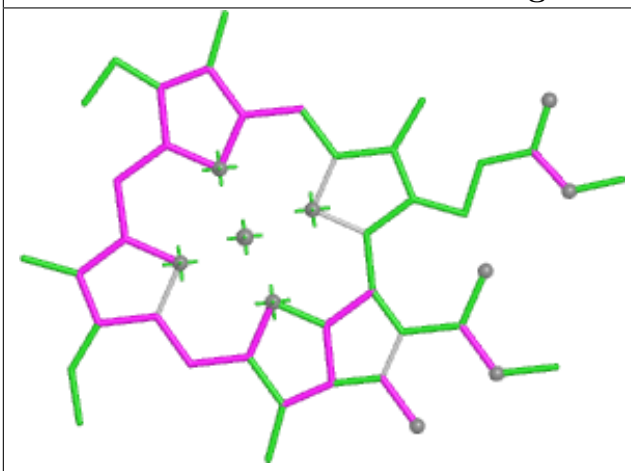


Rings

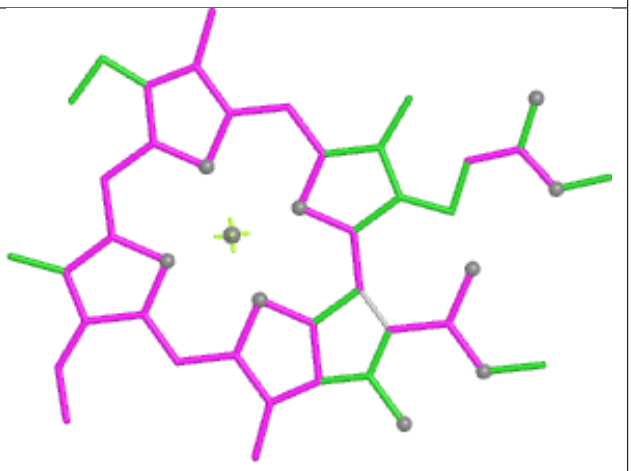
Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA F 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

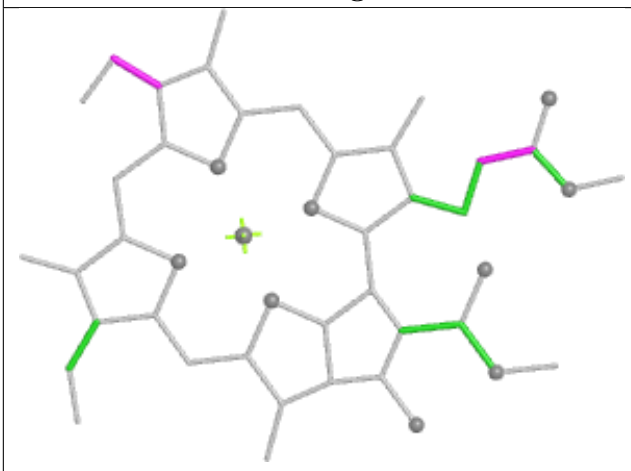
Ligand CLA 3 612



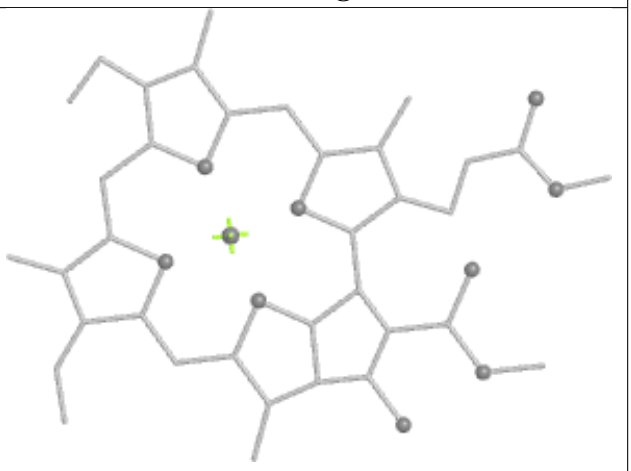
Bond lengths



Bond angles



Torsions

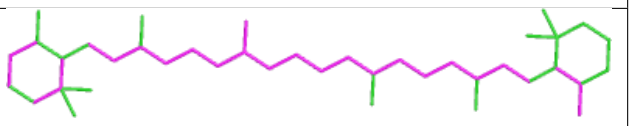


Rings

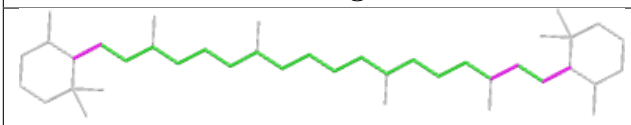
Ligand BCR K 4004



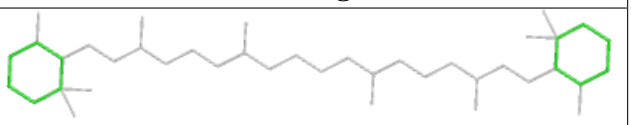
Bond lengths



Bond angles

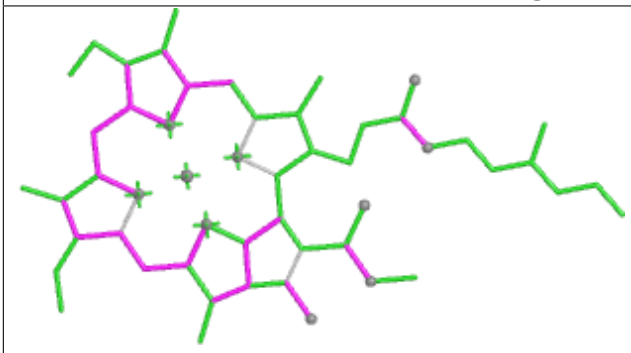


Torsions

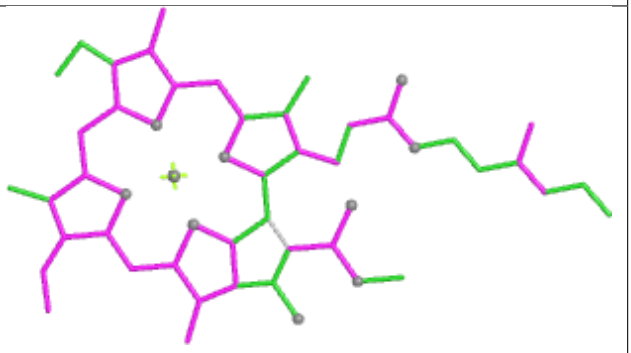


Rings

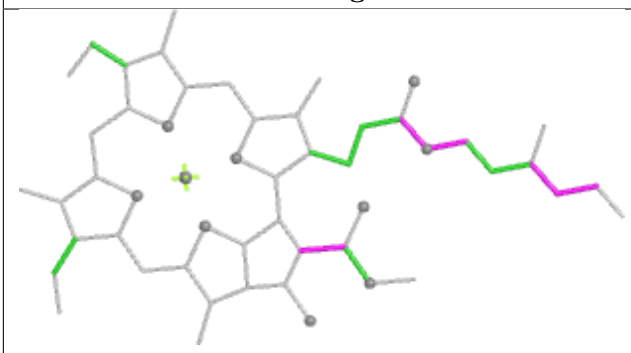
Ligand CLA 7 612



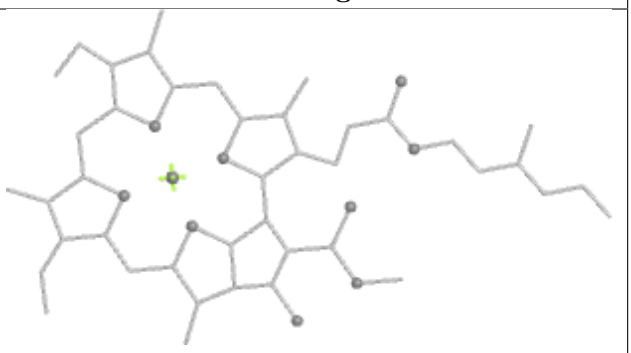
Bond lengths



Bond angles

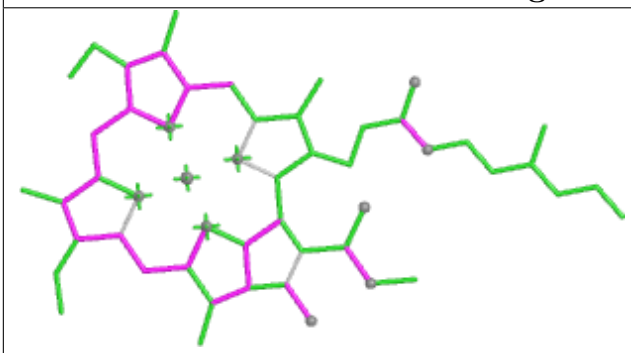


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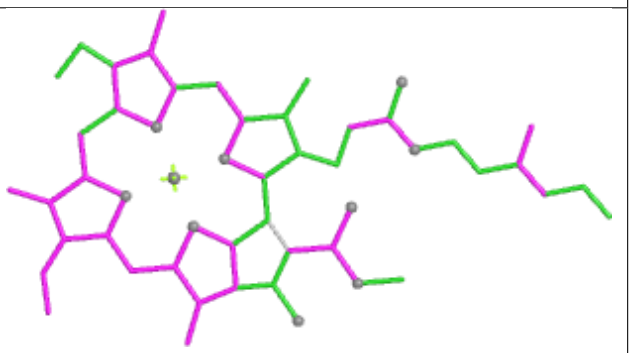


Rings

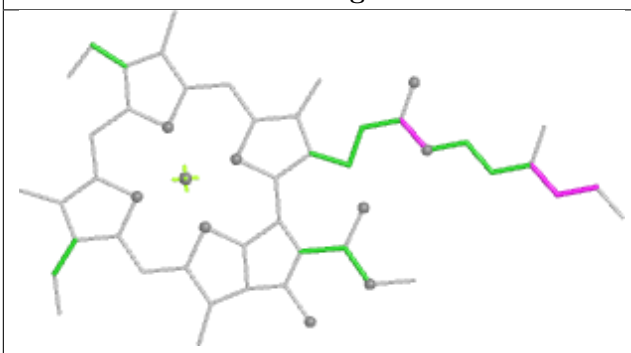
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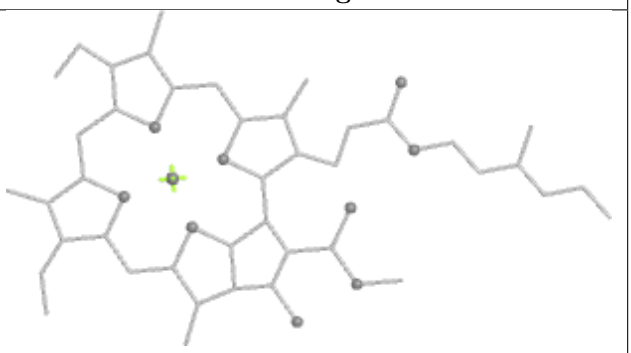
Bond lengths



Bond angles

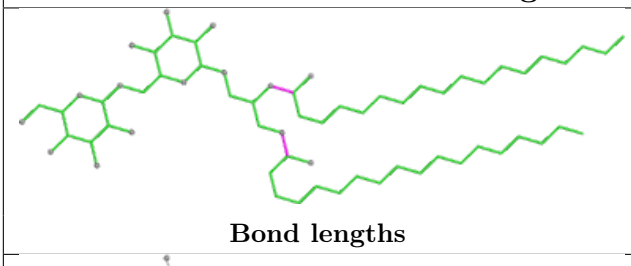


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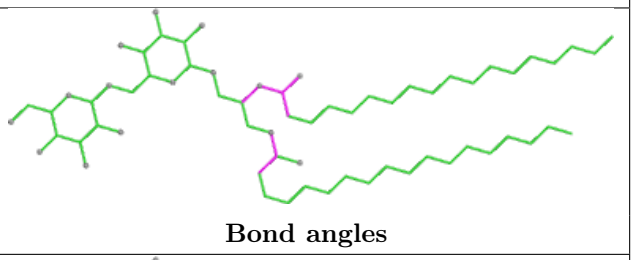


Rings

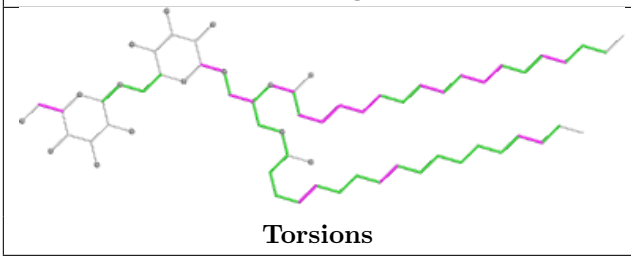
Ligand DGD B 850



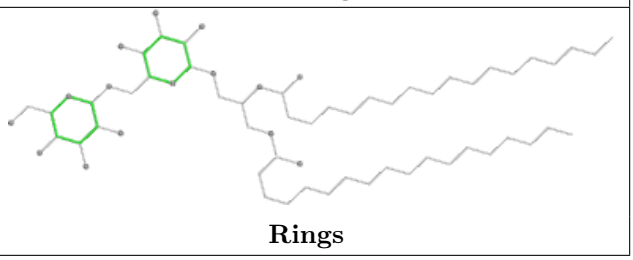
Bond lengths



Bond angles

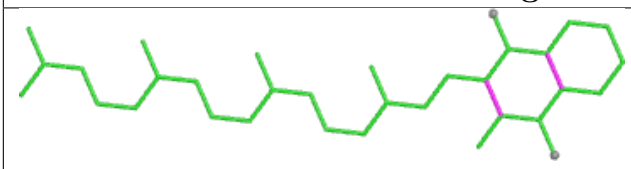


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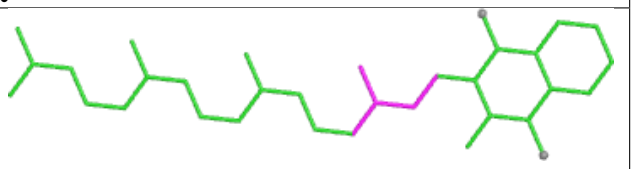


Rings

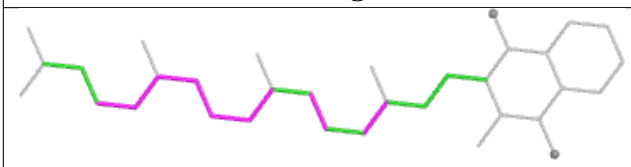
Ligand PQN A 844



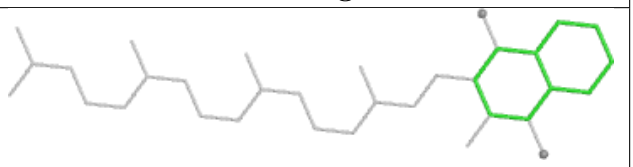
Bond lengths



Bond angles

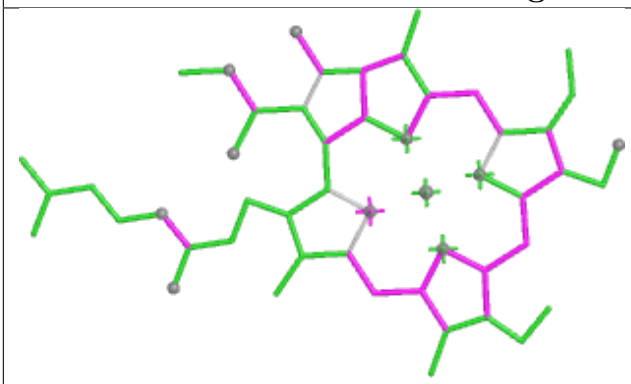


Torsions

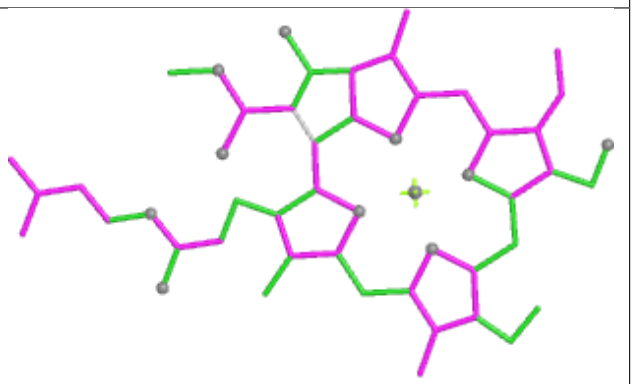


Rings

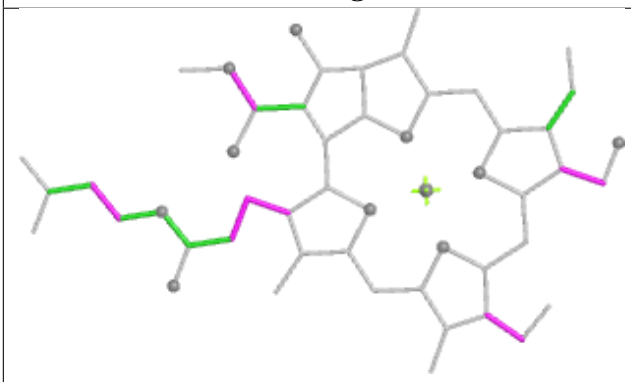
Ligand CHL 5 608



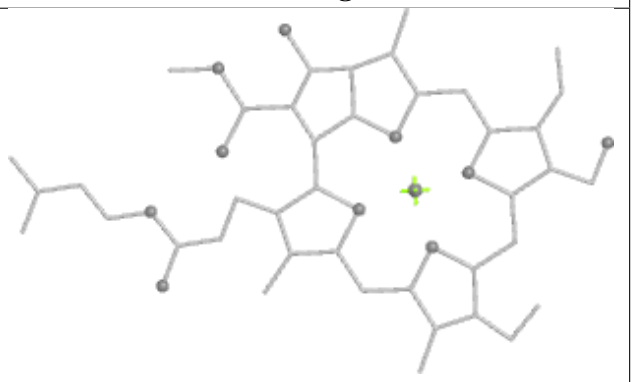
Bond lengths



Bond angles

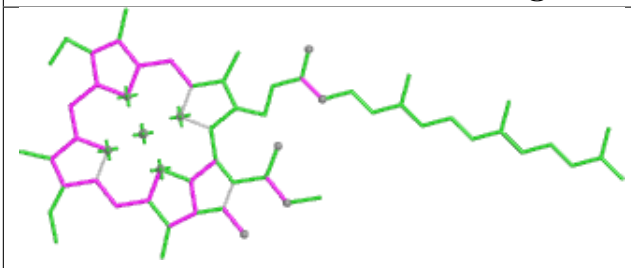


Torsions

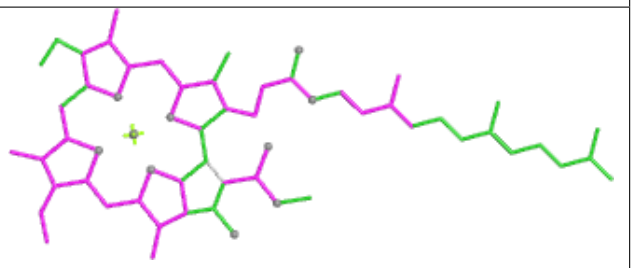


Rings

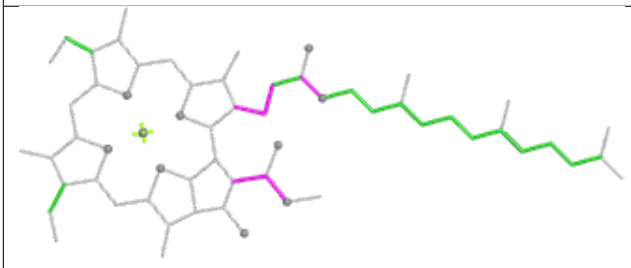
Ligand CLA 3 602



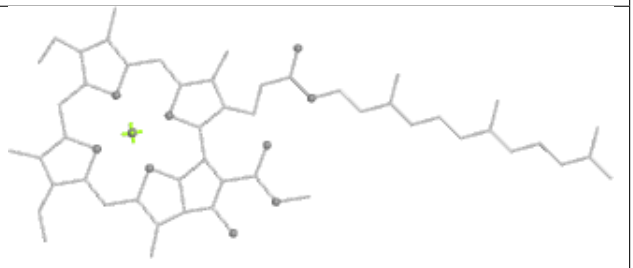
Bond lengths



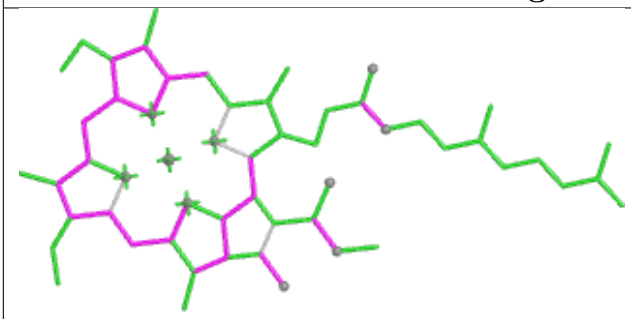
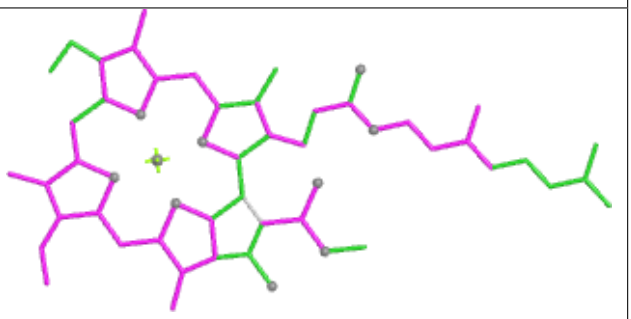
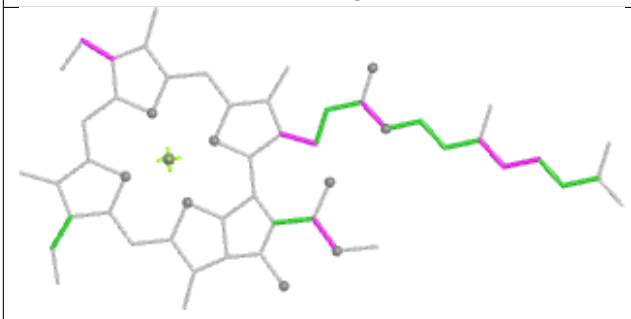
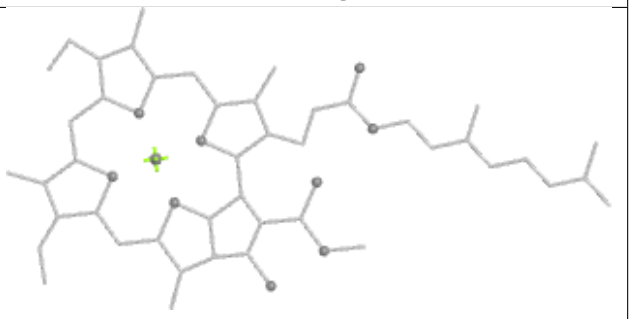
Bond angles

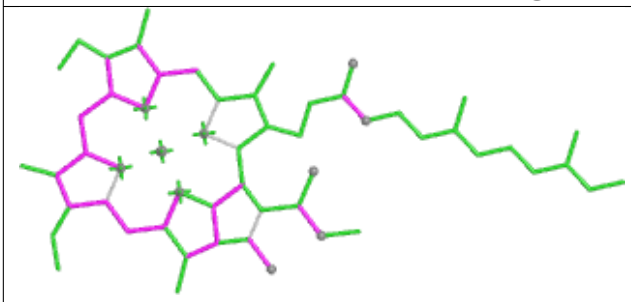
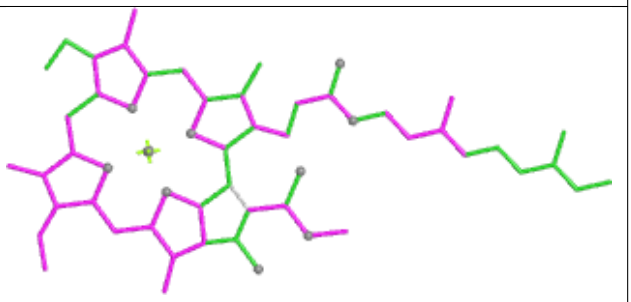
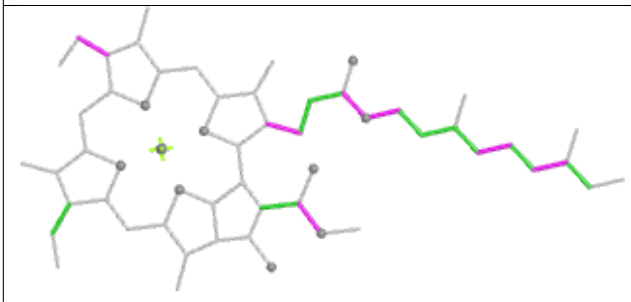
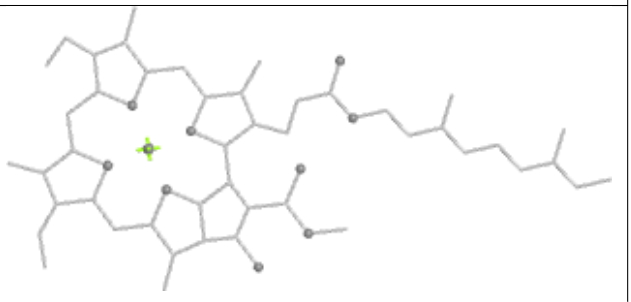


Torsions

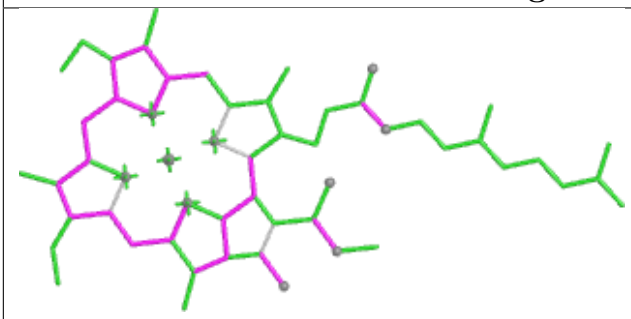


Rings

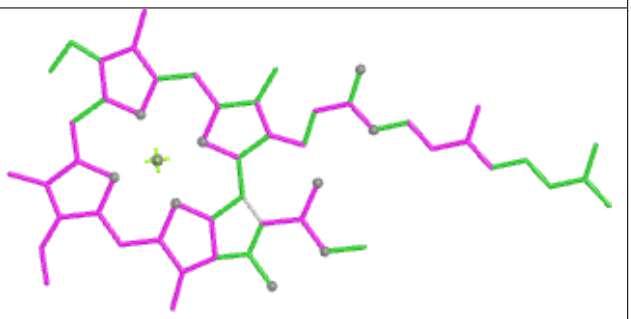
Ligand CLA 4 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

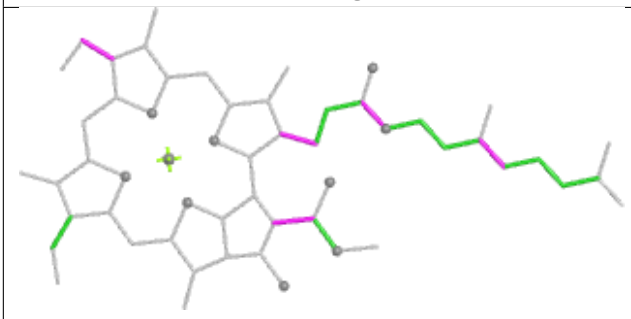
Ligand CLA 5 611



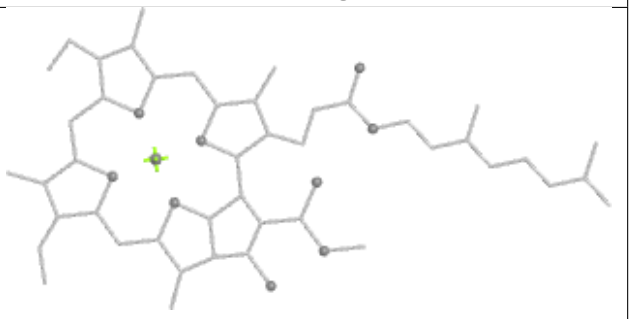
Bond lengths



Bond angles

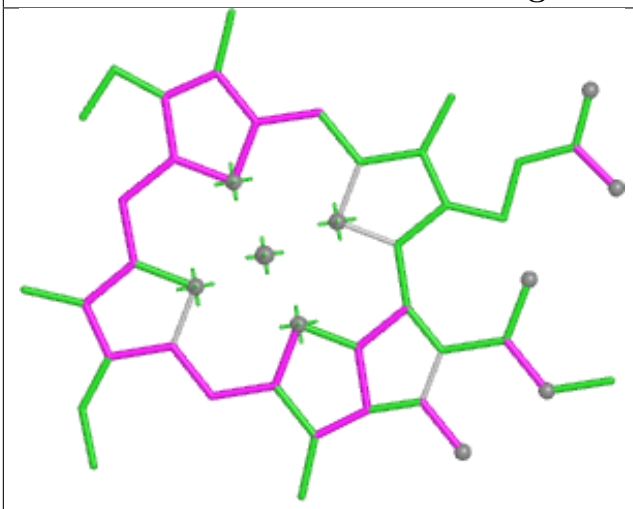


Torsions

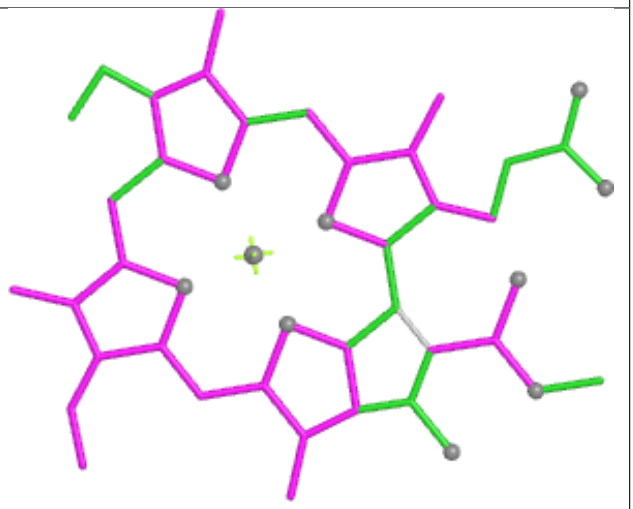


Rings

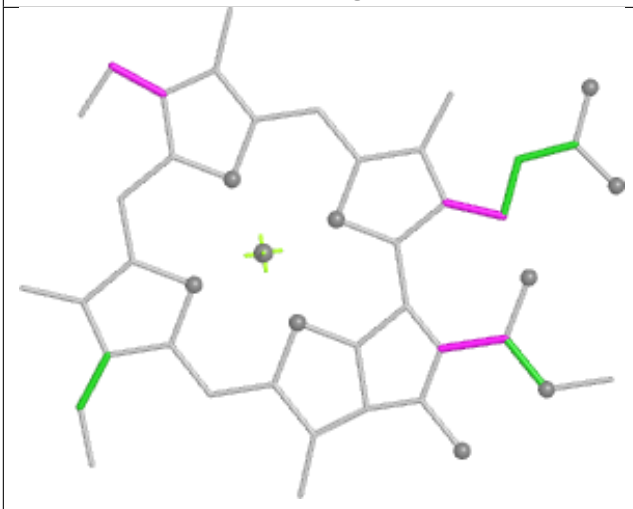
Ligand CLA 4 614



Bond lengths



Bond angles

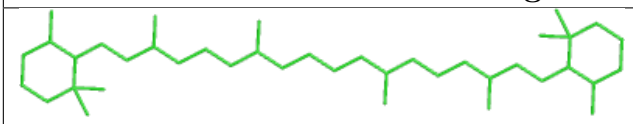


Torsions

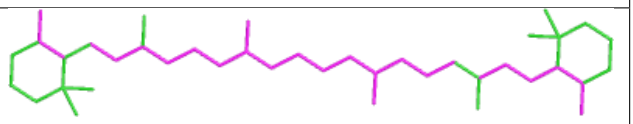


Rings

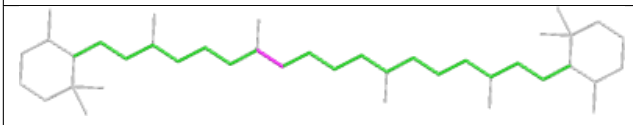
Ligand BCR F 305



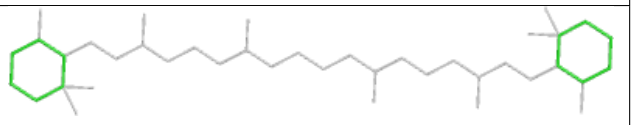
Bond lengths



Bond angles

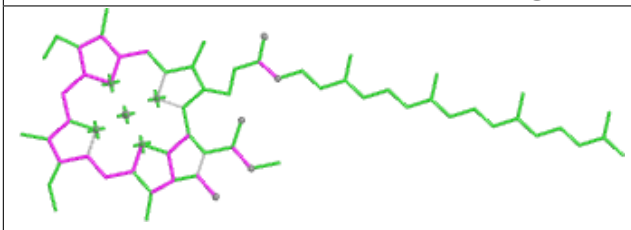


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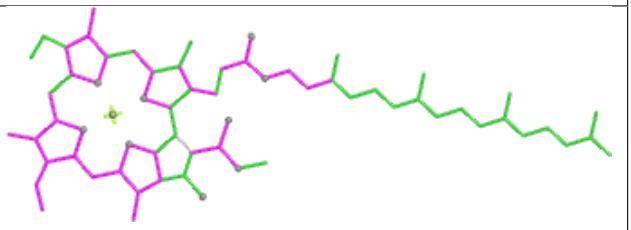


Rings

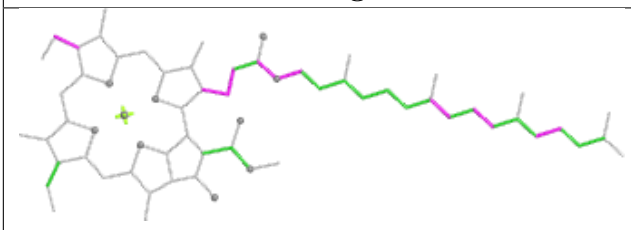
Ligand CLA 5 601



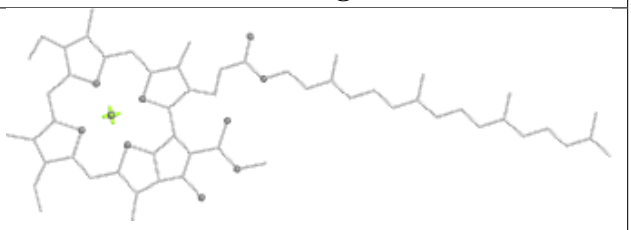
Bond lengths



Bond angles

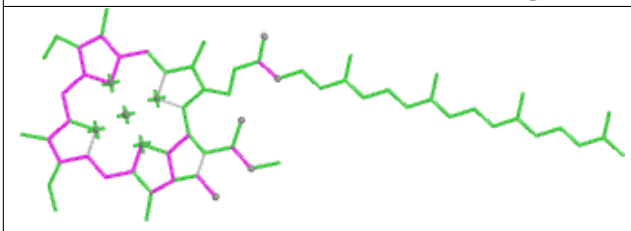


Torsions

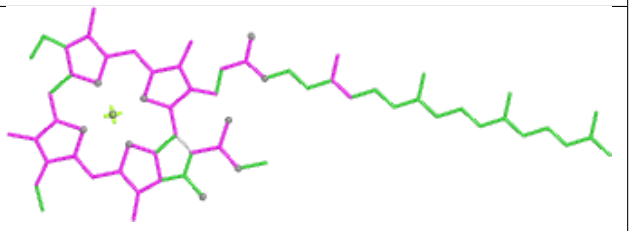


Rings

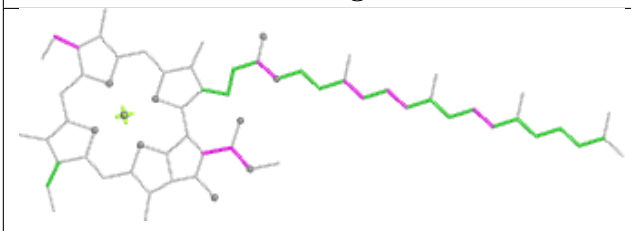
Ligand CLA B 829



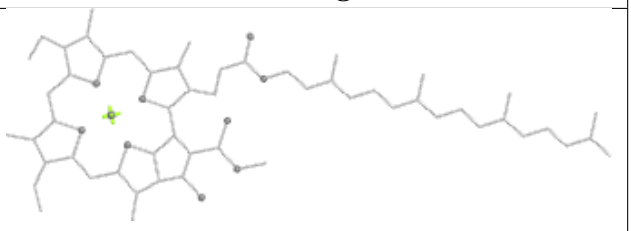
Bond lengths



Bond angles

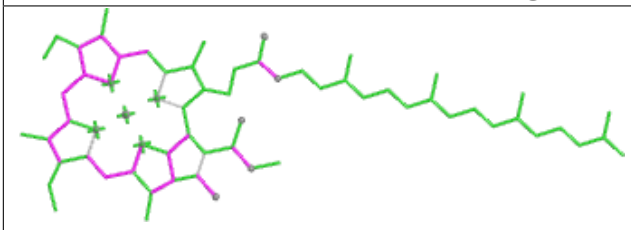


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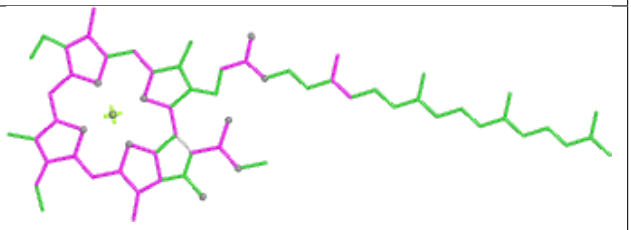


Rings

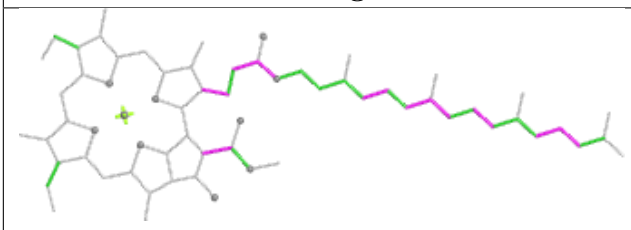
Ligand CLA B 805



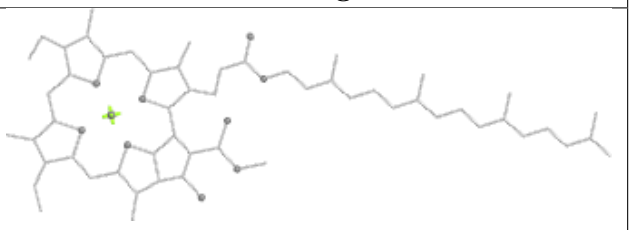
Bond lengths



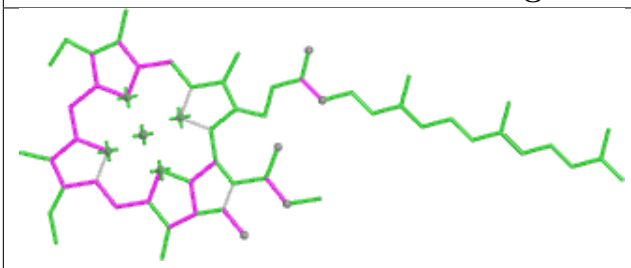
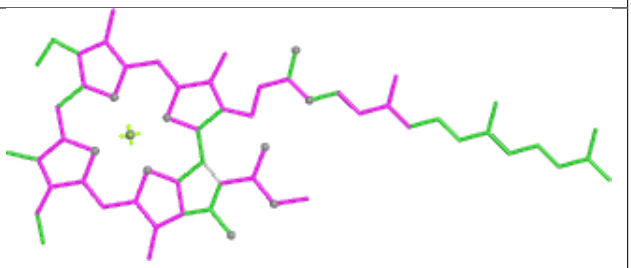
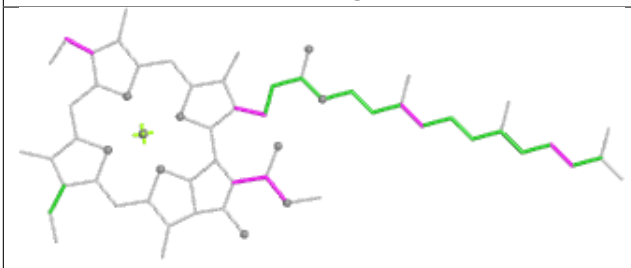
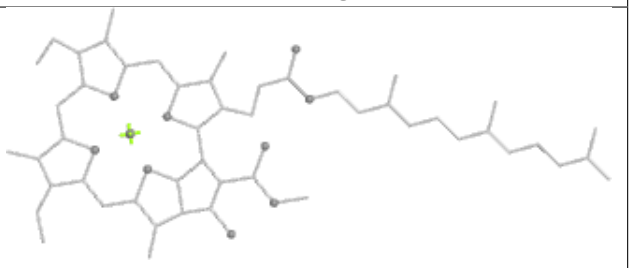
Bond angles

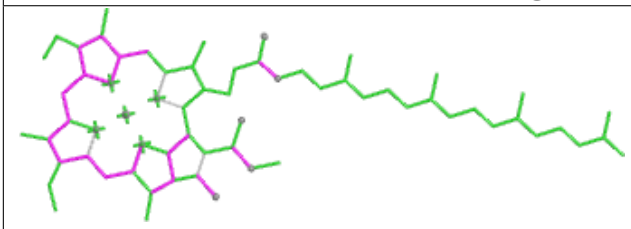
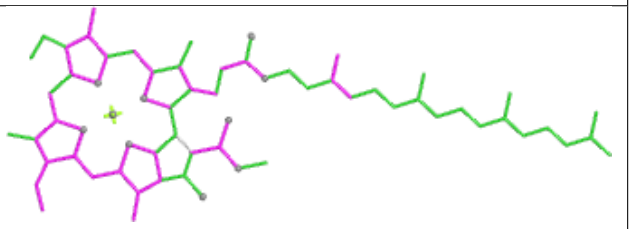
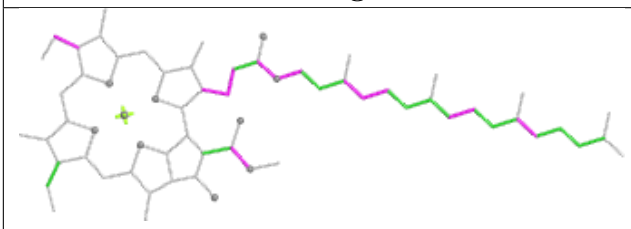
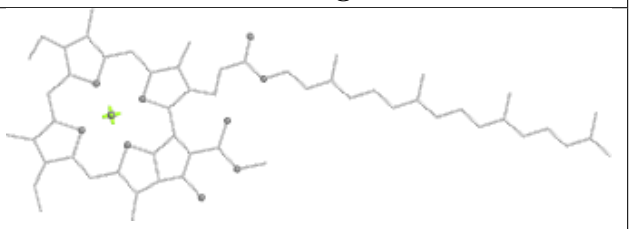


Torsions

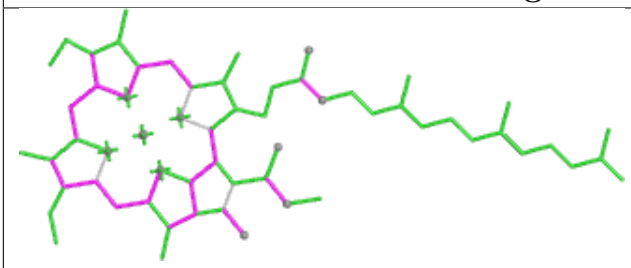


Rings

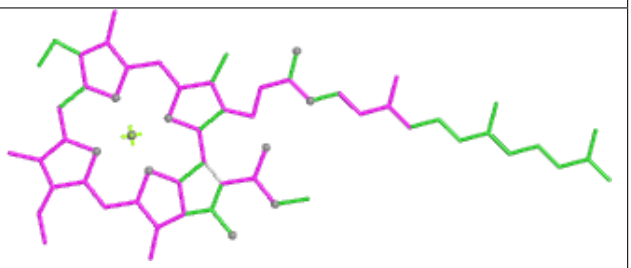
Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

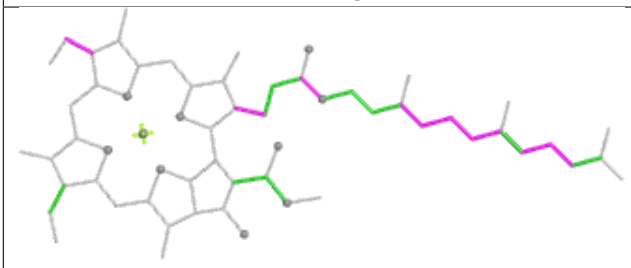
Ligand CLA B 818



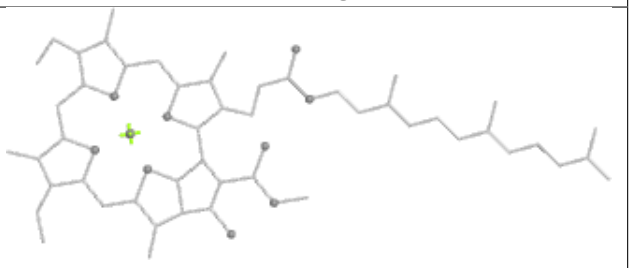
Bond lengths



Bond angles

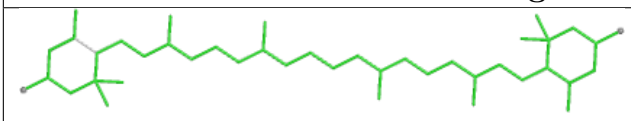


Torsions

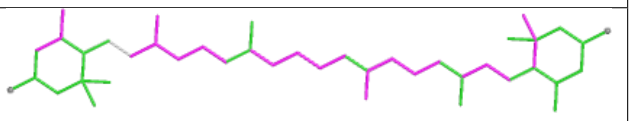


Rings

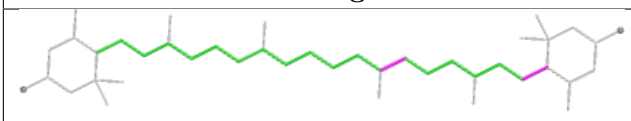
Ligand LUT 7 621



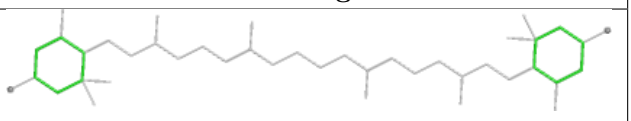
Bond lengths



Bond angles

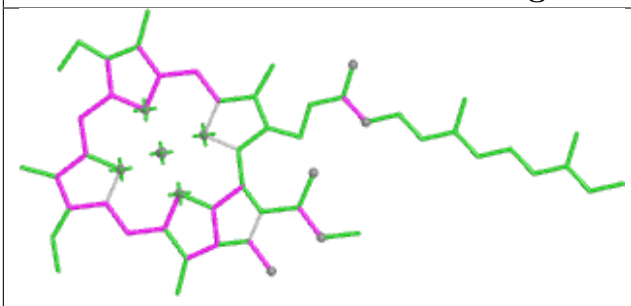


Torsions

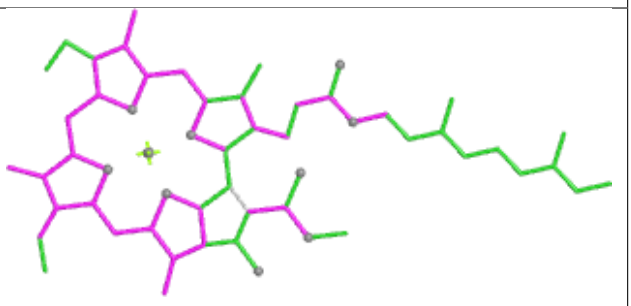


Rings

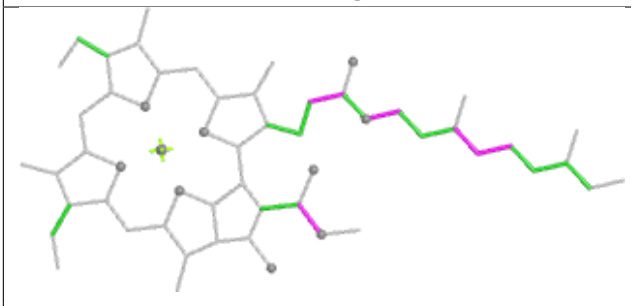
Ligand CLA 5 613



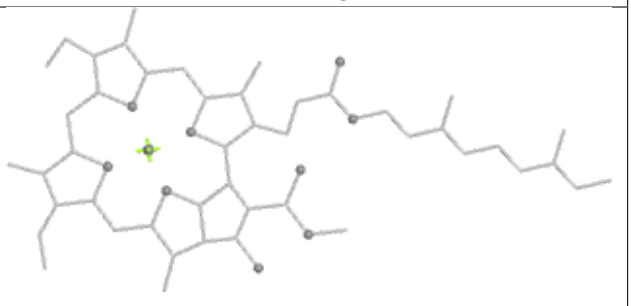
Bond lengths



Bond angles

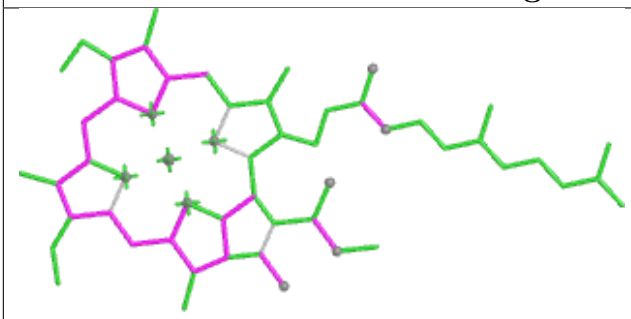


Torsions

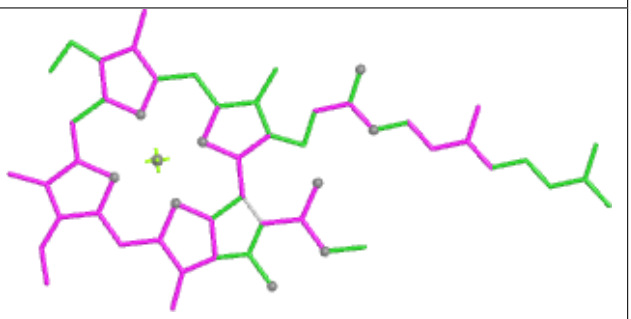


Rings

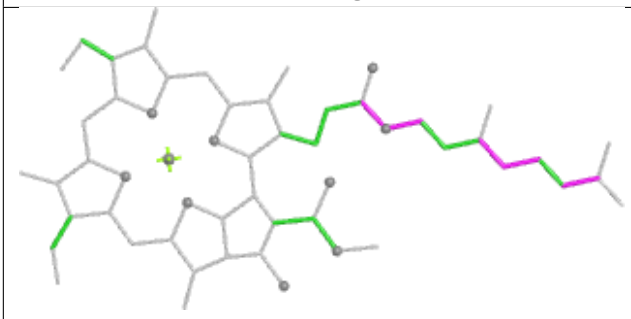
Ligand CLA A 805



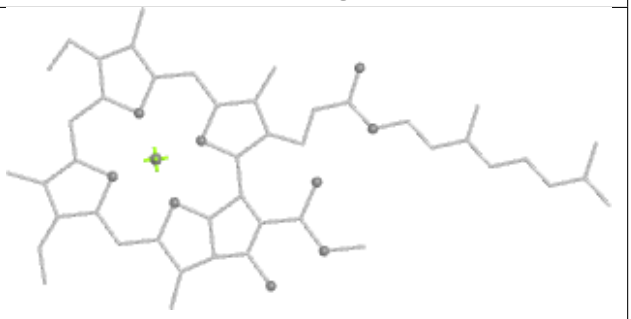
Bond lengths



Bond angles

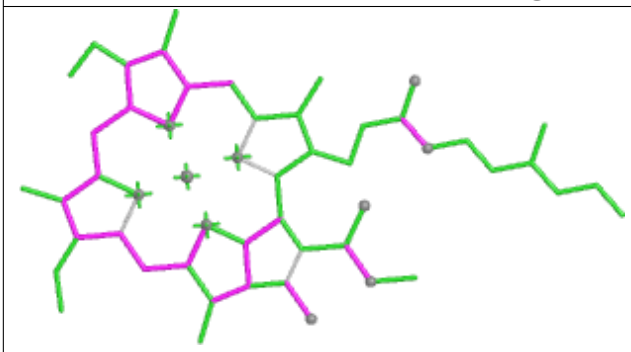


Torsions

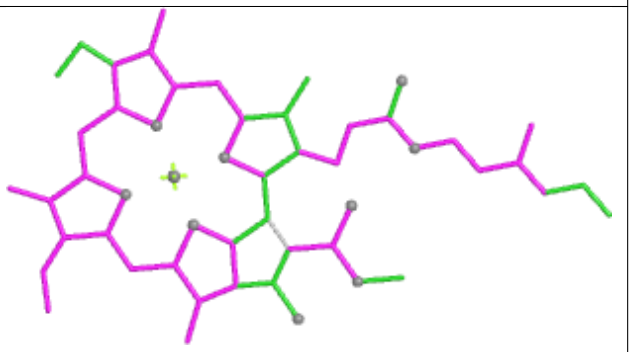


Rings

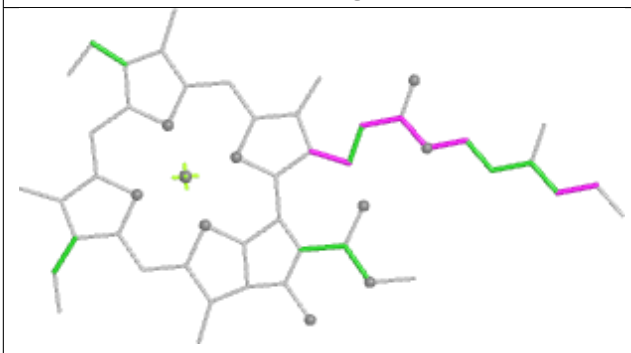
Ligand CLA 1 612



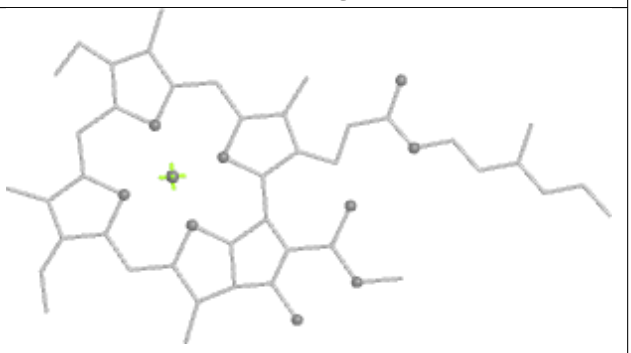
Bond lengths



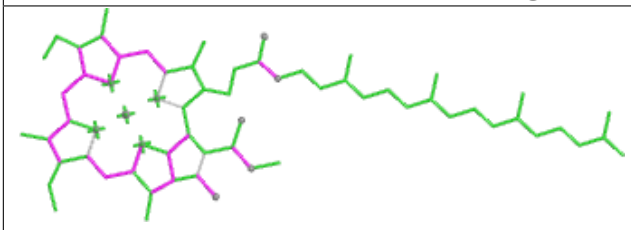
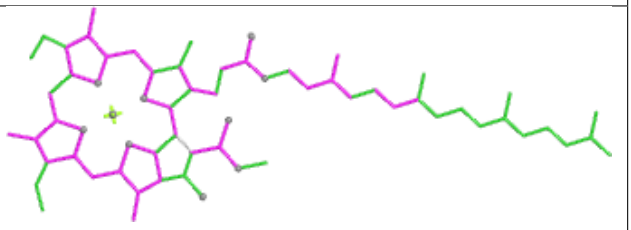
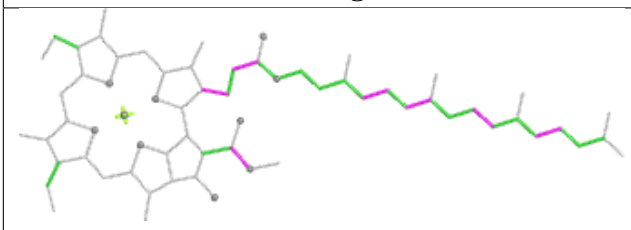
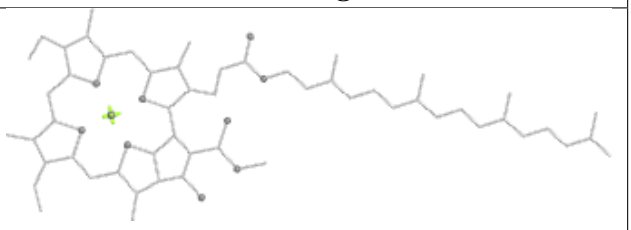
Bond angles

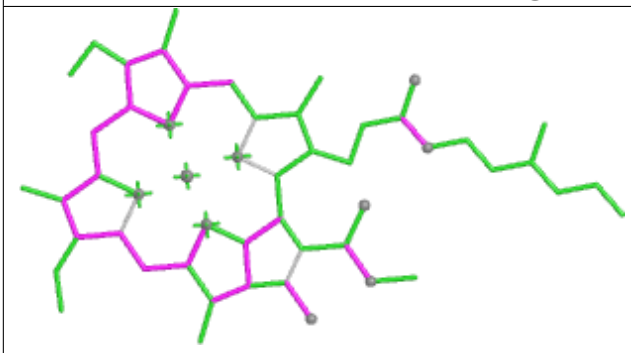
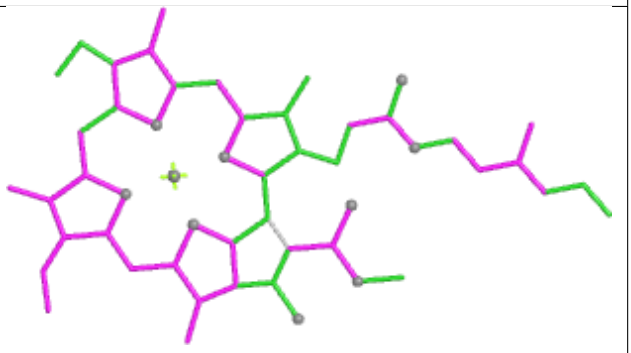
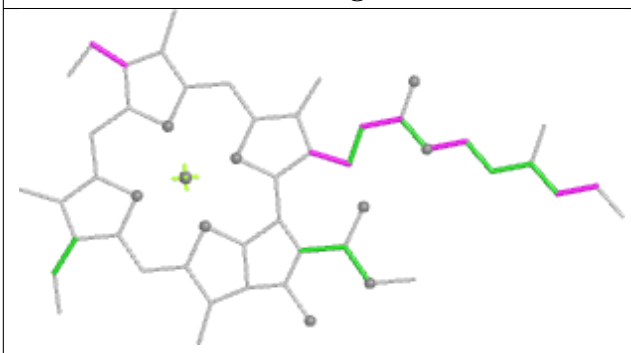
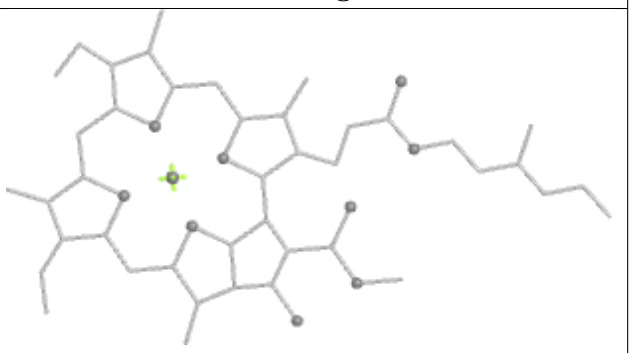


Torsions

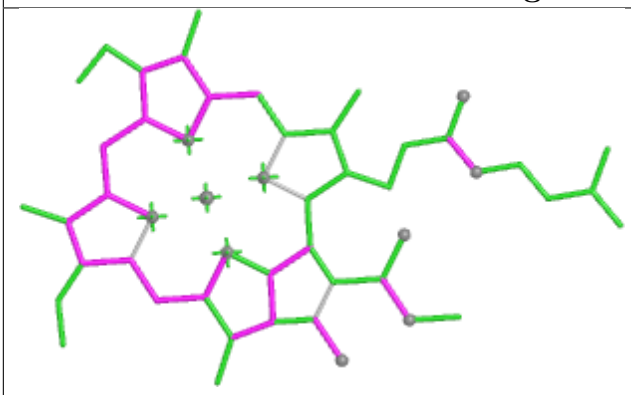


Rings

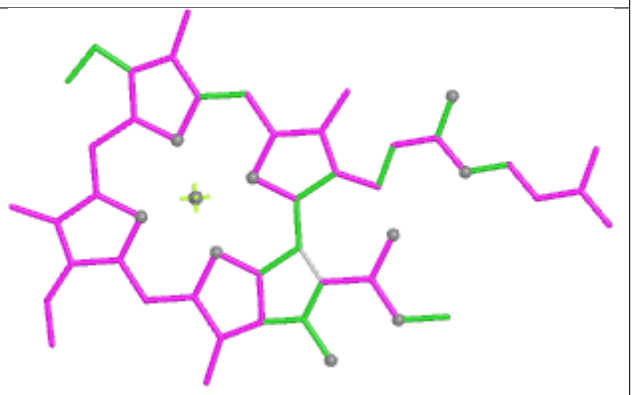
Ligand CLA B 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

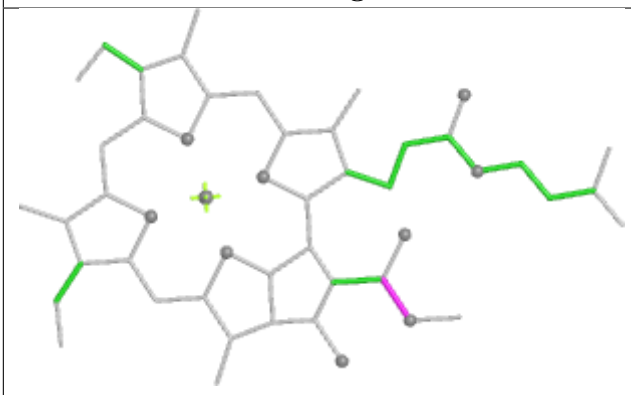
Ligand CLA A 836



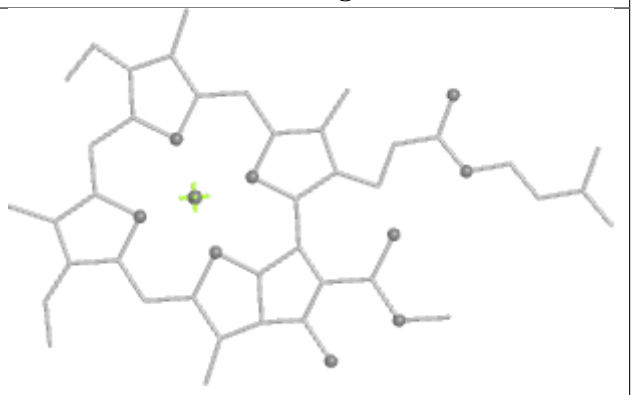
Bond lengths



Bond angles

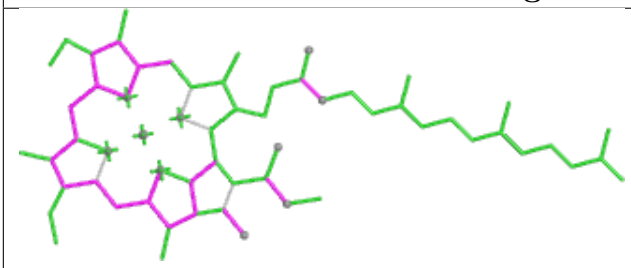


Torsions

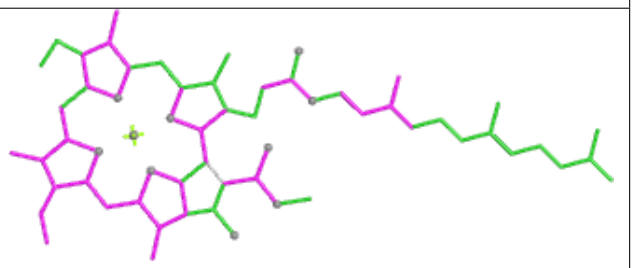


Rings

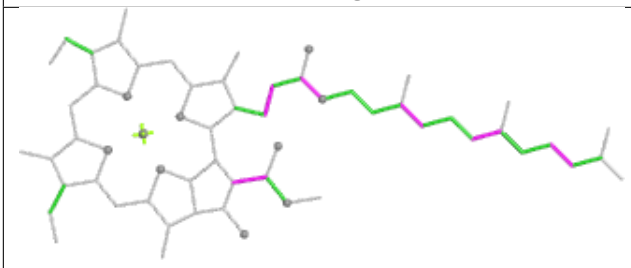
Ligand CLA A 815



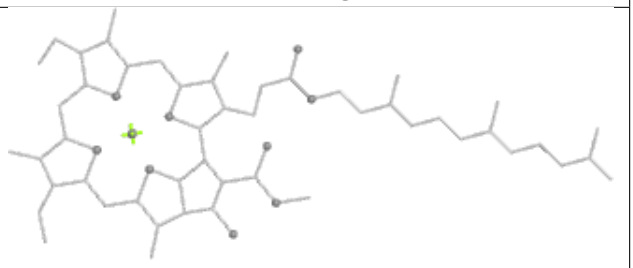
Bond lengths



Bond angles

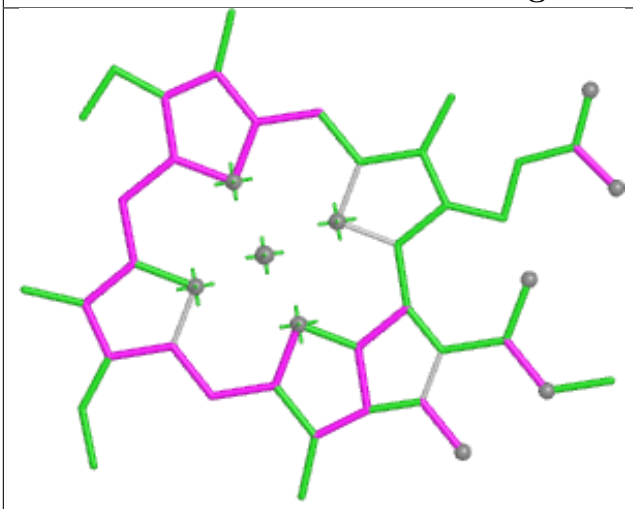


Torsions

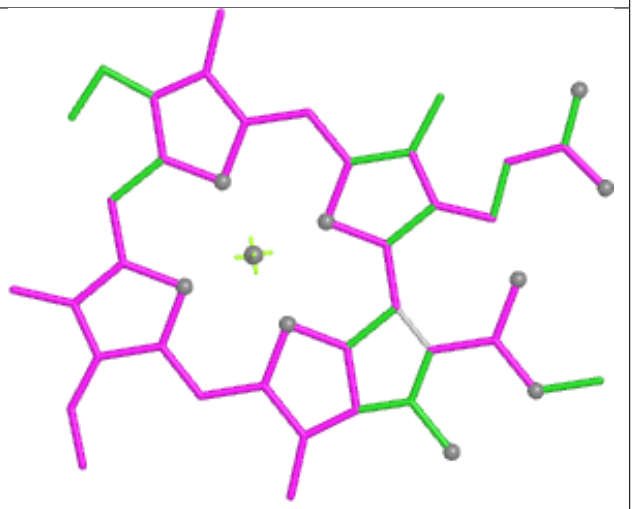


Rings

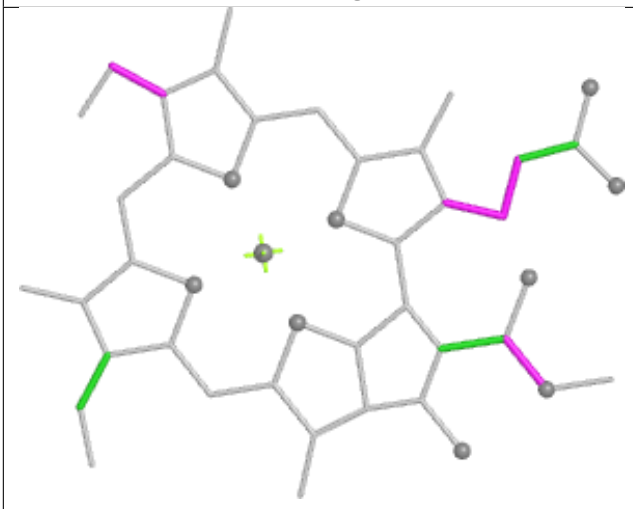
Ligand CLA 9 614



Bond lengths



Bond angles

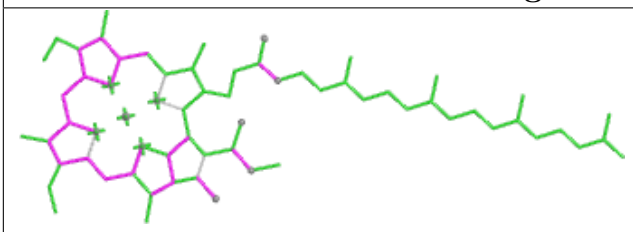


Torsions

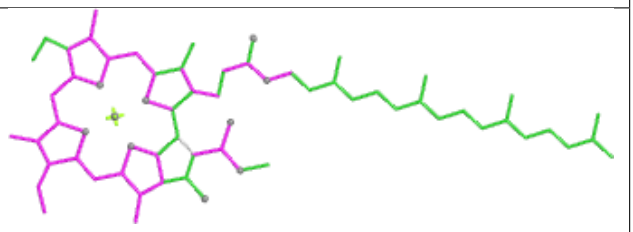


Rings

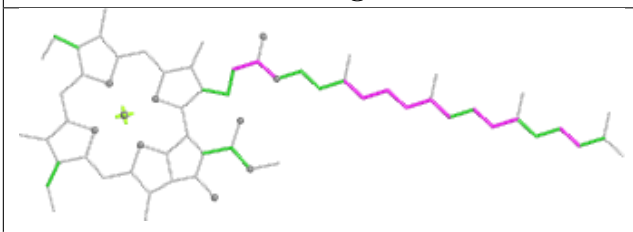
Ligand CLA B 812



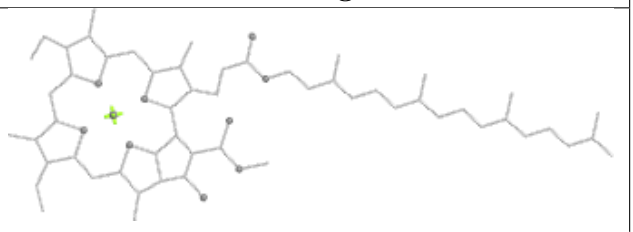
Bond lengths



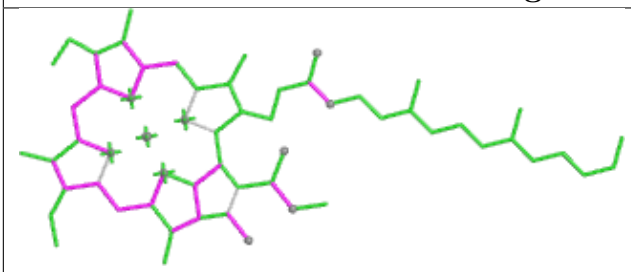
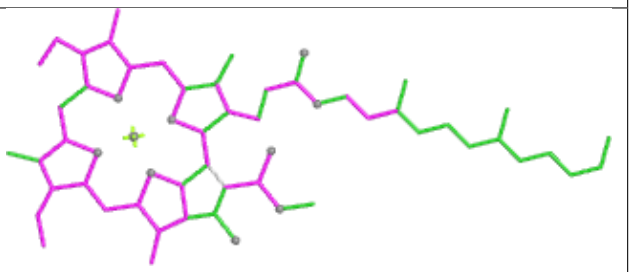
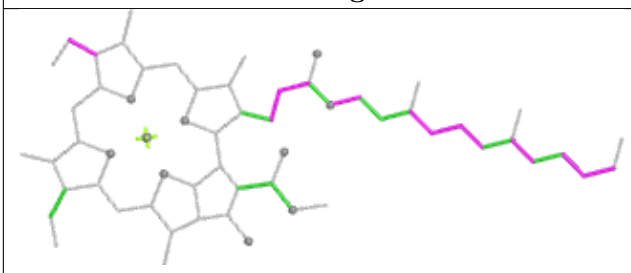
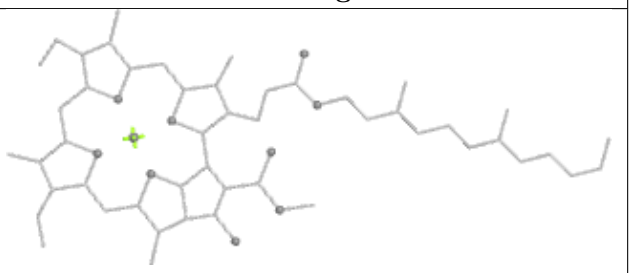
Bond angles

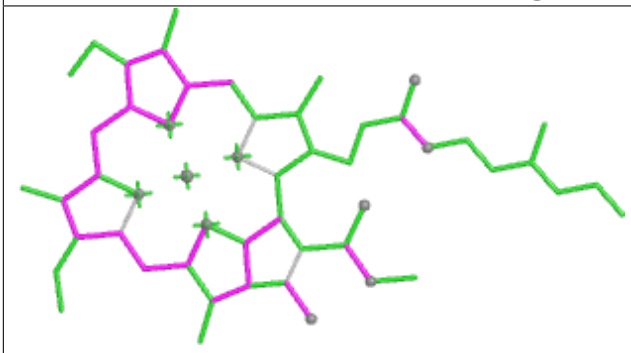
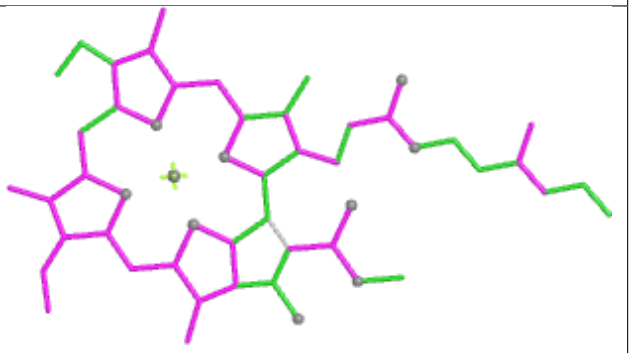
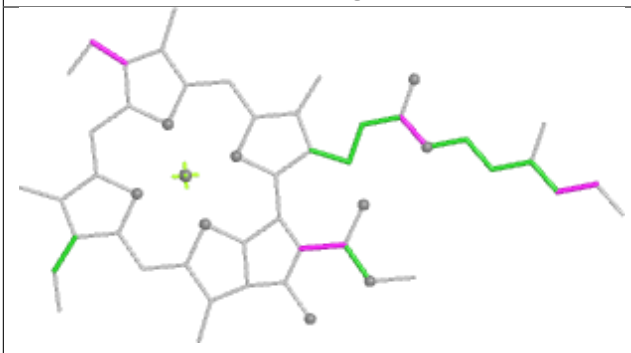
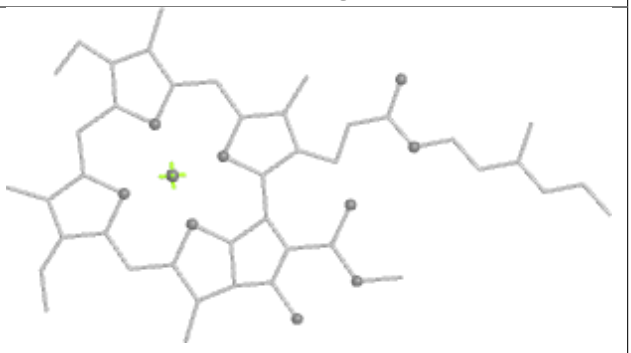


Torsions

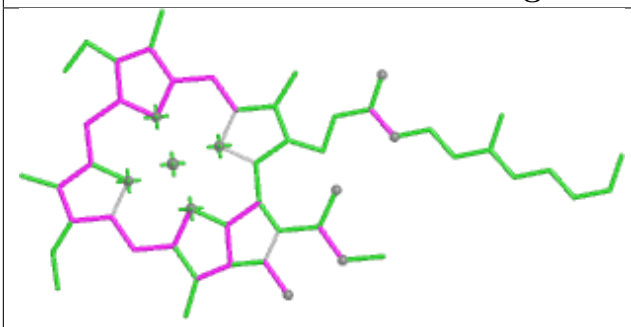


Rings

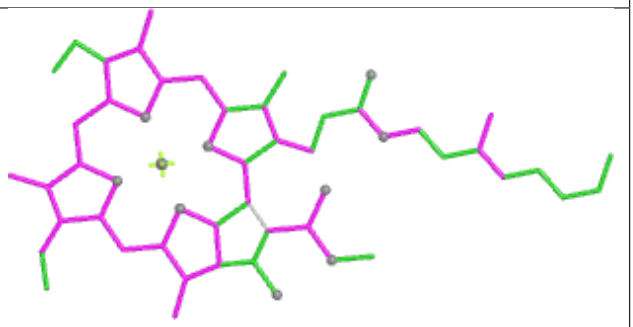
Ligand CLA B 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

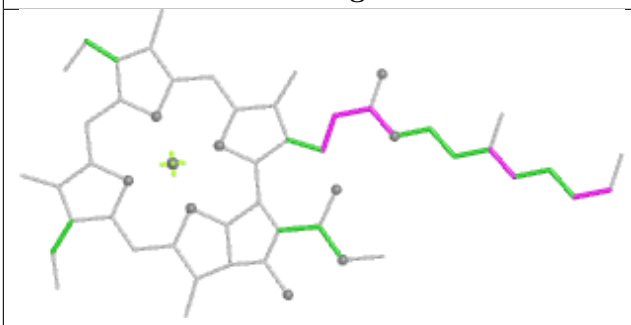
Ligand CLA A 813



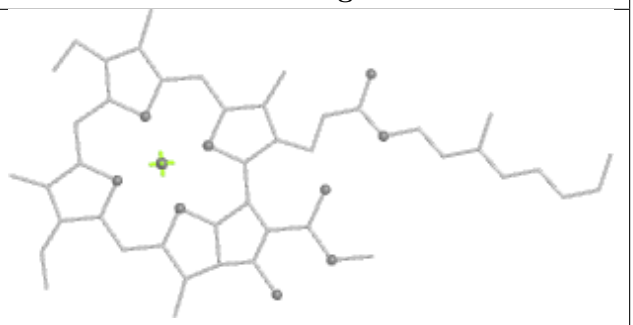
Bond lengths



Bond angles

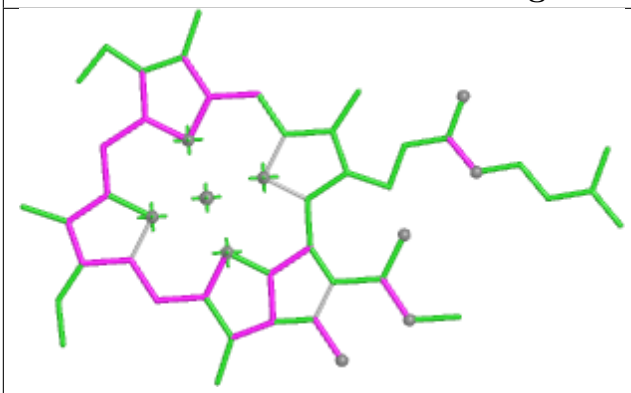


Torsions

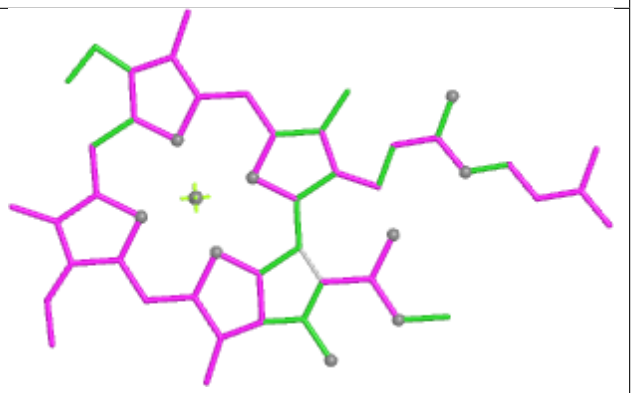


Rings

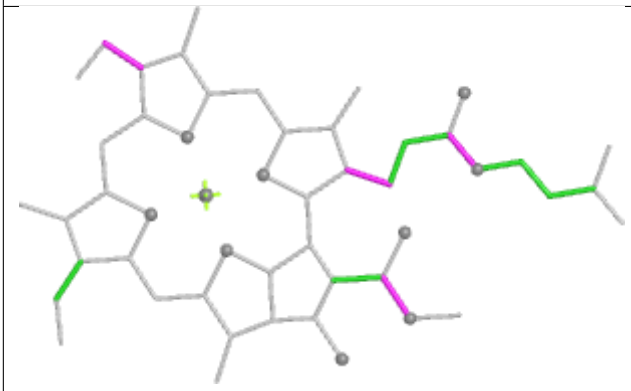
Ligand CLA 5 604



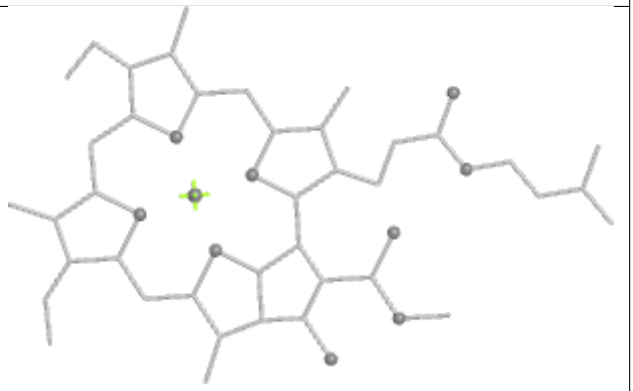
Bond lengths



Bond angles

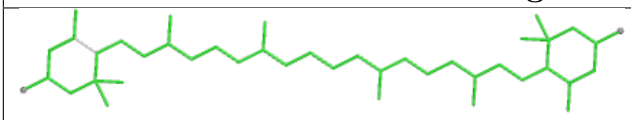


Torsions

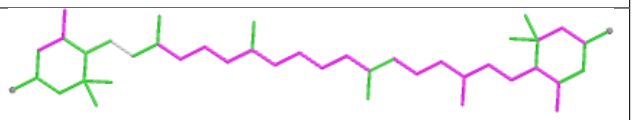


Rings

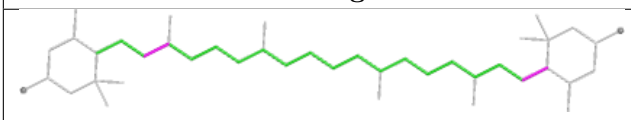
Ligand LUT Z 619



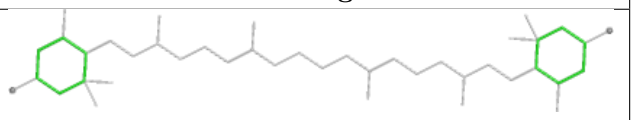
Bond lengths



Bond angles

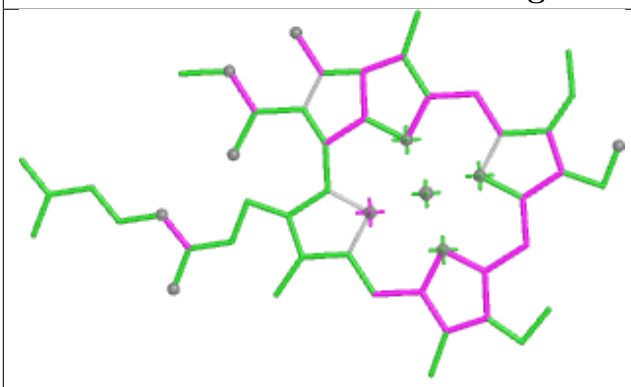


Torsions

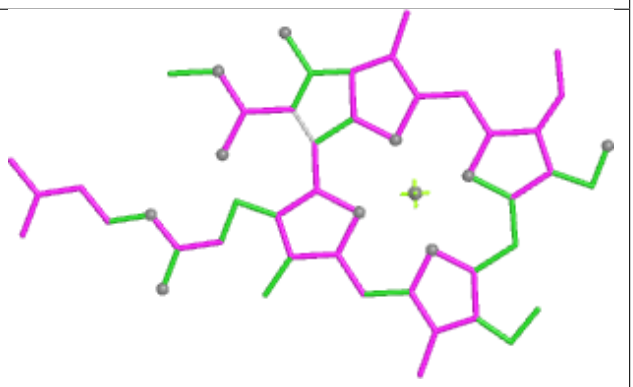


Rings

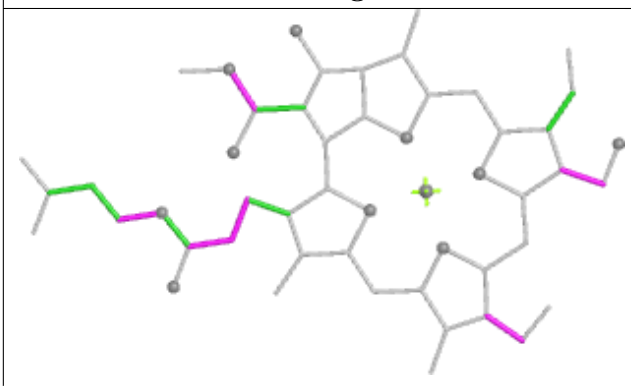
Ligand CHL 4 607



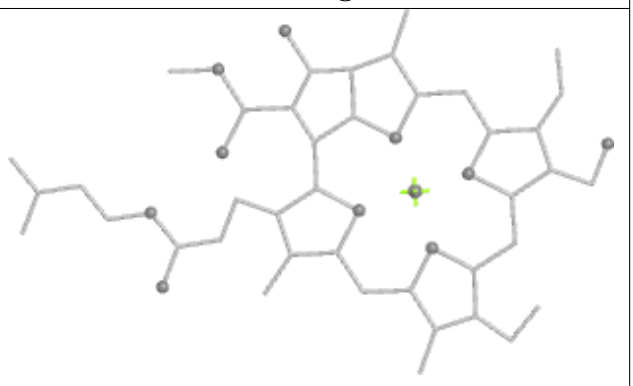
Bond lengths



Bond angles

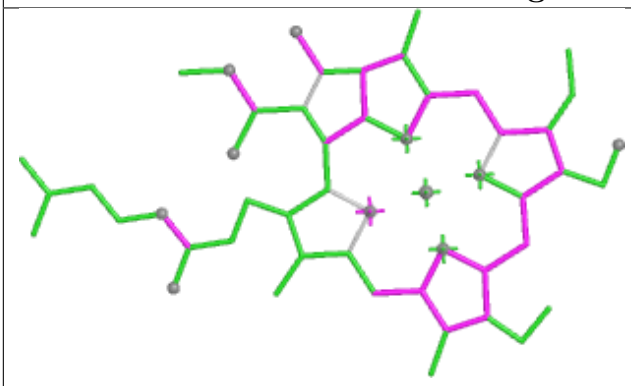


Torsions

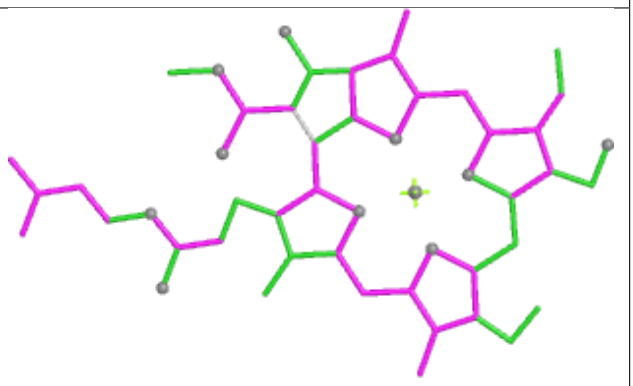


Rings

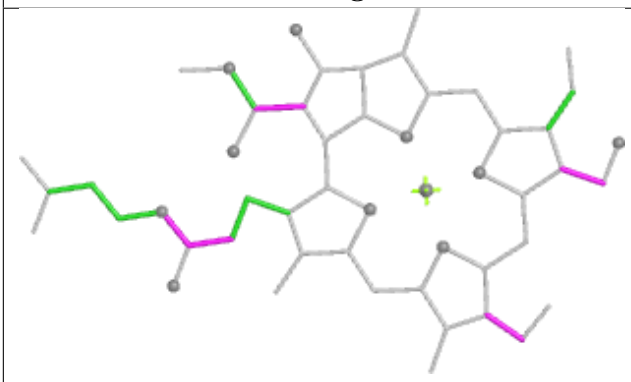
Ligand CHL 9 607



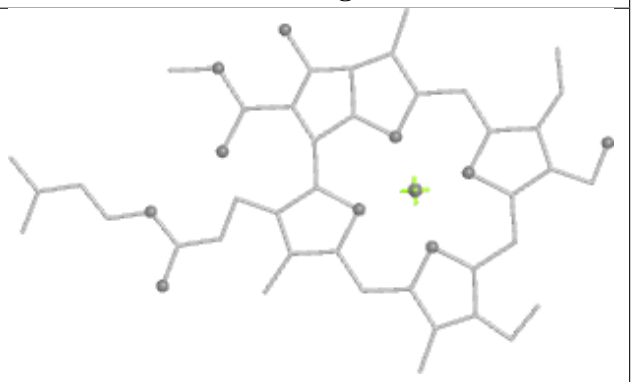
Bond lengths



Bond angles

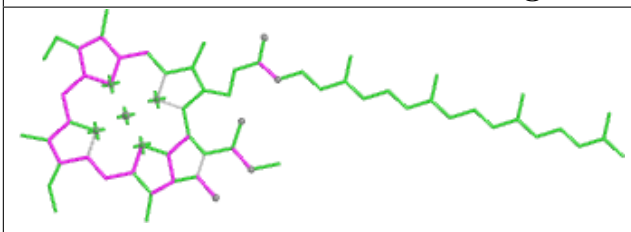


Torsions

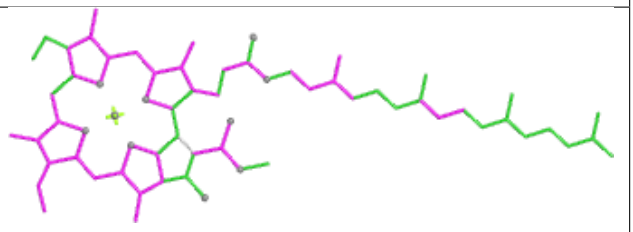


Rings

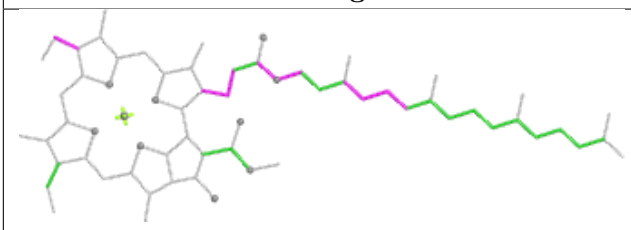
Ligand CLA A 834



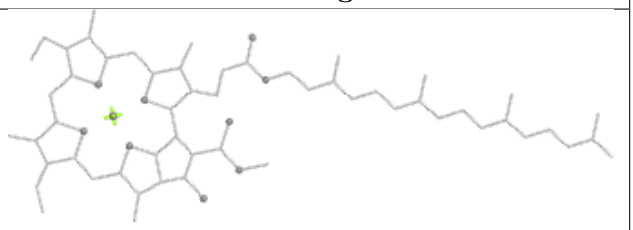
Bond lengths



Bond angles

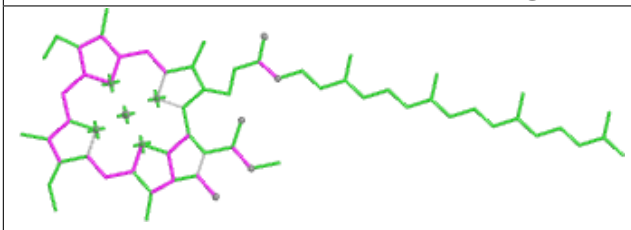


Torsions

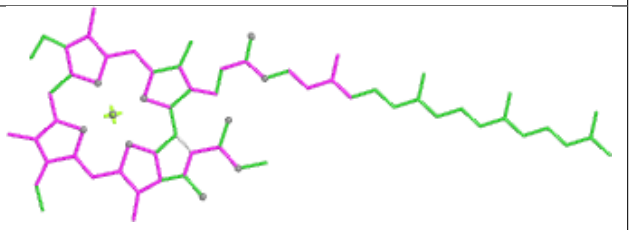


Rings

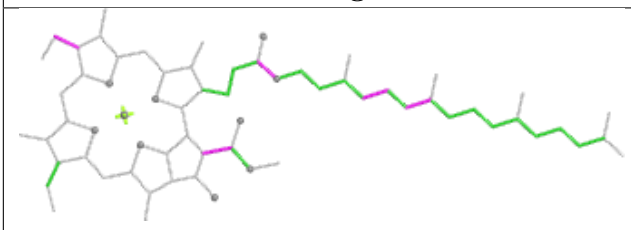
Ligand CLA A 827



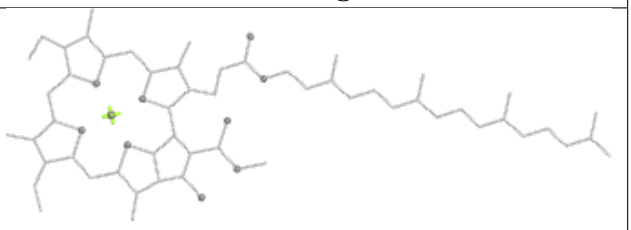
Bond lengths



Bond angles

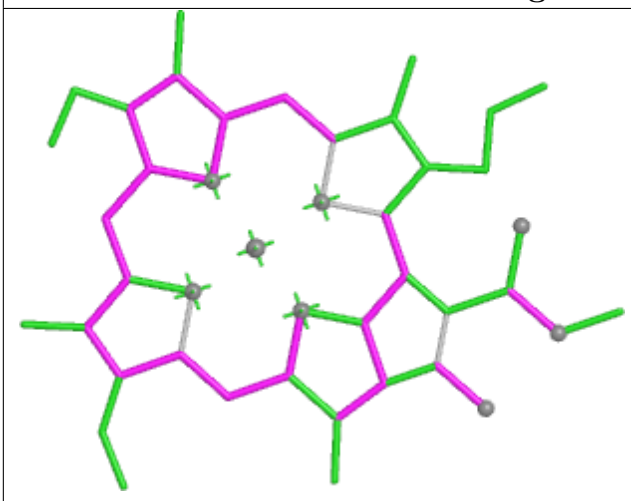


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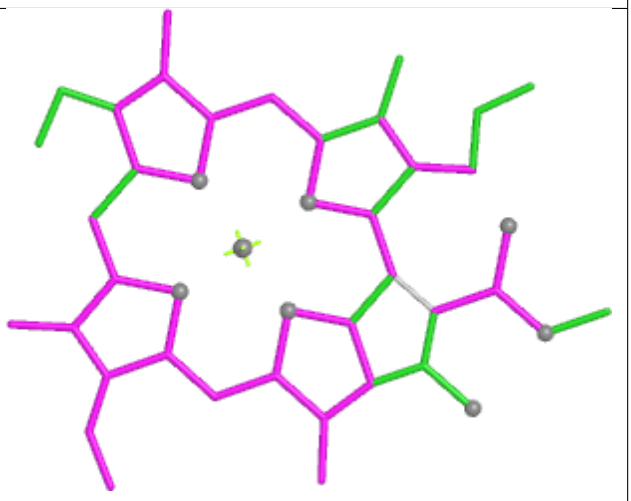


Rings

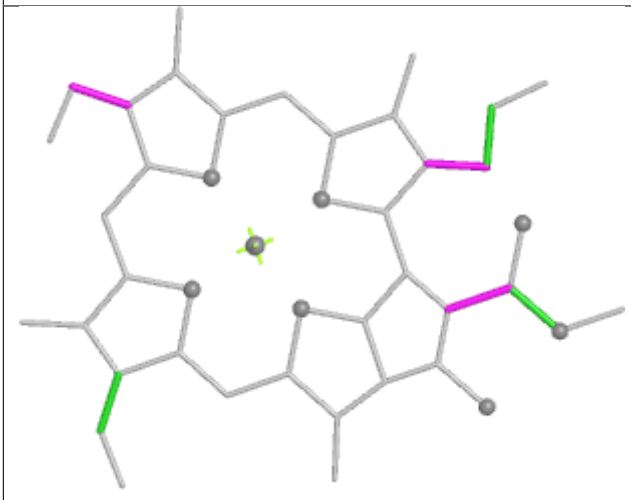
Ligand CLA 7 614



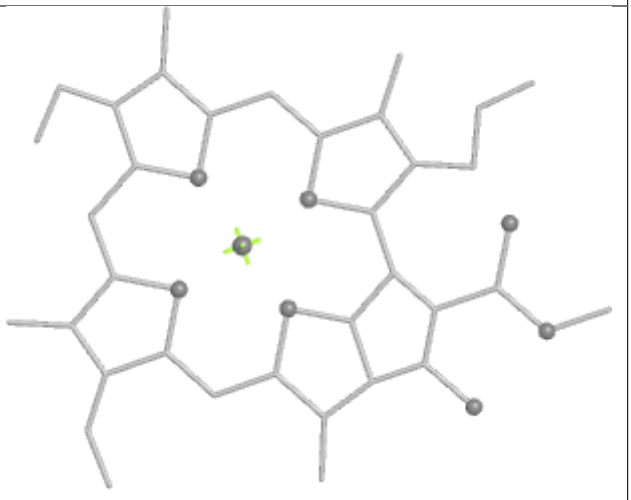
Bond lengths



Bond angles

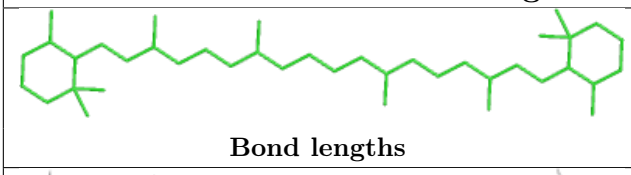


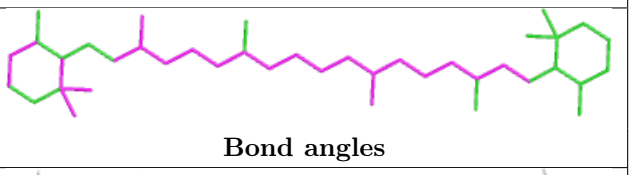
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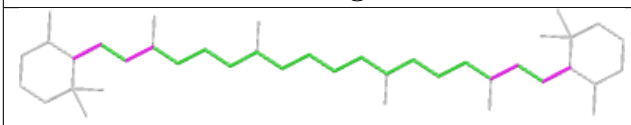


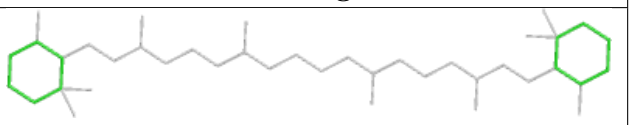
Rings

Ligand BCR B 847


Bond lengths


Bond angles

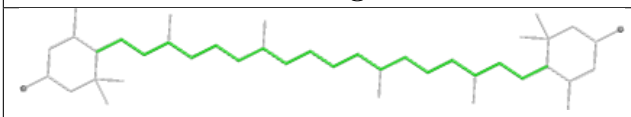

Torsions

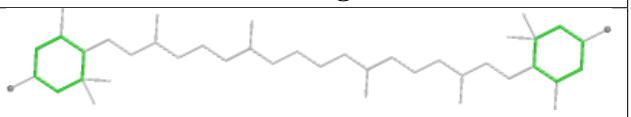

Rings

Ligand LUT 5 620

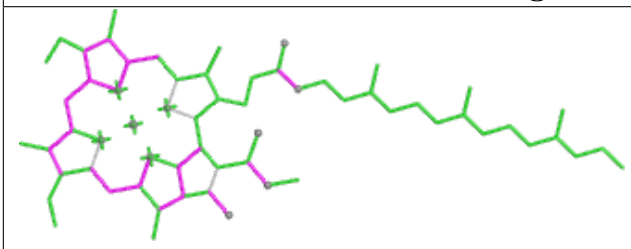

Bond lengths

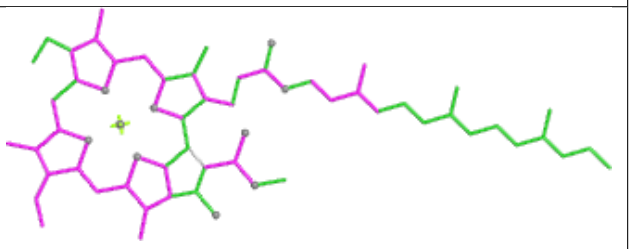

Bond angles

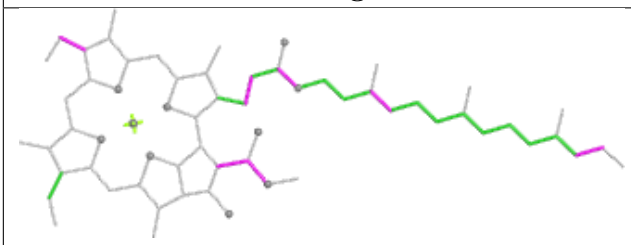

Torsions

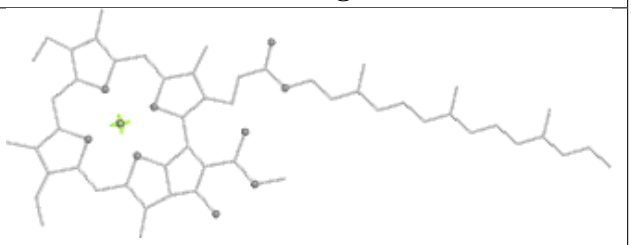

Rings

Ligand CLA 8 602

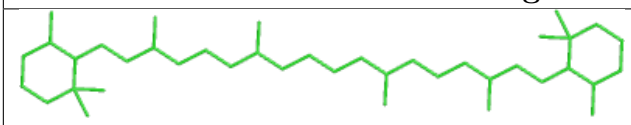

Bond lengths

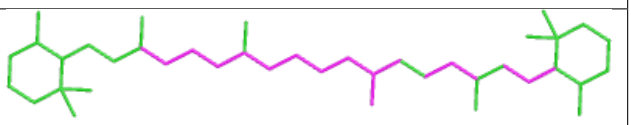

Bond angles

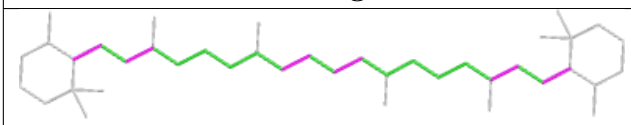

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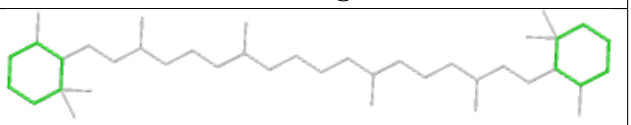

Rings

Ligand BCR B 843

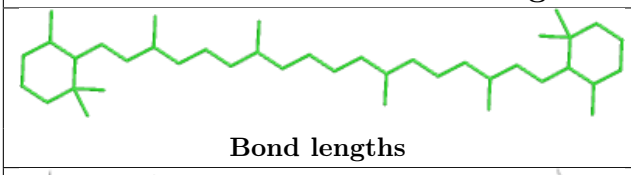

Bond lengths


Bond angles

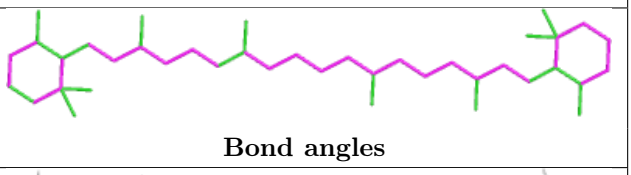

Torsions


Rings

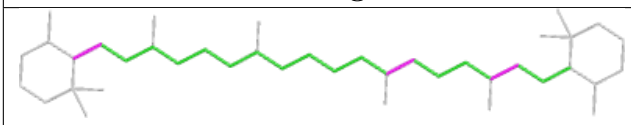
Ligand BCR I 172



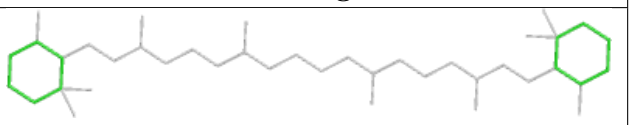
Bond lengths



Bond angles

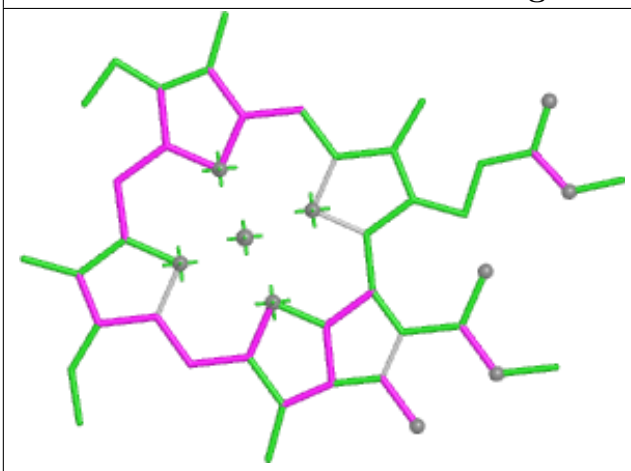


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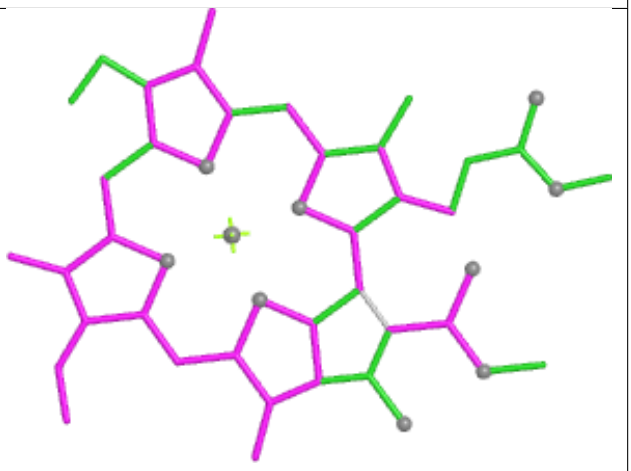


Rings

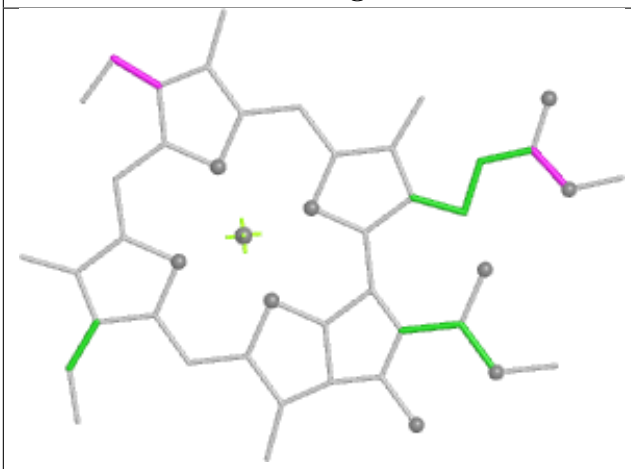
Ligand CLA 4 603



Bond lengths



Bond angles

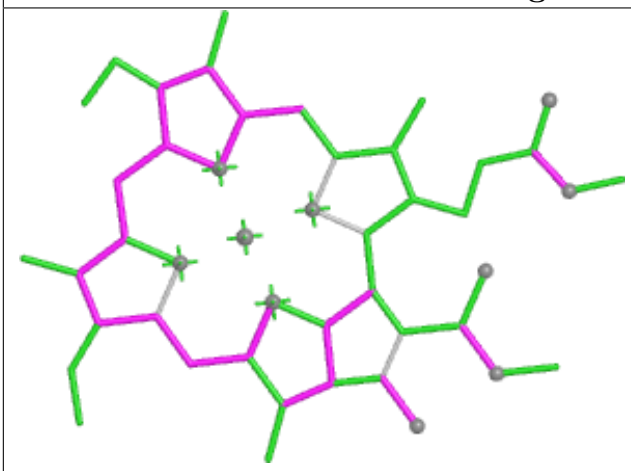


Torsions

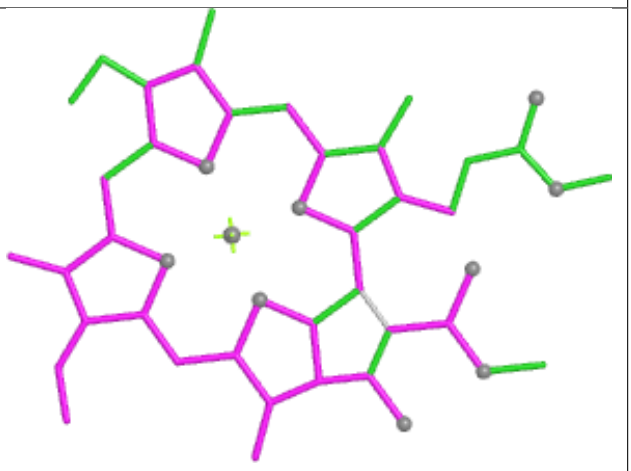


Rings

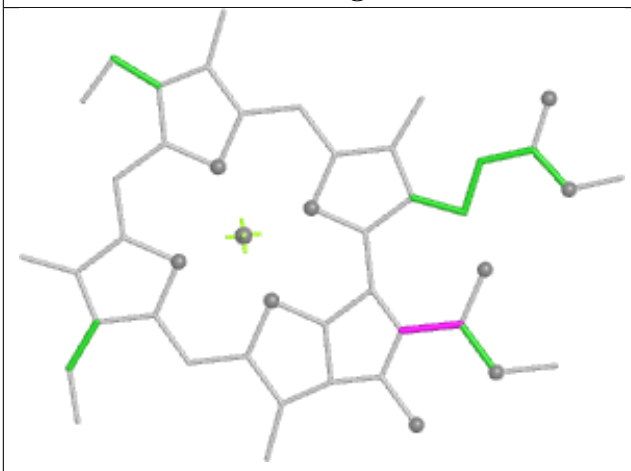
Ligand CLA 5 603



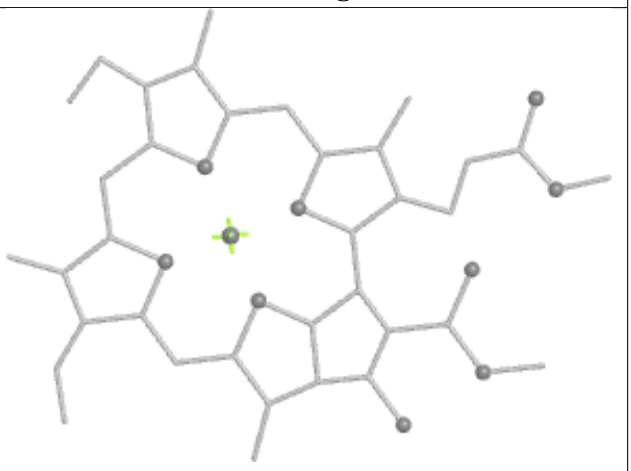
Bond lengths



Bond angles

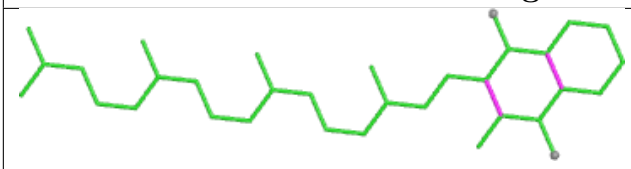


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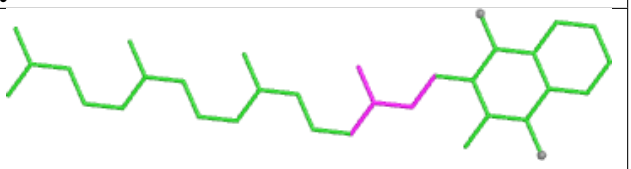


Rings

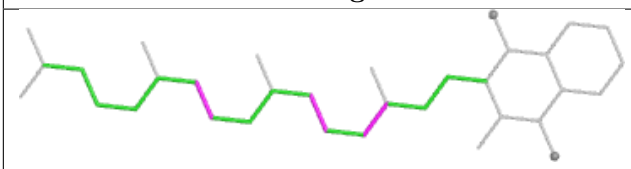
Ligand PQN B 842



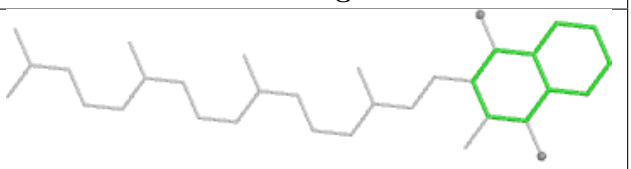
Bond lengths



Bond angles

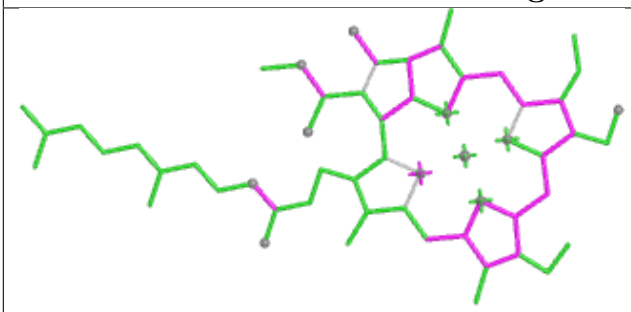


Torsions

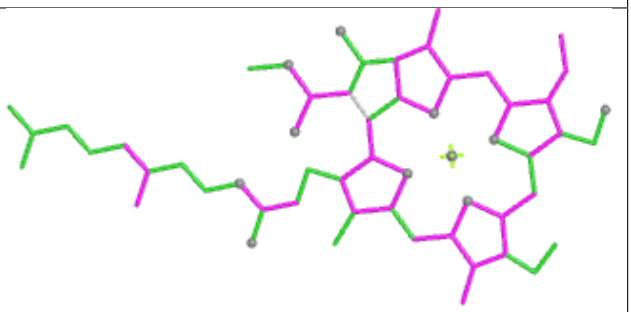


Rings

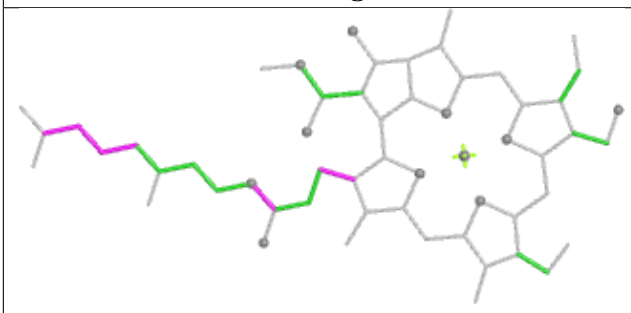
Ligand CHL 6 606



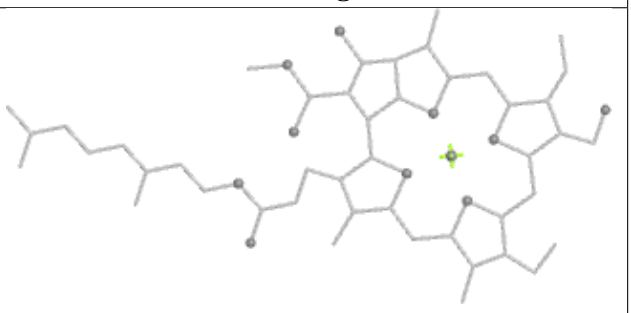
Bond lengths



Bond angles

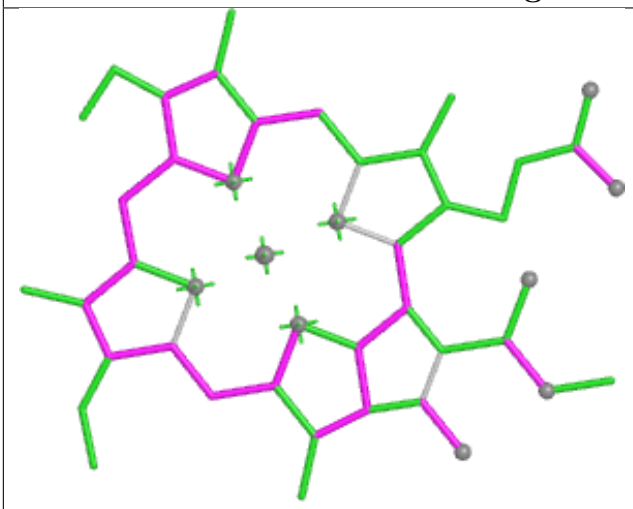


Torsions

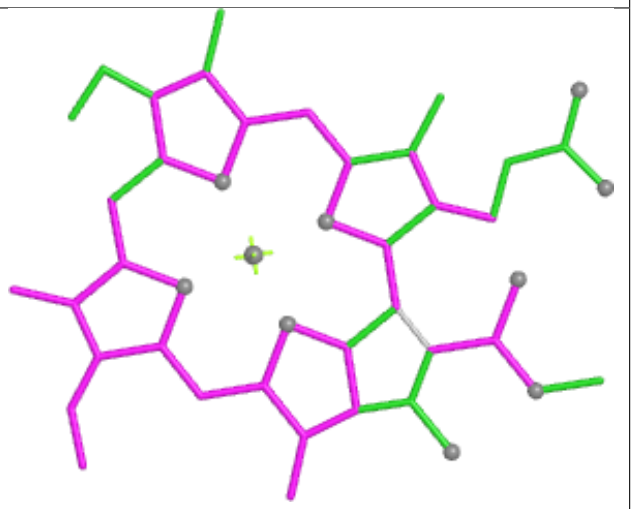


Rings

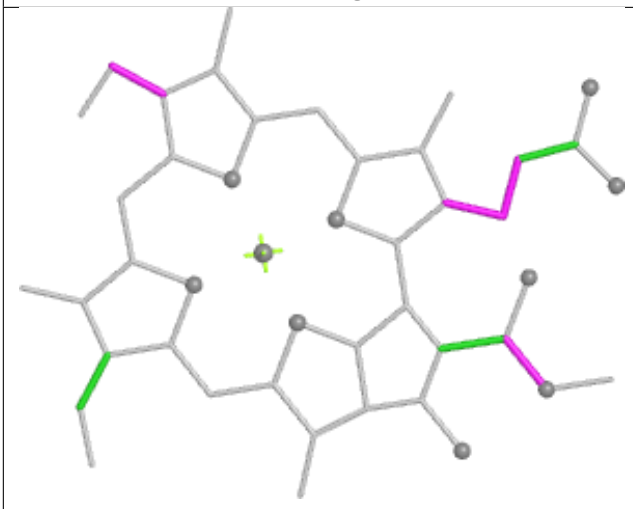
Ligand CLA B 835



Bond lengths



Bond angles

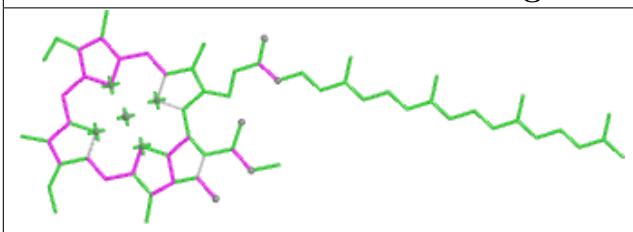


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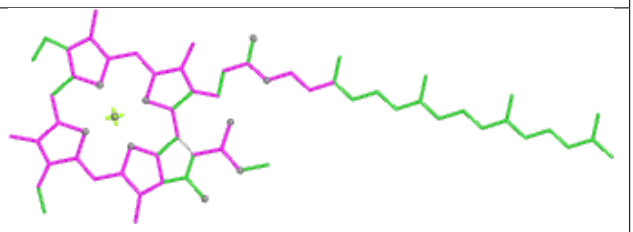


Rings

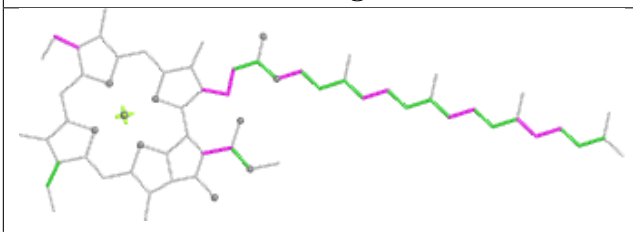
Ligand CLA A 854



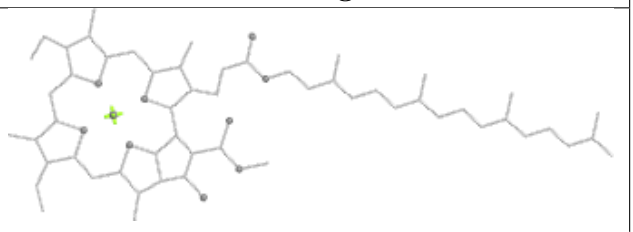
Bond lengths



Bond angles

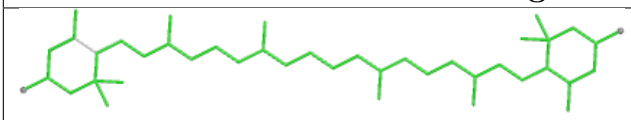


Torsions

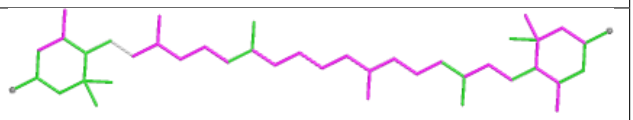


Rings

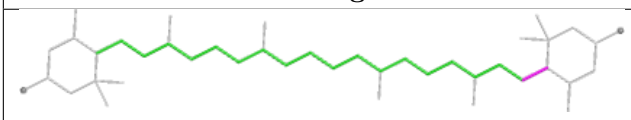
Ligand LUT 8 617



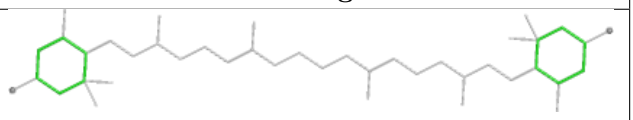
Bond lengths



Bond angles

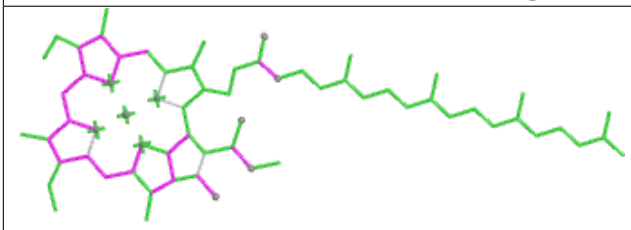


Torsions

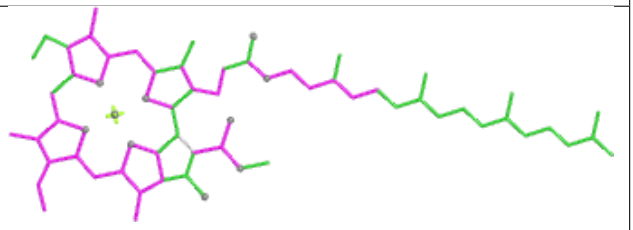


Rings

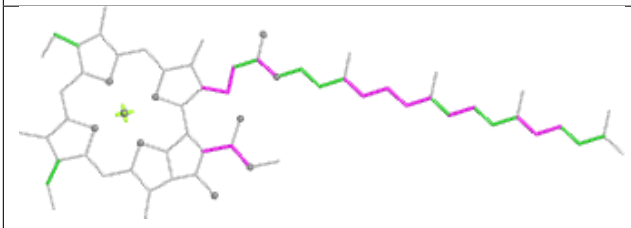
Ligand CLA A 809



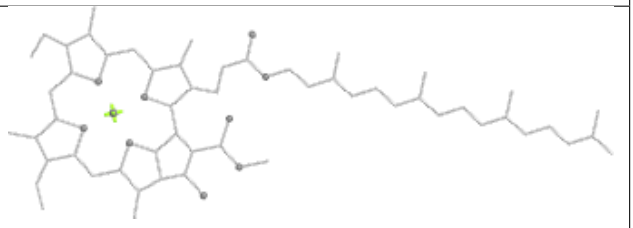
Bond lengths



Bond angles

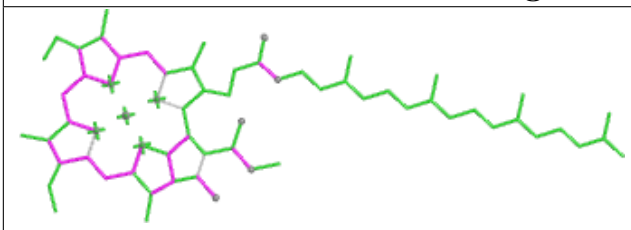


Torsions

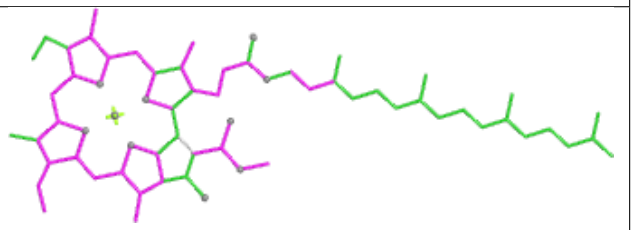


Rings

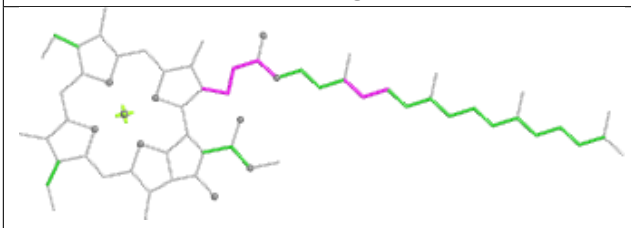
Ligand CLA B 828



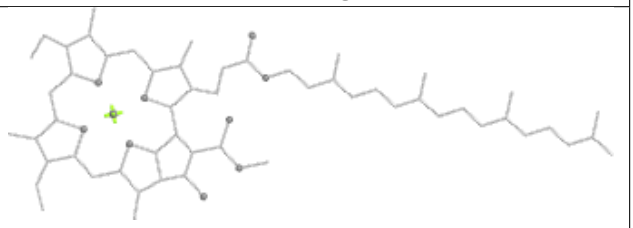
Bond lengths



Bond angles

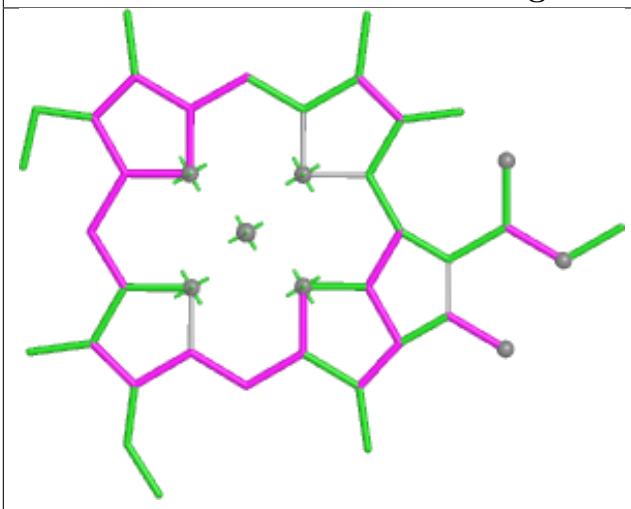


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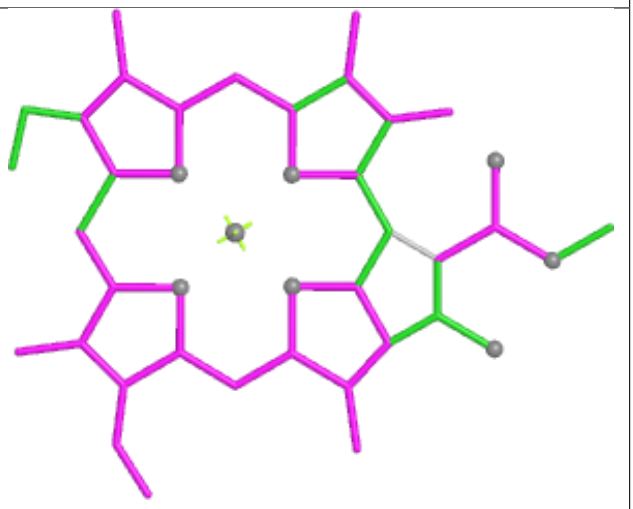


Rings

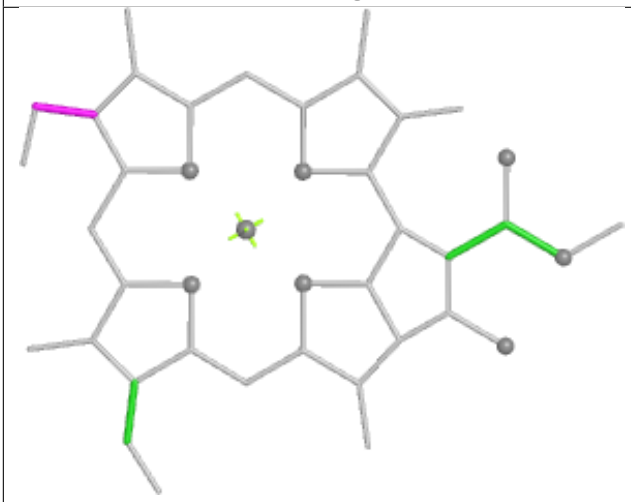
Ligand CLA 4 616



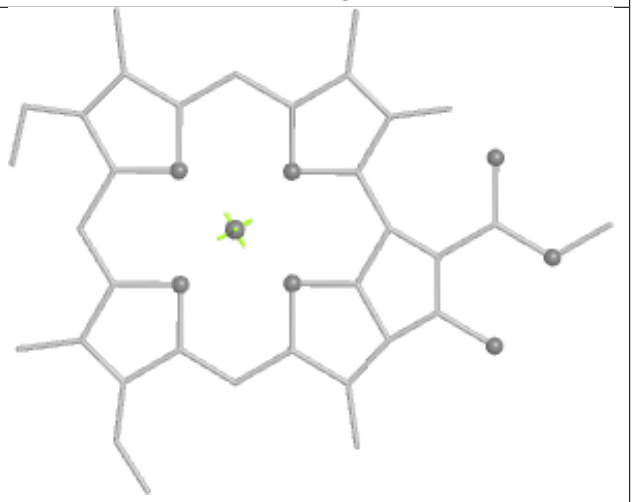
Bond lengths



Bond angles

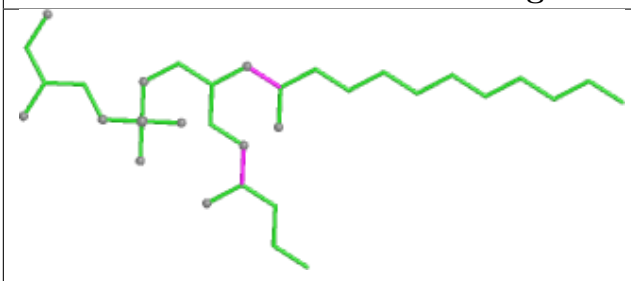


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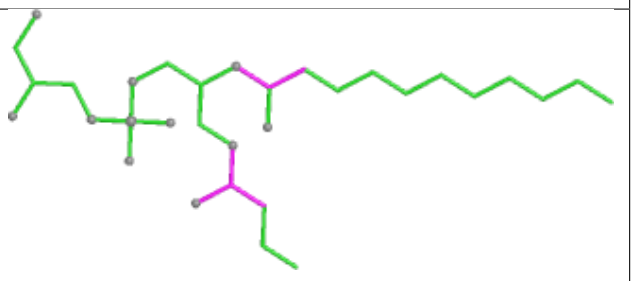


Rings

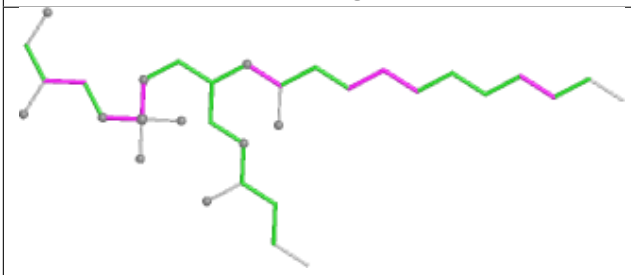
Ligand LHG 4 623



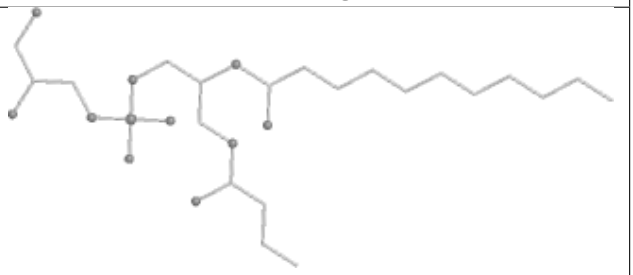
Bond lengths



Bond angles

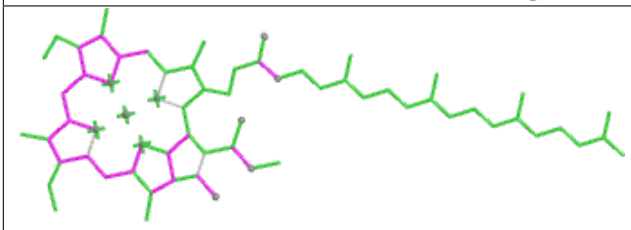


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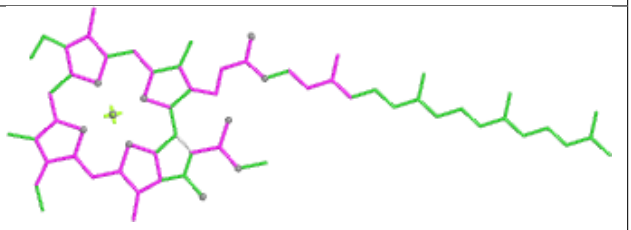


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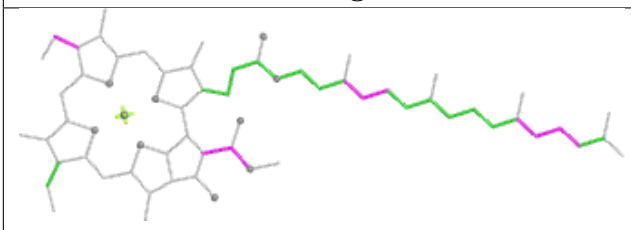
Ligand CLA B 808



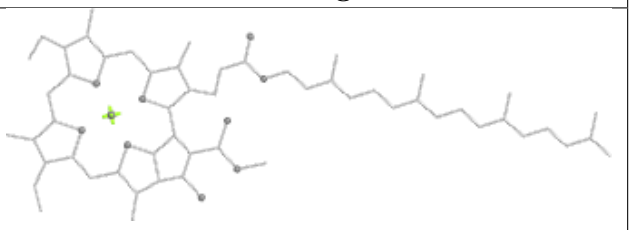
Bond lengths



Bond angles

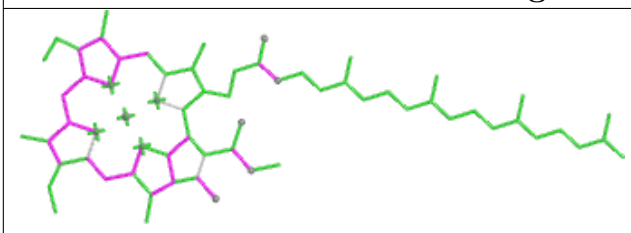


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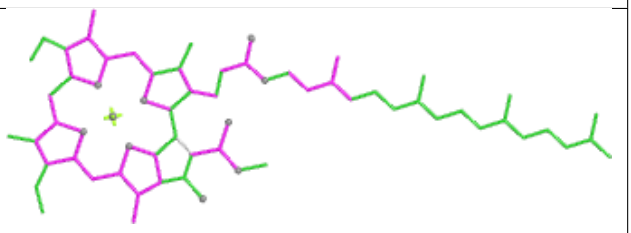


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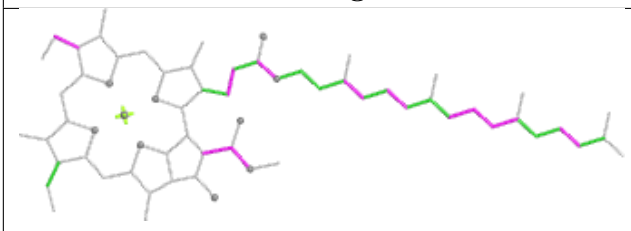
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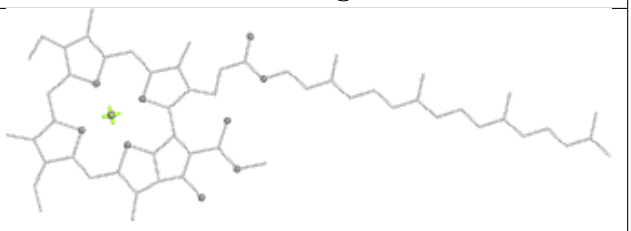
Bond lengths



Bond angles

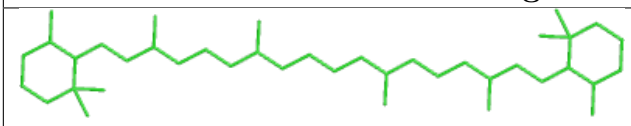


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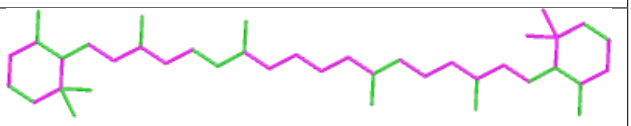


Rings

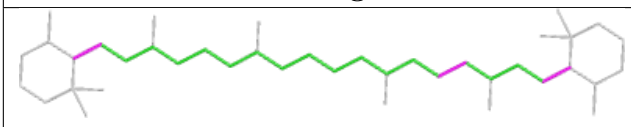
Ligand BCR B 846



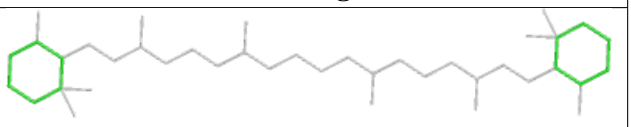
Bond lengths



Bond angles

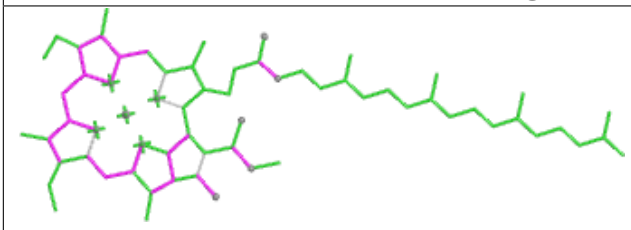


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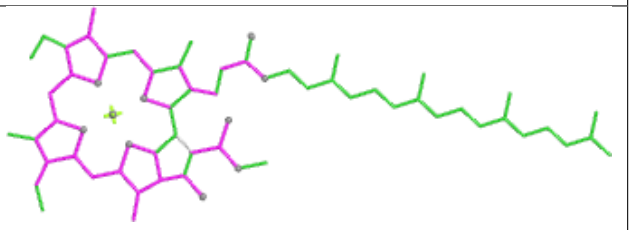


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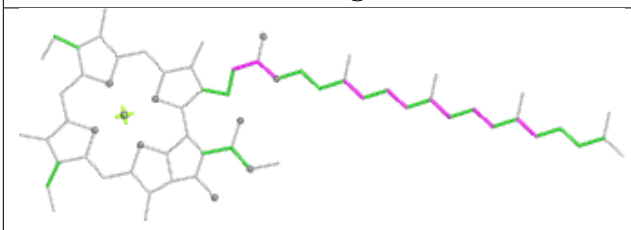
Ligand CLA A 828



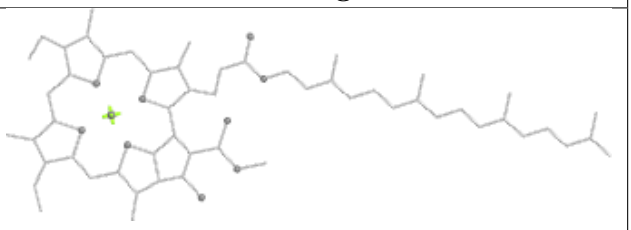
Bond lengths



Bond angles

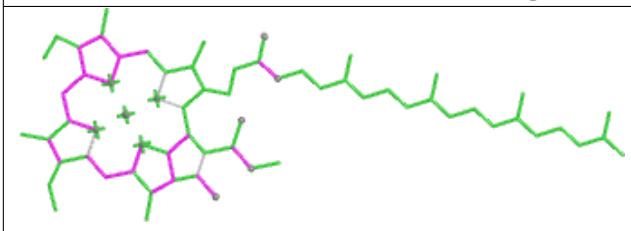


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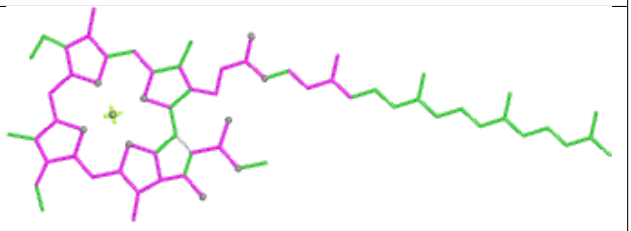


Rings

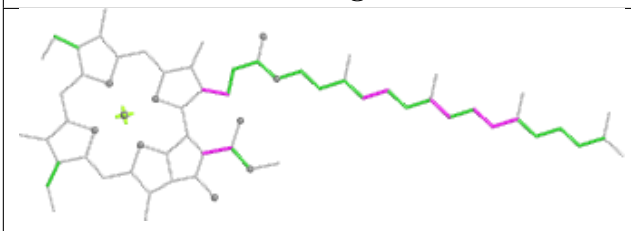
Ligand CLA B 826



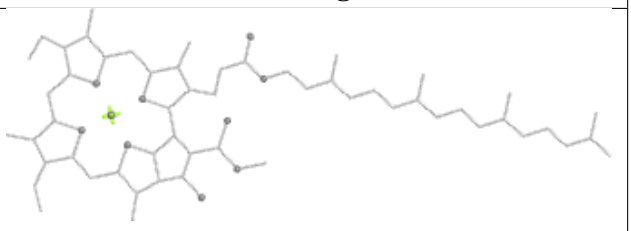
Bond lengths



Bond angles

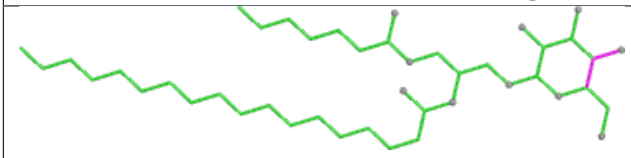


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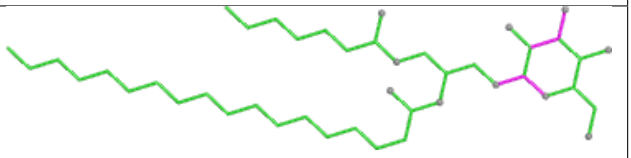


Rings

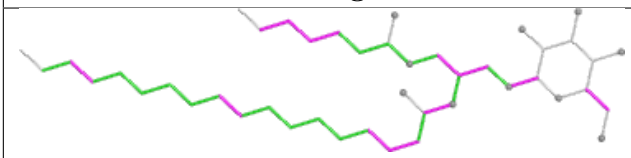
Ligand LMG 9 620



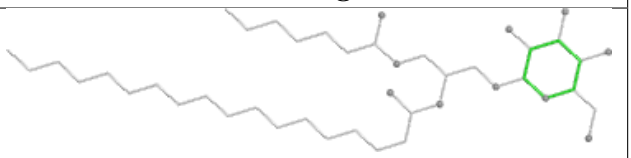
Bond lengths



Bond angles

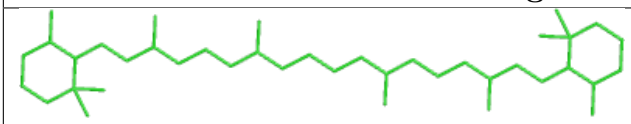


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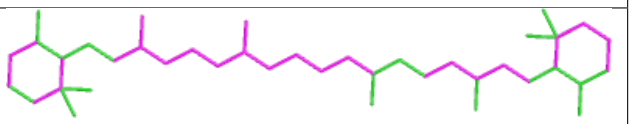


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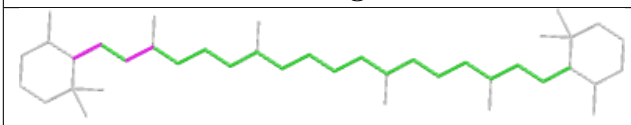
Ligand BCR 3 719



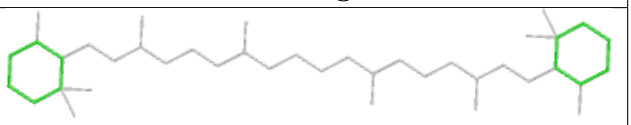
Bond lengths



Bond angles

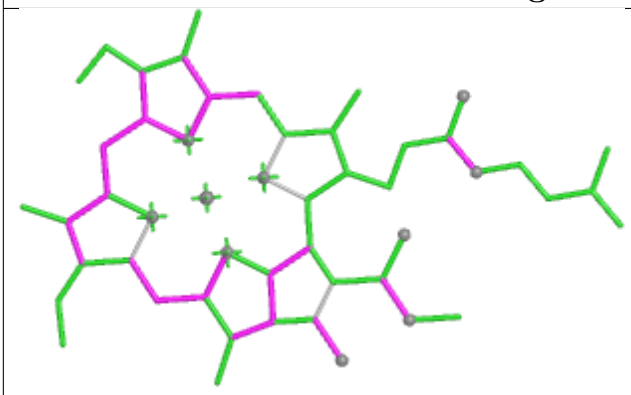


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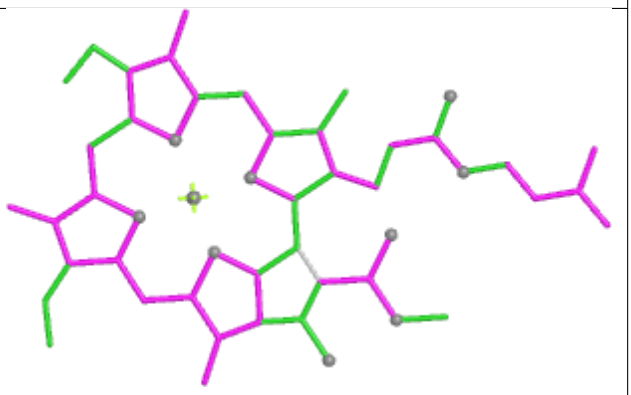


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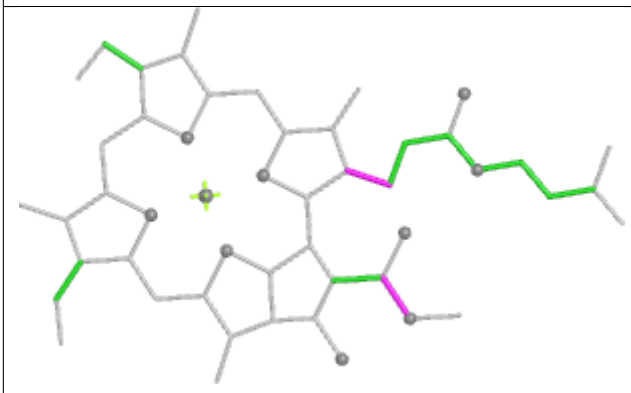
Ligand CLA 7 608



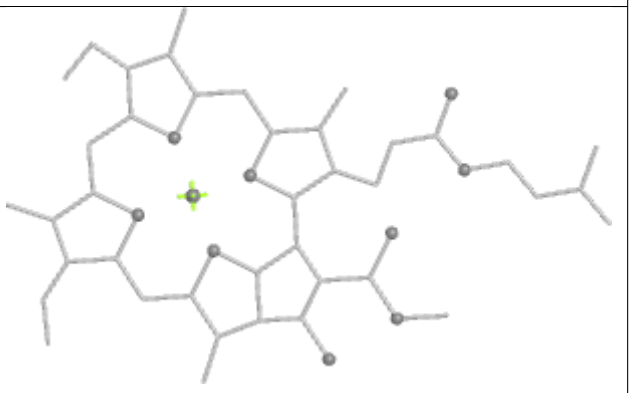
Bond lengths



Bond angles

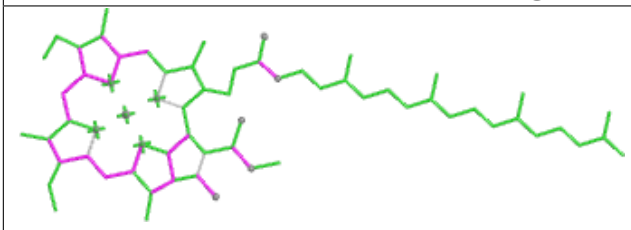


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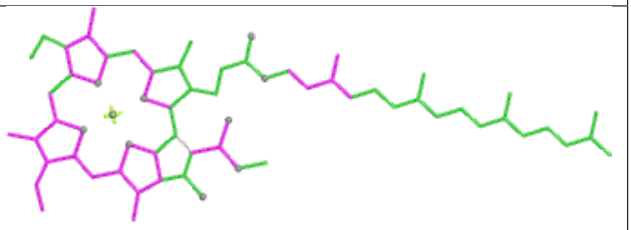


Rings

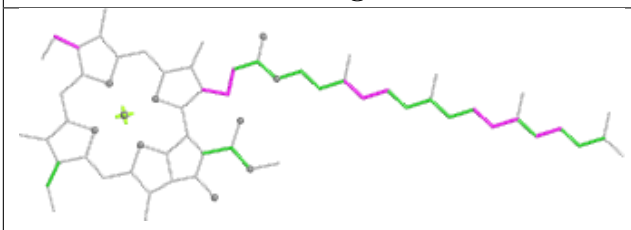
Ligand CLA 3 604



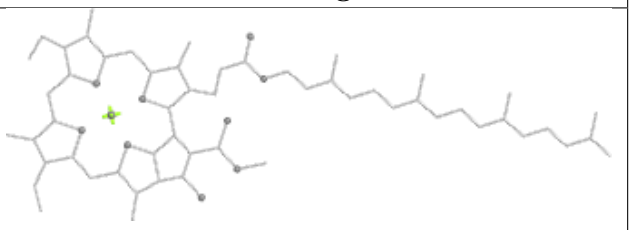
Bond lengths



Bond angles

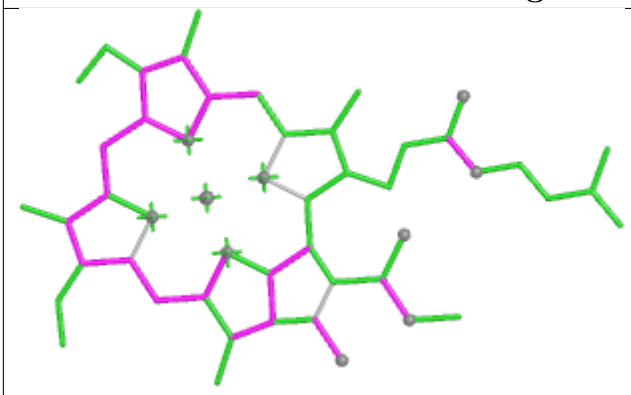


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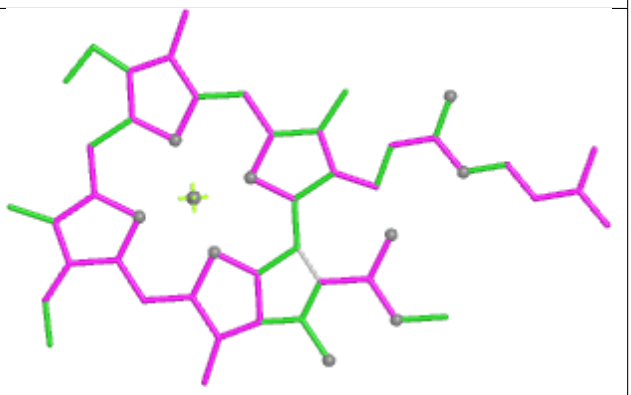


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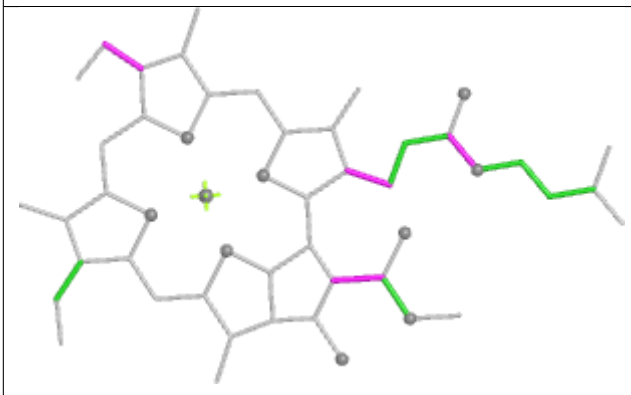
Ligand CLA L 204



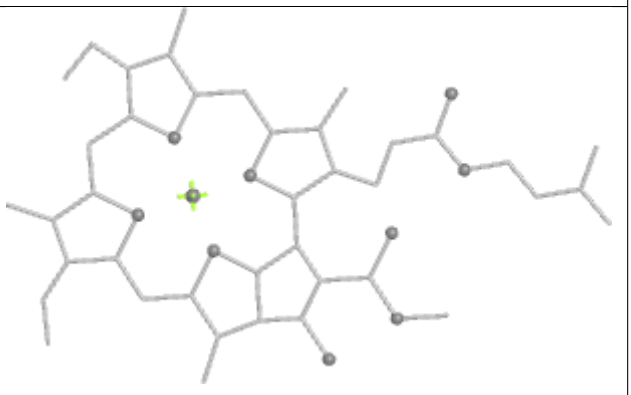
Bond lengths



Bond angles

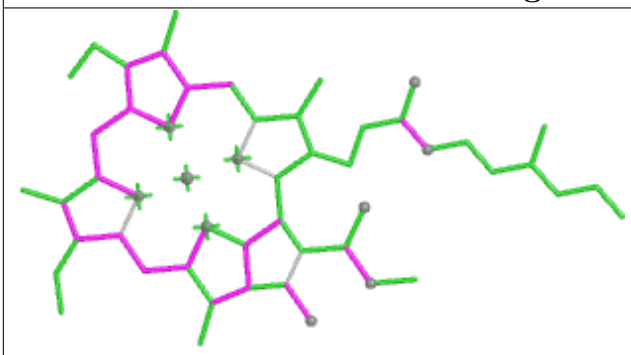


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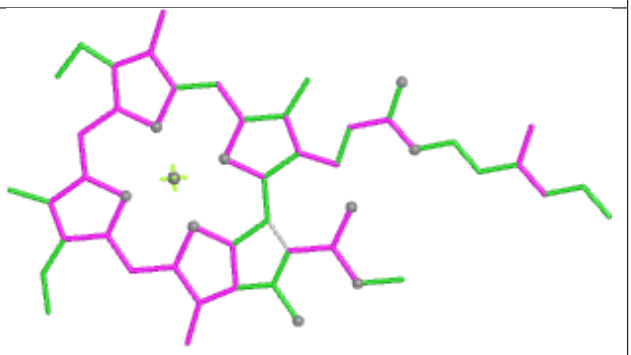


Rings

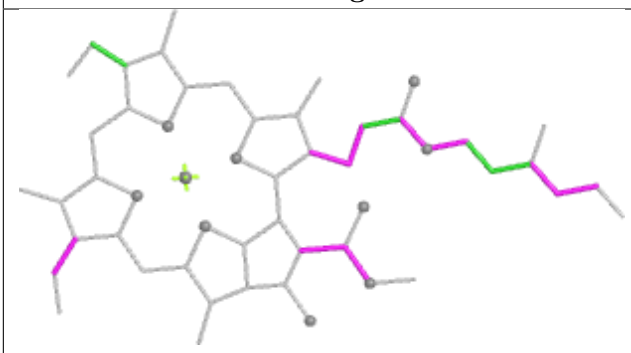
Ligand CLA A 845



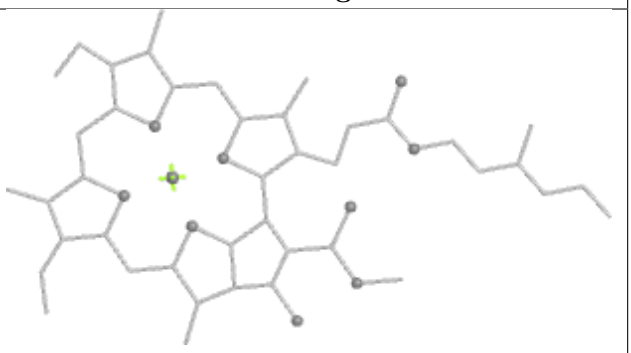
Bond lengths



Bond angles

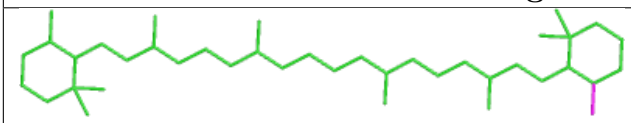


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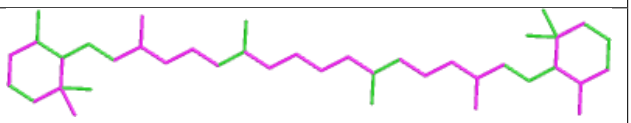


Rings

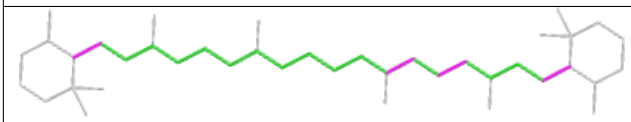
Ligand BCR 7 623



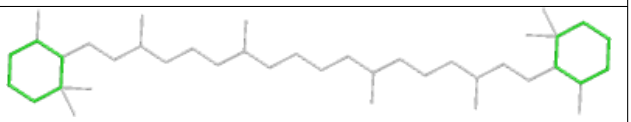
Bond lengths



Bond angles

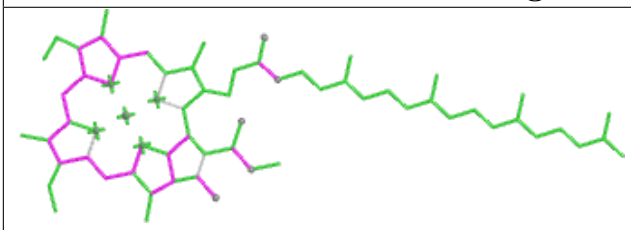


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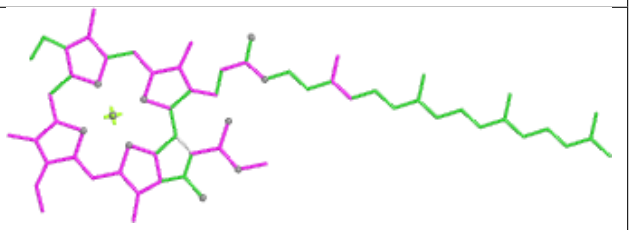


Rings

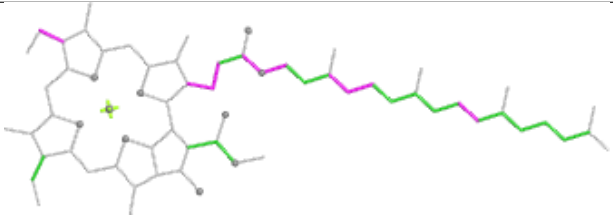
Ligand CLA Z 614



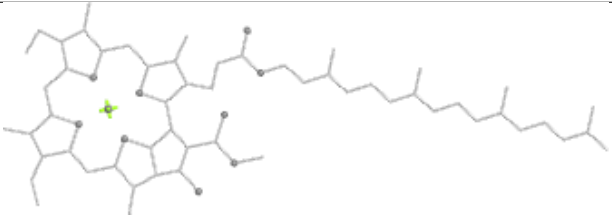
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Bond angles

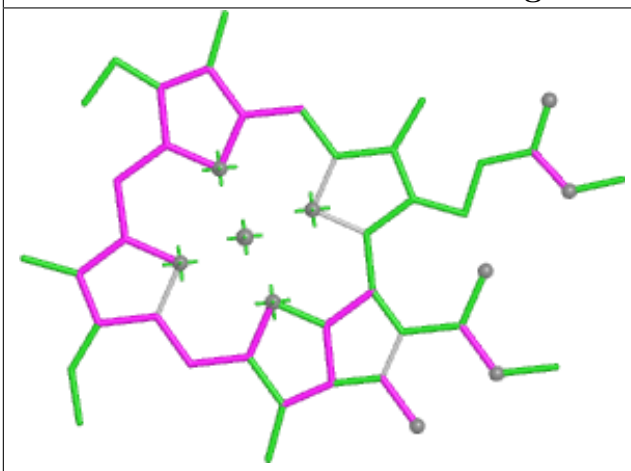


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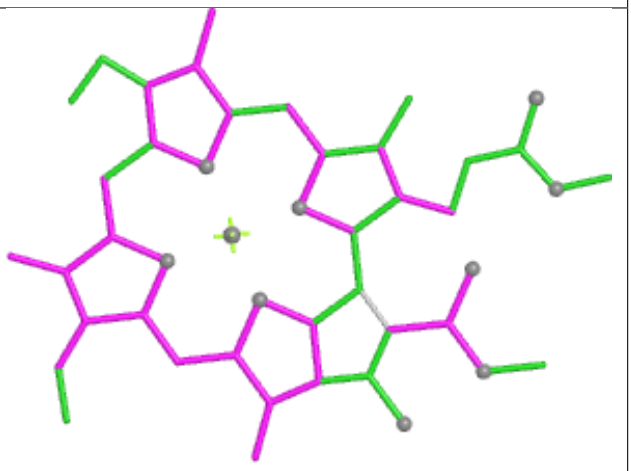


Rings

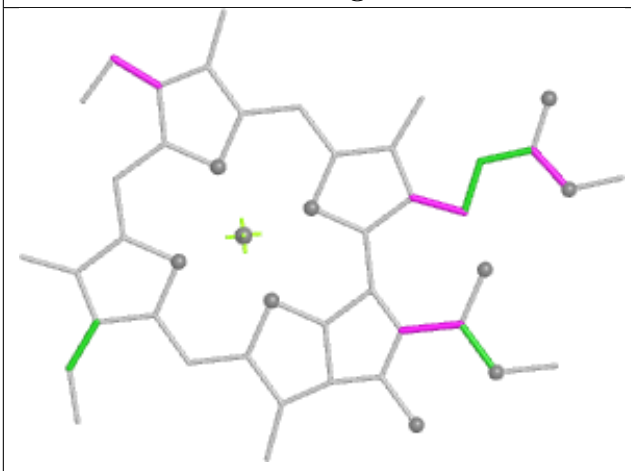
Ligand CLA B 821



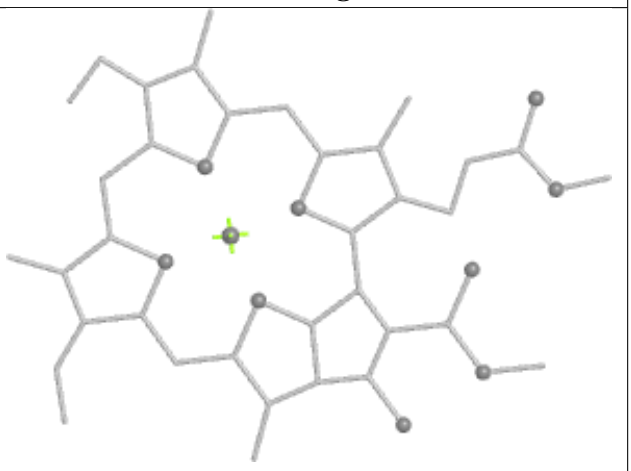
Bond lengths



Bond angles

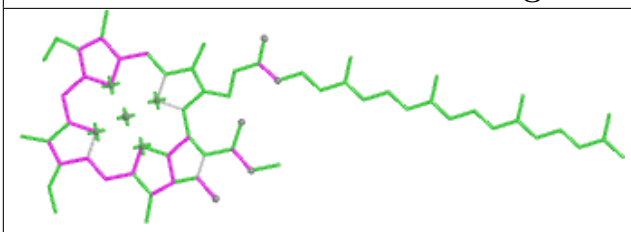


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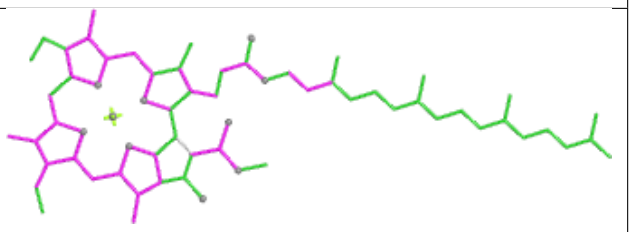


Rings

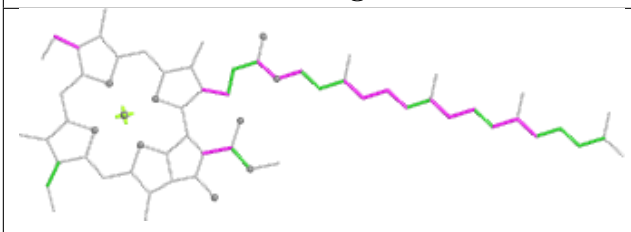
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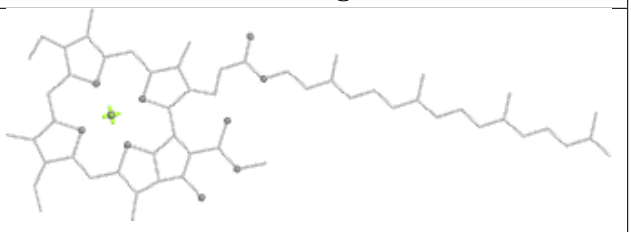
Bond lengths



Bond angles

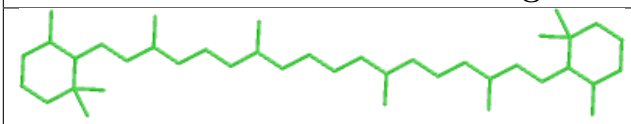


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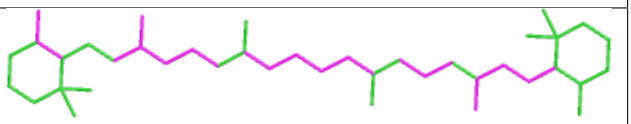


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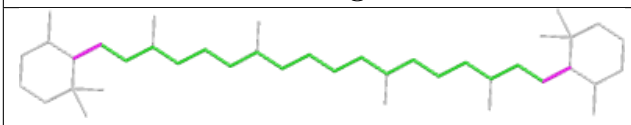
Ligand BCR B 848



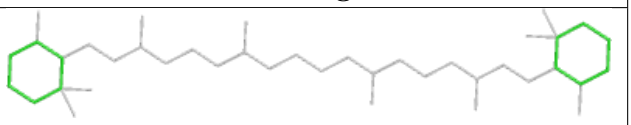
Bond lengths



Bond angles

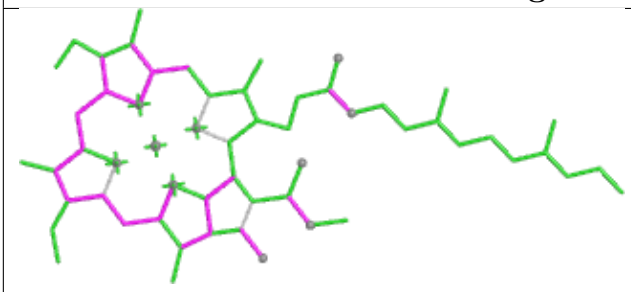


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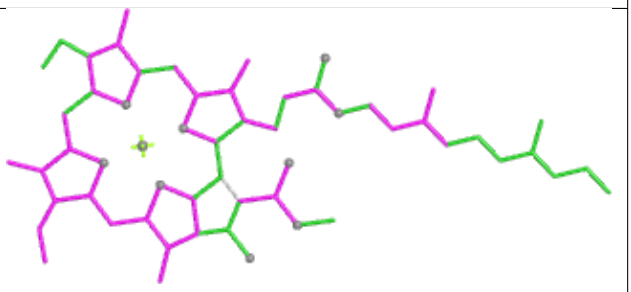


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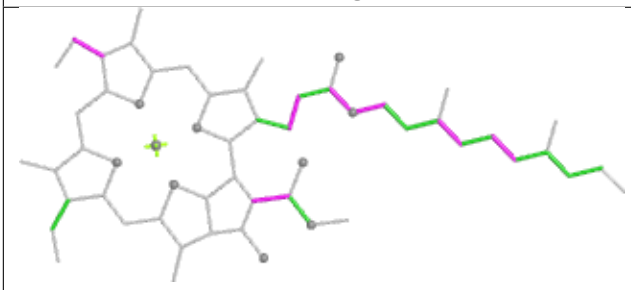
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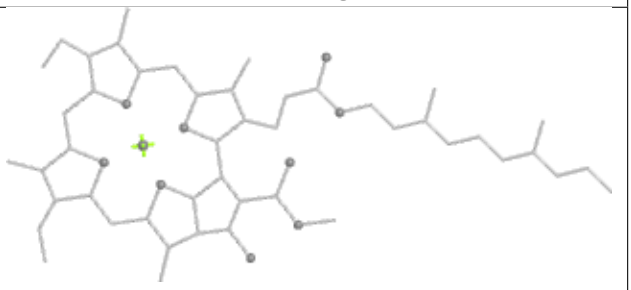
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Bond angles

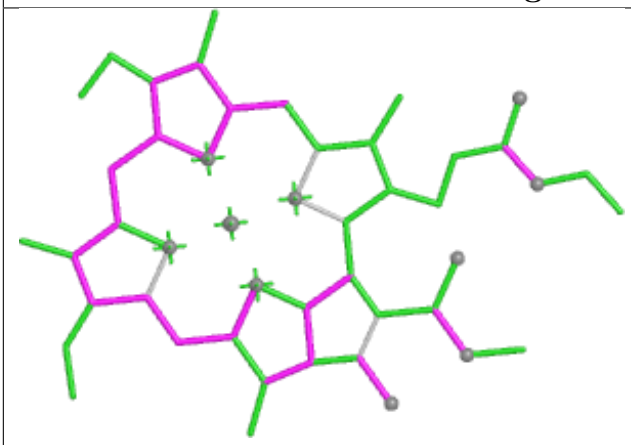


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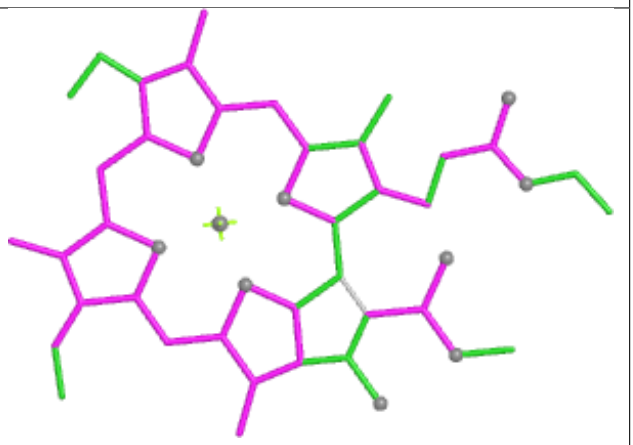


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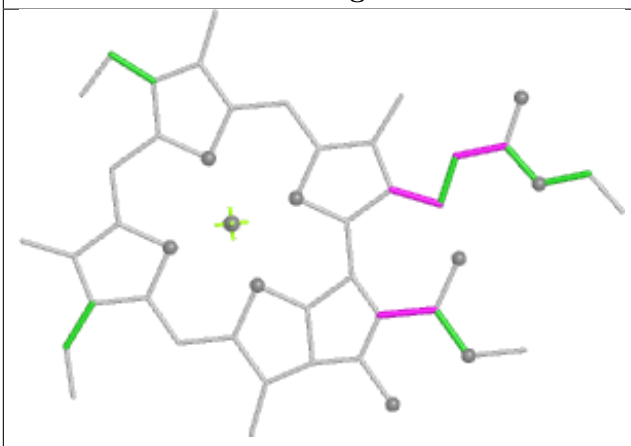
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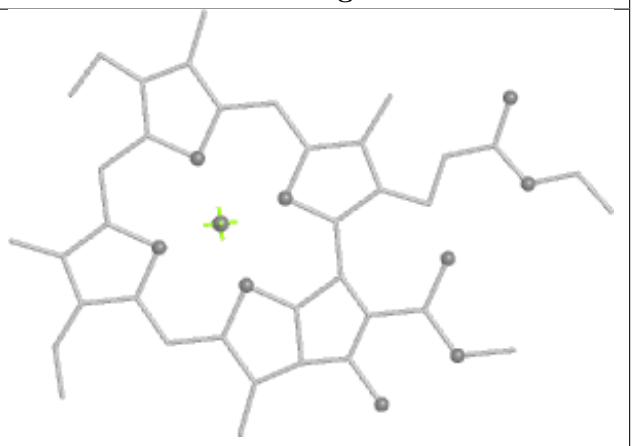
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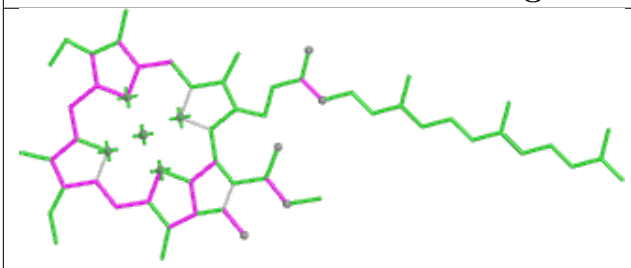


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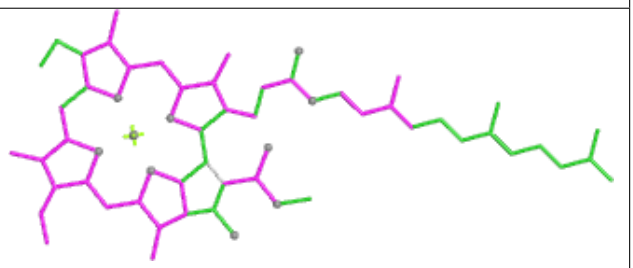


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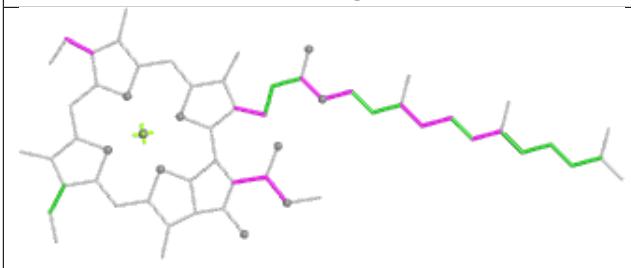
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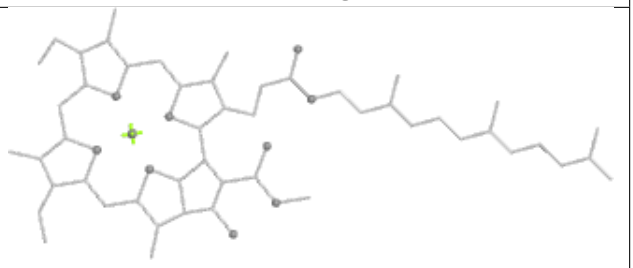
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Bond angles

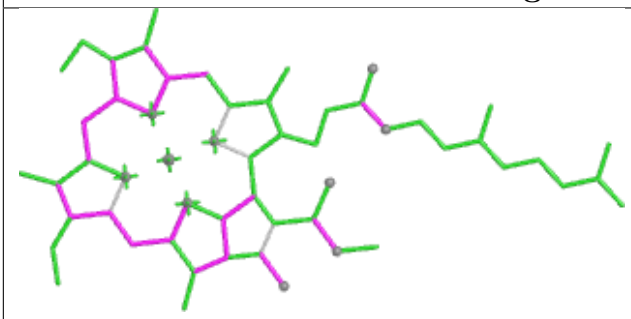


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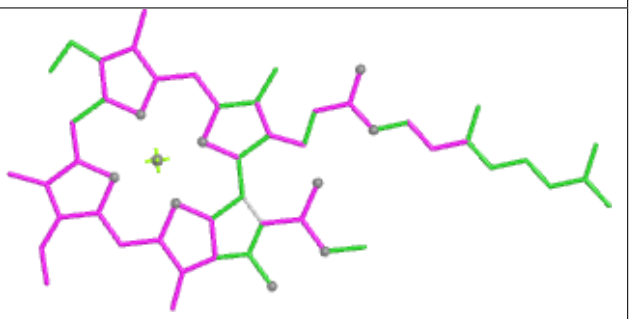


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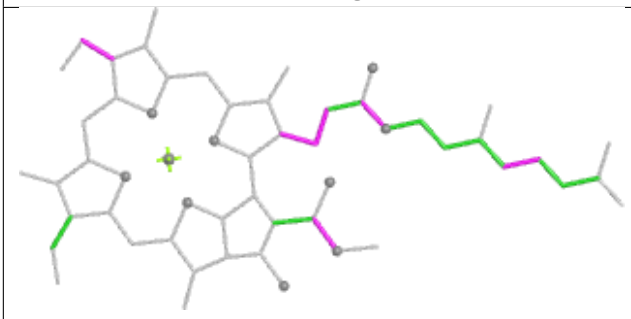
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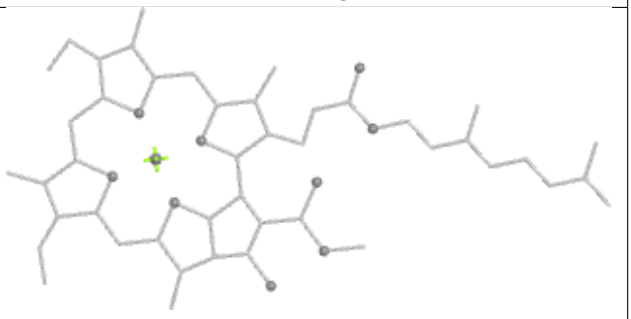
Bond lengths



Bond angles

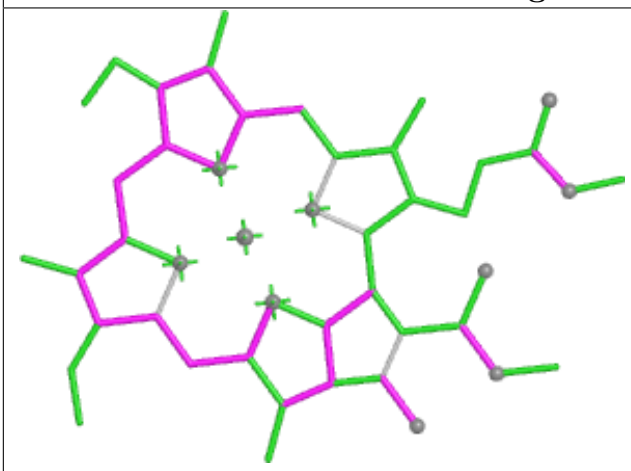


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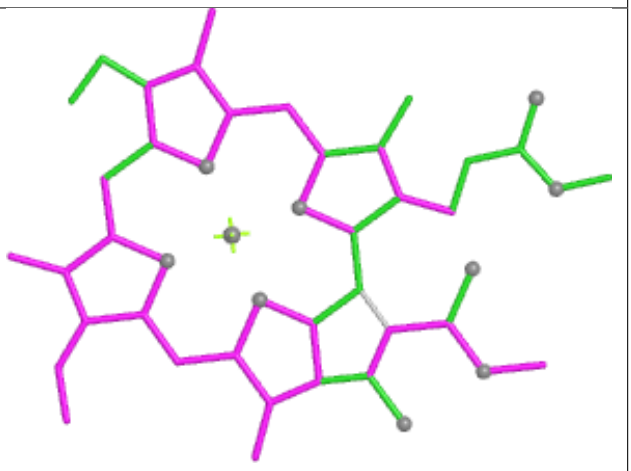


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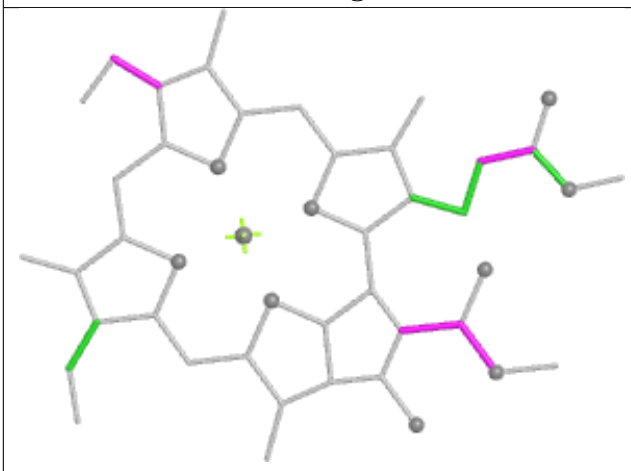
Ligand CLA 2 601



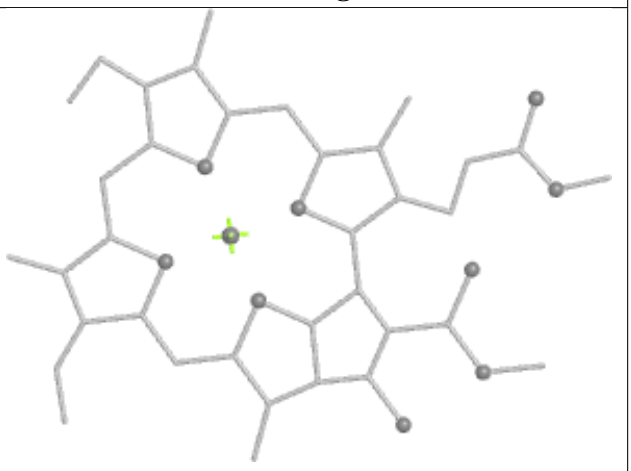
Bond lengths



Bond angles

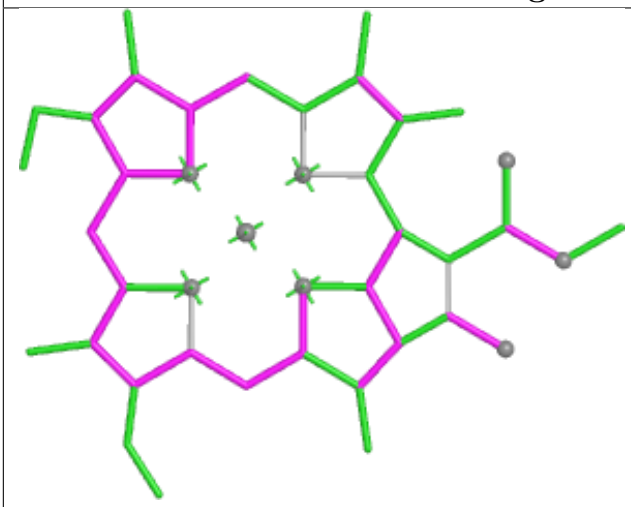


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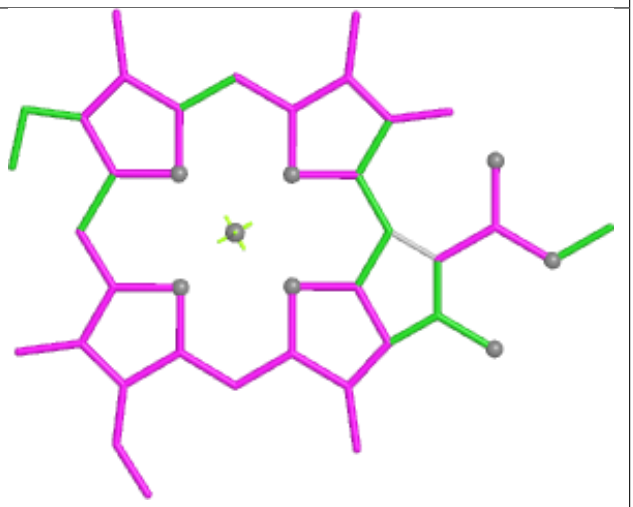


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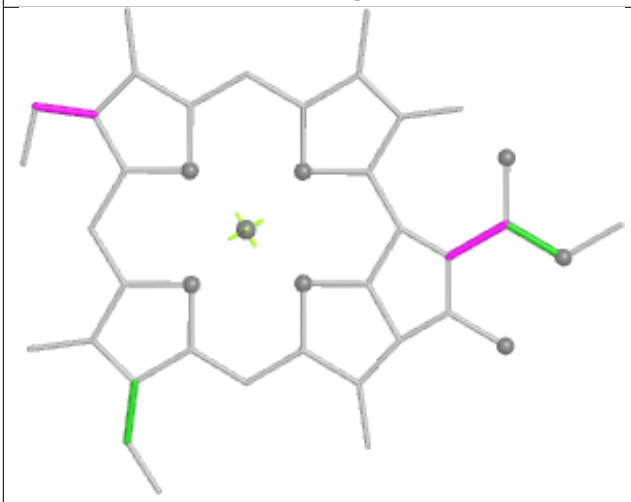
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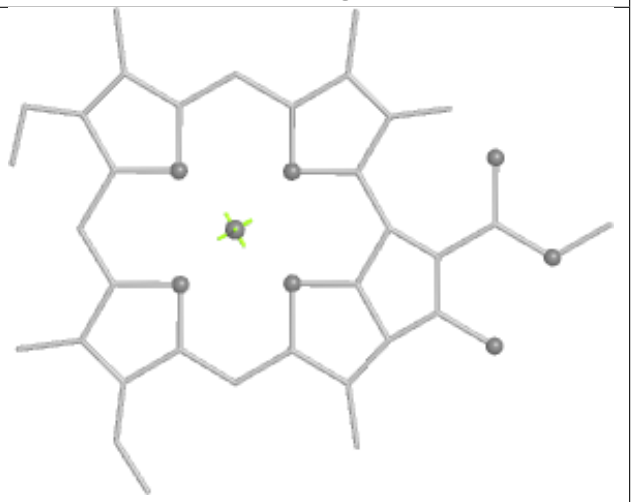
Bond lengths



Bond angles

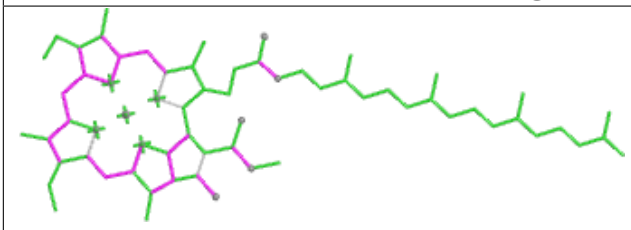


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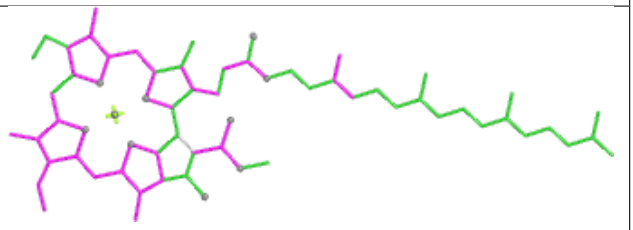


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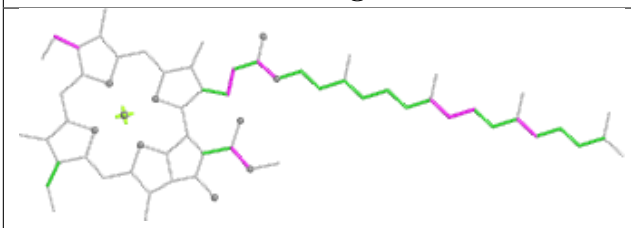
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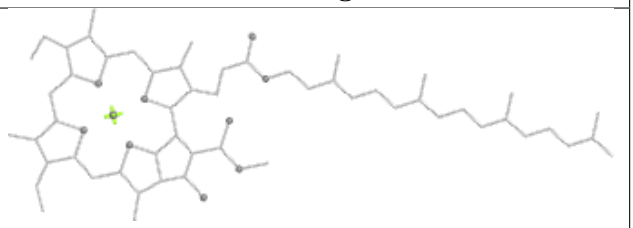
Bond lengths



Bond angles

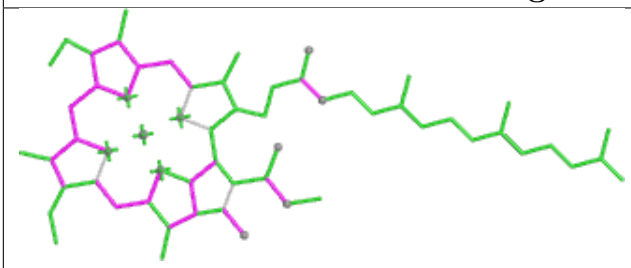


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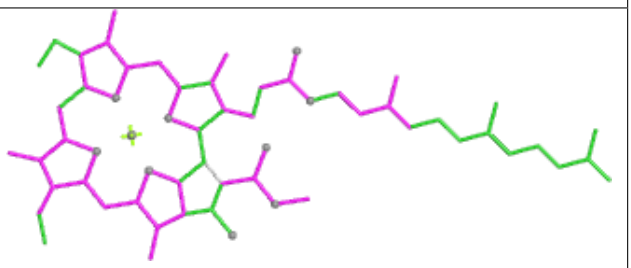


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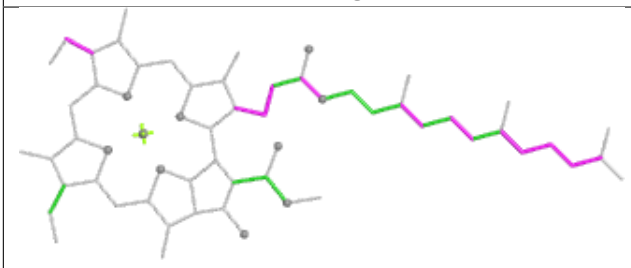
Ligand CLA 8 610



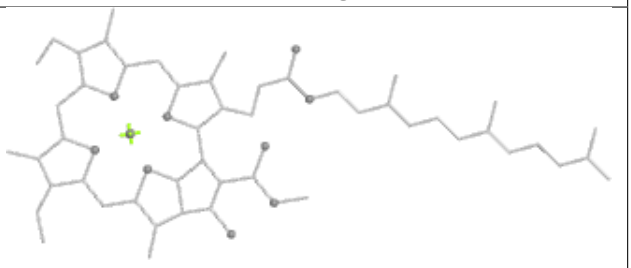
Bond lengths



Bond angles

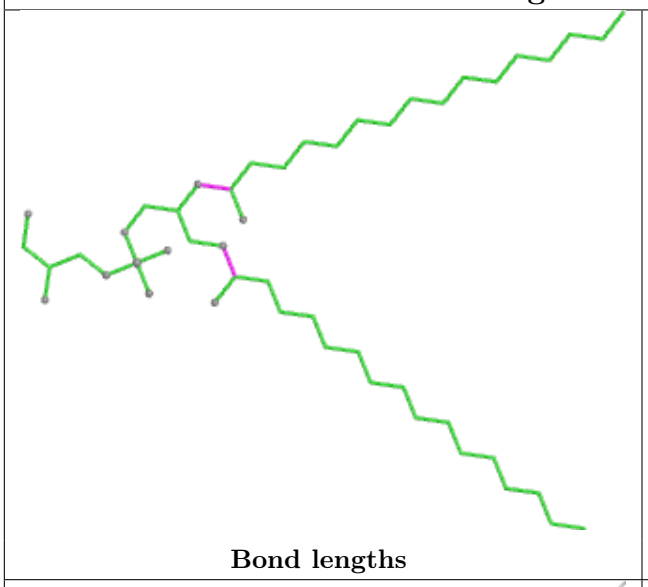


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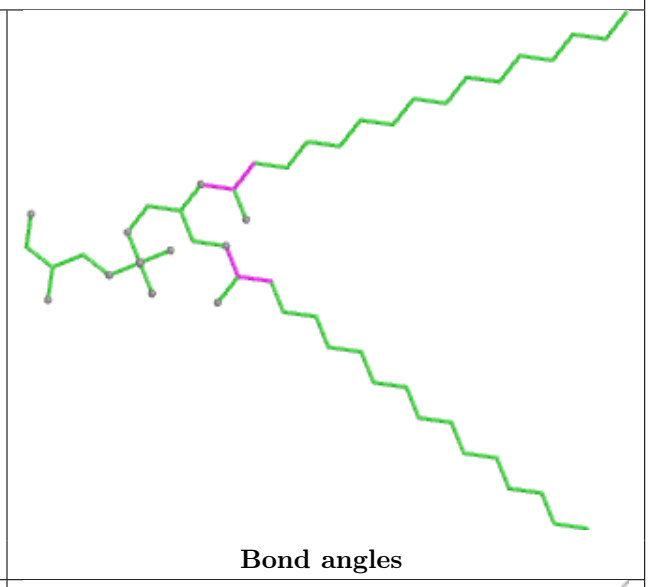


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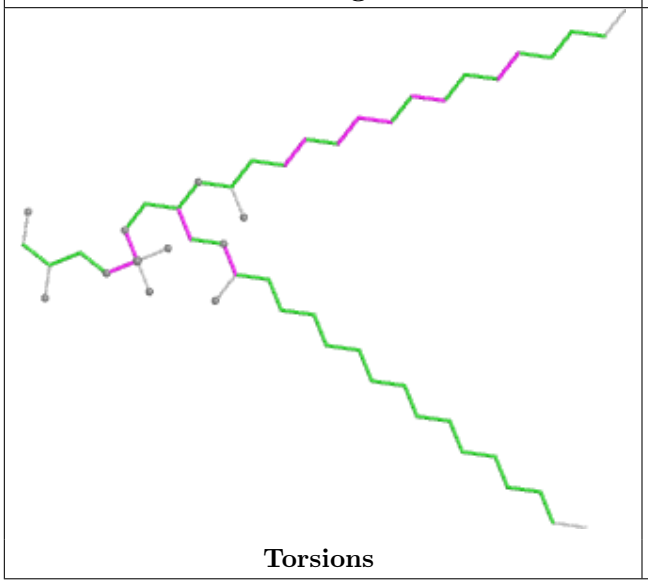
Ligand LHG 6 619



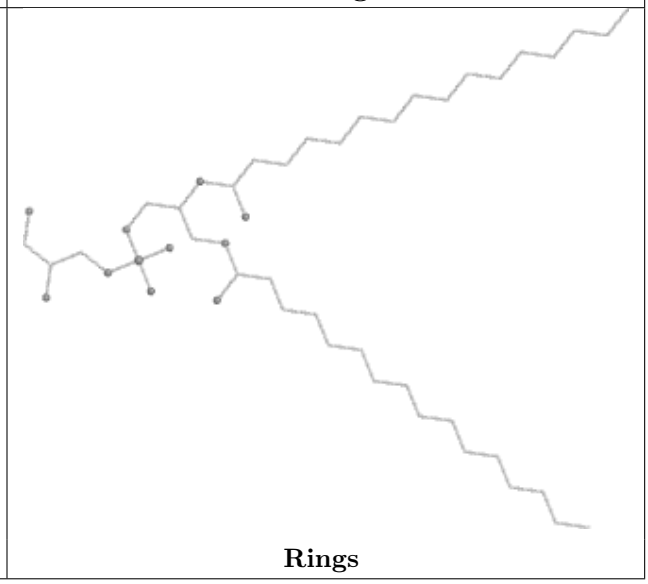
Bond lengths



Bond angles

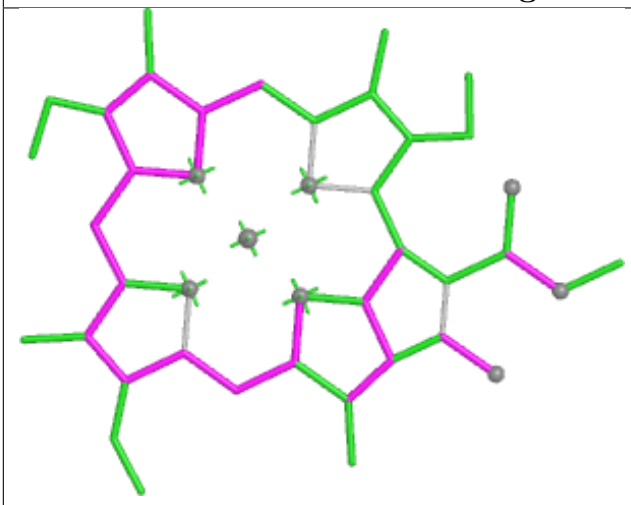


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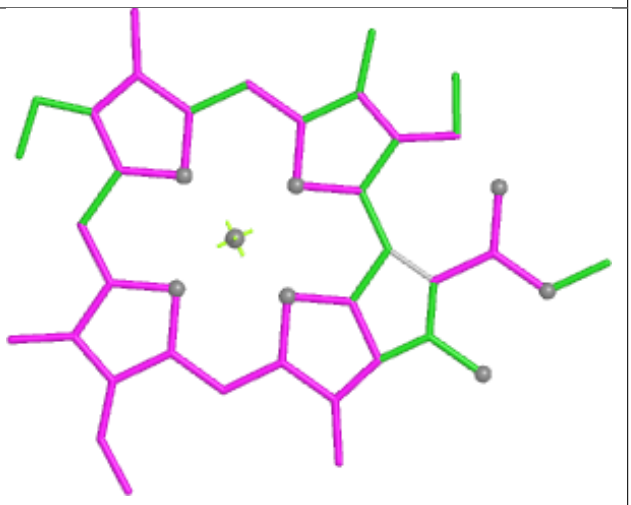


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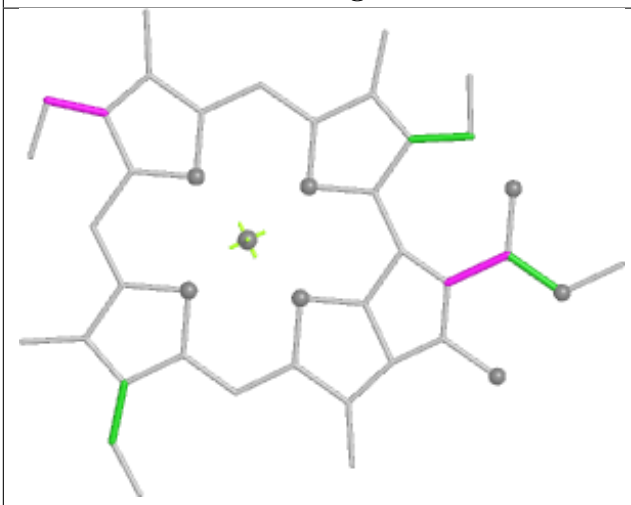
Ligand CLA J 3002



Bond lengths



Bond angles

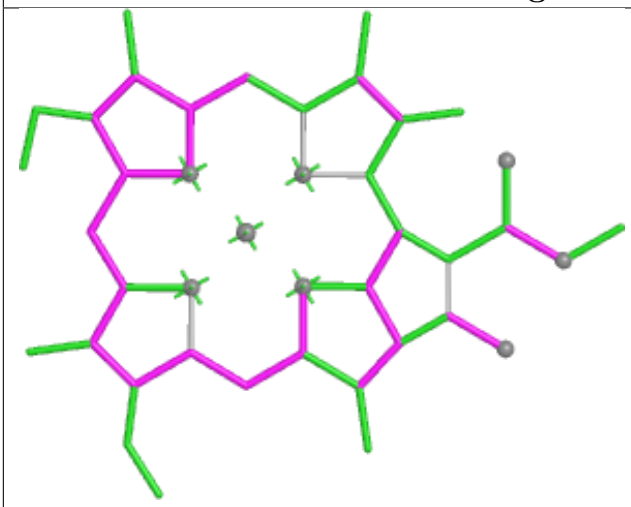


Torsions

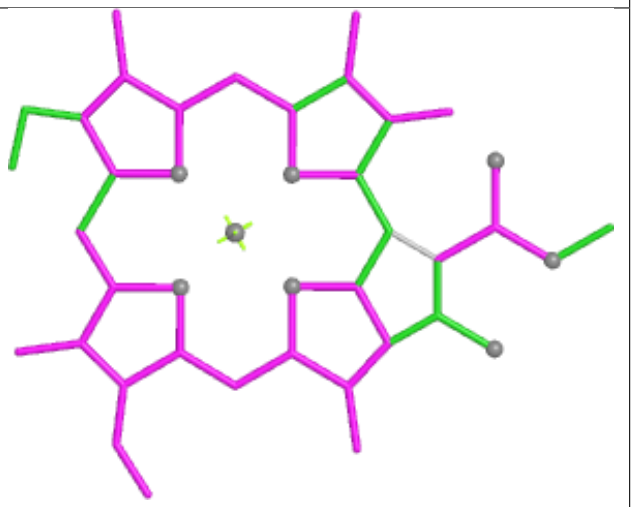


Rings

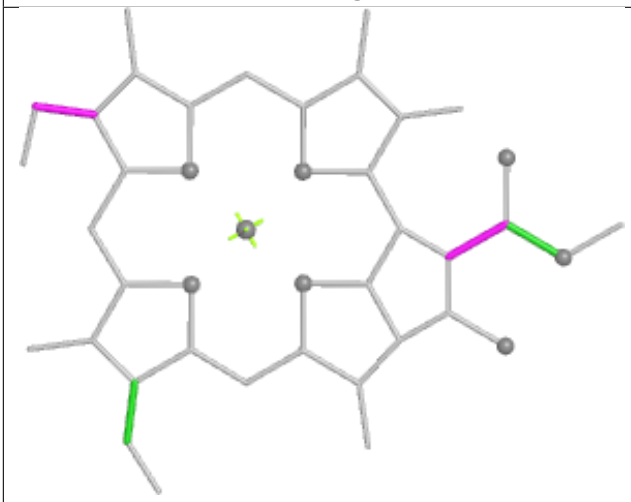
Ligand CLA 3 611



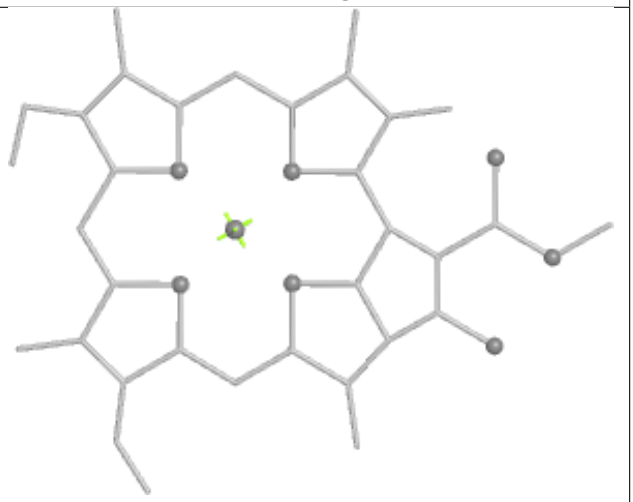
Bond lengths



Bond angles

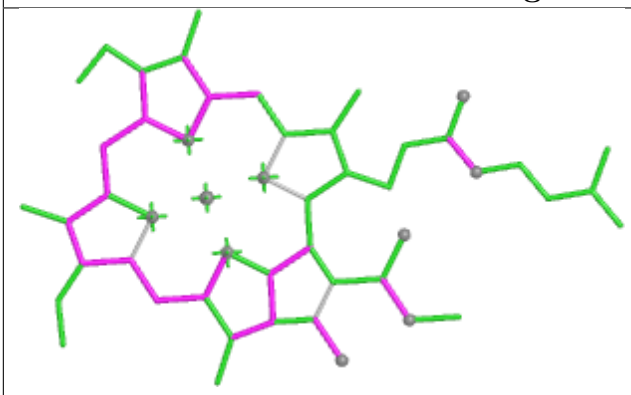


Torsions

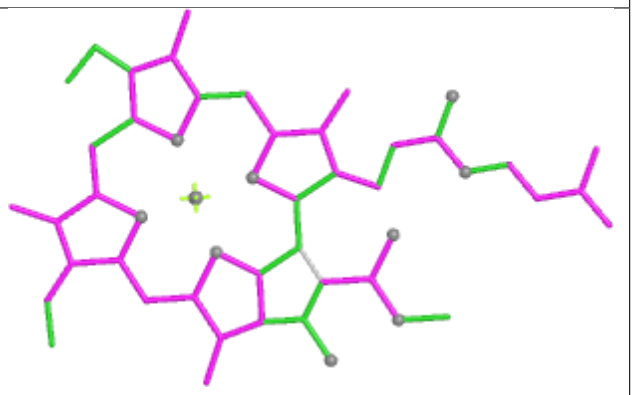


Rings

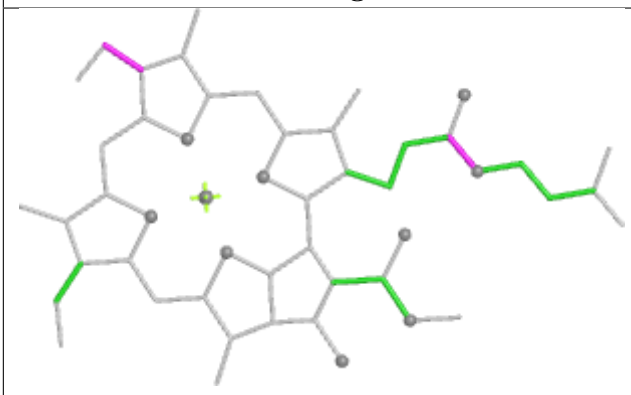
Ligand CLA A 832



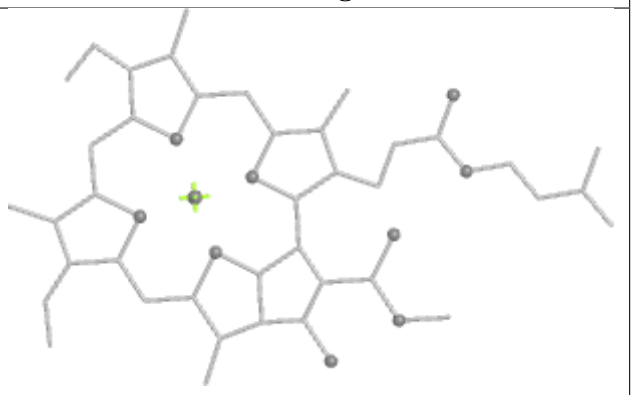
Bond lengths



Bond angles

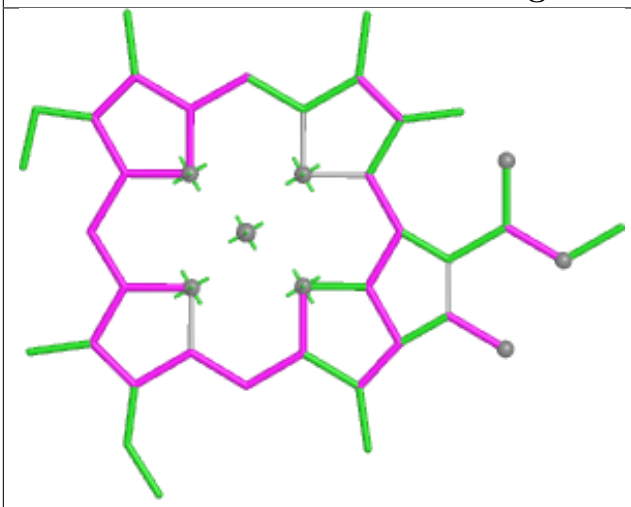


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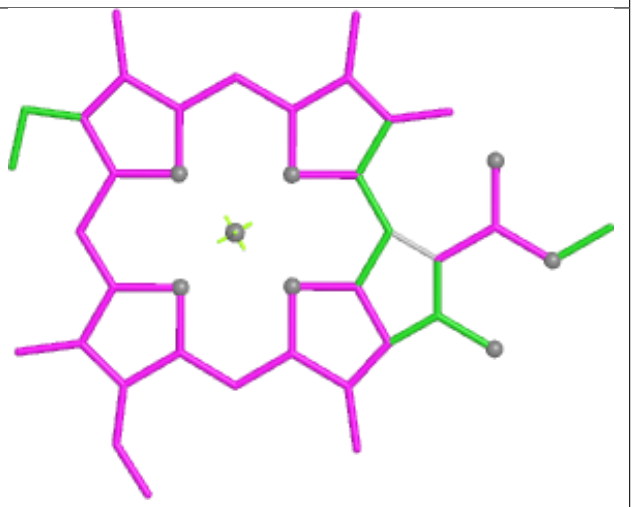


Rings

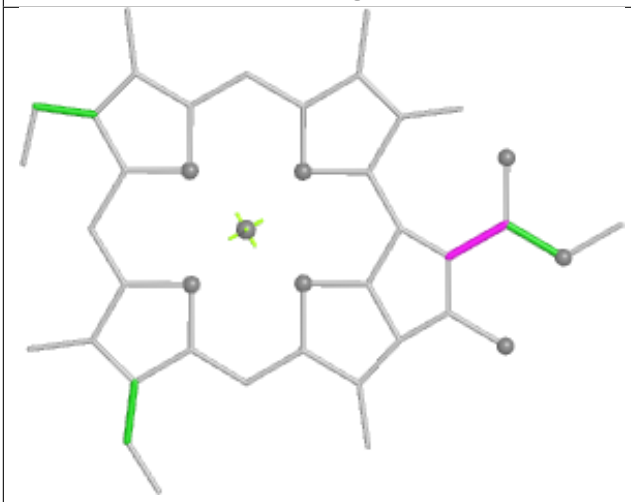
Ligand CLA 7 611



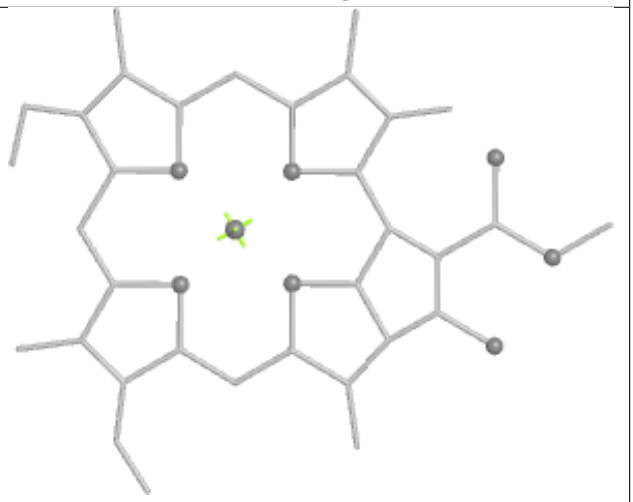
Bond lengths



Bond angles

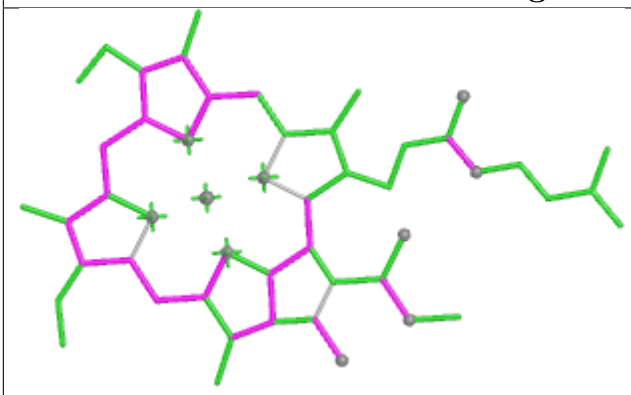


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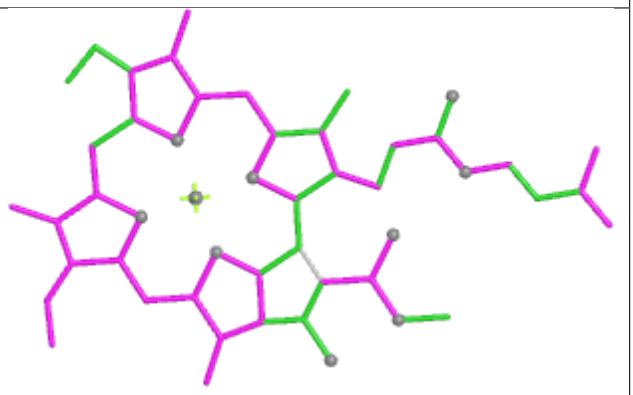


Rings

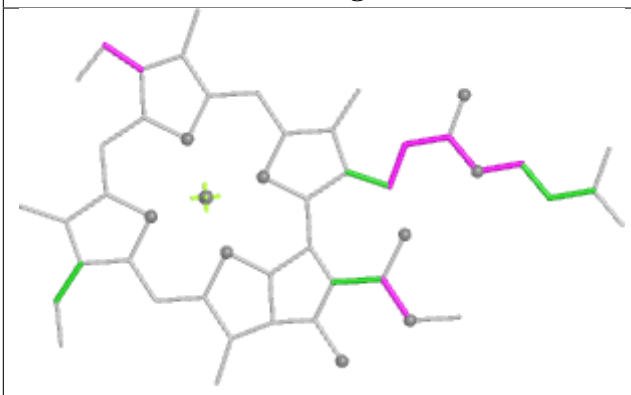
Ligand CLA 9 613



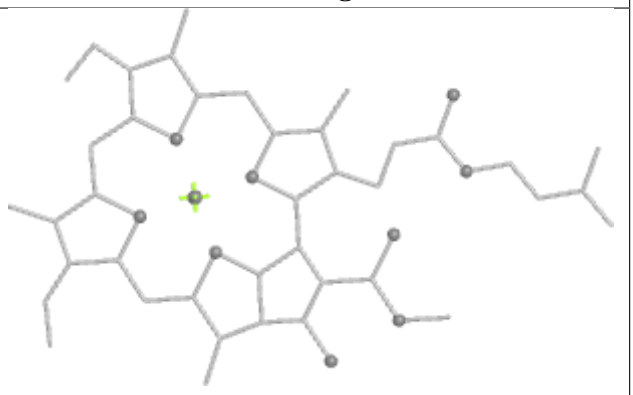
Bond lengths



Bond angles



Torsions

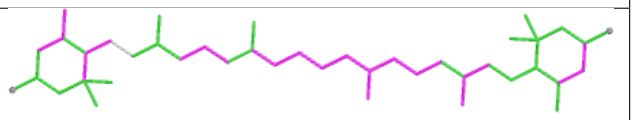


Rings

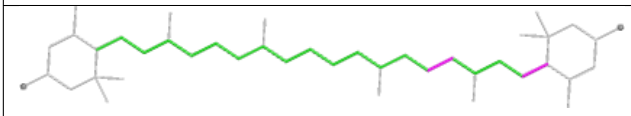
Ligand LUT 4 620



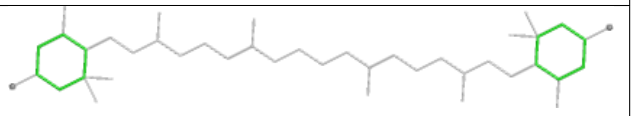
Bond lengths



Bond angles

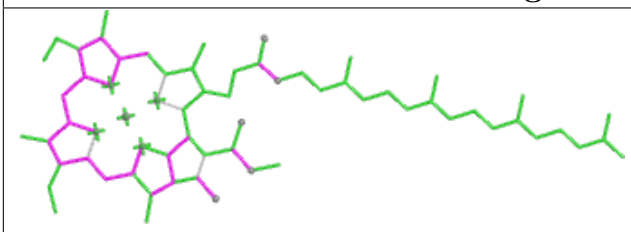


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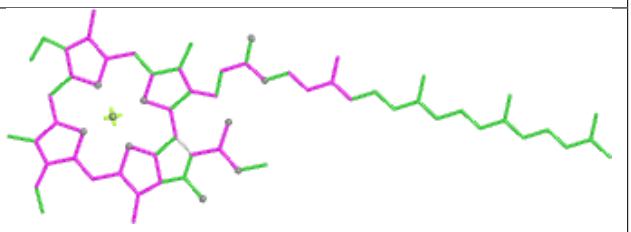


Rings

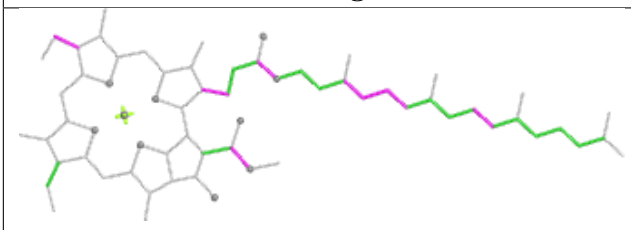
Ligand CLA B 810



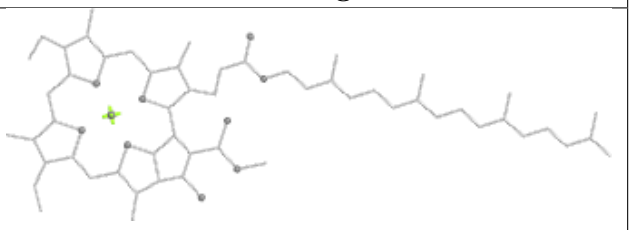
Bond lengths



Bond angles

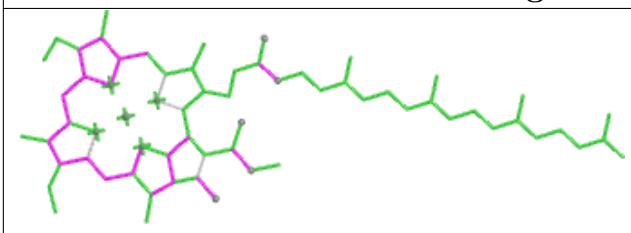


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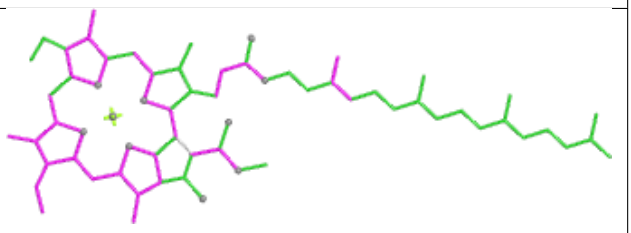


Rings

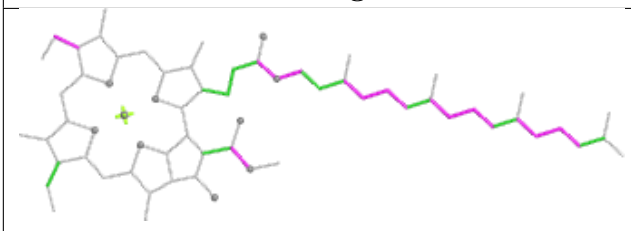
Ligand CLA Z 608



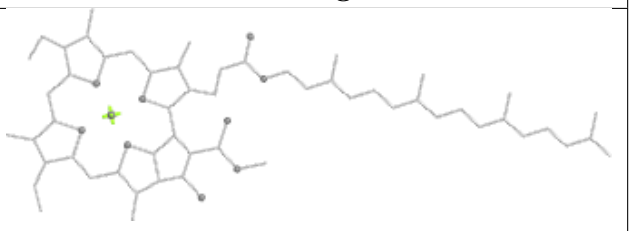
Bond lengths



Bond angles

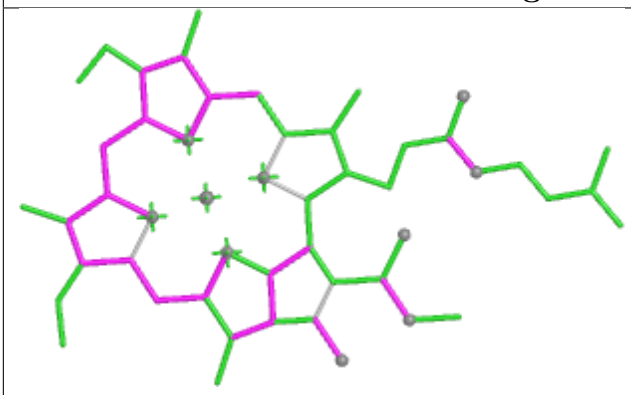


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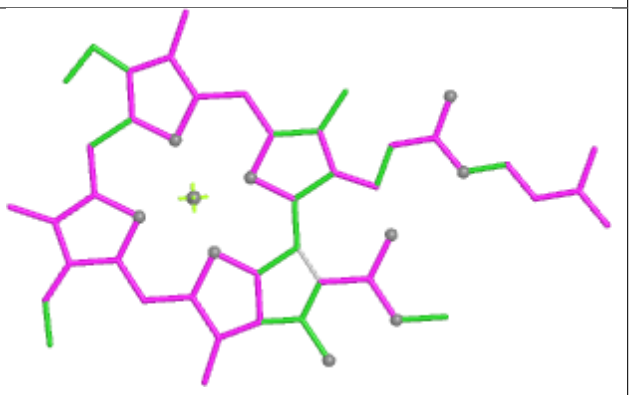


Rings

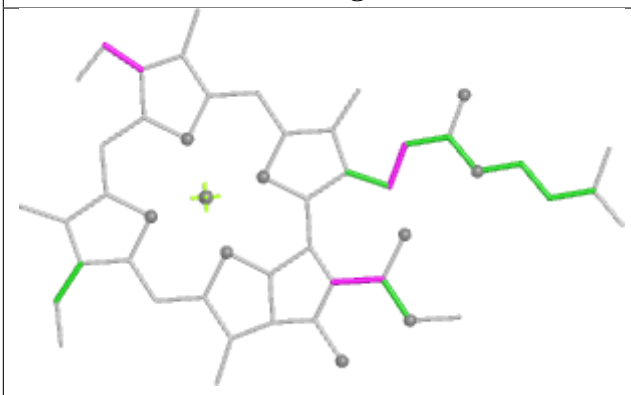
Ligand CLA G 203



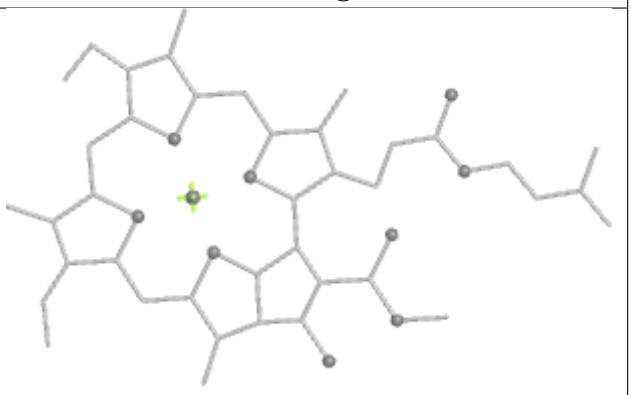
Bond lengths



Bond angles

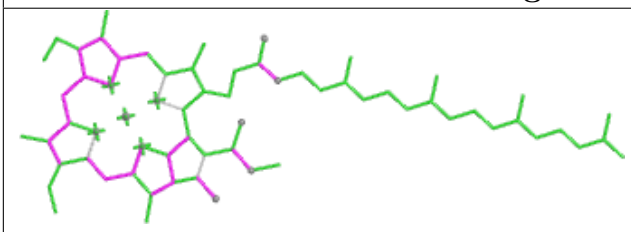


Torsions

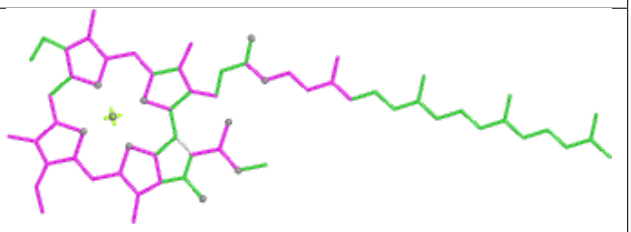


Rings

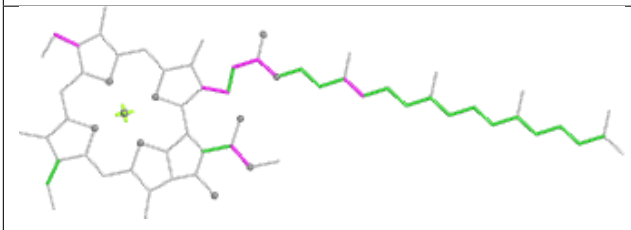
Ligand CLA A 811



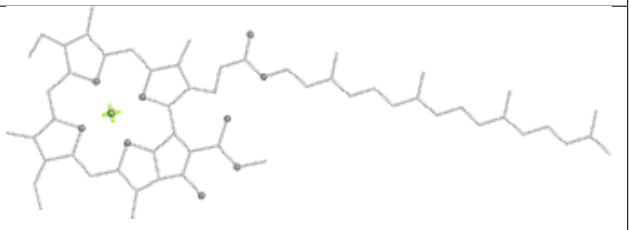
Bond lengths



Bond angles

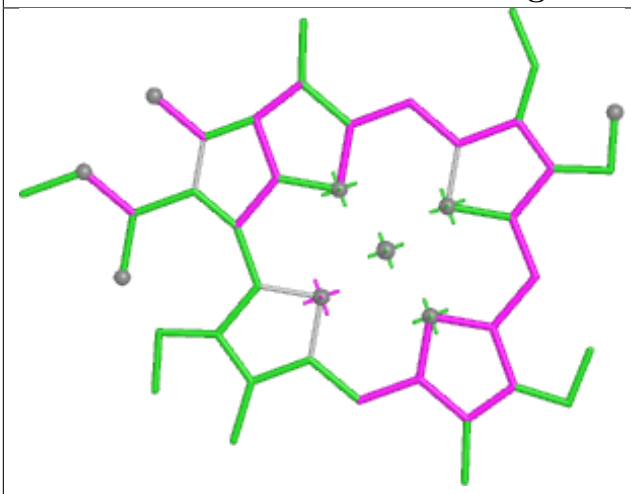


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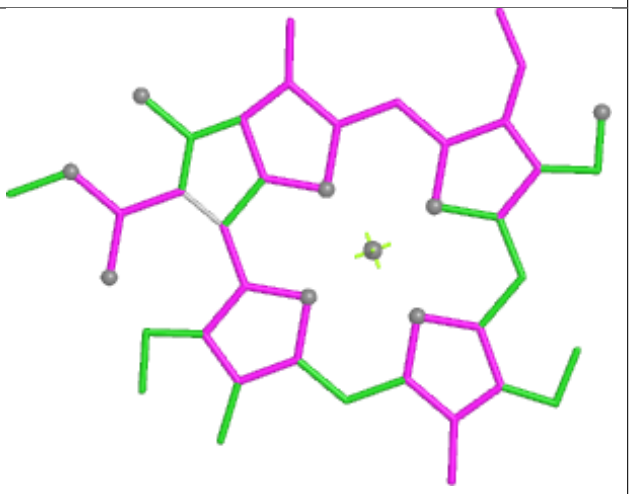


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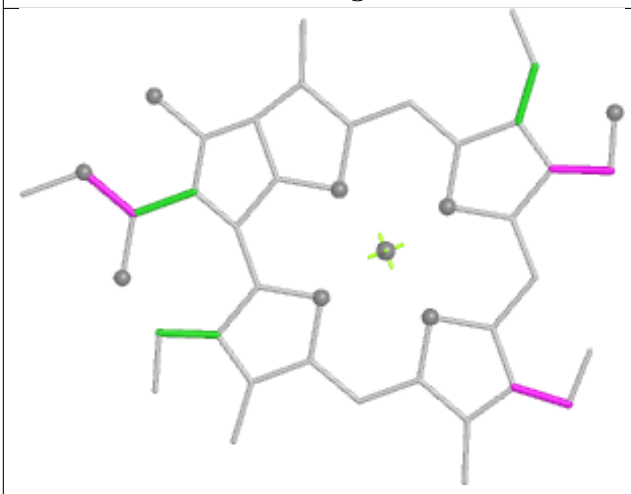
Ligand CHL 5 618



Bond lengths



Bond angles



Torsions

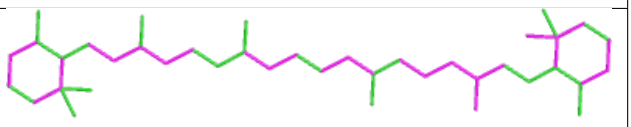


Rings

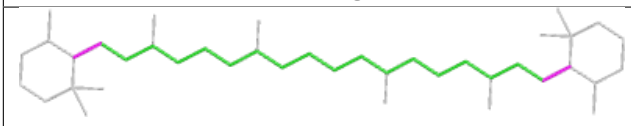
Ligand BCR 7 624



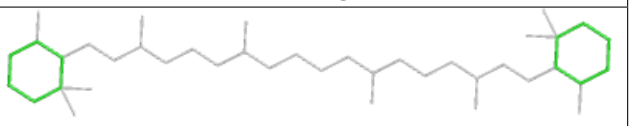
Bond lengths



Bond angles

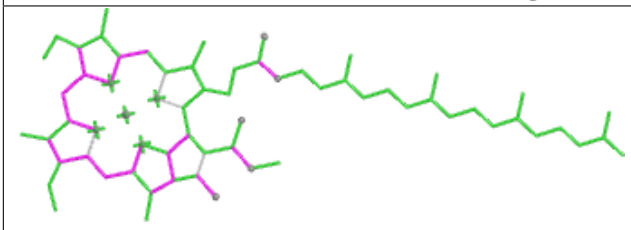


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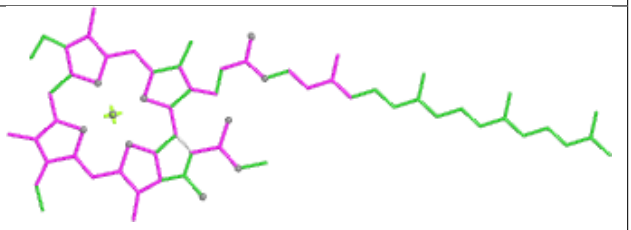


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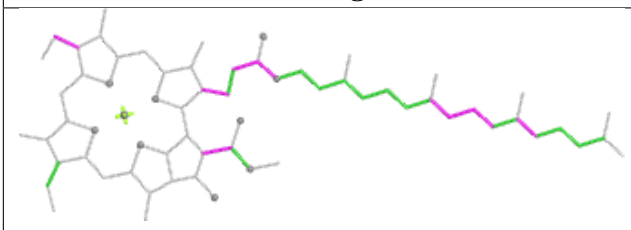
Ligand CLA B 813



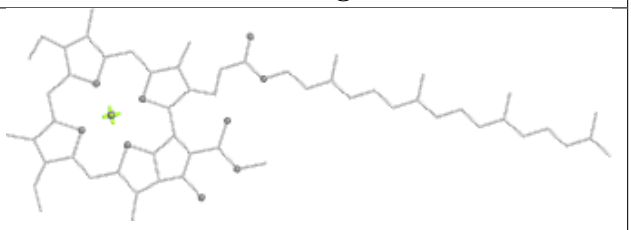
Bond lengths



Bond angles

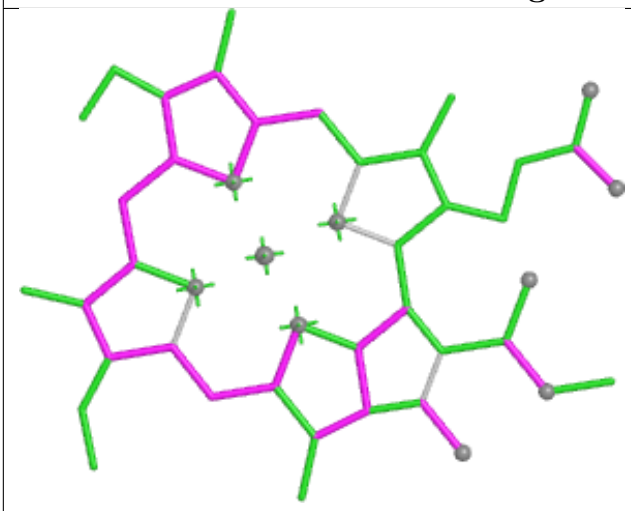


Torsions

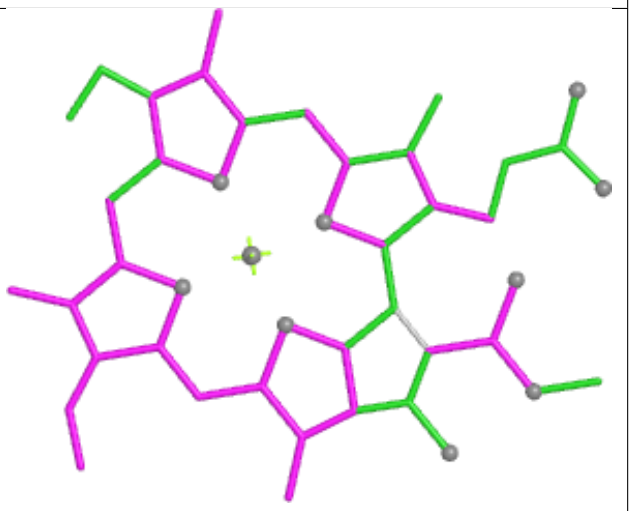


Rings

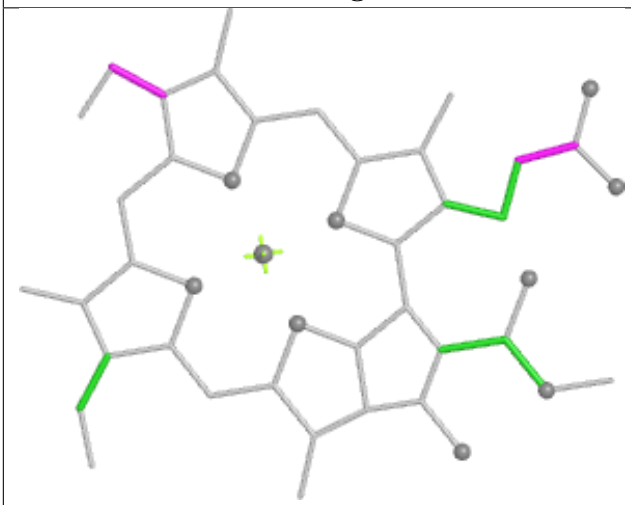
Ligand CLA 3 614



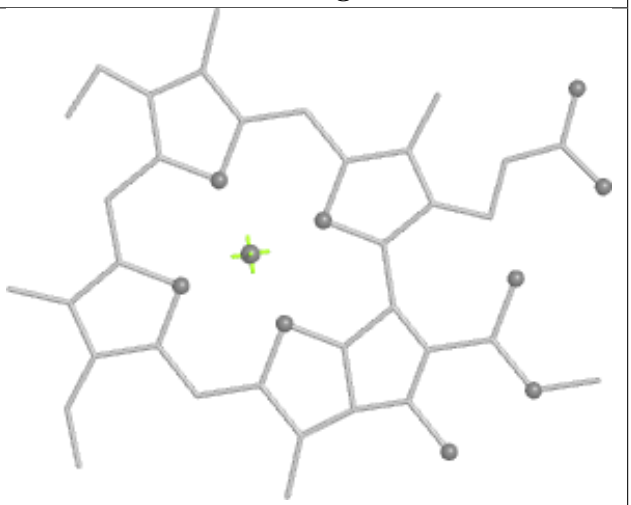
Bond lengths



Bond angles

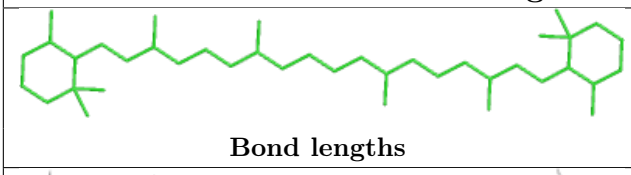


Torsions

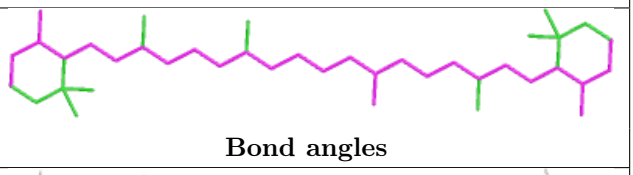


Rings

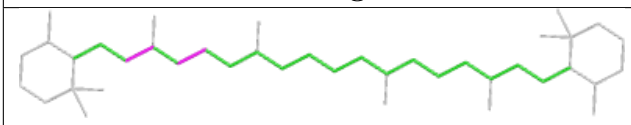
Ligand BCR 4 621



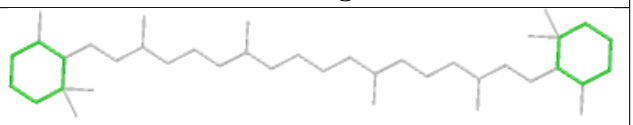
Bond lengths



Bond angles

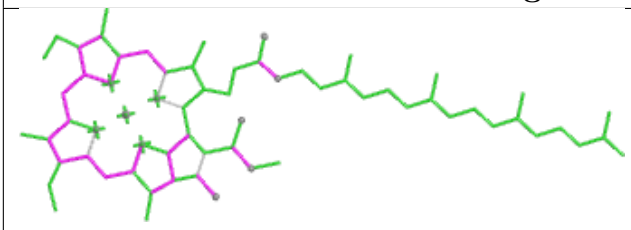


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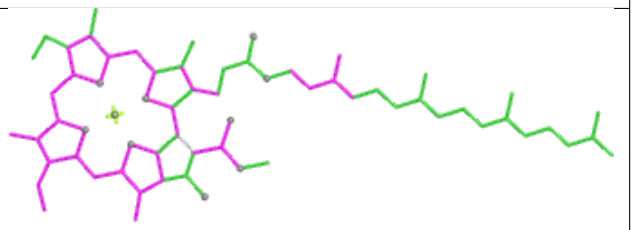


Rings

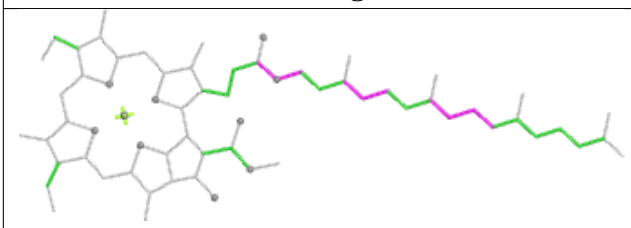
Ligand CLA A 833



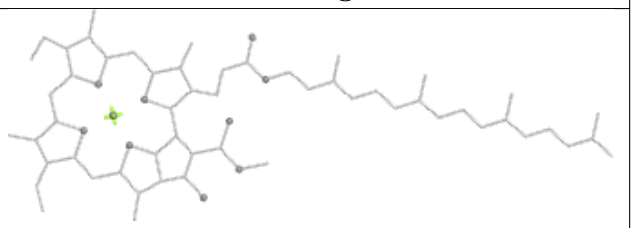
Bond lengths



Bond angles

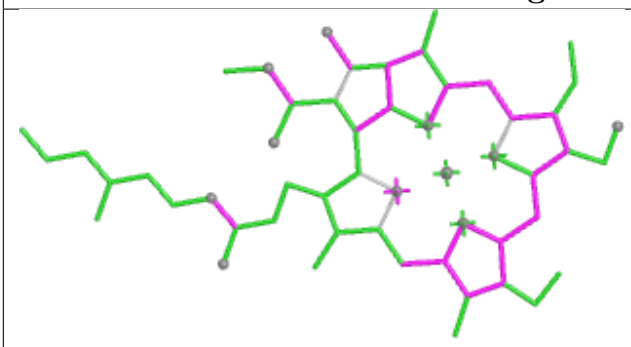


Torsions

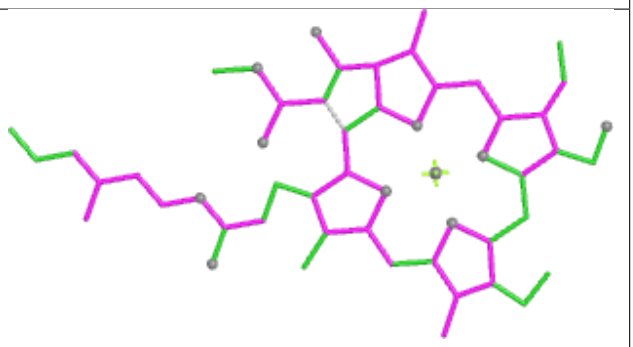


Rings

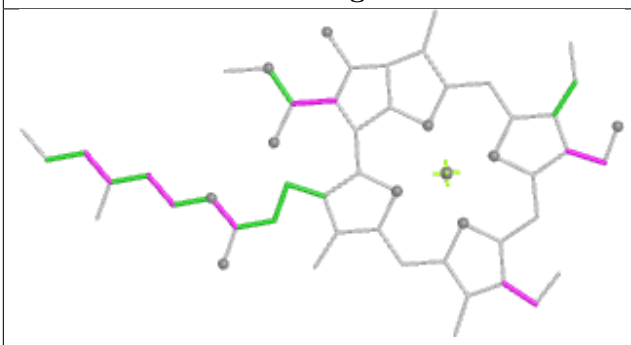
Ligand CHL 1 601



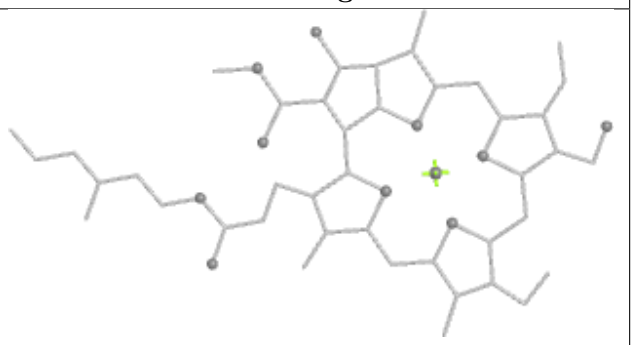
Bond lengths



Bond angles

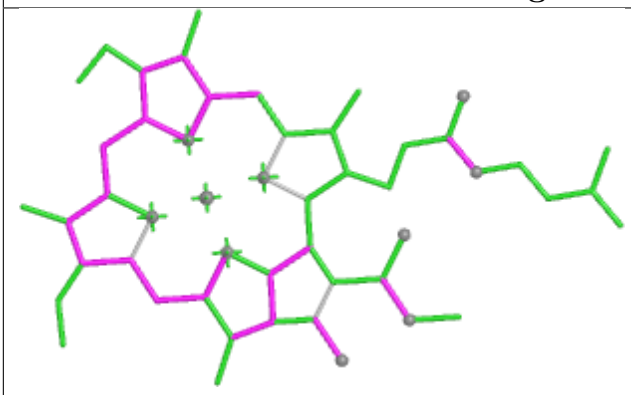


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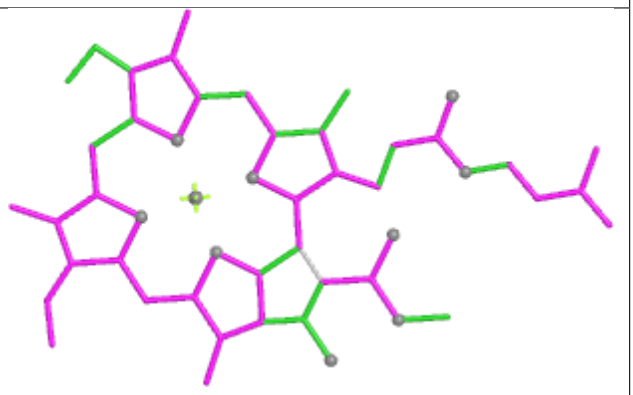


Rings

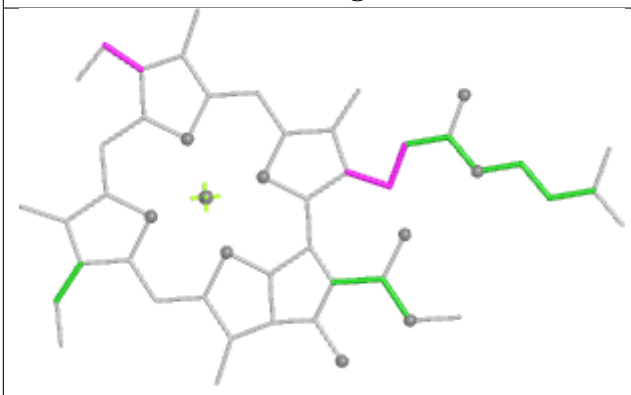
Ligand CLA 2 613



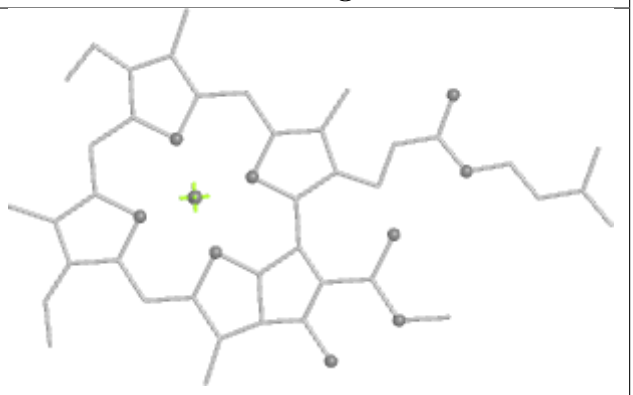
Bond lengths



Bond angles



Torsions

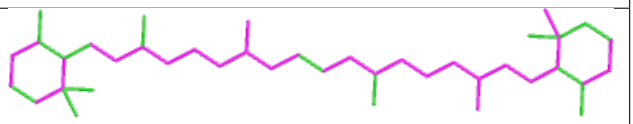


Rings

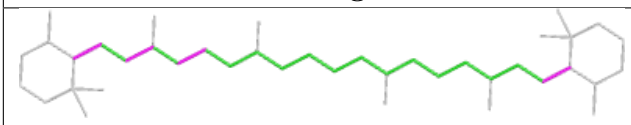
Ligand BCR 5 625



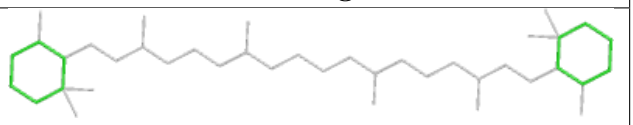
Bond lengths



Bond angles

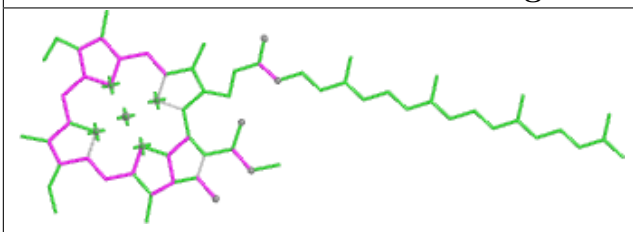


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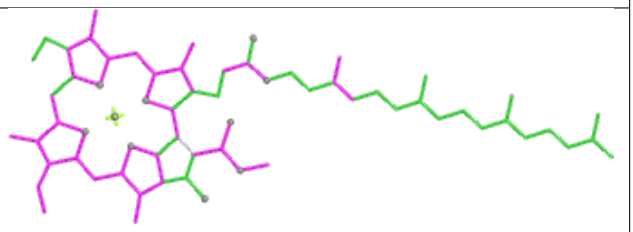


Rings

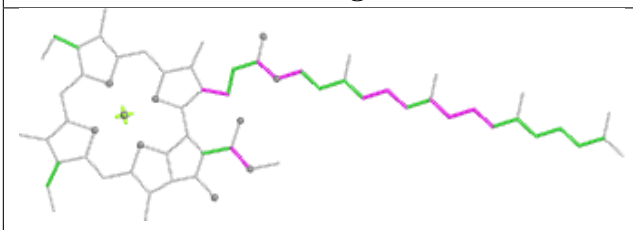
Ligand CLA B 834



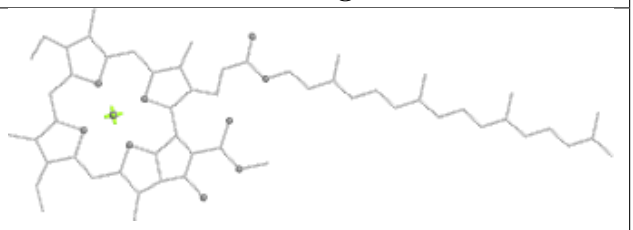
Bond lengths



Bond angles

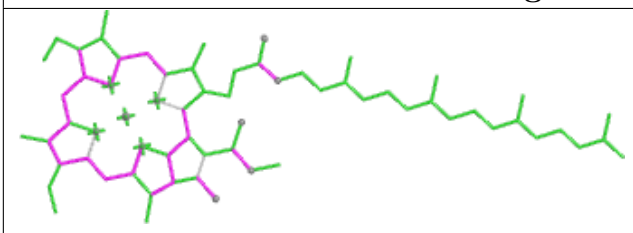


Torsions

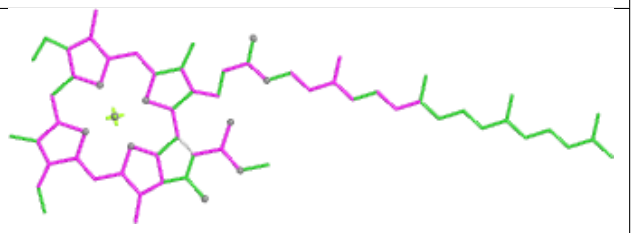


Rings

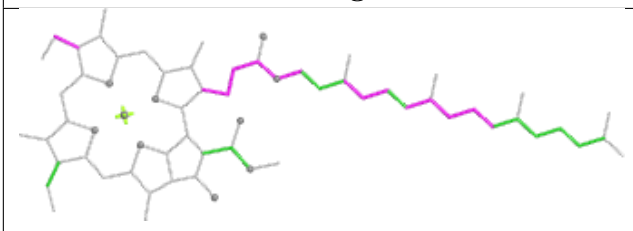
Ligand CLA B 827



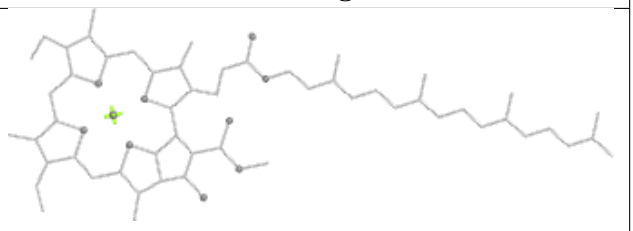
Bond lengths



Bond angles

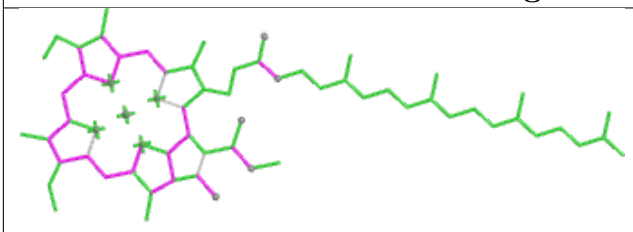


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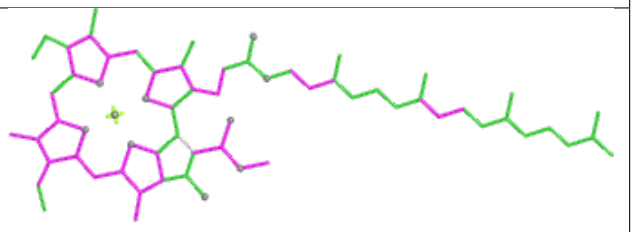


Rings

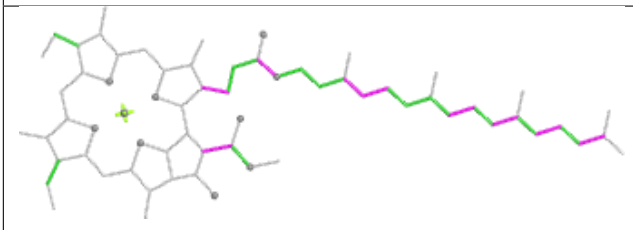
Ligand CLA A 820



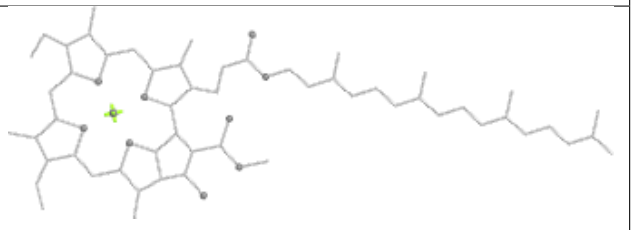
Bond lengths



Bond angles

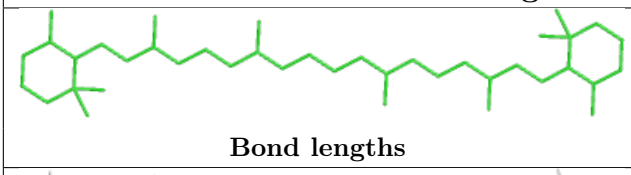


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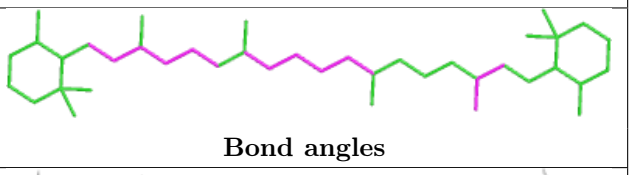


Rings

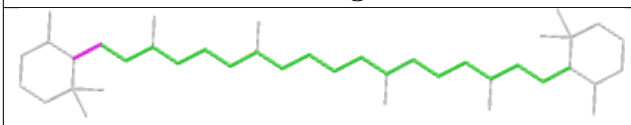
Ligand BCR G 205



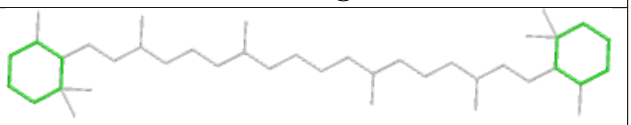
Bond lengths



Bond angles



Torsions



Rings

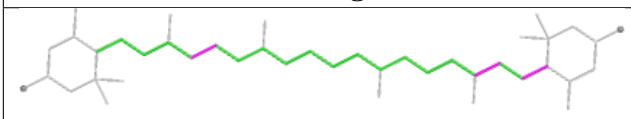
Ligand LUT 8 618



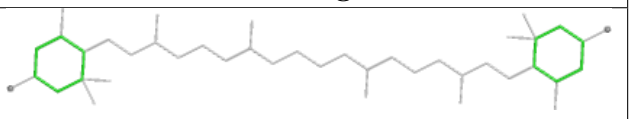
Bond lengths



Bond angles

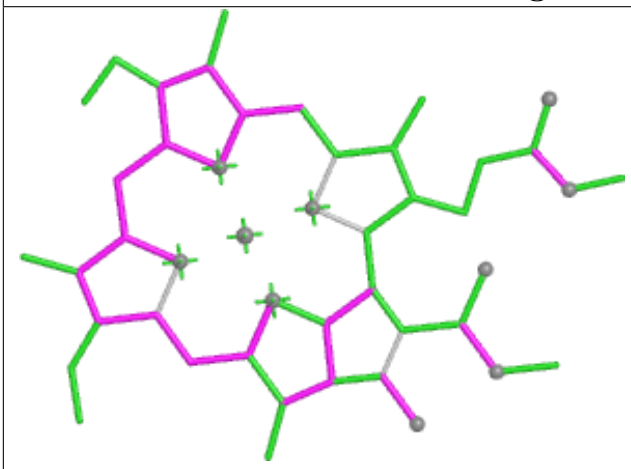


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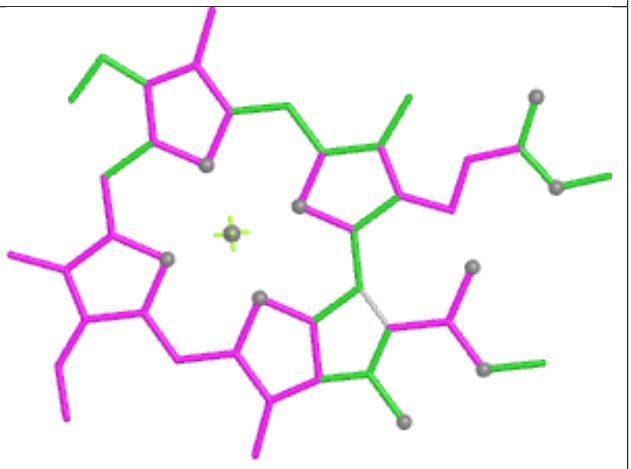


Rings

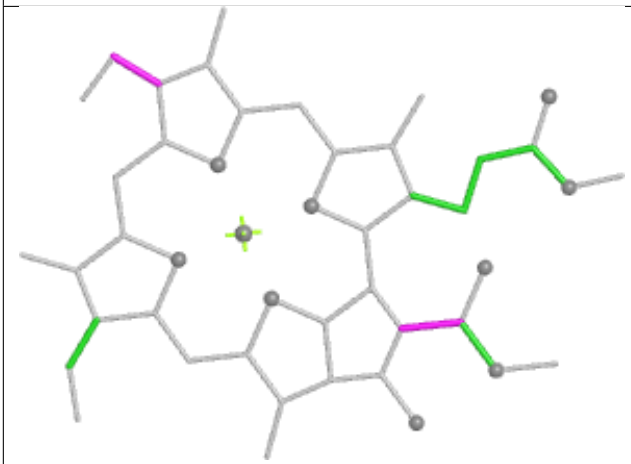
Ligand CLA 7 603



Bond lengths



Bond angles

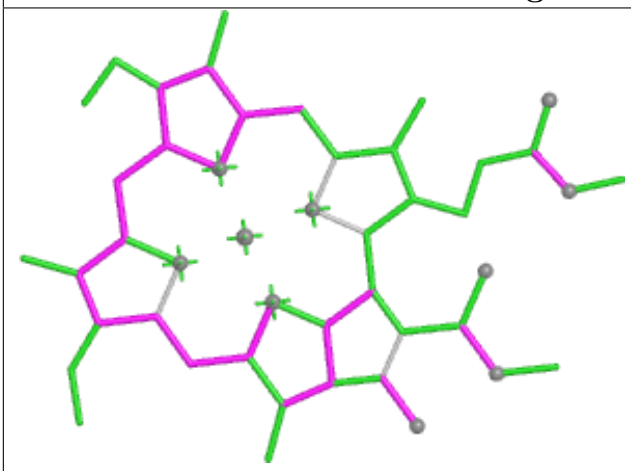


Torsions

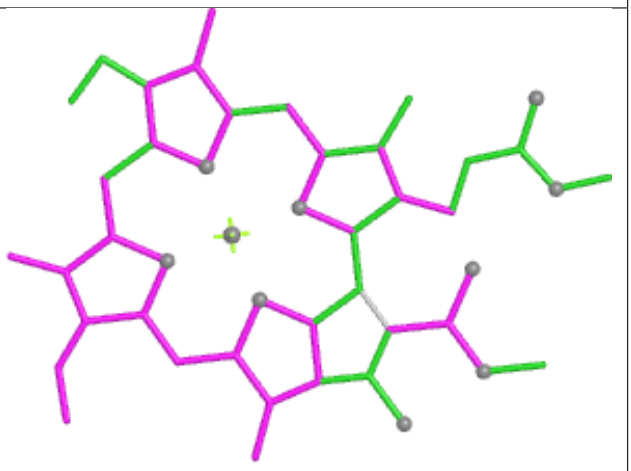


Rings

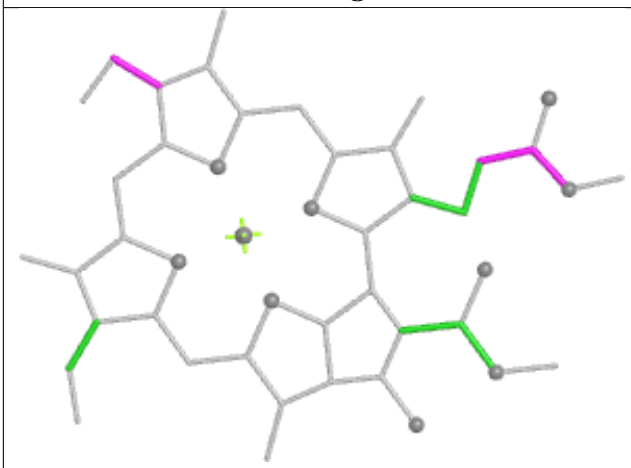
Ligand CLA Z 616



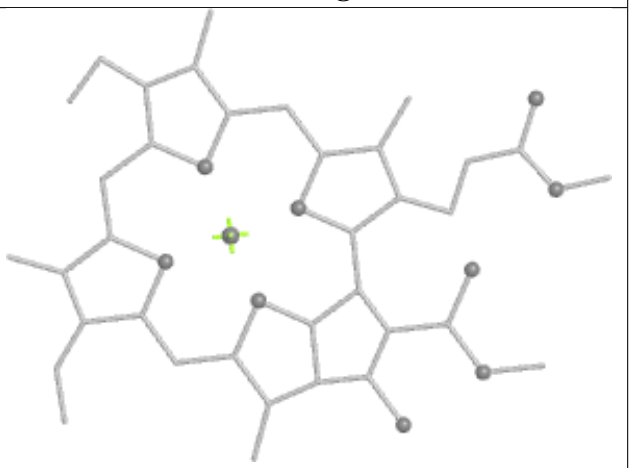
Bond lengths



Bond angles



Torsions

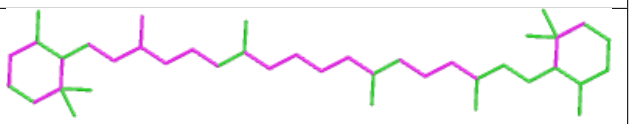


Rings

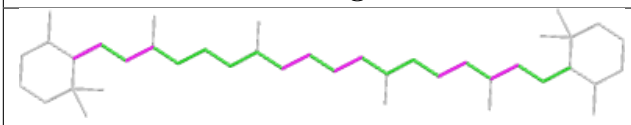
Ligand BCR B 801



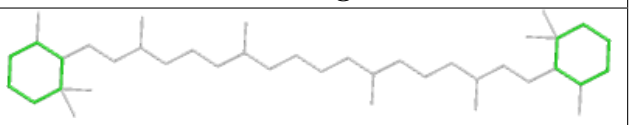
Bond lengths



Bond angles

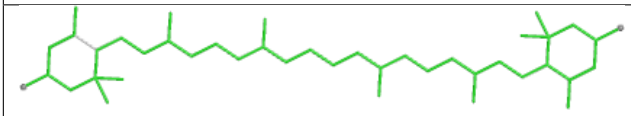


Torsions

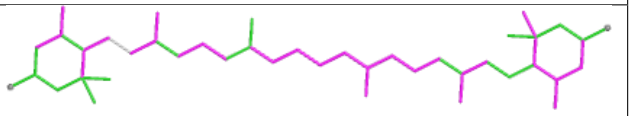


Rings

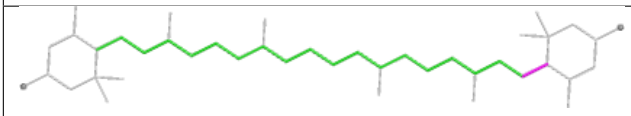
Ligand LUT 9 617



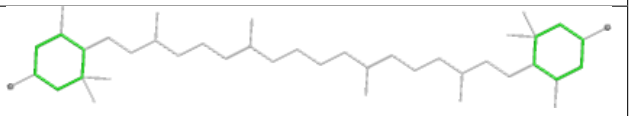
Bond lengths



Bond angles

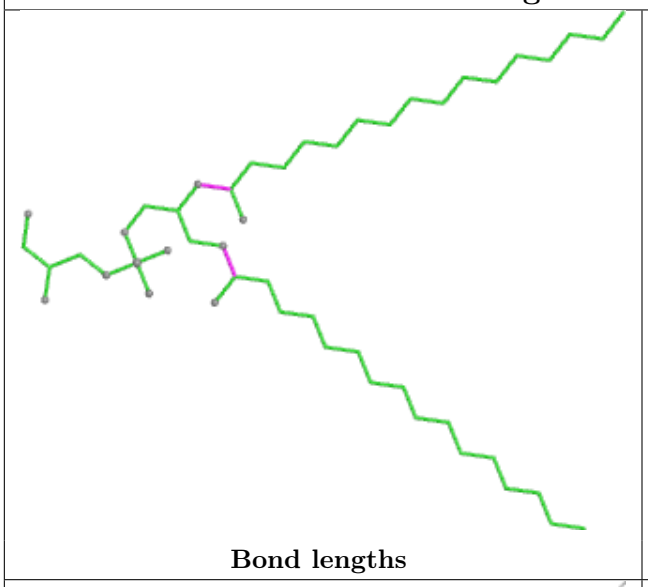


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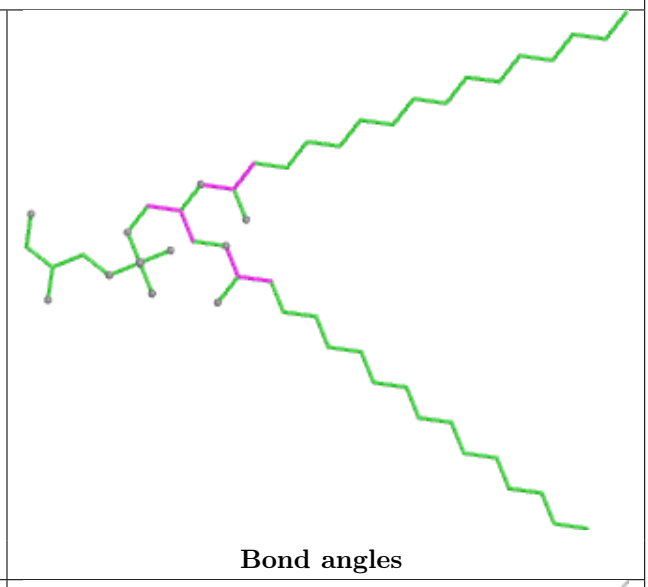


Rings

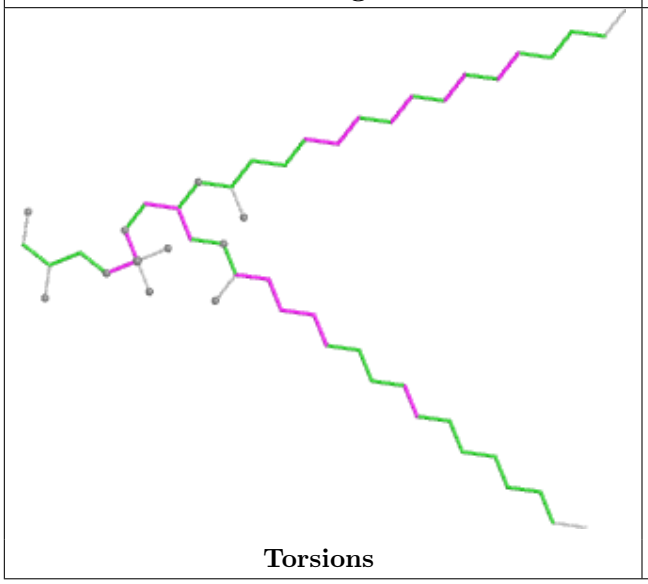
Ligand LHG A 846



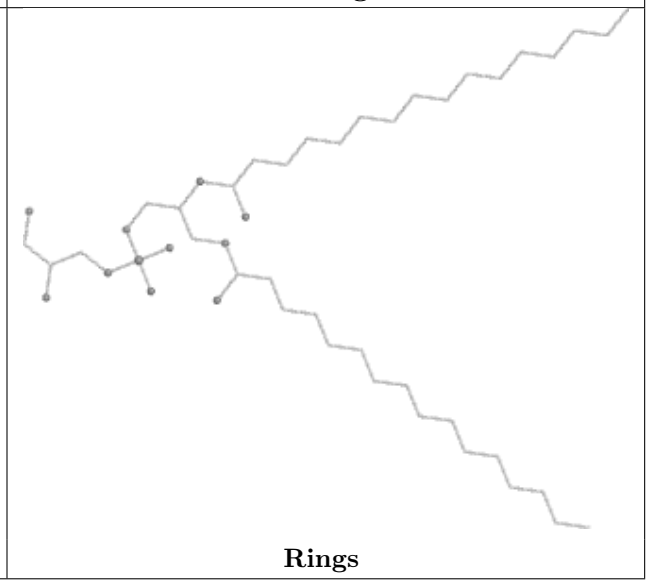
Bond lengths



Bond angles

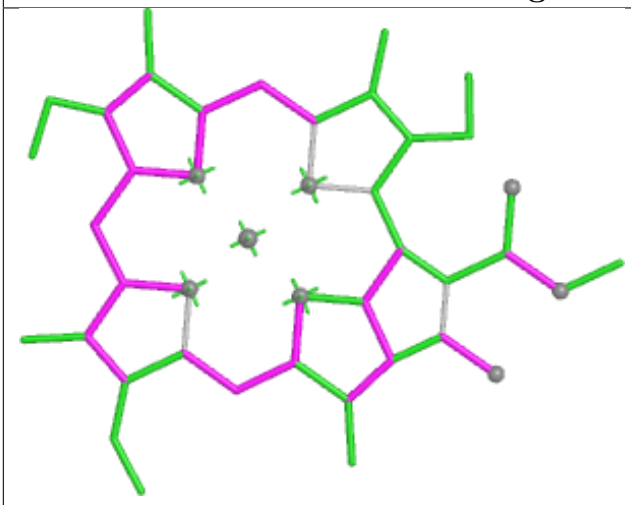


Torsions

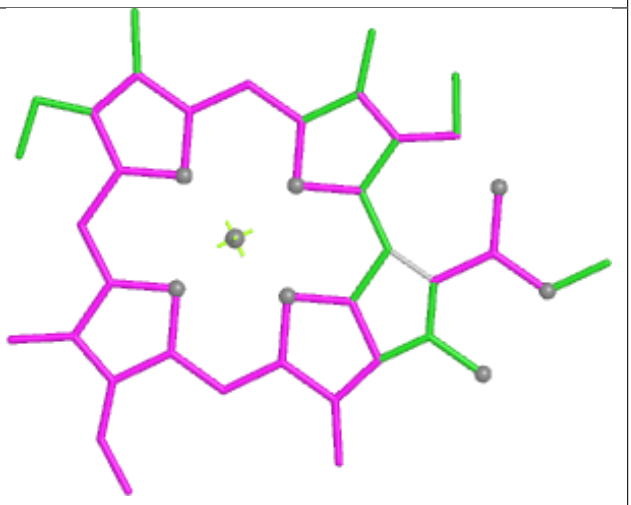


Rings

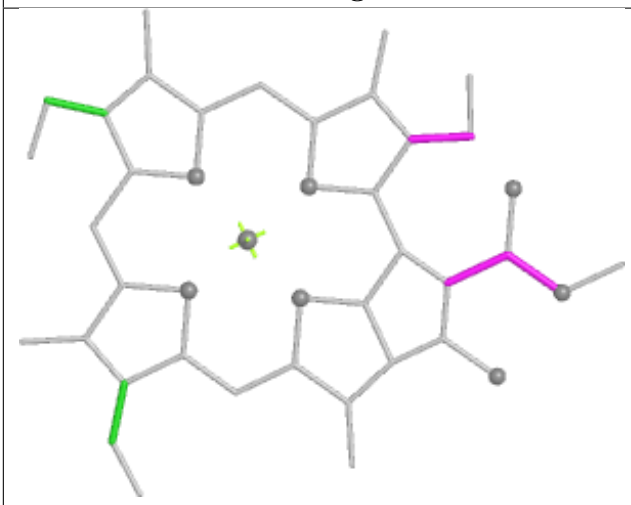
Ligand CLA 7 606



Bond lengths



Bond angles



Torsions

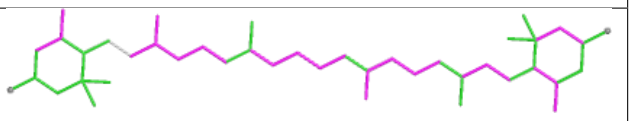


Rings

Ligand LUT 6 621



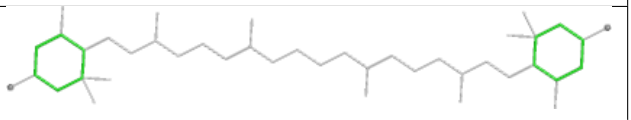
Bond lengths



Bond angles

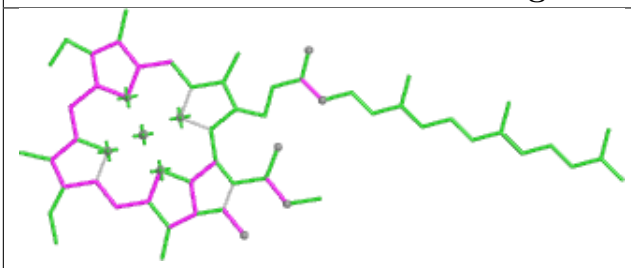


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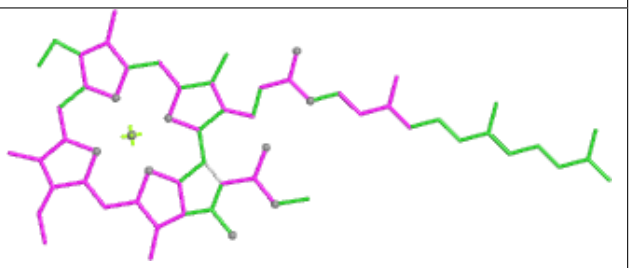


Rings

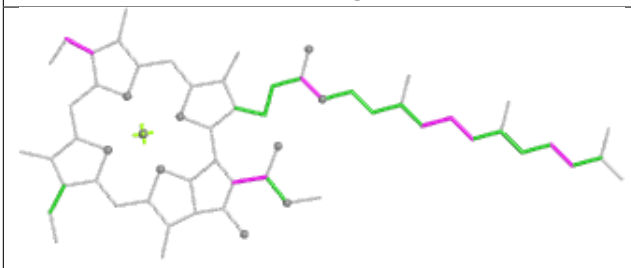
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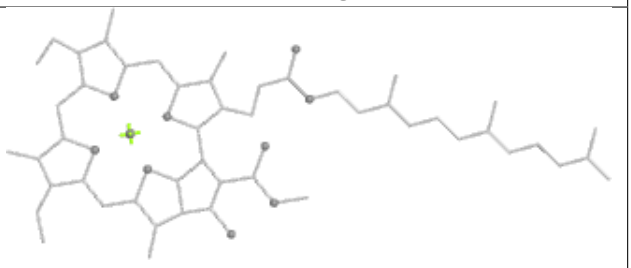
Bond lengths



Bond angles

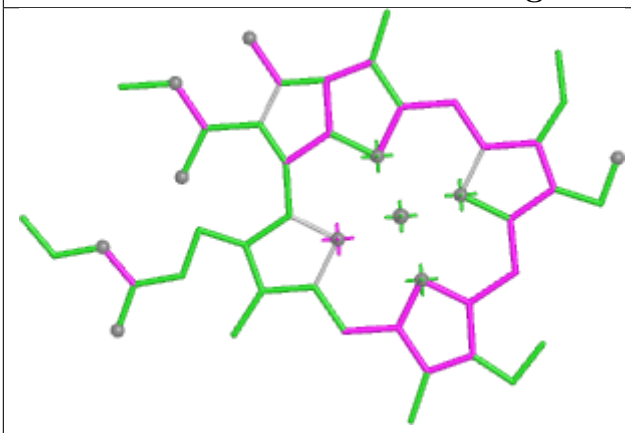


Torsions

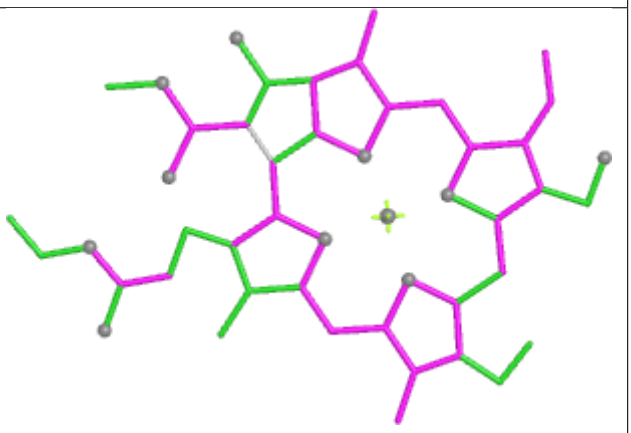


Rings

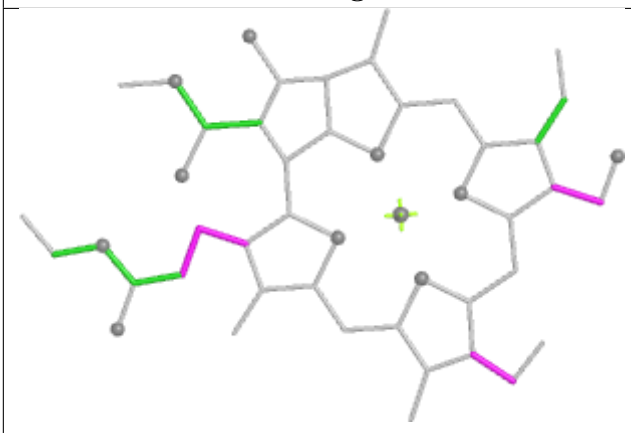
Ligand CHL Z 607



Bond lengths



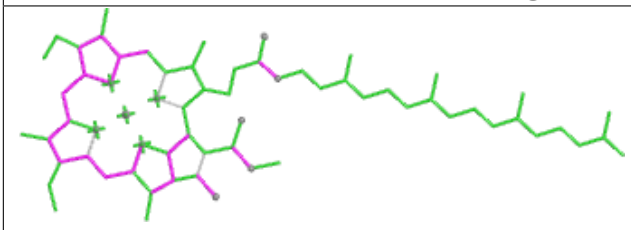
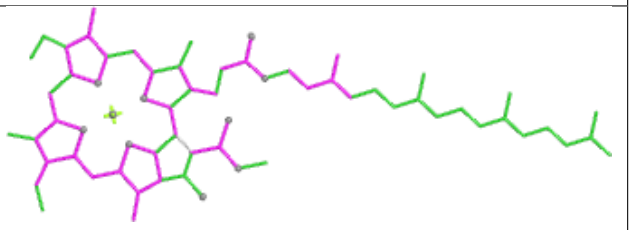
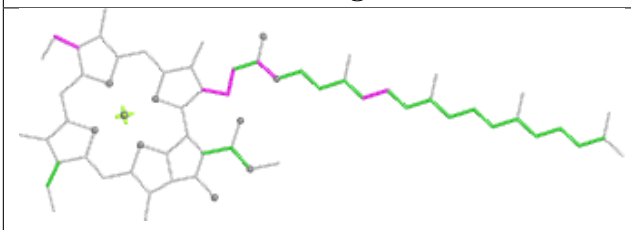
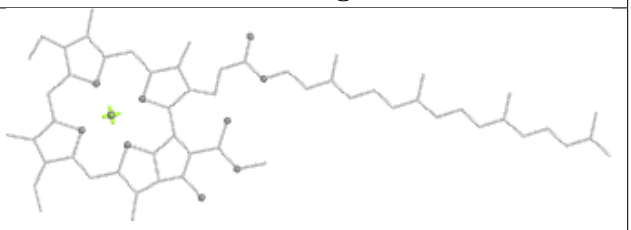
Bond angles

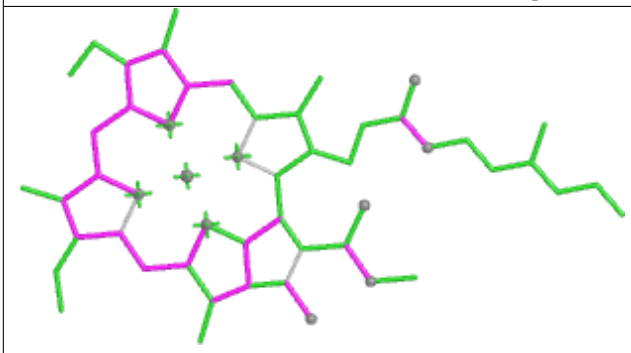
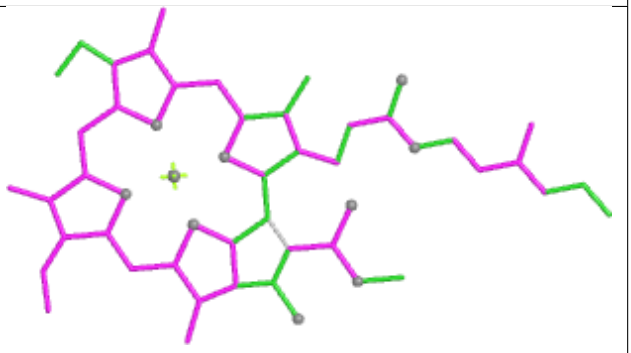
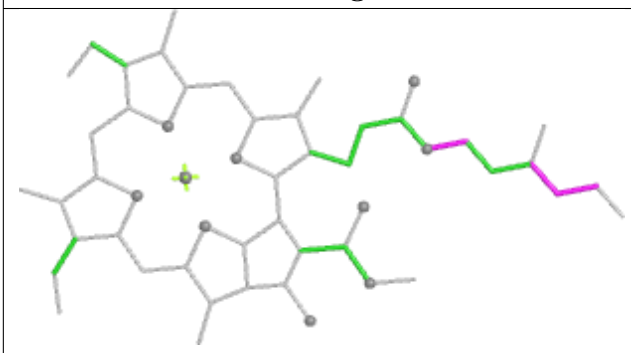
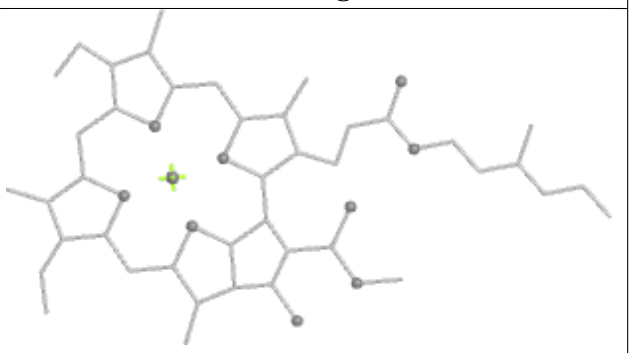


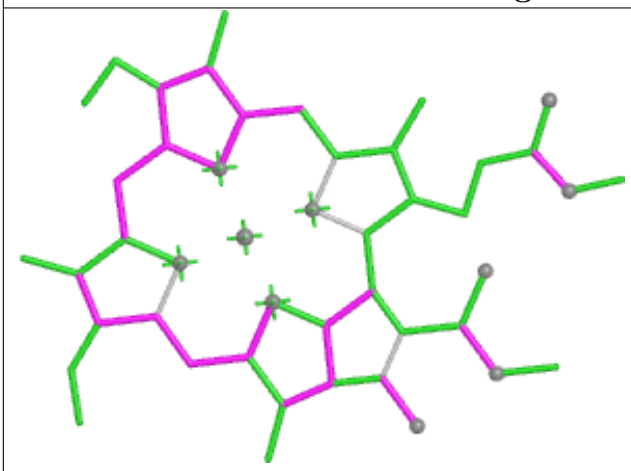
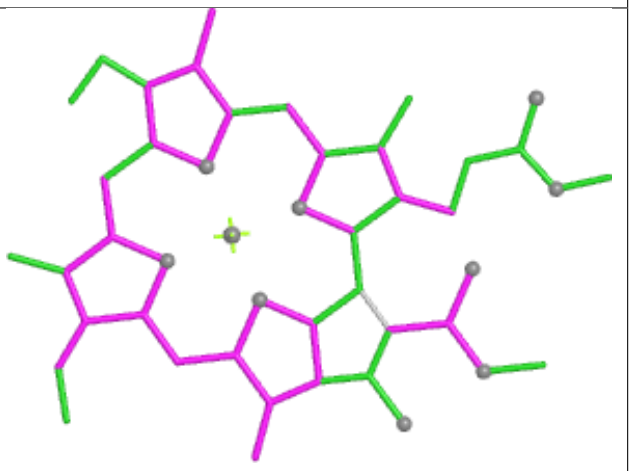
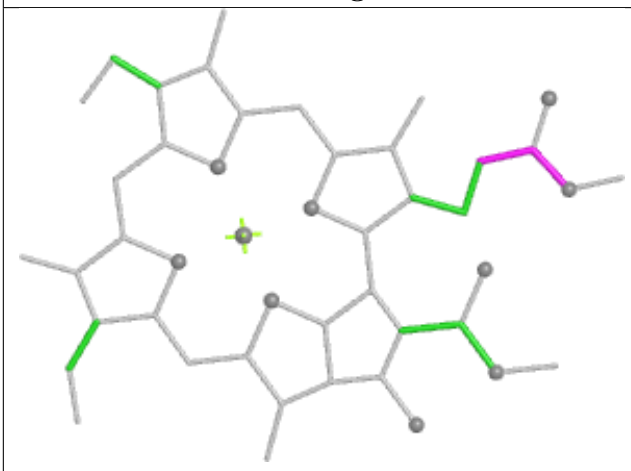
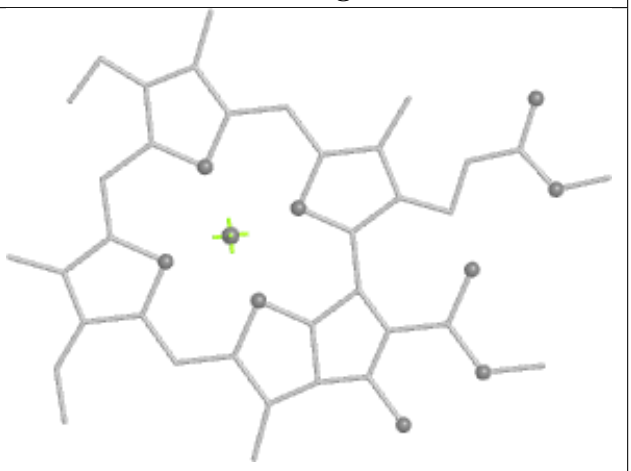
Torsions

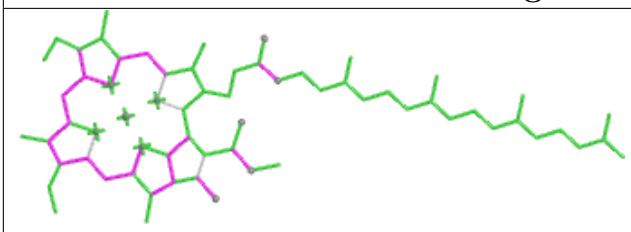
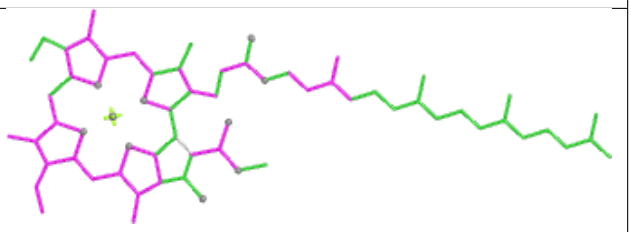
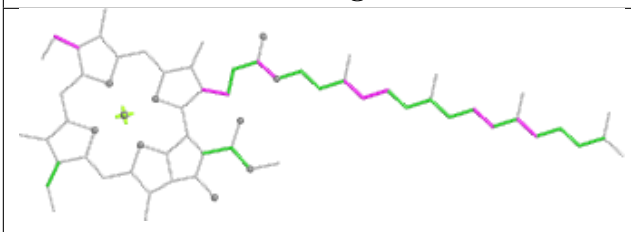
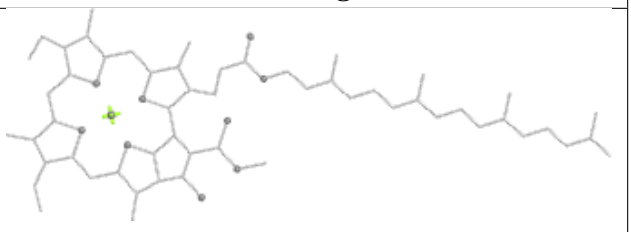


Rings

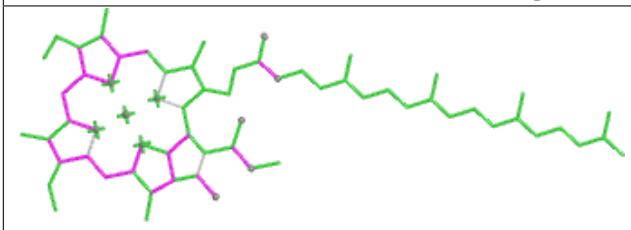
Ligand CLA B 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

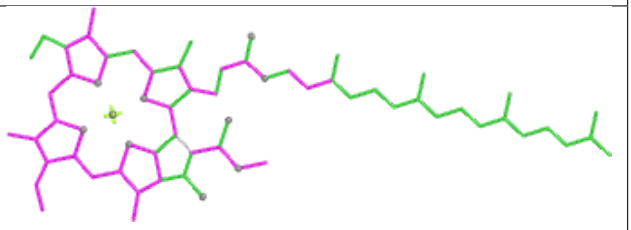
Ligand CLA K 4003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

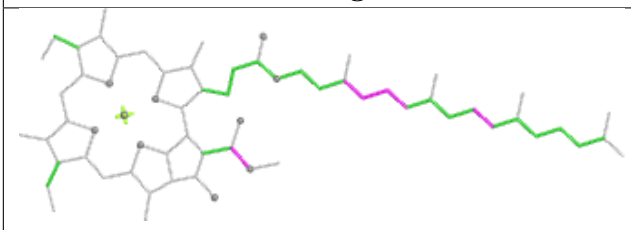
Ligand CLA 3 603



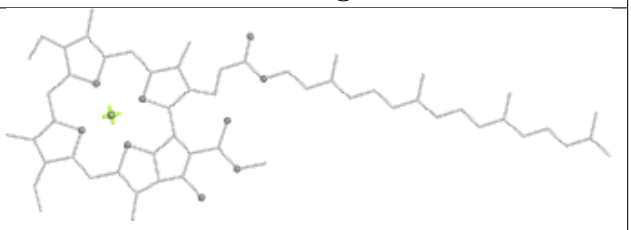
Bond lengths



Bond angles

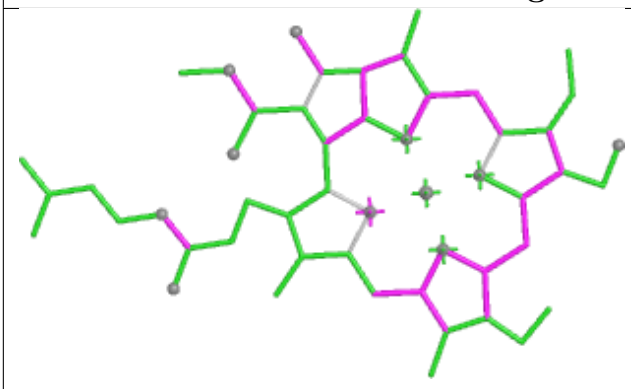


Torsions

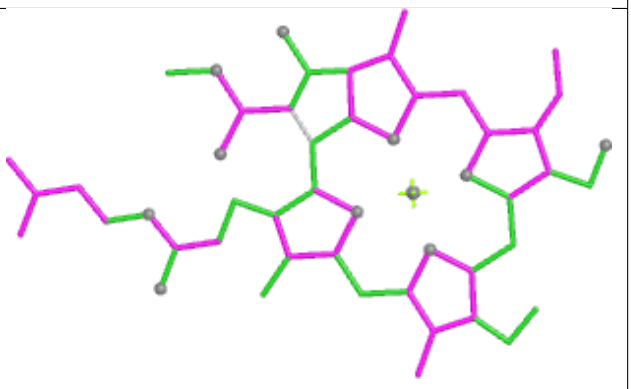


Rings

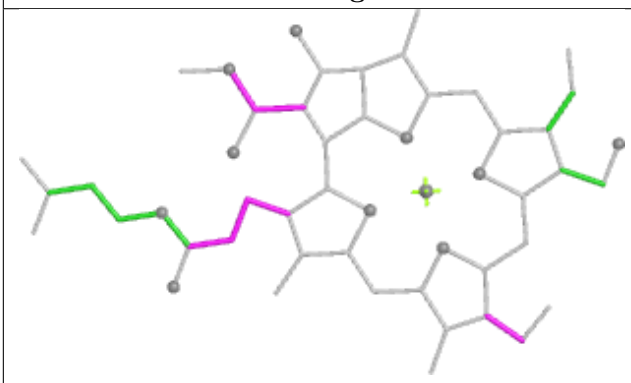
Ligand CHL 4 608



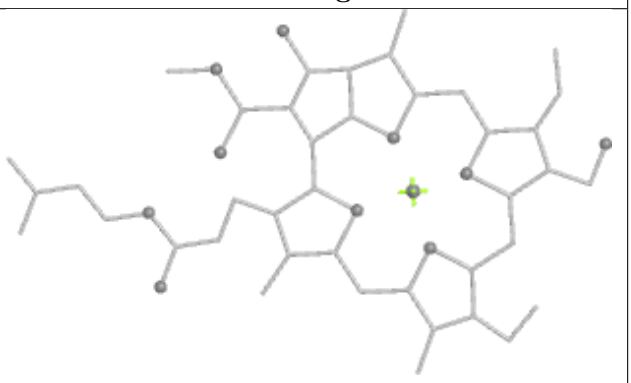
Bond lengths



Bond angles

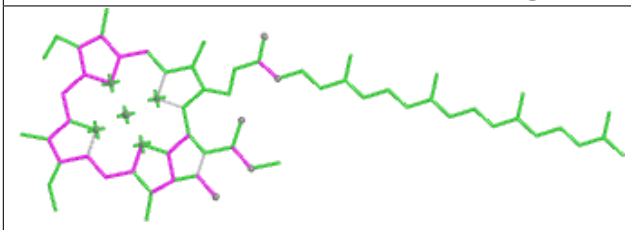


Torsions

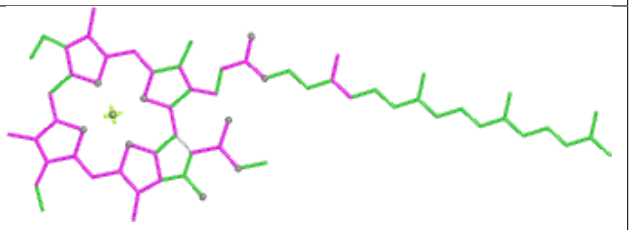


Rings

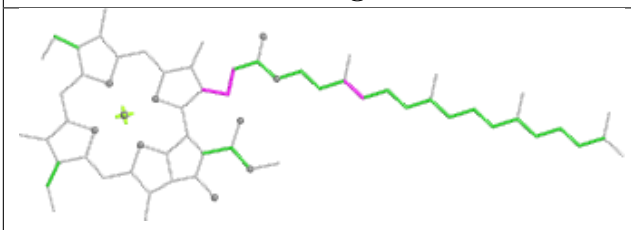
Ligand CLA A 803



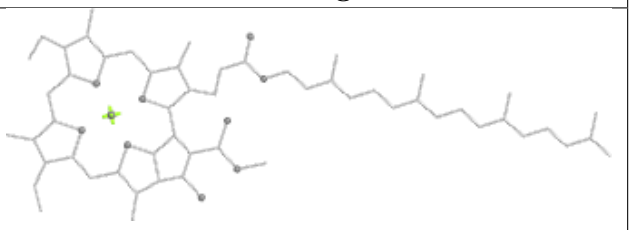
Bond lengths



Bond angles

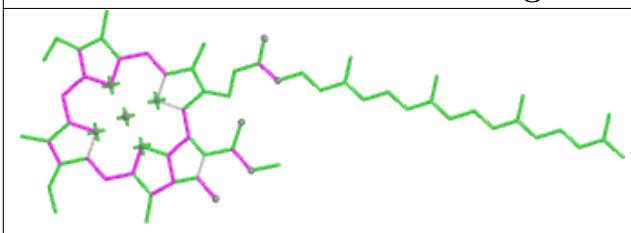


Torsions

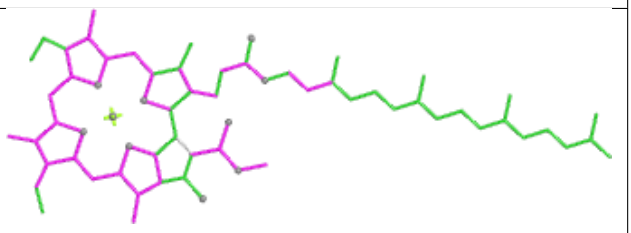


Rings

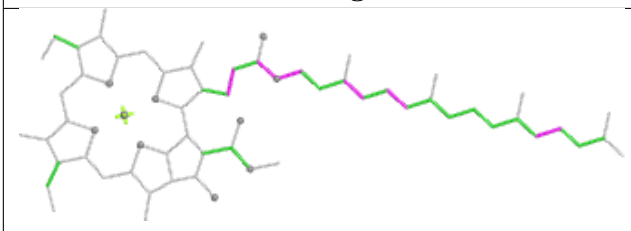
Ligand CLA A 830



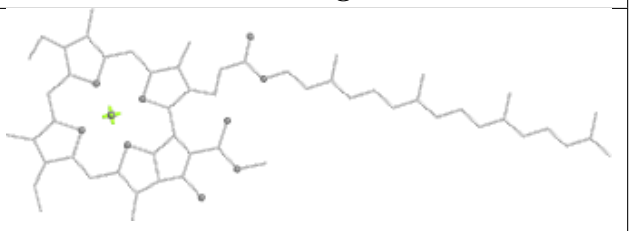
Bond lengths



Bond angles

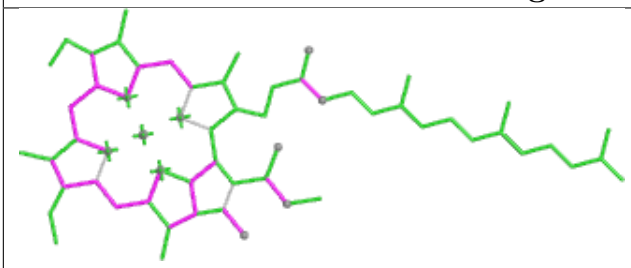


Torsions

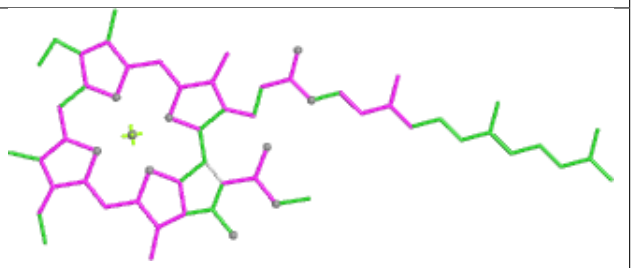


Rings

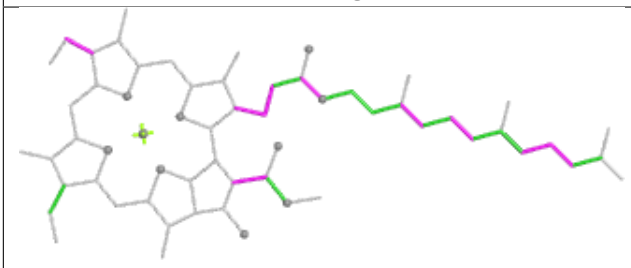
Ligand CLA 4 610



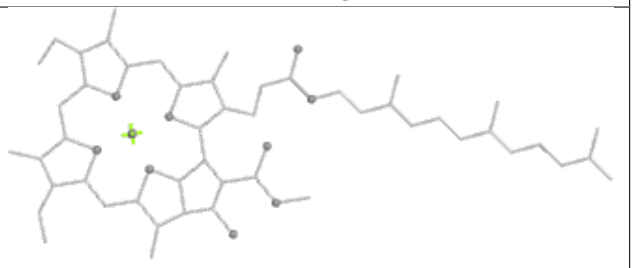
Bond lengths



Bond angles

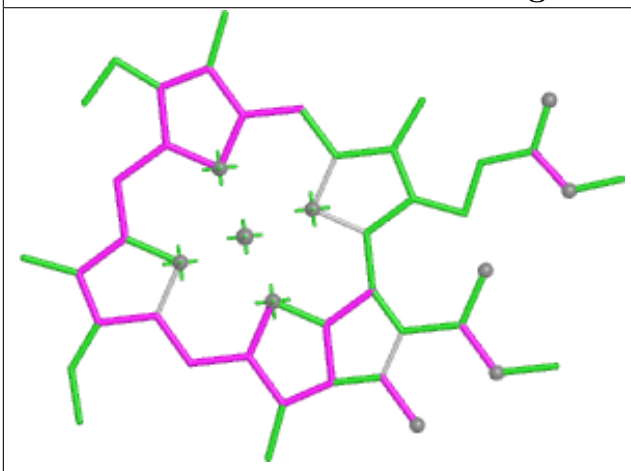


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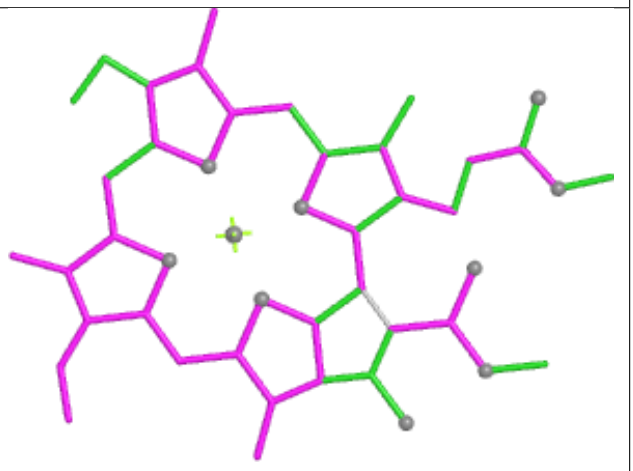


Rings

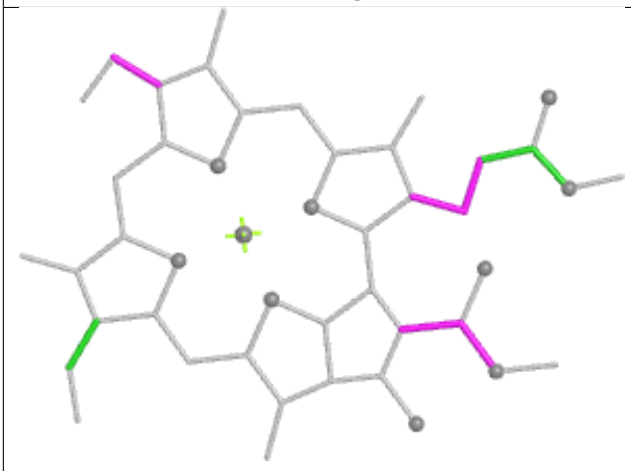
Ligand CLA 2 603



Bond lengths



Bond angles

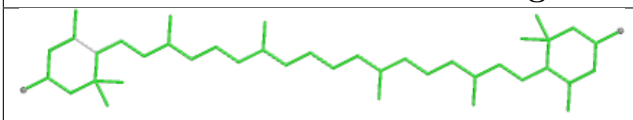


Torsions

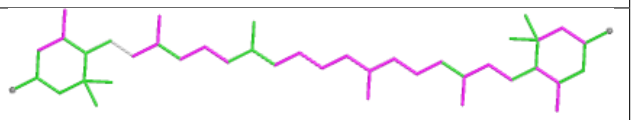


Rings

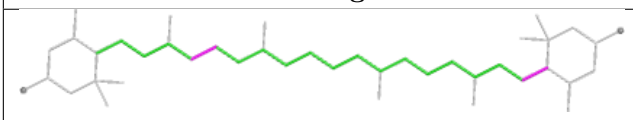
Ligand LUT 5 624



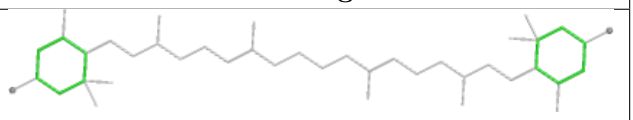
Bond lengths



Bond angles

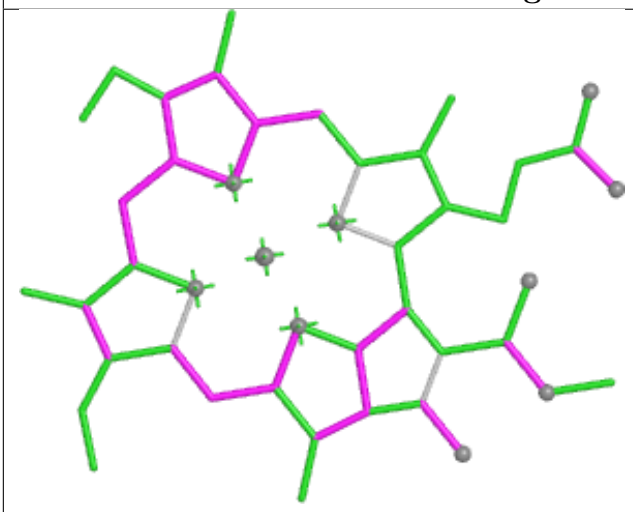


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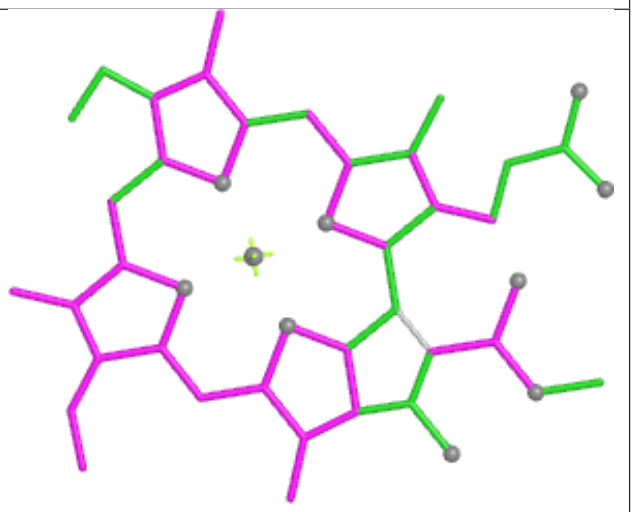


Rings

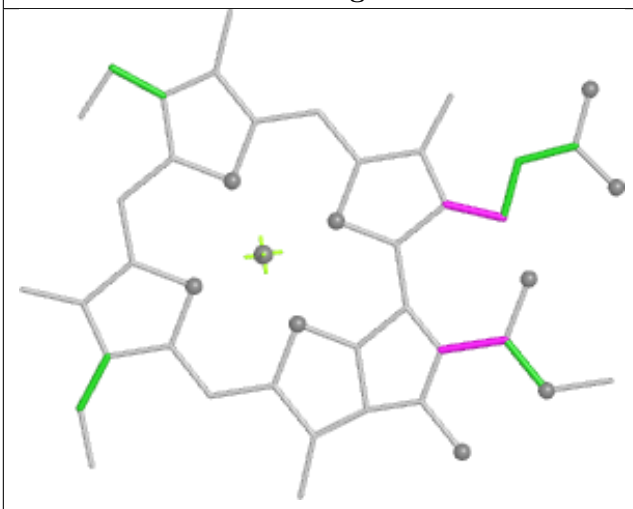
Ligand CLA A 821



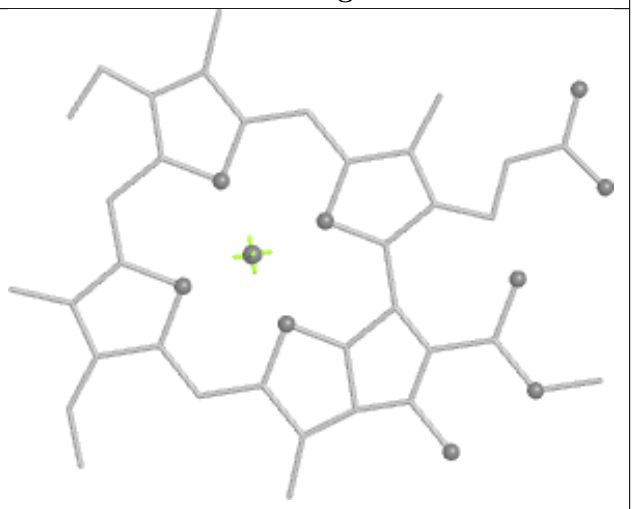
Bond lengths



Bond angles

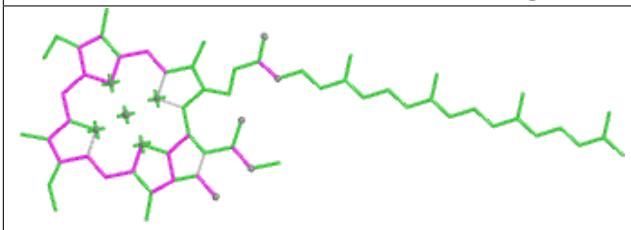


Torsions

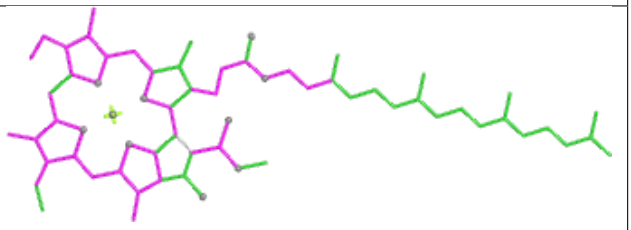


Rings

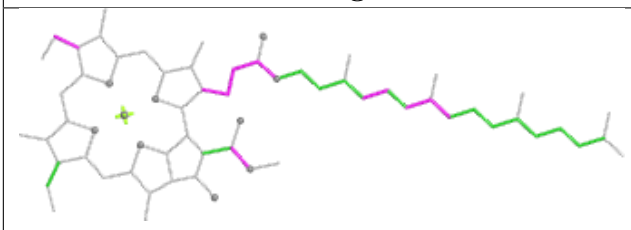
Ligand CLA A 819



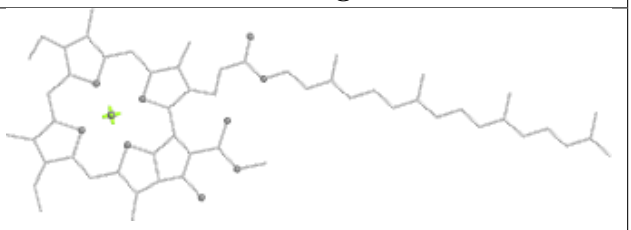
Bond lengths



Bond angles

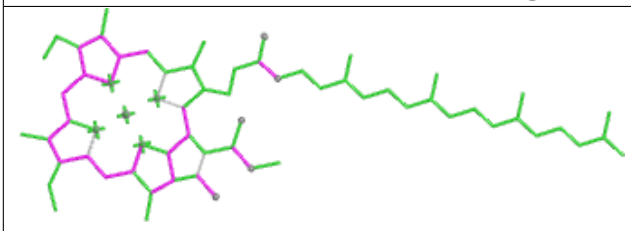


Torsions

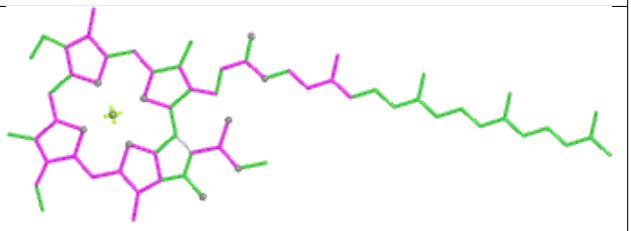


Rings

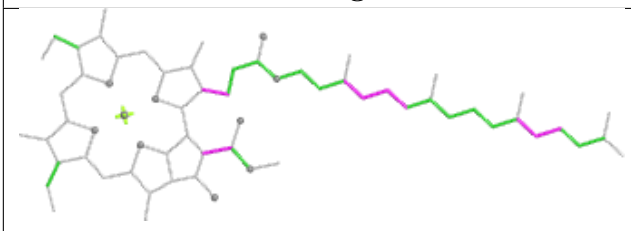
Ligand CLA A 816



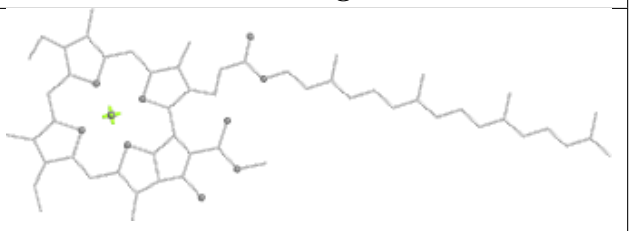
Bond lengths



Bond angles

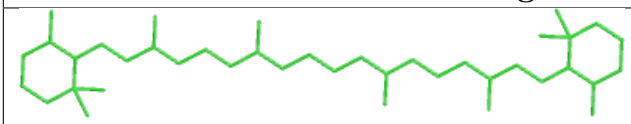


Torsions

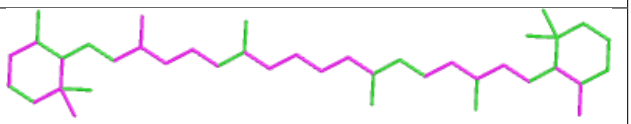


Rings

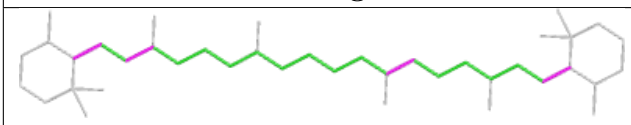
Ligand BCR J 3003



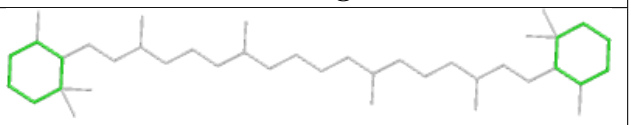
Bond lengths



Bond angles

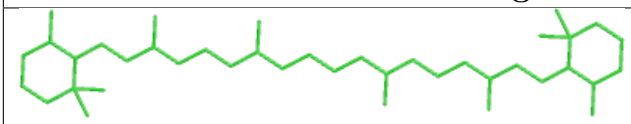


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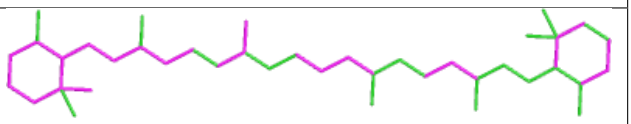


Rings

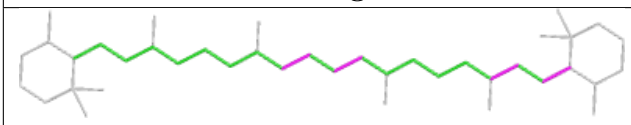
Ligand BCR K 4001



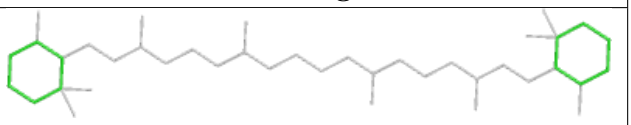
Bond lengths



Bond angles



Torsions

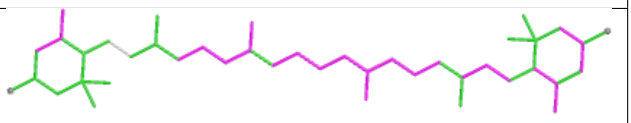


Rings

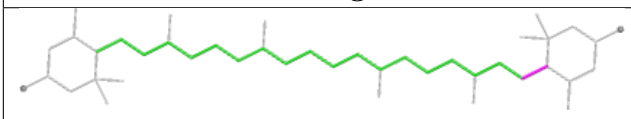
Ligand LUT 3 622



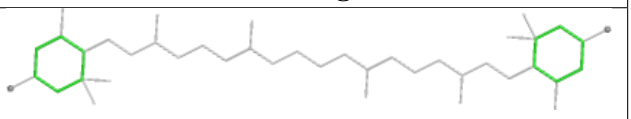
Bond lengths



Bond angles

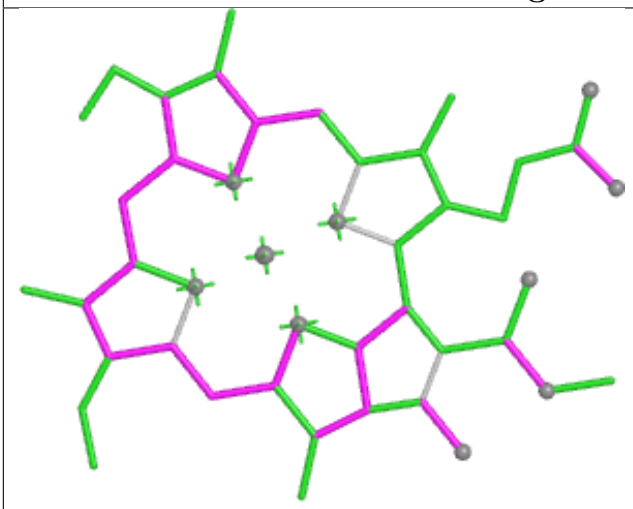


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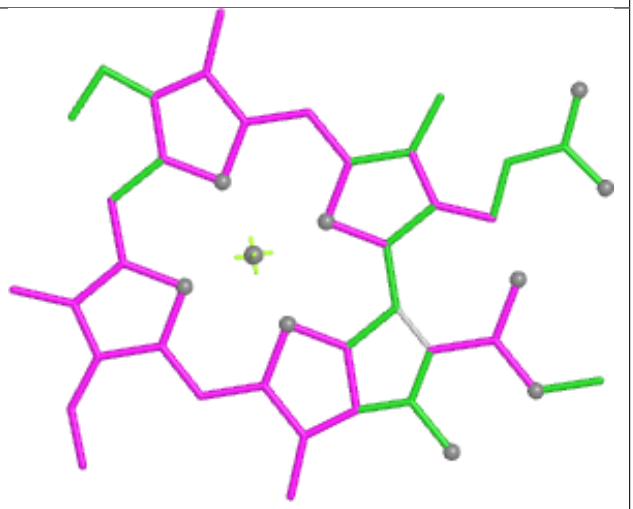


Rings

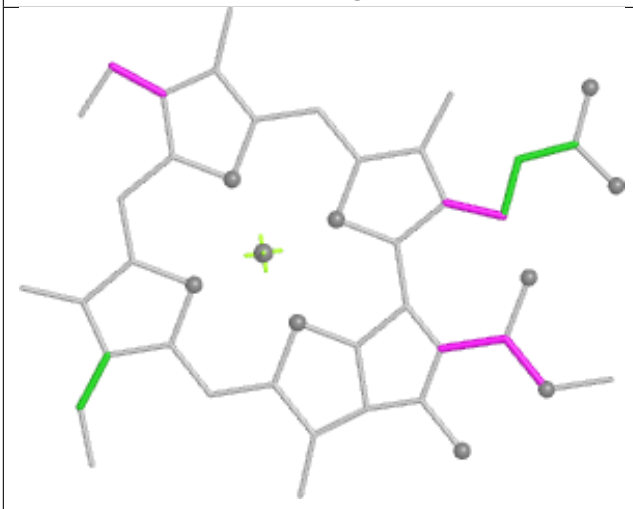
Ligand CLA 6 614



Bond lengths



Bond angles

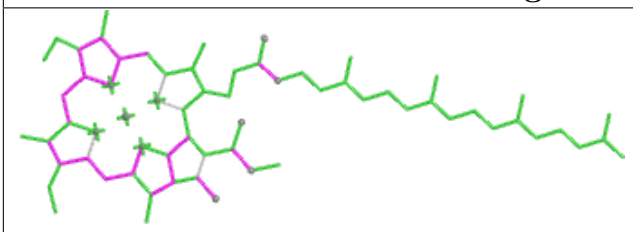


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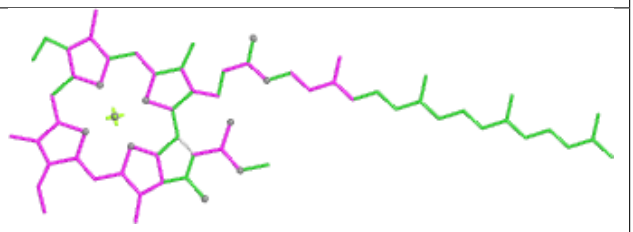


Rings

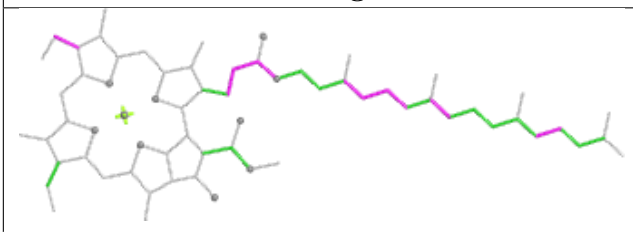
Ligand CLA B 807



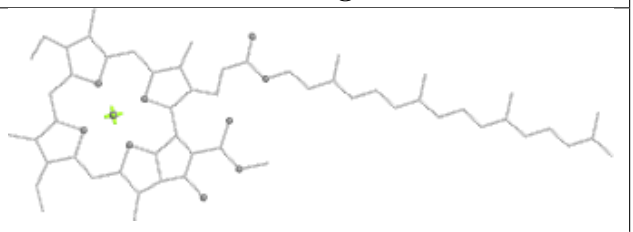
Bond lengths



Bond angles

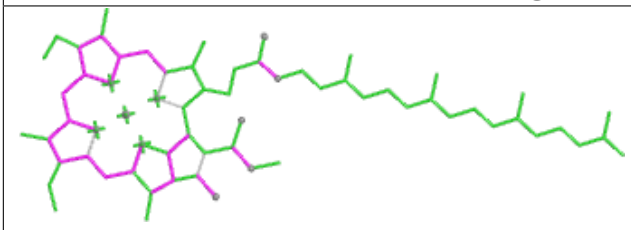


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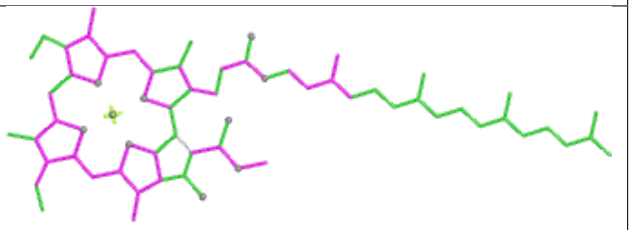


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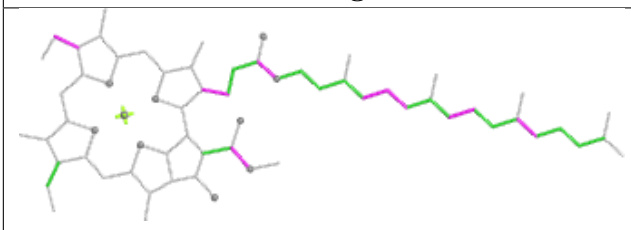
Ligand CLA 1 611



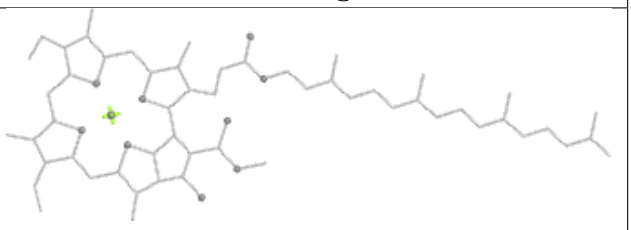
Bond lengths



Bond angles



Torsions



Rings

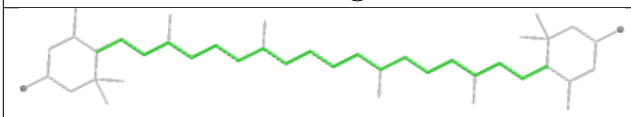
Ligand LUT 2 616



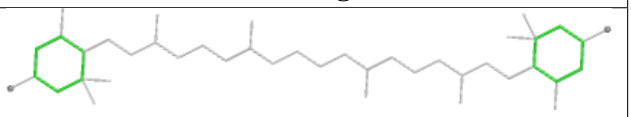
Bond lengths



Bond angles

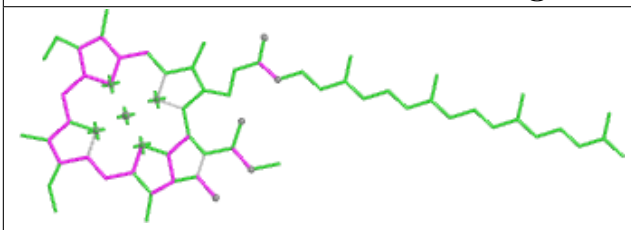


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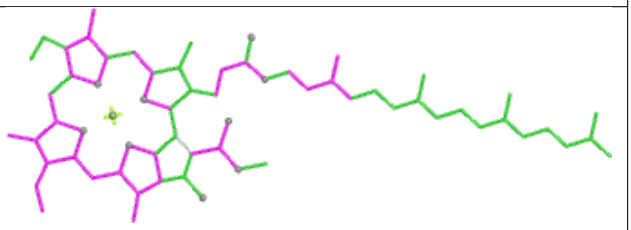


Rings

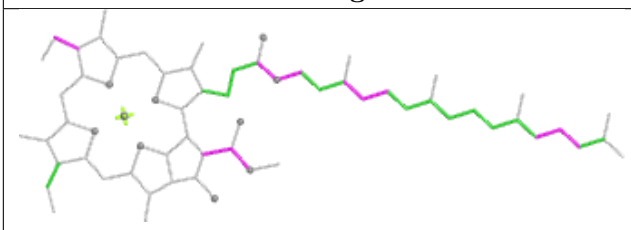
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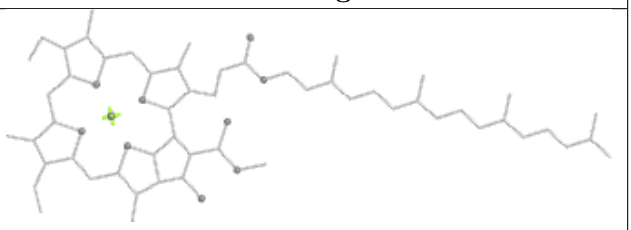
Bond lengths



Bond angles

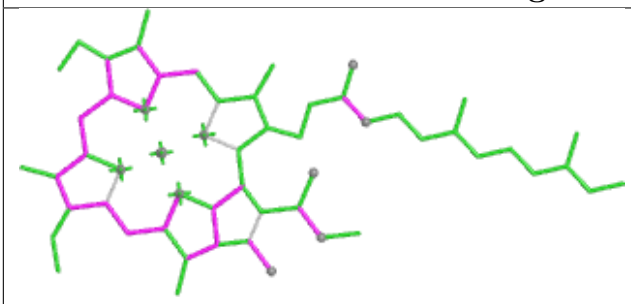


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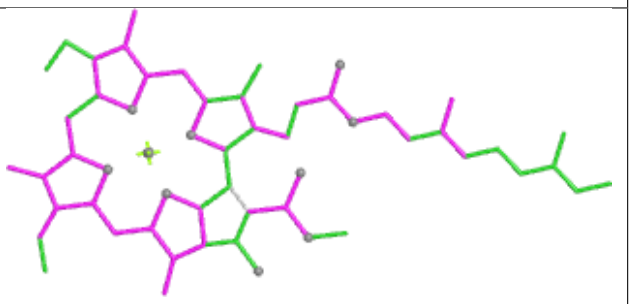


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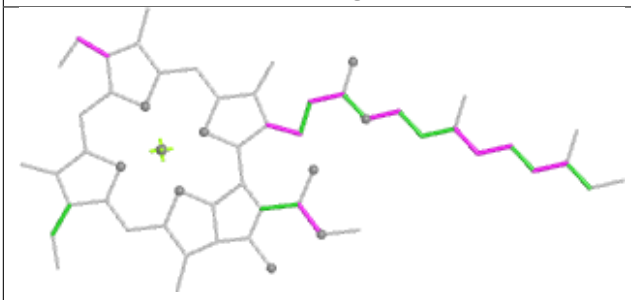
Ligand CLA 4 613



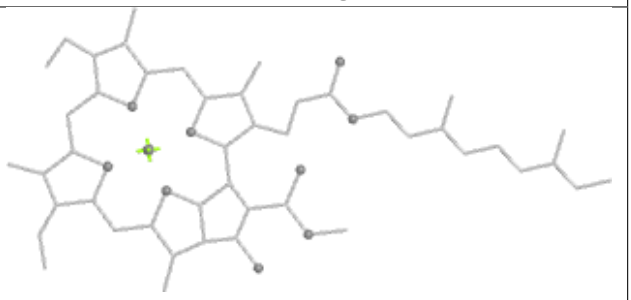
Bond lengths



Bond angles

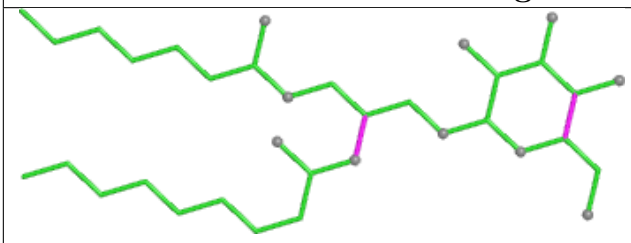


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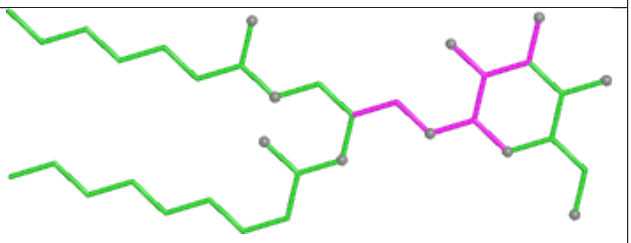


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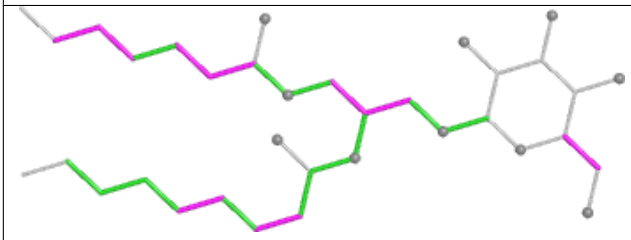
Ligand LMG J 3001



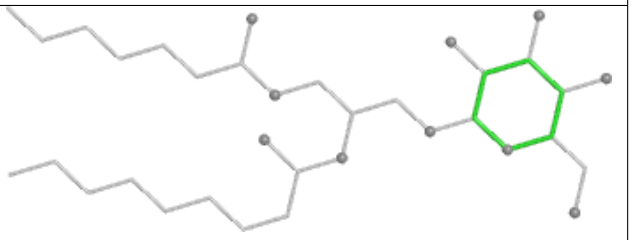
Bond lengths



Bond angles

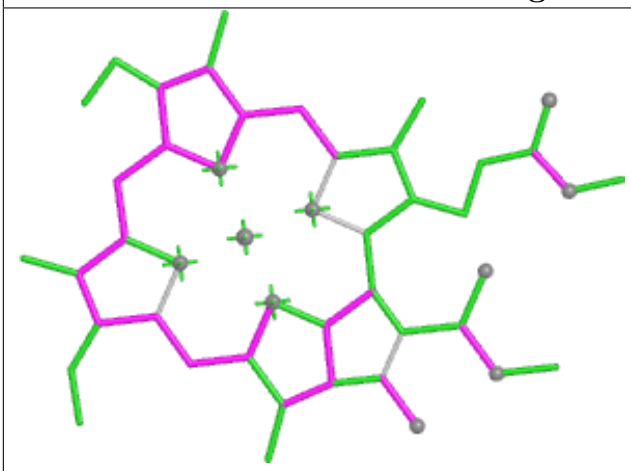


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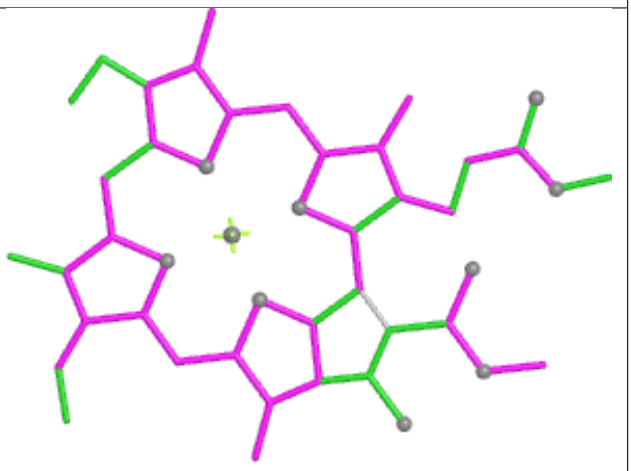


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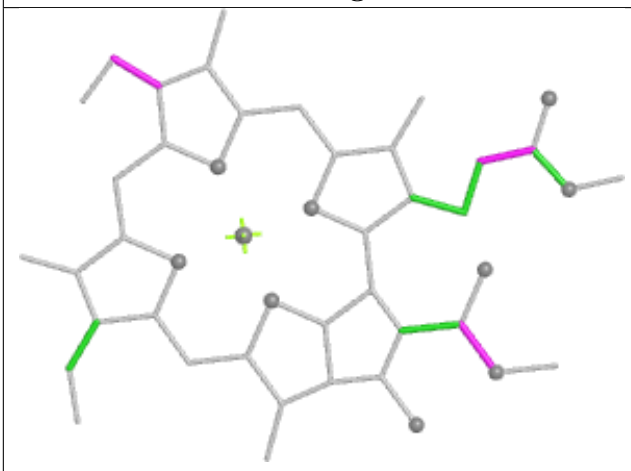
Ligand CLA 8 609



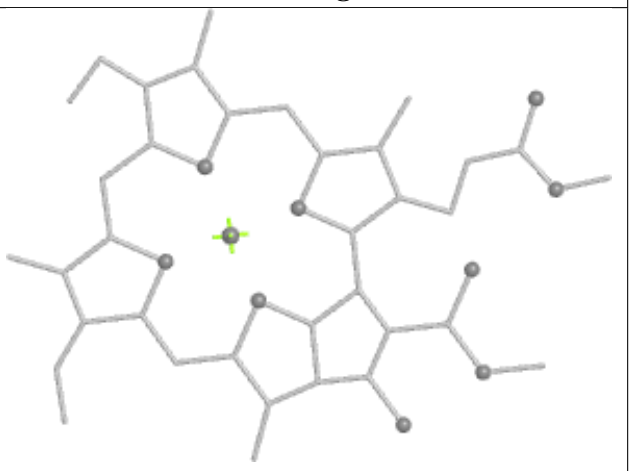
Bond lengths



Bond angles

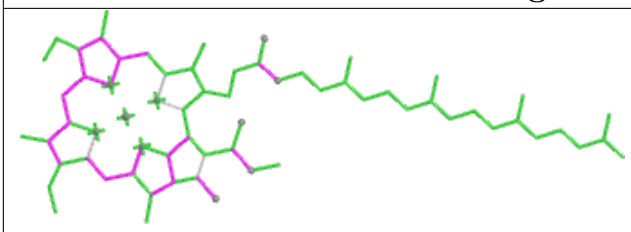


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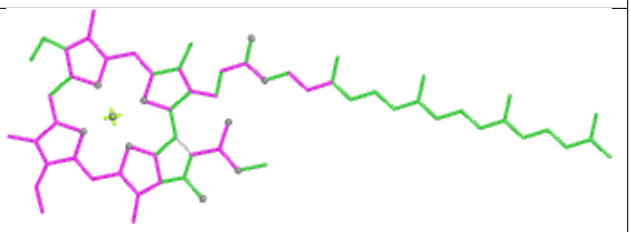


Rings

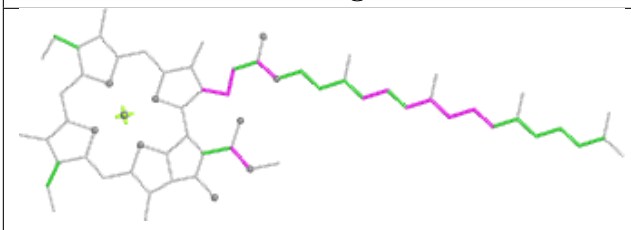
Ligand CLA 6 602



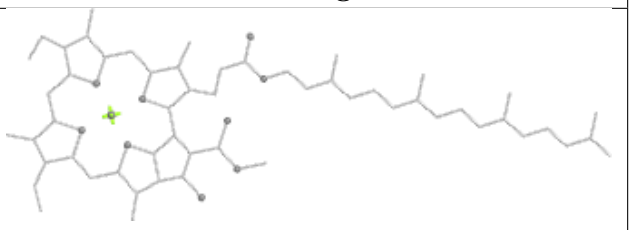
Bond lengths



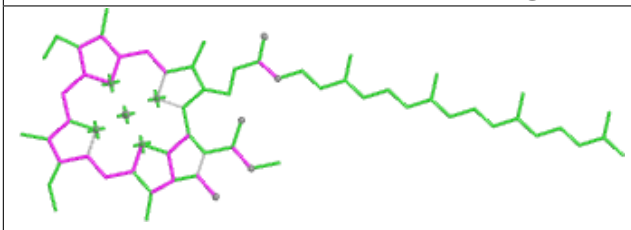
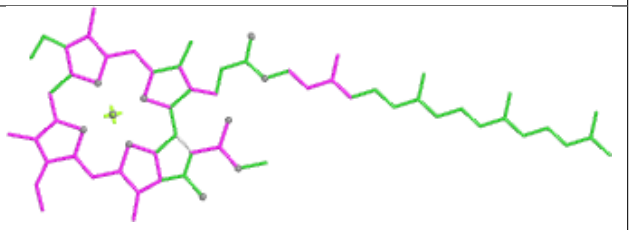
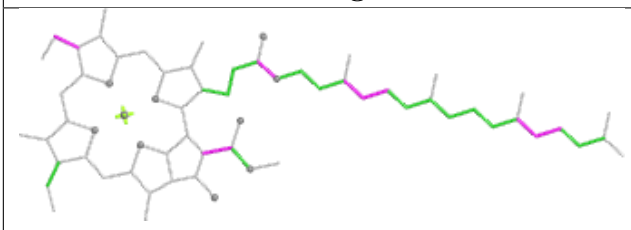
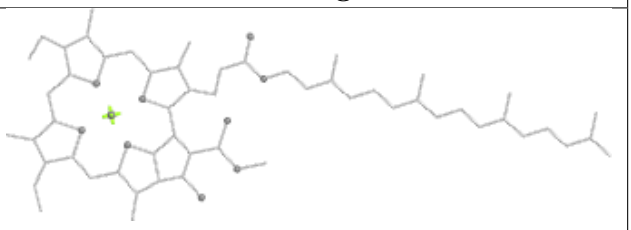
Bond angles

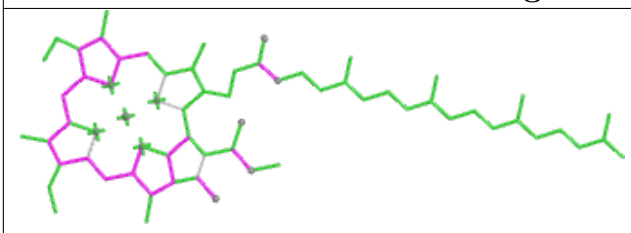
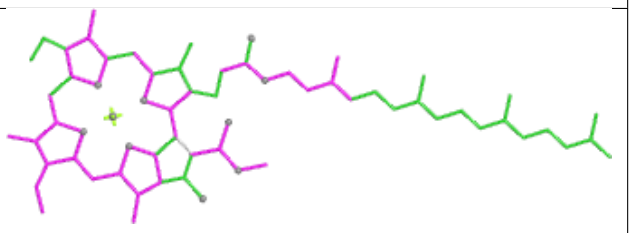
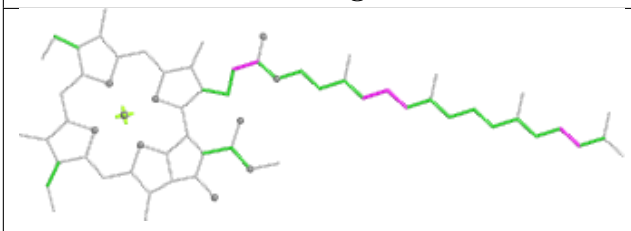
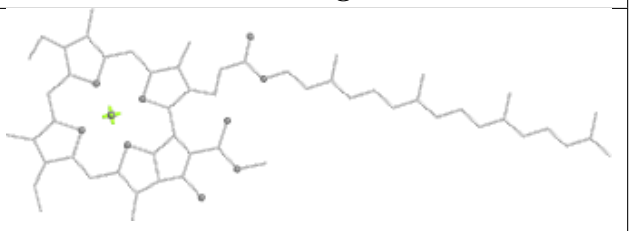


Torsions

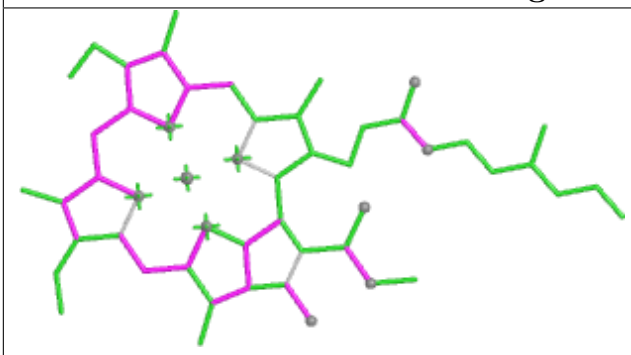


Rings

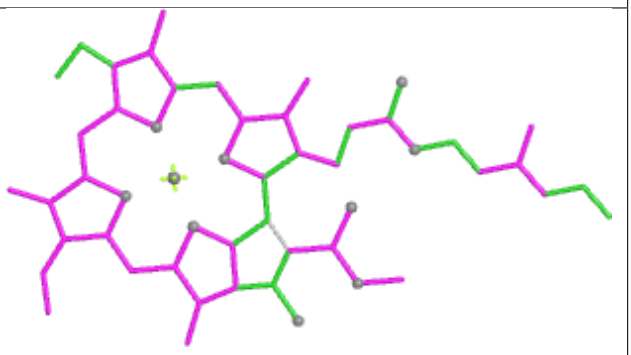
Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

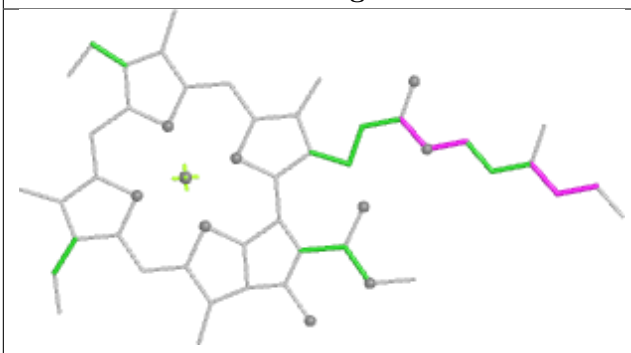
Ligand CLA 8 612



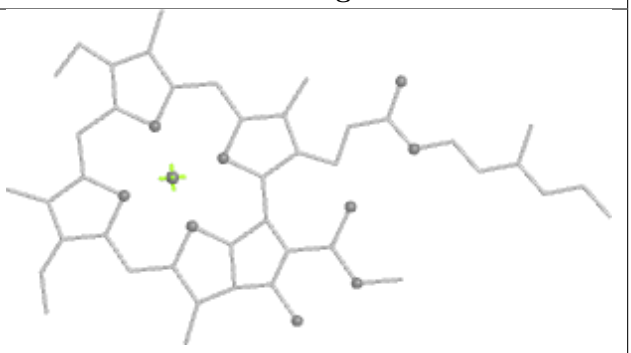
Bond lengths



Bond angles

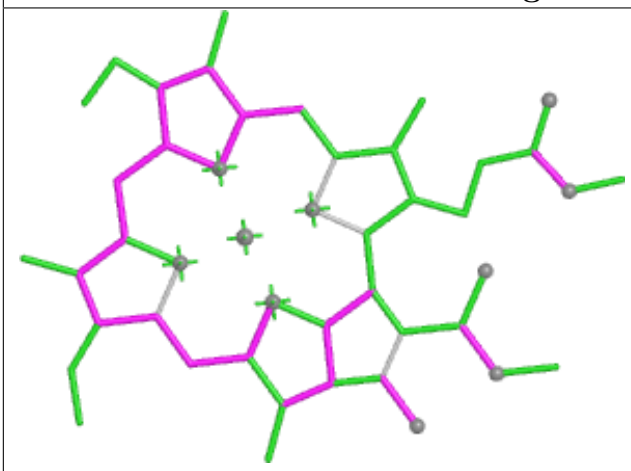


Torsions

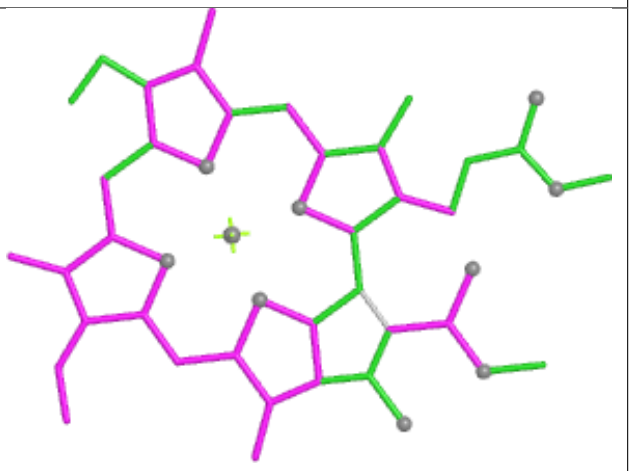


Rings

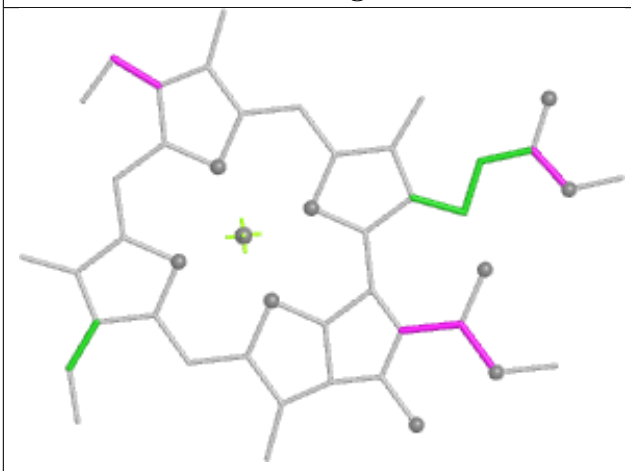
Ligand CLA G 204



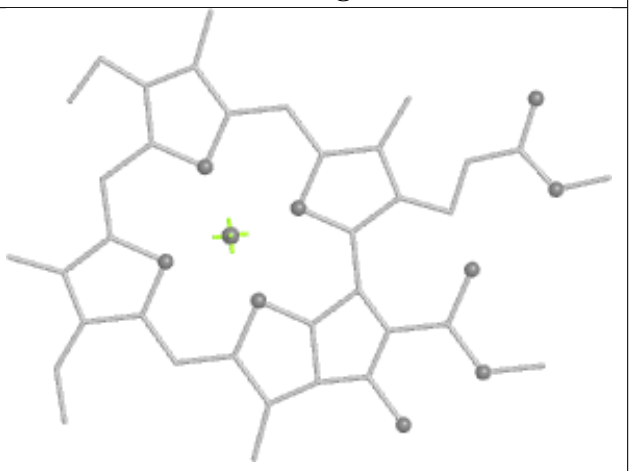
Bond lengths



Bond angles

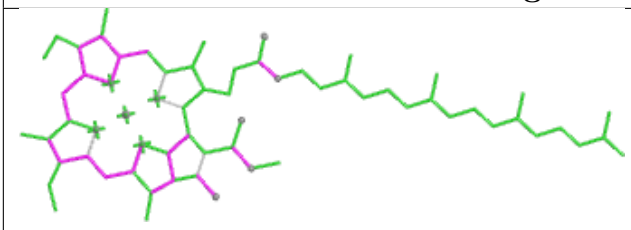


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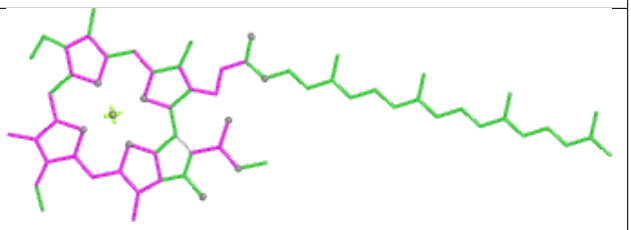


Rings

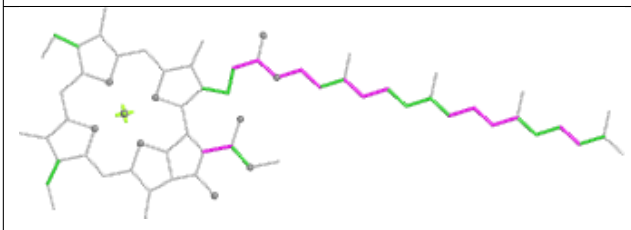
Ligand CLA A 806



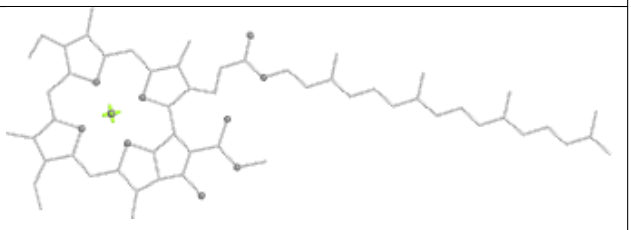
Bond lengths



Bond angles

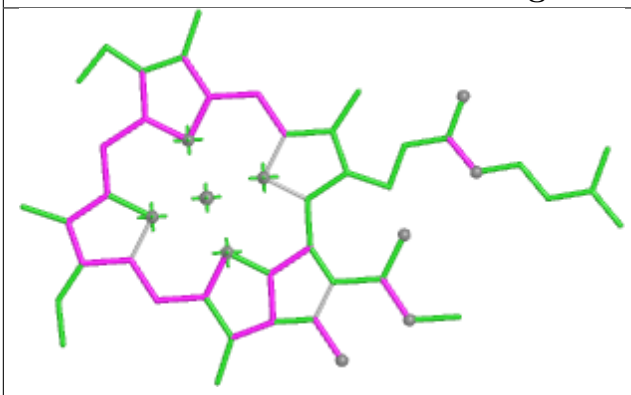


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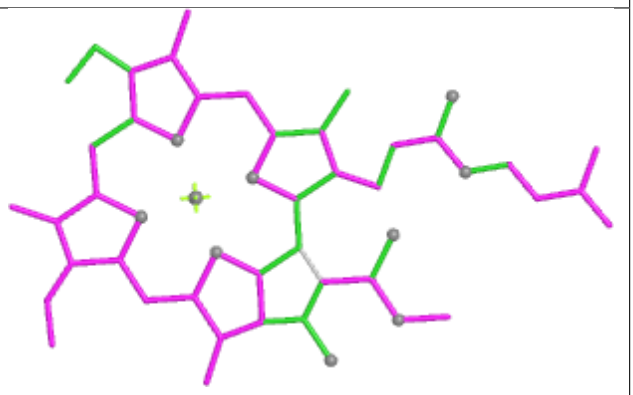


Rings

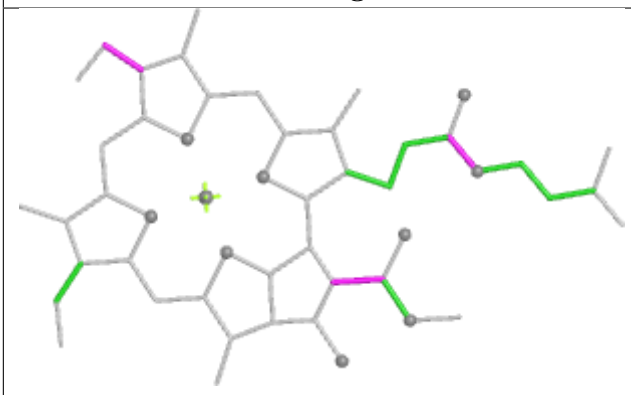
Ligand CLA 4 604



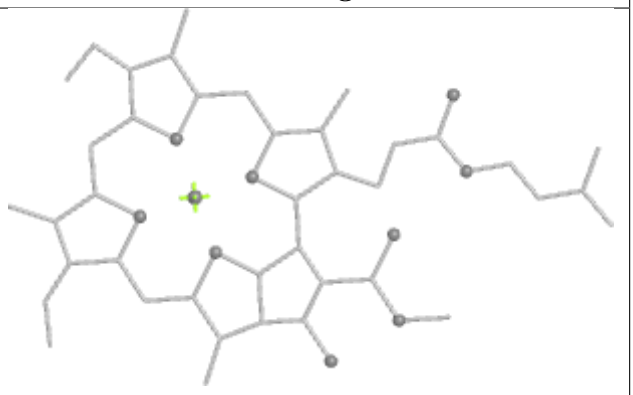
Bond lengths



Bond angles

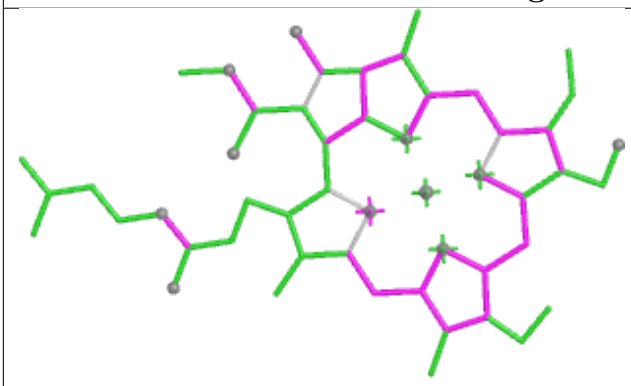


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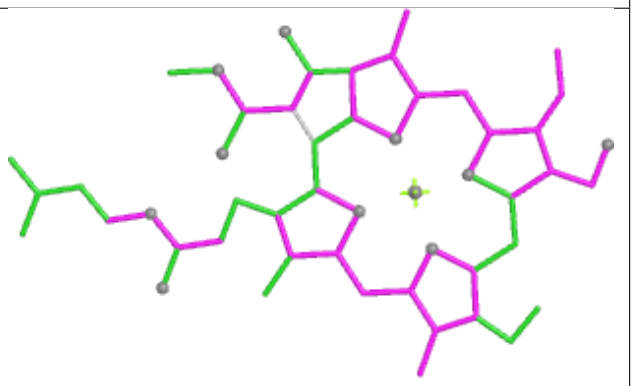


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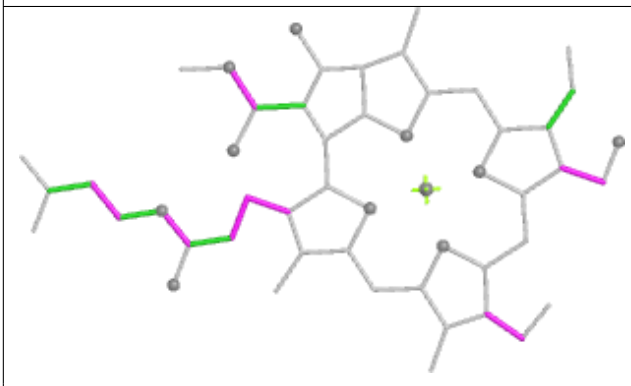
Ligand CHL 5 607



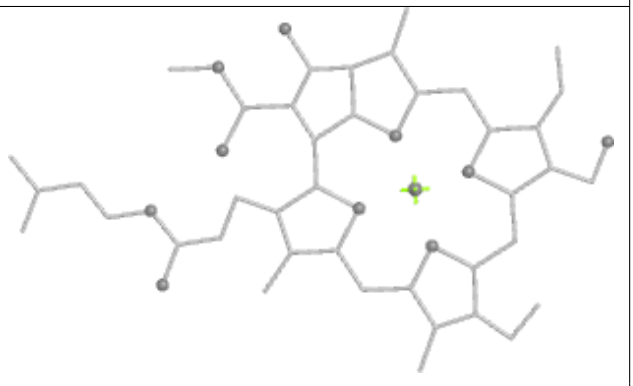
Bond lengths



Bond angles

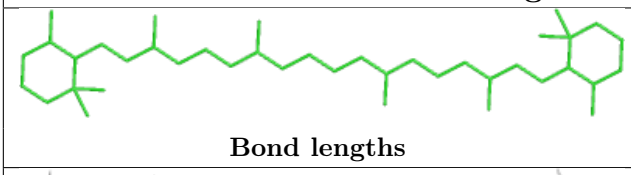


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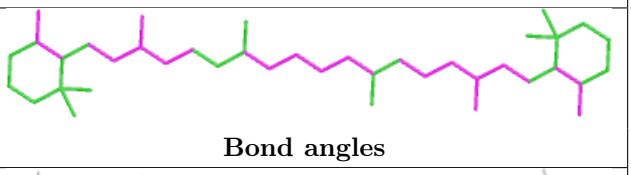


Rings

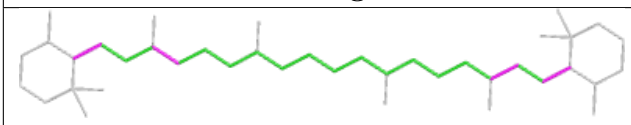
Ligand BCR L 201



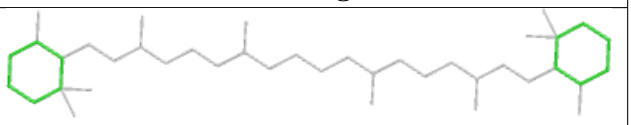
Bond lengths



Bond angles



Torsions



Rings

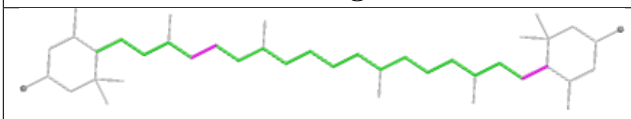
Ligand LUT 7 622



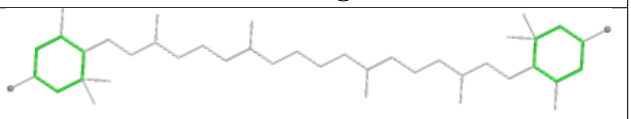
Bond lengths



Bond angles

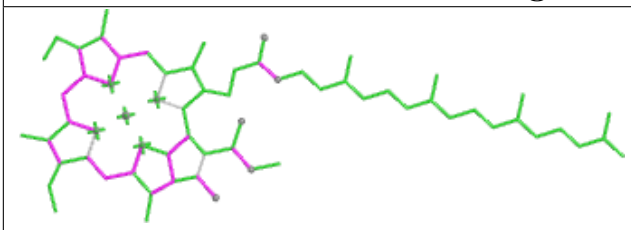


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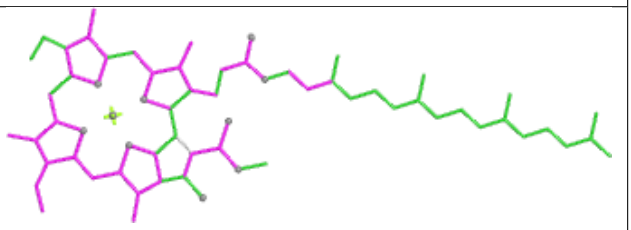


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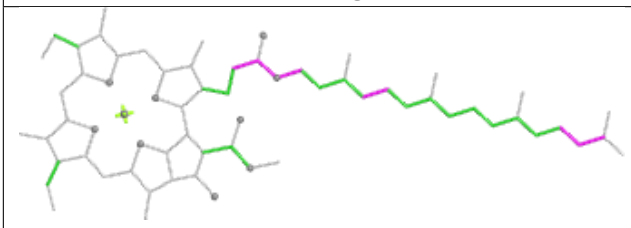
Ligand CL0 A 801



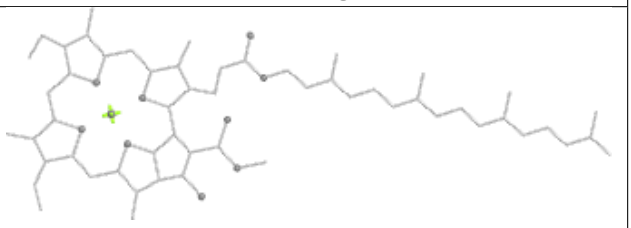
Bond lengths



Bond angles

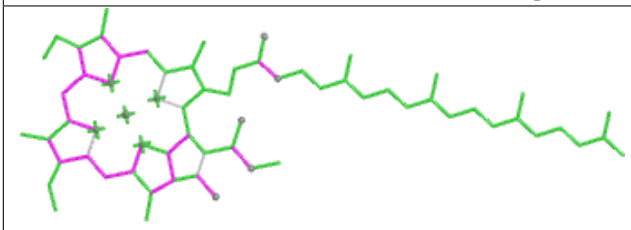


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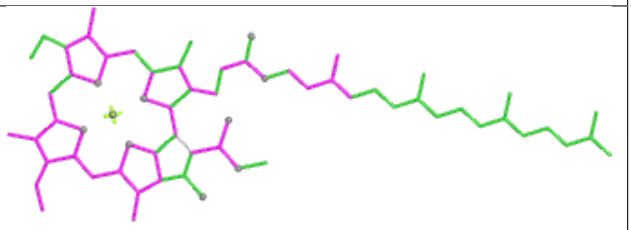


Rings

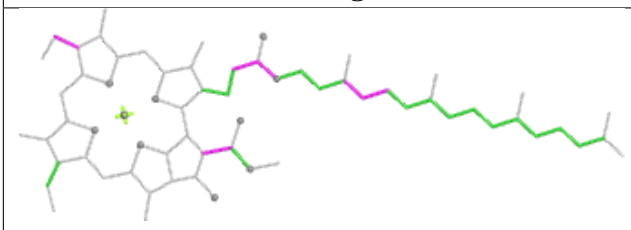
Ligand CLA 1 603



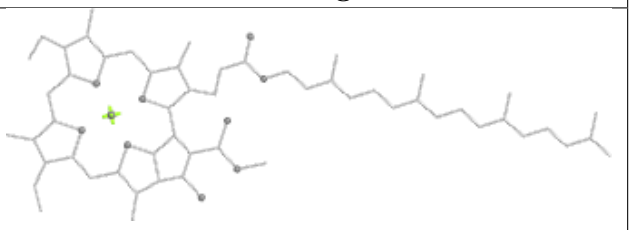
Bond lengths



Bond angles

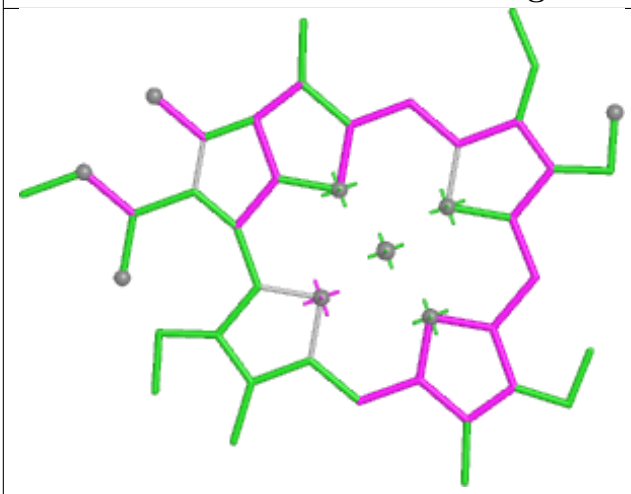


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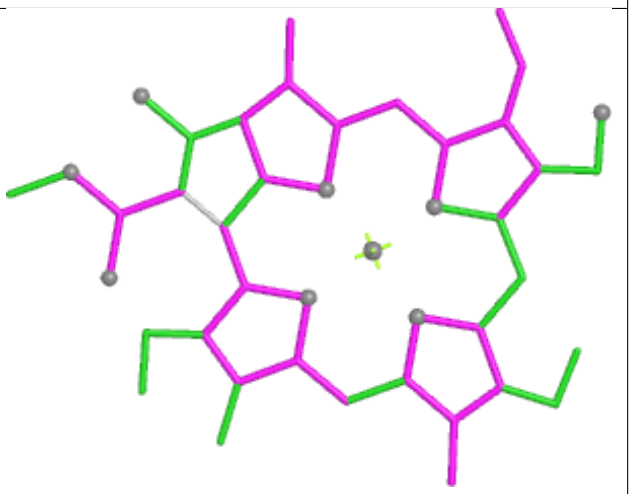


Rings

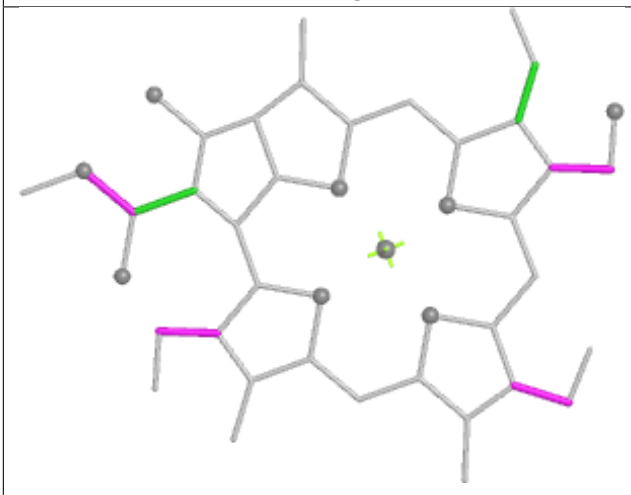
Ligand CHL 6 618



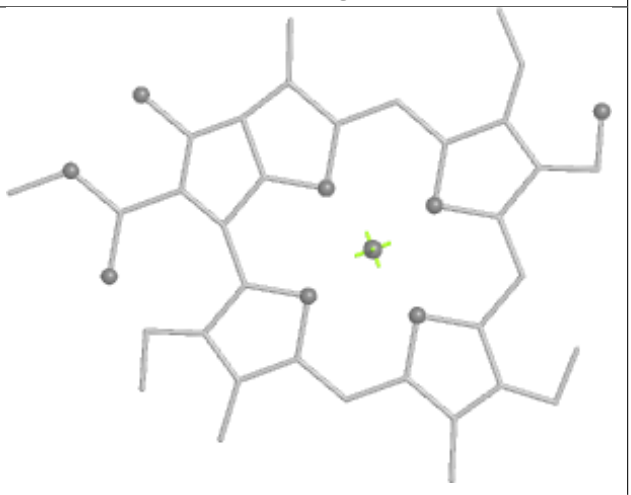
Bond lengths



Bond angles

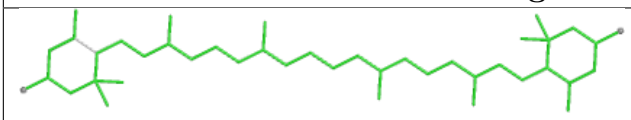


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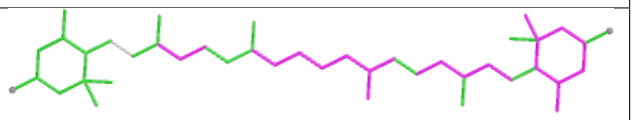


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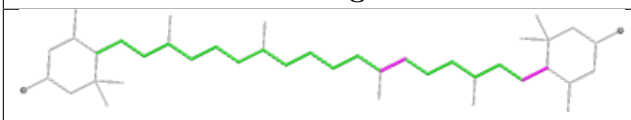
Ligand LUT 2 617



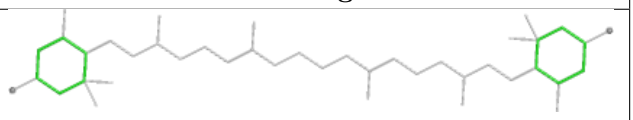
Bond lengths



Bond angles



Torsions

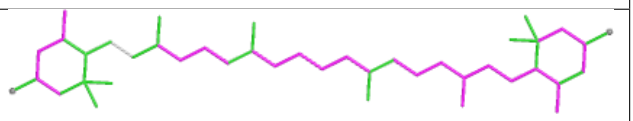


Rings

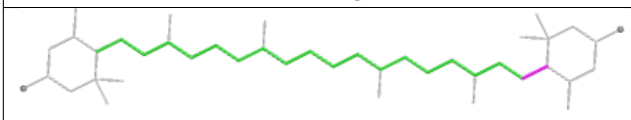
Ligand LUT 1 619



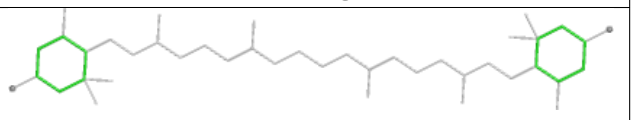
Bond lengths



Bond angles

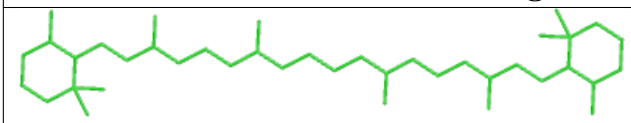


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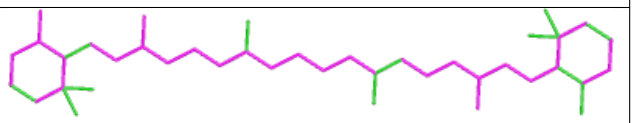


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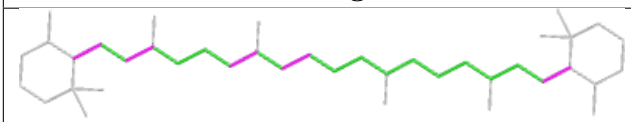
Ligand BCR 6 625



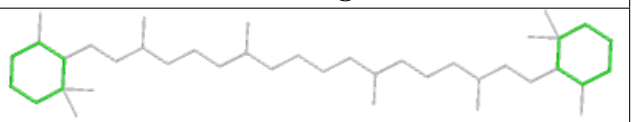
Bond lengths



Bond angles

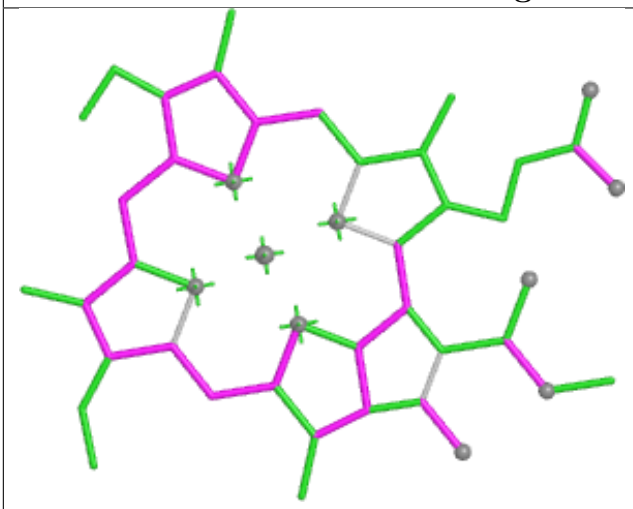


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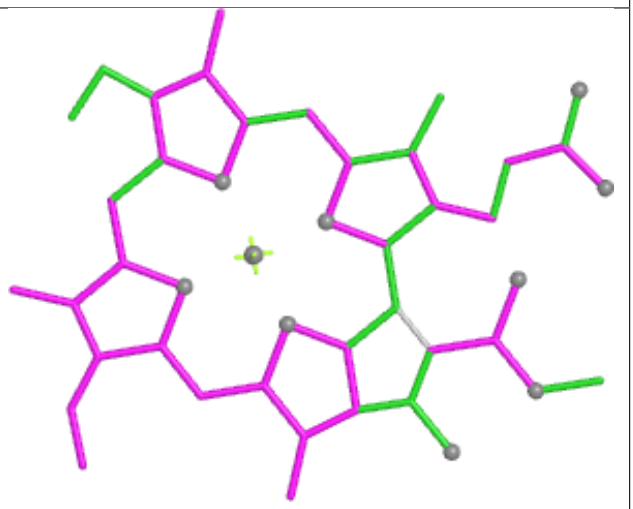


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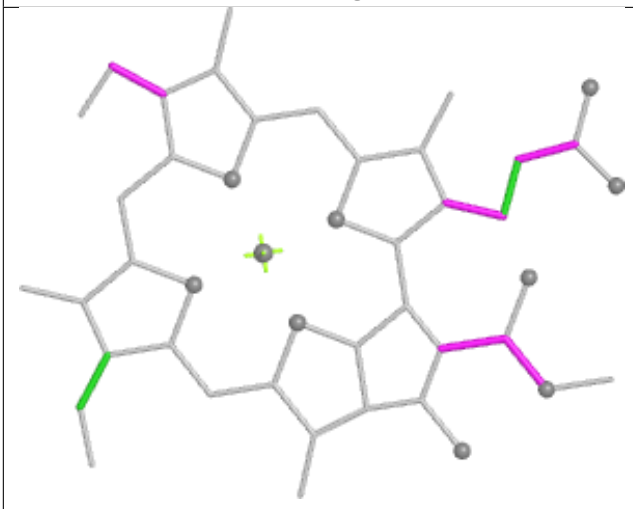
Ligand CLA K 4002



Bond lengths



Bond angles

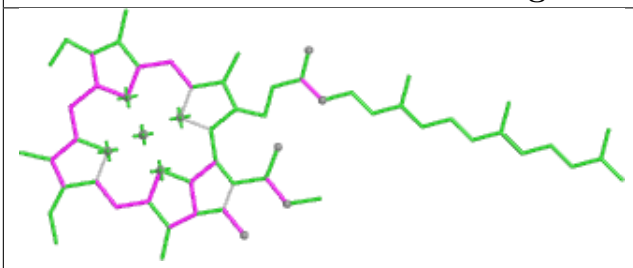


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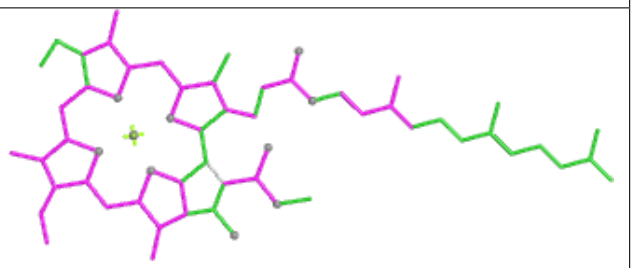


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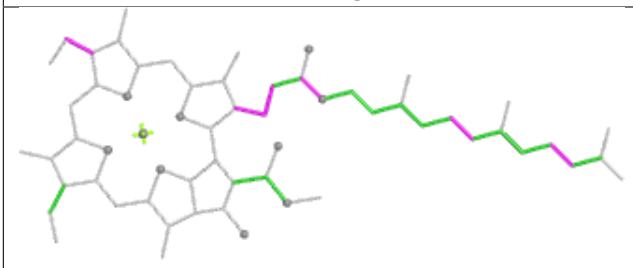
Ligand CLA 7 610



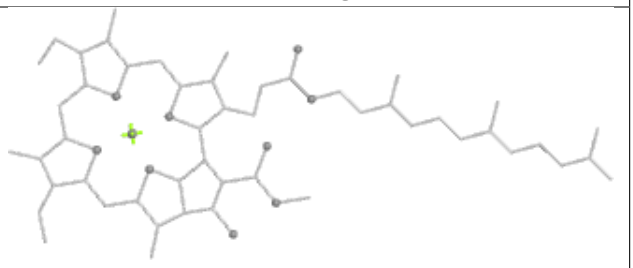
Bond lengths



Bond angles

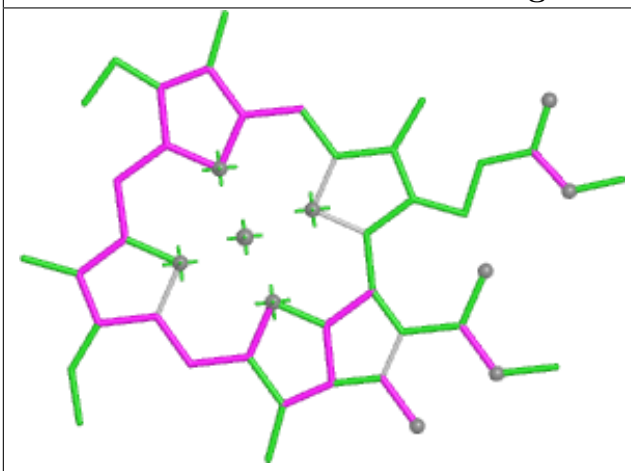


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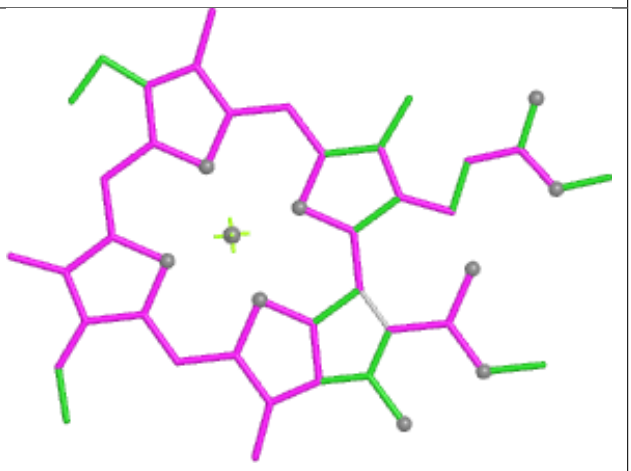


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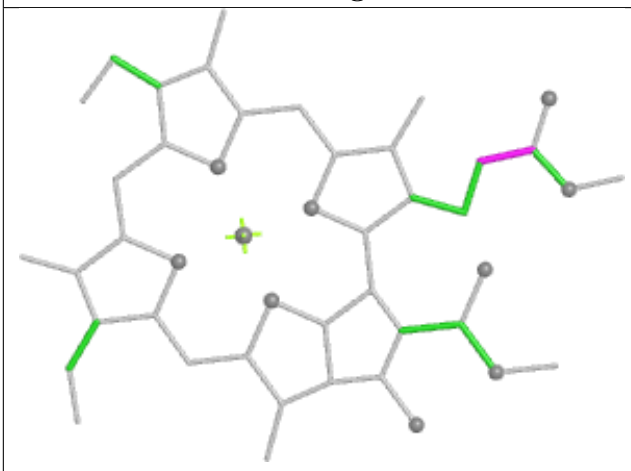
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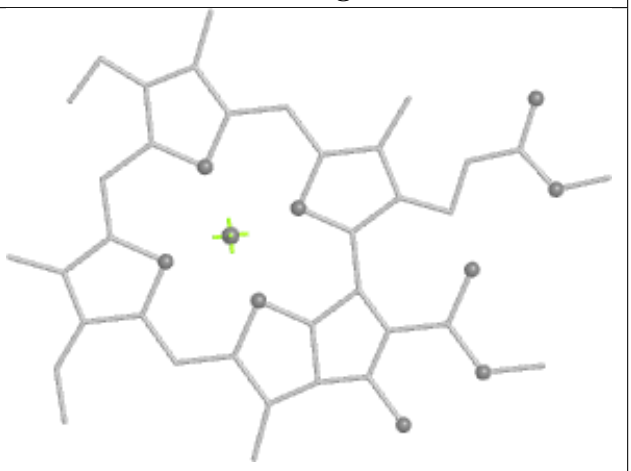
Bond lengths



Bond angles

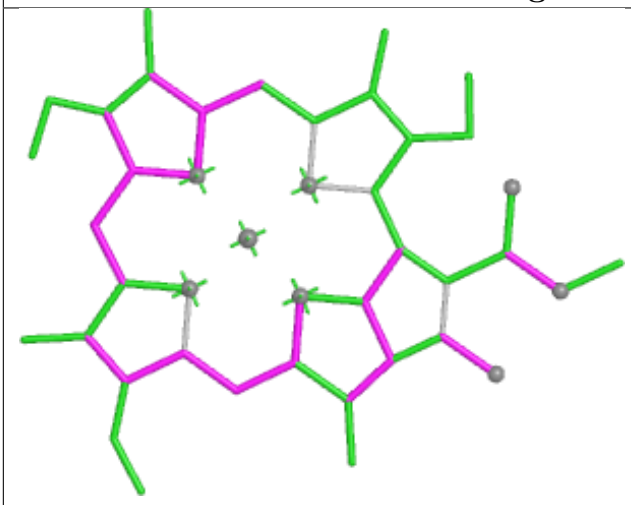


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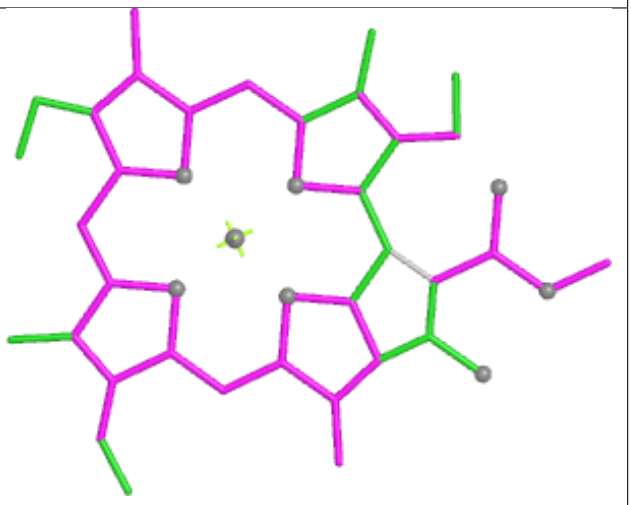


Rings

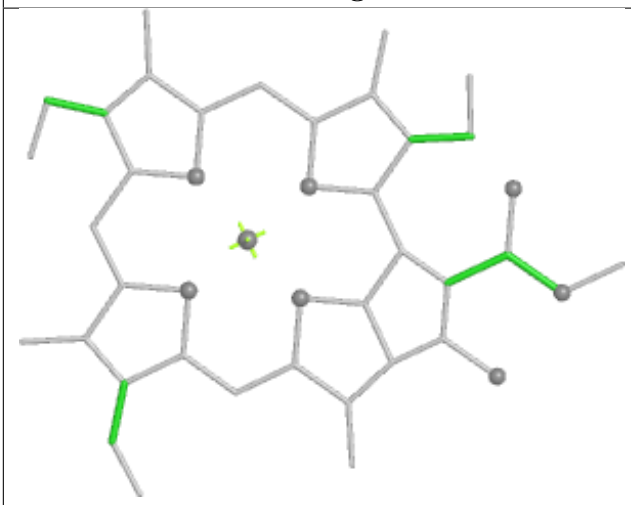
Ligand CLA 3 606



Bond lengths



Bond angles



Torsions

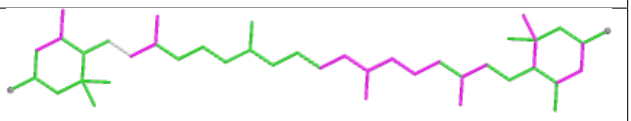


Rings

Ligand LUT 6 624



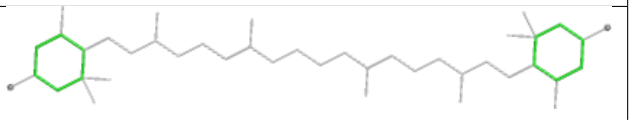
Bond lengths



Bond angles

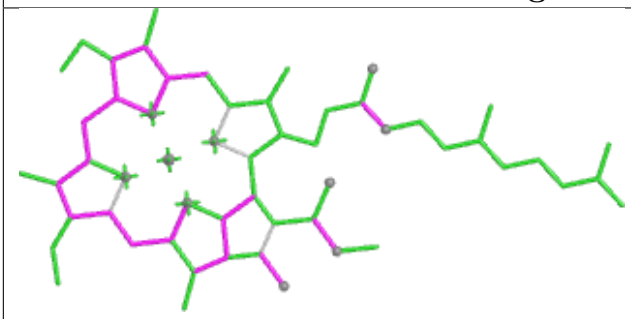


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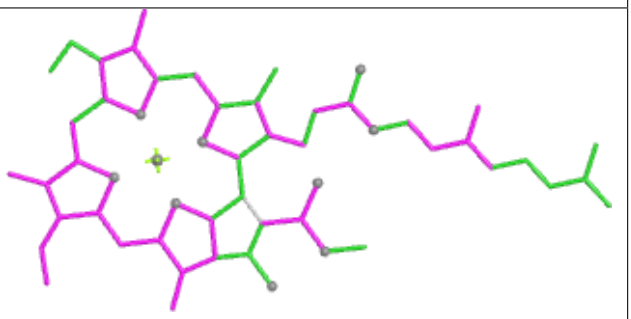


Rings

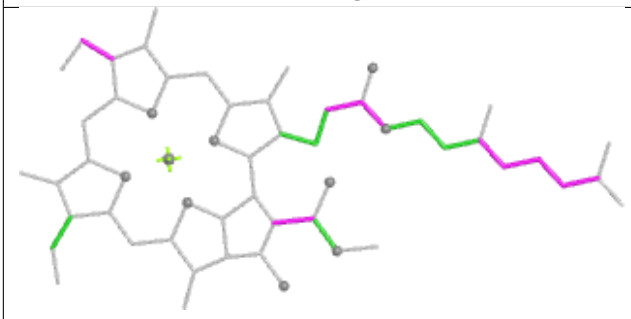
Ligand CLA 9 611



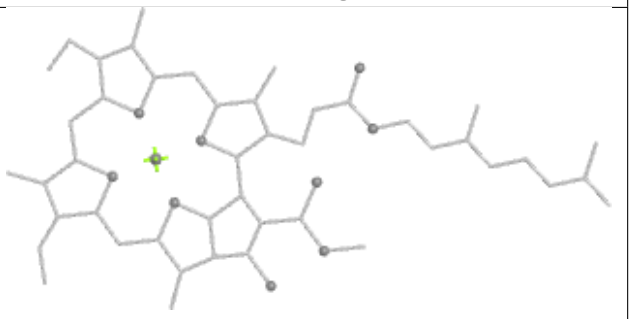
Bond lengths



Bond angles

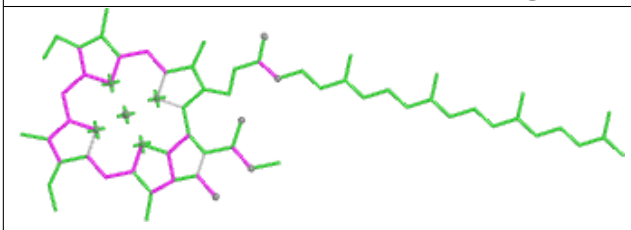


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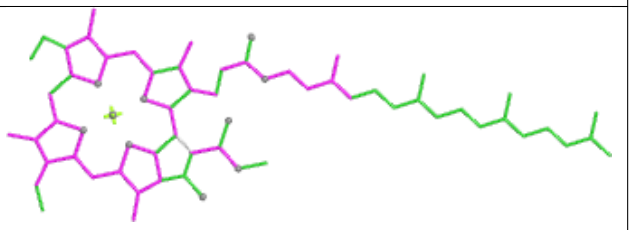


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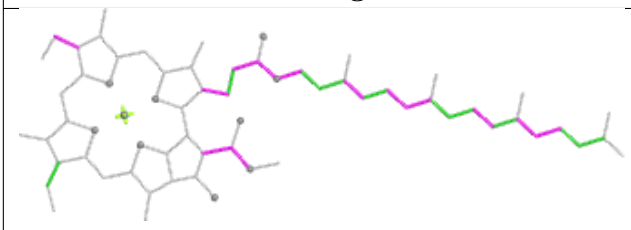
Ligand CLA A 829



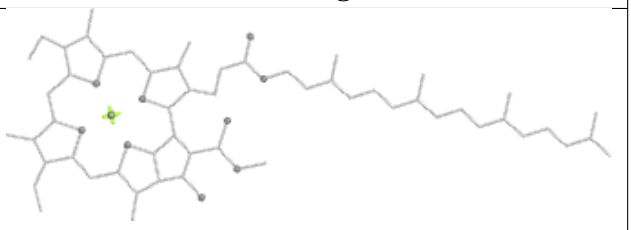
Bond lengths



Bond angles

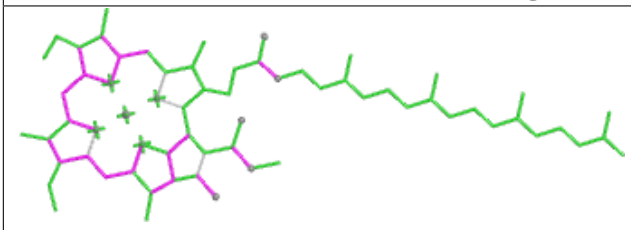


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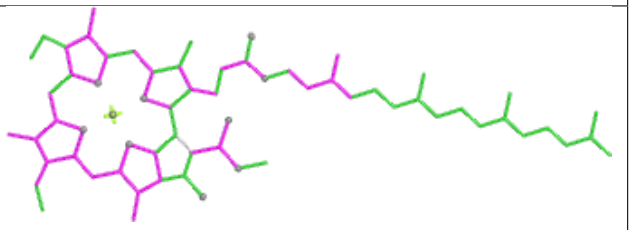


Rings

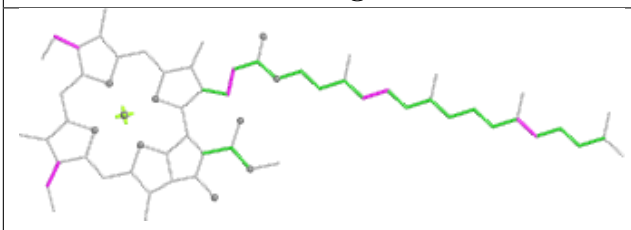
Ligand CLA B 840



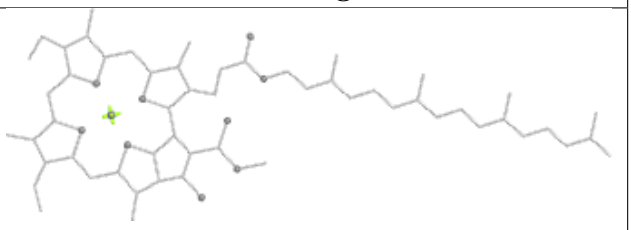
Bond lengths



Bond angles



Torsions



Rings

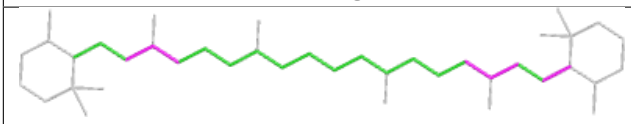
Ligand BCR B 845



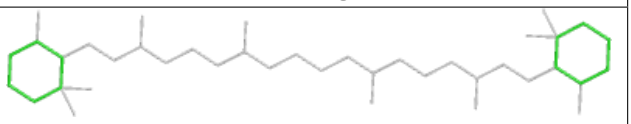
Bond lengths



Bond angles

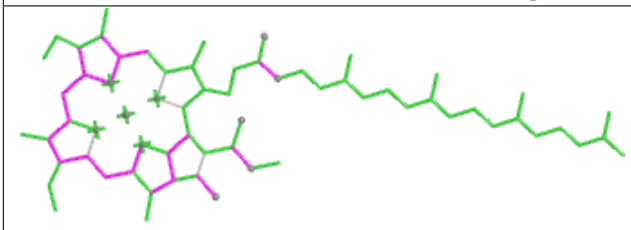


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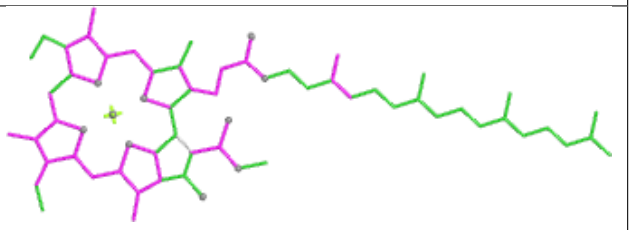


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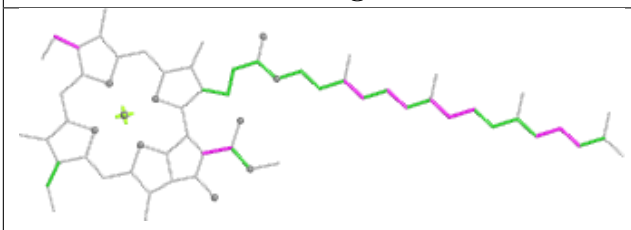
Ligand CLA B 837



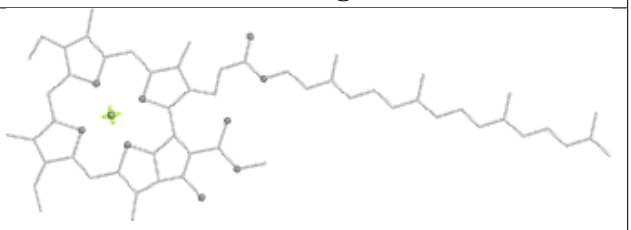
Bond lengths



Bond angles

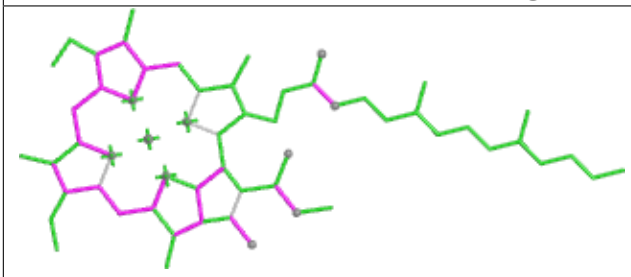


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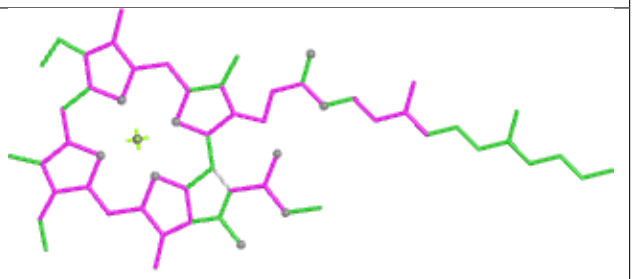


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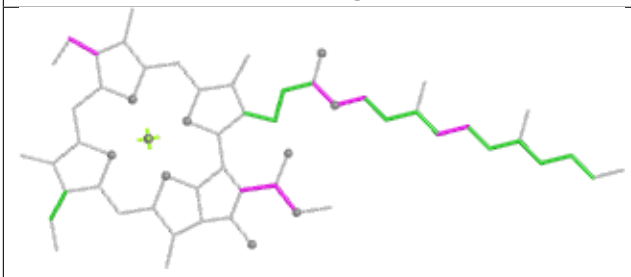
Ligand CLA B 833



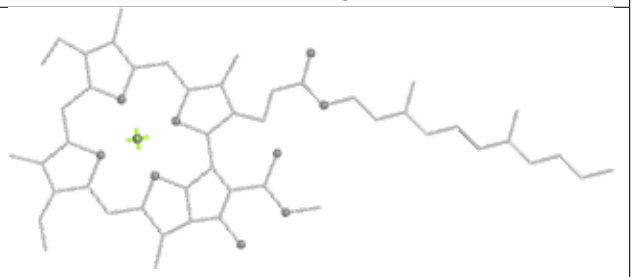
Bond lengths



Bond angles



Torsions

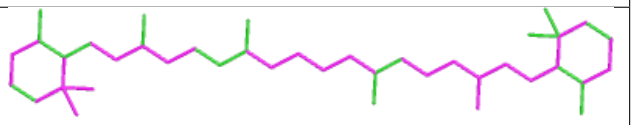


Rings

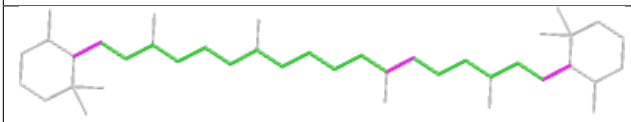
Ligand BCR 8 619



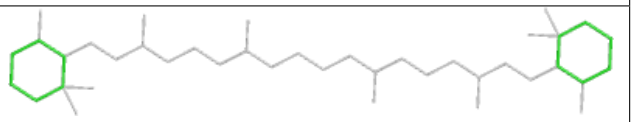
Bond lengths



Bond angles

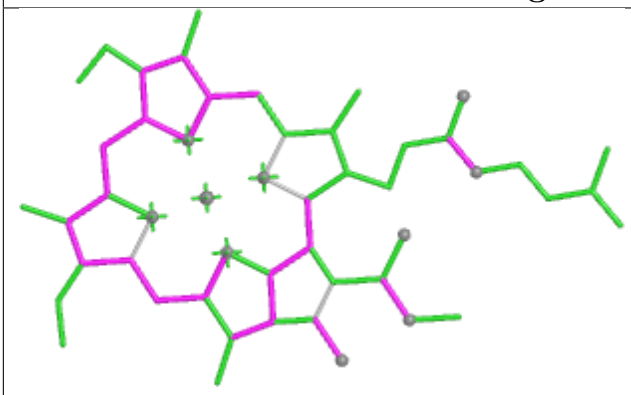


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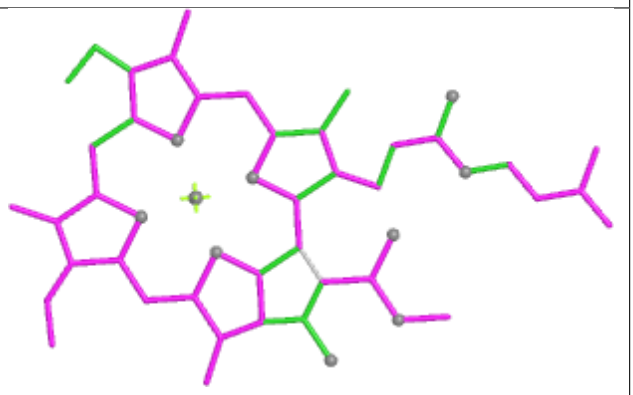


Rings

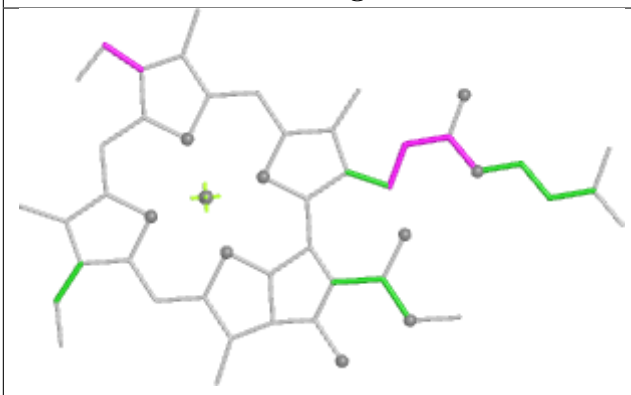
Ligand CLA 2 609



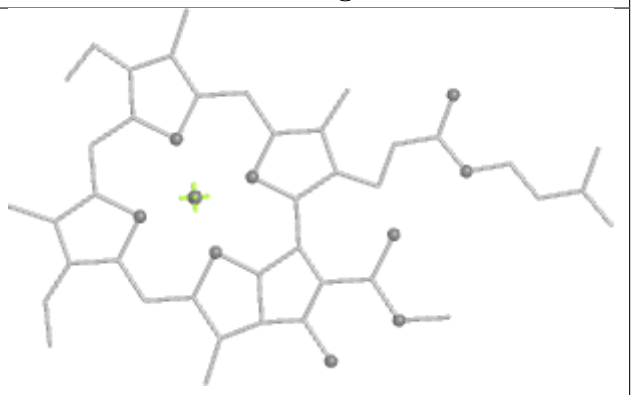
Bond lengths



Bond angles

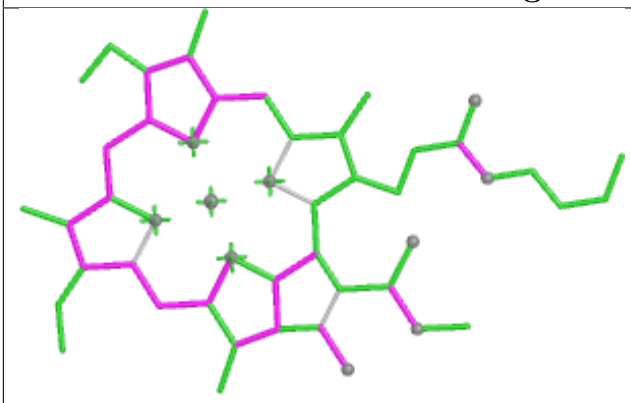


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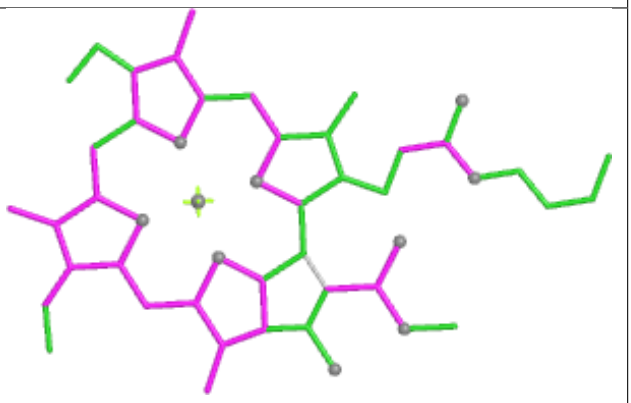


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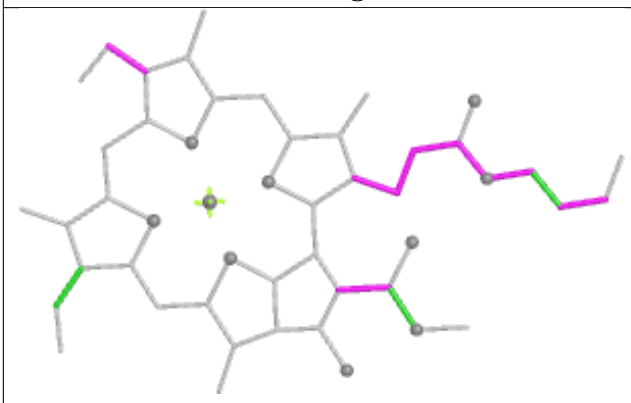
Ligand CLA A 823



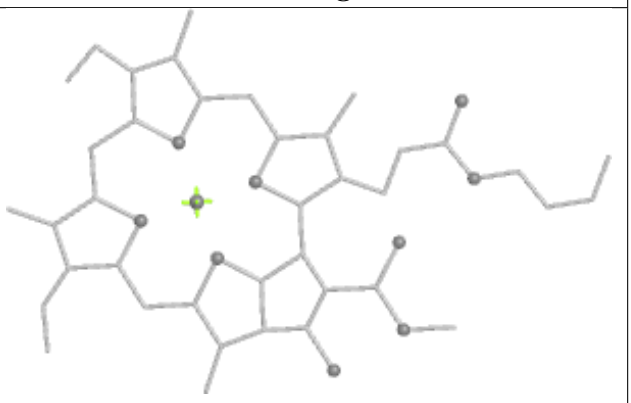
Bond lengths



Bond angles

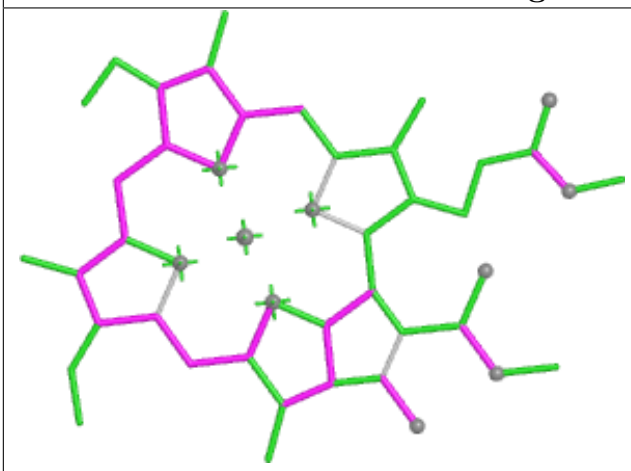


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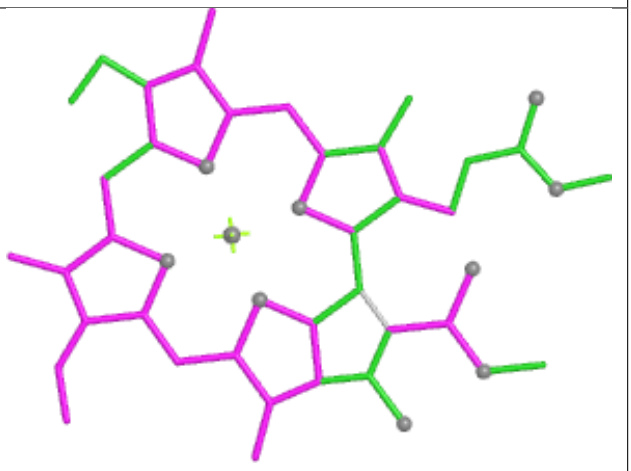


Rings

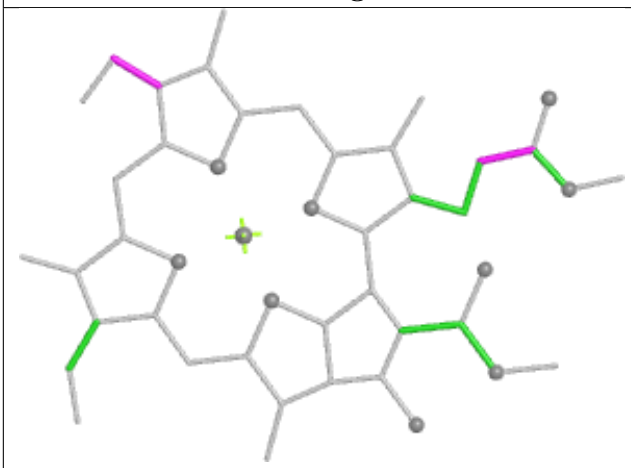
Ligand CLA 8 616



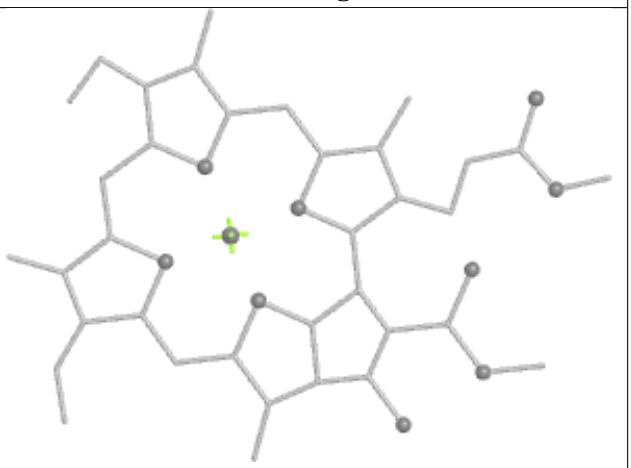
Bond lengths



Bond angles



Torsions

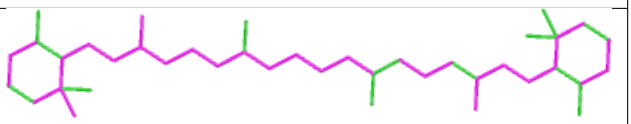


Rings

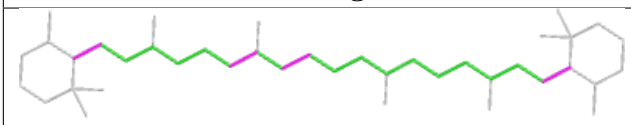
Ligand BCR 5 622



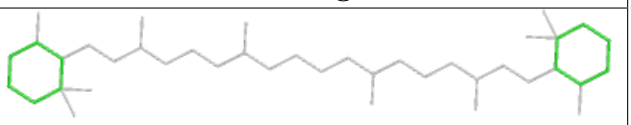
Bond lengths



Bond angles

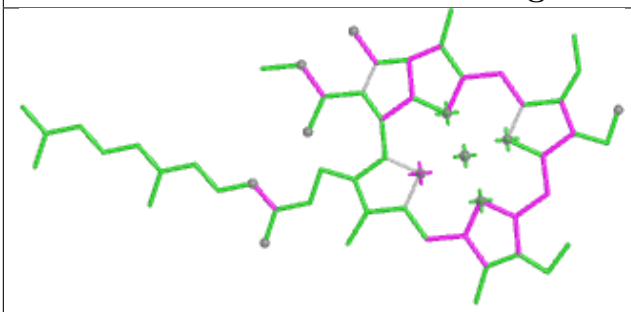


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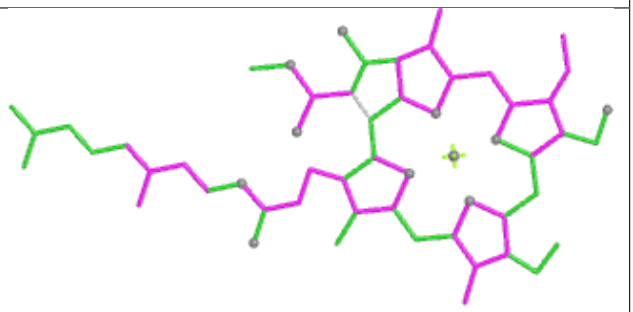


Rings

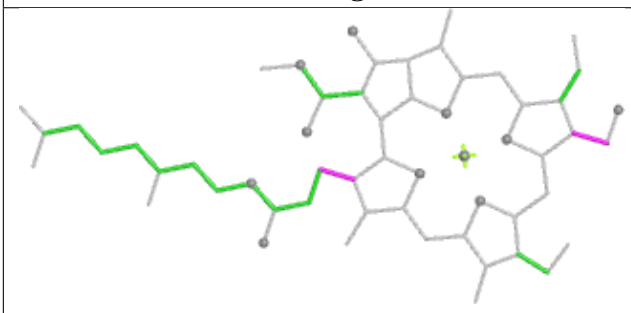
Ligand CHL 4 606



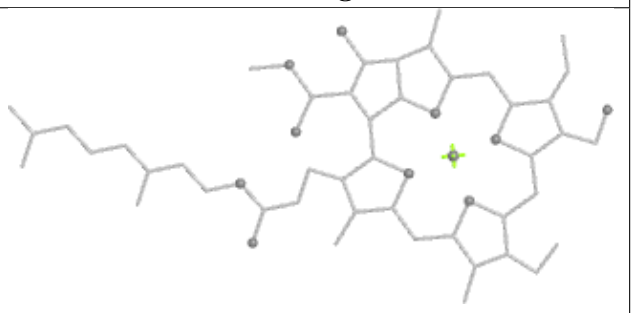
Bond lengths



Bond angles

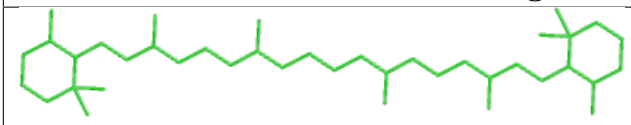


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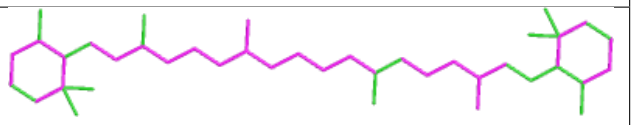


Rings

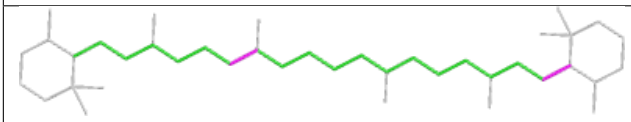
Ligand BCR 3 718



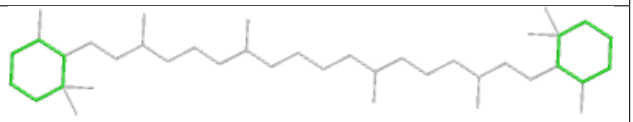
Bond lengths



Bond angles

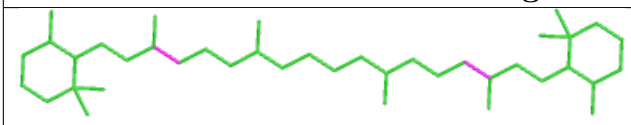


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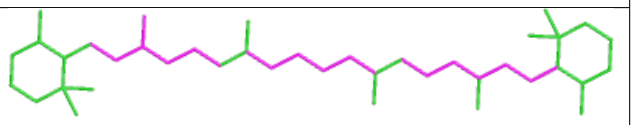


Rings

Ligand BCR A 851



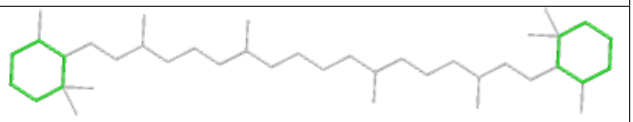
Bond lengths



Bond angles

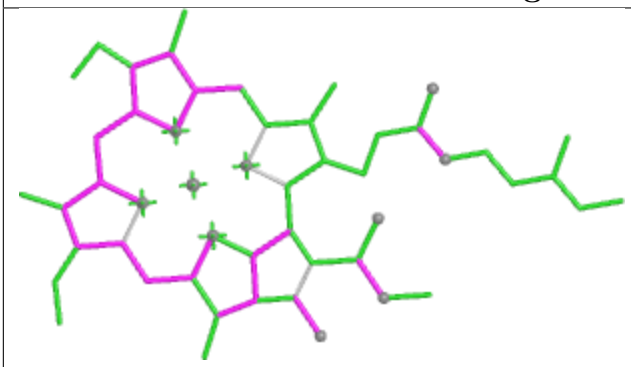


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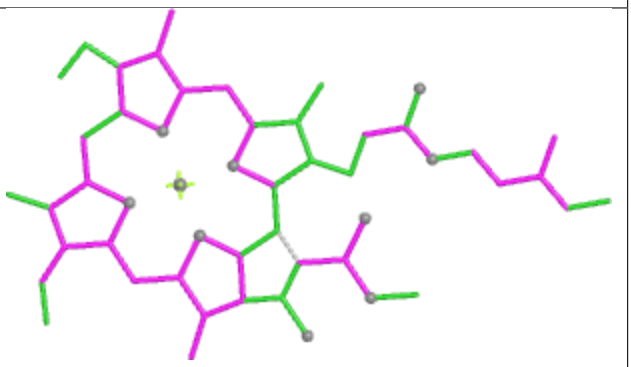


Rings

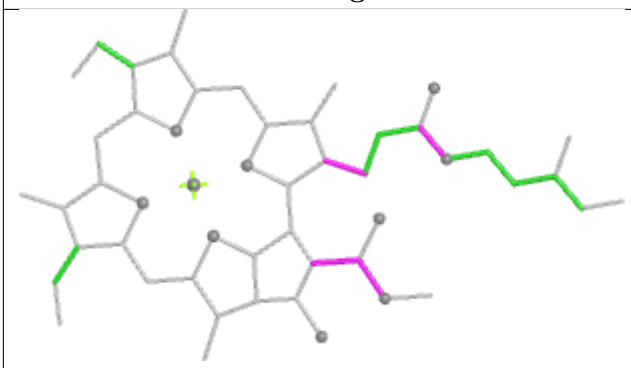
Ligand CLA A 824



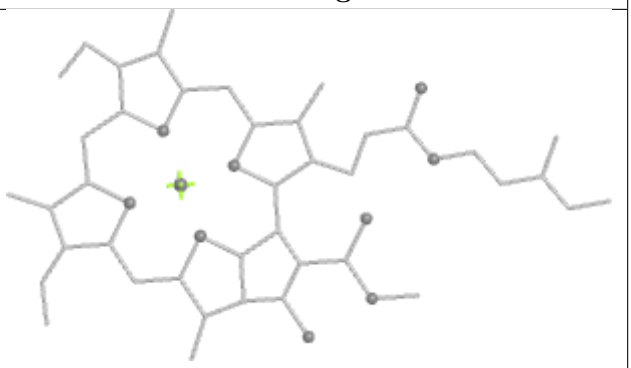
Bond lengths



Bond angles

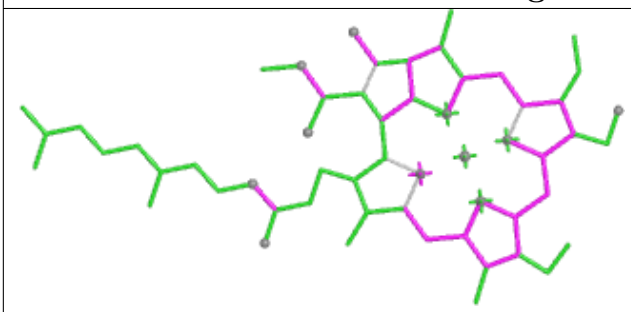


Torsions

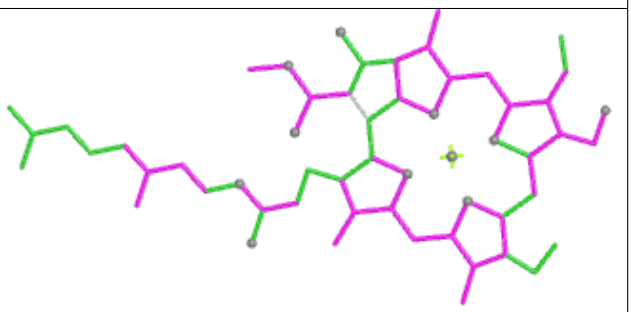


Rings

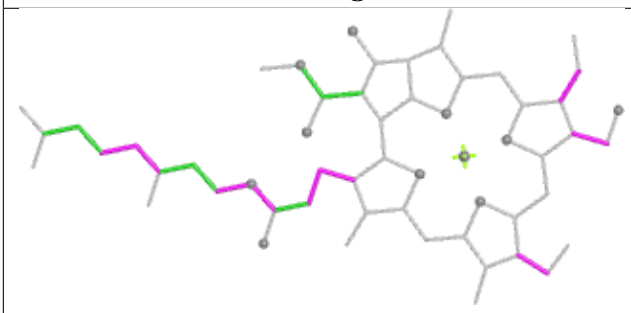
Ligand CHL 6 607



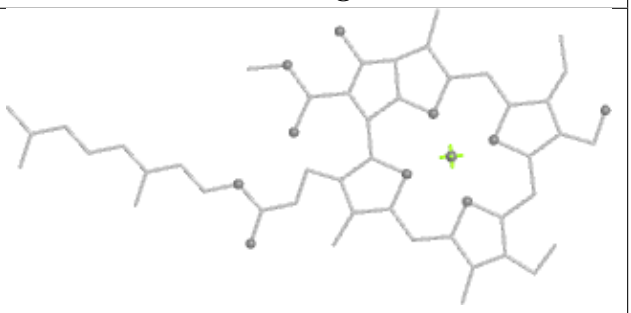
Bond lengths



Bond angles

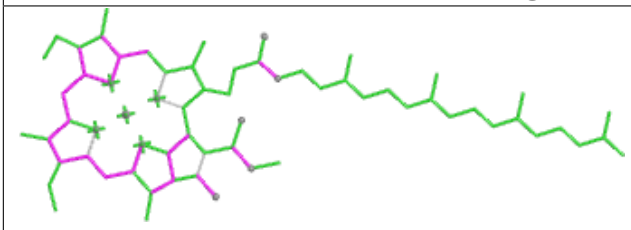


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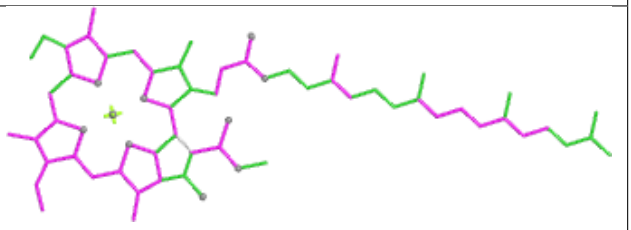


Rings

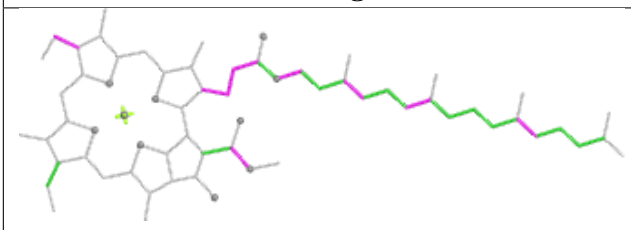
Ligand CLA A 810



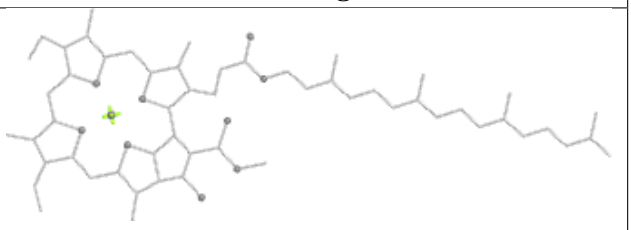
Bond lengths



Bond angles

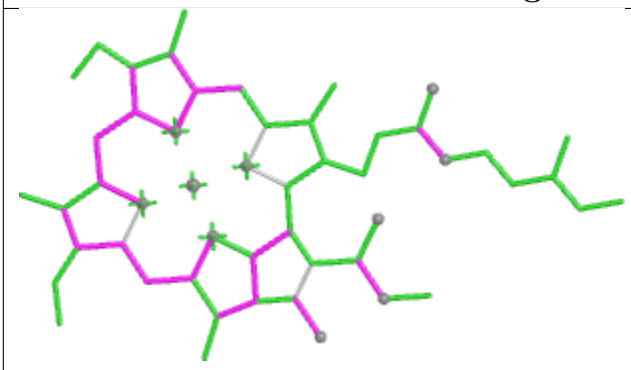


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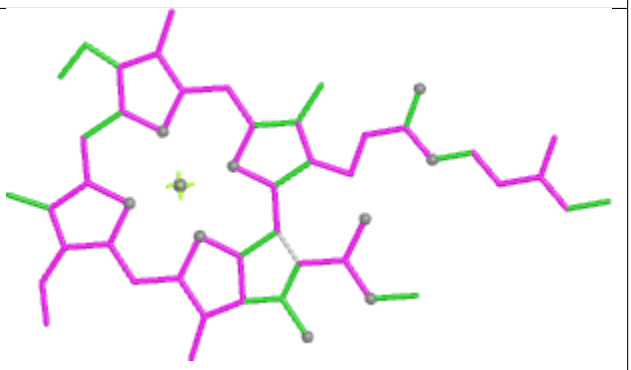


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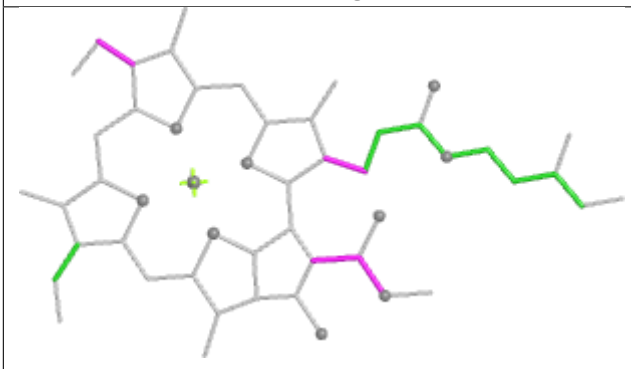
Ligand CLA A 838



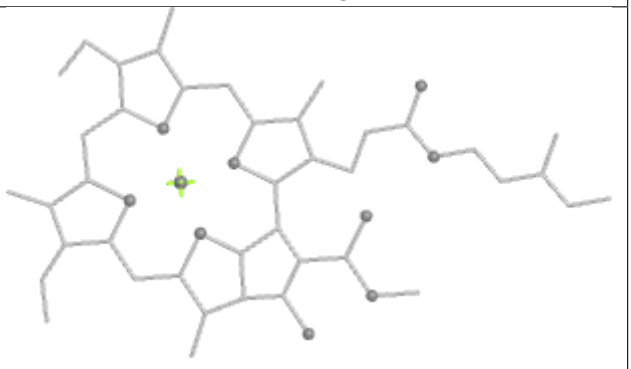
Bond lengths



Bond angles

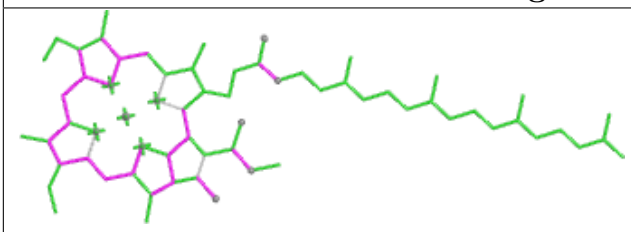


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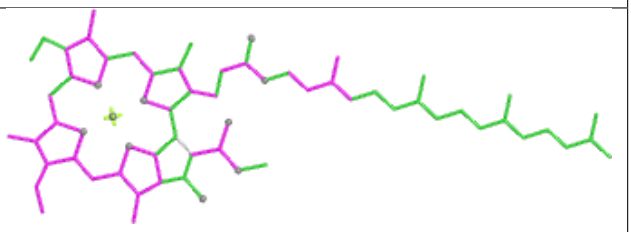


Rings

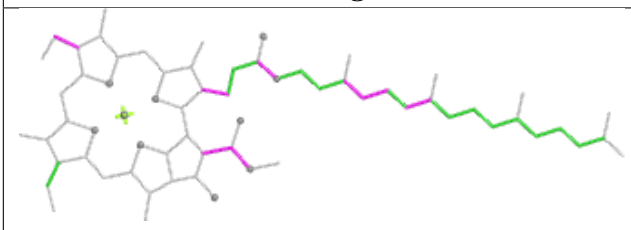
Ligand CLA 6 604



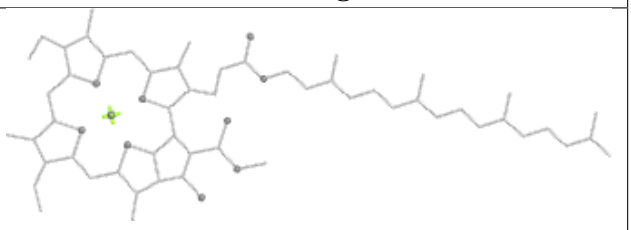
Bond lengths



Bond angles

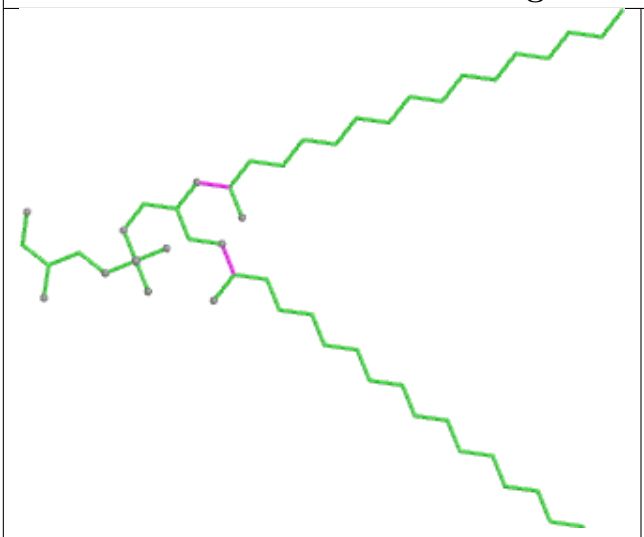


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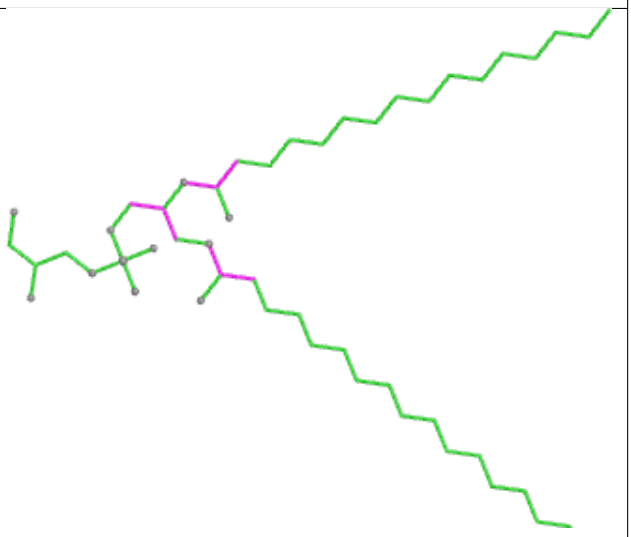


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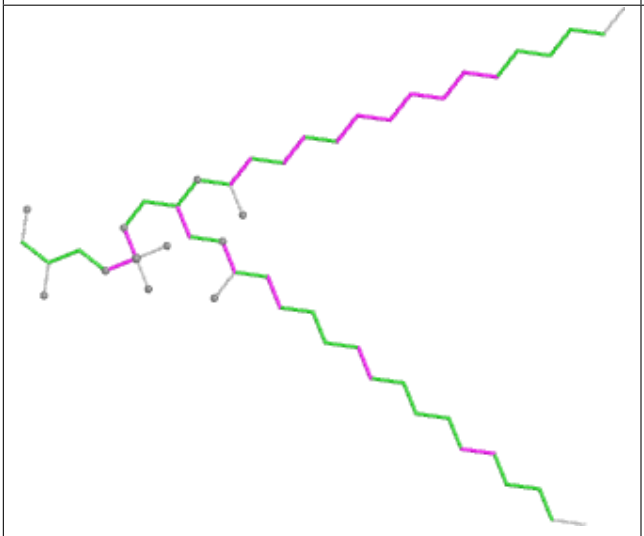
Ligand LHG 4 622



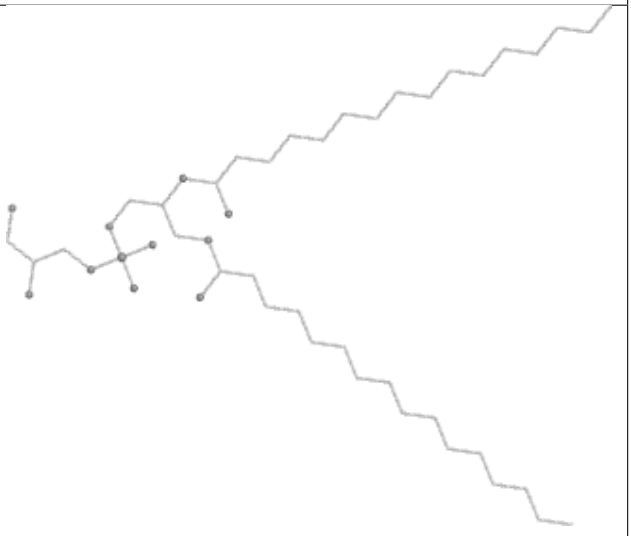
Bond lengths



Bond angles

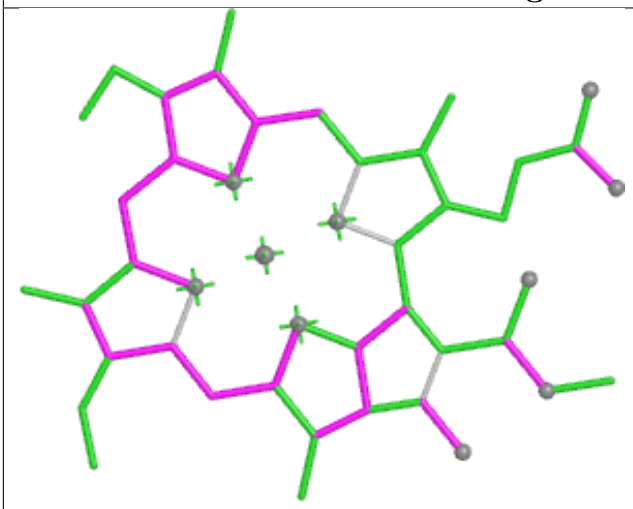


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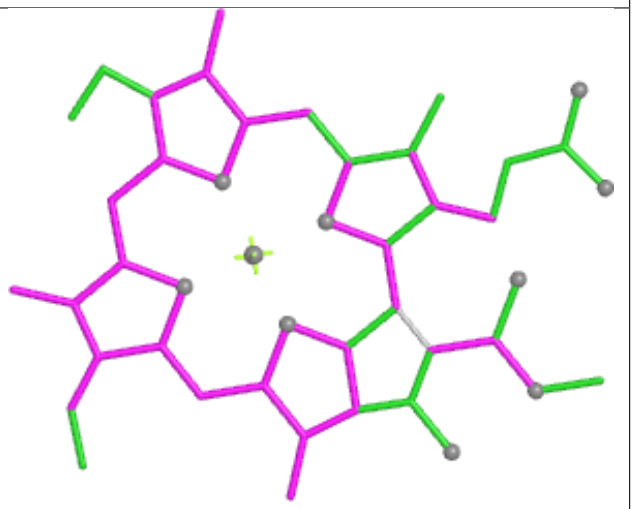


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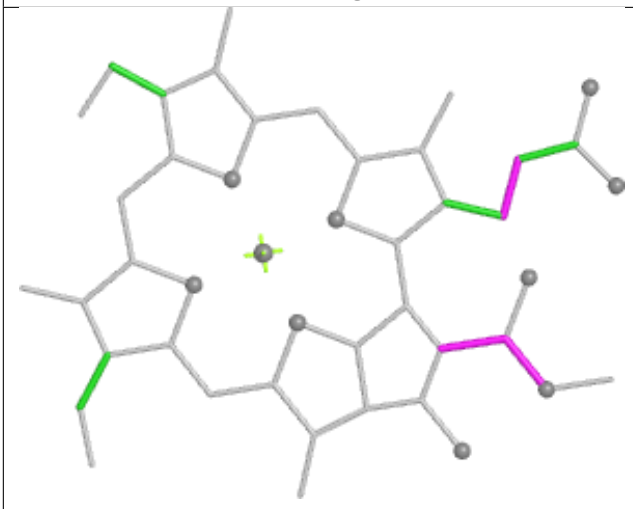
Ligand CLA F 303



Bond lengths



Bond angles

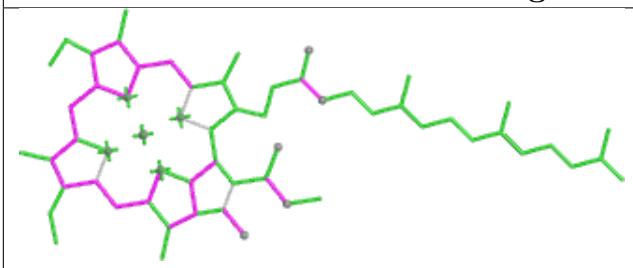


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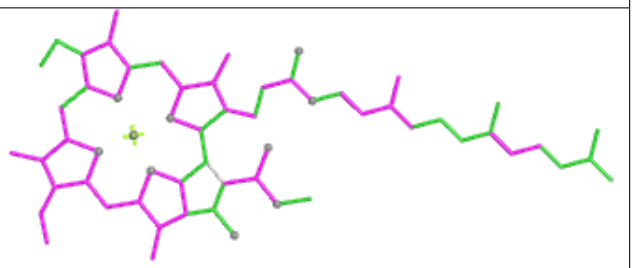


Rings

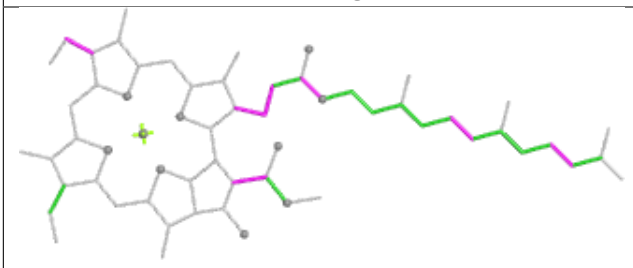
Ligand CLA 5 610



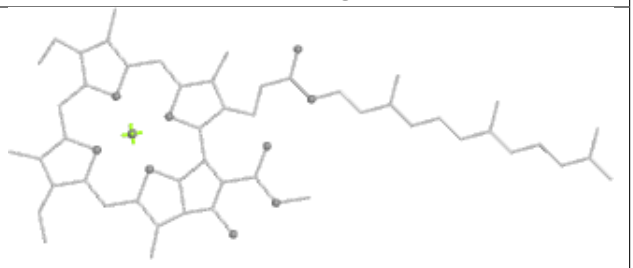
Bond lengths



Bond angles

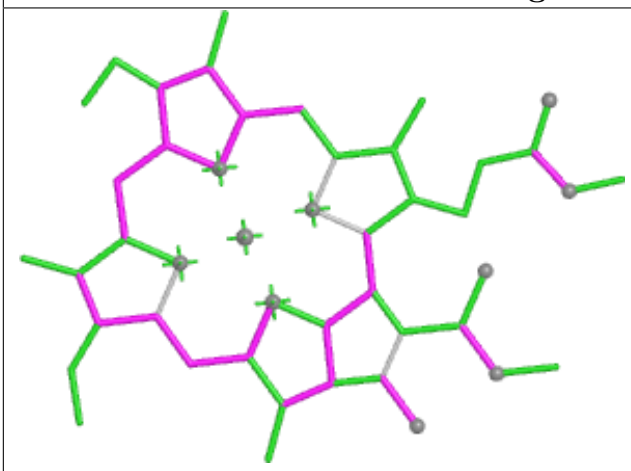


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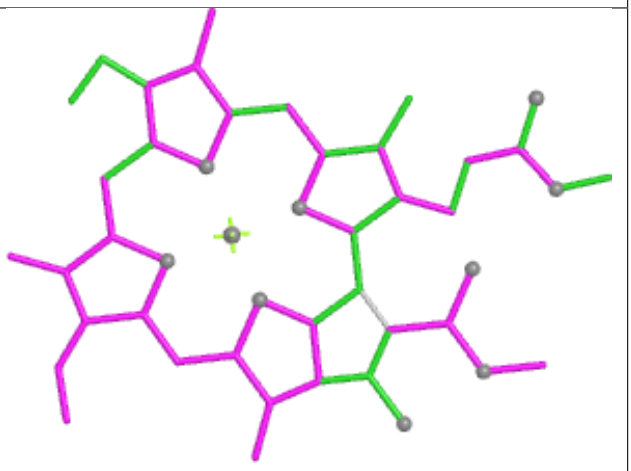


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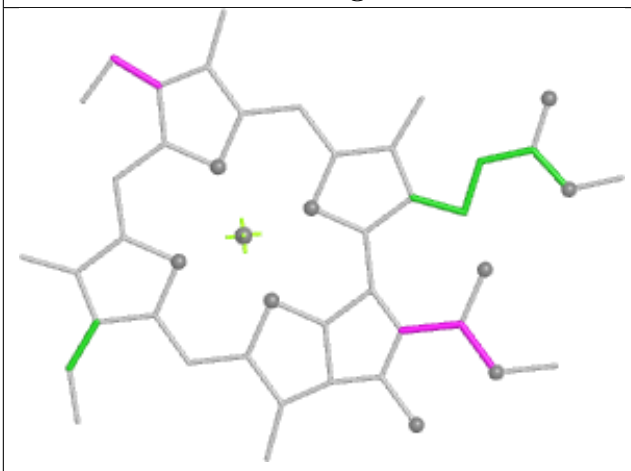
Ligand CLA 8 611



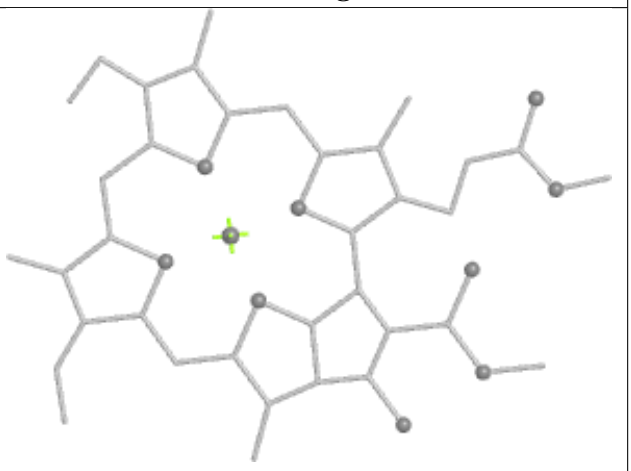
Bond lengths



Bond angles

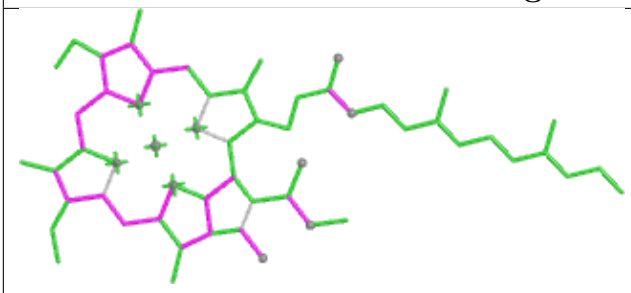


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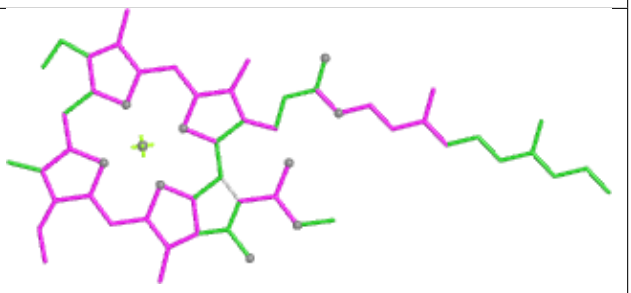


Rings

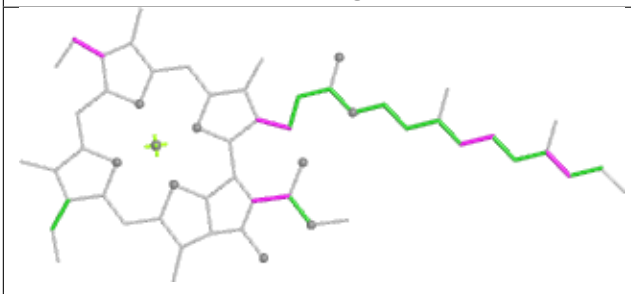
Ligand CLA B 815



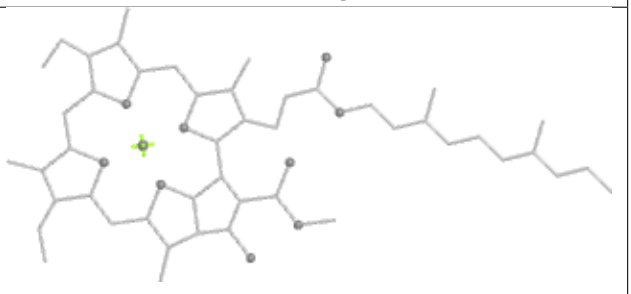
Bond lengths



Bond angles

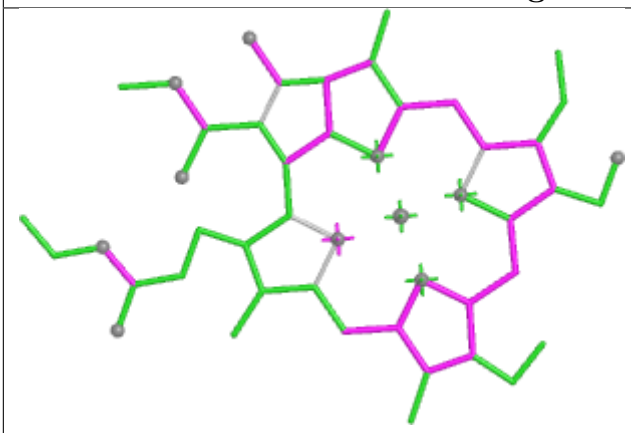


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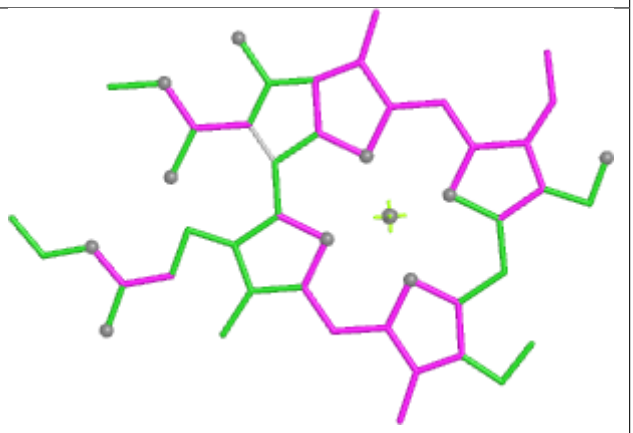


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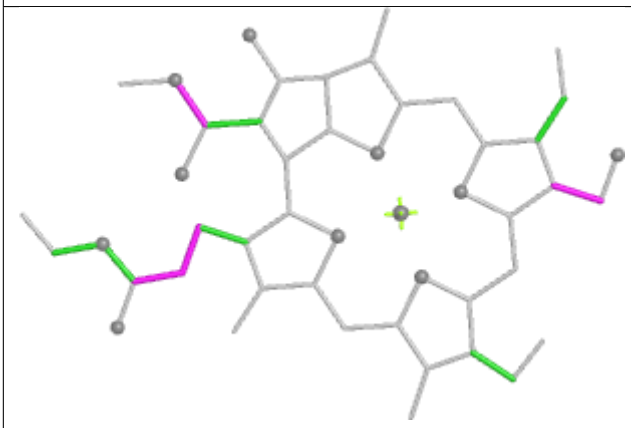
Ligand CHL 1 607



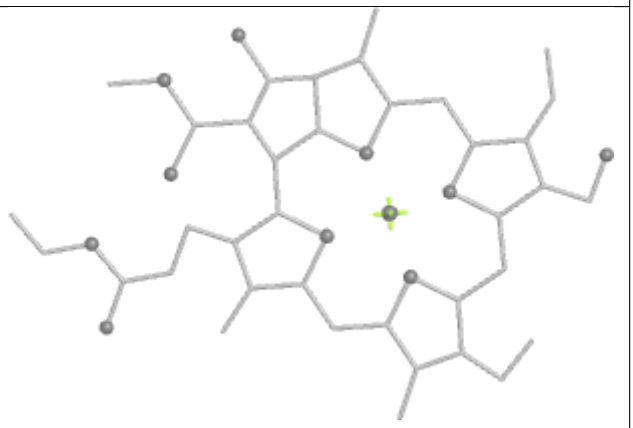
Bond lengths



Bond angles

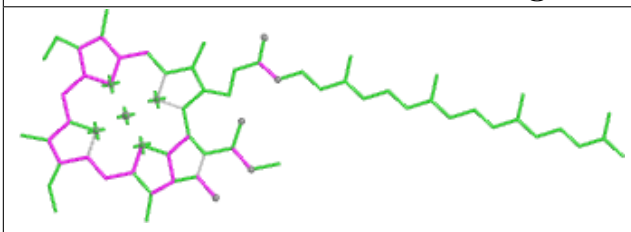


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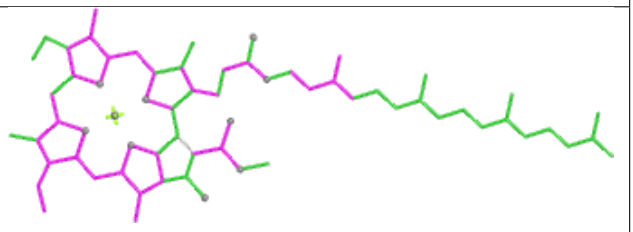


Rings

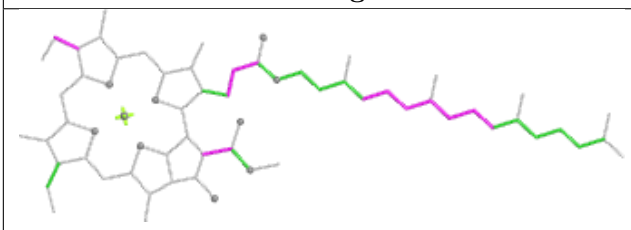
Ligand CLA 6 601



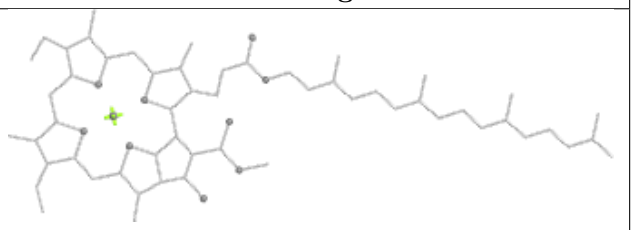
Bond lengths



Bond angles

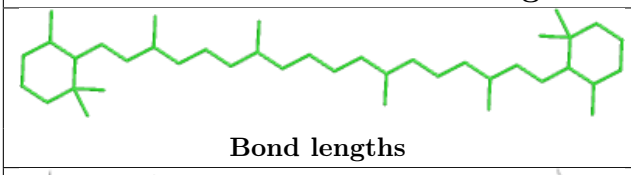


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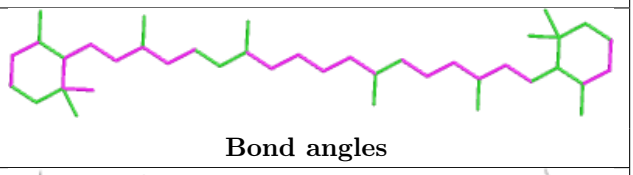


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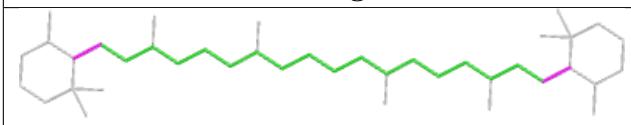
Ligand BCR A 850



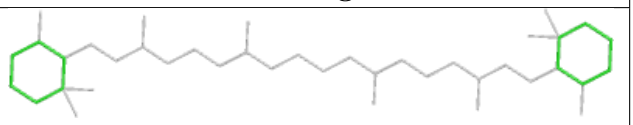
Bond lengths



Bond angles

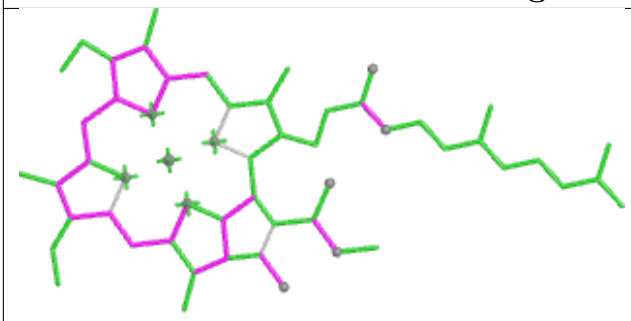


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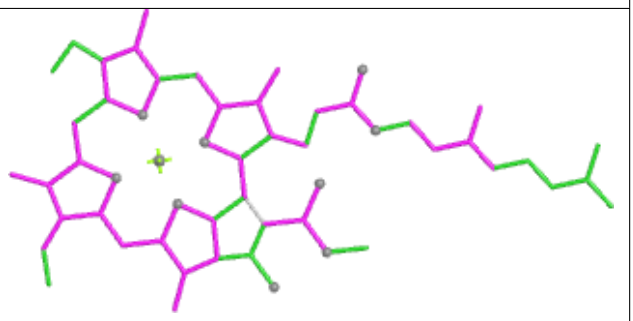


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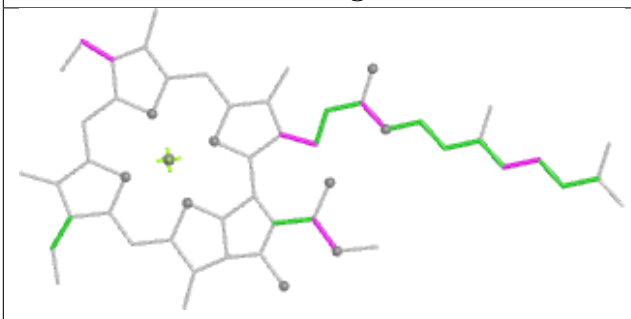
Ligand CLA 8 614



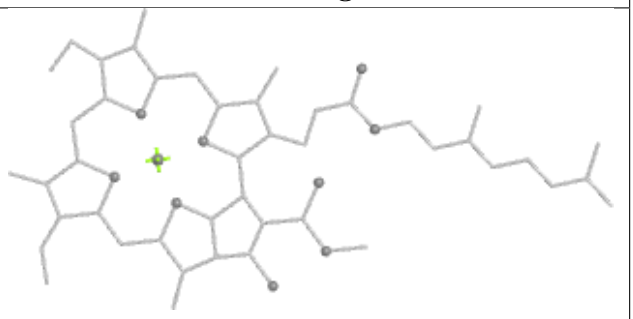
Bond lengths



Bond angles

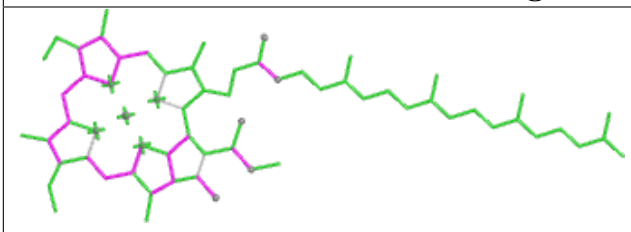


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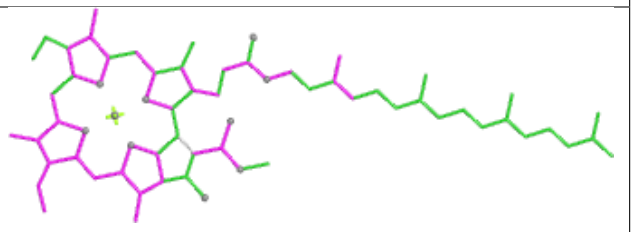


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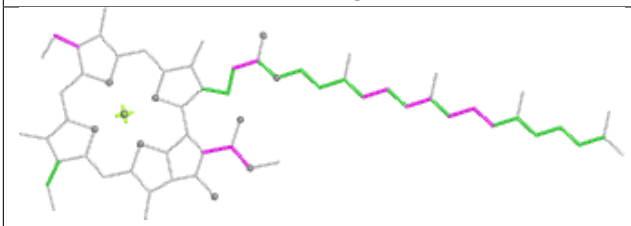
Ligand CLA Z 613



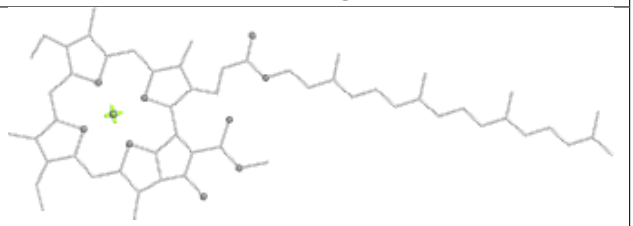
Bond lengths



Bond angles

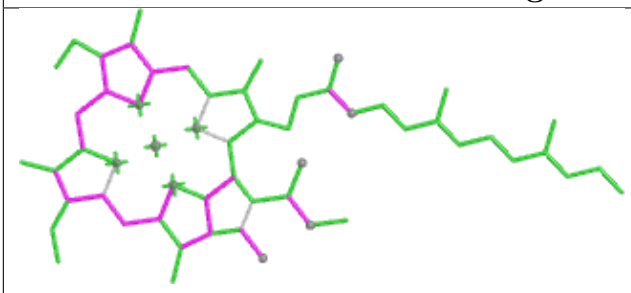


Torsions

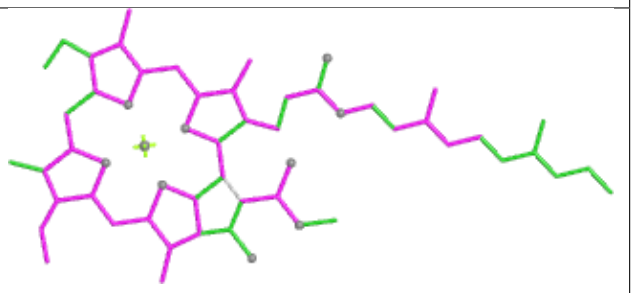


Rings

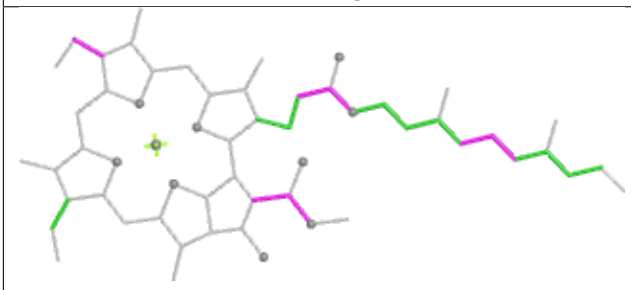
Ligand CLA Z 603



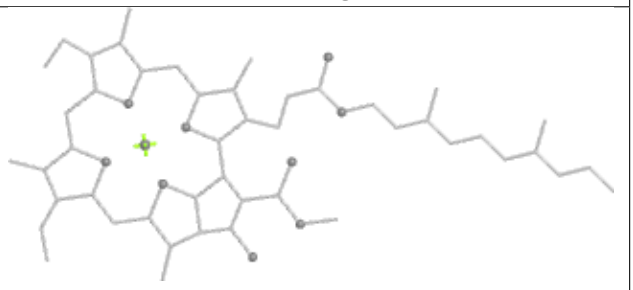
Bond lengths



Bond angles

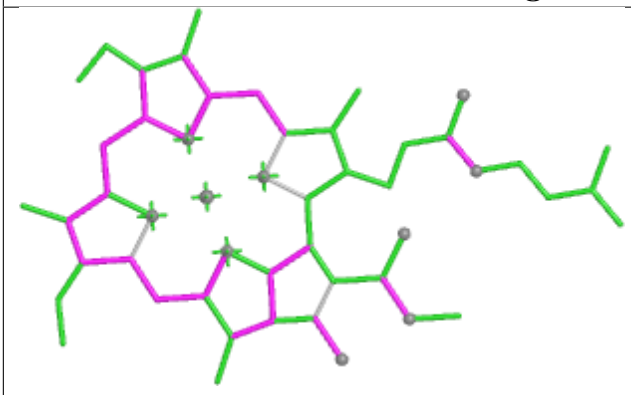


Torsions

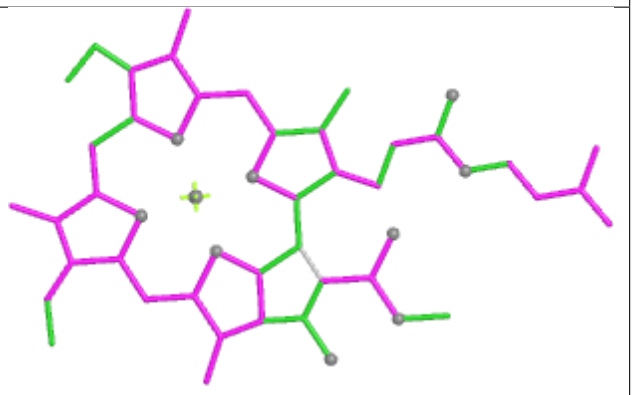


Rings

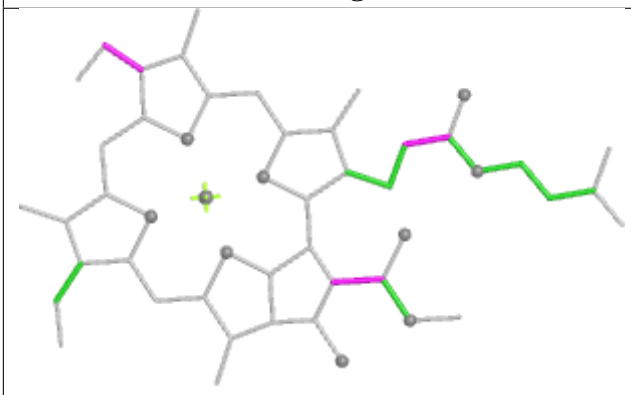
Ligand CLA B 830



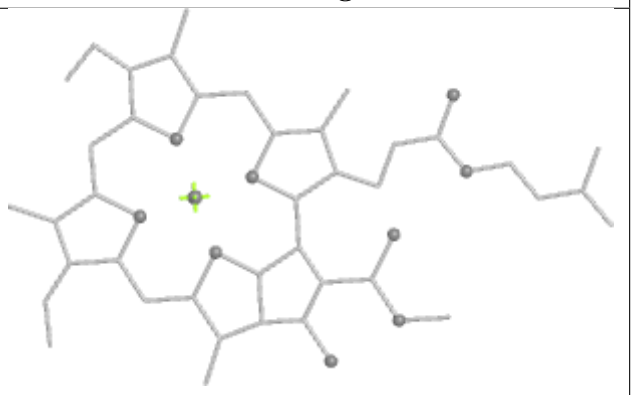
Bond lengths



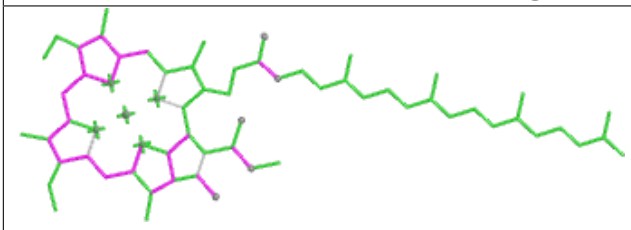
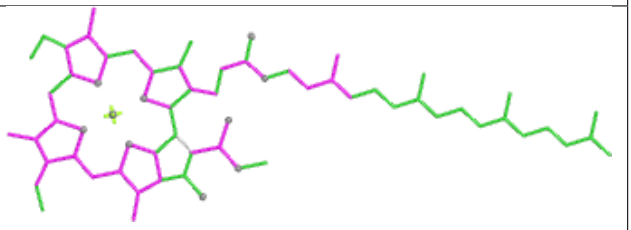
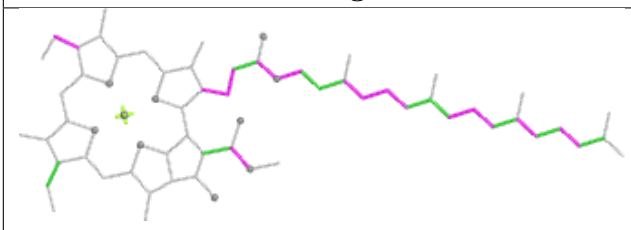
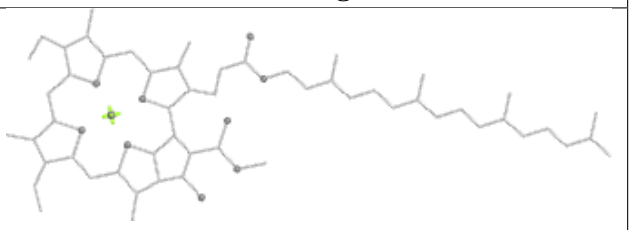
Bond angles

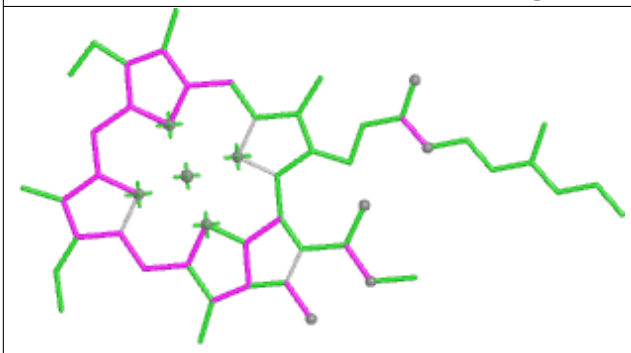
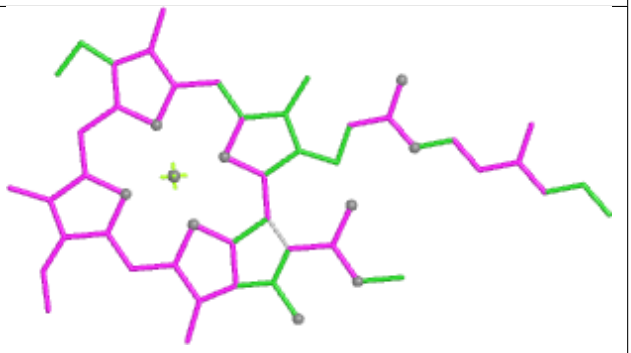
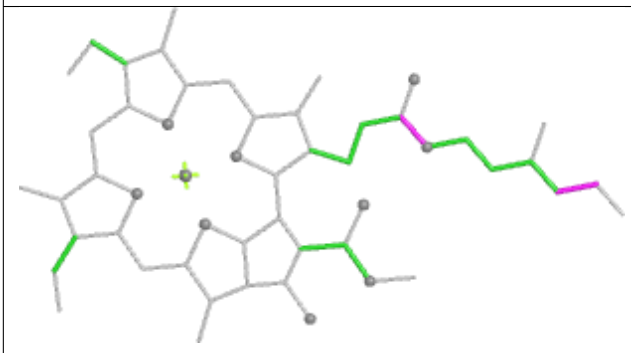
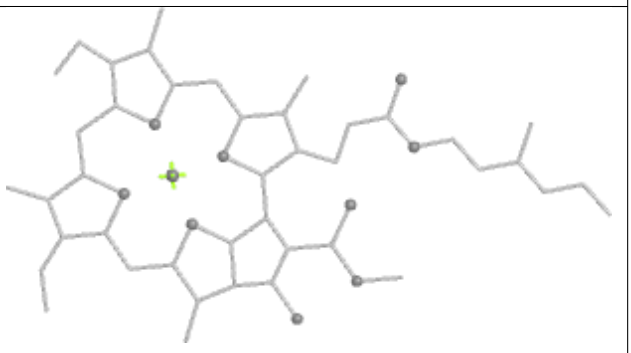


Torsions

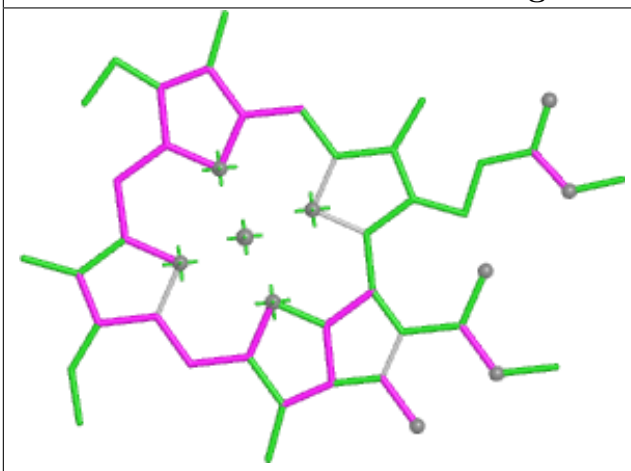


Rings

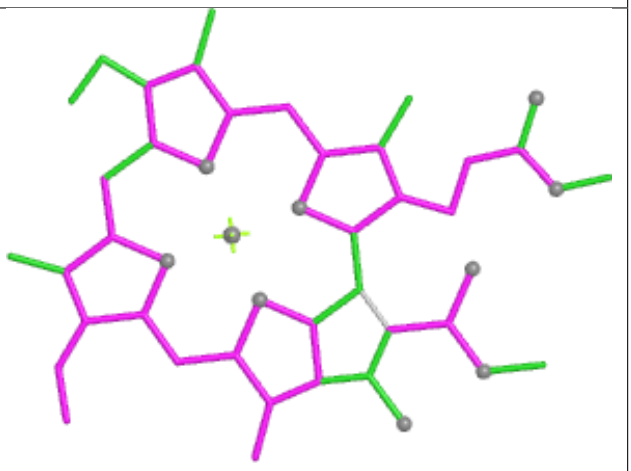
Ligand CLA Z 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

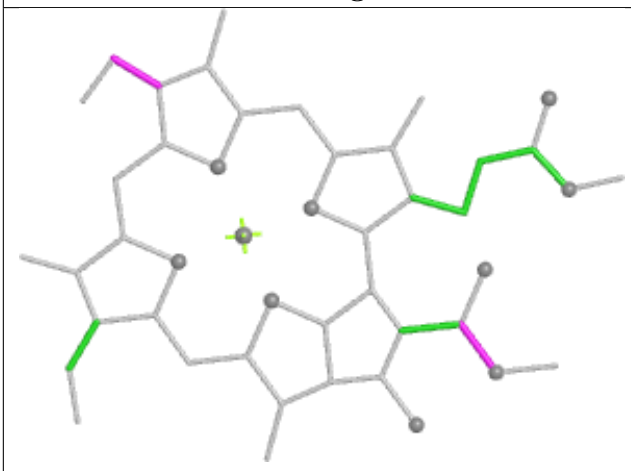
Ligand CLA 6 616



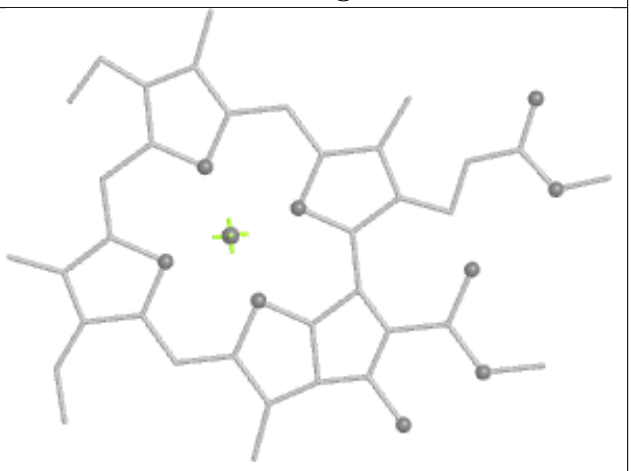
Bond lengths



Bond angles

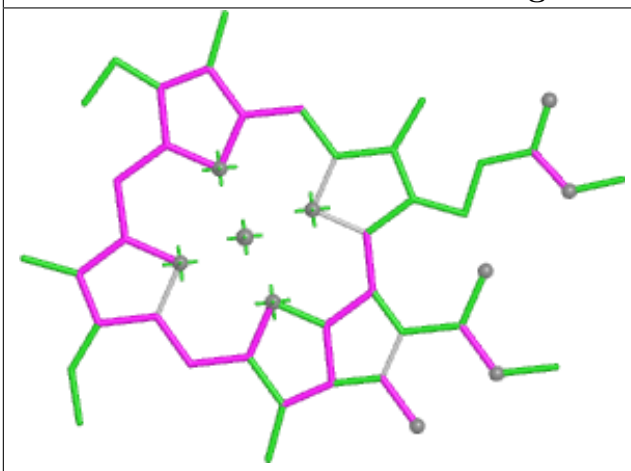


Torsions

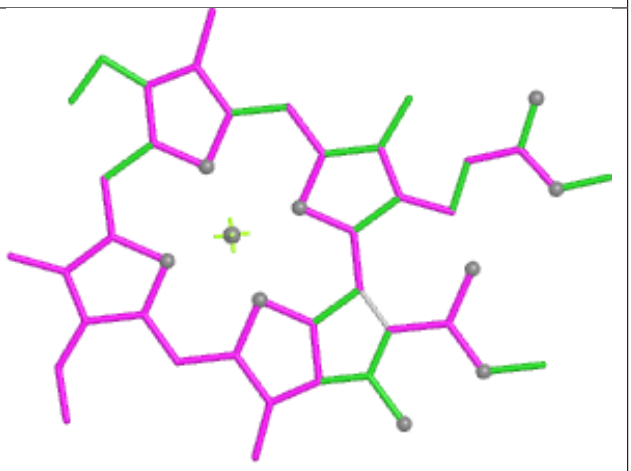


Rings

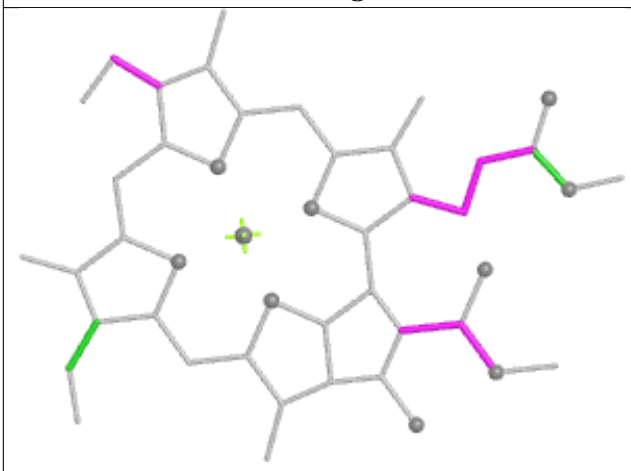
Ligand CLA 5 616



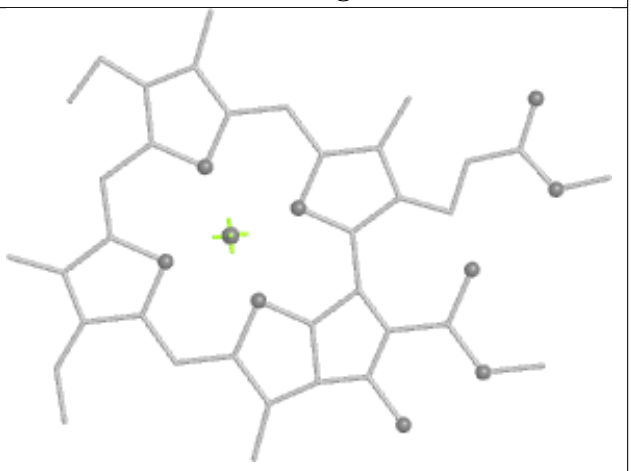
Bond lengths



Bond angles

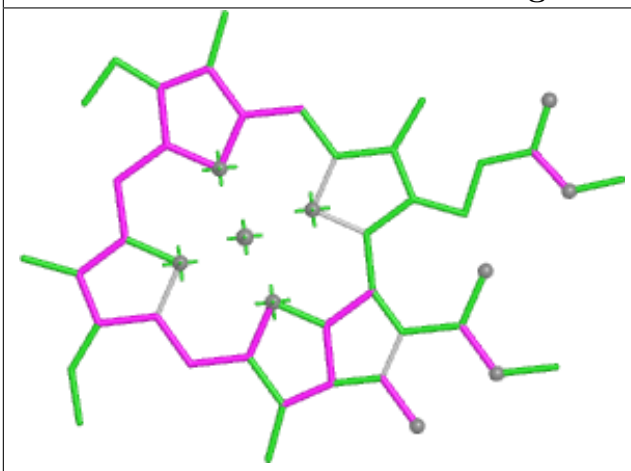


Torsions

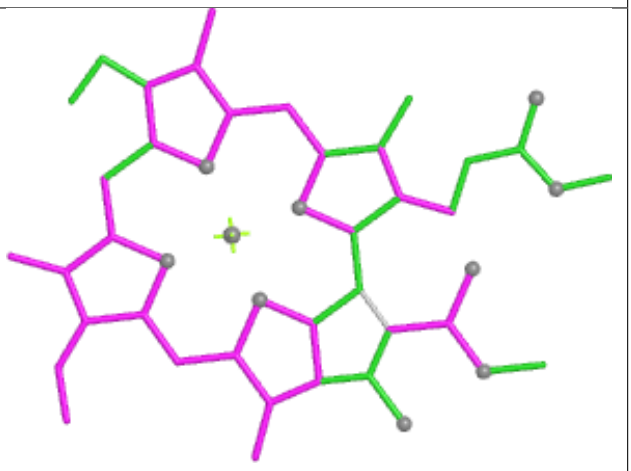


Rings

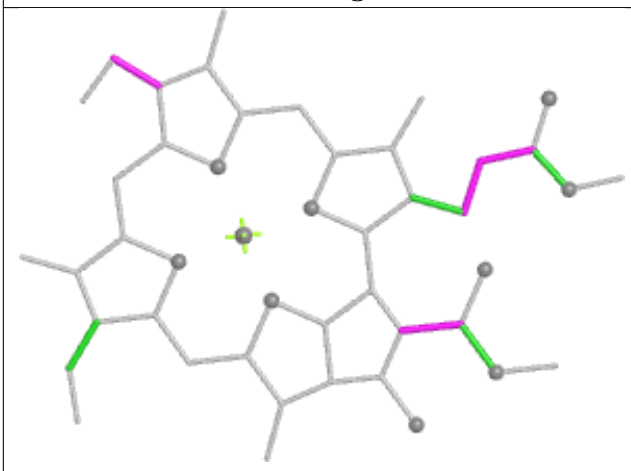
Ligand CLA 9 601



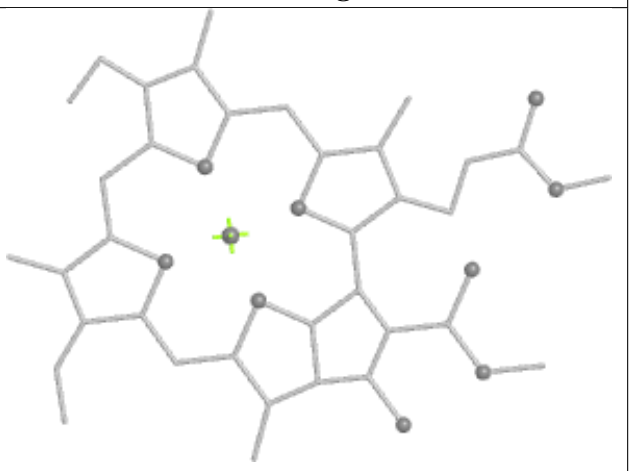
Bond lengths



Bond angles



Torsions



Rings

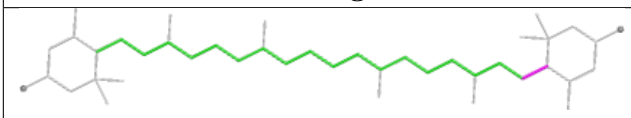
Ligand LUT 1 617



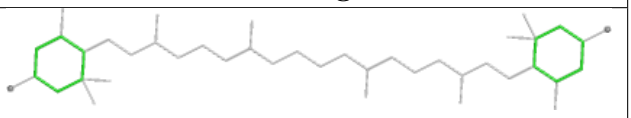
Bond lengths



Bond angles

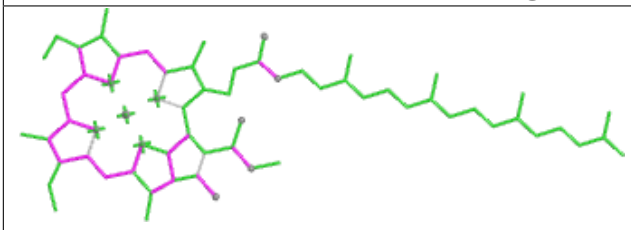


Torsions

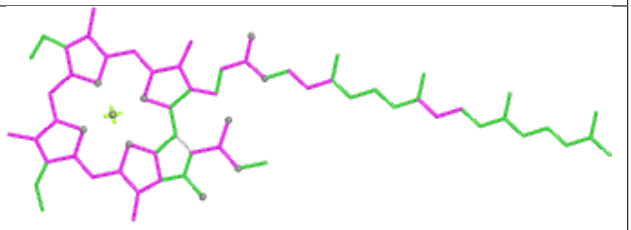


Rings

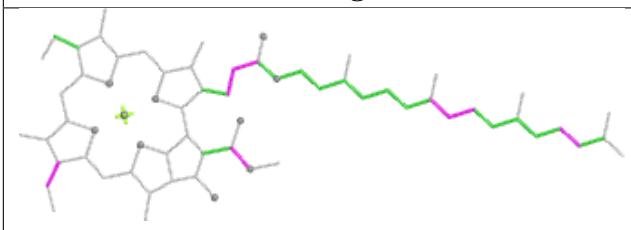
Ligand CLA A 841



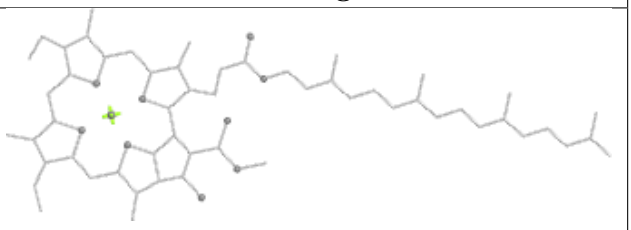
Bond lengths



Bond angles

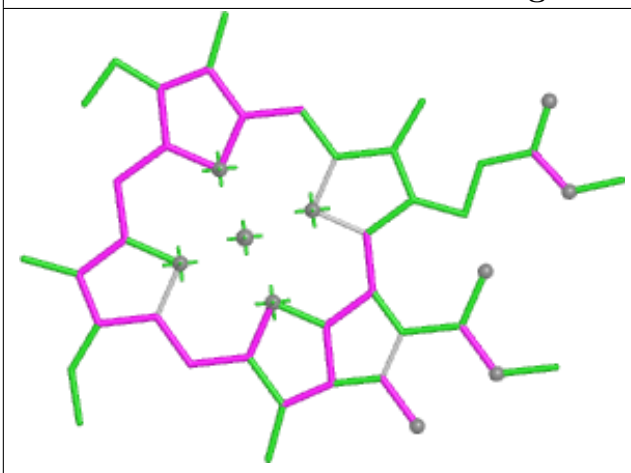


Torsions

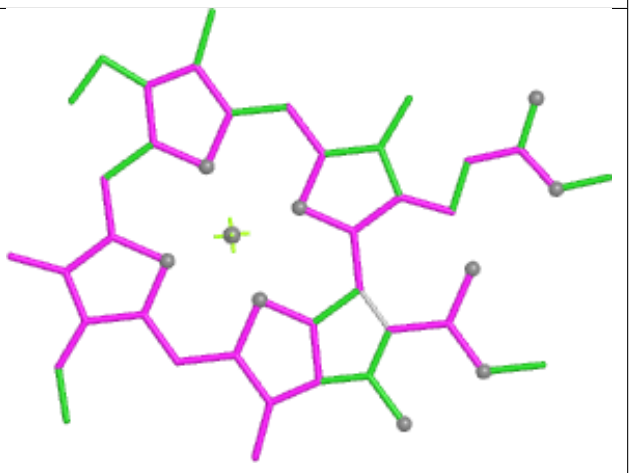


Rings

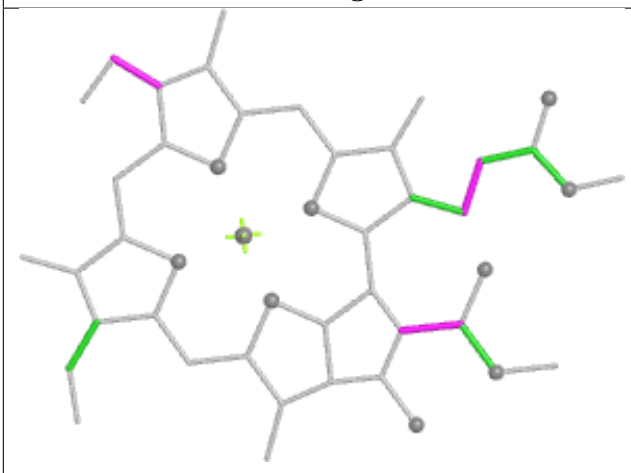
Ligand CLA 5 621



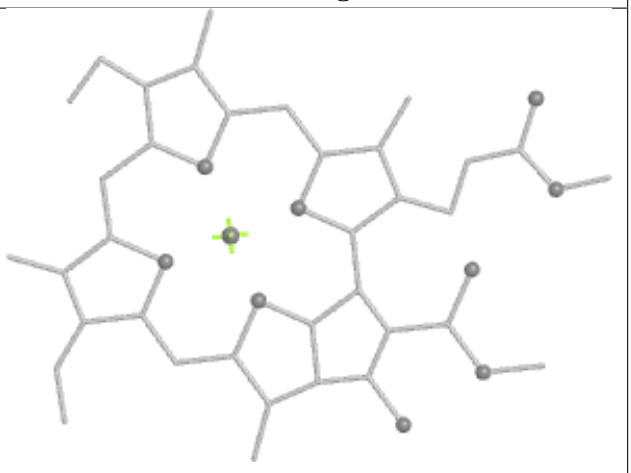
Bond lengths



Bond angles

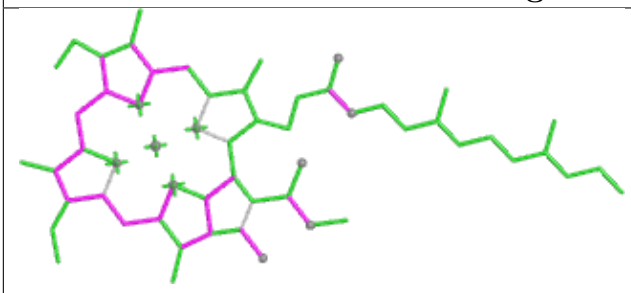


Torsions

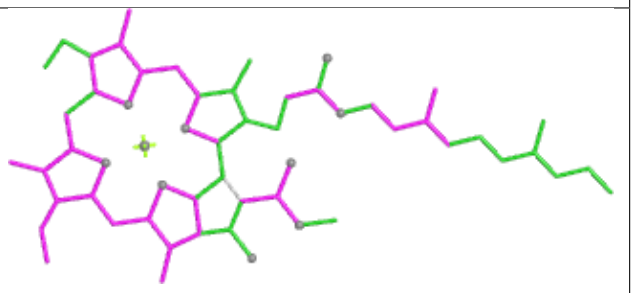


Rings

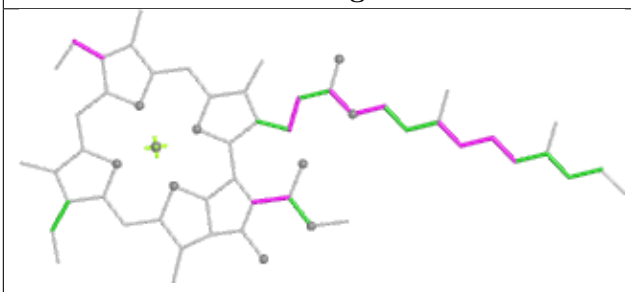
Ligand CLA Z 604



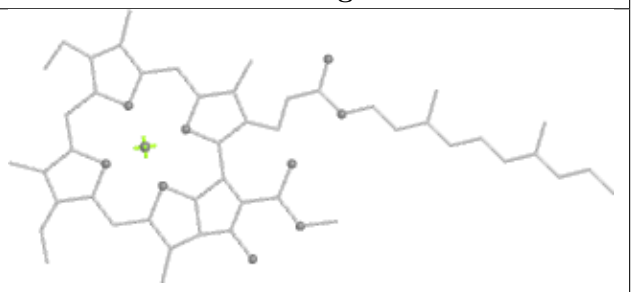
Bond lengths



Bond angles



Torsions

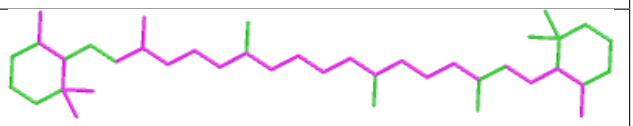


Rings

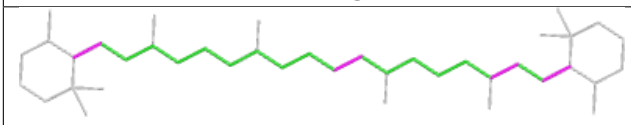
Ligand BCR A 856



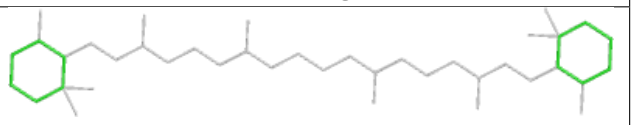
Bond lengths



Bond angles

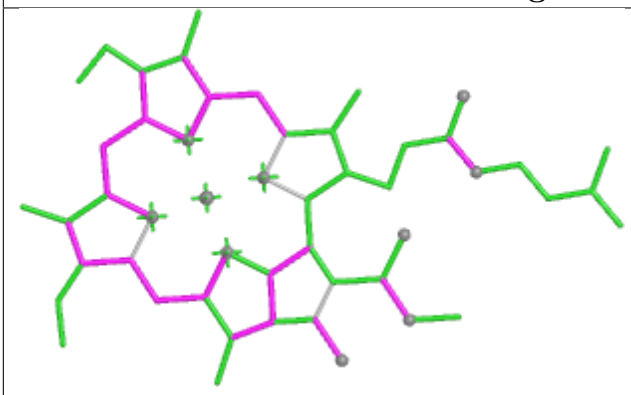


Torsions

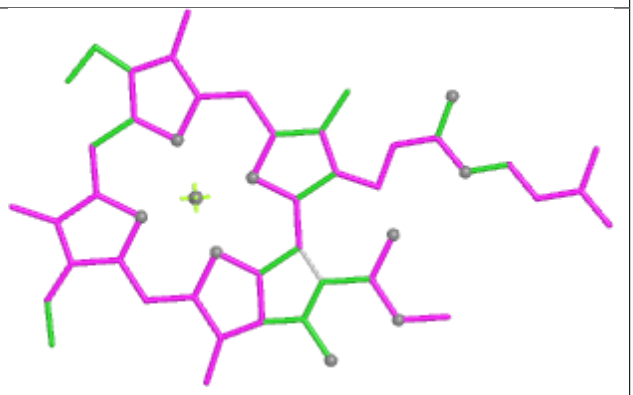


Rings

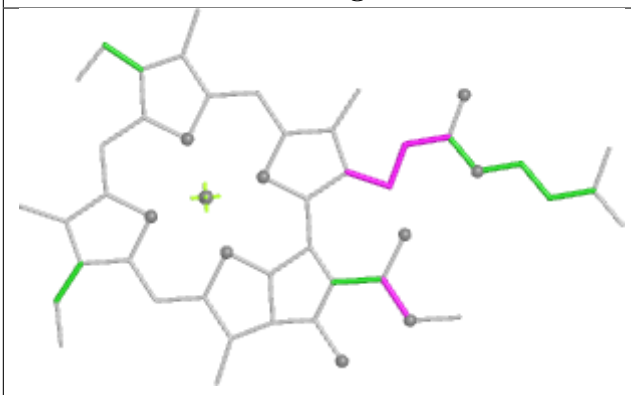
Ligand CLA 4 609



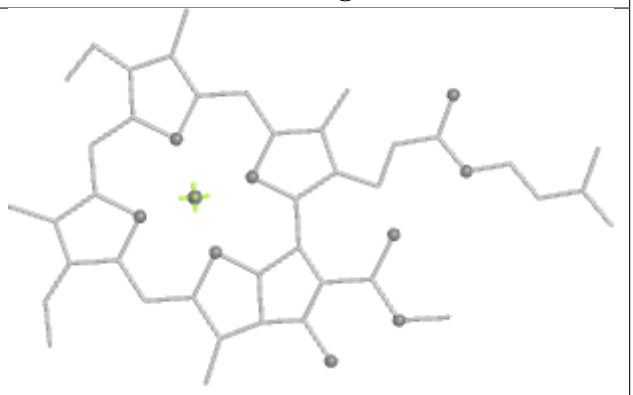
Bond lengths



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.

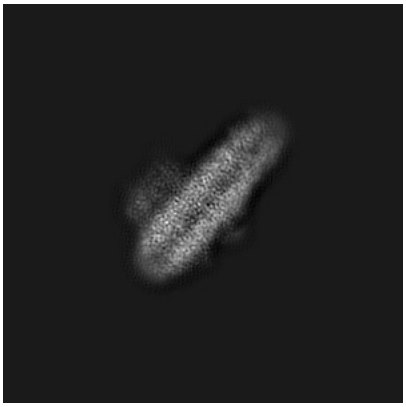
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9853. These allow visual inspection of the internal detail of the map and identification of artifacts.

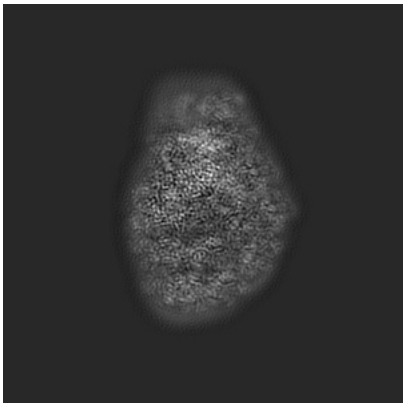
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

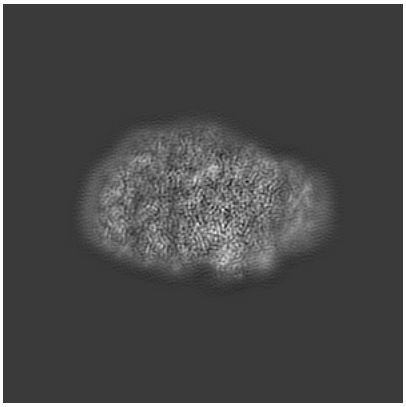
6.1.1 Primary map



X



Y

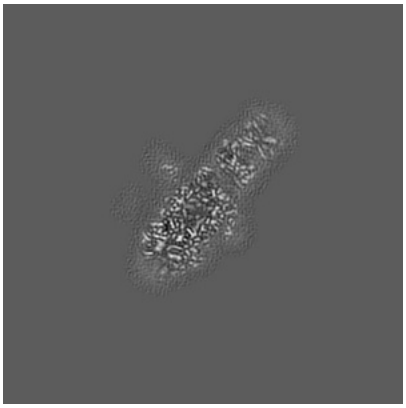


Z

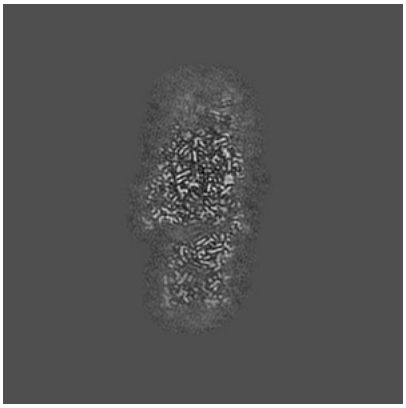
The images above show the map projected in three orthogonal directions.

6.2 Central slices

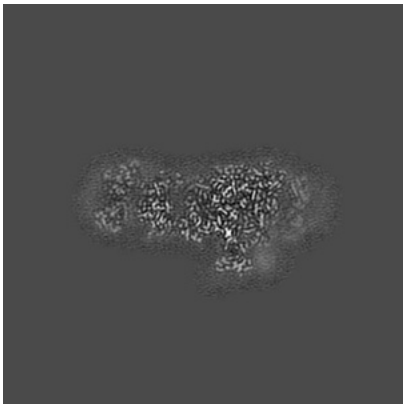
6.2.1 Primary map



X Index: 160



Y Index: 160

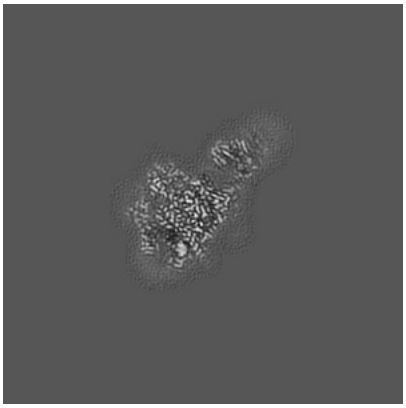


Z Index: 160

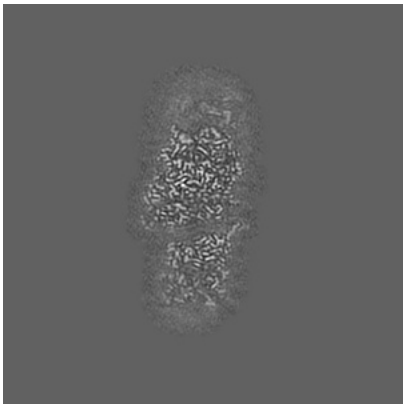
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

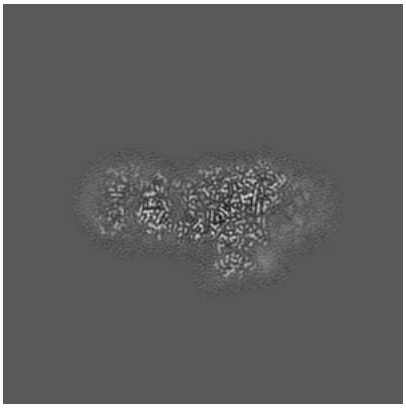
6.3.1 Primary map



X Index: 175



Y Index: 158

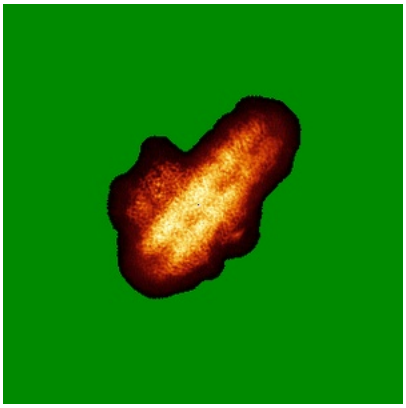


Z Index: 157

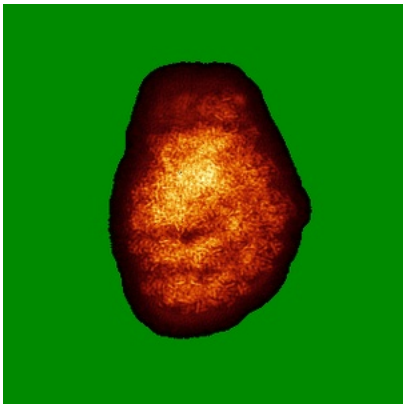
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

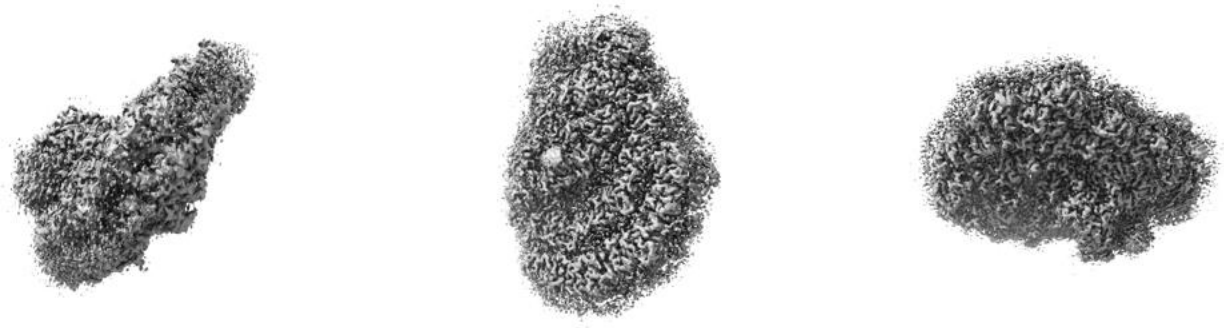


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

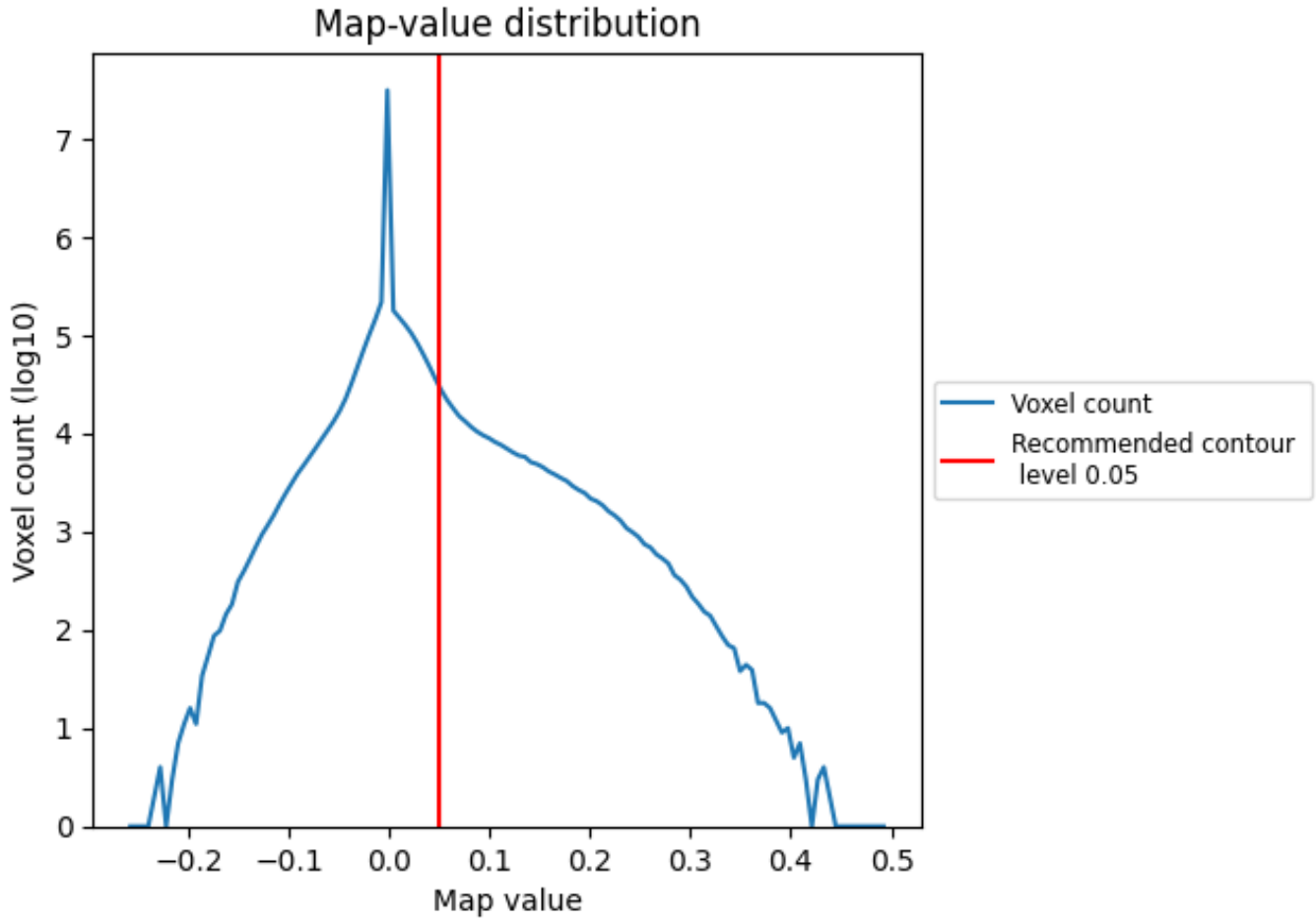
6.6 Mask visualisation (i)

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

7 Map analysis

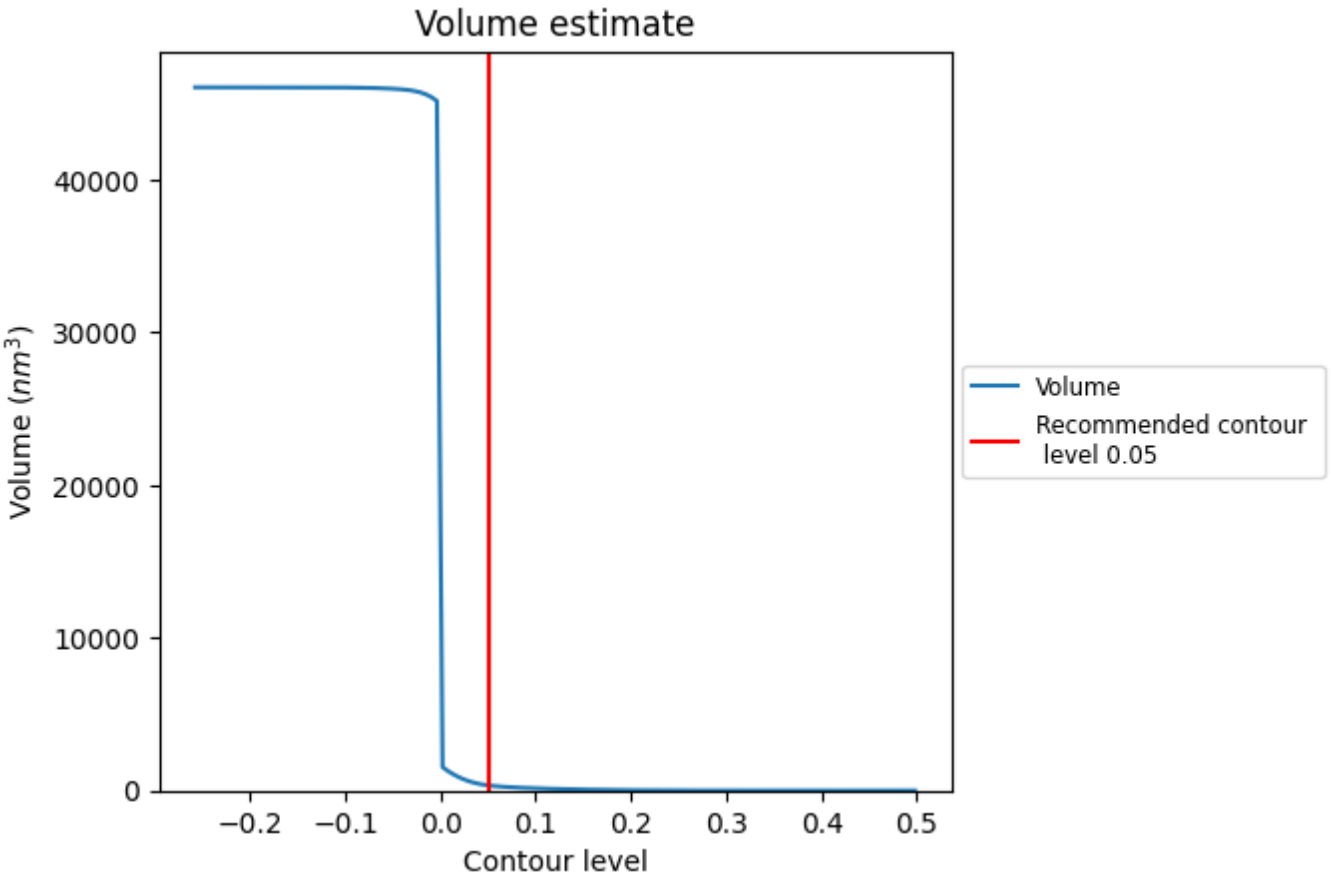
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

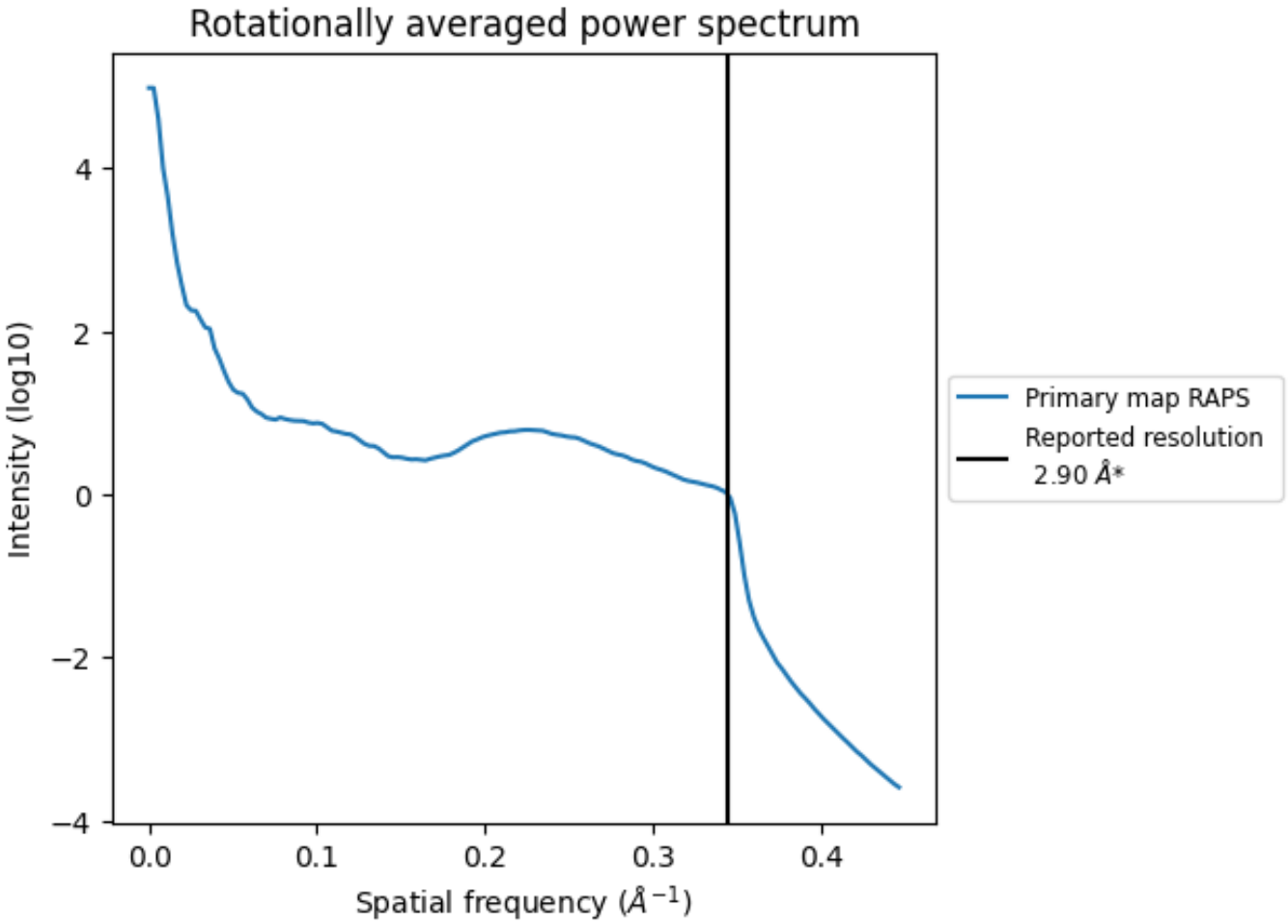
7.2 Volume estimate



The volume at the recommended contour level is 342 nm^3; this corresponds to an approximate mass of 309 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 0.345 $Å^{-1}$

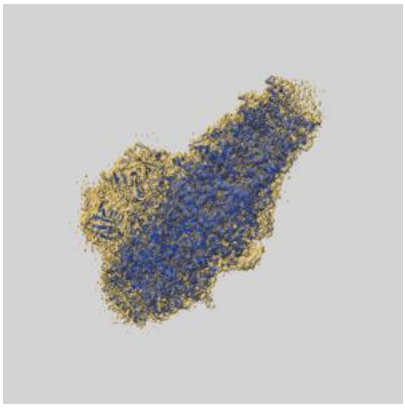
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

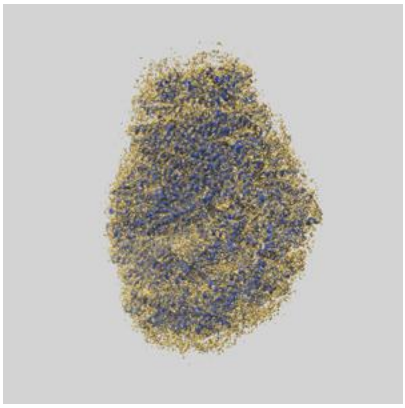
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9853 and PDB model 6JO5. Per-residue inclusion information can be found in section 3 on page 28.

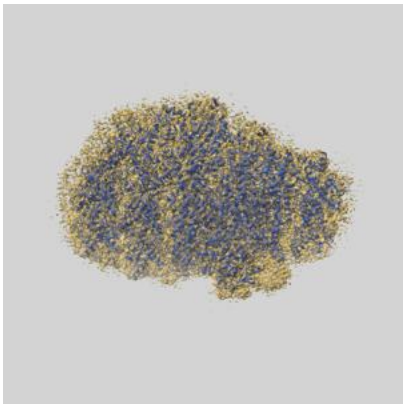
9.1 Map-model overlay



X



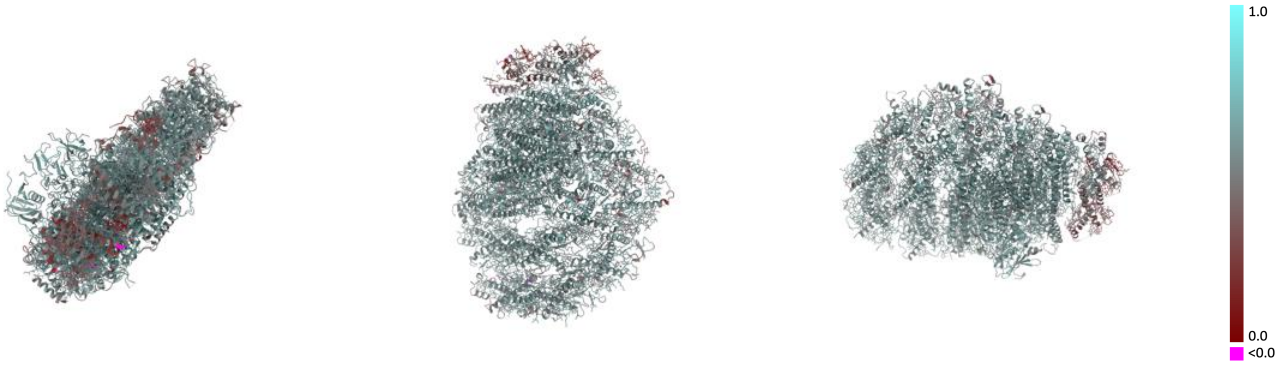
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

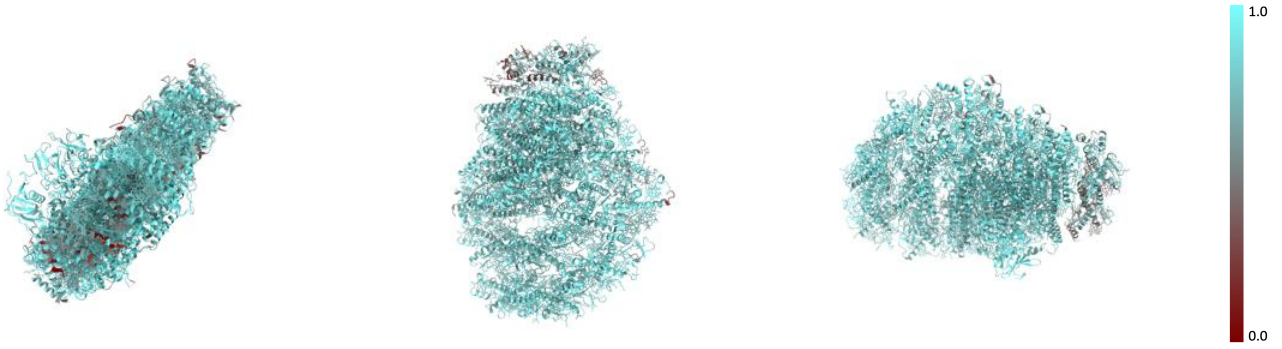
9.2 Q-score mapped to coordinate model (i)



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.

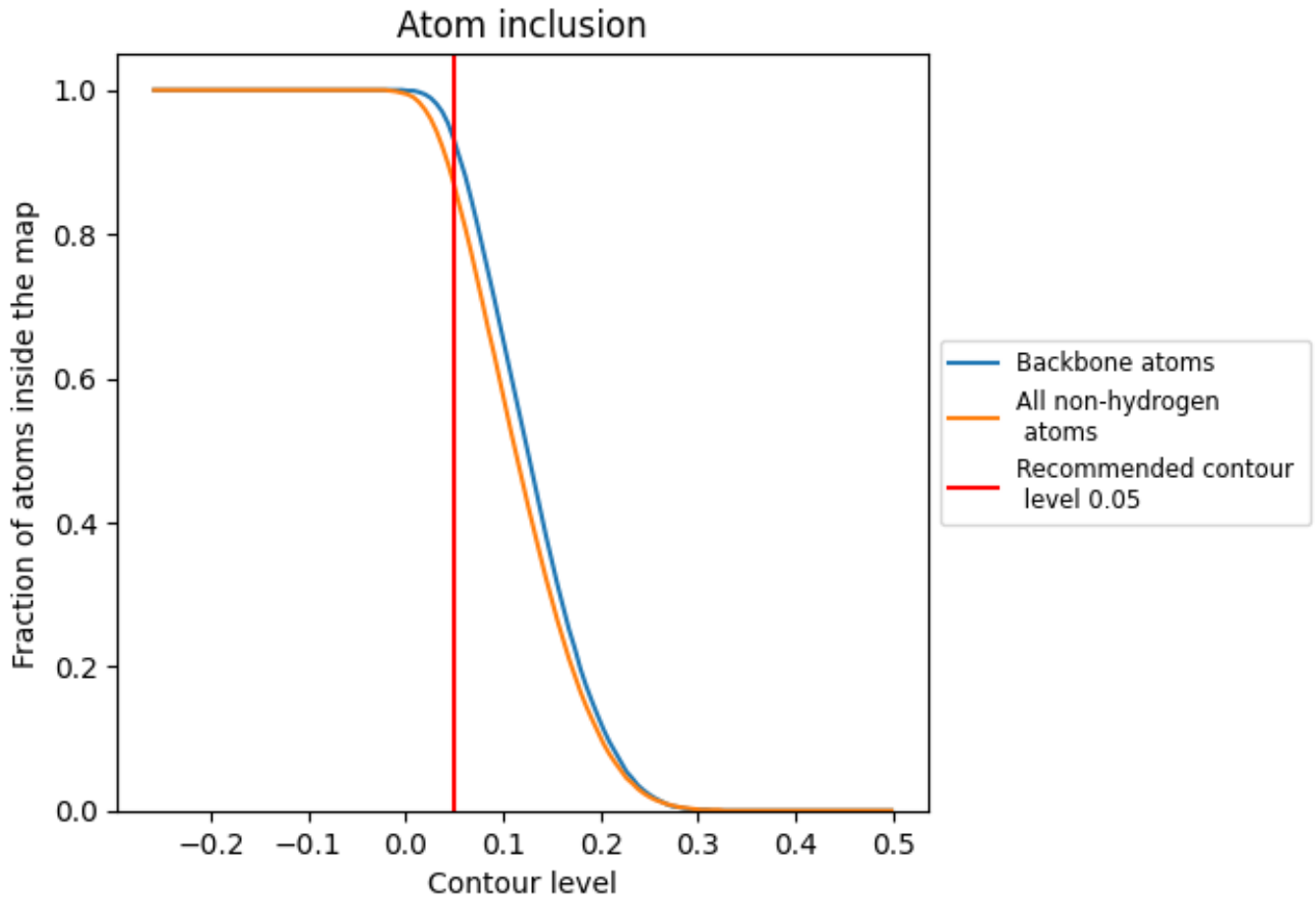
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.5670
1	0.8540	0.5660
2	0.5380	0.3290
3	0.8920	0.5820
4	0.8490	0.5440
5	0.8520	0.5470
6	0.8490	0.5510
7	0.8850	0.5860
8	0.8910	0.5830
9	0.6950	0.4490
A	0.9280	0.6080
B	0.9220	0.6090
C	0.9550	0.6010
D	0.9040	0.5730
E	0.8910	0.5830
F	0.8660	0.5660
G	0.8300	0.5500
I	0.8680	0.5680
J	0.9140	0.6010
K	0.7800	0.5270
L	0.8370	0.5420
Z	0.7810	0.5190

