Full wwPDB EM Validation Report

Mar 26, 2026 – 08:17 AM UTC

PDB ID	:	6L4U / pdb_00006l4u
EMDB ID	:	EMD-0835
Title	:	Structure of the PSI-FCPI supercomplex from diatom
Authors	:	Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.
Deposited on	:	2019-10-21
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

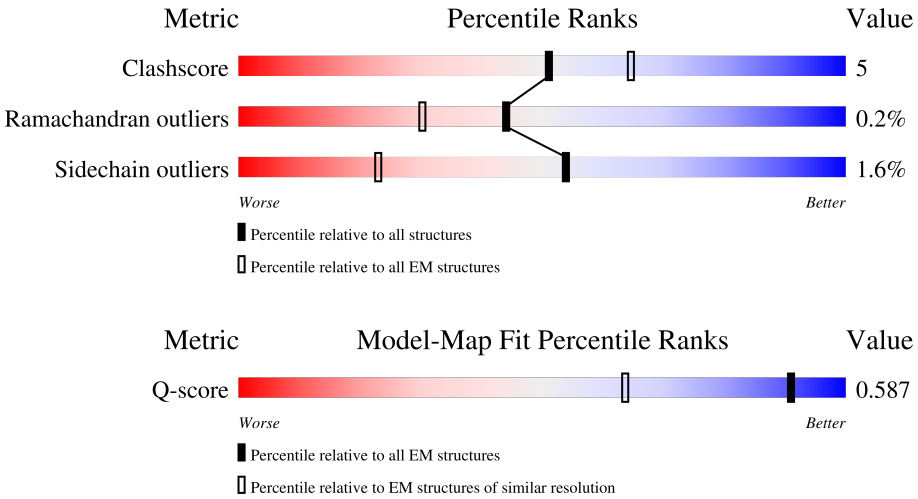
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



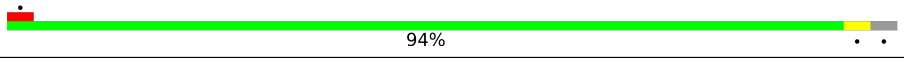
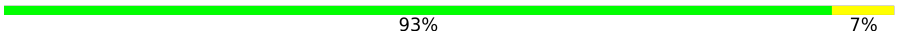
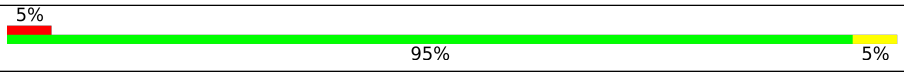
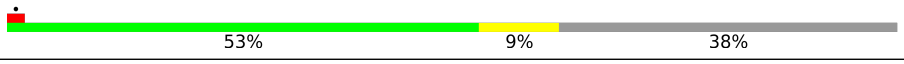
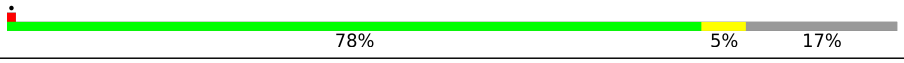
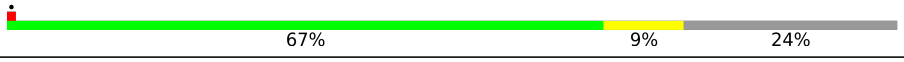
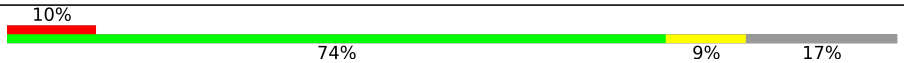
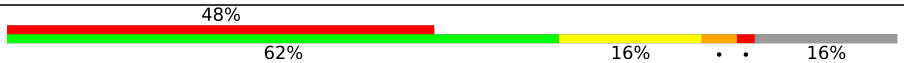
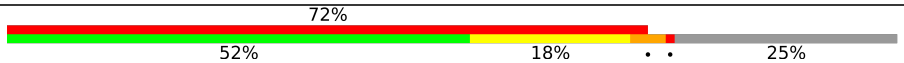
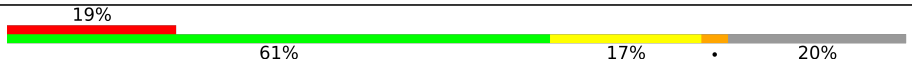
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	A	751	88% 10% •
2	B	733	89% 10%
3	C	81	81% 15% ••
4	D	139	81% 13% • 6%

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Mol	Chain	Length	Quality of chain
5	E	67	
6	F	185	
7	I	36	
8	J	41	
9	L	151	
10	M	30	
11	1u	130	
12	2u	121	
13	1	227	
14	2	205	
15	3	200	
16	4	215	
17	5	266	
18	6	208	
19	7	296	
20	8	270	
21	9	214	
22	10	207	
23	11	229	
24	12	204	
25	13	244	
26	14	249	
27	15	281	
28	16	218	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CL0	A	801	X	-	-	-
30	CLA	1	301	X	-	-	-
30	CLA	1	302	X	-	-	-
30	CLA	1	303	X	-	-	-
30	CLA	1	304	X	-	-	-
30	CLA	1	305	X	-	-	-
30	CLA	10	303	X	-	-	-
30	CLA	10	304	X	-	-	-
30	CLA	10	305	X	-	-	-
30	CLA	10	307	X	-	-	-
30	CLA	10	308	X	-	-	-
30	CLA	10	309	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	308	X	-	-	-
30	CLA	11	310	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	304	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	312	X	-	-	-
30	CLA	12	321	X	-	-	-
30	CLA	13	301	X	-	-	-
30	CLA	13	302	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	309	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	309	X	-	-	-
30	CLA	14	310	X	-	-	-
30	CLA	14	313	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	304	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-
30	CLA	15	308	X	-	-	-
30	CLA	15	310	X	-	-	-
30	CLA	15	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	15	312	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-
30	CLA	16	305	X	-	-	-
30	CLA	16	306	X	-	-	-
30	CLA	16	307	X	-	-	-
30	CLA	16	308	X	-	-	-
30	CLA	16	310	X	-	-	-
30	CLA	2	301	X	-	-	-
30	CLA	2	304	X	-	-	-
30	CLA	2	305	X	-	-	-
30	CLA	2	307	X	-	-	-
30	CLA	2	309	X	-	-	-
30	CLA	2	310	X	-	-	-
30	CLA	2u	202	X	-	-	-
30	CLA	3	301	X	-	-	-
30	CLA	3	302	X	-	-	-
30	CLA	3	303	X	-	-	-
30	CLA	3	305	X	-	-	-
30	CLA	3	306	X	-	-	-
30	CLA	3	307	X	-	-	-
30	CLA	4	301	X	-	-	-
30	CLA	4	302	X	-	-	-
30	CLA	4	303	X	-	-	-
30	CLA	4	304	X	-	-	-
30	CLA	4	305	X	-	-	-
30	CLA	4	306	X	-	-	-
30	CLA	4	309	X	-	-	-
30	CLA	4	311	X	-	-	-
30	CLA	5	302	X	-	-	-
30	CLA	5	303	X	-	-	-
30	CLA	5	304	X	-	-	-
30	CLA	5	307	X	-	-	-
30	CLA	5	309	X	-	-	-
30	CLA	5	311	X	-	-	-
30	CLA	6	304	X	-	-	-
30	CLA	6	305	X	-	-	-
30	CLA	6	306	X	-	-	-
30	CLA	6	307	X	-	-	-
30	CLA	6	309	X	-	-	-
30	CLA	6	310	X	-	-	-
30	CLA	6	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	6	316	X	-	-	-
30	CLA	6	317	X	-	-	-
30	CLA	7	303	X	-	-	-
30	CLA	7	304	X	-	-	-
30	CLA	7	305	X	-	-	-
30	CLA	7	306	X	-	-	-
30	CLA	7	309	X	-	-	-
30	CLA	7	311	X	-	-	-
30	CLA	7	312	X	-	-	-
30	CLA	8	301	X	-	-	-
30	CLA	8	302	X	-	-	-
30	CLA	8	304	X	-	-	-
30	CLA	8	308	X	-	-	-
30	CLA	9	301	X	-	-	-
30	CLA	9	302	X	-	-	-
30	CLA	9	305	X	-	-	-
30	CLA	9	306	X	-	-	-
30	CLA	9	307	X	-	-	-
30	CLA	9	308	X	-	-	-
30	CLA	9	309	X	-	-	-
30	CLA	A	802	X	-	-	-
30	CLA	A	803	X	-	-	-
30	CLA	A	804	X	-	-	-
30	CLA	A	805	X	-	-	-
30	CLA	A	806	X	-	-	-
30	CLA	A	807	X	-	-	-
30	CLA	A	808	X	-	-	-
30	CLA	A	809	X	-	-	-
30	CLA	A	810	X	-	-	-
30	CLA	A	811	X	-	-	-
30	CLA	A	812	X	-	-	-
30	CLA	A	813	X	-	-	-
30	CLA	A	814	X	-	-	-
30	CLA	A	815	X	-	-	-
30	CLA	A	816	X	-	-	-
30	CLA	A	820	X	-	-	-
30	CLA	A	821	X	-	-	-
30	CLA	A	822	X	-	-	-
30	CLA	A	824	X	-	-	-
30	CLA	A	825	X	-	-	-
30	CLA	A	826	X	-	-	-
30	CLA	A	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	A	828	X	-	-	-
30	CLA	A	829	X	-	-	-
30	CLA	A	830	X	-	-	-
30	CLA	A	831	X	-	-	-
30	CLA	A	833	X	-	-	-
30	CLA	A	834	X	-	-	-
30	CLA	A	835	X	-	-	-
30	CLA	A	836	X	-	-	-
30	CLA	A	837	X	-	-	-
30	CLA	A	838	X	-	-	-
30	CLA	A	839	X	-	-	-
30	CLA	A	840	X	-	-	-
30	CLA	A	841	X	-	-	-
30	CLA	A	842	X	-	-	-
30	CLA	A	843	X	-	-	-
30	CLA	A	844	X	-	-	-
30	CLA	B	801	X	-	-	-
30	CLA	B	802	X	-	-	-
30	CLA	B	803	X	-	-	-
30	CLA	B	804	X	-	-	-
30	CLA	B	805	X	-	-	-
30	CLA	B	806	X	-	-	-
30	CLA	B	807	X	-	-	-
30	CLA	B	808	X	-	-	-
30	CLA	B	809	X	-	-	-
30	CLA	B	810	X	-	-	-
30	CLA	B	811	X	-	-	-
30	CLA	B	812	X	-	-	-
30	CLA	B	813	X	-	-	-
30	CLA	B	814	X	-	-	-
30	CLA	B	815	X	-	-	-
30	CLA	B	817	X	-	-	-
30	CLA	B	818	X	-	-	-
30	CLA	B	819	X	-	-	-
30	CLA	B	821	X	-	-	-
30	CLA	B	823	X	-	-	-
30	CLA	B	824	X	-	-	-
30	CLA	B	825	X	-	-	-
30	CLA	B	826	X	-	-	-
30	CLA	B	827	X	-	-	-
30	CLA	B	828	X	-	-	-
30	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	B	830	X	-	-	-
30	CLA	B	832	X	-	-	-
30	CLA	B	833	X	-	-	-
30	CLA	B	834	X	-	-	-
30	CLA	B	835	X	-	-	-
30	CLA	B	836	X	-	-	-
30	CLA	B	837	X	-	-	-
30	CLA	B	838	X	-	-	-
30	CLA	B	839	X	-	-	-
30	CLA	F	201	X	-	-	-
30	CLA	F	202	X	-	-	-
30	CLA	F	203	X	-	-	-
30	CLA	J	101	X	-	-	-
30	CLA	L	202	X	-	-	-
30	CLA	L	203	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 62199 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5841	3816	991	1005	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5801	3814	977	992	18	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	131	1037	663	177	194	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	60	478	302	86	90	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1257	806	213	234	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	35	Total	C	N	O	S	0	0
			273	190	37	44	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			344	236	50	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	137	Total	C	N	O	S	0	0
			1030	680	169	179	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			227	151	35	40	1		

- Molecule 11 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	1u	130	Total	C	N	O	0	0
			650	390	130	130		

- Molecule 12 is a protein called Photosystem I reaction center subunit Psa28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2u	89	Total	C	N	O	S	0	0
			674	438	110	120	6		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	141	Total	C	N	O	S	0	0
			1086	692	184	201	9		

- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	172	Total	C	N	O	S	0	0
			1310	846	216	238	10		

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	164	Total	C	N	O	S	0	0
			1275	825	213	232	5		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	179	Total	C	N	O	S	0	0
			1368	878	227	250	13		

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	169	Total	C	N	O	S	0	0
			1304	834	222	236	12		

- Molecule 18 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 19 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 21 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	163	Total	C	N	O	S	0	0
			1267	816	211	233	7		

- Molecule 22 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 23 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

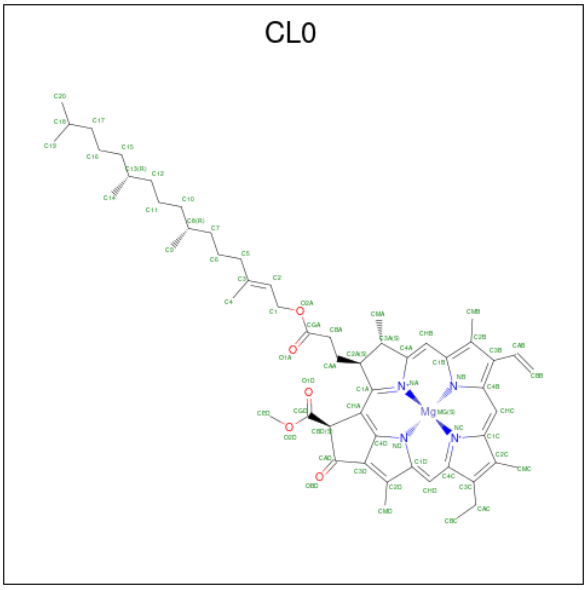
- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

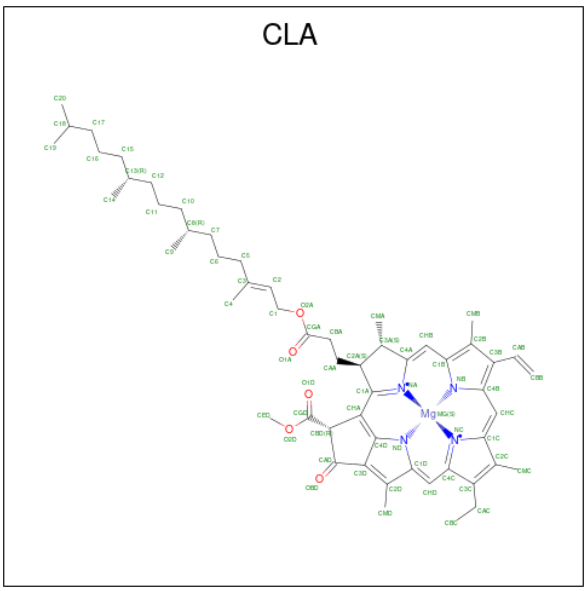
Mol	Chain	Residues	Atoms					AltConf	Trace
28	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 29 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	8	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	8	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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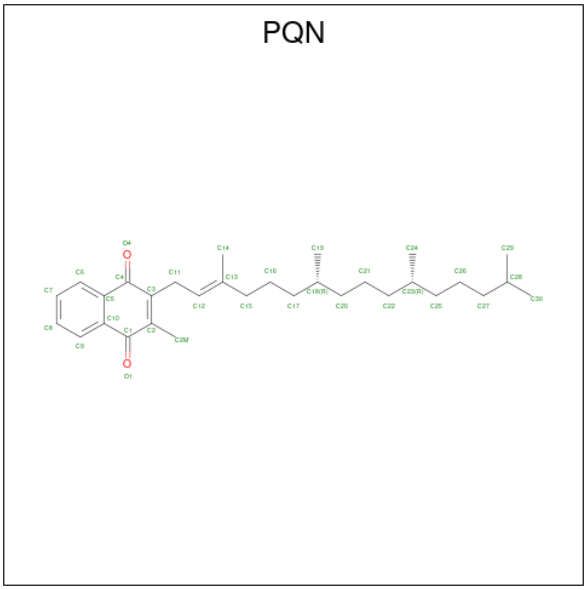
Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



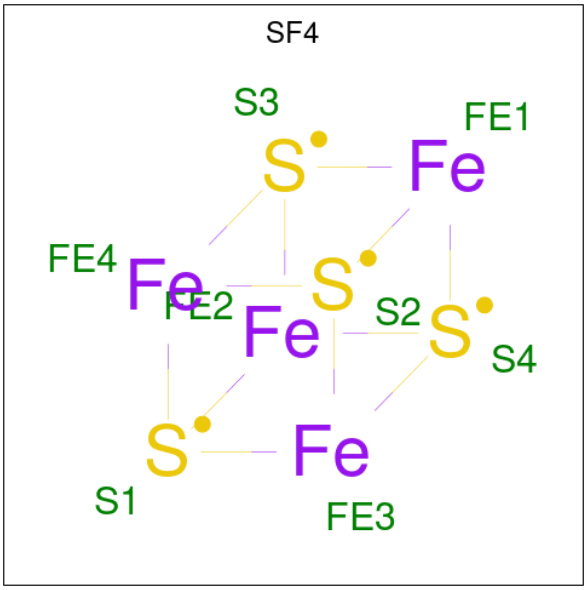
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			33	31	2	

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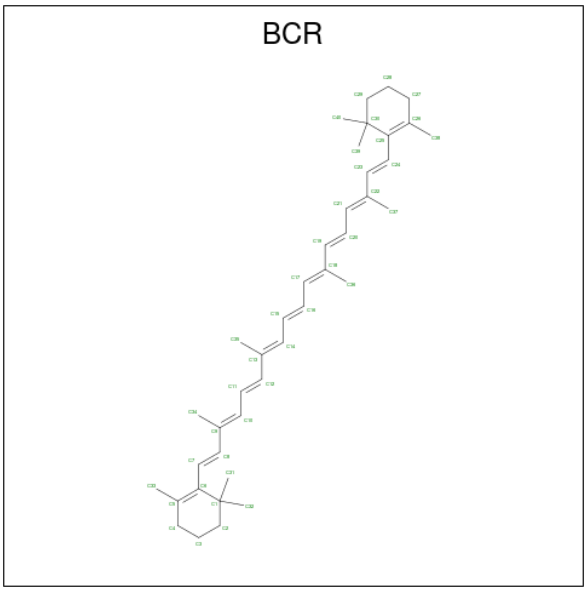
Mol	Chain	Residues	Atoms	AltConf
31	B	1	Total C O 33 31 2	0

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



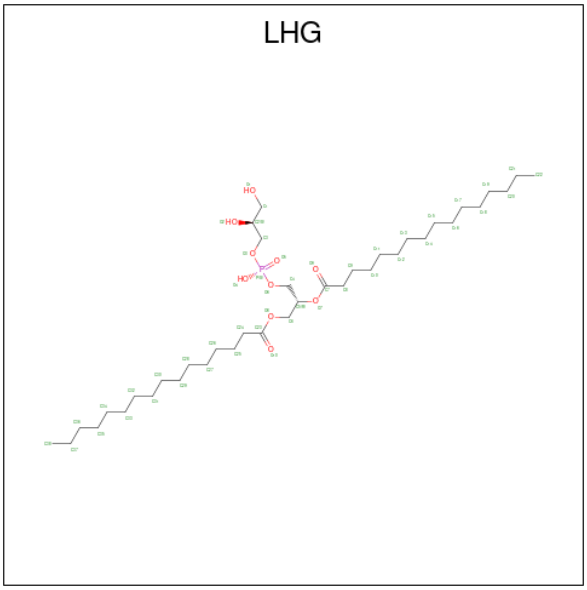
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	F	1	Total C 40 40	0
33	I	1	Total C 40 40	0
33	J	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
33	J	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	M	1	Total C 40 40	0
33	2u	1	Total C 40 40	0

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



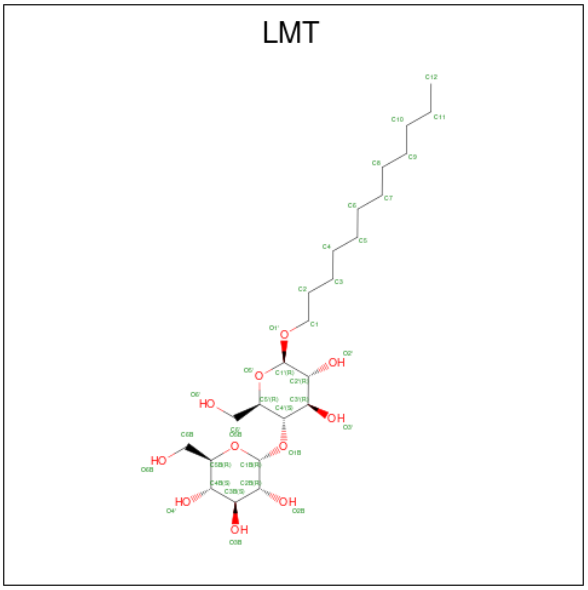
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C O P 49 38 10 1	0
34	A	1	Total C O P 27 16 10 1	0
34	B	1	Total C O P 27 16 10 1	0
34	2	1	Total C O P 27 16 10 1	0
34	5	1	Total C O P 27 16 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
34	6	1	Total	C	O	P	0
			27	16	10	1	
34	9	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



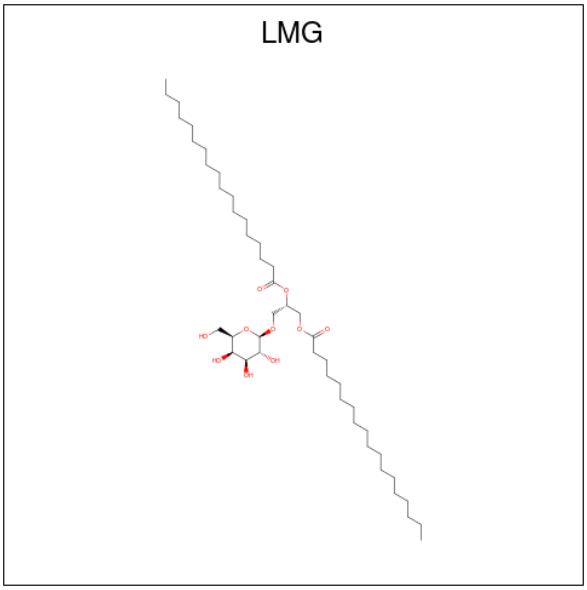
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			35	24	11	
35	A	1	Total	C	O	0
			35	24	11	
35	A	1	Total	C	O	0
			35	24	11	
35	B	1	Total	C	O	0
			35	24	11	
35	B	1	Total	C	O	0
			35	24	11	
35	1	1	Total	C	O	0
			35	24	11	
35	6	1	Total	C	O	0
			31	20	11	
35	7	1	Total	C	O	0
			35	24	11	
35	7	1	Total	C	O	0
			35	24	11	

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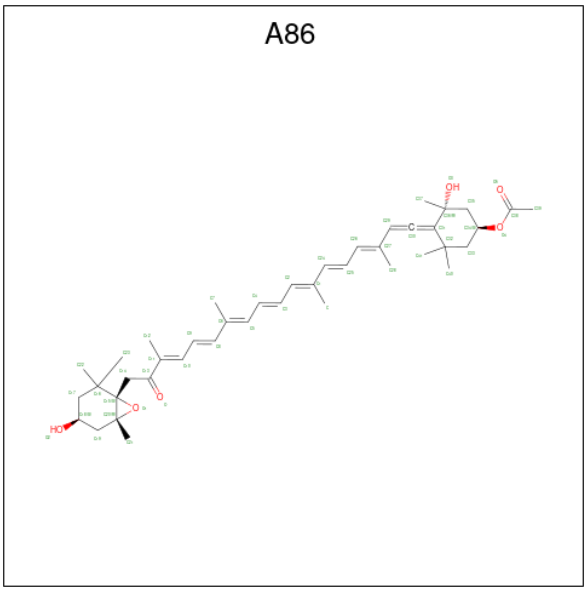
Mol	Chain	Residues	Atoms	AltConf
35	8	1	Total C O 35 24 11	0
35	9	1	Total C O 32 21 11	0
35	11	1	Total C O 35 24 11	0
35	11	1	Total C O 35 24 11	0
35	11	1	Total C O 35 24 11	0
35	11	1	Total C O 35 24 11	0
35	12	1	Total C O 35 24 11	0
35	12	1	Total C O 35 24 11	0
35	12	1	Total C O 35 24 11	0
35	12	1	Total C O 35 24 11	0
35	15	1	Total C O 35 24 11	0
35	16	1	Total C O 35 24 11	0

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			34	24	10	
36	B	1	Total	C	O	0
			55	45	10	
36	B	1	Total	C	O	0
			43	33	10	
36	F	1	Total	C	O	0
			27	17	10	
36	2u	1	Total	C	O	0
			31	21	10	
36	3	1	Total	C	O	0
			37	27	10	
36	5	1	Total	C	O	0
			33	23	10	
36	6	1	Total	C	O	0
			33	23	10	
36	7	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			42	32	10	
36	8	1	Total	C	O	0
			29	19	10	
36	14	1	Total	C	O	0
			38	28	10	

- Molecule 37 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms	AltConf
37	2u	1	Total C O 48 42 6	0
37	2u	1	Total C O 48 42 6	0
37	1	1	Total C O 48 42 6	0
37	2	1	Total C O 48 42 6	0
37	2	1	Total C O 48 42 6	0
37	2	1	Total C O 48 42 6	0
37	3	1	Total C O 48 42 6	0
37	3	1	Total C O 48 42 6	0
37	4	1	Total C O 48 42 6	0
37	4	1	Total C O 48 42 6	0
37	4	1	Total C O 48 42 6	0
37	4	1	Total C O 48 42 6	0
37	5	1	Total C O 48 42 6	0
37	5	1	Total C O 48 42 6	0

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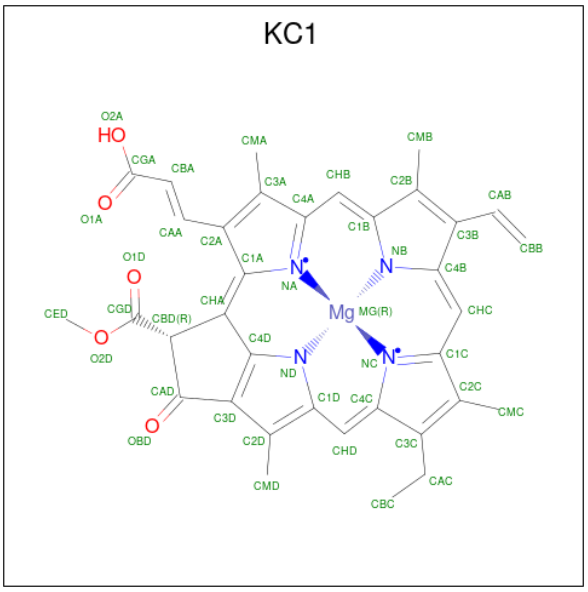
Mol	Chain	Residues	Atoms	AltConf
37	5	1	Total C O 48 42 6	0
37	6	1	Total C O 48 42 6	0
37	7	1	Total C O 48 42 6	0
37	7	1	Total C O 48 42 6	0
37	7	1	Total C O 48 42 6	0
37	8	1	Total C O 48 42 6	0
37	8	1	Total C O 48 42 6	0
37	9	1	Total C O 48 42 6	0
37	9	1	Total C O 48 42 6	0
37	9	1	Total C O 48 42 6	0
37	10	1	Total C O 48 42 6	0
37	10	1	Total C O 48 42 6	0
37	10	1	Total C O 48 42 6	0
37	10	1	Total C O 48 42 6	0
37	10	1	Total C O 48 42 6	0
37	11	1	Total C O 48 42 6	0
37	11	1	Total C O 48 42 6	0
37	11	1	Total C O 48 42 6	0
37	11	1	Total C O 48 42 6	0
37	12	1	Total C O 48 42 6	0
37	12	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
37	13	1	Total C O 45 40 5	0
37	13	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	14	1	Total C O 48 42 6	0
37	15	1	Total C O 48 42 6	0
37	15	1	Total C O 48 42 6	0
37	15	1	Total C O 48 42 6	0
37	15	1	Total C O 48 42 6	0
37	15	1	Total C O 48 42 6	0
37	15	1	Total C O 48 42 6	0
37	16	1	Total C O 48 42 6	0
37	16	1	Total C O 48 42 6	0

- Molecule 38 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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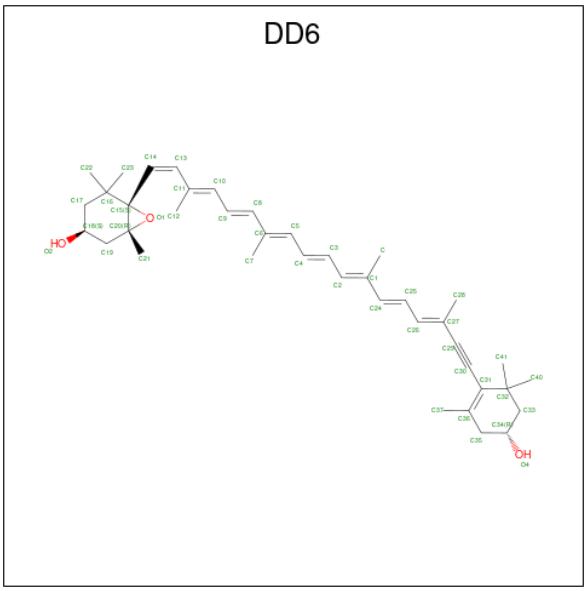
Mol	Chain	Residues	Atoms					AltConf
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	2	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	3	1	Total	C	O	0
			43	40	3	
39	4	1	Total	C	O	0
			43	40	3	
39	4	1	Total	C	O	0
			43	40	3	
39	5	1	Total	C	O	0
			43	40	3	
39	5	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	
39	6	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms	AltConf
39	6	1	Total C O 43 40 3	0
39	7	1	Total C O 43 40 3	0
39	7	1	Total C O 43 40 3	0
39	7	1	Total C O 43 40 3	0
39	7	1	Total C O 43 40 3	0
39	8	1	Total C O 43 40 3	0
39	8	1	Total C O 43 40 3	0
39	9	1	Total C O 43 40 3	0
39	10	1	Total C O 43 40 3	0
39	10	1	Total C O 43 40 3	0
39	11	1	Total C O 43 40 3	0
39	12	1	Total C O 43 40 3	0
39	12	1	Total C O 43 40 3	0
39	13	1	Total C O 43 40 3	0
39	15	1	Total C O 43 40 3	0
39	15	1	Total C O 43 40 3	0
39	16	1	Total C O 43 40 3	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	AltConf
40	A	42	Total O 42 42	0
40	B	53	Total O 53 53	0

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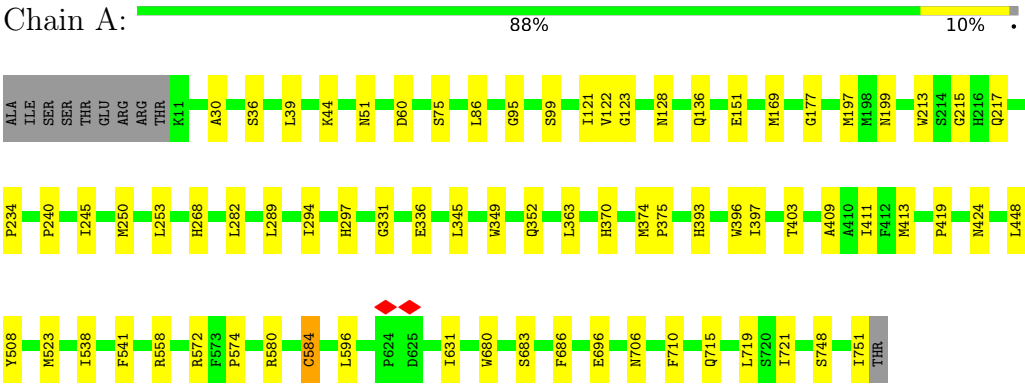
Mol	Chain	Residues	Atoms	AltConf
40	C	15	Total O 15 15	0
40	D	13	Total O 13 13	0
40	E	3	Total O 3 3	0
40	F	3	Total O 3 3	0
40	I	1	Total O 1 1	0
40	L	8	Total O 8 8	0
40	1	1	Total O 1 1	0
40	2	2	Total O 2 2	0
40	3	1	Total O 1 1	0
40	5	1	Total O 1 1	0
40	6	2	Total O 2 2	0
40	7	2	Total O 2 2	0
40	8	4	Total O 4 4	0
40	9	1	Total O 1 1	0
40	10	1	Total O 1 1	0
40	11	1	Total O 1 1	0
40	12	2	Total O 2 2	0

3 Residue-property plots (i)

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

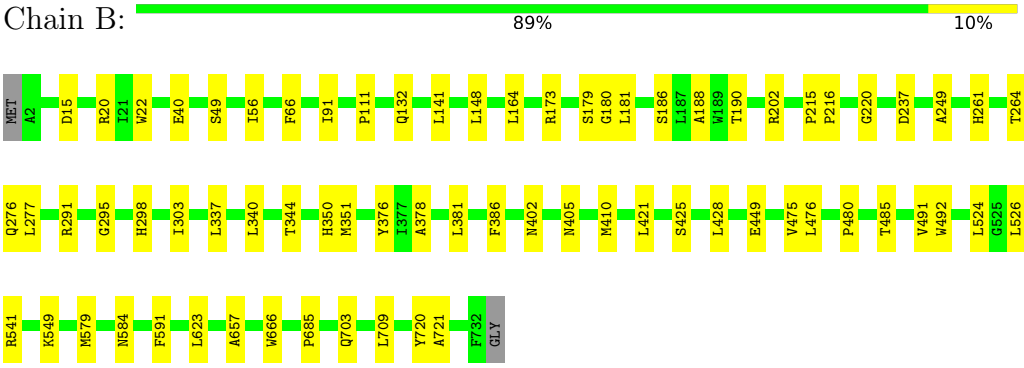
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



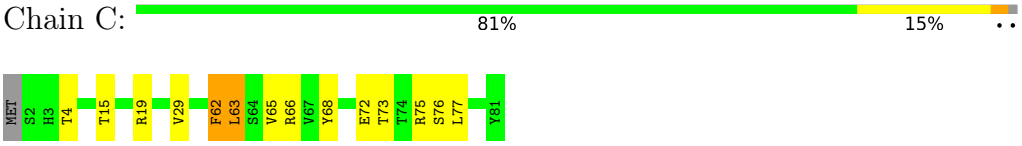
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



• Molecule 3: Photosystem I iron-sulfur center

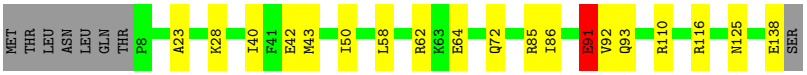
Chain C:



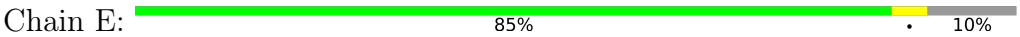
• Molecule 4: Photosystem I reaction center subunit II

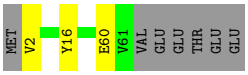
Chain D:



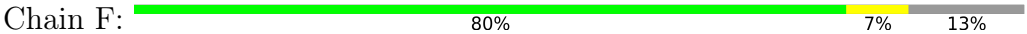


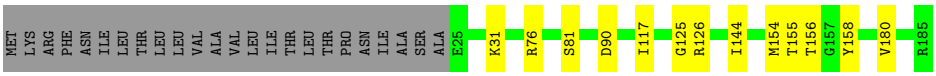
• Molecule 5: Photosystem I reaction center subunit IV





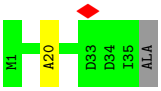
• Molecule 6: Photosystem I reaction center subunit III





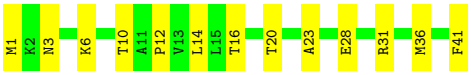
• Molecule 7: Photosystem I reaction center subunit VIII



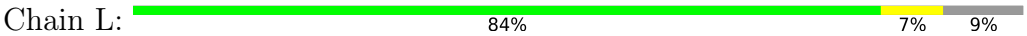


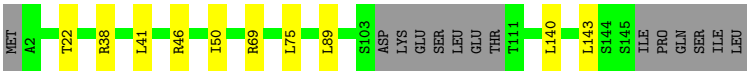
• Molecule 8: Photosystem I reaction center subunit IX





• Molecule 9: Photosystem I reaction center subunit XI





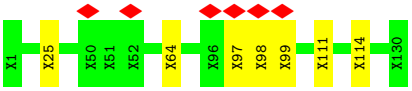
• Molecule 10: Photosystem I reaction center subunit XII





• Molecule 11: Unknown protein 1

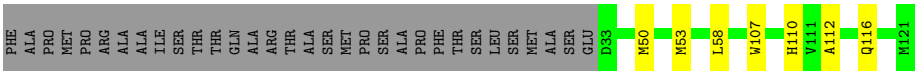




• Molecule 12: Photosystem I reaction center subunit Psa28

Chain 2u:



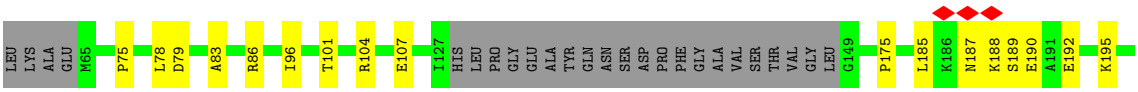


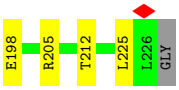
• Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcr15

Chain 1:





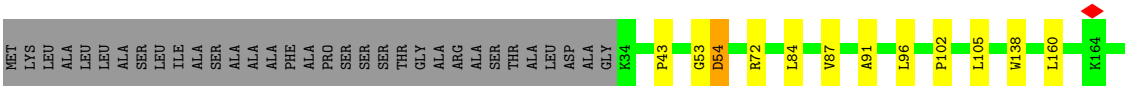


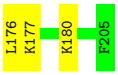


• Molecule 14: Fucoxanthin chlorophyll a/c-binding protein Lhcr8

Chain 2:



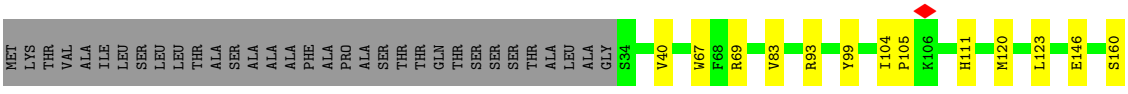


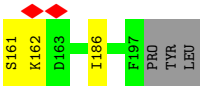


• Molecule 15: Fucoxanthin chlorophyll a/c-binding protein Lhcr2

Chain 3:



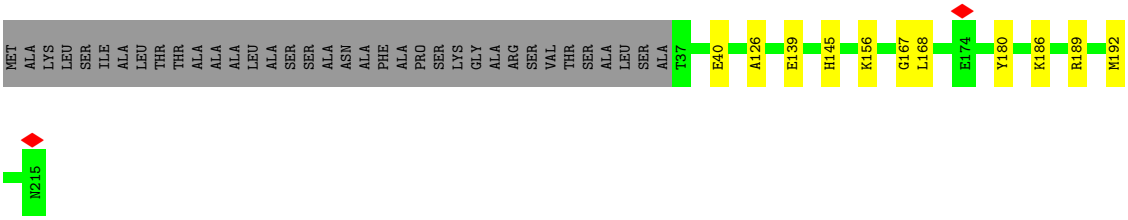




• Molecule 16: Fucoxanthin chlorophyll a/c-binding protein Lhcr9

Chain 4:

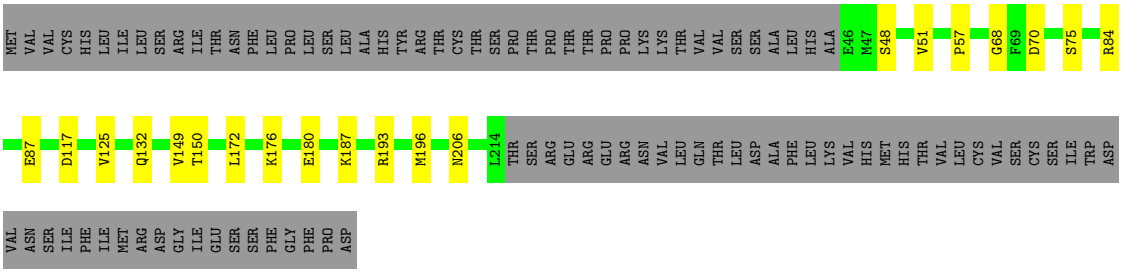




• Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lhcr11

Chain 5:

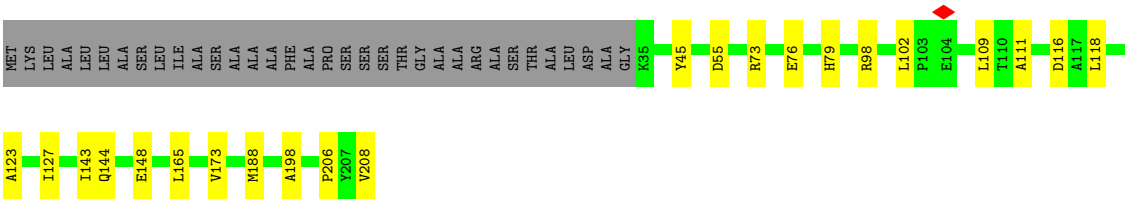




• Molecule 18: Fucoxanthin chlorophyll a/c-binding protein Lhcr12

Chain 6:

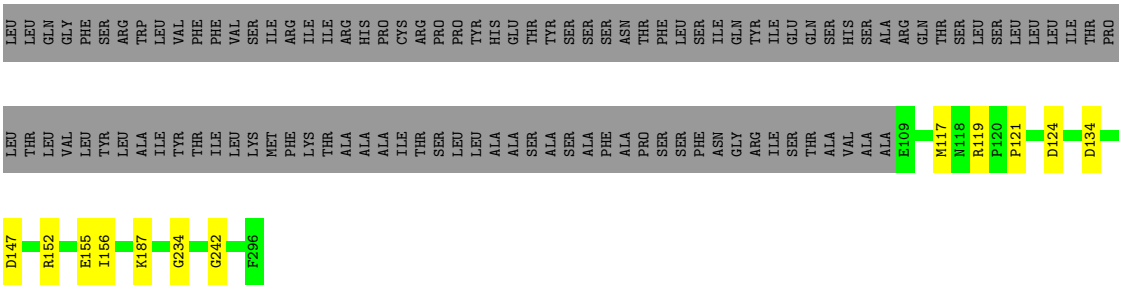




• Molecule 19: Fucoxanthin chlorophyll a/c-binding protein Lhcr10

Chain 7:





• Molecule 20: Fucoxanthin chlorophyll a/c-binding protein Lhcr4

Chain 8:





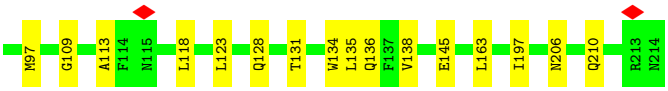


• Molecule 21: Fucoxanthin chlorophyll a/c-binding protein Lhcf6

Chain 9:



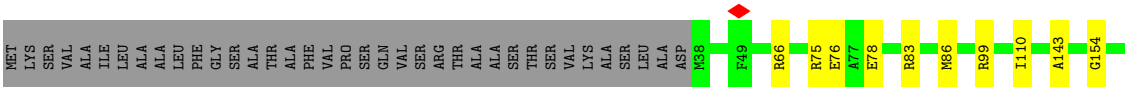


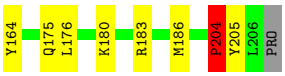


• Molecule 22: Fucoxanthin chlorophyll a/c-binding protein Lhcr3

Chain 10:



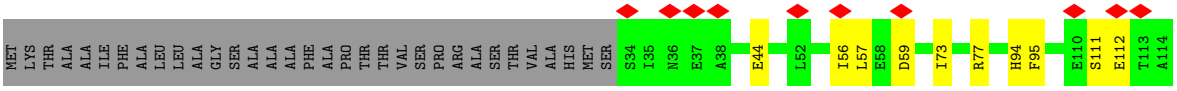


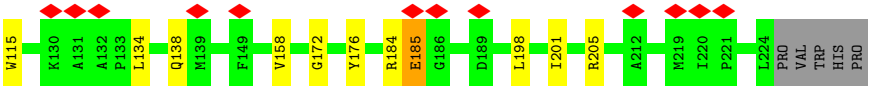


• Molecule 23: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

Chain 11:



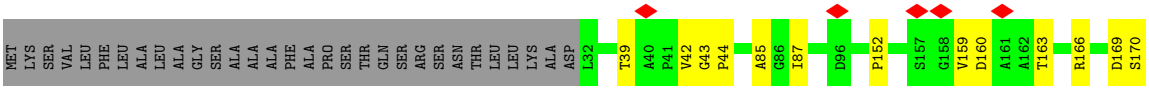


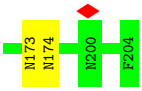


• Molecule 24: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

Chain 12:



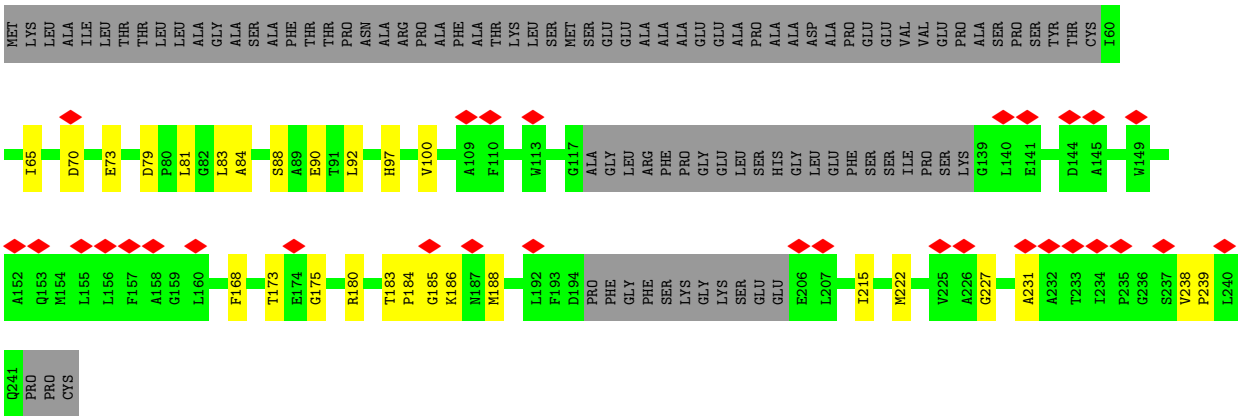




• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

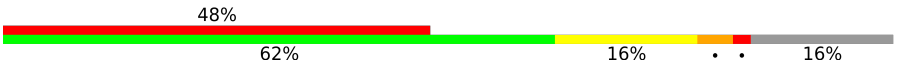
Chain 13:

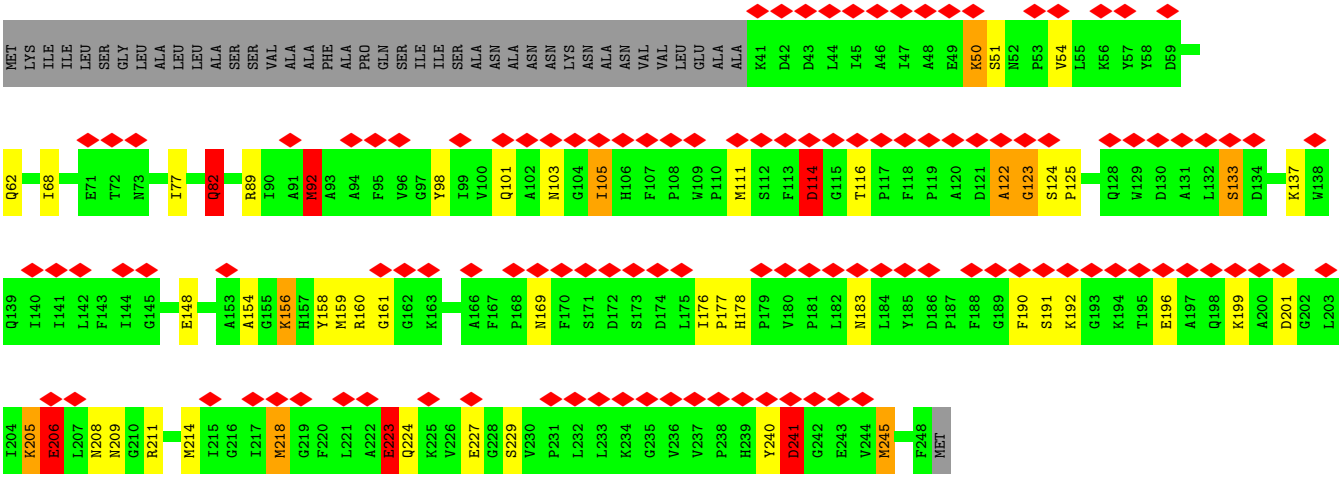




• Molecule 26: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

Chain 14:

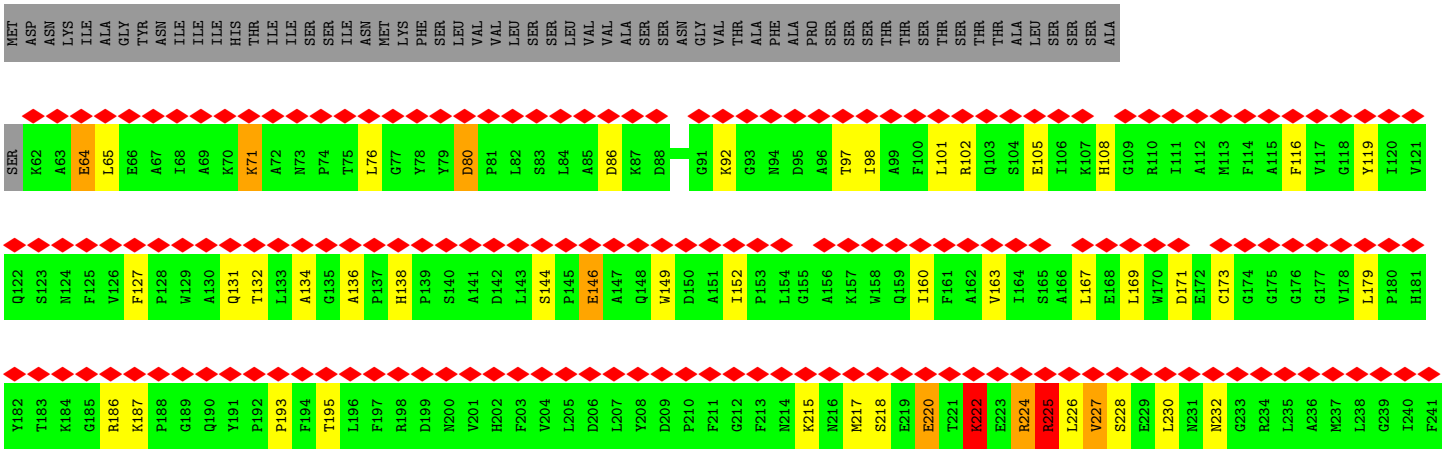


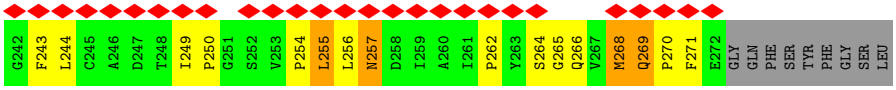


• Molecule 27: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain 15:



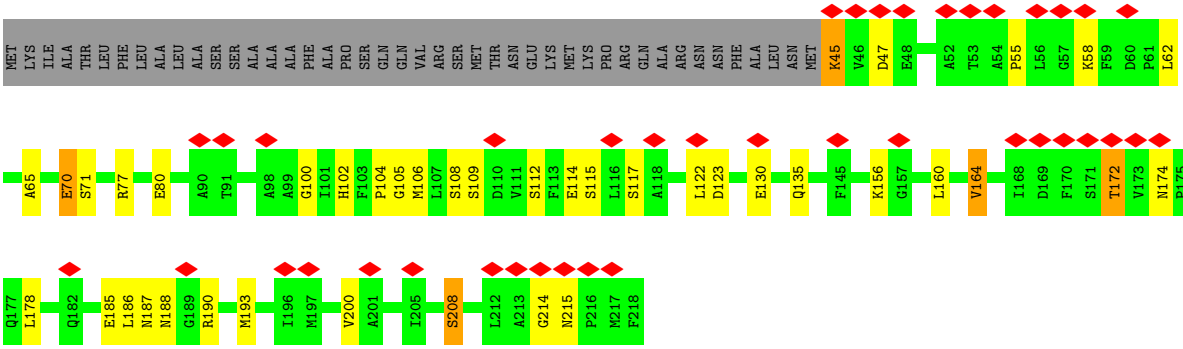




• Molecule 28: Fucoxanthin chlorophyll a/c-binding protein Lhcq5

Chain 16:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	0.401	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	560.952, 560.952, 560.952	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A86, SF4, BCR, LMG, LMT, KC1, CL0, PQN, LHG, DD6, CLA

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	0.33	0/6039	0.47	0/8220
2	B	0.33	0/6011	0.50	2/8209 (0.0%)
3	C	0.36	0/609	0.67	3/826 (0.4%)
4	D	0.32	0/1064	0.67	2/1437 (0.1%)
5	E	0.26	0/486	0.45	0/656
6	F	0.29	0/1287	0.47	0/1745
7	I	0.32	0/281	0.58	0/383
8	J	0.27	0/355	0.52	0/480
9	L	0.28	0/1054	0.48	0/1432
10	M	0.24	0/229	0.42	0/313
12	2u	0.26	0/696	0.40	0/948
13	1	0.21	0/1106	0.40	0/1490
14	2	0.28	0/1344	0.58	2/1818 (0.1%)
15	3	0.25	0/1309	0.55	0/1767
16	4	0.26	0/1404	0.48	0/1897
17	5	0.25	0/1336	0.49	0/1804
18	6	0.27	0/1391	0.47	0/1886
19	7	0.27	0/1445	0.48	0/1952
20	8	0.29	0/1706	0.50	0/2310
21	9	0.25	0/1302	0.52	0/1769
22	10	0.27	0/1344	0.52	0/1824
23	11	0.23	0/1522	0.56	2/2070 (0.1%)
24	12	0.29	0/1305	0.51	0/1776
25	13	0.23	0/1177	0.56	2/1592 (0.1%)
26	14	0.50	2/1660 (0.1%)	1.32	31/2255 (1.4%)
27	15	0.57	3/1705 (0.2%)	1.38	31/2319 (1.3%)
28	16	0.39	0/1347	0.98	8/1833 (0.4%)
All	All	0.32	5/40514 (0.0%)	0.64	83/55011 (0.2%)

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
4	D	0	1
11	1u	0	1
16	4	0	1
21	9	0	2
22	10	0	1
26	14	0	7
27	15	0	8
28	16	0	1
All	All	0	22

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	15	146	GLU	CB-CG	-6.90	1.31	1.52
26	14	245	MET	CB-CG	-6.32	1.33	1.52
26	14	50	LYS	CD-CE	-5.91	1.34	1.52
27	15	224	ARG	CD-NE	-5.43	1.38	1.46
27	15	224	ARG	CB-CG	-5.18	1.36	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	14	92	MET	CA-CB-CG	21.25	156.60	114.10
27	15	146	GLU	CA-CB-CG	17.81	149.72	114.10
27	15	224	ARG	NE-CZ-NH2	13.84	131.65	119.20
26	14	92	MET	CB-CG-SD	13.72	153.87	112.70
27	15	224	ARG	NE-CZ-NH1	-13.17	108.33	121.50
28	16	70	GLU	CA-CB-CG	10.37	134.83	114.10
27	15	269	GLN	CA-CB-CG	10.27	134.64	114.10
26	14	227	GLU	CA-CB-CG	9.54	133.18	114.10
26	14	206	GLU	CA-CB-CG	9.06	132.23	114.10
26	14	156	LYS	CB-CG-CD	-9.06	90.47	111.30
27	15	224	ARG	CD-NE-CZ	8.70	136.57	124.40
27	15	225	ARG	CD-NE-CZ	8.22	135.91	124.40
26	14	105	ILE	CG1-CB-CG2	-8.14	86.29	110.70
28	16	70	GLU	N-CA-CB	8.05	123.52	110.40
26	14	206	GLU	CB-CG-CD	7.80	125.87	112.60
26	14	92	MET	CB-CA-C	7.60	124.95	109.67
28	16	176	GLU	CA-CB-CG	7.37	128.84	114.10
26	14	227	GLU	CB-CA-C	7.33	121.89	109.50

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	14	82	GLN	CB-CG-CD	7.19	124.82	112.60
27	15	222	LYS	CB-CA-C	-7.12	97.68	110.70
27	15	225	ARG	CB-CG-CD	-6.91	95.40	111.30
27	15	269	GLN	CB-CG-CD	6.84	124.22	112.60
3	C	62	PHE	CA-C-N	6.82	134.56	121.54
3	C	62	PHE	C-N-CA	6.82	134.56	121.54
27	15	224	ARG	CB-CG-CD	6.79	126.93	111.30
26	14	206	GLU	CG-CD-OE2	-6.76	102.86	118.40
26	14	245	MET	CG-SD-CE	-6.68	86.19	100.90
26	14	105	ILE	CB-CG1-CD1	6.55	127.55	113.80
27	15	152	ILE	CA-C-N	6.51	142.62	127.00
27	15	152	ILE	C-N-CA	6.51	142.62	127.00
27	15	92	LYS	CD-CE-NZ	6.44	132.50	111.90
27	15	92	LYS	CA-CB-CG	6.35	126.80	114.10
26	14	223	GLU	CA-CB-CG	-6.29	101.53	114.10
26	14	122	ALA	CA-C-N	6.28	133.01	121.70
26	14	122	ALA	C-N-CA	6.28	133.01	121.70
27	15	254	PRO	CA-C-N	6.23	132.92	121.70
27	15	254	PRO	C-N-CA	6.23	132.92	121.70
26	14	156	LYS	CA-CB-CG	6.19	126.48	114.10
27	15	257	ASN	N-CA-CB	-6.10	100.18	110.49
27	15	71	LYS	CD-CE-NZ	6.07	131.33	111.90
28	16	214	GLY	CA-C-N	6.04	142.98	121.59
28	16	214	GLY	C-N-CA	6.04	142.98	121.59
26	14	114	ASP	CB-CA-C	-5.97	98.53	109.15
28	16	164	VAL	CG1-CB-CG2	-5.93	97.75	110.80
27	15	262	PRO	CA-C-N	5.92	132.84	121.54
27	15	262	PRO	C-N-CA	5.92	132.84	121.54
28	16	45	LYS	CB-CG-CD	5.87	124.80	111.30
4	D	91	GLU	CA-C-N	5.79	132.39	121.97
4	D	91	GLU	C-N-CA	5.79	132.39	121.97
27	15	152	ILE	C-N-CD	-5.65	108.17	120.60
26	14	178	HIS	CA-C-N	5.63	140.50	127.00
26	14	178	HIS	C-N-CA	5.63	140.50	127.00
27	15	169	LEU	CB-CG-CD1	-5.62	93.85	110.70
26	14	241	ASP	N-CA-CB	-5.61	103.72	112.41
26	14	199	LYS	CG-CD-CE	-5.54	98.57	111.30
27	15	179	LEU	CB-CG-CD2	5.51	127.23	110.70
27	15	265	GLY	N-CA-C	5.47	126.14	113.18
27	15	271	PHE	N-CA-CB	5.43	119.87	111.24
26	14	218	MET	CB-CG-SD	5.37	128.80	112.70
27	15	102	ARG	CG-CD-NE	-5.34	100.26	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	15	257	ASN	CB-CG-ND2	-5.33	108.40	116.40
26	14	116	THR	CA-CB-CG2	5.33	119.56	110.50
27	15	269	GLN	N-CA-C	5.32	121.56	109.81
27	15	215	LYS	CA-CB-CG	-5.29	103.51	114.10
26	14	241	ASP	CB-CA-C	5.29	119.98	111.36
27	15	71	LYS	CA-CB-CG	-5.24	103.62	114.10
28	16	215	ASN	N-CA-CB	-5.24	101.84	109.90
2	B	685	PRO	CA-C-N	5.18	131.44	121.54
2	B	685	PRO	C-N-CA	5.18	131.44	121.54
14	2	54	ASP	CA-C-N	-5.17	114.53	122.60
14	2	54	ASP	C-N-CA	-5.17	114.53	122.60
23	11	185	GLU	CA-C-N	5.17	131.00	121.70
23	11	185	GLU	C-N-CA	5.17	131.00	121.70
26	14	209	ASN	N-CA-CB	5.16	118.95	110.39
26	14	125	PRO	N-CA-C	5.15	116.98	110.70
27	15	220	GLU	CB-CA-C	-5.15	99.71	109.95
3	C	62	PHE	CA-CB-CG	-5.11	108.69	113.80
26	14	241	ASP	CA-CB-CG	5.09	117.69	112.60
26	14	156	LYS	CD-CE-NZ	-5.08	95.65	111.90
26	14	50	LYS	CG-CD-CE	5.03	122.87	111.30
25	13	239	PRO	CA-C-N	5.03	130.75	121.70
25	13	239	PRO	C-N-CA	5.03	130.75	121.70
26	14	82	GLN	CB-CA-C	-5.01	102.48	110.79

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	10	204	PRO	Peptide
26	14	123	GLY	Peptide
26	14	124	SER	Peptide
26	14	154	ALA	Peptide
26	14	161	GLY	Peptide
26	14	206	GLU	Sidechain
26	14	223	GLU	Sidechain
26	14	241	ASP	Sidechain
27	15	119	TYR	Sidechain
27	15	136	ALA	Peptide
27	15	225	ARG	Sidechain
27	15	257	ASN	Sidechain
27	15	264	SER	Peptide
27	15	268	MET	Peptide

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Mol	Chain	Res	Type	Group
27	15	270	PRO	Peptide
27	15	64	GLU	Sidechain
28	16	130	GLU	Sidechain
11	1u	97	UNK	Peptide
16	4	145	HIS	Sidechain
21	9	109	GLY	Peptide
21	9	113	ALA	Peptide
4	D	91	GLU	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	5841	0	5666	63	0
2	B	5801	0	5614	52	0
3	C	599	0	579	7	0
4	D	1037	0	1023	12	0
5	E	478	0	473	2	0
6	F	1257	0	1259	12	0
7	I	273	0	285	1	0
8	J	344	0	351	13	0
9	L	1030	0	1063	10	0
10	M	227	0	247	2	0
11	1u	650	0	138	4	0
12	2u	674	0	658	6	0
13	1	1086	0	1089	13	0
14	2	1310	0	1287	12	0
15	3	1275	0	1239	9	0
16	4	1368	0	1344	8	0
17	5	1304	0	1286	12	0
18	6	1354	0	1328	14	0
19	7	1416	0	1379	9	0
20	8	1660	0	1625	18	0
21	9	1267	0	1210	12	0
22	10	1302	0	1274	10	0
23	11	1479	0	1452	17	0
24	12	1274	0	1267	10	0
25	13	1148	0	1130	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	14	1609	0	1568	25	0
27	15	1654	0	1613	20	0
28	16	1313	0	1310	23	0
29	A	65	0	72	3	0
30	1	390	0	425	12	0
30	10	435	0	465	6	0
30	11	315	0	337	12	0
30	12	566	0	604	11	0
30	13	350	0	354	11	0
30	14	468	0	400	8	0
30	15	685	0	589	14	0
30	16	478	0	429	12	0
30	2	620	0	649	16	0
30	2u	65	0	72	3	0
30	3	472	0	474	7	0
30	4	484	0	495	12	0
30	5	455	0	499	12	0
30	6	620	0	656	10	0
30	7	566	0	609	13	0
30	8	420	0	427	7	0
30	9	486	0	503	12	0
30	A	2614	0	2694	85	0
30	B	2465	0	2570	85	0
30	F	175	0	177	7	0
30	J	45	0	33	1	0
30	L	110	0	105	6	0
31	A	33	0	46	5	0
31	B	33	0	46	1	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
33	2u	40	0	56	3	0
33	A	200	0	280	12	0
33	B	240	0	336	11	0
33	F	40	0	56	3	0
33	I	40	0	56	2	0
33	J	80	0	112	7	0
33	L	120	0	168	10	0
33	M	40	0	56	3	0
34	2	27	0	24	0	0
34	5	27	0	24	1	0
34	6	27	0	24	0	0
34	9	34	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	A	76	0	98	2	0
34	B	27	0	24	0	0
35	1	35	0	46	0	0
35	11	140	0	184	4	0
35	12	140	0	184	4	0
35	15	35	0	46	0	0
35	16	35	0	46	0	0
35	6	31	0	35	2	0
35	7	70	0	91	2	0
35	8	35	0	46	0	0
35	9	32	0	37	0	0
35	A	105	0	138	2	0
35	B	70	0	92	1	0
36	14	38	0	46	2	0
36	2u	31	0	31	0	0
36	3	37	0	44	2	0
36	5	33	0	36	0	0
36	6	33	0	34	0	0
36	7	37	0	44	0	0
36	8	108	0	123	1	0
36	A	34	0	38	3	0
36	B	98	0	141	3	0
36	F	27	0	24	0	0
37	1	48	0	0	0	0
37	10	240	0	0	0	0
37	11	192	0	0	1	0
37	12	96	0	0	0	0
37	13	93	0	0	0	0
37	14	384	0	0	2	0
37	15	336	0	0	0	0
37	16	96	0	0	0	0
37	2	144	0	0	0	0
37	2u	96	0	0	0	0
37	3	96	0	0	0	0
37	4	192	0	0	1	0
37	5	144	0	0	1	0
37	6	48	0	0	0	0
37	7	144	0	0	1	0
37	8	96	0	0	1	0
37	9	144	0	0	1	0
38	1	90	0	0	0	0
38	10	135	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	11	180	0	0	0	0
38	12	180	0	0	1	0
38	13	270	0	0	0	0
38	14	135	0	0	0	0
38	16	90	0	0	1	0
38	2	135	0	0	0	0
38	3	135	0	0	1	0
38	4	135	0	0	1	0
38	5	180	0	0	2	0
38	6	180	0	0	0	0
38	7	90	0	0	0	0
38	8	315	0	0	0	0
38	9	180	0	0	0	0
39	1	43	0	0	0	0
39	10	86	0	0	1	0
39	11	43	0	0	0	0
39	12	86	0	0	0	0
39	13	43	0	0	1	0
39	15	86	0	0	0	0
39	16	43	0	0	0	0
39	2	129	0	0	0	0
39	3	129	0	0	0	0
39	4	86	0	0	0	0
39	5	86	0	0	0	0
39	6	172	0	0	3	0
39	7	172	0	0	0	0
39	8	86	0	0	0	0
39	9	43	0	0	0	0
40	1	1	0	0	0	0
40	10	1	0	0	0	0
40	11	1	0	0	0	0
40	12	2	0	0	0	0
40	2	2	0	0	0	0
40	3	1	0	0	0	0
40	5	1	0	0	0	0
40	6	2	0	0	0	0
40	7	2	0	0	0	0
40	8	4	0	0	0	0
40	9	1	0	0	0	0
40	A	42	0	0	2	0
40	B	53	0	0	0	0
40	C	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	D	13	0	0	0	0
40	E	3	0	0	0	0
40	F	3	0	0	0	0
40	I	1	0	0	0	0
40	L	8	0	0	0	0
All	All	62199	0	55345	644	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (644) 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)
26:14:101:GLN:OE1	30:14:303:CLA:NA	2.01	0.94
23:11:44:GLU:OE1	30:11:310:CLA:NC	2.10	0.84
25:13:73:GLU:OE1	30:13:307:CLA:NC	2.11	0.83
27:15:105:GLU:OE1	30:15:302:CLA:NB	2.21	0.74
30:B:815:CLA:HBB1	33:B:841:BCR:H333	1.74	0.70
2:B:202:ARG:HG3	2:B:249:ALA:HB1	1.73	0.70
30:4:306:CLA:H42	30:4:306:CLA:HAA1	1.76	0.68
30:A:810:CLA:HBB1	33:J:102:BCR:HC7	1.76	0.68
30:A:802:CLA:H201	30:B:809:CLA:H2	1.75	0.68
27:15:127:PHE:O	27:15:138:HIS:NE2	2.26	0.67
4:D:42:GLU:H	4:D:72:GLN:HE22	1.41	0.66
2:B:402:ASN:HD22	2:B:405:ASN:HD21	1.43	0.66
21:9:59:ILE:O	21:9:86:ARG:NH2	2.29	0.66
30:3:302:CLA:HAC1	30:3:310:CLA:HAB	1.78	0.65
9:L:38:ARG:O	9:L:46:ARG:NH1	2.31	0.64
16:4:126:ALA:HB2	30:4:309:CLA:HBB1	1.79	0.64
30:A:843:CLA:H122	33:L:204:BCR:H19C	1.81	0.63
30:B:806:CLA:H162	30:B:827:CLA:HBB2	1.79	0.63
30:B:803:CLA:H13	33:I:101:BCR:H281	1.79	0.63
28:16:77:ARG:HG3	28:16:160:LEU:HD21	1.80	0.63
13:1:83:ALA:O	13:1:104:ARG:NH2	2.32	0.62
21:9:86:ARG:NH1	21:9:89:GLU:OE1	2.33	0.62
30:16:302:CLA:H202	30:16:302:CLA:HBB1	1.80	0.62
18:6:127:ILE:HB	30:6:314:CLA:HBC1	1.81	0.61
13:1:104:ARG:NH1	13:1:107:GLU:OE1	2.33	0.61
14:2:138:TRP:HB3	30:2:301:CLA:H2	1.81	0.61
18:6:73:ARG:NH2	18:6:76:GLU:OE1	2.33	0.61
15:3:123:LEU:HB2	30:3:310:CLA:HBC1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:188:LYS:HE3	13:1:192:GLU:HG3	1.81	0.61
28:16:55:PRO:HB3	30:16:307:CLA:HBB1	1.82	0.61
30:A:834:CLA:H142	33:B:846:BCR:H15C	1.82	0.61
26:14:224:GLN:HB3	26:14:240:TYR:HB3	1.81	0.61
30:A:816:CLA:HBB1	33:A:847:BCR:H333	1.83	0.61
3:C:73:THR:H	3:C:76:SER:HB3	1.66	0.61
30:2u:202:CLA:H8	30:2u:202:CLA:HBB1	1.83	0.61
22:10:75:ARG:NH2	22:10:78:GLU:OE1	2.34	0.61
27:15:217:MET:SD	27:15:225:ARG:NH2	2.74	0.60
30:B:821:CLA:H11	12:2u:112:ALA:HB2	1.83	0.60
17:5:84:ARG:NH1	17:5:87:GLU:OE1	2.34	0.60
30:B:836:CLA:HBC3	30:4:301:CLA:HAC1	1.83	0.60
20:8:58:MET:SD	20:8:58:MET:N	2.75	0.60
30:A:802:CLA:H13	33:B:846:BCR:H10C	1.83	0.60
25:13:84:ALA:HB2	30:13:301:CLA:HBA1	1.83	0.60
30:B:825:CLA:H112	33:B:844:BCR:H17C	1.83	0.60
23:11:56:ILE:HG13	23:11:57:LEU:HG	1.84	0.60
30:A:806:CLA:H12	30:A:807:CLA:HBB1	1.84	0.59
20:8:128:ARG:NH1	20:8:131:GLU:OE1	2.35	0.59
3:C:75:ARG:NH1	11:1u:25:UNK:O	2.35	0.59
26:14:245:MET:HG2	30:14:312:CLA:HBB1	1.85	0.59
30:7:309:CLA:H52	25:13:83:LEU:HD22	1.84	0.59
30:B:811:CLA:HAA2	13:1:96:ILE:HD13	1.85	0.58
26:14:101:GLN:OE1	30:14:303:CLA:C1A	2.50	0.58
27:15:232:ASN:ND2	30:15:309:CLA:OBD	2.36	0.58
2:B:337:LEU:HD21	30:B:828:CLA:HAB	1.85	0.58
14:2:72:ARG:NH1	30:2:303:CLA:O1D	2.37	0.58
30:B:809:CLA:H202	33:I:101:BCR:H353	1.85	0.58
1:A:715:GLN:NE2	5:E:16:TYR:OH	2.36	0.58
18:6:144:GLN:HA	18:6:148:GLU:HB2	1.86	0.58
23:11:134:LEU:O	23:11:138:GLN:NE2	2.37	0.58
14:2:91:ALA:HB1	14:2:96:LEU:HD23	1.86	0.57
30:A:842:CLA:H172	8:J:23:ALA:HB2	1.86	0.57
20:8:89:LEU:HB3	20:8:128:ARG:HH21	1.70	0.57
17:5:125:VAL:HG11	30:5:304:CLA:HAA2	1.86	0.57
15:3:111:HIS:HA	15:3:120:MET:HE2	1.86	0.57
30:A:804:CLA:H203	30:A:804:CLA:H101	1.86	0.57
1:A:30:ALA:HB1	8:J:6:LYS:HD2	1.88	0.56
30:A:842:CLA:H101	8:J:16:THR:HG23	1.88	0.56
30:A:839:CLA:H203	30:L:202:CLA:H171	1.88	0.56
18:6:79:HIS:HB3	18:6:188:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:309:CLA:H92	30:7:309:CLA:H2	1.87	0.56
20:8:187:LEU:HG	30:8:303:CLA:H12	1.88	0.56
36:A:856:LMG:HC62	8:J:3:ASN:HD22	1.71	0.56
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.87	0.56
26:14:98:TYR:OH	26:14:224:GLN:NE2	2.36	0.56
3:C:15:THR:OG1	3:C:19:ARG:NH1	2.39	0.56
28:16:135:GLN:OE1	38:16:304:KC1:ND	2.39	0.56
30:A:816:CLA:H8	33:A:848:BCR:H402	1.88	0.55
2:B:56:ILE:HD11	33:M:101:BCR:HC7	1.88	0.55
30:F:202:CLA:HED2	30:5:303:CLA:H93	1.88	0.55
17:5:57:PRO:HB3	17:5:70:ASP:HB3	1.89	0.55
36:8:319:LMG:HC8	36:8:321:LMG:H292	1.88	0.55
28:16:185:GLU:OE1	30:16:306:CLA:NA	2.39	0.55
1:A:349:TRP:HB3	30:A:806:CLA:HAC1	1.88	0.55
20:8:264:ASN:ND2	20:8:270:PHE:O	2.39	0.55
26:14:208:ASN:ND2	30:14:307:CLA:O1D	2.39	0.55
30:B:811:CLA:H171	30:1:303:CLA:H121	1.87	0.55
20:8:61:ARG:HH22	22:10:143:ALA:HB1	1.70	0.55
18:6:118:LEU:HB3	18:6:123:ALA:HB3	1.89	0.55
2:B:721:ALA:HB2	30:B:826:CLA:HBB1	1.87	0.55
18:6:98:ARG:NH2	18:6:109:LEU:O	2.40	0.55
1:A:121:ILE:O	1:A:123:GLY:N	2.40	0.54
2:B:190:THR:HG21	2:B:277:LEU:HB2	1.89	0.54
30:B:806:CLA:H102	30:B:806:CLA:H172	1.89	0.54
2:B:584:ASN:HB2	30:B:802:CLA:HBC2	1.89	0.54
1:A:60:ASP:N	1:A:60:ASP:OD1	2.40	0.54
4:D:62:ARG:NH2	4:D:64:GLU:OE2	2.39	0.54
26:14:159:MET:O	26:14:160:ARG:NH2	2.40	0.54
30:B:821:CLA:HHC	30:B:839:CLA:HED1	1.89	0.54
22:10:183:ARG:HA	22:10:186:MET:HE3	1.89	0.54
21:9:135:LEU:HA	21:9:138:VAL:HB	1.90	0.54
6:F:117:ILE:HG23	30:F:202:CLA:HAA1	1.90	0.54
18:6:165:LEU:HD22	18:6:173:VAL:HG12	1.89	0.54
2:B:180:GLY:HA3	30:B:813:CLA:HBB1	1.90	0.54
30:B:804:CLA:H2	33:M:101:BCR:HC21	1.91	0.54
1:A:151:GLU:HG2	1:A:213:TRP:HH2	1.73	0.53
30:B:821:CLA:H2	12:2u:50:MET:HE1	1.89	0.53
30:A:836:CLA:H2	33:A:851:BCR:H383	1.91	0.53
28:16:80:GLU:OE1	30:16:301:CLA:NA	2.41	0.53
6:F:155:THR:HG21	30:5:303:CLA:HED2	1.91	0.53
30:B:838:CLA:HAC2	33:B:846:BCR:H23C	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:70:ASP:OD1	25:13:70:ASP:N	2.40	0.53
25:13:183:THR:HG22	25:13:185:GLY:H	1.74	0.53
30:A:811:CLA:H172	30:A:813:CLA:H203	1.89	0.53
4:D:85:ARG:HB3	4:D:93:GLN:HB2	1.90	0.53
20:8:80:PRO:O	20:8:99:TYR:OH	2.25	0.53
25:13:173:THR:HG22	25:13:175:GLY:H	1.73	0.53
36:A:856:LMG:H142	35:6:302:LMT:H2'	1.91	0.53
6:F:154:MET:HE1	30:F:201:CLA:H8	1.91	0.53
14:2:87:VAL:HG12	30:2:305:CLA:HBC2	1.91	0.53
17:5:75:SER:HB3	30:5:302:CLA:HBA1	1.91	0.53
30:7:306:CLA:HHC	30:7:306:CLA:HBB1	1.91	0.53
1:A:336:GLU:HG2	1:A:424:ASN:HB3	1.91	0.52
35:11:318:LMT:H51	35:12:301:LMT:H62	1.91	0.52
1:A:501:ASN:HB2	30:A:837:CLA:HED2	1.91	0.52
2:B:173:ARG:HB2	30:B:813:CLA:HBC2	1.90	0.52
2:B:541:ARG:NH2	4:D:125:ASN:OD1	2.39	0.52
1:A:363:LEU:HD11	30:A:820:CLA:H71	1.89	0.52
30:A:805:CLA:HAB	30:A:812:CLA:H121	1.91	0.52
36:3:317:LMG:HC91	30:4:311:CLA:HAB	1.92	0.52
26:14:211:ARG:HA	26:14:214:MET:HE3	1.91	0.52
13:1:75:PRO:HB2	13:1:78:LEU:HB2	1.92	0.52
30:7:309:CLA:H122	30:13:301:CLA:H8	1.90	0.52
1:A:572:ARG:NH2	34:A:852:LHG:O2	2.42	0.52
2:B:66:PHE:HZ	10:M:7:VAL:HG13	1.75	0.52
23:11:158:VAL:HG22	35:11:303:LMT:H42	1.92	0.52
26:14:148:GLU:OE1	30:14:305:CLA:NA	2.43	0.52
30:A:820:CLA:HAB	30:A:820:CLA:H8	1.92	0.52
30:A:829:CLA:H161	30:A:842:CLA:H43	1.92	0.51
2:B:298:HIS:HB3	2:B:303:ILE:HD11	1.92	0.51
16:4:139:GLU:OE1	37:4:315:A86:O2	2.26	0.51
27:15:171:ASP:OD1	27:15:186:ARG:NH1	2.43	0.51
1:A:403:THR:HG21	1:A:596:LEU:HG	1.93	0.51
20:8:84:ASN:ND2	20:8:101:SER:O	2.43	0.51
23:11:205:ARG:NH2	30:11:304:CLA:O1D	2.42	0.51
2:B:428:LEU:HD11	30:B:835:CLA:HMB2	1.91	0.51
30:A:832:CLA:H42	30:9:308:CLA:H52	1.91	0.51
2:B:720:TYR:HB2	30:B:801:CLA:HED3	1.92	0.51
30:A:817:CLA:H2	30:A:817:CLA:HBD	1.92	0.51
30:B:806:CLA:H143	30:B:827:CLA:HBB2	1.92	0.51
4:D:116:ARG:HH22	4:D:138:GLU:HB2	1.75	0.51
13:1:101:THR:HG23	13:1:175:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:40:GLU:OE1	16:4:186:LYS:NZ	2.44	0.51
28:16:65:ALA:HB2	30:16:301:CLA:HBA1	1.93	0.51
30:A:813:CLA:H121	33:A:849:BCR:H343	1.93	0.51
14:2:54:ASP:HA	30:2:303:CLA:CGD	2.38	0.51
22:10:176:LEU:HG	22:10:180:LYS:HE2	1.92	0.51
30:A:833:CLA:H171	33:L:205:BCR:H333	1.92	0.51
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.92	0.51
30:A:833:CLA:H142	30:L:202:CLA:HAA2	1.92	0.51
18:6:45:TYR:OH	18:6:55:ASP:OD2	2.29	0.51
23:11:44:GLU:OE1	30:11:310:CLA:C4C	2.59	0.51
23:11:94:HIS:HB3	30:11:306:CLA:HED3	1.93	0.51
27:15:227:VAL:HG13	30:15:309:CLA:HED2	1.92	0.51
30:B:822:CLA:HBA2	33:2u:201:BCR:H17C	1.92	0.50
4:D:43:MET:HE1	4:D:58:LEU:HD21	1.93	0.50
19:7:152:ARG:NH2	19:7:155:GLU:OE1	2.42	0.50
1:A:748:SER:HA	1:A:751:ILE:HG12	1.93	0.50
30:B:826:CLA:HBC3	36:B:847:LMG:H421	1.93	0.50
17:5:172:LEU:HD22	30:5:308:CLA:H11	1.93	0.50
30:A:804:CLA:HHC	30:A:804:CLA:HBB1	1.94	0.50
11:1u:111:UNK:O	11:1u:114:UNK:N	2.44	0.50
19:7:124:ASP:OD1	19:7:124:ASP:N	2.42	0.50
23:11:115:TRP:O	35:11:317:LMT:O6'	2.29	0.50
30:B:824:CLA:HBB1	30:B:836:CLA:HHB	1.94	0.50
12:2u:53:MET:O	12:2u:116:GLN:NE2	2.39	0.50
17:5:176:LYS:HB3	17:5:180:GLU:HG3	1.93	0.50
30:A:821:CLA:HHC	30:A:821:CLA:HBB1	1.94	0.50
30:B:813:CLA:H112	30:B:818:CLA:H93	1.94	0.50
21:9:163:LEU:HD13	30:9:301:CLA:H91	1.94	0.50
2:B:291:ARG:NH1	2:B:295:GLY:O	2.44	0.50
30:7:303:CLA:H142	30:7:304:CLA:H161	1.93	0.50
27:15:193:PRO:HB2	27:15:195:THR:HG23	1.94	0.49
30:A:803:CLA:H91	31:A:845:PQN:H292	1.94	0.49
22:10:164:TYR:OH	22:10:175:GLN:NE2	2.44	0.49
1:A:470:ASP:OD1	9:L:69:ARG:NH2	2.45	0.49
30:B:827:CLA:H202	33:B:843:BCR:H17C	1.93	0.49
4:D:28:LYS:NZ	11:1u:64:UNK:O	2.45	0.49
18:6:98:ARG:HB3	18:6:102:LEU:HD13	1.94	0.49
21:9:206:ASN:HD22	21:9:210:GLN:HG3	1.77	0.49
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.93	0.49
21:9:118:LEU:HG	21:9:128:GLN:HB2	1.93	0.49
28:16:208:SER:HB3	30:16:309:CLA:C4D	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:HD13	30:A:831:CLA:HED3	1.93	0.49
30:A:817:CLA:H41	35:A:855:LMT:H6D	1.95	0.49
23:11:198:LEU:HD23	30:11:310:CLA:HED2	1.95	0.49
2:B:181:LEU:HD13	30:B:813:CLA:HHB	1.94	0.49
25:13:73:GLU:OE1	30:13:307:CLA:C1C	2.61	0.49
26:14:54:VAL:HG12	36:14:321:LMG:HC92	1.94	0.49
26:14:89:ARG:HA	26:14:92:MET:HE3	1.95	0.49
1:A:121:ILE:HD13	33:J:103:BCR:H313	1.94	0.49
1:A:396:TRP:CD1	30:A:829:CLA:HAB	2.47	0.49
1:A:696:GLU:OE1	2:B:549:LYS:NZ	2.39	0.49
9:L:143:LEU:HG	30:L:203:CLA:HED3	1.94	0.49
2:B:188:ALA:HA	30:B:815:CLA:HAB	1.95	0.48
2:B:340:LEU:HB3	2:B:381:LEU:HD13	1.95	0.48
13:1:187:ASN:ND2	13:1:192:GLU:OE2	2.46	0.48
2:B:22:TRP:CG	2:B:703:GLN:HE22	2.32	0.48
22:10:76:GLU:OE1	22:10:154:GLY:N	2.40	0.48
26:14:101:GLN:OE1	30:14:303:CLA:C4A	2.62	0.48
30:A:806:CLA:H72	33:A:849:BCR:H23C	1.94	0.48
27:15:222:LYS:O	27:15:226:LEU:N	2.43	0.48
23:11:77:ARG:NH1	23:11:172:GLY:O	2.47	0.48
1:A:217:GLN:HA	1:A:221:ALA:HB3	1.95	0.48
30:A:839:CLA:H201	30:L:202:CLA:H102	1.95	0.48
30:B:807:CLA:HBB1	30:B:807:CLA:H111	1.96	0.48
4:D:40:ILE:HG12	4:D:50:ILE:HG12	1.95	0.48
20:8:257:GLN:NE2	37:8:315:A86:O2	2.45	0.48
1:A:580:ARG:NH1	40:A:908:HOH:O	2.45	0.48
30:B:805:CLA:HBA1	30:B:805:CLA:H3A	1.74	0.48
30:B:817:CLA:HBC1	30:B:819:CLA:H193	1.96	0.48
36:B:849:LMG:H132	36:B:849:LMG:H301	1.96	0.48
13:1:86:ARG:NH2	13:1:198:GLU:OE2	2.44	0.48
27:15:228:SER:O	27:15:232:ASN:ND2	2.47	0.48
1:A:574:PRO:HB3	1:A:721:ILE:HB	1.96	0.47
8:J:20:THR:HG22	33:J:103:BCR:H15C	1.95	0.47
2:B:410:MET:HE2	33:2u:201:BCR:H323	1.96	0.47
11:1u:98:UNK:HA	11:1u:99:UNK:HA	1.76	0.47
26:14:68:ILE:O	37:14:317:A86:O2	2.32	0.47
26:14:82:GLN:HG2	26:14:158:TYR:CD1	2.49	0.47
27:15:80:ASP:HB3	30:15:302:CLA:HBA2	1.96	0.47
30:15:307:CLA:HHC	30:15:307:CLA:HBB1	1.96	0.47
1:A:289:LEU:HD21	1:A:374:MET:HB3	1.97	0.47
30:B:831:CLA:H61	30:B:831:CLA:H41	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:177:LYS:HD2	30:2:310:CLA:HBD	1.96	0.47
28:16:122:LEU:HD11	28:16:200:VAL:HG12	1.96	0.47
8:J:36:MET:HE1	8:J:41:PHE:HA	1.95	0.47
20:8:270:PHE:HA	30:8:308:CLA:HED2	1.95	0.47
23:11:59:ASP:OD2	23:11:59:ASP:N	2.43	0.47
2:B:449:GLU:OE1	6:F:76:ARG:NE	2.42	0.47
24:12:160:ASP:OD1	24:12:163:THR:OG1	2.31	0.47
30:A:829:CLA:H121	30:A:831:CLA:H18	1.97	0.47
30:A:839:CLA:H191	30:L:202:CLA:H72	1.96	0.47
14:2:53:GLY:HA2	14:2:176:LEU:HD13	1.97	0.47
30:7:311:CLA:H162	30:7:311:CLA:H122	1.67	0.47
28:16:187:ASN:HA	28:16:190:ARG:HD2	1.97	0.47
30:6:307:CLA:H61	30:6:307:CLA:H41	1.64	0.47
30:7:309:CLA:H52	30:7:309:CLA:H8	1.60	0.47
28:16:187:ASN:HA	28:16:190:ARG:HB2	1.95	0.47
29:A:801:CL0:H13	30:B:801:CLA:HAA1	1.97	0.47
30:A:833:CLA:H111	33:L:205:BCR:H312	1.97	0.47
16:4:189:ARG:HA	16:4:192:MET:HE3	1.96	0.47
17:5:187:LYS:NZ	38:5:310:KC1:O1A	2.39	0.47
30:A:836:CLA:H41	30:A:836:CLA:H62	1.73	0.47
30:B:808:CLA:H141	30:B:808:CLA:HBA2	1.96	0.47
30:B:851:CLA:H13	30:2:307:CLA:HBB1	1.97	0.47
24:12:39:THR:HG21	24:12:173:ASN:HD21	1.79	0.47
30:B:827:CLA:H3A	30:B:827:CLA:HBA2	1.64	0.46
4:D:23:ALA:HB1	4:D:28:LYS:HD2	1.97	0.46
13:1:205:ARG:NH2	30:1:301:CLA:O1D	2.47	0.46
30:12:310:CLA:H162	30:12:310:CLA:H122	1.69	0.46
1:A:538:ILE:HD12	29:A:801:CL0:H63	1.97	0.46
2:B:421:LEU:HD13	2:B:531:LEU:HA	1.97	0.46
30:B:811:CLA:HBA2	30:1:302:CLA:H52	1.98	0.46
15:3:93:ARG:HH12	15:3:104:ILE:HB	1.79	0.46
1:A:220:ILE:HG23	1:A:240:PRO:HB3	1.96	0.46
31:A:845:PQN:H141	30:F:201:CLA:HBB2	1.98	0.46
18:6:198:ALA:HA	18:6:208:VAL:HG12	1.97	0.46
25:13:97:HIS:ND1	25:13:184:PRO:O	2.49	0.46
26:14:51:SER:HB2	26:14:208:ASN:HD21	1.81	0.46
2:B:526:LEU:HD12	30:B:836:CLA:HED3	1.98	0.46
18:6:206:PRO:O	39:6:318:DD6:O2	2.33	0.46
26:14:114:ASP:OD2	26:14:114:ASP:N	2.45	0.46
30:B:830:CLA:H18	33:F:204:BCR:H17C	1.97	0.46
3:C:4:THR:HB	3:C:68:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:HE3	18:6:143:ILE:HG21	1.97	0.46
30:13:307:CLA:HHC	30:13:307:CLA:HBB1	1.97	0.46
1:A:508:TYR:HB2	1:A:523:MET:HG3	1.97	0.46
30:A:810:CLA:H152	30:A:812:CLA:H152	1.97	0.46
30:A:834:CLA:H161	30:B:838:CLA:HBA2	1.98	0.46
30:B:806:CLA:H41	30:B:806:CLA:H61	1.68	0.46
30:B:828:CLA:H192	30:B:838:CLA:H3A	1.98	0.46
30:B:838:CLA:H18	7:I:20:ALA:HB2	1.98	0.46
1:A:226:LYS:HG2	1:A:253:LEU:HD22	1.98	0.46
2:B:237:ASP:HB2	2:B:268:TRP:HZ3	1.81	0.46
30:2:303:CLA:HBA2	30:2:303:CLA:H3A	1.45	0.46
17:5:193:ARG:HA	17:5:196:MET:HE3	1.98	0.46
30:11:304:CLA:H41	30:11:304:CLA:H61	1.62	0.46
28:16:164:VAL:HG23	30:16:310:CLA:HED2	1.97	0.46
30:7:309:CLA:H162	25:13:81:LEU:HD11	1.98	0.46
35:12:320:LMT:H91	35:12:320:LMT:H62	1.79	0.46
1:A:370:HIS:ND1	30:A:819:CLA:OBD	2.49	0.46
30:A:804:CLA:H162	30:A:804:CLA:H122	1.72	0.46
2:B:350:HIS:ND1	30:B:817:CLA:OBD	2.46	0.46
30:B:835:CLA:H152	33:F:204:BCR:H23C	1.97	0.46
30:1:307:CLA:H162	30:1:307:CLA:H122	1.73	0.46
24:12:169:ASP:HB2	30:12:308:CLA:HED2	1.96	0.46
30:A:835:CLA:HHD	30:B:809:CLA:HBB2	1.98	0.45
9:L:41:LEU:HD21	30:9:302:CLA:HED1	1.97	0.45
21:9:72:GLY:HA3	22:10:66:ARG:HB3	1.98	0.45
28:16:188:ASN:ND2	30:16:307:CLA:OBD	2.49	0.45
1:A:413:MET:O	1:A:558:ARG:NH1	2.39	0.45
1:A:719:LEU:HD21	31:A:845:PQN:H151	1.99	0.45
2:B:132:GLN:NE2	10:M:1:MET:O	2.46	0.45
25:13:65:ILE:HG21	25:13:92:LEU:HG	1.98	0.45
26:14:183:ASN:O	37:14:320:A86:O2	2.35	0.45
1:A:363:LEU:HD21	30:A:820:CLA:H93	1.98	0.45
14:2:43:PRO:HG3	15:3:146:GLU:HG3	1.98	0.45
19:7:134:ASP:OD1	37:7:315:A86:O2	2.33	0.45
37:9:316:A86:O2	37:9:316:A86:O	2.35	0.45
24:12:170:SER:O	24:12:174:ASN:ND2	2.42	0.45
1:A:289:LEU:HB2	1:A:294:ILE:HD11	1.98	0.45
30:A:826:CLA:H143	30:A:826:CLA:H111	1.82	0.45
6:F:156:THR:HG22	17:5:150:THR:HB	1.98	0.45
2:B:524:LEU:HD21	30:B:802:CLA:HBB1	1.99	0.45
6:F:31:LYS:NZ	6:F:81:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:102:PRO:HG2	14:2:105:LEU:HD12	1.98	0.45
30:3:305:CLA:H61	30:3:305:CLA:H41	1.64	0.45
30:5:307:CLA:HBA2	30:5:307:CLA:H3A	1.65	0.45
24:12:159:VAL:HG13	26:14:62:GLN:HB2	1.97	0.45
36:A:856:LMG:H291	8:J:1:MET:HE2	1.98	0.45
9:L:75:LEU:HG	9:L:140:LEU:HD12	1.98	0.45
13:1:189:SER:OG	13:1:190:GLU:N	2.49	0.45
30:4:302:CLA:H3A	30:4:302:CLA:HBA2	1.76	0.45
25:13:90:GLU:OE1	25:13:180:ARG:NH1	2.48	0.45
28:16:77:ARG:NH2	30:16:301:CLA:O1D	2.44	0.45
1:A:95:GLY:O	1:A:99:SER:OG	2.28	0.45
31:B:840:PQN:H222	31:B:840:PQN:H261	1.75	0.45
5:E:2:VAL:HG12	5:E:60:GLU:HG2	1.98	0.45
6:F:158:TYR:HE1	30:5:307:CLA:HMB1	1.82	0.45
13:1:195:LYS:HA	13:1:198:GLU:HB2	1.98	0.45
30:15:313:CLA:H61	30:15:313:CLA:H41	1.74	0.45
28:16:104:PRO:HA	28:16:105:GLY:HA2	1.65	0.45
20:8:134:HIS:HB3	20:8:248:MET:HE3	1.97	0.45
30:F:202:CLA:H71	30:F:202:CLA:H111	1.65	0.45
30:6:316:CLA:H8	30:6:316:CLA:H52	1.79	0.45
30:12:321:CLA:HHC	30:12:321:CLA:HBB1	1.99	0.45
26:14:169:ASN:HB3	26:14:183:ASN:CG	2.42	0.45
28:16:102:HIS:NE2	28:16:114:GLU:HG2	2.32	0.45
33:A:847:BCR:H20C	33:A:847:BCR:H361	1.75	0.45
2:B:215:PRO:HA	2:B:216:PRO:HD3	1.90	0.45
30:12:308:CLA:H41	30:12:308:CLA:H62	1.79	0.45
30:A:809:CLA:H3A	30:A:809:CLA:HBA2	1.62	0.44
33:L:204:BCR:H20C	33:L:204:BCR:H361	1.78	0.44
15:3:99:TYR:OH	38:3:304:KC1:OBD	2.33	0.44
26:14:190:PHE:HA	26:14:191:SER:HA	1.72	0.44
16:4:180:TYR:CD2	30:4:306:CLA:H2	2.51	0.44
18:6:116:ASP:OD1	39:6:321:DD6:O2	2.35	0.44
37:11:315:A86:O3	35:11:317:LMT:O6'	2.35	0.44
27:15:132:THR:HG23	27:15:134:ALA:H	1.82	0.44
28:16:190:ARG:HA	28:16:193:MET:HE3	1.98	0.44
2:B:386:PHE:HZ	30:B:824:CLA:HAB	1.83	0.44
30:1:304:CLA:HBA2	30:1:304:CLA:H3A	1.78	0.44
16:4:167:GLY:HA3	16:4:168:LEU:HG	1.99	0.44
19:7:119:ARG:HH21	19:7:121:PRO:HA	1.82	0.44
30:9:307:CLA:HBA2	30:9:307:CLA:H3A	1.61	0.44
1:A:121:ILE:HB	33:J:103:BCR:H322	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:PHE:HA	31:A:845:PQN:H9	1.99	0.44
30:A:835:CLA:H152	33:L:201:BCR:H372	1.98	0.44
33:L:205:BCR:H323	30:9:306:CLA:HBA1	1.99	0.44
25:13:231:ALA:HA	25:13:238:VAL:HB	2.00	0.44
27:15:167:LEU:HD23	30:15:313:CLA:H43	2.00	0.44
30:15:303:CLA:HHC	30:15:303:CLA:HBB1	1.99	0.44
30:A:812:CLA:H111	30:A:812:CLA:H72	1.80	0.44
30:B:833:CLA:HBA2	30:B:833:CLA:H3A	1.65	0.44
30:4:306:CLA:H141	30:4:306:CLA:H162	1.86	0.44
25:13:79:ASP:OD2	39:13:314:DD6:O4	2.36	0.44
27:15:255:LEU:HA	27:15:256:LEU:HA	1.71	0.44
1:A:215:GLY:HA3	30:A:816:CLA:HAB	1.99	0.44
30:A:826:CLA:HBA1	30:A:830:CLA:H193	2.00	0.44
2:B:49:SER:HB2	30:B:805:CLA:HBB1	1.99	0.44
14:2:138:TRP:CE3	30:2:307:CLA:HHB	2.53	0.44
15:3:40:VAL:O	15:3:69:ARG:NH2	2.39	0.44
30:10:303:CLA:HBA2	30:10:303:CLA:H3A	1.75	0.44
24:12:166:ARG:NH2	38:12:309:KC1:OBD	2.51	0.44
21:9:131:THR:HA	21:9:134:TRP:HB2	2.00	0.44
30:9:307:CLA:H112	30:9:307:CLA:H71	1.70	0.44
23:11:184:ARG:HD3	23:11:185:GLU:HG2	1.99	0.44
30:11:308:CLA:H41	30:11:308:CLA:H92	1.99	0.44
33:A:850:BCR:H20C	33:A:850:BCR:H361	1.78	0.44
8:J:28:GLU:OE1	8:J:31:ARG:NH2	2.51	0.44
15:3:67:TRP:HB2	36:3:317:LMG:HC61	1.99	0.44
16:4:180:TYR:CG	30:4:306:CLA:H2	2.53	0.44
38:4:310:KC1:O1A	17:5:132:GLN:NE2	2.50	0.44
37:5:315:A86:O2	37:5:315:A86:O	2.36	0.44
27:15:149:TRP:NE1	27:15:266:GLN:O	2.49	0.44
1:A:297:HIS:HE2	30:A:820:CLA:C2B	2.31	0.43
30:A:813:CLA:H41	30:A:813:CLA:H62	1.80	0.43
30:A:814:CLA:H41	30:A:814:CLA:H61	1.80	0.43
2:B:344:THR:HB	2:B:378:ALA:HB2	2.00	0.43
30:B:813:CLA:H42	33:B:842:BCR:H19C	2.00	0.43
6:F:144:ILE:HG12	8:J:10:THR:HG22	2.00	0.43
9:L:41:LEU:HB3	9:L:46:ARG:HG2	2.00	0.43
13:1:212:THR:HG22	30:1:307:CLA:HBC2	2.00	0.43
30:9:307:CLA:H61	30:9:307:CLA:H41	1.70	0.43
1:A:409:ALA:HB1	33:A:850:BCR:HC42	2.00	0.43
26:14:82:GLN:HG2	26:14:158:TYR:CG	2.52	0.43
28:16:58:LYS:HE2	28:16:58:LYS:HB3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HG3	33:A:848:BCR:H322	2.00	0.43
30:A:821:CLA:H41	30:A:821:CLA:H62	1.63	0.43
30:B:837:CLA:H62	30:B:837:CLA:H41	1.83	0.43
6:F:90:ASP:OD2	6:F:90:ASP:N	2.45	0.43
28:16:186:LEU:O	28:16:190:ARG:N	2.50	0.43
1:A:86:LEU:HD22	30:A:810:CLA:H202	2.00	0.43
1:A:349:TRP:CD1	30:A:826:CLA:H202	2.53	0.43
30:4:305:CLA:H62	30:4:305:CLA:H41	1.68	0.43
30:A:810:CLA:H42	33:J:102:BCR:H21C	2.01	0.43
30:2:304:CLA:H2	30:2:304:CLA:HED2	2.01	0.43
30:10:303:CLA:H112	30:10:303:CLA:H151	1.68	0.43
30:10:309:CLA:H101	30:10:309:CLA:H62	1.73	0.43
1:A:51:ASN:ND2	40:A:909:HOH:O	2.50	0.43
1:A:250:MET:HE2	1:A:250:MET:HB3	1.96	0.43
1:A:393:HIS:CE1	30:A:829:CLA:ND	2.86	0.43
1:A:419:PRO:HG2	4:D:42:GLU:HB2	2.01	0.43
2:B:376:TYR:CD1	30:B:826:CLA:HAB	2.54	0.43
30:B:838:CLA:H62	30:B:838:CLA:H41	1.72	0.43
20:8:236:MET:HE1	30:8:305:CLA:H43	2.01	0.43
30:9:305:CLA:H91	30:9:305:CLA:H112	1.81	0.43
30:15:313:CLA:H122	30:15:313:CLA:H162	1.88	0.43
28:16:172:THR:HG22	28:16:174:ASN:H	1.83	0.43
1:A:268:HIS:NE2	35:A:857:LMT:O5B	2.47	0.43
1:A:680:TRP:O	1:A:683:SER:OG	2.32	0.43
30:B:824:CLA:H172	30:4:301:CLA:HBC1	2.00	0.43
23:11:95:PHE:N	30:11:306:CLA:OBD	2.48	0.43
24:12:85:ALA:HB3	24:12:87:ILE:HD12	2.00	0.43
30:16:301:CLA:H142	30:16:301:CLA:H112	1.85	0.43
30:A:833:CLA:H111	30:A:833:CLA:H91	1.91	0.43
33:2u:201:BCR:H373	30:2u:202:CLA:H152	2.01	0.43
1:A:631:ILE:HD13	1:A:751:ILE:HD12	2.01	0.43
29:A:801:CL0:C1A	30:B:801:CLA:HAB	2.49	0.43
30:A:830:CLA:HHC	30:A:830:CLA:HBB1	2.00	0.43
2:B:579:MET:HG3	2:B:709:LEU:HD21	2.01	0.43
30:B:804:CLA:H41	33:L:204:BCR:HC32	2.01	0.43
30:B:837:CLA:H52	30:B:838:CLA:H93	2.00	0.43
33:B:845:BCR:H361	33:B:845:BCR:H20C	1.77	0.43
30:3:303:CLA:H92	30:3:303:CLA:H61	1.84	0.43
30:16:301:CLA:H143	30:16:301:CLA:H161	1.88	0.43
30:7:311:CLA:H61	35:7:321:LMT:H42	2.01	0.43
20:8:170:THR:OG1	20:8:173:GLU:OE1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:10:99:ARG:HH12	22:10:110:ILE:HG13	1.83	0.43
23:11:176:TYR:HB3	30:11:309:CLA:HMD3	2.00	0.43
1:A:245:ILE:HG22	35:7:301:LMT:H51	2.01	0.42
30:A:841:CLA:H172	6:F:125:GLY:HA2	2.00	0.42
3:C:29:VAL:HG12	4:D:110:ARG:HB3	2.01	0.42
4:D:28:LYS:HB3	4:D:86:ILE:HB	2.01	0.42
30:6:309:CLA:H91	30:6:309:CLA:H112	1.82	0.42
30:11:308:CLA:H162	30:11:308:CLA:H122	1.68	0.42
24:12:174:ASN:ND2	30:12:308:CLA:OBD	2.52	0.42
30:A:811:CLA:H112	30:A:811:CLA:H72	1.75	0.42
30:2:311:CLA:H141	30:3:303:CLA:H171	2.00	0.42
17:5:48:SER:OG	17:5:68:GLY:O	2.35	0.42
18:6:111:ALA:O	39:6:319:DD6:O2	2.37	0.42
30:12:303:CLA:H2	30:12:303:CLA:HED3	2.01	0.42
30:13:307:CLA:H41	30:13:307:CLA:H62	1.86	0.42
27:15:64:GLU:HG2	27:15:65:LEU:N	2.33	0.42
30:A:829:CLA:H143	30:A:829:CLA:H112	1.85	0.42
31:A:845:PQN:H18	31:A:845:PQN:H222	1.79	0.42
2:B:181:LEU:HD21	30:B:813:CLA:H12	2.00	0.42
30:B:806:CLA:H51	30:B:828:CLA:H92	2.01	0.42
30:3:301:CLA:H61	30:3:301:CLA:H41	1.91	0.42
30:12:312:CLA:H193	30:12:312:CLA:H161	1.89	0.42
28:16:108:SER:OG	28:16:109:SER:N	2.53	0.42
1:A:199:ASN:HB3	30:A:821:CLA:HMD1	2.02	0.42
30:A:824:CLA:H52	30:A:824:CLA:H11	1.77	0.42
2:B:298:HIS:CE1	30:B:820:CLA:NA	2.87	0.42
2:B:351:MET:HB3	2:B:351:MET:HE2	1.82	0.42
30:B:812:CLA:HAC2	30:1:302:CLA:H13	2.01	0.42
30:2:308:CLA:HBA2	30:2:308:CLA:H3A	1.67	0.42
30:5:304:CLA:H3A	30:5:304:CLA:HBA2	1.74	0.42
30:6:314:CLA:H41	30:6:314:CLA:H62	1.57	0.42
26:14:133:SER:O	26:14:137:LYS:HE3	2.19	0.42
1:A:397:ILE:HG21	30:A:830:CLA:HHC	2.02	0.42
1:A:584:CYS:HB2	2:B:666:TRP:HB3	2.02	0.42
30:A:833:CLA:H61	30:A:833:CLA:H41	1.69	0.42
33:A:849:BCR:H15C	33:A:849:BCR:H351	1.86	0.42
17:5:117:ASP:OD2	17:5:206:ASN:ND2	2.51	0.42
30:6:309:CLA:H92	30:6:309:CLA:H62	1.85	0.42
20:8:223:SER:HB2	20:8:226:LYS:HB2	2.00	0.42
35:12:319:LMT:H6E	35:12:319:LMT:H5B	2.01	0.42
33:F:204:BCR:H353	30:4:301:CLA:H2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:12:PRO:HB2	33:J:103:BCR:H391	2.01	0.42
12:2u:50:MET:HG2	12:2u:58:LEU:HD21	2.01	0.42
30:10:304:CLA:H2	30:10:304:CLA:HED3	2.02	0.42
19:7:117:MET:HE2	19:7:117:MET:HB3	1.95	0.42
30:7:306:CLA:H3A	30:7:306:CLA:HBA1	1.82	0.42
30:7:307:CLA:HBA2	30:7:307:CLA:H3A	1.66	0.42
20:8:225:LEU:HD13	20:8:233:ILE:HG12	2.01	0.42
25:13:222:MET:HE1	30:13:301:CLA:HHC	2.00	0.42
27:15:163:VAL:O	27:15:167:LEU:N	2.47	0.42
30:A:805:CLA:H2	30:A:812:CLA:H92	2.01	0.42
30:A:811:CLA:H203	30:A:811:CLA:H161	1.89	0.42
2:B:274:HIS:HB3	30:B:817:CLA:HMB1	2.02	0.42
30:1:304:CLA:H101	30:1:304:CLA:H62	1.91	0.42
14:2:84:LEU:HD22	30:2:305:CLA:H93	2.01	0.42
30:2:309:CLA:H41	30:2:309:CLA:H62	1.75	0.42
30:3:306:CLA:H142	30:3:306:CLA:H111	1.88	0.42
30:7:307:CLA:H151	30:13:302:CLA:H8	2.00	0.42
23:11:111:SER:OG	23:11:112:GLU:N	2.53	0.42
28:16:106:MET:HA	28:16:112:SER:HA	2.00	0.42
30:A:822:CLA:HBC3	30:A:828:CLA:H193	2.02	0.42
2:B:91:ILE:HB	2:B:111:PRO:HB2	2.01	0.42
30:B:816:CLA:HBA2	30:B:816:CLA:H3A	1.70	0.42
33:B:844:BCR:H24C	33:B:844:BCR:H371	1.84	0.42
3:C:66:ARG:HA	3:C:66:ARG:HD2	1.86	0.42
30:F:201:CLA:H101	8:J:14:LEU:HD22	2.01	0.42
14:2:180:LYS:HD3	30:2:309:CLA:CAD	2.50	0.42
15:3:83:VAL:HG23	15:3:186:ILE:HD12	2.02	0.42
35:6:302:LMT:O3'	35:6:302:LMT:O2B	2.36	0.42
20:8:228:LYS:HB3	20:8:232:GLU:HG3	2.02	0.42
22:10:204:PRO:O	39:10:313:DD6:O2	2.36	0.42
26:14:122:ALA:H	26:14:123:GLY:HA2	1.83	0.42
30:A:820:CLA:HBA2	30:A:820:CLA:H3A	1.88	0.42
30:A:829:CLA:H91	30:A:831:CLA:H192	2.02	0.42
8:J:31:ARG:NH2	30:J:101:CLA:O1D	2.53	0.42
30:2:303:CLA:H61	30:2:303:CLA:H41	1.88	0.42
19:7:187:LYS:HA	19:7:187:LYS:HD3	1.86	0.42
30:15:304:CLA:H3A	30:15:304:CLA:HBA2	1.86	0.42
1:A:75:SER:OG	1:A:177:GLY:O	2.34	0.41
1:A:197:MET:HB3	30:A:826:CLA:HMD1	2.02	0.41
30:A:820:CLA:HAB	30:A:820:CLA:H111	2.01	0.41
30:B:807:CLA:HHB	30:B:808:CLA:HMB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:15:105:GLU:HA	27:15:108:HIS:HB2	2.00	0.41
1:A:44:LYS:HE3	1:A:44:LYS:HB2	1.81	0.41
2:B:480:PRO:HA	2:B:485:THR:HG21	2.02	0.41
30:B:830:CLA:H62	30:B:830:CLA:H2	1.75	0.41
25:13:183:THR:HB	25:13:186:LYS:HD3	2.00	0.41
30:13:301:CLA:H91	30:13:301:CLA:H112	1.85	0.41
30:15:302:CLA:H102	30:15:303:CLA:H61	2.01	0.41
2:B:141:LEU:HD21	33:B:843:BCR:H24C	2.03	0.41
2:B:476:LEU:O	2:B:485:THR:OG1	2.38	0.41
38:5:312:KC1:C4D	34:5:317:LHG:HC81	2.50	0.41
19:7:156:ILE:HG21	19:7:234:GLY:HA3	2.02	0.41
27:15:101:LEU:HD23	27:15:101:LEU:HA	1.89	0.41
28:16:100:GLY:O	28:16:102:HIS:ND1	2.51	0.41
9:L:89:LEU:HB3	33:L:204:BCR:H401	2.02	0.41
33:L:201:BCR:H20C	33:L:201:BCR:H361	1.86	0.41
30:L:203:CLA:HBA1	30:L:203:CLA:H3A	1.82	0.41
30:2:309:CLA:HBA2	30:2:310:CLA:HMD3	2.03	0.41
30:11:304:CLA:H3A	30:11:304:CLA:HBA2	1.82	0.41
30:12:302:CLA:H61	30:12:302:CLA:H41	1.65	0.41
1:A:710:PHE:HB3	6:F:126:ARG:HG3	2.03	0.41
30:A:833:CLA:HAA1	9:L:22:THR:HG22	2.02	0.41
33:A:849:BCR:H20C	33:A:849:BCR:H361	1.84	0.41
30:B:835:CLA:H142	30:B:835:CLA:H112	1.93	0.41
33:J:102:BCR:H15C	33:J:102:BCR:H351	1.90	0.41
24:12:152:PRO:HG3	30:12:321:CLA:H8	1.70	0.41
27:15:116:PHE:HE2	27:15:243:PHE:HE2	1.68	0.41
2:B:148:LEU:HD21	30:1:302:CLA:H201	2.01	0.41
2:B:261:HIS:HD2	2:B:264:THR:H	1.69	0.41
2:B:425:SER:HB3	2:B:528:VAL:HG22	2.01	0.41
30:5:302:CLA:H162	30:5:302:CLA:H122	1.81	0.41
30:8:305:CLA:H142	30:8:305:CLA:H112	1.85	0.41
21:9:145:GLU:OE1	30:9:307:CLA:NA	2.53	0.41
26:14:176:ILE:HA	26:14:177:PRO:HD3	1.86	0.41
36:14:321:LMG:HC71	27:15:173:CYS:SG	2.60	0.41
28:16:80:GLU:OE1	30:16:301:CLA:C4A	2.69	0.41
1:A:36:SER:HB3	1:A:39:LEU:HB2	2.02	0.41
1:A:393:HIS:HE2	30:A:830:CLA:C1B	2.34	0.41
30:A:819:CLA:HBA2	30:A:819:CLA:H3A	1.79	0.41
30:A:831:CLA:H142	30:A:831:CLA:H112	1.91	0.41
30:B:801:CLA:H102	30:B:801:CLA:H62	1.82	0.41
30:B:809:CLA:H101	30:B:826:CLA:H171	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:812:CLA:H121	30:B:812:CLA:H162	1.89	0.41
30:10:309:CLA:H41	30:10:309:CLA:H61	1.69	0.41
23:11:44:GLU:OE1	30:11:310:CLA:C1C	2.67	0.41
35:12:301:LMT:H71	35:12:301:LMT:H102	1.92	0.41
25:13:168:PHE:HB3	25:13:188:MET:HE2	2.03	0.41
30:14:302:CLA:H3A	30:14:302:CLA:HBA2	1.86	0.41
30:A:817:CLA:H11	30:6:316:CLA:CGA	2.51	0.41
2:B:186:SER:OG	2:B:276:GLN:O	2.39	0.41
30:B:828:CLA:H142	36:B:847:LMG:H212	2.03	0.41
12:2u:107:TRP:O	12:2u:110:HIS:ND1	2.53	0.41
30:1:303:CLA:H143	30:1:303:CLA:H112	1.83	0.41
15:3:160:SER:OG	15:3:161:SER:N	2.52	0.41
19:7:242:GLY:O	25:13:88:SER:OG	2.35	0.41
30:10:303:CLA:H192	30:10:307:CLA:H203	2.03	0.41
30:13:301:CLA:HBA2	30:13:301:CLA:H3A	1.77	0.41
30:A:822:CLA:H101	33:A:851:BCR:H10C	2.02	0.41
30:B:806:CLA:H111	30:B:806:CLA:H72	1.79	0.41
30:B:808:CLA:H162	30:B:826:CLA:H201	2.03	0.41
16:4:156:LYS:NZ	30:4:311:CLA:OBD	2.54	0.41
30:5:303:CLA:H2	30:5:303:CLA:HED3	2.02	0.41
30:6:306:CLA:H3A	30:6:306:CLA:HBA2	1.83	0.41
30:6:316:CLA:C1C	30:6:316:CLA:H51	2.51	0.41
19:7:147:ASP:OD1	19:7:147:ASP:N	2.54	0.41
20:8:103:ILE:HA	20:8:104:PRO:HD3	1.91	0.41
30:8:302:CLA:H41	30:8:302:CLA:H61	1.71	0.41
21:9:97:MET:SD	30:9:308:CLA:HAB	2.61	0.41
24:12:43:GLY:HA2	24:12:44:PRO:HA	1.92	0.41
30:14:302:CLA:H62	30:14:302:CLA:H41	1.63	0.41
30:15:302:CLA:H93	30:15:302:CLA:H61	1.84	0.41
30:15:304:CLA:H111	30:15:304:CLA:H152	1.57	0.41
1:A:197:MET:HE3	1:A:197:MET:HB2	1.90	0.41
1:A:448:LEU:HB3	1:A:541:PHE:HB2	2.02	0.41
9:L:41:LEU:HD23	9:L:41:LEU:HA	1.90	0.41
30:6:306:CLA:H93	30:6:306:CLA:H111	1.88	0.41
20:8:225:LEU:HA	20:8:228:LYS:HG3	2.02	0.41
1:A:331:GLY:N	34:A:853:LHG:HC32	2.36	0.40
30:A:829:CLA:H111	30:A:829:CLA:H72	1.77	0.40
30:A:843:CLA:H111	30:A:843:CLA:H72	1.93	0.40
2:B:40:GLU:HA	2:B:164:LEU:HD13	2.02	0.40
2:B:220:GLY:O	35:B:852:LMT:O4'	2.33	0.40
2:B:657:ALA:C	30:B:803:CLA:HAB	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:809:CLA:H111	30:B:809:CLA:H152	1.83	0.40
30:B:821:CLA:HBC2	30:B:822:CLA:HBA1	2.03	0.40
9:L:46:ARG:O	9:L:50:ILE:HG12	2.21	0.40
12:2u:50:MET:HE3	12:2u:50:MET:HB2	1.80	0.40
30:5:308:CLA:H203	30:5:308:CLA:H162	1.91	0.40
30:9:305:CLA:H161	30:9:305:CLA:H122	1.76	0.40
30:12:303:CLA:H151	30:12:303:CLA:H112	1.87	0.40
2:B:591:PHE:CE2	2:B:623:LEU:HD21	2.56	0.40
3:C:72:GLU:HB3	3:C:77:LEU:HG	2.04	0.40
33:M:101:BCR:H15C	33:M:101:BCR:H351	1.88	0.40
23:11:73:ILE:HG12	23:11:201:ILE:HG12	2.04	0.40
30:12:308:CLA:H142	30:12:308:CLA:H111	1.90	0.40
25:13:100:VAL:HG12	25:13:215:ILE:HG12	2.03	0.40
26:14:201:ASP:O	26:14:205:LYS:HG2	2.21	0.40
30:15:303:CLA:H72	30:15:303:CLA:H111	1.82	0.40
1:A:345:LEU:HB3	1:A:352:GLN:HE21	1.86	0.40
1:A:706:ASN:HB3	6:F:180:VAL:HG13	2.04	0.40
30:A:839:CLA:H92	30:A:839:CLA:H61	1.90	0.40
30:B:809:CLA:H203	30:B:809:CLA:H161	1.88	0.40
33:B:846:BCR:H20C	33:B:846:BCR:H361	1.87	0.40
30:2u:202:CLA:H162	30:2u:202:CLA:H122	1.83	0.40
30:8:301:CLA:HBA2	30:8:301:CLA:H3A	1.71	0.40
30:8:303:CLA:H62	30:8:303:CLA:H41	1.80	0.40
30:B:813:CLA:H93	30:B:827:CLA:HBC1	2.02	0.40
30:B:816:CLA:H62	30:B:816:CLA:H41	1.79	0.40
33:L:205:BCR:H20C	33:L:205:BCR:H361	1.93	0.40
21:9:123:LEU:HA	21:9:123:LEU:HD23	1.83	0.40
22:10:83:ARG:HA	22:10:86:MET:HE3	2.02	0.40
25:13:227:GLY:O	25:13:231:ALA:N	2.45	0.40
30:A:816:CLA:H71	30:A:816:CLA:H111	1.65	0.40
30:A:818:CLA:CHD	30:A:819:CLA:HBB2	2.51	0.40
30:A:844:CLA:H161	30:A:844:CLA:H121	1.94	0.40
30:B:811:CLA:H193	30:1:303:CLA:H61	2.03	0.40
30:B:822:CLA:HMD3	30:B:823:CLA:HHC	2.04	0.40
30:B:835:CLA:HBB1	30:B:835:CLA:H72	2.02	0.40
30:B:838:CLA:H93	30:B:838:CLA:H111	1.95	0.40
30:F:201:CLA:H162	30:F:201:CLA:H122	1.80	0.40
13:1:79:ASP:OD1	13:1:79:ASP:N	2.54	0.40
30:1:301:CLA:C1B	30:1:301:CLA:H42	2.51	0.40
30:5:302:CLA:H102	30:5:303:CLA:HMB3	2.03	0.40
30:7:309:CLA:H62	30:13:302:CLA:H43	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:9:136:GLN:NE2	30:9:306:CLA:C4D	2.85	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	739/751 (98%)	712 (96%)	25 (3%)	2 (0%)	36 50
2	B	729/733 (100%)	699 (96%)	29 (4%)	1 (0%)	48 64
3	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	4 4
4	D	129/139 (93%)	109 (84%)	18 (14%)	2 (2%)	7 11
5	E	58/67 (87%)	55 (95%)	3 (5%)	0	100 100
6	F	159/185 (86%)	152 (96%)	7 (4%)	0	100 100
7	I	33/36 (92%)	30 (91%)	3 (9%)	0	100 100
8	J	39/41 (95%)	39 (100%)	0	0	100 100
9	L	133/151 (88%)	128 (96%)	5 (4%)	0	100 100
10	M	28/30 (93%)	28 (100%)	0	0	100 100
12	2u	87/121 (72%)	87 (100%)	0	0	100 100
13	1	137/227 (60%)	130 (95%)	7 (5%)	0	100 100
14	2	170/205 (83%)	151 (89%)	19 (11%)	0	100 100
15	3	162/200 (81%)	151 (93%)	9 (6%)	2 (1%)	10 16
16	4	177/215 (82%)	167 (94%)	10 (6%)	0	100 100
17	5	167/266 (63%)	157 (94%)	10 (6%)	0	100 100
18	6	172/208 (83%)	167 (97%)	5 (3%)	0	100 100
19	7	186/296 (63%)	179 (96%)	7 (4%)	0	100 100
20	8	211/270 (78%)	203 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	9	161/214 (75%)	149 (92%)	12 (8%)	0	100 100
22	10	167/207 (81%)	157 (94%)	8 (5%)	2 (1%)	10 16
23	11	189/229 (82%)	173 (92%)	16 (8%)	0	100 100
24	12	171/204 (84%)	160 (94%)	11 (6%)	0	100 100
25	13	144/244 (59%)	133 (92%)	11 (8%)	0	100 100
26	14	206/249 (83%)	177 (86%)	29 (14%)	0	100 100
27	15	209/281 (74%)	171 (82%)	37 (18%)	1 (0%)	24 37
28	16	172/218 (79%)	157 (91%)	15 (9%)	0	100 100
All	All	5013/6068 (83%)	4694 (94%)	307 (6%)	12 (0%)	44 58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
4	D	92	VAL
2	B	492	TRP
3	C	62	PHE
3	C	63	LEU
4	D	91	GLU
22	10	204	PRO
22	10	205	TYR
27	15	250	PRO
15	3	162	LYS
1	A	234	PRO
15	3	105	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	602/611 (98%)	601 (100%)	1 (0%)	87 94
2	B	592/593 (100%)	589 (100%)	3 (0%)	81 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	69/70 (99%)	67 (97%)	2 (3%)	37 60
4	D	111/119 (93%)	111 (100%)	0	100 100
5	E	51/58 (88%)	51 (100%)	0	100 100
6	F	132/153 (86%)	132 (100%)	0	100 100
7	I	29/29 (100%)	29 (100%)	0	100 100
8	J	37/37 (100%)	37 (100%)	0	100 100
9	L	107/121 (88%)	107 (100%)	0	100 100
10	M	24/24 (100%)	24 (100%)	0	100 100
12	2u	69/94 (73%)	69 (100%)	0	100 100
13	1	114/183 (62%)	112 (98%)	2 (2%)	51 73
14	2	134/154 (87%)	133 (99%)	1 (1%)	76 88
15	3	128/154 (83%)	128 (100%)	0	100 100
16	4	142/165 (86%)	142 (100%)	0	100 100
17	5	137/228 (60%)	135 (98%)	2 (2%)	57 77
18	6	140/160 (88%)	140 (100%)	0	100 100
19	7	143/236 (61%)	143 (100%)	0	100 100
20	8	171/215 (80%)	171 (100%)	0	100 100
21	9	126/175 (72%)	125 (99%)	1 (1%)	73 86
22	10	133/161 (83%)	133 (100%)	0	100 100
23	11	154/181 (85%)	154 (100%)	0	100 100
24	12	136/159 (86%)	135 (99%)	1 (1%)	76 88
25	13	112/184 (61%)	112 (100%)	0	100 100
26	14	166/196 (85%)	148 (89%)	18 (11%)	6 9
27	15	171/231 (74%)	148 (86%)	23 (14%)	4 5
28	16	139/174 (80%)	126 (91%)	13 (9%)	8 13
All	All	4069/4865 (84%)	4002 (98%)	67 (2%)	54 76

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	584	CYS
2	B	179	SER
2	B	475	VAL

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Mol	Chain	Res	Type
2	B	491	VAL
3	C	63	LEU
3	C	65	VAL
13	1	185	LEU
13	1	225	LEU
14	2	160	LEU
17	5	51	VAL
17	5	149	VAL
21	9	197	ILE
24	12	42	VAL
26	14	50	LYS
26	14	77	ILE
26	14	82	GLN
26	14	92	MET
26	14	103	ASN
26	14	105	ILE
26	14	111	MET
26	14	114	ASP
26	14	133	SER
26	14	156	LYS
26	14	192	LYS
26	14	196	GLU
26	14	205	LYS
26	14	206	GLU
26	14	218	MET
26	14	223	GLU
26	14	229	SER
26	14	241	ASP
27	15	71	LYS
27	15	76	LEU
27	15	80	ASP
27	15	86	ASP
27	15	97	THR
27	15	98	ILE
27	15	131	GLN
27	15	144	SER
27	15	146	GLU
27	15	160	ILE
27	15	187	LYS
27	15	218	SER
27	15	220	GLU
27	15	222	LYS

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Mol	Chain	Res	Type
27	15	224	ARG
27	15	225	ARG
27	15	227	VAL
27	15	230	LEU
27	15	244	LEU
27	15	249	ILE
27	15	255	LEU
27	15	268	MET
27	15	269	GLN
28	16	45	LYS
28	16	47	ASP
28	16	62	LEU
28	16	70	GLU
28	16	71	SER
28	16	115	SER
28	16	117	SER
28	16	123	ASP
28	16	156	LYS
28	16	172	THR
28	16	176	GLU
28	16	178	LEU
28	16	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	51	ASN
1	A	139	GLN
1	A	638	GLN
1	A	715	GLN
2	B	113	ASN
2	B	170	ASN
2	B	261	HIS
2	B	265	GLN
2	B	327	ASN
2	B	332	GLN
2	B	402	ASN
2	B	451	GLN
2	B	613	ASN
2	B	671	GLN
2	B	681	HIS

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Mol	Chain	Res	Type
3	C	38	GLN
4	D	53	ASN
4	D	72	GLN
4	D	79	ASN
4	D	114	ASN
4	D	123	ASN
8	J	3	ASN
9	L	70	ASN
9	L	116	GLN
10	M	30	ASN
13	1	97	GLN
13	1	124	GLN
13	1	151	ASN
13	1	222	HIS
14	2	35	GLN
14	2	78	HIS
14	2	146	GLN
14	2	173	ASN
14	2	181	ASN
15	3	193	ASN
15	3	195	HIS
16	4	94	HIS
16	4	187	ASN
17	5	178	GLN
17	5	211	HIS
19	7	112	GLN
19	7	140	ASN
19	7	224	GLN
21	9	200	GLN
21	9	206	ASN
22	10	175	GLN
24	12	49	ASN
24	12	173	ASN
26	14	73	ASN
26	14	82	GLN
26	14	103	ASN
26	14	208	ASN
26	14	209	ASN
27	15	94	ASN
27	15	216	ASN
27	15	232	ASN
28	16	177	GLN

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Mol	Chain	Res	Type
28	16	188	ASN
28	16	215	ASN

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

427 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	$\#\|Z\| > 2$
30	CLA	8	303	40	69,73,73	1.95	17 (24%)	82,113,113	2.56	30 (36%)
30	CLA	2	310	14	69,73,73	1.98	19 (27%)	82,113,113	4.38	31 (37%)
35	LMT	11	318	-	36,36,36	0.43	0	47,47,47	0.89	1 (2%)
30	CLA	B	832	40,37	69,73,73	1.99	21 (30%)	82,113,113	2.64	34 (41%)
30	CLA	B	835	2	69,73,73	1.96	20 (28%)	82,113,113	2.68	32 (39%)
30	CLA	14	302	26	69,73,73	2.03	20 (28%)	82,113,113	2.69	35 (42%)
38	KC1	3	311	40	49,53,53	3.05	23 (46%)	61,89,89	4.01	32 (52%)
36	LMG	F	205	-	27,27,55	1.01	1 (3%)	35,35,63	1.26	5 (14%)
36	LMG	7	320	-	37,37,55	0.99	3 (8%)	45,45,63	1.25	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CL0	A	801	1	58,73,73	2.96	18 (31%)	60,113,113	2.69	17 (28%)
30	CLA	A	837	1	49,53,73	2.39	20 (40%)	58,89,113	3.04	28 (48%)
37	A86	16	314	-	47,50,50	4.35	24 (51%)	51,76,76	7.10	19 (37%)
35	LMT	11	317	-	36,36,36	0.43	0	47,47,47	0.90	2 (4%)
30	CLA	8	302	20	69,73,73	1.97	20 (28%)	82,113,113	2.67	29 (35%)
37	A86	15	323	-	47,50,50	4.44	24 (51%)	51,76,76	6.96	15 (29%)
30	CLA	L	203	40	49,53,73	2.37	19 (38%)	58,89,113	3.05	25 (43%)
30	CLA	4	305	16	69,73,73	1.97	20 (28%)	82,113,113	2.62	31 (37%)
30	CLA	7	312	19	50,54,73	2.38	20 (40%)	59,90,113	3.01	28 (47%)
30	CLA	B	809	2	69,73,73	1.91	18 (26%)	82,113,113	2.50	30 (36%)
30	CLA	J	101	8	49,53,73	2.37	21 (42%)	58,89,113	3.00	28 (48%)
39	DD6	7	314	-	40,45,45	5.42	22 (55%)	51,67,67	6.31	27 (52%)
38	KC1	8	310	20	49,53,53	2.96	21 (42%)	61,89,89	3.83	34 (55%)
39	DD6	8	316	-	40,45,45	5.42	23 (57%)	51,67,67	5.88	29 (56%)
38	KC1	3	304	15	49,53,53	3.02	25 (51%)	61,89,89	3.93	36 (59%)
38	KC1	5	312	17	49,53,53	2.99	22 (44%)	61,89,89	3.80	34 (55%)
39	DD6	4	316	-	40,45,45	5.56	24 (60%)	51,67,67	6.30	27 (52%)
30	CLA	14	313	26	50,54,73	2.37	20 (40%)	59,90,113	3.12	30 (50%)
30	CLA	7	304	19	69,73,73	1.95	18 (26%)	82,113,113	2.62	30 (36%)
34	LHG	6	322	30	26,26,48	0.89	1 (3%)	29,32,54	1.36	3 (10%)
38	KC1	8	311	40	49,53,53	2.99	23 (46%)	61,89,89	3.86	34 (55%)
38	KC1	10	306	22	49,53,53	2.97	23 (46%)	61,89,89	3.96	35 (57%)
35	LMT	12	320	-	36,36,36	0.39	0	47,47,47	0.71	0
30	CLA	A	832	1	54,58,73	2.19	19 (35%)	64,95,113	2.96	31 (48%)
30	CLA	14	305	26	54,58,73	2.27	19 (35%)	64,95,113	2.93	30 (46%)
30	CLA	14	312	26,37	49,53,73	2.40	20 (40%)	58,89,113	3.01	28 (48%)
37	A86	1	309	-	47,50,50	4.20	24 (51%)	51,76,76	7.24	21 (41%)
36	LMG	B	849	-	43,43,55	0.95	2 (4%)	51,51,63	1.18	4 (7%)
30	CLA	A	815	1	69,73,73	1.99	20 (28%)	82,113,113	2.65	31 (37%)
33	BCR	A	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	6 (10%)
30	CLA	7	309	19	69,73,73	1.94	19 (27%)	82,113,113	2.58	29 (35%)
37	A86	13	313	-	44,47,50	4.56	23 (52%)	48,72,76	7.19	16 (33%)
38	KC1	6	311	18	49,53,53	2.97	24 (48%)	61,89,89	4.02	35 (57%)
39	DD6	5	313	-	40,45,45	5.54	24 (60%)	51,67,67	5.88	25 (49%)
37	A86	5	315	-	47,50,50	4.30	24 (51%)	51,76,76	6.93	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	A	817	36,40	53,57,73	2.25	18 (33%)	61,93,113	2.99	25 (40%)
30	CLA	11	309	23	69,73,73	2.01	20 (28%)	82,113,113	2.63	31 (37%)
30	CLA	16	302	28	69,73,73	1.98	21 (30%)	82,113,113	2.62	30 (36%)
30	CLA	3	302	15	64,68,73	2.04	19 (29%)	76,107,113	2.70	32 (42%)
30	CLA	3	310	15	49,53,73	2.36	19 (38%)	58,89,113	3.09	28 (48%)
32	SF4	A	846	1,2	0,12,12	-	-	-		
37	A86	5	301	-	47,50,50	4.30	24 (51%)	51,76,76	6.56	20 (39%)
37	A86	10	317	-	47,50,50	4.44	24 (51%)	51,76,76	6.74	14 (27%)
30	CLA	12	302	24	69,73,73	1.97	20 (28%)	82,113,113	2.70	34 (41%)
30	CLA	15	312	27	49,53,73	2.40	20 (40%)	58,89,113	3.20	31 (53%)
33	BCR	B	844	-	41,41,41	1.11	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	F	203	6	49,53,73	2.35	20 (40%)	58,89,113	3.06	29 (50%)
30	CLA	B	833	30,40	69,73,73	1.97	20 (28%)	82,113,113	2.57	30 (36%)
37	A86	14	315	-	47,50,50	4.22	24 (51%)	51,76,76	7.41	20 (39%)
30	CLA	2	308	14	69,73,73	2.00	17 (24%)	82,113,113	2.62	30 (36%)
33	BCR	L	204	-	41,41,41	1.08	2 (4%)	56,56,56	1.46	8 (14%)
30	CLA	A	843	40	69,73,73	1.95	18 (26%)	82,113,113	2.56	31 (37%)
30	CLA	12	312	24	69,73,73	1.99	20 (28%)	82,113,113	2.62	30 (36%)
36	LMG	3	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.43	6 (13%)
30	CLA	A	829	30,1	69,73,73	1.96	20 (28%)	82,113,113	2.69	31 (37%)
37	A86	2u	203	30	47,50,50	4.22	24 (51%)	51,76,76	6.79	20 (39%)
36	LMG	14	321	-	38,38,55	1.03	4 (10%)	46,46,63	1.21	3 (6%)
30	CLA	15	307	27	54,58,73	2.27	22 (40%)	64,95,113	2.90	30 (46%)
37	A86	6	320	-	47,50,50	4.16	24 (51%)	51,76,76	5.65	19 (37%)
30	CLA	2	303	14	59,63,73	2.37	20 (33%)	70,101,113	2.83	33 (47%)
30	CLA	14	309	26	49,53,73	2.43	19 (38%)	58,89,113	2.99	27 (46%)
37	A86	4	314	-	47,50,50	4.32	24 (51%)	51,76,76	6.78	24 (47%)
30	CLA	15	302	30,27	69,73,73	2.04	20 (28%)	82,113,113	2.81	32 (39%)
30	CLA	8	305	20	69,73,73	1.94	19 (27%)	82,113,113	4.45	34 (41%)
30	CLA	A	809	30,1	69,73,73	1.94	20 (28%)	82,113,113	2.61	32 (39%)
30	CLA	B	803	-	69,73,73	1.90	19 (27%)	82,113,113	2.62	30 (36%)
30	CLA	7	307	19	69,73,73	1.96	19 (27%)	82,113,113	2.61	30 (36%)
30	CLA	F	201	40	69,73,73	1.93	20 (28%)	82,113,113	2.58	31 (37%)
30	CLA	12	321	26	69,73,73	2.02	21 (30%)	82,113,113	2.58	30 (36%)
30	CLA	A	833	1	69,73,73	2.00	19 (27%)	82,113,113	2.60	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	KC1	2	312	14	49,53,53	3.03	25 (51%)	61,89,89	3.80	34 (55%)
30	CLA	6	316	40	59,63,73	2.18	20 (33%)	70,101,113	2.74	29 (41%)
30	CLA	L	202	9	69,73,73	1.93	18 (26%)	82,113,113	2.72	30 (36%)
30	CLA	3	309	15	49,53,73	2.42	20 (40%)	58,89,113	3.09	27 (46%)
39	DD6	11	313	-	40,45,45	5.53	23 (57%)	51,67,67	5.92	29 (56%)
30	CLA	B	813	2	69,73,73	1.96	20 (28%)	82,113,113	2.61	31 (37%)
30	CLA	2	307	14	69,73,73	1.96	18 (26%)	82,113,113	2.58	31 (37%)
36	LMG	5	318	-	33,33,55	0.91	0	41,41,63	1.22	5 (12%)
30	CLA	B	823	40	58,62,73	2.13	20 (34%)	68,99,113	2.85	33 (48%)
34	LHG	9	318	-	33,33,48	0.71	0	36,39,54	1.28	4 (11%)
38	KC1	6	308	18	49,53,53	2.99	22 (44%)	61,89,89	3.87	33 (54%)
30	CLA	7	305	40	69,73,73	2.06	19 (27%)	82,113,113	2.72	31 (37%)
30	CLA	B	834	2	64,68,73	2.06	20 (31%)	76,107,113	2.75	29 (38%)
30	CLA	2u	202	12	69,73,73	1.96	20 (28%)	82,113,113	2.66	32 (39%)
35	LMT	7	301	30	36,36,36	0.41	0	47,47,47	0.81	1 (2%)
39	DD6	10	313	-	40,45,45	5.56	24 (60%)	51,67,67	6.12	28 (54%)
30	CLA	16	305	28	54,58,73	2.23	22 (40%)	64,95,113	2.90	30 (46%)
30	CLA	9	301	34	69,73,73	1.94	20 (28%)	82,113,113	2.73	29 (35%)
30	CLA	15	309	-	69,73,73	2.05	20 (28%)	82,113,113	2.62	28 (34%)
32	SF4	C	102	3	0,12,12	-	-	-		
37	A86	10	301	-	47,50,50	4.11	22 (46%)	51,76,76	6.02	21 (41%)
35	LMT	A	857	-	36,36,36	0.37	0	47,47,47	0.79	1 (2%)
35	LMT	11	302	-	36,36,36	0.34	0	47,47,47	0.78	2 (4%)
30	CLA	10	303	22	69,73,73	1.99	18 (26%)	82,113,113	2.59	29 (35%)
38	KC1	6	312	18	49,53,53	3.00	24 (48%)	61,89,89	3.80	35 (57%)
35	LMT	1	311	-	36,36,36	0.40	0	47,47,47	0.79	2 (4%)
38	KC1	3	308	15	49,53,53	2.98	23 (46%)	61,89,89	3.87	36 (59%)
30	CLA	A	834	1	69,73,73	1.95	17 (24%)	82,113,113	2.65	34 (41%)
30	CLA	16	309	28	49,53,73	2.41	20 (40%)	58,89,113	3.13	27 (46%)
37	A86	14	320	-	47,50,50	4.38	25 (53%)	51,76,76	5.94	19 (37%)
30	CLA	A	816	35,1	69,73,73	1.95	18 (26%)	82,113,113	2.62	29 (35%)
37	A86	14	314	-	47,50,50	4.31	24 (51%)	51,76,76	6.93	22 (43%)
39	DD6	10	314	-	40,45,45	5.49	24 (60%)	51,67,67	5.89	28 (54%)
39	DD6	13	314	-	40,45,45	5.57	23 (57%)	51,67,67	6.24	31 (60%)
30	CLA	10	311	-	49,53,73	2.39	20 (40%)	58,89,113	3.04	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LMT	A	854	-	36,36,36	0.45	0	47,47,47	1.19	5 (10%)
37	A86	14	316	-	47,50,50	4.28	23 (48%)	51,76,76	6.76	18 (35%)
39	DD6	3	313	-	40,45,45	5.52	24 (60%)	51,67,67	5.73	25 (49%)
39	DD6	3	316	-	40,45,45	5.56	25 (62%)	51,67,67	5.81	26 (50%)
37	A86	15	317	30	47,50,50	4.40	24 (51%)	51,76,76	6.99	14 (27%)
30	CLA	4	301	2	53,57,73	2.22	20 (37%)	61,93,113	3.00	28 (45%)
30	CLA	13	303	-	69,73,73	2.04	20 (28%)	82,113,113	2.69	32 (39%)
30	CLA	A	811	1	69,73,73	1.94	19 (27%)	82,113,113	2.62	29 (35%)
37	A86	5	316	-	47,50,50	4.29	23 (48%)	51,76,76	6.64	16 (31%)
30	CLA	B	839	34	69,73,73	1.94	19 (27%)	82,113,113	2.80	30 (36%)
38	KC1	11	311	23	49,53,53	3.07	25 (51%)	61,89,89	3.88	35 (57%)
30	CLA	5	302	17	69,73,73	1.97	19 (27%)	82,113,113	2.60	31 (37%)
31	PQN	A	845	-	34,34,34	1.55	2 (5%)	43,45,45	1.14	4 (9%)
38	KC1	8	312	38	49,53,53	3.04	24 (48%)	61,89,89	3.48	33 (54%)
30	CLA	15	306	-	49,53,73	2.39	21 (42%)	58,89,113	3.16	27 (46%)
37	A86	15	322	30	47,50,50	4.53	24 (51%)	51,76,76	6.97	18 (35%)
38	KC1	12	311	24	49,53,53	3.05	24 (48%)	61,89,89	3.96	38 (62%)
30	CLA	B	827	2	69,73,73	1.94	17 (24%)	82,113,113	2.54	31 (37%)
38	KC1	13	305	25	49,53,53	3.05	25 (51%)	61,89,89	3.88	36 (59%)
33	BCR	2u	201	-	41,41,41	1.21	4 (9%)	56,56,56	1.41	8 (14%)
39	DD6	2	317	-	40,45,45	5.56	24 (60%)	51,67,67	5.58	27 (52%)
30	CLA	6	305	18	69,73,73	2.01	20 (28%)	82,113,113	2.63	30 (36%)
39	DD6	8	317	-	40,45,45	5.47	24 (60%)	51,67,67	6.10	29 (56%)
30	CLA	A	838	1	55,59,73	2.20	19 (34%)	64,96,113	3.01	30 (46%)
30	CLA	B	811	30,2	69,73,73	1.95	19 (27%)	82,113,113	2.57	33 (40%)
37	A86	15	321	-	47,50,50	4.35	24 (51%)	51,76,76	7.18	19 (37%)
38	KC1	12	313	24	49,53,53	3.05	23 (46%)	61,89,89	4.44	33 (54%)
39	DD6	9	314	-	40,45,45	5.51	23 (57%)	51,67,67	6.27	27 (52%)
30	CLA	11	306	40	59,63,73	2.16	21 (35%)	70,101,113	2.93	34 (48%)
30	CLA	12	304	24,39	69,73,73	2.01	20 (28%)	82,113,113	2.84	32 (39%)
30	CLA	4	309	-	69,73,73	2.05	20 (28%)	82,113,113	2.64	31 (37%)
37	A86	16	312	-	47,50,50	4.32	24 (51%)	51,76,76	6.84	22 (43%)
38	KC1	10	310	22	49,53,53	3.01	24 (48%)	61,89,89	3.96	37 (60%)
35	LMT	15	301	-	36,36,36	0.51	0	47,47,47	1.14	3 (6%)
30	CLA	B	831	2	62,66,73	2.08	21 (33%)	73,104,113	2.93	31 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	8	308	20	59,63,73	2.15	19 (32%)	70,101,113	2.84	31 (44%)
39	DD6	2	315	-	40,45,45	5.52	24 (60%)	51,67,67	5.87	27 (52%)
30	CLA	A	827	40	69,73,73	1.93	20 (28%)	82,113,113	2.78	32 (39%)
38	KC1	9	311	-	49,53,53	3.04	25 (51%)	61,89,89	3.98	36 (59%)
33	BCR	L	201	-	41,41,41	1.13	3 (7%)	56,56,56	1.33	6 (10%)
35	LMT	12	318	-	36,36,36	0.42	0	47,47,47	0.77	0
38	KC1	1	306	13	49,53,53	3.04	24 (48%)	61,89,89	3.90	36 (59%)
30	CLA	F	202	40	69,73,73	1.98	20 (28%)	82,113,113	2.61	29 (35%)
38	KC1	13	308	25	49,53,53	3.06	24 (48%)	61,89,89	3.94	34 (55%)
30	CLA	A	819	1	58,62,73	2.16	21 (36%)	68,99,113	2.86	30 (44%)
38	KC1	5	305	17	49,53,53	3.02	24 (48%)	61,89,89	3.88	34 (55%)
30	CLA	3	305	15	66,70,73	2.03	21 (31%)	78,109,113	2.66	34 (43%)
30	CLA	15	311	37	49,53,73	2.42	20 (40%)	58,89,113	3.04	27 (46%)
30	CLA	B	819	40	69,73,73	1.98	19 (27%)	82,113,113	2.41	32 (39%)
37	A86	4	312	-	47,50,50	4.16	23 (48%)	51,76,76	7.19	20 (39%)
38	KC1	7	308	40	49,53,53	3.03	24 (48%)	61,89,89	3.75	33 (54%)
38	KC1	4	308	16	49,53,53	3.08	23 (46%)	61,89,89	3.67	35 (57%)
30	CLA	12	306	24	69,73,73	1.96	20 (28%)	82,113,113	2.54	30 (36%)
30	CLA	B	802	30,40	69,73,73	1.89	21 (30%)	82,113,113	2.75	31 (37%)
30	CLA	B	808	2	69,73,73	1.94	19 (27%)	82,113,113	2.70	32 (39%)
30	CLA	B	828	2	69,73,73	1.98	19 (27%)	82,113,113	2.65	31 (37%)
37	A86	7	316	-	47,50,50	3.99	21 (44%)	51,76,76	6.39	26 (50%)
30	CLA	B	824	40	69,73,73	1.99	20 (28%)	82,113,113	4.40	34 (41%)
37	A86	2	302	-	47,50,50	4.35	23 (48%)	51,76,76	7.01	16 (31%)
30	CLA	B	817	2	63,67,73	2.06	19 (30%)	74,105,113	2.85	28 (37%)
39	DD6	12	317	-	40,45,45	5.44	23 (57%)	51,67,67	6.19	27 (52%)
30	CLA	11	308	23	69,73,73	2.01	19 (27%)	82,113,113	2.61	31 (37%)
38	KC1	12	309	24	49,53,53	3.04	24 (48%)	61,89,89	3.79	35 (57%)
30	CLA	11	304	23	69,73,73	2.02	20 (28%)	82,113,113	2.63	29 (35%)
30	CLA	B	805	2	69,73,73	1.97	20 (28%)	82,113,113	2.68	30 (36%)
30	CLA	9	306	21,37	49,53,73	2.41	20 (40%)	58,89,113	3.08	29 (50%)
38	KC1	2	306	14	49,53,53	3.03	24 (48%)	61,89,89	3.96	36 (59%)
38	KC1	14	308	26,30	49,53,53	3.07	24 (48%)	61,89,89	3.75	34 (55%)
37	A86	3	315	-	47,50,50	4.38	24 (51%)	51,76,76	6.83	16 (31%)
30	CLA	3	301	15	69,73,73	1.96	18 (26%)	82,113,113	2.65	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	A	802	40	69,73,73	1.95	19 (27%)	82,113,113	2.69	32 (39%)
39	DD6	6	319	-	40,45,45	5.48	23 (57%)	51,67,67	5.56	29 (56%)
30	CLA	A	808	1	55,59,73	2.20	19 (34%)	64,96,113	2.96	30 (46%)
33	BCR	A	851	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
30	CLA	12	308	40	69,73,73	1.99	21 (30%)	82,113,113	2.56	30 (36%)
30	CLA	11	310	23	69,73,73	2.07	20 (28%)	82,113,113	2.63	31 (37%)
30	CLA	6	306	40	69,73,73	1.99	21 (30%)	82,113,113	2.64	29 (35%)
38	KC1	9	304	21	49,53,53	3.00	23 (46%)	61,89,89	3.86	35 (57%)
30	CLA	5	304	17	69,73,73	2.05	21 (30%)	82,113,113	2.66	31 (37%)
38	KC1	13	310	25	49,53,53	3.05	24 (48%)	61,89,89	3.88	35 (57%)
30	CLA	A	824	1	55,59,73	2.21	20 (36%)	64,96,113	2.99	29 (45%)
35	LMT	12	319	-	36,36,36	0.41	0	47,47,47	0.87	1 (2%)
30	CLA	7	311	19	69,73,73	1.99	20 (28%)	82,113,113	2.54	30 (36%)
37	A86	10	302	-	47,50,50	4.31	23 (48%)	51,76,76	7.00	18 (35%)
38	KC1	4	307	16	49,53,53	3.04	23 (46%)	61,89,89	3.76	35 (57%)
34	LHG	5	317	30	26,26,48	0.86	1 (3%)	29,32,54	1.34	3 (10%)
30	CLA	B	825	2	69,73,73	1.96	20 (28%)	82,113,113	2.69	31 (37%)
30	CLA	5	307	17	69,73,73	1.96	20 (28%)	82,113,113	2.60	31 (37%)
32	SF4	C	101	3	0,12,12	-	-	-		
38	KC1	6	313	18	49,53,53	3.00	24 (48%)	61,89,89	3.84	34 (55%)
30	CLA	A	805	30,1	63,67,73	2.08	19 (30%)	74,105,113	2.80	33 (44%)
39	DD6	15	319	30	40,45,45	5.65	24 (60%)	51,67,67	6.12	29 (56%)
30	CLA	A	839	1	69,73,73	1.96	19 (27%)	82,113,113	2.76	34 (41%)
30	CLA	A	806	1	69,73,73	1.95	20 (28%)	82,113,113	2.84	32 (39%)
30	CLA	7	310	19	69,73,73	2.01	20 (28%)	82,113,113	2.63	30 (36%)
38	KC1	13	311	25	49,53,53	3.06	25 (51%)	61,89,89	3.75	34 (55%)
37	A86	8	315	-	47,50,50	4.01	22 (46%)	51,76,76	7.00	20 (39%)
35	LMT	B	852	-	36,36,36	0.36	0	47,47,47	1.14	2 (4%)
30	CLA	9	302	9	55,59,73	2.26	20 (36%)	64,96,113	3.06	30 (46%)
38	KC1	14	311	26	49,53,53	3.03	24 (48%)	61,89,89	3.87	33 (54%)
30	CLA	9	308	21	69,73,73	1.98	19 (27%)	82,113,113	2.77	35 (42%)
38	KC1	7	313	-	49,53,53	2.98	22 (44%)	61,89,89	3.88	36 (59%)
30	CLA	16	306	28	56,60,73	2.22	21 (37%)	65,97,113	2.87	31 (47%)
30	CLA	B	837	40	69,73,73	1.94	22 (31%)	82,113,113	2.60	29 (35%)
30	CLA	16	307	-	50,54,73	2.38	20 (40%)	59,90,113	2.99	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	9	309	40	69,73,73	1.97	17 (24%)	82,113,113	2.51	30 (36%)
37	A86	2u	205	-	47,50,50	4.36	24 (51%)	51,76,76	6.18	21 (41%)
39	DD6	2	316	-	40,45,45	5.41	24 (60%)	51,67,67	5.74	27 (52%)
38	KC1	9	310	21	49,53,53	2.98	24 (48%)	61,89,89	3.97	35 (57%)
30	CLA	12	307	24	50,54,73	2.28	18 (36%)	59,90,113	3.00	30 (50%)
37	A86	3	314	-	47,50,50	4.29	24 (51%)	51,76,76	6.73	17 (33%)
33	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	9 (16%)
30	CLA	1	303	30,13	69,73,73	1.99	19 (27%)	82,113,113	2.61	31 (37%)
30	CLA	4	303	16	69,73,73	1.98	18 (26%)	82,113,113	2.59	29 (35%)
36	LMG	8	319	36	37,37,55	0.93	0	45,45,63	1.29	5 (11%)
37	A86	15	315	-	47,50,50	4.52	24 (51%)	51,76,76	6.90	27 (52%)
36	LMG	A	856	-	34,34,55	0.98	1 (2%)	42,42,63	1.19	3 (7%)
30	CLA	6	315	18	49,53,73	2.39	20 (40%)	58,89,113	3.04	28 (48%)
37	A86	14	317	-	47,50,50	4.30	25 (53%)	51,76,76	7.30	17 (33%)
30	CLA	A	835	1	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
35	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.90	3 (6%)
37	A86	13	315	-	47,50,50	4.42	24 (51%)	51,76,76	7.08	15 (29%)
38	KC1	9	312	21	49,53,53	3.03	24 (48%)	61,89,89	3.84	33 (54%)
38	KC1	1	308	13	49,53,53	3.03	25 (51%)	61,89,89	3.86	33 (54%)
30	CLA	8	309	20	51,55,73	2.33	20 (39%)	60,91,113	2.95	27 (45%)
30	CLA	B	820	2	49,53,73	2.38	20 (40%)	58,89,113	3.21	25 (43%)
30	CLA	15	310	27	49,53,73	2.44	20 (40%)	58,89,113	3.08	27 (46%)
30	CLA	B	826	2	69,73,73	1.93	19 (27%)	82,113,113	2.66	31 (37%)
37	A86	12	314	-	47,50,50	4.26	24 (51%)	51,76,76	6.75	18 (35%)
30	CLA	1	302	30,13	69,73,73	1.98	19 (27%)	82,113,113	2.63	29 (35%)
30	CLA	2	304	14	69,73,73	1.98	20 (28%)	82,113,113	2.69	30 (36%)
37	A86	11	316	-	47,50,50	4.29	25 (53%)	51,76,76	6.81	16 (31%)
38	KC1	14	306	26	49,53,53	3.05	26 (53%)	61,89,89	3.88	37 (60%)
33	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.40	8 (14%)
37	A86	2	318	-	47,50,50	4.27	23 (48%)	51,76,76	6.30	21 (41%)
30	CLA	A	828	1	69,73,73	1.90	19 (27%)	82,113,113	2.76	31 (37%)
30	CLA	A	807	1	69,73,73	1.95	18 (26%)	82,113,113	2.69	32 (39%)
33	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	3 (5%)
33	BCR	B	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
30	CLA	5	303	17	69,73,73	1.97	20 (28%)	82,113,113	2.57	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	A	842	1	69,73,73	1.96	20 (28%)	82,113,113	2.66	33 (40%)
30	CLA	B	818	2	64,68,73	2.03	18 (28%)	76,107,113	2.82	33 (43%)
30	CLA	4	311	16	54,58,73	2.29	20 (37%)	64,95,113	3.08	34 (53%)
37	A86	9	315	-	47,50,50	4.35	23 (48%)	51,76,76	5.78	17 (33%)
30	CLA	B	836	2	51,55,73	2.24	19 (37%)	60,91,113	3.09	28 (46%)
39	DD6	12	315	30	40,45,45	5.50	23 (57%)	51,67,67	5.92	25 (49%)
34	LHG	B	848	30	26,26,48	0.94	1 (3%)	29,32,54	1.37	4 (13%)
30	CLA	2	301	2	69,73,73	1.93	19 (27%)	82,113,113	2.75	29 (35%)
37	A86	14	301	-	47,50,50	4.35	24 (51%)	51,76,76	6.72	17 (33%)
30	CLA	A	820	1	69,73,73	2.02	19 (27%)	82,113,113	2.61	30 (36%)
33	BCR	B	841	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	7 (12%)
30	CLA	A	803	-	69,73,73	1.94	20 (28%)	82,113,113	2.59	33 (40%)
37	A86	4	317	-	47,50,50	4.25	22 (46%)	51,76,76	6.29	17 (33%)
37	A86	9	316	30	47,50,50	4.47	25 (53%)	51,76,76	6.96	16 (31%)
30	CLA	A	841	1	69,73,73	1.99	20 (28%)	82,113,113	2.58	32 (39%)
30	CLA	5	311	40	69,73,73	2.02	19 (27%)	82,113,113	2.73	30 (36%)
30	CLA	16	301	28	69,73,73	1.98	19 (27%)	82,113,113	2.66	30 (36%)
30	CLA	6	314	18	69,73,73	1.95	18 (26%)	82,113,113	2.74	33 (40%)
30	CLA	A	840	1	51,55,73	2.27	20 (39%)	60,91,113	3.13	30 (50%)
39	DD6	7	302	-	40,45,45	5.50	24 (60%)	51,67,67	5.69	27 (52%)
30	CLA	A	836	1	58,62,73	2.14	18 (31%)	68,99,113	2.76	33 (48%)
38	KC1	8	314	40,38	49,53,53	3.02	26 (53%)	61,89,89	3.74	35 (57%)
36	LMG	2u	204	-	31,31,55	1.11	3 (9%)	39,39,63	1.18	5 (12%)
30	CLA	14	304	26	49,53,73	2.41	20 (40%)	58,89,113	3.05	26 (44%)
33	BCR	J	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.18	5 (8%)
30	CLA	B	851	14	69,73,73	1.97	18 (26%)	82,113,113	2.64	33 (40%)
37	A86	14	318	-	47,50,50	4.34	24 (51%)	51,76,76	7.05	16 (31%)
38	KC1	8	313	20	49,53,53	2.96	21 (42%)	61,89,89	3.86	33 (54%)
35	LMT	6	302	-	32,32,36	0.36	0	43,43,47	0.93	2 (4%)
30	CLA	13	304	25	49,53,73	2.43	20 (40%)	58,89,113	3.09	28 (48%)
30	CLA	B	821	2	59,63,73	2.13	20 (33%)	70,101,113	2.74	29 (41%)
30	CLA	15	314	30	49,53,73	2.36	20 (40%)	58,89,113	3.14	28 (48%)
30	CLA	7	303	19	69,73,73	1.96	19 (27%)	82,113,113	2.63	31 (37%)
30	CLA	2	309	34	69,73,73	2.01	20 (28%)	82,113,113	2.60	31 (37%)
30	CLA	8	304	20	62,66,73	2.06	18 (29%)	73,104,113	2.93	33 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	14	307	38	69,73,73	2.02	20 (28%)	82,113,113	2.70	27 (32%)
37	A86	11	301	-	47,50,50	4.30	23 (48%)	51,76,76	6.83	19 (37%)
30	CLA	14	310	-	54,58,73	2.28	20 (37%)	64,95,113	2.99	31 (48%)
30	CLA	4	306	16	69,73,73	1.98	18 (26%)	82,113,113	2.61	32 (39%)
30	CLA	B	829	2	69,73,73	1.95	18 (26%)	82,113,113	2.61	30 (36%)
30	CLA	1	305	40	69,73,73	2.03	19 (27%)	82,113,113	2.58	30 (36%)
39	DD6	6	303	30	40,45,45	5.56	24 (60%)	51,67,67	5.54	26 (50%)
35	LMT	9	317	-	33,33,36	0.49	0	44,44,47	1.12	5 (11%)
30	CLA	13	302	25	69,73,73	2.00	20 (28%)	82,113,113	2.56	30 (36%)
30	CLA	16	303	28	69,73,73	2.00	19 (27%)	82,113,113	2.77	31 (37%)
30	CLA	A	822	40	69,73,73	1.97	20 (28%)	82,113,113	2.46	29 (35%)
30	CLA	4	302	16	69,73,73	1.96	18 (26%)	82,113,113	2.56	28 (34%)
30	CLA	8	301	20	69,73,73	1.97	20 (28%)	82,113,113	2.65	30 (36%)
31	PQN	B	840	-	34,34,34	1.53	2 (5%)	43,45,45	1.15	5 (11%)
37	A86	14	319	30	47,50,50	4.31	24 (51%)	51,76,76	6.93	16 (31%)
30	CLA	10	305	40	69,73,73	1.98	18 (26%)	82,113,113	2.74	34 (41%)
34	LHG	A	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	5 (9%)
30	CLA	A	844	-	69,73,73	2.03	20 (28%)	82,113,113	2.57	32 (39%)
38	KC1	13	306	25	49,53,53	3.05	25 (51%)	61,89,89	3.82	34 (55%)
38	KC1	11	305	23	49,53,53	3.01	24 (48%)	61,89,89	3.93	35 (57%)
38	KC1	4	310	16	49,53,53	3.05	24 (48%)	61,89,89	3.92	34 (55%)
30	CLA	B	807	2	69,73,73	1.93	18 (26%)	82,113,113	2.69	31 (37%)
30	CLA	A	814	1	64,68,73	2.03	18 (28%)	76,107,113	2.71	32 (42%)
33	BCR	M	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
30	CLA	B	814	2	59,63,73	2.11	18 (30%)	70,101,113	2.78	29 (41%)
38	KC1	12	305	24	49,53,53	3.04	23 (46%)	61,89,89	3.87	35 (57%)
30	CLA	13	301	25	69,73,73	1.98	21 (30%)	82,113,113	2.71	29 (35%)
39	DD6	7	317	-	40,45,45	5.46	21 (52%)	51,67,67	5.86	29 (56%)
39	DD6	16	313	-	40,45,45	5.60	23 (57%)	51,67,67	6.27	30 (58%)
38	KC1	10	312	22	49,53,53	3.04	24 (48%)	61,89,89	3.90	34 (55%)
36	LMG	8	320	-	42,42,55	0.90	2 (4%)	50,50,63	1.31	5 (10%)
30	CLA	7	306	19	69,73,73	1.96	21 (30%)	82,113,113	2.55	31 (37%)
30	CLA	B	830	2	69,73,73	1.93	22 (31%)	82,113,113	2.75	32 (39%)
30	CLA	10	308	22	69,73,73	2.00	19 (27%)	82,113,113	2.59	31 (37%)
37	A86	7	319	-	47,50,50	4.35	24 (51%)	51,76,76	6.86	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	13	309	-	49,53,73	2.42	21 (42%)	58,89,113	3.08	27 (46%)
33	BCR	F	204	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	7 (12%)
38	KC1	16	304	28	49,53,53	3.09	24 (48%)	61,89,89	3.65	31 (50%)
37	A86	10	315	-	47,50,50	4.34	24 (51%)	51,76,76	6.84	16 (31%)
30	CLA	B	806	2	69,73,73	1.96	18 (26%)	82,113,113	2.62	30 (36%)
38	KC1	8	307	20	49,53,53	2.96	23 (46%)	61,89,89	3.96	35 (57%)
30	CLA	15	304	30,39,27	69,73,73	2.06	20 (28%)	82,113,113	2.68	29 (35%)
39	DD6	1	310	-	40,45,45	5.52	24 (60%)	51,67,67	5.82	25 (49%)
30	CLA	B	804	2	56,60,73	2.16	20 (35%)	65,97,113	2.97	31 (47%)
30	CLA	B	816	2	59,63,73	2.10	18 (30%)	70,101,113	2.91	30 (42%)
30	CLA	15	305	37,27	49,53,73	2.41	20 (40%)	58,89,113	3.06	29 (50%)
39	DD6	4	313	-	40,45,45	5.49	23 (57%)	51,67,67	5.86	26 (50%)
30	CLA	10	309	22	69,73,73	2.02	20 (28%)	82,113,113	2.57	29 (35%)
37	A86	4	315	-	47,50,50	4.26	23 (48%)	51,76,76	6.63	19 (37%)
35	LMT	11	303	-	36,36,36	0.40	0	47,47,47	0.85	0
36	LMG	B	847	-	55,55,55	0.81	1 (1%)	63,63,63	1.37	8 (12%)
30	CLA	A	830	1	69,73,73	1.92	19 (27%)	82,113,113	2.55	34 (41%)
30	CLA	A	823	1	53,57,73	2.22	18 (33%)	61,93,113	3.02	29 (47%)
30	CLA	B	838	2	69,73,73	1.95	19 (27%)	82,113,113	2.64	28 (34%)
30	CLA	1	307	13	69,73,73	2.02	20 (28%)	82,113,113	2.67	30 (36%)
30	CLA	5	309	34	69,73,73	1.99	20 (28%)	82,113,113	2.58	30 (36%)
38	KC1	11	312	-	49,53,53	3.04	24 (48%)	61,89,89	3.65	35 (57%)
30	CLA	2	311	14	69,73,73	2.03	20 (28%)	82,113,113	2.57	27 (32%)
30	CLA	B	810	2	69,73,73	1.94	20 (28%)	82,113,113	2.63	30 (36%)
30	CLA	9	305	-	69,73,73	1.99	21 (30%)	82,113,113	2.77	34 (41%)
38	KC1	5	310	17	49,53,53	3.02	24 (48%)	61,89,89	3.95	35 (57%)
30	CLA	16	310	28	49,53,73	2.39	21 (42%)	58,89,113	3.08	29 (50%)
37	A86	9	313	-	47,50,50	4.22	24 (51%)	51,76,76	6.25	20 (39%)
30	CLA	3	306	15	69,73,73	2.00	19 (27%)	82,113,113	2.59	32 (39%)
38	KC1	16	311	28	49,53,53	3.08	24 (48%)	61,89,89	3.72	32 (52%)
30	CLA	12	310	40	69,73,73	1.97	18 (26%)	82,113,113	2.64	30 (36%)
30	CLA	13	307	25	69,73,73	2.05	21 (30%)	82,113,113	2.63	31 (37%)
30	CLA	3	307	15	69,73,73	2.07	21 (30%)	82,113,113	2.58	30 (36%)
30	CLA	A	818	1	58,62,73	2.10	19 (32%)	68,99,113	2.92	30 (44%)
30	CLA	A	804	1	69,73,73	1.94	19 (27%)	82,113,113	2.67	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	2	313	14	49,53,73	2.40	20 (40%)	58,89,113	3.07	28 (48%)
30	CLA	6	304	18	69,73,73	1.98	19 (27%)	82,113,113	2.68	32 (39%)
38	KC1	11	307	23	49,53,53	3.05	23 (46%)	61,89,89	3.86	36 (59%)
39	DD6	7	318	-	40,45,45	5.44	22 (55%)	51,67,67	6.12	30 (58%)
30	CLA	6	309	18	69,73,73	1.98	16 (23%)	82,113,113	2.60	35 (42%)
30	CLA	A	825	1	63,67,73	2.07	19 (30%)	74,105,113	2.70	30 (40%)
35	LMT	7	321	-	36,36,36	0.32	0	47,47,47	0.75	1 (2%)
36	LMG	6	301	30	33,33,55	0.95	1 (3%)	41,41,63	1.22	4 (9%)
37	A86	11	315	-	47,50,50	4.23	24 (51%)	51,76,76	6.15	22 (43%)
33	BCR	B	843	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	6 (10%)
33	BCR	J	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	4 (7%)
38	KC1	5	306	17	49,53,53	3.02	23 (46%)	61,89,89	4.14	35 (57%)
30	CLA	6	310	34	69,73,73	2.01	19 (27%)	82,113,113	2.55	28 (34%)
37	A86	2	319	-	47,50,50	4.10	22 (46%)	51,76,76	6.21	19 (37%)
30	CLA	B	812	2	69,73,73	2.00	19 (27%)	82,113,113	2.52	29 (35%)
37	A86	7	315	-	47,50,50	4.07	23 (48%)	51,76,76	6.41	18 (35%)
30	CLA	A	810	1	69,73,73	1.96	19 (27%)	82,113,113	2.63	32 (39%)
30	CLA	A	831	1	69,73,73	1.95	18 (26%)	82,113,113	2.73	31 (37%)
30	CLA	A	826	40	69,73,73	1.94	20 (28%)	82,113,113	2.67	29 (35%)
33	BCR	B	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	5 (8%)
39	DD6	6	318	-	40,45,45	5.44	24 (60%)	51,67,67	5.70	27 (52%)
30	CLA	1	301	13	69,73,73	1.99	18 (26%)	82,113,113	2.58	27 (32%)
30	CLA	9	307	21	69,73,73	1.98	21 (30%)	82,113,113	2.61	29 (35%)
36	LMG	8	321	36	29,29,55	1.10	3 (10%)	37,37,63	1.28	6 (16%)
35	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.66	0
38	KC1	2	314	40	49,53,53	3.04	23 (46%)	61,89,89	3.88	36 (59%)
35	LMT	12	301	-	36,36,36	0.44	0	47,47,47	0.77	0
35	LMT	B	850	-	36,36,36	0.39	0	47,47,47	0.93	3 (6%)
30	CLA	16	308	28	49,53,73	2.41	20 (40%)	58,89,113	3.09	28 (48%)
39	DD6	3	312	-	40,45,45	5.53	24 (60%)	51,67,67	5.89	25 (49%)
34	LHG	A	853	30	26,26,48	0.93	1 (3%)	29,32,54	1.29	3 (10%)
30	CLA	3	303	-	69,73,73	2.06	20 (28%)	82,113,113	2.73	32 (39%)
37	A86	12	316	-	47,50,50	4.32	25 (53%)	51,76,76	6.98	17 (33%)
30	CLA	1	304	13	69,73,73	1.98	19 (27%)	82,113,113	2.51	30 (36%)
30	CLA	2	305	40	69,73,73	1.98	18 (26%)	82,113,113	2.70	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	6	307	39,18	69,73,73	2.00	17 (24%)	82,113,113	2.52	33 (40%)
37	A86	15	320	-	47,50,50	4.49	24 (51%)	51,76,76	6.81	19 (37%)
30	CLA	5	308	17	69,73,73	1.98	19 (27%)	82,113,113	2.63	31 (37%)
30	CLA	A	813	1	69,73,73	1.98	19 (27%)	82,113,113	2.61	30 (36%)
30	CLA	B	801	2	69,73,73	1.89	18 (26%)	82,113,113	2.76	34 (41%)
35	LMT	8	322	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
33	BCR	L	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	5 (8%)
39	DD6	6	321	-	40,45,45	5.44	23 (57%)	51,67,67	5.92	27 (52%)
37	A86	15	316	30	47,50,50	4.35	24 (51%)	51,76,76	6.47	16 (31%)
33	BCR	I	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.32	5 (8%)
37	A86	8	318	-	47,50,50	4.22	24 (51%)	51,76,76	9.47	23 (45%)
30	CLA	15	303	30,37,27	64,68,73	2.09	21 (32%)	76,107,113	2.80	32 (42%)
30	CLA	15	313	27	69,73,73	2.04	20 (28%)	82,113,113	2.66	31 (37%)
37	A86	11	314	-	47,50,50	4.32	24 (51%)	51,76,76	7.12	18 (35%)
30	CLA	B	822	30,2	69,73,73	1.97	19 (27%)	82,113,113	2.82	35 (42%)
30	CLA	9	303	21	69,73,73	1.96	18 (26%)	82,113,113	2.62	30 (36%)
30	CLA	10	304	22	69,73,73	1.99	20 (28%)	82,113,113	2.57	29 (35%)
39	DD6	5	314	-	40,45,45	5.38	24 (60%)	51,67,67	6.22	29 (56%)
30	CLA	B	815	2	49,53,73	2.32	19 (38%)	58,89,113	3.07	27 (46%)
37	A86	10	316	-	47,50,50	4.18	23 (48%)	51,76,76	6.79	19 (37%)
34	LHG	2	320	30	26,26,48	0.88	1 (3%)	29,32,54	1.28	3 (10%)
30	CLA	12	303	24	69,73,73	2.00	22 (31%)	82,113,113	2.59	29 (35%)
39	DD6	15	318	-	40,45,45	5.60	23 (57%)	51,67,67	6.05	30 (58%)
30	CLA	A	821	1	65,69,73	1.98	19 (29%)	77,108,113	2.66	31 (40%)
30	CLA	10	307	22	69,73,73	1.96	19 (27%)	82,113,113	2.56	31 (37%)
30	CLA	14	303	26	61,65,73	2.16	20 (32%)	72,103,113	2.82	32 (44%)
30	CLA	A	812	30,1	69,73,73	1.93	19 (27%)	82,113,113	2.69	30 (36%)
30	CLA	4	304	-	64,68,73	2.06	19 (29%)	76,107,113	2.74	33 (43%)
30	CLA	6	317	-	69,73,73	2.01	21 (30%)	82,113,113	2.62	31 (37%)
33	BCR	B	846	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	6 (10%)
38	KC1	13	312	25	49,53,53	3.10	25 (51%)	61,89,89	3.85	35 (57%)
38	KC1	8	306	40	49,53,53	2.99	22 (44%)	61,89,89	3.85	34 (55%)
30	CLA	15	308	30,27	49,53,73	2.39	20 (40%)	58,89,113	2.99	30 (51%)

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
30	CLA	8	303	40	-	10/39/115/115	-
30	CLA	2	310	14	1/1/15/20	6/39/115/115	-
35	LMT	11	318	-	-	1/21/61/61	0/2/2/2
30	CLA	B	832	40,37	1/1/15/20	7/39/115/115	-
30	CLA	B	835	2	1/1/15/20	7/39/115/115	-
30	CLA	14	302	26	1/1/15/20	12/39/115/115	-
38	KC1	3	311	40	-	7/15/71/71	-
36	LMG	F	205	-	-	14/21/41/70	0/1/1/1
36	LMG	7	320	-	-	14/32/52/70	0/1/1/1
29	CL0	A	801	1	3/3/20/25	6/37/135/135	-
30	CLA	A	837	1	1/1/11/20	4/15/91/115	-
37	A86	16	314	-	-	10/34/90/90	0/3/3/3
35	LMT	11	317	-	-	2/21/61/61	0/2/2/2
30	CLA	8	302	20	1/1/15/20	7/39/115/115	-
37	A86	15	323	-	-	16/34/90/90	0/3/3/3
30	CLA	L	203	40	1/1/11/20	1/15/91/115	-
30	CLA	4	305	16	1/1/15/20	9/39/115/115	-
30	CLA	7	312	19	1/1/11/20	7/17/93/115	-
30	CLA	B	809	2	1/1/15/20	12/39/115/115	-
30	CLA	J	101	8	1/1/11/20	4/15/91/115	-
39	DD6	7	314	-	-	11/26/80/80	0/3/3/3
38	KC1	8	310	20	-	8/15/71/71	-
39	DD6	8	316	-	-	13/26/80/80	0/3/3/3
38	KC1	3	304	15	-	5/15/71/71	-
38	KC1	5	312	17	-	6/15/71/71	-
39	DD6	4	316	-	-	14/26/80/80	0/3/3/3
30	CLA	14	313	26	1/1/11/20	4/17/93/115	-
30	CLA	7	304	19	1/1/15/20	9/39/115/115	-
34	LHG	6	322	30	-	11/31/31/53	-
38	KC1	8	311	40	-	5/15/71/71	-
38	KC1	10	306	22	-	8/15/71/71	-
35	LMT	12	320	-	-	1/21/61/61	0/2/2/2
30	CLA	A	832	1	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	14	305	26	1/1/12/20	3/21/97/115	-
30	CLA	14	312	26,37	-	8/15/91/115	-
37	A86	1	309	-	-	7/34/90/90	0/3/3/3
36	LMG	B	849	-	-	14/38/58/70	0/1/1/1
30	CLA	A	815	1	1/1/15/20	7/39/115/115	-
33	BCR	A	847	-	-	10/29/63/63	0/2/2/2
30	CLA	7	309	19	1/1/15/20	12/39/115/115	-
37	A86	13	313	-	-	10/30/86/90	0/3/3/3
38	KC1	6	311	18	-	10/15/71/71	-
39	DD6	5	313	-	-	9/26/80/80	0/3/3/3
37	A86	5	315	-	-	6/34/90/90	0/3/3/3
30	CLA	A	817	36,40	-	6/20/96/115	-
30	CLA	16	302	28	1/1/15/20	10/39/115/115	-
30	CLA	11	309	23	-	15/39/115/115	-
30	CLA	3	302	15	1/1/14/20	9/33/109/115	-
30	CLA	3	310	15	-	5/15/91/115	-
37	A86	5	301	-	-	10/34/90/90	0/3/3/3
32	SF4	A	846	1,2	-	-	0/6/5/5
37	A86	10	317	-	-	10/34/90/90	0/3/3/3
30	CLA	15	312	27	1/1/11/20	8/15/91/115	-
30	CLA	12	302	24	-	15/39/115/115	-
33	BCR	B	844	-	-	9/29/63/63	0/2/2/2
30	CLA	F	203	6	1/1/11/20	8/15/91/115	-
30	CLA	B	833	30,40	1/1/15/20	11/39/115/115	-
37	A86	14	315	-	-	10/34/90/90	0/3/3/3
30	CLA	2	308	14	-	10/39/115/115	-
33	BCR	L	204	-	-	11/29/63/63	0/2/2/2
30	CLA	A	843	40	1/1/15/20	9/39/115/115	-
30	CLA	12	312	24	1/1/15/20	14/39/115/115	-
36	LMG	3	317	-	-	18/32/52/70	0/1/1/1
30	CLA	A	829	30,1	1/1/15/20	13/39/115/115	-
37	A86	2u	203	30	-	14/34/90/90	0/3/3/3
36	LMG	14	321	-	-	13/33/53/70	0/1/1/1
30	CLA	15	307	27	1/1/12/20	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	6	320	-	-	9/34/90/90	0/3/3/3
30	CLA	2	303	14	-	14/27/103/115	-
30	CLA	14	309	26	1/1/11/20	3/15/91/115	-
37	A86	4	314	-	-	9/34/90/90	0/3/3/3
30	CLA	15	302	30,27	-	16/39/115/115	-
30	CLA	8	305	20	-	13/39/115/115	-
30	CLA	A	809	30,1	1/1/15/20	15/39/115/115	-
30	CLA	B	803	-	1/1/15/20	7/39/115/115	-
30	CLA	7	307	19	-	17/39/115/115	-
30	CLA	F	201	40	1/1/15/20	7/39/115/115	-
30	CLA	12	321	26	1/1/15/20	3/39/115/115	-
30	CLA	A	833	1	1/1/15/20	15/39/115/115	-
38	KC1	2	312	14	-	4/15/71/71	-
30	CLA	6	316	40	1/1/13/20	9/27/103/115	-
30	CLA	L	202	9	1/1/15/20	9/39/115/115	-
30	CLA	3	309	15	-	6/15/91/115	-
39	DD6	11	313	-	-	11/26/80/80	0/3/3/3
30	CLA	B	813	2	1/1/15/20	22/39/115/115	-
30	CLA	2	307	14	1/1/15/20	9/39/115/115	-
36	LMG	5	318	-	-	11/28/48/70	0/1/1/1
30	CLA	B	823	40	1/1/12/20	5/26/102/115	-
34	LHG	9	318	-	-	19/38/38/53	-
38	KC1	6	308	18	-	6/15/71/71	-
30	CLA	7	305	40	1/1/15/20	8/39/115/115	-
30	CLA	B	834	2	1/1/14/20	8/33/109/115	-
30	CLA	2u	202	12	1/1/15/20	15/39/115/115	-
35	LMT	7	301	30	-	3/21/61/61	0/2/2/2
39	DD6	10	313	-	-	11/26/80/80	0/3/3/3
30	CLA	16	305	28	1/1/12/20	2/21/97/115	-
30	CLA	9	301	34	1/1/15/20	7/39/115/115	-
30	CLA	15	309	-	-	12/39/115/115	-
32	SF4	C	102	3	-	-	0/6/5/5
37	A86	10	301	-	-	6/34/90/90	0/3/3/3
35	LMT	A	857	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	11	302	-	-	0/21/61/61	0/2/2/2
30	CLA	10	303	22	1/1/15/20	14/39/115/115	-
38	KC1	6	312	18	-	5/15/71/71	-
35	LMT	1	311	-	-	5/21/61/61	0/2/2/2
38	KC1	3	308	15	-	8/15/71/71	-
30	CLA	A	834	1	1/1/15/20	11/39/115/115	-
30	CLA	16	309	28	-	6/15/91/115	-
37	A86	14	320	-	-	10/34/90/90	0/3/3/3
30	CLA	A	816	35,1	1/1/15/20	19/39/115/115	-
37	A86	14	314	-	-	10/34/90/90	0/3/3/3
39	DD6	10	314	-	-	9/26/80/80	0/3/3/3
39	DD6	13	314	-	-	13/26/80/80	0/3/3/3
30	CLA	10	311	-	-	8/15/91/115	-
35	LMT	A	854	-	-	16/21/61/61	0/2/2/2
37	A86	14	316	-	-	10/34/90/90	0/3/3/3
39	DD6	3	313	-	-	9/26/80/80	0/3/3/3
39	DD6	3	316	-	-	12/26/80/80	0/3/3/3
37	A86	15	317	30	-	15/34/90/90	0/3/3/3
30	CLA	4	301	2	1/1/11/20	8/20/96/115	-
30	CLA	13	303	-	-	9/39/115/115	-
30	CLA	A	811	1	1/1/15/20	11/39/115/115	-
37	A86	5	316	-	-	6/34/90/90	0/3/3/3
30	CLA	B	839	34	1/1/15/20	4/39/115/115	-
38	KC1	11	311	23	-	10/15/71/71	-
30	CLA	5	302	17	1/1/15/20	14/39/115/115	-
31	PQN	A	845	-	-	6/23/43/43	0/2/2/2
38	KC1	8	312	38	-	9/15/71/71	-
30	CLA	15	306	-	1/1/11/20	8/15/91/115	-
37	A86	15	322	30	-	15/34/90/90	0/3/3/3
38	KC1	12	311	24	-	5/15/71/71	-
30	CLA	B	827	2	1/1/15/20	7/39/115/115	-
38	KC1	13	305	25	-	8/15/71/71	-
33	BCR	2u	201	-	-	11/29/63/63	0/2/2/2
39	DD6	2	317	-	-	14/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	6	305	18	1/1/15/20	5/39/115/115	-
39	DD6	8	317	-	-	10/26/80/80	0/3/3/3
30	CLA	A	838	1	1/1/12/20	4/23/99/115	-
30	CLA	B	811	30,2	1/1/15/20	11/39/115/115	-
37	A86	15	321	-	-	13/34/90/90	0/3/3/3
38	KC1	12	313	24	-	7/15/71/71	-
39	DD6	9	314	-	-	12/26/80/80	0/3/3/3
30	CLA	11	306	40	1/1/13/20	10/27/103/115	-
30	CLA	12	304	24,39	1/1/15/20	15/39/115/115	-
30	CLA	4	309	-	1/1/15/20	10/39/115/115	-
37	A86	16	312	-	-	14/34/90/90	0/3/3/3
38	KC1	10	310	22	-	6/15/71/71	-
35	LMT	15	301	-	-	6/21/61/61	0/2/2/2
30	CLA	B	831	2	-	9/31/107/115	-
30	CLA	8	308	20	1/1/13/20	9/27/103/115	-
39	DD6	2	315	-	-	12/26/80/80	0/3/3/3
30	CLA	A	827	40	1/1/15/20	5/39/115/115	-
38	KC1	9	311	-	-	9/15/71/71	-
33	BCR	L	201	-	-	12/29/63/63	0/2/2/2
35	LMT	12	318	-	-	3/21/61/61	0/2/2/2
38	KC1	1	306	13	-	9/15/71/71	-
30	CLA	F	202	40	1/1/15/20	17/39/115/115	-
38	KC1	13	308	25	-	10/15/71/71	-
30	CLA	A	819	1	-	7/26/102/115	-
38	KC1	5	305	17	-	5/15/71/71	-
30	CLA	3	305	15	1/1/14/20	13/36/112/115	-
30	CLA	15	311	37	1/1/11/20	6/15/91/115	-
30	CLA	B	819	40	1/1/15/20	11/39/115/115	-
37	A86	4	312	-	-	9/34/90/90	0/3/3/3
38	KC1	7	308	40	-	7/15/71/71	-
38	KC1	4	308	16	-	2/15/71/71	-
30	CLA	12	306	24	1/1/15/20	6/39/115/115	-
30	CLA	B	802	30,40	1/1/15/20	9/39/115/115	-
30	CLA	B	808	2	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	828	2	1/1/15/20	13/39/115/115	-
37	A86	7	316	-	-	6/34/90/90	0/3/3/3
30	CLA	B	824	40	1/1/15/20	7/39/115/115	-
37	A86	2	302	-	-	10/34/90/90	0/3/3/3
30	CLA	B	817	2	1/1/13/20	5/32/108/115	-
39	DD6	12	317	-	-	13/26/80/80	0/3/3/3
30	CLA	11	308	23	1/1/15/20	12/39/115/115	-
38	KC1	12	309	24	-	9/15/71/71	-
30	CLA	11	304	23	1/1/15/20	11/39/115/115	-
30	CLA	B	805	2	1/1/15/20	11/39/115/115	-
30	CLA	9	306	21,37	1/1/11/20	7/15/91/115	-
38	KC1	2	306	14	-	5/15/71/71	-
38	KC1	14	308	26,30	-	9/15/71/71	-
37	A86	3	315	-	-	14/34/90/90	0/3/3/3
30	CLA	3	301	15	1/1/15/20	9/39/115/115	-
30	CLA	A	802	40	1/1/15/20	7/39/115/115	-
39	DD6	6	319	-	-	11/26/80/80	0/3/3/3
30	CLA	A	808	1	1/1/12/20	3/23/99/115	-
33	BCR	A	851	-	-	7/29/63/63	0/2/2/2
30	CLA	12	308	40	1/1/15/20	11/39/115/115	-
30	CLA	11	310	23	1/1/15/20	17/39/115/115	-
30	CLA	6	306	40	1/1/15/20	10/39/115/115	-
38	KC1	9	304	21	-	6/15/71/71	-
30	CLA	5	304	17	1/1/15/20	13/39/115/115	-
38	KC1	13	310	25	-	5/15/71/71	-
30	CLA	A	824	1	1/1/12/20	3/23/99/115	-
35	LMT	12	319	-	-	0/21/61/61	0/2/2/2
30	CLA	7	311	19	1/1/15/20	14/39/115/115	-
37	A86	10	302	-	-	12/34/90/90	0/3/3/3
38	KC1	4	307	16	-	6/15/71/71	-
34	LHG	5	317	30	-	4/31/31/53	-
30	CLA	B	825	2	1/1/15/20	10/39/115/115	-
30	CLA	5	307	17	1/1/15/20	13/39/115/115	-
32	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	6	313	18	-	5/15/71/71	-
30	CLA	A	805	30,1	1/1/13/20	9/32/108/115	-
39	DD6	15	319	30	-	13/26/80/80	0/3/3/3
30	CLA	A	839	1	1/1/15/20	11/39/115/115	-
30	CLA	A	806	1	1/1/15/20	14/39/115/115	-
30	CLA	7	310	19	-	11/39/115/115	-
38	KC1	13	311	25	-	2/15/71/71	-
37	A86	8	315	-	-	7/34/90/90	0/3/3/3
35	LMT	B	852	-	-	8/21/61/61	0/2/2/2
30	CLA	9	302	9	1/1/12/20	6/23/99/115	-
38	KC1	14	311	26	-	5/15/71/71	-
30	CLA	9	308	21	1/1/15/20	15/39/115/115	-
38	KC1	7	313	-	-	4/15/71/71	-
30	CLA	16	306	28	1/1/12/20	15/24/100/115	-
30	CLA	B	837	40	1/1/15/20	5/39/115/115	-
30	CLA	16	307	-	1/1/11/20	5/17/93/115	-
30	CLA	9	309	40	1/1/15/20	11/39/115/115	-
37	A86	2u	205	-	-	11/34/90/90	0/3/3/3
39	DD6	2	316	-	-	12/26/80/80	0/3/3/3
38	KC1	9	310	21	-	6/15/71/71	-
30	CLA	12	307	24	1/1/11/20	6/17/93/115	-
37	A86	3	314	-	-	8/34/90/90	0/3/3/3
33	BCR	A	850	-	-	11/29/63/63	0/2/2/2
30	CLA	1	303	30,13	1/1/15/20	15/39/115/115	-
30	CLA	4	303	16	1/1/15/20	5/39/115/115	-
36	LMG	8	319	36	-	17/32/52/70	0/1/1/1
37	A86	15	315	-	-	9/34/90/90	0/3/3/3
36	LMG	A	856	-	-	15/29/49/70	0/1/1/1
30	CLA	6	315	18	1/1/11/20	4/15/91/115	-
37	A86	14	317	-	-	15/34/90/90	0/3/3/3
30	CLA	A	835	1	1/1/15/20	11/39/115/115	-
35	LMT	A	855	-	-	4/21/61/61	0/2/2/2
37	A86	13	315	-	-	12/34/90/90	0/3/3/3
38	KC1	9	312	21	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	1	308	13	-	3/15/71/71	-
30	CLA	8	309	20	-	3/18/94/115	-
30	CLA	B	820	2	-	3/15/91/115	-
30	CLA	15	310	27	1/1/11/20	6/15/91/115	-
30	CLA	B	826	2	1/1/15/20	16/39/115/115	-
37	A86	12	314	-	-	12/34/90/90	0/3/3/3
30	CLA	1	302	30,13	1/1/15/20	9/39/115/115	-
30	CLA	2	304	14	1/1/15/20	10/39/115/115	-
37	A86	11	316	-	-	13/34/90/90	0/3/3/3
38	KC1	14	306	26	-	8/15/71/71	-
33	BCR	A	849	-	-	10/29/63/63	0/2/2/2
37	A86	2	318	-	-	8/34/90/90	0/3/3/3
30	CLA	A	828	1	1/1/15/20	13/39/115/115	-
30	CLA	A	807	1	1/1/15/20	13/39/115/115	-
33	BCR	A	848	-	-	10/29/63/63	0/2/2/2
33	BCR	B	842	-	-	8/29/63/63	0/2/2/2
30	CLA	5	303	17	1/1/15/20	7/39/115/115	-
30	CLA	A	842	1	1/1/15/20	10/39/115/115	-
30	CLA	B	818	2	1/1/14/20	7/33/109/115	-
30	CLA	4	311	16	1/1/12/20	2/21/97/115	-
37	A86	9	315	-	-	10/34/90/90	0/3/3/3
30	CLA	B	836	2	1/1/11/20	2/18/94/115	-
39	DD6	12	315	30	-	9/26/80/80	0/3/3/3
34	LHG	B	848	30	-	18/31/31/53	-
30	CLA	2	301	2	1/1/15/20	10/39/115/115	-
37	A86	14	301	-	-	7/34/90/90	0/3/3/3
30	CLA	A	820	1	1/1/15/20	18/39/115/115	-
33	BCR	B	841	-	-	10/29/63/63	0/2/2/2
30	CLA	A	803	-	1/1/15/20	7/39/115/115	-
37	A86	4	317	-	-	5/34/90/90	0/3/3/3
37	A86	9	316	30	-	9/34/90/90	0/3/3/3
30	CLA	A	841	1	1/1/15/20	10/39/115/115	-
30	CLA	5	311	40	1/1/15/20	15/39/115/115	-
30	CLA	16	301	28	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	6	314	18	-	18/39/115/115	-
30	CLA	A	840	1	1/1/11/20	3/18/94/115	-
39	DD6	7	302	-	-	12/26/80/80	0/3/3/3
30	CLA	A	836	1	1/1/12/20	9/26/102/115	-
38	KC1	8	314	40,38	-	5/15/71/71	-
36	LMG	2u	204	-	-	14/26/46/70	0/1/1/1
30	CLA	14	304	26	1/1/11/20	6/15/91/115	-
33	BCR	J	103	-	-	9/29/63/63	0/2/2/2
30	CLA	B	851	14	-	12/39/115/115	-
37	A86	14	318	-	-	16/34/90/90	0/3/3/3
38	KC1	8	313	20	-	5/15/71/71	-
35	LMT	6	302	-	-	2/17/57/61	0/2/2/2
30	CLA	13	304	25	-	8/15/91/115	-
30	CLA	B	821	2	1/1/13/20	15/27/103/115	-
30	CLA	15	314	30	-	6/15/91/115	-
30	CLA	7	303	19	1/1/15/20	12/39/115/115	-
30	CLA	2	309	34	1/1/15/20	11/39/115/115	-
30	CLA	8	304	20	1/1/13/20	10/31/107/115	-
30	CLA	14	307	38	-	8/39/115/115	-
37	A86	11	301	-	-	13/34/90/90	0/3/3/3
30	CLA	14	310	-	1/1/12/20	6/21/97/115	-
30	CLA	4	306	16	1/1/15/20	12/39/115/115	-
30	CLA	B	829	2	1/1/15/20	13/39/115/115	-
30	CLA	1	305	40	1/1/15/20	10/39/115/115	-
39	DD6	6	303	30	-	10/26/80/80	0/3/3/3
35	LMT	9	317	-	-	5/18/58/61	0/2/2/2
30	CLA	13	302	25	1/1/15/20	16/39/115/115	-
30	CLA	16	303	28	1/1/15/20	20/39/115/115	-
30	CLA	A	822	40	1/1/15/20	9/39/115/115	-
30	CLA	4	302	16	1/1/15/20	12/39/115/115	-
30	CLA	8	301	20	1/1/15/20	16/39/115/115	-
31	PQN	B	840	-	-	5/23/43/43	0/2/2/2
37	A86	14	319	30	-	10/34/90/90	0/3/3/3
30	CLA	10	305	40	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	A	852	-	-	25/53/53/53	-
30	CLA	A	844	-	1/1/15/20	14/39/115/115	-
38	KC1	13	306	25	-	9/15/71/71	-
38	KC1	11	305	23	-	7/15/71/71	-
38	KC1	4	310	16	-	4/15/71/71	-
30	CLA	B	807	2	1/1/15/20	9/39/115/115	-
30	CLA	A	814	1	1/1/14/20	11/33/109/115	-
33	BCR	M	101	-	-	10/29/63/63	0/2/2/2
30	CLA	B	814	2	1/1/13/20	5/27/103/115	-
38	KC1	12	305	24	-	7/15/71/71	-
30	CLA	13	301	25	1/1/15/20	17/39/115/115	-
39	DD6	7	317	-	-	10/26/80/80	0/3/3/3
39	DD6	16	313	-	-	13/26/80/80	0/3/3/3
38	KC1	10	312	22	-	5/15/71/71	-
36	LMG	8	320	-	-	20/37/57/70	0/1/1/1
30	CLA	7	306	19	1/1/15/20	8/39/115/115	-
30	CLA	B	830	2	1/1/15/20	10/39/115/115	-
30	CLA	10	308	22	1/1/15/20	13/39/115/115	-
37	A86	7	319	-	-	10/34/90/90	0/3/3/3
30	CLA	13	309	-	1/1/11/20	9/15/91/115	-
33	BCR	F	204	-	-	8/29/63/63	0/2/2/2
38	KC1	16	304	28	-	7/15/71/71	-
37	A86	10	315	-	-	13/34/90/90	0/3/3/3
30	CLA	B	806	2	1/1/15/20	9/39/115/115	-
38	KC1	8	307	20	-	8/15/71/71	-
30	CLA	15	304	30,39,27	1/1/15/20	20/39/115/115	-
39	DD6	1	310	-	-	12/26/80/80	0/3/3/3
30	CLA	B	804	2	1/1/12/20	7/24/100/115	-
30	CLA	B	816	2	-	9/27/103/115	-
30	CLA	15	305	37,27	1/1/11/20	10/15/91/115	-
39	DD6	4	313	-	-	14/26/80/80	0/3/3/3
30	CLA	10	309	22	1/1/15/20	12/39/115/115	-
37	A86	4	315	-	-	5/34/90/90	0/3/3/3
35	LMT	11	303	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	B	847	-	-	25/50/70/70	0/1/1/1
30	CLA	A	830	1	1/1/15/20	9/39/115/115	-
30	CLA	A	823	1	-	6/20/96/115	-
30	CLA	B	838	2	1/1/15/20	15/39/115/115	-
30	CLA	5	309	34	1/1/15/20	11/39/115/115	-
30	CLA	1	307	13	-	16/39/115/115	-
38	KC1	11	312	-	-	5/15/71/71	-
30	CLA	2	311	14	-	11/39/115/115	-
30	CLA	B	810	2	1/1/15/20	7/39/115/115	-
30	CLA	9	305	-	1/1/15/20	13/39/115/115	-
38	KC1	5	310	17	-	6/15/71/71	-
30	CLA	16	310	28	1/1/11/20	8/15/91/115	-
37	A86	9	313	-	-	8/34/90/90	0/3/3/3
30	CLA	3	306	15	1/1/15/20	11/39/115/115	-
38	KC1	16	311	28	-	6/15/71/71	-
30	CLA	12	310	40	-	10/39/115/115	-
30	CLA	13	307	25	1/1/15/20	6/39/115/115	-
30	CLA	3	307	15	1/1/15/20	13/39/115/115	-
30	CLA	A	804	1	1/1/15/20	11/39/115/115	-
30	CLA	A	818	1	-	6/26/102/115	-
30	CLA	2	313	14	-	5/15/91/115	-
30	CLA	6	304	18	1/1/15/20	12/39/115/115	-
38	KC1	11	307	23	-	10/15/71/71	-
39	DD6	7	318	-	-	14/26/80/80	0/3/3/3
30	CLA	6	309	18	1/1/15/20	14/39/115/115	-
30	CLA	A	825	1	1/1/13/20	13/32/108/115	-
35	LMT	7	321	-	-	4/21/61/61	0/2/2/2
36	LMG	6	301	30	-	16/28/48/70	0/1/1/1
37	A86	11	315	-	-	13/34/90/90	0/3/3/3
33	BCR	B	843	-	-	8/29/63/63	0/2/2/2
33	BCR	J	102	-	-	10/29/63/63	0/2/2/2
38	KC1	5	306	17	-	10/15/71/71	-
30	CLA	6	310	34	1/1/15/20	8/39/115/115	-
37	A86	2	319	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	812	2	1/1/15/20	7/39/115/115	-
37	A86	7	315	-	-	16/34/90/90	0/3/3/3
30	CLA	A	810	1	1/1/15/20	13/39/115/115	-
30	CLA	A	831	1	1/1/15/20	7/39/115/115	-
30	CLA	A	826	40	1/1/15/20	13/39/115/115	-
33	BCR	B	845	-	-	11/29/63/63	0/2/2/2
39	DD6	6	318	-	-	11/26/80/80	0/3/3/3
30	CLA	1	301	13	1/1/15/20	15/39/115/115	-
30	CLA	9	307	21	1/1/15/20	11/39/115/115	-
36	LMG	8	321	36	-	5/24/44/70	0/1/1/1
35	LMT	16	315	-	-	5/21/61/61	0/2/2/2
38	KC1	2	314	40	-	9/15/71/71	-
35	LMT	12	301	-	-	4/21/61/61	0/2/2/2
35	LMT	B	850	-	-	0/21/61/61	0/2/2/2
30	CLA	16	308	28	1/1/11/20	6/15/91/115	-
39	DD6	3	312	-	-	11/26/80/80	0/3/3/3
34	LHG	A	853	30	-	8/31/31/53	-
30	CLA	3	303	-	1/1/15/20	15/39/115/115	-
37	A86	12	316	-	-	16/34/90/90	0/3/3/3
30	CLA	1	304	13	1/1/15/20	12/39/115/115	-
30	CLA	2	305	40	1/1/15/20	12/39/115/115	-
30	CLA	6	307	39,18	1/1/15/20	13/39/115/115	-
37	A86	15	320	-	-	15/34/90/90	0/3/3/3
30	CLA	5	308	17	-	15/39/115/115	-
30	CLA	A	813	1	1/1/15/20	13/39/115/115	-
30	CLA	B	801	2	1/1/15/20	8/39/115/115	-
35	LMT	8	322	-	-	3/21/61/61	0/2/2/2
33	BCR	L	205	-	-	8/29/63/63	0/2/2/2
39	DD6	6	321	-	-	12/26/80/80	0/3/3/3
37	A86	15	316	30	-	13/34/90/90	0/3/3/3
33	BCR	I	101	-	-	4/29/63/63	0/2/2/2
37	A86	8	318	-	-	11/34/90/90	0/3/3/3
30	CLA	15	303	30,37,27	1/1/14/20	8/33/109/115	-
30	CLA	15	313	27	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	11	314	-	-	12/34/90/90	0/3/3/3
30	CLA	B	822	30,2	-	11/39/115/115	-
30	CLA	9	303	21	-	9/39/115/115	-
30	CLA	10	304	22	1/1/15/20	2/39/115/115	-
39	DD6	5	314	-	-	10/26/80/80	0/3/3/3
30	CLA	B	815	2	1/1/11/20	4/15/91/115	-
37	A86	10	316	-	-	11/34/90/90	0/3/3/3
34	LHG	2	320	30	-	12/31/31/53	-
30	CLA	12	303	24	1/1/15/20	6/39/115/115	-
39	DD6	15	318	-	-	13/26/80/80	0/3/3/3
30	CLA	A	821	1	1/1/14/20	9/35/111/115	-
30	CLA	10	307	22	1/1/15/20	12/39/115/115	-
30	CLA	14	303	26	1/1/13/20	10/30/106/115	-
30	CLA	A	812	30,1	1/1/15/20	16/39/115/115	-
30	CLA	4	304	-	1/1/14/20	10/33/109/115	-
30	CLA	6	317	-	1/1/15/20	15/39/115/115	-
33	BCR	B	846	-	-	7/29/63/63	0/2/2/2
38	KC1	13	312	25	-	6/15/71/71	-
38	KC1	8	306	40	-	8/15/71/71	-
30	CLA	15	308	30,27	1/1/11/20	10/15/91/115	-

All (7691) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	322	A86	C14-C13	16.41	1.69	1.51
37	15	315	A86	C14-C13	16.01	1.69	1.51
37	9	313	A86	C14-C13	15.74	1.68	1.51
37	16	314	A86	C14-C13	15.70	1.68	1.51
37	10	317	A86	C14-C13	15.54	1.68	1.51
37	2u	205	A86	C14-C13	15.53	1.68	1.51
37	15	320	A86	C14-C13	15.52	1.68	1.51
37	15	321	A86	C14-C13	15.45	1.68	1.51
37	9	316	A86	C14-C13	15.34	1.68	1.51
37	14	320	A86	C14-C13	15.32	1.68	1.51
37	13	315	A86	C14-C13	15.27	1.68	1.51
37	5	301	A86	C14-C13	15.24	1.68	1.51
37	7	319	A86	C14-C13	15.22	1.68	1.51
37	4	317	A86	C14-C13	15.22	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	301	A86	C14-C13	15.20	1.68	1.51
37	3	315	A86	C14-C13	15.19	1.68	1.51
37	2	318	A86	C14-C13	15.18	1.68	1.51
37	15	316	A86	C14-C13	15.15	1.68	1.51
37	5	315	A86	C14-C13	15.15	1.68	1.51
37	11	315	A86	C14-C13	15.14	1.68	1.51
37	11	314	A86	C14-C13	15.10	1.68	1.51
37	5	316	A86	C14-C13	15.10	1.68	1.51
37	4	315	A86	C14-C13	15.08	1.68	1.51
39	2	315	DD6	C10-C11	15.07	1.70	1.35
37	9	315	A86	C14-C13	15.03	1.68	1.51
37	14	318	A86	C14-C13	15.01	1.68	1.51
37	10	315	A86	C14-C13	14.99	1.68	1.51
37	8	318	A86	C14-C13	14.98	1.67	1.51
37	15	323	A86	C14-C13	14.96	1.67	1.51
37	14	316	A86	C14-C13	14.96	1.67	1.51
37	15	317	A86	C14-C13	14.96	1.67	1.51
37	2	319	A86	C14-C13	14.91	1.67	1.51
37	2	302	A86	C14-C13	14.90	1.67	1.51
39	11	313	DD6	C10-C11	14.88	1.70	1.35
37	14	315	A86	C14-C13	14.88	1.67	1.51
39	6	303	DD6	C10-C11	14.86	1.70	1.35
37	12	316	A86	C14-C13	14.85	1.67	1.51
37	14	317	A86	C14-C13	14.84	1.67	1.51
37	16	312	A86	C14-C13	14.83	1.67	1.51
37	12	314	A86	C14-C13	14.82	1.67	1.51
39	15	318	DD6	C10-C11	14.80	1.70	1.35
39	10	313	DD6	C10-C11	14.80	1.70	1.35
37	11	316	A86	C14-C13	14.78	1.67	1.51
39	3	313	DD6	C10-C11	14.78	1.70	1.35
39	13	314	DD6	C10-C11	14.75	1.69	1.35
37	13	313	A86	C14-C13	14.75	1.67	1.51
37	14	319	A86	C14-C13	14.75	1.67	1.51
39	15	319	DD6	C10-C11	14.74	1.69	1.35
37	10	301	A86	C14-C13	14.72	1.67	1.51
39	10	314	DD6	C10-C11	14.72	1.69	1.35
39	5	313	DD6	C10-C11	14.71	1.69	1.35
37	4	314	A86	C14-C13	14.71	1.67	1.51
37	10	316	A86	C14-C13	14.71	1.67	1.51
37	14	314	A86	C14-C13	14.71	1.67	1.51
39	7	318	DD6	C10-C11	14.70	1.69	1.35
37	3	314	A86	C14-C13	14.69	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	317	DD6	C10-C11	14.69	1.69	1.35
39	7	302	DD6	C10-C11	14.64	1.69	1.35
39	3	316	DD6	C10-C11	14.61	1.69	1.35
39	12	315	DD6	C10-C11	14.61	1.69	1.35
39	3	312	DD6	C10-C11	14.61	1.69	1.35
39	1	310	DD6	C10-C11	14.59	1.69	1.35
39	4	313	DD6	C10-C11	14.59	1.69	1.35
39	12	317	DD6	C10-C11	14.58	1.69	1.35
39	16	313	DD6	C10-C11	14.57	1.69	1.35
39	7	317	DD6	C10-C11	14.55	1.69	1.35
37	10	302	A86	C14-C13	14.54	1.67	1.51
37	4	312	A86	C14-C13	14.45	1.67	1.51
37	2u	203	A86	C14-C13	14.44	1.67	1.51
39	6	318	DD6	C10-C11	14.39	1.69	1.35
39	8	317	DD6	C10-C11	14.39	1.69	1.35
39	7	314	DD6	C10-C11	14.38	1.69	1.35
39	4	316	DD6	C10-C11	14.37	1.69	1.35
37	7	315	A86	C14-C13	14.36	1.67	1.51
39	6	319	DD6	C10-C11	14.36	1.69	1.35
37	1	309	A86	C14-C13	14.35	1.67	1.51
39	5	314	DD6	C10-C11	14.34	1.69	1.35
39	9	314	DD6	C10-C11	14.33	1.68	1.35
37	11	301	A86	C14-C13	14.31	1.67	1.51
37	7	316	A86	C14-C13	14.30	1.67	1.51
39	6	321	DD6	C10-C11	14.27	1.68	1.35
39	2	316	DD6	C10-C11	14.25	1.68	1.35
39	8	316	DD6	C10-C11	14.20	1.68	1.35
37	6	320	A86	C14-C13	14.10	1.67	1.51
39	4	316	DD6	C36-C31	14.09	1.50	1.35
39	15	319	DD6	C36-C31	14.08	1.50	1.35
39	3	316	DD6	C36-C31	13.87	1.50	1.35
37	8	315	A86	C14-C13	13.78	1.66	1.51
39	7	302	DD6	C36-C31	13.74	1.50	1.35
39	1	310	DD6	C36-C31	13.71	1.50	1.35
39	6	321	DD6	C36-C31	13.70	1.50	1.35
39	8	317	DD6	C36-C31	13.68	1.50	1.35
39	5	313	DD6	C36-C31	13.66	1.50	1.35
39	13	314	DD6	C36-C31	13.63	1.50	1.35
39	6	319	DD6	C36-C31	13.63	1.50	1.35
39	7	317	DD6	C36-C31	13.60	1.50	1.35
39	2	316	DD6	C36-C31	13.57	1.50	1.35
39	10	313	DD6	C36-C31	13.54	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	9	314	DD6	C36-C31	13.52	1.50	1.35
39	12	315	DD6	C36-C31	13.49	1.49	1.35
39	16	313	DD6	C36-C31	13.48	1.49	1.35
39	10	314	DD6	C36-C31	13.47	1.49	1.35
39	11	313	DD6	C36-C31	13.39	1.49	1.35
39	3	312	DD6	C36-C31	13.38	1.49	1.35
39	15	318	DD6	C36-C31	13.34	1.49	1.35
39	7	318	DD6	C36-C31	13.32	1.49	1.35
39	3	313	DD6	C36-C31	13.30	1.49	1.35
39	2	317	DD6	C36-C31	13.25	1.49	1.35
39	4	313	DD6	C36-C31	13.25	1.49	1.35
39	8	316	DD6	C36-C31	13.22	1.49	1.35
39	6	303	DD6	C36-C31	13.19	1.49	1.35
39	2	315	DD6	C36-C31	13.19	1.49	1.35
39	7	314	DD6	C36-C31	13.14	1.49	1.35
39	5	314	DD6	C36-C31	13.09	1.49	1.35
39	6	318	DD6	C36-C31	12.99	1.49	1.35
39	12	317	DD6	C36-C31	12.97	1.49	1.35
37	13	313	A86	C30-C31	12.22	1.44	1.30
37	15	320	A86	C30-C31	12.06	1.44	1.30
37	9	316	A86	C30-C31	11.97	1.44	1.30
37	15	323	A86	C30-C31	11.94	1.44	1.30
37	15	317	A86	C30-C31	11.93	1.44	1.30
37	10	317	A86	C30-C31	11.88	1.44	1.30
37	15	322	A86	C30-C31	11.83	1.44	1.30
37	15	315	A86	C30-C31	11.83	1.44	1.30
37	9	315	A86	C30-C31	11.78	1.44	1.30
37	3	315	A86	C30-C31	11.77	1.44	1.30
39	15	319	DD6	C28-C27	11.77	1.58	1.50
37	2	302	A86	C30-C31	11.74	1.44	1.30
37	14	320	A86	C30-C31	11.68	1.44	1.30
39	4	316	DD6	C28-C27	11.61	1.58	1.50
39	16	313	DD6	C28-C27	11.57	1.58	1.50
37	10	302	A86	C30-C31	11.57	1.44	1.30
37	3	314	A86	C30-C31	11.56	1.44	1.30
37	16	312	A86	C30-C31	11.54	1.44	1.30
37	13	315	A86	C30-C31	11.53	1.44	1.30
37	7	319	A86	C30-C31	11.53	1.44	1.30
37	14	317	A86	C30-C31	11.52	1.44	1.30
39	15	318	DD6	C28-C27	11.51	1.58	1.50
37	14	301	A86	C30-C31	11.47	1.44	1.30
37	6	320	A86	C30-C31	11.45	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	301	A86	C30-C31	11.45	1.43	1.30
37	10	315	A86	C30-C31	11.44	1.43	1.30
37	5	316	A86	C30-C31	11.43	1.43	1.30
39	2	315	DD6	C28-C27	11.40	1.58	1.50
37	14	318	A86	C30-C31	11.38	1.43	1.30
39	9	314	DD6	C28-C27	11.38	1.58	1.50
37	11	316	A86	C30-C31	11.35	1.43	1.30
37	5	301	A86	C30-C31	11.35	1.43	1.30
37	14	316	A86	C30-C31	11.35	1.43	1.30
37	12	316	A86	C30-C31	11.34	1.43	1.30
37	14	314	A86	C30-C31	11.34	1.43	1.30
39	3	312	DD6	C28-C27	11.33	1.58	1.50
37	4	317	A86	C30-C31	11.32	1.43	1.30
37	4	314	A86	C30-C31	11.29	1.43	1.30
37	15	316	A86	C30-C31	11.28	1.43	1.30
39	3	313	DD6	C28-C27	11.26	1.58	1.50
37	4	315	A86	C30-C31	11.26	1.43	1.30
37	15	321	A86	C30-C31	11.26	1.43	1.30
39	13	314	DD6	C28-C27	11.24	1.58	1.50
37	5	315	A86	C30-C31	11.23	1.43	1.30
37	11	314	A86	C30-C31	11.23	1.43	1.30
37	2u	205	A86	C30-C31	11.22	1.43	1.30
39	5	313	DD6	C28-C27	11.15	1.58	1.50
37	14	319	A86	C30-C31	11.12	1.43	1.30
37	12	314	A86	C30-C31	11.09	1.43	1.30
37	16	314	A86	C30-C31	11.07	1.43	1.30
37	11	315	A86	C30-C31	11.06	1.43	1.30
37	2	318	A86	C30-C31	11.06	1.43	1.30
39	6	303	DD6	C28-C27	11.06	1.58	1.50
39	1	310	DD6	C28-C27	11.05	1.58	1.50
39	8	316	DD6	C28-C27	11.03	1.58	1.50
39	10	313	DD6	C28-C27	11.03	1.58	1.50
39	3	316	DD6	C28-C27	11.02	1.58	1.50
37	10	316	A86	C30-C31	10.98	1.43	1.30
37	1	309	A86	C30-C31	10.96	1.43	1.30
37	4	312	A86	C30-C31	10.94	1.43	1.30
39	6	321	DD6	C28-C27	10.88	1.58	1.50
39	8	317	DD6	C28-C27	10.86	1.58	1.50
37	14	315	A86	C30-C31	10.81	1.43	1.30
39	2	317	DD6	C28-C27	10.81	1.58	1.50
39	4	313	DD6	C28-C27	10.80	1.58	1.50
39	12	315	DD6	C28-C27	10.80	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5	314	DD6	C28-C27	10.79	1.58	1.50
37	8	318	A86	C30-C31	10.78	1.43	1.30
39	2	316	DD6	C28-C27	10.75	1.58	1.50
39	11	313	DD6	C28-C27	10.72	1.58	1.50
39	6	319	DD6	C28-C27	10.70	1.58	1.50
37	2u	203	A86	C30-C31	10.67	1.43	1.30
37	10	301	A86	C30-C31	10.66	1.43	1.30
39	10	314	DD6	C28-C27	10.64	1.57	1.50
37	8	315	A86	C30-C31	10.64	1.43	1.30
39	6	318	DD6	C28-C27	10.62	1.57	1.50
37	9	313	A86	C30-C31	10.45	1.42	1.30
39	6	319	DD6	C5-C6	10.40	1.59	1.35
39	4	313	DD6	C5-C6	10.32	1.59	1.35
39	12	317	DD6	C28-C27	10.23	1.57	1.50
39	13	314	DD6	C5-C6	10.21	1.59	1.35
39	2	316	DD6	C5-C6	10.20	1.59	1.35
37	7	316	A86	C30-C31	10.19	1.42	1.30
37	2	319	A86	C30-C31	10.17	1.42	1.30
39	7	314	DD6	C28-C27	10.15	1.57	1.50
39	7	317	DD6	C28-C27	10.14	1.57	1.50
39	7	317	DD6	C5-C6	10.12	1.59	1.35
39	16	313	DD6	C5-C6	10.12	1.59	1.35
39	3	316	DD6	C5-C6	10.06	1.59	1.35
39	2	317	DD6	C5-C6	10.06	1.59	1.35
39	10	314	DD6	C5-C6	10.06	1.59	1.35
39	3	313	DD6	C5-C6	10.04	1.59	1.35
39	5	313	DD6	C5-C6	10.04	1.59	1.35
39	11	313	DD6	C5-C6	10.02	1.59	1.35
37	7	315	A86	C30-C31	10.01	1.42	1.30
39	6	318	DD6	C5-C6	10.01	1.58	1.35
39	10	313	DD6	C5-C6	10.00	1.58	1.35
39	12	317	DD6	C5-C6	9.98	1.58	1.35
39	9	314	DD6	C5-C6	9.98	1.58	1.35
39	6	303	DD6	C5-C6	9.97	1.58	1.35
39	8	316	DD6	C5-C6	9.97	1.58	1.35
39	3	312	DD6	C5-C6	9.96	1.58	1.35
39	7	302	DD6	C5-C6	9.96	1.58	1.35
39	7	314	DD6	C5-C6	9.95	1.58	1.35
39	15	319	DD6	C5-C6	9.92	1.58	1.35
39	7	318	DD6	C5-C6	9.90	1.58	1.35
39	12	315	DD6	C5-C6	9.89	1.58	1.35
39	15	318	DD6	C5-C6	9.86	1.58	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	315	DD6	C5-C6	9.86	1.58	1.35
39	6	321	DD6	C5-C6	9.86	1.58	1.35
39	1	310	DD6	C5-C6	9.84	1.58	1.35
39	4	316	DD6	C5-C6	9.84	1.58	1.35
39	8	317	DD6	C5-C6	9.84	1.58	1.35
37	13	313	A86	C30-C29	9.75	1.47	1.31
39	7	302	DD6	C28-C27	9.73	1.57	1.50
39	5	314	DD6	C5-C6	9.72	1.58	1.35
39	7	318	DD6	C28-C27	9.71	1.57	1.50
37	9	316	A86	C30-C29	9.66	1.47	1.31
37	15	317	A86	C30-C29	9.59	1.47	1.31
37	10	317	A86	C30-C29	9.56	1.47	1.31
37	15	322	A86	C30-C29	9.56	1.47	1.31
37	9	315	A86	C30-C29	9.56	1.47	1.31
37	15	320	A86	C30-C29	9.55	1.47	1.31
37	15	323	A86	C30-C29	9.51	1.47	1.31
29	A	801	CL0	C1A-CHA	9.50	1.50	1.40
37	13	315	A86	C30-C29	9.44	1.47	1.31
37	3	314	A86	C30-C29	9.43	1.47	1.31
37	7	319	A86	C30-C29	9.39	1.47	1.31
37	3	315	A86	C30-C29	9.38	1.47	1.31
37	2	302	A86	C30-C29	9.37	1.47	1.31
37	15	315	A86	C30-C29	9.35	1.47	1.31
37	14	320	A86	C30-C29	9.35	1.47	1.31
37	14	317	A86	C30-C29	9.34	1.47	1.31
37	14	316	A86	C30-C29	9.32	1.47	1.31
37	14	301	A86	C30-C29	9.30	1.47	1.31
37	10	315	A86	C30-C29	9.29	1.47	1.31
37	14	318	A86	C30-C29	9.28	1.47	1.31
37	16	312	A86	C30-C29	9.26	1.46	1.31
37	4	317	A86	C30-C29	9.24	1.46	1.31
37	10	302	A86	C30-C29	9.23	1.46	1.31
37	5	301	A86	C30-C29	9.21	1.46	1.31
37	12	316	A86	C30-C29	9.20	1.46	1.31
37	4	315	A86	C30-C29	9.18	1.46	1.31
37	6	320	A86	C30-C29	9.17	1.46	1.31
37	14	314	A86	C30-C29	9.17	1.46	1.31
37	11	314	A86	C30-C29	9.16	1.46	1.31
37	11	316	A86	C30-C29	9.15	1.46	1.31
37	4	314	A86	C30-C29	9.15	1.46	1.31
37	15	316	A86	C30-C29	9.13	1.46	1.31
37	5	315	A86	C30-C29	9.11	1.46	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	321	A86	C30-C29	9.11	1.46	1.31
39	15	319	DD6	C23-C16	9.11	1.71	1.53
37	5	316	A86	C30-C29	9.11	1.46	1.31
37	11	301	A86	C30-C29	9.10	1.46	1.31
39	2	317	DD6	C23-C16	9.06	1.71	1.53
37	12	314	A86	C30-C29	9.03	1.46	1.31
37	16	314	A86	C30-C29	9.02	1.46	1.31
39	12	315	DD6	C23-C16	9.00	1.71	1.53
37	14	319	A86	C30-C29	9.00	1.46	1.31
37	11	315	A86	C30-C29	8.99	1.46	1.31
37	10	316	A86	C30-C29	8.95	1.46	1.31
37	2	318	A86	C30-C29	8.94	1.46	1.31
39	10	313	DD6	C23-C16	8.94	1.70	1.53
37	2u	205	A86	C30-C29	8.92	1.46	1.31
37	1	309	A86	C30-C29	8.88	1.46	1.31
39	6	321	DD6	C13-C11	-8.84	1.27	1.46
37	8	318	A86	C30-C29	8.83	1.46	1.31
39	1	310	DD6	C23-C16	8.82	1.70	1.53
39	15	318	DD6	C23-C16	8.82	1.70	1.53
39	3	312	DD6	C23-C16	8.81	1.70	1.53
37	10	301	A86	C30-C29	8.81	1.46	1.31
37	4	312	A86	C30-C29	8.79	1.46	1.31
37	14	315	A86	C30-C29	8.79	1.46	1.31
39	5	314	DD6	C13-C11	-8.72	1.27	1.46
39	6	303	DD6	C23-C16	8.70	1.70	1.53
37	2u	203	A86	C30-C29	8.68	1.46	1.31
39	5	314	DD6	C23-C16	8.68	1.70	1.53
37	9	313	A86	C30-C29	8.64	1.45	1.31
39	5	313	DD6	C23-C16	8.64	1.70	1.53
39	3	316	DD6	C23-C16	8.62	1.70	1.53
39	5	313	DD6	C13-C11	-8.62	1.27	1.46
39	3	313	DD6	C23-C16	8.61	1.70	1.53
39	2	315	DD6	C23-C16	8.58	1.70	1.53
39	1	310	DD6	C13-C11	-8.57	1.27	1.46
39	2	317	DD6	C13-C11	-8.57	1.27	1.46
39	9	314	DD6	C23-C16	8.56	1.70	1.53
39	4	316	DD6	C23-C16	8.55	1.70	1.53
39	8	317	DD6	C13-C11	-8.52	1.27	1.46
37	8	315	A86	C30-C29	8.52	1.45	1.31
39	3	312	DD6	C13-C11	-8.50	1.27	1.46
39	6	318	DD6	C23-C16	8.49	1.70	1.53
39	11	313	DD6	C23-C16	8.48	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	318	DD6	C13-C11	-8.48	1.27	1.46
39	10	314	DD6	C13-C11	-8.48	1.27	1.46
39	7	318	DD6	C13-C11	-8.47	1.27	1.46
39	8	317	DD6	C23-C16	8.46	1.69	1.53
39	15	319	DD6	C13-C11	-8.46	1.27	1.46
39	7	317	DD6	C13-C11	-8.45	1.27	1.46
39	7	318	DD6	C23-C16	8.44	1.69	1.53
30	2	303	CLA	OBD-CAD	8.44	1.37	1.22
39	7	314	DD6	C23-C16	8.44	1.69	1.53
39	13	314	DD6	C23-C16	8.43	1.69	1.53
39	9	314	DD6	C13-C11	-8.43	1.27	1.46
37	2	319	A86	C30-C29	8.42	1.45	1.31
39	16	313	DD6	C13-C11	-8.42	1.27	1.46
39	12	317	DD6	C13-C11	-8.42	1.27	1.46
37	7	316	A86	C30-C29	8.41	1.45	1.31
39	4	313	DD6	C23-C16	8.40	1.69	1.53
39	6	303	DD6	C13-C11	-8.40	1.28	1.46
39	12	315	DD6	C13-C11	-8.39	1.28	1.46
39	7	317	DD6	C23-C16	8.38	1.69	1.53
39	4	313	DD6	C13-C11	-8.38	1.28	1.46
39	2	316	DD6	C23-C16	8.37	1.69	1.53
29	A	801	CL0	C1B-C2B	8.36	1.49	1.39
37	7	315	A86	C30-C29	8.35	1.45	1.31
39	11	313	DD6	C19-C20	8.35	1.63	1.52
39	15	318	DD6	C13-C11	-8.33	1.28	1.46
39	4	316	DD6	C13-C11	-8.28	1.28	1.46
39	12	317	DD6	C19-C20	8.25	1.63	1.52
39	6	321	DD6	C23-C16	8.25	1.69	1.53
39	12	317	DD6	C23-C16	8.24	1.69	1.53
39	8	316	DD6	C23-C16	8.20	1.69	1.53
39	3	316	DD6	C13-C11	-8.19	1.28	1.46
39	10	313	DD6	C13-C11	-8.19	1.28	1.46
39	10	314	DD6	C23-C16	8.17	1.69	1.53
39	10	313	DD6	C19-C20	8.13	1.63	1.52
39	11	313	DD6	C13-C11	-8.13	1.28	1.46
39	6	303	DD6	C19-C20	8.13	1.63	1.52
39	2	316	DD6	C13-C11	-8.11	1.28	1.46
39	7	302	DD6	C23-C16	8.06	1.69	1.53
39	7	302	DD6	C19-C20	8.05	1.63	1.52
39	6	318	DD6	C19-C20	8.04	1.63	1.52
39	3	313	DD6	C13-C11	-8.04	1.28	1.46
39	7	314	DD6	C13-C11	-8.04	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	319	DD6	C19-C20	8.04	1.63	1.52
39	13	314	DD6	C19-C20	8.04	1.63	1.52
37	2u	205	A86	C8-C6	8.02	1.63	1.46
37	4	314	A86	C8-C6	7.99	1.63	1.46
38	8	314	KC1	C2A-C3A	7.99	1.53	1.37
39	7	314	DD6	C19-C20	7.99	1.63	1.52
37	10	302	A86	C8-C6	7.96	1.63	1.46
37	14	314	A86	C4-C5	7.95	1.67	1.43
39	16	313	DD6	C21-C20	-7.95	1.39	1.51
39	7	318	DD6	C19-C20	7.93	1.63	1.52
37	15	315	A86	C4-C5	7.91	1.67	1.43
39	6	319	DD6	C13-C11	-7.89	1.29	1.46
39	16	313	DD6	C19-C20	7.89	1.63	1.52
37	11	301	A86	C8-C6	7.88	1.62	1.46
39	2	315	DD6	C13-C11	-7.88	1.29	1.46
39	7	302	DD6	C13-C11	-7.87	1.29	1.46
39	13	314	DD6	C13-C11	-7.87	1.29	1.46
37	15	315	A86	C8-C6	7.86	1.62	1.46
37	13	313	A86	C4-C5	7.86	1.67	1.43
38	11	312	KC1	C2A-C3A	7.84	1.53	1.37
38	4	308	KC1	C2A-C3A	7.84	1.53	1.37
37	2u	203	A86	C8-C6	7.83	1.62	1.46
39	11	313	DD6	C9-C10	7.82	1.67	1.43
39	10	314	DD6	C19-C20	7.81	1.63	1.52
39	3	313	DD6	C9-C10	7.79	1.67	1.43
39	15	318	DD6	C19-C20	7.78	1.63	1.52
38	16	311	KC1	C2A-C3A	7.76	1.52	1.37
39	6	319	DD6	C23-C16	7.76	1.68	1.53
39	8	316	DD6	C13-C11	-7.75	1.29	1.46
37	15	320	A86	C4-C5	7.75	1.67	1.43
39	16	313	DD6	C23-C16	7.74	1.68	1.53
37	15	322	A86	C4-C5	7.74	1.67	1.43
39	7	302	DD6	C9-C10	7.73	1.67	1.43
37	14	320	A86	C4-C5	7.72	1.67	1.43
39	2	317	DD6	C19-C20	7.72	1.63	1.52
39	13	314	DD6	C9-C10	7.72	1.67	1.43
37	9	316	A86	C4-C5	7.71	1.67	1.43
37	8	318	A86	C4-C5	7.69	1.67	1.43
39	12	317	DD6	C9-C10	7.69	1.67	1.43
39	6	319	DD6	C9-C10	7.69	1.67	1.43
39	3	316	DD6	C9-C10	7.68	1.67	1.43
39	2	317	DD6	C9-C10	7.68	1.67	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	320	A86	C8-C6	7.67	1.62	1.46
37	9	316	A86	C8-C6	7.66	1.62	1.46
39	5	313	DD6	C9-C10	7.66	1.66	1.43
37	10	317	A86	C4-C5	7.66	1.66	1.43
39	15	319	DD6	C19-C20	7.66	1.63	1.52
39	1	310	DD6	C19-C20	7.65	1.62	1.52
37	16	312	A86	C4-C5	7.65	1.66	1.43
39	16	313	DD6	C9-C10	7.65	1.66	1.43
37	14	319	A86	C4-C5	7.64	1.66	1.43
37	13	313	A86	C8-C6	7.64	1.62	1.46
37	13	315	A86	C4-C5	7.64	1.66	1.43
37	3	314	A86	C4-C5	7.64	1.66	1.43
37	15	323	A86	C4-C5	7.63	1.66	1.43
39	10	314	DD6	C9-C10	7.62	1.66	1.43
37	9	315	A86	C4-C5	7.62	1.66	1.43
39	7	318	DD6	C9-C10	7.62	1.66	1.43
39	3	312	DD6	C9-C10	7.61	1.66	1.43
37	15	317	A86	C4-C5	7.61	1.66	1.43
37	12	316	A86	C4-C5	7.60	1.66	1.43
39	12	315	DD6	C9-C10	7.60	1.66	1.43
39	7	317	DD6	C19-C20	7.60	1.62	1.52
39	7	317	DD6	C9-C10	7.60	1.66	1.43
37	15	316	A86	C4-C5	7.59	1.66	1.43
39	15	318	DD6	C9-C10	7.59	1.66	1.43
38	14	308	KC1	C2A-C3A	7.59	1.52	1.37
39	15	319	DD6	C9-C10	7.59	1.66	1.43
39	6	318	DD6	C9-C10	7.59	1.66	1.43
37	10	315	A86	C4-C5	7.59	1.66	1.43
37	14	317	A86	C4-C5	7.58	1.66	1.43
39	6	303	DD6	C9-C10	7.58	1.66	1.43
37	14	318	A86	C4-C5	7.57	1.66	1.43
37	11	314	A86	C4-C5	7.57	1.66	1.43
38	14	311	KC1	C2A-C3A	7.57	1.52	1.37
31	A	845	PQN	C3-C2	7.56	1.48	1.35
39	10	313	DD6	C9-C10	7.56	1.66	1.43
39	1	310	DD6	C9-C10	7.55	1.66	1.43
39	4	316	DD6	C9-C10	7.55	1.66	1.43
37	12	314	A86	C4-C5	7.55	1.66	1.43
39	4	316	DD6	C19-C20	7.55	1.62	1.52
37	5	316	A86	C4-C5	7.55	1.66	1.43
37	3	315	A86	C4-C5	7.54	1.66	1.43
39	3	313	DD6	C19-C20	7.54	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	309	KC1	C2A-C3A	7.54	1.52	1.37
37	5	301	A86	C4-C5	7.52	1.66	1.43
37	15	323	A86	C8-C6	7.52	1.62	1.46
38	13	312	KC1	C2A-C3A	7.52	1.52	1.37
37	2	302	A86	C4-C5	7.51	1.66	1.43
38	16	304	KC1	C2A-C3A	7.51	1.52	1.37
37	14	301	A86	C4-C5	7.50	1.66	1.43
37	13	315	A86	C8-C6	7.49	1.62	1.46
37	11	316	A86	C4-C5	7.49	1.66	1.43
37	1	309	A86	C4-C5	7.49	1.66	1.43
39	8	317	DD6	C9-C10	7.49	1.66	1.43
37	10	302	A86	C4-C5	7.48	1.66	1.43
39	3	312	DD6	C19-C20	7.48	1.62	1.52
37	15	322	A86	C8-C6	7.48	1.62	1.46
39	6	321	DD6	C9-C10	7.48	1.66	1.43
37	4	314	A86	C4-C5	7.47	1.66	1.43
37	5	315	A86	C4-C5	7.47	1.66	1.43
39	4	313	DD6	C9-C10	7.46	1.66	1.43
39	9	314	DD6	C19-C20	7.46	1.62	1.52
38	8	306	KC1	C2A-C3A	7.46	1.52	1.37
37	14	314	A86	C8-C6	7.45	1.61	1.46
39	9	314	DD6	C9-C10	7.45	1.66	1.43
37	7	315	A86	C4-C5	7.45	1.66	1.43
39	7	314	DD6	C9-C10	7.44	1.66	1.43
37	16	314	A86	C4-C5	7.44	1.66	1.43
39	3	316	DD6	C19-C20	7.44	1.62	1.52
38	11	311	KC1	C2A-C3A	7.44	1.52	1.37
37	11	315	A86	C4-C5	7.43	1.66	1.43
37	10	317	A86	C8-C6	7.43	1.61	1.46
38	7	308	KC1	C2A-C3A	7.42	1.52	1.37
37	2	319	A86	C4-C5	7.42	1.66	1.43
37	14	315	A86	C4-C5	7.42	1.66	1.43
37	14	316	A86	C4-C5	7.42	1.66	1.43
37	4	312	A86	C4-C5	7.41	1.66	1.43
37	9	315	A86	C8-C6	7.41	1.61	1.46
37	2	318	A86	C4-C5	7.41	1.66	1.43
37	9	316	A86	C19-C20	7.41	1.62	1.52
37	11	301	A86	C4-C5	7.41	1.66	1.43
37	16	314	A86	C19-C20	7.41	1.62	1.52
37	2u	205	A86	C4-C5	7.41	1.66	1.43
37	14	320	A86	C8-C6	7.41	1.61	1.46
37	15	321	A86	C4-C5	7.41	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	8	316	DD6	C9-C10	7.41	1.66	1.43
39	2	315	DD6	C9-C10	7.41	1.66	1.43
38	13	310	KC1	C2A-C3A	7.41	1.52	1.37
38	3	308	KC1	C2A-C3A	7.39	1.52	1.37
39	8	316	DD6	C21-C20	-7.39	1.40	1.51
37	5	316	A86	C8-C6	7.39	1.61	1.46
38	4	307	KC1	C2A-C3A	7.39	1.52	1.37
37	7	319	A86	C8-C6	7.38	1.61	1.46
37	10	315	A86	C8-C6	7.38	1.61	1.46
38	13	308	KC1	C2A-C3A	7.35	1.52	1.37
39	5	314	DD6	C9-C10	7.35	1.66	1.43
37	15	317	A86	C8-C6	7.34	1.61	1.46
37	13	315	A86	C19-C20	7.34	1.62	1.52
39	8	317	DD6	C19-C20	7.34	1.62	1.52
39	6	321	DD6	C19-C20	7.34	1.62	1.52
37	14	319	A86	C8-C6	7.34	1.61	1.46
38	11	307	KC1	C2A-C3A	7.33	1.52	1.37
37	10	316	A86	C4-C5	7.33	1.65	1.43
37	4	317	A86	C4-C5	7.33	1.65	1.43
37	7	319	A86	C4-C5	7.33	1.65	1.43
38	8	310	KC1	C2A-C3A	7.32	1.52	1.37
37	5	315	A86	C8-C6	7.32	1.61	1.46
37	2u	203	A86	C4-C5	7.32	1.65	1.43
38	2	312	KC1	C2A-C3A	7.31	1.52	1.37
39	2	315	DD6	C19-C20	7.31	1.62	1.52
31	B	840	PQN	C3-C2	7.31	1.48	1.35
37	2	302	A86	C8-C6	7.31	1.61	1.46
39	7	302	DD6	C24-C1	7.31	1.61	1.46
37	11	314	A86	C8-C6	7.31	1.61	1.46
37	12	316	A86	C8-C6	7.31	1.61	1.46
37	4	315	A86	C4-C5	7.30	1.65	1.43
37	15	316	A86	C8-C6	7.30	1.61	1.46
39	2	316	DD6	C9-C10	7.30	1.65	1.43
38	14	306	KC1	C2A-C3A	7.30	1.52	1.37
37	6	320	A86	C4-C5	7.29	1.65	1.43
38	12	311	KC1	C2A-C3A	7.29	1.52	1.37
39	5	313	DD6	C19-C20	7.29	1.62	1.52
37	15	321	A86	C19-C20	7.29	1.62	1.52
38	4	310	KC1	C2A-C3A	7.28	1.52	1.37
37	13	313	A86	C25-C26	7.28	1.65	1.43
37	16	312	A86	C8-C6	7.28	1.61	1.46
37	3	315	A86	C8-C6	7.28	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	305	KC1	C2A-C3A	7.28	1.51	1.37
38	8	312	KC1	C2A-C3A	7.26	1.51	1.37
39	4	316	DD6	C30-C29	7.26	1.40	1.20
37	14	301	A86	C8-C6	7.25	1.61	1.46
37	15	323	A86	C19-C20	7.25	1.62	1.52
37	3	314	A86	C8-C6	7.24	1.61	1.46
38	1	308	KC1	C2A-C3A	7.23	1.51	1.37
38	5	310	KC1	C2A-C3A	7.23	1.51	1.37
39	4	313	DD6	C19-C20	7.23	1.62	1.52
37	16	314	A86	C8-C6	7.22	1.61	1.46
37	9	313	A86	C4-C5	7.22	1.65	1.43
37	14	318	A86	C8-C6	7.22	1.61	1.46
38	3	304	KC1	C2A-C3A	7.21	1.51	1.37
37	15	321	A86	C8-C6	7.21	1.61	1.46
37	14	319	A86	C19-C20	7.21	1.62	1.52
37	5	301	A86	C8-C6	7.20	1.61	1.46
39	2	317	DD6	C24-C1	7.20	1.61	1.46
37	14	318	A86	C19-C20	7.20	1.62	1.52
39	12	315	DD6	C19-C20	7.20	1.62	1.52
37	14	317	A86	C8-C6	7.18	1.61	1.46
38	2	314	KC1	C2A-C3A	7.18	1.51	1.37
37	15	322	A86	C19-C20	7.18	1.62	1.52
39	15	318	DD6	C30-C29	7.18	1.40	1.20
37	13	313	A86	C19-C20	7.17	1.62	1.52
38	9	310	KC1	C2A-C3A	7.17	1.51	1.37
37	3	315	A86	C19-C20	7.17	1.62	1.52
38	13	311	KC1	C2A-C3A	7.17	1.51	1.37
39	13	314	DD6	C30-C29	7.16	1.40	1.20
37	11	315	A86	C8-C6	7.15	1.61	1.46
37	10	317	A86	C19-C20	7.14	1.62	1.52
38	8	311	KC1	C2A-C3A	7.14	1.51	1.37
38	6	312	KC1	C2A-C3A	7.13	1.51	1.37
38	13	306	KC1	C2A-C3A	7.13	1.51	1.37
38	10	310	KC1	C2A-C3A	7.13	1.51	1.37
37	11	316	A86	C8-C6	7.13	1.61	1.46
38	6	313	KC1	C2A-C3A	7.13	1.51	1.37
38	9	304	KC1	C2A-C3A	7.13	1.51	1.37
38	13	305	KC1	C2A-C3A	7.12	1.51	1.37
37	15	320	A86	C19-C20	7.12	1.62	1.52
39	12	315	DD6	C21-C20	-7.12	1.41	1.51
39	6	319	DD6	C24-C1	7.11	1.61	1.46
37	10	301	A86	C4-C5	7.11	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	313	DD6	C24-C1	7.11	1.61	1.46
38	10	312	KC1	C2A-C3A	7.11	1.51	1.37
37	1	309	A86	C19-C20	7.10	1.62	1.52
39	15	319	DD6	C30-C29	7.10	1.40	1.20
38	5	305	KC1	C2A-C3A	7.10	1.51	1.37
39	16	313	DD6	C30-C29	7.10	1.40	1.20
37	2	318	A86	C8-C6	7.10	1.61	1.46
38	1	306	KC1	C2A-C3A	7.10	1.51	1.37
38	6	311	KC1	C2A-C3A	7.09	1.51	1.37
39	2	315	DD6	C24-C1	7.09	1.61	1.46
39	3	316	DD6	C30-C29	7.08	1.40	1.20
39	2	315	DD6	C30-C29	7.08	1.40	1.20
39	15	318	DD6	C24-C1	7.08	1.61	1.46
39	15	319	DD6	C24-C1	7.08	1.61	1.46
38	2	306	KC1	C2A-C3A	7.08	1.51	1.37
38	7	313	KC1	C2A-C3A	7.08	1.51	1.37
37	14	315	A86	C19-C20	7.07	1.62	1.52
39	6	318	DD6	C24-C1	7.07	1.61	1.46
39	13	314	DD6	C24-C1	7.06	1.61	1.46
39	2	317	DD6	C30-C31	7.06	1.55	1.42
37	15	323	A86	C25-C26	7.06	1.65	1.43
37	15	317	A86	C19-C20	7.06	1.62	1.52
37	7	319	A86	C19-C20	7.05	1.62	1.52
37	11	316	A86	C19-C20	7.05	1.62	1.52
37	14	315	A86	C8-C6	7.04	1.61	1.46
37	14	316	A86	C8-C6	7.04	1.61	1.46
39	3	316	DD6	C24-C1	7.04	1.61	1.46
37	8	315	A86	C4-C5	7.03	1.65	1.43
39	15	318	DD6	C30-C31	7.03	1.55	1.42
37	4	312	A86	C8-C6	7.03	1.61	1.46
38	3	311	KC1	C2A-C3A	7.03	1.51	1.37
37	8	318	A86	C19-C20	7.03	1.62	1.52
39	12	315	DD6	C24-C1	7.03	1.61	1.46
38	5	312	KC1	C2A-C3A	7.03	1.51	1.37
39	4	313	DD6	C21-C20	-7.02	1.41	1.51
37	2	319	A86	C8-C6	7.02	1.61	1.46
37	15	320	A86	C25-C26	7.02	1.65	1.43
37	15	316	A86	C25-C26	7.02	1.65	1.43
37	14	314	A86	C19-C20	7.02	1.62	1.52
39	5	313	DD6	C30-C29	7.02	1.40	1.20
37	2	318	A86	C25-C26	7.02	1.64	1.43
37	15	317	A86	C25-C26	7.01	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	303	DD6	C30-C29	7.01	1.40	1.20
37	14	301	A86	C19-C20	7.01	1.62	1.52
37	6	320	A86	C8-C6	7.00	1.60	1.46
37	3	315	A86	C25-C26	7.00	1.64	1.43
37	1	309	A86	C8-C6	7.00	1.60	1.46
39	7	317	DD6	C24-C1	7.00	1.60	1.46
39	7	302	DD6	C30-C29	7.00	1.39	1.20
37	9	316	A86	C25-C26	7.00	1.64	1.43
38	6	308	KC1	C2A-C3A	7.00	1.51	1.37
39	1	310	DD6	C30-C29	6.99	1.39	1.20
37	2	302	A86	C19-C20	6.99	1.62	1.52
39	6	303	DD6	C24-C1	6.99	1.60	1.46
39	5	314	DD6	C21-C20	-6.99	1.41	1.51
39	3	313	DD6	C24-C1	6.99	1.60	1.46
37	11	314	A86	C19-C20	6.99	1.62	1.52
37	12	316	A86	C19-C20	6.98	1.62	1.52
39	3	312	DD6	C30-C29	6.98	1.39	1.20
37	15	316	A86	C19-C20	6.98	1.62	1.52
39	8	317	DD6	C30-C29	6.98	1.39	1.20
39	7	302	DD6	C21-C20	-6.98	1.41	1.51
39	2	316	DD6	C19-C20	6.98	1.62	1.52
37	10	316	A86	C8-C6	6.98	1.60	1.46
39	8	317	DD6	C24-C1	6.98	1.60	1.46
39	5	313	DD6	C24-C1	6.97	1.60	1.46
39	15	319	DD6	C30-C31	6.97	1.55	1.42
37	7	316	A86	C4-C5	6.97	1.64	1.43
39	2	316	DD6	C24-C1	6.97	1.60	1.46
37	12	314	A86	C19-C20	6.96	1.62	1.52
39	2	317	DD6	C30-C29	6.96	1.39	1.20
39	3	312	DD6	C24-C1	6.96	1.60	1.46
39	9	314	DD6	C21-C20	-6.96	1.41	1.51
37	4	315	A86	C8-C6	6.96	1.60	1.46
39	10	313	DD6	C30-C29	6.95	1.39	1.20
38	11	305	KC1	C2A-C3A	6.95	1.51	1.37
39	9	314	DD6	C30-C29	6.95	1.39	1.20
37	10	302	A86	C25-C26	6.94	1.64	1.43
39	10	314	DD6	C30-C29	6.94	1.39	1.20
38	12	311	KC1	CBA-CAA	6.94	1.53	1.33
38	12	313	KC1	C2A-C3A	6.94	1.51	1.37
39	10	314	DD6	C24-C1	6.94	1.60	1.46
37	4	317	A86	C8-C6	6.93	1.60	1.46
37	2u	203	A86	C19-C20	6.93	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	317	A86	C19-C20	6.93	1.61	1.52
37	15	315	A86	C19-C20	6.93	1.61	1.52
38	13	305	KC1	CBA-CAA	6.93	1.53	1.33
39	4	316	DD6	C24-C1	6.93	1.60	1.46
39	12	315	DD6	C30-C29	6.93	1.39	1.20
37	15	321	A86	C25-C26	6.93	1.64	1.43
39	7	317	DD6	C30-C29	6.92	1.39	1.20
37	9	315	A86	C25-C26	6.92	1.64	1.43
37	10	317	A86	C25-C26	6.92	1.64	1.43
39	16	313	DD6	C24-C1	6.92	1.60	1.46
39	9	314	DD6	C24-C1	6.91	1.60	1.46
39	3	313	DD6	C30-C29	6.91	1.39	1.20
38	8	307	KC1	C2A-C3A	6.91	1.51	1.37
37	11	316	A86	C25-C26	6.90	1.64	1.43
38	10	306	KC1	C2A-C3A	6.90	1.51	1.37
37	15	315	A86	C25-C26	6.90	1.64	1.43
37	15	322	A86	C25-C26	6.90	1.64	1.43
38	9	311	KC1	C2A-C3A	6.90	1.51	1.37
39	11	313	DD6	C30-C29	6.90	1.39	1.20
37	13	315	A86	C25-C26	6.89	1.64	1.43
37	5	315	A86	C19-C20	6.89	1.61	1.52
39	7	314	DD6	C24-C1	6.89	1.60	1.46
37	7	315	A86	C25-C26	6.89	1.64	1.43
39	8	316	DD6	C19-C20	6.88	1.61	1.52
39	6	303	DD6	C30-C31	6.88	1.55	1.42
37	10	315	A86	C25-C26	6.88	1.64	1.43
37	3	314	A86	C25-C26	6.88	1.64	1.43
39	6	321	DD6	C24-C1	6.87	1.60	1.46
39	6	319	DD6	C30-C29	6.87	1.39	1.20
39	7	318	DD6	C24-C1	6.87	1.60	1.46
39	13	314	DD6	C30-C31	6.87	1.55	1.42
39	4	316	DD6	C30-C31	6.87	1.55	1.42
37	14	317	A86	C25-C26	6.86	1.64	1.43
39	3	316	DD6	C21-C20	-6.86	1.41	1.51
39	12	317	DD6	C24-C1	6.86	1.60	1.46
37	10	315	A86	C19-C20	6.86	1.61	1.52
38	5	306	KC1	C2A-C3A	6.86	1.51	1.37
39	1	310	DD6	C24-C1	6.86	1.60	1.46
37	12	316	A86	C25-C26	6.85	1.64	1.43
37	14	320	A86	C25-C26	6.85	1.64	1.43
39	4	313	DD6	C30-C29	6.85	1.39	1.20
37	16	312	A86	C19-C20	6.85	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	318	A86	C25-C26	6.85	1.64	1.43
37	7	315	A86	C8-C6	6.85	1.60	1.46
39	10	313	DD6	C24-C1	6.85	1.60	1.46
39	5	314	DD6	C19-C20	6.84	1.61	1.52
39	8	316	DD6	C30-C29	6.84	1.39	1.20
39	11	313	DD6	C24-C1	6.84	1.60	1.46
37	7	319	A86	C25-C26	6.83	1.64	1.43
37	12	314	A86	C8-C6	6.83	1.60	1.46
39	16	313	DD6	C30-C31	6.83	1.55	1.42
37	11	314	A86	C25-C26	6.83	1.64	1.43
37	5	301	A86	C25-C26	6.82	1.64	1.43
39	3	316	DD6	C30-C31	6.82	1.55	1.42
38	8	313	KC1	C2A-C3A	6.82	1.51	1.37
38	8	312	KC1	CBA-CAA	6.81	1.53	1.33
38	13	306	KC1	CBA-CAA	6.81	1.53	1.33
39	2	316	DD6	C30-C29	6.80	1.39	1.20
38	6	308	KC1	CBA-CAA	6.80	1.53	1.33
37	4	315	A86	C25-C26	6.80	1.64	1.43
37	12	314	A86	C25-C26	6.80	1.64	1.43
37	9	313	A86	C8-C6	6.80	1.60	1.46
38	11	312	KC1	CBA-CAA	6.80	1.53	1.33
38	14	308	KC1	CBA-CAA	6.79	1.53	1.33
39	7	318	DD6	C30-C29	6.79	1.39	1.20
39	6	321	DD6	C30-C29	6.79	1.39	1.20
39	8	316	DD6	C24-C1	6.79	1.60	1.46
39	7	314	DD6	C30-C29	6.79	1.39	1.20
37	4	314	A86	C25-C26	6.79	1.64	1.43
39	12	317	DD6	C30-C29	6.79	1.39	1.20
37	14	319	A86	C25-C26	6.79	1.64	1.43
37	4	314	A86	C19-C20	6.79	1.61	1.52
39	7	317	DD6	C21-C20	-6.79	1.41	1.51
39	6	319	DD6	C21-C20	-6.78	1.41	1.51
39	3	313	DD6	C21-C20	-6.78	1.41	1.51
37	14	316	A86	C25-C26	6.77	1.64	1.43
39	7	318	DD6	C21-C20	-6.77	1.41	1.51
37	2	302	A86	C25-C26	6.76	1.64	1.43
38	12	305	KC1	CBA-CAA	6.76	1.53	1.33
39	7	302	DD6	C30-C31	6.76	1.55	1.42
37	6	320	A86	C25-C26	6.76	1.64	1.43
38	11	311	KC1	CBA-CAA	6.75	1.53	1.33
39	5	314	DD6	C24-C1	6.75	1.60	1.46
39	2	315	DD6	C30-C31	6.75	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	310	KC1	CBA-CAA	6.75	1.53	1.33
37	11	301	A86	C19-C20	6.75	1.61	1.52
39	6	318	DD6	C30-C29	6.74	1.39	1.20
37	5	315	A86	C25-C26	6.74	1.64	1.43
38	16	304	KC1	CBA-CAA	6.74	1.53	1.33
37	4	317	A86	C25-C26	6.74	1.64	1.43
38	7	313	KC1	CBA-CAA	6.73	1.53	1.33
37	8	318	A86	C8-C6	6.73	1.60	1.46
38	9	312	KC1	CBA-CAA	6.73	1.53	1.33
37	14	314	A86	C25-C26	6.73	1.64	1.43
37	11	301	A86	C25-C26	6.72	1.64	1.43
37	14	301	A86	C25-C26	6.72	1.64	1.43
38	13	310	KC1	CBA-CAA	6.71	1.53	1.33
37	4	312	A86	C19-C20	6.71	1.61	1.52
39	1	310	DD6	C21-C20	-6.71	1.41	1.51
38	3	311	KC1	CBA-CAA	6.70	1.53	1.33
37	11	315	A86	C25-C26	6.70	1.64	1.43
37	5	316	A86	C25-C26	6.70	1.64	1.43
37	16	312	A86	C25-C26	6.70	1.64	1.43
38	2	314	KC1	CBA-CAA	6.70	1.53	1.33
39	9	314	DD6	C30-C31	6.69	1.55	1.42
38	12	309	KC1	CBA-CAA	6.69	1.53	1.33
39	5	314	DD6	C30-C29	6.69	1.39	1.20
38	6	311	KC1	CBA-CAA	6.69	1.53	1.33
38	8	311	KC1	CBA-CAA	6.69	1.53	1.33
37	10	301	A86	C25-C26	6.68	1.63	1.43
38	4	310	KC1	CBA-CAA	6.68	1.53	1.33
38	5	305	KC1	CBA-CAA	6.67	1.53	1.33
37	1	309	A86	C25-C26	6.67	1.63	1.43
38	4	307	KC1	CBA-CAA	6.67	1.53	1.33
37	10	316	A86	C25-C26	6.67	1.63	1.43
37	4	315	A86	C19-C20	6.67	1.61	1.52
37	16	314	A86	C25-C26	6.67	1.63	1.43
38	9	312	KC1	C2A-C3A	6.66	1.50	1.37
38	5	306	KC1	CBA-CAA	6.66	1.52	1.33
38	6	312	KC1	CBA-CAA	6.66	1.52	1.33
37	2u	205	A86	C25-C26	6.65	1.63	1.43
37	14	315	A86	C25-C26	6.65	1.63	1.43
38	1	308	KC1	CBA-CAA	6.65	1.52	1.33
39	8	317	DD6	C30-C31	6.65	1.55	1.42
38	8	307	KC1	CBA-CAA	6.64	1.52	1.33
39	11	313	DD6	C21-C20	-6.64	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	313	KC1	CBA-CAA	6.63	1.52	1.33
39	3	312	DD6	C30-C31	6.63	1.55	1.42
38	13	308	KC1	CBA-CAA	6.63	1.52	1.33
38	16	311	KC1	CBA-CAA	6.63	1.52	1.33
38	10	310	KC1	CBA-CAA	6.63	1.52	1.33
38	14	311	KC1	CBA-CAA	6.62	1.52	1.33
37	10	301	A86	C8-C6	6.62	1.60	1.46
38	4	308	KC1	CBA-CAA	6.62	1.52	1.33
38	11	307	KC1	CBA-CAA	6.62	1.52	1.33
39	2	317	DD6	C21-C20	-6.61	1.41	1.51
38	10	312	KC1	CBA-CAA	6.61	1.52	1.33
38	2	306	KC1	CBA-CAA	6.61	1.52	1.33
39	15	318	DD6	C21-C20	-6.60	1.42	1.51
38	3	308	KC1	CBA-CAA	6.60	1.52	1.33
38	14	306	KC1	CBA-CAA	6.60	1.52	1.33
39	5	313	DD6	C30-C31	6.60	1.54	1.42
38	9	310	KC1	CBA-CAA	6.60	1.52	1.33
39	5	313	DD6	C21-C20	-6.59	1.42	1.51
38	5	312	KC1	CBA-CAA	6.59	1.52	1.33
38	1	306	KC1	CBA-CAA	6.59	1.52	1.33
38	7	308	KC1	CBA-CAA	6.58	1.52	1.33
38	8	306	KC1	CBA-CAA	6.57	1.52	1.33
39	12	315	DD6	C30-C31	6.57	1.54	1.42
39	7	314	DD6	C21-C20	-6.57	1.42	1.51
37	8	315	A86	C8-C6	6.57	1.60	1.46
39	2	316	DD6	C21-C20	-6.57	1.42	1.51
37	8	318	A86	C25-C26	6.57	1.63	1.43
37	4	312	A86	C25-C26	6.57	1.63	1.43
38	13	311	KC1	CBA-CAA	6.57	1.52	1.33
37	2u	203	A86	C25-C26	6.56	1.63	1.43
39	10	314	DD6	C21-C20	-6.56	1.42	1.51
38	13	312	KC1	CBA-CAA	6.56	1.52	1.33
39	6	321	DD6	C21-C20	-6.55	1.42	1.51
38	3	304	KC1	CBA-CAA	6.55	1.52	1.33
37	9	313	A86	C19-C20	6.55	1.61	1.52
39	8	317	DD6	C21-C20	-6.54	1.42	1.51
39	15	319	DD6	C21-C20	-6.53	1.42	1.51
38	9	304	KC1	CBA-CAA	6.53	1.52	1.33
38	9	311	KC1	CBA-CAA	6.53	1.52	1.33
39	7	317	DD6	C30-C31	6.52	1.54	1.42
38	2	312	KC1	CBA-CAA	6.52	1.52	1.33
38	8	313	KC1	CBA-CAA	6.52	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	318	DD6	C21-C20	-6.51	1.42	1.51
39	1	310	DD6	C30-C31	6.51	1.54	1.42
38	8	310	KC1	CBA-CAA	6.51	1.52	1.33
38	10	306	KC1	CBA-CAA	6.51	1.52	1.33
37	5	316	A86	C19-C20	6.50	1.61	1.52
39	10	313	DD6	C30-C31	6.49	1.54	1.42
38	11	305	KC1	CBA-CAA	6.49	1.52	1.33
39	10	314	DD6	C30-C31	6.48	1.54	1.42
37	8	315	A86	C19-C20	6.48	1.61	1.52
39	2	315	DD6	C21-C20	-6.48	1.42	1.51
37	14	316	A86	C19-C20	6.47	1.61	1.52
37	9	313	A86	C25-C26	6.47	1.63	1.43
37	10	316	A86	C19-C20	6.46	1.61	1.52
39	2	316	DD6	C30-C31	6.46	1.54	1.42
39	4	313	DD6	C30-C31	6.45	1.54	1.42
39	3	313	DD6	C30-C31	6.45	1.54	1.42
38	8	314	KC1	CBA-CAA	6.44	1.52	1.33
39	7	318	DD6	C30-C31	6.43	1.54	1.42
39	6	321	DD6	C30-C31	6.41	1.54	1.42
37	8	315	A86	C25-C26	6.41	1.63	1.43
39	6	319	DD6	C30-C31	6.40	1.54	1.42
37	5	301	A86	C19-C20	6.39	1.61	1.52
29	A	801	CL0	C3B-C4B	6.39	1.47	1.41
37	2	319	A86	C25-C26	6.39	1.63	1.43
39	3	312	DD6	C21-C20	-6.39	1.42	1.51
37	4	317	A86	C19-C20	6.38	1.61	1.52
37	10	302	A86	C19-C20	6.37	1.61	1.52
38	6	313	KC1	CBA-CAA	6.36	1.52	1.33
39	6	318	DD6	C30-C31	6.35	1.54	1.42
37	7	316	A86	C25-C26	6.35	1.62	1.43
39	11	313	DD6	C30-C31	6.35	1.54	1.42
37	14	320	A86	C19-C20	6.33	1.61	1.52
39	10	313	DD6	C21-C20	-6.33	1.42	1.51
39	8	316	DD6	C30-C31	6.32	1.54	1.42
39	7	314	DD6	C13-C14	6.32	1.46	1.32
37	2	318	A86	C19-C20	6.31	1.61	1.52
37	7	316	A86	C8-C6	6.30	1.59	1.46
37	7	316	A86	C19-C20	6.30	1.61	1.52
37	3	314	A86	C19-C20	6.30	1.61	1.52
39	4	316	DD6	C21-C20	-6.29	1.42	1.51
37	2u	205	A86	C19-C20	6.27	1.61	1.52
39	16	313	DD6	C13-C14	6.25	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	12	317	DD6	C30-C31	6.24	1.54	1.42
39	12	317	DD6	C21-C20	-6.24	1.42	1.51
39	6	303	DD6	C21-C20	-6.23	1.42	1.51
37	2	319	A86	C19-C20	6.20	1.60	1.52
39	5	314	DD6	C30-C31	6.20	1.54	1.42
29	A	801	CL0	C1D-C2D	6.17	1.46	1.39
37	7	315	A86	C19-C20	6.16	1.60	1.52
39	8	316	DD6	C13-C14	6.14	1.46	1.32
37	11	315	A86	C19-C20	6.14	1.60	1.52
39	13	314	DD6	C21-C20	-6.11	1.42	1.51
39	7	314	DD6	C30-C31	6.09	1.53	1.42
38	3	311	KC1	O2A-CGA	6.07	1.46	1.30
38	1	308	KC1	O2A-CGA	6.07	1.45	1.30
38	12	313	KC1	C4A-C3A	6.07	1.56	1.44
38	8	313	KC1	O2A-CGA	6.06	1.45	1.30
38	13	312	KC1	O2A-CGA	6.06	1.45	1.30
38	2	306	KC1	O2A-CGA	6.05	1.45	1.30
37	10	301	A86	C19-C20	6.05	1.60	1.52
38	2	312	KC1	O2A-CGA	6.04	1.45	1.30
38	9	304	KC1	O2A-CGA	6.04	1.45	1.30
38	5	306	KC1	O2A-CGA	6.04	1.45	1.30
38	5	305	KC1	O2A-CGA	6.04	1.45	1.30
38	5	312	KC1	O2A-CGA	6.04	1.45	1.30
38	12	311	KC1	O2A-CGA	6.04	1.45	1.30
38	6	308	KC1	O2A-CGA	6.03	1.45	1.30
30	7	305	CLA	OBD-CAD	6.02	1.32	1.22
38	4	308	KC1	O2A-CGA	6.02	1.45	1.30
38	9	312	KC1	O2A-CGA	6.02	1.45	1.30
38	11	311	KC1	O2A-CGA	6.02	1.45	1.30
38	14	311	KC1	O2A-CGA	6.01	1.45	1.30
38	5	310	KC1	O2A-CGA	6.01	1.45	1.30
38	8	310	KC1	O2A-CGA	6.01	1.45	1.30
38	10	306	KC1	O2A-CGA	6.01	1.45	1.30
38	11	307	KC1	O2A-CGA	6.00	1.45	1.30
38	16	311	KC1	O2A-CGA	6.00	1.45	1.30
38	12	309	KC1	O2A-CGA	6.00	1.45	1.30
38	4	310	KC1	O2A-CGA	6.00	1.45	1.30
38	14	306	KC1	O2A-CGA	6.00	1.45	1.30
38	13	308	KC1	O2A-CGA	6.00	1.45	1.30
38	10	312	KC1	O2A-CGA	6.00	1.45	1.30
38	1	306	KC1	O2A-CGA	5.99	1.45	1.30
38	13	305	KC1	O2A-CGA	5.99	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	306	KC1	O2A-CGA	5.99	1.45	1.30
38	16	304	KC1	O2A-CGA	5.99	1.45	1.30
38	11	305	KC1	O2A-CGA	5.98	1.45	1.30
38	12	305	KC1	O2A-CGA	5.98	1.45	1.30
38	2	314	KC1	O2A-CGA	5.98	1.45	1.30
38	9	311	KC1	O2A-CGA	5.98	1.45	1.30
38	13	310	KC1	O2A-CGA	5.97	1.45	1.30
38	4	307	KC1	O2A-CGA	5.97	1.45	1.30
38	10	310	KC1	O2A-CGA	5.96	1.45	1.30
38	3	304	KC1	O2A-CGA	5.96	1.45	1.30
38	8	311	KC1	O2A-CGA	5.96	1.45	1.30
38	3	308	KC1	O2A-CGA	5.96	1.45	1.30
39	13	314	DD6	C13-C14	5.95	1.45	1.32
38	13	311	KC1	O2A-CGA	5.95	1.45	1.30
37	9	315	A86	C19-C20	5.94	1.60	1.52
38	6	313	KC1	O2A-CGA	5.94	1.45	1.30
38	6	311	KC1	O2A-CGA	5.94	1.45	1.30
38	12	313	KC1	O2A-CGA	5.90	1.45	1.30
38	8	307	KC1	O2A-CGA	5.89	1.45	1.30
38	9	310	KC1	O2A-CGA	5.89	1.45	1.30
38	6	312	KC1	O2A-CGA	5.87	1.45	1.30
38	8	306	KC1	O2A-CGA	5.87	1.45	1.30
39	10	313	DD6	C13-C14	5.87	1.45	1.32
30	B	820	CLA	C3C-C2C	5.85	1.49	1.36
38	7	308	KC1	O2A-CGA	5.85	1.45	1.30
38	7	313	KC1	O2A-CGA	5.84	1.45	1.30
38	8	312	KC1	O2A-CGA	5.83	1.45	1.30
39	4	313	DD6	C13-C14	5.83	1.45	1.32
38	4	308	KC1	C3B-C2B	5.78	1.48	1.37
38	8	314	KC1	O2A-CGA	5.78	1.45	1.30
38	14	308	KC1	O2A-CGA	5.78	1.45	1.30
39	12	317	DD6	C13-C14	5.77	1.45	1.32
38	11	312	KC1	O2A-CGA	5.76	1.45	1.30
39	15	319	DD6	C13-C14	5.74	1.45	1.32
39	15	318	DD6	C13-C14	5.74	1.45	1.32
29	A	801	CL0	C3A-C2A	-5.71	1.49	1.54
37	6	320	A86	C19-C20	5.71	1.60	1.52
39	7	318	DD6	C13-C14	5.66	1.45	1.32
38	11	311	KC1	C3B-C2B	5.66	1.48	1.37
30	5	304	CLA	OBD-CAD	5.64	1.32	1.22
38	13	306	KC1	C3B-C2B	5.63	1.48	1.37
39	2	315	DD6	C13-C14	5.61	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	309	KC1	C3B-C2B	5.59	1.48	1.37
38	13	308	KC1	C3B-C2B	5.59	1.48	1.37
39	6	319	DD6	C13-C14	5.58	1.45	1.32
38	14	308	KC1	C3C-C2C	5.58	1.48	1.36
30	3	307	CLA	C3C-C2C	5.57	1.48	1.36
38	2	314	KC1	C3B-C2B	5.55	1.48	1.37
38	2	312	KC1	C3B-C2B	5.54	1.48	1.37
38	10	312	KC1	C3B-C2B	5.53	1.48	1.37
38	13	312	KC1	C3B-C2B	5.53	1.48	1.37
38	16	304	KC1	C3B-C2B	5.52	1.48	1.37
38	11	307	KC1	C3B-C2B	5.50	1.48	1.37
38	13	305	KC1	C3B-C2B	5.50	1.48	1.37
38	2	306	KC1	C3B-C2B	5.50	1.48	1.37
38	11	305	KC1	C3B-C2B	5.49	1.48	1.37
38	5	306	KC1	C3B-C2B	5.49	1.48	1.37
38	3	304	KC1	C3B-C2B	5.49	1.48	1.37
39	7	302	DD6	C13-C14	5.49	1.44	1.32
38	12	305	KC1	C3B-C2B	5.48	1.48	1.37
39	7	317	DD6	C13-C14	5.48	1.44	1.32
38	1	306	KC1	C3B-C2B	5.47	1.48	1.37
37	2u	205	A86	C9-C8	5.46	1.48	1.34
38	16	311	KC1	C3B-C2B	5.46	1.48	1.37
38	12	311	KC1	C3B-C2B	5.45	1.48	1.37
38	8	313	KC1	C3B-C2B	5.45	1.48	1.37
30	15	304	CLA	C3C-C2C	5.45	1.48	1.36
38	6	313	KC1	C3B-C2B	5.44	1.48	1.37
38	13	310	KC1	C3B-C2B	5.43	1.48	1.37
38	16	311	KC1	C3C-C2C	5.42	1.48	1.36
39	2	317	DD6	C13-C14	5.41	1.44	1.32
30	3	303	CLA	OBD-CAD	5.40	1.31	1.22
38	8	312	KC1	C3B-C2B	5.40	1.48	1.37
38	3	311	KC1	C3B-C2B	5.39	1.48	1.37
38	7	308	KC1	C3B-C2B	5.39	1.48	1.37
38	13	311	KC1	C3B-C2B	5.39	1.48	1.37
38	14	308	KC1	C3B-C2B	5.38	1.48	1.37
38	5	310	KC1	C3B-C2B	5.38	1.48	1.37
38	4	307	KC1	C3B-C2B	5.38	1.48	1.37
30	11	310	CLA	C3C-C2C	5.37	1.48	1.36
38	10	306	KC1	C3B-C2B	5.37	1.48	1.37
38	10	310	KC1	C3B-C2B	5.37	1.48	1.37
38	5	312	KC1	C3B-C2B	5.36	1.48	1.37
38	9	304	KC1	C3B-C2B	5.36	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	311	KC1	C3B-C2B	5.35	1.48	1.37
38	1	308	KC1	C3B-C2B	5.34	1.48	1.37
39	11	313	DD6	C13-C14	5.34	1.44	1.32
38	9	312	KC1	C3B-C2B	5.33	1.48	1.37
39	3	316	DD6	C13-C14	5.33	1.44	1.32
39	10	314	DD6	C13-C14	5.33	1.44	1.32
30	15	304	CLA	O2D-CGD	5.32	1.46	1.33
39	6	303	DD6	C3-C2	5.31	1.59	1.43
37	10	302	A86	C9-C8	5.31	1.48	1.34
38	6	311	KC1	C3B-C2B	5.31	1.47	1.37
38	9	310	KC1	C3B-C2B	5.31	1.47	1.37
29	A	801	CL0	C3B-C2B	5.31	1.47	1.40
38	8	314	KC1	C3B-C2B	5.30	1.47	1.37
39	2	316	DD6	C13-C14	5.30	1.44	1.32
30	16	308	CLA	C3C-C2C	5.30	1.48	1.36
30	16	310	CLA	O2D-CGD	5.29	1.46	1.33
38	14	306	KC1	C3B-C2B	5.28	1.47	1.37
30	13	304	CLA	C3C-C2C	5.28	1.48	1.36
37	4	314	A86	C9-C8	5.28	1.48	1.34
30	15	309	CLA	C3C-C2C	5.28	1.48	1.36
30	B	830	CLA	C3C-C2C	5.28	1.48	1.36
30	2	303	CLA	O2D-CGD	5.28	1.46	1.33
30	15	308	CLA	C3C-C2C	5.28	1.48	1.36
38	4	310	KC1	C3B-C2B	5.28	1.47	1.37
38	6	312	KC1	C3B-C2B	5.28	1.47	1.37
38	5	305	KC1	C3B-C2B	5.27	1.47	1.37
38	6	308	KC1	C3B-C2B	5.27	1.47	1.37
38	16	304	KC1	C3C-C2C	5.27	1.48	1.36
30	15	310	CLA	C3C-C2C	5.26	1.48	1.36
38	3	311	KC1	C3C-C2C	5.26	1.48	1.36
30	15	311	CLA	C3C-C2C	5.25	1.48	1.36
30	13	309	CLA	O2D-CGD	5.25	1.46	1.33
30	15	306	CLA	C3C-C2C	5.25	1.48	1.36
39	7	302	DD6	C3-C2	5.25	1.59	1.43
30	1	303	CLA	C3C-C2C	5.25	1.48	1.36
39	3	313	DD6	C13-C14	5.25	1.44	1.32
30	5	311	CLA	C3C-C2C	5.24	1.48	1.36
30	15	312	CLA	C3C-C2C	5.24	1.48	1.36
30	14	309	CLA	C3C-C2C	5.24	1.48	1.36
30	11	308	CLA	C3C-C2C	5.24	1.48	1.36
29	A	801	CL0	C3D-C2D	5.24	1.48	1.39
30	14	310	CLA	C3C-C2C	5.23	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	834	CLA	C3C-C2C	5.23	1.48	1.36
30	A	844	CLA	C3C-C2C	5.23	1.48	1.36
30	7	312	CLA	C3C-C2C	5.23	1.48	1.36
30	7	310	CLA	C3C-C2C	5.23	1.48	1.36
30	B	824	CLA	C3C-C2C	5.23	1.48	1.36
30	15	305	CLA	C3C-C2C	5.23	1.48	1.36
38	8	311	KC1	C3B-C2B	5.23	1.47	1.37
30	13	307	CLA	C3C-C2C	5.23	1.48	1.36
30	16	303	CLA	C3C-C2C	5.23	1.48	1.36
30	11	304	CLA	C3C-C2C	5.23	1.48	1.36
38	9	312	KC1	C3C-C2C	5.22	1.48	1.36
38	14	311	KC1	C3B-C2B	5.22	1.47	1.37
30	3	309	CLA	C3C-C2C	5.22	1.48	1.36
30	16	309	CLA	C3C-C2C	5.22	1.48	1.36
30	15	313	CLA	C3C-C2C	5.22	1.48	1.36
30	14	312	CLA	C3C-C2C	5.21	1.48	1.36
39	6	318	DD6	C13-C14	5.21	1.44	1.32
39	10	314	DD6	C3-C2	5.21	1.59	1.43
38	1	308	KC1	O2D-CGD	5.21	1.46	1.33
30	8	309	CLA	C3C-C2C	5.21	1.48	1.36
39	13	314	DD6	C3-C2	5.21	1.59	1.43
30	14	313	CLA	C3C-C2C	5.21	1.48	1.36
30	B	835	CLA	C3C-C2C	5.20	1.48	1.36
39	9	314	DD6	C13-C14	5.20	1.44	1.32
30	B	832	CLA	C3C-C2C	5.20	1.48	1.36
38	3	308	KC1	C3B-C2B	5.20	1.47	1.37
30	B	838	CLA	C3C-C2C	5.19	1.48	1.36
30	14	307	CLA	C3C-C2C	5.19	1.48	1.36
30	A	833	CLA	C3C-C2C	5.19	1.48	1.36
30	12	303	CLA	C3C-C2C	5.19	1.48	1.36
30	3	303	CLA	C3C-C2C	5.19	1.48	1.36
38	1	308	KC1	C3C-C2C	5.18	1.47	1.36
39	6	319	DD6	C3-C2	5.18	1.59	1.43
30	13	303	CLA	C3C-C2C	5.18	1.47	1.36
38	9	311	KC1	C3C-C2C	5.18	1.47	1.36
38	13	308	KC1	C3C-C2C	5.18	1.47	1.36
37	15	315	A86	C9-C8	5.17	1.48	1.34
38	3	304	KC1	C3C-C2C	5.17	1.47	1.36
30	4	304	CLA	C3C-C2C	5.17	1.47	1.36
30	F	202	CLA	C3C-C2C	5.17	1.47	1.36
30	2	305	CLA	C3C-C2C	5.17	1.47	1.36
30	A	839	CLA	C3C-C2C	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	303	DD6	C13-C14	5.17	1.44	1.32
30	A	827	CLA	C3C-C2C	5.17	1.47	1.36
38	13	311	KC1	C3C-C2C	5.17	1.47	1.36
39	6	318	DD6	C3-C2	5.17	1.59	1.43
30	4	301	CLA	C3C-C2C	5.16	1.47	1.36
30	10	309	CLA	C3C-C2C	5.16	1.47	1.36
30	13	304	CLA	O2D-CGD	5.16	1.45	1.33
39	11	313	DD6	C3-C2	5.16	1.59	1.43
30	6	310	CLA	C3C-C2C	5.16	1.47	1.36
38	2	306	KC1	C3C-C2C	5.16	1.47	1.36
38	13	312	KC1	C3C-C2C	5.16	1.47	1.36
38	4	307	KC1	C3C-C2C	5.16	1.47	1.36
37	2u	203	A86	C9-C8	5.16	1.48	1.34
39	15	318	DD6	C3-C2	5.16	1.59	1.43
39	3	313	DD6	C3-C2	5.16	1.59	1.43
30	1	305	CLA	C3C-C2C	5.15	1.47	1.36
30	B	819	CLA	C3C-C2C	5.15	1.47	1.36
30	10	305	CLA	C3C-C2C	5.15	1.47	1.36
30	14	305	CLA	C3C-C2C	5.15	1.47	1.36
30	16	307	CLA	C3C-C2C	5.15	1.47	1.36
39	2	315	DD6	C3-C2	5.15	1.59	1.43
30	4	309	CLA	O2D-CGD	5.15	1.45	1.33
30	7	305	CLA	C3C-C2C	5.15	1.47	1.36
30	A	844	CLA	O2D-CGD	5.15	1.45	1.33
38	5	306	KC1	C3C-C2C	5.15	1.47	1.36
30	9	306	CLA	C3C-C2C	5.15	1.47	1.36
39	3	312	DD6	C3-C2	5.15	1.59	1.43
30	15	302	CLA	C3C-C2C	5.15	1.47	1.36
39	1	310	DD6	C13-C14	5.15	1.44	1.32
39	15	319	DD6	C3-C2	5.15	1.59	1.43
30	B	831	CLA	C3C-C2C	5.15	1.47	1.36
38	13	312	KC1	O2D-CGD	5.14	1.45	1.33
38	7	308	KC1	C3C-C2C	5.14	1.47	1.36
30	14	304	CLA	C3C-C2C	5.14	1.47	1.36
30	4	305	CLA	C3C-C2C	5.14	1.47	1.36
30	15	303	CLA	C3C-C2C	5.14	1.47	1.36
38	4	310	KC1	C3C-C2C	5.14	1.47	1.36
30	10	304	CLA	C3C-C2C	5.14	1.47	1.36
39	10	313	DD6	C3-C2	5.14	1.59	1.43
30	15	313	CLA	O2D-CGD	5.13	1.45	1.33
38	13	311	KC1	O2D-CGD	5.13	1.45	1.33
38	2	314	KC1	C3C-C2C	5.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	312	KC1	C3C-C2C	5.13	1.47	1.36
30	A	835	CLA	C3C-C2C	5.13	1.47	1.36
38	11	305	KC1	C3C-C2C	5.13	1.47	1.36
30	12	304	CLA	C3C-C2C	5.13	1.47	1.36
39	16	313	DD6	C3-C2	5.13	1.59	1.43
38	11	312	KC1	C3B-C2B	5.13	1.47	1.37
39	4	316	DD6	C3-C2	5.13	1.59	1.43
30	A	813	CLA	C3C-C2C	5.12	1.47	1.36
30	15	310	CLA	O2D-CGD	5.12	1.45	1.33
30	15	307	CLA	C3C-C2C	5.12	1.47	1.36
38	13	306	KC1	O2D-CGD	5.12	1.45	1.33
30	B	825	CLA	C3C-C2C	5.12	1.47	1.36
30	2	308	CLA	O2D-CGD	5.12	1.45	1.33
30	6	315	CLA	C3C-C2C	5.12	1.47	1.36
30	14	303	CLA	C3C-C2C	5.12	1.47	1.36
38	5	305	KC1	C3C-C2C	5.12	1.47	1.36
38	6	313	KC1	C3C-C2C	5.12	1.47	1.36
38	2	314	KC1	O2D-CGD	5.12	1.45	1.33
30	1	301	CLA	C3C-C2C	5.12	1.47	1.36
39	2	317	DD6	C3-C2	5.12	1.59	1.43
30	6	316	CLA	C3C-C2C	5.12	1.47	1.36
38	8	311	KC1	C3C-C2C	5.12	1.47	1.36
39	12	315	DD6	C13-C14	5.12	1.43	1.32
30	7	304	CLA	C3C-C2C	5.12	1.47	1.36
30	2	313	CLA	C3C-C2C	5.12	1.47	1.36
30	L	203	CLA	C3C-C2C	5.11	1.47	1.36
30	16	302	CLA	O2D-CGD	5.11	1.45	1.33
39	3	316	DD6	C3-C2	5.11	1.59	1.43
30	13	302	CLA	O2D-CGD	5.11	1.45	1.33
38	11	305	KC1	O2D-CGD	5.11	1.45	1.33
38	8	306	KC1	C3C-C2C	5.11	1.47	1.36
38	13	305	KC1	C3C-C2C	5.11	1.47	1.36
39	12	315	DD6	C3-C2	5.11	1.59	1.43
30	4	303	CLA	C3C-C2C	5.11	1.47	1.36
30	6	307	CLA	C3C-C2C	5.10	1.47	1.36
30	8	302	CLA	C3C-C2C	5.10	1.47	1.36
38	7	313	KC1	C3B-C2B	5.10	1.47	1.37
30	15	305	CLA	O2D-CGD	5.10	1.45	1.33
38	11	311	KC1	C3C-C2C	5.10	1.47	1.36
30	3	306	CLA	C3C-C2C	5.10	1.47	1.36
30	16	310	CLA	C3C-C2C	5.10	1.47	1.36
39	9	314	DD6	C3-C2	5.10	1.59	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	321	CLA	C3C-C2C	5.10	1.47	1.36
30	4	309	CLA	C3C-C2C	5.09	1.47	1.36
30	11	309	CLA	C3C-C2C	5.09	1.47	1.36
38	11	311	KC1	O2D-CGD	5.09	1.45	1.33
30	B	822	CLA	C3C-C2C	5.09	1.47	1.36
39	4	313	DD6	C3-C2	5.09	1.59	1.43
30	13	307	CLA	O2D-CGD	5.09	1.45	1.33
38	8	313	KC1	O2D-CGD	5.09	1.45	1.33
38	10	312	KC1	C3C-C2C	5.09	1.47	1.36
30	13	302	CLA	C3C-C2C	5.09	1.47	1.36
30	14	302	CLA	O2D-CGD	5.09	1.45	1.33
38	12	313	KC1	C3B-C2B	5.09	1.47	1.37
30	J	101	CLA	O2D-CGD	5.09	1.45	1.33
38	11	312	KC1	O2D-CGD	5.09	1.45	1.33
38	8	307	KC1	C3C-C2C	5.08	1.47	1.36
30	5	304	CLA	O2D-CGD	5.08	1.45	1.33
30	2	307	CLA	C3C-C2C	5.08	1.47	1.36
38	10	312	KC1	O2D-CGD	5.08	1.45	1.33
30	15	311	CLA	O2D-CGD	5.08	1.45	1.33
30	A	820	CLA	C3C-C2C	5.08	1.47	1.36
30	13	309	CLA	C3C-C2C	5.08	1.47	1.36
38	8	307	KC1	C3B-C2B	5.08	1.47	1.37
30	14	309	CLA	O2D-CGD	5.08	1.45	1.33
38	3	308	KC1	O2D-CGD	5.08	1.45	1.33
38	8	306	KC1	C3B-C2B	5.08	1.47	1.37
30	3	310	CLA	O2D-CGD	5.08	1.45	1.33
30	1	307	CLA	C3C-C2C	5.08	1.47	1.36
30	B	851	CLA	O2D-CGD	5.08	1.45	1.33
30	2	311	CLA	O2D-CGD	5.08	1.45	1.33
30	14	307	CLA	O2D-CGD	5.07	1.45	1.33
38	10	310	KC1	C3C-C2C	5.07	1.47	1.36
39	3	312	DD6	C13-C14	5.07	1.43	1.32
30	6	306	CLA	C3C-C2C	5.07	1.47	1.36
38	10	306	KC1	C3C-C2C	5.07	1.47	1.36
38	13	308	KC1	O2D-CGD	5.07	1.45	1.33
30	9	302	CLA	C3C-C2C	5.07	1.47	1.36
30	8	303	CLA	C3C-C2C	5.07	1.47	1.36
38	1	306	KC1	C3C-C2C	5.07	1.47	1.36
30	3	305	CLA	C3C-C2C	5.07	1.47	1.36
39	2	316	DD6	C3-C2	5.07	1.58	1.43
39	5	313	DD6	C3-C2	5.07	1.58	1.43
30	14	304	CLA	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	311	KC1	O2D-CGD	5.07	1.45	1.33
39	12	317	DD6	C3-C2	5.07	1.58	1.43
30	B	833	CLA	C3C-C2C	5.07	1.47	1.36
38	8	310	KC1	C3B-C2B	5.07	1.47	1.37
39	8	317	DD6	C13-C14	5.07	1.43	1.32
30	9	306	CLA	O2D-CGD	5.06	1.45	1.33
30	L	202	CLA	C3C-C2C	5.06	1.47	1.36
30	9	309	CLA	C3C-C2C	5.06	1.47	1.36
30	11	310	CLA	O2D-CGD	5.06	1.45	1.33
30	15	303	CLA	O2D-CGD	5.06	1.45	1.33
30	J	101	CLA	C3C-C2C	5.06	1.47	1.36
30	12	321	CLA	O2D-CGD	5.06	1.45	1.33
30	12	310	CLA	C3C-C2C	5.06	1.47	1.36
30	7	312	CLA	O2D-CGD	5.06	1.45	1.33
30	B	815	CLA	C3C-C2C	5.06	1.47	1.36
30	A	834	CLA	C3C-C2C	5.06	1.47	1.36
30	3	302	CLA	C3C-C2C	5.06	1.47	1.36
30	14	302	CLA	C3C-C2C	5.06	1.47	1.36
30	16	309	CLA	O2D-CGD	5.06	1.45	1.33
39	7	314	DD6	C3-C2	5.06	1.58	1.43
30	A	824	CLA	C3C-C2C	5.06	1.47	1.36
38	11	307	KC1	O2D-CGD	5.06	1.45	1.33
30	B	828	CLA	C3C-C2C	5.05	1.47	1.36
30	16	306	CLA	C3C-C2C	5.05	1.47	1.36
30	B	820	CLA	CHC-C1C	5.05	1.48	1.38
30	8	308	CLA	C3C-C2C	5.05	1.47	1.36
30	A	838	CLA	C3C-C2C	5.05	1.47	1.36
30	B	829	CLA	C3C-C2C	5.05	1.47	1.36
38	5	305	KC1	O2D-CGD	5.05	1.45	1.33
38	9	311	KC1	O2D-CGD	5.05	1.45	1.33
30	16	306	CLA	O2D-CGD	5.05	1.45	1.33
30	9	305	CLA	C3C-C2C	5.05	1.47	1.36
30	A	822	CLA	C3C-C2C	5.05	1.47	1.36
30	4	306	CLA	O2D-CGD	5.05	1.45	1.33
30	6	305	CLA	C3C-C2C	5.05	1.47	1.36
39	5	313	DD6	C13-C14	5.04	1.43	1.32
30	F	203	CLA	C3C-C2C	5.04	1.47	1.36
38	4	310	KC1	O2D-CGD	5.04	1.45	1.33
30	16	305	CLA	C3C-C2C	5.04	1.47	1.36
30	A	816	CLA	C3C-C2C	5.04	1.47	1.36
30	5	304	CLA	C3C-C2C	5.04	1.47	1.36
30	14	312	CLA	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	305	KC1	C3C-C2C	5.04	1.47	1.36
39	8	316	DD6	C3-C2	5.04	1.58	1.43
30	11	306	CLA	C3C-C2C	5.04	1.47	1.36
38	13	310	KC1	O2D-CGD	5.04	1.45	1.33
30	5	309	CLA	C3C-C2C	5.04	1.47	1.36
38	13	310	KC1	C3C-C2C	5.04	1.47	1.36
30	6	309	CLA	O2D-CGD	5.04	1.45	1.33
38	12	309	KC1	C3C-C2C	5.03	1.47	1.36
30	3	309	CLA	O2D-CGD	5.03	1.45	1.33
30	A	817	CLA	C3C-C2C	5.03	1.47	1.36
37	11	301	A86	C9-C8	5.03	1.47	1.34
38	3	311	KC1	O2D-CGD	5.03	1.45	1.33
30	16	308	CLA	O2D-CGD	5.03	1.45	1.33
30	B	826	CLA	C3C-C2C	5.03	1.47	1.36
30	A	833	CLA	O2D-CGD	5.03	1.45	1.33
30	10	311	CLA	O2D-CGD	5.03	1.45	1.33
30	15	307	CLA	O2D-CGD	5.02	1.45	1.33
30	6	317	CLA	C3C-C2C	5.02	1.47	1.36
30	5	308	CLA	O2D-CGD	5.02	1.45	1.33
38	1	306	KC1	O2D-CGD	5.02	1.45	1.33
30	2	309	CLA	C3C-C2C	5.02	1.47	1.36
30	15	314	CLA	C3C-C2C	5.02	1.47	1.36
30	4	309	CLA	C1D-ND	5.02	1.44	1.37
30	12	308	CLA	O2D-CGD	5.02	1.45	1.33
30	5	311	CLA	O2D-CGD	5.02	1.45	1.33
30	14	310	CLA	O2D-CGD	5.02	1.45	1.33
30	7	303	CLA	C3C-C2C	5.01	1.47	1.36
30	A	819	CLA	C3C-C2C	5.01	1.47	1.36
30	F	201	CLA	C3C-C2C	5.01	1.47	1.36
38	9	312	KC1	O2D-CGD	5.01	1.45	1.33
30	5	303	CLA	C3C-C2C	5.01	1.47	1.36
30	16	302	CLA	C3C-C2C	5.01	1.47	1.36
30	15	312	CLA	O2D-CGD	5.01	1.45	1.33
30	A	841	CLA	O2D-CGD	5.01	1.45	1.33
30	B	810	CLA	C3C-C2C	5.01	1.47	1.36
30	10	307	CLA	C3C-C2C	5.01	1.47	1.36
38	10	310	KC1	O2D-CGD	5.01	1.45	1.33
30	B	836	CLA	C3C-C2C	5.01	1.47	1.36
30	14	303	CLA	O2D-CGD	5.01	1.45	1.33
30	2	313	CLA	O2D-CGD	5.00	1.45	1.33
30	15	309	CLA	O2D-CGD	5.00	1.45	1.33
30	A	841	CLA	C3C-C2C	5.00	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	805	CLA	C3C-C2C	5.00	1.47	1.36
30	3	306	CLA	O2D-CGD	5.00	1.45	1.33
38	14	308	KC1	O2D-CGD	5.00	1.45	1.33
30	10	309	CLA	O2D-CGD	5.00	1.45	1.33
38	4	308	KC1	O2D-CGD	5.00	1.45	1.33
38	6	312	KC1	C3C-C2C	5.00	1.47	1.36
30	3	301	CLA	C3C-C2C	5.00	1.47	1.36
30	12	307	CLA	O2D-CGD	5.00	1.45	1.33
30	A	836	CLA	C3C-C2C	5.00	1.47	1.36
38	16	304	KC1	O2D-CGD	5.00	1.45	1.33
30	9	307	CLA	C3C-C2C	5.00	1.47	1.36
30	2	304	CLA	C3C-C2C	5.00	1.47	1.36
30	A	831	CLA	C3C-C2C	5.00	1.47	1.36
38	12	311	KC1	C3C-C2C	4.99	1.47	1.36
30	12	303	CLA	O2D-CGD	4.99	1.45	1.33
30	10	311	CLA	C3C-C2C	4.99	1.47	1.36
39	7	317	DD6	C3-C2	4.99	1.58	1.43
30	A	805	CLA	C3C-C2C	4.99	1.47	1.36
30	11	306	CLA	CHC-C1C	4.99	1.48	1.38
38	8	313	KC1	C3C-C2C	4.99	1.47	1.36
38	8	314	KC1	C3C-C2C	4.99	1.47	1.36
30	A	815	CLA	C3C-C2C	4.99	1.47	1.36
30	12	308	CLA	C3C-C2C	4.99	1.47	1.36
30	10	308	CLA	O2D-CGD	4.99	1.45	1.33
39	7	318	DD6	C3-C2	4.99	1.58	1.43
30	4	311	CLA	O2D-CGD	4.99	1.45	1.33
30	1	307	CLA	O2D-CGD	4.98	1.45	1.33
30	15	302	CLA	CHC-C1C	4.98	1.48	1.38
30	1	302	CLA	C3C-C2C	4.98	1.47	1.36
30	16	307	CLA	O2D-CGD	4.98	1.45	1.33
30	A	812	CLA	C3C-C2C	4.98	1.47	1.36
30	14	313	CLA	O2D-CGD	4.98	1.45	1.33
30	B	812	CLA	C3C-C2C	4.98	1.47	1.36
38	6	311	KC1	C3C-C2C	4.98	1.47	1.36
38	9	304	KC1	O2D-CGD	4.98	1.45	1.33
30	6	315	CLA	O2D-CGD	4.98	1.45	1.33
30	16	301	CLA	O2D-CGD	4.98	1.45	1.33
30	11	306	CLA	O2D-CGD	4.98	1.45	1.33
38	14	311	KC1	C3C-C2C	4.98	1.47	1.36
30	2	309	CLA	O2D-CGD	4.97	1.45	1.33
30	13	303	CLA	O2D-CGD	4.97	1.45	1.33
30	11	304	CLA	O2D-CGD	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	304	CLA	O2D-CGD	4.97	1.45	1.33
30	6	316	CLA	O2D-CGD	4.97	1.45	1.33
39	6	321	DD6	C3-C2	4.97	1.58	1.43
38	9	310	KC1	C3C-C2C	4.97	1.47	1.36
30	A	808	CLA	C3C-C2C	4.97	1.47	1.36
30	12	312	CLA	C3C-C2C	4.97	1.47	1.36
30	10	305	CLA	O2D-CGD	4.97	1.45	1.33
30	11	309	CLA	O2D-CGD	4.97	1.45	1.33
30	7	310	CLA	O2D-CGD	4.96	1.45	1.33
30	6	314	CLA	O2D-CGD	4.96	1.45	1.33
38	5	310	KC1	O2D-CGD	4.96	1.45	1.33
30	7	304	CLA	O2D-CGD	4.96	1.45	1.33
30	B	827	CLA	C3C-C2C	4.96	1.47	1.36
30	10	303	CLA	C3C-C2C	4.96	1.47	1.36
30	2	310	CLA	O2D-CGD	4.96	1.45	1.33
37	9	316	A86	C9-C8	4.96	1.47	1.34
38	8	312	KC1	O2D-CGD	4.96	1.45	1.33
38	3	308	KC1	C3C-C2C	4.96	1.47	1.36
39	1	310	DD6	C3-C2	4.96	1.58	1.43
38	16	304	KC1	CHD-C4C	4.96	1.48	1.38
30	B	804	CLA	C3C-C2C	4.96	1.47	1.36
30	B	808	CLA	C3C-C2C	4.95	1.47	1.36
37	2	302	A86	C9-C8	4.95	1.47	1.34
30	10	304	CLA	O2D-CGD	4.95	1.45	1.33
30	9	302	CLA	O2A-CGA	4.95	1.47	1.33
38	13	312	KC1	C1D-ND	4.95	1.44	1.37
30	1	305	CLA	O2D-CGD	4.95	1.45	1.33
38	5	310	KC1	C3C-C2C	4.95	1.47	1.36
38	9	304	KC1	C3C-C2C	4.95	1.47	1.36
30	B	814	CLA	C3C-C2C	4.95	1.47	1.36
38	8	310	KC1	O2D-CGD	4.95	1.45	1.33
38	16	311	KC1	O2D-CGD	4.95	1.45	1.33
30	7	311	CLA	O2D-CGD	4.94	1.45	1.33
38	8	311	KC1	O2D-CGD	4.94	1.45	1.33
39	5	314	DD6	C3-C2	4.94	1.58	1.43
30	B	811	CLA	C3C-C2C	4.94	1.47	1.36
30	7	311	CLA	C3C-C2C	4.94	1.47	1.36
30	A	825	CLA	O2D-CGD	4.94	1.45	1.33
30	6	307	CLA	O2D-CGD	4.94	1.45	1.33
38	13	312	KC1	CHD-C4C	4.94	1.48	1.38
30	8	305	CLA	O2D-CGD	4.94	1.45	1.33
30	A	842	CLA	C3C-C2C	4.94	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	312	KC1	C3C-C2C	4.94	1.47	1.36
30	14	305	CLA	O2D-CGD	4.94	1.45	1.33
30	9	309	CLA	O2D-CGD	4.94	1.45	1.33
38	12	311	KC1	O2D-CGD	4.94	1.45	1.33
30	16	303	CLA	O2D-CGD	4.94	1.45	1.33
30	15	309	CLA	C1D-ND	4.94	1.44	1.37
38	7	313	KC1	C3C-C2C	4.93	1.47	1.36
30	F	203	CLA	O2D-CGD	4.93	1.45	1.33
30	2	311	CLA	C3C-C2C	4.93	1.47	1.36
39	8	317	DD6	C3-C2	4.93	1.58	1.43
30	12	304	CLA	O2D-CGD	4.93	1.45	1.33
38	12	305	KC1	O2D-CGD	4.93	1.45	1.33
30	B	839	CLA	C3C-C2C	4.93	1.47	1.36
30	12	310	CLA	O2D-CGD	4.93	1.45	1.33
30	A	817	CLA	O2D-CGD	4.93	1.45	1.33
30	2	308	CLA	CHC-C1C	4.93	1.48	1.38
30	3	310	CLA	C3C-C2C	4.93	1.47	1.36
30	16	301	CLA	C3C-C2C	4.93	1.47	1.36
30	6	305	CLA	O2D-CGD	4.92	1.45	1.33
30	3	301	CLA	O2D-CGD	4.92	1.45	1.33
38	3	311	KC1	CHD-C4C	4.92	1.48	1.38
38	14	306	KC1	CHD-C4C	4.92	1.48	1.38
30	13	301	CLA	O2D-CGD	4.92	1.45	1.33
30	A	825	CLA	C3C-C2C	4.92	1.47	1.36
37	3	315	A86	C9-C8	4.92	1.47	1.34
30	4	302	CLA	O2D-CGD	4.92	1.45	1.33
30	12	306	CLA	C3C-C2C	4.92	1.47	1.36
30	B	806	CLA	O2D-CGD	4.92	1.45	1.33
30	A	828	CLA	C3C-C2C	4.92	1.47	1.36
30	A	823	CLA	C3C-C2C	4.92	1.47	1.36
30	A	837	CLA	C3C-C2C	4.91	1.47	1.36
30	15	308	CLA	CHC-C1C	4.91	1.48	1.38
30	5	307	CLA	C3C-C2C	4.91	1.47	1.36
38	2	312	KC1	O2D-CGD	4.91	1.45	1.33
38	12	309	KC1	O2D-CGD	4.91	1.45	1.33
38	13	306	KC1	C3C-C2C	4.91	1.47	1.36
39	4	316	DD6	C13-C14	4.91	1.43	1.32
37	15	320	A86	C9-C8	4.91	1.47	1.34
30	7	307	CLA	O2D-CGD	4.91	1.45	1.33
38	5	306	KC1	CHD-C4C	4.91	1.48	1.38
30	3	307	CLA	O2D-CGD	4.91	1.45	1.33
30	9	307	CLA	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	819	CLA	O2D-CGD	4.91	1.45	1.33
30	2u	202	CLA	C3C-C2C	4.91	1.47	1.36
38	6	311	KC1	O2D-CGD	4.91	1.45	1.33
30	6	317	CLA	O2D-CGD	4.90	1.45	1.33
30	11	304	CLA	CHC-C1C	4.90	1.48	1.38
30	A	832	CLA	C3C-C2C	4.90	1.47	1.36
30	12	312	CLA	O2D-CGD	4.90	1.45	1.33
30	B	822	CLA	O2D-CGD	4.90	1.45	1.33
37	2u	205	A86	C17-C18	-4.90	1.45	1.52
38	12	313	KC1	C3C-C2C	4.90	1.47	1.36
30	9	303	CLA	O2D-CGD	4.90	1.45	1.33
30	4	306	CLA	C3C-C2C	4.90	1.47	1.36
30	15	311	CLA	C1D-ND	4.90	1.44	1.37
30	4	311	CLA	C3C-C2C	4.90	1.47	1.36
30	A	836	CLA	O2D-CGD	4.90	1.45	1.33
37	12	316	A86	C9-C8	4.90	1.47	1.34
30	A	843	CLA	O2D-CGD	4.90	1.45	1.33
37	15	322	A86	C9-C8	4.90	1.47	1.34
30	16	309	CLA	C1D-ND	4.90	1.44	1.37
30	7	306	CLA	C3C-C2C	4.89	1.47	1.36
38	2	312	KC1	C3C-C2C	4.89	1.47	1.36
30	13	304	CLA	C1D-ND	4.89	1.44	1.37
38	5	312	KC1	O2D-CGD	4.89	1.45	1.33
37	10	315	A86	C9-C8	4.89	1.47	1.34
37	13	313	A86	C9-C8	4.89	1.47	1.34
38	4	307	KC1	CHD-C4C	4.89	1.48	1.38
30	A	804	CLA	C3C-C2C	4.89	1.47	1.36
30	14	302	CLA	CHC-C1C	4.89	1.48	1.38
30	A	810	CLA	C3C-C2C	4.89	1.47	1.36
38	13	308	KC1	CHD-C4C	4.89	1.48	1.38
30	A	808	CLA	O2D-CGD	4.89	1.45	1.33
38	4	308	KC1	C3C-C2C	4.89	1.47	1.36
30	10	308	CLA	C3C-C2C	4.88	1.47	1.36
38	6	313	KC1	O2D-CGD	4.88	1.45	1.33
30	A	816	CLA	O2D-CGD	4.88	1.45	1.33
38	12	313	KC1	O2D-CGD	4.88	1.45	1.33
30	B	817	CLA	O2D-CGD	4.88	1.45	1.33
30	2	310	CLA	C3C-C2C	4.88	1.47	1.36
30	A	821	CLA	C3C-C2C	4.88	1.47	1.36
37	14	320	A86	C9-C8	4.88	1.47	1.34
30	15	306	CLA	O2D-CGD	4.88	1.45	1.33
30	A	803	CLA	C3C-C2C	4.88	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	308	CLA	O2D-CGD	4.88	1.45	1.33
30	12	306	CLA	O2D-CGD	4.88	1.45	1.33
38	11	307	KC1	C3C-C2C	4.88	1.47	1.36
38	5	306	KC1	O2D-CGD	4.88	1.45	1.33
30	1	301	CLA	O2D-CGD	4.88	1.45	1.33
30	A	822	CLA	O2D-CGD	4.87	1.45	1.33
30	6	309	CLA	C3C-C2C	4.87	1.47	1.36
38	13	311	KC1	C1D-ND	4.87	1.44	1.37
30	6	306	CLA	O2D-CGD	4.87	1.45	1.33
30	10	303	CLA	O2D-CGD	4.87	1.45	1.33
30	8	303	CLA	O2D-CGD	4.87	1.45	1.33
38	11	305	KC1	CHD-C4C	4.87	1.48	1.38
30	12	302	CLA	C3C-C2C	4.87	1.47	1.36
37	11	301	A86	C17-C18	-4.87	1.45	1.52
38	11	307	KC1	CHD-C4C	4.87	1.48	1.38
30	A	805	CLA	CHC-C1C	4.87	1.48	1.38
39	6	321	DD6	C13-C14	4.86	1.43	1.32
30	A	840	CLA	C3C-C2C	4.86	1.47	1.36
30	1	304	CLA	CHC-C1C	4.86	1.48	1.38
38	4	310	KC1	CHD-C4C	4.86	1.48	1.38
30	B	820	CLA	O2D-CGD	4.86	1.45	1.33
30	11	310	CLA	C1D-ND	4.86	1.44	1.37
30	A	811	CLA	C3C-C2C	4.86	1.47	1.36
30	B	821	CLA	C3C-C2C	4.86	1.47	1.36
30	5	302	CLA	C3C-C2C	4.86	1.47	1.36
30	3	302	CLA	O2D-CGD	4.86	1.45	1.33
37	14	316	A86	C17-C18	-4.86	1.45	1.52
38	10	312	KC1	CHD-C4C	4.86	1.48	1.38
38	6	308	KC1	C3C-C2C	4.86	1.47	1.36
30	15	309	CLA	CHC-C1C	4.86	1.48	1.38
30	13	307	CLA	C1D-ND	4.86	1.44	1.37
30	15	313	CLA	C1D-ND	4.86	1.44	1.37
37	13	315	A86	C9-C8	4.86	1.47	1.34
37	10	317	A86	C9-C8	4.85	1.47	1.34
30	A	818	CLA	O2D-CGD	4.85	1.45	1.33
30	B	831	CLA	O2D-CGD	4.85	1.45	1.33
30	14	309	CLA	C1D-ND	4.85	1.44	1.37
37	8	318	A86	C17-C18	-4.85	1.45	1.52
30	B	826	CLA	O2D-CGD	4.85	1.45	1.33
38	4	307	KC1	O2D-CGD	4.85	1.45	1.33
29	A	801	CL0	CHB-C1B	4.85	1.47	1.39
30	B	837	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	312	CLA	C1D-ND	4.85	1.44	1.37
30	A	824	CLA	O2D-CGD	4.85	1.45	1.33
30	A	837	CLA	O2D-CGD	4.85	1.45	1.33
30	2	304	CLA	O2D-CGD	4.84	1.45	1.33
30	A	829	CLA	C3C-C2C	4.84	1.47	1.36
30	16	305	CLA	O2D-CGD	4.84	1.45	1.33
37	9	313	A86	C17-C18	-4.84	1.45	1.52
38	12	313	KC1	C1D-ND	4.84	1.44	1.37
30	A	819	CLA	O2D-CGD	4.84	1.45	1.33
38	13	311	KC1	CHD-C4C	4.84	1.48	1.38
30	8	309	CLA	O2D-CGD	4.84	1.45	1.33
30	B	837	CLA	O2D-CGD	4.84	1.45	1.33
30	B	807	CLA	C3C-C2C	4.84	1.47	1.36
38	9	304	KC1	CHD-C4C	4.84	1.48	1.38
38	14	306	KC1	O2D-CGD	4.83	1.45	1.33
30	A	823	CLA	O2D-CGD	4.83	1.45	1.33
30	5	309	CLA	O2D-CGD	4.83	1.45	1.33
38	2	306	KC1	CHD-C4C	4.83	1.48	1.38
30	10	311	CLA	C1D-ND	4.83	1.44	1.37
30	16	303	CLA	CHC-C1C	4.83	1.48	1.38
38	9	311	KC1	CHD-C4C	4.83	1.48	1.38
30	5	303	CLA	O2D-CGD	4.83	1.45	1.33
30	13	303	CLA	C1D-ND	4.83	1.44	1.37
38	14	306	KC1	C3C-C2C	4.83	1.47	1.36
30	15	310	CLA	C1D-ND	4.83	1.44	1.37
30	2	308	CLA	C3C-C2C	4.83	1.47	1.36
30	B	829	CLA	O2D-CGD	4.83	1.45	1.33
30	7	312	CLA	C1D-ND	4.83	1.44	1.37
37	9	315	A86	C9-C8	4.83	1.47	1.34
30	13	301	CLA	C3C-C2C	4.82	1.47	1.36
30	16	308	CLA	C1D-ND	4.82	1.44	1.37
30	A	807	CLA	C3C-C2C	4.82	1.47	1.36
30	4	301	CLA	O2D-CGD	4.82	1.45	1.33
30	2	303	CLA	C3C-C2C	4.82	1.47	1.36
30	4	305	CLA	O2D-CGD	4.82	1.45	1.33
38	7	313	KC1	O2D-CGD	4.82	1.45	1.33
39	15	318	DD6	C2-C1	4.82	1.46	1.35
30	3	303	CLA	O2D-CGD	4.82	1.45	1.33
30	8	305	CLA	C3C-C2C	4.82	1.47	1.36
30	11	308	CLA	O2D-CGD	4.82	1.45	1.33
30	6	310	CLA	O2D-CGD	4.82	1.45	1.33
37	3	314	A86	C9-C8	4.82	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	310	KC1	O2D-CGD	4.82	1.45	1.33
30	B	811	CLA	O2D-CGD	4.82	1.45	1.33
37	15	323	A86	C9-C8	4.81	1.47	1.34
30	3	307	CLA	C1D-ND	4.81	1.44	1.37
38	8	307	KC1	O2D-CGD	4.81	1.45	1.33
30	F	202	CLA	O2D-CGD	4.81	1.45	1.33
30	7	309	CLA	O2D-CGD	4.81	1.45	1.33
30	2	301	CLA	O2D-CGD	4.81	1.45	1.33
30	B	817	CLA	C3C-C2C	4.81	1.47	1.36
38	11	311	KC1	CHD-C4C	4.81	1.48	1.38
30	3	305	CLA	O2D-CGD	4.81	1.45	1.33
38	13	311	KC1	CHC-C4B	4.81	1.47	1.38
30	A	826	CLA	C3C-C2C	4.81	1.47	1.36
30	6	304	CLA	C3C-C2C	4.81	1.47	1.36
30	8	302	CLA	O2D-CGD	4.81	1.45	1.33
37	5	301	A86	C17-C18	-4.81	1.45	1.52
38	1	306	KC1	CHD-C4C	4.80	1.48	1.38
38	13	310	KC1	CHD-C4C	4.80	1.48	1.38
30	12	321	CLA	C1D-ND	4.80	1.44	1.37
30	15	304	CLA	C1D-ND	4.80	1.44	1.37
30	8	304	CLA	O2D-CGD	4.80	1.45	1.33
30	15	302	CLA	O2D-CGD	4.80	1.45	1.33
37	16	312	A86	C17-C18	-4.80	1.45	1.52
30	A	830	CLA	C3C-C2C	4.80	1.47	1.36
38	9	312	KC1	CHD-C4C	4.80	1.48	1.38
30	9	308	CLA	C3C-C2C	4.80	1.47	1.36
38	13	305	KC1	CHD-C4C	4.80	1.48	1.38
30	15	306	CLA	C1D-ND	4.80	1.44	1.37
30	B	832	CLA	O2D-CGD	4.80	1.45	1.33
30	B	833	CLA	O2D-CGD	4.80	1.45	1.33
30	A	803	CLA	O2D-CGD	4.80	1.45	1.33
38	13	306	KC1	C1D-ND	4.79	1.44	1.37
38	4	308	KC1	CHD-C4C	4.79	1.48	1.38
30	5	308	CLA	C3C-C2C	4.79	1.47	1.36
38	5	305	KC1	CHD-C4C	4.79	1.48	1.38
37	5	315	A86	C9-C8	4.79	1.47	1.34
30	7	309	CLA	C3C-C2C	4.79	1.47	1.36
30	B	823	CLA	C3C-C2C	4.79	1.47	1.36
30	3	306	CLA	CHC-C1C	4.79	1.48	1.38
30	12	302	CLA	O2D-CGD	4.79	1.45	1.33
37	2	319	A86	C9-C8	4.79	1.47	1.34
30	4	304	CLA	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	835	CLA	O2D-CGD	4.78	1.45	1.33
38	14	306	KC1	CHC-C4B	4.78	1.47	1.38
30	4	304	CLA	CHC-C1C	4.78	1.48	1.38
38	16	311	KC1	CHD-C4C	4.78	1.48	1.38
37	14	319	A86	C9-C8	4.78	1.47	1.34
38	2	314	KC1	CHD-C4C	4.78	1.48	1.38
30	B	821	CLA	O2D-CGD	4.78	1.45	1.33
38	7	313	KC1	CHD-C4C	4.78	1.48	1.38
37	15	317	A86	C9-C8	4.78	1.47	1.34
30	8	304	CLA	C3C-C2C	4.78	1.47	1.36
30	B	825	CLA	O2D-CGD	4.78	1.45	1.33
30	4	302	CLA	C3C-C2C	4.77	1.47	1.36
30	9	308	CLA	O2D-CGD	4.77	1.45	1.33
38	9	311	KC1	CHC-C4B	4.77	1.47	1.38
38	7	308	KC1	O2D-CGD	4.77	1.45	1.33
30	B	813	CLA	C3C-C2C	4.77	1.47	1.36
38	11	312	KC1	CHD-C4C	4.77	1.48	1.38
30	A	843	CLA	C3C-C2C	4.77	1.47	1.36
37	5	316	A86	C9-C8	4.77	1.47	1.34
30	B	829	CLA	CHC-C1C	4.77	1.48	1.38
30	14	312	CLA	C1D-ND	4.77	1.44	1.37
30	2u	202	CLA	O2D-CGD	4.77	1.44	1.33
30	14	304	CLA	C1D-ND	4.76	1.44	1.37
38	6	312	KC1	O2D-CGD	4.76	1.44	1.33
38	16	304	KC1	C1D-ND	4.76	1.44	1.37
38	10	310	KC1	CHD-C4C	4.76	1.48	1.38
30	B	816	CLA	O2D-CGD	4.76	1.44	1.33
30	A	821	CLA	O2D-CGD	4.76	1.44	1.33
30	A	842	CLA	O2D-CGD	4.76	1.44	1.33
38	12	313	KC1	C1A-CHA	4.76	1.52	1.40
30	3	309	CLA	CHC-C1C	4.76	1.48	1.38
30	A	802	CLA	C3C-C2C	4.76	1.47	1.36
30	B	839	CLA	CHC-C1C	4.76	1.48	1.38
38	12	311	KC1	CHD-C4C	4.76	1.48	1.38
38	13	306	KC1	CHD-C4C	4.76	1.48	1.38
30	9	306	CLA	C1D-ND	4.76	1.44	1.37
38	13	306	KC1	CHC-C4B	4.76	1.47	1.38
38	10	306	KC1	O2D-CGD	4.76	1.44	1.33
38	3	304	KC1	CHD-C4C	4.75	1.48	1.38
38	12	309	KC1	CHD-C4C	4.75	1.48	1.38
38	12	305	KC1	CHD-C4C	4.75	1.48	1.38
30	A	811	CLA	O2D-CGD	4.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	315	A86	C10-C11	4.75	1.47	1.34
38	8	312	KC1	CHB-C1B	4.75	1.47	1.38
30	A	815	CLA	O2D-CGD	4.75	1.44	1.33
30	A	840	CLA	O2D-CGD	4.75	1.44	1.33
38	2	312	KC1	CHD-C4C	4.75	1.48	1.38
38	13	311	KC1	CHB-C1B	4.75	1.47	1.38
37	16	312	A86	C9-C8	4.75	1.47	1.34
30	B	836	CLA	O2D-CGD	4.75	1.44	1.33
30	9	301	CLA	C3C-C2C	4.74	1.47	1.36
30	2	313	CLA	C1D-ND	4.74	1.44	1.37
30	B	803	CLA	O2D-CGD	4.74	1.44	1.33
29	A	801	CL0	O2D-CGD	4.74	1.44	1.33
30	A	820	CLA	O2D-CGD	4.74	1.44	1.33
39	7	302	DD6	C2-C1	4.74	1.46	1.35
30	A	809	CLA	O2D-CGD	4.74	1.44	1.33
30	7	310	CLA	CHC-C1C	4.74	1.48	1.38
30	B	818	CLA	O2D-CGD	4.74	1.44	1.33
38	8	306	KC1	CHD-C4C	4.74	1.48	1.38
38	8	311	KC1	CHD-C4C	4.73	1.48	1.38
30	15	302	CLA	C1D-ND	4.73	1.44	1.37
30	10	308	CLA	CHC-C1C	4.73	1.48	1.38
30	A	831	CLA	C1B-NB	-4.73	1.31	1.37
37	14	301	A86	C9-C8	4.73	1.47	1.34
30	B	816	CLA	C3C-C2C	4.73	1.47	1.36
30	5	307	CLA	O2D-CGD	4.73	1.44	1.33
30	3	309	CLA	C1D-ND	4.73	1.44	1.37
38	5	312	KC1	C3C-C2C	4.73	1.47	1.36
30	15	314	CLA	C1D-ND	4.73	1.44	1.37
38	8	313	KC1	C1A-NA	-4.73	1.28	1.38
38	13	308	KC1	C1D-ND	4.73	1.44	1.37
30	13	309	CLA	C1D-ND	4.73	1.44	1.37
30	B	835	CLA	CHC-C1C	4.73	1.48	1.38
30	B	807	CLA	O2D-CGD	4.73	1.44	1.33
30	B	835	CLA	O2D-CGD	4.73	1.44	1.33
30	7	305	CLA	O2D-CGD	4.72	1.44	1.33
30	A	813	CLA	O2D-CGD	4.72	1.44	1.33
30	8	301	CLA	C3C-C2C	4.72	1.47	1.36
30	B	817	CLA	CHC-C1C	4.72	1.47	1.38
30	11	310	CLA	CHC-C1C	4.72	1.47	1.38
30	10	307	CLA	O2D-CGD	4.72	1.44	1.33
30	4	303	CLA	O2D-CGD	4.72	1.44	1.33
30	B	808	CLA	O2D-CGD	4.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	7	319	A86	C9-C8	4.72	1.47	1.34
30	3	310	CLA	C1D-ND	4.72	1.44	1.37
38	6	308	KC1	CHC-C4B	4.72	1.47	1.38
30	7	303	CLA	CHC-C1C	4.72	1.47	1.38
30	14	307	CLA	CHC-C1C	4.72	1.47	1.38
30	15	303	CLA	C1D-ND	4.71	1.44	1.37
30	A	806	CLA	O2D-CGD	4.71	1.44	1.33
30	B	806	CLA	C3C-C2C	4.71	1.46	1.36
38	6	308	KC1	O2D-CGD	4.71	1.44	1.33
38	8	314	KC1	CHD-C4C	4.71	1.47	1.38
30	16	307	CLA	C1D-ND	4.71	1.44	1.37
38	13	305	KC1	O2D-CGD	4.71	1.44	1.33
30	7	307	CLA	C3C-C2C	4.71	1.46	1.36
37	11	315	A86	C9-C8	4.71	1.47	1.34
30	B	838	CLA	O2D-CGD	4.71	1.44	1.33
30	B	827	CLA	O2D-CGD	4.71	1.44	1.33
37	15	316	A86	C9-C8	4.71	1.47	1.34
38	6	312	KC1	CHD-C4C	4.71	1.47	1.38
30	B	814	CLA	O2D-CGD	4.71	1.44	1.33
30	L	202	CLA	O2D-CGD	4.71	1.44	1.33
37	11	314	A86	C9-C8	4.71	1.47	1.34
30	14	313	CLA	C1D-ND	4.71	1.44	1.37
38	6	311	KC1	C1A-NA	-4.71	1.28	1.38
39	10	313	DD6	C2-C1	4.71	1.46	1.35
30	A	805	CLA	O2D-CGD	4.71	1.44	1.33
30	14	302	CLA	C1D-ND	4.71	1.44	1.37
39	5	314	DD6	C13-C14	4.71	1.43	1.32
38	2	306	KC1	O2D-CGD	4.71	1.44	1.33
30	B	812	CLA	O2D-CGD	4.70	1.44	1.33
38	12	311	KC1	C1D-ND	4.70	1.44	1.37
30	A	830	CLA	O2D-CGD	4.70	1.44	1.33
30	L	203	CLA	O2D-CGD	4.70	1.44	1.33
30	5	302	CLA	CHC-C1C	4.70	1.47	1.38
30	2	303	CLA	CHC-C1C	4.70	1.47	1.38
30	9	302	CLA	O2D-CGD	4.70	1.44	1.33
37	5	301	A86	C9-C8	4.70	1.46	1.34
30	B	810	CLA	O2D-CGD	4.70	1.44	1.33
30	B	809	CLA	C3C-C2C	4.70	1.46	1.36
30	8	301	CLA	O2D-CGD	4.70	1.44	1.33
38	11	311	KC1	C1D-ND	4.70	1.44	1.37
30	A	841	CLA	CHC-C1C	4.70	1.47	1.38
38	4	308	KC1	C1D-ND	4.69	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	307	CLA	O2D-CGD	4.69	1.44	1.33
37	10	315	A86	O4-C38	4.69	1.45	1.35
30	1	305	CLA	C1D-ND	4.69	1.44	1.37
30	9	308	CLA	CHC-C1C	4.69	1.47	1.38
30	14	313	CLA	CHC-C1C	4.69	1.47	1.38
30	5	311	CLA	C1D-ND	4.69	1.44	1.37
30	6	317	CLA	C1D-ND	4.69	1.44	1.37
30	10	303	CLA	CHC-C1C	4.69	1.47	1.38
30	16	301	CLA	CHC-C1C	4.68	1.47	1.38
38	9	310	KC1	CHD-C4C	4.68	1.47	1.38
38	8	307	KC1	CHD-C4C	4.68	1.47	1.38
30	1	303	CLA	CHC-C1C	4.68	1.47	1.38
30	A	828	CLA	O2D-CGD	4.68	1.44	1.33
38	13	305	KC1	CHC-C4B	4.68	1.47	1.38
37	14	318	A86	C9-C8	4.68	1.46	1.34
30	6	315	CLA	C1D-ND	4.68	1.44	1.37
30	15	304	CLA	CHC-C1C	4.68	1.47	1.38
30	A	829	CLA	O2D-CGD	4.68	1.44	1.33
30	A	812	CLA	O2D-CGD	4.67	1.44	1.33
38	8	306	KC1	O2D-CGD	4.67	1.44	1.33
30	1	304	CLA	C3C-C2C	4.67	1.46	1.36
30	B	828	CLA	C1B-NB	-4.67	1.31	1.37
37	15	321	A86	C9-C8	4.67	1.46	1.34
30	3	303	CLA	CHC-C1C	4.67	1.47	1.38
39	6	319	DD6	C2-C1	4.67	1.46	1.35
30	B	818	CLA	C3C-C2C	4.67	1.46	1.36
30	B	851	CLA	C3C-C2C	4.67	1.46	1.36
38	3	308	KC1	CHD-C4C	4.67	1.47	1.38
38	13	310	KC1	CHC-C4B	4.67	1.47	1.38
30	A	832	CLA	O2D-CGD	4.67	1.44	1.33
37	15	315	A86	C17-C18	-4.67	1.45	1.52
30	A	807	CLA	O2D-CGD	4.67	1.44	1.33
38	8	314	KC1	C1D-ND	4.67	1.44	1.37
38	3	304	KC1	C1D-ND	4.67	1.44	1.37
38	14	311	KC1	CHD-C4C	4.67	1.47	1.38
38	11	312	KC1	C1D-ND	4.67	1.44	1.37
30	6	306	CLA	CHC-C1C	4.67	1.47	1.38
30	A	844	CLA	C1D-ND	4.67	1.44	1.37
30	B	830	CLA	CHC-C1C	4.67	1.47	1.38
30	B	802	CLA	C3C-C2C	4.67	1.46	1.36
30	14	310	CLA	C1D-ND	4.66	1.44	1.37
30	13	309	CLA	CHC-C1C	4.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	310	KC1	CHD-C4C	4.66	1.47	1.38
30	2	303	CLA	O2A-CGA	4.66	1.46	1.33
39	13	314	DD6	C2-C1	4.66	1.46	1.35
38	9	312	KC1	C1D-ND	4.66	1.44	1.37
30	B	803	CLA	C3C-C2C	4.66	1.46	1.36
38	13	312	KC1	CHC-C4B	4.66	1.47	1.38
30	6	314	CLA	C3C-C2C	4.66	1.46	1.36
38	3	304	KC1	O2D-CGD	4.66	1.44	1.33
38	1	306	KC1	CHC-C4B	4.66	1.47	1.38
37	4	317	A86	C17-C18	-4.65	1.45	1.52
30	2	313	CLA	CHC-C1C	4.65	1.47	1.38
38	1	308	KC1	CHD-C4C	4.65	1.47	1.38
30	7	306	CLA	O2D-CGD	4.65	1.44	1.33
30	B	806	CLA	CHC-C1C	4.65	1.47	1.38
30	2	301	CLA	C3C-C2C	4.65	1.46	1.36
30	4	306	CLA	CHC-C1C	4.65	1.47	1.38
30	14	303	CLA	C1D-ND	4.65	1.44	1.37
37	16	314	A86	C9-C8	4.65	1.46	1.34
30	14	303	CLA	CHC-C1C	4.65	1.47	1.38
38	6	313	KC1	C1A-NA	-4.65	1.28	1.38
30	B	823	CLA	O2D-CGD	4.65	1.44	1.33
38	14	308	KC1	CHD-C4C	4.65	1.47	1.38
38	12	309	KC1	C1D-ND	4.65	1.44	1.37
39	2	317	DD6	C2-C1	4.65	1.46	1.35
30	15	310	CLA	CHC-C1C	4.65	1.47	1.38
39	3	313	DD6	C2-C1	4.64	1.46	1.35
37	8	315	A86	C17-C18	-4.64	1.45	1.52
37	14	315	A86	C9-C8	4.64	1.46	1.34
30	13	301	CLA	C1D-ND	4.64	1.44	1.37
30	6	310	CLA	C1D-ND	4.64	1.44	1.37
30	B	834	CLA	O2D-CGD	4.64	1.44	1.33
39	6	303	DD6	C2-C1	4.64	1.46	1.35
30	A	818	CLA	C3C-C2C	4.64	1.46	1.36
30	A	827	CLA	O2D-CGD	4.64	1.44	1.33
37	10	316	A86	C9-C8	4.64	1.46	1.34
30	A	838	CLA	O2D-CGD	4.64	1.44	1.33
30	14	305	CLA	CHC-C1C	4.64	1.47	1.38
37	14	317	A86	C9-C8	4.64	1.46	1.34
31	A	845	PQN	C10-C5	4.64	1.48	1.40
30	6	304	CLA	CHC-C1C	4.64	1.47	1.38
38	8	310	KC1	C3C-C2C	4.64	1.46	1.36
30	10	307	CLA	CHC-C1C	4.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	304	CLA	CHC-C1C	4.64	1.47	1.38
30	A	810	CLA	O2D-CGD	4.64	1.44	1.33
30	B	805	CLA	O2D-CGD	4.64	1.44	1.33
30	B	809	CLA	O2D-CGD	4.64	1.44	1.33
38	2	306	KC1	CHC-C4B	4.64	1.47	1.38
30	B	825	CLA	CHC-C1C	4.63	1.47	1.38
30	B	804	CLA	O2D-CGD	4.63	1.44	1.33
30	A	829	CLA	CHC-C1C	4.63	1.47	1.38
30	2	311	CLA	OBD-CAD	4.63	1.30	1.22
30	A	820	CLA	C1B-NB	-4.63	1.31	1.37
37	14	314	A86	C9-C8	4.63	1.46	1.34
30	A	837	CLA	CHC-C1C	4.63	1.47	1.38
30	15	305	CLA	C1D-ND	4.63	1.43	1.37
30	15	313	CLA	CHC-C1C	4.63	1.47	1.38
38	11	307	KC1	C1D-ND	4.63	1.43	1.37
30	B	824	CLA	CHC-C1C	4.62	1.47	1.38
30	A	809	CLA	C3C-C2C	4.62	1.46	1.36
30	14	312	CLA	CHC-C1C	4.62	1.47	1.38
37	9	316	A86	O4-C38	4.62	1.45	1.35
38	7	313	KC1	C1A-NA	-4.62	1.28	1.38
30	14	310	CLA	CHC-C1C	4.62	1.47	1.38
38	8	312	KC1	CHD-C4C	4.62	1.47	1.38
30	B	824	CLA	O2D-CGD	4.61	1.44	1.33
38	10	312	KC1	C1A-NA	-4.61	1.28	1.38
30	L	202	CLA	CHC-C1C	4.61	1.47	1.38
30	12	307	CLA	CHC-C1C	4.61	1.47	1.38
30	A	826	CLA	O2D-CGD	4.61	1.44	1.33
38	8	314	KC1	O2D-CGD	4.61	1.44	1.33
30	2	311	CLA	CHC-C1C	4.61	1.47	1.38
30	B	802	CLA	CHC-C1C	4.61	1.47	1.38
30	B	837	CLA	CHC-C1C	4.61	1.47	1.38
39	10	314	DD6	C2-C1	4.61	1.46	1.35
30	B	839	CLA	O2D-CGD	4.61	1.44	1.33
38	9	310	KC1	CHC-C4B	4.61	1.47	1.38
38	6	313	KC1	CHD-C4C	4.61	1.47	1.38
30	F	201	CLA	O2D-CGD	4.60	1.44	1.33
30	13	307	CLA	CHC-C1C	4.60	1.47	1.38
30	11	308	CLA	CHC-C1C	4.60	1.47	1.38
38	2	314	KC1	CHC-C4B	4.60	1.47	1.38
30	A	833	CLA	CHC-C1C	4.60	1.47	1.38
37	11	301	A86	C7-C6	4.60	1.60	1.50
37	4	312	A86	C17-C18	-4.60	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	12	314	A86	C17-C18	-4.60	1.45	1.52
30	5	304	CLA	CHC-C1C	4.60	1.47	1.38
39	5	313	DD6	C2-C1	4.60	1.46	1.35
30	B	801	CLA	O2D-CGD	4.60	1.44	1.33
30	15	308	CLA	O2D-CGD	4.60	1.44	1.33
38	5	306	KC1	C1A-NA	-4.60	1.28	1.38
38	7	308	KC1	CHD-C4C	4.60	1.47	1.38
38	5	306	KC1	CHC-C4B	4.60	1.47	1.38
38	10	312	KC1	CHC-C4B	4.60	1.47	1.38
30	7	303	CLA	O2D-CGD	4.60	1.44	1.33
38	8	307	KC1	C1A-NA	-4.59	1.28	1.38
38	10	306	KC1	CHD-C4C	4.59	1.47	1.38
30	12	307	CLA	C3C-C2C	4.59	1.46	1.36
30	3	305	CLA	C1D-ND	4.59	1.43	1.37
30	9	306	CLA	O2A-CGA	4.59	1.46	1.30
38	9	311	KC1	C1D-ND	4.59	1.43	1.37
39	6	318	DD6	C2-C1	4.59	1.46	1.35
30	7	307	CLA	CHC-C1C	4.59	1.47	1.38
37	7	316	A86	C17-C18	-4.59	1.45	1.52
30	13	301	CLA	CHC-C1C	4.59	1.47	1.38
30	16	307	CLA	CHC-C1C	4.59	1.47	1.38
30	A	844	CLA	CHC-C1C	4.59	1.47	1.38
30	15	312	CLA	CHC-C1C	4.58	1.47	1.38
30	B	815	CLA	O2D-CGD	4.58	1.44	1.33
30	9	305	CLA	CHC-C1C	4.58	1.47	1.38
38	2	312	KC1	CHC-C4B	4.58	1.47	1.38
37	3	314	A86	O4-C38	4.58	1.45	1.35
30	12	304	CLA	CHC-C1C	4.58	1.47	1.38
30	A	840	CLA	C1D-ND	4.58	1.43	1.37
38	13	310	KC1	C1D-ND	4.58	1.43	1.37
38	16	311	KC1	CHC-C4B	4.58	1.47	1.38
30	A	802	CLA	C1B-NB	-4.58	1.31	1.37
37	2u	205	A86	O4-C38	4.58	1.45	1.35
37	2	318	A86	C9-C8	4.58	1.46	1.34
30	16	301	CLA	C1D-ND	4.58	1.43	1.37
37	5	316	A86	C17-C18	-4.58	1.45	1.52
30	L	203	CLA	O2A-CGA	4.57	1.45	1.30
30	4	302	CLA	CHC-C1C	4.57	1.47	1.38
37	9	315	A86	O4-C38	4.57	1.45	1.35
30	12	312	CLA	C1D-ND	4.57	1.43	1.37
38	16	311	KC1	C1D-ND	4.57	1.43	1.37
30	15	305	CLA	CHC-C1C	4.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	316	DD6	C2-C1	4.57	1.46	1.35
37	11	316	A86	C9-C8	4.57	1.46	1.34
30	A	837	CLA	C1D-ND	4.57	1.43	1.37
38	12	311	KC1	CHC-C4B	4.57	1.47	1.38
38	8	310	KC1	C1A-NA	-4.57	1.28	1.38
38	9	304	KC1	C1A-NA	-4.57	1.28	1.38
38	9	311	KC1	C1A-NA	-4.57	1.28	1.38
30	L	203	CLA	CHC-C1C	4.57	1.47	1.38
30	3	310	CLA	O2A-CGA	4.57	1.45	1.30
30	15	307	CLA	C1D-ND	4.57	1.43	1.37
30	16	309	CLA	O2A-CGA	4.57	1.45	1.30
30	6	305	CLA	CHC-C1C	4.57	1.47	1.38
38	8	306	KC1	C1D-ND	4.57	1.43	1.37
38	11	305	KC1	C1D-ND	4.57	1.43	1.37
30	A	819	CLA	CHC-C1C	4.57	1.47	1.38
38	3	304	KC1	CHC-C4B	4.56	1.47	1.38
30	14	309	CLA	O2A-CGA	4.56	1.45	1.30
38	5	310	KC1	C1D-ND	4.56	1.43	1.37
30	14	304	CLA	O2A-CGA	4.56	1.45	1.30
38	9	310	KC1	C1A-NA	-4.56	1.28	1.38
37	12	314	A86	C9-C8	4.56	1.46	1.34
37	5	316	A86	O4-C38	4.56	1.45	1.35
30	2	309	CLA	CHC-C1C	4.56	1.47	1.38
30	6	304	CLA	O2D-CGD	4.56	1.44	1.33
30	A	804	CLA	O2D-CGD	4.56	1.44	1.33
30	10	311	CLA	O2A-CGA	4.56	1.45	1.30
30	B	804	CLA	CHC-C1C	4.56	1.47	1.38
30	F	202	CLA	CHC-C1C	4.56	1.47	1.38
37	6	320	A86	O4-C38	4.56	1.45	1.35
37	14	316	A86	C9-C8	4.56	1.46	1.34
30	15	314	CLA	O2A-CGA	4.56	1.45	1.30
38	4	310	KC1	C1D-ND	4.56	1.43	1.37
38	6	312	KC1	CHC-C4B	4.56	1.47	1.38
30	13	304	CLA	O2A-CGA	4.56	1.45	1.30
30	13	303	CLA	CHC-C1C	4.56	1.47	1.38
38	7	308	KC1	C1D-ND	4.56	1.43	1.37
38	14	311	KC1	C1D-ND	4.56	1.43	1.37
38	6	313	KC1	CHC-C4B	4.56	1.47	1.38
39	3	312	DD6	C2-C1	4.56	1.46	1.35
30	15	311	CLA	CHC-C1C	4.56	1.47	1.38
30	A	806	CLA	CHC-C1C	4.55	1.47	1.38
30	2	304	CLA	CHC-C1C	4.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	851	CLA	CHC-C1C	4.55	1.47	1.38
38	2	306	KC1	C1D-ND	4.55	1.43	1.37
38	1	306	KC1	C1A-NA	-4.55	1.28	1.38
38	12	305	KC1	CHC-C4B	4.55	1.47	1.38
30	A	803	CLA	C1B-NB	-4.55	1.31	1.37
30	12	304	CLA	C1D-ND	4.55	1.43	1.37
30	B	811	CLA	CHC-C1C	4.55	1.47	1.38
30	B	833	CLA	CHC-C1C	4.55	1.47	1.38
30	12	310	CLA	CHC-C1C	4.55	1.47	1.38
30	B	822	CLA	CHC-C1C	4.55	1.47	1.38
30	9	305	CLA	O2D-CGD	4.55	1.44	1.33
30	A	824	CLA	CHC-C1C	4.55	1.47	1.38
30	15	306	CLA	O2A-CGA	4.55	1.45	1.30
30	3	309	CLA	O2A-CGA	4.55	1.45	1.30
38	10	310	KC1	C1D-ND	4.55	1.43	1.37
38	10	310	KC1	C1A-NA	-4.55	1.28	1.38
30	10	305	CLA	CHC-C1C	4.54	1.47	1.38
37	9	313	A86	O4-C38	4.54	1.45	1.35
30	2	305	CLA	O2D-CGD	4.54	1.44	1.33
38	5	305	KC1	CHC-C4B	4.54	1.47	1.38
30	4	305	CLA	CHC-C1C	4.54	1.47	1.38
30	13	309	CLA	O2A-CGA	4.54	1.45	1.30
37	2	319	A86	O4-C38	4.54	1.45	1.35
37	4	312	A86	C9-C8	4.54	1.46	1.34
30	15	303	CLA	CHC-C1C	4.54	1.47	1.38
30	B	832	CLA	CHC-C1C	4.54	1.47	1.38
37	2	319	A86	C17-C18	-4.54	1.45	1.52
30	B	815	CLA	O2A-CGA	4.54	1.45	1.30
37	6	320	A86	C9-C8	4.54	1.46	1.34
37	2	302	A86	C7-C6	4.54	1.60	1.50
37	8	315	A86	O4-C38	4.54	1.45	1.35
30	2	313	CLA	O2A-CGA	4.54	1.45	1.30
37	14	301	A86	O4-C38	4.54	1.45	1.35
38	3	311	KC1	CHC-C4B	4.54	1.47	1.38
30	15	311	CLA	O2A-CGA	4.54	1.45	1.30
38	5	312	KC1	CHD-C4C	4.54	1.47	1.38
38	4	307	KC1	C1D-ND	4.54	1.43	1.37
30	2	305	CLA	CHC-C1C	4.54	1.47	1.38
38	5	310	KC1	C1A-NA	-4.54	1.28	1.38
30	6	307	CLA	CHC-C1C	4.54	1.47	1.38
38	8	312	KC1	CHC-C4B	4.54	1.47	1.38
38	13	308	KC1	CHC-C4B	4.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	303	CLA	CHC-C1C	4.53	1.47	1.38
30	5	309	CLA	C1D-ND	4.53	1.43	1.37
38	3	311	KC1	C1D-ND	4.53	1.43	1.37
38	8	312	KC1	C1D-ND	4.53	1.43	1.37
37	13	315	A86	C10-C11	4.53	1.46	1.34
30	9	307	CLA	C1D-ND	4.53	1.43	1.37
30	1	302	CLA	O2D-CGD	4.53	1.44	1.33
30	5	311	CLA	O2A-CGA	4.53	1.46	1.33
39	11	313	DD6	C2-C1	4.53	1.46	1.35
30	9	303	CLA	C3C-C2C	4.53	1.46	1.36
30	6	315	CLA	O2A-CGA	4.53	1.45	1.30
30	14	312	CLA	O2A-CGA	4.53	1.45	1.30
38	8	313	KC1	CHC-C4B	4.53	1.47	1.38
30	1	301	CLA	CHC-C1C	4.53	1.47	1.38
30	5	302	CLA	O2D-CGD	4.53	1.44	1.33
30	A	839	CLA	CHC-C1C	4.53	1.47	1.38
30	A	802	CLA	O2D-CGD	4.53	1.44	1.33
30	1	302	CLA	C1D-ND	4.53	1.43	1.37
30	5	303	CLA	CHC-C1C	4.53	1.47	1.38
30	A	807	CLA	CHC-C1C	4.53	1.47	1.38
30	16	310	CLA	O2A-CGA	4.52	1.45	1.30
30	F	201	CLA	CHC-C1C	4.52	1.47	1.38
37	14	320	A86	O4-C38	4.52	1.45	1.35
38	12	305	KC1	C1D-ND	4.52	1.43	1.37
38	14	308	KC1	C1D-ND	4.52	1.43	1.37
30	9	307	CLA	CHC-C1C	4.52	1.47	1.38
30	3	305	CLA	CHC-C1C	4.52	1.47	1.38
30	4	303	CLA	CHC-C1C	4.52	1.47	1.38
30	15	305	CLA	O2A-CGA	4.52	1.45	1.30
38	2	314	KC1	C1A-NA	-4.52	1.28	1.38
37	15	320	A86	O4-C38	4.52	1.45	1.35
30	B	809	CLA	C1B-NB	-4.52	1.31	1.37
39	12	315	DD6	C2-C1	4.52	1.46	1.35
37	4	312	A86	O4-C38	4.52	1.45	1.35
37	1	309	A86	C9-C8	4.52	1.46	1.34
30	B	819	CLA	CHC-C1C	4.52	1.47	1.38
38	4	308	KC1	C1A-CHA	4.52	1.51	1.40
30	6	306	CLA	C1D-ND	4.52	1.43	1.37
30	A	818	CLA	CHC-C1C	4.52	1.47	1.38
30	A	834	CLA	O2D-CGD	4.52	1.44	1.33
30	10	309	CLA	C1D-ND	4.52	1.43	1.37
30	4	301	CLA	CHC-C1C	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	314	A86	O4-C38	4.52	1.45	1.35
37	11	315	A86	O4-C38	4.52	1.45	1.35
38	5	312	KC1	C1A-NA	-4.52	1.28	1.38
30	2	311	CLA	C1D-ND	4.52	1.43	1.37
30	16	309	CLA	CHC-C1C	4.52	1.47	1.38
30	15	314	CLA	O2D-CGD	4.52	1.44	1.33
30	A	837	CLA	O2A-CGA	4.52	1.45	1.30
30	16	308	CLA	O2A-CGA	4.51	1.45	1.30
38	11	307	KC1	CHC-C4B	4.51	1.47	1.38
30	4	309	CLA	CHC-C1C	4.51	1.47	1.38
37	3	315	A86	C17-C18	-4.51	1.45	1.52
30	15	310	CLA	O2A-CGA	4.51	1.45	1.30
30	10	311	CLA	CHC-C1C	4.51	1.47	1.38
38	6	311	KC1	CHD-C4C	4.51	1.47	1.38
37	12	314	A86	O4-C38	4.51	1.45	1.35
30	6	315	CLA	CHC-C1C	4.51	1.47	1.38
37	11	316	A86	O4-C38	4.51	1.45	1.35
30	13	302	CLA	CHC-C1C	4.51	1.47	1.38
37	16	312	A86	O4-C38	4.51	1.45	1.35
38	11	305	KC1	CHC-C4B	4.51	1.47	1.38
30	14	309	CLA	CHD-C1D	4.51	1.47	1.38
30	14	309	CLA	CHC-C1C	4.51	1.47	1.38
38	4	310	KC1	CHC-C4B	4.51	1.47	1.38
30	15	312	CLA	O2A-CGA	4.51	1.45	1.30
30	5	308	CLA	CHC-C1C	4.51	1.47	1.38
30	6	317	CLA	CHC-C1C	4.51	1.47	1.38
30	16	306	CLA	CHC-C1C	4.51	1.47	1.38
30	A	806	CLA	C3C-C2C	4.51	1.46	1.36
30	16	310	CLA	C1D-ND	4.51	1.43	1.37
37	4	314	A86	C7-C6	4.51	1.60	1.50
30	B	831	CLA	CHC-C1C	4.51	1.47	1.38
30	10	309	CLA	CHC-C1C	4.51	1.47	1.38
30	15	308	CLA	O2A-CGA	4.51	1.45	1.30
30	13	302	CLA	C1D-ND	4.51	1.43	1.37
37	10	301	A86	O4-C38	4.51	1.45	1.35
37	10	317	A86	O4-C38	4.50	1.45	1.35
30	13	304	CLA	CHC-C1C	4.50	1.47	1.38
38	11	305	KC1	C1A-NA	-4.50	1.28	1.38
38	1	308	KC1	C1A-NA	-4.50	1.28	1.38
38	9	312	KC1	CHB-C1B	4.50	1.47	1.38
37	14	319	A86	O4-C38	4.50	1.45	1.35
37	4	317	A86	C9-C8	4.50	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	101	CLA	O2A-CGA	4.50	1.45	1.30
30	B	801	CLA	C3C-C2C	4.50	1.46	1.36
30	11	309	CLA	CHC-C1C	4.50	1.47	1.38
30	A	808	CLA	CHC-C1C	4.50	1.47	1.38
30	16	302	CLA	CHC-C1C	4.50	1.47	1.38
30	5	309	CLA	CHC-C1C	4.50	1.47	1.38
30	8	308	CLA	CHC-C1C	4.50	1.47	1.38
38	1	306	KC1	C1D-ND	4.50	1.43	1.37
39	7	314	DD6	C2-C1	4.50	1.46	1.35
30	4	311	CLA	C1D-ND	4.50	1.43	1.37
39	2	315	DD6	C2-C1	4.50	1.46	1.35
30	1	307	CLA	C1D-ND	4.50	1.43	1.37
30	3	302	CLA	CHC-C1C	4.49	1.47	1.38
38	9	312	KC1	CHC-C4B	4.49	1.47	1.38
39	16	313	DD6	C2-C1	4.49	1.46	1.35
38	7	308	KC1	CHC-C4B	4.49	1.47	1.38
30	2	301	CLA	O2A-CGA	4.49	1.46	1.33
30	16	303	CLA	O2A-CGA	4.49	1.46	1.33
30	B	819	CLA	C1B-NB	-4.49	1.32	1.37
38	5	306	KC1	C1D-ND	4.49	1.43	1.37
37	2	302	A86	O4-C38	4.49	1.45	1.35
38	14	308	KC1	CHC-C4B	4.49	1.47	1.38
30	6	309	CLA	CHC-C1C	4.49	1.47	1.38
30	15	314	CLA	CHC-C1C	4.49	1.47	1.38
38	2	306	KC1	C1A-NA	-4.49	1.28	1.38
30	J	101	CLA	C1D-ND	4.49	1.43	1.37
30	A	831	CLA	O2D-CGD	4.49	1.44	1.33
30	B	813	CLA	O2D-CGD	4.49	1.44	1.33
38	14	311	KC1	CHC-C4B	4.49	1.47	1.38
30	5	311	CLA	CHC-C1C	4.49	1.47	1.38
30	A	813	CLA	CHC-C1C	4.49	1.47	1.38
37	15	322	A86	C7-C6	4.49	1.59	1.50
30	11	310	CLA	CHD-C1D	4.49	1.47	1.38
37	2u	203	A86	C17-C18	-4.49	1.46	1.52
38	1	308	KC1	CHC-C4B	4.49	1.47	1.38
30	16	308	CLA	CHC-C1C	4.49	1.47	1.38
38	7	308	KC1	C1A-NA	-4.49	1.28	1.38
37	14	319	A86	C7-C6	4.49	1.59	1.50
38	11	311	KC1	C1A-NA	-4.49	1.28	1.38
30	B	820	CLA	O2A-CGA	4.49	1.45	1.30
37	14	315	A86	C17-C18	-4.49	1.46	1.52
30	8	301	CLA	CHC-C1C	4.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	203	CLA	O2A-CGA	4.49	1.45	1.30
30	1	307	CLA	OBD-CAD	4.48	1.30	1.22
39	12	317	DD6	C2-C1	4.48	1.46	1.35
37	5	315	A86	O4-C38	4.48	1.45	1.35
30	6	316	CLA	CHC-C1C	4.48	1.47	1.38
30	B	823	CLA	CHC-C1C	4.48	1.47	1.38
39	4	316	DD6	C2-C1	4.48	1.46	1.35
30	A	822	CLA	CHC-C1C	4.48	1.47	1.38
30	A	839	CLA	O2D-CGD	4.48	1.44	1.33
30	10	303	CLA	C1D-ND	4.48	1.43	1.37
37	10	302	A86	O4-C38	4.48	1.45	1.35
30	11	308	CLA	C1D-ND	4.48	1.43	1.37
30	2	309	CLA	C1D-ND	4.48	1.43	1.37
37	15	320	A86	C10-C11	4.48	1.46	1.34
30	B	812	CLA	O2A-CGA	4.48	1.46	1.33
30	B	810	CLA	CHC-C1C	4.48	1.47	1.38
37	8	318	A86	C9-C8	4.48	1.46	1.34
30	2	310	CLA	C1D-ND	4.48	1.43	1.37
30	3	303	CLA	C1D-ND	4.48	1.43	1.37
30	7	310	CLA	C1D-ND	4.48	1.43	1.37
37	7	319	A86	O4-C38	4.48	1.45	1.35
38	16	304	KC1	CHC-C4B	4.48	1.47	1.38
30	8	305	CLA	CHC-C1C	4.48	1.47	1.38
30	10	304	CLA	CHC-C1C	4.47	1.47	1.38
37	15	321	A86	C7-C6	4.47	1.59	1.50
37	10	316	A86	C17-C18	-4.47	1.46	1.52
38	9	312	KC1	C1A-NA	-4.47	1.28	1.38
37	4	315	A86	C9-C8	4.47	1.46	1.34
38	4	307	KC1	C1A-NA	-4.47	1.28	1.38
30	A	827	CLA	CHC-C1C	4.47	1.47	1.38
37	9	313	A86	C9-C8	4.47	1.46	1.34
39	7	317	DD6	C2-C1	4.47	1.46	1.35
37	14	301	A86	C21-C20	4.47	1.58	1.51
30	A	825	CLA	C1D-ND	4.47	1.43	1.37
30	9	305	CLA	C1D-ND	4.46	1.43	1.37
39	3	316	DD6	C2-C1	4.46	1.46	1.35
30	A	817	CLA	CHC-C1C	4.46	1.47	1.38
38	8	307	KC1	CHC-C4B	4.46	1.47	1.38
30	A	841	CLA	C1B-NB	-4.46	1.32	1.37
38	5	312	KC1	CHC-C4B	4.46	1.47	1.38
37	13	315	A86	O4-C38	4.46	1.45	1.35
30	A	802	CLA	CHC-C1C	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	308	KC1	C1A-NA	-4.46	1.28	1.38
30	7	303	CLA	O2A-CGA	4.46	1.46	1.33
30	6	306	CLA	O2A-CGA	4.46	1.46	1.33
30	11	304	CLA	C1D-ND	4.46	1.43	1.37
38	6	308	KC1	CHD-C4C	4.46	1.47	1.38
30	2u	202	CLA	CHC-C1C	4.46	1.47	1.38
30	7	311	CLA	CHC-C1C	4.46	1.47	1.38
30	1	305	CLA	CHD-C1D	4.46	1.47	1.38
38	7	313	KC1	CHC-C4B	4.46	1.47	1.38
37	14	314	A86	O4-C38	4.45	1.45	1.35
38	13	305	KC1	C1D-ND	4.45	1.43	1.37
30	A	835	CLA	C1D-ND	4.45	1.43	1.37
37	2	318	A86	C17-C18	-4.45	1.46	1.52
37	10	302	A86	C7-C6	4.45	1.59	1.50
38	11	312	KC1	C1A-CHA	4.45	1.51	1.40
37	14	320	A86	C7-C6	4.45	1.59	1.50
38	5	305	KC1	C1D-ND	4.45	1.43	1.37
37	16	312	A86	C10-C11	4.45	1.46	1.34
30	11	306	CLA	O2A-CGA	4.45	1.46	1.33
30	10	304	CLA	C1D-ND	4.45	1.43	1.37
38	10	312	KC1	C1D-ND	4.45	1.43	1.37
30	B	813	CLA	CHC-C1C	4.45	1.47	1.38
37	15	317	A86	O4-C38	4.45	1.45	1.35
30	8	302	CLA	CHC-C1C	4.45	1.47	1.38
37	14	318	A86	O4-C38	4.45	1.45	1.35
39	7	318	DD6	C2-C1	4.45	1.46	1.35
30	7	309	CLA	C1D-ND	4.45	1.43	1.37
30	2	303	CLA	C3D-C2D	4.45	1.51	1.39
38	13	305	KC1	C1A-CHA	4.45	1.51	1.40
30	9	301	CLA	O2D-CGD	4.45	1.44	1.33
37	7	315	A86	C9-C8	4.45	1.46	1.34
37	2u	203	A86	C7-C6	4.45	1.59	1.50
30	8	304	CLA	CHC-C1C	4.45	1.47	1.38
38	6	313	KC1	C1D-ND	4.44	1.43	1.37
30	14	305	CLA	C1D-ND	4.44	1.43	1.37
38	9	311	KC1	CHB-C1B	4.44	1.47	1.38
30	B	827	CLA	CHC-C1C	4.44	1.47	1.38
38	9	304	KC1	CHC-C4B	4.44	1.47	1.38
37	2	318	A86	O4-C38	4.44	1.45	1.35
30	1	303	CLA	O2D-CGD	4.44	1.44	1.33
37	15	317	A86	C17-C18	-4.44	1.46	1.52
37	15	323	A86	O4-C38	4.44	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	311	KC1	OBD-CAD	4.44	1.30	1.22
37	15	323	A86	C7-C6	4.44	1.59	1.50
38	8	311	KC1	CHC-C4B	4.44	1.47	1.38
38	10	306	KC1	CHC-C4B	4.44	1.47	1.38
31	B	840	PQN	C10-C5	4.44	1.47	1.40
30	A	814	CLA	C3C-C2C	4.44	1.46	1.36
39	8	317	DD6	C2-C1	4.44	1.46	1.35
38	8	306	KC1	C1A-NA	-4.44	1.28	1.38
30	A	803	CLA	CHC-C1C	4.43	1.47	1.38
30	7	305	CLA	C1D-ND	4.43	1.43	1.37
30	15	312	CLA	CHD-C1D	4.43	1.47	1.38
37	15	317	A86	C7-C6	4.43	1.59	1.50
30	7	305	CLA	CHC-C1C	4.43	1.47	1.38
30	1	305	CLA	CHC-C1C	4.43	1.47	1.38
30	16	305	CLA	C1D-ND	4.43	1.43	1.37
37	15	315	A86	O4-C38	4.43	1.45	1.35
37	2u	205	A86	C10-C11	4.43	1.46	1.34
37	15	323	A86	C17-C18	-4.43	1.46	1.52
30	12	312	CLA	CHC-C1C	4.43	1.47	1.38
39	1	310	DD6	C2-C1	4.43	1.46	1.35
37	12	316	A86	C17-C18	-4.43	1.46	1.52
38	6	312	KC1	C1A-NA	-4.43	1.28	1.38
38	12	313	KC1	CHC-C4B	4.43	1.47	1.38
30	15	304	CLA	O2A-CGA	4.43	1.46	1.33
30	A	823	CLA	CHC-C1C	4.42	1.47	1.38
30	16	302	CLA	C1D-ND	4.42	1.43	1.37
38	11	307	KC1	C1A-NA	-4.42	1.28	1.38
30	B	830	CLA	O2A-CGA	4.42	1.46	1.33
30	15	302	CLA	O2A-CGA	4.42	1.46	1.33
38	5	305	KC1	CHB-C1B	4.42	1.47	1.38
30	2	310	CLA	CHC-C1C	4.42	1.47	1.38
37	4	315	A86	O4-C38	4.42	1.45	1.35
30	12	310	CLA	C1D-ND	4.42	1.43	1.37
38	11	311	KC1	CHC-C4B	4.42	1.47	1.38
30	F	203	CLA	CHC-C1C	4.42	1.47	1.38
38	8	314	KC1	CHC-C4B	4.41	1.47	1.38
37	16	314	A86	O4-C38	4.41	1.45	1.35
37	11	316	A86	C7-C6	4.41	1.59	1.50
38	13	312	KC1	CHB-C1B	4.41	1.47	1.38
30	16	310	CLA	CHC-C1C	4.41	1.47	1.38
38	12	305	KC1	C1A-NA	-4.41	1.28	1.38
30	6	316	CLA	O2A-CGA	4.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	834	CLA	CHC-C1C	4.41	1.47	1.38
38	10	306	KC1	C1D-ND	4.41	1.43	1.37
37	9	316	A86	C7-C6	4.41	1.59	1.50
37	14	316	A86	O4-C38	4.41	1.44	1.35
38	12	313	KC1	CHD-C4C	4.41	1.47	1.38
30	1	302	CLA	CHC-C1C	4.41	1.47	1.38
30	A	832	CLA	CHC-C1C	4.41	1.47	1.38
38	3	311	KC1	C1A-NA	-4.41	1.28	1.38
37	14	317	A86	C17-C18	-4.41	1.46	1.52
38	8	311	KC1	C1A-NA	-4.40	1.28	1.38
38	14	306	KC1	C1A-NA	-4.40	1.28	1.38
37	3	315	A86	O4-C38	4.40	1.44	1.35
30	7	312	CLA	CHC-C1C	4.40	1.47	1.38
30	5	307	CLA	C1D-ND	4.40	1.43	1.37
30	6	314	CLA	C1D-ND	4.40	1.43	1.37
38	2	312	KC1	C1A-NA	-4.40	1.28	1.38
38	12	309	KC1	C1A-CHA	4.40	1.51	1.40
37	12	316	A86	O4-C38	4.40	1.44	1.35
38	8	310	KC1	C1D-ND	4.40	1.43	1.37
30	A	830	CLA	CHC-C1C	4.40	1.47	1.38
30	8	309	CLA	C1D-ND	4.40	1.43	1.37
37	11	314	A86	C7-C6	4.40	1.59	1.50
38	13	306	KC1	CHB-C1B	4.40	1.47	1.38
30	4	302	CLA	C1D-ND	4.40	1.43	1.37
30	B	851	CLA	C1D-ND	4.40	1.43	1.37
30	A	811	CLA	CHC-C1C	4.39	1.47	1.38
30	A	834	CLA	CHC-C1C	4.39	1.47	1.38
37	15	315	A86	C7-C6	4.39	1.59	1.50
30	A	810	CLA	CHC-C1C	4.39	1.47	1.38
30	12	303	CLA	CHC-C1C	4.39	1.47	1.38
30	2	307	CLA	CHC-C1C	4.39	1.47	1.38
37	14	315	A86	C7-C6	4.39	1.59	1.50
30	13	307	CLA	CHD-C1D	4.39	1.47	1.38
38	6	312	KC1	CHB-C1B	4.39	1.47	1.38
38	4	310	KC1	C1A-NA	-4.39	1.28	1.38
38	10	306	KC1	CHB-C1B	4.39	1.47	1.38
39	9	314	DD6	C2-C1	4.39	1.45	1.35
30	B	828	CLA	O2D-CGD	4.39	1.44	1.33
37	13	315	A86	C7-C6	4.39	1.59	1.50
30	8	308	CLA	C1D-ND	4.39	1.43	1.37
37	4	314	A86	C21-C20	4.38	1.58	1.51
30	12	308	CLA	C1D-ND	4.38	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	307	CLA	C1D-ND	4.38	1.43	1.37
38	11	305	KC1	CHB-C1B	4.38	1.47	1.38
30	A	814	CLA	O2D-CGD	4.38	1.44	1.33
30	A	814	CLA	C1D-ND	4.38	1.43	1.37
30	B	821	CLA	CHC-C1C	4.38	1.47	1.38
37	2u	203	A86	C10-C11	4.38	1.46	1.34
37	15	320	A86	C7-C6	4.38	1.59	1.50
30	3	307	CLA	CHC-C1C	4.38	1.47	1.38
30	12	308	CLA	CHC-C1C	4.38	1.47	1.38
30	A	835	CLA	O2A-CGA	4.38	1.46	1.33
30	10	305	CLA	O2A-CGA	4.38	1.46	1.33
30	8	309	CLA	CHC-C1C	4.38	1.47	1.38
38	2	314	KC1	C1D-ND	4.38	1.43	1.37
38	9	304	KC1	C1D-ND	4.38	1.43	1.37
37	4	317	A86	O4-C38	4.37	1.44	1.35
38	11	307	KC1	CHB-C1B	4.37	1.47	1.38
37	15	322	A86	O4-C38	4.37	1.44	1.35
37	14	301	A86	C7-C6	4.37	1.59	1.50
30	6	305	CLA	C1D-ND	4.37	1.43	1.37
38	8	310	KC1	CHD-C4C	4.37	1.47	1.38
38	3	308	KC1	CHB-C1B	4.37	1.47	1.38
39	8	316	DD6	C2-C1	4.37	1.45	1.35
38	6	313	KC1	CHB-C1B	4.37	1.46	1.38
37	14	317	A86	O4-C38	4.37	1.44	1.35
37	16	312	A86	C7-C6	4.37	1.59	1.50
30	13	304	CLA	CHD-C1D	4.37	1.46	1.38
37	4	315	A86	C7-C6	4.37	1.59	1.50
37	11	301	A86	O4-C38	4.37	1.44	1.35
37	10	317	A86	C7-C6	4.37	1.59	1.50
38	1	306	KC1	CHB-C1B	4.37	1.46	1.38
30	3	301	CLA	CHC-C1C	4.37	1.47	1.38
30	3	307	CLA	CHD-C1D	4.37	1.46	1.38
38	7	308	KC1	CHB-C1B	4.37	1.46	1.38
30	5	304	CLA	O2A-CGA	4.36	1.46	1.33
30	12	321	CLA	CHC-C1C	4.36	1.47	1.38
37	16	314	A86	C7-C6	4.36	1.59	1.50
30	5	303	CLA	O2A-CGA	4.36	1.46	1.33
37	14	320	A86	C21-C20	4.36	1.58	1.51
30	14	307	CLA	O2A-CGA	4.36	1.46	1.33
37	15	316	A86	C7-C6	4.36	1.59	1.50
39	4	313	DD6	C2-C1	4.36	1.45	1.35
30	B	826	CLA	CHC-C1C	4.36	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	307	KC1	CHC-C4B	4.36	1.46	1.38
30	A	842	CLA	CHC-C1C	4.36	1.47	1.38
38	3	308	KC1	C1D-ND	4.36	1.43	1.37
37	5	301	A86	O4-C38	4.36	1.44	1.35
38	14	311	KC1	CHB-C1B	4.36	1.46	1.38
30	B	802	CLA	O2D-CGD	4.36	1.43	1.33
37	13	313	A86	C10-C11	4.36	1.46	1.34
30	B	814	CLA	CHC-C1C	4.36	1.47	1.38
30	12	321	CLA	O2A-CGA	4.36	1.46	1.33
38	8	307	KC1	C1D-ND	4.36	1.43	1.37
30	B	818	CLA	CHC-C1C	4.35	1.47	1.38
37	16	312	A86	C21-C20	4.35	1.58	1.51
30	10	309	CLA	O2A-CGA	4.35	1.46	1.33
30	A	804	CLA	CHC-C1C	4.35	1.47	1.38
37	11	316	A86	C17-C18	-4.35	1.46	1.52
30	B	823	CLA	O2A-CGA	4.35	1.46	1.33
30	L	203	CLA	C1D-ND	4.35	1.43	1.37
37	9	313	A86	C7-C6	4.35	1.59	1.50
37	14	318	A86	C17-C18	-4.35	1.46	1.52
30	A	814	CLA	CHC-C1C	4.35	1.47	1.38
38	2	312	KC1	CHB-C1B	4.35	1.46	1.38
37	15	316	A86	O4-C38	4.35	1.44	1.35
37	14	319	A86	C21-C20	4.35	1.58	1.51
38	8	313	KC1	CHD-C4C	4.35	1.47	1.38
30	A	817	CLA	C1D-ND	4.35	1.43	1.37
37	2u	203	A86	O4-C38	4.34	1.44	1.35
37	1	309	A86	O4-C38	4.34	1.44	1.35
38	9	304	KC1	CHB-C1B	4.34	1.46	1.38
30	6	307	CLA	CHD-C1D	4.34	1.46	1.38
30	A	815	CLA	C1D-ND	4.34	1.43	1.37
30	10	305	CLA	C1D-ND	4.34	1.43	1.37
30	A	809	CLA	CHC-C1C	4.34	1.47	1.38
37	14	319	A86	C10-C11	4.34	1.46	1.34
38	13	312	KC1	C1A-CHA	4.34	1.51	1.40
38	6	311	KC1	C1D-ND	4.34	1.43	1.37
30	15	306	CLA	CHC-C1C	4.34	1.47	1.38
30	13	303	CLA	O2A-CGA	4.34	1.46	1.33
30	A	815	CLA	O2A-CGA	4.34	1.46	1.33
30	15	308	CLA	C1D-ND	4.34	1.43	1.37
30	10	308	CLA	C1D-ND	4.34	1.43	1.37
30	A	829	CLA	C1D-ND	4.34	1.43	1.37
30	1	307	CLA	CHC-C1C	4.34	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	314	A86	O4-C38	4.34	1.44	1.35
30	F	203	CLA	C1D-ND	4.34	1.43	1.37
38	6	308	KC1	C1A-CHA	4.34	1.51	1.40
30	1	303	CLA	C1D-ND	4.34	1.43	1.37
38	12	309	KC1	CHC-C4B	4.34	1.46	1.38
38	16	304	KC1	C1A-NA	-4.34	1.28	1.38
30	4	309	CLA	CHD-C1D	4.33	1.46	1.38
30	A	830	CLA	C1B-NB	-4.33	1.32	1.37
37	11	301	A86	C21-C20	4.33	1.58	1.51
30	15	303	CLA	O2A-CGA	4.33	1.46	1.33
37	10	301	A86	C17-C18	-4.33	1.46	1.52
30	2	308	CLA	O2A-CGA	4.33	1.46	1.33
38	13	308	KC1	CHB-C1B	4.33	1.46	1.38
37	1	309	A86	C7-C6	4.33	1.59	1.50
30	7	307	CLA	C1D-ND	4.33	1.43	1.37
30	B	803	CLA	CHC-C1C	4.33	1.47	1.38
30	9	306	CLA	CHD-C1D	4.33	1.46	1.38
30	A	820	CLA	CHC-C1C	4.33	1.47	1.38
30	12	303	CLA	C1D-ND	4.33	1.43	1.37
39	15	319	DD6	C2-C1	4.33	1.45	1.35
30	A	838	CLA	O2A-CGA	4.32	1.46	1.33
30	B	812	CLA	CHC-C1C	4.32	1.47	1.38
30	4	304	CLA	C1D-ND	4.32	1.43	1.37
38	6	312	KC1	C1D-ND	4.32	1.43	1.37
30	A	828	CLA	CHC-C1C	4.32	1.47	1.38
30	B	807	CLA	CHC-C1C	4.32	1.47	1.38
37	10	301	A86	C9-C8	4.32	1.46	1.34
38	2	312	KC1	C1D-ND	4.32	1.43	1.37
37	4	317	A86	C7-C6	4.32	1.59	1.50
30	13	303	CLA	CHD-C1D	4.32	1.46	1.38
38	8	314	KC1	C1A-CHA	4.32	1.51	1.40
37	14	318	A86	C21-C20	4.32	1.58	1.51
37	14	314	A86	C21-C20	4.32	1.58	1.51
30	8	303	CLA	CHC-C1C	4.32	1.47	1.38
37	12	314	A86	C21-C20	4.32	1.58	1.51
30	A	822	CLA	C1B-NB	-4.32	1.32	1.37
30	11	308	CLA	O2A-CGA	4.32	1.45	1.33
38	5	310	KC1	CHC-C4B	4.32	1.46	1.38
30	B	833	CLA	C1D-ND	4.32	1.43	1.37
37	14	314	A86	C10-C11	4.32	1.46	1.34
38	8	310	KC1	CHC-C4B	4.32	1.46	1.38
30	1	305	CLA	O2A-CGA	4.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	812	CLA	C1D-ND	4.31	1.43	1.37
30	14	312	CLA	CHD-C1D	4.31	1.46	1.38
38	11	312	KC1	CHB-C1B	4.31	1.46	1.38
37	15	323	A86	C21-C20	4.31	1.58	1.51
37	15	322	A86	C10-C11	4.31	1.46	1.34
38	14	306	KC1	C1D-ND	4.31	1.43	1.37
30	2	309	CLA	O2A-CGA	4.31	1.45	1.33
30	8	309	CLA	O2A-CGA	4.31	1.45	1.33
30	B	827	CLA	O2A-CGA	4.31	1.45	1.33
30	4	303	CLA	O2A-CGA	4.31	1.45	1.33
30	1	301	CLA	O2A-CGA	4.31	1.45	1.33
30	9	305	CLA	O2A-CGA	4.31	1.45	1.33
30	B	806	CLA	C1D-ND	4.31	1.43	1.37
38	3	304	KC1	C1A-CHA	4.31	1.51	1.40
30	6	304	CLA	C1D-ND	4.31	1.43	1.37
37	14	317	A86	C7-C6	4.31	1.59	1.50
38	14	311	KC1	C1A-CHA	4.30	1.51	1.40
30	A	825	CLA	CHD-C1D	4.30	1.46	1.38
30	B	816	CLA	CHC-C1C	4.30	1.47	1.38
30	16	306	CLA	O2A-CGA	4.30	1.45	1.33
30	6	310	CLA	CHD-C1D	4.30	1.46	1.38
38	8	306	KC1	CHC-C4B	4.30	1.46	1.38
30	1	304	CLA	O2A-CGA	4.30	1.45	1.33
30	14	303	CLA	CHD-C1D	4.30	1.46	1.38
30	16	307	CLA	CHD-C1D	4.30	1.46	1.38
38	6	308	KC1	C1A-NA	-4.30	1.29	1.38
37	14	315	A86	C21-C20	4.30	1.58	1.51
30	15	309	CLA	CHD-C1D	4.30	1.46	1.38
37	15	321	A86	O4-C38	4.30	1.44	1.35
38	12	311	KC1	C1A-NA	-4.30	1.29	1.38
30	B	816	CLA	C1D-ND	4.30	1.43	1.37
30	A	833	CLA	C1D-ND	4.30	1.43	1.37
30	2	304	CLA	C1D-ND	4.30	1.43	1.37
38	13	306	KC1	C1A-NA	-4.30	1.29	1.38
37	2u	205	A86	C7-C6	4.30	1.59	1.50
30	15	311	CLA	CHD-C1D	4.30	1.46	1.38
30	A	820	CLA	CHD-C1D	4.30	1.46	1.38
30	16	305	CLA	CHC-C1C	4.30	1.47	1.38
37	13	315	A86	C17-C18	-4.30	1.46	1.52
38	10	310	KC1	CHC-C4B	4.30	1.46	1.38
30	B	828	CLA	CHC-C1C	4.30	1.47	1.38
38	13	310	KC1	C1A-NA	-4.30	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5	314	DD6	C2-C1	4.30	1.45	1.35
30	B	836	CLA	CHC-C1C	4.29	1.47	1.38
30	A	834	CLA	C1D-ND	4.29	1.43	1.37
30	A	816	CLA	CHC-C1C	4.29	1.47	1.38
30	A	825	CLA	CHC-C1C	4.29	1.47	1.38
37	14	320	A86	C10-C11	4.29	1.46	1.34
30	A	813	CLA	O2A-CGA	4.29	1.45	1.33
30	7	305	CLA	O2A-CGA	4.29	1.45	1.33
30	A	804	CLA	O2A-CGA	4.29	1.45	1.33
37	15	317	A86	C21-C20	4.29	1.58	1.51
38	13	305	KC1	CHB-C1B	4.29	1.46	1.38
30	15	307	CLA	O2A-CGA	4.29	1.45	1.33
30	B	825	CLA	C1D-ND	4.29	1.43	1.37
30	2	305	CLA	O2A-CGA	4.29	1.45	1.33
30	2	303	CLA	CHD-C1D	4.29	1.46	1.38
30	7	310	CLA	CHD-C1D	4.29	1.46	1.38
30	A	822	CLA	O2A-CGA	4.29	1.45	1.33
30	B	816	CLA	O2A-CGA	4.29	1.45	1.33
30	J	101	CLA	CHC-C1C	4.29	1.47	1.38
38	8	310	KC1	C1A-CHA	4.29	1.51	1.40
37	10	317	A86	C10-C11	4.29	1.46	1.34
30	16	309	CLA	CHD-C1D	4.29	1.46	1.38
30	4	311	CLA	CHC-C1C	4.28	1.47	1.38
38	12	305	KC1	CHB-C1B	4.28	1.46	1.38
30	8	309	CLA	CHD-C1D	4.28	1.46	1.38
37	5	301	A86	C7-C6	4.28	1.59	1.50
30	A	838	CLA	CHC-C1C	4.28	1.47	1.38
30	B	805	CLA	CHC-C1C	4.28	1.47	1.38
30	7	312	CLA	CHD-C1D	4.28	1.46	1.38
38	16	311	KC1	C1A-CHA	4.28	1.51	1.40
30	A	825	CLA	O2A-CGA	4.28	1.45	1.33
30	B	814	CLA	O2A-CGA	4.28	1.45	1.33
38	11	307	KC1	C1A-CHA	4.28	1.51	1.40
30	14	305	CLA	O2A-CGA	4.28	1.45	1.33
30	7	304	CLA	CHC-C1C	4.28	1.47	1.38
37	12	316	A86	C7-C6	4.28	1.59	1.50
30	5	303	CLA	C1D-ND	4.28	1.43	1.37
37	2	318	A86	C21-C20	4.28	1.58	1.51
37	16	314	A86	C19-C18	4.28	1.58	1.52
30	2	307	CLA	O2A-CGA	4.28	1.45	1.33
37	14	316	A86	C7-C6	4.28	1.59	1.50
37	7	316	A86	C9-C8	4.28	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	311	CLA	O2A-CGA	4.28	1.45	1.33
38	3	308	KC1	C1A-NA	-4.28	1.29	1.38
37	9	315	A86	C7-C6	4.28	1.59	1.50
30	13	302	CLA	O2A-CGA	4.28	1.45	1.33
30	12	303	CLA	O2A-CGA	4.28	1.45	1.33
30	16	303	CLA	C1D-ND	4.28	1.43	1.37
30	B	834	CLA	O2A-CGA	4.28	1.45	1.33
38	3	304	KC1	CHB-C1B	4.28	1.46	1.38
30	15	313	CLA	CHD-C1D	4.27	1.46	1.38
37	2	318	A86	C7-C6	4.27	1.59	1.50
38	3	308	KC1	CHC-C4B	4.27	1.46	1.38
37	13	313	A86	C21-C20	4.27	1.58	1.51
30	6	310	CLA	CHC-C1C	4.27	1.47	1.38
37	10	316	A86	O4-C38	4.27	1.44	1.35
38	12	311	KC1	C1A-CHA	4.27	1.51	1.40
37	8	315	A86	C9-C8	4.27	1.45	1.34
30	A	844	CLA	CHD-C1D	4.27	1.46	1.38
38	7	313	KC1	C1D-ND	4.27	1.43	1.37
30	A	819	CLA	C1B-NB	-4.27	1.32	1.37
37	11	315	A86	C21-C20	4.27	1.58	1.51
30	B	832	CLA	C1D-ND	4.27	1.43	1.37
30	11	306	CLA	C1D-ND	4.27	1.43	1.37
30	11	304	CLA	O2A-CGA	4.27	1.45	1.33
30	A	812	CLA	CHC-C1C	4.27	1.47	1.38
30	3	307	CLA	O2A-CGA	4.27	1.45	1.33
30	9	306	CLA	CHC-C1C	4.27	1.47	1.38
37	14	315	A86	O4-C38	4.26	1.44	1.35
30	14	303	CLA	O2A-CGA	4.26	1.45	1.33
37	14	318	A86	C7-C6	4.26	1.59	1.50
30	14	310	CLA	O2A-CGA	4.26	1.45	1.33
37	6	320	A86	C7-C6	4.26	1.59	1.50
30	A	810	CLA	O2A-CGA	4.26	1.45	1.33
37	14	319	A86	C17-C18	-4.26	1.46	1.52
30	A	815	CLA	CHD-C1D	4.26	1.46	1.38
38	12	309	KC1	C1A-NA	-4.26	1.29	1.38
30	9	308	CLA	C1D-ND	4.26	1.43	1.37
37	15	316	A86	C21-C20	4.26	1.58	1.51
37	15	316	A86	C19-C18	4.26	1.58	1.52
38	14	308	KC1	C1A-CHA	4.26	1.51	1.40
30	3	309	CLA	CHD-C1D	4.26	1.46	1.38
30	9	302	CLA	CHC-C1C	4.26	1.47	1.38
30	8	304	CLA	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	323	A86	C10-C11	4.26	1.46	1.34
30	A	837	CLA	CHD-C1D	4.26	1.46	1.38
38	14	308	KC1	CHB-C1B	4.26	1.46	1.38
37	4	315	A86	C17-C18	-4.26	1.46	1.52
30	6	314	CLA	CHC-C1C	4.26	1.47	1.38
30	5	304	CLA	C1D-ND	4.26	1.43	1.37
37	13	313	A86	C7-C6	4.25	1.59	1.50
30	A	836	CLA	O2A-CGA	4.25	1.45	1.33
30	B	815	CLA	C1D-ND	4.25	1.43	1.37
30	3	303	CLA	CHD-C1D	4.25	1.46	1.38
30	2	310	CLA	O2A-CGA	4.25	1.45	1.33
30	15	309	CLA	O2A-CGA	4.25	1.45	1.33
30	B	821	CLA	O2A-CGA	4.25	1.45	1.33
30	12	302	CLA	C1D-ND	4.25	1.43	1.37
30	1	307	CLA	O2A-CGA	4.25	1.45	1.33
30	14	304	CLA	CHD-C1D	4.25	1.46	1.38
30	B	812	CLA	CHD-C1D	4.25	1.46	1.38
30	6	304	CLA	O2A-CGA	4.25	1.45	1.33
30	A	824	CLA	O2A-CGA	4.25	1.45	1.33
30	7	312	CLA	O2A-CGA	4.25	1.46	1.33
38	9	310	KC1	C1D-ND	4.25	1.43	1.37
30	6	305	CLA	O2A-CGA	4.25	1.45	1.33
38	16	304	KC1	CHB-C1B	4.25	1.46	1.38
38	8	310	KC1	CHB-C1B	4.25	1.46	1.38
30	4	309	CLA	O2A-CGA	4.25	1.45	1.33
37	11	315	A86	C7-C6	4.25	1.59	1.50
30	3	306	CLA	CHD-C1D	4.25	1.46	1.38
30	A	840	CLA	CHC-C1C	4.25	1.47	1.38
37	3	315	A86	C7-C6	4.25	1.59	1.50
38	13	310	KC1	CHB-C1B	4.25	1.46	1.38
30	F	202	CLA	O2A-CGA	4.25	1.45	1.33
30	9	309	CLA	O2A-CGA	4.24	1.45	1.33
30	2	308	CLA	C1D-ND	4.24	1.43	1.37
30	14	305	CLA	CHD-C1D	4.24	1.46	1.38
38	11	311	KC1	CHB-C1B	4.24	1.46	1.38
30	6	315	CLA	CHD-C1D	4.24	1.46	1.38
30	B	834	CLA	C1D-ND	4.24	1.43	1.37
37	15	321	A86	C21-C20	4.24	1.58	1.51
30	11	308	CLA	CHD-C1D	4.24	1.46	1.38
30	12	304	CLA	O2A-CGA	4.24	1.45	1.33
30	A	835	CLA	CHD-C1D	4.24	1.46	1.38
30	9	308	CLA	O2A-CGA	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	10	316	A86	C7-C6	4.24	1.59	1.50
30	10	303	CLA	O2A-CGA	4.24	1.45	1.33
30	10	304	CLA	O2A-CGA	4.24	1.45	1.33
30	7	307	CLA	O2A-CGA	4.24	1.45	1.33
30	B	831	CLA	C1D-ND	4.24	1.43	1.37
30	2	311	CLA	CHD-C1D	4.24	1.46	1.38
37	2	319	A86	C21-C20	4.24	1.58	1.51
38	5	312	KC1	C1A-CHA	4.24	1.51	1.40
30	14	302	CLA	CHD-C1D	4.24	1.46	1.38
30	7	311	CLA	C1D-ND	4.24	1.43	1.37
30	10	308	CLA	O2A-CGA	4.24	1.45	1.33
30	9	309	CLA	CHC-C1C	4.23	1.47	1.38
30	7	311	CLA	O2A-CGA	4.23	1.45	1.33
38	8	311	KC1	CHB-C1B	4.23	1.46	1.38
30	A	818	CLA	C1D-ND	4.23	1.43	1.37
30	9	302	CLA	C1D-ND	4.23	1.43	1.37
30	14	313	CLA	CHD-C1D	4.23	1.46	1.38
38	2	306	KC1	CHB-C1B	4.23	1.46	1.38
30	A	803	CLA	O2A-CGA	4.23	1.45	1.33
30	15	310	CLA	CHD-C1D	4.23	1.46	1.38
30	15	313	CLA	O2A-CGA	4.23	1.45	1.33
30	5	308	CLA	O2A-CGA	4.23	1.45	1.33
30	L	202	CLA	O2A-CGA	4.23	1.45	1.33
30	12	321	CLA	CHD-C1D	4.23	1.46	1.38
38	13	310	KC1	C1A-CHA	4.23	1.51	1.40
37	14	301	A86	C17-C18	-4.23	1.46	1.52
30	13	307	CLA	O2A-CGA	4.23	1.45	1.33
30	13	309	CLA	CHD-C1D	4.23	1.46	1.38
30	3	302	CLA	C1D-ND	4.23	1.43	1.37
37	2u	203	A86	C21-C20	4.23	1.58	1.51
37	3	314	A86	C21-C20	4.23	1.58	1.51
30	A	817	CLA	O2A-CGA	4.23	1.45	1.33
30	15	304	CLA	CHD-C1D	4.23	1.46	1.38
38	2	314	KC1	CHB-C1B	4.23	1.46	1.38
30	A	823	CLA	C1D-ND	4.23	1.43	1.37
30	2u	202	CLA	O2A-CGA	4.22	1.45	1.33
30	9	301	CLA	CHC-C1C	4.22	1.46	1.38
30	3	303	CLA	O2A-CGA	4.22	1.45	1.33
30	11	309	CLA	O2A-CGA	4.22	1.45	1.33
37	2	302	A86	C10-C11	4.22	1.46	1.34
37	3	314	A86	C7-C6	4.22	1.59	1.50
37	1	309	A86	C21-C20	4.22	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	3	314	A86	C10-C11	4.22	1.46	1.34
37	7	319	A86	C10-C11	4.22	1.46	1.34
37	10	317	A86	C21-C20	4.22	1.58	1.51
30	2u	202	CLA	C1D-ND	4.22	1.43	1.37
38	8	311	KC1	C1A-CHA	4.22	1.51	1.40
30	5	309	CLA	O2A-CGA	4.22	1.45	1.33
38	13	305	KC1	C1A-NA	-4.22	1.29	1.38
37	12	316	A86	C10-C11	4.22	1.46	1.34
30	12	302	CLA	CHC-C1C	4.22	1.46	1.38
38	4	307	KC1	CHB-C1B	4.22	1.46	1.38
30	10	308	CLA	CHD-C1D	4.22	1.46	1.38
38	3	311	KC1	CHB-C1B	4.22	1.46	1.38
30	4	304	CLA	O2A-CGA	4.22	1.45	1.33
30	1	304	CLA	C1D-ND	4.22	1.43	1.37
30	15	306	CLA	CHD-C1D	4.22	1.46	1.38
30	6	314	CLA	O2A-CGA	4.21	1.45	1.33
37	10	301	A86	C7-C6	4.21	1.59	1.50
38	4	308	KC1	C1B-NB	-4.21	1.32	1.37
30	A	835	CLA	CHC-C1C	4.21	1.46	1.38
30	12	306	CLA	CHC-C1C	4.21	1.46	1.38
37	10	315	A86	C21-C20	4.21	1.58	1.51
38	5	305	KC1	C1A-CHA	4.21	1.51	1.40
29	A	801	CL0	OBD-CAD	4.21	1.27	1.22
37	7	316	A86	C7-C6	4.21	1.59	1.50
38	7	308	KC1	C1A-CHA	4.21	1.51	1.40
30	8	302	CLA	O2A-CGA	4.21	1.45	1.33
37	15	320	A86	C21-C20	4.21	1.58	1.51
30	4	302	CLA	O2A-CGA	4.21	1.45	1.33
30	1	307	CLA	CHD-C1D	4.21	1.46	1.38
30	A	839	CLA	C1D-ND	4.21	1.43	1.37
30	5	302	CLA	C1D-ND	4.21	1.43	1.37
30	A	843	CLA	CHC-C1C	4.21	1.46	1.38
30	4	305	CLA	O2A-CGA	4.21	1.45	1.33
30	B	809	CLA	O2A-CGA	4.21	1.45	1.33
30	A	802	CLA	CHD-C1D	4.21	1.46	1.38
30	16	308	CLA	CHD-C1D	4.21	1.46	1.38
39	6	321	DD6	C2-C1	4.21	1.45	1.35
30	12	308	CLA	O2A-CGA	4.21	1.45	1.33
30	1	301	CLA	C1D-ND	4.20	1.43	1.37
38	5	312	KC1	C1B-NB	-4.20	1.32	1.37
38	4	307	KC1	C1A-CHA	4.20	1.51	1.40
38	8	313	KC1	CHB-C1B	4.20	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	844	CLA	O2A-CGA	4.20	1.45	1.33
38	10	306	KC1	C1A-CHA	4.20	1.51	1.40
38	10	306	KC1	C1A-NA	-4.20	1.29	1.38
30	9	307	CLA	O2A-CGA	4.20	1.45	1.33
30	B	821	CLA	C1B-NB	-4.20	1.32	1.37
30	11	309	CLA	C1D-ND	4.20	1.43	1.37
38	1	308	KC1	C1D-ND	4.20	1.43	1.37
37	2	302	A86	C19-C18	4.20	1.58	1.52
30	4	306	CLA	C1D-ND	4.20	1.43	1.37
30	6	310	CLA	O2A-CGA	4.20	1.45	1.33
30	A	815	CLA	CHC-C1C	4.20	1.46	1.38
38	5	305	KC1	C1A-NA	-4.20	1.29	1.38
30	11	310	CLA	O2A-CGA	4.20	1.45	1.33
30	14	302	CLA	O2A-CGA	4.20	1.45	1.33
38	8	306	KC1	CHB-C1B	4.20	1.46	1.38
30	B	832	CLA	O2A-CGA	4.20	1.45	1.33
30	5	302	CLA	O2A-CGA	4.20	1.45	1.33
30	A	841	CLA	CHD-C1D	4.20	1.46	1.38
30	3	310	CLA	CHC-C1C	4.19	1.46	1.38
37	10	315	A86	C7-C6	4.19	1.59	1.50
30	6	317	CLA	O2A-CGA	4.19	1.45	1.33
37	7	316	A86	C21-C20	4.19	1.58	1.51
30	4	303	CLA	C1D-ND	4.19	1.43	1.37
30	12	312	CLA	O2A-CGA	4.19	1.45	1.33
30	15	303	CLA	CHD-C1D	4.19	1.46	1.38
38	16	311	KC1	C1A-NA	-4.19	1.29	1.38
30	8	308	CLA	O2A-CGA	4.19	1.45	1.33
30	14	310	CLA	CHD-C1D	4.19	1.46	1.38
38	6	313	KC1	C1A-CHA	4.19	1.51	1.40
37	5	315	A86	C7-C6	4.19	1.59	1.50
37	11	316	A86	C21-C20	4.19	1.58	1.51
30	2	313	CLA	CHD-C1D	4.19	1.46	1.38
38	14	306	KC1	CHB-C1B	4.19	1.46	1.38
30	13	301	CLA	O2A-CGA	4.19	1.45	1.33
30	B	836	CLA	O2A-CGA	4.19	1.45	1.33
38	13	312	KC1	C1A-NA	-4.18	1.29	1.38
37	13	315	A86	C21-C20	4.18	1.58	1.51
38	10	312	KC1	CHB-C1B	4.18	1.46	1.38
30	A	811	CLA	C1D-ND	4.18	1.43	1.37
30	5	307	CLA	CHC-C1C	4.18	1.46	1.38
30	15	312	CLA	CHD-C4C	4.18	1.48	1.39
38	3	311	KC1	C1A-CHA	4.18	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	817	CLA	C1D-ND	4.18	1.43	1.37
38	11	311	KC1	C1A-CHA	4.18	1.51	1.40
30	A	820	CLA	O2A-CGA	4.18	1.45	1.33
38	14	308	KC1	C1A-NA	-4.18	1.29	1.38
30	A	805	CLA	C1B-NB	-4.18	1.32	1.37
38	2	306	KC1	C1A-CHA	4.18	1.51	1.40
30	A	831	CLA	CHC-C1C	4.18	1.46	1.38
30	3	305	CLA	O2A-CGA	4.18	1.45	1.33
30	12	302	CLA	O2A-CGA	4.17	1.45	1.33
30	16	301	CLA	O2A-CGA	4.17	1.45	1.33
37	11	301	A86	C10-C11	4.17	1.45	1.34
38	12	305	KC1	C1A-CHA	4.17	1.51	1.40
30	2	304	CLA	O2A-CGA	4.17	1.45	1.33
37	8	315	A86	C7-C6	4.17	1.59	1.50
30	2	301	CLA	C1B-NB	-4.17	1.32	1.37
37	15	317	A86	C10-C11	4.17	1.45	1.34
30	A	840	CLA	O2A-CGA	4.17	1.45	1.33
30	B	831	CLA	O2A-CGA	4.17	1.45	1.33
30	9	302	CLA	CHD-C1D	4.17	1.46	1.38
30	12	304	CLA	CHD-C1D	4.17	1.46	1.38
30	15	305	CLA	CHD-C1D	4.17	1.46	1.38
30	B	815	CLA	CHC-C1C	4.17	1.46	1.38
30	15	307	CLA	CHC-C1C	4.17	1.46	1.38
30	12	310	CLA	O2A-CGA	4.17	1.45	1.33
30	B	801	CLA	CHC-C1C	4.17	1.46	1.38
30	A	820	CLA	C1D-ND	4.17	1.43	1.37
37	14	316	A86	C21-C20	4.17	1.58	1.51
37	16	314	A86	C17-C18	-4.17	1.46	1.52
38	13	311	KC1	C1A-NA	-4.17	1.29	1.38
30	9	303	CLA	C1D-ND	4.17	1.43	1.37
38	1	308	KC1	CHB-C1B	4.16	1.46	1.38
38	2	312	KC1	C1A-CHA	4.16	1.51	1.40
38	16	304	KC1	C1A-CHA	4.16	1.51	1.40
30	7	311	CLA	CHD-C1D	4.16	1.46	1.38
30	B	832	CLA	CHD-C1D	4.16	1.46	1.38
30	A	807	CLA	C1D-ND	4.16	1.43	1.37
37	7	315	A86	O4-C38	4.16	1.44	1.35
30	6	317	CLA	CHD-C1D	4.16	1.46	1.38
30	B	824	CLA	CHD-C1D	4.16	1.46	1.38
37	13	313	A86	C17-C18	-4.16	1.46	1.52
30	A	816	CLA	C1D-ND	4.16	1.43	1.37
30	16	307	CLA	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	303	CLA	O2A-CGA	4.16	1.45	1.33
30	15	302	CLA	CHD-C1D	4.16	1.46	1.38
37	9	316	A86	C10-C11	4.15	1.45	1.34
30	7	310	CLA	O2A-CGA	4.15	1.45	1.33
37	1	309	A86	C10-C11	4.15	1.45	1.34
30	10	307	CLA	O2A-CGA	4.15	1.45	1.33
30	A	842	CLA	O2A-CGA	4.15	1.45	1.33
30	A	805	CLA	O2A-CGA	4.15	1.45	1.33
30	4	305	CLA	C1D-ND	4.15	1.43	1.37
30	10	309	CLA	CHD-C1D	4.15	1.46	1.38
38	5	312	KC1	CHB-C1B	4.15	1.46	1.38
30	A	823	CLA	O2A-CGA	4.15	1.45	1.33
37	9	315	A86	C10-C11	4.15	1.45	1.34
30	6	316	CLA	CHD-C1D	4.15	1.46	1.38
38	8	307	KC1	CHB-C1B	4.15	1.46	1.38
37	4	312	A86	C21-C20	4.15	1.58	1.51
30	3	310	CLA	CHD-C1D	4.15	1.46	1.38
38	6	311	KC1	CHB-C1B	4.15	1.46	1.38
30	B	830	CLA	O2D-CGD	4.15	1.43	1.33
30	B	821	CLA	CHD-C1D	4.15	1.46	1.38
37	15	316	A86	C10-C11	4.14	1.45	1.34
38	3	304	KC1	C1A-NA	-4.14	1.29	1.38
30	A	821	CLA	O2A-CGA	4.14	1.45	1.33
30	6	316	CLA	C1D-ND	4.14	1.43	1.37
30	F	202	CLA	C1D-ND	4.14	1.43	1.37
37	5	315	A86	C21-C20	4.14	1.58	1.51
30	B	828	CLA	O2A-CGA	4.14	1.45	1.33
30	B	823	CLA	C1D-ND	4.14	1.43	1.37
37	8	318	A86	C21-C20	4.14	1.58	1.51
37	2u	205	A86	C9-C10	4.14	1.56	1.43
30	3	302	CLA	O2A-CGA	4.14	1.45	1.33
38	5	310	KC1	CHB-C1B	4.14	1.46	1.38
30	A	811	CLA	O2A-CGA	4.14	1.45	1.33
30	A	815	CLA	C1B-NB	-4.14	1.32	1.37
38	3	308	KC1	C1A-CHA	4.14	1.51	1.40
30	B	838	CLA	O2A-CGA	4.14	1.45	1.33
30	10	305	CLA	CHD-C1D	4.14	1.46	1.38
30	6	307	CLA	O2A-CGA	4.14	1.45	1.33
37	2	319	A86	C7-C6	4.14	1.59	1.50
30	10	303	CLA	CHD-C1D	4.14	1.46	1.38
37	9	315	A86	C21-C20	4.14	1.58	1.51
30	A	810	CLA	C1D-ND	4.14	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	321	A86	C17-C18	-4.13	1.46	1.52
30	3	306	CLA	CHD-C4C	4.13	1.48	1.39
30	6	309	CLA	CHD-C1D	4.13	1.46	1.38
30	A	838	CLA	C1D-ND	4.13	1.43	1.37
37	14	314	A86	C19-C18	4.13	1.58	1.52
38	7	313	KC1	C1A-CHA	4.13	1.50	1.40
38	9	312	KC1	C1A-CHA	4.13	1.50	1.40
30	5	309	CLA	CHD-C1D	4.13	1.46	1.38
30	11	309	CLA	CHD-C1D	4.13	1.46	1.38
30	12	306	CLA	C1D-ND	4.13	1.43	1.37
30	B	827	CLA	C1B-NB	-4.13	1.32	1.37
38	6	311	KC1	CHC-C4B	4.13	1.46	1.38
38	11	312	KC1	CHC-C4B	4.13	1.46	1.38
30	1	303	CLA	O2A-CGA	4.13	1.45	1.33
30	7	305	CLA	CHD-C1D	4.13	1.46	1.38
30	A	826	CLA	CHC-C1C	4.13	1.46	1.38
30	4	301	CLA	O2A-CGA	4.12	1.45	1.33
37	9	316	A86	C9-C10	4.12	1.56	1.43
30	A	818	CLA	O2A-CGA	4.12	1.45	1.33
30	B	818	CLA	C1B-NB	-4.12	1.32	1.37
30	B	835	CLA	C1D-ND	4.12	1.43	1.37
30	16	305	CLA	O2A-CGA	4.12	1.45	1.33
30	J	101	CLA	CHD-C1D	4.12	1.46	1.38
30	15	307	CLA	CHD-C1D	4.12	1.46	1.38
30	9	301	CLA	O2A-CGA	4.12	1.45	1.33
30	7	309	CLA	O2A-CGA	4.12	1.45	1.33
30	2	307	CLA	CHD-C1D	4.12	1.46	1.38
30	8	305	CLA	C1B-NB	-4.12	1.32	1.37
30	9	303	CLA	O2A-CGA	4.12	1.45	1.33
37	1	309	A86	C17-C18	-4.12	1.46	1.52
37	9	313	A86	C21-C20	4.12	1.58	1.51
38	6	308	KC1	C1D-ND	4.12	1.43	1.37
30	B	839	CLA	O2A-CGA	4.12	1.45	1.33
30	A	839	CLA	O2A-CGA	4.12	1.45	1.33
30	5	311	CLA	CHD-C1D	4.12	1.46	1.38
30	3	301	CLA	C1D-ND	4.12	1.43	1.37
37	7	319	A86	C19-C18	4.12	1.58	1.52
30	10	311	CLA	CHD-C1D	4.12	1.46	1.38
38	8	312	KC1	C1A-NA	-4.12	1.29	1.38
37	7	319	A86	C7-C6	4.12	1.59	1.50
38	8	306	KC1	C1A-CHA	4.12	1.50	1.40
29	A	801	CL0	CHC-C4B	4.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	314	A86	C21-C20	4.11	1.57	1.51
38	4	310	KC1	C1A-CHA	4.11	1.50	1.40
37	11	314	A86	C17-C18	-4.11	1.46	1.52
30	4	304	CLA	CHD-C1D	4.11	1.46	1.38
37	5	316	A86	C10-C11	4.11	1.45	1.34
30	B	818	CLA	C1D-ND	4.11	1.43	1.37
37	14	314	A86	C9-C10	4.11	1.55	1.43
30	A	814	CLA	CHD-C1D	4.11	1.46	1.38
30	A	832	CLA	O2A-CGA	4.11	1.45	1.33
37	8	318	A86	O4-C38	4.11	1.44	1.35
38	13	308	KC1	C1A-CHA	4.11	1.50	1.40
30	A	819	CLA	O2A-CGA	4.11	1.45	1.33
30	B	817	CLA	O2A-CGA	4.11	1.45	1.33
38	1	308	KC1	C1A-CHA	4.11	1.50	1.40
37	10	317	A86	C19-C18	4.11	1.58	1.52
30	10	307	CLA	C1D-ND	4.11	1.43	1.37
30	3	306	CLA	O2A-CGA	4.11	1.45	1.33
30	4	306	CLA	O2A-CGA	4.11	1.45	1.33
30	8	305	CLA	O2A-CGA	4.11	1.45	1.33
30	B	828	CLA	CHD-C1D	4.11	1.46	1.38
30	B	819	CLA	O2A-CGA	4.10	1.45	1.33
38	1	306	KC1	C1A-CHA	4.10	1.50	1.40
30	A	836	CLA	CHD-C1D	4.10	1.46	1.38
30	B	829	CLA	O2A-CGA	4.10	1.45	1.33
38	13	306	KC1	C1A-CHA	4.10	1.50	1.40
30	A	806	CLA	O2A-CGA	4.10	1.45	1.33
30	12	306	CLA	O2A-CGA	4.10	1.45	1.33
37	4	314	A86	C9-C10	4.10	1.55	1.43
30	A	833	CLA	O2A-CGA	4.10	1.45	1.33
30	A	817	CLA	CHD-C1D	4.10	1.46	1.38
37	10	302	A86	C21-C20	4.10	1.57	1.51
30	9	301	CLA	C1D-ND	4.10	1.43	1.37
30	A	813	CLA	C1D-ND	4.10	1.43	1.37
30	14	309	CLA	CHD-C4C	4.10	1.48	1.39
30	B	837	CLA	C1D-ND	4.09	1.43	1.37
37	4	315	A86	C21-C20	4.09	1.57	1.51
30	B	825	CLA	O2A-CGA	4.09	1.45	1.33
30	A	816	CLA	O2A-CGA	4.09	1.45	1.33
30	4	305	CLA	CHD-C1D	4.09	1.46	1.38
30	B	838	CLA	C1D-ND	4.09	1.43	1.37
30	12	307	CLA	C1B-NB	-4.09	1.32	1.37
30	12	312	CLA	CHD-C1D	4.09	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	311	KC1	C1A-NA	-4.09	1.29	1.38
38	6	308	KC1	CHB-C1B	4.09	1.46	1.38
30	A	838	CLA	C1B-NB	-4.09	1.32	1.37
37	14	319	A86	C9-C10	4.09	1.55	1.43
30	9	305	CLA	CHD-C1D	4.09	1.46	1.38
38	12	311	KC1	CHB-C1B	4.09	1.46	1.38
30	B	806	CLA	O2A-CGA	4.09	1.45	1.33
30	15	302	CLA	CHD-C4C	4.09	1.48	1.39
37	12	314	A86	C10-C11	4.09	1.45	1.34
37	8	318	A86	C7-C6	4.09	1.59	1.50
30	5	308	CLA	CHD-C1D	4.09	1.46	1.38
30	3	301	CLA	O2A-CGA	4.08	1.45	1.33
30	B	851	CLA	CHD-C1D	4.08	1.46	1.38
30	6	305	CLA	CHD-C1D	4.08	1.46	1.38
30	14	313	CLA	O2A-CGA	4.08	1.45	1.33
30	6	314	CLA	CHD-C1D	4.08	1.46	1.38
30	A	843	CLA	O2A-CGA	4.08	1.45	1.33
38	11	312	KC1	C1A-NA	-4.08	1.29	1.38
30	6	309	CLA	C1D-ND	4.08	1.43	1.37
30	B	804	CLA	O2A-CGA	4.08	1.45	1.33
30	16	310	CLA	CHD-C1D	4.08	1.46	1.38
30	5	307	CLA	O2A-CGA	4.08	1.45	1.33
30	B	808	CLA	CHC-C1C	4.08	1.46	1.38
30	A	824	CLA	C1B-NB	-4.08	1.32	1.37
37	4	312	A86	C7-C6	4.08	1.59	1.50
30	A	809	CLA	C1D-ND	4.08	1.43	1.37
30	B	823	CLA	CHD-C1D	4.08	1.46	1.38
30	2	304	CLA	CHD-C1D	4.08	1.46	1.38
30	5	304	CLA	CHD-C1D	4.08	1.46	1.38
30	13	304	CLA	CHD-C4C	4.08	1.48	1.39
30	4	311	CLA	O2A-CGA	4.08	1.45	1.33
38	8	312	KC1	C1A-CHA	4.08	1.50	1.40
30	A	808	CLA	C1D-ND	4.07	1.43	1.37
37	13	315	A86	C9-C10	4.07	1.55	1.43
38	2	314	KC1	C1A-CHA	4.07	1.50	1.40
37	14	301	A86	C10-C11	4.07	1.45	1.34
30	16	302	CLA	O2A-CGA	4.07	1.45	1.33
30	7	310	CLA	CHD-C4C	4.07	1.48	1.39
30	9	309	CLA	C1B-NB	-4.07	1.32	1.37
30	9	309	CLA	CHD-C1D	4.07	1.46	1.38
30	8	308	CLA	CHD-C1D	4.07	1.46	1.38
30	8	304	CLA	C1B-NB	-4.07	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	10	310	KC1	CHB-C1B	4.07	1.46	1.38
30	B	836	CLA	C1D-ND	4.07	1.43	1.37
30	A	826	CLA	O2A-CGA	4.07	1.45	1.33
30	11	310	CLA	CHD-C4C	4.07	1.48	1.39
30	3	306	CLA	C1D-ND	4.06	1.43	1.37
30	13	302	CLA	CHD-C1D	4.06	1.46	1.38
30	A	804	CLA	C1B-NB	-4.06	1.32	1.37
30	6	304	CLA	CHD-C1D	4.06	1.46	1.38
30	12	308	CLA	CHD-C1D	4.06	1.46	1.38
30	4	309	CLA	CHD-C4C	4.06	1.48	1.39
30	9	307	CLA	CHD-C1D	4.06	1.46	1.38
30	A	836	CLA	CHC-C1C	4.06	1.46	1.38
38	5	306	KC1	CHB-C1B	4.06	1.46	1.38
30	15	309	CLA	CHD-C4C	4.06	1.48	1.39
37	11	314	A86	C10-C11	4.06	1.45	1.34
30	8	302	CLA	C1D-ND	4.06	1.43	1.37
30	2	310	CLA	CHD-C1D	4.06	1.46	1.38
30	A	843	CLA	CHD-C1D	4.06	1.46	1.38
30	5	308	CLA	C1D-ND	4.06	1.43	1.37
37	10	315	A86	C10-C11	4.06	1.45	1.34
30	13	303	CLA	CHD-C4C	4.06	1.48	1.39
30	B	833	CLA	O2A-CGA	4.05	1.45	1.33
30	B	829	CLA	CHD-C1D	4.05	1.46	1.38
30	B	833	CLA	C1B-NB	-4.05	1.32	1.37
30	6	307	CLA	C1B-NB	-4.05	1.32	1.37
30	B	811	CLA	O2A-CGA	4.05	1.45	1.33
30	A	822	CLA	CHD-C1D	4.05	1.46	1.38
30	6	307	CLA	C1D-ND	4.05	1.43	1.37
30	16	306	CLA	CHD-C1D	4.05	1.46	1.38
30	9	309	CLA	C1D-ND	4.05	1.43	1.37
30	16	306	CLA	C1D-ND	4.05	1.43	1.37
30	A	808	CLA	O2A-CGA	4.05	1.45	1.33
37	3	315	A86	C10-C11	4.05	1.45	1.34
30	9	308	CLA	C1B-NB	-4.05	1.32	1.37
30	A	809	CLA	O2A-CGA	4.05	1.45	1.33
37	9	315	A86	C9-C10	4.05	1.55	1.43
30	12	306	CLA	CHD-C1D	4.05	1.46	1.38
30	1	301	CLA	CHD-C1D	4.05	1.46	1.38
38	9	311	KC1	C1A-CHA	4.05	1.50	1.40
30	B	813	CLA	O2A-CGA	4.05	1.45	1.33
38	13	311	KC1	C1A-CHA	4.05	1.50	1.40
38	11	305	KC1	C1A-CHA	4.05	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	804	CLA	C1D-ND	4.05	1.43	1.37
37	15	315	A86	C9-C10	4.05	1.55	1.43
30	15	310	CLA	CHD-C4C	4.05	1.48	1.39
30	A	838	CLA	CHD-C1D	4.04	1.46	1.38
37	7	315	A86	C7-C6	4.04	1.59	1.50
30	13	309	CLA	CHD-C4C	4.04	1.48	1.39
30	A	806	CLA	C1B-NB	-4.04	1.32	1.37
30	6	304	CLA	C1B-NB	-4.04	1.32	1.37
30	2	309	CLA	CHD-C1D	4.04	1.46	1.38
37	2u	203	A86	C9-C10	4.04	1.55	1.43
30	F	201	CLA	O2A-CGA	4.04	1.45	1.33
30	2	305	CLA	C1D-ND	4.04	1.43	1.37
30	10	304	CLA	CHD-C1D	4.04	1.46	1.38
37	16	314	A86	C21-C20	4.04	1.57	1.51
38	14	306	KC1	C1A-CHA	4.04	1.50	1.40
30	A	814	CLA	O2A-CGA	4.04	1.45	1.33
37	15	320	A86	C9-C10	4.04	1.55	1.43
30	B	851	CLA	O2A-CGA	4.03	1.45	1.33
30	F	203	CLA	CHD-C1D	4.03	1.46	1.38
38	8	311	KC1	C1D-ND	4.03	1.43	1.37
30	A	831	CLA	O2A-CGA	4.03	1.45	1.33
38	9	310	KC1	CHB-C1B	4.03	1.46	1.38
37	5	315	A86	C10-C11	4.03	1.45	1.34
30	14	313	CLA	CHD-C4C	4.03	1.48	1.39
37	14	318	A86	C10-C11	4.03	1.45	1.34
30	7	312	CLA	CHD-C4C	4.03	1.48	1.39
30	4	311	CLA	C1B-NB	-4.03	1.32	1.37
30	12	303	CLA	CHD-C1D	4.03	1.46	1.38
30	A	827	CLA	C1D-ND	4.03	1.43	1.37
30	B	813	CLA	C1D-ND	4.03	1.43	1.37
30	A	810	CLA	CHD-C1D	4.03	1.46	1.38
30	B	806	CLA	C1B-NB	-4.02	1.32	1.37
30	3	307	CLA	CHD-C4C	4.02	1.48	1.39
30	14	302	CLA	CHD-C4C	4.02	1.48	1.39
30	4	311	CLA	CHD-C1D	4.02	1.46	1.38
30	16	308	CLA	CHD-C4C	4.02	1.48	1.39
30	B	820	CLA	CHC-C4B	4.02	1.48	1.39
30	A	814	CLA	C1B-NB	-4.02	1.32	1.37
37	11	315	A86	C10-C11	4.02	1.45	1.34
30	7	304	CLA	C1D-ND	4.02	1.43	1.37
37	5	301	A86	C10-C11	4.02	1.45	1.34
30	A	827	CLA	C1B-NB	-4.02	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	802	CLA	C1B-NB	-4.02	1.32	1.37
30	8	303	CLA	CHD-C1D	4.02	1.46	1.38
38	6	312	KC1	C1A-CHA	4.02	1.50	1.40
38	4	308	KC1	CHC-C4B	4.02	1.46	1.38
30	A	812	CLA	C1B-NB	-4.02	1.32	1.37
30	A	829	CLA	O2A-CGA	4.02	1.45	1.33
30	A	828	CLA	C1D-ND	4.02	1.43	1.37
30	6	306	CLA	CHD-C1D	4.02	1.46	1.38
30	15	308	CLA	CHD-C4C	4.02	1.48	1.39
30	B	815	CLA	CHD-C1D	4.02	1.46	1.38
30	B	810	CLA	O2A-CGA	4.02	1.45	1.33
38	7	313	KC1	CHB-C1B	4.02	1.46	1.38
30	11	308	CLA	CHD-C4C	4.02	1.48	1.39
30	B	825	CLA	C1B-NB	-4.02	1.32	1.37
30	15	304	CLA	CHD-C4C	4.02	1.48	1.39
30	B	818	CLA	CHD-C1D	4.02	1.46	1.38
30	16	305	CLA	CHD-C1D	4.01	1.46	1.38
30	14	304	CLA	CHD-C4C	4.01	1.48	1.39
30	12	307	CLA	O2A-CGA	4.01	1.45	1.33
30	8	301	CLA	C4B-NB	-4.01	1.32	1.37
30	B	824	CLA	C1D-ND	4.01	1.43	1.37
37	14	320	A86	C17-C18	-4.01	1.46	1.52
30	10	308	CLA	CHD-C4C	4.01	1.48	1.39
30	12	307	CLA	C1D-ND	4.01	1.43	1.37
37	11	301	A86	C9-C10	4.01	1.55	1.43
30	A	834	CLA	O2A-CGA	4.01	1.45	1.33
30	3	310	CLA	CHD-C4C	4.01	1.48	1.39
30	B	809	CLA	CHC-C1C	4.01	1.46	1.38
30	7	306	CLA	CHC-C1C	4.01	1.46	1.38
30	A	832	CLA	CHD-C1D	4.01	1.46	1.38
37	13	313	A86	C9-C10	4.01	1.55	1.43
30	A	841	CLA	C1D-ND	4.01	1.43	1.37
30	2	303	CLA	CHD-C4C	4.01	1.48	1.39
37	3	314	A86	C17-C18	-4.01	1.46	1.52
37	7	315	A86	C21-C20	4.01	1.57	1.51
30	9	306	CLA	CHD-C4C	4.01	1.48	1.39
30	1	302	CLA	CHD-C1D	4.00	1.46	1.38
30	3	303	CLA	CHD-C4C	4.00	1.48	1.39
30	B	838	CLA	C1B-NB	-4.00	1.32	1.37
38	1	308	KC1	C1B-NB	-4.00	1.32	1.37
38	10	310	KC1	C1A-CHA	4.00	1.50	1.40
30	B	805	CLA	C1B-NB	-4.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	844	CLA	CHD-C4C	4.00	1.48	1.39
38	8	313	KC1	C1A-CHA	4.00	1.50	1.40
30	7	306	CLA	CHD-C1D	4.00	1.46	1.38
30	8	303	CLA	C1B-NB	-4.00	1.32	1.37
37	7	319	A86	C9-C10	4.00	1.55	1.43
30	7	303	CLA	C1B-NB	-4.00	1.32	1.37
30	B	814	CLA	C1B-NB	-4.00	1.32	1.37
38	5	310	KC1	C1A-CHA	4.00	1.50	1.40
30	14	312	CLA	CHD-C4C	4.00	1.48	1.39
30	14	303	CLA	CHD-C4C	4.00	1.48	1.39
30	7	309	CLA	CHC-C1C	4.00	1.46	1.38
37	4	314	A86	C10-C11	4.00	1.45	1.34
30	8	301	CLA	O2A-CGA	4.00	1.45	1.33
37	15	321	A86	C10-C11	4.00	1.45	1.34
37	5	316	A86	C9-C10	4.00	1.55	1.43
37	10	317	A86	C9-C10	4.00	1.55	1.43
30	A	832	CLA	C1D-ND	4.00	1.43	1.37
30	A	826	CLA	C1B-NB	-4.00	1.32	1.37
30	2	305	CLA	C1B-NB	-4.00	1.32	1.37
30	7	304	CLA	C1B-NB	-4.00	1.32	1.37
38	9	310	KC1	C1A-CHA	4.00	1.50	1.40
30	B	834	CLA	C4B-NB	-3.99	1.32	1.37
30	4	303	CLA	CHD-C1D	3.99	1.46	1.38
30	1	305	CLA	CHD-C4C	3.99	1.48	1.39
30	14	307	CLA	CHD-C1D	3.99	1.46	1.38
30	B	838	CLA	CHD-C1D	3.99	1.46	1.38
37	2u	205	A86	C21-C20	3.99	1.57	1.51
30	B	822	CLA	O2A-CGA	3.99	1.45	1.33
30	B	813	CLA	CHD-C1D	3.99	1.46	1.38
38	12	309	KC1	CHB-C1B	3.99	1.46	1.38
37	9	316	A86	C19-C18	3.99	1.58	1.52
30	14	310	CLA	CHD-C4C	3.99	1.48	1.39
38	9	304	KC1	C1A-CHA	3.99	1.50	1.40
30	16	302	CLA	CHD-C1D	3.99	1.46	1.38
30	B	805	CLA	C1D-ND	3.99	1.43	1.37
30	11	309	CLA	CHD-C4C	3.99	1.48	1.39
30	B	836	CLA	C1B-NB	-3.99	1.32	1.37
30	8	305	CLA	C1D-ND	3.99	1.43	1.37
30	A	812	CLA	O2A-CGA	3.99	1.45	1.33
30	B	821	CLA	C1D-ND	3.99	1.43	1.37
30	B	807	CLA	O2A-CGA	3.99	1.45	1.33
30	A	840	CLA	CHD-C1D	3.99	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	308	CLA	C1B-NB	-3.98	1.32	1.37
30	A	807	CLA	O2A-CGA	3.98	1.45	1.33
30	B	802	CLA	O2A-CGA	3.98	1.45	1.33
30	15	308	CLA	CHD-C1D	3.98	1.46	1.38
30	B	826	CLA	O2A-CGA	3.98	1.45	1.33
37	5	316	A86	C7-C6	3.98	1.58	1.50
30	7	309	CLA	CHD-C1D	3.98	1.46	1.38
38	8	307	KC1	C1A-CHA	3.98	1.50	1.40
30	B	805	CLA	CHD-C1D	3.98	1.46	1.38
30	9	308	CLA	CHD-C1D	3.98	1.46	1.38
30	2	313	CLA	CHD-C4C	3.98	1.48	1.39
37	5	315	A86	C17-C18	-3.98	1.46	1.52
37	7	316	A86	O4-C38	3.98	1.44	1.35
30	12	310	CLA	CHD-C1D	3.98	1.46	1.38
37	10	301	A86	C21-C20	3.98	1.57	1.51
37	2	319	A86	C10-C11	3.98	1.45	1.34
37	14	317	A86	C21-C20	3.98	1.57	1.51
30	7	306	CLA	C1D-ND	3.98	1.43	1.37
37	12	316	A86	C9-C10	3.97	1.55	1.43
30	6	309	CLA	C1B-NB	-3.97	1.32	1.37
30	A	828	CLA	O2A-CGA	3.97	1.44	1.33
30	15	305	CLA	CHD-C4C	3.97	1.48	1.39
37	10	302	A86	C10-C11	3.97	1.45	1.34
30	A	839	CLA	CHD-C1D	3.97	1.46	1.38
30	B	837	CLA	O2A-CGA	3.97	1.44	1.33
38	5	312	KC1	C1D-ND	3.97	1.43	1.37
38	14	306	KC1	CHC-C1C	3.97	1.48	1.39
30	7	306	CLA	O2A-CGA	3.97	1.44	1.33
37	10	315	A86	C19-C18	3.97	1.57	1.52
37	15	320	A86	C19-C18	3.97	1.57	1.52
30	A	819	CLA	C1D-ND	3.97	1.43	1.37
30	15	311	CLA	CHD-C4C	3.97	1.48	1.39
37	15	322	A86	C9-C10	3.97	1.55	1.43
30	A	832	CLA	C1B-NB	-3.97	1.32	1.37
30	A	834	CLA	CHD-C1D	3.97	1.46	1.38
30	B	811	CLA	CHD-C1D	3.97	1.46	1.38
37	15	323	A86	C9-C10	3.97	1.55	1.43
30	16	309	CLA	CHD-C4C	3.97	1.48	1.39
37	15	315	A86	C21-C20	3.97	1.57	1.51
30	B	808	CLA	C1B-NB	-3.97	1.32	1.37
30	11	306	CLA	CHD-C1D	3.97	1.46	1.38
30	7	311	CLA	C1B-NB	-3.96	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	301	CLA	C1B-NB	-3.96	1.32	1.37
30	7	306	CLA	C1B-NB	-3.96	1.32	1.37
30	A	813	CLA	C1B-NB	-3.96	1.32	1.37
30	2	309	CLA	CHD-C4C	3.96	1.48	1.39
30	11	304	CLA	CHD-C4C	3.96	1.48	1.39
30	12	321	CLA	CHD-C4C	3.96	1.48	1.39
30	4	306	CLA	CHD-C1D	3.96	1.46	1.38
30	B	820	CLA	C1D-ND	3.96	1.43	1.37
30	6	305	CLA	C1B-NB	-3.96	1.32	1.37
37	8	315	A86	C21-C20	3.96	1.57	1.51
30	12	302	CLA	CHD-C1D	3.96	1.46	1.38
38	4	308	KC1	CHB-C1B	3.96	1.46	1.38
30	8	301	CLA	C1D-ND	3.96	1.43	1.37
30	B	807	CLA	C1D-ND	3.96	1.43	1.37
38	10	312	KC1	C1A-CHA	3.96	1.50	1.40
30	B	838	CLA	CHC-C1C	3.96	1.46	1.38
30	A	805	CLA	C1D-ND	3.96	1.43	1.37
30	6	307	CLA	CHD-C4C	3.96	1.48	1.39
30	A	842	CLA	C1D-ND	3.95	1.43	1.37
30	15	303	CLA	CHD-C4C	3.95	1.48	1.39
38	8	314	KC1	C1A-NA	-3.95	1.29	1.38
30	A	816	CLA	CHD-C1D	3.95	1.46	1.38
38	4	310	KC1	CHB-C1B	3.95	1.46	1.38
30	14	307	CLA	CHD-C4C	3.95	1.48	1.39
30	B	834	CLA	C1B-NB	-3.95	1.32	1.37
37	11	314	A86	C9-C10	3.95	1.55	1.43
30	A	843	CLA	C1D-ND	3.95	1.43	1.37
30	A	821	CLA	C1B-NB	-3.95	1.32	1.37
37	11	315	A86	C17-C18	-3.95	1.46	1.52
30	B	805	CLA	O2A-CGA	3.95	1.44	1.33
30	B	822	CLA	C1B-NB	-3.95	1.32	1.37
30	13	307	CLA	CHD-C4C	3.95	1.48	1.39
30	A	833	CLA	CHD-C1D	3.95	1.46	1.38
30	B	810	CLA	C1D-ND	3.95	1.43	1.37
30	15	313	CLA	CHD-C4C	3.95	1.48	1.39
37	14	316	A86	C10-C11	3.95	1.45	1.34
30	B	802	CLA	C3D-C2D	3.94	1.49	1.39
30	11	304	CLA	CHD-C1D	3.94	1.46	1.38
30	2	305	CLA	CHD-C1D	3.94	1.46	1.38
30	3	305	CLA	CHD-C1D	3.94	1.46	1.38
30	14	305	CLA	CHD-C4C	3.94	1.48	1.39
37	5	301	A86	C21-C20	3.94	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	306	KC1	C1A-CHA	3.94	1.50	1.40
30	B	824	CLA	CHD-C4C	3.94	1.48	1.39
37	14	320	A86	C9-C10	3.94	1.55	1.43
30	A	821	CLA	CHC-C1C	3.94	1.46	1.38
30	6	310	CLA	CHD-C4C	3.94	1.48	1.39
30	A	826	CLA	C1D-ND	3.94	1.43	1.37
30	11	306	CLA	CHD-C4C	3.94	1.48	1.39
29	A	801	CL0	CHD-C4C	3.93	1.46	1.39
37	11	316	A86	C10-C11	3.93	1.45	1.34
30	4	303	CLA	C1B-NB	-3.93	1.32	1.37
37	10	302	A86	C9-C10	3.93	1.55	1.43
30	7	304	CLA	CHD-C1D	3.93	1.46	1.38
37	10	316	A86	C21-C20	3.93	1.57	1.51
37	14	315	A86	C10-C11	3.93	1.45	1.34
38	8	313	KC1	C1D-ND	3.93	1.43	1.37
30	1	302	CLA	O2A-CGA	3.93	1.44	1.33
30	7	304	CLA	O2A-CGA	3.93	1.44	1.33
37	10	315	A86	C9-C10	3.93	1.55	1.43
30	B	839	CLA	C1B-NB	-3.93	1.32	1.37
29	A	801	CL0	O2A-CGA	3.93	1.44	1.33
30	16	307	CLA	CHD-C4C	3.93	1.48	1.39
38	4	308	KC1	C1A-NA	-3.93	1.29	1.38
30	2	308	CLA	CHD-C1D	3.93	1.46	1.38
37	12	316	A86	C21-C20	3.93	1.57	1.51
30	A	829	CLA	C1B-NB	-3.93	1.32	1.37
30	B	835	CLA	CHD-C4C	3.93	1.48	1.39
38	8	314	KC1	CHB-C1B	3.93	1.46	1.38
37	12	314	A86	C7-C6	3.93	1.58	1.50
30	A	811	CLA	C1B-NB	-3.93	1.32	1.37
30	B	839	CLA	C1D-ND	3.93	1.43	1.37
30	2	301	CLA	CHC-C1C	3.93	1.46	1.38
30	8	309	CLA	CHD-C4C	3.92	1.48	1.39
30	B	808	CLA	CHD-C1D	3.92	1.46	1.38
30	2u	202	CLA	CHD-C1D	3.92	1.46	1.38
37	3	315	A86	C21-C20	3.92	1.57	1.51
30	5	303	CLA	CHD-C1D	3.92	1.46	1.38
30	6	316	CLA	CHD-C4C	3.92	1.48	1.39
30	4	301	CLA	C1D-ND	3.92	1.43	1.37
30	A	803	CLA	C4B-NB	-3.92	1.32	1.37
37	9	316	A86	C21-C20	3.92	1.57	1.51
30	3	302	CLA	CHD-C1D	3.92	1.46	1.38
30	A	806	CLA	C1D-ND	3.92	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	303	CLA	C1B-NB	-3.92	1.32	1.37
30	A	837	CLA	CHD-C4C	3.92	1.48	1.39
30	15	314	CLA	CHD-C1D	3.92	1.46	1.38
30	A	842	CLA	C1B-NB	-3.92	1.32	1.37
30	B	818	CLA	O2A-CGA	3.92	1.44	1.33
30	A	811	CLA	CHD-C1D	3.92	1.46	1.38
30	10	309	CLA	CHD-C4C	3.92	1.48	1.39
30	1	303	CLA	CHD-C1D	3.92	1.46	1.38
30	15	314	CLA	CHD-C4C	3.91	1.48	1.39
37	15	317	A86	C9-C10	3.91	1.55	1.43
37	15	322	A86	C21-C20	3.91	1.57	1.51
30	10	303	CLA	CHD-C4C	3.91	1.48	1.39
37	2	318	A86	C10-C11	3.91	1.45	1.34
30	A	836	CLA	C1B-NB	-3.91	1.32	1.37
30	A	815	CLA	CHD-C4C	3.91	1.48	1.39
30	3	306	CLA	C3D-C2D	3.91	1.49	1.39
30	F	201	CLA	C1B-NB	-3.91	1.32	1.37
30	5	302	CLA	C1B-NB	-3.91	1.32	1.37
37	12	314	A86	C9-C10	3.91	1.55	1.43
30	12	312	CLA	CHD-C4C	3.91	1.48	1.39
37	2	302	A86	C9-C10	3.91	1.55	1.43
30	3	309	CLA	CHD-C4C	3.91	1.48	1.39
30	15	306	CLA	CHD-C4C	3.91	1.48	1.39
37	16	314	A86	C10-C11	3.91	1.45	1.34
30	A	804	CLA	C1D-ND	3.91	1.43	1.37
30	A	808	CLA	C1B-NB	-3.91	1.32	1.37
30	A	810	CLA	C1B-NB	-3.91	1.32	1.37
30	A	843	CLA	C1B-NB	-3.91	1.32	1.37
30	6	309	CLA	O2A-CGA	3.91	1.44	1.33
30	A	831	CLA	CHD-C1D	3.90	1.46	1.38
30	5	302	CLA	CHD-C1D	3.90	1.46	1.38
30	1	302	CLA	CHD-C4C	3.90	1.48	1.39
38	6	311	KC1	C1A-CHA	3.90	1.50	1.40
30	6	315	CLA	CHD-C4C	3.90	1.48	1.39
30	A	807	CLA	CHD-C1D	3.90	1.46	1.38
30	A	824	CLA	C1D-ND	3.90	1.43	1.37
30	1	304	CLA	CHD-C1D	3.90	1.46	1.38
37	16	314	A86	C9-C10	3.90	1.55	1.43
30	9	303	CLA	CHD-C1D	3.90	1.46	1.38
30	A	807	CLA	C1B-NB	-3.90	1.32	1.37
30	4	306	CLA	CHD-C4C	3.90	1.48	1.39
30	B	819	CLA	CHD-C1D	3.90	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	302	A86	C21-C20	3.90	1.57	1.51
30	B	816	CLA	CHD-C1D	3.90	1.46	1.38
30	5	308	CLA	C3D-C2D	3.90	1.49	1.39
30	B	808	CLA	C1D-ND	3.89	1.43	1.37
30	B	808	CLA	O2A-CGA	3.89	1.44	1.33
30	A	839	CLA	C1B-NB	-3.89	1.32	1.37
30	2	311	CLA	CHD-C4C	3.89	1.48	1.39
37	1	309	A86	C9-C10	3.89	1.55	1.43
37	16	312	A86	C9-C10	3.89	1.55	1.43
30	B	817	CLA	C1B-NB	-3.89	1.32	1.37
30	16	306	CLA	C1B-NB	-3.89	1.32	1.37
30	B	835	CLA	O2A-CGA	3.89	1.44	1.33
30	8	302	CLA	C4B-NB	-3.89	1.32	1.37
30	A	835	CLA	CHD-C4C	3.89	1.48	1.39
30	A	820	CLA	CHD-C4C	3.89	1.48	1.39
30	B	804	CLA	CHD-C1D	3.89	1.46	1.38
37	10	302	A86	C19-C18	3.89	1.57	1.52
30	4	311	CLA	CHD-C4C	3.88	1.48	1.39
30	B	811	CLA	C1B-NB	-3.88	1.32	1.37
30	B	801	CLA	O2A-CGA	3.88	1.44	1.33
37	3	314	A86	C9-C10	3.88	1.55	1.43
37	9	313	A86	C10-C11	3.88	1.45	1.34
30	B	824	CLA	C1B-NB	-3.88	1.32	1.37
30	A	840	CLA	C1B-NB	-3.88	1.32	1.37
38	7	308	KC1	C1B-NB	-3.88	1.32	1.37
30	4	302	CLA	CHD-C1D	3.88	1.46	1.38
30	B	822	CLA	CHD-C4C	3.88	1.48	1.39
30	2	301	CLA	CHD-C4C	3.88	1.48	1.39
38	8	311	KC1	C1B-NB	-3.88	1.32	1.37
30	8	304	CLA	CHD-C1D	3.88	1.46	1.38
38	12	313	KC1	C1B-NB	-3.88	1.32	1.37
30	B	835	CLA	CHD-C1D	3.88	1.46	1.38
30	B	824	CLA	O2A-CGA	3.88	1.44	1.33
30	5	311	CLA	CHD-C4C	3.88	1.48	1.39
30	7	304	CLA	CHD-C4C	3.88	1.48	1.39
30	A	824	CLA	CHD-C1D	3.88	1.46	1.38
30	A	830	CLA	O2A-CGA	3.88	1.44	1.33
37	3	315	A86	C9-C10	3.88	1.55	1.43
30	6	317	CLA	CHD-C4C	3.88	1.48	1.39
37	15	316	A86	C9-C10	3.88	1.55	1.43
30	B	833	CLA	CHD-C1D	3.87	1.46	1.38
30	2	308	CLA	C1B-NB	-3.87	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	802	CLA	O2A-CGA	3.87	1.44	1.33
30	B	805	CLA	CHD-C4C	3.87	1.48	1.39
30	12	304	CLA	CHD-C4C	3.87	1.48	1.39
30	4	303	CLA	CHD-C4C	3.87	1.48	1.39
30	A	825	CLA	CHD-C4C	3.87	1.48	1.39
30	B	806	CLA	CHD-C1D	3.87	1.46	1.38
30	L	203	CLA	CHD-C1D	3.87	1.46	1.38
30	B	831	CLA	CHD-C1D	3.86	1.46	1.38
30	8	305	CLA	C4B-NB	-3.86	1.32	1.37
38	8	313	KC1	CHC-C1C	3.86	1.48	1.39
30	15	310	CLA	C3D-C2D	3.86	1.49	1.39
30	B	815	CLA	C4B-NB	-3.86	1.32	1.37
38	13	310	KC1	CHC-C1C	3.86	1.48	1.39
30	A	833	CLA	CHD-C4C	3.86	1.48	1.39
30	12	302	CLA	C1B-NB	-3.86	1.32	1.37
30	6	309	CLA	C3D-C2D	3.86	1.49	1.39
30	16	301	CLA	CHD-C1D	3.86	1.45	1.38
30	6	305	CLA	CHD-C4C	3.86	1.48	1.39
38	11	312	KC1	C1B-NB	-3.86	1.32	1.37
30	14	309	CLA	C3D-C2D	3.86	1.49	1.39
30	2	304	CLA	CHD-C4C	3.86	1.48	1.39
30	A	809	CLA	CHD-C1D	3.86	1.45	1.38
30	B	851	CLA	CHD-C4C	3.86	1.48	1.39
30	A	838	CLA	C4B-NB	-3.85	1.32	1.37
30	6	314	CLA	C1B-NB	-3.85	1.32	1.37
30	1	307	CLA	CHD-C4C	3.85	1.48	1.39
30	7	305	CLA	CHD-C4C	3.85	1.48	1.39
30	A	812	CLA	C1D-ND	3.85	1.42	1.37
30	3	301	CLA	CHD-C1D	3.85	1.45	1.38
30	12	307	CLA	CHD-C1D	3.85	1.45	1.38
30	13	301	CLA	CHD-C1D	3.85	1.45	1.38
30	10	311	CLA	CHD-C4C	3.85	1.48	1.39
30	J	101	CLA	CHD-C4C	3.85	1.48	1.39
38	5	310	KC1	C1B-NB	-3.85	1.32	1.37
30	B	826	CLA	C1B-NB	-3.85	1.32	1.37
30	A	813	CLA	CHD-C1D	3.85	1.45	1.38
30	A	817	CLA	CHD-C4C	3.85	1.48	1.39
30	1	301	CLA	CHD-C4C	3.85	1.48	1.39
30	A	802	CLA	C3D-C2D	3.85	1.49	1.39
37	6	320	A86	C10-C11	3.85	1.45	1.34
30	A	827	CLA	O2A-CGA	3.85	1.44	1.33
30	B	813	CLA	C1B-NB	-3.85	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	307	CLA	C3D-C2D	3.84	1.49	1.39
37	7	319	A86	C21-C20	3.84	1.57	1.51
30	4	309	CLA	C3D-C2D	3.84	1.49	1.39
30	A	842	CLA	CHD-C1D	3.84	1.45	1.38
30	A	834	CLA	CHD-C4C	3.84	1.47	1.39
30	A	829	CLA	C4B-NB	-3.84	1.32	1.37
30	2	303	CLA	C1B-NB	-3.84	1.32	1.37
30	8	308	CLA	C1B-NB	-3.84	1.32	1.37
30	6	314	CLA	CHD-C4C	3.84	1.47	1.39
37	14	318	A86	C9-C10	3.84	1.55	1.43
37	5	315	A86	C9-C10	3.84	1.55	1.43
30	B	835	CLA	C1B-NB	-3.84	1.32	1.37
30	B	812	CLA	CHD-C4C	3.84	1.47	1.39
30	8	304	CLA	C1D-ND	3.84	1.42	1.37
30	B	821	CLA	CHD-C4C	3.84	1.47	1.39
30	6	304	CLA	CHD-C4C	3.83	1.47	1.39
30	2	307	CLA	C1D-ND	3.83	1.42	1.37
30	5	309	CLA	CHD-C4C	3.83	1.47	1.39
30	6	309	CLA	CHD-C4C	3.83	1.47	1.39
37	4	314	A86	C19-C18	3.83	1.57	1.52
30	3	301	CLA	CHD-C4C	3.83	1.47	1.39
30	13	302	CLA	C3D-C2D	3.83	1.49	1.39
38	6	311	KC1	C1B-NB	-3.83	1.32	1.37
30	11	309	CLA	C1B-NB	-3.83	1.32	1.37
37	7	315	A86	C10-C11	3.83	1.45	1.34
37	10	316	A86	C10-C11	3.83	1.45	1.34
30	A	806	CLA	C4B-NB	-3.83	1.32	1.37
30	8	302	CLA	C1B-NB	-3.83	1.32	1.37
30	9	305	CLA	CHD-C4C	3.83	1.47	1.39
38	10	312	KC1	CHC-C1C	3.83	1.47	1.39
30	10	305	CLA	CHD-C4C	3.83	1.47	1.39
30	4	301	CLA	C1B-NB	-3.83	1.32	1.37
30	4	304	CLA	CHD-C4C	3.83	1.47	1.39
37	15	322	A86	C19-C18	3.83	1.57	1.52
30	A	836	CLA	C1D-ND	3.83	1.42	1.37
30	L	202	CLA	C1D-ND	3.83	1.42	1.37
30	A	809	CLA	C1B-NB	-3.82	1.32	1.37
30	15	307	CLA	C3D-C2D	3.82	1.49	1.39
30	1	301	CLA	C1B-NB	-3.82	1.32	1.37
30	3	302	CLA	CHD-C4C	3.82	1.47	1.39
30	A	808	CLA	CHD-C1D	3.82	1.45	1.38
37	4	312	A86	C10-C11	3.82	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	801	CLA	C1D-ND	3.82	1.42	1.37
30	13	302	CLA	CHD-C4C	3.82	1.47	1.39
30	8	301	CLA	CHD-C1D	3.82	1.45	1.38
30	5	307	CLA	CHD-C1D	3.82	1.45	1.38
30	B	803	CLA	C1B-NB	-3.82	1.32	1.37
30	8	308	CLA	CHD-C4C	3.82	1.47	1.39
30	B	837	CLA	C1B-NB	-3.82	1.32	1.37
30	4	305	CLA	CHD-C4C	3.82	1.47	1.39
30	15	308	CLA	C3D-C2D	3.82	1.49	1.39
30	B	837	CLA	CHD-C1D	3.82	1.45	1.38
30	16	302	CLA	CHD-C4C	3.82	1.47	1.39
30	A	836	CLA	C4B-NB	-3.82	1.32	1.37
30	A	802	CLA	CHD-C4C	3.82	1.47	1.39
30	3	301	CLA	C1B-NB	-3.82	1.32	1.37
30	6	310	CLA	C1B-NB	-3.82	1.32	1.37
30	A	843	CLA	CHD-C4C	3.82	1.47	1.39
30	16	303	CLA	CHD-C4C	3.82	1.47	1.39
30	B	823	CLA	C1B-NB	-3.82	1.32	1.37
30	A	833	CLA	C1B-NB	-3.81	1.32	1.37
30	13	303	CLA	C3D-C2D	3.81	1.49	1.39
30	A	805	CLA	CHD-C1D	3.81	1.45	1.38
30	B	832	CLA	CHD-C4C	3.81	1.47	1.39
30	B	812	CLA	C3D-C2D	3.81	1.49	1.39
29	A	801	CL0	CHB-C4A	-3.81	1.34	1.38
38	13	312	KC1	CHC-C1C	3.81	1.47	1.39
30	A	823	CLA	CHD-C4C	3.81	1.47	1.39
37	15	321	A86	C9-C10	3.81	1.55	1.43
37	10	302	A86	C17-C18	-3.81	1.46	1.52
30	L	203	CLA	CHD-C4C	3.81	1.47	1.39
30	4	306	CLA	C1B-NB	-3.81	1.32	1.37
30	14	305	CLA	C3D-C2D	3.81	1.49	1.39
30	2	305	CLA	CHD-C4C	3.81	1.47	1.39
30	5	303	CLA	C1B-NB	-3.81	1.32	1.37
30	B	830	CLA	CHC-C4B	3.81	1.48	1.39
30	B	812	CLA	C1B-NB	-3.81	1.32	1.37
37	8	318	A86	C9-C10	3.81	1.55	1.43
30	6	315	CLA	C3D-C2D	3.81	1.49	1.39
30	2	305	CLA	C3D-C2D	3.80	1.49	1.39
30	2	310	CLA	CHD-C4C	3.80	1.47	1.39
30	B	814	CLA	CHD-C1D	3.80	1.45	1.38
30	5	302	CLA	CHD-C4C	3.80	1.47	1.39
30	A	818	CLA	CHD-C1D	3.80	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	818	CLA	CHD-C4C	3.80	1.47	1.39
30	A	829	CLA	CHD-C1D	3.80	1.45	1.38
30	9	306	CLA	C3D-C2D	3.80	1.49	1.39
30	B	839	CLA	CHC-C4B	3.80	1.47	1.39
38	12	313	KC1	CHB-C1B	3.80	1.45	1.38
30	14	312	CLA	C3D-C2D	3.80	1.49	1.39
30	A	831	CLA	C3D-C2D	3.80	1.49	1.39
37	4	317	A86	C10-C11	3.80	1.44	1.34
30	A	837	CLA	C1B-NB	-3.80	1.32	1.37
30	A	804	CLA	CHD-C1D	3.80	1.45	1.38
30	12	302	CLA	C4B-NB	-3.80	1.32	1.37
30	15	304	CLA	C3D-C2D	3.80	1.49	1.39
30	16	306	CLA	CHD-C4C	3.80	1.47	1.39
38	4	310	KC1	CHC-C1C	3.79	1.47	1.39
30	8	304	CLA	C3D-C2D	3.79	1.49	1.39
30	12	308	CLA	CHD-C4C	3.79	1.47	1.39
30	A	803	CLA	C3D-C2D	3.79	1.49	1.39
30	A	814	CLA	C4B-NB	-3.79	1.32	1.37
30	15	302	CLA	CHC-C4B	3.79	1.47	1.39
30	5	308	CLA	CHD-C4C	3.79	1.47	1.39
37	14	315	A86	C9-C10	3.79	1.54	1.43
37	2	319	A86	C9-C10	3.79	1.54	1.43
37	11	316	A86	C9-C10	3.79	1.54	1.43
30	F	203	CLA	C1B-NB	-3.79	1.32	1.37
30	2	304	CLA	C1B-NB	-3.79	1.32	1.37
30	12	303	CLA	C1B-NB	-3.79	1.32	1.37
30	10	311	CLA	C3D-C2D	3.79	1.49	1.39
30	7	306	CLA	C3D-C2D	3.79	1.49	1.39
37	5	301	A86	C9-C10	3.79	1.54	1.43
30	B	834	CLA	CHD-C1D	3.79	1.45	1.38
30	B	828	CLA	CHD-C4C	3.79	1.47	1.39
30	16	305	CLA	C3D-C2D	3.79	1.49	1.39
30	15	309	CLA	C3D-C2D	3.78	1.49	1.39
30	15	306	CLA	C3D-C2D	3.78	1.49	1.39
37	14	301	A86	C9-C10	3.78	1.54	1.43
30	6	310	CLA	C3D-C2D	3.78	1.49	1.39
30	10	304	CLA	CHD-C4C	3.78	1.47	1.39
30	B	830	CLA	C1D-ND	3.78	1.42	1.37
30	5	304	CLA	CHD-C4C	3.78	1.47	1.39
37	11	315	A86	C9-C10	3.78	1.54	1.43
37	4	315	A86	C10-C11	3.78	1.44	1.34
30	4	302	CLA	CHD-C4C	3.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	809	CLA	C4B-NB	-3.78	1.32	1.37
30	2	308	CLA	CHD-C4C	3.78	1.47	1.39
30	9	303	CLA	CHD-C4C	3.78	1.47	1.39
30	13	304	CLA	OBD-CAD	3.78	1.29	1.22
30	14	303	CLA	C3D-C2D	3.78	1.49	1.39
30	15	313	CLA	C3D-C2D	3.78	1.49	1.39
30	8	309	CLA	C1B-NB	-3.77	1.32	1.37
37	14	317	A86	C10-C11	3.77	1.44	1.34
30	13	307	CLA	CHC-C4B	3.77	1.47	1.39
30	A	841	CLA	C3D-C2D	3.77	1.49	1.39
38	4	310	KC1	C1B-NB	-3.77	1.32	1.37
30	B	816	CLA	CHD-C4C	3.77	1.47	1.39
30	13	307	CLA	C3D-C2D	3.77	1.49	1.39
30	8	301	CLA	C3D-C2D	3.77	1.49	1.39
30	9	302	CLA	CHD-C4C	3.77	1.47	1.39
38	13	306	KC1	CHC-C1C	3.77	1.47	1.39
38	16	311	KC1	C1B-NB	-3.77	1.32	1.37
38	8	313	KC1	C1B-NB	-3.77	1.32	1.37
37	1	309	A86	C19-C18	3.77	1.57	1.52
30	B	810	CLA	C1B-NB	-3.77	1.32	1.37
30	12	306	CLA	C1B-NB	-3.77	1.32	1.37
30	2	311	CLA	C3D-C2D	3.77	1.49	1.39
38	8	314	KC1	C1B-NB	-3.77	1.32	1.37
30	9	301	CLA	C4B-NB	-3.77	1.32	1.37
30	A	819	CLA	CHC-C4B	3.77	1.47	1.39
30	1	303	CLA	CHD-C4C	3.77	1.47	1.39
30	16	310	CLA	CHD-C4C	3.77	1.47	1.39
30	B	805	CLA	C4B-NB	-3.77	1.32	1.37
30	6	316	CLA	C1B-NB	-3.77	1.32	1.37
30	13	303	CLA	OBD-CAD	3.77	1.29	1.22
30	16	309	CLA	C3D-C2D	3.76	1.49	1.39
30	3	301	CLA	C3D-C2D	3.76	1.49	1.39
30	B	826	CLA	C1D-ND	3.76	1.42	1.37
30	2	310	CLA	C1B-NB	-3.76	1.32	1.37
30	6	306	CLA	CHD-C4C	3.76	1.47	1.39
37	6	320	A86	C17-C18	-3.76	1.47	1.52
30	B	822	CLA	CHD-C1D	3.76	1.45	1.38
30	10	307	CLA	CHD-C1D	3.76	1.45	1.38
30	9	309	CLA	CHD-C4C	3.76	1.47	1.39
30	3	309	CLA	C3D-C2D	3.76	1.49	1.39
30	15	311	CLA	OBD-CAD	3.76	1.29	1.22
30	B	804	CLA	C1B-NB	-3.76	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	311	KC1	CHC-C1C	3.76	1.47	1.39
30	14	309	CLA	OBD-CAD	3.76	1.29	1.22
37	14	317	A86	C9-C10	3.76	1.54	1.43
30	B	807	CLA	C1B-NB	-3.76	1.32	1.37
30	A	841	CLA	O2A-CGA	3.76	1.44	1.33
30	B	817	CLA	CHC-C4B	3.76	1.47	1.39
30	3	305	CLA	CHD-C4C	3.76	1.47	1.39
30	10	308	CLA	C1B-NB	-3.76	1.32	1.37
30	5	311	CLA	C3D-C2D	3.76	1.49	1.39
30	15	303	CLA	C3D-C2D	3.76	1.49	1.39
38	14	311	KC1	CHC-C1C	3.76	1.47	1.39
38	8	310	KC1	C1B-NB	-3.76	1.32	1.37
30	2	308	CLA	C3D-C2D	3.76	1.49	1.39
30	12	312	CLA	C3D-C2D	3.76	1.49	1.39
30	12	303	CLA	C3D-C2D	3.76	1.49	1.39
30	L	202	CLA	CHD-C4C	3.76	1.47	1.39
30	A	839	CLA	CHD-C4C	3.75	1.47	1.39
30	15	302	CLA	C3D-C2D	3.75	1.49	1.39
30	15	311	CLA	C3D-C2D	3.75	1.49	1.39
30	3	310	CLA	C3D-C2D	3.75	1.49	1.39
30	13	304	CLA	C3D-C2D	3.75	1.49	1.39
30	B	829	CLA	C1D-ND	3.75	1.42	1.37
30	13	309	CLA	C3D-C2D	3.75	1.49	1.39
30	14	307	CLA	C3D-C2D	3.75	1.49	1.39
30	2	310	CLA	C3D-C2D	3.75	1.49	1.39
30	14	304	CLA	C3D-C2D	3.75	1.49	1.39
30	3	302	CLA	C3D-C2D	3.75	1.49	1.39
30	15	305	CLA	C3D-C2D	3.75	1.49	1.39
30	6	317	CLA	C3D-C2D	3.75	1.49	1.39
30	B	828	CLA	C1D-ND	3.75	1.42	1.37
30	12	321	CLA	C3D-C2D	3.75	1.49	1.39
38	8	312	KC1	CHC-C1C	3.75	1.47	1.39
30	B	817	CLA	CHD-C1D	3.75	1.45	1.38
30	10	308	CLA	C3D-C2D	3.75	1.49	1.39
30	15	310	CLA	OBD-CAD	3.75	1.28	1.22
38	8	311	KC1	CHC-C1C	3.75	1.47	1.39
30	1	305	CLA	C3D-C2D	3.75	1.49	1.39
30	15	312	CLA	C1B-NB	-3.75	1.32	1.37
37	2	318	A86	C9-C10	3.75	1.54	1.43
30	A	819	CLA	CHD-C1D	3.75	1.45	1.38
30	3	305	CLA	C3D-C2D	3.74	1.49	1.39
30	9	308	CLA	CHD-C4C	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	310	CLA	CHD-C4C	3.74	1.47	1.39
30	B	803	CLA	C3D-C2D	3.74	1.49	1.39
30	4	305	CLA	C1B-NB	-3.74	1.32	1.37
30	A	838	CLA	CHD-C4C	3.74	1.47	1.39
30	8	303	CLA	CHD-C4C	3.74	1.47	1.39
30	A	809	CLA	CHD-C4C	3.74	1.47	1.39
30	15	314	CLA	OBD-CAD	3.74	1.28	1.22
30	A	840	CLA	CHD-C4C	3.74	1.47	1.39
30	B	833	CLA	CHD-C4C	3.74	1.47	1.39
30	8	302	CLA	CHD-C4C	3.74	1.47	1.39
30	7	311	CLA	CHD-C4C	3.74	1.47	1.39
30	15	307	CLA	OBD-CAD	3.74	1.28	1.22
38	13	312	KC1	OBD-CAD	3.74	1.28	1.22
30	B	813	CLA	C3D-C2D	3.74	1.49	1.39
30	10	307	CLA	C3D-C2D	3.74	1.49	1.39
30	14	304	CLA	OBD-CAD	3.74	1.28	1.22
30	A	813	CLA	CHD-C4C	3.74	1.47	1.39
30	A	816	CLA	C1B-NB	-3.74	1.33	1.37
30	A	828	CLA	C1B-NB	-3.74	1.33	1.37
30	15	308	CLA	OBD-CAD	3.74	1.28	1.22
37	4	314	A86	C17-C18	-3.74	1.47	1.52
30	15	302	CLA	OBD-CAD	3.74	1.28	1.22
38	16	311	KC1	CHB-C1B	3.74	1.45	1.38
30	16	307	CLA	C3D-C2D	3.74	1.49	1.39
30	2	304	CLA	C3D-C2D	3.73	1.49	1.39
30	B	832	CLA	C1B-NB	-3.73	1.33	1.37
38	5	306	KC1	CHC-C1C	3.73	1.47	1.39
30	A	836	CLA	C3D-C2D	3.73	1.49	1.39
30	9	307	CLA	CHD-C4C	3.73	1.47	1.39
30	7	307	CLA	C1B-NB	-3.73	1.33	1.37
38	3	304	KC1	C1B-NB	-3.73	1.33	1.37
30	13	309	CLA	OBD-CAD	3.73	1.28	1.22
30	13	307	CLA	OBD-CAD	3.73	1.28	1.22
30	B	829	CLA	CHD-C4C	3.73	1.47	1.39
30	9	303	CLA	C3D-C2D	3.73	1.49	1.39
37	2	302	A86	C17-C18	-3.73	1.47	1.52
30	A	826	CLA	CHD-C1D	3.73	1.45	1.38
30	5	303	CLA	CHD-C4C	3.73	1.47	1.39
30	15	307	CLA	CHD-C4C	3.73	1.47	1.39
38	16	311	KC1	CHC-C1C	3.73	1.47	1.39
30	5	309	CLA	C3D-C2D	3.73	1.49	1.39
37	14	319	A86	C19-C18	3.73	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	810	CLA	CHD-C1D	3.73	1.45	1.38
30	12	307	CLA	CHC-C4B	3.73	1.47	1.39
30	B	812	CLA	C4B-NB	-3.73	1.33	1.37
38	6	308	KC1	C1B-NB	-3.73	1.33	1.37
38	2	306	KC1	CHC-C1C	3.72	1.47	1.39
30	12	304	CLA	C3D-C2D	3.72	1.49	1.39
30	14	313	CLA	C3D-C2D	3.72	1.49	1.39
30	A	813	CLA	C4B-NB	-3.72	1.33	1.37
30	A	818	CLA	C1B-NB	-3.72	1.33	1.37
30	B	830	CLA	CHD-C4C	3.72	1.47	1.39
37	9	316	A86	C17-C18	-3.72	1.47	1.52
30	A	826	CLA	C4B-NB	-3.72	1.33	1.37
30	7	307	CLA	CHD-C4C	3.72	1.47	1.39
30	9	305	CLA	C1B-NB	-3.72	1.33	1.37
30	9	308	CLA	C3D-C2D	3.72	1.49	1.39
37	7	315	A86	C17-C18	-3.72	1.47	1.52
30	B	831	CLA	CHD-C4C	3.72	1.47	1.39
38	16	304	KC1	CHC-C1C	3.72	1.47	1.39
30	B	823	CLA	CHD-C4C	3.72	1.47	1.39
30	10	304	CLA	C3D-C2D	3.72	1.49	1.39
30	15	311	CLA	CHC-C4B	3.72	1.47	1.39
30	2	308	CLA	CHC-C4B	3.72	1.47	1.39
38	8	306	KC1	C1B-NB	-3.72	1.33	1.37
30	16	308	CLA	OBD-CAD	3.72	1.28	1.22
38	8	307	KC1	CHC-C1C	3.72	1.47	1.39
30	7	311	CLA	C3D-C2D	3.72	1.49	1.39
30	A	821	CLA	CHD-C1D	3.72	1.45	1.38
37	14	316	A86	C9-C10	3.72	1.54	1.43
38	6	312	KC1	C1B-NB	-3.72	1.33	1.37
38	4	307	KC1	C1B-NB	-3.71	1.33	1.37
38	2	314	KC1	CHC-C1C	3.71	1.47	1.39
38	14	308	KC1	OBD-CAD	3.71	1.28	1.22
30	7	312	CLA	C3D-C2D	3.71	1.49	1.39
38	12	313	KC1	C1A-NA	-3.71	1.30	1.38
30	11	304	CLA	OBD-CAD	3.71	1.28	1.22
30	B	825	CLA	CHC-C4B	3.71	1.47	1.39
30	10	307	CLA	CHD-C4C	3.71	1.47	1.39
30	2	313	CLA	OBD-CAD	3.71	1.28	1.22
30	16	301	CLA	C3D-C2D	3.71	1.49	1.39
30	10	303	CLA	C3D-C2D	3.71	1.49	1.39
30	15	303	CLA	CHC-C4B	3.71	1.47	1.39
30	16	301	CLA	CHD-C4C	3.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	829	CLA	C3D-C2D	3.71	1.49	1.39
30	B	804	CLA	CHD-C4C	3.71	1.47	1.39
30	12	303	CLA	CHD-C4C	3.71	1.47	1.39
30	11	308	CLA	C3D-C2D	3.71	1.49	1.39
30	A	811	CLA	CHD-C4C	3.70	1.47	1.39
30	F	203	CLA	C3D-C2D	3.70	1.49	1.39
30	B	818	CLA	C3D-C2D	3.70	1.49	1.39
30	7	304	CLA	C3D-C2D	3.70	1.49	1.39
30	12	302	CLA	C3D-C2D	3.70	1.49	1.39
30	F	203	CLA	CHD-C4C	3.70	1.47	1.39
30	A	830	CLA	C3D-C2D	3.70	1.49	1.39
30	16	308	CLA	C3D-C2D	3.70	1.49	1.39
38	10	312	KC1	C1B-NB	-3.70	1.33	1.37
30	11	306	CLA	CHC-C4B	3.70	1.47	1.39
30	A	823	CLA	CHD-C1D	3.70	1.45	1.38
30	7	307	CLA	CHD-C1D	3.70	1.45	1.38
30	12	306	CLA	CHD-C4C	3.70	1.47	1.39
30	A	833	CLA	C3D-C2D	3.70	1.49	1.39
30	A	814	CLA	CHD-C4C	3.70	1.47	1.39
30	B	809	CLA	CHD-C1D	3.70	1.45	1.38
38	9	310	KC1	CHC-C1C	3.70	1.47	1.39
30	B	806	CLA	CHD-C4C	3.70	1.47	1.39
38	6	308	KC1	CHC-C1C	3.70	1.47	1.39
30	3	306	CLA	CHC-C4B	3.70	1.47	1.39
30	A	835	CLA	C1B-NB	-3.70	1.33	1.37
38	10	306	KC1	C1B-NB	-3.70	1.33	1.37
30	1	302	CLA	C1B-NB	-3.70	1.33	1.37
30	9	301	CLA	CHD-C4C	3.70	1.47	1.39
37	4	312	A86	C9-C10	3.70	1.54	1.43
30	14	302	CLA	OBD-CAD	3.70	1.28	1.22
37	7	315	A86	C9-C10	3.70	1.54	1.43
30	A	805	CLA	CHD-C4C	3.70	1.47	1.39
30	A	841	CLA	CHD-C4C	3.70	1.47	1.39
30	3	309	CLA	OBD-CAD	3.70	1.28	1.22
30	A	842	CLA	CHC-C4B	3.70	1.47	1.39
30	1	302	CLA	C3D-C2D	3.70	1.49	1.39
38	11	311	KC1	CHC-C1C	3.69	1.47	1.39
30	A	843	CLA	C3D-C2D	3.69	1.49	1.39
30	A	821	CLA	C1D-ND	3.69	1.42	1.37
30	F	201	CLA	C3D-C2D	3.69	1.49	1.39
30	4	305	CLA	C3D-C2D	3.69	1.49	1.39
30	A	817	CLA	C1B-NB	-3.69	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	305	CLA	CHD-C4C	3.69	1.47	1.39
39	15	319	DD6	C35-C34	3.69	1.58	1.52
30	A	814	CLA	C3D-C2D	3.69	1.49	1.39
30	F	202	CLA	C1B-NB	-3.69	1.33	1.37
30	2	313	CLA	CHC-C4B	3.69	1.47	1.39
30	1	303	CLA	C1B-NB	-3.69	1.33	1.37
30	1	304	CLA	C3D-C2D	3.69	1.49	1.39
30	B	803	CLA	CHD-C1D	3.69	1.45	1.38
30	B	831	CLA	C1B-NB	-3.69	1.33	1.37
30	1	304	CLA	CHC-C4B	3.69	1.47	1.39
30	B	814	CLA	C1D-ND	3.69	1.42	1.37
30	3	303	CLA	C3D-C2D	3.69	1.49	1.39
30	B	805	CLA	C3D-C2D	3.69	1.49	1.39
37	10	316	A86	C9-C10	3.69	1.54	1.43
30	B	804	CLA	C3D-C2D	3.69	1.49	1.39
30	B	810	CLA	CHD-C4C	3.69	1.47	1.39
38	10	310	KC1	C1B-NB	-3.68	1.33	1.37
38	14	306	KC1	C1B-NB	-3.68	1.33	1.37
38	12	305	KC1	OBD-CAD	3.68	1.28	1.22
30	7	310	CLA	C1B-NB	-3.68	1.33	1.37
30	9	302	CLA	C1B-NB	-3.68	1.33	1.37
30	A	822	CLA	CHD-C4C	3.68	1.47	1.39
30	16	307	CLA	OBD-CAD	3.68	1.28	1.22
30	1	301	CLA	C3D-C2D	3.68	1.49	1.39
30	6	316	CLA	C4B-NB	-3.68	1.33	1.37
37	15	323	A86	C19-C18	3.68	1.57	1.52
30	B	838	CLA	CHD-C4C	3.68	1.47	1.39
30	6	306	CLA	C1B-NB	-3.68	1.33	1.37
30	B	833	CLA	C3D-C2D	3.68	1.49	1.39
30	3	307	CLA	C3D-C2D	3.68	1.49	1.39
30	2	313	CLA	C3D-C2D	3.68	1.49	1.39
38	7	313	KC1	CHC-C1C	3.68	1.47	1.39
38	3	311	KC1	C1B-NB	-3.68	1.33	1.37
30	4	309	CLA	OBD-CAD	3.68	1.28	1.22
30	6	305	CLA	C3D-C2D	3.68	1.49	1.39
38	13	305	KC1	CHC-C1C	3.68	1.47	1.39
30	3	309	CLA	CHC-C4B	3.68	1.47	1.39
30	3	310	CLA	OBD-CAD	3.68	1.28	1.22
29	A	801	CL0	CHC-C1C	3.68	1.46	1.39
30	2	307	CLA	CHD-C4C	3.68	1.47	1.39
30	14	305	CLA	C1B-NB	-3.67	1.33	1.37
30	B	815	CLA	CHD-C4C	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	833	CLA	CHC-C4B	3.67	1.47	1.39
30	B	807	CLA	C3D-C2D	3.67	1.49	1.39
30	15	313	CLA	CHC-C4B	3.67	1.47	1.39
30	10	311	CLA	OBD-CAD	3.67	1.28	1.22
37	14	314	A86	C7-C6	3.67	1.58	1.50
37	5	315	A86	C19-C18	3.67	1.57	1.52
30	A	825	CLA	C1B-NB	-3.67	1.33	1.37
30	A	824	CLA	CHD-C4C	3.67	1.47	1.39
30	13	301	CLA	CHD-C4C	3.67	1.47	1.39
38	8	314	KC1	CHC-C1C	3.67	1.47	1.39
30	A	807	CLA	C3D-C2D	3.67	1.49	1.39
37	10	315	A86	C17-C18	-3.67	1.47	1.52
30	11	309	CLA	OBD-CAD	3.67	1.28	1.22
30	B	815	CLA	C3D-C2D	3.67	1.49	1.39
30	B	810	CLA	CHC-C4B	3.67	1.47	1.39
38	13	308	KC1	CHC-C1C	3.67	1.47	1.39
30	8	303	CLA	C3D-C2D	3.67	1.49	1.39
30	16	303	CLA	C3D-C2D	3.67	1.49	1.39
30	14	304	CLA	CHC-C4B	3.67	1.47	1.39
30	A	820	CLA	C3D-C2D	3.67	1.49	1.39
30	8	302	CLA	CHD-C1D	3.67	1.45	1.38
30	11	306	CLA	C3D-C2D	3.67	1.49	1.39
30	A	844	CLA	C3D-C2D	3.67	1.49	1.39
38	5	306	KC1	OBD-CAD	3.67	1.28	1.22
30	B	807	CLA	CHD-C4C	3.67	1.47	1.39
30	16	301	CLA	CHC-C4B	3.67	1.47	1.39
30	B	838	CLA	C3D-C2D	3.67	1.49	1.39
30	14	313	CLA	OBD-CAD	3.67	1.28	1.22
30	5	307	CLA	CHB-C1B	3.67	1.47	1.39
30	15	305	CLA	OBD-CAD	3.67	1.28	1.22
38	2	312	KC1	CHC-C1C	3.67	1.47	1.39
30	11	310	CLA	OBD-CAD	3.67	1.28	1.22
30	8	303	CLA	C1D-ND	3.67	1.42	1.37
30	16	305	CLA	C1B-NB	-3.67	1.33	1.37
38	3	311	KC1	CHC-C1C	3.67	1.47	1.39
30	14	303	CLA	OBD-CAD	3.67	1.28	1.22
30	6	306	CLA	C3D-C2D	3.67	1.49	1.39
30	9	305	CLA	C3D-C2D	3.67	1.49	1.39
38	8	307	KC1	C1B-NB	-3.66	1.33	1.37
30	A	830	CLA	CHC-C4B	3.66	1.47	1.39
30	B	830	CLA	C1B-NB	-3.66	1.33	1.37
30	10	309	CLA	C3D-C2D	3.66	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	311	CLA	C3D-C2D	3.66	1.49	1.39
30	2u	202	CLA	C1B-NB	-3.66	1.33	1.37
30	B	817	CLA	CHD-C4C	3.66	1.47	1.39
38	12	309	KC1	CHC-C1C	3.66	1.47	1.39
30	A	837	CLA	C3D-C2D	3.66	1.49	1.39
30	7	305	CLA	C1B-NB	-3.66	1.33	1.37
38	2	312	KC1	C1B-NB	-3.66	1.33	1.37
30	15	314	CLA	C3D-C2D	3.66	1.49	1.39
30	1	303	CLA	C3D-C2D	3.66	1.49	1.39
37	10	301	A86	C10-C11	3.66	1.44	1.34
30	10	307	CLA	C1B-NB	-3.66	1.33	1.37
30	15	313	CLA	OBD-CAD	3.66	1.28	1.22
30	A	816	CLA	C3D-C2D	3.66	1.49	1.39
30	6	316	CLA	C3D-C2D	3.66	1.49	1.39
30	15	308	CLA	CHC-C4B	3.66	1.47	1.39
38	1	308	KC1	CHC-C1C	3.66	1.47	1.39
30	A	818	CLA	CHC-C4B	3.66	1.47	1.39
30	11	304	CLA	CHC-C4B	3.66	1.47	1.39
30	14	307	CLA	CHC-C4B	3.66	1.47	1.39
30	9	306	CLA	OBD-CAD	3.66	1.28	1.22
38	9	310	KC1	C1B-NB	-3.66	1.33	1.37
38	6	312	KC1	CHC-C1C	3.66	1.47	1.39
38	13	311	KC1	CHC-C1C	3.66	1.47	1.39
30	A	832	CLA	CHD-C4C	3.66	1.47	1.39
30	J	101	CLA	C1B-NB	-3.66	1.33	1.37
30	4	302	CLA	C1B-NB	-3.66	1.33	1.37
30	A	805	CLA	CHC-C4B	3.66	1.47	1.39
30	2u	202	CLA	C3D-C2D	3.66	1.49	1.39
30	14	302	CLA	CHC-C4B	3.66	1.47	1.39
37	13	313	A86	C19-C18	3.66	1.57	1.52
30	B	813	CLA	C4B-NB	-3.65	1.33	1.37
37	4	315	A86	C9-C10	3.65	1.54	1.43
30	A	823	CLA	C3D-C2D	3.65	1.49	1.39
30	16	306	CLA	CHC-C4B	3.65	1.47	1.39
30	12	307	CLA	C3D-C2D	3.65	1.49	1.39
37	7	316	A86	C10-C11	3.65	1.44	1.34
30	14	312	CLA	OBD-CAD	3.65	1.28	1.22
38	3	311	KC1	OBD-CAD	3.65	1.28	1.22
30	7	303	CLA	C3D-C2D	3.65	1.48	1.39
30	A	802	CLA	C1D-ND	3.65	1.42	1.37
30	2	309	CLA	C3D-C2D	3.65	1.48	1.39
37	4	317	A86	C21-C20	3.65	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	823	CLA	C1B-NB	-3.65	1.33	1.37
30	3	307	CLA	OBD-CAD	3.65	1.28	1.22
30	7	309	CLA	C1B-NB	-3.65	1.33	1.37
30	B	825	CLA	CHD-C1D	3.65	1.45	1.38
30	8	308	CLA	C3D-C2D	3.65	1.48	1.39
30	A	828	CLA	C4B-NB	-3.65	1.33	1.37
30	B	829	CLA	C1B-NB	-3.65	1.33	1.37
30	8	309	CLA	C3D-C2D	3.64	1.48	1.39
38	2	314	KC1	C1B-NB	-3.64	1.33	1.37
30	12	306	CLA	C3D-C2D	3.64	1.48	1.39
30	16	302	CLA	C3D-C2D	3.64	1.48	1.39
38	1	306	KC1	C1B-NB	-3.64	1.33	1.37
30	B	807	CLA	CHD-C1D	3.64	1.45	1.38
30	16	309	CLA	OBD-CAD	3.64	1.28	1.22
37	6	320	A86	C9-C10	3.64	1.54	1.43
30	B	834	CLA	C3D-C2D	3.64	1.48	1.39
30	4	304	CLA	C1B-NB	-3.64	1.33	1.37
30	B	836	CLA	CHD-C4C	3.64	1.47	1.39
30	9	309	CLA	C3D-C2D	3.64	1.48	1.39
30	4	301	CLA	CHD-C4C	3.64	1.47	1.39
37	8	318	A86	C10-C11	3.64	1.44	1.34
38	10	312	KC1	OBD-CAD	3.64	1.28	1.22
30	4	306	CLA	C3D-C2D	3.64	1.48	1.39
30	A	813	CLA	C3D-C2D	3.64	1.48	1.39
38	8	310	KC1	CHC-C1C	3.64	1.47	1.39
30	A	844	CLA	CHC-C4B	3.64	1.47	1.39
39	6	303	DD6	C35-C34	3.64	1.58	1.52
30	15	302	CLA	C1B-NB	-3.64	1.33	1.37
38	13	311	KC1	OBD-CAD	3.64	1.28	1.22
30	16	308	CLA	CHC-C4B	3.64	1.47	1.39
30	F	202	CLA	CHD-C1D	3.64	1.45	1.38
30	2	301	CLA	C1D-ND	3.64	1.42	1.37
30	F	201	CLA	CHC-C4B	3.64	1.47	1.39
30	B	851	CLA	C1B-NB	-3.63	1.33	1.37
38	11	311	KC1	OBD-CAD	3.63	1.28	1.22
30	16	307	CLA	CHC-C4B	3.63	1.47	1.39
30	6	314	CLA	OBD-CAD	3.63	1.28	1.22
30	16	303	CLA	CHD-C1D	3.63	1.45	1.38
30	6	305	CLA	C4B-NB	-3.63	1.33	1.37
30	A	812	CLA	CHD-C1D	3.63	1.45	1.38
30	F	202	CLA	CHD-C4C	3.63	1.47	1.39
38	6	313	KC1	CHC-C1C	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	307	CLA	CHD-C4C	3.63	1.47	1.39
30	4	303	CLA	C3D-C2D	3.63	1.48	1.39
30	9	305	CLA	OBD-CAD	3.63	1.28	1.22
38	11	312	KC1	OBD-CAD	3.63	1.28	1.22
30	7	306	CLA	CHD-C4C	3.63	1.47	1.39
30	B	808	CLA	CHD-C4C	3.63	1.47	1.39
30	10	304	CLA	C1B-NB	-3.63	1.33	1.37
30	11	310	CLA	C3D-C2D	3.63	1.48	1.39
30	B	801	CLA	C1B-NB	-3.63	1.33	1.37
30	10	303	CLA	C1B-NB	-3.63	1.33	1.37
30	10	309	CLA	OBD-CAD	3.63	1.28	1.22
30	1	303	CLA	CHC-C4B	3.63	1.47	1.39
37	7	319	A86	C17-C18	-3.63	1.47	1.52
37	5	316	A86	C21-C20	3.63	1.57	1.51
37	6	320	A86	C21-C20	3.63	1.57	1.51
30	A	843	CLA	CHB-C1B	3.63	1.47	1.39
30	15	306	CLA	OBD-CAD	3.62	1.28	1.22
30	15	312	CLA	OBD-CAD	3.62	1.28	1.22
30	7	310	CLA	C3D-C2D	3.62	1.48	1.39
30	2	307	CLA	C1B-NB	-3.62	1.33	1.37
30	2u	202	CLA	CHD-C4C	3.62	1.47	1.39
30	B	837	CLA	CHC-C4B	3.62	1.47	1.39
30	B	834	CLA	CHC-C4B	3.62	1.47	1.39
30	11	304	CLA	C3D-C2D	3.62	1.48	1.39
38	12	309	KC1	C1B-NB	-3.62	1.33	1.37
30	F	202	CLA	CHB-C1B	3.62	1.47	1.39
30	8	308	CLA	CHC-C4B	3.62	1.47	1.39
30	A	808	CLA	CHD-C4C	3.62	1.47	1.39
30	A	827	CLA	CHC-C4B	3.62	1.47	1.39
30	1	307	CLA	C3D-C2D	3.62	1.48	1.39
30	1	305	CLA	C1B-NB	-3.62	1.33	1.37
30	A	842	CLA	C3D-C2D	3.62	1.48	1.39
30	B	839	CLA	C3D-C2D	3.62	1.48	1.39
30	A	844	CLA	OBD-CAD	3.62	1.28	1.22
37	13	315	A86	C19-C18	3.62	1.57	1.52
30	6	315	CLA	OBD-CAD	3.62	1.28	1.22
37	4	317	A86	C9-C10	3.62	1.54	1.43
30	A	833	CLA	C4B-NB	-3.62	1.33	1.37
30	B	814	CLA	C4B-NB	-3.62	1.33	1.37
30	2	309	CLA	C1B-NB	-3.62	1.33	1.37
38	13	306	KC1	C1B-NB	-3.62	1.33	1.37
30	B	803	CLA	O2A-CGA	3.61	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	307	CLA	OBD-CAD	3.61	1.28	1.22
30	16	306	CLA	C3D-C2D	3.61	1.48	1.39
38	11	307	KC1	OBD-CAD	3.61	1.28	1.22
30	8	301	CLA	C1B-NB	-3.61	1.33	1.37
30	8	301	CLA	CHD-C4C	3.61	1.47	1.39
30	6	317	CLA	OBD-CAD	3.61	1.28	1.22
30	14	305	CLA	OBD-CAD	3.61	1.28	1.22
30	A	816	CLA	CHD-C4C	3.61	1.47	1.39
30	L	202	CLA	C1B-NB	-3.61	1.33	1.37
38	12	305	KC1	CHC-C1C	3.61	1.47	1.39
30	5	304	CLA	C3D-C2D	3.61	1.48	1.39
30	5	307	CLA	C3D-C2D	3.61	1.48	1.39
30	A	836	CLA	CHD-C4C	3.61	1.47	1.39
30	A	815	CLA	C4B-NB	-3.61	1.33	1.37
30	B	816	CLA	C3D-C2D	3.61	1.48	1.39
30	12	308	CLA	OBD-CAD	3.61	1.28	1.22
30	6	307	CLA	C3D-C2D	3.61	1.48	1.39
30	15	307	CLA	CHC-C4B	3.61	1.47	1.39
30	14	310	CLA	OBD-CAD	3.61	1.28	1.22
30	13	301	CLA	OBD-CAD	3.61	1.28	1.22
30	B	815	CLA	C1B-NB	-3.61	1.33	1.37
30	A	803	CLA	CHD-C4C	3.61	1.47	1.39
30	J	101	CLA	CHC-C4B	3.61	1.47	1.39
30	B	836	CLA	CHC-C4B	3.61	1.47	1.39
30	A	809	CLA	C3D-C2D	3.61	1.48	1.39
30	B	827	CLA	CHD-C1D	3.61	1.45	1.38
30	A	823	CLA	C4B-NB	-3.61	1.33	1.37
30	B	832	CLA	C4B-NB	-3.61	1.33	1.37
38	6	313	KC1	C1B-NB	-3.61	1.33	1.37
30	A	835	CLA	C3D-C2D	3.61	1.48	1.39
30	9	307	CLA	C3D-C2D	3.61	1.48	1.39
30	14	310	CLA	C3D-C2D	3.61	1.48	1.39
30	A	825	CLA	C3D-C2D	3.60	1.48	1.39
30	11	309	CLA	C3D-C2D	3.60	1.48	1.39
30	A	819	CLA	CHD-C4C	3.60	1.47	1.39
30	7	303	CLA	CHC-C4B	3.60	1.47	1.39
30	13	301	CLA	CHC-C4B	3.60	1.47	1.39
30	16	301	CLA	OBD-CAD	3.60	1.28	1.22
30	A	810	CLA	CHD-C4C	3.60	1.47	1.39
30	B	837	CLA	CHD-C4C	3.60	1.47	1.39
30	2	311	CLA	CHC-C4B	3.60	1.47	1.39
30	11	310	CLA	CHC-C4B	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	304	CLA	OBD-CAD	3.60	1.28	1.22
38	4	310	KC1	OBD-CAD	3.60	1.28	1.22
38	9	312	KC1	OBD-CAD	3.60	1.28	1.22
30	9	302	CLA	C3D-C2D	3.60	1.48	1.39
38	16	304	KC1	OBD-CAD	3.60	1.28	1.22
30	B	831	CLA	C3D-C2D	3.60	1.48	1.39
37	14	314	A86	C17-C18	-3.60	1.47	1.52
30	B	803	CLA	C1D-ND	3.59	1.42	1.37
30	A	824	CLA	CHC-C4B	3.59	1.47	1.39
30	A	804	CLA	CHD-C4C	3.59	1.47	1.39
30	A	805	CLA	C3D-C2D	3.59	1.48	1.39
30	A	811	CLA	C3D-C2D	3.59	1.48	1.39
30	B	809	CLA	C3D-C2D	3.59	1.48	1.39
30	12	302	CLA	OBD-CAD	3.59	1.28	1.22
30	6	304	CLA	C3D-C2D	3.59	1.48	1.39
30	A	835	CLA	C4B-NB	-3.59	1.33	1.37
30	4	309	CLA	CHC-C4B	3.59	1.47	1.39
30	A	834	CLA	C1B-NB	-3.59	1.33	1.37
30	L	203	CLA	C1B-NB	-3.59	1.33	1.37
30	A	815	CLA	C3D-C2D	3.59	1.48	1.39
30	B	819	CLA	CHD-C4C	3.59	1.47	1.39
30	1	307	CLA	C1B-NB	-3.59	1.33	1.37
30	A	830	CLA	CHD-C1D	3.59	1.45	1.38
30	6	317	CLA	CHC-C4B	3.59	1.47	1.39
30	A	807	CLA	CHD-C4C	3.59	1.47	1.39
30	12	308	CLA	CHC-C4B	3.59	1.47	1.39
38	5	305	KC1	CHC-C1C	3.59	1.47	1.39
30	A	838	CLA	C3D-C2D	3.59	1.48	1.39
30	B	839	CLA	CHD-C1D	3.59	1.45	1.38
30	A	822	CLA	C1D-ND	3.59	1.42	1.37
30	13	307	CLA	C1B-NB	-3.59	1.33	1.37
30	10	305	CLA	C3D-C2D	3.59	1.48	1.39
30	6	315	CLA	CHC-C4B	3.58	1.47	1.39
30	A	812	CLA	CHD-C4C	3.58	1.47	1.39
30	5	308	CLA	OBD-CAD	3.58	1.28	1.22
38	8	306	KC1	OBD-CAD	3.58	1.28	1.22
30	L	202	CLA	C3D-C2D	3.58	1.48	1.39
30	A	826	CLA	CHD-C4C	3.58	1.47	1.39
39	11	313	DD6	O2-C18	3.58	1.53	1.43
38	1	306	KC1	CHC-C1C	3.58	1.47	1.39
30	3	303	CLA	C1B-NB	-3.58	1.33	1.37
38	12	311	KC1	C1B-NB	-3.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	806	CLA	CHD-C4C	3.58	1.47	1.39
30	7	309	CLA	C3D-C2D	3.58	1.48	1.39
38	5	305	KC1	C1B-NB	-3.58	1.33	1.37
37	15	322	A86	C17-C18	-3.58	1.47	1.52
30	F	203	CLA	CHC-C4B	3.58	1.47	1.39
30	B	831	CLA	C4B-NB	-3.58	1.33	1.37
30	7	311	CLA	CHC-C4B	3.58	1.47	1.39
30	B	834	CLA	CHD-C4C	3.58	1.47	1.39
30	11	308	CLA	CHC-C4B	3.58	1.47	1.39
30	B	824	CLA	C4B-NB	-3.58	1.33	1.37
38	14	306	KC1	OBD-CAD	3.58	1.28	1.22
38	12	305	KC1	C1B-NB	-3.58	1.33	1.37
30	A	842	CLA	CHD-C4C	3.57	1.47	1.39
30	12	321	CLA	CHC-C4B	3.57	1.47	1.39
30	7	312	CLA	OBD-CAD	3.57	1.28	1.22
38	11	305	KC1	C1B-NB	-3.57	1.33	1.37
30	10	309	CLA	CHC-C4B	3.57	1.47	1.39
38	2	306	KC1	OBD-CAD	3.57	1.28	1.22
30	5	303	CLA	C3D-C2D	3.57	1.48	1.39
30	14	313	CLA	CHC-C4B	3.57	1.47	1.39
30	A	831	CLA	CHD-C4C	3.57	1.47	1.39
38	9	304	KC1	CHC-C1C	3.57	1.47	1.39
38	1	306	KC1	OBD-CAD	3.57	1.28	1.22
30	10	308	CLA	OBD-CAD	3.57	1.28	1.22
30	14	313	CLA	CHB-C1B	3.57	1.47	1.39
38	4	308	KC1	OBD-CAD	3.57	1.28	1.22
30	9	308	CLA	CHC-C4B	3.57	1.47	1.39
30	14	303	CLA	CHC-C4B	3.57	1.47	1.39
30	L	203	CLA	C3D-C2D	3.57	1.48	1.39
30	A	832	CLA	C3D-C2D	3.57	1.48	1.39
30	B	809	CLA	CHD-C4C	3.57	1.47	1.39
30	A	839	CLA	C3D-C2D	3.56	1.48	1.39
30	A	834	CLA	C3D-C2D	3.56	1.48	1.39
30	A	837	CLA	CHC-C4B	3.56	1.47	1.39
37	14	318	A86	C19-C18	3.56	1.57	1.52
38	11	307	KC1	CHC-C1C	3.56	1.47	1.39
30	16	303	CLA	CHC-C4B	3.56	1.47	1.39
30	14	309	CLA	CHC-C4B	3.56	1.47	1.39
30	3	305	CLA	C1B-NB	-3.56	1.33	1.37
30	13	302	CLA	CHC-C4B	3.56	1.47	1.39
30	14	310	CLA	CHC-C4B	3.56	1.47	1.39
38	2	314	KC1	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	831	CLA	C1D-ND	3.56	1.42	1.37
30	15	305	CLA	CHC-C4B	3.56	1.47	1.39
30	15	309	CLA	CHC-C4B	3.56	1.47	1.39
39	2	315	DD6	C35-C34	3.56	1.58	1.52
30	13	303	CLA	CHC-C4B	3.56	1.47	1.39
37	8	315	A86	C10-C11	3.56	1.44	1.34
30	14	303	CLA	C1B-NB	-3.56	1.33	1.37
30	15	307	CLA	C1B-NB	-3.56	1.33	1.37
30	1	304	CLA	OBD-CAD	3.56	1.28	1.22
30	16	310	CLA	C3D-C2D	3.56	1.48	1.39
30	10	308	CLA	CHC-C4B	3.56	1.47	1.39
30	13	309	CLA	CHC-C4B	3.56	1.47	1.39
30	1	304	CLA	CHD-C4C	3.56	1.47	1.39
30	7	303	CLA	CHD-C4C	3.56	1.47	1.39
30	4	305	CLA	CHC-C4B	3.56	1.47	1.39
38	5	310	KC1	OBD-CAD	3.56	1.28	1.22
30	A	807	CLA	C4B-NB	-3.56	1.33	1.37
30	1	304	CLA	C1B-NB	-3.56	1.33	1.37
30	5	304	CLA	C1B-NB	-3.56	1.33	1.37
30	14	302	CLA	C1B-NB	-3.56	1.33	1.37
30	15	309	CLA	OBD-CAD	3.56	1.28	1.22
30	B	839	CLA	CHD-C4C	3.56	1.47	1.39
38	8	306	KC1	CHC-C1C	3.56	1.47	1.39
30	B	807	CLA	C4B-NB	-3.56	1.33	1.37
30	1	302	CLA	CHC-C4B	3.56	1.47	1.39
38	14	311	KC1	OBD-CAD	3.55	1.28	1.22
38	10	310	KC1	CHC-C1C	3.55	1.47	1.39
30	B	826	CLA	CHD-C1D	3.55	1.45	1.38
30	B	835	CLA	C3D-C2D	3.55	1.48	1.39
30	14	312	CLA	CHC-C4B	3.55	1.47	1.39
30	12	308	CLA	C3D-C2D	3.55	1.48	1.39
38	10	306	KC1	CHC-C1C	3.55	1.47	1.39
30	12	310	CLA	C3D-C2D	3.55	1.48	1.39
30	14	302	CLA	C3D-C2D	3.55	1.48	1.39
30	4	301	CLA	C4B-NB	-3.55	1.33	1.37
30	13	302	CLA	CHB-C1B	3.55	1.47	1.39
30	7	309	CLA	CHD-C4C	3.55	1.47	1.39
30	7	307	CLA	CHC-C4B	3.55	1.47	1.39
30	B	851	CLA	OBD-CAD	3.55	1.28	1.22
30	12	312	CLA	OBD-CAD	3.55	1.28	1.22
37	9	315	A86	C17-C18	-3.55	1.47	1.52
37	14	301	A86	C19-C18	3.55	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	309	CLA	OBD-CAD	3.55	1.28	1.22
38	13	310	KC1	OBD-CAD	3.55	1.28	1.22
30	F	202	CLA	C3D-C2D	3.55	1.48	1.39
30	10	311	CLA	CHC-C4B	3.55	1.47	1.39
30	A	817	CLA	C3D-C2D	3.55	1.48	1.39
30	4	302	CLA	C3D-C2D	3.55	1.48	1.39
30	8	304	CLA	CHD-C4C	3.55	1.47	1.39
30	B	819	CLA	C4B-NB	-3.55	1.33	1.37
30	B	825	CLA	CHD-C4C	3.55	1.47	1.39
38	9	304	KC1	C1B-NB	-3.55	1.33	1.37
38	13	305	KC1	C1B-NB	-3.55	1.33	1.37
39	2	317	DD6	O2-C18	3.55	1.53	1.43
38	9	312	KC1	CHC-C1C	3.54	1.47	1.39
30	B	832	CLA	C3D-C2D	3.54	1.48	1.39
39	15	318	DD6	C-C1	3.54	1.58	1.50
30	15	304	CLA	CHC-C4B	3.54	1.47	1.39
30	B	811	CLA	C1D-ND	3.54	1.42	1.37
30	3	302	CLA	C1B-NB	-3.54	1.33	1.37
30	13	304	CLA	CHC-C4B	3.54	1.47	1.39
30	7	307	CLA	C3D-C2D	3.54	1.48	1.39
38	10	306	KC1	OBD-CAD	3.54	1.28	1.22
30	L	203	CLA	OBD-CAD	3.54	1.28	1.22
30	A	832	CLA	C4B-NB	-3.54	1.33	1.37
30	9	302	CLA	CHC-C4B	3.54	1.47	1.39
38	16	304	KC1	C1B-NB	-3.54	1.33	1.37
30	A	818	CLA	CHD-C4C	3.54	1.47	1.39
30	5	302	CLA	CHC-C4B	3.54	1.47	1.39
30	A	841	CLA	CHC-C4B	3.54	1.47	1.39
30	B	811	CLA	CHD-C4C	3.54	1.47	1.39
30	A	837	CLA	OBD-CAD	3.54	1.28	1.22
30	6	316	CLA	OBD-CAD	3.54	1.28	1.22
30	3	307	CLA	CHC-C4B	3.54	1.47	1.39
38	5	312	KC1	OBD-CAD	3.53	1.28	1.22
30	2	311	CLA	C1B-NB	-3.53	1.33	1.37
38	11	305	KC1	CHC-C1C	3.53	1.47	1.39
30	B	806	CLA	C3D-C2D	3.53	1.48	1.39
38	2	312	KC1	OBD-CAD	3.53	1.28	1.22
30	A	829	CLA	CHD-C4C	3.53	1.47	1.39
30	2	309	CLA	CHC-C4B	3.53	1.47	1.39
30	12	307	CLA	CHD-C4C	3.53	1.47	1.39
30	B	801	CLA	C4B-NB	-3.53	1.33	1.37
30	12	303	CLA	C4B-NB	-3.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	808	CLA	C3D-C2D	3.53	1.48	1.39
38	6	311	KC1	C4B-NB	-3.53	1.33	1.37
30	10	304	CLA	CHC-C4B	3.53	1.47	1.39
30	A	806	CLA	CHD-C1D	3.53	1.45	1.38
38	5	312	KC1	CHC-C1C	3.53	1.47	1.39
30	15	313	CLA	C1B-NB	-3.53	1.33	1.37
30	A	804	CLA	C3D-C2D	3.53	1.48	1.39
30	A	820	CLA	C4B-NB	-3.53	1.33	1.37
38	7	313	KC1	C1B-NB	-3.53	1.33	1.37
33	A	847	BCR	C1-C6	-3.53	1.49	1.53
30	A	812	CLA	C3D-C2D	3.53	1.48	1.39
38	14	308	KC1	CHC-C1C	3.53	1.47	1.39
30	9	307	CLA	OBD-CAD	3.53	1.28	1.22
30	11	308	CLA	C1B-NB	-3.53	1.33	1.37
30	A	810	CLA	CHB-C1B	3.53	1.47	1.39
30	7	303	CLA	CHD-C1D	3.53	1.45	1.38
30	9	307	CLA	CHC-C4B	3.53	1.47	1.39
30	11	308	CLA	OBD-CAD	3.53	1.28	1.22
38	9	304	KC1	OBD-CAD	3.53	1.28	1.22
37	11	314	A86	C19-C18	3.52	1.57	1.52
30	12	302	CLA	CHD-C4C	3.52	1.47	1.39
30	15	304	CLA	C1B-NB	-3.52	1.33	1.37
30	2	309	CLA	OBD-CAD	3.52	1.28	1.22
38	13	305	KC1	OBD-CAD	3.52	1.28	1.22
30	B	820	CLA	C3D-C2D	3.52	1.48	1.39
37	15	321	A86	C19-C18	3.52	1.57	1.52
30	F	202	CLA	C4B-NB	-3.52	1.33	1.37
30	B	803	CLA	C4B-NB	-3.52	1.33	1.37
30	16	305	CLA	OBD-CAD	3.52	1.28	1.22
30	A	826	CLA	C3D-C2D	3.52	1.48	1.39
30	7	310	CLA	CHC-C4B	3.52	1.47	1.39
37	6	320	A86	C19-C18	3.52	1.57	1.52
30	15	312	CLA	C3D-C2D	3.52	1.48	1.39
29	A	801	CL0	CHD-C1D	3.51	1.45	1.39
30	5	303	CLA	CHC-C4B	3.51	1.47	1.39
30	15	314	CLA	CHC-C4B	3.51	1.47	1.39
38	11	311	KC1	C1B-NB	-3.51	1.33	1.37
38	13	308	KC1	C1B-NB	-3.51	1.33	1.37
39	7	318	DD6	O2-C18	3.51	1.53	1.43
30	A	810	CLA	C3D-C2D	3.51	1.48	1.39
30	12	308	CLA	C1B-NB	-3.51	1.33	1.37
39	12	317	DD6	O2-C18	3.51	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	301	CLA	C3D-C2D	3.51	1.48	1.39
30	5	307	CLA	C1B-NB	-3.51	1.33	1.37
30	B	824	CLA	C3D-C2D	3.51	1.48	1.39
30	B	822	CLA	C4B-NB	-3.51	1.33	1.37
30	4	301	CLA	CHD-C1D	3.51	1.45	1.38
30	9	302	CLA	OBD-CAD	3.51	1.28	1.22
30	10	303	CLA	OBD-CAD	3.51	1.28	1.22
38	13	308	KC1	OBD-CAD	3.51	1.28	1.22
30	B	836	CLA	C3D-C2D	3.51	1.48	1.39
30	13	301	CLA	C3D-C2D	3.51	1.48	1.39
30	3	305	CLA	CHC-C4B	3.51	1.47	1.39
37	9	313	A86	C9-C10	3.51	1.54	1.43
37	15	316	A86	C17-C18	-3.51	1.47	1.52
38	4	307	KC1	CHC-C1C	3.51	1.47	1.39
38	7	308	KC1	CHC-C1C	3.51	1.47	1.39
30	A	829	CLA	CHC-C4B	3.51	1.47	1.39
30	3	307	CLA	C1B-NB	-3.51	1.33	1.37
38	8	310	KC1	OBD-CAD	3.50	1.28	1.22
30	B	826	CLA	C3D-C2D	3.50	1.48	1.39
30	B	827	CLA	C1D-ND	3.50	1.42	1.37
30	16	301	CLA	C1B-NB	-3.50	1.33	1.37
30	B	826	CLA	C4B-NB	-3.50	1.33	1.37
30	B	813	CLA	CHD-C4C	3.50	1.47	1.39
38	14	311	KC1	C1B-NB	-3.50	1.33	1.37
39	6	303	DD6	O2-C18	3.50	1.53	1.43
38	8	312	KC1	OBD-CAD	3.50	1.28	1.22
30	10	305	CLA	CHB-C1B	3.50	1.47	1.39
30	11	306	CLA	C1B-NB	-3.50	1.33	1.37
30	A	822	CLA	C3D-C2D	3.50	1.48	1.39
30	9	301	CLA	C3D-C2D	3.50	1.48	1.39
30	9	307	CLA	C1B-NB	-3.50	1.33	1.37
30	B	827	CLA	CHD-C4C	3.50	1.47	1.39
30	B	801	CLA	CHB-C1B	3.50	1.47	1.39
30	12	310	CLA	CHC-C4B	3.50	1.47	1.39
30	6	310	CLA	CHC-C4B	3.50	1.47	1.39
30	B	811	CLA	CHB-C1B	3.50	1.47	1.39
30	B	814	CLA	C3D-C2D	3.49	1.48	1.39
38	12	309	KC1	OBD-CAD	3.49	1.28	1.22
30	B	827	CLA	C3D-C2D	3.49	1.48	1.39
39	3	312	DD6	C-C1	3.49	1.57	1.50
30	13	301	CLA	CHB-C1B	3.49	1.47	1.39
37	14	315	A86	C19-C18	3.49	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	302	CLA	C3D-C2D	3.49	1.48	1.39
30	B	814	CLA	CHD-C4C	3.49	1.47	1.39
37	10	301	A86	C9-C10	3.49	1.54	1.43
30	16	302	CLA	CHC-C4B	3.49	1.47	1.39
30	16	302	CLA	C1B-NB	-3.49	1.33	1.37
38	9	311	KC1	C1B-NB	-3.49	1.33	1.37
30	L	203	CLA	C4B-NB	-3.49	1.33	1.37
30	7	312	CLA	C1B-NB	-3.49	1.33	1.37
30	B	801	CLA	CHD-C1D	3.49	1.45	1.38
30	4	304	CLA	OBD-CAD	3.49	1.28	1.22
30	B	816	CLA	C1B-NB	-3.49	1.33	1.37
38	3	304	KC1	CHC-C1C	3.49	1.47	1.39
30	13	302	CLA	OBD-CAD	3.48	1.28	1.22
30	9	303	CLA	C4B-NB	-3.48	1.33	1.37
30	12	321	CLA	C1B-NB	-3.48	1.33	1.37
30	2	301	CLA	C3D-C2D	3.48	1.48	1.39
30	9	302	CLA	C4B-NB	-3.48	1.33	1.37
30	12	310	CLA	C1B-NB	-3.48	1.33	1.37
30	6	309	CLA	CHC-C4B	3.48	1.47	1.39
30	A	828	CLA	C3D-C2D	3.48	1.48	1.39
30	A	841	CLA	C4B-NB	-3.48	1.33	1.37
30	14	304	CLA	CHB-C1B	3.48	1.47	1.39
30	A	831	CLA	C4B-NB	-3.48	1.33	1.37
30	16	305	CLA	CHC-C4B	3.48	1.47	1.39
30	15	311	CLA	CHB-C1B	3.48	1.47	1.39
30	A	821	CLA	C3D-C2D	3.48	1.48	1.39
30	7	303	CLA	OBD-CAD	3.48	1.28	1.22
30	A	827	CLA	C4B-NB	-3.48	1.33	1.37
39	13	314	DD6	O2-C18	3.48	1.53	1.43
30	F	201	CLA	CHD-C1D	3.48	1.45	1.38
38	12	311	KC1	CHC-C1C	3.48	1.47	1.39
39	15	318	DD6	C35-C34	3.47	1.58	1.52
39	3	312	DD6	O2-C18	3.47	1.53	1.43
30	4	306	CLA	CHC-C4B	3.47	1.47	1.39
30	3	306	CLA	OBD-CAD	3.47	1.28	1.22
30	A	810	CLA	C4B-NB	-3.47	1.33	1.37
30	4	304	CLA	CHC-C4B	3.47	1.47	1.39
30	B	828	CLA	C4B-NB	-3.47	1.33	1.37
30	5	311	CLA	C1B-NB	-3.47	1.33	1.37
30	A	826	CLA	OBD-CAD	3.47	1.28	1.22
30	7	307	CLA	OBD-CAD	3.47	1.28	1.22
30	8	308	CLA	OBD-CAD	3.47	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	302	CLA	CHB-C1B	3.47	1.47	1.39
30	15	310	CLA	CHC-C4B	3.47	1.47	1.39
30	16	310	CLA	CHC-C4B	3.47	1.47	1.39
30	A	804	CLA	CHC-C4B	3.47	1.47	1.39
30	B	835	CLA	CHC-C4B	3.47	1.47	1.39
30	12	304	CLA	C1B-NB	-3.47	1.33	1.37
30	10	307	CLA	CHC-C4B	3.47	1.47	1.39
30	2	305	CLA	OBD-CAD	3.47	1.28	1.22
30	B	817	CLA	C3D-C2D	3.46	1.48	1.39
37	8	315	A86	C9-C10	3.46	1.53	1.43
30	A	817	CLA	OBD-CAD	3.46	1.28	1.22
39	1	310	DD6	O2-C18	3.46	1.53	1.43
30	6	309	CLA	C4B-NB	-3.46	1.33	1.37
30	A	821	CLA	CHB-C1B	3.46	1.47	1.39
30	B	851	CLA	C3D-C2D	3.46	1.48	1.39
30	15	306	CLA	C1B-NB	-3.46	1.33	1.37
38	5	306	KC1	C1B-NB	-3.46	1.33	1.37
30	4	303	CLA	CHC-C4B	3.46	1.47	1.39
30	B	822	CLA	C1D-ND	3.46	1.42	1.37
30	A	812	CLA	C4B-NB	-3.46	1.33	1.37
30	B	836	CLA	CHD-C1D	3.46	1.45	1.38
30	F	202	CLA	CHC-C4B	3.46	1.47	1.39
33	2u	201	BCR	C1-C6	-3.46	1.49	1.53
30	A	807	CLA	CHC-C4B	3.46	1.47	1.39
30	A	833	CLA	CHC-C4B	3.46	1.47	1.39
30	6	305	CLA	CHC-C4B	3.46	1.47	1.39
30	16	309	CLA	CHC-C4B	3.46	1.47	1.39
37	10	301	A86	C19-C18	3.46	1.57	1.52
30	3	303	CLA	CHC-C4B	3.46	1.47	1.39
30	1	301	CLA	OBD-CAD	3.46	1.28	1.22
37	12	314	A86	C19-C18	3.46	1.57	1.52
37	11	315	A86	C19-C18	3.46	1.57	1.52
30	3	306	CLA	C1B-NB	-3.46	1.33	1.37
39	15	318	DD6	O2-C18	3.46	1.53	1.43
30	J	101	CLA	C3D-C2D	3.46	1.48	1.39
30	8	303	CLA	C4B-NB	-3.46	1.33	1.37
30	8	309	CLA	CHC-C4B	3.46	1.47	1.39
30	B	802	CLA	CHC-C4B	3.46	1.47	1.39
38	6	312	KC1	OBD-CAD	3.46	1.28	1.22
30	B	806	CLA	C4B-NB	-3.46	1.33	1.37
30	12	312	CLA	CHC-C4B	3.46	1.47	1.39
37	15	320	A86	C17-C18	-3.46	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	304	CLA	C4B-NB	-3.45	1.33	1.37
30	5	309	CLA	CHC-C4B	3.45	1.47	1.39
30	10	304	CLA	CHB-C1B	3.45	1.47	1.39
30	L	203	CLA	CHB-C1B	3.45	1.47	1.39
38	2	306	KC1	C1B-NB	-3.45	1.33	1.37
30	B	804	CLA	CHC-C4B	3.45	1.47	1.39
30	12	310	CLA	CHB-C1B	3.45	1.47	1.39
37	7	316	A86	C9-C10	3.45	1.53	1.43
38	16	311	KC1	OBD-CAD	3.45	1.28	1.22
30	2u	202	CLA	CHC-C4B	3.45	1.47	1.39
30	A	802	CLA	C4B-NB	-3.45	1.33	1.37
30	5	309	CLA	C1B-NB	-3.45	1.33	1.37
30	B	828	CLA	OBD-CAD	3.45	1.28	1.22
38	12	313	KC1	OBD-CAD	3.45	1.28	1.22
33	J	103	BCR	C1-C6	-3.45	1.49	1.53
39	7	317	DD6	O2-C18	3.45	1.53	1.43
30	B	806	CLA	CHC-C4B	3.45	1.47	1.39
30	12	312	CLA	CHB-C1B	3.45	1.47	1.39
30	7	310	CLA	OBD-CAD	3.45	1.28	1.22
30	9	309	CLA	OBD-CAD	3.45	1.28	1.22
38	6	313	KC1	OBD-CAD	3.44	1.28	1.22
30	A	839	CLA	CHC-C4B	3.44	1.47	1.39
30	10	303	CLA	CHC-C4B	3.44	1.47	1.39
30	13	303	CLA	CHB-C1B	3.44	1.47	1.39
30	3	301	CLA	C4B-NB	-3.44	1.33	1.37
33	B	841	BCR	C1-C6	-3.44	1.49	1.53
30	F	203	CLA	OBD-CAD	3.44	1.28	1.22
30	A	808	CLA	CHC-C4B	3.44	1.47	1.39
30	A	814	CLA	OBD-CAD	3.44	1.28	1.22
30	16	303	CLA	OBD-CAD	3.44	1.28	1.22
30	5	302	CLA	OBD-CAD	3.44	1.28	1.22
30	9	308	CLA	C4B-NB	-3.44	1.33	1.37
38	5	305	KC1	OBD-CAD	3.44	1.28	1.22
30	1	304	CLA	CHB-C1B	3.44	1.47	1.39
30	2	308	CLA	OBD-CAD	3.44	1.28	1.22
38	7	313	KC1	C4B-NB	-3.44	1.33	1.37
30	B	802	CLA	CHD-C1D	3.44	1.45	1.38
30	B	851	CLA	C4B-NB	-3.44	1.33	1.37
30	6	306	CLA	CHC-C4B	3.44	1.47	1.39
37	3	314	A86	C19-C18	3.44	1.57	1.52
30	6	310	CLA	OBD-CAD	3.44	1.28	1.22
30	B	831	CLA	CHC-C4B	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	805	CLA	OBD-CAD	3.44	1.28	1.22
30	5	311	CLA	OBD-CAD	3.43	1.28	1.22
30	A	826	CLA	CHB-C1B	3.43	1.47	1.39
30	6	314	CLA	C3D-C2D	3.43	1.48	1.39
30	8	301	CLA	CHC-C4B	3.43	1.47	1.39
30	12	304	CLA	CHC-C4B	3.43	1.47	1.39
30	B	802	CLA	CHD-C4C	3.43	1.47	1.39
38	5	310	KC1	CHC-C1C	3.43	1.47	1.39
30	8	304	CLA	C4B-NB	-3.43	1.33	1.37
30	7	306	CLA	CHC-C4B	3.43	1.47	1.39
30	10	311	CLA	CHB-C1B	3.43	1.47	1.39
30	4	311	CLA	OBD-CAD	3.43	1.28	1.22
30	6	306	CLA	C4B-NB	-3.43	1.33	1.37
30	9	303	CLA	OBD-CAD	3.43	1.28	1.22
30	4	302	CLA	CHC-C4B	3.43	1.47	1.39
30	14	305	CLA	CHC-C4B	3.43	1.47	1.39
30	B	811	CLA	C3D-C2D	3.43	1.48	1.39
38	4	307	KC1	OBD-CAD	3.43	1.28	1.22
38	11	307	KC1	C1B-NB	-3.43	1.33	1.37
30	2	303	CLA	CHC-C4B	3.43	1.47	1.39
30	A	818	CLA	C3D-C2D	3.43	1.48	1.39
37	14	320	A86	C19-C18	3.43	1.57	1.52
38	7	313	KC1	OBD-CAD	3.43	1.28	1.22
38	12	311	KC1	OBD-CAD	3.43	1.28	1.22
30	J	101	CLA	OBD-CAD	3.43	1.28	1.22
30	5	309	CLA	OBD-CAD	3.43	1.28	1.22
30	7	304	CLA	C4B-NB	-3.43	1.33	1.37
30	7	312	CLA	CHC-C4B	3.42	1.47	1.39
30	3	310	CLA	C1B-NB	-3.42	1.33	1.37
30	12	308	CLA	CHB-C1B	3.42	1.47	1.39
38	4	308	KC1	CHC-C1C	3.42	1.47	1.39
30	7	303	CLA	C1D-ND	3.42	1.42	1.37
30	A	840	CLA	CHC-C4B	3.42	1.47	1.39
38	1	308	KC1	OBD-CAD	3.42	1.28	1.22
30	5	307	CLA	C4B-NB	-3.42	1.33	1.37
30	16	307	CLA	C1B-NB	-3.42	1.33	1.37
30	5	304	CLA	CHC-C4B	3.42	1.47	1.39
30	13	309	CLA	CHB-C1B	3.42	1.47	1.39
30	A	829	CLA	C3D-C2D	3.42	1.48	1.39
30	B	830	CLA	OBD-CAD	3.42	1.28	1.22
30	14	310	CLA	C1B-NB	-3.42	1.33	1.37
30	15	310	CLA	C1B-NB	-3.42	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	808	CLA	OBD-CAD	3.42	1.28	1.22
30	B	809	CLA	CHB-C1B	3.42	1.47	1.39
30	B	804	CLA	OBD-CAD	3.42	1.28	1.22
30	B	821	CLA	C3D-C2D	3.42	1.48	1.39
37	15	317	A86	C19-C18	3.42	1.57	1.52
30	15	308	CLA	C1B-NB	-3.42	1.33	1.37
30	B	837	CLA	C3D-C2D	3.42	1.48	1.39
30	1	302	CLA	OBD-CAD	3.42	1.28	1.22
37	9	315	A86	C19-C18	3.42	1.57	1.52
30	1	305	CLA	OBD-CAD	3.42	1.28	1.22
30	5	308	CLA	C4B-NB	-3.42	1.33	1.37
30	B	820	CLA	CHB-C1B	3.42	1.47	1.39
30	16	308	CLA	C1B-NB	-3.42	1.33	1.37
30	B	826	CLA	CHD-C4C	3.42	1.47	1.39
30	B	825	CLA	C4B-NB	-3.42	1.33	1.37
37	8	318	A86	C19-C18	3.41	1.57	1.52
30	5	302	CLA	C3D-C2D	3.41	1.48	1.39
30	16	309	CLA	C1B-NB	-3.41	1.33	1.37
30	3	305	CLA	OBD-CAD	3.41	1.28	1.22
39	7	302	DD6	C-C1	3.41	1.57	1.50
39	2	317	DD6	C35-C34	3.41	1.58	1.52
30	B	851	CLA	CHC-C4B	3.41	1.47	1.39
39	15	319	DD6	O2-C18	3.41	1.53	1.43
30	10	309	CLA	C1B-NB	-3.41	1.33	1.37
39	10	314	DD6	O2-C18	3.41	1.53	1.43
30	A	830	CLA	CHD-C4C	3.41	1.47	1.39
30	B	829	CLA	CHC-C4B	3.41	1.47	1.39
30	4	304	CLA	C3D-C2D	3.41	1.48	1.39
38	12	313	KC1	CHC-C1C	3.41	1.47	1.39
30	1	305	CLA	CHC-C4B	3.41	1.47	1.39
30	A	827	CLA	CHD-C4C	3.41	1.47	1.39
30	A	815	CLA	OBD-CAD	3.41	1.28	1.22
30	9	303	CLA	CHC-C4B	3.41	1.47	1.39
30	11	309	CLA	C4B-NB	-3.41	1.33	1.37
30	A	808	CLA	OBD-CAD	3.41	1.28	1.22
30	9	306	CLA	CHC-C4B	3.40	1.47	1.39
30	L	202	CLA	CHD-C1D	3.40	1.45	1.38
30	16	310	CLA	CHB-C1B	3.40	1.47	1.39
30	13	302	CLA	C1B-NB	-3.40	1.33	1.37
30	A	805	CLA	OBD-CAD	3.40	1.28	1.22
30	10	311	CLA	C1B-NB	-3.40	1.33	1.37
30	14	309	CLA	C1B-NB	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	303	CLA	C1B-NB	-3.40	1.33	1.37
30	16	309	CLA	CHB-C1B	3.40	1.47	1.39
30	B	823	CLA	CHC-C4B	3.40	1.47	1.39
30	3	302	CLA	CHB-C1B	3.40	1.47	1.39
30	5	311	CLA	CHB-C1B	3.40	1.47	1.39
30	6	309	CLA	OBD-CAD	3.40	1.28	1.22
38	13	306	KC1	OBD-CAD	3.40	1.28	1.22
30	4	301	CLA	CHC-C4B	3.40	1.47	1.39
30	A	821	CLA	CHD-C4C	3.40	1.46	1.39
30	L	203	CLA	CHC-C4B	3.40	1.47	1.39
38	7	308	KC1	OBD-CAD	3.40	1.28	1.22
30	B	814	CLA	OBD-CAD	3.40	1.28	1.22
30	B	807	CLA	CHB-C1B	3.40	1.47	1.39
30	2	301	CLA	CHB-C1B	3.40	1.47	1.39
38	8	311	KC1	OBD-CAD	3.40	1.28	1.22
30	3	302	CLA	C4B-NB	-3.40	1.33	1.37
39	3	316	DD6	O2-C18	3.40	1.53	1.43
30	9	305	CLA	CHC-C4B	3.40	1.47	1.39
30	4	302	CLA	OBD-CAD	3.40	1.28	1.22
30	4	306	CLA	OBD-CAD	3.40	1.28	1.22
30	A	827	CLA	CHD-C1D	3.40	1.45	1.38
39	5	313	DD6	O2-C18	3.40	1.53	1.43
30	1	307	CLA	CHC-C4B	3.40	1.47	1.39
30	3	309	CLA	C1B-NB	-3.40	1.33	1.37
30	5	311	CLA	C4B-NB	-3.40	1.33	1.37
30	2	301	CLA	CHD-C1D	3.40	1.45	1.38
30	L	202	CLA	CHC-C4B	3.39	1.47	1.39
30	10	309	CLA	CHB-C1B	3.39	1.47	1.39
30	8	305	CLA	CHC-C4B	3.39	1.47	1.39
30	A	819	CLA	C3D-C2D	3.39	1.48	1.39
30	9	301	CLA	CHD-C1D	3.39	1.45	1.38
30	B	823	CLA	C3D-C2D	3.39	1.48	1.39
30	A	842	CLA	OBD-CAD	3.39	1.28	1.22
30	6	304	CLA	OBD-CAD	3.39	1.28	1.22
30	16	307	CLA	CHB-C1B	3.39	1.47	1.39
30	15	306	CLA	CHC-C4B	3.39	1.47	1.39
39	12	315	DD6	O2-C18	3.39	1.53	1.43
38	16	304	KC1	CHD-C1D	3.39	1.47	1.39
30	2	310	CLA	OBD-CAD	3.39	1.28	1.22
39	9	314	DD6	C-C1	3.39	1.57	1.50
30	A	811	CLA	OBD-CAD	3.39	1.28	1.22
30	B	808	CLA	C4B-NB	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	309	CLA	CHC-C4B	3.38	1.47	1.39
30	8	305	CLA	CHD-C4C	3.38	1.46	1.39
30	15	306	CLA	CHB-C1B	3.38	1.47	1.39
30	2u	202	CLA	CHB-C1B	3.38	1.47	1.39
30	B	835	CLA	C4B-NB	-3.38	1.33	1.37
39	9	314	DD6	O2-C18	3.38	1.53	1.43
30	B	824	CLA	CHC-C4B	3.38	1.47	1.39
38	9	310	KC1	OBD-CAD	3.38	1.28	1.22
30	7	305	CLA	C3D-C2D	3.38	1.48	1.39
30	1	303	CLA	OBD-CAD	3.38	1.28	1.22
39	15	319	DD6	C-C1	3.38	1.57	1.50
30	2	305	CLA	C4B-NB	-3.38	1.33	1.37
30	4	306	CLA	C4B-NB	-3.38	1.33	1.37
30	6	307	CLA	OBD-CAD	3.38	1.28	1.22
30	6	304	CLA	CHC-C4B	3.38	1.47	1.39
30	14	309	CLA	CHB-C1B	3.38	1.47	1.39
30	A	812	CLA	CHC-C4B	3.38	1.47	1.39
30	6	317	CLA	C1B-NB	-3.38	1.33	1.37
30	A	803	CLA	CHC-C4B	3.38	1.47	1.39
30	A	817	CLA	CHC-C4B	3.38	1.47	1.39
30	12	303	CLA	CHC-C4B	3.38	1.47	1.39
30	A	822	CLA	C4B-NB	-3.38	1.33	1.37
30	9	306	CLA	C1B-NB	-3.38	1.33	1.37
30	12	312	CLA	C1B-NB	-3.38	1.33	1.37
39	4	316	DD6	O2-C18	3.37	1.53	1.43
30	L	202	CLA	OBD-CAD	3.37	1.28	1.22
30	A	817	CLA	CHB-C1B	3.37	1.47	1.39
30	5	311	CLA	CHC-C4B	3.37	1.47	1.39
30	6	315	CLA	CHB-C1B	3.37	1.47	1.39
30	B	818	CLA	C4B-NB	-3.37	1.33	1.37
38	4	308	KC1	C4B-NB	-3.37	1.33	1.37
30	A	834	CLA	CHC-C4B	3.37	1.47	1.39
30	A	840	CLA	C3D-C2D	3.37	1.48	1.39
39	6	318	DD6	O2-C18	3.37	1.53	1.43
30	B	822	CLA	CHC-C4B	3.37	1.47	1.39
39	3	313	DD6	O2-C18	3.37	1.53	1.43
30	7	307	CLA	C4B-NB	-3.37	1.33	1.37
30	4	311	CLA	CHC-C4B	3.37	1.47	1.39
30	16	303	CLA	C1B-NB	-3.37	1.33	1.37
37	16	312	A86	C19-C18	3.37	1.57	1.52
30	B	819	CLA	OBD-CAD	3.36	1.28	1.22
30	B	809	CLA	C4B-NB	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	309	CLA	C1B-NB	-3.36	1.33	1.37
30	8	303	CLA	OBD-CAD	3.36	1.28	1.22
30	13	304	CLA	CHB-C1B	3.36	1.47	1.39
30	6	315	CLA	C1B-NB	-3.36	1.33	1.37
30	B	825	CLA	C3D-C2D	3.36	1.48	1.39
30	15	305	CLA	C1B-NB	-3.36	1.33	1.37
37	7	315	A86	C19-C18	3.36	1.57	1.52
30	B	832	CLA	CHC-C4B	3.36	1.47	1.39
30	15	310	CLA	CHB-C1B	3.36	1.47	1.39
30	B	820	CLA	C1B-NB	-3.36	1.33	1.37
37	15	322	A86	C14-C15	3.36	1.59	1.52
30	11	304	CLA	C1B-NB	-3.36	1.33	1.37
30	7	305	CLA	C4B-NB	-3.36	1.33	1.37
30	10	305	CLA	OBD-CAD	3.36	1.28	1.22
30	4	311	CLA	CAA-C2A	3.36	1.60	1.54
30	B	829	CLA	OBD-CAD	3.36	1.28	1.22
30	A	816	CLA	C4B-NB	-3.36	1.33	1.37
30	8	301	CLA	OBD-CAD	3.36	1.28	1.22
30	B	819	CLA	CHC-C4B	3.36	1.46	1.39
38	9	312	KC1	C1B-NB	-3.36	1.33	1.37
30	A	816	CLA	CHB-C1B	3.36	1.46	1.39
38	4	307	KC1	CHD-C1D	3.36	1.46	1.39
37	10	317	A86	C17-C18	-3.36	1.47	1.52
39	7	314	DD6	O2-C18	3.36	1.53	1.43
30	B	827	CLA	C4B-NB	-3.36	1.33	1.37
30	J	101	CLA	C4B-NB	-3.36	1.33	1.37
30	5	302	CLA	C4B-NB	-3.36	1.33	1.37
38	8	307	KC1	OBD-CAD	3.35	1.28	1.22
30	10	307	CLA	OBD-CAD	3.35	1.28	1.22
30	2	313	CLA	C1B-NB	-3.35	1.33	1.37
39	10	313	DD6	O2-C18	3.35	1.53	1.43
30	2	307	CLA	OBD-CAD	3.35	1.28	1.22
30	15	305	CLA	CHB-C1B	3.35	1.46	1.39
30	A	844	CLA	CHB-C1B	3.35	1.46	1.39
30	6	316	CLA	CHC-C4B	3.35	1.46	1.39
38	14	308	KC1	CHD-C1D	3.35	1.46	1.39
30	B	821	CLA	C4B-NB	-3.35	1.33	1.37
30	B	802	CLA	C1D-ND	3.35	1.42	1.37
30	A	823	CLA	CHC-C4B	3.35	1.46	1.39
30	A	810	CLA	OBD-CAD	3.35	1.28	1.22
30	A	827	CLA	C3D-C2D	3.35	1.48	1.39
30	A	803	CLA	CHD-C1D	3.35	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	302	CLA	CHC-C4B	3.35	1.46	1.39
30	A	838	CLA	CHC-C4B	3.35	1.46	1.39
30	A	813	CLA	OBD-CAD	3.35	1.28	1.22
39	3	313	DD6	C-C1	3.35	1.57	1.50
39	7	302	DD6	O2-C18	3.35	1.53	1.43
39	6	321	DD6	O2-C18	3.35	1.53	1.43
30	3	309	CLA	CHB-C1B	3.35	1.46	1.39
30	A	816	CLA	OBD-CAD	3.34	1.28	1.22
38	3	304	KC1	OBD-CAD	3.34	1.28	1.22
30	9	301	CLA	OBD-CAD	3.34	1.28	1.22
30	B	826	CLA	CHB-C1B	3.34	1.46	1.39
30	A	843	CLA	OBD-CAD	3.34	1.28	1.22
39	2	315	DD6	O2-C18	3.34	1.53	1.43
30	A	825	CLA	CHC-C4B	3.34	1.46	1.39
39	3	312	DD6	C35-C34	3.34	1.58	1.52
30	B	820	CLA	CHD-C1D	3.34	1.44	1.38
30	A	819	CLA	C4B-NB	-3.34	1.33	1.37
30	A	839	CLA	C4B-NB	-3.34	1.33	1.37
30	B	811	CLA	C4B-NB	-3.34	1.33	1.37
30	2	304	CLA	CHC-C4B	3.34	1.46	1.39
30	B	807	CLA	CHC-C4B	3.34	1.46	1.39
30	B	801	CLA	CHC-C4B	3.34	1.46	1.39
30	16	310	CLA	C1B-NB	-3.34	1.33	1.37
30	12	304	CLA	OBD-CAD	3.34	1.28	1.22
30	A	824	CLA	C3D-C2D	3.34	1.48	1.39
30	B	826	CLA	OBD-CAD	3.34	1.28	1.22
30	A	834	CLA	OBD-CAD	3.33	1.28	1.22
38	16	311	KC1	CHD-C1D	3.33	1.46	1.39
38	14	308	KC1	C1B-NB	-3.33	1.33	1.37
30	A	836	CLA	OBD-CAD	3.33	1.28	1.22
30	B	812	CLA	OBD-CAD	3.33	1.28	1.22
30	A	806	CLA	OBD-CAD	3.33	1.28	1.22
30	B	820	CLA	CHD-C4C	3.33	1.46	1.39
38	3	308	KC1	CHC-C1C	3.33	1.46	1.39
30	8	305	CLA	CHD-C1D	3.33	1.44	1.38
30	15	314	CLA	C4B-NB	-3.33	1.33	1.37
30	B	820	CLA	OBD-CAD	3.33	1.28	1.22
38	10	310	KC1	OBD-CAD	3.33	1.28	1.22
30	14	312	CLA	C1B-NB	-3.33	1.33	1.37
33	J	102	BCR	C1-C6	-3.33	1.49	1.53
30	B	817	CLA	OBD-CAD	3.33	1.28	1.22
30	3	310	CLA	CHC-C4B	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	307	CLA	CHB-C1B	3.33	1.46	1.39
39	16	313	DD6	C-C1	3.33	1.57	1.50
30	4	311	CLA	C4B-NB	-3.33	1.33	1.37
30	7	305	CLA	CHC-C4B	3.33	1.46	1.39
39	16	313	DD6	O2-C18	3.33	1.53	1.43
30	9	306	CLA	C4B-NB	-3.33	1.33	1.37
30	2	311	CLA	CHB-C1B	3.33	1.46	1.39
30	7	311	CLA	OBD-CAD	3.33	1.28	1.22
33	B	841	BCR	C30-C25	-3.33	1.49	1.53
30	1	301	CLA	CHC-C4B	3.33	1.46	1.39
30	2	307	CLA	CHC-C4B	3.33	1.46	1.39
30	7	306	CLA	C4B-NB	-3.32	1.33	1.37
30	B	822	CLA	C3D-C2D	3.32	1.48	1.39
30	A	844	CLA	C1B-NB	-3.32	1.33	1.37
30	5	307	CLA	CHC-C4B	3.32	1.46	1.39
30	4	309	CLA	CHB-C1B	3.32	1.46	1.39
30	5	308	CLA	CHC-C4B	3.32	1.46	1.39
30	A	803	CLA	OBD-CAD	3.32	1.28	1.22
30	B	823	CLA	C4B-NB	-3.32	1.33	1.37
30	2	309	CLA	CHB-C1B	3.32	1.46	1.39
38	13	312	KC1	CHD-C1D	3.32	1.46	1.39
30	2u	202	CLA	OBD-CAD	3.32	1.28	1.22
30	7	312	CLA	CHB-C1B	3.32	1.46	1.39
30	B	839	CLA	OBD-CAD	3.32	1.28	1.22
30	15	303	CLA	CHB-C1B	3.32	1.46	1.39
30	B	811	CLA	CHC-C4B	3.32	1.46	1.39
30	B	803	CLA	CHC-C4B	3.32	1.46	1.39
30	1	307	CLA	CHB-C1B	3.32	1.46	1.39
30	12	302	CLA	CHC-C4B	3.32	1.46	1.39
30	2	310	CLA	C4B-NB	-3.32	1.33	1.37
30	2	313	CLA	CHB-C1B	3.31	1.46	1.39
30	A	817	CLA	C4B-NB	-3.31	1.33	1.37
30	2	310	CLA	CHC-C4B	3.31	1.46	1.39
30	A	806	CLA	CHC-C4B	3.31	1.46	1.39
30	9	309	CLA	C4B-NB	-3.31	1.33	1.37
38	9	311	KC1	CHD-C1D	3.31	1.46	1.39
30	A	842	CLA	CHB-C1B	3.31	1.46	1.39
30	B	810	CLA	CHB-C1B	3.31	1.46	1.39
30	B	824	CLA	OBD-CAD	3.31	1.28	1.22
30	15	312	CLA	CHC-C4B	3.31	1.46	1.39
30	7	309	CLA	CHB-C1B	3.31	1.46	1.39
30	F	201	CLA	CHD-C4C	3.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	307	CLA	C1B-NB	-3.31	1.33	1.37
38	11	312	KC1	CHC-C1C	3.31	1.46	1.39
30	B	816	CLA	OBD-CAD	3.31	1.28	1.22
39	6	319	DD6	O2-C18	3.31	1.53	1.43
30	12	303	CLA	CHB-C1B	3.31	1.46	1.39
30	10	307	CLA	C4B-NB	-3.30	1.33	1.37
30	2	305	CLA	CHB-C1B	3.30	1.46	1.39
30	2	305	CLA	CHC-C4B	3.30	1.46	1.39
38	3	308	KC1	OBD-CAD	3.30	1.28	1.22
30	12	306	CLA	CHC-C4B	3.30	1.46	1.39
30	A	806	CLA	C3D-C2D	3.30	1.48	1.39
30	B	810	CLA	C3D-C2D	3.30	1.48	1.39
30	B	809	CLA	C1D-ND	3.30	1.42	1.37
30	15	309	CLA	CHB-C1B	3.30	1.46	1.39
30	11	310	CLA	C1B-NB	-3.30	1.33	1.37
30	A	823	CLA	OBD-CAD	3.30	1.28	1.22
30	B	827	CLA	CHC-C4B	3.30	1.46	1.39
30	B	817	CLA	C4B-NB	-3.30	1.33	1.37
30	6	317	CLA	CHB-C1B	3.30	1.46	1.39
30	A	823	CLA	CHB-C1B	3.30	1.46	1.39
30	B	813	CLA	CHC-C4B	3.30	1.46	1.39
30	11	310	CLA	CHB-C1B	3.29	1.46	1.39
38	6	311	KC1	CHC-C1C	3.29	1.46	1.39
30	B	801	CLA	C3D-C2D	3.29	1.48	1.39
30	F	201	CLA	C1D-ND	3.29	1.42	1.37
39	7	317	DD6	C-C1	3.29	1.57	1.50
30	16	301	CLA	CHB-C1B	3.29	1.46	1.39
38	13	310	KC1	C1B-NB	-3.29	1.33	1.37
30	A	822	CLA	CHC-C4B	3.29	1.46	1.39
30	B	825	CLA	CHB-C1B	3.29	1.46	1.39
30	8	302	CLA	CHC-C4B	3.29	1.46	1.39
30	A	821	CLA	OBD-CAD	3.29	1.28	1.22
30	A	820	CLA	CHC-C4B	3.29	1.46	1.39
30	A	822	CLA	OBD-CAD	3.29	1.28	1.22
38	13	311	KC1	C1B-NB	-3.29	1.33	1.37
30	8	305	CLA	C3D-C2D	3.29	1.48	1.39
39	6	319	DD6	C-C1	3.29	1.57	1.50
30	B	819	CLA	C3D-C2D	3.29	1.48	1.39
30	A	813	CLA	CHC-C4B	3.29	1.46	1.39
38	3	308	KC1	C1B-NB	-3.29	1.33	1.37
30	B	822	CLA	OBD-CAD	3.29	1.28	1.22
30	A	805	CLA	C4B-NB	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	812	CLA	CHC-C4B	3.29	1.46	1.39
39	7	318	DD6	C-C1	3.29	1.57	1.50
30	B	801	CLA	CHD-C4C	3.29	1.46	1.39
30	A	834	CLA	C4B-NB	-3.29	1.33	1.37
38	8	313	KC1	C4B-NB	-3.29	1.33	1.37
39	2	315	DD6	C-C1	3.29	1.57	1.50
30	4	304	CLA	C4B-NB	-3.28	1.33	1.37
30	7	309	CLA	CHC-C4B	3.28	1.46	1.39
30	A	832	CLA	CHC-C4B	3.28	1.46	1.39
30	5	309	CLA	CHB-C1B	3.28	1.46	1.39
30	6	307	CLA	CHC-C4B	3.28	1.46	1.39
30	2	310	CLA	CHB-C1B	3.28	1.46	1.39
30	4	305	CLA	OBD-CAD	3.28	1.28	1.22
30	7	309	CLA	C4B-NB	-3.28	1.33	1.37
30	8	305	CLA	CHB-C1B	3.28	1.46	1.39
30	B	830	CLA	C3D-C2D	3.28	1.47	1.39
30	15	313	CLA	CHB-C1B	3.28	1.46	1.39
30	2	304	CLA	OBD-CAD	3.28	1.28	1.22
30	B	814	CLA	CHC-C4B	3.28	1.46	1.39
39	13	314	DD6	C-C1	3.28	1.57	1.50
38	8	312	KC1	C1B-NB	-3.28	1.33	1.37
30	2	304	CLA	C4B-NB	-3.28	1.33	1.37
30	12	306	CLA	OBD-CAD	3.28	1.28	1.22
30	15	309	CLA	C1B-NB	-3.28	1.33	1.37
30	6	314	CLA	CHC-C4B	3.28	1.46	1.39
30	12	310	CLA	OBD-CAD	3.28	1.28	1.22
30	B	820	CLA	C4B-NB	-3.28	1.33	1.37
30	13	307	CLA	CHB-C1B	3.27	1.46	1.39
30	2	301	CLA	OBD-CAD	3.27	1.28	1.22
30	7	303	CLA	C4B-NB	-3.27	1.33	1.37
38	4	310	KC1	CHD-C1D	3.27	1.46	1.39
37	14	317	A86	C19-C18	3.27	1.56	1.52
30	16	306	CLA	CHB-C1B	3.27	1.46	1.39
30	A	811	CLA	C4B-NB	-3.27	1.33	1.37
30	5	303	CLA	CHB-C1B	3.27	1.46	1.39
30	12	307	CLA	CHB-C1B	3.27	1.46	1.39
30	1	302	CLA	CHB-C1B	3.27	1.46	1.39
30	6	304	CLA	C4B-NB	-3.27	1.33	1.37
30	10	305	CLA	C1B-NB	-3.27	1.33	1.37
30	3	301	CLA	CHC-C4B	3.27	1.46	1.39
30	B	836	CLA	CHB-C1B	3.27	1.46	1.39
30	10	305	CLA	CHC-C4B	3.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	3	315	A86	C19-C18	3.27	1.56	1.52
30	2	307	CLA	C4B-NB	-3.27	1.33	1.37
30	A	830	CLA	OBD-CAD	3.27	1.28	1.22
30	B	834	CLA	CHB-C1B	3.27	1.46	1.39
30	A	824	CLA	CHB-C1B	3.27	1.46	1.39
30	5	304	CLA	CHB-C1B	3.27	1.46	1.39
30	B	818	CLA	OBD-CAD	3.26	1.28	1.22
30	4	303	CLA	CHB-C1B	3.26	1.46	1.39
30	8	304	CLA	CHC-C4B	3.26	1.46	1.39
30	A	828	CLA	CHC-C4B	3.26	1.46	1.39
39	3	316	DD6	C35-C34	3.26	1.57	1.52
30	5	307	CLA	OBD-CAD	3.26	1.28	1.22
39	12	315	DD6	C-C1	3.26	1.57	1.50
30	2	301	CLA	CHC-C4B	3.26	1.46	1.39
30	2	303	CLA	C1D-ND	3.26	1.42	1.37
39	1	310	DD6	C-C1	3.26	1.57	1.50
30	12	321	CLA	OBD-CAD	3.26	1.28	1.22
30	B	828	CLA	CHB-C1B	3.26	1.46	1.39
30	A	821	CLA	CHC-C4B	3.26	1.46	1.39
30	14	307	CLA	CHB-C1B	3.26	1.46	1.39
30	B	816	CLA	CHB-C1B	3.26	1.46	1.39
39	12	317	DD6	C-C1	3.26	1.57	1.50
30	A	834	CLA	CHB-C1B	3.26	1.46	1.39
33	B	845	BCR	C30-C25	-3.25	1.49	1.53
30	14	304	CLA	C1B-NB	-3.25	1.33	1.37
39	8	317	DD6	O2-C18	3.25	1.52	1.43
30	F	203	CLA	CHB-C1B	3.25	1.46	1.39
30	4	303	CLA	OBD-CAD	3.25	1.28	1.22
30	B	828	CLA	CHC-C4B	3.25	1.46	1.39
38	3	311	KC1	CHD-C1D	3.25	1.46	1.39
30	B	816	CLA	C4B-NB	-3.25	1.33	1.37
38	6	313	KC1	C4B-NB	-3.25	1.33	1.37
30	A	828	CLA	CHD-C1D	3.25	1.44	1.38
30	3	310	CLA	CHB-C1B	3.25	1.46	1.39
30	A	820	CLA	OBD-CAD	3.25	1.28	1.22
30	A	833	CLA	OBD-CAD	3.25	1.28	1.22
30	9	309	CLA	CHB-C1B	3.25	1.46	1.39
30	B	813	CLA	OBD-CAD	3.25	1.28	1.22
30	13	301	CLA	C1B-NB	-3.25	1.33	1.37
30	12	321	CLA	CHB-C1B	3.25	1.46	1.39
39	4	316	DD6	C-C1	3.25	1.57	1.50
37	13	313	A86	C25-C24	3.25	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	301	CLA	CHB-C1B	3.25	1.46	1.39
38	2	306	KC1	CHD-C1D	3.25	1.46	1.39
37	15	320	A86	C25-C24	3.24	1.43	1.34
30	16	308	CLA	CHB-C1B	3.24	1.46	1.39
38	13	308	KC1	CHD-C1D	3.24	1.46	1.39
39	8	317	DD6	C-C1	3.24	1.57	1.50
37	2u	203	A86	C19-C18	3.24	1.56	1.52
30	B	838	CLA	C4B-NB	-3.24	1.33	1.37
30	F	201	CLA	CHB-C1B	3.24	1.46	1.39
30	16	310	CLA	OBD-CAD	3.24	1.28	1.22
30	B	818	CLA	CHC-C4B	3.24	1.46	1.39
30	5	302	CLA	CHB-C1B	3.24	1.46	1.39
30	16	303	CLA	CHB-C1B	3.24	1.46	1.39
38	5	306	KC1	CHD-C1D	3.24	1.46	1.39
30	F	201	CLA	OBD-CAD	3.24	1.28	1.22
30	B	829	CLA	C4B-NB	-3.24	1.33	1.37
30	15	314	CLA	CHB-C1B	3.24	1.46	1.39
30	A	812	CLA	OBD-CAD	3.24	1.28	1.22
30	A	835	CLA	CHC-C4B	3.24	1.46	1.39
30	A	811	CLA	CHC-C4B	3.24	1.46	1.39
30	B	826	CLA	CHC-C4B	3.23	1.46	1.39
30	B	810	CLA	OBD-CAD	3.23	1.28	1.22
30	A	818	CLA	OBD-CAD	3.23	1.28	1.22
37	2	318	A86	C19-C18	3.23	1.56	1.52
30	B	832	CLA	OBD-CAD	3.23	1.28	1.22
30	3	307	CLA	CHB-C1B	3.23	1.46	1.39
39	6	303	DD6	C-C1	3.23	1.57	1.50
30	A	804	CLA	CHB-C1B	3.23	1.46	1.39
30	8	303	CLA	CHB-C1B	3.23	1.46	1.39
30	13	303	CLA	C1B-NB	-3.23	1.33	1.37
39	10	313	DD6	C-C1	3.23	1.57	1.50
30	L	202	CLA	C4B-NB	-3.23	1.33	1.37
30	10	305	CLA	C4B-NB	-3.23	1.33	1.37
30	B	827	CLA	CHB-C1B	3.23	1.46	1.39
30	14	312	CLA	CHB-C1B	3.23	1.46	1.39
30	A	816	CLA	CHC-C4B	3.23	1.46	1.39
30	A	825	CLA	C4B-NB	-3.23	1.33	1.37
38	8	310	KC1	C4B-NB	-3.23	1.33	1.37
30	A	843	CLA	CHC-C4B	3.23	1.46	1.39
30	A	804	CLA	OBD-CAD	3.23	1.28	1.22
38	11	305	KC1	OBD-CAD	3.23	1.28	1.22
33	M	101	BCR	C1-C6	-3.23	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	11	313	DD6	C-C1	3.22	1.57	1.50
30	A	810	CLA	CHC-C4B	3.22	1.46	1.39
30	7	306	CLA	OBD-CAD	3.22	1.28	1.22
38	13	312	KC1	C1B-NB	-3.22	1.33	1.37
30	B	823	CLA	CHB-C1B	3.22	1.46	1.39
30	B	821	CLA	OBD-CAD	3.22	1.28	1.22
30	9	308	CLA	OBD-CAD	3.22	1.28	1.22
30	B	803	CLA	CHD-C4C	3.22	1.46	1.39
30	8	302	CLA	CHB-C1B	3.22	1.46	1.39
30	7	312	CLA	C4B-NB	-3.22	1.33	1.37
30	A	831	CLA	OBD-CAD	3.22	1.28	1.22
37	13	313	A86	C26-C27	3.22	1.43	1.35
30	B	805	CLA	CHC-C4B	3.22	1.46	1.39
30	4	302	CLA	CHB-C1B	3.22	1.46	1.39
38	13	311	KC1	CHD-C1D	3.22	1.46	1.39
30	5	303	CLA	C4B-NB	-3.22	1.33	1.37
30	B	808	CLA	CHC-C4B	3.22	1.46	1.39
30	11	304	CLA	CHB-C1B	3.21	1.46	1.39
30	A	825	CLA	OBD-CAD	3.21	1.28	1.22
38	9	312	KC1	CHD-C1D	3.21	1.46	1.39
38	10	312	KC1	CHD-C1D	3.21	1.46	1.39
39	3	316	DD6	C-C1	3.21	1.57	1.50
38	5	312	KC1	C4B-NB	-3.21	1.33	1.37
37	12	316	A86	C19-C18	3.21	1.56	1.52
30	9	305	CLA	CHB-C1B	3.21	1.46	1.39
30	F	201	CLA	C4B-NB	-3.21	1.33	1.37
38	11	311	KC1	CHD-C1D	3.21	1.46	1.39
30	9	305	CLA	C4B-NB	-3.21	1.33	1.37
30	A	840	CLA	CHB-C1B	3.20	1.46	1.39
30	B	816	CLA	CHC-C4B	3.20	1.46	1.39
30	12	306	CLA	C4B-NB	-3.20	1.33	1.37
30	7	311	CLA	CHB-C1B	3.20	1.46	1.39
39	4	313	DD6	O2-C18	3.20	1.52	1.43
30	1	305	CLA	CHB-C1B	3.20	1.46	1.39
30	16	305	CLA	CHB-C1B	3.20	1.46	1.39
30	B	811	CLA	OBD-CAD	3.20	1.28	1.22
30	B	837	CLA	C4B-NB	-3.20	1.33	1.37
37	11	316	A86	C19-C18	3.20	1.56	1.52
30	B	804	CLA	CHB-C1B	3.20	1.46	1.39
30	7	305	CLA	CHB-C1B	3.20	1.46	1.39
30	15	311	CLA	C1B-NB	-3.20	1.33	1.37
38	2	312	KC1	C4B-NB	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	2	314	KC1	C4B-NB	-3.20	1.33	1.37
30	8	309	CLA	CHB-C1B	3.20	1.46	1.39
30	A	833	CLA	CHB-C1B	3.20	1.46	1.39
30	12	306	CLA	CHB-C1B	3.20	1.46	1.39
39	8	316	DD6	O2-C18	3.20	1.52	1.43
30	B	838	CLA	OBD-CAD	3.20	1.28	1.22
30	A	813	CLA	CHB-C1B	3.20	1.46	1.39
30	A	827	CLA	CHB-C1B	3.20	1.46	1.39
38	14	306	KC1	CHD-C1D	3.20	1.46	1.39
39	10	314	DD6	C-C1	3.20	1.57	1.50
38	8	314	KC1	C4B-NB	-3.20	1.33	1.37
30	5	309	CLA	C4B-NB	-3.19	1.33	1.37
30	13	304	CLA	C1B-NB	-3.19	1.33	1.37
37	9	315	A86	C25-C24	3.19	1.43	1.34
30	B	802	CLA	CHB-C1B	3.19	1.46	1.39
30	1	301	CLA	CHB-C1B	3.19	1.46	1.39
30	A	806	CLA	CHB-C1B	3.19	1.46	1.39
30	B	814	CLA	CHB-C1B	3.19	1.46	1.39
30	6	305	CLA	CHB-C1B	3.19	1.46	1.39
37	9	316	A86	C25-C24	3.19	1.43	1.34
30	F	203	CLA	C4B-NB	-3.19	1.33	1.37
30	15	308	CLA	CHB-C1B	3.19	1.46	1.39
38	11	311	KC1	C4B-NB	-3.19	1.33	1.37
38	3	304	KC1	CHD-C1D	3.19	1.46	1.39
38	10	310	KC1	CHD-C1D	3.19	1.46	1.39
38	13	305	KC1	CHD-C1D	3.19	1.46	1.39
30	8	309	CLA	C4B-NB	-3.19	1.33	1.37
37	4	312	A86	C19-C18	3.19	1.56	1.52
30	A	828	CLA	CHD-C4C	3.19	1.46	1.39
39	5	313	DD6	C-C1	3.19	1.57	1.50
30	B	803	CLA	OBD-CAD	3.19	1.28	1.22
30	A	835	CLA	OBD-CAD	3.19	1.28	1.22
30	10	304	CLA	OBD-CAD	3.18	1.28	1.22
30	6	307	CLA	CHB-C1B	3.18	1.46	1.39
38	1	308	KC1	CHD-C1D	3.18	1.46	1.39
39	7	302	DD6	C35-C34	3.18	1.57	1.52
33	L	204	BCR	C30-C25	-3.18	1.49	1.53
30	4	302	CLA	C4B-NB	-3.18	1.33	1.37
30	B	851	CLA	CHB-C1B	3.18	1.46	1.39
30	A	825	CLA	CHB-C1B	3.18	1.46	1.39
30	3	303	CLA	CHB-C1B	3.18	1.46	1.39
38	8	313	KC1	OBD-CAD	3.18	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	7	308	KC1	C4B-NB	-3.18	1.33	1.37
37	15	323	A86	C25-C24	3.18	1.43	1.34
30	11	309	CLA	CHB-C1B	3.18	1.46	1.39
37	11	301	A86	C19-C18	3.18	1.56	1.52
30	9	306	CLA	CHB-C1B	3.18	1.46	1.39
30	3	307	CLA	C4B-NB	-3.18	1.33	1.37
30	7	306	CLA	CHB-C1B	3.18	1.46	1.39
30	9	309	CLA	CHC-C4B	3.18	1.46	1.39
30	B	809	CLA	OBD-CAD	3.18	1.28	1.22
30	A	826	CLA	CHC-C4B	3.18	1.46	1.39
39	2	317	DD6	C-C1	3.18	1.57	1.50
30	14	302	CLA	CHB-C1B	3.17	1.46	1.39
38	12	305	KC1	CHD-C1D	3.17	1.46	1.39
30	B	801	CLA	OBD-CAD	3.17	1.28	1.22
33	A	849	BCR	C1-C6	-3.17	1.49	1.53
30	A	841	CLA	OBD-CAD	3.17	1.27	1.22
38	8	311	KC1	C4B-NB	-3.17	1.33	1.37
30	6	306	CLA	CHB-C1B	3.17	1.46	1.39
39	6	321	DD6	C-C1	3.17	1.57	1.50
38	8	314	KC1	CHD-C1D	3.17	1.46	1.39
30	B	808	CLA	C3D-C2D	3.17	1.47	1.39
38	10	312	KC1	C4B-NB	-3.17	1.33	1.37
38	12	309	KC1	C4B-NB	-3.17	1.33	1.37
37	13	313	A86	C24-C1	3.17	1.52	1.46
30	A	802	CLA	CHC-C4B	3.17	1.46	1.39
37	7	319	A86	C25-C24	3.17	1.42	1.34
30	B	821	CLA	CHC-C4B	3.17	1.46	1.39
37	15	322	A86	C25-C24	3.17	1.42	1.34
30	15	314	CLA	C1B-NB	-3.17	1.33	1.37
38	6	308	KC1	OBD-CAD	3.17	1.27	1.22
33	J	103	BCR	C30-C25	-3.17	1.49	1.53
38	1	306	KC1	CHD-C1D	3.17	1.46	1.39
30	6	307	CLA	C4B-NB	-3.16	1.33	1.37
30	9	303	CLA	CHB-C1B	3.16	1.46	1.39
30	A	809	CLA	OBD-CAD	3.16	1.27	1.22
30	A	818	CLA	CHB-C1B	3.16	1.46	1.39
37	2u	205	A86	C25-C24	3.16	1.42	1.34
30	2	301	CLA	C4B-NB	-3.16	1.33	1.37
30	B	804	CLA	C4B-NB	-3.16	1.33	1.37
30	9	307	CLA	CHB-C1B	3.16	1.46	1.39
38	4	308	KC1	CHD-C1D	3.16	1.46	1.39
38	11	307	KC1	CHD-C1D	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	305	KC1	CHD-C1D	3.16	1.46	1.39
30	6	310	CLA	CHB-C1B	3.16	1.46	1.39
39	12	317	DD6	C35-C34	3.16	1.57	1.52
30	A	830	CLA	C1D-ND	3.16	1.42	1.37
30	12	304	CLA	CHB-C1B	3.15	1.46	1.39
38	11	312	KC1	CHD-C1D	3.15	1.46	1.39
39	7	314	DD6	C-C1	3.15	1.57	1.50
38	4	310	KC1	C4B-NB	-3.15	1.33	1.37
30	14	305	CLA	C4B-NB	-3.15	1.33	1.37
30	B	806	CLA	CHB-C1B	3.15	1.46	1.39
39	4	313	DD6	C-C1	3.15	1.57	1.50
38	16	311	KC1	C4B-NB	-3.15	1.33	1.37
30	B	812	CLA	CHB-C1B	3.15	1.46	1.39
30	7	304	CLA	CHC-C4B	3.15	1.46	1.39
38	13	310	KC1	CHD-C1D	3.15	1.46	1.39
30	B	808	CLA	CHB-C1B	3.15	1.46	1.39
39	5	314	DD6	C-C1	3.15	1.57	1.50
30	B	827	CLA	OBD-CAD	3.15	1.27	1.22
30	A	809	CLA	CHC-C4B	3.15	1.46	1.39
39	2	316	DD6	C-C1	3.15	1.57	1.50
39	7	314	DD6	C26-C27	-3.15	1.30	1.37
30	3	310	CLA	C4B-NB	-3.14	1.33	1.37
37	15	315	A86	C19-C18	3.14	1.56	1.52
33	A	850	BCR	C30-C25	-3.14	1.49	1.53
38	6	313	KC1	CHD-C1D	3.14	1.46	1.39
30	10	308	CLA	C4B-NB	-3.14	1.33	1.37
30	A	824	CLA	OBD-CAD	3.14	1.27	1.22
30	6	305	CLA	OBD-CAD	3.14	1.27	1.22
30	16	306	CLA	OBD-CAD	3.14	1.27	1.22
30	L	202	CLA	CHB-C1B	3.14	1.46	1.39
30	10	303	CLA	C4B-NB	-3.14	1.33	1.37
30	7	304	CLA	CHB-C1B	3.14	1.46	1.39
30	A	808	CLA	C4B-NB	-3.14	1.33	1.37
30	3	301	CLA	CHB-C1B	3.14	1.46	1.39
39	5	314	DD6	O2-C18	3.14	1.52	1.43
30	B	828	CLA	C3D-C2D	3.14	1.47	1.39
30	B	819	CLA	C1D-ND	3.14	1.42	1.37
30	A	814	CLA	CHC-C4B	3.13	1.46	1.39
30	8	308	CLA	C4B-NB	-3.13	1.33	1.37
38	8	307	KC1	C4B-NB	-3.13	1.33	1.37
30	B	838	CLA	CHB-C1B	3.13	1.46	1.39
38	5	312	KC1	CHD-C1D	3.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	813	CLA	CHB-C1B	3.13	1.46	1.39
38	8	307	KC1	CHD-C1D	3.13	1.46	1.39
30	8	304	CLA	CHB-C1B	3.13	1.46	1.39
30	10	303	CLA	CHB-C1B	3.13	1.46	1.39
30	12	310	CLA	C4B-NB	-3.13	1.33	1.37
30	3	306	CLA	C4B-NB	-3.13	1.33	1.37
30	6	315	CLA	C4B-NB	-3.13	1.33	1.37
37	13	315	A86	C25-C24	3.12	1.42	1.34
38	9	304	KC1	CHD-C1D	3.12	1.46	1.39
30	A	838	CLA	CHB-C1B	3.12	1.46	1.39
30	7	311	CLA	C4B-NB	-3.12	1.33	1.37
30	3	303	CLA	C4B-NB	-3.12	1.33	1.37
37	14	320	A86	C25-C24	3.12	1.42	1.34
39	2	316	DD6	O2-C18	3.12	1.52	1.43
30	2	307	CLA	CHB-C1B	3.12	1.46	1.39
30	1	303	CLA	CHB-C1B	3.12	1.46	1.39
30	15	310	CLA	C4B-NB	-3.12	1.33	1.37
38	3	304	KC1	C4B-NB	-3.12	1.33	1.37
30	9	302	CLA	CHB-C1B	3.12	1.46	1.39
30	B	823	CLA	OBD-CAD	3.12	1.27	1.22
38	16	304	KC1	C4B-NB	-3.12	1.33	1.37
38	10	306	KC1	CHD-C1D	3.12	1.46	1.39
30	A	808	CLA	CHB-C1B	3.12	1.46	1.39
30	11	306	CLA	OBD-CAD	3.12	1.27	1.22
30	2u	202	CLA	C4B-NB	-3.12	1.33	1.37
30	11	310	CLA	C4B-NB	-3.11	1.33	1.37
30	1	303	CLA	C4B-NB	-3.11	1.33	1.37
38	6	311	KC1	OBD-CAD	3.11	1.27	1.22
37	8	315	A86	C19-C18	3.11	1.56	1.52
30	3	305	CLA	CHB-C1B	3.11	1.46	1.39
39	8	316	DD6	C-C1	3.11	1.57	1.50
30	7	309	CLA	OBD-CAD	3.11	1.27	1.22
39	6	318	DD6	C-C1	3.11	1.57	1.50
30	7	303	CLA	CHB-C1B	3.11	1.46	1.39
30	B	807	CLA	OBD-CAD	3.11	1.27	1.22
30	B	830	CLA	CHD-C1D	3.11	1.44	1.38
30	2	309	CLA	C4B-NB	-3.11	1.33	1.37
38	2	306	KC1	C4B-NB	-3.11	1.33	1.37
37	15	317	A86	C25-C24	3.11	1.42	1.34
30	14	303	CLA	CHB-C1B	3.11	1.46	1.39
38	11	305	KC1	C4B-NB	-3.11	1.33	1.37
30	A	836	CLA	CHB-C1B	3.11	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	316	A86	C25-C24	3.11	1.42	1.34
30	B	833	CLA	OBD-CAD	3.11	1.27	1.22
30	B	837	CLA	OBD-CAD	3.10	1.27	1.22
30	A	843	CLA	C4B-NB	-3.10	1.33	1.37
38	12	305	KC1	C4B-NB	-3.10	1.33	1.37
30	15	303	CLA	OBD-CAD	3.10	1.27	1.22
38	8	314	KC1	OBD-CAD	3.10	1.27	1.22
38	8	306	KC1	C4B-NB	-3.10	1.33	1.37
30	7	307	CLA	CHB-C1B	3.10	1.46	1.39
38	13	310	KC1	C4B-NB	-3.10	1.33	1.37
37	10	317	A86	C25-C24	3.10	1.42	1.34
37	4	314	A86	C25-C24	3.10	1.42	1.34
33	L	201	BCR	C1-C6	-3.10	1.49	1.53
30	4	301	CLA	CHB-C1B	3.10	1.46	1.39
30	4	309	CLA	C4B-NB	-3.10	1.33	1.37
38	3	308	KC1	C4B-NB	-3.10	1.33	1.37
30	2	308	CLA	CHB-C1B	3.09	1.46	1.39
38	9	312	KC1	C4B-NB	-3.09	1.33	1.37
39	10	313	DD6	C9-C8	3.09	1.42	1.34
30	B	815	CLA	CHC-C4B	3.09	1.46	1.39
30	4	306	CLA	CHB-C1B	3.09	1.46	1.39
38	12	309	KC1	CHD-C1D	3.09	1.46	1.39
33	A	847	BCR	C30-C25	-3.09	1.49	1.53
33	A	851	BCR	C30-C25	-3.09	1.49	1.53
30	B	819	CLA	C3D-C4D	-3.09	1.37	1.44
30	8	303	CLA	CHC-C4B	3.09	1.46	1.39
38	12	311	KC1	CHD-C1D	3.09	1.46	1.39
30	8	304	CLA	OBD-CAD	3.09	1.27	1.22
38	9	304	KC1	C4B-NB	-3.09	1.33	1.37
30	8	301	CLA	CHB-C1B	3.09	1.46	1.39
30	A	837	CLA	C4B-NB	-3.09	1.33	1.37
30	A	828	CLA	CHB-C1B	3.08	1.46	1.39
30	B	838	CLA	CHC-C4B	3.08	1.46	1.39
30	9	301	CLA	CHC-C4B	3.08	1.46	1.39
30	14	310	CLA	CHB-C1B	3.08	1.46	1.39
30	A	840	CLA	C4B-NB	-3.08	1.33	1.37
30	15	302	CLA	CHB-C1B	3.08	1.46	1.39
38	11	312	KC1	C4B-NB	-3.08	1.33	1.37
30	B	818	CLA	CHB-C1B	3.08	1.46	1.39
37	3	315	A86	C25-C24	3.08	1.42	1.34
30	12	302	CLA	CHB-C1B	3.08	1.46	1.39
38	5	305	KC1	CHD-C1D	3.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	313	CLA	C1B-NB	-3.08	1.33	1.37
38	5	305	KC1	C4B-NB	-3.08	1.33	1.37
37	10	302	A86	C25-C24	3.08	1.42	1.34
30	11	306	CLA	C4B-NB	-3.07	1.33	1.37
30	J	101	CLA	CHB-C1B	3.07	1.46	1.39
30	13	309	CLA	C1B-NB	-3.07	1.33	1.37
38	13	306	KC1	CHD-C1D	3.07	1.46	1.39
30	2	304	CLA	CHB-C1B	3.07	1.46	1.39
30	8	302	CLA	OBD-CAD	3.07	1.27	1.22
39	11	313	DD6	C35-C34	3.07	1.57	1.52
30	15	312	CLA	C4B-NB	-3.07	1.33	1.37
30	13	309	CLA	C4B-NB	-3.07	1.33	1.37
39	13	314	DD6	C9-C8	3.07	1.42	1.34
38	4	307	KC1	C4B-NB	-3.07	1.33	1.37
33	A	851	BCR	C1-C6	-3.07	1.49	1.53
33	B	846	BCR	C30-C25	-3.07	1.49	1.53
37	12	316	A86	C25-C24	3.07	1.42	1.34
30	B	809	CLA	CHC-C4B	3.07	1.46	1.39
30	B	831	CLA	CHB-C1B	3.07	1.46	1.39
38	5	310	KC1	CHD-C1D	3.07	1.46	1.39
38	13	311	KC1	C4A-C3A	3.06	1.50	1.44
30	4	305	CLA	C4B-NB	-3.06	1.33	1.37
30	7	310	CLA	C4B-NB	-3.06	1.33	1.37
30	B	831	CLA	OBD-CAD	3.06	1.27	1.22
30	1	301	CLA	C4B-NB	-3.06	1.33	1.37
30	1	305	CLA	C4B-NB	-3.06	1.33	1.37
30	16	310	CLA	C4B-NB	-3.06	1.33	1.37
30	10	307	CLA	CHB-C1B	3.06	1.46	1.39
30	11	306	CLA	CHB-C1B	3.06	1.46	1.39
30	A	831	CLA	CHB-C1B	3.06	1.46	1.39
30	1	307	CLA	C4B-NB	-3.06	1.33	1.37
37	13	313	A86	C-C1	3.06	1.57	1.50
33	A	848	BCR	C1-C6	-3.06	1.49	1.53
30	B	837	CLA	CHB-C1B	3.05	1.46	1.39
30	A	819	CLA	OBD-CAD	3.05	1.27	1.22
30	A	807	CLA	CHB-C1B	3.05	1.46	1.39
39	6	321	DD6	C35-C34	3.05	1.57	1.52
30	A	831	CLA	CHC-C4B	3.05	1.46	1.39
37	5	301	A86	C25-C24	3.05	1.42	1.34
30	6	314	CLA	CHB-C1B	3.05	1.46	1.39
30	B	810	CLA	C4B-NB	-3.05	1.33	1.37
30	A	832	CLA	OBD-CAD	3.05	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	313	KC1	C4B-NB	-3.05	1.33	1.37
37	14	318	A86	C25-C24	3.05	1.42	1.34
30	10	311	CLA	C4B-NB	-3.04	1.33	1.37
37	15	315	A86	C25-C24	3.04	1.42	1.34
38	4	308	KC1	C2A-C1A	3.04	1.54	1.44
38	8	312	KC1	C4A-C3A	3.04	1.50	1.44
30	3	301	CLA	OBD-CAD	3.04	1.27	1.22
30	A	836	CLA	CHC-C4B	3.04	1.46	1.39
38	8	312	KC1	CHD-C1D	3.04	1.46	1.39
38	6	308	KC1	C4B-NB	-3.04	1.33	1.37
30	9	308	CLA	CHB-C1B	3.04	1.46	1.39
30	A	837	CLA	CHB-C1B	3.04	1.46	1.39
30	11	308	CLA	C4B-NB	-3.04	1.33	1.37
38	5	306	KC1	C4B-NB	-3.04	1.33	1.37
38	2	314	KC1	CHD-C1D	3.04	1.46	1.39
39	7	318	DD6	C35-C34	3.03	1.57	1.52
38	3	308	KC1	CHD-C1D	3.03	1.46	1.39
30	B	815	CLA	OBD-CAD	3.03	1.27	1.22
30	4	304	CLA	CHB-C1B	3.03	1.46	1.39
30	B	817	CLA	CHB-C1B	3.03	1.46	1.39
30	11	304	CLA	C4B-NB	-3.03	1.33	1.37
38	9	310	KC1	C4B-NB	-3.03	1.33	1.37
30	5	308	CLA	CHB-C1B	3.03	1.46	1.39
30	2	311	CLA	C4B-NB	-3.03	1.33	1.37
30	A	832	CLA	CHB-C1B	3.03	1.46	1.39
30	A	807	CLA	OBD-CAD	3.02	1.27	1.22
30	B	822	CLA	CHB-C1B	3.02	1.46	1.39
30	15	304	CLA	CHB-C1B	3.02	1.46	1.39
30	6	309	CLA	CHB-C1B	3.02	1.46	1.39
38	14	311	KC1	CHD-C1D	3.02	1.46	1.39
37	15	316	A86	C25-C24	3.02	1.42	1.34
30	A	809	CLA	CHB-C1B	3.02	1.46	1.39
30	15	305	CLA	C4B-NB	-3.02	1.33	1.37
38	2	312	KC1	CHD-C1D	3.02	1.46	1.39
38	8	306	KC1	CHD-C1D	3.02	1.46	1.39
30	B	802	CLA	C4B-NB	-3.02	1.33	1.37
38	3	311	KC1	C4B-NB	-3.02	1.33	1.37
37	15	321	A86	C25-C24	3.02	1.42	1.34
30	B	835	CLA	CHB-C1B	3.02	1.46	1.39
38	5	310	KC1	C4B-NB	-3.02	1.33	1.37
30	14	310	CLA	C4B-NB	-3.02	1.33	1.37
30	16	306	CLA	C4B-NB	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	833	CLA	CHB-C1B	3.01	1.46	1.39
38	7	308	KC1	CHD-C1D	3.01	1.46	1.39
30	15	304	CLA	C4B-NB	-3.01	1.33	1.37
37	9	316	A86	C26-C27	3.01	1.42	1.35
30	A	812	CLA	CHB-C1B	3.01	1.46	1.39
38	7	313	KC1	CHD-C1D	3.01	1.46	1.39
30	16	302	CLA	C4B-NB	-3.01	1.33	1.37
30	16	303	CLA	C4B-NB	-3.01	1.33	1.37
30	6	304	CLA	CHB-C1B	3.01	1.46	1.39
38	11	307	KC1	C4B-NB	-3.01	1.33	1.37
38	10	310	KC1	C4B-NB	-3.01	1.33	1.37
38	6	312	KC1	CHD-C1D	3.01	1.46	1.39
30	A	804	CLA	C4B-NB	-3.01	1.33	1.37
37	3	314	A86	C25-C24	3.00	1.42	1.34
38	8	312	KC1	C4B-NB	-3.00	1.33	1.37
37	5	316	A86	C19-C18	3.00	1.56	1.52
37	2u	205	A86	C19-C18	3.00	1.56	1.52
30	9	307	CLA	C4B-NB	-3.00	1.33	1.37
30	A	830	CLA	CHB-C1B	3.00	1.46	1.39
30	B	830	CLA	CHB-C1B	3.00	1.46	1.39
37	14	314	A86	C25-C24	3.00	1.42	1.34
37	2	318	A86	C14-C15	3.00	1.58	1.52
37	9	316	A86	C14-C15	3.00	1.58	1.52
33	B	843	BCR	C1-C6	-3.00	1.49	1.53
37	15	315	A86	C26-C27	3.00	1.42	1.35
30	2	308	CLA	C4B-NB	-3.00	1.33	1.37
39	11	313	DD6	C9-C8	3.00	1.42	1.34
37	14	319	A86	C25-C24	3.00	1.42	1.34
30	A	819	CLA	CHB-C1B	3.00	1.46	1.39
37	15	316	A86	C26-C27	3.00	1.42	1.35
30	A	814	CLA	CHB-C1B	3.00	1.46	1.39
30	B	836	CLA	C4B-NB	-2.99	1.33	1.37
30	16	305	CLA	C4B-NB	-2.99	1.33	1.37
30	B	839	CLA	CHB-C1B	2.99	1.46	1.39
30	6	314	CLA	C4B-NB	-2.99	1.33	1.37
30	A	815	CLA	CHB-C1B	2.99	1.46	1.39
39	4	316	DD6	C35-C34	2.99	1.57	1.52
37	2	318	A86	C25-C24	2.99	1.42	1.34
37	15	315	A86	C14-C15	2.99	1.58	1.52
30	15	306	CLA	C4B-NB	-2.99	1.33	1.37
37	15	315	A86	C24-C1	2.99	1.52	1.46
30	A	811	CLA	CHB-C1B	2.99	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	315	A86	C19-C18	2.98	1.56	1.52
39	8	317	DD6	C35-C34	2.98	1.57	1.52
30	A	824	CLA	C4B-NB	-2.98	1.33	1.37
37	9	315	A86	O-C13	-2.98	1.17	1.23
30	12	307	CLA	OBD-CAD	2.98	1.27	1.22
30	4	311	CLA	CHB-C1B	2.98	1.46	1.39
33	L	205	BCR	C1-C6	-2.98	1.50	1.53
30	7	310	CLA	CHB-C1B	2.98	1.46	1.39
37	2	319	A86	C19-C18	2.98	1.56	1.52
30	5	303	CLA	OBD-CAD	2.98	1.27	1.22
37	9	313	A86	C19-C18	2.98	1.56	1.52
37	14	316	A86	C19-C18	2.98	1.56	1.52
30	4	301	CLA	OBD-CAD	2.98	1.27	1.22
30	4	305	CLA	CHB-C1B	2.97	1.46	1.39
39	10	314	DD6	C9-C8	2.97	1.42	1.34
37	16	312	A86	C25-C24	2.97	1.42	1.34
38	1	308	KC1	C4B-NB	-2.97	1.34	1.37
30	B	802	CLA	OBD-CAD	2.97	1.27	1.22
30	5	304	CLA	C4B-NB	-2.97	1.34	1.37
30	B	833	CLA	C4B-NB	-2.97	1.34	1.37
39	6	319	DD6	C9-C8	2.97	1.42	1.34
30	14	307	CLA	C4B-NB	-2.97	1.34	1.37
30	6	306	CLA	OBD-CAD	2.97	1.27	1.22
37	9	313	A86	C14-C15	2.97	1.58	1.52
30	12	312	CLA	C4B-NB	-2.96	1.34	1.37
30	A	803	CLA	C1D-ND	2.96	1.41	1.37
30	15	312	CLA	CHB-C1B	2.96	1.46	1.39
30	6	310	CLA	C4B-NB	-2.96	1.34	1.37
38	6	311	KC1	CHD-C1D	2.96	1.46	1.39
30	A	818	CLA	C4B-NB	-2.95	1.34	1.37
38	9	310	KC1	CHD-C1D	2.95	1.46	1.39
30	B	815	CLA	CHB-C1B	2.95	1.46	1.39
30	B	806	CLA	OBD-CAD	2.95	1.27	1.22
30	A	839	CLA	CHB-C1B	2.95	1.46	1.39
30	13	301	CLA	C4B-NB	-2.95	1.34	1.37
39	16	313	DD6	C9-C8	2.95	1.42	1.34
37	11	301	A86	C25-C24	2.95	1.42	1.34
30	10	308	CLA	CHB-C1B	2.95	1.46	1.39
37	14	316	A86	C25-C24	2.94	1.42	1.34
30	A	821	CLA	C4B-NB	-2.94	1.34	1.37
39	7	317	DD6	C26-C27	-2.94	1.31	1.37
37	10	315	A86	C25-C24	2.94	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	309	CLA	C4B-NB	-2.94	1.34	1.37
30	A	829	CLA	CHB-C1B	2.94	1.46	1.39
37	9	315	A86	C24-C1	2.94	1.52	1.46
30	A	822	CLA	CHB-C1B	2.94	1.46	1.39
37	15	320	A86	C26-C27	2.94	1.42	1.35
30	1	302	CLA	C4B-NB	-2.94	1.34	1.37
30	14	313	CLA	C4B-NB	-2.94	1.34	1.37
37	14	301	A86	C25-C24	2.94	1.42	1.34
37	8	318	A86	O-C13	-2.94	1.17	1.23
37	15	320	A86	C24-C1	2.94	1.52	1.46
37	9	315	A86	C14-C15	2.94	1.58	1.52
30	14	302	CLA	C4B-NB	-2.93	1.34	1.37
30	10	309	CLA	C4B-NB	-2.93	1.34	1.37
30	16	309	CLA	C4B-NB	-2.93	1.34	1.37
33	A	850	BCR	C1-C6	-2.93	1.50	1.53
37	15	315	A86	C2-C1	2.93	1.42	1.35
30	13	303	CLA	C4B-NB	-2.93	1.34	1.37
30	A	820	CLA	CHB-C1B	2.93	1.46	1.39
30	3	306	CLA	CHB-C1B	2.93	1.46	1.39
37	6	320	A86	O-C13	-2.92	1.17	1.23
30	16	302	CLA	OBD-CAD	2.92	1.27	1.22
39	13	314	DD6	C35-C34	2.92	1.57	1.52
30	B	829	CLA	CHB-C1B	2.92	1.46	1.39
37	5	315	A86	C25-C24	2.92	1.42	1.34
39	9	314	DD6	C9-C8	2.92	1.42	1.34
30	A	805	CLA	CHB-C1B	2.92	1.46	1.39
38	6	308	KC1	CAA-C2A	2.92	1.55	1.46
30	6	316	CLA	CHB-C1B	2.92	1.46	1.39
37	5	316	A86	C25-C24	2.92	1.42	1.34
30	8	305	CLA	C3D-C4D	-2.92	1.37	1.44
30	11	308	CLA	CHB-C1B	2.92	1.46	1.39
36	14	321	LMG	O7-C8	-2.92	1.39	1.46
39	3	312	DD6	C9-C8	2.91	1.42	1.34
38	14	311	KC1	C4B-NB	-2.91	1.34	1.37
30	B	805	CLA	CHB-C1B	2.91	1.46	1.39
38	10	306	KC1	C4B-NB	-2.91	1.34	1.37
39	1	310	DD6	C35-C34	2.91	1.57	1.52
30	B	803	CLA	C1C-NC	-2.91	1.33	1.37
30	A	829	CLA	OBD-CAD	2.91	1.27	1.22
30	16	307	CLA	C4B-NB	-2.91	1.34	1.37
39	7	302	DD6	C9-C8	2.91	1.42	1.34
30	B	824	CLA	CHB-C1B	2.90	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	9	315	A86	C26-C27	2.90	1.42	1.35
30	B	832	CLA	CHB-C1B	2.90	1.45	1.39
30	A	815	CLA	CHC-C4B	2.90	1.45	1.39
30	B	821	CLA	CHB-C1B	2.90	1.45	1.39
37	15	323	A86	C24-C1	2.90	1.52	1.46
30	1	304	CLA	C4B-NB	-2.90	1.34	1.37
30	10	304	CLA	C4B-NB	-2.90	1.34	1.37
30	12	308	CLA	C4B-NB	-2.90	1.34	1.37
30	15	308	CLA	C4B-NB	-2.90	1.34	1.37
37	4	315	A86	C25-C24	2.90	1.42	1.34
37	15	322	A86	C24-C1	2.90	1.52	1.46
38	6	308	KC1	CHD-C1D	2.90	1.45	1.39
39	6	303	DD6	C9-C8	2.90	1.42	1.34
37	12	314	A86	C25-C24	2.90	1.42	1.34
39	7	314	DD6	C35-C34	2.90	1.57	1.52
38	12	313	KC1	CAA-C2A	2.90	1.55	1.46
37	11	314	A86	C25-C24	2.89	1.42	1.34
37	2	302	A86	C25-C24	2.89	1.42	1.34
39	2	317	DD6	C9-C8	2.89	1.42	1.34
39	5	313	DD6	C9-C8	2.89	1.42	1.34
37	15	323	A86	C26-C27	2.88	1.42	1.35
38	8	314	KC1	C2A-C1A	2.88	1.53	1.44
39	2	315	DD6	C9-C8	2.88	1.42	1.34
30	A	830	CLA	C4B-NB	-2.88	1.34	1.37
37	4	317	A86	C25-C24	2.88	1.42	1.34
37	9	316	A86	C24-C1	2.88	1.52	1.46
33	B	846	BCR	C1-C6	-2.88	1.50	1.53
30	B	839	CLA	C4B-NB	-2.88	1.34	1.37
37	15	322	A86	C-C1	2.88	1.56	1.50
30	14	312	CLA	C4B-NB	-2.88	1.34	1.37
30	14	307	CLA	C4C-C3C	2.88	1.49	1.45
37	16	314	A86	C14-C15	2.88	1.58	1.52
33	B	842	BCR	C1-C6	-2.88	1.50	1.53
38	4	310	KC1	CHB-C4A	-2.87	1.32	1.39
38	12	311	KC1	C4B-NB	-2.87	1.34	1.37
30	6	317	CLA	C4B-NB	-2.87	1.34	1.37
37	11	315	A86	C25-C24	2.87	1.42	1.34
30	A	840	CLA	OBD-CAD	2.87	1.27	1.22
30	15	309	CLA	C4B-NB	-2.86	1.34	1.37
39	12	317	DD6	C26-C27	-2.86	1.31	1.37
38	14	306	KC1	C4C-C3C	2.86	1.49	1.45
37	6	320	A86	C25-C24	2.86	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	10	313	DD6	C35-C34	2.86	1.57	1.52
30	8	308	CLA	CHB-C1B	2.86	1.45	1.39
38	9	311	KC1	C4B-NB	-2.86	1.34	1.37
30	14	305	CLA	CHB-C1B	2.86	1.45	1.39
37	15	317	A86	C26-C27	2.86	1.42	1.35
38	13	305	KC1	CAA-C2A	2.86	1.55	1.46
39	5	314	DD6	C26-C27	-2.85	1.31	1.37
30	13	302	CLA	C4B-NB	-2.85	1.34	1.37
30	B	828	CLA	C3D-C4D	-2.85	1.37	1.44
39	6	303	DD6	O1-C20	2.85	1.50	1.46
39	3	313	DD6	C9-C8	2.85	1.42	1.34
39	12	317	DD6	C9-C8	2.85	1.42	1.34
37	15	322	A86	C26-C27	2.85	1.42	1.35
37	7	315	A86	C25-C24	2.85	1.42	1.34
37	11	316	A86	C26-C27	2.85	1.42	1.35
30	14	304	CLA	C4B-NB	-2.85	1.34	1.37
38	12	313	KC1	CHD-C1D	2.85	1.45	1.39
30	3	305	CLA	C4B-NB	-2.85	1.34	1.37
30	13	304	CLA	C4B-NB	-2.85	1.34	1.37
38	14	308	KC1	C4C-C3C	2.85	1.49	1.45
37	2	318	A86	C26-C27	2.85	1.42	1.35
38	6	312	KC1	C4B-NB	-2.84	1.34	1.37
38	13	308	KC1	C4B-NB	-2.84	1.34	1.37
30	A	828	CLA	C1C-NC	-2.84	1.33	1.37
37	2	318	A86	O-C13	-2.84	1.17	1.23
39	16	313	DD6	C35-C34	2.84	1.57	1.52
37	7	319	A86	C26-C27	2.84	1.42	1.35
37	9	315	A86	C-C1	2.84	1.56	1.50
37	14	320	A86	C-C1	2.84	1.56	1.50
30	B	803	CLA	CHB-C1B	2.84	1.45	1.39
39	15	318	DD6	C9-C8	2.84	1.42	1.34
38	14	306	KC1	C3B-C4B	2.84	1.51	1.46
39	3	316	DD6	C9-C8	2.84	1.42	1.34
37	10	301	A86	C-C1	2.83	1.56	1.50
30	3	307	CLA	C4D-CHA	2.83	1.48	1.38
30	4	303	CLA	C4B-NB	-2.83	1.34	1.37
37	3	315	A86	C26-C27	2.83	1.42	1.35
39	15	319	DD6	C9-C8	2.83	1.42	1.34
38	1	308	KC1	CHB-C4A	-2.82	1.32	1.39
37	10	317	A86	C24-C1	2.82	1.52	1.46
30	15	306	CLA	C4D-CHA	2.82	1.48	1.38
37	14	301	A86	C-C1	2.82	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	842	CLA	C4B-NB	-2.82	1.34	1.37
30	13	307	CLA	C3B-C4B	2.82	1.50	1.42
37	15	321	A86	C26-C27	2.82	1.42	1.35
39	3	313	DD6	C35-C34	2.82	1.57	1.52
37	15	316	A86	C24-C1	2.82	1.52	1.46
30	12	307	CLA	C4B-NB	-2.82	1.34	1.37
30	A	840	CLA	C3D-C4D	-2.82	1.37	1.44
37	14	320	A86	C26-C27	2.81	1.42	1.35
30	A	827	CLA	C3D-C4D	-2.81	1.37	1.44
37	10	317	A86	C14-C15	2.81	1.58	1.52
30	B	830	CLA	C4B-NB	-2.81	1.34	1.37
30	4	309	CLA	C4D-CHA	2.81	1.48	1.38
39	1	310	DD6	C9-C8	2.81	1.42	1.34
37	14	317	A86	C25-C24	2.81	1.42	1.34
39	4	313	DD6	C9-C8	2.81	1.42	1.34
37	14	316	A86	C-C1	2.81	1.56	1.50
39	4	316	DD6	C9-C8	2.80	1.42	1.34
30	15	303	CLA	C4D-CHA	2.80	1.48	1.38
30	15	308	CLA	C4D-CHA	2.80	1.48	1.38
30	A	802	CLA	CHB-C1B	2.80	1.45	1.39
38	14	306	KC1	CHB-C4A	-2.80	1.32	1.39
37	10	315	A86	C-C1	2.80	1.56	1.50
30	15	311	CLA	C4D-CHA	2.80	1.48	1.38
30	14	309	CLA	C4D-CHA	2.80	1.48	1.38
37	13	315	A86	C24-C1	2.80	1.51	1.46
30	B	825	CLA	C3D-C4D	-2.80	1.37	1.44
37	14	320	A86	C24-C1	2.80	1.51	1.46
37	1	309	A86	C25-C24	2.80	1.42	1.34
39	6	318	DD6	C9-C8	2.80	1.42	1.34
30	9	306	CLA	C4D-CHA	2.80	1.48	1.38
30	B	824	CLA	C3D-C4D	-2.80	1.37	1.44
37	15	317	A86	C-C1	2.79	1.56	1.50
37	10	301	A86	C25-C24	2.79	1.42	1.34
37	15	323	A86	C-C1	2.79	1.56	1.50
37	2u	203	A86	C25-C24	2.79	1.42	1.34
37	13	315	A86	C-C1	2.79	1.56	1.50
37	16	314	A86	C25-C24	2.79	1.42	1.34
37	15	317	A86	C24-C1	2.79	1.51	1.46
37	4	317	A86	C19-C18	2.79	1.56	1.52
39	6	303	DD6	C26-C27	-2.79	1.31	1.37
30	B	834	CLA	C3D-C4D	-2.79	1.37	1.44
30	3	307	CLA	C4C-C3C	2.79	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	305	CLA	C4D-CHA	2.78	1.47	1.38
38	10	310	KC1	CHB-C4A	-2.78	1.32	1.39
30	A	838	CLA	C3D-C4D	-2.78	1.37	1.44
30	13	309	CLA	C4D-CHA	2.78	1.47	1.38
39	8	316	DD6	C26-C27	-2.78	1.31	1.37
30	6	315	CLA	C4D-CHA	2.78	1.47	1.38
39	6	321	DD6	C26-C27	-2.78	1.31	1.37
37	7	316	A86	C19-C18	2.78	1.56	1.52
30	16	307	CLA	C4D-CHA	2.78	1.47	1.38
39	12	315	DD6	C9-C8	2.78	1.41	1.34
39	7	317	DD6	C9-C8	2.78	1.41	1.34
38	10	312	KC1	CHB-C4A	-2.78	1.32	1.39
30	B	811	CLA	C3D-C4D	-2.77	1.37	1.44
39	8	317	DD6	C9-C8	2.77	1.41	1.34
30	15	307	CLA	C4B-NB	-2.77	1.34	1.37
30	15	305	CLA	C4D-CHA	2.77	1.47	1.38
39	8	316	DD6	C9-C8	2.77	1.41	1.34
37	4	317	A86	C14-C15	2.77	1.58	1.52
38	8	310	KC1	CHD-C1D	2.77	1.45	1.39
30	A	824	CLA	C3D-C4D	-2.77	1.38	1.44
38	16	311	KC1	C2A-C1A	2.77	1.53	1.44
30	B	819	CLA	CHB-C1B	2.77	1.45	1.39
30	A	828	CLA	OBD-CAD	2.77	1.27	1.22
38	8	313	KC1	CHD-C1D	2.77	1.45	1.39
30	2	313	CLA	C4B-NB	-2.77	1.34	1.37
37	9	313	A86	O-C13	-2.76	1.17	1.23
37	15	320	A86	C-C1	2.76	1.56	1.50
30	A	844	CLA	C4B-NB	-2.76	1.34	1.37
39	7	314	DD6	C9-C8	2.76	1.41	1.34
30	A	835	CLA	CHB-C1B	2.76	1.45	1.39
30	A	822	CLA	C3D-C4D	-2.76	1.38	1.44
30	15	303	CLA	C3B-C4B	2.76	1.50	1.42
30	B	801	CLA	C1B-C2B	2.76	1.49	1.43
39	7	318	DD6	C26-C27	-2.76	1.31	1.37
38	5	306	KC1	CHB-C4A	-2.76	1.32	1.39
37	4	315	A86	O-C13	-2.76	1.17	1.23
30	A	825	CLA	C4D-CHA	2.76	1.47	1.38
30	16	301	CLA	C4B-NB	-2.76	1.34	1.37
38	13	312	KC1	C4B-NB	-2.75	1.34	1.37
37	4	317	A86	C-C1	2.75	1.56	1.50
30	14	303	CLA	C4D-CHA	2.75	1.47	1.38
30	3	306	CLA	C4D-CHA	2.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	303	CLA	CHB-C1B	2.75	1.45	1.39
30	15	309	CLA	C4D-CHA	2.75	1.47	1.38
30	B	825	CLA	OBD-CAD	2.75	1.27	1.22
30	A	838	CLA	C4D-CHA	2.75	1.47	1.38
33	A	849	BCR	C30-C25	-2.75	1.50	1.53
33	2u	201	BCR	C30-C25	-2.75	1.50	1.53
30	A	827	CLA	OBD-CAD	2.75	1.27	1.22
39	12	315	DD6	C35-C34	2.75	1.57	1.52
37	5	315	A86	C-C1	2.75	1.56	1.50
30	7	312	CLA	C4D-CHA	2.75	1.47	1.38
37	10	316	A86	C19-C18	2.75	1.56	1.52
30	2	303	CLA	C4B-NB	-2.75	1.34	1.37
30	7	304	CLA	OBD-CAD	2.75	1.27	1.22
39	6	318	DD6	C26-C27	-2.75	1.31	1.37
37	15	316	A86	C14-C15	2.75	1.58	1.52
37	16	314	A86	O-C13	-2.74	1.17	1.23
37	2u	205	A86	C24-C1	2.74	1.51	1.46
39	5	313	DD6	C35-C34	2.74	1.57	1.52
37	4	314	A86	C26-C27	2.74	1.42	1.35
38	8	311	KC1	CHD-C1D	2.74	1.45	1.39
37	10	315	A86	C24-C1	2.74	1.51	1.46
39	1	310	DD6	C26-C27	-2.74	1.31	1.37
30	9	305	CLA	C4D-CHA	2.74	1.47	1.38
30	14	312	CLA	C4D-CHA	2.74	1.47	1.38
38	11	312	KC1	C2A-C1A	2.74	1.53	1.44
38	13	306	KC1	C4B-NB	-2.74	1.34	1.37
37	15	316	A86	C-C1	2.74	1.56	1.50
30	3	302	CLA	C4D-CHA	2.74	1.47	1.38
30	14	303	CLA	C4B-NB	-2.74	1.34	1.37
37	2u	205	A86	C26-C27	2.74	1.42	1.35
30	B	823	CLA	C4D-CHA	2.74	1.47	1.38
38	4	308	KC1	C4A-C3A	2.73	1.50	1.44
37	10	317	A86	C26-C27	2.73	1.42	1.35
39	9	314	DD6	C35-C34	2.73	1.57	1.52
37	10	316	A86	C25-C24	2.73	1.41	1.34
30	A	828	CLA	C3D-C4D	-2.73	1.38	1.44
30	16	308	CLA	C4B-NB	-2.73	1.34	1.37
30	B	815	CLA	C4D-CHA	2.73	1.47	1.38
37	14	318	A86	C-C1	2.73	1.56	1.50
37	2	302	A86	C24-C1	2.73	1.51	1.46
37	14	315	A86	C25-C24	2.73	1.41	1.34
37	4	315	A86	C-C1	2.73	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	12	316	A86	C26-C27	2.73	1.42	1.35
30	2	313	CLA	C4D-CHA	2.73	1.47	1.38
30	12	321	CLA	C4D-CHA	2.73	1.47	1.38
30	12	321	CLA	C3B-C4B	2.73	1.50	1.42
30	A	841	CLA	C4D-CHA	2.73	1.47	1.38
30	16	305	CLA	C4D-CHA	2.73	1.47	1.38
37	7	316	A86	O4-C34	-2.73	1.40	1.46
30	12	303	CLA	C4D-CHA	2.73	1.47	1.38
38	16	311	KC1	CHB-C4A	-2.73	1.33	1.39
37	7	315	A86	C24-C1	2.72	1.51	1.46
33	B	845	BCR	C1-C6	-2.72	1.50	1.53
37	13	315	A86	C26-C27	2.72	1.42	1.35
37	2	302	A86	C-C1	2.72	1.56	1.50
30	4	302	CLA	C4D-CHA	2.72	1.47	1.38
39	7	317	DD6	C35-C34	2.72	1.57	1.52
37	2	302	A86	C26-C27	2.72	1.42	1.35
37	10	316	A86	C-C1	2.72	1.56	1.50
30	A	831	CLA	C4D-CHA	2.72	1.47	1.38
38	6	308	KC1	CHB-C4A	-2.72	1.33	1.39
30	13	302	CLA	C4D-CHA	2.72	1.47	1.38
39	6	318	DD6	C35-C34	2.72	1.57	1.52
37	13	313	A86	C2-C1	2.72	1.42	1.35
30	15	310	CLA	C4D-CHA	2.72	1.47	1.38
39	8	316	DD6	C35-C34	2.72	1.57	1.52
37	3	314	A86	C24-C1	2.72	1.51	1.46
38	5	312	KC1	CHB-C4A	-2.72	1.33	1.39
39	2	317	DD6	C26-C27	-2.72	1.31	1.37
37	10	315	A86	C26-C27	2.72	1.42	1.35
30	15	311	CLA	C4B-NB	-2.72	1.34	1.37
37	7	319	A86	C14-C15	2.72	1.58	1.52
30	3	310	CLA	C4D-CHA	2.72	1.47	1.38
30	13	304	CLA	C4D-CHA	2.72	1.47	1.38
30	10	305	CLA	C1B-C2B	2.72	1.49	1.43
39	3	313	DD6	C26-C27	-2.72	1.31	1.37
30	A	826	CLA	C4D-CHA	2.72	1.47	1.38
30	13	307	CLA	C4D-CHA	2.72	1.47	1.38
39	13	314	DD6	C4-C5	2.72	1.51	1.43
38	9	312	KC1	C4A-C3A	2.71	1.50	1.44
30	B	822	CLA	C3D-C4D	-2.71	1.38	1.44
37	3	315	A86	C-C1	2.71	1.56	1.50
30	6	310	CLA	C4D-CHA	2.71	1.47	1.38
37	14	318	A86	C26-C27	2.71	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5	314	DD6	C9-C8	2.71	1.41	1.34
37	10	315	A86	C2-C1	2.71	1.42	1.35
30	14	310	CLA	C4D-CHA	2.71	1.47	1.38
33	B	844	BCR	C1-C6	-2.71	1.50	1.53
39	11	313	DD6	C26-C27	-2.71	1.31	1.37
30	11	310	CLA	C4D-CHA	2.71	1.47	1.38
37	3	314	A86	C-C1	2.71	1.56	1.50
39	5	313	DD6	C26-C27	-2.71	1.31	1.37
30	1	301	CLA	C4D-CHA	2.71	1.47	1.38
37	7	315	A86	C26-C27	2.71	1.42	1.35
37	4	312	A86	C25-C24	2.71	1.41	1.34
30	A	806	CLA	C3D-C4D	-2.71	1.38	1.44
37	3	315	A86	C24-C1	2.71	1.51	1.46
37	15	321	A86	C-C1	2.71	1.56	1.50
37	12	314	A86	C-C1	2.70	1.56	1.50
30	12	321	CLA	C4B-NB	-2.70	1.34	1.37
38	13	312	KC1	C4A-C3A	2.70	1.50	1.44
30	A	837	CLA	C4D-CHA	2.70	1.47	1.38
30	15	304	CLA	C4D-CHA	2.70	1.47	1.38
37	11	316	A86	C-C1	2.70	1.56	1.50
30	A	835	CLA	C3D-C4D	-2.70	1.38	1.44
37	16	314	A86	C-C1	2.70	1.56	1.50
30	5	311	CLA	C4D-CHA	2.70	1.47	1.38
30	A	807	CLA	C4D-CHA	2.70	1.47	1.38
38	8	313	KC1	CHB-C4A	-2.70	1.33	1.39
30	B	804	CLA	C4D-CHA	2.70	1.47	1.38
30	8	308	CLA	C4D-CHA	2.70	1.47	1.38
37	7	319	A86	C24-C1	2.70	1.51	1.46
30	B	833	CLA	C4D-CHA	2.70	1.47	1.38
30	A	841	CLA	CHB-C1B	2.70	1.45	1.39
37	6	320	A86	O1-C15	2.70	1.50	1.45
30	15	313	CLA	C4D-CHA	2.70	1.47	1.38
37	8	318	A86	C-C1	2.70	1.56	1.50
30	1	304	CLA	C4D-CHA	2.70	1.47	1.38
34	A	853	LHG	O7-C5	-2.69	1.40	1.46
37	5	301	A86	C24-C1	2.69	1.51	1.46
30	16	309	CLA	C4D-CHA	2.69	1.47	1.38
38	1	306	KC1	C3B-C4B	2.69	1.50	1.46
30	A	844	CLA	C4D-CHA	2.69	1.47	1.38
38	6	311	KC1	CHB-C4A	-2.69	1.33	1.39
37	10	301	A86	C24-C1	2.69	1.51	1.46
30	5	308	CLA	C4D-CHA	2.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	307	CLA	C4D-CHA	2.69	1.47	1.38
39	2	316	DD6	C35-C34	2.69	1.56	1.52
33	L	201	BCR	C30-C25	-2.69	1.50	1.53
30	A	828	CLA	C4D-CHA	2.69	1.47	1.38
30	7	307	CLA	C4D-CHA	2.69	1.47	1.38
30	9	307	CLA	C4D-CHA	2.69	1.47	1.38
38	9	310	KC1	CHB-C4A	-2.69	1.33	1.39
30	B	821	CLA	C3D-C4D	-2.69	1.38	1.44
30	11	308	CLA	C4D-CHA	2.69	1.47	1.38
30	6	316	CLA	C4D-CHA	2.69	1.47	1.38
37	15	323	A86	C2-C1	2.69	1.42	1.35
37	7	315	A86	O-C13	-2.69	1.17	1.23
38	16	304	KC1	C4A-C3A	2.69	1.50	1.44
30	6	306	CLA	C4D-CHA	2.69	1.47	1.38
37	5	301	A86	C-C1	2.69	1.56	1.50
30	9	308	CLA	C4D-CHA	2.69	1.47	1.38
30	A	815	CLA	C4D-CHA	2.69	1.47	1.38
30	14	305	CLA	C4D-CHA	2.69	1.47	1.38
37	7	315	A86	C-C1	2.69	1.56	1.50
30	B	812	CLA	C4D-CHA	2.69	1.47	1.38
38	14	311	KC1	C2A-C1A	2.69	1.53	1.44
37	10	301	A86	O-C13	-2.68	1.17	1.23
37	14	318	A86	C24-C1	2.68	1.51	1.46
37	14	319	A86	C26-C27	2.68	1.42	1.35
30	16	301	CLA	C4D-CHA	2.68	1.47	1.38
37	9	316	A86	C-C1	2.68	1.56	1.50
30	A	802	CLA	OBD-CAD	2.68	1.27	1.22
30	A	809	CLA	C4D-CHA	2.68	1.47	1.38
38	7	313	KC1	CHB-C4A	-2.68	1.33	1.39
30	16	308	CLA	C4D-CHA	2.68	1.47	1.38
30	B	835	CLA	C3D-C4D	-2.68	1.38	1.44
37	15	320	A86	C14-C15	2.68	1.58	1.52
37	12	316	A86	C-C1	2.68	1.56	1.50
39	11	313	DD6	O1-C20	2.68	1.49	1.46
38	2	314	KC1	CHB-C4A	-2.68	1.33	1.39
30	B	837	CLA	C3D-C4D	-2.68	1.38	1.44
30	5	303	CLA	C4D-CHA	2.68	1.47	1.38
30	B	805	CLA	C4D-CHA	2.68	1.47	1.38
30	B	830	CLA	C3B-C4B	2.68	1.50	1.42
37	10	302	A86	C-C1	2.68	1.56	1.50
30	16	302	CLA	C4D-CHA	2.68	1.47	1.38
39	10	314	DD6	C35-C34	2.67	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	12	316	A86	C24-C1	2.67	1.51	1.46
30	2	305	CLA	C4D-CHA	2.67	1.47	1.38
38	5	310	KC1	CHB-C4A	-2.67	1.33	1.39
39	2	316	DD6	C26-C27	-2.67	1.31	1.37
30	B	818	CLA	C4D-CHA	2.67	1.47	1.38
30	A	842	CLA	C3D-C4D	-2.67	1.38	1.44
30	A	836	CLA	C4D-CHA	2.67	1.47	1.38
37	11	315	A86	C-C1	2.67	1.56	1.50
30	14	309	CLA	C4B-NB	-2.67	1.34	1.37
38	16	304	KC1	CHB-C4A	-2.67	1.33	1.39
37	11	301	A86	O-C13	-2.67	1.17	1.23
30	3	305	CLA	C4D-CHA	2.67	1.47	1.38
30	A	820	CLA	C4D-CHA	2.67	1.47	1.38
30	10	307	CLA	C4D-CHA	2.67	1.47	1.38
30	3	309	CLA	C4D-CHA	2.67	1.47	1.38
30	10	303	CLA	C4D-CHA	2.67	1.47	1.38
39	7	318	DD6	C9-C8	2.67	1.41	1.34
37	7	316	A86	O-C13	-2.67	1.17	1.23
30	15	312	CLA	C4D-CHA	2.67	1.47	1.38
30	F	202	CLA	C4D-CHA	2.67	1.47	1.38
39	3	316	DD6	C26-C27	-2.67	1.31	1.37
30	10	304	CLA	C4D-CHA	2.67	1.47	1.38
39	3	312	DD6	O1-C20	2.67	1.49	1.46
38	8	307	KC1	CHB-C4A	-2.67	1.33	1.39
30	A	819	CLA	C4D-CHA	2.67	1.47	1.38
30	A	805	CLA	C4D-CHA	2.66	1.47	1.38
38	9	312	KC1	CAA-C2A	2.66	1.54	1.46
38	13	312	KC1	CAA-C2A	2.66	1.54	1.46
38	6	308	KC1	C2A-C1A	2.66	1.52	1.44
30	A	819	CLA	C3D-C4D	-2.66	1.38	1.44
37	2u	203	A86	O-C13	-2.66	1.17	1.23
37	5	316	A86	C-C1	2.66	1.56	1.50
30	B	813	CLA	C4D-CHA	2.66	1.47	1.38
37	14	315	A86	C-C1	2.66	1.56	1.50
30	A	807	CLA	C3D-C4D	-2.66	1.38	1.44
30	A	831	CLA	C3D-C4D	-2.66	1.38	1.44
30	A	829	CLA	C3D-C4D	-2.66	1.38	1.44
30	12	308	CLA	C4D-CHA	2.66	1.47	1.38
38	12	311	KC1	CAA-C2A	2.66	1.54	1.46
30	2	304	CLA	C4D-CHA	2.66	1.47	1.38
37	11	301	A86	C-C1	2.66	1.56	1.50
30	6	314	CLA	C3D-C4D	-2.66	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	312	CLA	C4D-CHA	2.66	1.47	1.38
30	A	816	CLA	C4D-CHA	2.66	1.47	1.38
30	3	303	CLA	C4D-CHA	2.66	1.47	1.38
37	10	302	A86	C26-C27	2.66	1.41	1.35
37	3	315	A86	C14-C15	2.66	1.57	1.52
30	6	309	CLA	C4D-CHA	2.66	1.47	1.38
36	A	856	LMG	O7-C8	-2.65	1.40	1.46
30	4	311	CLA	C4D-CHA	2.65	1.47	1.38
30	6	307	CLA	C4D-CHA	2.65	1.47	1.38
38	4	307	KC1	CHB-C4A	-2.65	1.33	1.39
30	B	817	CLA	C3D-C4D	-2.65	1.38	1.44
30	13	303	CLA	C4D-CHA	2.65	1.47	1.38
30	12	306	CLA	C4D-CHA	2.65	1.47	1.38
30	15	302	CLA	C4B-NB	-2.65	1.34	1.37
37	15	320	A86	C2-C1	2.65	1.41	1.35
30	15	313	CLA	C4B-NB	-2.65	1.34	1.37
30	15	308	CLA	C4C-C3C	2.65	1.49	1.45
38	12	309	KC1	C2A-C1A	2.65	1.52	1.44
30	2	310	CLA	C4D-CHA	2.65	1.47	1.38
30	A	837	CLA	C3B-C4B	2.65	1.50	1.42
39	5	313	DD6	O1-C20	2.65	1.49	1.46
30	A	817	CLA	C3D-C4D	-2.65	1.38	1.44
30	6	317	CLA	C4D-CHA	2.65	1.47	1.38
30	3	301	CLA	C4D-CHA	2.65	1.47	1.38
30	1	307	CLA	C4D-CHA	2.65	1.47	1.38
30	F	202	CLA	OBD-CAD	2.65	1.27	1.22
30	A	813	CLA	C4D-CHA	2.65	1.47	1.38
30	7	311	CLA	C4D-CHA	2.65	1.47	1.38
30	15	303	CLA	C4B-NB	-2.65	1.34	1.37
30	B	808	CLA	C3D-C4D	-2.64	1.38	1.44
30	2	308	CLA	C4D-CHA	2.64	1.47	1.38
30	8	305	CLA	OBD-CAD	2.64	1.27	1.22
30	F	203	CLA	C4D-CHA	2.64	1.47	1.38
30	J	101	CLA	C4D-CHA	2.64	1.47	1.38
30	4	306	CLA	C4D-CHA	2.64	1.47	1.38
39	2	316	DD6	C9-C8	2.64	1.41	1.34
30	A	820	CLA	C3D-C4D	-2.64	1.38	1.44
37	11	314	A86	C26-C27	2.64	1.41	1.35
30	8	304	CLA	C3D-C4D	-2.64	1.38	1.44
38	3	311	KC1	CAA-C2A	2.64	1.54	1.46
37	3	314	A86	C26-C27	2.64	1.41	1.35
30	10	309	CLA	C4D-CHA	2.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	314	KC1	CHB-C4A	-2.64	1.33	1.39
30	B	838	CLA	C3D-C4D	-2.64	1.38	1.44
37	10	317	A86	C-C1	2.64	1.56	1.50
30	5	307	CLA	C1B-C2B	2.64	1.49	1.43
37	14	314	A86	C26-C27	2.64	1.41	1.35
37	14	301	A86	C26-C27	2.64	1.41	1.35
30	B	814	CLA	C3D-C4D	-2.64	1.38	1.44
30	B	838	CLA	C4D-CHA	2.64	1.47	1.38
30	1	303	CLA	C4D-CHA	2.64	1.47	1.38
30	8	303	CLA	C3D-C4D	-2.64	1.38	1.44
37	15	315	A86	C5-C6	2.64	1.41	1.35
38	13	310	KC1	C2A-C1A	2.63	1.52	1.44
30	A	832	CLA	C3D-C4D	-2.63	1.38	1.44
37	7	319	A86	O-C13	-2.63	1.17	1.23
30	A	832	CLA	C4D-CHA	2.63	1.47	1.38
37	5	315	A86	C24-C1	2.63	1.51	1.46
30	B	806	CLA	C3D-C4D	-2.63	1.38	1.44
37	14	316	A86	C26-C27	2.63	1.41	1.35
37	14	319	A86	C-C1	2.63	1.56	1.50
30	B	806	CLA	C4D-CHA	2.63	1.47	1.38
30	9	303	CLA	C4D-CHA	2.63	1.47	1.38
30	7	306	CLA	C4D-CHA	2.63	1.47	1.38
30	14	313	CLA	C1B-C2B	2.63	1.49	1.43
37	8	315	A86	O-C13	-2.63	1.17	1.23
38	12	309	KC1	CHB-C4A	-2.63	1.33	1.39
37	14	319	A86	C2-C1	2.63	1.41	1.35
30	12	304	CLA	C4D-CHA	2.63	1.47	1.38
37	15	316	A86	C2-C1	2.63	1.41	1.35
30	4	301	CLA	C3D-C4D	-2.63	1.38	1.44
30	8	302	CLA	C3D-C4D	-2.63	1.38	1.44
30	16	310	CLA	O1D-CGD	2.63	1.27	1.21
37	5	301	A86	C26-C27	2.63	1.41	1.35
30	1	302	CLA	C3B-C4B	2.63	1.50	1.42
33	F	204	BCR	C1-C6	-2.63	1.50	1.53
30	A	825	CLA	C3D-C4D	-2.63	1.38	1.44
37	5	301	A86	C19-C18	2.63	1.56	1.52
30	F	202	CLA	C1B-C2B	2.62	1.49	1.43
33	B	844	BCR	C30-C25	-2.62	1.50	1.53
30	A	814	CLA	C4D-CHA	2.62	1.47	1.38
37	14	317	A86	C24-C1	2.62	1.51	1.46
38	1	306	KC1	CHB-C4A	-2.62	1.33	1.39
30	2	309	CLA	C4D-CHA	2.62	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	834	CLA	C4D-CHA	2.62	1.47	1.38
30	15	314	CLA	C1B-C2B	2.62	1.49	1.43
38	14	308	KC1	C4A-C3A	2.62	1.49	1.44
30	A	826	CLA	C1B-C2B	2.62	1.49	1.43
36	6	301	LMG	O7-C8	-2.62	1.40	1.46
30	5	309	CLA	C4D-CHA	2.62	1.47	1.38
37	1	309	A86	C-C1	2.62	1.56	1.50
30	A	810	CLA	C4D-CHA	2.62	1.47	1.38
30	B	824	CLA	C4D-CHA	2.62	1.47	1.38
30	15	302	CLA	C3B-C4B	2.62	1.50	1.42
39	10	313	DD6	C26-C27	-2.62	1.31	1.37
30	B	810	CLA	C3D-C4D	-2.62	1.38	1.44
30	16	310	CLA	C1B-C2B	2.62	1.49	1.43
30	6	305	CLA	C4D-CHA	2.62	1.47	1.38
30	4	311	CLA	C3D-C4D	-2.62	1.38	1.44
30	6	305	CLA	C3D-C4D	-2.62	1.38	1.44
30	7	304	CLA	C4D-CHA	2.62	1.47	1.38
39	6	303	DD6	C4-C5	2.62	1.51	1.43
30	2	307	CLA	C4D-CHA	2.62	1.47	1.38
37	9	313	A86	C25-C24	2.62	1.41	1.34
30	15	306	CLA	C1B-C2B	2.62	1.49	1.43
38	1	306	KC1	C4B-NB	-2.62	1.34	1.37
30	B	816	CLA	C4D-CHA	2.62	1.47	1.38
30	4	305	CLA	C4D-CHA	2.62	1.47	1.38
30	10	311	CLA	C4D-CHA	2.62	1.47	1.38
30	B	836	CLA	C4D-CHA	2.61	1.47	1.38
30	15	310	CLA	C1B-C2B	2.61	1.49	1.43
37	8	318	A86	C14-C15	2.61	1.57	1.52
30	7	303	CLA	C3D-C4D	-2.61	1.38	1.44
30	15	313	CLA	C3B-C4B	2.61	1.50	1.42
30	5	307	CLA	C4D-CHA	2.61	1.47	1.38
30	4	303	CLA	C4C-C3C	2.61	1.49	1.45
37	14	301	A86	C24-C1	2.61	1.51	1.46
30	B	832	CLA	C4D-CHA	2.61	1.47	1.38
30	2	311	CLA	C4D-CHA	2.61	1.47	1.38
30	A	808	CLA	C3D-C4D	-2.61	1.38	1.44
30	5	304	CLA	C4D-CHA	2.61	1.47	1.38
38	8	310	KC1	CHB-C4A	-2.61	1.33	1.39
37	7	316	A86	C-C1	2.61	1.56	1.50
30	2	301	CLA	C3D-C4D	-2.61	1.38	1.44
38	3	311	KC1	CHB-C4A	-2.61	1.33	1.39
36	F	205	LMG	C1-C2	2.61	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	322	A86	C2-C1	2.61	1.41	1.35
30	B	831	CLA	C3D-C4D	-2.61	1.38	1.44
39	9	314	DD6	C26-C27	-2.61	1.31	1.37
38	3	308	KC1	C4A-C3A	2.61	1.49	1.44
37	4	314	A86	C24-C1	2.61	1.51	1.46
38	13	308	KC1	CHB-C4A	-2.61	1.33	1.39
30	7	304	CLA	C3D-C4D	-2.61	1.38	1.44
37	10	302	A86	C24-C1	2.61	1.51	1.46
30	B	839	CLA	C3B-C4B	2.61	1.50	1.42
37	10	316	A86	C14-C15	2.61	1.57	1.52
30	13	301	CLA	C1B-C2B	2.61	1.49	1.43
39	7	302	DD6	C26-C27	-2.61	1.31	1.37
30	10	308	CLA	C4D-CHA	2.61	1.47	1.38
37	11	301	A86	C26-C27	2.61	1.41	1.35
37	12	314	A86	C24-C1	2.61	1.51	1.46
30	B	835	CLA	C4D-CHA	2.61	1.47	1.38
38	6	312	KC1	CHB-C4A	-2.60	1.33	1.39
38	12	311	KC1	CHB-C4A	-2.60	1.33	1.39
30	B	825	CLA	C4D-CHA	2.60	1.47	1.38
37	4	314	A86	O-C13	-2.60	1.17	1.23
30	15	314	CLA	C4D-CHA	2.60	1.47	1.38
30	B	807	CLA	C3D-C4D	-2.60	1.38	1.44
38	7	308	KC1	CHB-C4A	-2.60	1.33	1.39
30	A	833	CLA	C3D-C4D	-2.60	1.38	1.44
37	13	315	A86	C2-C1	2.60	1.41	1.35
30	14	309	CLA	C3B-C4B	2.60	1.50	1.42
30	15	302	CLA	C4D-CHA	2.60	1.47	1.38
38	8	311	KC1	CHB-C4A	-2.60	1.33	1.39
30	A	839	CLA	OBD-CAD	2.60	1.27	1.22
37	14	314	A86	C24-C1	2.60	1.51	1.46
30	14	304	CLA	C4D-CHA	2.60	1.47	1.38
30	14	307	CLA	C4D-CHA	2.60	1.47	1.38
37	4	315	A86	C14-C15	2.60	1.57	1.52
37	7	315	A86	C2-C1	2.60	1.41	1.35
30	8	309	CLA	C4D-CHA	2.60	1.47	1.38
30	13	301	CLA	C4D-CHA	2.60	1.47	1.38
30	A	814	CLA	C1C-NC	-2.60	1.33	1.37
39	4	316	DD6	C26-C27	-2.59	1.31	1.37
33	I	101	BCR	C1-C6	-2.59	1.50	1.53
30	14	302	CLA	C4D-CHA	2.59	1.47	1.38
38	2	306	KC1	CHB-C4A	-2.59	1.33	1.39
30	A	802	CLA	C3D-C4D	-2.59	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	310	CLA	C3D-C4D	-2.59	1.38	1.44
30	A	840	CLA	C4D-CHA	2.59	1.47	1.38
37	2	302	A86	C14-C15	2.59	1.57	1.52
30	7	310	CLA	C4D-CHA	2.59	1.47	1.38
30	A	833	CLA	C4D-CHA	2.59	1.47	1.38
39	4	316	DD6	O1-C20	2.59	1.49	1.46
30	A	819	CLA	C3B-C4B	2.59	1.50	1.42
30	7	309	CLA	C4D-CHA	2.59	1.47	1.38
30	8	304	CLA	C4D-CHA	2.59	1.47	1.38
30	2u	202	CLA	C4D-CHA	2.59	1.47	1.38
37	8	315	A86	C25-C24	2.59	1.41	1.34
33	B	843	BCR	C30-C25	-2.59	1.50	1.53
30	A	815	CLA	C3D-C4D	-2.59	1.38	1.44
30	A	835	CLA	C4D-CHA	2.59	1.47	1.38
30	8	309	CLA	C3D-C4D	-2.59	1.38	1.44
38	14	311	KC1	C4A-C3A	2.59	1.49	1.44
37	14	314	A86	C2-C1	2.59	1.41	1.35
30	B	816	CLA	C3D-C4D	-2.59	1.38	1.44
37	5	316	A86	C26-C27	2.59	1.41	1.35
30	6	304	CLA	C4D-CHA	2.59	1.47	1.38
30	A	821	CLA	C4D-CHA	2.59	1.47	1.38
38	8	312	KC1	C2A-C1A	2.59	1.52	1.44
30	12	307	CLA	C4D-CHA	2.59	1.47	1.38
30	12	303	CLA	OBD-CAD	2.59	1.26	1.22
30	B	836	CLA	C3D-C4D	-2.59	1.38	1.44
30	11	310	CLA	C4C-C3C	2.59	1.49	1.45
34	2	320	LHG	O7-C5	-2.58	1.40	1.46
37	14	317	A86	C-C1	2.58	1.56	1.50
30	A	808	CLA	C4D-CHA	2.58	1.47	1.38
34	5	317	LHG	O7-C5	-2.58	1.40	1.46
37	6	320	A86	C-C1	2.58	1.56	1.50
30	B	821	CLA	C4D-CHA	2.58	1.47	1.38
30	12	303	CLA	C3D-C4D	-2.58	1.38	1.44
30	A	834	CLA	C4D-CHA	2.58	1.47	1.38
39	10	314	DD6	C26-C27	-2.58	1.31	1.37
39	2	317	DD6	C4-C5	2.58	1.51	1.43
38	4	310	KC1	CAA-C2A	2.58	1.54	1.46
33	F	204	BCR	C30-C25	-2.58	1.50	1.53
39	3	316	DD6	O1-C20	2.58	1.49	1.46
36	B	847	LMG	O7-C8	-2.58	1.40	1.46
30	B	801	CLA	C3D-C4D	-2.58	1.38	1.44
30	9	309	CLA	C3D-C4D	-2.58	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	301	CLA	C4D-CHA	2.58	1.47	1.38
30	A	844	CLA	C1B-C2B	2.58	1.49	1.43
30	4	304	CLA	C4D-CHA	2.58	1.47	1.38
37	11	316	A86	C24-C1	2.58	1.51	1.46
37	2	318	A86	C24-C1	2.58	1.51	1.46
37	5	315	A86	C14-C15	2.57	1.57	1.52
30	16	306	CLA	C3D-C4D	-2.57	1.38	1.44
39	3	313	DD6	O1-C20	2.57	1.49	1.46
30	15	305	CLA	C4C-C3C	2.57	1.49	1.45
38	16	304	KC1	C4C-C3C	2.57	1.49	1.45
30	A	839	CLA	C4D-CHA	2.57	1.47	1.38
39	4	313	DD6	C35-C34	2.57	1.56	1.52
30	16	310	CLA	C4D-CHA	2.57	1.47	1.38
38	14	308	KC1	C4B-NB	-2.57	1.34	1.37
30	B	829	CLA	C3D-C4D	-2.57	1.38	1.44
30	9	302	CLA	C4D-CHA	2.57	1.47	1.38
30	4	303	CLA	C4D-CHA	2.57	1.47	1.38
30	L	203	CLA	C1B-C2B	2.57	1.49	1.43
30	13	309	CLA	C1B-C2B	2.57	1.49	1.43
30	J	101	CLA	C3D-C4D	-2.57	1.38	1.44
30	L	203	CLA	C4D-CHA	2.57	1.47	1.38
38	3	304	KC1	CHB-C4A	-2.57	1.33	1.39
30	A	822	CLA	C4D-CHA	2.57	1.47	1.38
30	A	843	CLA	C4D-CHA	2.57	1.47	1.38
30	6	307	CLA	C3D-C4D	-2.57	1.38	1.44
37	13	315	A86	C14-C15	2.57	1.57	1.52
37	6	320	A86	C26-C27	2.57	1.41	1.35
38	13	306	KC1	CHB-C4A	-2.57	1.33	1.39
38	11	305	KC1	CHB-C4A	-2.57	1.33	1.39
30	A	804	CLA	C3B-C4B	2.57	1.50	1.42
38	2	312	KC1	CHB-C4A	-2.57	1.33	1.39
30	B	837	CLA	C4D-CHA	2.57	1.47	1.38
30	5	302	CLA	C4D-CHA	2.57	1.47	1.38
37	14	316	A86	C24-C1	2.57	1.51	1.46
30	15	304	CLA	C3B-C4B	2.57	1.50	1.42
30	15	304	CLA	C4C-C3C	2.57	1.49	1.45
30	A	803	CLA	C4D-CHA	2.56	1.47	1.38
38	13	312	KC1	C2A-C1A	2.56	1.52	1.44
37	8	318	A86	C25-C24	2.56	1.41	1.34
30	4	301	CLA	C4D-CHA	2.56	1.47	1.38
30	15	311	CLA	C1B-C2B	2.56	1.49	1.43
37	5	301	A86	O-C13	-2.56	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	831	CLA	C4D-CHA	2.56	1.47	1.38
30	7	305	CLA	C4D-CHA	2.56	1.47	1.38
30	11	304	CLA	C4D-CHA	2.56	1.47	1.38
39	3	316	DD6	C4-C5	2.56	1.51	1.43
30	1	302	CLA	C4D-CHA	2.56	1.47	1.38
37	10	317	A86	C2-C1	2.56	1.41	1.35
30	B	813	CLA	C1C-NC	-2.56	1.33	1.37
30	B	809	CLA	C4D-CHA	2.56	1.47	1.38
37	5	315	A86	C26-C27	2.56	1.41	1.35
37	4	315	A86	C24-C1	2.56	1.51	1.46
39	15	319	DD6	C4-C5	2.56	1.51	1.43
38	13	312	KC1	C1D-C2D	2.56	1.49	1.43
30	12	312	CLA	C1B-C2B	2.56	1.49	1.43
30	A	839	CLA	C3D-C4D	-2.56	1.38	1.44
30	A	823	CLA	C4D-CHA	2.56	1.47	1.38
30	A	829	CLA	C4D-CHA	2.56	1.47	1.38
37	11	314	A86	C-C1	2.56	1.56	1.50
30	15	307	CLA	C3B-C4B	2.55	1.50	1.42
30	B	809	CLA	C3D-C4D	-2.55	1.38	1.44
37	9	316	A86	O-C13	-2.55	1.17	1.23
30	B	838	CLA	C1C-NC	-2.55	1.33	1.37
39	9	314	DD6	O1-C20	2.55	1.49	1.46
37	2	319	A86	C25-C24	2.55	1.41	1.34
39	6	321	DD6	C9-C8	2.55	1.41	1.34
30	B	832	CLA	C3D-C4D	-2.55	1.38	1.44
38	14	306	KC1	C4A-C3A	2.55	1.49	1.44
30	B	807	CLA	C4D-CHA	2.55	1.47	1.38
37	7	316	A86	C14-C15	2.55	1.57	1.52
37	14	317	A86	O-C13	-2.55	1.17	1.23
30	A	810	CLA	C3D-C4D	-2.55	1.38	1.44
38	16	311	KC1	C4A-C3A	2.55	1.49	1.44
38	2	314	KC1	CAA-C2A	2.55	1.54	1.46
30	A	830	CLA	C3B-C4B	2.55	1.50	1.42
30	A	842	CLA	C3B-C4B	2.55	1.50	1.42
30	A	818	CLA	C4D-CHA	2.55	1.47	1.38
30	B	836	CLA	OBD-CAD	2.55	1.26	1.22
30	3	302	CLA	C3D-C4D	-2.55	1.38	1.44
30	13	303	CLA	C1B-C2B	2.55	1.49	1.43
30	15	305	CLA	C1B-C2B	2.55	1.49	1.43
37	9	315	A86	C2-C1	2.55	1.41	1.35
38	11	307	KC1	C4A-C3A	2.55	1.49	1.44
39	3	313	DD6	C4-C5	2.55	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	319	DD6	C4-C5	2.55	1.51	1.43
30	B	827	CLA	C4D-CHA	2.55	1.47	1.38
30	A	811	CLA	C4D-CHA	2.55	1.47	1.38
30	16	308	CLA	C4C-C3C	2.55	1.49	1.45
37	11	301	A86	C24-C1	2.55	1.51	1.46
37	11	315	A86	C24-C1	2.55	1.51	1.46
37	3	315	A86	O-C13	-2.55	1.17	1.23
38	13	308	KC1	C4A-C3A	2.55	1.49	1.44
38	11	311	KC1	C4A-C3A	2.55	1.49	1.44
39	15	318	DD6	C26-C27	-2.55	1.31	1.37
30	9	309	CLA	C4D-CHA	2.55	1.47	1.38
38	6	312	KC1	CAA-C2A	2.54	1.54	1.46
30	2u	202	CLA	C3D-C4D	-2.54	1.38	1.44
38	13	306	KC1	C2A-C1A	2.54	1.52	1.44
30	B	816	CLA	C1B-C2B	2.54	1.49	1.43
38	13	305	KC1	C4B-NB	-2.54	1.34	1.37
39	13	314	DD6	C26-C27	-2.54	1.31	1.37
30	A	842	CLA	C4D-CHA	2.54	1.47	1.38
30	B	851	CLA	C4D-CHA	2.54	1.47	1.38
38	9	312	KC1	C4C-C3C	2.54	1.49	1.45
30	B	829	CLA	C4D-CHA	2.54	1.47	1.38
39	16	313	DD6	C4-C5	2.54	1.51	1.43
38	8	306	KC1	CHB-C4A	-2.54	1.33	1.39
30	8	303	CLA	C4D-CHA	2.54	1.47	1.38
30	A	812	CLA	C3D-C4D	-2.54	1.38	1.44
30	A	830	CLA	C4D-CHA	2.54	1.47	1.38
30	13	302	CLA	C1B-C2B	2.54	1.49	1.43
38	4	307	KC1	C4A-C3A	2.54	1.49	1.44
30	7	309	CLA	C1B-C2B	2.54	1.49	1.43
37	11	314	A86	C24-C1	2.54	1.51	1.46
37	7	315	A86	O4-C34	-2.54	1.40	1.46
30	16	309	CLA	C1B-C2B	2.54	1.49	1.43
37	11	315	A86	O-C13	-2.53	1.18	1.23
37	15	315	A86	C-C1	2.53	1.56	1.50
39	1	310	DD6	O1-C20	2.53	1.49	1.46
39	3	312	DD6	C26-C27	-2.53	1.31	1.37
30	8	301	CLA	C4D-CHA	2.53	1.47	1.38
34	A	852	LHG	O7-C5	-2.53	1.40	1.46
30	B	820	CLA	C1B-C2B	2.53	1.49	1.43
30	12	307	CLA	C3D-C4D	-2.53	1.38	1.44
37	15	321	A86	C24-C1	2.53	1.51	1.46
30	B	808	CLA	C4D-CHA	2.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	813	CLA	C3D-C4D	-2.53	1.38	1.44
30	3	307	CLA	C1B-C2B	2.53	1.49	1.43
39	12	315	DD6	C26-C27	-2.53	1.31	1.37
38	12	305	KC1	CHB-C4A	-2.53	1.33	1.39
38	12	313	KC1	C2A-C1A	2.53	1.52	1.44
38	13	311	KC1	C2A-C1A	2.53	1.52	1.44
30	B	819	CLA	C4D-CHA	2.53	1.47	1.38
38	13	305	KC1	CHB-C4A	-2.53	1.33	1.39
39	8	317	DD6	C26-C27	-2.53	1.31	1.37
30	6	314	CLA	C4D-CHA	2.53	1.47	1.38
30	A	812	CLA	C4D-CHA	2.53	1.47	1.38
30	12	310	CLA	C4D-CHA	2.53	1.47	1.38
37	9	316	A86	C2-C1	2.53	1.41	1.35
37	5	315	A86	O-C13	-2.53	1.18	1.23
30	2	301	CLA	C4D-CHA	2.53	1.47	1.38
37	2u	205	A86	O-C13	-2.53	1.18	1.23
37	12	314	A86	O-C13	-2.53	1.18	1.23
38	4	308	KC1	CAA-C2A	2.53	1.54	1.46
38	7	313	KC1	CAA-C2A	2.53	1.54	1.46
38	9	311	KC1	CHB-C4A	-2.53	1.33	1.39
30	14	303	CLA	C3B-C4B	2.53	1.50	1.42
39	4	313	DD6	C26-C27	-2.53	1.31	1.37
38	6	313	KC1	CHB-C4A	-2.53	1.33	1.39
37	2	318	A86	C-C1	2.52	1.55	1.50
37	15	322	A86	O-C13	-2.52	1.18	1.23
37	3	314	A86	C2-C1	2.52	1.41	1.35
33	J	102	BCR	C30-C25	-2.52	1.50	1.53
30	A	810	CLA	C1B-C2B	2.52	1.49	1.43
30	2	303	CLA	C3B-C4B	2.52	1.50	1.42
30	A	817	CLA	C4D-CHA	2.52	1.47	1.38
30	B	815	CLA	C1C-NC	-2.52	1.33	1.37
30	16	306	CLA	C4D-CHA	2.52	1.47	1.38
39	5	313	DD6	C4-C5	2.52	1.51	1.43
37	10	302	A86	O-C13	-2.52	1.18	1.23
39	11	313	DD6	C4-C5	2.52	1.51	1.43
30	B	820	CLA	C4D-CHA	2.52	1.47	1.38
30	1	305	CLA	C4C-C3C	2.52	1.49	1.45
38	16	304	KC1	C2A-C1A	2.52	1.52	1.44
30	A	823	CLA	C3D-C4D	-2.52	1.38	1.44
30	8	302	CLA	C4D-CHA	2.52	1.47	1.38
38	11	311	KC1	CHB-C4A	-2.52	1.33	1.39
30	13	304	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	830	CLA	C3D-C4D	-2.52	1.38	1.44
30	9	301	CLA	C1B-C2B	2.52	1.49	1.43
37	7	319	A86	C2-C1	2.52	1.41	1.35
30	14	304	CLA	C1B-C2B	2.52	1.49	1.43
30	A	804	CLA	C3D-C4D	-2.52	1.38	1.44
30	A	809	CLA	C3D-C4D	-2.52	1.38	1.44
30	B	814	CLA	C4D-CHA	2.52	1.47	1.38
30	A	816	CLA	C1B-C2B	2.52	1.49	1.43
30	8	305	CLA	C4D-CHA	2.52	1.47	1.38
30	B	833	CLA	C3B-C4B	2.52	1.50	1.42
37	2	319	A86	C14-C15	2.52	1.57	1.52
37	15	317	A86	C2-C1	2.52	1.41	1.35
38	9	304	KC1	CHB-C4A	-2.52	1.33	1.39
37	8	315	A86	C-C1	2.52	1.55	1.50
30	A	821	CLA	C3D-C4D	-2.52	1.38	1.44
37	4	317	A86	O-C13	-2.52	1.18	1.23
39	10	314	DD6	C4-C5	2.52	1.51	1.43
30	13	307	CLA	C4B-NB	-2.52	1.34	1.37
39	10	314	DD6	O1-C20	2.52	1.49	1.46
39	4	313	DD6	C4-C5	2.52	1.51	1.43
39	6	318	DD6	C4-C5	2.52	1.51	1.43
30	B	823	CLA	C3D-C4D	-2.52	1.38	1.44
30	10	305	CLA	C4D-CHA	2.52	1.47	1.38
38	4	308	KC1	CHB-C4A	-2.52	1.33	1.39
30	6	315	CLA	C1B-C2B	2.52	1.49	1.43
37	10	315	A86	C14-C15	2.52	1.57	1.52
37	15	321	A86	C14-C15	2.52	1.57	1.52
37	14	314	A86	C-C1	2.51	1.55	1.50
37	6	320	A86	C24-C1	2.51	1.51	1.46
37	9	313	A86	C20-C15	2.51	1.51	1.48
38	13	310	KC1	CHB-C4A	-2.51	1.33	1.39
39	6	319	DD6	C26-C27	-2.51	1.31	1.37
37	4	312	A86	C-C1	2.51	1.55	1.50
39	4	316	DD6	C4-C5	2.51	1.51	1.43
38	9	304	KC1	C4A-C3A	2.51	1.49	1.44
30	A	821	CLA	C1C-NC	-2.51	1.33	1.37
30	A	815	CLA	C1C-NC	-2.51	1.33	1.37
37	10	317	A86	O-C13	-2.51	1.18	1.23
30	11	309	CLA	C4D-CHA	2.51	1.47	1.38
37	16	312	A86	C26-C27	2.51	1.41	1.35
39	15	319	DD6	C26-C27	-2.51	1.31	1.37
30	3	301	CLA	C3D-C4D	-2.51	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	316	A86	C24-C1	2.51	1.51	1.46
30	F	201	CLA	C4D-CHA	2.51	1.47	1.38
37	4	315	A86	C26-C27	2.51	1.41	1.35
30	12	310	CLA	C1B-C2B	2.50	1.49	1.43
30	A	804	CLA	C4D-CHA	2.50	1.47	1.38
38	12	309	KC1	C4A-C3A	2.50	1.49	1.44
30	A	804	CLA	C1C-NC	-2.50	1.34	1.37
37	10	302	A86	C14-C15	2.50	1.57	1.52
37	14	320	A86	C14-C15	2.50	1.57	1.52
30	A	827	CLA	C4D-CHA	2.50	1.47	1.38
37	10	316	A86	O-C13	-2.50	1.18	1.23
37	14	314	A86	O-C13	-2.50	1.18	1.23
30	B	817	CLA	C3B-C4B	2.50	1.50	1.42
30	L	203	CLA	C3D-C4D	-2.50	1.38	1.44
37	11	314	A86	C14-C15	2.50	1.57	1.52
30	11	306	CLA	C4D-CHA	2.50	1.47	1.38
30	16	303	CLA	C1B-C2B	2.50	1.49	1.43
39	16	313	DD6	C26-C27	-2.50	1.31	1.37
30	12	302	CLA	C4D-CHA	2.50	1.47	1.38
30	B	839	CLA	C4D-CHA	2.50	1.47	1.38
37	7	316	A86	C25-C24	2.50	1.41	1.34
39	10	313	DD6	C4-C5	2.50	1.50	1.43
37	5	316	A86	C14-C15	2.50	1.57	1.52
30	B	827	CLA	C3D-C4D	-2.50	1.38	1.44
30	B	851	CLA	C3D-C4D	-2.50	1.38	1.44
37	11	314	A86	C2-C1	2.50	1.41	1.35
30	11	309	CLA	C3D-C4D	-2.50	1.38	1.44
30	8	308	CLA	C3D-C4D	-2.50	1.38	1.44
38	11	312	KC1	C4A-C3A	2.50	1.49	1.44
38	5	305	KC1	CHB-C4A	-2.50	1.33	1.39
30	6	316	CLA	C3D-C4D	-2.50	1.38	1.44
38	4	310	KC1	C2A-C1A	2.50	1.52	1.44
38	7	308	KC1	C4A-C3A	2.50	1.49	1.44
39	12	315	DD6	O1-C20	2.50	1.49	1.46
30	A	836	CLA	C3D-C4D	-2.50	1.38	1.44
30	A	837	CLA	C3D-C4D	-2.50	1.38	1.44
37	1	309	A86	O-C13	-2.49	1.18	1.23
30	10	311	CLA	C1B-C2B	2.49	1.49	1.43
30	B	820	CLA	C1C-C2C	2.49	1.49	1.44
30	A	818	CLA	C3D-C4D	-2.49	1.38	1.44
30	9	306	CLA	C1B-C2B	2.49	1.49	1.43
38	1	308	KC1	CAA-C2A	2.49	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	818	CLA	C3D-C4D	-2.49	1.38	1.44
30	7	306	CLA	C3B-C4B	2.49	1.50	1.42
30	12	303	CLA	C1B-C2B	2.49	1.49	1.43
38	10	306	KC1	CHB-C4A	-2.49	1.33	1.39
30	2	304	CLA	C3D-C4D	-2.49	1.38	1.44
37	14	320	A86	C2-C1	2.49	1.41	1.35
30	3	307	CLA	C3B-C4B	2.49	1.50	1.42
30	B	826	CLA	C3D-C4D	-2.49	1.38	1.44
38	13	311	KC1	C1D-C2D	2.49	1.49	1.43
38	13	306	KC1	C4A-C3A	2.49	1.49	1.44
30	16	302	CLA	C1B-C2B	2.49	1.49	1.43
38	3	311	KC1	C4C-C3C	2.49	1.49	1.45
37	12	316	A86	C14-C15	2.49	1.57	1.52
38	11	307	KC1	CHB-C4A	-2.49	1.33	1.39
38	1	306	KC1	C4A-C3A	2.49	1.49	1.44
30	B	805	CLA	C3D-C4D	-2.49	1.38	1.44
30	A	813	CLA	C3D-C4D	-2.49	1.38	1.44
30	A	811	CLA	C3D-C4D	-2.49	1.38	1.44
30	2	313	CLA	C1B-C2B	2.49	1.49	1.43
39	2	315	DD6	O1-C20	2.49	1.49	1.46
37	2	319	A86	O-C13	-2.48	1.18	1.23
38	14	308	KC1	C2A-C1A	2.48	1.52	1.44
30	11	310	CLA	C1B-C2B	2.48	1.49	1.43
38	5	306	KC1	C1D-C2D	2.48	1.49	1.43
38	14	308	KC1	CHB-C4A	-2.48	1.33	1.39
37	4	317	A86	C24-C1	2.48	1.51	1.46
30	6	310	CLA	C3B-C4B	2.48	1.50	1.42
37	2	319	A86	C-C1	2.48	1.55	1.50
30	A	843	CLA	C1B-C2B	2.48	1.49	1.43
30	A	814	CLA	C3D-C4D	-2.48	1.38	1.44
30	5	302	CLA	C3D-C4D	-2.48	1.38	1.44
30	14	304	CLA	C3B-C4B	2.48	1.50	1.42
37	14	316	A86	O-C13	-2.48	1.18	1.23
30	13	309	CLA	C4C-C3C	2.48	1.49	1.45
38	13	310	KC1	C4A-C3A	2.48	1.49	1.44
30	5	311	CLA	C1B-C2B	2.48	1.48	1.43
38	13	308	KC1	C1D-C2D	2.48	1.48	1.43
38	5	305	KC1	CAA-C2A	2.48	1.53	1.46
30	B	839	CLA	C3D-C4D	-2.48	1.38	1.44
39	13	314	DD6	O1-C20	2.48	1.49	1.46
37	14	301	A86	C14-C15	2.48	1.57	1.52
30	11	308	CLA	C3B-C4B	2.48	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	844	CLA	C3B-C4B	2.48	1.49	1.42
30	16	303	CLA	C4D-CHA	2.48	1.46	1.38
30	L	202	CLA	C1B-C2B	2.48	1.48	1.43
30	F	202	CLA	C3D-C4D	-2.48	1.38	1.44
38	10	312	KC1	C1D-C2D	2.48	1.48	1.43
30	2	301	CLA	C1B-C2B	2.48	1.48	1.43
30	5	304	CLA	C1B-C2B	2.48	1.48	1.43
30	10	305	CLA	C3D-C4D	-2.48	1.38	1.44
30	13	303	CLA	C4C-C3C	2.47	1.49	1.45
38	3	304	KC1	C2A-C1A	2.47	1.52	1.44
30	15	309	CLA	C3B-C4B	2.47	1.49	1.42
30	2	307	CLA	C1B-C2B	2.47	1.48	1.43
37	15	323	A86	O-C13	-2.47	1.18	1.23
30	2	310	CLA	C1B-C2B	2.47	1.48	1.43
37	14	301	A86	C2-C1	2.47	1.41	1.35
30	10	308	CLA	C3D-C4D	-2.47	1.38	1.44
30	A	803	CLA	CHB-C1B	2.47	1.45	1.39
39	15	319	DD6	C35-C36	2.47	1.54	1.51
39	2	316	DD6	C4-C5	2.47	1.50	1.43
30	16	307	CLA	C3B-C4B	2.47	1.49	1.42
30	A	802	CLA	C4D-CHA	2.47	1.46	1.38
30	B	810	CLA	C4D-CHA	2.47	1.46	1.38
33	B	842	BCR	C30-C25	-2.47	1.50	1.53
30	14	313	CLA	C4D-CHA	2.47	1.46	1.38
30	A	808	CLA	C3B-C4B	2.47	1.49	1.42
30	B	803	CLA	C4D-CHA	2.47	1.46	1.38
38	3	304	KC1	CAA-C2A	2.47	1.53	1.46
38	13	312	KC1	CHB-C4A	-2.47	1.33	1.39
38	8	311	KC1	CAA-C2A	2.47	1.53	1.46
30	5	309	CLA	C1B-C2B	2.47	1.48	1.43
30	3	309	CLA	C3B-C4B	2.47	1.49	1.42
30	2	308	CLA	C3D-C4D	-2.47	1.38	1.44
39	8	316	DD6	C15-C14	2.47	1.54	1.50
37	14	320	A86	O-C13	-2.47	1.18	1.23
37	4	317	A86	C26-C27	2.47	1.41	1.35
39	7	302	DD6	C4-C5	2.47	1.50	1.43
30	5	303	CLA	C3D-C4D	-2.47	1.38	1.44
30	F	201	CLA	C3B-C4B	2.47	1.49	1.42
30	16	307	CLA	C1B-C2B	2.47	1.48	1.43
38	12	311	KC1	C2A-C1A	2.46	1.52	1.44
30	4	309	CLA	C1B-C2B	2.46	1.48	1.43
30	B	835	CLA	OBD-CAD	2.46	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	817	CLA	C4D-CHA	2.46	1.46	1.38
30	7	303	CLA	C4D-CHA	2.46	1.46	1.38
37	12	316	A86	C2-C1	2.46	1.41	1.35
30	A	834	CLA	C3D-C4D	-2.46	1.38	1.44
30	1	302	CLA	C3D-C4D	-2.46	1.38	1.44
30	12	308	CLA	C1B-C2B	2.46	1.48	1.43
38	12	305	KC1	C2A-C1A	2.46	1.52	1.44
39	3	312	DD6	C4-C5	2.46	1.50	1.43
30	A	830	CLA	C3D-C4D	-2.46	1.38	1.44
30	16	307	CLA	C4C-C3C	2.46	1.49	1.45
30	14	309	CLA	C4C-C3C	2.46	1.49	1.45
30	15	309	CLA	C4C-C3C	2.46	1.49	1.45
30	15	311	CLA	C3B-C4B	2.46	1.49	1.42
30	A	826	CLA	C3D-C4D	-2.46	1.38	1.44
38	14	306	KC1	C4B-NB	-2.46	1.34	1.37
30	16	308	CLA	C1B-C2B	2.46	1.48	1.43
30	16	302	CLA	C3D-C4D	-2.46	1.38	1.44
37	12	316	A86	O-C13	-2.46	1.18	1.23
37	14	315	A86	O-C13	-2.46	1.18	1.23
39	6	319	DD6	C35-C34	2.46	1.56	1.52
37	11	315	A86	C26-C27	2.46	1.41	1.35
30	B	812	CLA	C3D-C4D	-2.46	1.38	1.44
30	6	317	CLA	C1B-C2B	2.46	1.48	1.43
36	B	849	LMG	O1-C1	2.46	1.44	1.40
37	5	316	A86	C2-C1	2.46	1.41	1.35
30	15	310	CLA	C4C-C3C	2.46	1.49	1.45
37	10	316	A86	C24-C1	2.46	1.51	1.46
30	B	826	CLA	C4D-CHA	2.46	1.46	1.38
38	13	305	KC1	C2A-C1A	2.46	1.52	1.44
30	9	301	CLA	C1C-NC	-2.46	1.34	1.37
37	4	314	A86	C14-C15	2.46	1.57	1.52
39	15	318	DD6	C4-C5	2.46	1.50	1.43
38	1	306	KC1	C4C-C3C	2.45	1.49	1.45
30	B	801	CLA	C1C-NC	-2.45	1.34	1.37
30	A	816	CLA	C3D-C4D	-2.45	1.38	1.44
30	L	202	CLA	C4D-CHA	2.45	1.46	1.38
38	11	307	KC1	C4C-C3C	2.45	1.49	1.45
37	3	314	A86	O-C13	-2.45	1.18	1.23
30	A	834	CLA	C1B-C2B	2.45	1.48	1.43
30	7	310	CLA	C3D-C4D	-2.45	1.38	1.44
30	12	310	CLA	C3D-C4D	-2.45	1.38	1.44
37	12	314	A86	C26-C27	2.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	319	A86	C24-C1	2.45	1.51	1.46
38	2	312	KC1	C4A-C3A	2.45	1.49	1.44
30	B	834	CLA	OBD-CAD	2.45	1.26	1.22
30	16	305	CLA	C1B-C2B	2.45	1.48	1.43
39	5	314	DD6	C35-C34	2.45	1.56	1.52
38	14	311	KC1	CHB-C4A	-2.45	1.33	1.39
30	B	808	CLA	C1C-NC	-2.45	1.34	1.37
30	1	301	CLA	C3D-C4D	-2.45	1.38	1.44
30	12	304	CLA	C1B-C2B	2.45	1.48	1.43
37	2	302	A86	O-C13	-2.45	1.18	1.23
30	4	304	CLA	C3D-C4D	-2.45	1.38	1.44
38	5	312	KC1	CAA-C2A	2.45	1.53	1.46
37	5	316	A86	O-C13	-2.45	1.18	1.23
38	11	312	KC1	CHB-C4A	-2.45	1.33	1.39
38	8	310	KC1	CAA-C2A	2.45	1.53	1.46
37	2u	205	A86	C14-C15	2.45	1.57	1.52
30	10	309	CLA	C1B-C2B	2.45	1.48	1.43
30	B	820	CLA	C3D-C4D	-2.45	1.38	1.44
38	9	312	KC1	C1D-C2D	2.45	1.48	1.43
37	7	319	A86	C-C1	2.45	1.55	1.50
30	6	304	CLA	C3B-C4B	2.45	1.49	1.42
30	6	304	CLA	C3D-C4D	-2.45	1.38	1.44
38	11	307	KC1	C1D-C2D	2.45	1.48	1.43
38	3	308	KC1	C4C-C3C	2.44	1.49	1.45
30	B	807	CLA	C1B-C2B	2.44	1.48	1.43
30	2	313	CLA	C3B-C4B	2.44	1.49	1.42
37	11	316	A86	C2-C1	2.44	1.41	1.35
38	6	312	KC1	C4A-C3A	2.44	1.49	1.44
38	13	311	KC1	C4B-NB	-2.44	1.34	1.37
37	16	312	A86	O-C13	-2.44	1.18	1.23
39	10	313	DD6	C22-C16	-2.44	1.49	1.53
30	1	307	CLA	C3B-C4B	2.44	1.49	1.42
39	7	317	DD6	C4-C5	2.44	1.50	1.43
30	B	827	CLA	C1B-C2B	2.44	1.48	1.43
37	14	318	A86	O-C13	-2.44	1.18	1.23
37	14	318	A86	C2-C1	2.44	1.41	1.35
37	4	314	A86	C2-C1	2.44	1.41	1.35
30	15	309	CLA	C1B-C2B	2.44	1.48	1.43
37	10	301	A86	C14-C15	2.44	1.57	1.52
38	11	311	KC1	C2A-C1A	2.44	1.52	1.44
39	2	315	DD6	C4-C5	2.44	1.50	1.43
30	16	309	CLA	C4C-C3C	2.44	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	305	KC1	C4C-C3C	2.44	1.49	1.45
30	B	836	CLA	C3B-C4B	2.44	1.49	1.42
39	6	319	DD6	O1-C20	2.44	1.49	1.46
39	7	318	DD6	C4-C5	2.44	1.50	1.43
30	6	309	CLA	C3D-C4D	-2.44	1.38	1.44
30	16	306	CLA	C4C-C3C	2.44	1.49	1.45
30	A	824	CLA	C4D-CHA	2.44	1.46	1.38
30	B	811	CLA	C4D-CHA	2.44	1.46	1.38
30	4	306	CLA	C3D-C4D	-2.44	1.38	1.44
30	7	311	CLA	C3D-C4D	-2.44	1.38	1.44
30	1	307	CLA	C1B-C2B	2.44	1.48	1.43
37	2u	203	A86	C14-C15	2.44	1.57	1.52
38	9	312	KC1	CHB-C4A	-2.43	1.33	1.39
37	1	309	A86	C26-C27	2.43	1.41	1.35
30	3	302	CLA	OBD-CAD	2.43	1.26	1.22
30	16	306	CLA	C3B-C4B	2.43	1.49	1.42
30	B	801	CLA	C4D-CHA	2.43	1.46	1.38
30	10	304	CLA	C3D-C4D	-2.43	1.38	1.44
30	B	802	CLA	C4D-CHA	2.43	1.46	1.38
30	A	831	CLA	C1C-NC	-2.43	1.34	1.37
30	4	303	CLA	C3D-C4D	-2.43	1.38	1.44
39	9	314	DD6	C4-C5	2.43	1.50	1.43
30	15	310	CLA	C3B-C2B	2.43	1.49	1.41
30	9	303	CLA	C3D-C4D	-2.43	1.38	1.44
30	16	308	CLA	C3B-C4B	2.43	1.49	1.42
38	7	308	KC1	C2A-C1A	2.43	1.52	1.44
38	13	308	KC1	C2A-C1A	2.43	1.52	1.44
38	5	305	KC1	C4A-C3A	2.43	1.49	1.44
30	11	310	CLA	C3B-C4B	2.43	1.49	1.42
30	A	823	CLA	C1B-C2B	2.43	1.48	1.43
37	16	314	A86	C24-C1	2.43	1.51	1.46
37	2u	203	A86	O4-C34	-2.43	1.40	1.46
36	14	321	LMG	C4-C3	2.43	1.58	1.52
30	A	841	CLA	C3D-C4D	-2.43	1.38	1.44
37	11	316	A86	O-C13	-2.42	1.18	1.23
30	12	307	CLA	C3B-C4B	2.42	1.49	1.42
37	11	314	A86	O-C13	-2.42	1.18	1.23
30	13	303	CLA	C3B-C4B	2.42	1.49	1.42
30	14	309	CLA	C1B-C2B	2.42	1.48	1.43
30	7	312	CLA	C4C-C3C	2.42	1.49	1.45
30	16	305	CLA	C3B-C4B	2.42	1.49	1.42
37	15	320	A86	O-C13	-2.42	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	10	309	CLA	C4C-C3C	2.42	1.49	1.45
37	14	320	A86	C5-C6	2.42	1.41	1.35
30	6	317	CLA	C3B-C4B	2.42	1.49	1.42
30	A	843	CLA	C3D-C4D	-2.42	1.38	1.44
30	1	303	CLA	C3B-C4B	2.42	1.49	1.42
30	10	311	CLA	C3B-C4B	2.42	1.49	1.42
37	14	318	A86	C14-C15	2.42	1.57	1.52
38	2	312	KC1	C2A-C1A	2.42	1.52	1.44
30	A	806	CLA	C1C-NC	-2.42	1.34	1.37
37	16	314	A86	C26-C27	2.42	1.41	1.35
30	A	821	CLA	C1B-C2B	2.42	1.48	1.43
30	A	844	CLA	C3D-C4D	-2.42	1.38	1.44
37	10	315	A86	O-C13	-2.42	1.18	1.23
30	15	306	CLA	C4C-C3C	2.42	1.49	1.45
38	2	306	KC1	C4A-C3A	2.42	1.49	1.44
37	5	301	A86	C14-C15	2.41	1.57	1.52
30	7	312	CLA	C1B-C2B	2.41	1.48	1.43
37	13	313	A86	C5-C6	2.41	1.41	1.35
37	15	320	A86	C5-C6	2.41	1.41	1.35
37	15	321	A86	C2-C1	2.41	1.41	1.35
37	2	302	A86	C2-C1	2.41	1.41	1.35
30	A	805	CLA	C3D-C4D	-2.41	1.38	1.44
30	9	301	CLA	C3B-C2B	2.41	1.49	1.41
30	L	203	CLA	C3B-C2B	2.41	1.49	1.41
38	5	310	KC1	C4A-C3A	2.41	1.49	1.44
38	4	307	KC1	C2A-C1A	2.41	1.52	1.44
30	15	311	CLA	C4C-C3C	2.41	1.49	1.45
30	A	818	CLA	C3B-C4B	2.41	1.49	1.42
38	16	311	KC1	C1D-C2D	2.41	1.48	1.43
39	6	321	DD6	C35-C36	2.41	1.54	1.51
37	5	301	A86	C2-C1	2.41	1.41	1.35
30	1	305	CLA	C1B-C2B	2.41	1.48	1.43
30	2	309	CLA	C1B-C2B	2.41	1.48	1.43
36	8	321	LMG	C3-C2	2.41	1.58	1.52
30	F	203	CLA	C3D-C4D	-2.41	1.38	1.44
38	8	310	KC1	C2A-C1A	2.41	1.52	1.44
30	A	838	CLA	OBD-CAD	2.41	1.26	1.22
38	12	305	KC1	C1D-C2D	2.41	1.48	1.43
30	7	309	CLA	C3D-C4D	-2.41	1.38	1.44
37	14	319	A86	O-C13	-2.41	1.18	1.23
30	3	306	CLA	C3D-C4D	-2.41	1.38	1.44
38	10	310	KC1	C4A-C3A	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	306	CLA	C4C-C3C	2.41	1.49	1.45
38	12	311	KC1	C3B-C4B	2.41	1.50	1.46
30	14	303	CLA	C1B-C2B	2.41	1.48	1.43
30	F	201	CLA	C1C-NC	-2.41	1.34	1.37
30	9	305	CLA	C3D-C4D	-2.40	1.38	1.44
37	13	313	A86	O-C13	-2.40	1.18	1.23
30	A	807	CLA	C1C-NC	-2.40	1.34	1.37
30	15	313	CLA	C4C-C3C	2.40	1.49	1.45
30	12	308	CLA	C3B-C4B	2.40	1.49	1.42
30	12	306	CLA	C3D-C4D	-2.40	1.38	1.44
30	3	302	CLA	C1B-C2B	2.40	1.48	1.43
38	3	304	KC1	C4A-C3A	2.40	1.49	1.44
38	10	310	KC1	C4C-C3C	2.40	1.49	1.45
38	11	305	KC1	C4A-C3A	2.40	1.49	1.44
38	6	313	KC1	C4A-C3A	2.40	1.49	1.44
30	1	305	CLA	C3B-C4B	2.40	1.49	1.42
30	F	201	CLA	C3D-C4D	-2.40	1.38	1.44
30	11	306	CLA	C3D-C4D	-2.40	1.38	1.44
30	3	306	CLA	C3B-C4B	2.40	1.49	1.42
38	11	305	KC1	C1D-C2D	2.40	1.48	1.43
30	14	302	CLA	C3D-C4D	-2.40	1.38	1.44
38	11	307	KC1	C2A-C1A	2.40	1.52	1.44
30	8	308	CLA	C3B-C4B	2.40	1.49	1.42
38	6	312	KC1	C2A-C1A	2.40	1.52	1.44
30	10	304	CLA	C3B-C4B	2.40	1.49	1.42
30	12	302	CLA	C3D-C4D	-2.40	1.38	1.44
30	12	306	CLA	C1B-C2B	2.39	1.48	1.43
38	3	311	KC1	C1D-C2D	2.39	1.48	1.43
30	B	820	CLA	C3B-C4B	2.39	1.49	1.42
30	4	303	CLA	C3B-C4B	2.39	1.49	1.42
38	10	310	KC1	C2A-C1A	2.39	1.52	1.44
30	7	306	CLA	C1C-NC	-2.39	1.34	1.37
38	5	306	KC1	CAA-C2A	2.39	1.53	1.46
30	B	819	CLA	C1C-NC	-2.39	1.34	1.37
30	15	307	CLA	C1B-C2B	2.39	1.48	1.43
37	4	312	A86	O-C13	-2.39	1.18	1.23
38	5	306	KC1	C4C-C3C	2.39	1.49	1.45
36	2u	204	LMG	C4-C3	2.39	1.58	1.52
37	3	314	A86	C14-C15	2.39	1.57	1.52
37	14	301	A86	O-C13	-2.39	1.18	1.23
38	3	311	KC1	C2A-C1A	2.39	1.52	1.44
30	A	840	CLA	C3B-C4B	2.39	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	16	304	KC1	C1D-C2D	2.39	1.48	1.43
30	8	305	CLA	C3B-C2B	2.39	1.49	1.41
39	5	314	DD6	C22-C16	-2.39	1.49	1.53
37	11	315	A86	C14-C15	2.39	1.57	1.52
30	7	305	CLA	C1B-C2B	2.39	1.48	1.43
38	13	305	KC1	C3B-C4B	2.39	1.50	1.46
38	5	310	KC1	C2A-C1A	2.39	1.52	1.44
38	12	311	KC1	C4C-C3C	2.39	1.49	1.45
30	3	310	CLA	C1B-C2B	2.39	1.48	1.43
30	8	309	CLA	C3B-C4B	2.39	1.49	1.42
39	5	314	DD6	O1-C20	2.39	1.49	1.46
30	B	830	CLA	C4D-CHA	2.39	1.46	1.38
37	15	317	A86	C14-C15	2.39	1.57	1.52
39	7	314	DD6	C4-C5	2.39	1.50	1.43
38	11	312	KC1	C4C-C3C	2.38	1.49	1.45
38	5	305	KC1	C4C-C3C	2.38	1.49	1.45
30	15	306	CLA	C3B-C4B	2.38	1.49	1.42
38	2	314	KC1	C4A-C3A	2.38	1.49	1.44
30	8	302	CLA	C3B-C2B	2.38	1.49	1.41
30	B	839	CLA	C1C-C2C	2.38	1.49	1.44
38	8	306	KC1	C2A-C1A	2.38	1.52	1.44
30	14	307	CLA	C3B-C4B	2.38	1.49	1.42
30	14	312	CLA	C4C-C3C	2.38	1.49	1.45
30	4	309	CLA	C3B-C4B	2.38	1.49	1.42
37	14	315	A86	C14-C15	2.38	1.57	1.52
38	11	311	KC1	C1D-C2D	2.38	1.48	1.43
38	10	306	KC1	CAA-C2A	2.38	1.53	1.46
30	8	301	CLA	C3D-C4D	-2.38	1.38	1.44
30	13	304	CLA	C4C-C3C	2.38	1.49	1.45
30	13	307	CLA	C4C-C3C	2.38	1.49	1.45
38	12	313	KC1	CBD-CAD	-2.38	1.45	1.56
30	12	303	CLA	C3B-C2B	2.38	1.49	1.41
38	3	308	KC1	CHB-C4A	-2.38	1.33	1.39
37	11	316	A86	C14-C15	2.38	1.57	1.52
30	A	820	CLA	C4C-C3C	2.38	1.49	1.45
39	12	317	DD6	C4-C5	2.38	1.50	1.43
30	14	310	CLA	C1B-C2B	2.38	1.48	1.43
37	2u	203	A86	C-C1	2.38	1.55	1.50
37	12	314	A86	C2-C1	2.38	1.41	1.35
33	L	205	BCR	C30-C25	-2.38	1.50	1.53
38	8	310	KC1	C4A-C3A	2.38	1.49	1.44
38	3	308	KC1	C2A-C1A	2.38	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	10	310	KC1	C3B-C4B	2.37	1.50	1.46
30	7	306	CLA	C3D-C4D	-2.37	1.38	1.44
30	A	805	CLA	C3B-C4B	2.37	1.49	1.42
30	9	305	CLA	C1B-C2B	2.37	1.48	1.43
30	15	302	CLA	C3D-C4D	-2.37	1.38	1.44
38	12	305	KC1	C4A-C3A	2.37	1.49	1.44
30	10	309	CLA	C3B-C4B	2.37	1.49	1.42
39	6	319	DD6	C22-C16	-2.37	1.49	1.53
30	B	810	CLA	C1C-C2C	2.37	1.49	1.44
30	6	306	CLA	C3D-C4D	-2.37	1.38	1.44
30	3	303	CLA	C1B-C2B	2.37	1.48	1.43
37	15	316	A86	O-C13	-2.37	1.18	1.23
30	9	302	CLA	C3B-C4B	2.37	1.49	1.42
38	11	305	KC1	C4C-C3C	2.37	1.49	1.45
38	6	311	KC1	C2A-C1A	2.37	1.51	1.44
30	13	304	CLA	C3B-C4B	2.37	1.49	1.42
30	7	312	CLA	C3D-C4D	-2.37	1.38	1.44
30	3	309	CLA	C1B-C2B	2.37	1.48	1.43
30	B	814	CLA	C1C-NC	-2.37	1.34	1.37
37	10	302	A86	O4-C34	-2.37	1.41	1.46
37	9	313	A86	C-C1	2.37	1.55	1.50
30	16	309	CLA	C3B-C4B	2.37	1.49	1.42
30	16	303	CLA	C3D-C4D	-2.37	1.38	1.44
39	7	302	DD6	C22-C16	-2.37	1.49	1.53
36	8	320	LMG	O7-C8	-2.37	1.41	1.46
30	12	302	CLA	C1B-C2B	2.37	1.48	1.43
30	5	308	CLA	C3D-C4D	-2.37	1.38	1.44
30	12	304	CLA	C3D-C4D	-2.37	1.38	1.44
38	5	312	KC1	C2A-C1A	2.37	1.51	1.44
39	12	315	DD6	C4-C5	2.37	1.50	1.43
39	3	316	DD6	C35-C36	2.37	1.54	1.51
30	B	828	CLA	C4D-CHA	2.37	1.46	1.38
37	4	317	A86	C2-C1	2.37	1.41	1.35
30	F	202	CLA	C3B-C2B	2.37	1.49	1.41
30	9	307	CLA	C1B-C2B	2.37	1.48	1.43
38	5	305	KC1	C2A-C1A	2.36	1.51	1.44
38	2	306	KC1	C1D-C2D	2.36	1.48	1.43
30	11	304	CLA	C3D-C4D	-2.36	1.38	1.44
30	B	808	CLA	C1B-C2B	2.36	1.48	1.43
38	2	312	KC1	CAA-C2A	2.36	1.53	1.46
38	13	306	KC1	C3B-C4B	2.36	1.50	1.46
30	1	307	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	304	CLA	C1C-NC	-2.36	1.34	1.37
30	3	310	CLA	C3D-C4D	-2.36	1.38	1.44
37	16	312	A86	C24-C1	2.36	1.51	1.46
38	9	311	KC1	C1D-C2D	2.36	1.48	1.43
37	2u	203	A86	C24-C1	2.36	1.51	1.46
30	2	310	CLA	C3D-C4D	-2.36	1.38	1.44
30	7	307	CLA	C3D-C4D	-2.36	1.38	1.44
30	B	834	CLA	C3B-C2B	2.36	1.49	1.41
30	11	304	CLA	C3B-C4B	2.36	1.49	1.42
36	8	320	LMG	O8-C9	-2.36	1.39	1.45
30	2	307	CLA	C3D-C4D	-2.36	1.38	1.44
30	2	313	CLA	C4C-C3C	2.36	1.49	1.45
30	5	304	CLA	C1A-CHA	2.36	1.52	1.43
37	14	317	A86	C2-C1	2.36	1.41	1.35
37	2u	203	A86	C26-C27	2.35	1.41	1.35
30	B	837	CLA	C3B-C4B	2.35	1.49	1.42
30	A	826	CLA	C3B-C2B	2.35	1.49	1.41
30	8	309	CLA	C1B-C2B	2.35	1.48	1.43
33	M	101	BCR	C30-C25	-2.35	1.50	1.53
38	13	312	KC1	C4C-C3C	2.35	1.49	1.45
38	9	311	KC1	C4A-C3A	2.35	1.49	1.44
30	9	302	CLA	C4C-C3C	2.35	1.49	1.45
37	14	314	A86	C14-C15	2.35	1.57	1.52
30	15	314	CLA	C4C-C3C	2.35	1.49	1.45
39	4	316	DD6	C22-C16	-2.35	1.49	1.53
39	15	318	DD6	C22-C16	-2.35	1.49	1.53
30	15	304	CLA	C1B-C2B	2.35	1.48	1.43
38	14	306	KC1	CAA-C2A	2.35	1.53	1.46
30	A	806	CLA	C4D-CHA	2.35	1.46	1.38
30	8	305	CLA	C1C-NC	-2.35	1.34	1.37
39	6	321	DD6	O1-C20	2.35	1.49	1.46
30	A	803	CLA	C1C-NC	-2.35	1.34	1.37
30	B	826	CLA	C1B-C2B	2.35	1.48	1.43
30	2u	202	CLA	C1B-C2B	2.35	1.48	1.43
38	11	312	KC1	C1D-C2D	2.34	1.48	1.43
30	2	309	CLA	C3D-C4D	-2.34	1.38	1.44
36	B	849	LMG	C7-C8	2.34	1.58	1.50
30	9	308	CLA	C3D-C4D	-2.34	1.38	1.44
30	11	306	CLA	C3B-C4B	2.34	1.49	1.42
39	11	313	DD6	C35-C36	2.34	1.54	1.51
38	13	308	KC1	C4C-C3C	2.34	1.49	1.45
30	A	813	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	302	DD6	O1-C20	2.34	1.49	1.46
30	14	304	CLA	C4C-C3C	2.34	1.49	1.45
38	8	314	KC1	C4A-C3A	2.34	1.49	1.44
38	14	306	KC1	C2A-C1A	2.34	1.51	1.44
30	14	310	CLA	C3B-C4B	2.34	1.49	1.42
30	15	312	CLA	C3D-C4D	-2.34	1.38	1.44
38	10	306	KC1	C2A-C1A	2.34	1.51	1.44
30	14	310	CLA	C4C-C3C	2.34	1.49	1.45
38	12	311	KC1	C1D-C2D	2.34	1.48	1.43
37	4	314	A86	C-C1	2.34	1.55	1.50
30	14	302	CLA	C1B-C2B	2.34	1.48	1.43
30	A	844	CLA	C4C-C3C	2.34	1.49	1.45
37	14	315	A86	C2-C1	2.34	1.41	1.35
37	2	302	A86	C5-C6	2.34	1.41	1.35
37	3	315	A86	C2-C1	2.34	1.41	1.35
30	B	822	CLA	C4D-CHA	2.34	1.46	1.38
38	8	311	KC1	C2A-C1A	2.34	1.51	1.44
30	4	302	CLA	C1B-C2B	2.34	1.48	1.43
38	9	304	KC1	C1D-C2D	2.34	1.48	1.43
37	7	315	A86	C14-C15	2.34	1.57	1.52
30	8	301	CLA	C1C-C2C	2.34	1.49	1.44
37	11	301	A86	C2-C1	2.34	1.41	1.35
30	11	304	CLA	C1B-C2B	2.34	1.48	1.43
38	13	306	KC1	CAA-C2A	2.33	1.53	1.46
30	6	316	CLA	C4C-C3C	2.33	1.49	1.45
30	2	303	CLA	C4D-CHA	2.33	1.46	1.38
30	2	303	CLA	C3D-CAD	2.33	1.53	1.45
30	3	305	CLA	C1B-C2B	2.33	1.48	1.43
30	10	304	CLA	C1B-C2B	2.33	1.48	1.43
38	10	312	KC1	C4A-C3A	2.33	1.49	1.44
39	10	313	DD6	O1-C20	2.33	1.49	1.46
30	B	810	CLA	C3B-C4B	2.33	1.49	1.42
30	14	302	CLA	C3B-C4B	2.33	1.49	1.42
38	4	310	KC1	C1D-C2D	2.33	1.48	1.43
30	A	821	CLA	C3B-C4B	2.33	1.49	1.42
38	5	312	KC1	C4A-C3A	2.33	1.49	1.44
30	5	309	CLA	C4C-C3C	2.33	1.49	1.45
30	10	309	CLA	C3D-C4D	-2.33	1.38	1.44
30	B	823	CLA	C1B-C2B	2.33	1.48	1.43
39	12	317	DD6	O1-C20	2.33	1.49	1.46
37	14	314	A86	C5-C6	2.33	1.41	1.35
30	13	301	CLA	C3D-C4D	-2.33	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	305	CLA	C3D-C4D	-2.33	1.38	1.44
30	6	306	CLA	C1B-C2B	2.33	1.48	1.43
30	1	305	CLA	C3D-C4D	-2.33	1.38	1.44
30	14	313	CLA	C3D-C4D	-2.33	1.38	1.44
30	B	802	CLA	C3D-C4D	-2.33	1.38	1.44
30	14	312	CLA	C1B-C2B	2.33	1.48	1.43
30	13	309	CLA	C3B-C4B	2.33	1.49	1.42
38	8	312	KC1	CAA-C2A	2.33	1.53	1.46
38	13	311	KC1	CHB-C4A	-2.33	1.33	1.39
30	13	301	CLA	C1C-C2C	2.33	1.49	1.44
37	14	316	A86	C2-C1	2.33	1.41	1.35
30	5	309	CLA	C3D-C4D	-2.33	1.39	1.44
30	7	306	CLA	C1B-C2B	2.33	1.48	1.43
30	B	804	CLA	C1B-C2B	2.33	1.48	1.43
37	11	301	A86	O4-C34	-2.33	1.41	1.46
30	2	311	CLA	C1B-C2B	2.33	1.48	1.43
30	14	303	CLA	C4C-C3C	2.33	1.49	1.45
30	B	811	CLA	C1B-C2B	2.32	1.48	1.43
30	A	841	CLA	CHB-C4A	-2.32	1.31	1.37
30	5	311	CLA	C3D-C4D	-2.32	1.39	1.44
30	8	301	CLA	C1B-C2B	2.32	1.48	1.43
30	A	835	CLA	C1B-C2B	2.32	1.48	1.43
30	B	815	CLA	C3D-C4D	-2.32	1.39	1.44
30	14	312	CLA	C3D-C4D	-2.32	1.39	1.44
30	10	303	CLA	C3D-C4D	-2.32	1.39	1.44
30	1	304	CLA	C1C-C2C	2.32	1.49	1.44
37	1	309	A86	C24-C1	2.32	1.50	1.46
30	12	312	CLA	C3D-C4D	-2.32	1.39	1.44
30	11	306	CLA	C1C-C2C	2.32	1.49	1.44
37	11	301	A86	C14-C15	2.32	1.57	1.52
30	L	202	CLA	C3D-C4D	-2.32	1.39	1.44
30	A	838	CLA	C3B-C2B	2.32	1.49	1.41
30	10	307	CLA	C1B-C2B	2.32	1.48	1.43
38	1	306	KC1	CAA-C2A	2.32	1.53	1.46
39	8	316	DD6	C22-C16	-2.32	1.49	1.53
30	5	307	CLA	C3B-C2B	2.32	1.49	1.41
37	15	321	A86	O-C13	-2.32	1.18	1.23
38	9	312	KC1	C2A-C1A	2.32	1.51	1.44
30	15	302	CLA	C1C-C2C	2.32	1.49	1.44
30	2	305	CLA	C3D-C4D	-2.32	1.39	1.44
30	2	310	CLA	C3B-C2B	2.32	1.49	1.41
37	2	318	A86	C2-C1	2.32	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	10	306	KC1	C4A-C3A	2.32	1.49	1.44
30	4	302	CLA	C3D-C4D	-2.32	1.39	1.44
39	8	316	DD6	C4-C5	2.32	1.50	1.43
36	7	320	LMG	O1-C7	-2.32	1.39	1.43
30	14	305	CLA	C1B-C2B	2.32	1.48	1.43
30	6	315	CLA	C3B-C4B	2.31	1.49	1.42
30	9	302	CLA	C3D-C4D	-2.31	1.39	1.44
30	A	824	CLA	C3B-C4B	2.31	1.49	1.42
37	11	315	A86	C2-C1	2.31	1.41	1.35
38	13	310	KC1	C1C-C2C	2.31	1.49	1.44
30	15	303	CLA	C1B-C2B	2.31	1.48	1.43
37	4	312	A86	C14-C15	2.31	1.57	1.52
30	11	310	CLA	C3D-C4D	-2.31	1.39	1.44
38	2	306	KC1	C4C-C3C	2.31	1.49	1.45
30	12	321	CLA	C1B-C2B	2.31	1.48	1.43
38	4	307	KC1	C4C-C3C	2.31	1.49	1.45
30	A	830	CLA	C1C-C2C	2.31	1.49	1.44
37	8	315	A86	O4-C34	-2.31	1.41	1.46
39	3	313	DD6	C22-C16	-2.31	1.49	1.53
30	8	309	CLA	C4C-C3C	2.31	1.49	1.45
38	5	310	KC1	C3B-C4B	2.31	1.50	1.46
30	A	825	CLA	C1B-C2B	2.31	1.48	1.43
37	14	317	A86	C14-C15	2.31	1.57	1.52
30	8	301	CLA	C1C-NC	-2.31	1.34	1.37
30	9	302	CLA	C1C-NC	-2.31	1.34	1.37
30	12	321	CLA	C4C-C3C	2.31	1.49	1.45
38	2	312	KC1	C4C-C3C	2.31	1.49	1.45
38	6	311	KC1	C4A-C3A	2.31	1.49	1.44
30	15	308	CLA	C3B-C4B	2.31	1.49	1.42
37	12	314	A86	C14-C15	2.31	1.57	1.52
30	15	307	CLA	C4C-C3C	2.31	1.49	1.45
30	15	308	CLA	C1C-C2C	2.30	1.49	1.44
30	B	831	CLA	C1C-NC	-2.30	1.34	1.37
37	15	317	A86	O-C13	-2.30	1.18	1.23
38	8	311	KC1	C4A-C3A	2.30	1.49	1.44
38	16	311	KC1	C1C-C2C	2.30	1.49	1.44
37	15	323	A86	C14-C15	2.30	1.57	1.52
30	16	303	CLA	C3B-C4B	2.30	1.49	1.42
36	7	320	LMG	C4-C5	2.30	1.57	1.53
39	8	317	DD6	C4-C5	2.30	1.50	1.43
30	B	830	CLA	C4C-C3C	2.30	1.48	1.45
30	1	303	CLA	C3D-C4D	-2.30	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	313	CLA	C1B-C2B	2.30	1.48	1.43
30	F	203	CLA	C1B-C2B	2.30	1.48	1.43
30	16	301	CLA	C1C-C2C	2.30	1.49	1.44
37	13	313	A86	C14-C15	2.30	1.57	1.52
30	6	305	CLA	C1B-C2B	2.30	1.48	1.43
38	2	314	KC1	C2A-C1A	2.30	1.51	1.44
30	7	310	CLA	C1C-C2C	2.30	1.49	1.44
37	15	321	A86	O4-C34	-2.30	1.41	1.46
30	9	301	CLA	C4C-C3C	2.30	1.48	1.45
30	8	305	CLA	C1B-C2B	2.30	1.48	1.43
37	14	315	A86	O4-C34	-2.30	1.41	1.46
30	B	814	CLA	C1B-C2B	2.30	1.48	1.43
30	B	812	CLA	C4C-C3C	2.30	1.48	1.45
38	13	306	KC1	C4C-C3C	2.30	1.48	1.45
30	B	833	CLA	C3D-C4D	-2.30	1.39	1.44
30	12	302	CLA	C1C-NC	-2.30	1.34	1.37
37	2u	205	A86	C2-C1	2.30	1.41	1.35
30	2	304	CLA	C1B-C2B	2.30	1.48	1.43
30	1	301	CLA	C4C-C3C	2.30	1.48	1.45
38	8	313	KC1	C4A-C3A	2.30	1.49	1.44
36	2u	204	LMG	O7-C8	-2.30	1.41	1.46
33	A	848	BCR	C30-C25	-2.30	1.50	1.53
30	1	304	CLA	C1B-C2B	2.30	1.48	1.43
30	3	305	CLA	C3B-C4B	2.30	1.49	1.42
37	16	312	A86	C-C1	2.30	1.55	1.50
30	A	839	CLA	CBD-CAD	-2.30	1.46	1.56
30	10	308	CLA	C3B-C4B	2.29	1.49	1.42
37	14	315	A86	C26-C27	2.29	1.41	1.35
30	10	303	CLA	C1B-C2B	2.29	1.48	1.43
30	B	834	CLA	C1B-C2B	2.29	1.48	1.43
30	15	304	CLA	C3D-C4D	-2.29	1.39	1.44
30	B	815	CLA	C4C-C3C	2.29	1.48	1.45
37	9	316	A86	C15-C16	-2.29	1.51	1.55
37	9	313	A86	C26-C27	2.29	1.41	1.35
30	6	307	CLA	C4C-C3C	2.29	1.48	1.45
37	4	312	A86	C2-C1	2.29	1.41	1.35
30	1	301	CLA	C1B-C2B	2.29	1.48	1.43
30	7	311	CLA	C3B-C4B	2.29	1.49	1.42
39	6	321	DD6	C4-C5	2.29	1.50	1.43
37	10	301	A86	C26-C27	2.29	1.41	1.35
37	13	315	A86	O-C13	-2.29	1.18	1.23
30	B	819	CLA	CHB-C4A	-2.29	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	813	CLA	C3B-C2B	2.29	1.48	1.41
38	12	313	KC1	C1D-C2D	2.29	1.48	1.43
37	2	319	A86	O4-C34	-2.29	1.41	1.46
38	14	311	KC1	C1C-C2C	2.29	1.49	1.44
30	4	309	CLA	C4C-C3C	2.29	1.48	1.45
38	3	304	KC1	C1D-C2D	2.29	1.48	1.43
30	B	822	CLA	C3A-C2A	-2.29	1.48	1.54
30	7	305	CLA	C3B-C2B	2.29	1.48	1.41
30	2	309	CLA	C4C-C3C	2.29	1.48	1.45
36	2u	204	LMG	C4-C5	2.29	1.57	1.53
30	1	304	CLA	C3D-C4D	-2.28	1.39	1.44
30	2	311	CLA	C3B-C4B	2.28	1.49	1.42
38	7	313	KC1	C1D-C2D	2.28	1.48	1.43
38	10	310	KC1	C1D-C2D	2.28	1.48	1.43
30	B	822	CLA	C1C-NC	-2.28	1.34	1.37
30	B	851	CLA	C1B-C2B	2.28	1.48	1.43
30	14	305	CLA	C4C-C3C	2.28	1.48	1.45
30	6	314	CLA	C3B-C4B	2.28	1.49	1.42
30	5	309	CLA	C3B-C4B	2.28	1.49	1.42
30	B	812	CLA	C3B-C2B	2.28	1.48	1.41
39	4	316	DD6	C35-C36	2.28	1.54	1.51
30	A	819	CLA	C1C-NC	-2.28	1.34	1.37
30	A	842	CLA	C1C-NC	-2.28	1.34	1.37
30	A	839	CLA	C3B-C4B	2.28	1.49	1.42
30	B	831	CLA	C1B-C2B	2.28	1.48	1.43
30	A	813	CLA	C1C-NC	-2.28	1.34	1.37
37	9	316	A86	C5-C6	2.28	1.41	1.35
30	5	307	CLA	C3D-C4D	-2.28	1.39	1.44
30	14	304	CLA	C3D-C4D	-2.28	1.39	1.44
30	16	309	CLA	C3D-C4D	-2.28	1.39	1.44
37	1	309	A86	C2-C1	2.28	1.41	1.35
30	11	308	CLA	C3D-C4D	-2.28	1.39	1.44
30	A	836	CLA	C1C-NC	-2.28	1.34	1.37
39	8	317	DD6	C35-C36	2.28	1.54	1.51
37	16	314	A86	C2-C1	2.28	1.41	1.35
30	5	303	CLA	C1B-C2B	2.28	1.48	1.43
30	A	811	CLA	C1C-NC	-2.28	1.34	1.37
30	3	305	CLA	C3D-C4D	-2.28	1.39	1.44
30	2	308	CLA	C3B-C4B	2.28	1.49	1.42
30	11	304	CLA	C4C-C3C	2.28	1.48	1.45
30	A	806	CLA	C3B-C2B	2.28	1.48	1.41
38	4	307	KC1	CAA-C2A	2.27	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	306	KC1	C4A-C3A	2.27	1.49	1.44
37	14	319	A86	C14-C15	2.27	1.57	1.52
37	15	323	A86	C5-C6	2.27	1.41	1.35
30	13	303	CLA	C3D-C4D	-2.27	1.39	1.44
30	B	802	CLA	C1B-C2B	2.27	1.48	1.43
30	F	201	CLA	C1C-C2C	2.27	1.49	1.44
30	11	306	CLA	C1B-C2B	2.27	1.48	1.43
38	11	307	KC1	CAA-C2A	2.27	1.53	1.46
30	A	805	CLA	C1C-C2C	2.27	1.49	1.44
30	15	313	CLA	C3D-C4D	-2.27	1.39	1.44
37	15	315	A86	O-C13	-2.27	1.18	1.23
38	1	306	KC1	C2A-C1A	2.27	1.51	1.44
38	4	310	KC1	C4C-C3C	2.27	1.48	1.45
30	A	829	CLA	C1B-C2B	2.27	1.48	1.43
30	2	309	CLA	C3B-C4B	2.27	1.49	1.42
30	11	309	CLA	C4C-C3C	2.27	1.48	1.45
30	J	101	CLA	C3B-C4B	2.27	1.49	1.42
30	1	302	CLA	C1B-C2B	2.27	1.48	1.43
39	2	317	DD6	C41-C32	-2.27	1.49	1.53
30	12	312	CLA	C3B-C4B	2.27	1.49	1.42
37	4	312	A86	C26-C27	2.27	1.41	1.35
30	1	304	CLA	C3B-C4B	2.27	1.49	1.42
39	5	313	DD6	C22-C16	-2.27	1.49	1.53
30	3	307	CLA	C1C-NC	-2.27	1.34	1.37
37	15	317	A86	C5-C6	2.27	1.41	1.35
30	B	824	CLA	C4C-C3C	2.27	1.48	1.45
38	13	305	KC1	C4A-C3A	2.27	1.49	1.44
30	3	309	CLA	C4C-C3C	2.26	1.48	1.45
30	7	303	CLA	C1C-C2C	2.26	1.49	1.44
30	11	308	CLA	C1B-C2B	2.26	1.48	1.43
30	14	312	CLA	C3B-C4B	2.26	1.49	1.42
30	B	815	CLA	C1B-C2B	2.26	1.48	1.43
30	B	812	CLA	C1B-C2B	2.26	1.48	1.43
38	2	306	KC1	C2A-C1A	2.26	1.51	1.44
30	A	818	CLA	C1B-C2B	2.26	1.48	1.43
30	12	306	CLA	C3B-C4B	2.26	1.49	1.42
30	2	311	CLA	C3D-C4D	-2.26	1.39	1.44
30	10	304	CLA	C4C-C3C	2.26	1.48	1.45
38	3	304	KC1	C4C-C3C	2.26	1.48	1.45
30	A	808	CLA	C1C-C2C	2.26	1.49	1.44
30	3	309	CLA	C1C-C2C	2.26	1.49	1.44
30	8	302	CLA	C1B-C2B	2.26	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	302	CLA	C3B-C4B	2.26	1.49	1.42
37	5	315	A86	C2-C1	2.26	1.41	1.35
30	7	309	CLA	C1C-NC	-2.26	1.34	1.37
39	1	310	DD6	C4-C5	2.26	1.50	1.43
30	15	303	CLA	C4C-C3C	2.26	1.48	1.45
38	8	311	KC1	C4C-C3C	2.26	1.48	1.45
30	4	304	CLA	C1B-C2B	2.26	1.48	1.43
39	6	303	DD6	C35-C36	2.26	1.54	1.51
30	9	301	CLA	C3D-C4D	-2.26	1.39	1.44
30	9	306	CLA	C3D-C4D	-2.26	1.39	1.44
30	B	835	CLA	CBD-CAD	-2.26	1.46	1.56
39	3	316	DD6	C22-C16	-2.26	1.49	1.53
30	B	814	CLA	C3B-C2B	2.26	1.48	1.41
39	10	313	DD6	C35-C36	2.26	1.54	1.51
30	2	303	CLA	C1A-CHA	2.26	1.52	1.43
30	B	836	CLA	C1B-C2B	2.26	1.48	1.43
38	13	310	KC1	C1D-C2D	2.25	1.48	1.43
30	3	309	CLA	C3D-C4D	-2.25	1.39	1.44
30	14	313	CLA	C3B-C4B	2.25	1.49	1.42
30	12	308	CLA	C3D-C4D	-2.25	1.39	1.44
38	8	307	KC1	C2A-C1A	2.25	1.51	1.44
30	F	203	CLA	C3B-C4B	2.25	1.49	1.42
38	13	308	KC1	C3B-C4B	2.25	1.49	1.46
37	2u	205	A86	O4-C34	-2.25	1.41	1.46
30	A	806	CLA	C1B-C2B	2.25	1.48	1.43
38	10	312	KC1	CAA-C2A	2.25	1.53	1.46
30	16	303	CLA	C1C-C2C	2.25	1.49	1.44
30	1	307	CLA	C4C-C3C	2.25	1.48	1.45
38	6	312	KC1	C1D-C2D	2.25	1.48	1.43
37	15	322	A86	C5-C6	2.25	1.41	1.35
30	6	305	CLA	C3B-C2B	2.25	1.48	1.41
30	A	828	CLA	C1B-C2B	2.25	1.48	1.43
30	2	313	CLA	C3D-C4D	-2.25	1.39	1.44
30	13	304	CLA	C3D-C4D	-2.25	1.39	1.44
30	11	309	CLA	C3B-C2B	2.25	1.48	1.41
38	4	307	KC1	C1D-C2D	2.25	1.48	1.43
30	12	306	CLA	C1C-NC	-2.25	1.34	1.37
30	14	302	CLA	C4C-C3C	2.25	1.48	1.45
38	11	311	KC1	CAA-C2A	2.25	1.53	1.46
30	6	310	CLA	C3D-C4D	-2.25	1.39	1.44
30	6	310	CLA	C4C-C3C	2.25	1.48	1.45
37	16	312	A86	C14-C15	2.25	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	305	CLA	C3B-C4B	2.25	1.49	1.42
30	15	311	CLA	C1C-C2C	2.25	1.49	1.44
38	1	306	KC1	C1D-C2D	2.25	1.48	1.43
38	4	308	KC1	C1D-C2D	2.25	1.48	1.43
33	A	847	BCR	C33-C5	-2.25	1.47	1.50
30	B	836	CLA	C1C-NC	-2.25	1.34	1.37
30	F	202	CLA	CBD-CAD	-2.25	1.46	1.56
37	10	302	A86	C2-C1	2.25	1.41	1.35
30	15	306	CLA	C3B-C2B	2.24	1.48	1.41
30	7	306	CLA	C4C-C3C	2.24	1.48	1.45
30	7	312	CLA	C3B-C4B	2.24	1.49	1.42
38	8	306	KC1	C1D-C2D	2.24	1.48	1.43
30	2	305	CLA	C1B-C2B	2.24	1.48	1.43
30	A	825	CLA	C4C-C3C	2.24	1.48	1.45
30	A	803	CLA	CHB-C4A	-2.24	1.32	1.37
37	13	315	A86	O4-C34	-2.24	1.41	1.46
30	6	315	CLA	C3D-C4D	-2.24	1.39	1.44
38	16	311	KC1	C4C-C3C	2.24	1.48	1.45
37	1	309	A86	O4-C34	-2.24	1.41	1.46
30	9	302	CLA	C1B-C2B	2.24	1.48	1.43
30	B	832	CLA	C1C-NC	-2.24	1.34	1.37
30	2	301	CLA	C3B-C4B	2.24	1.49	1.42
30	13	301	CLA	C3B-C4B	2.24	1.49	1.42
30	15	314	CLA	C1C-C2C	2.24	1.49	1.44
30	B	822	CLA	C1B-C2B	2.24	1.48	1.43
38	11	311	KC1	C4C-C3C	2.24	1.48	1.45
38	13	311	KC1	C4C-C3C	2.24	1.48	1.45
37	10	316	A86	C26-C27	2.24	1.41	1.35
30	15	309	CLA	C3B-C2B	2.24	1.48	1.41
30	A	836	CLA	C4C-C3C	2.24	1.48	1.45
30	J	101	CLA	C4C-C3C	2.24	1.48	1.45
38	8	312	KC1	C4C-C3C	2.24	1.48	1.45
30	16	307	CLA	C3D-C4D	-2.24	1.39	1.44
38	8	312	KC1	C1D-C2D	2.24	1.48	1.43
33	I	101	BCR	C30-C25	-2.24	1.50	1.53
30	A	812	CLA	C1B-C2B	2.24	1.48	1.43
38	1	308	KC1	C2A-C1A	2.24	1.51	1.44
38	8	307	KC1	C1D-C2D	2.24	1.48	1.43
30	7	311	CLA	C4C-C3C	2.24	1.48	1.45
30	B	826	CLA	C1C-NC	-2.23	1.34	1.37
30	7	307	CLA	C1B-C2B	2.23	1.48	1.43
30	4	309	CLA	C3B-C2B	2.23	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	314	CLA	C1B-C2B	2.23	1.48	1.43
30	1	302	CLA	C1C-NC	-2.23	1.34	1.37
30	4	306	CLA	C1B-C2B	2.23	1.48	1.43
38	13	312	KC1	C3B-C4B	2.23	1.49	1.46
30	4	305	CLA	C3B-C4B	2.23	1.49	1.42
30	A	815	CLA	C4C-C3C	2.23	1.48	1.45
38	8	314	KC1	C1D-C2D	2.23	1.48	1.43
30	15	302	CLA	C4C-C3C	2.23	1.48	1.45
37	2	319	A86	C2-C1	2.23	1.41	1.35
30	11	309	CLA	C1B-C2B	2.23	1.48	1.43
39	9	314	DD6	C22-C16	-2.23	1.49	1.53
38	14	308	KC1	C3B-C4B	2.23	1.49	1.46
30	B	839	CLA	CHB-C4A	-2.23	1.32	1.37
30	7	310	CLA	C3B-C4B	2.23	1.49	1.42
30	B	805	CLA	C1C-NC	-2.23	1.34	1.37
39	8	317	DD6	C22-C16	-2.23	1.49	1.53
30	4	309	CLA	C3D-C4D	-2.23	1.39	1.44
30	11	308	CLA	C4C-C3C	2.23	1.48	1.45
30	9	307	CLA	C3B-C4B	2.23	1.49	1.42
30	2	308	CLA	C1C-C2C	2.23	1.49	1.44
38	5	310	KC1	C1D-C2D	2.23	1.48	1.43
38	14	311	KC1	CAA-C2A	2.23	1.53	1.46
38	12	305	KC1	C4C-C3C	2.23	1.48	1.45
38	10	312	KC1	C2A-C1A	2.23	1.51	1.44
37	8	318	A86	C24-C1	2.23	1.50	1.46
38	8	314	KC1	CAA-C2A	2.23	1.53	1.46
30	2	305	CLA	C4C-C3C	2.22	1.48	1.45
30	8	301	CLA	C3B-C2B	2.22	1.48	1.41
34	6	322	LHG	O7-C5	-2.22	1.41	1.46
38	9	310	KC1	C2A-C1A	2.22	1.51	1.44
30	15	308	CLA	C1B-C2B	2.22	1.48	1.43
30	10	311	CLA	C3D-C4D	-2.22	1.39	1.44
30	B	810	CLA	C1B-C2B	2.22	1.48	1.43
37	13	315	A86	C5-C6	2.22	1.40	1.35
30	2	304	CLA	C3B-C2B	2.22	1.48	1.41
36	3	317	LMG	C1-C2	2.22	1.59	1.52
30	11	310	CLA	C3B-C2B	2.22	1.48	1.41
30	16	301	CLA	C3B-C4B	2.22	1.49	1.42
30	13	307	CLA	C3B-C2B	2.22	1.48	1.41
37	4	312	A86	C24-C1	2.22	1.50	1.46
37	11	314	A86	C5-C6	2.22	1.40	1.35
34	B	848	LHG	O7-C5	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	307	CLA	C3D-C4D	-2.22	1.39	1.44
30	A	826	CLA	C1C-NC	-2.22	1.34	1.37
30	A	837	CLA	C4C-C3C	2.22	1.48	1.45
30	10	307	CLA	C3D-C4D	-2.22	1.39	1.44
37	10	317	A86	C5-C6	2.22	1.40	1.35
30	7	305	CLA	C3D-C4D	-2.22	1.39	1.44
30	13	302	CLA	C1C-C2C	2.22	1.49	1.44
37	14	316	A86	C14-C15	2.22	1.57	1.52
30	9	307	CLA	C1C-C2C	2.21	1.49	1.44
38	6	311	KC1	CAA-C2A	2.21	1.53	1.46
30	A	839	CLA	C1C-NC	-2.21	1.34	1.37
38	8	312	KC1	C1C-C2C	2.21	1.49	1.44
39	16	313	DD6	C15-C14	2.21	1.54	1.50
38	5	310	KC1	CAA-C2A	2.21	1.53	1.46
30	2	303	CLA	C1B-C2B	2.21	1.48	1.43
30	15	310	CLA	C3B-C4B	2.21	1.49	1.42
37	15	316	A86	C5-C6	2.21	1.40	1.35
38	14	308	KC1	CAA-C2A	2.21	1.53	1.46
30	9	303	CLA	C3B-C2B	2.21	1.48	1.41
30	10	309	CLA	C1C-C2C	2.21	1.49	1.44
30	11	304	CLA	C1C-C2C	2.21	1.49	1.44
38	7	308	KC1	CAA-C2A	2.21	1.53	1.46
39	6	318	DD6	C22-C16	-2.21	1.49	1.53
38	13	311	KC1	C1C-C2C	2.21	1.49	1.44
37	13	313	A86	C35-C34	2.21	1.55	1.52
38	8	313	KC1	C2A-C1A	2.21	1.51	1.44
30	13	302	CLA	C3D-C4D	-2.21	1.39	1.44
39	2	315	DD6	C35-C36	2.21	1.54	1.51
30	A	820	CLA	CHB-C4A	-2.21	1.32	1.37
30	B	828	CLA	C4C-C3C	2.21	1.48	1.45
30	A	816	CLA	C1C-NC	-2.21	1.34	1.37
38	13	311	KC1	C3B-C4B	2.21	1.49	1.46
30	15	310	CLA	C1C-C2C	2.21	1.49	1.44
37	11	316	A86	O4-C34	-2.21	1.41	1.46
30	4	301	CLA	C1C-NC	-2.21	1.34	1.37
30	5	311	CLA	C4C-C3C	2.21	1.48	1.45
30	1	303	CLA	C1C-C2C	2.21	1.49	1.44
37	5	301	A86	O4-C34	-2.21	1.41	1.46
30	B	805	CLA	C1B-C2B	2.21	1.48	1.43
38	11	312	KC1	CAA-C2A	2.21	1.53	1.46
30	A	825	CLA	C3B-C4B	2.21	1.49	1.42
38	13	306	KC1	C1D-C2D	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	309	CLA	C3D-C4D	-2.21	1.39	1.44
38	14	306	KC1	C1D-C2D	2.21	1.48	1.43
30	14	313	CLA	C1C-C2C	2.21	1.49	1.44
36	7	320	LMG	O8-C9	-2.21	1.40	1.45
37	14	319	A86	C5-C6	2.20	1.40	1.35
38	4	310	KC1	C4A-C3A	2.20	1.49	1.44
30	16	307	CLA	C3B-C2B	2.20	1.48	1.41
30	2	303	CLA	C4C-C3C	2.20	1.48	1.45
38	5	306	KC1	C2A-C1A	2.20	1.51	1.44
30	6	317	CLA	C3D-C4D	-2.20	1.39	1.44
38	5	305	KC1	C1D-C2D	2.20	1.48	1.43
38	16	304	KC1	CAA-C2A	2.20	1.53	1.46
29	A	801	CL0	C3D-C4D	-2.20	1.38	1.41
30	5	307	CLA	C1A-CHA	2.20	1.52	1.43
38	2	306	KC1	CAA-C2A	2.20	1.53	1.46
30	6	317	CLA	C1C-C2C	2.20	1.49	1.44
30	7	303	CLA	C3B-C4B	2.20	1.49	1.42
30	B	805	CLA	C4C-C3C	2.20	1.48	1.45
30	5	302	CLA	C1B-C2B	2.20	1.48	1.43
30	14	310	CLA	C1C-C2C	2.20	1.49	1.44
30	10	307	CLA	C1C-C2C	2.20	1.49	1.44
38	12	309	KC1	C1D-C2D	2.20	1.48	1.43
30	14	305	CLA	C3D-C4D	-2.20	1.39	1.44
30	13	307	CLA	C3D-C4D	-2.20	1.39	1.44
30	B	813	CLA	C4C-C3C	2.20	1.48	1.45
30	16	305	CLA	C3D-C4D	-2.20	1.39	1.44
30	16	310	CLA	C3B-C4B	2.20	1.49	1.42
37	10	301	A86	O4-C34	-2.20	1.41	1.46
38	9	310	KC1	CAA-C2A	2.20	1.53	1.46
37	12	314	A86	C5-C6	2.20	1.40	1.35
30	B	834	CLA	C1C-C2C	2.20	1.49	1.44
38	9	310	KC1	C4A-C3A	2.20	1.49	1.44
39	2	316	DD6	C22-C16	-2.20	1.49	1.53
37	6	320	A86	C2-C1	2.20	1.40	1.35
39	5	314	DD6	C4-C5	2.19	1.50	1.43
30	B	835	CLA	C1B-C2B	2.19	1.48	1.43
30	B	826	CLA	C3B-C2B	2.19	1.48	1.41
30	12	304	CLA	C3B-C2B	2.19	1.48	1.41
39	3	312	DD6	C35-C36	2.19	1.54	1.51
38	11	305	KC1	CAA-C2A	2.19	1.53	1.46
30	15	312	CLA	C3B-C4B	2.19	1.49	1.42
30	12	312	CLA	C4C-C3C	2.19	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	311	KC1	CAA-C2A	2.19	1.53	1.46
30	B	803	CLA	C1B-C2B	2.19	1.48	1.43
30	9	303	CLA	C1B-C2B	2.19	1.48	1.43
37	15	316	A86	O4-C34	-2.19	1.41	1.46
30	B	804	CLA	C3D-C4D	-2.19	1.39	1.44
30	A	802	CLA	CBD-CAD	-2.19	1.46	1.56
30	13	309	CLA	C3D-C4D	-2.19	1.39	1.44
39	6	303	DD6	C22-C16	-2.19	1.49	1.53
30	2	313	CLA	C1C-C2C	2.19	1.49	1.44
38	13	312	KC1	C1C-C2C	2.19	1.49	1.44
30	15	312	CLA	C4C-C3C	2.19	1.48	1.45
30	6	306	CLA	CBD-CAD	-2.19	1.46	1.56
37	14	317	A86	C26-C27	2.19	1.40	1.35
30	15	305	CLA	C1C-C2C	2.19	1.49	1.44
30	15	309	CLA	C3D-C4D	-2.19	1.39	1.44
30	4	301	CLA	C1B-C2B	2.19	1.48	1.43
37	12	316	A86	O4-C34	-2.19	1.41	1.46
30	B	813	CLA	C1B-C2B	2.19	1.48	1.43
37	4	312	A86	O4-C34	-2.19	1.41	1.46
30	14	313	CLA	C4C-C3C	2.19	1.48	1.45
30	13	304	CLA	C3B-C2B	2.19	1.48	1.41
37	14	317	A86	O4-C34	-2.19	1.41	1.46
30	A	841	CLA	C3B-C4B	2.19	1.49	1.42
30	3	303	CLA	C4C-C3C	2.19	1.48	1.45
37	16	312	A86	C5-C6	2.19	1.40	1.35
30	12	308	CLA	C3B-C2B	2.19	1.48	1.41
30	7	312	CLA	C3B-C2B	2.19	1.48	1.41
30	A	836	CLA	C1B-C2B	2.19	1.48	1.43
30	8	304	CLA	C1B-C2B	2.19	1.48	1.43
38	2	314	KC1	C4C-C3C	2.19	1.48	1.45
38	8	306	KC1	CAA-C2A	2.19	1.53	1.46
30	B	804	CLA	C3B-C2B	2.19	1.48	1.41
37	16	312	A86	C2-C1	2.19	1.40	1.35
30	13	302	CLA	C4C-C3C	2.19	1.48	1.45
38	2	314	KC1	C1D-C2D	2.18	1.48	1.43
33	J	103	BCR	C33-C5	-2.18	1.47	1.50
39	8	317	DD6	O1-C20	2.18	1.49	1.46
30	16	302	CLA	C4C-C3C	2.18	1.48	1.45
30	B	835	CLA	C3B-C4B	2.18	1.49	1.42
30	B	802	CLA	C3B-C2B	2.18	1.48	1.41
30	3	307	CLA	C3D-C4D	-2.18	1.39	1.44
30	2u	202	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	302	DD6	C35-C36	2.18	1.54	1.51
30	14	303	CLA	C1C-C2C	2.18	1.49	1.44
37	14	315	A86	C24-C1	2.18	1.50	1.46
30	F	203	CLA	C1C-NC	-2.18	1.34	1.37
38	13	310	KC1	CAA-C2A	2.18	1.53	1.46
37	2u	205	A86	C-C1	2.18	1.55	1.50
39	2	315	DD6	C26-C27	-2.18	1.32	1.37
37	4	315	A86	O4-C34	-2.18	1.41	1.46
39	1	310	DD6	C35-C36	2.18	1.54	1.51
30	4	311	CLA	C4C-C3C	2.18	1.48	1.45
30	1	303	CLA	C1B-C2B	2.18	1.48	1.43
38	6	311	KC1	C1D-C2D	2.18	1.48	1.43
30	3	307	CLA	C3B-C2B	2.18	1.48	1.41
38	6	313	KC1	C1D-C2D	2.18	1.48	1.43
30	6	317	CLA	C4C-C3C	2.18	1.48	1.45
30	B	810	CLA	C1C-NC	-2.18	1.34	1.37
30	B	824	CLA	C1C-NC	-2.18	1.34	1.37
38	1	308	KC1	C4A-C3A	2.18	1.48	1.44
33	M	101	BCR	C33-C5	-2.18	1.47	1.50
38	13	305	KC1	C1D-C2D	2.18	1.48	1.43
30	16	301	CLA	C1B-C2B	2.18	1.48	1.43
30	9	307	CLA	C3D-C4D	-2.17	1.39	1.44
30	16	301	CLA	C3D-C4D	-2.17	1.39	1.44
30	B	821	CLA	C1C-NC	-2.17	1.34	1.37
30	A	842	CLA	C1C-C2C	2.17	1.48	1.44
30	J	101	CLA	C1B-C2B	2.17	1.48	1.43
30	14	302	CLA	C1C-C2C	2.17	1.48	1.44
30	A	808	CLA	C1B-C2B	2.17	1.48	1.43
30	15	309	CLA	C1C-C2C	2.17	1.48	1.44
30	B	821	CLA	C4C-C3C	2.17	1.48	1.45
30	B	811	CLA	C3B-C2B	2.17	1.48	1.41
30	10	303	CLA	C3B-C4B	2.17	1.49	1.42
37	2	318	A86	O4-C34	-2.17	1.41	1.46
30	6	304	CLA	CHB-C4A	-2.17	1.32	1.37
38	13	308	KC1	CAA-C2A	2.17	1.52	1.46
30	12	310	CLA	C1C-C2C	2.17	1.48	1.44
30	A	844	CLA	C3B-C2B	2.17	1.48	1.41
30	16	302	CLA	C3B-C4B	2.17	1.49	1.42
30	6	317	CLA	C3B-C2B	2.17	1.48	1.41
30	B	834	CLA	C1C-NC	-2.17	1.34	1.37
30	9	306	CLA	C3B-C2B	2.17	1.48	1.41
30	14	304	CLA	C3B-C2B	2.17	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	304	CLA	C1C-C2C	2.17	1.48	1.44
38	3	311	KC1	C4A-C3A	2.17	1.48	1.44
30	B	831	CLA	C3B-C4B	2.17	1.49	1.42
30	A	817	CLA	C1B-C2B	2.17	1.48	1.43
39	2	315	DD6	C22-C16	-2.16	1.49	1.53
30	B	828	CLA	C3B-C2B	2.16	1.48	1.41
30	16	310	CLA	C3B-C2B	2.16	1.48	1.41
30	12	321	CLA	C3D-C4D	-2.16	1.39	1.44
30	15	303	CLA	C3D-C4D	-2.16	1.39	1.44
38	9	304	KC1	C2A-C1A	2.16	1.51	1.44
39	3	312	DD6	C22-C16	-2.16	1.49	1.53
38	9	304	KC1	CAA-C2A	2.16	1.52	1.46
30	A	812	CLA	C1C-NC	-2.16	1.34	1.37
30	9	308	CLA	C3B-C4B	2.16	1.49	1.42
30	F	202	CLA	C4C-C3C	2.16	1.48	1.45
30	A	833	CLA	C1B-C2B	2.16	1.48	1.43
30	16	308	CLA	C3D-C4D	-2.16	1.39	1.44
30	A	829	CLA	C3B-C2B	2.16	1.48	1.41
38	13	311	KC1	CAA-C2A	2.16	1.52	1.46
38	8	312	KC1	CHB-C4A	-2.16	1.34	1.39
30	8	303	CLA	C1B-C2B	2.16	1.48	1.43
30	15	310	CLA	C3D-C4D	-2.16	1.39	1.44
30	A	814	CLA	C4C-C3C	2.16	1.48	1.45
36	14	321	LMG	O4-C4	-2.16	1.37	1.43
30	5	303	CLA	C3B-C4B	2.16	1.49	1.42
30	A	840	CLA	C1B-C2B	2.16	1.48	1.43
30	12	321	CLA	C1C-NC	-2.16	1.34	1.37
30	15	303	CLA	C1C-C2C	2.16	1.48	1.44
30	15	311	CLA	C3D-C4D	-2.16	1.39	1.44
30	A	824	CLA	C1C-NC	-2.16	1.34	1.37
30	7	305	CLA	C1A-CHA	2.16	1.52	1.43
37	5	315	A86	O4-C34	-2.16	1.41	1.46
38	7	313	KC1	C2A-C1A	2.16	1.51	1.44
30	A	829	CLA	C1C-NC	-2.16	1.34	1.37
30	A	822	CLA	C1C-NC	-2.16	1.34	1.37
30	A	838	CLA	C1C-NC	-2.16	1.34	1.37
30	14	309	CLA	C3B-C2B	2.15	1.48	1.41
38	12	305	KC1	CAA-C2A	2.15	1.52	1.46
30	13	307	CLA	C1C-C2C	2.15	1.48	1.44
30	B	815	CLA	CBD-CAD	-2.15	1.46	1.56
30	A	838	CLA	C1B-C2B	2.15	1.48	1.43
30	15	311	CLA	C3B-C2B	2.15	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	818	CLA	C1B-C2B	2.15	1.48	1.43
37	12	316	A86	C5-C6	2.15	1.40	1.35
30	A	809	CLA	C3B-C2B	2.15	1.48	1.41
30	4	311	CLA	C1B-C2B	2.15	1.48	1.43
30	A	805	CLA	C3B-C2B	2.15	1.48	1.41
30	B	802	CLA	C1C-C2C	2.15	1.48	1.44
37	14	318	A86	C5-C6	2.15	1.40	1.35
30	12	308	CLA	C4C-C3C	2.15	1.48	1.45
30	B	806	CLA	C1B-C2B	2.15	1.48	1.43
30	B	824	CLA	C1B-C2B	2.15	1.48	1.43
30	B	817	CLA	C1C-NC	-2.15	1.34	1.37
30	B	825	CLA	C3B-C2B	2.15	1.48	1.41
30	A	826	CLA	C4C-C3C	2.15	1.48	1.45
30	10	311	CLA	C3B-C2B	2.15	1.48	1.41
39	6	318	DD6	C35-C36	2.15	1.54	1.51
38	5	306	KC1	C1C-C2C	2.15	1.48	1.44
30	13	303	CLA	C3B-C2B	2.15	1.48	1.41
38	8	313	KC1	CAA-C2A	2.15	1.52	1.46
38	10	310	KC1	CAA-C2A	2.15	1.52	1.46
30	8	308	CLA	C1C-C2C	2.15	1.48	1.44
30	B	825	CLA	C1C-NC	-2.15	1.34	1.37
30	2	307	CLA	C1C-NC	-2.15	1.34	1.37
30	10	309	CLA	C3B-C2B	2.15	1.48	1.41
37	8	318	A86	O4-C34	-2.15	1.41	1.46
38	13	310	KC1	C4C-C3C	2.15	1.48	1.45
37	14	301	A86	C5-C6	2.15	1.40	1.35
37	8	318	A86	C26-C27	2.15	1.40	1.35
30	A	815	CLA	C1B-C2B	2.15	1.48	1.43
30	3	303	CLA	C3D-C4D	-2.15	1.39	1.44
30	B	827	CLA	C1C-NC	-2.15	1.34	1.37
37	3	315	A86	O4-C34	-2.15	1.41	1.46
37	15	315	A86	O4-C34	-2.15	1.41	1.46
30	6	315	CLA	C4C-C3C	2.15	1.48	1.45
37	10	316	A86	O4-C34	-2.14	1.41	1.46
30	8	309	CLA	C1C-NC	-2.14	1.34	1.37
30	15	305	CLA	C3D-C4D	-2.14	1.39	1.44
30	14	313	CLA	C3B-C2B	2.14	1.48	1.41
37	14	320	A86	O4-C34	-2.14	1.41	1.46
30	A	830	CLA	CHB-C4A	-2.14	1.32	1.37
30	5	302	CLA	C1C-C2C	2.14	1.48	1.44
30	15	305	CLA	C3B-C4B	2.14	1.49	1.42
30	3	302	CLA	CBD-CAD	-2.14	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	313	CLA	C3B-C2B	2.14	1.48	1.41
30	6	305	CLA	C4C-C3C	2.14	1.48	1.45
30	2	311	CLA	C1C-C2C	2.14	1.48	1.44
30	14	310	CLA	C3D-C4D	-2.14	1.39	1.44
30	10	308	CLA	C1B-C2B	2.14	1.48	1.43
30	5	304	CLA	C4C-C3C	2.14	1.48	1.45
30	B	832	CLA	C3B-C4B	2.14	1.49	1.42
38	10	306	KC1	C1C-C2C	2.14	1.48	1.44
37	3	314	A86	O4-C34	-2.14	1.41	1.46
30	A	842	CLA	C1B-C2B	2.14	1.48	1.43
30	16	306	CLA	C1C-C2C	2.14	1.48	1.44
30	B	828	CLA	C1C-NC	-2.14	1.34	1.37
38	5	305	KC1	C1C-C2C	2.14	1.48	1.44
37	9	313	A86	C2-C1	2.14	1.40	1.35
30	16	307	CLA	C1C-C2C	2.14	1.48	1.44
30	16	309	CLA	C3B-C2B	2.14	1.48	1.41
30	A	807	CLA	C3B-C4B	2.14	1.49	1.42
30	12	312	CLA	C3B-C2B	2.14	1.48	1.41
30	3	301	CLA	C1B-C2B	2.14	1.48	1.43
38	2	312	KC1	C1D-C2D	2.14	1.48	1.43
37	10	317	A86	O4-C34	-2.14	1.41	1.46
39	5	314	DD6	C41-C32	-2.14	1.49	1.53
30	12	310	CLA	C3B-C4B	2.14	1.49	1.42
30	16	306	CLA	C3B-C2B	2.14	1.48	1.41
30	B	832	CLA	C1B-C2B	2.14	1.48	1.43
30	A	810	CLA	C1C-NC	-2.14	1.34	1.37
30	14	307	CLA	C1C-C2C	2.14	1.48	1.44
30	15	307	CLA	C3D-C4D	-2.14	1.39	1.44
30	2	309	CLA	C1C-C2C	2.14	1.48	1.44
30	15	307	CLA	C3B-C2B	2.14	1.48	1.41
30	3	309	CLA	C3B-C2B	2.14	1.48	1.41
30	15	305	CLA	C3B-C2B	2.14	1.48	1.41
30	9	308	CLA	C1C-C2C	2.14	1.48	1.44
30	B	829	CLA	CHB-C4A	-2.14	1.32	1.37
30	A	814	CLA	C1B-C2B	2.14	1.48	1.43
30	A	825	CLA	C1C-NC	-2.14	1.34	1.37
37	2u	203	A86	C39-C38	2.14	1.56	1.49
30	A	808	CLA	C1C-NC	-2.14	1.34	1.37
30	15	313	CLA	C1C-C2C	2.14	1.48	1.44
30	B	820	CLA	C3B-C2B	2.13	1.48	1.41
38	6	312	KC1	C3B-C4B	2.13	1.49	1.46
30	A	827	CLA	C3B-C4B	2.13	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	309	CLA	C3B-C4B	2.13	1.49	1.42
38	11	305	KC1	C2A-C1A	2.13	1.51	1.44
30	B	802	CLA	CBD-CAD	-2.13	1.46	1.56
39	16	313	DD6	C35-C36	2.13	1.54	1.51
30	4	305	CLA	C1C-C2C	2.13	1.48	1.44
30	3	303	CLA	C3B-C4B	2.13	1.49	1.42
37	4	315	A86	C2-C1	2.13	1.40	1.35
30	A	844	CLA	C1C-C2C	2.13	1.48	1.44
30	A	809	CLA	C1B-C2B	2.13	1.48	1.43
30	13	309	CLA	C1C-C2C	2.13	1.48	1.44
30	B	816	CLA	C1C-NC	-2.13	1.34	1.37
30	A	819	CLA	C1C-C2C	2.13	1.48	1.44
37	7	319	A86	O4-C34	-2.13	1.41	1.46
37	16	314	A86	C15-C16	-2.13	1.52	1.55
30	15	306	CLA	C3D-C4D	-2.13	1.39	1.44
30	8	303	CLA	C1C-NC	-2.13	1.34	1.37
30	5	302	CLA	C3B-C4B	2.13	1.48	1.42
30	A	819	CLA	CHB-C4A	-2.13	1.32	1.37
30	13	307	CLA	C1B-C2B	2.13	1.48	1.43
30	A	823	CLA	C3B-C2B	2.13	1.48	1.41
30	15	313	CLA	C3B-C2B	2.13	1.48	1.41
38	8	307	KC1	CAA-C2A	2.13	1.52	1.46
30	A	822	CLA	CHB-C4A	-2.13	1.32	1.37
30	5	304	CLA	C1C-C2C	2.13	1.48	1.44
37	6	320	A86	C14-C15	2.13	1.56	1.52
37	3	314	A86	C5-C6	2.13	1.40	1.35
37	9	313	A86	O4-C34	-2.13	1.41	1.46
30	16	308	CLA	C3B-C2B	2.13	1.48	1.41
30	15	314	CLA	C3D-C4D	-2.13	1.39	1.44
30	6	315	CLA	C3B-C2B	2.13	1.48	1.41
38	14	308	KC1	C1C-C2C	2.13	1.48	1.44
30	B	837	CLA	CBD-CAD	-2.12	1.47	1.56
30	A	832	CLA	C1C-NC	-2.12	1.34	1.37
30	7	310	CLA	C1B-C2B	2.12	1.48	1.43
30	B	830	CLA	C1C-C2C	2.12	1.48	1.44
30	2	311	CLA	C4C-C3C	2.12	1.48	1.45
30	6	316	CLA	C3B-C2B	2.12	1.48	1.41
30	7	304	CLA	C1B-C2B	2.12	1.48	1.43
30	14	312	CLA	C1C-C2C	2.12	1.48	1.44
30	F	202	CLA	C1C-C2C	2.12	1.48	1.44
30	14	303	CLA	C3D-C4D	-2.12	1.39	1.44
30	14	307	CLA	C1B-C2B	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	310	KC1	C1D-C2D	2.12	1.48	1.43
30	B	838	CLA	C3B-C4B	2.12	1.48	1.42
30	B	833	CLA	C4C-C3C	2.12	1.48	1.45
30	9	305	CLA	C3B-C4B	2.12	1.48	1.42
39	12	315	DD6	C22-C16	-2.12	1.49	1.53
37	16	312	A86	O4-C34	-2.12	1.41	1.46
30	9	305	CLA	C1C-C2C	2.12	1.48	1.44
30	2	301	CLA	C1C-NC	-2.12	1.34	1.37
37	1	309	A86	C14-C15	2.12	1.56	1.52
30	A	811	CLA	C1B-C2B	2.12	1.48	1.43
30	7	309	CLA	C4C-C3C	2.12	1.48	1.45
37	16	314	A86	O4-C34	-2.12	1.41	1.46
30	B	803	CLA	C3D-C4D	-2.12	1.39	1.44
37	8	318	A86	C5-C6	2.12	1.40	1.35
30	3	306	CLA	CHB-C4A	-2.12	1.32	1.37
38	14	311	KC1	C1D-C2D	2.12	1.48	1.43
38	6	308	KC1	C4A-C3A	2.12	1.48	1.44
30	16	310	CLA	C4C-C3C	2.12	1.48	1.45
30	L	203	CLA	C1C-NC	-2.12	1.34	1.37
30	1	307	CLA	C3B-C2B	2.12	1.48	1.41
30	B	801	CLA	CBD-CAD	-2.12	1.47	1.56
30	F	201	CLA	CBD-CAD	-2.12	1.47	1.56
37	11	314	A86	O4-C34	-2.12	1.41	1.46
30	16	310	CLA	C1C-C2C	2.12	1.48	1.44
30	1	305	CLA	C3B-C2B	2.11	1.48	1.41
30	A	822	CLA	C4C-C3C	2.11	1.48	1.45
38	10	306	KC1	C4C-C3C	2.11	1.48	1.45
38	8	314	KC1	C4C-C3C	2.11	1.48	1.45
38	9	304	KC1	C4C-C3C	2.11	1.48	1.45
30	5	311	CLA	C3B-C2B	2.11	1.48	1.41
30	16	302	CLA	C1C-C2C	2.11	1.48	1.44
30	2	304	CLA	C1C-C2C	2.11	1.48	1.44
39	4	313	DD6	C22-C16	-2.11	1.49	1.53
30	B	809	CLA	C1C-NC	-2.11	1.34	1.37
30	10	305	CLA	C4C-C3C	2.11	1.48	1.45
30	12	304	CLA	C4C-C3C	2.11	1.48	1.45
30	4	303	CLA	C1B-C2B	2.11	1.48	1.43
30	15	304	CLA	C1C-C2C	2.11	1.48	1.44
30	4	305	CLA	C4C-C3C	2.11	1.48	1.45
30	A	803	CLA	C3D-C4D	-2.11	1.39	1.44
30	B	818	CLA	CBD-CAD	-2.11	1.47	1.56
30	A	802	CLA	CHB-C4A	-2.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	302	CLA	C1C-C2C	2.11	1.48	1.44
37	2	319	A86	C26-C27	2.11	1.40	1.35
39	15	319	DD6	C22-C16	-2.11	1.49	1.53
30	B	806	CLA	C3B-C4B	2.11	1.48	1.42
30	A	804	CLA	C1B-C2B	2.11	1.48	1.43
30	9	302	CLA	C3B-C2B	2.11	1.48	1.41
30	15	312	CLA	C1C-C2C	2.11	1.48	1.44
39	10	314	DD6	C22-C16	-2.11	1.49	1.53
30	4	305	CLA	C1B-C2B	2.11	1.48	1.43
30	15	314	CLA	C3B-C4B	2.11	1.48	1.42
30	B	824	CLA	CHB-C4A	-2.11	1.32	1.37
38	5	310	KC1	C4C-C3C	2.11	1.48	1.45
30	16	305	CLA	C1C-NC	-2.11	1.34	1.37
30	B	824	CLA	C3B-C4B	2.11	1.48	1.42
38	6	313	KC1	C4C-C3C	2.11	1.48	1.45
30	A	828	CLA	C3B-C2B	2.10	1.48	1.41
30	14	307	CLA	C3B-C2B	2.10	1.48	1.41
30	A	803	CLA	C3B-C2B	2.10	1.48	1.41
30	3	301	CLA	C1C-NC	-2.10	1.34	1.37
37	4	314	A86	O4-C34	-2.10	1.41	1.46
30	10	308	CLA	C4C-C3C	2.10	1.48	1.45
30	2	309	CLA	C3B-C2B	2.10	1.48	1.41
30	B	851	CLA	C1C-NC	-2.10	1.34	1.37
30	12	303	CLA	C4C-C3C	2.10	1.48	1.45
30	A	806	CLA	C3B-C4B	2.10	1.48	1.42
30	B	835	CLA	C1C-NC	-2.10	1.34	1.37
30	12	308	CLA	C1C-C2C	2.10	1.48	1.44
30	16	309	CLA	C1C-C2C	2.10	1.48	1.44
30	12	321	CLA	C3B-C2B	2.10	1.48	1.41
30	7	307	CLA	C3B-C4B	2.10	1.48	1.42
30	A	818	CLA	C1C-NC	-2.10	1.34	1.37
30	A	840	CLA	C1C-NC	-2.10	1.34	1.37
37	14	314	A86	O4-C34	-2.10	1.41	1.46
30	8	302	CLA	C1C-NC	-2.10	1.34	1.37
37	5	301	A86	C5-C6	2.10	1.40	1.35
30	14	310	CLA	C3B-C2B	2.10	1.48	1.41
30	10	307	CLA	C1A-CHA	2.10	1.51	1.43
30	5	303	CLA	CBD-CAD	-2.10	1.47	1.56
30	B	820	CLA	C1C-NC	-2.10	1.34	1.37
30	11	306	CLA	C4C-C3C	2.10	1.48	1.45
30	A	812	CLA	C3B-C4B	2.10	1.48	1.42
30	B	830	CLA	C1C-NC	-2.10	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	309	CLA	C3B-C2B	2.10	1.48	1.41
30	14	303	CLA	C3B-C2B	2.10	1.48	1.41
30	6	310	CLA	C3B-C2B	2.10	1.48	1.41
30	A	824	CLA	C1C-C2C	2.10	1.48	1.44
30	10	311	CLA	C4C-C3C	2.10	1.48	1.45
30	9	309	CLA	C1C-NC	-2.10	1.34	1.37
30	A	824	CLA	C1B-C2B	2.10	1.48	1.43
30	14	304	CLA	C1C-C2C	2.10	1.48	1.44
38	6	311	KC1	C4C-C3C	2.10	1.48	1.45
30	B	830	CLA	CBD-CAD	-2.10	1.47	1.56
37	10	316	A86	C2-C1	2.10	1.40	1.35
30	12	307	CLA	C1C-C2C	2.10	1.48	1.44
39	3	316	DD6	C41-C32	-2.10	1.49	1.53
37	15	322	A86	O4-C34	-2.10	1.41	1.46
30	A	835	CLA	C4C-C3C	2.10	1.48	1.45
39	10	314	DD6	C35-C36	2.10	1.54	1.51
30	L	202	CLA	C3B-C4B	2.10	1.48	1.42
33	2u	201	BCR	C38-C26	-2.10	1.47	1.50
30	7	304	CLA	CBD-CAD	-2.10	1.47	1.56
33	I	101	BCR	C27-C26	-2.09	1.47	1.51
30	9	305	CLA	C3B-C2B	2.09	1.48	1.41
30	10	311	CLA	C1C-NC	-2.09	1.34	1.37
30	9	307	CLA	C1A-CHA	2.09	1.51	1.43
30	5	307	CLA	CBD-CAD	-2.09	1.47	1.56
38	9	310	KC1	C1C-C2C	2.09	1.48	1.44
38	12	313	KC1	C1C-C2C	2.09	1.48	1.44
37	6	320	A86	O4-C34	-2.09	1.41	1.46
30	B	808	CLA	CBD-CAD	-2.09	1.47	1.56
38	4	308	KC1	C4C-C3C	2.09	1.48	1.45
30	12	307	CLA	C3B-C2B	2.09	1.48	1.41
37	14	317	A86	C5-C6	2.09	1.40	1.35
38	6	313	KC1	C2A-C1A	2.09	1.51	1.44
30	5	311	CLA	C3B-C4B	2.09	1.48	1.42
37	2u	203	A86	C2-C1	2.09	1.40	1.35
38	1	308	KC1	C4C-C3C	2.09	1.48	1.45
37	14	319	A86	O4-C34	-2.09	1.41	1.46
38	16	304	KC1	C3B-C4B	2.09	1.49	1.46
38	11	311	KC1	C1C-C2C	2.09	1.48	1.44
30	B	833	CLA	CBD-CAD	-2.09	1.47	1.56
30	A	815	CLA	C3B-C2B	2.09	1.48	1.41
30	13	309	CLA	C3B-C2B	2.09	1.48	1.41
30	4	304	CLA	C3B-C4B	2.09	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	801	CL0	CBD-CGD	-2.09	1.49	1.52
30	B	803	CLA	CBD-CAD	-2.09	1.47	1.56
30	B	825	CLA	C3B-C4B	2.09	1.48	1.42
30	15	304	CLA	C3B-C2B	2.09	1.48	1.41
30	7	303	CLA	C1B-C2B	2.09	1.48	1.43
30	16	305	CLA	C4C-C3C	2.09	1.48	1.45
30	16	302	CLA	CBD-CAD	-2.09	1.47	1.56
30	A	809	CLA	C1C-NC	-2.09	1.34	1.37
30	12	303	CLA	CBD-CAD	-2.09	1.47	1.56
30	14	305	CLA	C1C-C2C	2.09	1.48	1.44
33	L	204	BCR	C1-C6	-2.09	1.51	1.53
37	9	315	A86	C5-C6	2.09	1.40	1.35
39	15	318	DD6	O1-C20	2.09	1.49	1.46
30	5	302	CLA	CBD-CAD	-2.09	1.47	1.56
33	2u	201	BCR	C33-C5	-2.09	1.47	1.50
30	15	307	CLA	C1C-NC	-2.09	1.34	1.37
30	4	301	CLA	CBD-CAD	-2.09	1.47	1.56
30	B	813	CLA	C3B-C2B	2.09	1.48	1.41
30	7	306	CLA	C3B-C2B	2.09	1.48	1.41
30	6	306	CLA	C1C-C2C	2.09	1.48	1.44
37	15	323	A86	O4-C34	-2.08	1.41	1.46
30	B	821	CLA	CBD-CAD	-2.08	1.47	1.56
30	13	302	CLA	C3B-C2B	2.08	1.48	1.41
30	16	302	CLA	C3B-C2B	2.08	1.48	1.41
30	5	307	CLA	C1C-C2C	2.08	1.48	1.44
38	12	311	KC1	C4A-C3A	2.08	1.48	1.44
30	A	827	CLA	C1B-C2B	2.08	1.48	1.43
30	B	837	CLA	C1C-NC	-2.08	1.34	1.37
30	5	308	CLA	C1B-C2B	2.08	1.48	1.43
30	B	802	CLA	C4C-C3C	2.08	1.48	1.45
30	B	823	CLA	CBD-CAD	-2.08	1.47	1.56
30	B	807	CLA	C1C-C2C	2.08	1.48	1.44
30	6	315	CLA	C1C-C2C	2.08	1.48	1.44
30	10	304	CLA	C1C-C2C	2.08	1.48	1.44
30	3	310	CLA	C3B-C4B	2.08	1.48	1.42
38	12	309	KC1	C4C-C3C	2.08	1.48	1.45
30	1	303	CLA	C3B-C2B	2.08	1.48	1.41
30	A	824	CLA	CBD-CAD	-2.08	1.47	1.56
30	1	301	CLA	C3B-C4B	2.08	1.48	1.42
30	12	304	CLA	C3B-C4B	2.08	1.48	1.42
30	15	307	CLA	C1C-C2C	2.08	1.48	1.44
37	4	314	A86	C5-C6	2.08	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	305	CLA	C1A-CHA	2.08	1.51	1.43
30	B	819	CLA	C3B-C4B	2.08	1.48	1.42
30	A	831	CLA	C4C-C3C	2.08	1.48	1.45
30	A	840	CLA	C1C-C2C	2.08	1.48	1.44
30	B	830	CLA	C1B-C2B	2.08	1.48	1.43
30	A	835	CLA	C1C-NC	-2.08	1.34	1.37
30	B	821	CLA	CHB-C4A	-2.08	1.32	1.37
30	B	838	CLA	C1B-C2B	2.08	1.48	1.43
30	B	805	CLA	C3B-C2B	2.08	1.48	1.41
30	12	302	CLA	C1C-C2C	2.08	1.48	1.44
30	3	306	CLA	C1C-C2C	2.08	1.48	1.44
30	9	306	CLA	C3B-C4B	2.08	1.48	1.42
38	10	312	KC1	C4C-C3C	2.08	1.48	1.45
30	A	819	CLA	C3B-C2B	2.08	1.48	1.41
30	J	101	CLA	C3B-C2B	2.08	1.48	1.41
30	16	305	CLA	C3B-C2B	2.08	1.48	1.41
30	F	203	CLA	C1C-C2C	2.08	1.48	1.44
30	3	302	CLA	C3B-C2B	2.08	1.48	1.41
30	A	829	CLA	C3B-C4B	2.07	1.48	1.42
30	11	310	CLA	C1C-C2C	2.07	1.48	1.44
38	8	307	KC1	C4A-C3A	2.07	1.48	1.44
37	12	314	A86	O4-C34	-2.07	1.41	1.46
30	3	305	CLA	C3B-C2B	2.07	1.48	1.41
38	9	311	KC1	C4C-C3C	2.07	1.48	1.45
30	15	312	CLA	C1B-C2B	2.07	1.48	1.43
30	6	306	CLA	C3B-C4B	2.07	1.48	1.42
37	9	313	A86	C24-C1	2.07	1.50	1.46
30	2	301	CLA	C3B-C2B	2.07	1.48	1.41
30	11	304	CLA	C3B-C2B	2.07	1.48	1.41
30	A	833	CLA	C4C-C3C	2.07	1.48	1.45
38	8	307	KC1	C1C-C2C	2.07	1.48	1.44
30	2	310	CLA	C3B-C4B	2.07	1.48	1.42
37	8	315	A86	C26-C27	2.07	1.40	1.35
30	L	202	CLA	C3B-C2B	2.07	1.48	1.41
37	9	316	A86	O4-C34	-2.07	1.41	1.46
30	B	829	CLA	C3B-C4B	2.07	1.48	1.42
30	4	311	CLA	C1C-NC	-2.07	1.34	1.37
38	14	311	KC1	C4C-C3C	2.07	1.48	1.45
30	5	304	CLA	C3D-C4D	-2.07	1.39	1.44
37	14	317	A86	C15-C16	-2.07	1.52	1.55
30	5	304	CLA	C3B-C2B	2.07	1.48	1.41
30	4	309	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	308	KC1	C1C-C2C	2.07	1.48	1.44
38	8	311	KC1	C1D-C2D	2.07	1.48	1.43
30	13	301	CLA	C4C-C3C	2.07	1.48	1.45
30	A	822	CLA	C3B-C4B	2.07	1.48	1.42
30	4	311	CLA	C3B-C4B	2.07	1.48	1.42
30	8	309	CLA	C3B-C2B	2.07	1.48	1.41
30	12	302	CLA	C3B-C2B	2.07	1.48	1.41
38	2	306	KC1	C1C-C2C	2.07	1.48	1.44
30	6	310	CLA	C1B-C2B	2.07	1.48	1.43
30	9	308	CLA	CHB-C4A	-2.07	1.32	1.37
39	6	318	DD6	O1-C20	2.07	1.48	1.46
37	14	315	A86	C5-C6	2.07	1.40	1.35
30	10	304	CLA	C3B-C2B	2.07	1.48	1.41
30	F	203	CLA	C3B-C2B	2.07	1.48	1.41
30	14	312	CLA	C3B-C2B	2.07	1.48	1.41
30	A	802	CLA	C1C-NC	-2.07	1.34	1.37
30	9	305	CLA	C4C-C3C	2.07	1.48	1.45
38	6	313	KC1	C1C-C2C	2.07	1.48	1.44
30	B	804	CLA	C1C-C2C	2.06	1.48	1.44
30	7	306	CLA	C1A-CHA	2.06	1.51	1.43
38	16	311	KC1	CAA-C2A	2.06	1.52	1.46
30	A	827	CLA	C1C-C2C	2.06	1.48	1.44
30	10	308	CLA	CHB-C4A	-2.06	1.32	1.37
30	A	807	CLA	C1B-C2B	2.06	1.48	1.43
30	15	308	CLA	C3D-C4D	-2.06	1.39	1.44
30	9	307	CLA	CBD-CAD	-2.06	1.47	1.56
30	B	803	CLA	C1A-CHA	2.06	1.51	1.43
30	B	804	CLA	C1A-CHA	2.06	1.51	1.43
30	A	841	CLA	C1C-C2C	2.06	1.48	1.44
30	1	302	CLA	C3B-C2B	2.06	1.48	1.41
30	14	302	CLA	C3B-C2B	2.06	1.48	1.41
30	B	817	CLA	CHB-C4A	-2.06	1.32	1.37
30	7	310	CLA	C4C-C3C	2.06	1.48	1.45
38	5	312	KC1	C3D-C2D	2.06	1.49	1.42
30	B	836	CLA	CBD-CAD	-2.06	1.47	1.56
30	4	306	CLA	C3B-C4B	2.06	1.48	1.42
30	2u	202	CLA	C1C-NC	-2.06	1.34	1.37
30	3	305	CLA	C4C-C3C	2.06	1.48	1.45
30	A	803	CLA	C3B-C4B	2.06	1.48	1.42
30	B	802	CLA	C3B-C4B	2.06	1.48	1.42
30	A	829	CLA	CBD-CAD	-2.06	1.47	1.56
30	9	309	CLA	C4C-C3C	2.06	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	309	CLA	C3B-C4B	2.06	1.48	1.42
30	12	308	CLA	C1C-NC	-2.06	1.34	1.37
33	B	844	BCR	C33-C5	-2.06	1.47	1.50
30	A	809	CLA	C1A-CHA	2.06	1.51	1.43
36	3	317	LMG	O6-C1	2.06	1.47	1.41
30	8	308	CLA	C1B-C2B	2.06	1.48	1.43
30	B	811	CLA	C1C-C2C	2.06	1.48	1.44
30	15	303	CLA	C3B-C2B	2.06	1.48	1.41
38	1	308	KC1	C1D-C2D	2.06	1.48	1.43
30	13	303	CLA	C1C-C2C	2.06	1.48	1.44
30	6	314	CLA	C4C-C3C	2.06	1.48	1.45
30	2	310	CLA	C4C-C3C	2.06	1.48	1.45
38	3	304	KC1	CBD-CAD	-2.06	1.47	1.56
37	14	318	A86	O4-C34	-2.06	1.41	1.46
30	15	302	CLA	CHB-C4A	-2.06	1.32	1.37
38	7	313	KC1	C4A-C3A	2.06	1.48	1.44
30	8	304	CLA	C3B-C4B	2.06	1.48	1.42
30	A	820	CLA	CBD-CAD	-2.06	1.47	1.56
30	4	304	CLA	C1C-C2C	2.06	1.48	1.44
30	7	303	CLA	CHB-C4A	-2.06	1.32	1.37
38	6	312	KC1	C4C-C3C	2.06	1.48	1.45
37	15	321	A86	C5-C6	2.05	1.40	1.35
30	A	810	CLA	C4C-C3C	2.05	1.48	1.45
30	4	301	CLA	C4C-C3C	2.05	1.48	1.45
30	B	825	CLA	C1C-C2C	2.05	1.48	1.44
30	9	301	CLA	CBD-CAD	-2.05	1.47	1.56
37	7	316	A86	C20-C15	2.05	1.50	1.48
39	2	316	DD6	C41-C32	-2.05	1.49	1.53
30	7	307	CLA	C1C-NC	-2.05	1.34	1.37
30	5	308	CLA	C4C-C3C	2.05	1.48	1.45
37	11	316	A86	C5-C6	2.05	1.40	1.35
38	6	311	KC1	CBD-CAD	-2.05	1.47	1.56
36	14	321	LMG	O1-C7	-2.05	1.40	1.43
38	1	308	KC1	C3B-C4B	2.05	1.49	1.46
30	15	303	CLA	CBD-CAD	-2.05	1.47	1.56
30	A	826	CLA	C1A-CHA	2.05	1.51	1.43
38	7	308	KC1	C1D-C2D	2.05	1.47	1.43
30	12	306	CLA	C4C-C3C	2.05	1.48	1.45
30	A	832	CLA	CHB-C4A	-2.05	1.32	1.37
30	6	306	CLA	C3B-C2B	2.05	1.48	1.41
30	A	838	CLA	C1C-C2C	2.05	1.48	1.44
30	A	827	CLA	C1C-NC	-2.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	10	312	KC1	C1C-C2C	2.05	1.48	1.44
39	2	317	DD6	C22-C16	-2.05	1.49	1.53
37	10	315	A86	C5-C6	2.05	1.40	1.35
30	7	304	CLA	C4C-C3C	2.05	1.48	1.45
39	4	313	DD6	C15-C14	2.05	1.54	1.50
30	12	302	CLA	C3B-C4B	2.05	1.48	1.42
38	6	313	KC1	CAA-C2A	2.05	1.52	1.46
30	A	837	CLA	CHB-C4A	-2.05	1.32	1.37
30	B	812	CLA	C1C-NC	-2.05	1.34	1.37
30	B	809	CLA	CBD-CAD	-2.05	1.47	1.56
30	12	312	CLA	C1C-C2C	2.05	1.48	1.44
30	B	807	CLA	C1C-NC	-2.05	1.34	1.37
30	11	309	CLA	C1C-NC	-2.05	1.34	1.37
30	B	810	CLA	C3B-C2B	2.05	1.48	1.41
30	2	304	CLA	C4C-C3C	2.05	1.48	1.45
30	6	307	CLA	C3B-C4B	2.05	1.48	1.42
30	B	806	CLA	CBD-CAD	-2.05	1.47	1.56
30	2	303	CLA	CHB-C4A	-2.04	1.32	1.37
30	B	832	CLA	C4C-C3C	2.04	1.48	1.45
39	1	310	DD6	C22-C16	-2.04	1.49	1.53
30	A	837	CLA	C1B-C2B	2.04	1.47	1.43
36	8	321	LMG	C4-C3	2.04	1.57	1.52
30	B	833	CLA	C1A-CHA	2.04	1.51	1.43
30	B	804	CLA	CBD-CAD	-2.04	1.47	1.56
30	A	842	CLA	C3B-C2B	2.04	1.48	1.41
30	4	302	CLA	C3B-C4B	2.04	1.48	1.42
30	2	305	CLA	C3B-C2B	2.04	1.48	1.41
38	9	311	KC1	C1C-C2C	2.04	1.48	1.44
30	A	833	CLA	C1C-NC	-2.04	1.34	1.37
30	1	307	CLA	C1C-NC	-2.04	1.34	1.37
30	A	833	CLA	C1C-C2C	2.04	1.48	1.44
30	A	812	CLA	C4C-C3C	2.04	1.48	1.45
38	9	310	KC1	C4C-C3C	2.04	1.48	1.45
39	13	314	DD6	C35-C36	2.04	1.54	1.51
30	A	810	CLA	C3B-C2B	2.04	1.48	1.41
30	B	821	CLA	C3B-C4B	2.04	1.48	1.42
30	5	303	CLA	C1C-NC	-2.04	1.34	1.37
30	6	317	CLA	C1A-CHA	2.04	1.51	1.43
30	A	831	CLA	CHB-C4A	-2.04	1.32	1.37
30	B	831	CLA	CBD-CAD	-2.04	1.47	1.56
38	4	310	KC1	C1C-C2C	2.04	1.48	1.44
37	5	316	A86	O4-C34	-2.04	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	815	CLA	CBD-CAD	-2.04	1.47	1.56
30	B	828	CLA	CBD-CAD	-2.04	1.47	1.56
30	B	851	CLA	C3B-C4B	2.04	1.48	1.42
30	7	311	CLA	C1B-C2B	2.04	1.47	1.43
30	5	308	CLA	C3B-C2B	2.04	1.48	1.41
30	11	306	CLA	CBD-CAD	-2.04	1.47	1.56
30	8	308	CLA	CHB-C4A	-2.04	1.32	1.37
30	9	303	CLA	C1C-C2C	2.04	1.48	1.44
38	2	312	KC1	C1C-C2C	2.04	1.48	1.44
30	3	301	CLA	C3B-C4B	2.04	1.48	1.42
30	A	816	CLA	C4C-C3C	2.04	1.48	1.45
37	7	319	A86	C5-C6	2.04	1.40	1.35
39	2	316	DD6	O1-C20	2.04	1.48	1.46
30	7	310	CLA	CHB-C4A	-2.04	1.32	1.37
30	3	303	CLA	C3B-C2B	2.04	1.48	1.41
30	16	306	CLA	C1C-NC	-2.04	1.34	1.37
30	1	304	CLA	C3B-C2B	2.04	1.48	1.41
30	A	821	CLA	C4C-C3C	2.03	1.48	1.45
37	11	316	A86	C39-C38	2.03	1.56	1.49
39	3	313	DD6	C35-C36	2.03	1.54	1.51
30	A	843	CLA	C1C-NC	-2.03	1.34	1.37
30	A	822	CLA	CBD-CAD	-2.03	1.47	1.56
30	16	305	CLA	C1A-CHA	2.03	1.51	1.43
30	3	310	CLA	C4C-C3C	2.03	1.48	1.45
30	4	302	CLA	C1A-CHA	2.03	1.51	1.43
30	3	303	CLA	C1A-CHA	2.03	1.51	1.43
37	11	315	A86	C39-C38	2.03	1.56	1.49
30	B	808	CLA	C3B-C4B	2.03	1.48	1.42
30	2	307	CLA	C4C-C3C	2.03	1.48	1.45
30	A	809	CLA	CBD-CAD	-2.03	1.47	1.56
30	B	823	CLA	C4C-C3C	2.03	1.48	1.45
38	9	311	KC1	C2A-C1A	2.03	1.50	1.44
30	16	303	CLA	C3B-C2B	2.03	1.48	1.41
30	7	312	CLA	C1C-NC	-2.03	1.34	1.37
30	10	307	CLA	C4C-C3C	2.03	1.48	1.45
37	8	315	A86	C14-C15	2.03	1.56	1.52
30	A	830	CLA	CBD-CAD	-2.03	1.47	1.56
30	A	817	CLA	C3B-C2B	2.03	1.48	1.41
37	8	315	A86	C39-C38	2.03	1.56	1.49
36	8	321	LMG	O7-C8	-2.03	1.41	1.46
37	14	316	A86	O4-C34	-2.03	1.41	1.46
30	A	835	CLA	CHB-C4A	-2.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	823	CLA	C1C-NC	-2.03	1.34	1.37
37	10	315	A86	C39-C38	2.03	1.56	1.49
30	B	819	CLA	CBD-CAD	-2.03	1.47	1.56
30	A	817	CLA	C4C-C3C	2.03	1.48	1.45
30	B	831	CLA	CHB-C4A	-2.03	1.32	1.37
30	A	841	CLA	CBD-CAD	-2.03	1.47	1.56
30	10	305	CLA	C1C-C2C	2.03	1.48	1.44
30	B	811	CLA	CBD-CAD	-2.03	1.47	1.56
38	7	308	KC1	C3B-C4B	2.03	1.49	1.46
38	14	306	KC1	C1C-C2C	2.03	1.48	1.44
37	15	317	A86	O4-C34	-2.03	1.41	1.46
37	15	320	A86	O4-C34	-2.03	1.41	1.46
30	A	832	CLA	C1B-C2B	2.03	1.47	1.43
39	5	313	DD6	C35-C36	2.03	1.54	1.51
30	B	833	CLA	C1C-NC	-2.03	1.34	1.37
30	12	303	CLA	C1C-C2C	2.03	1.48	1.44
38	1	308	KC1	C3D-C2D	2.03	1.49	1.42
30	A	803	CLA	CBD-CAD	-2.03	1.47	1.56
37	14	301	A86	O4-C34	-2.03	1.41	1.46
30	B	837	CLA	CHB-C4A	-2.03	1.32	1.37
30	15	312	CLA	CHB-C4A	-2.03	1.32	1.37
30	8	302	CLA	CBD-CAD	-2.03	1.47	1.56
30	B	832	CLA	C3B-C2B	2.03	1.48	1.41
37	2u	205	A86	C5-C6	2.03	1.40	1.35
38	8	314	KC1	CBD-CAD	-2.03	1.47	1.56
30	A	834	CLA	CBD-CAD	-2.03	1.47	1.56
38	14	306	KC1	C3D-C2D	2.03	1.49	1.42
37	1	309	A86	C5-C6	2.03	1.40	1.35
30	12	303	CLA	C1C-NC	-2.03	1.34	1.37
38	13	306	KC1	C1C-C2C	2.03	1.48	1.44
30	4	306	CLA	C3B-C2B	2.03	1.48	1.41
30	11	306	CLA	C3B-C2B	2.03	1.48	1.41
30	15	302	CLA	C3B-C2B	2.03	1.48	1.41
30	12	321	CLA	CBD-CAD	-2.03	1.47	1.56
30	B	835	CLA	CHB-C4A	-2.03	1.32	1.37
30	3	305	CLA	C1C-C2C	2.03	1.48	1.44
30	15	308	CLA	C1A-CHA	2.02	1.51	1.43
30	5	309	CLA	C1C-C2C	2.02	1.48	1.44
30	7	311	CLA	C1C-C2C	2.02	1.48	1.44
30	B	816	CLA	CBD-CAD	-2.02	1.47	1.56
30	A	841	CLA	C1C-NC	-2.02	1.34	1.37
37	11	315	A86	O4-C34	-2.02	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	203	CLA	C4C-C3C	2.02	1.48	1.45
30	9	307	CLA	C4C-C3C	2.02	1.48	1.45
38	2	312	KC1	C3B-C4B	2.02	1.49	1.46
30	5	304	CLA	C3B-C4B	2.02	1.48	1.42
30	A	805	CLA	CBD-CAD	-2.02	1.47	1.56
30	7	307	CLA	C1C-C2C	2.02	1.48	1.44
30	12	304	CLA	C1C-C2C	2.02	1.48	1.44
38	3	308	KC1	C1B-C2B	2.02	1.49	1.45
33	B	846	BCR	C38-C26	-2.02	1.47	1.50
30	A	843	CLA	CBD-CAD	-2.02	1.47	1.56
30	16	308	CLA	C1C-C2C	2.02	1.48	1.44
38	11	305	KC1	C1C-C2C	2.02	1.48	1.44
30	4	305	CLA	CHB-C4A	-2.02	1.32	1.37
30	A	818	CLA	C1C-C2C	2.02	1.48	1.44
30	3	307	CLA	C1C-C2C	2.02	1.48	1.44
30	B	817	CLA	CBD-CAD	-2.02	1.47	1.56
30	A	811	CLA	C3B-C4B	2.02	1.48	1.42
30	11	308	CLA	C3B-C2B	2.02	1.48	1.41
30	6	304	CLA	C1C-NC	-2.02	1.34	1.37
30	2u	202	CLA	CBD-CAD	-2.02	1.47	1.56
37	5	315	A86	C5-C6	2.02	1.40	1.35
30	16	305	CLA	C1C-C2C	2.02	1.48	1.44
30	A	837	CLA	C3B-C2B	2.02	1.48	1.41
30	6	309	CLA	CHB-C4A	-2.02	1.32	1.37
30	B	832	CLA	CBD-CAD	-2.02	1.47	1.56
30	16	306	CLA	CBD-CAD	-2.02	1.47	1.56
30	A	832	CLA	C1C-C2C	2.02	1.48	1.44
30	3	306	CLA	C4C-C3C	2.02	1.48	1.45
30	12	306	CLA	C3B-C2B	2.02	1.48	1.41
30	13	301	CLA	C3B-C2B	2.02	1.48	1.41
38	7	308	KC1	CBD-CAD	-2.02	1.47	1.56
30	B	837	CLA	C1C-C2C	2.02	1.48	1.44
38	8	314	KC1	C3B-C4B	2.02	1.49	1.46
30	A	839	CLA	CHB-C4A	-2.02	1.32	1.37
30	A	840	CLA	CBD-CAD	-2.02	1.47	1.56
30	4	301	CLA	C3B-C4B	2.02	1.48	1.42
30	15	306	CLA	C1C-C2C	2.02	1.48	1.44
30	B	809	CLA	C1A-CHA	2.02	1.51	1.43
39	7	318	DD6	C35-C36	2.02	1.54	1.51
38	8	314	KC1	C1C-C2C	2.02	1.48	1.44
30	B	839	CLA	C1C-NC	-2.02	1.34	1.37
30	8	305	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	307	CLA	C1A-CHA	2.02	1.51	1.43
38	3	308	KC1	C1C-C2C	2.02	1.48	1.44
30	15	306	CLA	C1A-CHA	2.02	1.51	1.43
30	A	819	CLA	CBD-CAD	-2.02	1.47	1.56
30	A	806	CLA	CBD-CAD	-2.02	1.47	1.56
39	2	317	DD6	C35-C36	2.01	1.54	1.51
30	F	201	CLA	C1B-C2B	2.01	1.47	1.43
37	8	318	A86	C2-C1	2.01	1.40	1.35
38	9	312	KC1	C1C-C2C	2.01	1.48	1.44
30	13	307	CLA	C1A-CHA	2.01	1.51	1.43
38	13	305	KC1	C1C-C2C	2.01	1.48	1.44
30	B	813	CLA	C3B-C4B	2.01	1.48	1.42
30	J	101	CLA	C1C-C2C	2.01	1.48	1.44
30	B	837	CLA	C1B-C2B	2.01	1.47	1.43
30	B	830	CLA	C1A-CHA	2.01	1.51	1.43
30	7	311	CLA	CHB-C4A	-2.01	1.32	1.37
30	6	316	CLA	C1C-C2C	2.01	1.48	1.44
30	5	308	CLA	CHB-C4A	-2.01	1.32	1.37
30	B	837	CLA	C3B-C2B	2.01	1.48	1.41
30	4	304	CLA	CBD-CAD	-2.01	1.47	1.56
30	B	823	CLA	C3B-C2B	2.01	1.47	1.41
30	B	822	CLA	CHB-C4A	-2.01	1.32	1.37
30	3	310	CLA	C1C-NC	-2.01	1.34	1.37
30	2	311	CLA	C3B-C2B	2.01	1.47	1.41
30	8	302	CLA	C1C-C2C	2.01	1.48	1.44
38	12	309	KC1	CBD-CAD	-2.01	1.47	1.56
38	12	309	KC1	C1C-C2C	2.01	1.48	1.44
39	12	317	DD6	C41-C32	-2.01	1.50	1.53
30	B	838	CLA	C4C-C3C	2.01	1.48	1.45
30	A	820	CLA	C1C-NC	-2.01	1.34	1.37
30	5	303	CLA	C1C-C2C	2.01	1.48	1.44
30	13	301	CLA	C1A-CHA	2.01	1.51	1.43
30	8	301	CLA	C3B-C4B	2.01	1.48	1.42
30	B	829	CLA	C1B-C2B	2.01	1.47	1.43
30	6	316	CLA	C1B-C2B	2.01	1.47	1.43
30	2	304	CLA	C3B-C4B	2.01	1.48	1.42
30	B	825	CLA	C1B-C2B	2.01	1.47	1.43
37	12	316	A86	C15-C16	-2.01	1.52	1.55
38	3	304	KC1	C3B-C4B	2.01	1.49	1.46
30	13	309	CLA	C1A-CHA	2.01	1.51	1.43
30	B	826	CLA	CBD-CAD	-2.01	1.47	1.56
30	A	804	CLA	C3B-C2B	2.01	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	305	CLA	C3B-C4B	2.01	1.48	1.42
30	9	305	CLA	C1A-CHA	2.01	1.51	1.43
30	6	304	CLA	C1C-C2C	2.01	1.48	1.44
38	11	311	KC1	C3D-C2D	2.01	1.49	1.42
30	B	805	CLA	CHB-C4A	-2.01	1.32	1.37
33	L	201	BCR	C33-C5	-2.01	1.47	1.50
30	B	818	CLA	C3B-C4B	2.01	1.48	1.42
30	A	827	CLA	CBD-CAD	-2.01	1.47	1.56
30	16	301	CLA	C1A-CHA	2.01	1.51	1.43
30	B	831	CLA	C3B-C2B	2.00	1.47	1.41
30	A	823	CLA	C3B-C4B	2.00	1.48	1.42
38	11	312	KC1	CBD-CAD	-2.00	1.47	1.56
30	2u	202	CLA	C1C-C2C	2.00	1.48	1.44
30	B	834	CLA	CBD-CAD	-2.00	1.47	1.56
37	3	315	A86	C5-C6	2.00	1.40	1.35
30	J	101	CLA	C1C-NC	-2.00	1.34	1.37
30	A	828	CLA	C3B-C4B	2.00	1.48	1.42
39	7	314	DD6	C22-C16	-2.00	1.50	1.53
30	6	316	CLA	CHB-C4A	-2.00	1.32	1.37
30	9	308	CLA	C3B-C2B	2.00	1.47	1.41
30	12	303	CLA	C3B-C4B	2.00	1.48	1.42
37	14	320	A86	C39-C38	2.00	1.56	1.49
30	6	305	CLA	C1C-C2C	2.00	1.48	1.44
39	15	319	DD6	O1-C20	2.00	1.48	1.46
30	9	306	CLA	C1A-CHA	2.00	1.51	1.43
30	10	303	CLA	C3B-C2B	2.00	1.47	1.41
30	A	813	CLA	C3B-C4B	2.00	1.48	1.42
30	15	314	CLA	C3B-C2B	2.00	1.47	1.41
30	A	802	CLA	C4C-C3C	2.00	1.48	1.45
30	A	811	CLA	CBD-CAD	-2.00	1.47	1.56
30	6	305	CLA	C3B-C4B	2.00	1.48	1.42
30	6	306	CLA	C1A-CHA	2.00	1.51	1.43
38	9	311	KC1	C3D-C2D	2.00	1.49	1.42

All (10713) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	315	A86	O1-C20-C19	46.49	157.06	113.49
37	14	317	A86	O1-C20-C19	45.77	156.39	113.49
37	15	321	A86	O1-C20-C19	45.61	156.24	113.49
37	8	318	A86	O1-C20-C19	45.45	156.09	113.49
37	4	312	A86	O1-C20-C19	45.21	155.87	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	16	314	A86	O1-C20-C19	44.96	155.63	113.49
37	1	309	A86	O1-C20-C19	44.92	155.59	113.49
37	11	314	A86	O1-C20-C19	44.72	155.41	113.49
37	13	315	A86	O1-C20-C19	44.70	155.39	113.49
37	8	315	A86	O1-C20-C19	44.70	155.38	113.49
37	14	318	A86	O1-C20-C19	44.70	155.38	113.49
37	15	317	A86	O1-C20-C19	44.52	155.22	113.49
37	13	313	A86	O1-C20-C19	44.40	155.10	113.49
37	9	316	A86	O1-C20-C19	44.39	155.10	113.49
37	15	323	A86	O1-C20-C19	44.28	154.99	113.49
37	5	315	A86	O1-C20-C19	44.02	154.75	113.49
37	12	316	A86	O1-C20-C19	43.99	154.72	113.49
37	15	322	A86	O1-C20-C19	43.86	154.60	113.49
37	3	315	A86	O1-C20-C19	43.72	154.47	113.49
37	11	316	A86	O1-C20-C19	43.50	154.26	113.49
37	14	319	A86	O1-C20-C19	43.41	154.18	113.49
37	10	315	A86	O1-C20-C19	43.38	154.15	113.49
37	2	302	A86	O1-C20-C19	43.37	154.14	113.49
37	10	302	A86	O1-C20-C19	43.35	154.12	113.49
37	15	320	A86	O1-C20-C19	43.29	154.06	113.49
37	10	317	A86	O1-C20-C19	43.06	153.85	113.49
37	2u	203	A86	O1-C20-C19	42.89	153.69	113.49
37	7	319	A86	O1-C20-C19	42.88	153.68	113.49
37	14	301	A86	O1-C20-C19	42.72	153.53	113.49
37	14	316	A86	O1-C20-C19	42.67	153.48	113.49
37	11	301	A86	O1-C20-C19	42.63	153.45	113.49
37	4	314	A86	O1-C20-C19	42.62	153.44	113.49
37	12	314	A86	O1-C20-C19	42.50	153.32	113.49
37	14	314	A86	O1-C20-C19	42.45	153.28	113.49
37	10	316	A86	O1-C20-C19	42.29	153.13	113.49
37	3	314	A86	O1-C20-C19	41.84	152.71	113.49
37	5	316	A86	O1-C20-C19	41.81	152.68	113.49
37	16	312	A86	O1-C20-C19	41.43	152.32	113.49
37	4	315	A86	O1-C20-C19	41.30	152.20	113.49
37	15	315	A86	O1-C20-C19	41.19	152.09	113.49
37	5	301	A86	O1-C20-C19	41.17	152.08	113.49
37	15	316	A86	O1-C20-C19	40.96	151.88	113.49
37	7	315	A86	O1-C20-C19	40.15	151.12	113.49
37	7	316	A86	O1-C20-C19	39.44	150.45	113.49
37	4	317	A86	O1-C20-C19	38.97	150.01	113.49
37	2	319	A86	O1-C20-C19	38.95	150.00	113.49
37	2	318	A86	O1-C20-C19	38.87	149.92	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	9	313	A86	O1-C20-C19	38.48	149.56	113.49
37	11	315	A86	O1-C20-C19	37.90	149.01	113.49
37	2u	205	A86	O1-C20-C19	37.25	148.40	113.49
37	9	315	A86	O1-C20-C19	36.17	147.39	113.49
37	14	320	A86	O1-C20-C19	35.88	147.12	113.49
37	10	301	A86	O1-C20-C19	35.78	147.02	113.49
37	6	320	A86	O1-C20-C19	34.50	145.83	113.49
37	8	318	A86	C-C1-C2	-28.50	76.65	122.82
37	8	318	A86	C-C1-C24	-27.51	76.06	118.09
39	9	314	DD6	O1-C20-C19	27.45	139.22	113.49
39	4	316	DD6	O1-C20-C19	27.12	138.91	113.49
39	7	314	DD6	O1-C20-C19	26.76	138.57	113.49
39	13	314	DD6	O1-C20-C19	26.02	137.88	113.49
39	5	314	DD6	O1-C20-C19	25.55	137.44	113.49
39	8	317	DD6	O1-C20-C19	25.36	137.26	113.49
39	5	313	DD6	O1-C20-C19	24.93	136.85	113.49
39	12	317	DD6	O1-C20-C19	24.79	136.72	113.49
39	2	315	DD6	O1-C20-C19	24.79	136.72	113.49
39	16	313	DD6	O1-C20-C19	24.32	136.29	113.49
39	15	318	DD6	O1-C20-C19	24.29	136.26	113.49
39	10	313	DD6	O1-C20-C19	24.22	136.19	113.49
39	12	315	DD6	O1-C20-C19	24.03	136.01	113.49
39	2	316	DD6	O1-C20-C19	23.99	135.97	113.49
39	3	312	DD6	O1-C20-C19	23.90	135.89	113.49
39	3	316	DD6	O1-C20-C19	23.85	135.84	113.49
39	6	303	DD6	O1-C20-C19	23.73	135.73	113.49
39	8	316	DD6	O1-C20-C19	23.55	135.56	113.49
39	4	313	DD6	O1-C20-C19	23.33	135.35	113.49
39	6	319	DD6	O1-C20-C19	23.24	135.27	113.49
39	7	318	DD6	O1-C20-C19	22.81	134.87	113.49
39	11	313	DD6	O1-C20-C19	22.67	134.74	113.49
39	7	302	DD6	O1-C20-C19	22.53	134.61	113.49
39	10	314	DD6	O1-C20-C19	22.52	134.59	113.49
39	3	313	DD6	O1-C20-C19	22.31	134.40	113.49
39	1	310	DD6	O1-C20-C19	22.26	134.36	113.49
39	15	319	DD6	O1-C20-C19	21.99	134.10	113.49
39	6	321	DD6	O1-C20-C19	21.79	133.91	113.49
39	6	318	DD6	O1-C20-C19	21.68	133.81	113.49
39	2	317	DD6	O1-C20-C19	21.41	133.56	113.49
37	8	318	A86	C24-C1-C2	21.38	152.64	119.01
30	8	305	CLA	C4-C3-C5	-21.11	78.59	115.23
39	7	317	DD6	O1-C20-C19	20.89	133.07	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	310	CLA	C4-C3-C5	-20.03	80.47	115.23
30	B	824	CLA	C4-C3-C5	-19.78	80.90	115.23
38	12	313	KC1	C2A-C3A-C4A	-19.60	91.70	106.41
30	2	310	CLA	C5-C3-C2	17.77	161.05	121.17
39	3	312	DD6	C29-C30-C31	-17.55	134.61	175.48
30	B	824	CLA	C5-C3-C2	17.46	160.37	121.17
39	15	319	DD6	C29-C30-C31	-17.24	135.34	175.48
30	B	824	CLA	C4-C3-C2	-17.16	79.57	123.63
30	8	305	CLA	C4-C3-C2	-17.02	79.91	123.63
30	2	310	CLA	C4-C3-C2	-16.71	80.71	123.63
30	8	305	CLA	C5-C3-C2	16.61	158.46	121.17
39	7	318	DD6	C29-C30-C31	-16.60	136.83	175.48
39	12	317	DD6	C29-C30-C31	-16.51	137.03	175.48
39	11	313	DD6	C29-C30-C31	-16.19	137.79	175.48
39	9	314	DD6	C29-C30-C31	-16.10	137.98	175.48
39	15	318	DD6	C29-C30-C31	-15.88	138.49	175.48
39	8	317	DD6	C29-C30-C31	-15.83	138.61	175.48
39	6	321	DD6	C29-C30-C31	-15.81	138.66	175.48
39	5	314	DD6	C29-C30-C31	-15.77	138.77	175.48
39	7	314	DD6	C29-C30-C31	-15.70	138.92	175.48
39	6	318	DD6	C29-C30-C31	-15.66	139.01	175.48
39	16	313	DD6	C29-C30-C31	-15.63	139.08	175.48
39	1	310	DD6	C29-C30-C31	-15.60	139.17	175.48
39	13	314	DD6	C29-C30-C31	-15.59	139.18	175.48
39	5	313	DD6	C29-C30-C31	-15.54	139.31	175.48
39	10	314	DD6	C29-C30-C31	-15.49	139.41	175.48
39	10	313	DD6	C29-C30-C31	-15.42	139.57	175.48
39	12	315	DD6	C29-C30-C31	-15.42	139.58	175.48
39	2	316	DD6	C29-C30-C31	-15.28	139.89	175.48
39	4	313	DD6	C29-C30-C31	-14.95	140.68	175.48
39	3	313	DD6	C29-C30-C31	-14.93	140.72	175.48
39	8	316	DD6	C29-C30-C31	-14.90	140.78	175.48
39	7	302	DD6	C29-C30-C31	-14.80	141.02	175.48
39	4	316	DD6	C29-C30-C31	-14.78	141.07	175.48
39	6	319	DD6	C29-C30-C31	-14.49	141.73	175.48
38	5	306	KC1	CMA-C3A-C4A	-13.80	103.46	125.03
37	9	313	A86	C21-C20-C19	-13.79	98.75	114.24
39	3	316	DD6	C29-C30-C31	-13.74	143.49	175.48
39	7	317	DD6	C29-C30-C31	-13.71	143.55	175.48
37	16	314	A86	O1-C20-C21	-13.62	99.83	115.05
37	3	315	A86	C21-C20-C19	-13.02	99.62	114.24
39	2	315	DD6	C9-C10-C11	-12.95	109.12	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	7	317	DD6	C9-C10-C11	-12.88	109.21	127.28
37	9	316	A86	O1-C20-C21	-12.79	100.75	115.05
38	3	311	KC1	CMA-C3A-C4A	-12.74	105.13	125.03
37	8	318	A86	O1-C20-C21	-12.61	100.96	115.05
39	6	303	DD6	C29-C30-C31	-12.59	146.16	175.48
37	10	316	A86	C21-C20-C19	-12.59	100.10	114.24
37	15	321	A86	C21-C20-C19	-12.47	100.23	114.24
39	4	316	DD6	C3-C2-C1	-12.40	109.89	127.28
37	5	316	A86	C21-C20-C19	-12.26	100.47	114.24
37	5	301	A86	C21-C20-C19	-12.25	100.48	114.24
37	5	315	A86	O1-C20-C21	-12.24	101.37	115.05
37	15	322	A86	C21-C20-C19	-12.17	100.57	114.24
37	11	314	A86	C21-C20-C19	-12.12	100.63	114.24
37	4	312	A86	C21-C20-C19	-12.09	100.66	114.24
39	3	313	DD6	C9-C10-C11	-12.08	110.34	127.28
37	14	315	A86	O1-C20-C21	-11.96	101.68	115.05
37	14	315	A86	C21-C20-C19	-11.96	100.81	114.24
37	12	316	A86	C21-C20-C19	-11.95	100.82	114.24
37	13	315	A86	O1-C20-C21	-11.93	101.72	115.05
37	14	316	A86	C21-C20-C19	-11.91	100.86	114.24
37	15	317	A86	O1-C20-C21	-11.86	101.80	115.05
37	14	317	A86	O1-C20-C21	-11.82	101.84	115.05
37	11	316	A86	C21-C20-C19	-11.75	101.04	114.24
39	10	313	DD6	C12-C11-C10	-11.73	103.81	122.82
39	7	314	DD6	C13-C11-C10	-11.70	100.61	119.01
37	15	323	A86	O1-C20-C21	-11.65	102.02	115.05
39	4	316	DD6	C4-C5-C6	-11.63	110.97	127.28
37	1	309	A86	O1-C20-C21	-11.62	102.06	115.05
39	3	316	DD6	C9-C10-C11	-11.58	111.04	127.28
38	12	313	KC1	CMA-C3A-C4A	-11.57	106.95	125.03
37	14	317	A86	C21-C20-C19	-11.57	101.25	114.24
37	13	313	A86	O1-C20-C21	-11.56	102.12	115.05
37	16	312	A86	C4-C5-C6	-11.52	111.12	127.28
37	14	318	A86	O1-C20-C21	-11.50	102.19	115.05
39	2	317	DD6	C3-C2-C1	-11.48	111.17	127.28
37	14	314	A86	C21-C20-C19	-11.45	101.38	114.24
37	1	309	A86	C21-C20-C19	-11.38	101.46	114.24
37	15	315	A86	C21-C20-C19	-11.37	101.47	114.24
38	12	311	KC1	CMA-C3A-C4A	-11.36	107.28	125.03
38	9	310	KC1	CMA-C3A-C4A	-11.36	107.28	125.03
37	2u	203	A86	O1-C20-C21	-11.35	102.36	115.05
38	9	311	KC1	CMA-C3A-C4A	-11.33	107.33	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	318	A86	C21-C20-C19	-11.32	101.52	114.24
37	2	302	A86	C21-C20-C19	-11.31	101.54	114.24
37	10	315	A86	C21-C20-C19	-11.31	101.54	114.24
38	10	306	KC1	CMA-C3A-C4A	-11.31	107.37	125.03
38	4	310	KC1	CMA-C3A-C4A	-11.28	107.41	125.03
39	7	318	DD6	C9-C10-C11	-11.27	111.47	127.28
39	13	314	DD6	C12-C11-C10	-11.26	104.57	122.82
39	7	317	DD6	C3-C2-C1	-11.26	111.49	127.28
37	8	315	A86	C21-C20-C19	-11.25	101.60	114.24
37	10	317	A86	O1-C20-C21	-11.25	102.48	115.05
39	5	314	DD6	C13-C11-C10	-11.21	101.38	119.01
38	5	305	KC1	CMA-C3A-C4A	-11.16	107.60	125.03
38	8	307	KC1	CMA-C3A-C4A	-11.15	107.60	125.03
37	8	315	A86	O1-C20-C21	-11.15	102.59	115.05
37	15	321	A86	O1-C20-C21	-11.12	102.62	115.05
37	10	302	A86	O1-C20-C21	-11.11	102.63	115.05
38	2	314	KC1	CMA-C3A-C4A	-11.11	107.68	125.03
37	4	315	A86	C21-C20-C19	-11.09	101.78	114.24
37	10	301	A86	C25-C26-C27	-11.09	111.73	127.28
37	15	320	A86	C21-C20-C19	-11.06	101.81	114.24
37	14	319	A86	O1-C20-C21	-11.05	102.69	115.05
38	11	305	KC1	CMA-C3A-C4A	-11.05	107.76	125.03
38	5	310	KC1	CMA-C3A-C4A	-11.04	107.78	125.03
39	8	316	DD6	C12-C11-C10	-11.04	104.94	122.82
37	7	319	A86	O1-C20-C21	-11.03	102.72	115.05
38	16	311	KC1	C2A-C3A-C4A	-11.03	98.13	106.41
39	11	313	DD6	C9-C10-C11	-11.02	111.83	127.28
37	14	301	A86	O1-C20-C21	-10.97	102.79	115.05
38	6	308	KC1	CMA-C3A-C4A	-10.97	107.90	125.03
39	15	319	DD6	C3-C2-C1	-10.95	111.92	127.28
38	6	311	KC1	CMA-C3A-C4A	-10.94	107.94	125.03
37	11	314	A86	O1-C20-C21	-10.94	102.82	115.05
39	8	317	DD6	C13-C11-C10	-10.93	101.81	119.01
39	10	313	DD6	C9-C10-C11	-10.92	111.96	127.28
38	3	304	KC1	CMA-C3A-C4A	-10.91	107.98	125.03
37	13	313	A86	C21-C20-C19	-10.91	101.98	114.24
37	4	312	A86	O1-C20-C21	-10.87	102.90	115.05
37	14	319	A86	C21-C20-C19	-10.87	102.03	114.24
38	5	312	KC1	CMA-C3A-C4A	-10.85	108.08	125.03
38	13	305	KC1	CMA-C3A-C4A	-10.83	108.11	125.03
37	13	315	A86	C21-C20-C19	-10.83	102.08	114.24
39	15	319	DD6	C9-C10-C11	-10.79	112.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	303	CLA	C1D-ND-C4D	-10.78	98.75	106.31
39	6	321	DD6	C9-C10-C11	-10.78	112.16	127.28
37	15	323	A86	C21-C20-C19	-10.77	102.14	114.24
38	8	311	KC1	CMA-C3A-C4A	-10.76	108.21	125.03
38	2	306	KC1	CMA-C3A-C4A	-10.76	108.22	125.03
37	11	301	A86	O1-C20-C21	-10.75	103.04	115.05
37	4	314	A86	O1-C20-C21	-10.71	103.08	115.05
39	2	317	DD6	C29-C30-C31	-10.71	150.54	175.48
30	L	202	CLA	C1D-ND-C4D	-10.71	98.80	106.31
37	4	317	A86	C21-C20-C19	-10.70	102.22	114.24
38	8	313	KC1	CMA-C3A-C4A	-10.65	108.39	125.03
37	12	314	A86	O1-C20-C21	-10.65	103.15	115.05
38	10	312	KC1	CMA-C3A-C4A	-10.64	108.41	125.03
38	1	308	KC1	CMA-C3A-C4A	-10.63	108.42	125.03
37	8	318	A86	C21-C20-C19	-10.60	102.33	114.24
39	3	312	DD6	C13-C11-C10	-10.59	102.36	119.01
39	2	315	DD6	C29-C30-C31	-10.58	150.84	175.48
37	15	317	A86	C21-C20-C19	-10.58	102.36	114.24
39	11	313	DD6	C4-C5-C6	-10.57	112.45	127.28
39	12	317	DD6	C3-C2-C1	-10.57	112.45	127.28
38	12	305	KC1	CMA-C3A-C4A	-10.57	108.52	125.03
37	12	316	A86	O1-C20-C21	-10.56	103.25	115.05
37	16	312	A86	C21-C20-C19	-10.55	102.39	114.24
37	1	309	A86	C4-C5-C6	-10.55	112.49	127.28
39	15	318	DD6	C4-C5-C6	-10.54	112.50	127.28
37	15	320	A86	O1-C20-C21	-10.54	103.27	115.05
38	12	309	KC1	C2A-C3A-C4A	-10.54	98.50	106.41
38	13	308	KC1	CMA-C3A-C4A	-10.53	108.58	125.03
39	9	314	DD6	C4-C5-C6	-10.53	112.51	127.28
37	14	301	A86	C21-C20-C19	-10.50	102.45	114.24
37	11	301	A86	C21-C20-C19	-10.47	102.48	114.24
38	13	310	KC1	CMA-C3A-C4A	-10.45	108.70	125.03
38	4	308	KC1	C2A-C3A-C4A	-10.45	98.56	106.41
39	13	314	DD6	C4-C5-C6	-10.45	112.62	127.28
38	6	313	KC1	CMA-C3A-C4A	-10.43	108.74	125.03
38	2	312	KC1	CMA-C3A-C4A	-10.42	108.75	125.03
39	7	318	DD6	C4-C5-C6	-10.41	112.68	127.28
30	A	806	CLA	C1D-ND-C4D	-10.40	99.01	106.31
37	10	315	A86	O1-C20-C21	-10.39	103.44	115.05
37	12	314	A86	C21-C20-C19	-10.38	102.58	114.24
30	B	830	CLA	C1D-ND-C4D	-10.37	99.04	106.31
37	14	314	A86	C33-C32-C31	10.36	119.28	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	2	302	A86	O1-C20-C21	-10.36	103.47	115.05
30	14	307	CLA	C1D-ND-C4D	-10.35	99.05	106.31
37	7	315	A86	C21-C20-C19	-10.35	102.61	114.24
37	5	315	A86	C21-C20-C19	-10.35	102.62	114.24
37	2	319	A86	C21-C20-C19	-10.35	102.62	114.24
37	7	319	A86	C21-C20-C19	-10.34	102.63	114.24
37	4	314	A86	C21-C20-C19	-10.33	102.63	114.24
38	8	306	KC1	CMA-C3A-C4A	-10.33	108.89	125.03
38	8	310	KC1	CMA-C3A-C4A	-10.32	108.91	125.03
37	15	322	A86	O1-C20-C21	-10.32	103.52	115.05
30	B	820	CLA	C1D-ND-C4D	-10.31	99.08	106.31
38	11	307	KC1	CMA-C3A-C4A	-10.30	108.94	125.03
39	10	314	DD6	C13-C11-C10	-10.29	102.82	119.01
39	2	317	DD6	C9-C10-C11	-10.29	112.85	127.28
37	10	302	A86	C21-C20-C19	-10.28	102.70	114.24
30	16	303	CLA	C1D-ND-C4D	-10.27	99.10	106.31
39	7	314	DD6	C3-C2-C1	-10.27	112.87	127.28
38	9	312	KC1	CMA-C3A-C2A	-10.24	103.64	128.43
38	9	304	KC1	CMA-C3A-C4A	-10.23	109.04	125.03
38	11	311	KC1	CMA-C3A-C4A	-10.22	109.06	125.03
37	11	316	A86	O1-C20-C21	-10.22	103.62	115.05
37	15	316	A86	O1-C20-C21	-10.22	103.63	115.05
38	1	306	KC1	CMA-C3A-C4A	-10.21	109.08	125.03
38	14	311	KC1	CMA-C3A-C4A	-10.20	109.09	125.03
37	10	317	A86	C21-C20-C19	-10.20	102.78	114.24
37	9	316	A86	C21-C20-C19	-10.19	102.79	114.24
37	2	318	A86	O1-C20-C21	-10.18	103.67	115.05
37	3	314	A86	C21-C20-C19	-10.17	102.81	114.24
39	3	316	DD6	C4-C5-C6	-10.17	113.02	127.28
39	12	317	DD6	C9-C10-C11	-10.16	113.03	127.28
39	7	302	DD6	C9-C10-C11	-10.15	113.04	127.28
39	16	313	DD6	C13-C11-C10	-10.10	103.12	119.01
38	10	310	KC1	CMA-C3A-C4A	-10.10	109.25	125.03
37	2	318	A86	C33-C32-C31	10.08	119.01	109.21
39	16	313	DD6	C3-C2-C1	-10.08	113.14	127.28
39	2	315	DD6	C8-C6-C5	-10.08	103.16	119.01
39	15	319	DD6	C4-C5-C6	-10.07	113.15	127.28
39	5	314	DD6	C4-C5-C6	-10.07	113.15	127.28
30	15	302	CLA	C1D-ND-C4D	-10.07	99.25	106.31
37	3	314	A86	O1-C20-C21	-10.04	103.82	115.05
39	15	318	DD6	C9-C10-C11	-10.04	113.19	127.28
38	13	312	KC1	CMA-C3A-C4A	-10.03	109.36	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	5	313	DD6	C4-C5-C6	-10.02	113.22	127.28
37	2u	203	A86	C21-C20-C19	-10.02	102.99	114.24
39	5	313	DD6	C13-C11-C10	-10.01	103.26	119.01
39	6	318	DD6	C9-C10-C11	-10.01	113.25	127.28
30	A	827	CLA	C1D-ND-C4D	-9.99	99.30	106.31
38	12	313	KC1	C1D-ND-C4D	-9.99	99.30	106.31
30	B	822	CLA	C1D-ND-C4D	-9.98	99.31	106.31
38	3	308	KC1	C2A-C3A-C4A	-9.97	98.93	106.41
38	11	311	KC1	C2A-C3A-C4A	-9.94	98.95	106.41
39	4	313	DD6	C9-C10-C11	-9.93	113.36	127.28
37	7	316	A86	C21-C20-C19	-9.92	103.09	114.24
39	10	313	DD6	C8-C6-C5	-9.92	103.40	119.01
39	12	315	DD6	C4-C5-C6	-9.91	113.38	127.28
38	3	308	KC1	CMA-C3A-C4A	-9.90	109.56	125.03
38	10	310	KC1	C2A-C3A-C4A	-9.89	98.98	106.41
30	15	314	CLA	C1D-ND-C4D	-9.88	99.38	106.31
39	6	318	DD6	C4-C5-C6	-9.87	113.44	127.28
30	B	817	CLA	C1D-ND-C4D	-9.87	99.39	106.31
30	A	818	CLA	C1D-ND-C4D	-9.87	99.39	106.31
38	8	313	KC1	C2A-C3A-C4A	-9.85	99.01	106.41
38	13	308	KC1	C2A-C3A-C4A	-9.82	99.04	106.41
37	16	312	A86	O1-C20-C21	-9.80	104.10	115.05
30	A	817	CLA	C1D-ND-C4D	-9.79	99.45	106.31
38	6	313	KC1	C2A-C3A-C4A	-9.78	99.07	106.41
30	B	816	CLA	C1D-ND-C4D	-9.78	99.45	106.31
37	15	316	A86	C21-C20-C19	-9.78	103.26	114.24
38	7	313	KC1	CMA-C3A-C4A	-9.77	109.76	125.03
30	13	301	CLA	C1D-ND-C4D	-9.77	99.46	106.31
39	6	321	DD6	C12-C11-C10	-9.77	106.99	122.82
38	7	308	KC1	CMA-C3A-C4A	-9.77	109.77	125.03
39	4	313	DD6	C3-C2-C1	-9.77	113.58	127.28
39	6	303	DD6	C3-C2-C1	-9.77	113.58	127.28
38	4	307	KC1	C2A-C3A-C4A	-9.76	99.08	106.41
39	1	310	DD6	C9-C10-C11	-9.75	113.60	127.28
30	8	305	CLA	C1D-ND-C4D	-9.73	99.48	106.31
37	14	315	A86	C4-C5-C6	-9.73	113.63	127.28
39	6	319	DD6	C9-C10-C11	-9.72	113.64	127.28
39	10	314	DD6	C4-C5-C6	-9.72	113.64	127.28
38	6	312	KC1	CMA-C3A-C4A	-9.72	109.84	125.03
39	8	316	DD6	C4-C5-C6	-9.72	113.65	127.28
39	6	319	DD6	C12-C11-C10	-9.71	107.08	122.82
30	16	301	CLA	C1D-ND-C4D	-9.70	99.50	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	1	306	KC1	C2A-C3A-C4A	-9.70	99.13	106.41
30	7	305	CLA	C1D-ND-C4D	-9.69	99.51	106.31
38	6	311	KC1	C2A-C3A-C4A	-9.69	99.13	106.41
38	7	308	KC1	C2A-C3A-C4A	-9.69	99.13	106.41
30	11	304	CLA	C1D-ND-C4D	-9.69	99.51	106.31
30	A	823	CLA	C1D-ND-C4D	-9.69	99.52	106.31
39	2	316	DD6	C13-C11-C10	-9.68	103.78	119.01
38	14	308	KC1	C2A-C3A-C4A	-9.68	99.14	106.41
39	2	316	DD6	C12-C11-C10	-9.67	107.15	122.82
38	2	306	KC1	C2A-C3A-C4A	-9.66	99.16	106.41
38	14	311	KC1	C2A-C3A-C4A	-9.66	99.16	106.41
39	16	313	DD6	C37-C36-C31	-9.63	106.15	124.16
30	13	303	CLA	C1D-ND-C4D	-9.62	99.56	106.31
30	2	311	CLA	C1D-ND-C4D	-9.62	99.56	106.31
39	6	318	DD6	C3-C2-C1	-9.62	113.79	127.28
39	9	314	DD6	C37-C36-C31	-9.61	106.19	124.16
39	11	313	DD6	C3-C2-C1	-9.59	113.83	127.28
37	15	315	A86	C3-C2-C1	-9.59	113.83	127.28
30	13	304	CLA	C1D-ND-C4D	-9.59	99.59	106.31
38	9	311	KC1	C2A-C3A-C4A	-9.57	99.22	106.41
37	14	314	A86	C4-C5-C6	-9.56	113.87	127.28
39	6	321	DD6	C3-C2-C1	-9.55	113.88	127.28
38	13	306	KC1	CMA-C3A-C4A	-9.55	110.10	125.03
30	1	307	CLA	C1D-ND-C4D	-9.55	99.61	106.31
30	12	310	CLA	C1D-ND-C4D	-9.54	99.61	106.31
39	5	314	DD6	C3-C2-C1	-9.54	113.89	127.28
38	13	305	KC1	C2A-C3A-C4A	-9.53	99.26	106.41
30	3	309	CLA	C1D-ND-C4D	-9.52	99.63	106.31
30	14	313	CLA	C1D-ND-C4D	-9.52	99.63	106.31
37	14	314	A86	O1-C20-C21	-9.52	104.41	115.05
38	5	310	KC1	C2A-C3A-C4A	-9.51	99.27	106.41
39	3	316	DD6	C3-C2-C1	-9.51	113.94	127.28
38	9	304	KC1	C2A-C3A-C4A	-9.49	99.28	106.41
37	4	315	A86	O1-C20-C21	-9.49	104.44	115.05
37	2u	205	A86	C21-C20-C19	-9.49	103.59	114.24
38	10	312	KC1	C2A-C3A-C4A	-9.49	99.29	106.41
37	3	315	A86	O1-C20-C21	-9.48	104.45	115.05
37	7	316	A86	O1-C20-C21	-9.48	104.45	115.05
38	5	312	KC1	C2A-C3A-C4A	-9.47	99.30	106.41
39	15	319	DD6	C-C1-C2	-9.46	107.49	122.82
30	7	307	CLA	C1D-ND-C4D	-9.46	99.68	106.31
30	B	836	CLA	C1D-ND-C4D	-9.45	99.68	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	14	306	KC1	C2A-C3A-C4A	-9.45	99.31	106.41
38	11	307	KC1	C2A-C3A-C4A	-9.45	99.32	106.41
30	15	309	CLA	C1D-ND-C4D	-9.45	99.68	106.31
38	8	312	KC1	C1D-ND-C4D	-9.44	99.69	106.31
38	8	306	KC1	C1D-ND-C4D	-9.44	99.69	106.31
30	B	801	CLA	C1D-ND-C4D	-9.43	99.70	106.31
38	9	310	KC1	C2A-C3A-C4A	-9.43	99.33	106.41
39	12	317	DD6	C12-C11-C10	-9.43	107.54	122.82
39	1	310	DD6	C4-C5-C6	-9.43	114.06	127.28
39	9	314	DD6	C3-C2-C1	-9.43	114.06	127.28
38	14	308	KC1	CMA-C3A-C4A	-9.42	110.31	125.03
38	8	311	KC1	C1D-ND-C4D	-9.42	99.70	106.31
38	4	310	KC1	C2A-C3A-C4A	-9.41	99.35	106.41
30	10	311	CLA	C1D-ND-C4D	-9.41	99.71	106.31
30	14	310	CLA	C1D-ND-C4D	-9.41	99.71	106.31
30	A	812	CLA	C1D-ND-C4D	-9.41	99.71	106.31
30	15	304	CLA	C1D-ND-C4D	-9.40	99.72	106.31
30	B	839	CLA	C1D-ND-C4D	-9.40	99.72	106.31
30	7	303	CLA	C1D-ND-C4D	-9.39	99.72	106.31
39	8	316	DD6	C3-C2-C1	-9.39	114.11	127.28
39	6	321	DD6	C37-C36-C31	-9.38	106.62	124.16
30	16	309	CLA	C1D-ND-C4D	-9.38	99.73	106.31
37	14	316	A86	O1-C20-C21	-9.38	104.57	115.05
30	A	828	CLA	C1D-ND-C4D	-9.38	99.73	106.31
39	7	317	DD6	C12-C11-C10	-9.38	107.63	122.82
30	3	307	CLA	C1D-ND-C4D	-9.37	99.73	106.31
39	10	313	DD6	C3-C2-C1	-9.37	114.13	127.28
38	8	310	KC1	C2A-C3A-C4A	-9.37	99.38	106.41
38	12	305	KC1	C2A-C3A-C4A	-9.37	99.38	106.41
39	2	315	DD6	C3-C2-C1	-9.36	114.15	127.28
30	9	301	CLA	C1D-ND-C4D	-9.36	99.74	106.31
30	B	810	CLA	C1D-ND-C4D	-9.34	99.76	106.31
30	4	311	CLA	C1D-ND-C4D	-9.34	99.76	106.31
30	L	203	CLA	C1D-ND-C4D	-9.34	99.76	106.31
30	1	303	CLA	C1D-ND-C4D	-9.33	99.76	106.31
30	10	309	CLA	C1D-ND-C4D	-9.33	99.76	106.31
38	6	312	KC1	C1D-ND-C4D	-9.32	99.77	106.31
30	A	808	CLA	C1D-ND-C4D	-9.32	99.77	106.31
30	2	313	CLA	C1D-ND-C4D	-9.32	99.77	106.31
30	F	201	CLA	C1D-ND-C4D	-9.32	99.78	106.31
30	B	831	CLA	C1D-ND-C4D	-9.32	99.78	106.31
30	14	302	CLA	C1D-ND-C4D	-9.31	99.78	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	9	312	KC1	CMA-C3A-C4A	-9.31	110.48	125.03
39	10	314	DD6	C37-C36-C31	-9.31	106.76	124.16
39	16	313	DD6	C12-C11-C10	-9.31	107.73	122.82
30	A	811	CLA	C1D-ND-C4D	-9.31	99.78	106.31
30	2	309	CLA	C1D-ND-C4D	-9.31	99.78	106.31
30	9	302	CLA	C1D-ND-C4D	-9.31	99.78	106.31
37	10	301	A86	C21-C20-C19	-9.31	103.79	114.24
38	5	306	KC1	C1D-ND-C4D	-9.29	99.79	106.31
30	5	311	CLA	C1D-ND-C4D	-9.29	99.79	106.31
30	10	305	CLA	C1D-ND-C4D	-9.29	99.79	106.31
38	13	312	KC1	C2A-C3A-C4A	-9.29	99.44	106.41
30	15	313	CLA	C1D-ND-C4D	-9.28	99.80	106.31
30	A	842	CLA	C1D-ND-C4D	-9.28	99.80	106.31
37	2	302	A86	C4-C5-C6	-9.28	114.26	127.28
37	16	314	A86	C21-C20-C19	-9.28	103.82	114.24
38	7	313	KC1	C1D-ND-C4D	-9.28	99.80	106.31
38	1	308	KC1	C2A-C3A-C4A	-9.27	99.45	106.41
37	14	317	A86	C33-C32-C31	9.27	118.22	109.21
37	4	312	A86	C33-C32-C31	9.27	118.22	109.21
30	7	310	CLA	C1D-ND-C4D	-9.26	99.81	106.31
30	A	816	CLA	C1D-ND-C4D	-9.26	99.81	106.31
38	14	306	KC1	CMA-C3A-C4A	-9.26	110.56	125.03
30	2u	202	CLA	C1D-ND-C4D	-9.26	99.81	106.31
39	3	313	DD6	C3-C2-C1	-9.25	114.30	127.28
30	B	837	CLA	C1D-ND-C4D	-9.25	99.82	106.31
30	1	302	CLA	C1D-ND-C4D	-9.25	99.82	106.31
38	9	311	KC1	C1D-ND-C4D	-9.24	99.83	106.31
39	7	302	DD6	C4-C5-C6	-9.24	114.32	127.28
30	5	304	CLA	C1D-ND-C4D	-9.23	99.83	106.31
38	11	305	KC1	C2A-C3A-C4A	-9.23	99.48	106.41
30	15	311	CLA	C1D-ND-C4D	-9.23	99.84	106.31
30	2	301	CLA	C1D-ND-C4D	-9.22	99.84	106.31
39	12	315	DD6	C3-C2-C1	-9.22	114.35	127.28
30	12	308	CLA	C1D-ND-C4D	-9.22	99.84	106.31
30	6	317	CLA	C1D-ND-C4D	-9.21	99.85	106.31
30	6	314	CLA	C1D-ND-C4D	-9.21	99.85	106.31
30	11	309	CLA	C1D-ND-C4D	-9.21	99.85	106.31
30	B	802	CLA	C1D-ND-C4D	-9.21	99.85	106.31
38	13	311	KC1	C1D-ND-C4D	-9.21	99.85	106.31
30	4	305	CLA	C1D-ND-C4D	-9.19	99.86	106.31
30	15	303	CLA	C1D-ND-C4D	-9.19	99.87	106.31
38	7	313	KC1	C2A-C3A-C4A	-9.18	99.51	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	306	CLA	C1D-ND-C4D	-9.18	99.87	106.31
39	13	314	DD6	C13-C11-C10	-9.18	104.56	119.01
30	8	302	CLA	C1D-ND-C4D	-9.18	99.87	106.31
39	1	310	DD6	C37-C36-C31	-9.18	106.99	124.16
30	14	304	CLA	C1D-ND-C4D	-9.18	99.87	106.31
39	8	317	DD6	C12-C11-C10	-9.18	107.95	122.82
37	4	315	A86	C33-C32-C31	9.17	118.13	109.21
30	11	308	CLA	C1D-ND-C4D	-9.17	99.88	106.31
39	7	318	DD6	C3-C2-C1	-9.17	114.42	127.28
30	A	833	CLA	C1D-ND-C4D	-9.16	99.88	106.31
38	13	310	KC1	C2A-C3A-C4A	-9.16	99.53	106.41
30	A	810	CLA	C1D-ND-C4D	-9.15	99.89	106.31
30	A	804	CLA	C1D-ND-C4D	-9.15	99.89	106.31
39	7	317	DD6	C37-C36-C31	-9.15	107.06	124.16
38	1	306	KC1	C1D-ND-C4D	-9.14	99.90	106.31
39	3	312	DD6	C3-C2-C1	-9.14	114.46	127.28
30	4	301	CLA	C1D-ND-C4D	-9.13	99.90	106.31
30	8	301	CLA	C1D-ND-C4D	-9.13	99.91	106.31
39	10	314	DD6	C3-C2-C1	-9.12	114.48	127.28
30	3	310	CLA	C1D-ND-C4D	-9.12	99.91	106.31
30	16	308	CLA	C1D-ND-C4D	-9.11	99.92	106.31
37	15	315	A86	O1-C20-C21	-9.11	104.87	115.05
39	4	313	DD6	C37-C36-C31	-9.11	107.13	124.16
39	3	313	DD6	C12-C11-C10	-9.10	108.07	122.82
39	6	318	DD6	C12-C11-C10	-9.10	108.07	122.82
37	11	315	A86	C33-C32-C31	9.10	118.05	109.21
30	B	803	CLA	C1D-ND-C4D	-9.09	99.93	106.31
39	7	314	DD6	C12-C11-C10	-9.09	108.09	122.82
38	8	307	KC1	C1D-ND-C4D	-9.09	99.94	106.31
30	6	306	CLA	C1D-ND-C4D	-9.08	99.94	106.31
30	5	302	CLA	C1D-ND-C4D	-9.08	99.94	106.31
38	16	304	KC1	C2A-C3A-C4A	-9.08	99.59	106.41
29	A	801	CL0	C1B-CHB-C4A	9.08	127.16	121.32
30	3	303	CLA	C1D-ND-C4D	-9.08	99.94	106.31
38	3	311	KC1	C1D-ND-C4D	-9.07	99.95	106.31
30	14	312	CLA	C1D-ND-C4D	-9.07	99.95	106.31
38	13	311	KC1	C2A-C3A-C4A	-9.07	99.60	106.41
30	F	202	CLA	C1D-ND-C4D	-9.07	99.95	106.31
39	10	313	DD6	C37-C36-C31	-9.06	107.22	124.16
30	9	308	CLA	C1D-ND-C4D	-9.06	99.95	106.31
39	8	317	DD6	C37-C36-C31	-9.05	107.23	124.16
30	2	308	CLA	C1D-ND-C4D	-9.05	99.96	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	301	CLA	C1D-ND-C4D	-9.05	99.96	106.31
30	B	851	CLA	C1D-ND-C4D	-9.04	99.97	106.31
38	14	311	KC1	C1D-ND-C4D	-9.04	99.97	106.31
30	15	310	CLA	C1D-ND-C4D	-9.04	99.97	106.31
38	9	310	KC1	C1D-ND-C4D	-9.03	99.98	106.31
30	A	829	CLA	C1D-ND-C4D	-9.03	99.98	106.31
30	4	303	CLA	C1D-ND-C4D	-9.03	99.98	106.31
38	13	306	KC1	C1D-ND-C4D	-9.03	99.98	106.31
37	11	314	A86	C4-C5-C6	-9.03	114.62	127.28
38	5	305	KC1	C1D-ND-C4D	-9.03	99.98	106.31
30	B	826	CLA	C1D-ND-C4D	-9.02	99.98	106.31
39	9	314	DD6	C13-C11-C10	-9.02	104.81	119.01
30	12	312	CLA	C1D-ND-C4D	-9.02	99.98	106.31
38	6	311	KC1	C1D-ND-C4D	-9.01	99.99	106.31
30	6	315	CLA	C1D-ND-C4D	-9.01	99.99	106.31
30	10	308	CLA	C1D-ND-C4D	-9.01	99.99	106.31
30	A	824	CLA	C1D-ND-C4D	-9.01	99.99	106.31
30	16	307	CLA	C1D-ND-C4D	-9.00	100.00	106.31
38	2	306	KC1	C1D-ND-C4D	-9.00	100.00	106.31
30	1	304	CLA	C1D-ND-C4D	-9.00	100.00	106.31
38	12	311	KC1	C1D-ND-C4D	-9.00	100.00	106.31
30	F	203	CLA	C1D-ND-C4D	-9.00	100.00	106.31
39	2	316	DD6	C8-C6-C5	-9.00	104.86	119.01
30	8	303	CLA	C1D-ND-C4D	-8.99	100.00	106.31
38	9	312	KC1	C1D-ND-C4D	-8.99	100.00	106.31
38	13	312	KC1	C1D-ND-C4D	-8.99	100.00	106.31
30	5	309	CLA	C1D-ND-C4D	-8.99	100.00	106.31
30	9	303	CLA	C1D-ND-C4D	-8.99	100.00	106.31
38	2	312	KC1	C2A-C3A-C4A	-8.99	99.66	106.41
30	A	819	CLA	C1D-ND-C4D	-8.98	100.01	106.31
39	7	302	DD6	C3-C2-C1	-8.98	114.68	127.28
30	11	306	CLA	C1D-ND-C4D	-8.98	100.01	106.31
39	2	316	DD6	C3-C2-C1	-8.98	114.68	127.28
38	5	306	KC1	CMA-C3A-C2A	-8.98	106.70	128.43
30	16	302	CLA	C1D-ND-C4D	-8.98	100.01	106.31
30	A	839	CLA	C1D-ND-C4D	-8.98	100.01	106.31
38	6	308	KC1	CMA-C3A-C2A	-8.98	106.71	128.43
30	14	303	CLA	C1D-ND-C4D	-8.97	100.02	106.31
30	11	310	CLA	C1D-ND-C4D	-8.97	100.02	106.31
39	13	314	DD6	C9-C10-C11	-8.97	114.70	127.28
30	B	806	CLA	C1D-ND-C4D	-8.97	100.02	106.31
30	B	835	CLA	C1D-ND-C4D	-8.96	100.02	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	804	CLA	C1D-ND-C4D	-8.96	100.02	106.31
30	5	308	CLA	C1D-ND-C4D	-8.96	100.03	106.31
30	A	803	CLA	C1D-ND-C4D	-8.96	100.03	106.31
30	B	808	CLA	C1D-ND-C4D	-8.95	100.03	106.31
30	16	310	CLA	C1D-ND-C4D	-8.95	100.03	106.31
30	A	834	CLA	C1D-ND-C4D	-8.95	100.03	106.31
30	4	304	CLA	C1D-ND-C4D	-8.95	100.03	106.31
39	12	315	DD6	C37-C36-C31	-8.95	107.43	124.16
38	8	307	KC1	C2A-C3A-C4A	-8.95	99.69	106.41
30	8	308	CLA	C1D-ND-C4D	-8.94	100.04	106.31
30	A	844	CLA	C1D-ND-C4D	-8.94	100.04	106.31
30	13	309	CLA	C1D-ND-C4D	-8.94	100.04	106.31
30	A	840	CLA	C1D-ND-C4D	-8.94	100.04	106.31
30	12	304	CLA	C1D-ND-C4D	-8.94	100.04	106.31
39	8	317	DD6	C4-C5-C6	-8.94	114.75	127.28
38	11	307	KC1	C1D-ND-C4D	-8.93	100.04	106.31
30	8	309	CLA	C1D-ND-C4D	-8.93	100.05	106.31
39	15	319	DD6	C12-C11-C10	-8.93	108.35	122.82
38	9	304	KC1	C1D-ND-C4D	-8.93	100.05	106.31
39	12	315	DD6	C9-C10-C11	-8.93	114.76	127.28
38	2	314	KC1	C1D-ND-C4D	-8.93	100.05	106.31
30	15	306	CLA	C1D-ND-C4D	-8.93	100.05	106.31
38	11	305	KC1	C1D-ND-C4D	-8.92	100.05	106.31
37	7	315	A86	O1-C20-C21	-8.92	105.08	115.05
30	6	304	CLA	C1D-ND-C4D	-8.92	100.06	106.31
30	13	307	CLA	C1D-ND-C4D	-8.92	100.06	106.31
38	3	308	KC1	C1D-ND-C4D	-8.91	100.06	106.31
37	15	315	A86	C25-C26-C27	-8.91	114.79	127.28
39	6	321	DD6	C13-C11-C10	-8.90	105.01	119.01
30	12	321	CLA	C1D-ND-C4D	-8.90	100.07	106.31
30	2	305	CLA	C1D-ND-C4D	-8.90	100.07	106.31
30	A	805	CLA	C1D-ND-C4D	-8.89	100.07	106.31
30	4	302	CLA	C1D-ND-C4D	-8.89	100.07	106.31
38	1	308	KC1	C1D-ND-C4D	-8.89	100.08	106.31
38	13	310	KC1	C1D-ND-C4D	-8.89	100.08	106.31
38	10	306	KC1	CMA-C3A-C2A	-8.88	106.93	128.43
30	9	307	CLA	C1D-ND-C4D	-8.88	100.08	106.31
30	12	302	CLA	C1D-ND-C4D	-8.88	100.08	106.31
38	8	306	KC1	C2A-C3A-C4A	-8.88	99.74	106.41
38	12	313	KC1	CMD-C2D-C1D	8.88	138.94	125.42
30	15	305	CLA	C1D-ND-C4D	-8.88	100.08	106.31
30	1	301	CLA	C1D-ND-C4D	-8.88	100.08	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	813	CLA	C1D-ND-C4D	-8.88	100.08	106.31
30	B	807	CLA	C1D-ND-C4D	-8.88	100.08	106.31
39	4	316	DD6	C12-C11-C10	-8.86	108.46	122.82
30	B	825	CLA	C1D-ND-C4D	-8.86	100.09	106.31
38	5	310	KC1	C1D-ND-C4D	-8.86	100.09	106.31
37	14	320	A86	C21-C20-C19	-8.86	104.29	114.24
38	10	312	KC1	C1D-ND-C4D	-8.85	100.10	106.31
30	5	303	CLA	C1D-ND-C4D	-8.85	100.10	106.31
30	15	307	CLA	C1D-ND-C4D	-8.85	100.11	106.31
38	6	312	KC1	C2A-C3A-C4A	-8.84	99.77	106.41
30	10	303	CLA	C1D-ND-C4D	-8.84	100.11	106.31
30	9	305	CLA	C1D-ND-C4D	-8.84	100.11	106.31
39	4	316	DD6	C9-C10-C11	-8.84	114.89	127.28
38	10	310	KC1	C1D-ND-C4D	-8.84	100.11	106.31
38	8	310	KC1	C1D-ND-C4D	-8.83	100.11	106.31
30	B	814	CLA	C1D-ND-C4D	-8.83	100.12	106.31
30	2	310	CLA	C1D-ND-C4D	-8.83	100.12	106.31
38	8	313	KC1	C1D-ND-C4D	-8.83	100.12	106.31
39	8	316	DD6	C37-C36-C31	-8.83	107.66	124.16
37	11	315	A86	O1-C20-C21	-8.82	105.19	115.05
38	6	308	KC1	C2A-C3A-C4A	-8.82	99.79	106.41
39	1	310	DD6	C12-C11-C10	-8.82	108.52	122.82
39	5	314	DD6	C8-C6-C5	-8.82	105.14	119.01
30	B	805	CLA	C1D-ND-C4D	-8.82	100.12	106.31
37	9	315	A86	O1-C20-C21	-8.82	105.19	115.05
38	11	311	KC1	C1D-ND-C4D	-8.82	100.13	106.31
30	12	307	CLA	C1D-ND-C4D	-8.81	100.13	106.31
30	13	302	CLA	C1D-ND-C4D	-8.81	100.13	106.31
39	4	316	DD6	C13-C11-C10	-8.80	105.16	119.01
30	7	309	CLA	C1D-ND-C4D	-8.80	100.14	106.31
39	9	314	DD6	C12-C11-C10	-8.80	108.56	122.82
38	6	313	KC1	C1D-ND-C4D	-8.80	100.14	106.31
38	3	311	KC1	CMA-C3A-C2A	-8.79	107.15	128.43
30	3	302	CLA	C1D-ND-C4D	-8.79	100.15	106.31
30	4	309	CLA	C1D-ND-C4D	-8.79	100.15	106.31
30	B	811	CLA	C1D-ND-C4D	-8.78	100.15	106.31
30	7	311	CLA	C1D-ND-C4D	-8.78	100.15	106.31
38	12	309	KC1	C1D-ND-C4D	-8.78	100.15	106.31
30	B	827	CLA	C1D-ND-C4D	-8.78	100.15	106.31
38	2	314	KC1	C2A-C3A-C4A	-8.78	99.82	106.41
39	8	317	DD6	C8-C6-C5	-8.78	105.20	119.01
38	11	312	KC1	C2A-C3A-C4A	-8.77	99.82	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	307	KC1	C1D-ND-C4D	-8.77	100.16	106.31
30	B	832	CLA	C1D-ND-C4D	-8.77	100.16	106.31
30	10	304	CLA	C1D-ND-C4D	-8.76	100.16	106.31
38	3	304	KC1	C1D-ND-C4D	-8.76	100.17	106.31
30	A	830	CLA	C1D-ND-C4D	-8.75	100.17	106.31
30	7	312	CLA	C1D-ND-C4D	-8.74	100.18	106.31
30	16	305	CLA	C1D-ND-C4D	-8.74	100.18	106.31
30	3	305	CLA	C1D-ND-C4D	-8.74	100.18	106.31
38	13	305	KC1	C1D-ND-C4D	-8.74	100.18	106.31
30	A	843	CLA	C1D-ND-C4D	-8.74	100.18	106.31
39	7	318	DD6	C12-C11-C10	-8.73	108.67	122.82
30	B	838	CLA	C1D-ND-C4D	-8.73	100.19	106.31
38	12	305	KC1	C1D-ND-C4D	-8.73	100.19	106.31
38	12	311	KC1	C2A-C3A-C4A	-8.72	99.86	106.41
38	4	307	KC1	CMA-C3A-C4A	-8.72	111.41	125.03
39	3	313	DD6	C37-C36-C31	-8.72	107.86	124.16
30	6	305	CLA	C1D-ND-C4D	-8.72	100.20	106.31
30	7	304	CLA	C1D-ND-C4D	-8.71	100.20	106.31
38	8	311	KC1	C2A-C3A-C4A	-8.71	99.87	106.41
30	16	306	CLA	C1D-ND-C4D	-8.70	100.20	106.31
30	B	833	CLA	C1D-ND-C4D	-8.70	100.21	106.31
30	9	306	CLA	C1D-ND-C4D	-8.70	100.21	106.31
38	14	306	KC1	C1D-ND-C4D	-8.68	100.22	106.31
30	A	821	CLA	C1D-ND-C4D	-8.68	100.22	106.31
39	11	313	DD6	C37-C36-C31	-8.68	107.94	124.16
39	3	313	DD6	C4-C5-C6	-8.67	115.11	127.28
39	5	313	DD6	C37-C36-C31	-8.67	107.95	124.16
37	14	319	A86	C33-C32-C31	8.67	117.64	109.21
39	2	315	DD6	C7-C6-C5	-8.67	108.78	122.82
38	2	312	KC1	C1D-ND-C4D	-8.66	100.24	106.31
37	11	315	A86	C21-C20-C19	-8.66	104.52	114.24
38	13	308	KC1	C1D-ND-C4D	-8.65	100.24	106.31
30	14	305	CLA	C1D-ND-C4D	-8.65	100.25	106.31
39	1	310	DD6	C3-C2-C1	-8.65	115.15	127.28
39	12	317	DD6	C37-C36-C31	-8.64	108.00	124.16
39	13	314	DD6	C37-C36-C31	-8.64	108.00	124.16
38	8	307	KC1	CMA-C3A-C2A	-8.64	107.52	128.43
30	15	308	CLA	C1D-ND-C4D	-8.63	100.25	106.31
38	9	312	KC1	C2A-C3A-C4A	-8.63	99.93	106.41
38	5	306	KC1	C2A-C3A-C4A	-8.63	99.93	106.41
38	5	305	KC1	CMA-C3A-C2A	-8.63	107.55	128.43
37	2	302	A86	C25-C26-C27	-8.63	115.18	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	829	CLA	C1D-ND-C4D	-8.62	100.26	106.31
37	14	320	A86	C33-C32-C31	8.62	117.59	109.21
30	B	824	CLA	C1D-ND-C4D	-8.62	100.26	106.31
30	A	814	CLA	C1D-ND-C4D	-8.62	100.27	106.31
30	15	312	CLA	C1D-ND-C4D	-8.62	100.27	106.31
30	6	310	CLA	C1D-ND-C4D	-8.61	100.27	106.31
39	12	315	DD6	C12-C11-C10	-8.61	108.87	122.82
39	12	317	DD6	C8-C6-C5	-8.60	105.48	119.01
38	7	308	KC1	C1D-ND-C4D	-8.60	100.28	106.31
30	1	305	CLA	C1D-ND-C4D	-8.59	100.28	106.31
30	A	807	CLA	C1D-ND-C4D	-8.59	100.28	106.31
30	A	825	CLA	C1D-ND-C4D	-8.58	100.30	106.31
30	2	304	CLA	C1D-ND-C4D	-8.58	100.30	106.31
37	10	316	A86	O1-C20-C21	-8.57	105.47	115.05
38	16	304	KC1	C1D-ND-C4D	-8.57	100.30	106.31
30	A	831	CLA	O2D-CGD-CBD	8.57	126.20	111.23
30	5	307	CLA	C1D-ND-C4D	-8.57	100.30	106.31
38	3	304	KC1	C2A-C3A-C4A	-8.56	99.98	106.41
39	1	310	DD6	C13-C11-C10	-8.56	105.55	119.01
39	6	319	DD6	C3-C2-C1	-8.56	115.28	127.28
39	3	312	DD6	C37-C36-C31	-8.55	108.17	124.16
29	A	801	CL0	O2D-CGD-CBD	8.54	120.33	110.95
39	10	313	DD6	C7-C6-C5	-8.54	108.98	122.82
30	A	837	CLA	C1D-ND-C4D	-8.53	100.33	106.31
30	B	818	CLA	C1D-ND-C4D	-8.53	100.33	106.31
39	2	316	DD6	C37-C36-C31	-8.53	108.22	124.16
30	12	306	CLA	C1D-ND-C4D	-8.52	100.33	106.31
37	2	318	A86	C21-C20-C19	-8.52	104.67	114.24
30	A	826	CLA	C1D-ND-C4D	-8.52	100.33	106.31
38	13	311	KC1	CMA-C3A-C2A	-8.52	107.82	128.43
30	A	832	CLA	C1D-ND-C4D	-8.52	100.34	106.31
39	11	313	DD6	C7-C6-C5	-8.50	109.05	122.82
37	13	313	A86	C4-C5-C6	-8.49	115.37	127.28
37	5	316	A86	O1-C20-C21	-8.49	105.56	115.05
30	10	307	CLA	C1D-ND-C4D	-8.49	100.36	106.31
30	A	809	CLA	C1D-ND-C4D	-8.49	100.36	106.31
39	6	321	DD6	C4-C5-C6	-8.49	115.38	127.28
37	3	314	A86	C4-C5-C6	-8.48	115.39	127.28
37	5	316	A86	C33-C32-C31	8.48	117.45	109.21
38	6	308	KC1	C1D-ND-C4D	-8.47	100.37	106.31
39	7	314	DD6	C4-C5-C6	-8.46	115.41	127.28
38	10	306	KC1	C2A-C3A-C4A	-8.46	100.06	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	12	315	DD6	C13-C11-C10	-8.46	105.71	119.01
38	9	311	KC1	CMA-C3A-C2A	-8.45	107.97	128.43
30	B	809	CLA	C1D-ND-C4D	-8.45	100.38	106.31
30	9	309	CLA	C1D-ND-C4D	-8.45	100.38	106.31
39	5	314	DD6	C12-C11-C10	-8.45	109.12	122.82
30	14	309	CLA	C1D-ND-C4D	-8.44	100.39	106.31
39	4	313	DD6	C12-C11-C10	-8.44	109.14	122.82
39	5	313	DD6	C3-C2-C1	-8.44	115.44	127.28
38	4	308	KC1	C1D-ND-C4D	-8.44	100.39	106.31
30	A	835	CLA	C1D-ND-C4D	-8.43	100.40	106.31
38	10	306	KC1	C1D-ND-C4D	-8.42	100.40	106.31
30	B	815	CLA	C1D-ND-C4D	-8.42	100.41	106.31
39	10	314	DD6	C12-C11-C10	-8.41	109.19	122.82
38	13	306	KC1	C2A-C3A-C4A	-8.41	100.10	106.41
38	5	305	KC1	C2A-C3A-C4A	-8.40	100.10	106.41
38	8	314	KC1	C1D-ND-C4D	-8.40	100.42	106.31
38	4	310	KC1	C1D-ND-C4D	-8.39	100.42	106.31
30	8	304	CLA	C1D-ND-C4D	-8.39	100.43	106.31
38	11	312	KC1	C1D-ND-C4D	-8.38	100.43	106.31
30	J	101	CLA	C1D-ND-C4D	-8.38	100.43	106.31
38	5	312	KC1	C1D-ND-C4D	-8.37	100.44	106.31
30	2	307	CLA	C1D-ND-C4D	-8.37	100.44	106.31
39	3	312	DD6	C12-C11-C10	-8.35	109.29	122.82
37	9	315	A86	C25-C26-C27	-8.35	115.57	127.28
39	6	303	DD6	C9-C10-C11	-8.35	115.57	127.28
38	16	311	KC1	CMA-C3A-C4A	-8.35	111.99	125.03
39	16	313	DD6	C4-C5-C6	-8.35	115.57	127.28
37	14	319	A86	C4-C5-C6	-8.34	115.58	127.28
38	12	309	KC1	CMA-C3A-C4A	-8.33	112.02	125.03
39	2	317	DD6	C12-C11-C10	-8.33	109.33	122.82
30	12	303	CLA	C1D-ND-C4D	-8.32	100.47	106.31
30	B	813	CLA	C1D-ND-C4D	-8.32	100.48	106.31
39	7	318	DD6	C37-C36-C31	-8.32	108.61	124.16
30	6	309	CLA	C1D-ND-C4D	-8.31	100.48	106.31
39	16	313	DD6	C8-C6-C5	-8.31	105.94	119.01
39	7	317	DD6	C4-C5-C6	-8.31	115.63	127.28
39	4	313	DD6	C4-C5-C6	-8.30	115.63	127.28
37	14	315	A86	C33-C32-C31	8.30	117.28	109.21
39	3	316	DD6	C12-C11-C10	-8.29	109.38	122.82
30	B	828	CLA	C1D-ND-C4D	-8.27	100.51	106.31
30	7	306	CLA	C1D-ND-C4D	-8.27	100.51	106.31
39	5	314	DD6	C37-C36-C31	-8.27	108.70	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	812	CLA	C1D-ND-C4D	-8.26	100.51	106.31
37	14	318	A86	C4-C5-C6	-8.26	115.69	127.28
39	7	318	DD6	C7-C6-C5	-8.26	109.44	122.82
39	8	317	DD6	C3-C2-C1	-8.25	115.71	127.28
38	11	305	KC1	CMA-C3A-C2A	-8.24	108.48	128.43
39	7	302	DD6	C12-C11-C10	-8.23	109.48	122.82
39	7	314	DD6	C37-C36-C31	-8.23	108.78	124.16
37	4	317	A86	O1-C20-C21	-8.22	105.86	115.05
30	A	836	CLA	C1D-ND-C4D	-8.22	100.54	106.31
30	A	822	CLA	C1D-ND-C4D	-8.22	100.54	106.31
39	16	313	DD6	C-C1-C2	-8.20	109.52	122.82
38	3	311	KC1	C2A-C3A-C4A	-8.20	100.26	106.41
37	5	301	A86	O1-C20-C21	-8.19	105.89	115.05
39	6	318	DD6	C37-C36-C31	-8.18	108.86	124.16
37	10	302	A86	C33-C32-C31	8.18	117.16	109.21
37	14	317	A86	C4-C5-C6	-8.17	115.81	127.28
39	15	318	DD6	C3-C2-C1	-8.17	115.82	127.28
30	B	834	CLA	C1D-ND-C4D	-8.17	100.58	106.31
39	7	318	DD6	C-C1-C2	-8.17	109.59	122.82
30	A	841	CLA	C1D-ND-C4D	-8.16	100.59	106.31
30	B	821	CLA	C1D-ND-C4D	-8.15	100.59	106.31
37	7	315	A86	C33-C32-C31	8.15	117.13	109.21
37	2	319	A86	C33-C32-C31	8.15	117.13	109.21
39	15	319	DD6	C7-C6-C5	-8.14	109.63	122.82
30	A	831	CLA	C1D-ND-C4D	-8.14	100.60	106.31
39	16	313	DD6	C7-C6-C5	-8.14	109.63	122.82
30	B	823	CLA	C1D-ND-C4D	-8.14	100.60	106.31
30	3	306	CLA	C1D-ND-C4D	-8.13	100.61	106.31
30	6	316	CLA	C1D-ND-C4D	-8.13	100.61	106.31
30	A	838	CLA	C1D-ND-C4D	-8.13	100.61	106.31
37	15	317	A86	C4-C5-C6	-8.13	115.88	127.28
39	4	316	DD6	C37-C36-C31	-8.12	108.97	124.16
39	2	315	DD6	C12-C11-C10	-8.10	109.69	122.82
39	5	314	DD6	C9-C10-C11	-8.10	115.92	127.28
39	15	318	DD6	C12-C11-C10	-8.10	109.69	122.82
38	11	312	KC1	CMA-C3A-C4A	-8.10	112.38	125.03
38	16	311	KC1	C1D-ND-C4D	-8.10	100.63	106.31
38	2	314	KC1	CMA-C3A-C2A	-8.09	108.84	128.43
30	6	307	CLA	C1D-ND-C4D	-8.09	100.64	106.31
38	5	312	KC1	CMA-C3A-C2A	-8.08	108.87	128.43
39	12	317	DD6	C-C1-C2	-8.08	109.73	122.82
30	A	815	CLA	C1D-ND-C4D	-8.07	100.65	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	12	317	DD6	C4-C5-C6	-8.07	115.96	127.28
39	7	317	DD6	O1-C15-C14	-8.06	93.78	116.88
38	8	314	KC1	O2D-CGD-CBD	8.06	125.32	111.23
38	14	308	KC1	C1D-ND-C4D	-8.05	100.66	106.31
39	10	313	DD6	C13-C11-C10	-8.05	106.35	119.01
38	3	304	KC1	CMD-C2D-C1D	8.04	137.66	125.42
39	4	316	DD6	C28-C27-C26	-8.03	108.59	124.18
39	15	318	DD6	C7-C6-C5	-8.02	109.82	122.82
30	12	304	CLA	CAA-C2A-C3A	-8.02	91.32	113.00
39	2	317	DD6	C-C1-C2	-8.00	109.86	122.82
39	7	302	DD6	C28-C27-C26	-7.99	108.66	124.18
38	13	305	KC1	CMA-C3A-C2A	-7.98	109.13	128.43
37	12	314	A86	C33-C32-C31	7.97	116.96	109.21
37	10	302	A86	C25-C26-C27	-7.97	116.11	127.28
39	6	319	DD6	C37-C36-C31	-7.97	109.27	124.16
30	8	304	CLA	CAA-C2A-C3A	-7.96	91.48	113.00
39	10	314	DD6	C28-C27-C26	-7.96	108.72	124.18
39	6	321	DD6	C8-C6-C5	-7.95	106.50	119.01
39	4	316	DD6	C-C1-C2	-7.95	109.93	122.82
39	15	318	DD6	C37-C36-C31	-7.95	109.29	124.16
38	12	311	KC1	CMA-C3A-C2A	-7.95	109.19	128.43
39	4	313	DD6	C-C1-C2	-7.95	109.94	122.82
37	13	315	A86	C33-C32-C31	7.94	116.93	109.21
38	13	306	KC1	CMA-C3A-C2A	-7.94	109.20	128.43
39	2	317	DD6	C28-C27-C26	-7.94	108.75	124.18
39	7	317	DD6	C28-C27-C26	-7.94	108.75	124.18
39	8	317	DD6	C9-C10-C11	-7.92	116.16	127.28
39	5	313	DD6	C9-C10-C11	-7.92	116.17	127.28
39	16	313	DD6	O1-C15-C14	-7.92	94.19	116.88
39	13	314	DD6	C3-C2-C1	-7.92	116.17	127.28
39	7	302	DD6	C37-C36-C31	-7.91	109.36	124.16
39	13	314	DD6	C28-C27-C26	-7.91	108.81	124.18
30	A	820	CLA	C1D-ND-C4D	-7.91	100.76	106.31
39	8	317	DD6	C28-C27-C26	-7.91	108.82	124.18
37	2	319	A86	O1-C20-C21	-7.90	106.22	115.05
37	12	314	A86	C4-C5-C6	-7.90	116.20	127.28
37	2u	205	A86	O1-C20-C21	-7.90	106.22	115.05
39	7	318	DD6	C28-C27-C26	-7.88	108.86	124.18
39	3	312	DD6	C4-C5-C6	-7.88	116.22	127.28
37	9	315	A86	C21-C20-C19	-7.88	105.39	114.24
39	16	313	DD6	C28-C27-C26	-7.87	108.88	124.18
39	3	313	DD6	C7-C6-C5	-7.84	110.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	839	CLA	O2D-CGD-CBD	7.83	124.93	111.23
39	3	312	DD6	C9-C10-C11	-7.83	116.29	127.28
39	6	303	DD6	C28-C27-C26	-7.83	108.96	124.18
38	8	313	KC1	CMA-C3A-C2A	-7.83	109.47	128.43
39	4	316	DD6	C7-C6-C5	-7.83	110.13	122.82
39	11	313	DD6	C12-C11-C10	-7.83	110.13	122.82
39	3	316	DD6	C37-C36-C31	-7.83	109.53	124.16
39	13	314	DD6	C7-C6-C5	-7.82	110.14	122.82
39	10	314	DD6	C7-C6-C5	-7.82	110.14	122.82
39	1	310	DD6	C28-C27-C26	-7.82	108.99	124.18
37	15	321	A86	C33-C32-C31	7.82	116.81	109.21
37	7	316	A86	C33-C32-C31	7.82	116.81	109.21
38	8	311	KC1	CMA-C3A-C2A	-7.81	109.52	128.43
39	8	316	DD6	O1-C15-C14	-7.81	94.49	116.88
39	8	316	DD6	C8-C6-C5	-7.81	106.72	119.01
39	10	314	DD6	C9-C10-C11	-7.81	116.33	127.28
39	5	314	DD6	C7-C6-C5	-7.81	110.17	122.82
38	8	314	KC1	C2A-C3A-C4A	-7.80	100.55	106.41
39	12	317	DD6	C28-C27-C26	-7.79	109.04	124.18
30	15	312	CLA	CMD-C2D-C1D	7.79	138.44	124.73
39	1	310	DD6	C7-C6-C5	-7.79	110.20	122.82
39	6	303	DD6	C8-C6-C5	-7.78	106.78	119.01
39	11	313	DD6	C28-C27-C26	-7.77	109.09	124.18
38	3	304	KC1	CMA-C3A-C2A	-7.77	109.63	128.43
39	5	313	DD6	C28-C27-C26	-7.76	109.10	124.18
39	9	314	DD6	C-C1-C2	-7.76	110.25	122.82
38	6	311	KC1	CMA-C3A-C2A	-7.75	109.66	128.43
38	11	312	KC1	CMD-C2D-C1D	7.75	137.22	125.42
37	12	316	A86	C4-C5-C6	-7.74	116.42	127.28
39	3	316	DD6	C7-C6-C5	-7.74	110.27	122.82
38	8	310	KC1	CMA-C3A-C2A	-7.74	109.70	128.43
39	12	315	DD6	C28-C27-C26	-7.73	109.16	124.18
39	12	317	DD6	C7-C6-C5	-7.73	110.29	122.82
39	3	316	DD6	C28-C27-C26	-7.73	109.17	124.18
37	14	320	A86	C25-C26-C27	-7.72	116.45	127.28
38	1	308	KC1	CMA-C3A-C2A	-7.71	109.76	128.43
30	A	802	CLA	C1D-ND-C4D	-7.71	100.90	106.31
38	3	311	KC1	CMD-C2D-C1D	7.69	137.13	125.42
38	7	313	KC1	CMA-C3A-C2A	-7.69	109.83	128.43
39	15	318	DD6	C28-C27-C26	-7.68	109.25	124.18
39	10	313	DD6	C28-C27-C26	-7.68	109.26	124.18
39	2	316	DD6	C28-C27-C26	-7.67	109.28	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	9	310	KC1	CMA-C3A-C2A	-7.67	109.88	128.43
39	9	314	DD6	C28-C27-C26	-7.66	109.30	124.18
39	7	302	DD6	C7-C6-C5	-7.65	110.42	122.82
37	14	301	A86	C33-C32-C31	7.65	116.65	109.21
38	2	306	KC1	CMA-C3A-C2A	-7.64	109.93	128.43
30	B	819	CLA	C1D-ND-C4D	-7.64	100.95	106.31
37	2u	205	A86	C33-C32-C31	7.63	116.63	109.21
39	3	313	DD6	C28-C27-C26	-7.63	109.36	124.18
37	14	318	A86	C33-C32-C31	7.63	116.62	109.21
39	6	321	DD6	C-C1-C2	-7.62	110.47	122.82
38	9	312	KC1	CMD-C2D-C1D	7.62	137.02	125.42
39	2	317	DD6	O1-C15-C14	-7.62	95.05	116.88
39	6	319	DD6	C28-C27-C26	-7.62	109.39	124.18
38	16	304	KC1	CMD-C2D-C1D	7.61	137.01	125.42
38	6	312	KC1	CMA-C3A-C2A	-7.61	110.01	128.43
39	7	314	DD6	C8-C6-C5	-7.60	107.05	119.01
39	7	314	DD6	C15-C14-C13	7.60	142.06	125.99
39	6	303	DD6	C13-C11-C10	-7.60	107.06	119.01
39	7	302	DD6	C-C1-C2	-7.59	110.52	122.82
39	12	315	DD6	C7-C6-C5	-7.59	110.52	122.82
38	12	305	KC1	CMA-C3A-C2A	-7.59	110.06	128.43
37	12	316	A86	C33-C32-C31	7.59	116.58	109.21
39	6	318	DD6	C28-C27-C26	-7.59	109.44	124.18
39	2	315	DD6	C28-C27-C26	-7.59	109.44	124.18
39	8	316	DD6	C28-C27-C26	-7.58	109.46	124.18
39	12	315	DD6	C-C1-C2	-7.58	110.54	122.82
39	11	313	DD6	C-C1-C2	-7.58	110.54	122.82
39	16	313	DD6	C15-C14-C13	7.58	142.01	125.99
39	7	317	DD6	C-C1-C2	-7.57	110.55	122.82
39	15	319	DD6	C28-C27-C26	-7.56	109.50	124.18
38	11	305	KC1	CMD-C2D-C1D	7.55	136.92	125.42
37	10	302	A86	C4-C5-C6	-7.54	116.70	127.28
38	8	311	KC1	CMD-C2D-C1D	7.54	136.90	125.42
38	10	312	KC1	CMA-C3A-C2A	-7.54	110.19	128.43
39	3	312	DD6	C28-C27-C26	-7.54	109.54	124.18
37	5	301	A86	C4-C5-C6	-7.54	116.71	127.28
38	13	312	KC1	CMD-C2D-C1D	7.54	136.89	125.42
38	12	311	KC1	CMD-C2D-C1D	7.53	136.89	125.42
39	6	321	DD6	C28-C27-C26	-7.53	109.56	124.18
37	13	313	A86	C33-C32-C31	7.52	116.52	109.21
30	B	828	CLA	CMD-C2D-C1D	7.52	137.97	124.73
38	16	311	KC1	CMD-C2D-C1D	7.52	136.86	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	310	KC1	CMA-C3A-C2A	-7.51	110.25	128.43
39	6	303	DD6	C7-C6-C5	-7.50	110.66	122.82
39	2	315	DD6	C-C1-C2	-7.50	110.67	122.82
37	11	301	A86	C33-C32-C31	7.50	116.50	109.21
38	1	306	KC1	CMA-C3A-C2A	-7.49	110.29	128.43
39	4	313	DD6	C28-C27-C26	-7.49	109.64	124.18
37	2	302	A86	C33-C32-C31	7.48	116.48	109.21
38	8	306	KC1	CMD-C2D-C1D	7.48	136.81	125.42
39	5	314	DD6	C28-C27-C26	-7.47	109.66	124.18
37	10	316	A86	C33-C32-C31	7.47	116.47	109.21
39	7	314	DD6	C28-C27-C26	-7.46	109.69	124.18
39	9	314	DD6	C7-C6-C5	-7.45	110.74	122.82
37	16	312	A86	C3-C2-C1	-7.45	116.83	127.28
39	6	318	DD6	C12-C11-C13	-7.44	106.72	118.09
38	8	312	KC1	C1A-C2A-C3A	-7.44	100.44	107.28
38	6	313	KC1	CMA-C3A-C2A	-7.43	110.44	128.43
38	13	311	KC1	CMD-C2D-C1D	7.43	136.73	125.42
39	8	317	DD6	C7-C6-C5	-7.42	110.79	122.82
30	A	840	CLA	CMD-C2D-C1D	7.42	137.80	124.73
37	3	314	A86	C3-C2-C1	-7.42	116.87	127.28
38	2	312	KC1	CMA-C3A-C2A	-7.41	110.51	128.43
38	10	306	KC1	O2D-CGD-CBD	7.41	124.18	111.23
38	13	312	KC1	CMA-C3A-C2A	-7.40	110.51	128.43
39	10	313	DD6	C-C1-C2	-7.40	110.83	122.82
38	10	310	KC1	CMA-C3A-C2A	-7.40	110.53	128.43
38	13	308	KC1	CMA-C3A-C2A	-7.40	110.53	128.43
38	10	312	KC1	CMD-C2D-C1D	7.39	136.68	125.42
38	5	306	KC1	CMD-C2D-C1D	7.39	136.67	125.42
38	5	310	KC1	CMA-C3A-C2A	-7.38	110.57	128.43
38	3	308	KC1	CMA-C3A-C2A	-7.37	110.60	128.43
39	2	317	DD6	C8-C6-C5	-7.37	107.42	119.01
39	12	315	DD6	C8-C6-C5	-7.36	107.42	119.01
38	8	314	KC1	CMD-C2D-C1D	7.35	136.61	125.42
38	4	310	KC1	CMD-C2D-C1D	7.35	136.61	125.42
39	2	315	DD6	C37-C36-C31	-7.34	110.44	124.16
30	14	302	CLA	CMD-C2D-C1D	7.34	137.65	124.73
39	2	317	DD6	C37-C36-C31	-7.33	110.46	124.16
30	7	305	CLA	CMD-C2D-C1D	7.33	137.63	124.73
38	9	304	KC1	CMA-C3A-C2A	-7.33	110.70	128.43
37	14	320	A86	O1-C20-C21	-7.32	106.86	115.05
38	7	313	KC1	CMD-C2D-C1D	7.32	136.56	125.42
38	11	307	KC1	CMA-C3A-C2A	-7.32	110.72	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	820	CLA	C2D-C1D-ND	7.31	117.36	110.13
38	12	305	KC1	CMD-C2D-C1D	7.30	136.54	125.42
39	3	316	DD6	C-C1-C2	-7.29	111.01	122.82
38	13	310	KC1	CMA-C3A-C2A	-7.29	110.79	128.43
30	L	202	CLA	C2D-C1D-ND	7.29	117.34	110.13
38	2	306	KC1	CMD-C2D-C1D	7.28	136.51	125.42
39	7	317	DD6	C8-C6-C5	-7.28	107.55	119.01
39	3	312	DD6	C-C1-C2	-7.28	111.03	122.82
37	7	319	A86	C33-C32-C31	7.27	116.27	109.21
38	4	308	KC1	CMD-C2D-C1D	7.26	136.48	125.42
39	4	313	DD6	O1-C15-C14	-7.26	96.06	116.88
39	15	318	DD6	C8-C6-C5	-7.26	107.58	119.01
39	15	319	DD6	C8-C6-C5	-7.26	107.59	119.01
39	10	314	DD6	C-C1-C2	-7.25	111.06	122.82
38	14	311	KC1	CMD-C2D-C1D	7.25	136.46	125.42
30	B	830	CLA	C2D-C1D-ND	7.24	117.29	110.13
38	12	309	KC1	CMD-C2D-C1D	7.23	136.44	125.42
39	7	318	DD6	C24-C1-C2	-7.23	107.64	119.01
30	A	815	CLA	CMD-C2D-C1D	7.22	137.45	124.73
39	5	313	DD6	C12-C11-C10	-7.22	111.11	122.82
38	13	308	KC1	CMD-C2D-C1D	7.21	136.39	125.42
39	4	313	DD6	C8-C6-C5	-7.20	107.69	119.01
38	13	306	KC1	CMD-C2D-C1D	7.20	136.38	125.42
39	1	310	DD6	C24-C1-C2	-7.20	107.69	119.01
39	15	319	DD6	O1-C15-C14	-7.19	96.27	116.88
38	6	312	KC1	CMD-C2D-C1D	7.18	136.36	125.42
39	7	318	DD6	O1-C15-C14	-7.18	96.30	116.88
37	4	314	A86	C33-C32-C31	7.18	116.19	109.21
38	8	312	KC1	CMD-C2D-C1D	7.18	136.35	125.42
39	8	316	DD6	C7-C6-C5	-7.18	111.18	122.82
37	6	320	A86	C21-C20-C19	-7.18	106.18	114.24
39	13	314	DD6	C-C1-C2	-7.17	111.20	122.82
39	8	316	DD6	C9-C10-C11	-7.17	117.23	127.28
30	6	314	CLA	CMD-C2D-C1D	7.17	137.35	124.73
39	2	315	DD6	C4-C5-C6	-7.16	117.23	127.28
39	2	317	DD6	C12-C11-C13	-7.16	107.15	118.09
39	4	313	DD6	C13-C11-C10	-7.16	107.75	119.01
38	10	306	KC1	CMD-C2D-C1D	7.16	136.32	125.42
38	8	314	KC1	C1A-C2A-C3A	-7.16	100.70	107.28
38	11	311	KC1	CMA-C3A-C2A	-7.15	111.12	128.43
39	1	310	DD6	C8-C6-C5	-7.15	107.77	119.01
30	11	310	CLA	CMD-C2D-C1D	7.14	137.31	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	11	307	KC1	CMD-C2D-C1D	7.14	136.29	125.42
39	6	319	DD6	C4-C5-C6	-7.14	117.27	127.28
30	B	830	CLA	CMD-C2D-C1D	7.14	137.30	124.73
38	14	311	KC1	CMA-C3A-C2A	-7.13	111.17	128.43
37	16	312	A86	C33-C32-C31	7.13	116.14	109.21
39	2	316	DD6	C-C1-C2	-7.12	111.27	122.82
30	14	310	CLA	CMD-C2D-C1D	7.12	137.27	124.73
39	5	314	DD6	C-C1-C2	-7.12	111.28	122.82
38	4	310	KC1	CHB-C4A-C3A	-7.11	113.81	125.03
30	B	839	CLA	O2D-CGD-CBD	7.11	123.65	111.23
38	8	307	KC1	CMD-C2D-C1D	7.10	136.24	125.42
30	A	828	CLA	CHD-C4C-C3C	-7.10	114.42	124.77
37	14	316	A86	C33-C32-C31	7.10	116.11	109.21
30	A	826	CLA	O2D-CGD-CBD	7.10	123.64	111.23
37	15	323	A86	C4-C5-C6	-7.09	117.33	127.28
30	6	304	CLA	CMD-C2D-C1D	7.09	137.21	124.73
38	12	309	KC1	CHB-C4A-C3A	-7.09	113.84	125.03
37	15	315	A86	C33-C32-C31	7.08	116.10	109.21
38	2	314	KC1	CMD-C2D-C1D	7.08	136.20	125.42
37	6	320	A86	C33-C32-C31	7.08	116.09	109.21
38	16	311	KC1	CHB-C4A-C3A	-7.07	113.86	125.03
39	12	317	DD6	C13-C11-C10	-7.07	107.89	119.01
38	5	305	KC1	CMD-C2D-C1D	7.06	136.17	125.42
39	6	303	DD6	C-C1-C2	-7.05	111.39	122.82
38	4	308	KC1	CHB-C4A-C3A	-7.05	113.90	125.03
38	11	311	KC1	CMD-C2D-C1D	7.04	136.15	125.42
39	15	319	DD6	C37-C36-C31	-7.04	110.99	124.16
30	B	835	CLA	CMD-C2D-C1D	7.04	137.13	124.73
38	9	304	KC1	CMD-C2D-C1D	7.04	136.14	125.42
39	2	317	DD6	C7-C6-C5	-7.04	111.41	122.82
39	10	314	DD6	C8-C6-C5	-7.03	107.95	119.01
37	10	316	A86	C4-C5-C6	-7.03	117.42	127.28
30	15	306	CLA	O2D-CGD-CBD	7.03	123.52	111.23
30	B	825	CLA	CMD-C2D-C1D	7.02	137.10	124.73
37	4	317	A86	C33-C32-C31	7.02	116.04	109.21
30	B	832	CLA	CMD-C2D-C1D	7.01	137.08	124.73
30	B	820	CLA	CHD-C4C-C3C	-7.01	114.55	124.77
38	5	310	KC1	CMD-C2D-C1D	7.01	136.09	125.42
30	A	827	CLA	CMD-C2D-C1D	7.00	137.06	124.73
30	B	823	CLA	O2D-CGD-CBD	7.00	123.47	111.23
37	10	315	A86	C33-C32-C31	7.00	116.02	109.21
30	A	835	CLA	O2D-CGD-CBD	7.00	123.47	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	3	313	DD6	C-C1-C2	-7.00	111.47	122.82
30	16	308	CLA	CMD-C2D-C1D	7.00	137.05	124.73
39	7	314	DD6	C14-C13-C11	6.98	136.37	125.53
30	A	817	CLA	CMD-C2D-C1D	6.98	137.01	124.73
30	B	831	CLA	O2D-CGD-CBD	6.97	123.42	111.23
38	8	310	KC1	CMD-C2D-C1D	6.97	136.03	125.42
38	8	314	KC1	CMA-C3A-C4A	-6.97	114.15	125.03
30	15	314	CLA	CMD-C2D-C1D	6.96	136.98	124.73
38	6	311	KC1	CHB-C4A-C3A	-6.95	114.05	125.03
39	8	317	DD6	C24-C1-C2	-6.95	108.08	119.01
30	16	310	CLA	CMD-C2D-C1D	6.95	136.96	124.73
39	6	321	DD6	C12-C11-C13	-6.94	107.48	118.09
30	A	803	CLA	C2D-C1D-ND	6.94	117.00	110.13
38	8	314	KC1	CHB-C4A-C3A	-6.94	114.07	125.03
37	11	314	A86	C33-C32-C31	6.93	115.94	109.21
38	8	312	KC1	C2A-C3A-C4A	-6.92	101.22	106.41
30	A	828	CLA	C2D-C1D-ND	6.92	116.97	110.13
38	7	313	KC1	CHB-C4A-C3A	-6.91	114.11	125.03
30	9	302	CLA	O2D-CGD-CBD	6.91	123.31	111.23
39	13	314	DD6	C7-C6-C8	-6.90	107.54	118.09
37	6	320	A86	O1-C20-C21	-6.90	107.33	115.05
39	15	319	DD6	C13-C11-C10	-6.90	108.15	119.01
37	3	314	A86	C33-C32-C31	6.90	115.92	109.21
39	6	303	DD6	C37-C36-C31	-6.90	111.26	124.16
38	1	306	KC1	CMD-C2D-C1D	6.90	135.93	125.42
38	12	311	KC1	CHB-C4A-C3A	-6.90	114.14	125.03
38	3	304	KC1	O2D-CGD-CBD	6.90	123.29	111.23
30	3	310	CLA	CMD-C2D-C1D	6.89	136.87	124.73
39	1	310	DD6	C-C1-C2	-6.89	111.65	122.82
38	6	308	KC1	CHB-C4A-C3A	-6.89	114.15	125.03
38	13	310	KC1	CMD-C2D-C1D	6.89	135.91	125.42
30	15	302	CLA	CMD-C2D-C1D	6.88	136.85	124.73
37	4	312	A86	C4-C5-C6	-6.88	117.62	127.28
30	3	303	CLA	O2D-CGD-CBD	6.88	123.26	111.23
30	7	312	CLA	CMD-C2D-C1D	6.88	136.84	124.73
39	6	303	DD6	C12-C11-C10	-6.88	111.68	122.82
30	7	310	CLA	CMD-C2D-C1D	6.87	136.83	124.73
38	10	310	KC1	CHB-C4A-C3A	-6.87	114.18	125.03
39	7	302	DD6	C8-C6-C5	-6.87	108.20	119.01
39	7	317	DD6	C7-C6-C5	-6.86	111.69	122.82
30	15	309	CLA	CMD-C2D-C1D	6.86	136.80	124.73
30	A	835	CLA	CMD-C2D-C1D	6.86	136.80	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	316	A86	C33-C32-C31	6.85	115.87	109.21
30	B	802	CLA	C2D-C1D-ND	6.85	116.91	110.13
38	13	305	KC1	CHB-C4A-C3A	-6.85	114.22	125.03
30	B	817	CLA	CMD-C2D-C1D	6.84	136.78	124.73
39	10	313	DD6	C-C1-C24	-6.84	107.64	118.09
38	10	310	KC1	CMD-C2D-C1D	6.84	135.83	125.42
37	10	301	A86	O1-C20-C21	-6.83	107.41	115.05
30	13	301	CLA	CMD-C2D-C1D	6.83	136.76	124.73
30	B	824	CLA	CMD-C2D-C1D	6.83	136.75	124.73
30	13	309	CLA	CMD-C2D-C1D	6.83	136.75	124.73
38	13	311	KC1	CMA-C3A-C4A	-6.83	114.37	125.03
30	B	803	CLA	C2D-C1D-ND	6.83	116.88	110.13
30	A	827	CLA	CHD-C4C-C3C	-6.82	114.82	124.77
30	J	101	CLA	CMD-C2D-C1D	6.82	136.74	124.73
39	5	313	DD6	C-C1-C2	-6.82	111.77	122.82
38	9	310	KC1	CHB-C4A-C3A	-6.81	114.27	125.03
30	A	827	CLA	C2D-C1D-ND	6.81	116.86	110.13
39	3	313	DD6	C12-C11-C13	-6.80	107.69	118.09
37	15	315	A86	C24-C1-C2	6.80	129.71	119.01
30	2	313	CLA	CMD-C2D-C1D	6.80	136.70	124.73
30	14	304	CLA	CMD-C2D-C1D	6.80	136.70	124.73
30	2	305	CLA	O2D-CGD-CBD	6.79	123.11	111.23
30	4	304	CLA	CMD-C2D-C1D	6.79	136.69	124.73
30	A	837	CLA	CMD-C2D-C1D	6.79	136.69	124.73
30	1	305	CLA	CMD-C2D-C1D	6.79	136.69	124.73
37	5	301	A86	C33-C32-C31	6.79	115.81	109.21
38	4	307	KC1	CMD-C2D-C1D	6.78	135.75	125.42
30	13	304	CLA	CMD-C2D-C1D	6.78	136.67	124.73
38	2	312	KC1	CMD-C2D-C1D	6.78	135.74	125.42
38	14	306	KC1	CMA-C3A-C2A	-6.78	112.02	128.43
30	6	317	CLA	CMD-C2D-C1D	6.77	136.66	124.73
29	A	801	CL0	C4D-ND-C1D	-6.77	100.08	105.22
30	14	313	CLA	CMD-C2D-C1D	6.77	136.66	124.73
39	6	321	DD6	C7-C6-C5	-6.77	111.84	122.82
30	A	806	CLA	CMD-C2D-C1D	6.77	136.66	124.73
30	B	837	CLA	CMD-C2D-C1D	6.77	136.65	124.73
38	14	311	KC1	CHB-C4A-C3A	-6.77	114.34	125.03
30	9	306	CLA	CMD-C2D-C1D	6.77	136.65	124.73
30	A	829	CLA	CMD-C2D-C1D	6.76	136.64	124.73
30	A	819	CLA	CMD-C2D-C1D	6.76	136.64	124.73
39	11	313	DD6	C12-C11-C13	-6.76	107.76	118.09
39	6	318	DD6	C-C1-C2	-6.76	111.86	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	836	CLA	C2D-C1D-ND	6.76	116.82	110.13
30	9	305	CLA	O2D-CGD-CBD	6.75	123.04	111.23
30	L	203	CLA	CMD-C2D-C1D	6.75	136.62	124.73
30	A	844	CLA	CMD-C2D-C1D	6.75	136.62	124.73
30	13	303	CLA	CMD-C2D-C1D	6.75	136.62	124.73
30	15	304	CLA	CMD-C2D-C1D	6.75	136.62	124.73
30	A	810	CLA	CMD-C2D-C1D	6.75	136.61	124.73
30	12	304	CLA	CMD-C2D-C1D	6.75	136.61	124.73
37	1	309	A86	C33-C32-C31	6.75	115.77	109.21
30	B	823	CLA	CMD-C2D-C1D	6.74	136.59	124.73
38	2	306	KC1	CHB-C4A-C3A	-6.74	114.39	125.03
30	4	302	CLA	CMD-C2D-C1D	6.74	136.59	124.73
30	9	301	CLA	O2D-CGD-CBD	6.73	123.00	111.23
30	A	824	CLA	CMD-C2D-C1D	6.73	136.59	124.73
38	11	311	KC1	CHB-C4A-C3A	-6.73	114.40	125.03
30	9	302	CLA	CMD-C2D-C1D	6.73	136.58	124.73
30	6	305	CLA	CMD-C2D-C1D	6.73	136.57	124.73
39	15	318	DD6	O1-C15-C14	-6.73	97.61	116.88
38	13	308	KC1	CHB-C4A-C3A	-6.71	114.43	125.03
38	9	311	KC1	CMD-C2D-C1D	6.71	135.64	125.42
37	7	319	A86	C25-C26-C27	-6.71	117.87	127.28
38	8	307	KC1	CHB-C4A-C3A	-6.71	114.44	125.03
30	A	834	CLA	CMD-C2D-C1D	6.71	136.54	124.73
39	12	317	DD6	C12-C11-C13	-6.70	107.85	118.09
38	11	312	KC1	CHB-C4A-C3A	-6.70	114.44	125.03
30	8	305	CLA	C2D-C1D-ND	6.70	116.76	110.13
38	6	311	KC1	CMD-C2D-C1D	6.70	135.62	125.42
30	9	307	CLA	CMD-C2D-C1D	6.70	136.53	124.73
38	5	310	KC1	CHB-C4A-C3A	-6.70	114.45	125.03
38	12	305	KC1	CHB-C4A-C3A	-6.70	114.45	125.03
38	16	304	KC1	CHB-C4A-C3A	-6.69	114.46	125.03
30	8	302	CLA	CMD-C2D-C1D	6.69	136.51	124.73
30	B	808	CLA	CMD-C2D-C1D	6.69	136.51	124.73
30	B	828	CLA	O2D-CGD-CBD	6.69	122.92	111.23
38	5	306	KC1	CHB-C4A-C3A	-6.68	114.48	125.03
37	15	322	A86	C25-C26-C27	-6.68	117.91	127.28
38	1	308	KC1	CHB-C4A-C3A	-6.68	114.48	125.03
38	13	312	KC1	CHB-C4A-C3A	-6.68	114.48	125.03
30	16	303	CLA	C2D-C1D-ND	6.68	116.74	110.13
30	10	305	CLA	CMD-C2D-C1D	6.68	136.49	124.73
39	6	318	DD6	C7-C6-C5	-6.68	112.00	122.82
30	8	305	CLA	CMD-C2D-C1D	6.67	136.48	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	317	A86	C36-C31-C32	-6.67	113.08	119.70
30	B	851	CLA	CMD-C2D-C1D	6.67	136.48	124.73
30	15	311	CLA	CMD-C2D-C1D	6.67	136.48	124.73
38	14	308	KC1	CHB-C4A-C3A	-6.67	114.50	125.03
30	4	311	CLA	CMD-C2D-C1D	6.66	136.46	124.73
30	B	839	CLA	CHD-C4C-C3C	-6.66	115.06	124.77
38	13	305	KC1	CMD-C2D-C1D	6.66	135.56	125.42
30	15	313	CLA	CMD-C2D-C1D	6.66	136.46	124.73
38	13	310	KC1	CHB-C4A-C3A	-6.66	114.51	125.03
30	14	312	CLA	CMD-C2D-C1D	6.66	136.46	124.73
30	B	816	CLA	CMD-C2D-C1D	6.66	136.45	124.73
38	8	306	KC1	CHB-C4A-C3A	-6.65	114.53	125.03
30	2	309	CLA	CMD-C2D-C1D	6.65	136.44	124.73
38	7	308	KC1	CMD-C2D-C1D	6.65	135.54	125.42
38	4	307	KC1	CHB-C4A-C3A	-6.64	114.54	125.03
39	4	313	DD6	C21-C20-C19	-6.64	106.78	114.24
38	3	308	KC1	CHB-C4A-C3A	-6.64	114.55	125.03
37	4	317	A86	C3-C2-C1	-6.64	117.97	127.28
30	A	808	CLA	CMD-C2D-C1D	6.64	136.41	124.73
30	11	304	CLA	CMD-C2D-C1D	6.63	136.41	124.73
30	14	309	CLA	CMD-C2D-C1D	6.63	136.41	124.73
37	4	317	A86	C25-C26-C27	-6.63	117.97	127.28
30	3	303	CLA	CMD-C2D-C1D	6.63	136.41	124.73
30	4	301	CLA	CMD-C2D-C1D	6.63	136.40	124.73
30	10	311	CLA	CMD-C2D-C1D	6.63	136.40	124.73
30	14	307	CLA	C2D-C1D-ND	6.63	116.69	110.13
30	5	311	CLA	O2D-CGD-CBD	6.63	122.82	111.23
30	9	301	CLA	C2D-C1D-ND	6.63	116.69	110.13
37	11	316	A86	C33-C32-C31	6.63	115.65	109.21
38	3	311	KC1	CHB-C4A-C3A	-6.63	114.56	125.03
39	6	319	DD6	C-C1-C2	-6.63	112.08	122.82
37	5	315	A86	C33-C32-C31	6.62	115.65	109.21
39	12	317	DD6	C24-C1-C2	-6.62	108.59	119.01
30	3	309	CLA	CMD-C2D-C1D	6.62	136.39	124.73
38	1	306	KC1	CHB-C4A-C3A	-6.61	114.59	125.03
30	15	303	CLA	CMD-C2D-C1D	6.61	136.36	124.73
39	8	316	DD6	C-C1-C2	-6.61	112.11	122.82
30	B	804	CLA	O2D-CGD-CBD	6.61	122.78	111.23
30	B	836	CLA	CMD-C2D-C1D	6.60	136.36	124.73
30	8	308	CLA	CMD-C2D-C1D	6.60	136.36	124.73
38	4	310	KC1	C3B-C2B-C1B	-6.60	100.80	107.05
30	B	821	CLA	CMD-C2D-C1D	6.60	136.35	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	312	CLA	CMD-C2D-C1D	6.59	136.34	124.73
39	2	315	DD6	C-C1-C24	-6.59	108.02	118.09
30	A	806	CLA	C2D-C1D-ND	6.59	116.65	110.13
30	2	301	CLA	CBC-CAC-C3C	-6.59	94.55	112.42
30	A	825	CLA	CMD-C2D-C1D	6.59	136.33	124.73
38	5	312	KC1	CHB-C4A-C3A	-6.59	114.62	125.03
39	15	318	DD6	C13-C11-C10	-6.58	108.65	119.01
30	16	309	CLA	CMD-C2D-C1D	6.58	136.32	124.73
30	15	305	CLA	CMD-C2D-C1D	6.58	136.31	124.73
39	7	318	DD6	C12-C11-C13	-6.58	108.04	118.09
30	B	818	CLA	CMD-C2D-C1D	6.58	136.31	124.73
30	7	309	CLA	CMD-C2D-C1D	6.58	136.31	124.73
30	B	831	CLA	CMD-C2D-C1D	6.58	136.31	124.73
39	8	317	DD6	C-C1-C2	-6.58	112.16	122.82
30	B	806	CLA	CMD-C2D-C1D	6.58	136.31	124.73
38	6	313	KC1	CMD-C2D-C1D	6.57	135.42	125.42
38	8	313	KC1	CHB-C4A-C3A	-6.57	114.66	125.03
30	16	301	CLA	C2D-C1D-ND	6.57	116.63	110.13
37	16	314	A86	C33-C32-C31	6.57	115.59	109.21
30	11	308	CLA	CMD-C2D-C1D	6.57	136.29	124.73
30	A	818	CLA	CMD-C2D-C1D	6.56	136.28	124.73
39	5	314	DD6	C24-C1-C2	-6.56	108.69	119.01
30	1	307	CLA	CMD-C2D-C1D	6.55	136.27	124.73
30	15	310	CLA	CMD-C2D-C1D	6.55	136.27	124.73
38	3	304	KC1	CHB-C4A-C3A	-6.55	114.69	125.03
30	7	307	CLA	C2D-C1D-ND	6.55	116.61	110.13
37	15	323	A86	C33-C32-C31	6.55	115.57	109.21
30	7	305	CLA	O2D-CGD-CBD	6.54	122.67	111.23
30	6	315	CLA	CMD-C2D-C1D	6.54	136.25	124.73
30	B	834	CLA	CHD-C4C-C3C	-6.54	115.24	124.77
30	14	303	CLA	CMD-C2D-C1D	6.53	136.24	124.73
38	10	312	KC1	CHB-C4A-C3A	-6.53	114.71	125.03
38	7	308	KC1	CHB-C4A-C3A	-6.53	114.72	125.03
30	B	801	CLA	CHD-C4C-C3C	-6.53	115.25	124.77
30	1	304	CLA	CHD-C4C-C3C	-6.52	115.26	124.77
30	16	301	CLA	CHD-C4C-C3C	-6.52	115.26	124.77
30	4	309	CLA	CMD-C2D-C1D	6.52	136.21	124.73
39	9	314	DD6	C7-C6-C8	-6.52	108.13	118.09
38	7	308	KC1	CMA-C3A-C2A	-6.51	112.67	128.43
38	7	313	KC1	C3B-C2B-C1B	-6.51	100.88	107.05
30	A	812	CLA	CMD-C2D-C1D	6.51	136.20	124.73
30	6	306	CLA	CMD-C2D-C1D	6.51	136.19	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	823	CLA	C2D-C1D-ND	6.51	116.57	110.13
30	3	305	CLA	CMD-C2D-C1D	6.51	136.19	124.73
38	14	308	KC1	CMA-C3A-C2A	-6.51	112.68	128.43
30	5	302	CLA	CMD-C2D-C1D	6.51	136.19	124.73
38	16	304	KC1	CMA-C3A-C4A	-6.50	114.87	125.03
38	16	311	KC1	C3A-C4A-NA	6.50	118.50	110.45
38	5	306	KC1	C3B-C2B-C1B	-6.50	100.90	107.05
38	14	306	KC1	CHB-C4A-C3A	-6.50	114.77	125.03
30	A	818	CLA	C2D-C1D-ND	6.49	116.55	110.13
30	13	307	CLA	CMD-C2D-C1D	6.49	136.16	124.73
30	6	316	CLA	CMD-C2D-C1D	6.49	136.16	124.73
30	5	304	CLA	CMD-C2D-C1D	6.49	136.16	124.73
38	9	310	KC1	CMD-C2D-C1D	6.49	135.30	125.42
30	B	833	CLA	CMD-C2D-C1D	6.49	136.15	124.73
38	12	309	KC1	C3B-C2B-C1B	-6.48	100.91	107.05
38	8	310	KC1	CHB-C4A-C3A	-6.48	114.80	125.03
38	2	312	KC1	CHB-C4A-C3A	-6.48	114.80	125.03
38	9	311	KC1	O2D-CGD-CBD	6.48	122.56	111.23
39	3	312	DD6	C7-C6-C5	-6.48	112.32	122.82
39	7	317	DD6	C12-C11-C13	-6.48	108.19	118.09
30	10	304	CLA	CMD-C2D-C1D	6.48	136.13	124.73
38	3	311	KC1	C1A-C2A-C3A	-6.48	101.33	107.28
30	9	308	CLA	O2D-CGD-CBD	6.47	122.54	111.23
37	9	316	A86	C33-C32-C31	6.47	115.50	109.21
37	6	320	A86	C4-C5-C6	-6.47	118.21	127.28
30	10	308	CLA	CMD-C2D-C1D	6.47	136.12	124.73
38	13	306	KC1	C1A-C2A-C3A	-6.47	101.34	107.28
37	7	315	A86	C3-C2-C1	-6.46	118.21	127.28
30	16	302	CLA	CMD-C2D-C1D	6.46	136.11	124.73
37	15	315	A86	C3-C4-C5	-6.46	110.29	123.52
30	A	833	CLA	CMD-C2D-C1D	6.46	136.11	124.73
38	3	308	KC1	CMD-C2D-C1D	6.45	135.24	125.42
39	11	313	DD6	C-C1-C24	-6.45	108.23	118.09
38	10	306	KC1	CHB-C4A-C3A	-6.45	114.85	125.03
30	A	820	CLA	CMD-C2D-C1D	6.44	136.07	124.73
30	9	305	CLA	CMD-C2D-C1D	6.44	136.07	124.73
39	7	314	DD6	C9-C10-C11	-6.44	118.24	127.28
37	11	315	A86	C4-C5-C6	-6.44	118.25	127.28
30	F	201	CLA	C2D-C1D-ND	6.44	116.50	110.13
30	A	832	CLA	O2D-CGD-CBD	6.44	122.49	111.23
38	11	307	KC1	CHB-C4A-C3A	-6.44	114.86	125.03
30	3	307	CLA	CMD-C2D-C1D	6.44	136.07	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	307	CLA	CMD-C2D-C1D	6.44	136.06	124.73
30	A	806	CLA	O2D-CGD-CBD	6.44	122.48	111.23
30	A	839	CLA	CMD-C2D-C1D	6.44	136.06	124.73
30	F	202	CLA	C2D-C1D-ND	6.43	116.49	110.13
30	15	302	CLA	O2D-CGD-CBD	6.43	122.47	111.23
30	B	825	CLA	O2D-CGD-CBD	6.43	122.47	111.23
38	6	313	KC1	CHB-C4A-C3A	-6.43	114.88	125.03
30	F	202	CLA	CMD-C2D-C1D	6.43	136.04	124.73
39	3	316	DD6	C24-C1-C2	-6.43	108.90	119.01
38	13	306	KC1	CHB-C4A-C3A	-6.42	114.89	125.03
30	9	301	CLA	CMD-C2D-C1D	6.42	136.04	124.73
38	2	314	KC1	CHB-C4A-C3A	-6.42	114.89	125.03
37	10	317	A86	C33-C32-C31	6.42	115.45	109.21
30	A	811	CLA	CMD-C2D-C1D	6.41	136.03	124.73
38	10	310	KC1	C3A-C4A-NA	6.41	118.39	110.45
38	8	311	KC1	CHB-C4A-C3A	-6.41	114.90	125.03
38	5	305	KC1	CHB-C4A-C3A	-6.41	114.91	125.03
38	9	304	KC1	CHB-C4A-C3A	-6.41	114.91	125.03
30	7	307	CLA	CMD-C2D-C1D	6.41	136.01	124.73
30	12	321	CLA	CMD-C2D-C1D	6.41	136.01	124.73
30	16	303	CLA	CMD-C2D-C1D	6.41	136.01	124.73
38	4	308	KC1	CMA-C3A-C4A	-6.41	115.02	125.03
39	3	313	DD6	C8-C6-C5	-6.40	108.94	119.01
38	8	312	KC1	CMA-C3A-C2A	-6.40	112.94	128.43
39	4	316	DD6	C-C1-C24	-6.40	108.31	118.09
39	2	316	DD6	C9-C10-C11	-6.40	118.31	127.28
38	16	311	KC1	C3B-C2B-C1B	-6.40	100.99	107.05
30	B	815	CLA	CMD-C2D-C1D	6.40	135.99	124.73
30	B	838	CLA	CMD-C2D-C1D	6.39	135.99	124.73
30	8	309	CLA	CMD-C2D-C1D	6.39	135.99	124.73
30	2	303	CLA	C2D-C1D-ND	6.39	116.45	110.13
30	1	303	CLA	CMD-C2D-C1D	6.39	135.98	124.73
30	15	306	CLA	CMD-C2D-C1D	6.39	135.98	124.73
30	A	823	CLA	CMD-C2D-C1D	6.39	135.98	124.73
30	8	305	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
30	B	839	CLA	C2D-C1D-ND	6.38	116.44	110.13
30	12	310	CLA	CMD-C2D-C1D	6.38	135.97	124.73
39	5	313	DD6	C24-C1-C2	-6.38	108.97	119.01
39	15	318	DD6	C-C1-C2	-6.38	112.48	122.82
38	11	305	KC1	CHB-C4A-C3A	-6.38	114.95	125.03
30	A	828	CLA	O2D-CGD-CBD	6.38	122.39	111.23
30	A	818	CLA	CHD-C4C-C3C	-6.38	115.47	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	310	CLA	CMD-C2D-C1D	6.38	135.96	124.73
38	8	314	KC1	C3B-C2B-C1B	-6.37	101.02	107.05
30	A	830	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
37	10	301	A86	C-C1-C24	6.37	127.82	118.09
39	15	319	DD6	C12-C11-C13	-6.37	108.36	118.09
39	7	318	DD6	C7-C6-C8	-6.37	108.36	118.09
30	11	306	CLA	CMD-C2D-C1D	6.37	135.94	124.73
39	6	321	DD6	C24-C1-C2	-6.36	109.00	119.01
30	B	815	CLA	O2D-CGD-CBD	6.36	122.35	111.23
30	1	302	CLA	CMD-C2D-C1D	6.36	135.92	124.73
30	10	303	CLA	CMD-C2D-C1D	6.36	135.92	124.73
30	16	307	CLA	CMD-C2D-C1D	6.36	135.92	124.73
30	4	303	CLA	CMD-C2D-C1D	6.35	135.92	124.73
30	7	303	CLA	C2D-C1D-ND	6.35	116.41	110.13
30	B	804	CLA	C2D-C1D-ND	6.35	116.41	110.13
38	5	306	KC1	C1A-C2A-C3A	-6.35	101.44	107.28
38	2	306	KC1	O2D-CGD-CBD	6.35	122.33	111.23
37	2u	203	A86	C33-C32-C31	6.35	115.38	109.21
30	B	822	CLA	CMD-C2D-C1D	6.34	135.90	124.73
30	10	309	CLA	CMD-C2D-C1D	6.34	135.90	124.73
30	A	838	CLA	CMD-C2D-C1D	6.34	135.89	124.73
30	A	805	CLA	O2D-CGD-CBD	6.34	122.31	111.23
30	14	305	CLA	CMD-C2D-C1D	6.34	135.89	124.73
30	B	807	CLA	CMD-C2D-C1D	6.34	135.88	124.73
38	14	306	KC1	CMD-C2D-C1D	6.33	135.06	125.42
39	2	317	DD6	C4-C5-C6	-6.33	118.40	127.28
38	9	311	KC1	CHB-C4A-C3A	-6.33	115.04	125.03
30	6	307	CLA	CMD-C2D-C1D	6.33	135.87	124.73
30	F	201	CLA	CHD-C4C-C3C	-6.32	115.55	124.77
30	B	805	CLA	CMD-C2D-C1D	6.32	135.86	124.73
30	5	311	CLA	CMD-C2D-C1D	6.32	135.86	124.73
39	7	314	DD6	C7-C6-C5	-6.32	112.58	122.82
39	6	303	DD6	C35-C36-C31	-6.31	107.37	120.50
30	A	831	CLA	O2D-CGD-O1D	-6.31	111.56	123.85
37	2u	205	A86	O4-C38-C39	6.31	122.34	111.09
38	2	306	KC1	C3B-C2B-C1B	-6.31	101.08	107.05
30	4	301	CLA	C2D-C1D-ND	6.31	116.37	110.13
30	15	314	CLA	C2D-C1D-ND	6.31	116.37	110.13
30	A	807	CLA	CMD-C2D-C1D	6.30	135.83	124.73
39	7	318	DD6	C8-C6-C5	-6.30	109.10	119.01
30	B	810	CLA	CMD-C2D-C1D	6.30	135.82	124.73
38	12	313	KC1	C3B-C2B-C1B	-6.30	101.09	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	6	312	KC1	CHB-C4A-C3A	-6.29	115.09	125.03
39	13	314	DD6	C14-C13-C11	6.29	135.29	125.53
30	B	826	CLA	C2D-C1D-ND	6.29	116.35	110.13
30	B	813	CLA	CMD-C2D-C1D	6.29	135.81	124.73
39	7	314	DD6	O1-C20-C21	-6.29	108.02	115.05
30	11	309	CLA	CMD-C2D-C1D	6.28	135.78	124.73
37	10	301	A86	C4-C5-C6	-6.27	118.48	127.28
30	13	301	CLA	C2D-C1D-ND	6.27	116.33	110.13
30	A	814	CLA	CMD-C2D-C1D	6.27	135.77	124.73
30	16	301	CLA	CMD-C2D-C1D	6.27	135.77	124.73
37	2u	203	A86	O4-C38-C39	6.27	122.27	111.09
30	A	832	CLA	CMD-C2D-C1D	6.26	135.76	124.73
30	B	834	CLA	CMD-C2D-C1D	6.26	135.75	124.73
37	15	320	A86	C4-C5-C6	-6.26	118.50	127.28
39	5	313	DD6	C7-C6-C5	-6.26	112.68	122.82
30	A	812	CLA	C2D-C1D-ND	6.25	116.31	110.13
30	F	203	CLA	CMD-C2D-C1D	6.25	135.73	124.73
30	9	307	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
30	9	308	CLA	CMD-C2D-C1D	6.25	135.73	124.73
30	2	304	CLA	O2D-CGD-CBD	6.25	122.15	111.23
30	4	306	CLA	CMD-C2D-C1D	6.24	135.72	124.73
38	6	311	KC1	C3A-C4A-NA	6.24	118.18	110.45
38	6	308	KC1	C3B-C2B-C1B	-6.24	101.14	107.05
30	4	305	CLA	CMD-C2D-C1D	6.24	135.72	124.73
38	14	306	KC1	CAC-C3C-C4C	6.24	132.91	124.79
30	5	309	CLA	CMD-C2D-C1D	6.24	135.71	124.73
30	A	819	CLA	CHD-C4C-C3C	-6.24	115.68	124.77
38	9	310	KC1	C3B-C2B-C1B	-6.24	101.15	107.05
30	B	839	CLA	C4A-NA-C1A	-6.23	103.84	106.68
38	5	306	KC1	C2B-C1B-NB	6.23	116.29	110.13
30	B	816	CLA	C2D-C1D-ND	6.23	116.29	110.13
38	11	312	KC1	C1A-C2A-C3A	-6.23	101.56	107.28
30	A	804	CLA	CMD-C2D-C1D	6.22	135.69	124.73
30	5	303	CLA	CMD-C2D-C1D	6.22	135.68	124.73
30	12	302	CLA	CMD-C2D-C1D	6.22	135.68	124.73
30	A	809	CLA	CMD-C2D-C1D	6.22	135.68	124.73
38	4	310	KC1	C3A-C4A-NA	6.21	118.14	110.45
30	1	301	CLA	CMD-C2D-C1D	6.21	135.66	124.73
30	16	309	CLA	O2D-CGD-CBD	6.21	122.08	111.23
30	2	304	CLA	CMD-C2D-C1D	6.21	135.66	124.73
30	A	842	CLA	C2D-C1D-ND	6.20	116.27	110.13
30	2	311	CLA	CMD-C2D-C1D	6.20	135.65	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	313	KC1	C2B-C1B-NB	6.20	116.26	110.13
38	12	311	KC1	C1A-C2A-C3A	-6.20	101.58	107.28
39	16	313	DD6	C9-C10-C11	-6.20	118.59	127.28
37	11	301	A86	C3-C2-C1	-6.19	118.59	127.28
38	4	308	KC1	C3B-C2B-C1B	-6.19	101.19	107.05
38	8	314	KC1	C2B-C1B-NB	6.19	116.25	110.13
30	8	301	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
30	13	301	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
30	B	817	CLA	C2D-C1D-ND	6.19	116.25	110.13
30	A	842	CLA	CHD-C4C-C3C	-6.18	115.76	124.77
30	5	307	CLA	CHD-C4C-C3C	-6.18	115.76	124.77
38	6	308	KC1	CMD-C2D-C1D	6.18	134.83	125.42
30	A	821	CLA	O2D-CGD-CBD	6.18	122.04	111.23
30	2	301	CLA	C2D-C1D-ND	6.18	116.24	110.13
39	7	318	DD6	C13-C11-C10	-6.18	109.29	119.01
38	8	306	KC1	CMA-C3A-C2A	-6.18	113.47	128.43
39	1	310	DD6	C12-C11-C13	-6.18	108.65	118.09
39	6	319	DD6	C7-C6-C5	-6.17	112.81	122.82
30	B	807	CLA	C2D-C1D-ND	6.17	116.23	110.13
30	A	804	CLA	C2D-C1D-ND	6.17	116.23	110.13
37	1	309	A86	C4-C3-C2	-6.17	110.90	123.52
30	7	304	CLA	CMD-C2D-C1D	6.17	135.59	124.73
38	16	304	KC1	C1A-C2A-C3A	-6.17	101.61	107.28
30	12	307	CLA	CHD-C4C-C3C	-6.17	115.78	124.77
38	13	310	KC1	C3B-C2B-C1B	-6.17	101.21	107.05
30	15	302	CLA	C2D-C1D-ND	6.17	116.23	110.13
30	B	802	CLA	O2D-CGD-CBD	6.16	122.00	111.23
38	12	309	KC1	C3A-C4A-NA	6.16	118.08	110.45
30	B	804	CLA	CMD-C2D-C1D	6.15	135.57	124.73
30	A	837	CLA	O2D-CGD-CBD	6.15	121.98	111.23
38	2	314	KC1	C1A-C2A-C3A	-6.15	101.63	107.28
30	8	303	CLA	O2D-CGD-CBD	6.15	121.98	111.23
30	B	820	CLA	CMD-C2D-C1D	6.15	135.55	124.73
39	11	313	DD6	C24-C1-C2	-6.14	109.34	119.01
30	B	817	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
30	A	811	CLA	C2D-C1D-ND	6.14	116.20	110.13
30	A	807	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
38	8	306	KC1	C1A-C2A-C3A	-6.14	101.64	107.28
30	5	307	CLA	CMD-C2D-C1D	6.14	135.54	124.73
38	9	312	KC1	CHB-C4A-C3A	-6.14	115.34	125.03
30	A	841	CLA	CMD-C2D-C1D	6.14	135.54	124.73
30	10	307	CLA	C2D-C1D-ND	6.14	116.20	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2u	202	CLA	CHD-C4C-C3C	-6.14	115.83	124.77
30	A	808	CLA	C2D-C1D-ND	6.14	116.20	110.13
30	A	816	CLA	CMD-C2D-C1D	6.14	135.53	124.73
38	8	313	KC1	C3B-C2B-C1B	-6.13	101.24	107.05
30	5	307	CLA	C2D-C1D-ND	6.13	116.20	110.13
37	11	301	A86	C7-C6-C8	6.13	127.46	118.09
30	8	302	CLA	C2D-C1D-ND	6.13	116.19	110.13
39	7	314	DD6	O1-C15-C14	-6.13	99.31	116.88
30	A	805	CLA	CMD-C2D-C1D	6.13	135.52	124.73
30	A	813	CLA	CMD-C2D-C1D	6.13	135.52	124.73
30	A	828	CLA	CMD-C2D-C1D	6.13	135.52	124.73
30	B	806	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
30	A	804	CLA	O2D-CGD-CBD	6.13	121.94	111.23
30	3	306	CLA	CMD-C2D-C1D	6.12	135.51	124.73
30	B	825	CLA	CHD-C4C-C3C	-6.12	115.84	124.77
30	2	310	CLA	CMD-C2D-C1D	6.12	135.51	124.73
30	7	307	CLA	CHD-C4C-C3C	-6.12	115.85	124.77
39	2	316	DD6	C4-C5-C6	-6.12	118.70	127.28
30	A	816	CLA	C2D-C1D-ND	6.11	116.18	110.13
30	1	303	CLA	C2D-C1D-ND	6.11	116.17	110.13
30	A	810	CLA	C2D-C1D-ND	6.11	116.17	110.13
30	8	301	CLA	C2D-C1D-ND	6.10	116.17	110.13
30	9	307	CLA	C2D-C1D-ND	6.10	116.17	110.13
38	4	307	KC1	C3B-C2B-C1B	-6.10	101.28	107.05
39	3	312	DD6	C8-C6-C5	-6.09	109.43	119.01
30	A	817	CLA	C2D-C1D-ND	6.09	116.15	110.13
37	10	315	A86	C3-C2-C1	-6.09	118.74	127.28
30	L	202	CLA	CMD-C2D-C1D	6.08	135.44	124.73
30	12	308	CLA	CMD-C2D-C1D	6.08	135.44	124.73
38	11	311	KC1	C3B-C2B-C1B	-6.08	101.29	107.05
39	2	315	DD6	C35-C36-C31	-6.08	107.84	120.50
30	A	838	CLA	O2D-CGD-CBD	6.08	121.86	111.23
38	14	311	KC1	C3A-C4A-NA	6.08	117.97	110.45
30	9	308	CLA	C2D-C1D-ND	6.08	116.14	110.13
38	8	307	KC1	C3B-C2B-C1B	-6.08	101.30	107.05
38	13	308	KC1	C3A-C4A-NA	6.07	117.97	110.45
30	11	304	CLA	C2D-C1D-ND	6.07	116.14	110.13
30	A	819	CLA	C2D-C1D-ND	6.07	116.14	110.13
30	12	303	CLA	CMD-C2D-C1D	6.07	135.42	124.73
30	A	813	CLA	C2D-C1D-ND	6.07	116.13	110.13
38	5	305	KC1	C1A-C2A-C3A	-6.07	101.70	107.28
30	A	838	CLA	CHD-C4C-C3C	-6.07	115.93	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	311	CLA	C2D-C1D-ND	6.07	116.13	110.13
30	5	308	CLA	C2D-C1D-ND	6.07	116.13	110.13
38	2	314	KC1	C3B-C2B-C1B	-6.06	101.31	107.05
38	8	313	KC1	CMD-C2D-C1D	6.06	134.65	125.42
30	3	309	CLA	C2D-C1D-ND	6.06	116.13	110.13
38	12	305	KC1	C3B-C2B-C1B	-6.06	101.31	107.05
38	16	304	KC1	C3B-C2B-C1B	-6.06	101.32	107.05
30	5	311	CLA	C2D-C1D-ND	6.05	116.12	110.13
30	A	842	CLA	CMD-C2D-C1D	6.05	135.38	124.73
30	B	829	CLA	CMD-C2D-C1D	6.05	135.38	124.73
30	3	301	CLA	C2D-C1D-ND	6.05	116.11	110.13
30	2	308	CLA	C2D-C1D-ND	6.05	116.11	110.13
37	8	315	A86	O4-C38-C39	6.05	121.87	111.09
38	6	312	KC1	C1A-C2A-C3A	-6.05	101.72	107.28
39	6	321	DD6	C7-C6-C8	-6.05	108.85	118.09
30	A	824	CLA	CHD-C4C-C3C	-6.04	115.96	124.77
30	3	302	CLA	CHD-C4C-C3C	-6.04	115.96	124.77
38	4	308	KC1	C3A-C4A-NA	6.04	117.93	110.45
38	5	310	KC1	C3A-C4A-NA	6.04	117.93	110.45
38	6	308	KC1	C1A-C2A-C3A	-6.04	101.73	107.28
30	A	829	CLA	C2D-C1D-ND	6.04	116.10	110.13
30	B	825	CLA	C2D-C1D-ND	6.04	116.10	110.13
39	6	319	DD6	C8-C6-C5	-6.04	109.51	119.01
38	8	313	KC1	C3A-C4A-NA	6.04	117.92	110.45
30	2u	202	CLA	CMD-C2D-C1D	6.03	135.35	124.73
38	13	310	KC1	C1A-C2A-C3A	-6.03	101.73	107.28
30	7	303	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
38	6	308	KC1	C3A-C4A-NA	6.03	117.92	110.45
38	9	310	KC1	C3A-C4A-NA	6.03	117.91	110.45
38	4	310	KC1	C2B-C1B-NB	6.03	116.09	110.13
30	1	303	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
38	11	311	KC1	C3A-C4A-NA	6.03	117.91	110.45
30	B	826	CLA	CHD-C4C-C3C	-6.03	115.99	124.77
30	3	305	CLA	C2D-C1D-ND	6.02	116.09	110.13
30	5	302	CLA	CHD-C4C-C3C	-6.02	115.99	124.77
39	9	314	DD6	C12-C11-C13	-6.02	108.89	118.09
30	2	308	CLA	CMD-C2D-C1D	6.02	135.32	124.73
30	1	304	CLA	C2D-C1D-ND	6.02	116.08	110.13
38	14	306	KC1	C3A-C4A-NA	6.01	117.89	110.45
30	2	311	CLA	C2D-C1D-ND	6.01	116.08	110.13
38	11	307	KC1	C3B-C2B-C1B	-6.01	101.36	107.05
30	A	826	CLA	CMD-C2D-C1D	6.01	135.31	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	311	CLA	C2D-C1D-ND	6.01	116.07	110.13
38	10	312	KC1	C3A-C4A-NA	6.01	117.89	110.45
30	L	203	CLA	C2D-C1D-ND	6.01	116.07	110.13
30	2	301	CLA	C2C-C1C-NC	6.01	116.29	109.98
30	9	302	CLA	C2D-C1D-ND	6.01	116.07	110.13
38	9	304	KC1	C3B-C2B-C1B	-6.01	101.36	107.05
30	B	801	CLA	C2D-C1D-ND	6.00	116.07	110.13
30	10	307	CLA	CHD-C4C-C3C	-6.00	116.02	124.77
38	1	308	KC1	C1A-C2A-C3A	-6.00	101.77	107.28
38	8	307	KC1	C1A-C2A-C3A	-6.00	101.77	107.28
39	4	313	DD6	C12-C11-C13	-6.00	108.93	118.09
38	1	306	KC1	C3A-C4A-NA	6.00	117.87	110.45
30	15	303	CLA	C2D-C1D-ND	5.99	116.06	110.13
38	13	310	KC1	C3A-C4A-NA	5.99	117.87	110.45
38	14	306	KC1	O2D-CGD-CBD	5.99	121.71	111.23
30	A	809	CLA	C2D-C1D-ND	5.99	116.06	110.13
38	3	304	KC1	C1A-C2A-C3A	-5.99	101.77	107.28
30	A	823	CLA	O2D-CGD-CBD	5.99	121.70	111.23
30	4	305	CLA	C2D-C1D-ND	5.99	116.05	110.13
38	4	307	KC1	CMA-C3A-C2A	-5.99	113.94	128.43
39	12	315	DD6	C-C1-C24	-5.98	108.95	118.09
39	7	302	DD6	C13-C11-C10	-5.98	109.60	119.01
37	10	315	A86	C25-C26-C27	-5.98	118.89	127.28
30	B	833	CLA	C2D-C1D-ND	5.98	116.05	110.13
30	6	306	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
30	A	805	CLA	C2D-C1D-ND	5.98	116.05	110.13
39	16	313	DD6	C-C1-C24	-5.98	108.95	118.09
30	F	202	CLA	CHD-C4C-C3C	-5.98	116.06	124.77
30	10	309	CLA	C2D-C1D-ND	5.98	116.04	110.13
30	9	303	CLA	CMD-C2D-C1D	5.98	135.25	124.73
30	4	306	CLA	C2D-C1D-ND	5.98	116.04	110.13
30	2	308	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
30	4	303	CLA	C2D-C1D-ND	5.97	116.04	110.13
30	13	302	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
30	16	303	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
30	7	311	CLA	CMD-C2D-C1D	5.97	135.25	124.73
30	A	803	CLA	C2B-C1B-NB	5.97	116.52	110.33
37	5	315	A86	C25-C26-C27	-5.97	118.91	127.28
30	A	833	CLA	C2D-C1D-ND	5.97	116.03	110.13
37	11	301	A86	C4-C5-C6	-5.97	118.91	127.28
38	1	308	KC1	CMD-C2D-C1D	5.97	134.50	125.42
30	2u	202	CLA	C2D-C1D-ND	5.97	116.03	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	301	CLA	CMD-C2D-C1D	5.96	135.23	124.73
30	2	303	CLA	C2B-C1B-NB	5.96	116.51	110.33
30	A	840	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
30	A	826	CLA	C2D-C1D-ND	5.96	116.02	110.13
30	B	814	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
37	11	316	A86	O4-C38-C39	5.96	121.71	111.09
30	7	305	CLA	C2D-C1D-ND	5.95	116.02	110.13
38	14	308	KC1	CMD-C2D-C1D	5.95	134.48	125.42
38	7	308	KC1	C3A-C4A-NA	5.95	117.81	110.45
30	3	302	CLA	C2D-C1D-ND	5.95	116.01	110.13
30	15	302	CLA	C4A-NA-C1A	-5.95	103.97	106.68
30	13	303	CLA	O2D-CGD-CBD	5.95	121.62	111.23
30	B	816	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
39	10	314	DD6	C-C1-C24	-5.94	109.01	118.09
30	B	827	CLA	C2D-C1D-ND	5.94	116.01	110.13
30	9	305	CLA	C2D-C1D-ND	5.94	116.01	110.13
30	15	308	CLA	C2D-C1D-ND	5.94	116.00	110.13
38	3	311	KC1	C3B-C2B-C1B	-5.94	101.43	107.05
39	15	318	DD6	C12-C11-C13	-5.94	109.02	118.09
39	3	313	DD6	C7-C6-C8	-5.94	109.02	118.09
38	10	310	KC1	C1A-NA-C4A	-5.94	103.97	106.68
30	15	304	CLA	C2D-C1D-ND	5.94	116.00	110.13
30	B	808	CLA	O2D-CGD-CBD	5.93	121.60	111.23
30	A	834	CLA	C2D-C1D-ND	5.93	116.00	110.13
30	3	305	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
30	B	810	CLA	C2D-C1D-ND	5.93	116.00	110.13
39	5	313	DD6	C8-C6-C5	-5.93	109.68	119.01
30	12	303	CLA	CHD-C4C-C3C	-5.93	116.13	124.77
30	13	302	CLA	C2D-C1D-ND	5.93	115.99	110.13
30	A	841	CLA	C2B-C1B-NB	5.93	116.47	110.33
39	4	313	DD6	C-C1-C24	-5.93	109.04	118.09
30	2	309	CLA	C2D-C1D-ND	5.92	115.99	110.13
30	A	829	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
38	12	309	KC1	C2B-C1B-NB	5.92	115.99	110.13
38	13	308	KC1	O2D-CGD-CBD	5.92	121.58	111.23
30	15	309	CLA	C2D-C1D-ND	5.92	115.98	110.13
30	9	303	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
30	2	305	CLA	C2D-C1D-ND	5.92	115.98	110.13
39	4	316	DD6	C7-C6-C8	-5.92	109.05	118.09
38	9	310	KC1	C1A-C2A-C3A	-5.92	101.84	107.28
30	B	810	CLA	CHD-C4C-C3C	-5.92	116.15	124.77
38	1	308	KC1	C3A-C4A-NA	5.92	117.77	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	302	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
39	2	317	DD6	C35-C36-C31	-5.91	108.20	120.50
38	14	306	KC1	C1A-C2A-C3A	-5.91	101.85	107.28
39	6	303	DD6	C-C1-C24	-5.91	109.06	118.09
30	11	306	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
30	A	813	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
30	B	837	CLA	C2D-C1D-ND	5.91	115.97	110.13
30	5	304	CLA	C2D-C1D-ND	5.91	115.97	110.13
30	16	302	CLA	C2D-C1D-ND	5.90	115.97	110.13
30	13	302	CLA	CMD-C2D-C1D	5.90	135.12	124.73
30	F	203	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
30	B	831	CLA	C2D-C1D-ND	5.90	115.97	110.13
30	1	307	CLA	C2D-C1D-ND	5.90	115.97	110.13
39	16	313	DD6	C24-C1-C2	-5.90	109.73	119.01
38	4	310	KC1	C1A-C2A-C3A	-5.90	101.86	107.28
30	12	310	CLA	C2D-C1D-ND	5.90	115.96	110.13
30	4	302	CLA	C2D-C1D-ND	5.90	115.96	110.13
30	A	834	CLA	CHD-C4C-C3C	-5.90	116.18	124.77
38	10	306	KC1	C1A-C2A-C3A	-5.90	101.86	107.28
30	B	829	CLA	O2D-CGD-CBD	5.90	121.54	111.23
30	14	313	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
38	3	308	KC1	C3A-C4A-NA	5.89	117.74	110.45
30	B	806	CLA	C2D-C1D-ND	5.89	115.96	110.13
30	2	303	CLA	C3D-C4D-ND	5.89	119.56	109.99
30	A	808	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
30	16	302	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
30	A	807	CLA	CAA-C2A-C3A	-5.89	97.09	113.00
30	F	203	CLA	C2D-C1D-ND	5.89	115.95	110.13
30	5	303	CLA	C2D-C1D-ND	5.89	115.95	110.13
38	7	313	KC1	C1A-C2A-C3A	-5.89	101.87	107.28
38	13	305	KC1	C3A-C4A-NA	5.88	117.73	110.45
30	15	311	CLA	C2D-C1D-ND	5.88	115.95	110.13
38	10	312	KC1	C1A-C2A-C3A	-5.88	101.87	107.28
38	2	312	KC1	C3B-C2B-C1B	-5.88	101.48	107.05
38	5	305	KC1	C3B-C2B-C1B	-5.88	101.48	107.05
30	9	305	CLA	CHD-C4C-C3C	-5.88	116.20	124.77
39	15	319	DD6	C7-C6-C8	-5.88	109.10	118.09
30	9	308	CLA	CHD-C4C-C3C	-5.88	116.20	124.77
38	2	306	KC1	C3A-C4A-NA	5.88	117.73	110.45
38	14	308	KC1	C3A-C4A-NA	5.88	117.73	110.45
30	6	315	CLA	C2D-C1D-ND	5.88	115.94	110.13
30	8	302	CLA	CHD-C4C-C3C	-5.88	116.20	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	809	CLA	C2D-C1D-ND	5.88	115.94	110.13
30	A	805	CLA	C2B-C1B-NB	5.88	116.42	110.33
30	14	313	CLA	O2D-CGD-CBD	5.87	121.50	111.23
30	6	317	CLA	C2D-C1D-ND	5.87	115.94	110.13
30	15	303	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
38	6	313	KC1	C3B-C2B-C1B	-5.87	101.49	107.05
30	A	822	CLA	CMD-C2D-C1D	5.87	135.07	124.73
38	10	310	KC1	C2B-C1B-NB	5.87	115.94	110.13
38	2	312	KC1	C1A-C2A-C3A	-5.87	101.88	107.28
30	A	802	CLA	C4A-NA-C1A	-5.87	104.00	106.68
38	4	307	KC1	C2B-C1B-NB	5.87	115.94	110.13
30	9	309	CLA	CMD-C2D-C1D	5.87	135.06	124.73
30	10	311	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
30	B	811	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
38	16	311	KC1	C2B-C1B-NB	5.87	115.93	110.13
39	9	314	DD6	C24-C1-C2	-5.86	109.79	119.01
30	8	308	CLA	C2D-C1D-ND	5.86	115.93	110.13
38	13	312	KC1	C3A-C4A-NA	5.86	117.70	110.45
38	8	311	KC1	C1A-C2A-C3A	-5.86	101.89	107.28
30	15	313	CLA	C2D-C1D-ND	5.86	115.92	110.13
38	4	307	KC1	C3A-C4A-NA	5.86	117.70	110.45
30	A	840	CLA	O2D-CGD-CBD	5.86	121.47	111.23
30	16	305	CLA	C2D-C1D-ND	5.86	115.92	110.13
38	6	311	KC1	C1A-C2A-C3A	-5.86	101.90	107.28
39	13	314	DD6	C21-C20-C19	-5.86	107.66	114.24
30	2	313	CLA	C2D-C1D-ND	5.86	115.92	110.13
30	13	304	CLA	C2D-C1D-ND	5.86	115.92	110.13
38	14	311	KC1	C3B-C2B-C1B	-5.85	101.51	107.05
30	A	831	CLA	C2D-C1D-ND	5.85	115.92	110.13
30	A	804	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
30	B	812	CLA	CMD-C2D-C1D	5.85	135.03	124.73
30	12	310	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
30	15	307	CLA	CMD-C2D-C1D	5.85	135.03	124.73
30	7	304	CLA	C2D-C1D-ND	5.85	115.92	110.13
39	10	313	DD6	C21-C20-C19	-5.85	107.67	114.24
30	12	312	CLA	C2D-C1D-ND	5.85	115.91	110.13
39	2	315	DD6	C13-C11-C10	-5.85	109.81	119.01
30	7	309	CLA	C2D-C1D-ND	5.85	115.91	110.13
38	5	310	KC1	C1A-C2A-C3A	-5.85	101.91	107.28
30	B	822	CLA	C2D-C1D-ND	5.85	115.91	110.13
30	13	303	CLA	C2D-C1D-ND	5.85	115.91	110.13
30	B	826	CLA	CMD-C2D-C1D	5.84	135.02	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	3	314	A86	C25-C26-C27	-5.84	119.08	127.28
30	16	309	CLA	C2D-C1D-ND	5.84	115.91	110.13
38	8	311	KC1	C3B-C2B-C1B	-5.84	101.52	107.05
39	13	314	DD6	C24-C1-C2	-5.84	109.82	119.01
30	A	816	CLA	O2D-CGD-CBD	5.84	121.44	111.23
30	9	303	CLA	C2D-C1D-ND	5.84	115.91	110.13
38	5	312	KC1	C3A-C4A-NA	5.84	117.68	110.45
38	8	306	KC1	C3B-C2B-C1B	-5.84	101.52	107.05
30	B	802	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
30	8	304	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
30	2u	202	CLA	O2D-CGD-CBD	5.83	121.43	111.23
30	4	301	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
30	A	807	CLA	C2D-C1D-ND	5.83	115.90	110.13
30	12	308	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
38	3	304	KC1	C3B-C2B-C1B	-5.83	101.53	107.05
30	14	310	CLA	C2D-C1D-ND	5.83	115.89	110.13
38	12	311	KC1	C3A-C4A-NA	5.83	117.66	110.45
38	12	305	KC1	C3A-C4A-NA	5.82	117.66	110.45
30	B	814	CLA	O2D-CGD-CBD	5.82	121.41	111.23
39	6	318	DD6	C-C1-C24	-5.82	109.20	118.09
39	13	314	DD6	C-C1-C24	-5.82	109.20	118.09
30	A	830	CLA	C2D-C1D-ND	5.82	115.89	110.13
30	5	309	CLA	C2D-C1D-ND	5.82	115.89	110.13
30	15	310	CLA	C2D-C1D-ND	5.82	115.89	110.13
30	7	306	CLA	C2D-C1D-ND	5.82	115.88	110.13
37	14	320	A86	C4-C3-C2	-5.82	111.61	123.52
30	10	304	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
30	B	824	CLA	O2D-CGD-CBD	5.82	121.40	111.23
30	B	813	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
30	16	305	CLA	CMD-C2D-C1D	5.82	134.97	124.73
38	14	308	KC1	O2D-CGD-CBD	5.82	121.40	111.23
30	B	805	CLA	C2D-C1D-ND	5.81	115.88	110.13
37	11	315	A86	O4-C38-C39	5.81	121.46	111.09
38	6	311	KC1	C3B-C2B-C1B	-5.81	101.55	107.05
30	A	843	CLA	CMD-C2D-C1D	5.81	134.96	124.73
30	16	308	CLA	C2D-C1D-ND	5.81	115.88	110.13
30	14	302	CLA	O2D-CGD-CBD	5.81	121.39	111.23
30	B	815	CLA	C2D-C1D-ND	5.81	115.87	110.13
30	9	306	CLA	C2C-C1C-NC	5.81	116.08	109.98
30	B	838	CLA	C2D-C1D-ND	5.81	115.87	110.13
30	4	304	CLA	CHD-C4C-C3C	-5.81	116.31	124.77
30	12	307	CLA	C2D-C1D-ND	5.81	115.87	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	310	CLA	C2D-C1D-ND	5.80	115.87	110.13
30	3	302	CLA	CMD-C2D-C1D	5.80	134.95	124.73
30	13	307	CLA	O2D-CGD-CBD	5.80	121.38	111.23
38	12	313	KC1	C2D-C1D-ND	5.80	116.34	110.33
30	A	839	CLA	C2D-C1D-ND	5.80	115.87	110.13
30	15	306	CLA	C2D-C1D-ND	5.80	115.87	110.13
30	B	837	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
30	A	814	CLA	C2D-C1D-ND	5.80	115.87	110.13
30	12	302	CLA	C2D-C1D-ND	5.80	115.87	110.13
37	13	315	A86	C3-C2-C1	-5.80	119.14	127.28
30	B	803	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
30	2	301	CLA	CMD-C2D-C1D	5.80	134.94	124.73
30	16	310	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
30	15	312	CLA	O2D-CGD-CBD	5.80	121.36	111.23
30	12	302	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
38	12	311	KC1	C2B-C1B-NB	5.80	115.86	110.13
38	13	312	KC1	C1A-C2A-C3A	-5.80	101.95	107.28
39	10	313	DD6	C24-C1-C2	-5.79	109.90	119.01
30	B	834	CLA	O2D-CGD-CBD	5.79	121.36	111.23
39	9	314	DD6	C9-C10-C11	-5.79	119.15	127.28
30	5	303	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
38	13	311	KC1	C1A-C2A-C3A	-5.79	101.96	107.28
30	13	309	CLA	C2D-C1D-ND	5.79	115.86	110.13
39	5	313	DD6	C12-C11-C13	-5.79	109.24	118.09
38	13	311	KC1	CHB-C4A-C3A	-5.79	115.89	125.03
37	9	313	A86	C33-C32-C31	5.79	114.84	109.21
37	8	318	A86	C10-C9-C8	-5.79	106.43	123.20
38	13	308	KC1	C3B-C2B-C1B	-5.79	101.57	107.05
30	B	823	CLA	CHD-C4C-C3C	-5.79	116.34	124.77
30	6	306	CLA	C2D-C1D-ND	5.79	115.85	110.13
38	9	311	KC1	C3B-C2B-C1B	-5.78	101.57	107.05
39	12	315	DD6	C12-C11-C13	-5.78	109.25	118.09
30	B	839	CLA	C2B-C1B-NB	5.78	116.33	110.33
30	6	315	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
39	9	314	DD6	O1-C20-C21	-5.78	108.59	115.05
38	13	305	KC1	C2B-C1B-NB	5.78	115.85	110.13
30	8	308	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
30	B	838	CLA	C2C-C1C-NC	5.78	116.05	109.98
30	2	301	CLA	O2D-CGD-CBD	5.78	121.33	111.23
38	8	307	KC1	C3A-C4A-NA	5.78	117.60	110.45
38	4	308	KC1	C2B-C1B-NB	5.78	115.84	110.13
37	14	319	A86	O4-C38-C39	5.78	121.39	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	304	CLA	C2D-C1D-ND	5.78	115.84	110.13
39	3	316	DD6	C8-C6-C5	-5.77	109.93	119.01
30	12	308	CLA	C2D-C1D-ND	5.77	115.84	110.13
30	15	307	CLA	C2D-C1D-ND	5.77	115.84	110.13
37	9	313	A86	O4-C38-C39	5.77	121.38	111.09
30	B	835	CLA	C2D-C1D-ND	5.77	115.83	110.13
30	B	831	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
30	1	307	CLA	O2D-CGD-CBD	5.77	121.31	111.23
30	B	805	CLA	C2B-C1B-NB	5.77	116.31	110.33
30	B	804	CLA	CHD-C4C-C3C	-5.77	116.37	124.77
30	A	829	CLA	C2B-C1B-NB	5.77	116.31	110.33
30	A	832	CLA	CHD-C4C-C3C	-5.77	116.37	124.77
30	16	306	CLA	CMD-C2D-C1D	5.76	134.88	124.73
30	B	836	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
39	8	316	DD6	C24-C1-C2	-5.76	109.94	119.01
30	2	310	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
30	A	829	CLA	C3B-C2B-C1B	-5.76	100.38	107.17
37	15	322	A86	C4-C3-C2	-5.76	111.73	123.52
37	2u	205	A86	C25-C26-C27	-5.76	119.20	127.28
37	2	319	A86	C4-C5-C6	-5.76	119.20	127.28
30	13	309	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
38	13	305	KC1	O2D-CGD-CBD	5.76	121.29	111.23
37	16	314	A86	C25-C26-C27	-5.76	119.20	127.28
39	6	303	DD6	C4-C5-C6	-5.75	119.21	127.28
30	1	302	CLA	C2D-C1D-ND	5.75	115.82	110.13
30	12	321	CLA	C2D-C1D-ND	5.75	115.82	110.13
30	10	307	CLA	CMD-C2D-C1D	5.75	134.86	124.73
30	11	306	CLA	C2D-C1D-ND	5.75	115.82	110.13
37	14	320	A86	O4-C38-C39	5.75	121.34	111.09
30	7	305	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
30	6	304	CLA	C2D-C1D-ND	5.75	115.81	110.13
38	13	312	KC1	C3B-C2B-C1B	-5.75	101.61	107.05
30	3	307	CLA	C2D-C1D-ND	5.75	115.81	110.13
38	3	308	KC1	C3B-C2B-C1B	-5.75	101.61	107.05
30	B	834	CLA	C2D-C1D-ND	5.75	115.81	110.13
30	10	305	CLA	O2D-CGD-CBD	5.75	121.28	111.23
30	A	840	CLA	C2D-C1D-ND	5.75	115.81	110.13
30	5	304	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
38	12	311	KC1	C3B-C2B-C1B	-5.74	101.61	107.05
38	8	311	KC1	C2D-C1D-ND	5.74	116.28	110.33
37	14	317	A86	C41-C32-C31	-5.74	105.33	110.47
30	15	305	CLA	C2D-C1D-ND	5.74	115.81	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	304	CLA	C2D-C1D-ND	5.74	115.81	110.13
30	12	303	CLA	C2D-C1D-ND	5.74	115.81	110.13
30	B	807	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
30	15	305	CLA	O2D-CGD-CBD	5.74	121.26	111.23
30	A	805	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
39	9	314	DD6	C-C1-C24	-5.74	109.33	118.09
30	2	304	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
30	10	305	CLA	C2D-C1D-ND	5.73	115.80	110.13
38	7	313	KC1	C3A-C4A-NA	5.73	117.55	110.45
38	9	304	KC1	C3A-C4A-NA	5.73	117.55	110.45
38	7	313	KC1	C2B-C1B-NB	5.73	115.80	110.13
38	10	312	KC1	C3B-C2B-C1B	-5.73	101.62	107.05
30	A	816	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
30	11	308	CLA	C2D-C1D-ND	5.73	115.80	110.13
39	5	314	DD6	C12-C11-C13	-5.73	109.34	118.09
37	10	302	A86	C7-C6-C8	5.73	126.83	118.09
38	14	308	KC1	C3B-C2B-C1B	-5.72	101.63	107.05
30	B	813	CLA	C2D-C1D-ND	5.72	115.79	110.13
30	1	301	CLA	C2D-C1D-ND	5.72	115.79	110.13
30	7	311	CLA	C2D-C1D-ND	5.72	115.79	110.13
38	8	313	KC1	C2D-C1D-ND	5.72	116.25	110.33
30	B	839	CLA	CMD-C2D-C1D	5.72	134.79	124.73
37	2u	205	A86	C4-C3-C2	-5.71	111.83	123.52
38	5	306	KC1	C3A-C4A-NA	5.71	117.52	110.45
39	12	317	DD6	C-C1-C24	-5.71	109.37	118.09
30	1	302	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
30	10	303	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
30	B	810	CLA	O2D-CGD-CBD	5.71	121.21	111.23
30	14	303	CLA	C2B-C1B-NB	5.71	116.24	110.33
30	A	811	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
30	A	841	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
38	16	304	KC1	C3A-C4A-NA	5.71	117.51	110.45
30	14	313	CLA	C2D-C1D-ND	5.70	115.77	110.13
30	B	832	CLA	C2D-C1D-ND	5.70	115.77	110.13
30	15	313	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
30	4	306	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
30	B	836	CLA	O2D-CGD-CBD	5.70	121.19	111.23
38	14	308	KC1	C2B-C1B-NB	5.70	115.77	110.13
30	8	304	CLA	C2D-C1D-ND	5.70	115.76	110.13
30	3	309	CLA	CHD-C4C-C3C	-5.70	116.47	124.77
30	B	818	CLA	O2D-CGD-CBD	5.70	121.19	111.23
30	6	314	CLA	O2D-CGD-CBD	5.69	121.18	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	9	312	KC1	C1A-C2A-C3A	-5.69	102.05	107.28
38	6	313	KC1	C3A-C4A-NA	5.69	117.50	110.45
30	L	203	CLA	CHD-C4C-C3C	-5.69	116.47	124.77
38	9	310	KC1	C2B-C1B-NB	5.69	115.75	110.13
38	8	310	KC1	C3A-C4A-NA	5.69	117.49	110.45
30	B	827	CLA	CHD-C4C-C3C	-5.68	116.48	124.77
30	B	835	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
30	8	301	CLA	C3B-C2B-C1B	-5.68	100.47	107.17
38	10	310	KC1	C1A-C2A-C3A	-5.68	102.06	107.28
30	B	833	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
30	10	305	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
30	2	304	CLA	C2D-C1D-ND	5.68	115.75	110.13
30	B	818	CLA	CHD-C4C-C3C	-5.68	116.50	124.77
38	13	308	KC1	C2B-C1B-NB	5.68	115.74	110.13
30	7	310	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
38	11	307	KC1	C3A-C4A-NA	5.67	117.47	110.45
30	A	826	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
38	9	312	KC1	C3B-C2B-C1B	-5.67	101.68	107.05
30	3	309	CLA	O2D-CGD-CBD	5.67	121.14	111.23
30	12	306	CLA	CMD-C2D-C1D	5.67	134.71	124.73
38	16	304	KC1	C2B-C1B-NB	5.67	115.74	110.13
37	14	314	A86	C8-C6-C5	5.67	127.93	119.01
39	2	316	DD6	C24-C1-C2	-5.67	110.09	119.01
30	16	310	CLA	C2D-C1D-ND	5.67	115.73	110.13
30	12	312	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
30	14	312	CLA	C2D-C1D-ND	5.66	115.73	110.13
30	7	310	CLA	C2D-C1D-ND	5.66	115.73	110.13
30	15	302	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
30	6	317	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
39	4	316	DD6	O1-C20-C21	-5.66	108.72	115.05
30	15	311	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
37	10	302	A86	O4-C38-C39	5.66	121.18	111.09
30	5	308	CLA	O2D-CGD-CBD	5.65	121.12	111.23
38	3	308	KC1	O2D-CGD-CBD	5.65	121.11	111.23
38	11	305	KC1	C1A-C2A-C3A	-5.65	102.08	107.28
38	8	310	KC1	C2D-C1D-ND	5.65	116.19	110.33
30	B	826	CLA	O2D-CGD-CBD	5.65	121.11	111.23
30	11	309	CLA	O2D-CGD-CBD	5.65	121.11	111.23
30	9	306	CLA	C2D-C1D-ND	5.65	115.72	110.13
30	6	309	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
30	15	312	CLA	CBA-CAA-C2A	-5.65	96.99	113.79
30	15	304	CLA	C2B-C1B-NB	5.64	116.18	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	821	CLA	C2C-C1C-NC	5.64	115.91	109.98
38	13	306	KC1	C3A-C4A-NA	5.64	117.44	110.45
30	B	829	CLA	C2D-C1D-ND	5.64	115.71	110.13
38	2	306	KC1	C2B-C1B-NB	5.64	115.71	110.13
38	3	311	KC1	C2B-C1B-NB	5.64	115.71	110.13
30	8	303	CLA	C2D-C1D-ND	5.64	115.71	110.13
30	2	313	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
38	11	305	KC1	C3A-C4A-NA	5.64	117.43	110.45
30	5	302	CLA	C2D-C1D-ND	5.64	115.70	110.13
38	13	305	KC1	C3B-C2B-C1B	-5.64	101.71	107.05
38	5	310	KC1	O2D-CGD-CBD	5.64	121.08	111.23
30	14	303	CLA	C2D-C1D-ND	5.64	115.70	110.13
38	9	311	KC1	C3A-C4A-NA	5.64	117.43	110.45
37	4	312	A86	O4-C38-C39	5.63	121.14	111.09
38	8	310	KC1	C3B-C2B-C1B	-5.63	101.72	107.05
30	3	306	CLA	C2B-C1B-NB	5.63	116.17	110.33
38	9	310	KC1	O2D-CGD-CBD	5.63	121.07	111.23
30	A	832	CLA	C2D-C1D-ND	5.63	115.70	110.13
37	4	314	A86	O4-C38-C39	5.63	121.13	111.09
39	4	313	DD6	C7-C6-C5	-5.63	113.70	122.82
30	10	303	CLA	C2D-C1D-ND	5.63	115.70	110.13
39	5	313	DD6	C-C1-C24	-5.63	109.49	118.09
30	3	303	CLA	C2D-C1D-ND	5.63	115.69	110.13
37	2u	205	A86	C24-C1-C2	5.63	127.86	119.01
38	6	312	KC1	C3A-C4A-NA	5.63	117.41	110.45
30	A	806	CLA	C2B-C1B-NB	5.63	116.16	110.33
30	A	835	CLA	CHD-C4C-C3C	-5.63	116.57	124.77
30	A	802	CLA	O2D-CGD-CBD	5.62	121.06	111.23
30	A	839	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
30	A	835	CLA	C3B-C2B-C1B	-5.62	100.54	107.17
30	11	308	CLA	C2B-C1B-NB	5.62	116.15	110.33
30	7	312	CLA	C2D-C1D-ND	5.62	115.69	110.13
39	7	317	DD6	C13-C11-C10	-5.62	110.17	119.01
30	B	803	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
30	B	801	CLA	CMD-C2D-C1D	5.62	134.62	124.73
30	15	306	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
30	16	305	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
38	9	304	KC1	C1A-C2A-C3A	-5.62	102.12	107.28
30	2	310	CLA	C2D-C1D-ND	5.61	115.68	110.13
38	8	310	KC1	C1A-C2A-C3A	-5.61	102.12	107.28
30	B	805	CLA	O2D-CGD-CBD	5.61	121.05	111.23
38	13	311	KC1	C3A-C4A-NA	5.61	117.40	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	817	CLA	C2B-C1B-NB	5.61	116.15	110.33
30	A	815	CLA	O2D-CGD-CBD	5.61	121.04	111.23
30	A	843	CLA	C2D-C1D-ND	5.61	115.68	110.13
30	15	308	CLA	CMD-C2D-C1D	5.61	134.61	124.73
30	4	309	CLA	C2D-C1D-ND	5.61	115.68	110.13
38	8	312	KC1	C2D-C1D-ND	5.61	116.14	110.33
38	11	305	KC1	C3B-C2B-C1B	-5.60	101.74	107.05
30	14	305	CLA	C2D-C1D-ND	5.60	115.67	110.13
30	2	313	CLA	O2D-CGD-CBD	5.60	121.03	111.23
30	8	303	CLA	CHD-C4C-C3C	-5.60	116.60	124.77
39	15	318	DD6	C-C1-C24	-5.60	109.53	118.09
30	5	308	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
30	2	309	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
30	6	310	CLA	C2D-C1D-ND	5.60	115.67	110.13
30	10	308	CLA	C2B-C1B-NB	5.59	116.13	110.33
39	7	314	DD6	C-C1-C2	-5.59	113.75	122.82
30	2	305	CLA	CMD-C2D-C1D	5.59	134.58	124.73
30	2	304	CLA	C2B-C1B-NB	5.59	116.12	110.33
30	7	306	CLA	C2C-C1C-NC	5.59	115.86	109.98
30	B	820	CLA	O2D-CGD-CBD	5.59	121.00	111.23
39	7	317	DD6	C24-C1-C2	-5.59	110.22	119.01
38	8	306	KC1	C3A-C4A-NA	5.59	117.37	110.45
30	15	314	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
30	2	307	CLA	C2D-C1D-ND	5.59	115.66	110.13
37	4	314	A86	C4-C5-C6	-5.59	119.44	127.28
39	1	310	DD6	C-C1-C24	-5.59	109.55	118.09
30	B	831	CLA	C2B-C1B-NB	5.59	116.12	110.33
30	A	809	CLA	CHD-C4C-C3C	-5.59	116.63	124.77
39	10	314	DD6	C24-C1-C2	-5.58	110.22	119.01
30	B	808	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
38	6	311	KC1	C2B-C1B-NB	5.58	115.65	110.13
38	7	308	KC1	C1A-C2A-C3A	-5.58	102.15	107.28
37	5	316	A86	C3-C2-C1	-5.58	119.45	127.28
30	12	307	CLA	CMD-C2D-C1D	5.58	134.56	124.73
38	11	312	KC1	C3A-C4A-NA	5.58	117.36	110.45
30	14	304	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
30	A	833	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
30	3	303	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
38	12	311	KC1	C2D-C1D-ND	5.58	116.11	110.33
30	A	821	CLA	C2D-C1D-ND	5.58	115.65	110.13
39	11	313	DD6	C8-C6-C5	-5.58	110.24	119.01
30	15	307	CLA	CHD-C4C-C3C	-5.58	116.64	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	312	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
30	3	307	CLA	C2C-C1C-NC	5.57	115.84	109.98
38	6	308	KC1	C2D-C1D-ND	5.57	116.11	110.33
30	A	802	CLA	CMD-C2D-C1D	5.57	134.54	124.73
38	12	305	KC1	C1A-C2A-C3A	-5.57	102.16	107.28
38	14	308	KC1	C3C-C4C-NC	5.57	115.87	109.90
30	3	301	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
30	13	307	CLA	C2D-C1D-ND	5.57	115.64	110.13
30	14	305	CLA	C2B-C1B-NB	5.57	116.10	110.33
37	2	302	A86	C4-C3-C2	-5.57	112.12	123.52
39	15	319	DD6	C24-C1-C2	-5.57	110.25	119.01
30	B	851	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
30	B	818	CLA	C2D-C1D-ND	5.57	115.63	110.13
38	2	312	KC1	C3A-C4A-NA	5.56	117.34	110.45
38	6	312	KC1	C2D-C1D-ND	5.56	116.09	110.33
38	6	308	KC1	C2B-C1B-NB	5.56	115.63	110.13
38	7	313	KC1	C2D-C1D-ND	5.56	116.09	110.33
38	12	309	KC1	CMA-C3A-C2A	-5.56	114.97	128.43
39	10	313	DD6	C4-C5-C6	-5.56	119.48	127.28
39	7	302	DD6	C24-C1-C2	-5.56	110.27	119.01
30	B	838	CLA	CHD-C4C-C3C	-5.56	116.67	124.77
38	12	313	KC1	C3A-C4A-NA	5.56	117.33	110.45
30	6	316	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
30	12	304	CLA	C2D-C1D-ND	5.55	115.62	110.13
37	9	313	A86	C4-C5-C6	-5.55	119.49	127.28
30	8	308	CLA	C2B-C1B-NB	5.55	116.08	110.33
30	10	309	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
30	14	310	CLA	C2B-C1B-NB	5.55	116.08	110.33
30	16	309	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
30	4	305	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
30	5	308	CLA	CMD-C2D-C1D	5.54	134.49	124.73
30	6	304	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
30	11	304	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
30	9	309	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
30	B	818	CLA	C4A-NA-C1A	-5.54	104.15	106.68
38	1	306	KC1	C1A-C2A-C3A	-5.54	102.19	107.28
39	2	316	DD6	C7-C6-C5	-5.54	113.84	122.82
37	15	316	A86	C3-C2-C1	-5.54	119.51	127.28
30	5	311	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
30	15	304	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
30	A	803	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
38	10	306	KC1	C3B-C2B-C1B	-5.54	101.81	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	819	CLA	C2B-C1B-NB	5.53	116.06	110.33
30	15	307	CLA	C2C-C1C-NC	5.53	115.79	109.98
29	A	801	CL0	CBC-CAC-C3C	-5.53	104.95	112.87
30	A	838	CLA	C2D-C1D-ND	5.53	115.60	110.13
38	13	306	KC1	C2D-C1D-ND	5.53	116.06	110.33
38	5	312	KC1	C3B-C2B-C1B	-5.53	101.81	107.05
30	15	310	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
30	6	305	CLA	C2D-C1D-ND	5.53	115.60	110.13
30	A	825	CLA	C2D-C1D-ND	5.53	115.60	110.13
30	14	302	CLA	CHD-C4C-C3C	-5.53	116.72	124.77
30	B	832	CLA	C2B-C1B-NB	5.53	116.06	110.33
30	14	305	CLA	CHD-C4C-C3C	-5.53	116.72	124.77
37	13	315	A86	O4-C38-C39	5.52	120.94	111.09
30	J	101	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
30	B	812	CLA	C3B-C2B-C1B	-5.52	100.66	107.17
30	A	812	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
38	3	304	KC1	C3A-C4A-NA	5.52	117.28	110.45
30	16	307	CLA	C2D-C1D-ND	5.52	115.59	110.13
30	12	306	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
30	9	308	CLA	C2B-C1B-NB	5.52	116.05	110.33
39	7	317	DD6	C7-C6-C8	-5.52	109.66	118.09
39	8	316	DD6	C13-C11-C10	-5.52	110.33	119.01
30	14	303	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
30	A	843	CLA	CHD-C4C-C3C	-5.51	116.73	124.77
38	12	305	KC1	C2B-C1B-NB	5.51	115.58	110.13
30	2	311	CLA	CHD-C4C-C3C	-5.51	116.73	124.77
30	7	310	CLA	C2B-C1B-NB	5.51	116.04	110.33
30	A	838	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
30	A	841	CLA	C2D-C1D-ND	5.51	115.58	110.13
30	9	306	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
38	3	304	KC1	C2B-C1B-NB	5.51	115.58	110.13
30	B	811	CLA	CMD-C2D-C1D	5.51	134.43	124.73
30	A	822	CLA	CHD-C4C-C3C	-5.51	116.75	124.77
30	7	309	CLA	CHD-C4C-C3C	-5.51	116.75	124.77
30	B	812	CLA	C2D-C1D-ND	5.50	115.57	110.13
30	14	302	CLA	C2D-C1D-ND	5.50	115.57	110.13
38	11	307	KC1	C2B-C1B-NB	5.50	115.57	110.13
30	6	305	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
30	15	306	CLA	C2C-C1C-NC	5.50	115.76	109.98
30	12	304	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
30	1	302	CLA	O2D-CGD-CBD	5.50	120.85	111.23
38	14	306	KC1	C2B-C1B-NB	5.50	115.57	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	308	CLA	C2D-C1D-ND	5.50	115.57	110.13
30	12	306	CLA	C2D-C1D-ND	5.50	115.57	110.13
38	7	308	KC1	C2D-C1D-ND	5.50	116.03	110.33
38	2	314	KC1	C3A-C4A-NA	5.50	117.25	110.45
39	15	318	DD6	C24-C1-C2	-5.50	110.36	119.01
30	B	830	CLA	O2D-CGD-CBD	5.50	120.84	111.23
30	A	806	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
38	8	306	KC1	C2D-C1D-ND	5.49	116.02	110.33
30	8	302	CLA	C3B-C2B-C1B	-5.49	100.69	107.17
30	14	310	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
30	8	309	CLA	C2D-C1D-ND	5.49	115.56	110.13
38	4	307	KC1	O2D-CGD-CBD	5.49	120.83	111.23
38	11	311	KC1	C2B-C1B-NB	5.49	115.56	110.13
37	6	320	A86	C25-C26-C27	-5.49	119.58	127.28
38	8	306	KC1	C2B-C1B-NB	5.49	115.56	110.13
30	12	304	CLA	C3B-C2B-C1B	-5.49	100.70	107.17
38	13	308	KC1	C1A-C2A-C3A	-5.49	102.24	107.28
38	6	312	KC1	C3B-C2B-C1B	-5.49	101.86	107.05
30	B	829	CLA	CHD-C4C-C3C	-5.49	116.78	124.77
37	9	316	A86	C4-C5-C6	-5.49	119.58	127.28
30	B	830	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
39	8	316	DD6	C-C1-C24	-5.48	109.71	118.09
39	9	314	DD6	C8-C6-C5	-5.48	110.38	119.01
30	A	809	CLA	O2D-CGD-CBD	5.48	120.81	111.23
30	1	307	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
30	A	828	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
38	10	310	KC1	C3B-C2B-C1B	-5.48	101.86	107.05
30	5	309	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
38	2	314	KC1	C2B-C1B-NB	5.48	115.55	110.13
30	15	303	CLA	C2B-C1B-NB	5.48	116.01	110.33
39	3	312	DD6	C-C1-C24	-5.48	109.72	118.09
39	15	319	DD6	C-C1-C24	-5.48	109.72	118.09
30	A	835	CLA	C2B-C1B-NB	5.48	116.00	110.33
38	11	307	KC1	C1A-C2A-C3A	-5.47	102.25	107.28
30	7	303	CLA	O2D-CGD-CBD	5.47	120.80	111.23
39	3	316	DD6	C-C1-C24	-5.47	109.73	118.09
37	3	315	A86	C33-C32-C31	5.47	114.53	109.21
30	A	837	CLA	C2B-C1B-NB	5.47	116.00	110.33
30	6	309	CLA	C2D-C1D-ND	5.47	115.54	110.13
30	B	809	CLA	CHD-C4C-C3C	-5.47	116.80	124.77
30	13	304	CLA	CHD-C4C-C3C	-5.47	116.80	124.77
37	14	316	A86	C25-C26-C27	-5.47	119.61	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	309	CLA	C2B-C1B-NB	5.47	116.00	110.33
30	11	309	CLA	C2D-C1D-ND	5.47	115.54	110.13
30	16	307	CLA	CHD-C4C-C3C	-5.47	116.80	124.77
30	12	307	CLA	O2D-CGD-CBD	5.47	120.78	111.23
30	A	807	CLA	C4A-NA-C1A	-5.46	104.19	106.68
30	A	806	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
30	6	305	CLA	C4A-NA-C1A	-5.46	104.19	106.68
38	12	309	KC1	O2D-CGD-CBD	5.46	120.77	111.23
38	13	311	KC1	C2D-C1D-ND	5.46	115.98	110.33
30	L	202	CLA	O2D-CGD-CBD	5.45	120.77	111.23
39	2	317	DD6	C13-C11-C10	-5.45	110.43	119.01
38	1	306	KC1	C2D-C1D-ND	5.45	115.98	110.33
30	A	836	CLA	CMD-C2D-C1D	5.45	134.33	124.73
30	11	308	CLA	CHD-C4C-C3C	-5.45	116.82	124.77
38	6	311	KC1	C1A-NA-C4A	-5.45	104.19	106.68
30	13	309	CLA	C2C-C1C-NC	5.45	115.71	109.98
30	B	802	CLA	C4A-NA-C1A	-5.45	104.19	106.68
30	B	818	CLA	C2B-C1B-NB	5.45	115.98	110.33
30	13	307	CLA	C2B-C1B-NB	5.45	115.98	110.33
38	6	311	KC1	O2D-CGD-CBD	5.45	120.75	111.23
30	7	306	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
30	15	308	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
38	14	311	KC1	C1A-C2A-C3A	-5.45	102.27	107.28
30	1	301	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
38	10	306	KC1	C3A-C4A-NA	5.45	117.19	110.45
30	11	310	CLA	C4A-NA-C1A	-5.44	104.19	106.68
30	10	308	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
30	6	306	CLA	O2D-CGD-CBD	5.44	120.74	111.23
39	3	316	DD6	C13-C11-C10	-5.44	110.45	119.01
30	F	203	CLA	O2D-CGD-CBD	5.44	120.74	111.23
30	2	305	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
38	5	312	KC1	C2B-C1B-NB	5.44	115.51	110.13
30	6	314	CLA	C2B-C1B-NB	5.44	115.97	110.33
30	A	844	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
30	B	819	CLA	CMD-C2D-C1D	5.44	134.30	124.73
38	12	311	KC1	O2D-CGD-CBD	5.44	120.73	111.23
30	B	819	CLA	CHD-C4C-C3C	-5.43	116.85	124.77
30	L	202	CLA	CHD-C4C-C3C	-5.43	116.85	124.77
30	4	306	CLA	O2D-CGD-CBD	5.43	120.72	111.23
38	5	312	KC1	C1A-C2A-C3A	-5.43	102.29	107.28
38	5	310	KC1	C2B-C1B-NB	5.43	115.50	110.13
30	A	842	CLA	O2D-CGD-CBD	5.43	120.72	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	313	KC1	O2D-CGD-CBD	5.43	120.72	111.23
37	14	316	A86	C4-C5-C6	-5.43	119.67	127.28
30	A	827	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
30	B	813	CLA	O2D-CGD-CBD	5.42	120.70	111.23
38	9	304	KC1	C2B-C1B-NB	5.42	115.49	110.13
30	2	304	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
30	A	833	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
30	7	309	CLA	C2C-C1C-NC	5.41	115.67	109.98
37	9	316	A86	C25-C26-C27	-5.41	119.69	127.28
30	4	303	CLA	C4A-NA-C1A	-5.41	104.21	106.68
30	B	832	CLA	CHD-C4C-C3C	-5.41	116.88	124.77
30	7	305	CLA	C2B-C1B-NB	5.41	115.93	110.33
30	B	820	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
30	A	808	CLA	O2D-CGD-CBD	5.41	120.68	111.23
30	15	309	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
30	3	306	CLA	CHD-C4C-C3C	-5.40	116.89	124.77
30	B	831	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
30	B	832	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
30	6	314	CLA	CHD-C4C-C3C	-5.40	116.89	124.77
30	13	307	CLA	CHD-C4C-C3C	-5.40	116.89	124.77
38	7	308	KC1	C3B-C2B-C1B	-5.40	101.93	107.05
30	4	301	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
30	A	824	CLA	C4A-NA-C1A	-5.40	104.22	106.68
38	8	312	KC1	CHB-C4A-C3A	-5.40	116.50	125.03
39	7	318	DD6	C-C1-C24	-5.40	109.84	118.09
38	3	311	KC1	C3A-C4A-NA	5.40	117.13	110.45
30	1	303	CLA	C2B-C1B-NB	5.39	115.92	110.33
30	8	305	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
39	4	316	DD6	C8-C6-C5	-5.39	110.53	119.01
30	B	821	CLA	CHD-C4C-C3C	-5.39	116.91	124.77
30	B	808	CLA	C2D-C1D-ND	5.39	115.46	110.13
30	15	312	CLA	CHD-C4C-C3C	-5.39	116.91	124.77
30	15	312	CLA	C2B-C1B-NB	5.39	115.92	110.33
30	A	814	CLA	C2B-C1B-NB	5.39	115.91	110.33
30	12	321	CLA	CHD-C4C-C3C	-5.39	116.92	124.77
30	A	814	CLA	CHD-C4C-C3C	-5.39	116.92	124.77
30	A	817	CLA	CHD-C4C-C3C	-5.39	116.92	124.77
30	7	304	CLA	CHD-C4C-C3C	-5.38	116.92	124.77
30	2	307	CLA	CHD-C4C-C3C	-5.38	116.92	124.77
39	6	303	DD6	C24-C1-C2	-5.38	110.54	119.01
30	6	309	CLA	O2D-CGD-CBD	5.38	120.64	111.23
38	6	311	KC1	C2D-C1D-ND	5.38	115.91	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	323	A86	O4-C38-C39	5.38	120.68	111.09
30	B	830	CLA	C2B-C1B-NB	5.38	115.90	110.33
38	4	307	KC1	C1A-C2A-C3A	-5.38	102.34	107.28
38	14	308	KC1	C1A-C2A-C3A	-5.38	102.34	107.28
30	B	824	CLA	CAA-C2A-C3A	-5.38	98.47	113.00
30	1	304	CLA	CMD-C2D-C1D	5.38	134.20	124.73
38	12	313	KC1	CHD-C4C-C3C	-5.38	115.31	125.23
30	A	838	CLA	C2B-C1B-NB	5.38	115.90	110.33
30	B	803	CLA	C2B-C1B-NB	5.38	115.90	110.33
30	11	304	CLA	C2B-C1B-NB	5.38	115.90	110.33
38	8	307	KC1	C2B-C1B-NB	5.38	115.45	110.13
30	12	307	CLA	C4A-NA-C1A	-5.37	104.23	106.68
30	6	314	CLA	C2D-C1D-ND	5.37	115.44	110.13
38	10	312	KC1	C2B-C1B-NB	5.37	115.44	110.13
30	12	321	CLA	C2B-C1B-NB	5.37	115.90	110.33
30	B	851	CLA	C2D-C1D-ND	5.37	115.44	110.13
30	B	805	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
38	9	310	KC1	C2D-C1D-ND	5.37	115.90	110.33
37	5	315	A86	C4-C5-C6	-5.37	119.75	127.28
30	A	836	CLA	C2D-C1D-ND	5.37	115.44	110.13
30	B	834	CLA	C4A-NA-C1A	-5.37	104.23	106.68
37	13	315	A86	C4-C5-C6	-5.37	119.75	127.28
30	3	310	CLA	CHD-C4C-C3C	-5.37	116.94	124.77
38	13	312	KC1	C2B-C1B-NB	5.37	115.44	110.13
39	3	312	DD6	C24-C1-C2	-5.37	110.57	119.01
38	8	311	KC1	C3A-C4A-NA	5.37	117.09	110.45
30	B	836	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
30	A	836	CLA	C2C-C1C-NC	5.36	115.62	109.98
38	1	308	KC1	C2D-C1D-ND	5.36	115.89	110.33
39	2	316	DD6	C-C1-C24	-5.36	109.90	118.09
30	B	809	CLA	CMD-C2D-C1D	5.36	134.16	124.73
30	A	833	CLA	C2B-C1B-NB	5.36	115.88	110.33
38	11	307	KC1	C2D-C1D-ND	5.36	115.88	110.33
29	A	801	CL0	CHA-C1A-C2A	-5.36	120.73	133.31
30	4	309	CLA	O2D-CGD-CBD	5.36	120.60	111.23
30	B	814	CLA	C2D-C1D-ND	5.36	115.43	110.13
30	16	308	CLA	CHD-C4C-C3C	-5.36	116.96	124.77
30	2	304	CLA	C4A-NA-C1A	-5.35	104.24	106.68
38	2	312	KC1	C2D-C1D-ND	5.35	115.88	110.33
30	A	823	CLA	CHD-C4C-C3C	-5.35	116.97	124.77
38	8	312	KC1	C3B-C2B-C1B	-5.35	101.98	107.05
38	13	306	KC1	C3B-C2B-C1B	-5.35	101.98	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	5	305	KC1	C3A-C4A-NA	5.35	117.07	110.45
30	3	306	CLA	C2D-C1D-ND	5.35	115.42	110.13
38	11	305	KC1	C2D-C1D-ND	5.35	115.87	110.33
30	B	816	CLA	O2D-CGD-CBD	5.35	120.58	111.23
30	11	310	CLA	C2B-C1B-NB	5.35	115.87	110.33
30	12	304	CLA	C2B-C1B-NB	5.35	115.87	110.33
38	13	310	KC1	C2D-C1D-ND	5.35	115.87	110.33
30	A	826	CLA	C2C-C1C-NC	5.35	115.60	109.98
38	2	314	KC1	C2D-C1D-ND	5.34	115.87	110.33
30	A	813	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
30	6	306	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
30	10	307	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
30	4	311	CLA	CHD-C4C-C3C	-5.34	116.98	124.77
30	15	310	CLA	C2B-C1B-NB	5.34	115.87	110.33
30	4	309	CLA	CHD-C4C-C3C	-5.34	116.98	124.77
30	9	309	CLA	C2D-C1D-ND	5.34	115.41	110.13
30	7	312	CLA	CHD-C4C-C3C	-5.34	116.98	124.77
38	2	306	KC1	C2D-C1D-ND	5.34	115.86	110.33
30	B	812	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
39	2	317	DD6	C-C1-C24	-5.34	109.93	118.09
30	A	821	CLA	CMD-C2D-C1D	5.34	134.13	124.73
37	11	315	A86	C25-C26-C27	-5.34	119.80	127.28
37	5	316	A86	O4-C38-C39	5.34	120.60	111.09
30	8	303	CLA	CMD-C2D-C1D	5.34	134.12	124.73
38	13	305	KC1	C2D-C1D-ND	5.34	115.86	110.33
39	3	316	DD6	C12-C11-C13	-5.33	109.94	118.09
39	6	318	DD6	C8-C6-C5	-5.33	110.62	119.01
38	8	311	KC1	C2B-C1B-NB	5.33	115.41	110.13
30	B	814	CLA	CMD-C2D-C1D	5.33	134.12	124.73
39	3	313	DD6	C24-C1-C2	-5.33	110.62	119.01
30	5	307	CLA	C2C-C1C-NC	5.33	115.58	109.98
38	11	311	KC1	C1A-C2A-C3A	-5.33	102.38	107.28
37	2u	203	A86	C7-C6-C8	5.33	126.23	118.09
30	14	305	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
30	12	304	CLA	O2D-CGD-CBD	5.33	120.55	111.23
30	A	810	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
30	15	310	CLA	O2D-CGD-CBD	5.33	120.55	111.23
30	14	309	CLA	C2D-C1D-ND	5.33	115.40	110.13
38	8	314	KC1	C3A-C4A-NA	5.33	117.04	110.45
38	5	306	KC1	C2D-C1D-ND	5.33	115.85	110.33
38	9	311	KC1	C2D-C1D-ND	5.33	115.85	110.33
38	9	311	KC1	C2B-C1B-NB	5.33	115.40	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	301	CLA	O2D-CGD-CBD	5.33	120.54	111.23
30	1	305	CLA	C2D-C1D-ND	5.32	115.40	110.13
38	8	313	KC1	C1A-C2A-C3A	-5.32	102.39	107.28
38	6	313	KC1	C2D-C1D-ND	5.32	115.85	110.33
30	A	802	CLA	CHD-C4C-C3C	-5.32	117.01	124.77
30	14	307	CLA	C2B-C1B-NB	5.32	115.84	110.33
38	8	307	KC1	C2D-C1D-ND	5.32	115.84	110.33
30	A	824	CLA	C2D-C1D-ND	5.32	115.39	110.13
30	3	306	CLA	O2D-CGD-CBD	5.32	120.53	111.23
30	16	306	CLA	CHD-C4C-C3C	-5.32	117.02	124.77
39	12	317	DD6	C21-C20-C19	-5.32	108.27	114.24
39	16	313	DD6	C14-C13-C11	5.32	133.78	125.53
30	4	303	CLA	O2D-CGD-CBD	5.32	120.53	111.23
30	A	805	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
38	13	310	KC1	C3C-C4C-NC	5.32	115.60	109.90
30	4	304	CLA	C2D-C1D-ND	5.32	115.39	110.13
38	2	306	KC1	C1A-C2A-C3A	-5.31	102.39	107.28
38	13	310	KC1	C2B-C1B-NB	5.31	115.38	110.13
30	9	308	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
30	8	309	CLA	O2D-CGD-CBD	5.31	120.51	111.23
30	A	837	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
30	11	306	CLA	C4A-NA-C1A	-5.31	104.26	106.68
38	12	309	KC1	C2D-C1D-ND	5.31	115.83	110.33
30	16	308	CLA	C2B-C1B-NB	5.31	115.83	110.33
30	6	316	CLA	C2B-C1B-NB	5.30	115.83	110.33
30	7	311	CLA	CHD-C4C-C3C	-5.30	117.04	124.77
30	7	306	CLA	CMD-C2D-C1D	5.30	134.06	124.73
38	8	310	KC1	CHD-C4C-C3C	-5.30	115.45	125.23
38	1	308	KC1	C2B-C1B-NB	5.30	115.37	110.13
30	15	314	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
30	6	309	CLA	CMD-C2D-C1D	5.30	134.06	124.73
37	10	317	A86	O4-C38-C39	5.30	120.53	111.09
30	B	851	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
38	14	311	KC1	C2D-C1D-ND	5.29	115.82	110.33
38	8	313	KC1	C3C-C4C-NC	5.29	115.57	109.90
30	14	309	CLA	C2B-C1B-NB	5.29	115.81	110.33
30	4	311	CLA	C2C-C1C-NC	5.29	115.54	109.98
30	A	802	CLA	C2D-C1D-ND	5.29	115.36	110.13
30	A	844	CLA	C2D-C1D-ND	5.29	115.36	110.13
38	8	314	KC1	C2D-C1D-ND	5.29	115.81	110.33
30	A	821	CLA	CHD-C4C-C3C	-5.29	117.06	124.77
30	A	802	CLA	CAA-C2A-C3A	-5.29	98.71	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	837	CLA	C2D-C1D-ND	5.29	115.36	110.13
30	A	814	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
38	13	312	KC1	C2D-C1D-ND	5.28	115.81	110.33
30	2	301	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
39	1	310	DD6	C7-C6-C8	-5.28	110.02	118.09
38	5	310	KC1	C3B-C2B-C1B	-5.28	102.05	107.05
30	B	835	CLA	O2D-CGD-CBD	5.28	120.47	111.23
30	14	302	CLA	C2B-C1B-NB	5.28	115.80	110.33
30	9	305	CLA	CAA-C2A-C3A	-5.28	98.73	113.00
30	6	316	CLA	CHD-C4C-C3C	-5.28	117.07	124.77
30	B	823	CLA	C2D-C1D-ND	5.28	115.35	110.13
30	11	306	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
38	2	312	KC1	C2B-C1B-NB	5.28	115.35	110.13
30	J	101	CLA	C2B-C1B-NB	5.28	115.80	110.33
39	8	317	DD6	O1-C15-C14	-5.28	101.76	116.88
30	B	803	CLA	CMD-C2D-C1D	5.28	134.02	124.73
30	A	835	CLA	C2D-C1D-ND	5.28	115.35	110.13
30	6	305	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
30	7	305	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
38	5	312	KC1	C2D-C1D-ND	5.27	115.80	110.33
30	B	813	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
39	3	316	DD6	C7-C6-C8	-5.27	110.03	118.09
30	4	309	CLA	C2B-C1B-NB	5.27	115.79	110.33
30	11	304	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
30	13	304	CLA	C2B-C1B-NB	5.27	115.79	110.33
37	15	321	A86	O4-C38-C39	5.27	120.49	111.09
30	7	310	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
30	7	303	CLA	CMD-C2D-C1D	5.27	134.01	124.73
30	11	306	CLA	CAA-C2A-C3A	-5.27	98.76	113.00
38	8	313	KC1	C2B-C1B-NB	5.27	115.34	110.13
30	7	312	CLA	C2B-C1B-NB	5.27	115.79	110.33
30	B	809	CLA	C2C-C1C-NC	5.27	115.51	109.98
38	5	305	KC1	C2D-C1D-ND	5.27	115.79	110.33
30	1	305	CLA	C2C-C1C-NC	5.27	115.51	109.98
38	1	306	KC1	C2B-C1B-NB	5.26	115.33	110.13
38	9	311	KC1	C1A-C2A-C3A	-5.26	102.44	107.28
30	10	303	CLA	C2B-C1B-NB	5.26	115.78	110.33
30	15	302	CLA	C2B-C1B-NB	5.26	115.78	110.33
30	4	304	CLA	C2B-C1B-NB	5.26	115.78	110.33
30	15	305	CLA	C2B-C1B-NB	5.26	115.78	110.33
39	2	317	DD6	C21-C20-C15	-5.26	113.64	122.30
38	6	312	KC1	C2B-C1B-NB	5.26	115.33	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	303	CLA	CHD-C4C-C3C	-5.26	117.10	124.77
30	A	841	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
38	11	312	KC1	CHC-C1C-C2C	-5.26	116.72	125.03
30	7	312	CLA	C2C-C1C-NC	5.26	115.50	109.98
38	3	311	KC1	O2D-CGD-CBD	5.26	120.42	111.23
30	1	305	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
30	2	310	CLA	C4A-NA-C1A	-5.26	104.28	106.68
37	8	315	A86	C10-C9-C8	-5.26	107.97	123.20
39	10	314	DD6	O1-C15-C14	-5.25	101.82	116.88
30	6	310	CLA	C2B-C1B-NB	5.25	115.77	110.33
30	9	302	CLA	CHD-C4C-C3C	-5.25	117.11	124.77
38	13	306	KC1	C2B-C1B-NB	5.25	115.32	110.13
30	8	305	CLA	O2D-CGD-CBD	5.25	120.41	111.23
30	16	306	CLA	C4A-NA-C1A	-5.25	104.28	106.68
37	3	315	A86	C36-C31-C32	-5.25	114.49	119.70
38	11	311	KC1	C2D-C1D-ND	5.25	115.77	110.33
39	7	302	DD6	C21-C20-C15	-5.25	113.67	122.30
30	A	803	CLA	CHD-C4C-C3C	-5.25	117.12	124.77
37	10	301	A86	O4-C38-C39	5.24	120.44	111.09
30	8	301	CLA	C2B-C1B-NB	5.24	115.76	110.33
30	4	304	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
38	10	310	KC1	C2D-C1D-ND	5.24	115.76	110.33
38	12	313	KC1	C3C-C4C-NC	5.24	115.52	109.90
30	B	829	CLA	C2B-C1B-NB	5.24	115.76	110.33
30	12	306	CLA	O2D-CGD-CBD	5.24	120.39	111.23
37	10	317	A86	C3-C2-C1	-5.24	119.93	127.28
38	1	308	KC1	C3B-C2B-C1B	-5.24	102.09	107.05
30	A	815	CLA	C2D-C1D-ND	5.24	115.31	110.13
30	11	308	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
30	B	830	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
30	B	835	CLA	C2B-C1B-NB	5.24	115.75	110.33
30	6	306	CLA	C2B-C1B-NB	5.24	115.75	110.33
38	6	308	KC1	C3C-C4C-NC	5.23	115.51	109.90
30	B	813	CLA	C2B-C1B-NB	5.23	115.75	110.33
30	9	302	CLA	C2B-C1B-NB	5.23	115.75	110.33
30	6	316	CLA	C2D-C1D-ND	5.23	115.30	110.13
30	11	310	CLA	C2D-C1D-ND	5.23	115.30	110.13
37	15	320	A86	O4-C38-C39	5.23	120.41	111.09
30	15	305	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
30	8	302	CLA	C2B-C1B-NB	5.23	115.75	110.33
38	14	306	KC1	C2D-C1D-ND	5.23	115.75	110.33
30	10	308	CLA	C3B-C2B-C1B	-5.22	101.01	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	11	312	KC1	C3B-C2B-C1B	-5.22	102.10	107.05
30	A	820	CLA	O2D-CGD-CBD	5.22	120.36	111.23
30	B	805	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
30	11	306	CLA	C2B-C1B-NB	5.22	115.74	110.33
30	8	301	CLA	CMD-C2D-C1D	5.22	133.92	124.73
30	A	826	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
30	9	306	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
30	11	310	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
38	6	313	KC1	C1A-C2A-C3A	-5.22	102.48	107.28
30	B	807	CLA	C2C-C1C-NC	5.22	115.46	109.98
30	B	834	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
38	9	304	KC1	C2D-C1D-ND	5.22	115.74	110.33
30	J	101	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
30	3	306	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
30	8	309	CLA	CHD-C4C-C3C	-5.22	117.17	124.77
37	14	301	A86	O4-C38-C39	5.22	120.39	111.09
38	13	306	KC1	O2D-CGD-CBD	5.22	120.35	111.23
39	7	302	DD6	O1-C15-C14	-5.22	101.94	116.88
39	7	314	DD6	C-C1-C24	-5.21	110.12	118.09
30	A	834	CLA	C3B-C2B-C1B	-5.21	101.02	107.17
38	3	308	KC1	C2D-C1D-ND	5.21	115.73	110.33
30	14	309	CLA	CHD-C4C-C3C	-5.21	117.17	124.77
39	7	314	DD6	C24-C1-C2	-5.21	110.81	119.01
30	14	310	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
30	14	309	CLA	C2C-C1C-NC	5.21	115.45	109.98
30	15	303	CLA	C2C-C1C-NC	5.21	115.45	109.98
30	A	802	CLA	C2B-C1B-NB	5.21	115.73	110.33
30	A	831	CLA	C2C-C1C-NC	5.21	115.45	109.98
30	B	824	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
30	15	305	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
38	12	305	KC1	C2D-C1D-ND	5.21	115.73	110.33
38	8	313	KC1	CHD-C4C-C3C	-5.21	115.62	125.23
30	B	815	CLA	C2C-C1C-NC	5.21	115.45	109.98
30	A	836	CLA	CHD-C4C-C3C	-5.21	117.18	124.77
30	B	836	CLA	C2C-C1C-NC	5.21	115.45	109.98
30	9	303	CLA	C3B-C2B-C1B	-5.20	101.03	107.17
38	5	305	KC1	C2B-C1B-NB	5.20	115.28	110.13
37	4	315	A86	C40-C32-C31	-5.20	105.82	110.47
30	6	310	CLA	CHD-C4C-C3C	-5.20	117.19	124.77
30	3	310	CLA	C2C-C1C-NC	5.20	115.45	109.98
37	9	316	A86	O4-C38-C39	5.20	120.36	111.09
30	B	817	CLA	C3B-C2B-C1B	-5.20	101.04	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	304	CLA	C2C-C1C-NC	5.20	115.44	109.98
37	2u	205	A86	C-C1-C2	-5.20	114.39	122.82
38	16	304	KC1	O2D-CGD-CBD	5.20	120.32	111.23
38	3	304	KC1	C2D-C1D-ND	5.20	115.72	110.33
30	6	315	CLA	O2D-CGD-CBD	5.20	120.32	111.23
39	5	314	DD6	C-C1-C24	-5.20	110.15	118.09
30	3	303	CLA	C2B-C1B-NB	5.20	115.72	110.33
30	14	312	CLA	C2B-C1B-NB	5.20	115.72	110.33
30	B	811	CLA	O2D-CGD-CBD	5.20	120.32	111.23
30	5	311	CLA	C2B-C1B-NB	5.20	115.71	110.33
38	14	311	KC1	C2B-C1B-NB	5.20	115.27	110.13
38	14	311	KC1	CHD-C4C-C3C	-5.20	115.65	125.23
38	7	308	KC1	C2B-C1B-NB	5.19	115.27	110.13
38	10	306	KC1	C2B-C1B-NB	5.19	115.27	110.13
37	15	320	A86	C3-C4-C5	-5.19	112.90	123.52
30	A	831	CLA	CHD-C4C-C3C	-5.19	117.20	124.77
30	4	305	CLA	O2D-CGD-CBD	5.19	120.30	111.23
30	15	310	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
30	A	815	CLA	C2C-C1C-NC	5.19	115.43	109.98
30	6	305	CLA	C2B-C1B-NB	5.19	115.71	110.33
38	6	308	KC1	CHD-C4C-C3C	-5.19	115.66	125.23
30	9	307	CLA	C2B-C1B-NB	5.19	115.70	110.33
30	A	820	CLA	C4A-NA-C1A	-5.18	104.31	106.68
37	16	314	A86	O4-C38-C39	5.18	120.33	111.09
37	4	315	A86	C4-C5-C6	-5.18	120.01	127.28
30	A	814	CLA	O2D-CGD-CBD	5.18	120.29	111.23
30	B	824	CLA	C4A-NA-C1A	-5.18	104.31	106.68
30	4	301	CLA	C2B-C1B-NB	5.18	115.70	110.33
38	8	307	KC1	O2D-CGD-CBD	5.18	120.29	111.23
30	6	317	CLA	C2B-C1B-NB	5.18	115.70	110.33
30	12	303	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
38	5	312	KC1	CMD-C2D-C1D	5.18	133.30	125.42
38	2	312	KC1	C3C-C4C-NC	5.18	115.45	109.90
30	4	303	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
37	7	319	A86	O4-C38-C39	5.18	120.32	111.09
39	3	313	DD6	C-C1-C24	-5.18	110.18	118.09
30	5	304	CLA	O2D-CGD-CBD	5.18	120.28	111.23
38	9	312	KC1	C3A-C4A-NA	5.17	116.86	110.45
37	1	309	A86	C41-C32-C31	-5.17	105.84	110.47
38	6	313	KC1	C2B-C1B-NB	5.17	115.25	110.13
39	7	317	DD6	C-C1-C24	-5.17	110.18	118.09
30	9	302	CLA	C2C-C1C-NC	5.17	115.42	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	3	315	A86	O4-C38-C39	5.17	120.31	111.09
30	12	302	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
39	11	313	DD6	C21-C20-C15	-5.17	113.79	122.30
30	6	307	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
39	16	313	DD6	C12-C11-C13	-5.17	110.19	118.09
30	A	815	CLA	C2B-C1B-NB	5.17	115.69	110.33
30	16	305	CLA	O2D-CGD-CBD	5.17	120.27	111.23
38	5	310	KC1	C2D-C1D-ND	5.17	115.69	110.33
30	5	308	CLA	C2B-C1B-NB	5.17	115.68	110.33
38	4	308	KC1	C2D-C1D-ND	5.17	115.68	110.33
30	B	833	CLA	C2B-C1B-NB	5.16	115.68	110.33
30	B	814	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
30	B	824	CLA	C2D-C1D-ND	5.16	115.23	110.13
30	16	307	CLA	O2D-CGD-CBD	5.16	120.25	111.23
38	10	310	KC1	O2D-CGD-CBD	5.16	120.25	111.23
30	5	304	CLA	C2B-C1B-NB	5.16	115.68	110.33
30	A	828	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
30	B	822	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
37	10	316	A86	C25-C26-C27	-5.16	120.05	127.28
30	B	818	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
30	15	314	CLA	C2C-C1C-NC	5.16	115.40	109.98
30	3	302	CLA	C3B-C2B-C1B	-5.15	101.09	107.17
39	6	303	DD6	C21-C20-C19	-5.15	108.45	114.24
30	L	202	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
38	3	308	KC1	C2B-C1B-NB	5.15	115.23	110.13
37	14	317	A86	O4-C38-C39	5.15	120.28	111.09
30	6	310	CLA	C2C-C1C-NC	5.15	115.39	109.98
30	B	824	CLA	C2B-C1B-NB	5.15	115.67	110.33
30	F	202	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
38	14	311	KC1	C3C-C4C-NC	5.15	115.42	109.90
30	14	307	CLA	C4A-NA-C1A	-5.15	104.33	106.68
30	1	305	CLA	C2B-C1B-NB	5.15	115.67	110.33
30	5	304	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
30	3	306	CLA	C4A-NA-C1A	-5.14	104.33	106.68
30	12	306	CLA	C2C-C1C-NC	5.14	115.39	109.98
38	8	310	KC1	O2D-CGD-CBD	5.14	120.22	111.23
30	A	839	CLA	C2B-C1B-NB	5.14	115.66	110.33
38	3	311	KC1	C2D-C1D-ND	5.14	115.66	110.33
38	10	312	KC1	C2D-C1D-ND	5.14	115.66	110.33
30	3	301	CLA	O2D-CGD-CBD	5.14	120.22	111.23
39	10	314	DD6	C7-C6-C8	-5.14	110.24	118.09
30	2	310	CLA	C2B-C1B-NB	5.14	115.66	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	5	314	DD6	C21-C20-C19	-5.14	108.47	114.24
30	A	813	CLA	C2B-C1B-NB	5.14	115.65	110.33
30	A	808	CLA	C2B-C1B-NB	5.14	115.65	110.33
30	A	825	CLA	C2B-C1B-NB	5.14	115.65	110.33
30	B	820	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
30	B	829	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
30	9	308	CLA	CAA-C2A-C3A	-5.13	99.12	113.00
30	8	308	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	14	302	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
38	10	312	KC1	C1A-NA-C4A	-5.13	104.34	106.68
30	11	310	CLA	CHD-C4C-C3C	-5.13	117.29	124.77
30	B	812	CLA	C2B-C1B-NB	5.13	115.65	110.33
39	6	319	DD6	C24-C1-C2	-5.13	110.94	119.01
30	A	812	CLA	C2C-C1C-NC	5.13	115.37	109.98
30	8	305	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	B	828	CLA	C2C-C1C-NC	5.13	115.37	109.98
30	15	304	CLA	C2C-C1C-NC	5.13	115.37	109.98
38	13	305	KC1	C1A-C2A-C3A	-5.13	102.56	107.28
30	10	303	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	14	303	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	B	835	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	13	309	CLA	C2B-C1B-NB	5.13	115.64	110.33
30	A	832	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	5	302	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
30	B	821	CLA	O2D-CGD-CBD	5.13	120.19	111.23
30	3	303	CLA	C3B-C2B-C1B	-5.13	101.13	107.17
39	6	321	DD6	O1-C15-C14	-5.13	102.19	116.88
30	16	309	CLA	C2B-C1B-NB	5.13	115.64	110.33
30	16	306	CLA	C2D-C1D-ND	5.13	115.20	110.13
30	B	815	CLA	C2B-C1B-NB	5.12	115.64	110.33
30	9	306	CLA	C2B-C1B-NB	5.12	115.64	110.33
37	9	315	A86	C4-C3-C2	-5.12	113.04	123.52
30	B	815	CLA	CHD-C4C-C3C	-5.12	117.30	124.77
37	10	316	A86	O4-C38-C39	5.12	120.22	111.09
30	8	304	CLA	CMD-C2D-C1D	5.12	133.75	124.73
30	15	313	CLA	C2B-C1B-NB	5.12	115.64	110.33
38	8	312	KC1	C3C-C4C-NC	5.12	115.39	109.90
38	9	312	KC1	C2B-C1B-NB	5.12	115.19	110.13
30	16	306	CLA	O2D-CGD-CBD	5.12	120.18	111.23
37	2u	203	A86	C25-C26-C27	-5.12	120.10	127.28
38	13	308	KC1	C2D-C1D-ND	5.12	115.64	110.33
30	16	305	CLA	C2C-C1C-NC	5.12	115.36	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	11	312	KC1	C2D-C1D-ND	5.12	115.63	110.33
30	16	309	CLA	C2C-C1C-NC	5.12	115.36	109.98
30	L	203	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
37	2	318	A86	O4-C38-C39	5.12	120.21	111.09
30	B	825	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
30	B	801	CLA	O2D-CGD-CBD	5.12	120.17	111.23
30	A	815	CLA	CHD-C4C-C3C	-5.12	117.31	124.77
37	2	319	A86	O4-C38-C39	5.12	120.21	111.09
37	14	315	A86	O4-C38-C39	5.12	120.21	111.09
37	15	322	A86	O4-C38-C39	5.11	120.21	111.09
30	A	820	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
30	6	304	CLA	C2B-C1B-NB	5.11	115.63	110.33
37	11	314	A86	C41-C32-C31	-5.11	105.90	110.47
30	16	303	CLA	C2B-C1B-NB	5.11	115.63	110.33
30	5	311	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
30	B	824	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
30	6	314	CLA	C4A-NA-C1A	-5.11	104.35	106.68
38	11	305	KC1	C2B-C1B-NB	5.11	115.18	110.13
30	12	303	CLA	C2C-C1C-NC	5.11	115.35	109.98
30	B	814	CLA	C2B-C1B-NB	5.11	115.62	110.33
30	B	851	CLA	C2B-C1B-NB	5.11	115.62	110.33
30	F	203	CLA	C2B-C1B-NB	5.11	115.62	110.33
37	11	314	A86	O4-C38-C39	5.11	120.19	111.09
30	A	802	CLA	C2C-C1C-NC	5.11	115.34	109.98
30	15	304	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
39	6	318	DD6	C13-C11-C10	-5.10	110.98	119.01
30	A	811	CLA	C2B-C1B-NB	5.10	115.62	110.33
30	2	308	CLA	C2B-C1B-NB	5.10	115.62	110.33
30	5	311	CLA	C2C-C1C-NC	5.10	115.34	109.98
37	10	302	A86	C36-C31-C32	-5.10	114.63	119.70
30	9	303	CLA	C2B-C1B-NB	5.10	115.62	110.33
38	9	312	KC1	C2D-C1D-ND	5.10	115.62	110.33
30	11	306	CLA	O2D-CGD-CBD	5.10	120.15	111.23
37	12	316	A86	C3-C2-C1	-5.10	120.12	127.28
30	16	302	CLA	C4A-NA-C1A	-5.10	104.35	106.68
38	14	306	KC1	C1A-NA-C4A	-5.10	104.35	106.68
30	15	311	CLA	C2B-C1B-NB	5.10	115.61	110.33
30	B	837	CLA	C2B-C1B-NB	5.10	115.61	110.33
30	A	840	CLA	C4A-NA-C1A	-5.10	104.35	106.68
39	6	318	DD6	C21-C20-C15	-5.10	113.92	122.30
30	1	307	CLA	C2C-C1C-NC	5.10	115.33	109.98
39	6	318	DD6	C24-C1-C2	-5.10	110.99	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	839	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
30	4	306	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
30	A	840	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
30	A	844	CLA	C2B-C1B-NB	5.09	115.61	110.33
30	9	309	CLA	C2C-C1C-NC	5.09	115.33	109.98
30	1	307	CLA	C2B-C1B-NB	5.09	115.61	110.33
30	B	804	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
30	7	312	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
29	A	801	CL0	CMA-C3A-C4A	-5.09	103.64	114.61
30	11	309	CLA	CHD-C4C-C3C	-5.09	117.35	124.77
30	A	820	CLA	C2D-C1D-ND	5.09	115.16	110.13
30	4	301	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
37	2	318	A86	C3-C2-C1	-5.09	120.15	127.28
30	B	815	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
30	12	321	CLA	C4A-NA-C1A	-5.09	104.36	106.68
39	6	321	DD6	C-C1-C24	-5.09	110.32	118.09
30	9	301	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
30	4	309	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
30	1	303	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
30	3	305	CLA	C2B-C1B-NB	5.08	115.60	110.33
30	B	817	CLA	O2D-CGD-CBD	5.08	120.11	111.23
30	5	302	CLA	C2B-C1B-NB	5.08	115.59	110.33
30	14	312	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
37	6	320	A86	C4-C3-C2	-5.08	113.13	123.52
30	11	309	CLA	C2B-C1B-NB	5.08	115.59	110.33
30	15	309	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
37	14	314	A86	O4-C38-C39	5.07	120.14	111.09
30	2	307	CLA	CMD-C2D-C1D	5.07	133.66	124.73
37	15	316	A86	O4-C38-C39	5.07	120.14	111.09
38	13	310	KC1	O2D-CGD-CBD	5.07	120.10	111.23
30	F	202	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
30	9	307	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
30	A	828	CLA	C2B-C1B-NB	5.07	115.59	110.33
37	4	317	A86	O4-C38-C39	5.07	120.13	111.09
30	15	311	CLA	C2C-C1C-NC	5.07	115.31	109.98
30	13	309	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
30	B	803	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
38	4	307	KC1	C2D-C1D-ND	5.07	115.58	110.33
30	A	809	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
38	11	307	KC1	O2D-CGD-CBD	5.07	120.09	111.23
30	16	303	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
30	5	309	CLA	C2B-C1B-NB	5.07	115.58	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	305	KC1	O2D-CGD-CBD	5.07	120.09	111.23
38	8	310	KC1	C3C-C4C-NC	5.07	115.33	109.90
30	2	313	CLA	C2B-C1B-NB	5.07	115.58	110.33
30	2	305	CLA	CAA-C2A-C3A	-5.07	99.31	113.00
30	B	807	CLA	O2D-CGD-CBD	5.06	120.08	111.23
30	B	806	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
30	5	308	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
30	B	821	CLA	C2B-C1B-NB	5.06	115.58	110.33
30	15	303	CLA	C4A-NA-C1A	-5.06	104.37	106.68
39	2	315	DD6	C24-C1-C2	-5.06	111.05	119.01
30	15	312	CLA	C2D-C1D-ND	5.06	115.13	110.13
30	A	804	CLA	C2B-C1B-NB	5.06	115.57	110.33
39	12	317	DD6	C7-C6-C8	-5.06	110.36	118.09
30	2	310	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
37	10	316	A86	C4-C3-C2	-5.06	113.17	123.52
38	1	306	KC1	O2D-CGD-CBD	5.06	120.07	111.23
38	5	306	KC1	C3D-C4D-ND	5.06	117.25	110.20
30	7	307	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
38	11	311	KC1	O2D-CGD-CBD	5.05	120.06	111.23
30	10	304	CLA	C2C-C1C-NC	5.05	115.29	109.98
37	5	301	A86	O4-C38-C39	5.05	120.10	111.09
30	12	302	CLA	C2C-C1C-NC	5.05	115.29	109.98
30	A	840	CLA	C2C-C1C-NC	5.05	115.29	109.98
30	2	303	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
39	6	319	DD6	C-C1-C24	-5.05	110.37	118.09
37	4	315	A86	O4-C38-C39	5.05	120.09	111.09
30	B	826	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
37	6	320	A86	O4-C38-C39	5.05	120.09	111.09
30	A	829	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
30	8	309	CLA	C2B-C1B-NB	5.05	115.56	110.33
30	J	101	CLA	C2C-C1C-NC	5.05	115.28	109.98
30	16	308	CLA	C2C-C1C-NC	5.05	115.28	109.98
30	7	304	CLA	C4A-NA-C1A	-5.05	104.38	106.68
30	12	310	CLA	O2D-CGD-CBD	5.05	120.05	111.23
30	B	812	CLA	C2C-C1C-NC	5.04	115.28	109.98
30	4	304	CLA	O2D-CGD-CBD	5.04	120.05	111.23
30	A	823	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
30	A	822	CLA	C2D-C1D-ND	5.04	115.12	110.13
37	15	315	A86	O4-C38-C39	5.04	120.08	111.09
30	A	810	CLA	C2C-C1C-NC	5.04	115.28	109.98
30	14	307	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
37	5	315	A86	O4-C38-C39	5.04	120.08	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	303	CLA	C2B-C1B-NB	5.04	115.55	110.33
30	16	308	CLA	O2D-CGD-CBD	5.04	120.04	111.23
30	B	802	CLA	CAA-C2A-C3A	-5.04	99.39	113.00
37	7	316	A86	C3-C2-C1	-5.04	120.22	127.28
37	16	312	A86	C36-C31-C32	-5.04	114.70	119.70
30	A	810	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
38	1	306	KC1	C3B-C2B-C1B	-5.03	102.28	107.05
30	7	311	CLA	C2B-C1B-NB	5.03	115.54	110.33
38	11	312	KC1	C2B-C1B-NB	5.03	115.10	110.13
30	14	303	CLA	O2D-CGD-CBD	5.03	120.02	111.23
30	9	301	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
30	15	306	CLA	C2B-C1B-NB	5.03	115.54	110.33
30	B	816	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
39	12	315	DD6	C24-C1-C2	-5.03	111.10	119.01
38	13	312	KC1	O2D-CGD-CBD	5.03	120.02	111.23
39	6	319	DD6	C21-C20-C19	-5.03	108.59	114.24
30	16	306	CLA	C2B-C1B-NB	5.02	115.54	110.33
30	A	823	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
30	A	814	CLA	CAC-C3C-C4C	5.02	131.33	124.79
30	6	314	CLA	C2C-C1C-NC	5.02	115.26	109.98
30	2	307	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
30	B	806	CLA	C2B-C1B-NB	5.02	115.54	110.33
30	12	303	CLA	C2B-C1B-NB	5.02	115.53	110.33
30	B	808	CLA	C2C-C1C-NC	5.02	115.26	109.98
30	J	101	CLA	C2D-C1D-ND	5.02	115.10	110.13
30	14	307	CLA	CAC-C3C-C4C	5.02	131.32	124.79
30	A	820	CLA	C2C-C1C-NC	5.02	115.26	109.98
30	2	307	CLA	C2C-C1C-NC	5.02	115.26	109.98
30	B	822	CLA	CHD-C4C-C3C	-5.02	117.45	124.77
37	2	318	A86	C4-C5-C6	-5.02	120.24	127.28
30	9	301	CLA	CHD-C4C-C3C	-5.02	117.46	124.77
39	10	314	DD6	C12-C11-C13	-5.02	110.42	118.09
30	B	820	CLA	C2B-C1B-NB	5.02	115.53	110.33
37	6	320	A86	O1-C20-C15	5.02	61.24	59.23
38	14	306	KC1	C3B-C2B-C1B	-5.01	102.30	107.05
38	5	306	KC1	O2D-CGD-CBD	5.01	119.99	111.23
39	12	315	DD6	C21-C20-C19	-5.01	108.61	114.24
30	12	304	CLA	C4A-NA-C1A	-5.01	104.39	106.68
30	A	825	CLA	C2C-C1C-NC	5.01	115.24	109.98
30	3	307	CLA	CHD-C4C-C3C	-5.01	117.47	124.77
30	3	307	CLA	C2B-C1B-NB	5.01	115.52	110.33
38	3	308	KC1	C1A-C2A-C3A	-5.01	102.68	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	309	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
37	11	301	A86	O4-C38-C39	5.01	120.02	111.09
30	A	840	CLA	C2B-C1B-NB	5.01	115.52	110.33
30	B	801	CLA	CMB-C2B-C1B	5.01	133.04	125.42
38	4	308	KC1	CHC-C1C-C2C	-5.01	117.13	125.03
30	1	302	CLA	C2B-C1B-NB	5.00	115.51	110.33
39	2	316	DD6	C7-C6-C8	-5.00	110.45	118.09
30	B	811	CLA	C2D-C1D-ND	5.00	115.07	110.13
38	13	305	KC1	C3C-C4C-NC	5.00	115.26	109.90
38	9	311	KC1	C3D-C4D-ND	5.00	117.17	110.20
30	A	819	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
30	A	831	CLA	CMD-C2D-C1D	5.00	133.53	124.73
30	B	805	CLA	C2C-C1C-NC	5.00	115.23	109.98
37	8	318	A86	O4-C38-C39	4.99	120.00	111.09
30	5	309	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
39	4	316	DD6	C21-C20-C19	-4.99	108.63	114.24
30	A	830	CLA	C2B-C1B-NB	4.99	115.50	110.33
37	4	317	A86	C41-C32-C31	-4.99	106.01	110.47
38	10	306	KC1	C3C-C4C-NC	4.99	115.25	109.90
38	4	308	KC1	C1A-C2A-C3A	-4.99	102.69	107.28
30	2	301	CLA	CHD-C4C-C3C	-4.99	117.50	124.77
39	15	318	DD6	C35-C36-C31	-4.99	110.12	120.50
30	B	828	CLA	CHD-C4C-C3C	-4.99	117.50	124.77
39	3	312	DD6	C7-C6-C8	-4.99	110.47	118.09
38	1	306	KC1	C1A-NA-C4A	-4.99	104.40	106.68
30	10	309	CLA	C2B-C1B-NB	4.99	115.50	110.33
30	16	301	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
30	B	804	CLA	C2B-C1B-NB	4.98	115.50	110.33
37	3	315	A86	C4-C5-C6	-4.98	120.29	127.28
30	B	807	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
30	6	315	CLA	C2B-C1B-NB	4.98	115.49	110.33
30	7	307	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
30	2	311	CLA	C2B-C1B-NB	4.98	115.49	110.33
37	15	317	A86	O4-C38-C39	4.98	119.97	111.09
30	A	820	CLA	C2B-C1B-NB	4.98	115.49	110.33
38	16	304	KC1	CMA-C3A-C2A	-4.98	116.37	128.43
30	4	306	CLA	C2B-C1B-NB	4.98	115.49	110.33
30	B	821	CLA	C2C-C1C-NC	4.98	115.21	109.98
38	14	306	KC1	C3C-C4C-NC	4.98	115.23	109.90
30	4	301	CLA	O2D-CGD-CBD	4.98	119.93	111.23
30	A	832	CLA	C2B-C1B-NB	4.98	115.49	110.33
30	7	310	CLA	C4A-NA-C1A	-4.98	104.41	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	823	CLA	C2B-C1B-NB	4.97	115.48	110.33
30	7	307	CLA	C2B-C1B-NB	4.97	115.48	110.33
30	A	818	CLA	C2B-C1B-NB	4.97	115.48	110.33
30	4	305	CLA	C2B-C1B-NB	4.97	115.48	110.33
30	J	101	CLA	C4A-NA-C1A	-4.97	104.41	106.68
30	2	305	CLA	C2B-C1B-NB	4.97	115.48	110.33
30	8	309	CLA	C2C-C1C-NC	4.97	115.20	109.98
30	16	310	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
30	3	302	CLA	C4A-NA-C1A	-4.97	104.41	106.68
39	4	313	DD6	C24-C1-C2	-4.97	111.20	119.01
30	3	301	CLA	C2C-C1C-NC	4.97	115.20	109.98
39	7	317	DD6	C21-C20-C15	-4.97	114.13	122.30
39	8	317	DD6	O1-C20-C21	-4.97	109.50	115.05
30	2	305	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
37	14	318	A86	C41-C32-C31	-4.96	106.03	110.47
30	A	837	CLA	C2C-C1C-NC	4.96	115.20	109.98
30	14	309	CLA	O2D-CGD-CBD	4.96	119.91	111.23
30	B	810	CLA	C2B-C1B-NB	4.96	115.47	110.33
30	9	302	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
30	12	308	CLA	C2C-C1C-NC	4.96	115.19	109.98
38	13	310	KC1	CHD-C4C-C3C	-4.96	116.08	125.23
30	14	304	CLA	O2D-CGD-CBD	4.96	119.90	111.23
30	B	826	CLA	C2C-C1C-NC	4.96	115.19	109.98
30	8	302	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
30	15	308	CLA	O2D-CGD-CBD	4.96	119.90	111.23
30	B	836	CLA	C2B-C1B-NB	4.96	115.47	110.33
30	12	302	CLA	C2B-C1B-NB	4.96	115.47	110.33
39	15	318	DD6	C7-C6-C8	-4.96	110.51	118.09
30	A	839	CLA	C4A-NA-C1A	-4.95	104.42	106.68
30	6	307	CLA	C4A-NA-C1A	-4.95	104.42	106.68
38	4	310	KC1	C2D-C1D-ND	4.95	115.46	110.33
30	3	310	CLA	C2B-C1B-NB	4.95	115.46	110.33
30	7	304	CLA	C2C-C1C-NC	4.95	115.18	109.98
30	A	827	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
39	11	313	DD6	C7-C6-C8	-4.95	110.53	118.09
30	12	303	CLA	C4A-NA-C1A	-4.95	104.42	106.68
30	B	822	CLA	C2B-C1B-NB	4.95	115.46	110.33
30	B	834	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
30	10	307	CLA	C2B-C1B-NB	4.95	115.46	110.33
30	10	304	CLA	C4A-NA-C1A	-4.95	104.42	106.68
30	6	315	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
38	16	311	KC1	O2D-CGD-CBD	4.94	119.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	843	CLA	C2C-C1C-NC	4.94	115.17	109.98
38	9	310	KC1	C1A-NA-C4A	-4.94	104.42	106.68
38	8	311	KC1	C3C-C4C-NC	4.94	115.19	109.90
30	14	310	CLA	C2C-C1C-NC	4.94	115.17	109.98
30	A	809	CLA	C2B-C1B-NB	4.94	115.45	110.33
30	14	304	CLA	C2B-C1B-NB	4.94	115.45	110.33
30	16	303	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
30	14	313	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
37	2u	205	A86	C25-C24-C1	-4.94	112.82	126.36
37	6	320	A86	C21-C20-C15	-4.94	107.41	123.35
37	13	315	A86	C25-C26-C27	-4.94	120.35	127.28
38	8	314	KC1	C3C-C4C-NC	4.94	115.19	109.90
30	3	309	CLA	C2B-C1B-NB	4.94	115.44	110.33
30	B	822	CLA	C4A-NA-C1A	-4.94	104.43	106.68
30	A	835	CLA	C2C-C1C-NC	4.94	115.17	109.98
30	15	307	CLA	C2B-C1B-NB	4.94	115.44	110.33
38	16	311	KC1	C3C-C4C-NC	4.93	115.19	109.90
30	9	305	CLA	C2B-C1B-NB	4.93	115.44	110.33
30	16	307	CLA	C2B-C1B-NB	4.93	115.44	110.33
37	4	312	A86	C41-C32-C31	-4.93	106.06	110.47
30	5	307	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
37	16	312	A86	C9-C10-C11	-4.93	112.70	126.64
30	A	838	CLA	C2C-C1C-NC	4.93	115.16	109.98
30	10	305	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
30	A	819	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
37	9	315	A86	O4-C38-C39	4.93	119.88	111.09
30	A	807	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
30	B	825	CLA	C2B-C1B-NB	4.93	115.44	110.33
37	9	313	A86	C3-C2-C1	-4.93	120.36	127.28
30	6	309	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
37	14	316	A86	O4-C38-C39	4.93	119.87	111.09
30	6	304	CLA	C4A-NA-C1A	-4.93	104.43	106.68
38	13	306	KC1	CHD-C4C-C3C	-4.92	116.15	125.23
30	F	203	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
37	15	315	A86	C4-C3-C2	4.92	133.59	123.52
30	A	824	CLA	O2D-CGD-CBD	4.92	119.83	111.23
30	6	315	CLA	C2C-C1C-NC	4.92	115.15	109.98
30	7	306	CLA	O2D-CGD-CBD	4.92	119.83	111.23
30	2	309	CLA	C2B-C1B-NB	4.92	115.43	110.33
38	8	314	KC1	CHD-C4C-C3C	-4.92	116.16	125.23
30	B	807	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
30	13	304	CLA	C3B-C2B-C1B	-4.92	101.37	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	818	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
30	L	202	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
30	B	814	CLA	C2C-C1C-NC	4.92	115.15	109.98
30	15	305	CLA	C2C-C1C-NC	4.92	115.15	109.98
30	B	833	CLA	O2D-CGD-CBD	4.92	119.83	111.23
37	4	314	A86	C7-C6-C8	4.92	125.60	118.09
30	B	825	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
38	13	311	KC1	C3B-C2B-C1B	-4.91	102.40	107.05
30	4	305	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
30	A	812	CLA	C2B-C1B-NB	4.91	115.42	110.33
30	6	317	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
30	A	825	CLA	CHD-C4C-C3C	-4.91	117.61	124.77
38	4	308	KC1	O2D-CGD-CBD	4.91	119.81	111.23
30	A	842	CLA	C2B-C1B-NB	4.91	115.42	110.33
30	A	838	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
30	2	309	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
37	14	318	A86	O4-C38-C39	4.91	119.84	111.09
39	6	318	DD6	O1-C15-C14	-4.90	102.83	116.88
30	16	307	CLA	C2C-C1C-NC	4.90	115.13	109.98
30	A	809	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
37	14	301	A86	C41-C32-C31	-4.90	106.08	110.47
30	12	303	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
30	A	813	CLA	C2C-C1C-NC	4.90	115.13	109.98
30	B	838	CLA	O2D-CGD-CBD	4.90	119.80	111.23
39	16	313	DD6	C21-C20-C19	-4.90	108.74	114.24
38	1	308	KC1	O2D-CGD-CBD	4.90	119.79	111.23
37	2	319	A86	C3-C2-C1	-4.90	120.41	127.28
30	15	312	CLA	C2C-C1C-NC	4.90	115.13	109.98
30	2	313	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
39	6	319	DD6	C21-C20-C15	-4.90	114.24	122.30
30	2	310	CLA	O2D-CGD-CBD	4.90	119.79	111.23
30	B	837	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
30	8	305	CLA	C2B-C1B-NB	4.89	115.40	110.33
30	16	310	CLA	C2C-C1C-NC	4.89	115.12	109.98
38	8	310	KC1	C2B-C1B-NB	4.89	114.97	110.13
37	11	301	A86	C25-C26-C27	-4.89	120.42	127.28
30	A	844	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
30	14	305	CLA	C2C-C1C-NC	4.89	115.12	109.98
30	A	812	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
30	16	308	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
30	9	308	CLA	C4A-NA-C1A	-4.89	104.45	106.68
30	B	821	CLA	C2D-C1D-ND	4.89	114.97	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	827	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
38	8	307	KC1	C3D-C4D-ND	4.89	117.02	110.20
38	6	313	KC1	CHD-C4C-C3C	-4.89	116.21	125.23
37	1	309	A86	O4-C38-C39	4.89	119.81	111.09
38	6	308	KC1	O2D-CGD-CBD	4.89	119.77	111.23
38	10	306	KC1	C2D-C1D-ND	4.89	115.39	110.33
30	9	305	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
38	5	310	KC1	C1A-NA-C4A	-4.88	104.45	106.68
30	14	307	CLA	C2C-C1C-NC	4.88	115.11	109.98
30	B	835	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
38	7	308	KC1	CHD-C4C-C3C	-4.88	116.23	125.23
30	A	826	CLA	C2B-C1B-NB	4.88	115.39	110.33
30	B	823	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
30	A	807	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
30	12	312	CLA	C2C-C1C-NC	4.88	115.11	109.98
30	15	314	CLA	C2B-C1B-NB	4.88	115.39	110.33
30	3	305	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
30	2	310	CLA	C2C-C1C-NC	4.88	115.11	109.98
38	5	306	KC1	C1A-NA-C4A	-4.88	104.45	106.68
38	8	312	KC1	C2A-C1A-NA	4.88	117.15	109.34
30	A	808	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
37	14	316	A86	C3-C2-C1	-4.88	120.44	127.28
38	6	311	KC1	C3C-C4C-NC	4.87	115.12	109.90
37	13	315	A86	C41-C32-C31	-4.87	106.11	110.47
30	1	301	CLA	C2B-C1B-NB	4.87	115.38	110.33
30	7	306	CLA	C2B-C1B-NB	4.87	115.38	110.33
38	2	314	KC1	C3C-C4C-NC	4.87	115.12	109.90
30	B	822	CLA	C3D-C4D-ND	4.87	117.91	109.99
30	B	811	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
30	8	304	CLA	O2D-CGD-CBD	4.87	119.74	111.23
30	9	307	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
30	B	830	CLA	CHD-C1D-ND	-4.87	117.95	124.80
30	A	836	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
37	10	315	A86	O4-C38-C39	4.87	119.77	111.09
30	5	303	CLA	C2B-C1B-NB	4.87	115.37	110.33
30	6	309	CLA	C2B-C1B-NB	4.87	115.37	110.33
37	15	322	A86	C36-C31-C32	-4.87	114.87	119.70
30	A	834	CLA	C2B-C1B-NB	4.87	115.37	110.33
38	6	311	KC1	C3D-C4D-ND	4.87	116.98	110.20
38	10	312	KC1	C3D-C4D-ND	4.87	116.98	110.20
30	10	305	CLA	C2C-C1C-NC	4.87	115.09	109.98
30	16	305	CLA	C2B-C1B-NB	4.86	115.37	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	312	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
30	4	309	CLA	C2C-C1C-NC	4.86	115.09	109.98
39	3	312	DD6	C12-C11-C13	-4.86	110.66	118.09
38	7	308	KC1	C3C-C4C-NC	4.86	115.11	109.90
30	4	311	CLA	C2B-C1B-NB	4.86	115.37	110.33
39	12	317	DD6	C35-C36-C31	-4.86	110.38	120.50
30	4	301	CLA	C2C-C1C-NC	4.86	115.09	109.98
30	12	321	CLA	C2C-C1C-NC	4.86	115.09	109.98
30	B	802	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
38	8	307	KC1	CHD-C4C-C3C	-4.86	116.27	125.23
30	5	307	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
30	12	312	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
30	2	311	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
30	3	310	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
30	2	308	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
38	12	309	KC1	CHD-C4C-C3C	-4.86	116.27	125.23
30	16	308	CLA	C4A-NA-C1A	-4.86	104.46	106.68
38	13	306	KC1	C3C-C4C-NC	4.86	115.10	109.90
30	B	804	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
30	A	807	CLA	C2B-C1B-NB	4.86	115.36	110.33
30	7	311	CLA	O2D-CGD-CBD	4.85	119.72	111.23
30	15	313	CLA	C2C-C1C-NC	4.85	115.08	109.98
37	8	315	A86	C4-C5-C6	-4.85	120.47	127.28
30	9	301	CLA	C2B-C1B-NB	4.85	115.36	110.33
30	16	301	CLA	C2B-C1B-NB	4.85	115.36	110.33
37	7	315	A86	C23-C16-C22	-4.85	100.32	107.37
39	7	314	DD6	C21-C20-C19	-4.85	108.79	114.24
30	13	303	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
30	15	310	CLA	C2C-C1C-NC	4.85	115.08	109.98
30	14	310	CLA	O2D-CGD-CBD	4.85	119.71	111.23
30	16	309	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
38	6	312	KC1	C3D-C4D-ND	4.85	116.96	110.20
30	4	311	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
38	8	306	KC1	C3D-C4D-ND	4.85	116.96	110.20
30	B	823	CLA	C2C-C1C-NC	4.85	115.07	109.98
37	12	316	A86	O4-C38-C39	4.85	119.73	111.09
30	13	301	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
30	A	811	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
39	9	314	DD6	C21-C20-C19	-4.85	108.80	114.24
30	F	201	CLA	C2B-C1B-NB	4.85	115.35	110.33
30	A	810	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
38	3	311	KC1	C3D-C4D-ND	4.85	116.96	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	15	319	DD6	C35-C36-C31	-4.85	110.42	120.50
39	2	315	DD6	C7-C6-C8	-4.85	110.69	118.09
37	2u	205	A86	C4-C5-C6	-4.84	120.48	127.28
30	L	203	CLA	O2D-CGD-CBD	4.84	119.70	111.23
29	A	801	CL0	CAA-C2A-C3A	-4.84	99.91	113.00
30	15	308	CLA	C2C-C1C-NC	4.84	115.07	109.98
38	9	310	KC1	C3D-C4D-ND	4.84	116.95	110.20
30	9	305	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
30	8	304	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
30	L	202	CLA	C2B-C1B-NB	4.84	115.34	110.33
38	13	311	KC1	C1A-NA-C4A	-4.84	104.47	106.68
30	B	816	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
39	8	316	DD6	C21-C20-C19	-4.84	108.81	114.24
30	B	834	CLA	C2C-C1C-NC	4.84	115.06	109.98
30	A	834	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
30	7	304	CLA	C2B-C1B-NB	4.83	115.34	110.33
30	6	309	CLA	C4A-NA-C1A	-4.83	104.47	106.68
30	A	833	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
30	L	203	CLA	C2B-C1B-NB	4.83	115.34	110.33
37	16	312	A86	O4-C38-C39	4.83	119.70	111.09
38	5	312	KC1	C3C-C4C-NC	4.83	115.08	109.90
30	2	305	CLA	C2C-C1C-NC	4.83	115.06	109.98
38	13	311	KC1	CHD-C4C-C3C	-4.83	116.32	125.23
30	14	304	CLA	C2C-C1C-NC	4.83	115.05	109.98
30	8	302	CLA	C4A-NA-C1A	-4.83	104.48	106.68
30	11	308	CLA	O2D-CGD-CBD	4.83	119.67	111.23
30	B	816	CLA	C2B-C1B-NB	4.83	115.33	110.33
38	10	306	KC1	CHD-C4C-C3C	-4.83	116.33	125.23
30	3	307	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
38	14	308	KC1	C2D-C1D-ND	4.83	115.33	110.33
30	12	310	CLA	C2C-C1C-NC	4.83	115.05	109.98
38	8	312	KC1	C3D-C4D-ND	4.83	116.93	110.20
30	8	303	CLA	C2C-C1C-NC	4.82	115.05	109.98
30	13	303	CLA	C2C-C1C-NC	4.82	115.05	109.98
30	2	301	CLA	C1-O2A-CGA	4.82	128.32	116.65
30	12	306	CLA	C2B-C1B-NB	4.82	115.33	110.33
30	5	309	CLA	C2C-C1C-NC	4.82	115.05	109.98
38	9	304	KC1	C3D-C4D-ND	4.82	116.92	110.20
30	A	806	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
38	5	310	KC1	C3C-C4C-NC	4.82	115.06	109.90
30	14	307	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
30	B	827	CLA	C2C-C1C-NC	4.82	115.04	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	314	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
30	B	827	CLA	CMD-C2D-C1D	4.82	133.21	124.73
30	7	303	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
30	B	833	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
30	10	309	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
37	3	314	A86	C41-C32-C31	-4.82	106.16	110.47
30	B	802	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
30	4	303	CLA	C2C-C1C-NC	4.81	115.04	109.98
30	3	301	CLA	C2B-C1B-NB	4.81	115.32	110.33
30	A	804	CLA	C4A-NA-C1A	-4.81	104.48	106.68
30	A	825	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
30	5	303	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
30	7	304	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
39	2	317	DD6	C7-C6-C8	-4.81	110.74	118.09
38	6	313	KC1	C3C-C4C-NC	4.81	115.05	109.90
30	A	842	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
30	15	302	CLA	CHD-C1D-ND	-4.81	118.03	124.80
30	15	302	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
30	A	817	CLA	O2D-CGD-CBD	4.81	119.64	111.23
30	B	801	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
38	7	313	KC1	C3D-C4D-ND	4.81	116.90	110.20
38	10	312	KC1	CHD-C4C-C3C	-4.81	116.36	125.23
39	7	314	DD6	C35-C36-C31	-4.81	110.50	120.50
30	A	804	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
30	A	813	CLA	O2D-CGD-CBD	4.81	119.63	111.23
30	14	307	CLA	CHD-C1D-ND	-4.80	118.04	124.80
30	15	306	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
30	15	302	CLA	C3D-C4D-ND	4.80	117.79	109.99
30	2	309	CLA	C2C-C1C-NC	4.80	115.03	109.98
30	3	302	CLA	C2C-C1C-NC	4.80	115.03	109.98
30	A	814	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
30	B	838	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
30	4	303	CLA	C2B-C1B-NB	4.80	115.30	110.33
30	A	812	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
38	9	312	KC1	C3D-C4D-ND	4.80	116.89	110.20
30	6	317	CLA	C2C-C1C-NC	4.80	115.02	109.98
38	6	312	KC1	CHD-C4C-C3C	-4.80	116.38	125.23
30	12	312	CLA	C2B-C1B-NB	4.80	115.30	110.33
30	A	839	CLA	C3B-C2B-C1B	-4.80	101.52	107.17
30	10	307	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
30	14	304	CLA	C3B-C2B-C1B	-4.80	101.52	107.17
38	1	306	KC1	C3D-C4D-ND	4.79	116.89	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	301	CLA	C2C-C1C-NC	4.79	115.02	109.98
38	13	311	KC1	C3D-C4D-ND	4.79	116.88	110.20
30	13	302	CLA	C2C-C1C-NC	4.79	115.02	109.98
30	A	817	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
30	1	305	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
30	6	307	CLA	C2C-C1C-NC	4.79	115.01	109.98
30	15	308	CLA	C2B-C1B-NB	4.79	115.29	110.33
30	10	311	CLA	O2D-CGD-CBD	4.79	119.60	111.23
30	15	311	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
30	A	811	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
38	10	310	KC1	C3D-C4D-ND	4.79	116.87	110.20
30	2u	202	CLA	C2C-C1C-NC	4.79	115.01	109.98
30	A	822	CLA	C2C-C1C-NC	4.78	115.01	109.98
30	F	202	CLA	C2C-C1C-NC	4.78	115.01	109.98
38	2	314	KC1	C3D-C4D-ND	4.78	116.87	110.20
30	9	303	CLA	O2D-CGD-CBD	4.78	119.59	111.23
38	9	310	KC1	C3C-C4C-NC	4.78	115.02	109.90
30	B	802	CLA	C2B-C1B-NB	4.78	115.28	110.33
38	1	308	KC1	C3D-C4D-ND	4.78	116.87	110.20
30	A	835	CLA	C4A-NA-C1A	-4.78	104.50	106.68
38	5	305	KC1	O2D-CGD-CBD	4.78	119.59	111.23
30	B	839	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
30	8	304	CLA	C2B-C1B-NB	4.78	115.28	110.33
38	8	312	KC1	CHD-C4C-C3C	-4.78	116.42	125.23
30	2	308	CLA	O2D-CGD-CBD	4.78	119.58	111.23
30	B	815	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
30	4	302	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
30	16	302	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
30	B	806	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
30	B	808	CLA	C2B-C1B-NB	4.78	115.28	110.33
38	9	310	KC1	CHD-C4C-C3C	-4.77	116.42	125.23
30	2	313	CLA	C2C-C1C-NC	4.77	115.00	109.98
38	1	308	KC1	C3C-C4C-NC	4.77	115.01	109.90
30	10	311	CLA	C2B-C1B-NB	4.77	115.28	110.33
38	3	308	KC1	C3D-C4D-ND	4.77	116.86	110.20
30	3	305	CLA	C2C-C1C-NC	4.77	114.99	109.98
30	B	810	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
30	B	832	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
30	9	308	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
30	B	826	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
30	5	302	CLA	O2D-CGD-CBD	4.77	119.57	111.23
30	2	303	CLA	O2D-CGD-CBD	4.77	119.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	2u	205	A86	C7-C6-C8	4.77	125.37	118.09
30	L	203	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
38	5	310	KC1	CHD-C4C-C3C	-4.77	116.44	125.23
38	4	307	KC1	C3D-C4D-ND	4.76	116.84	110.20
30	A	834	CLA	C2C-C1C-NC	4.76	114.98	109.98
30	3	309	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
37	12	314	A86	O4-C38-C39	4.76	119.58	111.09
30	7	312	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
30	A	827	CLA	C2B-C1B-NB	4.76	115.27	110.33
30	3	302	CLA	C2B-C1B-NB	4.76	115.27	110.33
30	3	302	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
30	4	311	CLA	CBA-CAA-C2A	-4.76	99.63	113.79
30	10	311	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
30	A	813	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
38	10	312	KC1	O2D-CGD-CBD	4.76	119.55	111.23
30	5	307	CLA	C2B-C1B-NB	4.76	115.26	110.33
30	2	304	CLA	C2C-C1C-NC	4.76	114.98	109.98
30	A	831	CLA	C2B-C1B-NB	4.76	115.26	110.33
30	3	305	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
30	5	308	CLA	C2C-C1C-NC	4.76	114.98	109.98
38	5	305	KC1	C3D-C4D-ND	4.76	116.83	110.20
30	7	309	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
38	16	311	KC1	C2D-C1D-ND	4.75	115.26	110.33
39	8	317	DD6	C7-C6-C8	-4.75	110.83	118.09
30	8	302	CLA	C2C-C1C-NC	4.75	114.97	109.98
39	13	314	DD6	O1-C20-C21	-4.75	109.74	115.05
30	6	307	CLA	C2D-C1D-ND	4.75	114.83	110.13
39	2	316	DD6	O1-C15-C14	-4.75	103.26	116.88
30	B	828	CLA	C2B-C1B-NB	4.75	115.25	110.33
30	15	311	CLA	O2D-CGD-CBD	4.75	119.53	111.23
30	2	308	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
30	B	833	CLA	C2C-C1C-NC	4.75	114.97	109.98
30	B	817	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
30	B	824	CLA	C1-C2-C3	-4.75	118.42	126.20
38	14	306	KC1	C3D-C4D-ND	4.75	116.82	110.20
30	A	815	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
38	16	304	KC1	CHC-C1C-C2C	-4.75	117.53	125.03
30	11	308	CLA	C2C-C1C-NC	4.75	114.97	109.98
30	16	302	CLA	C2C-C1C-NC	4.75	114.97	109.98
38	2	312	KC1	CHD-C4C-C3C	-4.75	116.48	125.23
37	15	316	A86	C41-C32-C31	-4.74	106.23	110.47
38	8	311	KC1	O2D-CGD-CBD	4.74	119.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	307	CLA	C2B-C1B-NB	4.74	115.25	110.33
30	B	820	CLA	C3C-C4C-NC	4.74	116.51	110.43
30	16	310	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
38	3	311	KC1	CHC-C1C-C2C	-4.74	117.54	125.03
30	6	310	CLA	O2D-CGD-CBD	4.74	119.52	111.23
30	5	307	CLA	C3B-C4B-NB	4.74	114.76	110.53
30	1	302	CLA	C2C-C1C-NC	4.74	114.96	109.98
38	5	310	KC1	C3D-C4D-ND	4.74	116.81	110.20
30	6	304	CLA	O2D-CGD-CBD	4.74	119.52	111.23
30	3	301	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
37	16	314	A86	C3-C2-C1	-4.74	120.63	127.28
30	A	816	CLA	C2C-C1C-NC	4.74	114.96	109.98
38	8	311	KC1	C3D-C4D-ND	4.74	116.81	110.20
30	A	810	CLA	C2B-C1B-NB	4.74	115.24	110.33
30	16	307	CLA	C3B-C2B-C1B	-4.74	101.59	107.17
30	B	830	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
30	10	309	CLA	C2C-C1C-NC	4.73	114.95	109.98
30	16	302	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
30	1	301	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
30	5	303	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
30	14	307	CLA	C3D-C4D-ND	4.73	117.68	109.99
39	11	313	DD6	O1-C15-C14	-4.73	103.32	116.88
38	11	311	KC1	C3D-C4D-ND	4.73	116.80	110.20
30	B	811	CLA	C2C-C1C-NC	4.73	114.95	109.98
37	15	322	A86	C33-C32-C31	4.73	113.81	109.21
30	B	829	CLA	C4A-NA-C1A	-4.73	104.52	106.68
38	4	310	KC1	O2D-CGD-CBD	4.73	119.49	111.23
30	A	816	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
30	L	202	CLA	C3D-C4D-ND	4.72	117.67	109.99
39	16	313	DD6	C7-C6-C8	-4.72	110.87	118.09
30	1	303	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
39	3	313	DD6	C21-C20-C15	-4.72	114.53	122.30
30	A	826	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
30	8	308	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
38	13	311	KC1	C2B-C1B-NB	4.72	114.80	110.13
30	8	309	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
38	11	307	KC1	C3D-C4D-ND	4.72	116.78	110.20
38	4	307	KC1	CHC-C1C-C2C	-4.72	117.58	125.03
30	11	310	CLA	C2C-C1C-NC	4.72	114.94	109.98
30	14	313	CLA	C2B-C1B-NB	4.72	115.22	110.33
30	A	841	CLA	C4A-NA-C1A	-4.72	104.53	106.68
30	5	303	CLA	C4A-NA-C1A	-4.72	104.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	304	CLA	O2D-CGD-CBD	4.72	119.48	111.23
38	16	304	KC1	C3D-C4D-ND	4.72	116.78	110.20
30	B	818	CLA	C2C-C1C-NC	4.72	114.94	109.98
30	4	302	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
37	10	316	A86	C10-C9-C8	-4.71	109.54	123.20
38	2	306	KC1	C3D-C4D-ND	4.71	116.77	110.20
30	A	818	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
30	2u	202	CLA	C2B-C1B-NB	4.71	115.21	110.33
30	3	309	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
30	8	308	CLA	O2D-CGD-CBD	4.71	119.47	111.23
30	16	302	CLA	C2B-C1B-NB	4.71	115.21	110.33
30	4	303	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
30	2	307	CLA	O2D-CGD-CBD	4.71	119.47	111.23
30	F	203	CLA	C2C-C1C-NC	4.71	114.93	109.98
30	12	312	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
30	15	313	CLA	O2D-CGD-CBD	4.71	119.46	111.23
38	13	312	KC1	C3D-C4D-ND	4.71	116.77	110.20
30	B	823	CLA	C2B-C1B-NB	4.71	115.21	110.33
30	4	302	CLA	C2B-C1B-NB	4.71	115.21	110.33
30	A	803	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
30	A	809	CLA	C2C-C1C-NC	4.71	114.93	109.98
30	6	305	CLA	C2C-C1C-NC	4.71	114.93	109.98
37	8	318	A86	C4-C3-C2	-4.71	113.89	123.52
37	5	315	A86	C40-C32-C31	-4.71	106.26	110.47
30	A	811	CLA	C2C-C1C-NC	4.71	114.92	109.98
30	7	311	CLA	C2C-C1C-NC	4.71	114.92	109.98
30	15	313	CLA	C4A-NA-C1A	-4.71	104.53	106.68
30	A	818	CLA	O2D-CGD-CBD	4.71	119.46	111.23
30	B	808	CLA	C3B-C2B-C1B	-4.70	101.62	107.17
38	10	310	KC1	C3C-C4C-NC	4.70	114.94	109.90
38	11	311	KC1	C3C-C4C-NC	4.70	114.94	109.90
38	8	313	KC1	C1A-NA-C4A	-4.70	104.53	106.68
30	4	304	CLA	O2A-CGA-CBA	4.70	126.18	111.83
30	16	310	CLA	C2B-C1B-NB	4.70	115.20	110.33
37	3	314	A86	O4-C38-C39	4.70	119.47	111.09
30	12	302	CLA	O2D-CGD-CBD	4.70	119.45	111.23
30	15	308	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
30	B	813	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
30	B	838	CLA	C2B-C1B-NB	4.70	115.20	110.33
30	9	306	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
38	11	311	KC1	CHD-C4C-C3C	-4.70	116.56	125.23
38	5	312	KC1	CHD-C4C-C3C	-4.70	116.56	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	311	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
30	B	807	CLA	C2B-C1B-NB	4.70	115.20	110.33
38	8	306	KC1	CHD-C4C-C3C	-4.70	116.56	125.23
39	5	314	DD6	O1-C15-C14	-4.70	103.42	116.88
30	12	306	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
38	16	311	KC1	CMA-C3A-C2A	-4.70	117.06	128.43
30	F	201	CLA	C2C-C1C-NC	4.69	114.91	109.98
30	13	309	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
30	3	302	CLA	O2D-CGD-CBD	4.69	119.44	111.23
30	A	839	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
38	13	306	KC1	C1A-NA-C4A	-4.69	104.54	106.68
30	6	309	CLA	C2C-C1C-NC	4.69	114.91	109.98
30	B	801	CLA	CAA-C2A-C3A	-4.69	100.32	113.00
30	15	309	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
30	A	827	CLA	O2D-CGD-CBD	4.69	119.43	111.23
30	A	844	CLA	C2C-C1C-NC	4.69	114.91	109.98
30	14	312	CLA	C4A-NA-C1A	-4.69	104.54	106.68
30	B	832	CLA	C2C-C1C-NC	4.69	114.91	109.98
30	1	307	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
37	2	302	A86	C41-C32-C31	-4.69	106.28	110.47
38	13	310	KC1	C3D-C4D-ND	4.69	116.74	110.20
30	15	313	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
30	B	811	CLA	C2B-C1B-NB	4.69	115.19	110.33
30	B	819	CLA	C2B-C1B-NB	4.69	115.19	110.33
38	8	307	KC1	C1A-NA-C4A	-4.69	104.54	106.68
30	6	304	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
30	14	309	CLA	C3B-C2B-C1B	-4.69	101.65	107.17
38	13	311	KC1	C3C-C4C-NC	4.69	114.92	109.90
30	16	303	CLA	C3D-C4D-ND	4.68	117.60	109.99
38	2	314	KC1	CHD-C4C-C3C	-4.68	116.59	125.23
38	16	311	KC1	CHD-C4C-C3C	-4.68	116.59	125.23
30	5	311	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	6	314	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
30	16	307	CLA	C4A-NA-C1A	-4.68	104.54	106.68
38	3	311	KC1	C3C-C4C-NC	4.68	114.92	109.90
30	15	304	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
37	5	316	A86	C4-C5-C6	-4.68	120.71	127.28
30	10	304	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	6	315	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	F	203	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
30	9	307	CLA	C2C-C1C-NC	4.68	114.90	109.98
30	A	815	CLA	C3D-C2D-C1D	-4.68	99.45	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	311	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
30	16	303	CLA	O2D-CGD-CBD	4.68	119.41	111.23
30	14	313	CLA	C3D-C4D-ND	4.68	117.59	109.99
38	11	307	KC1	CHC-C1C-C2C	-4.68	117.64	125.03
30	F	201	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
30	12	310	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
30	A	843	CLA	O2D-CGD-CBD	4.68	119.41	111.23
38	6	312	KC1	C3C-C4C-NC	4.68	114.91	109.90
30	B	822	CLA	CAA-C2A-C1A	-4.67	96.65	111.97
30	7	312	CLA	O2D-CGD-CBD	4.67	119.40	111.23
30	3	310	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
30	13	302	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
38	11	305	KC1	O2D-CGD-CBD	4.67	119.40	111.23
37	7	319	A86	C9-C8-C6	-4.67	113.55	126.36
38	9	311	KC1	CHD-C4C-C3C	-4.67	116.61	125.23
38	16	304	KC1	C2D-C1D-ND	4.67	115.17	110.33
30	A	817	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
37	15	320	A86	C33-C32-C31	4.67	113.75	109.21
30	10	305	CLA	CAA-C2A-C3A	-4.67	100.38	113.00
30	15	311	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
38	13	305	KC1	CHD-C4C-C3C	-4.67	116.62	125.23
30	14	312	CLA	C2C-C1C-NC	4.67	114.89	109.98
30	13	302	CLA	C2B-C1B-NB	4.67	115.17	110.33
38	13	308	KC1	C3D-C4D-ND	4.67	116.70	110.20
30	2u	202	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
30	6	317	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
30	3	301	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
30	15	303	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
30	A	828	CLA	C1D-CHD-C4C	-4.66	116.11	126.02
38	12	305	KC1	C3D-C4D-ND	4.66	116.70	110.20
30	5	303	CLA	C2C-C1C-NC	4.66	114.88	109.98
38	6	313	KC1	C3D-C4D-ND	4.66	116.70	110.20
38	13	308	KC1	CHD-C4C-C3C	-4.66	116.64	125.23
30	A	837	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
30	A	824	CLA	C2C-C1C-NC	4.66	114.87	109.98
30	7	303	CLA	C2B-C1B-NB	4.66	115.16	110.33
39	8	317	DD6	C21-C20-C19	-4.66	109.01	114.24
30	B	834	CLA	C2B-C1B-NB	4.66	115.15	110.33
30	14	313	CLA	C4A-NA-C1A	-4.66	104.56	106.68
37	10	301	A86	C33-C32-C31	4.65	113.73	109.21
38	12	305	KC1	C3C-C4C-NC	4.65	114.89	109.90
30	15	304	CLA	C4A-NA-C1A	-4.65	104.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	309	KC1	CBA-CAA-C2A	-4.65	106.78	125.45
38	13	311	KC1	O2D-CGD-CBD	4.65	119.36	111.23
30	13	307	CLA	C2C-C1C-NC	4.65	114.87	109.98
30	4	311	CLA	C4A-NA-C1A	-4.65	104.56	106.68
30	3	303	CLA	C2C-C1C-NC	4.65	114.87	109.98
30	13	307	CLA	C4A-NA-C1A	-4.65	104.56	106.68
38	11	305	KC1	C3D-C4D-ND	4.65	116.68	110.20
38	14	311	KC1	O2D-CGD-CBD	4.65	119.36	111.23
30	13	301	CLA	C2C-C1C-NC	4.65	114.86	109.98
30	B	826	CLA	C2B-C1B-NB	4.65	115.15	110.33
38	9	304	KC1	CHD-C4C-C3C	-4.64	116.66	125.23
30	15	306	CLA	C4A-NA-C1A	-4.64	104.56	106.68
30	B	831	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
30	1	304	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
30	12	308	CLA	C2B-C1B-NB	4.64	115.14	110.33
39	1	310	DD6	O1-C15-C14	-4.64	103.58	116.88
30	2	309	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
30	B	819	CLA	C2C-C1C-NC	4.64	114.86	109.98
30	15	310	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
38	4	310	KC1	C1A-NA-C4A	-4.64	104.56	106.68
30	15	314	CLA	CHD-C1D-ND	-4.64	118.28	124.80
30	7	305	CLA	C2C-C1C-NC	4.64	114.85	109.98
38	6	311	KC1	CHD-C4C-C3C	-4.64	116.68	125.23
30	A	823	CLA	C2C-C1C-NC	4.63	114.85	109.98
30	11	309	CLA	C2C-C1C-NC	4.63	114.85	109.98
30	A	822	CLA	O2D-CGD-CBD	4.63	119.33	111.23
30	B	813	CLA	C4A-NA-C1A	-4.63	104.56	106.68
38	8	306	KC1	CHC-C1C-C2C	-4.63	117.71	125.03
30	13	302	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
30	2	313	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
30	13	303	CLA	C3D-C4D-ND	4.63	117.52	109.99
30	16	308	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
38	7	313	KC1	CHD-C4C-C3C	-4.63	116.69	125.23
30	A	832	CLA	C2C-C1C-NC	4.63	114.84	109.98
38	11	305	KC1	CHD-C4C-C3C	-4.63	116.69	125.23
30	F	202	CLA	O2D-CGD-CBD	4.63	119.32	111.23
30	A	817	CLA	C2B-C1B-NB	4.63	115.12	110.33
30	2	301	CLA	C2B-C1B-NB	4.63	115.12	110.33
30	6	316	CLA	O2D-CGD-CBD	4.63	119.32	111.23
30	F	203	CLA	C4A-NA-C1A	-4.62	104.57	106.68
38	13	308	KC1	C1A-NA-C4A	-4.62	104.57	106.68
30	9	306	CLA	O2D-CGD-CBD	4.62	119.31	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	316	A86	C41-C32-C31	-4.62	106.33	110.47
30	2	304	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
30	14	303	CLA	C2C-C1C-NC	4.62	114.84	109.98
30	B	801	CLA	C1D-CHD-C4C	-4.62	116.20	126.02
30	L	202	CLA	CHD-C1D-ND	-4.62	118.30	124.80
30	B	835	CLA	C4A-NA-C1A	-4.62	104.57	106.68
30	A	808	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
30	1	301	CLA	O2D-CGD-CBD	4.62	119.31	111.23
30	3	310	CLA	O2D-CGD-CBD	4.62	119.31	111.23
38	3	304	KC1	C3C-C4C-NC	4.62	114.85	109.90
30	5	308	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
39	2	317	DD6	C24-C1-C2	-4.62	111.75	119.01
30	5	304	CLA	C2C-C1C-NC	4.62	114.83	109.98
39	8	317	DD6	C-C1-C24	-4.62	111.04	118.09
30	9	301	CLA	C2C-C1C-NC	4.61	114.83	109.98
30	B	819	CLA	C4A-NA-C1A	-4.61	104.57	106.68
30	6	306	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
30	15	314	CLA	O2D-CGD-CBD	4.61	119.29	111.23
37	13	313	A86	C41-C32-C31	-4.61	106.34	110.47
30	A	840	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
30	A	830	CLA	C2C-C1C-NC	4.61	114.83	109.98
39	2	317	DD6	C21-C20-C19	-4.61	109.06	114.24
38	3	304	KC1	CHD-C4C-C3C	-4.61	116.73	125.23
30	14	304	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
37	7	315	A86	O4-C38-C39	4.61	119.31	111.09
37	4	315	A86	C25-C26-C27	-4.61	120.81	127.28
30	A	806	CLA	C3D-C4D-ND	4.61	117.48	109.99
30	6	305	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
38	13	312	KC1	CHD-C4C-C3C	-4.61	116.73	125.23
30	9	302	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
30	9	305	CLA	C2C-C1C-NC	4.61	114.82	109.98
30	7	309	CLA	O2D-CGD-CBD	4.61	119.28	111.23
38	14	308	KC1	CHD-C4C-C3C	-4.60	116.74	125.23
30	2	303	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
30	10	309	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	B	818	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
38	11	312	KC1	C3C-C4C-NC	4.60	114.83	109.90
38	12	309	KC1	C1A-C2A-C3A	-4.60	103.05	107.28
30	2u	202	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
37	15	321	A86	C3-C2-C1	-4.60	120.83	127.28
30	B	837	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	A	829	CLA	O2D-CGD-CBD	4.60	119.27	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	805	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
30	A	825	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
30	A	825	CLA	O2D-CGD-CBD	4.60	119.27	111.23
38	9	312	KC1	C3C-C4C-NC	4.60	114.83	109.90
38	12	309	KC1	C3C-C4C-NC	4.60	114.83	109.90
30	16	301	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
38	11	312	KC1	O2D-CGD-CBD	4.60	119.27	111.23
30	15	303	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
30	14	305	CLA	O2D-CGD-CBD	4.60	119.26	111.23
30	3	309	CLA	C4A-NA-C1A	-4.59	104.58	106.68
30	14	309	CLA	C4A-NA-C1A	-4.59	104.58	106.68
30	11	304	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
30	A	811	CLA	O2D-CGD-CBD	4.59	119.26	111.23
38	1	308	KC1	C1A-NA-C4A	-4.59	104.58	106.68
38	3	308	KC1	C3C-C4C-NC	4.59	114.82	109.90
30	F	202	CLA	C2B-C1B-NB	4.59	115.09	110.33
30	A	835	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
30	11	310	CLA	O2D-CGD-CBD	4.59	119.25	111.23
38	4	308	KC1	CHD-C4C-C3C	-4.59	116.77	125.23
39	6	303	DD6	C7-C6-C8	-4.59	111.08	118.09
38	5	312	KC1	C3D-C4D-ND	4.59	116.60	110.20
30	4	306	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
37	4	312	A86	C36-C31-C32	-4.59	115.14	119.70
39	10	314	DD6	C21-C20-C15	-4.59	114.75	122.30
39	6	319	DD6	C12-C11-C13	-4.59	111.08	118.09
30	11	309	CLA	C3D-C4D-ND	4.59	117.44	109.99
30	8	308	CLA	C2C-C1C-NC	4.58	114.80	109.98
39	8	316	DD6	C15-C14-C13	4.58	135.69	125.99
30	A	831	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
30	9	305	CLA	O2D-CGD-O1D	-4.58	114.93	123.85
38	1	308	KC1	CHD-C4C-C3C	-4.58	116.78	125.23
30	15	309	CLA	C2C-C1C-NC	4.58	114.79	109.98
38	16	311	KC1	C1A-C2A-C3A	-4.58	103.07	107.28
38	14	311	KC1	C3D-C4D-ND	4.58	116.59	110.20
37	16	314	A86	C4-C5-C6	-4.58	120.86	127.28
30	7	311	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
30	B	836	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
30	10	304	CLA	C2B-C1B-NB	4.58	115.07	110.33
30	12	307	CLA	C2B-C1B-NB	4.58	115.07	110.33
30	13	304	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
30	4	309	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
38	9	304	KC1	C1A-NA-C4A	-4.58	104.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	5	305	KC1	CHD-C4C-C3C	-4.58	116.79	125.23
30	A	816	CLA	C3B-C2B-C1B	-4.58	101.78	107.17
30	11	304	CLA	O2D-CGD-CBD	4.58	119.23	111.23
30	2	310	CLA	C1D-CHD-C4C	-4.57	116.30	126.02
30	4	305	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
39	5	314	DD6	C7-C6-C8	-4.57	111.10	118.09
30	16	301	CLA	C2C-C1C-NC	4.57	114.78	109.98
38	5	305	KC1	C3C-C4C-NC	4.57	114.80	109.90
30	7	304	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
30	16	305	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
30	12	304	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
39	5	313	DD6	O1-C20-C21	-4.57	109.94	115.05
30	12	321	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
30	A	832	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
30	F	201	CLA	C4A-NA-C1A	-4.57	104.60	106.68
30	B	803	CLA	CHD-C1D-ND	-4.57	118.38	124.80
30	13	303	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
30	6	316	CLA	C2C-C1C-NC	4.56	114.78	109.98
30	A	819	CLA	C4A-NA-C1A	-4.56	104.60	106.68
37	7	319	A86	C25-C24-C1	-4.56	113.85	126.36
38	11	312	KC1	C2C-C1C-NC	4.56	116.09	110.45
38	12	305	KC1	CHD-C4C-C3C	-4.56	116.82	125.23
38	14	308	KC1	CHC-C1C-C2C	-4.56	117.83	125.03
37	11	316	A86	C4-C5-C6	-4.56	120.89	127.28
30	B	827	CLA	C2B-C1B-NB	4.56	115.05	110.33
39	12	315	DD6	C7-C6-C8	-4.56	111.13	118.09
30	A	808	CLA	C2C-C1C-NC	4.56	114.77	109.98
38	12	305	KC1	CHC-C1C-C2C	-4.56	117.83	125.03
39	10	314	DD6	C21-C20-C19	-4.56	109.12	114.24
38	4	310	KC1	C3D-C4D-ND	4.56	116.55	110.20
38	6	313	KC1	O2D-CGD-CBD	4.55	119.19	111.23
39	3	313	DD6	O1-C15-C14	-4.55	103.83	116.88
30	A	841	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
30	B	816	CLA	C2C-C1C-NC	4.55	114.76	109.98
30	1	302	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
30	A	817	CLA	C3D-C4D-ND	4.55	117.39	109.99
30	A	824	CLA	C2B-C1B-NB	4.55	115.05	110.33
30	L	203	CLA	C2C-C1C-NC	4.55	114.76	109.98
37	2u	205	A86	C7-C6-C5	-4.55	115.45	122.82
38	9	311	KC1	C3C-C4C-NC	4.55	114.77	109.90
30	A	838	CLA	C4A-NA-C1A	-4.55	104.60	106.68
38	8	311	KC1	CHD-C4C-C3C	-4.55	116.84	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	827	CLA	CAA-C2A-C3A	-4.55	100.72	113.00
30	A	803	CLA	CMD-C2D-C1D	4.55	132.73	124.73
30	2	311	CLA	C3D-C4D-ND	4.54	117.38	109.99
30	15	305	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
30	A	839	CLA	C2C-C1C-NC	4.54	114.75	109.98
30	5	309	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
30	A	842	CLA	C4A-NA-C1A	-4.54	104.61	106.68
30	14	312	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
30	6	304	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
38	13	305	KC1	CHC-C1C-C2C	-4.54	117.86	125.03
30	A	817	CLA	C2C-C1C-NC	4.54	114.75	109.98
30	8	301	CLA	C2C-C1C-NC	4.54	114.75	109.98
30	A	816	CLA	C2B-C1B-NB	4.54	115.04	110.33
39	1	310	DD6	C21-C20-C15	-4.54	114.83	122.30
30	6	307	CLA	C2B-C1B-NB	4.54	115.03	110.33
30	16	309	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
30	7	306	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
30	2	303	CLA	C2C-C1C-NC	4.54	114.75	109.98
38	5	306	KC1	CHD-C4C-C3C	-4.53	116.87	125.23
38	13	305	KC1	C3D-C4D-ND	4.53	116.52	110.20
30	B	805	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
39	7	318	DD6	C35-C36-C31	-4.53	111.07	120.50
38	12	313	KC1	CMA-C3A-C2A	-4.53	117.46	128.43
30	B	812	CLA	O2D-CGD-CBD	4.53	119.15	111.23
39	7	302	DD6	C21-C20-C19	-4.53	109.15	114.24
30	B	838	CLA	C1C-C2C-C3C	-4.53	102.22	106.98
38	4	310	KC1	CHD-C4C-C3C	-4.53	116.88	125.23
38	12	309	KC1	C3D-C4D-ND	4.53	116.52	110.20
37	10	317	A86	C4-C5-C6	-4.53	120.93	127.28
38	10	312	KC1	C2A-C1A-NA	4.53	116.60	109.34
30	A	817	CLA	CHD-C1D-ND	-4.53	118.43	124.80
30	B	817	CLA	C3D-C4D-ND	4.53	117.35	109.99
30	12	312	CLA	O2D-CGD-CBD	4.53	119.14	111.23
30	9	309	CLA	C2B-C1B-NB	4.53	115.02	110.33
38	13	306	KC1	C3D-C4D-ND	4.53	116.51	110.20
38	13	306	KC1	C2A-C1A-NA	4.53	116.59	109.34
38	14	308	KC1	C3D-C4D-ND	4.52	116.51	110.20
38	14	306	KC1	C2A-C1A-NA	4.52	116.59	109.34
30	16	306	CLA	C2C-C1C-NC	4.52	114.73	109.98
30	B	811	CLA	C3D-C4D-ND	4.52	117.34	109.99
30	13	304	CLA	C3D-C4D-ND	4.52	117.34	109.99
30	12	302	CLA	C3D-C2D-C1D	-4.52	99.66	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	301	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
30	9	303	CLA	C2C-C1C-NC	4.52	114.73	109.98
38	10	310	KC1	C2A-C1A-NA	4.52	116.58	109.34
35	B	852	LMT	O1B-C4'-C3'	4.52	118.72	107.23
30	11	306	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
30	15	306	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
38	2	312	KC1	C3D-C4D-ND	4.52	116.50	110.20
37	8	315	A86	C12-C11-C13	4.52	123.33	116.00
38	8	312	KC1	C3A-C4A-NA	4.52	116.04	110.45
30	A	833	CLA	C2C-C1C-NC	4.52	114.73	109.98
38	16	304	KC1	C3C-C4C-NC	4.52	114.74	109.90
37	10	316	A86	C12-C11-C13	4.52	123.33	116.00
38	13	308	KC1	CHC-C1C-C2C	-4.52	117.89	125.03
30	B	812	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
30	15	314	CLA	C3D-C4D-ND	4.52	117.33	109.99
30	B	816	CLA	C3D-C4D-ND	4.52	117.33	109.99
30	B	801	CLA	CMA-C3A-C2A	-4.51	96.53	113.98
37	2	302	A86	O4-C38-C39	4.51	119.14	111.09
30	16	305	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
39	10	313	DD6	C12-C11-C13	-4.51	111.20	118.09
30	2	308	CLA	C4A-NA-C1A	-4.51	104.62	106.68
30	10	305	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
30	6	304	CLA	C2C-C1C-NC	4.51	114.72	109.98
30	7	306	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
30	11	304	CLA	C3D-C4D-ND	4.51	117.32	109.99
30	15	312	CLA	C4A-NA-C1A	-4.51	104.62	106.68
37	11	314	A86	C25-C26-C27	-4.51	120.96	127.28
30	A	820	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
39	3	312	DD6	O1-C15-C14	-4.51	103.97	116.88
30	B	829	CLA	C2C-C1C-NC	4.51	114.71	109.98
30	15	313	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
38	3	308	KC1	CHC-C1C-C2C	-4.50	117.92	125.03
38	3	308	KC1	CHD-C4C-C3C	-4.50	116.92	125.23
38	12	313	KC1	C3D-C4D-ND	4.50	116.48	110.20
30	A	830	CLA	C4A-NA-C1A	-4.50	104.62	106.68
30	B	817	CLA	C4A-NA-C1A	-4.50	104.62	106.68
38	3	311	KC1	CHD-C4C-C3C	-4.50	116.93	125.23
30	7	303	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	15	308	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	12	308	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
38	8	307	KC1	C3C-C4C-NC	4.50	114.72	109.90
30	14	305	CLA	C3D-C2D-C1D	-4.50	99.69	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	6	311	KC1	C2A-C1A-NA	4.50	116.55	109.34
30	9	303	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
38	12	311	KC1	CHD-C4C-C3C	-4.50	116.93	125.23
30	14	310	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
30	B	803	CLA	C1D-CHD-C4C	-4.50	116.46	126.02
30	3	309	CLA	C2C-C1C-NC	4.50	114.70	109.98
30	2	301	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
38	11	305	KC1	C1A-NA-C4A	-4.50	104.63	106.68
38	1	306	KC1	C3C-C4C-NC	4.49	114.72	109.90
30	10	307	CLA	C2C-C1C-NC	4.49	114.70	109.98
38	9	312	KC1	CHC-C1C-C2C	-4.49	117.93	125.03
30	13	307	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
30	2	301	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
30	10	308	CLA	C3D-C4D-ND	4.49	117.29	109.99
30	A	807	CLA	C2C-C1C-NC	4.49	114.70	109.98
30	A	805	CLA	C4A-NA-C1A	-4.49	104.63	106.68
30	6	316	CLA	C4A-NA-C1A	-4.49	104.63	106.68
38	12	311	KC1	C3D-C4D-ND	4.49	116.46	110.20
30	B	830	CLA	C4A-NA-C1A	-4.49	104.63	106.68
30	A	812	CLA	CHD-C1D-ND	-4.49	118.48	124.80
30	4	305	CLA	CHD-C1D-ND	-4.49	118.49	124.80
30	6	310	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
30	A	830	CLA	O2D-CGD-CBD	4.49	119.08	111.23
38	11	305	KC1	C3C-C4C-NC	4.49	114.71	109.90
30	3	303	CLA	CAA-C2A-C3A	-4.49	100.88	113.00
30	A	802	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
30	1	304	CLA	C2B-C1B-NB	4.49	114.98	110.33
38	2	306	KC1	CHD-C4C-C3C	-4.48	116.96	125.23
39	6	319	DD6	C13-C11-C10	-4.48	111.96	119.01
30	15	312	CLA	CHD-C1D-ND	-4.48	118.49	124.80
30	1	301	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
30	8	304	CLA	C1D-CHD-C4C	-4.48	116.49	126.02
30	14	302	CLA	C3D-C4D-ND	4.48	117.27	109.99
30	12	321	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
30	13	301	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
30	9	301	CLA	C3B-C4B-NB	4.48	114.53	110.53
30	B	837	CLA	O2D-CGD-CBD	4.48	119.06	111.23
30	B	837	CLA	C2C-C1C-NC	4.48	114.69	109.98
30	10	308	CLA	C4A-NA-C1A	-4.48	104.64	106.68
30	B	802	CLA	C2C-C1C-NC	4.48	114.69	109.98
38	4	308	KC1	C3C-C4C-NC	4.48	114.70	109.90
30	14	313	CLA	C3D-C2D-C1D	-4.48	99.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	10	310	KC1	CHC-C1C-C2C	-4.48	117.96	125.03
30	8	303	CLA	C3D-C4D-ND	4.48	117.27	109.99
38	13	308	KC1	C3C-C4C-NC	4.48	114.70	109.90
30	12	310	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
30	8	308	CLA	C4A-NA-C1A	-4.48	104.64	106.68
30	5	309	CLA	O2D-CGD-CBD	4.47	119.05	111.23
30	B	829	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
38	4	308	KC1	C4B-C3B-C2B	-4.47	102.94	106.81
30	6	310	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
30	B	809	CLA	O2D-CGD-CBD	4.47	119.05	111.23
30	A	820	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
30	7	309	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
30	10	303	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
38	13	311	KC1	C2A-C1A-NA	4.47	116.50	109.34
30	7	310	CLA	CHD-C1D-ND	-4.47	118.51	124.80
38	3	304	KC1	CHC-C1C-C2C	-4.47	117.97	125.03
37	2u	203	A86	C7-C6-C5	-4.47	115.58	122.82
30	15	303	CLA	O2D-CGD-CBD	4.47	119.04	111.23
30	7	305	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
30	1	303	CLA	C2C-C1C-NC	4.47	114.67	109.98
30	12	304	CLA	C2C-C1C-NC	4.47	114.67	109.98
30	B	813	CLA	C2C-C1C-NC	4.47	114.67	109.98
30	B	835	CLA	CHD-C1D-ND	-4.46	118.52	124.80
30	6	314	CLA	C3D-C4D-ND	4.46	117.24	109.99
38	5	306	KC1	C2A-C1A-NA	4.46	116.49	109.34
39	5	314	DD6	C35-C36-C31	-4.46	111.21	120.50
30	B	819	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
30	B	804	CLA	C2C-C1C-NC	4.46	114.67	109.98
38	6	311	KC1	CHC-C1C-C2C	-4.46	117.98	125.03
38	8	310	KC1	CHC-C1C-C2C	-4.46	117.98	125.03
30	15	307	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
38	4	310	KC1	C3C-C4C-NC	4.46	114.68	109.90
30	13	302	CLA	O2D-CGD-CBD	4.46	119.03	111.23
30	2	305	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
38	8	306	KC1	C3C-C4C-NC	4.46	114.68	109.90
30	A	827	CLA	CHD-C1D-ND	-4.46	118.53	124.80
38	7	313	KC1	O2D-CGD-CBD	4.46	119.02	111.23
39	10	314	DD6	C15-C14-C13	-4.46	116.57	125.99
30	16	306	CLA	C3D-C4D-ND	4.46	117.23	109.99
30	12	307	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
30	7	311	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
30	12	310	CLA	C3D-C4D-ND	4.46	117.23	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	6	322	LHG	O4-P-O5	4.45	133.17	112.44
30	A	837	CLA	C4A-NA-C1A	-4.45	104.65	106.68
30	8	304	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
38	10	310	KC1	CHD-C4C-C3C	-4.45	117.02	125.23
38	2	312	KC1	CHC-C1C-C2C	-4.45	118.00	125.03
30	3	306	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
34	9	318	LHG	O4-P-O5	4.45	133.15	112.44
30	B	831	CLA	C2C-C1C-NC	4.45	114.66	109.98
38	9	312	KC1	CHD-C4C-C3C	-4.45	117.02	125.23
38	11	312	KC1	CHD-C4C-C3C	-4.45	117.03	125.23
38	5	310	KC1	C4B-C3B-C2B	-4.45	102.96	106.81
30	1	305	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
38	8	313	KC1	C3D-C4D-ND	4.45	116.40	110.20
38	8	314	KC1	CHC-C1C-C2C	-4.45	118.01	125.03
30	9	301	CLA	CAC-C3C-C4C	4.45	130.58	124.79
30	14	307	CLA	CHD-C4C-C3C	-4.45	118.29	124.77
30	A	826	CLA	C3B-C4B-NB	4.45	114.50	110.53
30	2	311	CLA	O2D-CGD-CBD	4.45	119.00	111.23
39	11	313	DD6	C21-C20-C19	-4.44	109.25	114.24
30	16	303	CLA	C4A-NA-C1A	-4.44	104.65	106.68
38	16	304	KC1	C2A-C1A-NA	4.44	116.46	109.34
30	10	305	CLA	C3D-C4D-ND	4.44	117.21	109.99
37	11	315	A86	C41-C32-C31	-4.44	106.50	110.47
38	5	306	KC1	C3C-C4C-NC	4.44	114.66	109.90
30	B	802	CLA	C3C-C4C-NC	4.44	116.12	110.43
30	2	311	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
30	6	317	CLA	O2D-CGD-CBD	4.44	118.99	111.23
30	2	305	CLA	C4A-NA-C1A	-4.44	104.65	106.68
30	B	822	CLA	CAA-C2A-C3A	-4.44	101.00	113.00
30	11	308	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
30	1	302	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
30	1	307	CLA	C3D-C4D-ND	4.44	117.20	109.99
30	A	802	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
39	4	316	DD6	C24-C1-C2	-4.44	112.03	119.01
38	9	304	KC1	C2A-C1A-NA	4.44	116.45	109.34
37	7	316	A86	C35-C34-C33	4.44	117.86	109.89
30	A	837	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
37	12	316	A86	C40-C32-C31	-4.43	106.50	110.47
38	10	310	KC1	C4B-C3B-C2B	-4.43	102.97	106.81
38	9	310	KC1	C2A-C1A-NA	4.43	116.44	109.34
39	3	316	DD6	C37-C36-C35	-4.43	106.27	114.42
30	8	301	CLA	O2D-CGD-CBD	4.43	118.98	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	313	CLA	C2C-C1C-NC	4.43	114.64	109.98
30	15	309	CLA	CHD-C1D-ND	-4.43	118.56	124.80
38	12	313	KC1	CHC-C1C-C2C	-4.43	118.03	125.03
30	1	304	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
30	10	303	CLA	C2C-C1C-NC	4.43	114.64	109.98
38	5	312	KC1	CHC-C1C-C2C	-4.43	118.04	125.03
30	7	310	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
30	7	305	CLA	C3D-C4D-ND	4.43	117.19	109.99
30	A	834	CLA	C4A-NA-C1A	-4.43	104.66	106.68
30	B	821	CLA	C4A-NA-C1A	-4.43	104.66	106.68
38	12	311	KC1	C3C-C4C-NC	4.43	114.64	109.90
30	B	809	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
30	1	302	CLA	C3D-C4D-ND	4.43	117.18	109.99
37	10	315	A86	C40-C32-C31	-4.43	106.51	110.47
30	B	810	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
38	2	306	KC1	C1A-NA-C4A	-4.43	104.66	106.68
34	5	317	LHG	O4-P-O5	4.43	133.03	112.44
38	6	311	KC1	C2C-C1C-NC	4.42	115.93	110.45
30	4	304	CLA	C2C-C1C-NC	4.42	114.63	109.98
30	1	303	CLA	O2D-CGD-CBD	4.42	118.96	111.23
30	15	307	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
37	16	312	A86	C8-C6-C5	4.42	125.96	119.01
30	3	309	CLA	C3D-C4D-ND	4.42	117.17	109.99
37	10	302	A86	C7-C6-C5	-4.42	115.66	122.82
30	7	310	CLA	C3D-C4D-ND	4.42	117.17	109.99
30	B	833	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
38	13	312	KC1	C3C-C4C-NC	4.42	114.63	109.90
30	12	304	CLA	C3D-C4D-ND	4.42	117.17	109.99
30	4	305	CLA	C2C-C1C-NC	4.42	114.62	109.98
30	B	828	CLA	C2D-C1D-ND	4.42	114.50	110.13
30	1	307	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
30	14	309	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
30	A	804	CLA	C2C-C1C-NC	4.41	114.62	109.98
38	8	311	KC1	CHC-C1C-C2C	-4.41	118.06	125.03
37	14	301	A86	C3-C2-C1	-4.41	121.09	127.28
30	A	842	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
38	12	311	KC1	CHC-C1C-C2C	-4.41	118.06	125.03
30	B	821	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
34	A	852	LHG	O4-P-O5	4.41	132.96	112.44
30	B	806	CLA	C4A-NA-C1A	-4.41	104.67	106.68
30	B	824	CLA	C2C-C1C-NC	4.41	114.61	109.98
30	4	311	CLA	O2D-CGD-CBD	4.40	118.93	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	822	CLA	C2B-C1B-NB	4.40	114.89	110.33
30	B	827	CLA	C4A-NA-C1A	-4.40	104.67	106.68
30	2	310	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
30	B	831	CLA	C3D-C4D-ND	4.40	117.14	109.99
30	14	310	CLA	CHD-C1D-ND	-4.40	118.61	124.80
38	1	306	KC1	C2A-C1A-NA	4.40	116.39	109.34
30	14	302	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
30	A	804	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
30	7	303	CLA	C3D-C4D-ND	4.40	117.14	109.99
30	A	836	CLA	C2B-C1B-NB	4.40	114.89	110.33
37	10	301	A86	C4-C3-C2	-4.40	114.52	123.52
37	14	320	A86	C9-C8-C6	-4.40	114.30	126.36
30	B	851	CLA	C3D-C4D-ND	4.40	117.14	109.99
30	1	305	CLA	C4A-NA-C1A	-4.40	104.67	106.68
39	2	315	DD6	C21-C20-C19	-4.40	109.30	114.24
30	A	824	CLA	C3D-C4D-ND	4.39	117.13	109.99
30	15	304	CLA	C3D-C4D-ND	4.39	117.13	109.99
38	2	314	KC1	C2A-C1A-NA	4.39	116.38	109.34
37	7	316	A86	C4-C5-C6	-4.39	121.12	127.28
30	3	310	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
30	15	309	CLA	C3D-C4D-ND	4.39	117.12	109.99
30	11	308	CLA	C3D-C4D-ND	4.39	117.12	109.99
39	3	316	DD6	C21-C20-C19	-4.39	109.31	114.24
30	13	309	CLA	CHD-C1D-ND	-4.39	118.63	124.80
38	5	310	KC1	C2A-C1A-NA	4.39	116.37	109.34
30	14	304	CLA	CHD-C1D-ND	-4.39	118.63	124.80
30	16	303	CLA	CHD-C1D-ND	-4.38	118.63	124.80
30	A	828	CLA	C3C-C4C-NC	4.38	116.05	110.43
30	B	810	CLA	C4A-NA-C1A	-4.38	104.68	106.68
38	1	306	KC1	CHC-C1C-C2C	-4.38	118.11	125.03
30	3	303	CLA	C3D-C4D-ND	4.38	117.11	109.99
30	3	307	CLA	C3D-C4D-ND	4.38	117.11	109.99
38	12	309	KC1	CHC-C1C-C2C	-4.38	118.11	125.03
38	8	310	KC1	C3D-C4D-ND	4.38	116.31	110.20
37	14	315	A86	C10-C9-C8	-4.38	110.51	123.20
30	14	303	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
30	4	302	CLA	C2C-C1C-NC	4.38	114.58	109.98
30	5	302	CLA	C4A-NA-C1A	-4.38	104.68	106.68
30	10	311	CLA	C2C-C1C-NC	4.38	114.58	109.98
30	2	311	CLA	C2C-C1C-NC	4.38	114.58	109.98
30	7	303	CLA	C4A-NA-C1A	-4.38	104.68	106.68
30	14	310	CLA	C3D-C4D-ND	4.37	117.10	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	9	304	KC1	C3C-C4C-NC	4.37	114.59	109.90
30	J	101	CLA	O2D-CGD-CBD	4.37	118.88	111.23
38	5	310	KC1	CHC-C1C-C2C	-4.37	118.12	125.03
39	4	313	DD6	C7-C6-C8	-4.37	111.41	118.09
38	2	314	KC1	CHC-C1C-C2C	-4.37	118.12	125.03
30	B	831	CLA	C4A-NA-C1A	-4.37	104.68	106.68
38	8	312	KC1	O2D-CGD-CBD	4.37	118.87	111.23
30	8	309	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
38	1	308	KC1	C2A-C1A-NA	4.37	116.34	109.34
38	7	308	KC1	C3D-C4D-ND	4.37	116.30	110.20
38	1	306	KC1	C4B-C3B-C2B	-4.37	103.02	106.81
30	15	302	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
30	14	312	CLA	O2D-CGD-CBD	4.37	118.87	111.23
38	6	312	KC1	C2A-C1A-NA	4.37	116.34	109.34
37	14	317	A86	C12-C11-C13	4.37	123.08	116.00
37	10	316	A86	C40-C32-C31	-4.37	106.56	110.47
30	B	814	CLA	C3D-C4D-ND	4.37	117.09	109.99
38	11	312	KC1	CMA-C3A-C2A	-4.37	117.86	128.43
38	8	307	KC1	C2A-C1A-NA	4.37	116.34	109.34
30	13	307	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
30	12	304	CLA	CHD-C1D-ND	-4.37	118.66	124.80
30	3	307	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
38	11	305	KC1	C2A-C1A-NA	4.37	116.34	109.34
30	L	202	CLA	C2C-C1C-NC	4.37	114.57	109.98
38	8	312	KC1	CMA-C3A-C4A	-4.36	118.21	125.03
30	9	302	CLA	C3D-C4D-ND	4.36	117.08	109.99
30	A	842	CLA	C2C-C1C-NC	4.36	114.56	109.98
30	15	313	CLA	C3D-C4D-ND	4.36	117.08	109.99
30	A	844	CLA	C3D-C4D-ND	4.36	117.08	109.99
30	2u	202	CLA	C3D-C4D-ND	4.36	117.08	109.99
38	11	312	KC1	C4B-C3B-C2B	-4.36	103.03	106.81
30	F	201	CLA	C3C-C4C-NC	4.36	116.02	110.43
30	2	309	CLA	C3D-C4D-ND	4.36	117.08	109.99
30	11	309	CLA	C4A-NA-C1A	-4.36	104.69	106.68
39	13	314	DD6	C15-C14-C13	4.36	135.21	125.99
38	3	304	KC1	C3D-C4D-ND	4.36	116.27	110.20
30	A	830	CLA	C3C-C4C-NC	4.36	116.01	110.43
39	2	315	DD6	O1-C15-C14	-4.36	104.40	116.88
30	B	802	CLA	CMD-C2D-C1D	4.36	132.40	124.73
38	10	306	KC1	C3D-C4D-ND	4.35	116.27	110.20
37	15	320	A86	C41-C32-C31	-4.35	106.58	110.47
37	2	319	A86	C26-C25-C24	-4.35	110.58	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	844	CLA	O2D-CGD-CBD	4.35	118.84	111.23
38	16	311	KC1	C3D-C4D-ND	4.35	116.27	110.20
30	10	307	CLA	O2D-CGD-CBD	4.35	118.84	111.23
30	12	310	CLA	C2B-C1B-NB	4.35	114.84	110.33
30	14	304	CLA	C3D-C4D-ND	4.35	117.06	109.99
38	9	304	KC1	CHC-C1C-C2C	-4.35	118.16	125.03
30	B	828	CLA	C4A-NA-C1A	-4.35	104.69	106.68
30	A	833	CLA	O2D-CGD-CBD	4.35	118.84	111.23
30	10	308	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
30	B	823	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
30	A	812	CLA	C3D-C4D-ND	4.35	117.06	109.99
30	15	304	CLA	CHD-C1D-ND	-4.35	118.68	124.80
30	B	816	CLA	CHD-C1D-ND	-4.35	118.69	124.80
38	2	306	KC1	C3C-C4C-NC	4.34	114.56	109.90
30	4	306	CLA	C2C-C1C-NC	4.34	114.55	109.98
30	13	301	CLA	C3D-C4D-ND	4.34	117.05	109.99
30	13	304	CLA	CHD-C1D-ND	-4.34	118.69	124.80
30	11	310	CLA	C3D-C4D-ND	4.34	117.05	109.99
30	6	317	CLA	C3D-C4D-ND	4.34	117.04	109.99
30	8	301	CLA	C3D-C4D-ND	4.34	117.04	109.99
38	8	314	KC1	O2D-CGD-O1D	-4.34	115.40	123.85
30	7	309	CLA	C2B-C1B-NB	4.34	114.83	110.33
37	9	313	A86	C21-C20-C15	-4.34	109.34	123.35
38	1	306	KC1	CHD-C4C-C3C	-4.34	117.23	125.23
30	8	304	CLA	C4A-NA-C1A	-4.34	104.70	106.68
30	A	835	CLA	CHD-C1D-ND	-4.34	118.70	124.80
37	14	320	A86	C25-C24-C1	-4.34	114.47	126.36
30	12	308	CLA	C3D-C4D-ND	4.34	117.04	109.99
34	A	853	LHG	O4-P-O5	4.34	132.61	112.44
30	10	305	CLA	C2B-C1B-NB	4.34	114.82	110.33
30	6	305	CLA	O2D-CGD-CBD	4.34	118.81	111.23
30	10	311	CLA	C3D-C4D-ND	4.33	117.03	109.99
30	A	834	CLA	O2D-CGD-CBD	4.33	118.81	111.23
30	14	313	CLA	CHD-C1D-ND	-4.33	118.70	124.80
30	B	839	CLA	C2C-C1C-NC	4.33	114.53	109.98
30	3	306	CLA	CHD-C1D-ND	-4.33	118.71	124.80
38	3	308	KC1	CBA-CAA-C2A	-4.33	108.07	125.45
38	11	312	KC1	C3D-C4D-ND	4.33	116.24	110.20
30	10	303	CLA	O2D-CGD-CBD	4.33	118.80	111.23
38	4	308	KC1	C3D-C4D-ND	4.33	116.24	110.20
38	13	312	KC1	CHC-C1C-C2C	-4.33	118.19	125.03
37	9	315	A86	C33-C32-C31	4.33	113.42	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	304	CLA	CHD-C1D-ND	-4.33	118.71	124.80
30	2	313	CLA	C3D-C4D-ND	4.33	117.02	109.99
30	14	312	CLA	C3D-C4D-ND	4.33	117.02	109.99
38	5	305	KC1	CHC-C1C-C2C	-4.33	118.19	125.03
30	F	201	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
30	6	306	CLA	C2C-C1C-NC	4.33	114.53	109.98
30	6	309	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
38	14	306	KC1	CHC-C1C-C2C	-4.32	118.20	125.03
30	1	303	CLA	C3D-C4D-ND	4.32	117.02	109.99
30	A	823	CLA	C3D-C4D-ND	4.32	117.02	109.99
30	B	828	CLA	C3D-C4D-ND	4.32	117.02	109.99
38	11	305	KC1	CHC-C1C-C2C	-4.32	118.20	125.03
30	16	301	CLA	O2D-CGD-CBD	4.32	118.79	111.23
39	12	317	DD6	O1-C20-C21	-4.32	110.22	115.05
30	B	827	CLA	O2D-CGD-CBD	4.32	118.78	111.23
30	8	302	CLA	O2D-CGD-CBD	4.32	118.78	111.23
30	6	316	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
39	2	315	DD6	C25-C24-C1	-4.32	114.52	126.36
38	9	312	KC1	C2A-C1A-NA	4.32	116.26	109.34
30	9	303	CLA	C3D-C4D-ND	4.32	117.01	109.99
38	10	312	KC1	C3C-C4C-NC	4.32	114.53	109.90
30	B	835	CLA	C3D-C4D-ND	4.32	117.00	109.99
30	4	305	CLA	C3D-C4D-ND	4.32	117.00	109.99
30	16	307	CLA	C3D-C4D-ND	4.32	117.00	109.99
30	16	306	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
30	15	312	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
30	7	310	CLA	O2D-CGD-CBD	4.32	118.78	111.23
30	B	851	CLA	C4A-NA-C1A	-4.32	104.71	106.68
38	10	306	KC1	CHC-C1C-C2C	-4.32	118.22	125.03
30	A	827	CLA	C2C-C1C-NC	4.31	114.51	109.98
38	13	310	KC1	C1A-NA-C4A	-4.31	104.71	106.68
30	5	304	CLA	C3D-C4D-ND	4.31	117.00	109.99
30	10	309	CLA	C3D-C4D-ND	4.31	117.00	109.99
30	A	838	CLA	C1D-CHD-C4C	-4.31	116.85	126.02
30	8	305	CLA	C2C-C1C-NC	4.31	114.51	109.98
30	11	306	CLA	C3D-C4D-ND	4.31	117.00	109.99
30	9	309	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
30	B	835	CLA	C2C-C1C-NC	4.31	114.51	109.98
38	11	311	KC1	CHC-C1C-C2C	-4.31	118.22	125.03
30	1	303	CLA	CHD-C1D-ND	-4.31	118.74	124.80
30	A	818	CLA	C3D-C4D-ND	4.31	116.99	109.99
38	6	308	KC1	C1A-NA-C4A	-4.31	104.71	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	320	A86	C9-C10-C11	-4.31	114.46	126.64
30	A	819	CLA	O2D-CGD-CBD	4.31	118.76	111.23
30	8	309	CLA	C3D-C4D-ND	4.31	116.99	109.99
30	B	801	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
30	10	304	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
30	B	830	CLA	C2C-C1C-NC	4.31	114.51	109.98
30	5	302	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
30	6	307	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
30	15	312	CLA	C1C-C2C-C3C	-4.30	102.45	106.98
39	15	318	DD6	O1-C20-C21	-4.30	110.24	115.05
30	5	304	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
30	B	822	CLA	CAA-CBA-CGA	-4.30	100.99	113.21
30	14	304	CLA	C4A-NA-C1A	-4.30	104.72	106.68
30	L	203	CLA	C3D-C4D-ND	4.30	116.98	109.99
30	12	308	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
30	A	816	CLA	C3D-C4D-ND	4.30	116.98	109.99
30	B	806	CLA	C2C-C1C-NC	4.30	114.50	109.98
38	13	312	KC1	C1A-NA-C4A	-4.30	104.72	106.68
30	B	831	CLA	CHD-C1D-ND	-4.30	118.75	124.80
30	B	825	CLA	C2C-C1C-NC	4.30	114.50	109.98
30	4	311	CLA	CHD-C1D-ND	-4.30	118.75	124.80
37	14	314	A86	C4-C3-C2	-4.30	114.72	123.52
30	13	303	CLA	CHD-C1D-ND	-4.30	118.75	124.80
37	9	313	A86	C25-C24-C1	-4.30	114.58	126.36
30	3	303	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
30	A	812	CLA	O2D-CGD-CBD	4.30	118.74	111.23
38	9	312	KC1	O2D-CGD-CBD	4.29	118.74	111.23
30	B	824	CLA	C3D-C4D-ND	4.29	116.97	109.99
38	16	304	KC1	C1A-NA-C4A	-4.29	104.72	106.68
30	3	310	CLA	C3D-C4D-ND	4.29	116.97	109.99
30	B	829	CLA	C3D-C4D-ND	4.29	116.96	109.99
38	11	311	KC1	C1A-NA-C4A	-4.29	104.72	106.68
39	7	302	DD6	C-C1-C24	-4.29	111.53	118.09
30	A	843	CLA	C3D-C4D-ND	4.29	116.96	109.99
37	10	317	A86	C25-C26-C27	-4.29	121.26	127.28
38	5	312	KC1	O2D-CGD-CBD	4.29	118.73	111.23
30	16	307	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
39	7	302	DD6	C7-C6-C8	-4.29	111.53	118.09
38	3	311	KC1	C2A-C1A-NA	4.29	116.21	109.34
30	16	309	CLA	C3D-C4D-ND	4.29	116.96	109.99
30	13	309	CLA	O2D-CGD-CBD	4.29	118.73	111.23
30	14	303	CLA	C3D-C4D-ND	4.29	116.96	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	828	CLA	C4C-C3C-C2C	-4.28	100.65	106.89
30	6	306	CLA	C3D-C4D-ND	4.28	116.95	109.99
39	7	317	DD6	C15-C14-C13	4.28	135.05	125.99
38	2	312	KC1	O2D-CGD-CBD	4.28	118.72	111.23
38	7	308	KC1	O2D-CGD-CBD	4.28	118.72	111.23
30	A	821	CLA	C1-C2-C3	-4.28	119.18	126.20
37	12	316	A86	C10-C9-C8	-4.28	110.79	123.20
30	2	305	CLA	C3D-C4D-ND	4.28	116.95	109.99
30	4	304	CLA	C3D-C4D-ND	4.28	116.95	109.99
37	13	313	A86	C9-C10-C11	-4.28	114.54	126.64
30	F	201	CLA	C3D-C4D-ND	4.28	116.95	109.99
38	7	308	KC1	CHC-C1C-C2C	-4.28	118.27	125.03
30	14	302	CLA	C4A-NA-C1A	-4.28	104.73	106.68
37	15	316	A86	C9-C8-C6	-4.28	114.63	126.36
37	4	314	A86	C25-C26-C27	-4.28	121.28	127.28
39	6	319	DD6	O1-C15-C14	-4.28	104.62	116.88
38	13	308	KC1	CBA-CAA-C2A	-4.28	108.28	125.45
38	5	305	KC1	C2A-C1A-NA	4.28	116.19	109.34
30	12	312	CLA	C3D-C4D-ND	4.28	116.94	109.99
38	6	308	KC1	C3D-C4D-ND	4.28	116.16	110.20
30	16	309	CLA	C4A-NA-C1A	-4.27	104.73	106.68
30	8	303	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
30	5	308	CLA	C3D-C4D-ND	4.27	116.93	109.99
30	B	822	CLA	C2C-C1C-NC	4.27	114.47	109.98
30	B	814	CLA	C1D-CHD-C4C	-4.27	116.94	126.02
30	16	301	CLA	C3D-C4D-ND	4.27	116.93	109.99
30	15	310	CLA	C4A-NA-C1A	-4.27	104.73	106.68
38	8	312	KC1	C2B-C1B-NB	4.27	114.35	110.13
38	16	304	KC1	CHD-C4C-C3C	-4.27	117.35	125.23
30	2	310	CLA	C3D-C4D-ND	4.27	116.93	109.99
30	7	309	CLA	C1D-CHD-C4C	-4.27	116.94	126.02
30	7	307	CLA	O2D-CGD-CBD	4.27	118.69	111.23
38	9	304	KC1	O2D-CGD-CBD	4.27	118.69	111.23
39	6	303	DD6	C21-C20-C15	-4.27	115.28	122.30
30	10	308	CLA	O2D-CGD-CBD	4.27	118.69	111.23
38	13	312	KC1	C2A-C1A-NA	4.27	116.18	109.34
30	B	839	CLA	C3D-C4D-ND	4.27	116.93	109.99
30	14	302	CLA	CHD-C1D-ND	-4.27	118.80	124.80
30	A	830	CLA	C3D-C4D-ND	4.27	116.92	109.99
30	B	817	CLA	CHD-C1D-ND	-4.27	118.80	124.80
39	5	313	DD6	O1-C15-C14	-4.27	104.65	116.88
30	B	834	CLA	C3C-C4C-NC	4.27	115.89	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	310	KC1	CHC-C1C-C2C	-4.27	118.29	125.03
30	A	815	CLA	C3B-C4B-NB	4.27	114.34	110.53
30	1	305	CLA	O2D-CGD-CBD	4.27	118.69	111.23
37	1	309	A86	C25-C26-C27	-4.27	121.30	127.28
30	15	307	CLA	CAA-C2A-C3A	-4.26	101.48	113.00
30	10	308	CLA	CHD-C1D-ND	-4.26	118.80	124.80
38	14	308	KC1	C2C-C1C-NC	4.26	115.72	110.45
30	B	810	CLA	C1D-CHD-C4C	-4.26	116.97	126.02
38	6	312	KC1	C1A-NA-C4A	-4.26	104.74	106.68
30	3	310	CLA	CHD-C1D-ND	-4.26	118.81	124.80
30	15	310	CLA	C3D-C4D-ND	4.26	116.91	109.99
30	15	311	CLA	C3D-C4D-ND	4.26	116.91	109.99
30	3	309	CLA	CHD-C1D-ND	-4.26	118.81	124.80
30	15	303	CLA	CHD-C1D-ND	-4.26	118.81	124.80
30	B	832	CLA	CHD-C1D-ND	-4.26	118.81	124.80
37	14	319	A86	C36-C31-C32	-4.25	115.47	119.70
30	A	808	CLA	C3D-C4D-ND	4.25	116.90	109.99
30	A	811	CLA	C3D-C4D-ND	4.25	116.90	109.99
30	A	833	CLA	C3D-C4D-ND	4.25	116.90	109.99
30	3	301	CLA	C3D-C4D-ND	4.25	116.90	109.99
30	B	820	CLA	C3D-C4D-ND	4.25	116.90	109.99
38	1	308	KC1	CHC-C1C-C2C	-4.25	118.31	125.03
38	13	308	KC1	C2A-C1A-NA	4.25	116.16	109.34
30	2	307	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
30	4	311	CLA	C3D-C4D-ND	4.25	116.90	109.99
30	13	301	CLA	C2B-C1B-NB	4.25	114.73	110.33
30	4	303	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
37	15	322	A86	C9-C8-C6	-4.25	114.71	126.36
39	7	318	DD6	C15-C14-C13	4.25	134.97	125.99
30	B	820	CLA	CBC-CAC-C3C	-4.25	100.91	112.42
38	3	308	KC1	C2C-C1C-NC	4.25	115.70	110.45
37	7	316	A86	C26-C25-C24	-4.25	110.90	123.20
30	B	815	CLA	C1D-CHD-C4C	-4.24	117.00	126.02
30	A	836	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
30	B	809	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
37	12	314	A86	C4-C3-C2	-4.24	114.84	123.52
38	2	306	KC1	CHC-C1C-C2C	-4.24	118.33	125.03
30	A	812	CLA	CAA-C2A-C3A	-4.24	101.54	113.00
37	11	301	A86	C36-C31-C32	-4.24	115.49	119.70
30	A	821	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
30	B	813	CLA	C3C-C4C-NC	4.24	115.86	110.43
30	4	306	CLA	C3D-C4D-ND	4.24	116.88	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	303	CLA	C3D-C4D-ND	4.24	116.88	109.99
30	9	306	CLA	CHD-C1D-ND	-4.24	118.83	124.80
30	6	314	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
39	12	315	DD6	O1-C15-C14	-4.24	104.73	116.88
38	7	313	KC1	C2A-C1A-NA	4.24	116.13	109.34
30	A	843	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
30	6	304	CLA	C3D-C4D-ND	4.24	116.88	109.99
30	A	830	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
38	4	307	KC1	CHD-C4C-C3C	-4.24	117.41	125.23
30	14	305	CLA	CHD-C1D-ND	-4.24	118.84	124.80
39	6	318	DD6	C15-C14-C13	-4.24	117.04	125.99
30	15	307	CLA	C1C-C2C-C3C	-4.24	102.53	106.98
30	16	308	CLA	C3D-C4D-ND	4.23	116.87	109.99
30	7	311	CLA	C4A-NA-C1A	-4.23	104.75	106.68
39	3	316	DD6	C35-C36-C31	-4.23	111.69	120.50
39	2	317	DD6	C15-C14-C13	4.23	134.94	125.99
30	7	305	CLA	CHD-C1D-ND	-4.23	118.85	124.80
38	7	313	KC1	C3C-C4C-NC	4.23	114.43	109.90
38	1	308	KC1	C4B-C3B-C2B	-4.23	103.14	106.81
38	6	311	KC1	C1C-C2C-C3C	-4.23	102.53	106.98
30	A	823	CLA	CHD-C1D-ND	-4.23	118.85	124.80
30	1	305	CLA	C3D-C4D-ND	4.23	116.86	109.99
30	15	304	CLA	C1D-CHD-C4C	-4.23	117.03	126.02
30	16	303	CLA	CAA-C2A-C3A	-4.23	101.57	113.00
30	10	304	CLA	O2D-CGD-CBD	4.23	118.62	111.23
38	13	310	KC1	C2A-C1A-NA	4.23	116.12	109.34
38	12	311	KC1	C2A-C1A-NA	4.23	116.12	109.34
30	B	827	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
30	A	815	CLA	CHD-C1D-ND	-4.23	118.86	124.80
30	2	308	CLA	C3D-C4D-ND	4.23	116.86	109.99
39	7	302	DD6	C35-C36-C31	-4.23	111.71	120.50
34	B	848	LHG	O4-P-O5	4.22	132.09	112.44
38	12	311	KC1	C1A-NA-C4A	-4.22	104.75	106.68
30	1	301	CLA	C3D-C4D-ND	4.22	116.85	109.99
30	15	308	CLA	C3C-C4C-NC	4.22	115.84	110.43
30	A	839	CLA	CHD-C1D-ND	-4.22	118.86	124.80
30	5	302	CLA	C3D-C4D-ND	4.22	116.85	109.99
30	13	302	CLA	C4A-NA-C1A	-4.22	104.75	106.68
38	6	313	KC1	CHC-C1C-C2C	-4.22	118.36	125.03
30	5	302	CLA	C2C-C1C-NC	4.22	114.42	109.98
30	14	310	CLA	C1D-CHD-C4C	-4.22	117.05	126.02
30	9	309	CLA	C3D-C4D-ND	4.22	116.85	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	829	CLA	C2C-C1C-NC	4.22	114.41	109.98
37	8	318	A86	C33-C32-C31	4.22	113.31	109.21
37	2	318	A86	C25-C24-C1	-4.22	114.79	126.36
30	B	830	CLA	C3D-C4D-ND	4.22	116.85	109.99
30	6	317	CLA	CHD-C1D-ND	-4.22	118.86	124.80
39	15	318	DD6	C23-C16-C15	4.22	121.44	110.05
30	B	819	CLA	O2D-CGD-CBD	4.22	118.61	111.23
30	A	842	CLA	C3D-C4D-ND	4.22	116.84	109.99
38	11	307	KC1	C3C-C4C-NC	4.22	114.42	109.90
30	A	839	CLA	O2D-CGD-O1D	-4.22	115.64	123.85
38	8	313	KC1	C2A-C1A-NA	4.22	116.10	109.34
37	14	319	A86	C41-C32-C31	-4.22	106.70	110.47
30	B	837	CLA	C3D-C4D-ND	4.22	116.84	109.99
30	A	840	CLA	CHD-C1D-ND	-4.21	118.87	124.80
38	10	306	KC1	C2A-C1A-NA	4.21	116.09	109.34
38	10	310	KC1	C2C-C1C-NC	4.21	115.67	110.45
30	8	303	CLA	C2B-C1B-NB	4.21	114.70	110.33
30	F	203	CLA	C3D-C4D-ND	4.21	116.84	109.99
30	A	834	CLA	CHD-C1D-ND	-4.21	118.87	124.80
30	A	811	CLA	CHD-C1D-ND	-4.21	118.87	124.80
30	B	824	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
30	11	310	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
38	8	314	KC1	C3D-C4D-ND	4.21	116.07	110.20
30	16	308	CLA	CHD-C1D-ND	-4.21	118.88	124.80
39	6	303	DD6	O1-C15-C14	-4.21	104.81	116.88
30	B	833	CLA	C4A-NA-C1A	-4.21	104.76	106.68
37	10	301	A86	C36-C31-C32	-4.21	115.52	119.70
30	A	804	CLA	C3D-C4D-ND	4.21	116.83	109.99
30	A	839	CLA	C3D-C4D-ND	4.21	116.83	109.99
37	3	315	A86	C4-C3-C2	-4.21	114.91	123.52
30	A	833	CLA	CHD-C1D-ND	-4.21	118.88	124.80
30	12	310	CLA	C4A-NA-C1A	-4.21	104.76	106.68
37	14	318	A86	C3-C2-C1	-4.21	121.38	127.28
38	4	310	KC1	C2A-C1A-NA	4.21	116.08	109.34
30	B	834	CLA	C1D-CHD-C4C	-4.21	117.08	126.02
30	16	303	CLA	C2C-C1C-NC	4.21	114.40	109.98
38	6	312	KC1	O2D-CGD-CBD	4.21	118.58	111.23
30	A	827	CLA	C3D-C4D-ND	4.21	116.83	109.99
30	A	824	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
30	11	308	CLA	CHD-C1D-ND	-4.21	118.88	124.80
37	7	315	A86	C25-C26-C27	-4.21	121.38	127.28
38	9	311	KC1	CHC-C1C-C2C	-4.21	118.39	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	822	CLA	C3D-C4D-ND	4.20	116.82	109.99
30	15	312	CLA	C3D-C4D-ND	4.20	116.82	109.99
30	15	306	CLA	C1D-CHD-C4C	-4.20	117.08	126.02
30	B	805	CLA	C3D-C4D-ND	4.20	116.82	109.99
39	4	313	DD6	C15-C14-C13	4.20	134.88	125.99
37	16	312	A86	C26-C25-C24	-4.20	111.02	123.20
30	B	824	CLA	CHD-C1D-ND	-4.20	118.89	124.80
30	6	315	CLA	C3D-C4D-ND	4.20	116.82	109.99
30	12	302	CLA	C3D-C4D-ND	4.20	116.82	109.99
30	14	305	CLA	C3D-C4D-ND	4.20	116.82	109.99
39	8	316	DD6	C23-C16-C17	-4.20	101.59	108.97
30	11	304	CLA	C2C-C1C-NC	4.20	114.39	109.98
30	3	301	CLA	C4A-NA-C1A	-4.20	104.76	106.68
38	11	307	KC1	CHD-C4C-C3C	-4.20	117.49	125.23
30	B	810	CLA	C3D-C4D-ND	4.20	116.81	109.99
30	15	307	CLA	C3D-C4D-ND	4.20	116.81	109.99
38	9	311	KC1	C2A-C1A-NA	4.20	116.07	109.34
38	6	311	KC1	C1D-CHD-C4C	-4.20	116.38	126.25
39	3	316	DD6	C21-C20-C15	-4.20	115.40	122.30
37	15	315	A86	C41-C32-C31	-4.20	106.72	110.47
38	8	306	KC1	C2A-C1A-NA	4.20	116.06	109.34
30	15	303	CLA	C3D-C4D-ND	4.20	116.81	109.99
30	A	810	CLA	CHD-C1D-ND	-4.20	118.90	124.80
30	9	308	CLA	C3D-C4D-ND	4.19	116.81	109.99
38	8	306	KC1	O2D-CGD-CBD	4.19	118.56	111.23
38	5	312	KC1	C4B-C3B-C2B	-4.19	103.18	106.81
37	15	322	A86	C25-C24-C1	-4.19	114.87	126.36
30	B	808	CLA	C3D-C4D-ND	4.19	116.80	109.99
30	15	303	CLA	C1D-CHD-C4C	-4.19	117.11	126.02
38	9	311	KC1	C1A-NA-C4A	-4.19	104.77	106.68
30	B	818	CLA	CHD-C1D-ND	-4.19	118.91	124.80
30	5	311	CLA	C3D-C4D-ND	4.19	116.80	109.99
30	1	303	CLA	C4A-NA-C1A	-4.19	104.77	106.68
30	8	302	CLA	C3D-C4D-ND	4.19	116.79	109.99
30	6	310	CLA	C1C-C2C-C3C	-4.19	102.58	106.98
39	9	314	DD6	C37-C36-C35	-4.19	106.72	114.42
30	J	101	CLA	C3D-C2D-C1D	-4.19	100.12	105.83
30	5	307	CLA	C1D-CHD-C4C	-4.18	117.13	126.02
30	4	311	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
39	11	313	DD6	C13-C11-C10	-4.18	112.43	119.01
30	B	818	CLA	C3D-C4D-ND	4.18	116.79	109.99
38	2	306	KC1	C2A-C1A-NA	4.18	116.04	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	305	CLA	C3D-C4D-ND	4.18	116.78	109.99
37	7	316	A86	C41-C32-C31	-4.18	106.73	110.47
30	16	310	CLA	C3D-C4D-ND	4.18	116.78	109.99
30	F	202	CLA	C4A-NA-C1A	-4.18	104.77	106.68
38	6	313	KC1	C2A-C1A-NA	4.18	116.04	109.34
30	2	310	CLA	C1-C2-C3	-4.18	119.35	126.20
30	4	303	CLA	C3D-C4D-ND	4.18	116.78	109.99
37	14	315	A86	C36-C31-C32	-4.18	115.55	119.70
30	B	819	CLA	C2D-C1D-ND	4.18	114.26	110.13
30	2	313	CLA	CHD-C1D-ND	-4.18	118.92	124.80
30	11	309	CLA	CHD-C1D-ND	-4.18	118.92	124.80
30	9	301	CLA	CHD-C1D-ND	-4.18	118.92	124.80
30	7	311	CLA	C3D-C4D-ND	4.18	116.78	109.99
30	A	803	CLA	O2D-CGD-CBD	4.18	118.53	111.23
37	15	321	A86	C4-C5-C6	-4.17	121.42	127.28
30	6	307	CLA	C3D-C4D-ND	4.17	116.77	109.99
30	B	802	CLA	C3D-C4D-ND	4.17	116.77	109.99
30	A	820	CLA	CHD-C1D-ND	-4.17	118.93	124.80
30	2	313	CLA	C4A-NA-C1A	-4.17	104.78	106.68
30	5	309	CLA	C3D-C4D-ND	4.17	116.77	109.99
39	6	321	DD6	C21-C20-C15	-4.17	115.44	122.30
39	7	314	DD6	C37-C36-C35	-4.17	106.75	114.42
38	14	306	KC1	C4B-C3B-C2B	-4.17	103.20	106.81
30	A	829	CLA	CHD-C1D-ND	-4.17	118.93	124.80
30	13	307	CLA	C3D-C4D-ND	4.17	116.77	109.99
38	10	306	KC1	C1A-NA-C4A	-4.17	104.78	106.68
30	15	305	CLA	C3D-C4D-ND	4.17	116.76	109.99
30	B	851	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
30	15	302	CLA	C2C-C1C-NC	4.17	114.36	109.98
39	7	318	DD6	C21-C20-C15	-4.17	115.44	122.30
30	10	305	CLA	CMB-C2B-C1B	4.17	131.76	125.42
38	12	313	KC1	C1C-C2C-C3C	-4.17	102.60	106.98
30	12	306	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
30	B	819	CLA	C3D-C4D-ND	4.16	116.76	109.99
30	2	307	CLA	CAA-C2A-C3A	-4.16	101.75	113.00
38	11	312	KC1	C1C-C2C-C3C	-4.16	102.60	106.98
38	2	312	KC1	C2A-C1A-NA	4.16	116.01	109.34
30	B	831	CLA	C1D-CHD-C4C	-4.16	117.17	126.02
30	12	307	CLA	C1D-CHD-C4C	-4.16	117.17	126.02
30	13	309	CLA	C3D-C4D-ND	4.16	116.75	109.99
30	3	303	CLA	CHD-C1D-ND	-4.16	118.95	124.80
30	5	311	CLA	C4A-NA-C1A	-4.16	104.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	315	A86	C36-C31-C32	-4.16	115.57	119.70
30	B	801	CLA	C2C-C1C-NC	4.16	114.35	109.98
30	6	309	CLA	C3D-C4D-ND	4.16	116.75	109.99
30	B	822	CLA	CHD-C1D-ND	-4.16	118.95	124.80
30	A	806	CLA	CAA-C2A-C3A	-4.16	101.76	113.00
30	6	307	CLA	O2D-CGD-CBD	4.16	118.50	111.23
37	10	301	A86	C24-C1-C2	-4.16	112.47	119.01
30	10	305	CLA	CHD-C1D-ND	-4.15	118.95	124.80
30	11	304	CLA	CHD-C1D-ND	-4.15	118.96	124.80
30	6	314	CLA	CBC-CAC-C3C	-4.15	101.17	112.42
37	15	323	A86	C25-C24-C1	-4.15	114.98	126.36
30	12	307	CLA	C3D-C4D-ND	4.15	116.73	109.99
38	4	307	KC1	C3C-C4C-NC	4.15	114.35	109.90
30	7	303	CLA	C2C-C1C-NC	4.15	114.34	109.98
38	8	306	KC1	C1C-C2C-C3C	-4.15	102.62	106.98
38	13	306	KC1	C4B-C3B-C2B	-4.15	103.22	106.81
30	9	306	CLA	C3D-C4D-ND	4.15	116.73	109.99
30	10	303	CLA	C4A-NA-C1A	-4.15	104.79	106.68
30	B	808	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
30	B	801	CLA	C3D-C4D-ND	4.15	116.73	109.99
30	8	308	CLA	CHD-C1D-ND	-4.14	118.97	124.80
30	10	305	CLA	C4A-NA-C1A	-4.14	104.79	106.68
38	12	313	KC1	C2C-C1C-NC	4.14	115.58	110.45
38	11	311	KC1	C2A-C1A-NA	4.14	115.98	109.34
30	A	805	CLA	C2C-C1C-NC	4.14	114.33	109.98
30	4	303	CLA	CHD-C1D-ND	-4.14	118.97	124.80
30	B	808	CLA	C1D-CHD-C4C	-4.14	117.21	126.02
38	3	304	KC1	C2A-C1A-NA	4.14	115.98	109.34
39	5	313	DD6	C37-C36-C35	-4.14	106.80	114.42
30	16	310	CLA	CHD-C1D-ND	-4.14	118.97	124.80
38	13	311	KC1	C4B-C3B-C2B	-4.14	103.22	106.81
30	F	201	CLA	C1D-CHD-C4C	-4.14	117.22	126.02
30	12	321	CLA	C3D-C4D-ND	4.14	116.72	109.99
30	A	802	CLA	CHD-C1D-ND	-4.14	118.97	124.80
30	7	304	CLA	C3D-C4D-ND	4.14	116.72	109.99
38	7	308	KC1	C4B-C3B-C2B	-4.14	103.22	106.81
30	9	306	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
30	8	301	CLA	C1-C2-C3	-4.14	119.42	126.20
30	B	807	CLA	CHD-C1D-ND	-4.14	118.98	124.80
39	5	314	DD6	O1-C20-C21	-4.14	110.42	115.05
30	10	309	CLA	C4A-NA-C1A	-4.14	104.79	106.68
30	10	311	CLA	C4A-NA-C1A	-4.14	104.79	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	312	CLA	C3D-C4D-ND	4.14	116.71	109.99
30	A	840	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
30	A	836	CLA	C3D-C4D-ND	4.14	116.71	109.99
30	A	818	CLA	C2C-C1C-NC	4.14	114.33	109.98
37	14	315	A86	C12-C11-C13	4.14	122.71	116.00
30	7	304	CLA	O2D-CGD-CBD	4.13	118.45	111.23
37	15	317	A86	C33-C32-C31	4.13	113.23	109.21
39	6	318	DD6	C7-C6-C8	-4.13	111.78	118.09
38	7	313	KC1	C1A-NA-C4A	-4.13	104.79	106.68
30	A	844	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
30	2	301	CLA	C3D-C4D-ND	4.13	116.70	109.99
30	A	838	CLA	CHD-C1D-ND	-4.13	118.99	124.80
30	9	308	CLA	CHD-C1D-ND	-4.13	118.99	124.80
30	B	838	CLA	C3D-C4D-ND	4.13	116.70	109.99
30	9	301	CLA	CAA-C2A-C3A	-4.13	101.84	113.00
30	14	302	CLA	C2C-C1C-NC	4.13	114.32	109.98
30	1	304	CLA	C3D-C4D-ND	4.13	116.70	109.99
30	3	310	CLA	CBC-CAC-C3C	-4.13	101.23	112.42
37	15	316	A86	C12-C11-C13	4.13	122.69	116.00
38	6	311	KC1	C4B-C3B-C2B	-4.13	103.23	106.81
30	A	837	CLA	C3D-C4D-ND	4.13	116.70	109.99
30	B	851	CLA	C2C-C1C-NC	4.13	114.32	109.98
30	8	301	CLA	C1D-CHD-C4C	-4.13	117.25	126.02
30	12	304	CLA	O2A-CGA-CBA	4.13	124.42	111.83
38	7	308	KC1	C2A-C1A-NA	4.13	115.95	109.34
30	6	305	CLA	CHD-C1D-ND	-4.13	119.00	124.80
30	A	829	CLA	C1D-CHD-C4C	-4.13	117.25	126.02
30	A	836	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
37	16	314	A86	C40-C32-C31	-4.13	106.78	110.47
30	6	314	CLA	CHD-C1D-ND	-4.13	119.00	124.80
30	12	306	CLA	C1D-CHD-C4C	-4.12	117.25	126.02
30	11	306	CLA	CHD-C1D-ND	-4.12	119.00	124.80
30	4	309	CLA	C3D-C4D-ND	4.12	116.69	109.99
30	B	826	CLA	C3C-C4C-NC	4.12	115.71	110.43
30	15	314	CLA	C4A-NA-C1A	-4.12	104.80	106.68
30	A	806	CLA	CHD-C1D-ND	-4.12	119.00	124.80
30	16	309	CLA	CHD-C1D-ND	-4.12	119.00	124.80
30	B	819	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
30	4	309	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
30	14	309	CLA	CHD-C1D-ND	-4.12	119.00	124.80
39	6	319	DD6	C35-C36-C31	-4.12	111.92	120.50
30	A	831	CLA	C3B-C2B-C1B	-4.12	102.31	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	807	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
39	15	319	DD6	C15-C14-C13	4.12	134.70	125.99
37	15	323	A86	C41-C32-C31	-4.12	106.79	110.47
30	8	305	CLA	C1D-CHD-C4C	-4.12	117.27	126.02
30	B	807	CLA	C4A-NA-C1A	-4.12	104.80	106.68
30	A	827	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
30	15	309	CLA	C4A-NA-C1A	-4.11	104.80	106.68
38	13	306	KC1	CHC-C1C-C2C	-4.11	118.53	125.03
37	4	317	A86	C12-C11-C13	4.11	122.67	116.00
30	2	307	CLA	C3D-C4D-ND	4.11	116.67	109.99
30	16	302	CLA	C3D-C4D-ND	4.11	116.67	109.99
30	16	305	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
30	1	304	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
30	F	203	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
37	11	314	A86	C36-C31-C32	-4.11	115.62	119.70
38	8	314	KC1	C2A-C1A-NA	4.11	115.93	109.34
30	A	818	CLA	CHD-C1D-ND	-4.11	119.02	124.80
30	A	835	CLA	C3D-C4D-ND	4.11	116.67	109.99
30	10	311	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
30	A	841	CLA	C2C-C1C-NC	4.11	114.30	109.98
39	1	310	DD6	C21-C20-C19	-4.11	109.63	114.24
30	16	302	CLA	O2D-CGD-CBD	4.11	118.41	111.23
30	11	309	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
39	2	316	DD6	O1-C20-C21	-4.11	110.46	115.05
30	A	810	CLA	C3D-C4D-ND	4.11	116.66	109.99
30	B	805	CLA	C3B-C4B-NB	4.11	114.20	110.53
30	8	303	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
30	A	821	CLA	C3D-C4D-ND	4.11	116.66	109.99
30	9	309	CLA	C3B-C2B-C1B	-4.11	102.33	107.17
38	16	311	KC1	CBA-CAA-C2A	-4.11	108.97	125.45
30	13	301	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
30	15	310	CLA	CHD-C1D-ND	-4.11	119.03	124.80
30	16	301	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
30	5	307	CLA	C1C-C2C-C3C	-4.10	102.66	106.98
38	2	312	KC1	C2C-C1C-NC	4.10	115.53	110.45
30	15	306	CLA	C3D-C4D-ND	4.10	116.66	109.99
30	9	302	CLA	CHD-C1D-ND	-4.10	119.03	124.80
38	8	307	KC1	CHC-C1C-C2C	-4.10	118.55	125.03
30	A	834	CLA	C3D-C4D-ND	4.10	116.66	109.99
30	14	309	CLA	C3D-C4D-ND	4.10	116.65	109.99
30	3	306	CLA	C3D-C4D-ND	4.10	116.65	109.99
30	12	302	CLA	C1D-CHD-C4C	-4.10	117.31	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	7	313	KC1	CHC-C1C-C2C	-4.10	118.56	125.03
30	B	825	CLA	C4A-NA-C1A	-4.10	104.81	106.68
30	7	304	CLA	CHD-C1D-ND	-4.10	119.04	124.80
30	B	832	CLA	O2D-CGD-CBD	4.10	118.39	111.23
37	15	321	A86	C12-C11-C13	4.09	122.64	116.00
38	13	310	KC1	C2C-C1C-NC	4.09	115.52	110.45
30	7	306	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
30	A	844	CLA	C4A-NA-C1A	-4.09	104.81	106.68
30	A	824	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
39	3	316	DD6	O1-C15-C14	-4.09	105.16	116.88
30	7	309	CLA	C1C-C2C-C3C	-4.09	102.68	106.98
30	5	307	CLA	O2D-CGD-CBD	4.09	118.38	111.23
30	12	310	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
30	15	307	CLA	C4A-NA-C1A	-4.09	104.81	106.68
30	B	838	CLA	C3B-C4B-NB	4.09	114.18	110.53
30	13	302	CLA	C3D-C4D-ND	4.09	116.64	109.99
39	13	314	DD6	C8-C6-C5	-4.09	112.58	119.01
30	1	305	CLA	CHD-C1D-ND	-4.09	119.05	124.80
30	B	818	CLA	CBA-CAA-C2A	4.09	125.96	113.79
38	6	313	KC1	CAA-CBA-CGA	-4.09	106.26	127.05
30	11	308	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
39	2	315	DD6	C12-C11-C13	-4.09	111.84	118.09
30	15	313	CLA	CHD-C1D-ND	-4.09	119.05	124.80
38	14	306	KC1	CHD-C4C-C3C	-4.09	117.69	125.23
30	A	823	CLA	C1C-C2C-C3C	-4.09	102.68	106.98
30	3	301	CLA	C1C-C2C-C3C	-4.09	102.68	106.98
30	14	312	CLA	CHD-C1D-ND	-4.09	119.05	124.80
30	4	301	CLA	C3D-C4D-ND	4.09	116.63	109.99
37	5	316	A86	C36-C31-C32	-4.09	115.64	119.70
38	3	308	KC1	C1C-C2C-C3C	-4.08	102.68	106.98
30	3	306	CLA	C2C-C1C-NC	4.08	114.27	109.98
30	1	304	CLA	C3C-C4C-NC	4.08	115.66	110.43
30	7	310	CLA	C2C-C1C-NC	4.08	114.27	109.98
30	5	311	CLA	CHD-C1D-ND	-4.08	119.06	124.80
30	13	301	CLA	C4A-NA-C1A	-4.08	104.82	106.68
30	B	810	CLA	C2C-C1C-NC	4.08	114.27	109.98
37	4	317	A86	C3-C4-C5	-4.08	115.18	123.52
30	12	302	CLA	C4A-NA-C1A	-4.08	104.82	106.68
30	13	304	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
38	10	312	KC1	CHC-C1C-C2C	-4.08	118.59	125.03
30	B	832	CLA	C3D-C4D-ND	4.07	116.61	109.99
30	8	308	CLA	C3D-C4D-ND	4.07	116.61	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	314	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
38	4	308	KC1	CBA-CAA-C2A	-4.07	109.10	125.45
30	J	101	CLA	C3D-C4D-ND	4.07	116.61	109.99
30	B	836	CLA	C1C-C2C-C3C	-4.07	102.69	106.98
30	B	821	CLA	C3D-C4D-ND	4.07	116.61	109.99
38	11	311	KC1	C1D-CHD-C4C	-4.07	116.67	126.25
30	3	302	CLA	C3D-C4D-ND	4.07	116.61	109.99
30	A	836	CLA	O2D-CGD-CBD	4.07	118.35	111.23
37	14	317	A86	C36-C31-C32	-4.07	115.66	119.70
38	11	307	KC1	C1C-C2C-C3C	-4.07	102.70	106.98
30	B	801	CLA	C3C-C4C-NC	4.07	115.65	110.43
30	B	807	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
30	1	301	CLA	C1-C2-C3	-4.07	119.53	126.20
30	8	304	CLA	C2C-C1C-NC	4.07	114.26	109.98
38	13	311	KC1	CHC-C1C-C2C	-4.07	118.61	125.03
30	1	304	CLA	O2D-CGD-CBD	4.07	118.34	111.23
30	10	304	CLA	C3D-C4D-ND	4.07	116.60	109.99
30	13	309	CLA	C4A-NA-C1A	-4.07	104.82	106.68
30	B	838	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
30	L	203	CLA	C4A-NA-C1A	-4.07	104.82	106.68
37	2	318	A86	C36-C31-C32	-4.06	115.66	119.70
30	B	827	CLA	C3D-C4D-ND	4.06	116.59	109.99
37	15	317	A86	C3-C2-C1	-4.06	121.58	127.28
30	F	203	CLA	CHD-C1D-ND	-4.06	119.09	124.80
30	J	101	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
30	12	306	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
39	2	316	DD6	C21-C20-C19	-4.06	109.68	114.24
30	B	828	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
30	4	304	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
30	9	303	CLA	C4A-NA-C1A	-4.06	104.83	106.68
39	3	312	DD6	C35-C36-C31	-4.06	112.05	120.50
30	F	201	CLA	CMD-C2D-C1D	4.06	131.88	124.73
30	6	316	CLA	C3D-C4D-ND	4.06	116.58	109.99
30	B	807	CLA	C3D-C4D-ND	4.06	116.58	109.99
30	9	307	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
30	8	302	CLA	CHD-C1D-ND	-4.06	119.09	124.80
38	13	305	KC1	C4B-C3B-C2B	-4.06	103.30	106.81
38	14	308	KC1	CBA-CAA-C2A	-4.06	109.17	125.45
30	A	811	CLA	C1D-CHD-C4C	-4.06	117.40	126.02
30	2	311	CLA	CHD-C1D-ND	-4.06	119.09	124.80
30	9	309	CLA	C4A-NA-C1A	-4.06	104.83	106.68
30	A	841	CLA	CHD-C1D-ND	-4.05	119.10	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	304	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
30	A	804	CLA	C1D-CHD-C4C	-4.05	117.40	126.02
30	A	819	CLA	C2C-C1C-NC	4.05	114.24	109.98
30	A	805	CLA	CHD-C1D-ND	-4.05	119.10	124.80
30	2	308	CLA	CHD-C1D-ND	-4.05	119.10	124.80
38	9	312	KC1	C1A-NA-C4A	-4.05	104.83	106.68
38	11	307	KC1	C2A-C1A-NA	4.05	115.83	109.34
30	B	818	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
30	2	304	CLA	C3D-C4D-ND	4.05	116.57	109.99
38	8	311	KC1	C2A-C1A-NA	4.05	115.83	109.34
30	B	801	CLA	C2B-C1B-NB	4.05	114.53	110.33
30	15	307	CLA	O2D-CGD-CBD	4.05	118.31	111.23
30	15	304	CLA	O2D-CGD-CBD	4.05	118.31	111.23
30	12	306	CLA	C3D-C4D-ND	4.05	116.57	109.99
37	16	314	A86	C36-C31-C32	-4.05	115.68	119.70
30	B	828	CLA	C4B-C3B-C2B	-4.05	102.27	107.30
30	3	307	CLA	O2D-CGD-CBD	4.05	118.30	111.23
39	15	318	DD6	C15-C14-C13	4.05	134.55	125.99
37	13	315	A86	C36-C31-C32	-4.05	115.68	119.70
30	2	305	CLA	CBA-CAA-C2A	4.04	125.83	113.79
30	A	830	CLA	CMD-C2D-C1D	4.04	131.85	124.73
38	13	305	KC1	C2C-C1C-NC	4.04	115.45	110.45
30	6	314	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
30	16	305	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
38	8	310	KC1	C2A-C1A-NA	4.04	115.82	109.34
33	L	204	BCR	C24-C23-C22	-4.04	120.26	126.23
38	6	308	KC1	C2A-C1A-NA	4.04	115.82	109.34
30	16	306	CLA	CAA-C2A-C3A	-4.04	102.08	113.00
30	5	303	CLA	C3D-C4D-ND	4.04	116.56	109.99
30	B	805	CLA	CHD-C1D-ND	-4.04	119.12	124.80
30	B	836	CLA	CHD-C1D-ND	-4.04	119.12	124.80
30	15	306	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
30	2u	202	CLA	C4A-NA-C1A	-4.04	104.84	106.68
30	2	307	CLA	C4A-NA-C1A	-4.04	104.84	106.68
30	12	308	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
30	6	310	CLA	C3D-C4D-ND	4.04	116.55	109.99
30	1	302	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
30	8	305	CLA	C3D-C4D-ND	4.04	116.55	109.99
30	9	301	CLA	C3D-C4D-ND	4.04	116.55	109.99
30	A	825	CLA	CHD-C1D-ND	-4.03	119.12	124.80
30	A	805	CLA	C3D-C4D-ND	4.03	116.55	109.99
30	A	807	CLA	O2A-CGA-CBA	4.03	124.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	851	CLA	O2D-CGD-CBD	4.03	118.28	111.23
38	10	306	KC1	C2C-C1C-NC	4.03	115.44	110.45
38	11	307	KC1	C2C-C1C-NC	4.03	115.44	110.45
30	10	305	CLA	CBA-CAA-C2A	4.03	125.79	113.79
30	A	837	CLA	CHD-C1D-ND	-4.03	119.13	124.80
39	10	314	DD6	C37-C36-C35	-4.03	107.00	114.42
38	16	311	KC1	CHC-C1C-C2C	-4.03	118.66	125.03
30	12	303	CLA	O2D-CGD-CBD	4.03	118.28	111.23
30	B	851	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
30	7	307	CLA	C3D-C4D-ND	4.03	116.54	109.99
30	A	822	CLA	C3B-C2B-C1B	-4.03	102.42	107.17
30	A	838	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
30	A	814	CLA	C3D-C4D-ND	4.03	116.54	109.99
37	7	319	A86	C9-C10-C11	-4.03	115.25	126.64
30	12	312	CLA	CHD-C1D-ND	-4.03	119.13	124.80
37	15	315	A86	C-C1-C24	-4.03	111.93	118.09
30	6	306	CLA	O2A-CGA-CBA	4.03	124.12	111.83
30	8	302	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
30	2	309	CLA	CHD-C1D-ND	-4.03	119.13	124.80
38	6	312	KC1	CHC-C1C-C2C	-4.03	118.67	125.03
38	12	313	KC1	CHB-C4A-C3A	-4.03	118.67	125.03
30	A	830	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
39	11	313	DD6	C35-C36-C31	-4.03	112.12	120.50
30	4	309	CLA	C4A-NA-C1A	-4.03	104.84	106.68
30	9	308	CLA	C2C-C1C-NC	4.03	114.21	109.98
30	B	812	CLA	C3D-C4D-ND	4.03	116.53	109.99
30	2	304	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
30	4	301	CLA	CHD-C1D-ND	-4.02	119.14	124.80
30	6	306	CLA	CHD-C1D-ND	-4.02	119.14	124.80
39	3	313	DD6	C21-C20-C19	-4.02	109.72	114.24
38	12	305	KC1	C2A-C1A-NA	4.02	115.79	109.34
30	J	101	CLA	CAA-C2A-C3A	-4.02	102.13	113.00
30	7	309	CLA	C3D-C4D-ND	4.02	116.53	109.99
30	12	321	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
30	14	303	CLA	CHD-C1D-ND	-4.02	119.14	124.80
30	7	306	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
37	7	319	A86	C36-C31-C32	-4.02	115.71	119.70
30	14	305	CLA	CAA-C2A-C3A	-4.02	102.14	113.00
30	6	315	CLA	CHD-C1D-ND	-4.02	119.15	124.80
30	B	806	CLA	C3D-C4D-ND	4.02	116.52	109.99
38	10	306	KC1	C1C-C2C-C3C	-4.02	102.75	106.98
30	13	304	CLA	C1D-CHD-C4C	-4.02	117.48	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	843	CLA	CMB-C2B-C1B	4.02	131.54	125.42
38	12	305	KC1	C2C-C1C-NC	4.02	115.42	110.45
30	4	302	CLA	C3D-C4D-ND	4.02	116.52	109.99
30	15	314	CLA	C1D-CHD-C4C	-4.02	117.48	126.02
30	B	822	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
30	A	808	CLA	CHD-C1D-ND	-4.02	119.15	124.80
30	A	816	CLA	C3B-C4B-NB	4.02	114.12	110.53
39	7	317	DD6	C22-C16-C15	4.02	120.89	110.05
38	16	311	KC1	C1C-C2C-C3C	-4.01	102.76	106.98
39	8	316	DD6	C7-C6-C8	-4.01	111.96	118.09
39	4	316	DD6	O1-C15-C14	-4.01	105.38	116.88
39	15	318	DD6	C21-C20-C19	-4.01	109.73	114.24
30	9	306	CLA	C1D-CHD-C4C	-4.01	117.49	126.02
30	16	306	CLA	C1D-CHD-C4C	-4.01	117.49	126.02
30	B	805	CLA	C4A-NA-C1A	-4.01	104.85	106.68
30	13	303	CLA	C4A-NA-C1A	-4.01	104.85	106.68
37	15	323	A86	C3-C4-C5	-4.01	115.31	123.52
38	5	312	KC1	C2A-C1A-NA	4.01	115.77	109.34
38	5	310	KC1	C1D-CHD-C4C	-4.01	116.82	126.25
30	A	813	CLA	C3D-C4D-ND	4.01	116.51	109.99
30	A	820	CLA	C3D-C4D-ND	4.01	116.51	109.99
30	15	310	CLA	C3B-C4B-NB	4.01	114.11	110.53
38	4	307	KC1	C2A-C1A-NA	4.01	115.77	109.34
30	16	305	CLA	C3D-C4D-ND	4.01	116.50	109.99
37	1	309	A86	C10-C9-C8	-4.01	111.59	123.20
38	4	307	KC1	C1C-C2C-C3C	-4.01	102.77	106.98
30	3	307	CLA	CHD-C1D-ND	-4.01	119.17	124.80
30	9	307	CLA	O2D-CGD-CBD	4.01	118.23	111.23
30	A	814	CLA	C1D-CHD-C4C	-4.01	117.51	126.02
30	11	310	CLA	CHD-C1D-ND	-4.00	119.17	124.80
30	8	301	CLA	C4A-NA-C1A	-4.00	104.85	106.68
30	F	202	CLA	C3C-C4C-NC	4.00	115.56	110.43
30	B	837	CLA	C4A-NA-C1A	-4.00	104.85	106.68
38	8	310	KC1	C1D-CHD-C4C	-4.00	116.84	126.25
37	14	314	A86	C10-C9-C8	-4.00	111.61	123.20
38	13	310	KC1	C1D-CHD-C4C	-4.00	116.84	126.25
38	2	314	KC1	O2D-CGD-CBD	4.00	118.22	111.23
30	7	312	CLA	C4A-NA-C1A	-4.00	104.85	106.68
30	4	309	CLA	CHD-C1D-ND	-4.00	119.17	124.80
30	A	813	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
30	B	809	CLA	C3D-C4D-ND	4.00	116.49	109.99
30	15	311	CLA	CHD-C1D-ND	-4.00	119.17	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	307	CLA	C3B-C2B-C1B	-4.00	102.46	107.17
30	A	832	CLA	C3D-C4D-ND	4.00	116.48	109.99
37	3	314	A86	C9-C10-C11	-4.00	115.34	126.64
38	13	308	KC1	C4B-C3B-C2B	-4.00	103.35	106.81
38	3	308	KC1	C1A-NA-C4A	-4.00	104.86	106.68
38	14	308	KC1	C2A-C1A-NA	4.00	115.74	109.34
30	8	301	CLA	C3C-C4C-NC	3.99	115.55	110.43
30	3	302	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
39	16	313	DD6	C37-C36-C35	-3.99	107.08	114.42
34	2	320	LHG	O4-P-O5	3.99	131.02	112.44
30	6	310	CLA	CHD-C1D-ND	-3.99	119.18	124.80
30	7	312	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
30	16	308	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
30	J	101	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
30	A	841	CLA	C3D-C4D-ND	3.99	116.47	109.99
30	1	304	CLA	C2C-C1C-NC	3.99	114.17	109.98
30	B	820	CLA	C4C-C3C-C2C	-3.99	101.08	106.89
30	B	828	CLA	C3B-C4B-NB	3.99	114.09	110.53
30	B	804	CLA	C3D-C4D-ND	3.99	116.47	109.99
30	12	308	CLA	O2D-CGD-CBD	3.99	118.20	111.23
30	B	838	CLA	CHD-C1D-ND	-3.99	119.19	124.80
30	15	308	CLA	C3D-C4D-ND	3.99	116.47	109.99
30	10	308	CLA	C2C-C1C-NC	3.99	114.17	109.98
30	5	308	CLA	C4A-NA-C1A	-3.99	104.86	106.68
39	5	313	DD6	C7-C6-C8	-3.99	112.00	118.09
30	A	819	CLA	C3D-C4D-ND	3.99	116.47	109.99
37	14	301	A86	C12-C11-C13	3.99	122.46	116.00
30	7	307	CLA	C1D-CHD-C4C	-3.99	117.55	126.02
30	B	825	CLA	C3C-C4C-NC	3.99	115.53	110.43
37	15	322	A86	C9-C10-C11	-3.98	115.38	126.64
30	A	802	CLA	C3D-C4D-ND	3.98	116.46	109.99
30	B	817	CLA	CAA-C2A-C3A	-3.98	102.23	113.00
30	3	305	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
30	B	826	CLA	C3D-C4D-ND	3.98	116.46	109.99
30	B	839	CLA	C3C-C4C-NC	3.98	115.53	110.43
37	7	316	A86	O4-C38-C39	3.98	118.19	111.09
30	A	812	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
30	A	831	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
37	2	318	A86	C40-C32-C31	-3.98	106.91	110.47
30	B	822	CLA	CMA-C3A-C2A	-3.98	98.59	113.98
30	A	843	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
30	8	304	CLA	CAA-CBA-CGA	-3.98	101.90	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	307	CLA	C2C-C1C-NC	3.98	114.16	109.98
37	4	315	A86	C12-C11-C13	3.98	122.45	116.00
30	A	812	CLA	C4A-NA-C1A	-3.98	104.86	106.68
30	10	303	CLA	CHD-C1D-ND	-3.98	119.20	124.80
30	2u	202	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
30	A	827	CLA	C1D-CHD-C4C	-3.98	117.57	126.02
38	9	312	KC1	C2C-C1C-NC	3.98	115.37	110.45
30	14	307	CLA	O2D-CGD-CBD	3.98	118.18	111.23
30	B	802	CLA	C1D-CHD-C4C	-3.97	117.57	126.02
30	7	312	CLA	CHD-C1D-ND	-3.97	119.21	124.80
30	10	311	CLA	CHD-C1D-ND	-3.97	119.21	124.80
38	16	304	KC1	C2C-C1C-NC	3.97	115.37	110.45
38	10	306	KC1	C4B-C3B-C2B	-3.97	103.37	106.81
30	A	814	CLA	C2C-C1C-NC	3.97	114.16	109.98
38	13	310	KC1	CHC-C1C-C2C	-3.97	118.75	125.03
38	10	310	KC1	C1D-CHD-C4C	-3.97	116.90	126.25
30	B	839	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
30	A	840	CLA	C3D-C4D-ND	3.97	116.44	109.99
38	13	311	KC1	CBA-CAA-C2A	-3.97	109.51	125.45
30	4	305	CLA	C4A-NA-C1A	-3.97	104.87	106.68
30	A	821	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
30	6	317	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
30	4	303	CLA	CAC-C3C-C4C	3.97	129.96	124.79
30	A	835	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
30	10	307	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
30	B	815	CLA	C3B-C4B-NB	3.97	114.07	110.53
30	B	817	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
37	9	316	A86	C36-C31-C32	-3.97	115.76	119.70
37	9	313	A86	C12-C11-C13	3.97	122.43	116.00
30	6	309	CLA	O2A-CGA-CBA	3.97	123.93	111.83
30	A	807	CLA	C3D-C4D-ND	3.97	116.44	109.99
30	2	304	CLA	CHD-C1D-ND	-3.97	119.22	124.80
30	A	842	CLA	C1D-CHD-C4C	-3.97	117.59	126.02
30	9	305	CLA	C3D-C4D-ND	3.97	116.44	109.99
30	A	803	CLA	CHD-C1D-ND	-3.97	119.22	124.80
30	B	813	CLA	CHD-C1D-ND	-3.97	119.22	124.80
30	A	806	CLA	C1D-CHD-C4C	-3.97	117.59	126.02
30	B	808	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
30	13	309	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
38	14	311	KC1	C1A-NA-C4A	-3.96	104.87	106.68
30	A	819	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
30	A	815	CLA	C3D-C4D-ND	3.96	116.43	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	813	CLA	C3D-C4D-ND	3.96	116.43	109.99
30	3	301	CLA	CHD-C1D-ND	-3.96	119.23	124.80
39	7	302	DD6	C12-C11-C13	-3.96	112.04	118.09
30	12	310	CLA	CHD-C1D-ND	-3.96	119.23	124.80
30	11	306	CLA	C2C-C1C-NC	3.96	114.14	109.98
38	9	310	KC1	CBA-CAA-C2A	-3.96	109.56	125.45
30	A	841	CLA	O2D-CGD-CBD	3.96	118.15	111.23
38	12	311	KC1	C4B-C3B-C2B	-3.96	103.38	106.81
30	F	203	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
38	11	312	KC1	C2A-C1A-NA	3.96	115.68	109.34
30	B	806	CLA	C1D-CHD-C4C	-3.95	117.61	126.02
30	4	304	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
39	6	303	DD6	C12-C11-C13	-3.95	112.05	118.09
30	B	803	CLA	C3D-C4D-ND	3.95	116.41	109.99
30	5	311	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
30	1	301	CLA	CHD-C1D-ND	-3.95	119.24	124.80
30	A	818	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
30	14	310	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
30	5	311	CLA	O2D-CGD-O1D	-3.95	116.16	123.85
30	8	304	CLA	C3D-C4D-ND	3.95	116.41	109.99
37	2	318	A86	C41-C32-C31	-3.95	106.94	110.47
39	15	319	DD6	C21-C20-C15	-3.95	115.80	122.30
30	A	831	CLA	C3C-C4C-NC	3.95	115.49	110.43
30	B	813	CLA	C4C-C3C-C2C	-3.95	101.14	106.89
30	A	822	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
30	10	304	CLA	CHD-C1D-ND	-3.95	119.25	124.80
30	B	836	CLA	C3D-C4D-ND	3.95	116.40	109.99
30	3	305	CLA	CHD-C1D-ND	-3.95	119.25	124.80
30	A	802	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
30	B	804	CLA	CHD-C1D-ND	-3.95	119.25	124.80
30	B	837	CLA	CHD-C1D-ND	-3.95	119.25	124.80
30	9	309	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
30	10	307	CLA	C4A-NA-C1A	-3.95	104.88	106.68
30	14	303	CLA	C4A-NA-C1A	-3.95	104.88	106.68
33	L	204	BCR	C31-C1-C6	3.95	116.43	110.24
30	A	825	CLA	C3D-C4D-ND	3.95	116.40	109.99
30	B	820	CLA	C2C-C1C-NC	3.94	114.12	109.98
30	1	301	CLA	C4A-NA-C1A	-3.94	104.88	106.68
37	14	301	A86	C4-C5-C6	-3.94	121.75	127.28
38	4	308	KC1	C2C-C1C-NC	3.94	115.33	110.45
30	B	833	CLA	C3D-C4D-ND	3.94	116.39	109.99
38	8	306	KC1	CBA-CAA-C2A	-3.94	109.64	125.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	310	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
38	7	308	KC1	C2C-C1C-NC	3.94	115.33	110.45
30	5	302	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
30	16	309	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
30	A	810	CLA	C3B-C4B-NB	3.94	114.05	110.53
30	14	304	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
38	3	311	KC1	C2C-C1C-NC	3.94	115.32	110.45
38	12	305	KC1	C1C-C2C-C3C	-3.94	102.84	106.98
38	11	305	KC1	C2C-C1C-NC	3.94	115.32	110.45
30	15	305	CLA	CHD-C1D-ND	-3.94	119.26	124.80
30	4	304	CLA	C4A-NA-C1A	-3.94	104.88	106.68
30	A	803	CLA	C3D-C4D-ND	3.94	116.39	109.99
30	2	310	CLA	CHD-C1D-ND	-3.94	119.26	124.80
30	9	303	CLA	C1D-CHD-C4C	-3.94	117.66	126.02
30	A	802	CLA	C3B-C4B-NB	3.94	114.04	110.53
38	1	308	KC1	CAA-CBA-CGA	-3.94	107.04	127.05
38	8	313	KC1	O2D-CGD-CBD	3.93	118.11	111.23
30	15	302	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
38	14	311	KC1	C1D-CHD-C4C	-3.93	117.00	126.25
30	A	843	CLA	C1-C2-C3	-3.93	119.75	126.20
30	6	305	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
37	15	316	A86	C4-C5-C6	-3.93	121.76	127.28
38	3	304	KC1	C1C-C2C-C3C	-3.93	102.84	106.98
30	3	305	CLA	C4A-NA-C1A	-3.93	104.89	106.68
30	7	305	CLA	C3B-C4B-NB	3.93	114.04	110.53
30	16	302	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
30	16	309	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
30	13	309	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
37	15	321	A86	C36-C31-C32	-3.93	115.80	119.70
38	3	308	KC1	C2A-C1A-NA	3.93	115.64	109.34
30	16	307	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
30	F	202	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
30	2	310	CLA	C3B-C4B-NB	3.93	114.04	110.53
30	1	307	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
30	3	307	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
30	7	312	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
30	15	303	CLA	C3C-C4C-NC	3.93	115.46	110.43
38	13	310	KC1	C1C-C2C-C3C	-3.93	102.85	106.98
37	15	317	A86	C25-C26-C27	-3.93	121.77	127.28
30	A	831	CLA	C3B-C4B-NB	3.93	114.04	110.53
30	4	302	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
37	10	301	A86	C12-C11-C13	3.93	122.37	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	303	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
39	16	313	DD6	C21-C20-C15	-3.93	115.84	122.30
38	3	304	KC1	C2C-C1C-NC	3.93	115.31	110.45
30	B	821	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
30	B	822	CLA	O2D-CGD-CBD	3.92	118.09	111.23
38	4	307	KC1	C2C-C1C-NC	3.92	115.31	110.45
39	6	319	DD6	C7-C6-C8	-3.92	112.09	118.09
30	15	312	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
38	13	311	KC1	C1C-C2C-C3C	-3.92	102.86	106.98
30	10	309	CLA	CHD-C1D-ND	-3.92	119.28	124.80
38	8	306	KC1	C2C-C1C-NC	3.92	115.30	110.45
30	15	311	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
38	5	305	KC1	C1A-NA-C4A	-3.92	104.89	106.68
30	1	302	CLA	CHD-C1D-ND	-3.92	119.28	124.80
30	9	302	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
30	14	309	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
30	6	315	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
38	11	305	KC1	C1C-C2C-C3C	-3.92	102.86	106.98
30	1	305	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
30	5	304	CLA	CHD-C1D-ND	-3.92	119.29	124.80
38	14	311	KC1	CBA-CAA-C2A	-3.92	109.72	125.45
30	16	301	CLA	CHD-C1D-ND	-3.92	119.29	124.80
30	15	311	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
30	A	803	CLA	C2C-C1C-NC	3.92	114.10	109.98
30	A	844	CLA	CHD-C1D-ND	-3.92	119.29	124.80
30	B	820	CLA	CHD-C1D-ND	-3.92	119.29	124.80
30	A	819	CLA	C3C-C4C-NC	3.92	115.45	110.43
30	B	851	CLA	CAA-C2A-C3A	-3.92	102.42	113.00
30	F	202	CLA	C3D-C4D-ND	3.92	116.35	109.99
30	13	307	CLA	CHD-C1D-ND	-3.92	119.29	124.80
30	1	302	CLA	C4A-NA-C1A	-3.91	104.89	106.68
30	11	304	CLA	C4A-NA-C1A	-3.91	104.89	106.68
30	9	303	CLA	CHD-C1D-ND	-3.91	119.29	124.80
30	8	305	CLA	C3C-C4C-NC	3.91	115.44	110.43
30	7	307	CLA	CHD-C1D-ND	-3.91	119.30	124.80
30	A	836	CLA	C4A-NA-C1A	-3.91	104.89	106.68
30	10	303	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
30	L	203	CLA	CHD-C1D-ND	-3.91	119.30	124.80
30	8	308	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
30	12	302	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
38	10	310	KC1	C1C-C2C-C3C	-3.91	102.87	106.98
38	3	304	KC1	C4B-C3B-C2B	-3.91	103.42	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	829	CLA	CHD-C1D-ND	-3.91	119.30	124.80
38	6	313	KC1	C1A-NA-C4A	-3.91	104.89	106.68
37	2u	203	A86	C25-C24-C1	-3.91	115.64	126.36
39	2	315	DD6	O1-C20-C21	-3.91	110.68	115.05
38	8	312	KC1	CHC-C1C-C2C	-3.91	118.86	125.03
30	B	807	CLA	C3C-C4C-NC	3.91	115.44	110.43
37	7	316	A86	C4-C3-C2	-3.91	115.52	123.52
38	9	310	KC1	CHC-C1C-C2C	-3.91	118.86	125.03
30	6	315	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
30	15	314	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
30	B	832	CLA	C4A-NA-C1A	-3.91	104.90	106.68
37	2u	205	A86	C36-C31-C32	-3.91	115.82	119.70
38	4	308	KC1	C1D-CHD-C4C	-3.91	117.06	126.25
30	B	837	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
30	7	307	CLA	C2C-C1C-NC	3.91	114.08	109.98
30	6	316	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
37	5	301	A86	C41-C32-C31	-3.91	106.98	110.47
39	8	316	DD6	C35-C36-C31	-3.90	112.37	120.50
30	6	304	CLA	C1C-C2C-C3C	-3.90	102.87	106.98
30	B	808	CLA	CAA-C2A-C3A	-3.90	102.45	113.00
37	5	315	A86	C12-C11-C13	3.90	122.33	116.00
38	5	306	KC1	CHC-C1C-C2C	-3.90	118.86	125.03
30	9	305	CLA	CHD-C1D-ND	-3.90	119.31	124.80
30	12	303	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
30	B	833	CLA	CHD-C1D-ND	-3.90	119.31	124.80
30	8	309	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
33	L	201	BCR	C2-C1-C6	3.90	116.11	110.44
35	A	854	LMT	C1B-O5B-C5B	3.90	121.34	113.72
30	3	310	CLA	C4A-NA-C1A	-3.90	104.90	106.68
30	8	303	CLA	C4A-NA-C1A	-3.90	104.90	106.68
30	12	304	CLA	CBA-CAA-C2A	3.90	125.39	113.79
30	2	308	CLA	C2C-C1C-NC	3.90	114.08	109.98
30	3	302	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
30	B	823	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
30	13	302	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
30	15	313	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
30	B	815	CLA	C3D-C4D-ND	3.90	116.32	109.99
30	4	306	CLA	CHD-C1D-ND	-3.90	119.32	124.80
30	16	301	CLA	C3C-C4C-NC	3.90	115.42	110.43
37	2u	203	A86	C3-C2-C1	-3.90	121.81	127.28
30	5	311	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
30	3	307	CLA	C1D-CHD-C4C	-3.89	117.74	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	316	A86	C25-C26-C27	-3.89	121.82	127.28
39	7	318	DD6	C22-C16-C15	3.89	120.56	110.05
30	B	828	CLA	CHD-C1D-ND	-3.89	119.32	124.80
30	1	307	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
30	14	309	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
30	10	307	CLA	C3C-C4C-NC	3.89	115.42	110.43
30	B	809	CLA	CAA-C2A-C3A	-3.89	102.48	113.00
30	4	302	CLA	O2D-CGD-CBD	3.89	118.03	111.23
30	B	827	CLA	C3C-C4C-NC	3.89	115.41	110.43
30	A	842	CLA	CHD-C1D-ND	-3.89	119.33	124.80
30	B	830	CLA	C3C-C4C-NC	3.89	115.41	110.43
30	A	820	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
30	A	839	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
30	9	309	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
30	B	815	CLA	CHD-C1D-ND	-3.89	119.33	124.80
30	15	308	CLA	CAC-C3C-C4C	3.89	129.85	124.79
30	A	825	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
30	12	312	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
30	3	305	CLA	C3D-C4D-ND	3.89	116.30	109.99
38	2	306	KC1	C1C-C2C-C3C	-3.88	102.89	106.98
30	B	833	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
30	7	306	CLA	C3C-C4C-NC	3.88	115.40	110.43
30	A	829	CLA	C3D-C4D-ND	3.88	116.30	109.99
30	8	302	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
30	2	304	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
30	A	815	CLA	C4A-NA-C1A	-3.88	104.91	106.68
30	6	317	CLA	C4A-NA-C1A	-3.88	104.91	106.68
30	8	309	CLA	C4A-NA-C1A	-3.88	104.91	106.68
38	1	306	KC1	C2C-C1C-NC	3.88	115.25	110.45
30	8	303	CLA	C3B-C4B-NB	3.88	113.99	110.53
39	12	315	DD6	C37-C36-C35	-3.88	107.29	114.42
30	1	307	CLA	CHD-C1D-ND	-3.88	119.34	124.80
30	5	307	CLA	C3C-C4C-NC	3.88	115.40	110.43
38	1	308	KC1	CAA-C2A-C1A	-3.88	107.65	124.64
30	5	309	CLA	CHD-C1D-ND	-3.88	119.35	124.80
38	6	313	KC1	C1C-C2C-C3C	-3.88	102.90	106.98
30	A	816	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
30	A	840	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
30	B	821	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
30	12	304	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
30	16	310	CLA	C4A-NA-C1A	-3.88	104.91	106.68
30	B	811	CLA	C1D-CHD-C4C	-3.87	117.78	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	806	CLA	CAC-C3C-C4C	3.87	129.83	124.79
30	A	824	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
30	9	307	CLA	C3D-C4D-ND	3.87	116.28	109.99
30	B	811	CLA	C4A-NA-C1A	-3.87	104.91	106.68
38	2	314	KC1	C1A-NA-C4A	-3.87	104.91	106.68
30	5	311	CLA	C3B-C4B-NB	3.87	113.99	110.53
30	12	310	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
30	11	309	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
30	12	303	CLA	C3D-C4D-ND	3.87	116.28	109.99
30	9	307	CLA	CHD-C1D-ND	-3.87	119.36	124.80
30	2	305	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
38	7	308	KC1	C1C-C2C-C3C	-3.87	102.91	106.98
30	10	305	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
30	A	826	CLA	C3C-C4C-NC	3.87	115.39	110.43
38	8	310	KC1	CAA-CBA-CGA	-3.87	107.37	127.05
30	L	203	CLA	C3B-C4B-NB	3.87	113.98	110.53
38	11	305	KC1	C4B-C3B-C2B	-3.87	103.46	106.81
38	14	311	KC1	CHC-C1C-C2C	-3.87	118.92	125.03
37	5	301	A86	C36-C31-C32	-3.87	115.86	119.70
38	14	308	KC1	C4B-C3B-C2B	-3.87	103.46	106.81
30	A	829	CLA	CAA-C2A-C3A	-3.87	102.55	113.00
38	14	311	KC1	C2A-C1A-NA	3.87	115.54	109.34
39	8	317	DD6	C37-C36-C35	-3.87	107.31	114.42
30	6	306	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
30	6	304	CLA	CBC-CAC-C3C	-3.86	101.94	112.42
30	B	851	CLA	CHD-C1D-ND	-3.86	119.37	124.80
30	5	308	CLA	CHD-C1D-ND	-3.86	119.37	124.80
30	F	201	CLA	O2D-CGD-CBD	3.86	117.98	111.23
30	A	826	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
38	5	305	KC1	C1C-C2C-C3C	-3.86	102.92	106.98
30	9	307	CLA	C3C-C4C-NC	3.86	115.38	110.43
30	B	814	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
30	8	303	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
30	12	312	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
30	L	203	CLA	C1D-CHD-C4C	-3.86	117.82	126.02
30	B	825	CLA	CHD-C1D-ND	-3.86	119.37	124.80
30	4	309	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
30	2u	202	CLA	CHD-C1D-ND	-3.86	119.37	124.80
39	16	313	DD6	O1-C20-C21	-3.86	110.74	115.05
38	16	311	KC1	C1D-CHD-C4C	-3.86	117.18	126.25
38	11	307	KC1	CAC-C3C-C4C	3.86	129.81	124.79
30	4	302	CLA	CHD-C1D-ND	-3.86	119.38	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	835	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
30	A	809	CLA	C1D-CHD-C4C	-3.86	117.82	126.02
30	B	839	CLA	CHD-C1D-ND	-3.86	119.38	124.80
30	5	302	CLA	CHD-C1D-ND	-3.86	119.38	124.80
39	15	318	DD6	C21-C20-C15	-3.86	115.96	122.30
30	A	831	CLA	C4B-C3B-C2B	-3.85	102.51	107.30
38	2	314	KC1	C2C-C1C-NC	3.85	115.22	110.45
38	13	306	KC1	C1D-CHD-C4C	-3.85	117.19	126.25
30	7	306	CLA	C3D-C4D-ND	3.85	116.25	109.99
30	13	307	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
30	16	303	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
37	11	315	A86	C3-C2-C1	-3.85	121.88	127.28
30	4	301	CLA	C3C-C4C-NC	3.85	115.36	110.43
30	3	310	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
30	15	307	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
30	A	842	CLA	C3C-C4C-NC	3.85	115.36	110.43
30	7	303	CLA	C3C-C4C-NC	3.85	115.36	110.43
29	A	801	CL0	CMA-C3A-C2A	-3.85	99.27	114.13
30	A	810	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
30	15	304	CLA	C3C-C4C-NC	3.85	115.36	110.43
30	9	305	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
38	13	308	KC1	C2C-C1C-NC	3.85	115.21	110.45
37	7	315	A86	C9-C10-C11	-3.85	115.77	126.64
30	15	310	CLA	C1D-CHD-C4C	-3.85	117.85	126.02
30	B	809	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
38	8	313	KC1	C1D-CHD-C4C	-3.84	117.21	126.25
30	2	307	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
38	13	308	KC1	C1C-C2C-C3C	-3.84	102.94	106.98
37	6	320	A86	C9-C8-C6	-3.84	115.83	126.36
37	11	316	A86	C36-C31-C32	-3.84	115.88	119.70
30	A	843	CLA	CHD-C1D-ND	-3.84	119.39	124.80
37	9	313	A86	O1-C20-C21	-3.84	110.75	115.05
30	16	310	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
38	12	309	KC1	C1C-C2C-C3C	-3.84	102.94	106.98
30	2	301	CLA	CHD-C1D-ND	-3.84	119.40	124.80
30	9	302	CLA	C1-O2A-CGA	3.84	125.95	116.65
30	16	306	CLA	CAC-C3C-C4C	3.84	129.79	124.79
30	A	832	CLA	CHD-C1D-ND	-3.84	119.40	124.80
30	15	309	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
30	9	305	CLA	C4A-NA-C1A	-3.84	104.93	106.68
37	7	319	A86	C24-C1-C2	3.84	125.05	119.01
30	15	306	CLA	CHD-C1D-ND	-3.84	119.40	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	9	310	KC1	C1D-CHD-C4C	-3.84	117.22	126.25
38	6	313	KC1	C2C-C1C-NC	3.84	115.20	110.45
30	A	812	CLA	C3C-C4C-NC	3.84	115.35	110.43
38	13	312	KC1	C1C-C2C-C3C	-3.84	102.94	106.98
30	5	308	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
30	A	823	CLA	C3B-C4B-NB	3.84	113.95	110.53
30	A	815	CLA	C1D-CHD-C4C	-3.84	117.87	126.02
38	5	310	KC1	C2C-C1C-NC	3.84	115.20	110.45
30	12	303	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
30	B	816	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
30	14	313	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
30	3	301	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
30	A	830	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
30	2	307	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
30	13	301	CLA	CHD-C1D-ND	-3.83	119.41	124.80
30	A	826	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
30	B	821	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
30	B	832	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
30	B	828	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
30	6	305	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
38	5	312	KC1	C2C-C1C-NC	3.83	115.19	110.45
38	7	313	KC1	CAA-C2A-C1A	-3.83	107.87	124.64
30	12	321	CLA	CHD-C1D-ND	-3.83	119.42	124.80
30	A	827	CLA	C3C-C4C-NC	3.83	115.33	110.43
30	A	825	CLA	C4A-NA-C1A	-3.83	104.93	106.68
30	13	304	CLA	C4A-NA-C1A	-3.83	104.93	106.68
30	B	811	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
38	2	312	KC1	CAA-CBA-CGA	-3.83	107.59	127.05
30	B	836	CLA	C3C-C4C-NC	3.83	115.33	110.43
39	15	318	DD6	C37-C36-C35	-3.83	107.39	114.42
30	A	809	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
30	B	810	CLA	C3C-C4C-NC	3.82	115.33	110.43
38	16	311	KC1	C2C-C1C-NC	3.82	115.18	110.45
30	B	806	CLA	CHD-C1D-ND	-3.82	119.42	124.80
30	2	305	CLA	CHD-C1D-ND	-3.82	119.42	124.80
30	16	306	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
37	14	317	A86	C3-C2-C1	-3.82	121.92	127.28
30	12	303	CLA	C3B-C4B-NB	3.82	113.94	110.53
38	5	305	KC1	C2C-C1C-NC	3.82	115.18	110.45
38	3	308	KC1	CMB-C2B-C1B	3.82	131.45	124.73
30	B	804	CLA	C1D-CHD-C4C	-3.82	117.91	126.02
30	B	839	CLA	C1C-C2C-C3C	-3.82	102.97	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	316	A86	C8-C6-C5	-3.82	113.00	119.01
30	2	307	CLA	CMB-C2B-C1B	3.82	131.23	125.42
38	2	314	KC1	C1C-C2C-C3C	-3.82	102.97	106.98
30	15	308	CLA	C4A-NA-C1A	-3.82	104.94	106.68
30	B	814	CLA	C3C-C4C-NC	3.81	115.32	110.43
30	8	308	CLA	C1D-CHD-C4C	-3.81	117.91	126.02
30	5	309	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
30	10	304	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
30	A	822	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
37	4	314	A86	C3-C2-C1	-3.81	121.93	127.28
30	9	308	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
30	2	303	CLA	CHD-C1D-ND	-3.81	119.44	124.80
30	16	302	CLA	CHD-C1D-ND	-3.81	119.44	124.80
30	B	803	CLA	C4C-C3C-C2C	-3.81	101.34	106.89
30	A	838	CLA	C3D-C4D-ND	3.81	116.18	109.99
30	9	306	CLA	C3C-C4C-NC	3.81	115.31	110.43
38	11	311	KC1	CBA-CAA-C2A	-3.81	110.16	125.45
30	A	828	CLA	C3D-C4D-ND	3.81	116.18	109.99
30	8	309	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
30	A	809	CLA	CHD-C1D-ND	-3.81	119.44	124.80
30	A	816	CLA	CHD-C1D-ND	-3.81	119.44	124.80
30	6	317	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
30	A	802	CLA	C3C-C4C-NC	3.81	115.31	110.43
30	B	827	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
39	7	318	DD6	C21-C20-C19	-3.81	109.97	114.24
37	12	314	A86	C40-C32-C31	-3.81	107.07	110.47
30	3	303	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
30	14	312	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
38	16	304	KC1	CBA-CAA-C2A	-3.81	110.18	125.45
30	8	309	CLA	CHD-C1D-ND	-3.80	119.45	124.80
38	13	311	KC1	C2C-C1C-NC	3.80	115.16	110.45
30	15	313	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
30	A	817	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
30	6	309	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
30	A	824	CLA	C1-C2-C3	-3.80	119.97	126.20
30	A	807	CLA	CHD-C1D-ND	-3.80	119.46	124.80
39	10	313	DD6	C21-C20-C15	-3.80	116.05	122.30
38	3	308	KC1	C1D-CHD-C4C	-3.80	117.32	126.25
30	B	811	CLA	C3C-C4C-NC	3.80	115.29	110.43
30	A	819	CLA	CHD-C1D-ND	-3.79	119.46	124.80
30	A	809	CLA	C3D-C4D-ND	3.79	116.16	109.99
38	7	308	KC1	C1A-NA-C4A	-3.79	104.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	306	CLA	C1D-CHD-C4C	-3.79	117.96	126.02
30	A	838	CLA	C3C-C4C-NC	3.79	115.29	110.43
38	14	308	KC1	C1A-NA-C4A	-3.79	104.95	106.68
30	9	309	CLA	CHD-C1D-ND	-3.79	119.47	124.80
30	12	303	CLA	C3C-C4C-NC	3.79	115.29	110.43
30	13	309	CLA	C3C-C4C-NC	3.79	115.29	110.43
30	B	825	CLA	C3D-C4D-ND	3.79	116.15	109.99
38	11	311	KC1	C4B-C3B-C2B	-3.79	103.53	106.81
30	B	805	CLA	C1C-C2C-C3C	-3.79	103.00	106.98
30	7	304	CLA	CAA-C2A-C3A	-3.79	102.76	113.00
30	7	304	CLA	C3B-C4B-NB	3.79	113.91	110.53
30	A	825	CLA	CAC-C3C-C4C	3.79	129.72	124.79
38	8	313	KC1	CHC-C1C-C2C	-3.79	119.05	125.03
30	A	834	CLA	C1C-C2C-C3C	-3.79	103.00	106.98
30	15	306	CLA	C3C-C4C-NC	3.79	115.28	110.43
30	A	821	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
37	14	301	A86	C25-C26-C27	-3.79	121.97	127.28
38	6	311	KC1	CBA-CAA-C2A	-3.79	110.26	125.45
30	B	803	CLA	O2D-CGD-CBD	3.79	117.85	111.23
38	12	311	KC1	C2C-C1C-NC	3.78	115.13	110.45
30	14	305	CLA	C4A-NA-C1A	-3.78	104.95	106.68
30	5	309	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
30	A	812	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
38	10	312	KC1	C4B-C3B-C2B	-3.78	103.53	106.81
30	A	835	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
38	10	310	KC1	CBA-CAA-C2A	-3.78	110.27	125.45
30	15	303	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
30	10	309	CLA	O2D-CGD-CBD	3.78	117.84	111.23
30	A	844	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
30	14	305	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
38	4	308	KC1	C1C-C2C-C3C	-3.78	103.00	106.98
30	2	313	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
30	16	307	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
39	6	318	DD6	C21-C20-C19	-3.78	110.00	114.24
30	6	309	CLA	CHD-C1D-ND	-3.78	119.49	124.80
30	13	301	CLA	C1-C2-C3	-3.78	120.01	126.20
37	14	314	A86	C41-C32-C31	-3.78	107.09	110.47
30	B	838	CLA	C4A-NA-C1A	-3.78	104.96	106.68
30	A	832	CLA	C3C-C4C-NC	3.78	115.27	110.43
39	5	313	DD6	C21-C20-C19	-3.78	110.00	114.24
38	9	304	KC1	C1C-C2C-C3C	-3.78	103.01	106.98
38	4	307	KC1	C4B-C3B-C2B	-3.78	103.54	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	307	CLA	CHD-C1D-ND	-3.78	119.49	124.80
30	A	843	CLA	C3B-C4B-NB	3.78	113.90	110.53
30	A	824	CLA	CHD-C1D-ND	-3.77	119.49	124.80
30	6	316	CLA	CHD-C1D-ND	-3.77	119.49	124.80
38	1	308	KC1	C1C-C2C-C3C	-3.77	103.01	106.98
37	7	315	A86	C40-C32-C31	-3.77	107.09	110.47
30	2	309	CLA	C4A-NA-C1A	-3.77	104.96	106.68
30	5	303	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
30	B	812	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
38	9	312	KC1	C1C-C2C-C3C	-3.77	103.01	106.98
38	11	307	KC1	CBA-CAA-C2A	-3.77	110.31	125.45
30	B	826	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
30	5	308	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
30	1	304	CLA	C4A-NA-C1A	-3.77	104.96	106.68
38	5	312	KC1	C1A-NA-C4A	-3.77	104.96	106.68
30	A	818	CLA	C3C-C4C-NC	3.77	115.26	110.43
38	7	308	KC1	C1D-CHD-C4C	-3.77	117.38	126.25
30	A	831	CLA	C3D-C4D-ND	3.77	116.12	109.99
30	12	308	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
38	5	312	KC1	CAC-C3C-C4C	3.77	129.70	124.79
30	15	305	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
37	12	314	A86	C36-C31-C32	-3.77	115.96	119.70
30	6	314	CLA	C3B-C4B-NB	3.77	113.89	110.53
30	A	829	CLA	C4A-NA-C1A	-3.77	104.96	106.68
30	8	303	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
30	13	301	CLA	C3C-C4C-NC	3.77	115.26	110.43
30	B	825	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
30	A	818	CLA	C4A-NA-C1A	-3.77	104.96	106.68
30	11	308	CLA	C4A-NA-C1A	-3.77	104.96	106.68
30	4	304	CLA	CHD-C1D-ND	-3.77	119.50	124.80
30	4	311	CLA	C1D-CHD-C4C	-3.77	118.02	126.02
30	4	311	CLA	CAA-C2A-C3A	-3.76	102.83	113.00
30	10	309	CLA	C1D-CHD-C4C	-3.76	118.02	126.02
30	13	303	CLA	C1D-CHD-C4C	-3.76	118.02	126.02
30	15	305	CLA	C4A-NA-C1A	-3.76	104.96	106.68
39	4	316	DD6	C37-C36-C35	-3.76	107.50	114.42
30	4	305	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
30	14	303	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
30	10	305	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
30	A	843	CLA	C3B-C2B-C1B	-3.76	102.74	107.17
33	B	844	BCR	C15-C16-C17	-3.76	115.82	123.52
30	6	307	CLA	C3D-C2D-C1D	-3.76	100.70	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	303	CLA	C1-C2-C3	-3.76	120.04	126.20
30	14	307	CLA	C3C-C4C-NC	3.76	115.25	110.43
30	A	813	CLA	C4A-NA-C1A	-3.76	104.96	106.68
30	15	314	CLA	C3C-C4C-NC	3.76	115.25	110.43
38	12	309	KC1	C2C-C1C-NC	3.76	115.10	110.45
30	B	806	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
30	11	308	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
38	1	306	KC1	C1C-C2C-C3C	-3.76	103.03	106.98
30	15	307	CLA	CHD-C1D-ND	-3.76	119.52	124.80
30	16	310	CLA	C1D-CHD-C4C	-3.76	118.04	126.02
33	A	850	BCR	C2-C1-C6	3.76	115.89	110.44
38	1	308	KC1	C2C-C1C-NC	3.76	115.10	110.45
30	1	305	CLA	C1D-CHD-C4C	-3.76	118.04	126.02
30	3	302	CLA	CHD-C1D-ND	-3.76	119.52	124.80
30	3	309	CLA	C1D-CHD-C4C	-3.76	118.04	126.02
30	6	304	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
30	1	302	CLA	C1C-C2C-C3C	-3.75	103.03	106.98
30	B	821	CLA	C3B-C4B-NB	3.75	113.88	110.53
30	B	826	CLA	CHD-C1D-ND	-3.75	119.52	124.80
30	2	311	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
30	A	808	CLA	C3C-C4C-NC	3.75	115.23	110.43
30	6	307	CLA	C1C-C2C-C3C	-3.75	103.03	106.98
39	3	312	DD6	C21-C20-C19	-3.75	110.03	114.24
30	A	826	CLA	C3D-C4D-ND	3.75	116.08	109.99
30	B	823	CLA	C3D-C4D-ND	3.75	116.08	109.99
30	14	303	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
30	8	305	CLA	C1-C2-C3	-3.75	120.06	126.20
30	A	837	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
38	6	312	KC1	C1C-C2C-C3C	-3.75	103.04	106.98
30	5	303	CLA	CHD-C1D-ND	-3.75	119.53	124.80
37	11	301	A86	C7-C6-C5	-3.75	116.75	122.82
30	B	819	CLA	C3C-C4C-NC	3.75	115.23	110.43
37	9	313	A86	C23-C16-C22	-3.74	101.93	107.37
30	A	821	CLA	C4B-C3B-C2B	-3.74	102.65	107.30
30	A	802	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
38	9	312	KC1	C4B-C3B-C2B	-3.74	103.57	106.81
38	6	308	KC1	CHC-C1C-C2C	-3.74	119.12	125.03
37	14	320	A86	C9-C10-C11	-3.74	116.06	126.64
30	A	837	CLA	C1D-CHD-C4C	-3.74	118.07	126.02
30	A	822	CLA	C4A-NA-C1A	-3.74	104.97	106.68
30	B	823	CLA	C4A-NA-C1A	-3.74	104.97	106.68
30	B	836	CLA	C4A-NA-C1A	-3.74	104.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	303	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
30	B	817	CLA	C3C-C4C-NC	3.74	115.22	110.43
30	A	821	CLA	CMB-C2B-C1B	3.74	131.11	125.42
30	10	304	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
30	13	302	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
30	B	802	CLA	CHD-C1D-ND	-3.74	119.54	124.80
30	10	307	CLA	C3D-C4D-ND	3.74	116.06	109.99
30	A	824	CLA	C3C-C4C-NC	3.74	115.22	110.43
30	A	807	CLA	O2D-CGD-CBD	3.74	117.77	111.23
30	A	833	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
39	15	319	DD6	C37-C36-C35	-3.74	107.55	114.42
38	11	311	KC1	C2C-C1C-NC	3.74	115.08	110.45
30	A	827	CLA	C4A-NA-C1A	-3.74	104.97	106.68
30	16	308	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
30	B	808	CLA	CHD-C1D-ND	-3.74	119.55	124.80
30	F	201	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
30	2u	202	CLA	C3C-C4C-NC	3.73	115.21	110.43
30	9	303	CLA	CMC-C2C-C1C	3.73	130.87	125.03
30	12	303	CLA	CHD-C1D-ND	-3.73	119.55	124.80
30	1	303	CLA	C1D-CHD-C4C	-3.73	118.08	126.02
39	8	316	DD6	O1-C20-C21	-3.73	110.88	115.05
38	6	312	KC1	C4B-C3B-C2B	-3.73	103.58	106.81
37	9	313	A86	C3-C4-C5	-3.73	115.88	123.52
38	3	304	KC1	C1A-NA-C4A	-3.73	104.98	106.68
37	2	302	A86	C3-C2-C1	-3.73	122.04	127.28
30	A	822	CLA	CHD-C1D-ND	-3.73	119.55	124.80
38	13	305	KC1	C1C-C2C-C3C	-3.73	103.06	106.98
30	F	201	CLA	CAA-C2A-C3A	-3.73	102.92	113.00
38	8	313	KC1	CAA-CBA-CGA	-3.73	108.07	127.05
30	A	813	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
38	2	312	KC1	C1C-C2C-C3C	-3.73	103.06	106.98
30	B	828	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
30	3	305	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
30	13	307	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
38	10	306	KC1	C1D-CHD-C4C	-3.73	117.48	126.25
30	F	202	CLA	CHD-C1D-ND	-3.73	119.56	124.80
30	B	809	CLA	C4B-C3B-C2B	-3.73	102.67	107.30
38	5	310	KC1	CBA-CAA-C2A	-3.73	110.49	125.45
38	8	314	KC1	C2C-C1C-NC	3.73	115.06	110.45
30	14	302	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
30	7	305	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
30	J	101	CLA	CHD-C1D-ND	-3.73	119.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	838	CLA	C4B-C3B-C2B	-3.73	102.67	107.30
30	7	305	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
30	B	810	CLA	CHD-C1D-ND	-3.72	119.56	124.80
30	12	307	CLA	C3C-C4C-NC	3.72	115.20	110.43
30	6	309	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
30	A	813	CLA	C3C-C4C-NC	3.72	115.20	110.43
30	10	304	CLA	C3C-C4C-NC	3.72	115.20	110.43
38	13	312	KC1	C2C-C1C-NC	3.72	115.06	110.45
38	3	311	KC1	C4B-C3B-C2B	-3.72	103.59	106.81
38	12	309	KC1	C1D-CHD-C4C	-3.72	117.50	126.25
30	B	838	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
30	11	306	CLA	CBA-CAA-C2A	3.72	124.86	113.79
30	4	306	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
30	2	309	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
30	15	310	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
30	A	821	CLA	C2B-C1B-NB	3.72	114.18	110.33
30	L	202	CLA	CBC-CAC-C3C	-3.72	102.34	112.42
30	12	307	CLA	CAC-C3C-C4C	3.72	129.63	124.79
30	3	307	CLA	C3C-C4C-NC	3.72	115.19	110.43
30	A	814	CLA	C4C-C3C-C2C	-3.72	101.48	106.89
30	A	844	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
30	B	820	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
30	A	806	CLA	C2C-C1C-NC	3.72	113.89	109.98
30	15	306	CLA	C3B-C4B-NB	3.72	113.85	110.53
30	7	309	CLA	CHD-C1D-ND	-3.72	119.57	124.80
30	3	303	CLA	C1C-C2C-C3C	-3.71	103.07	106.98
38	8	311	KC1	C2C-C1C-NC	3.71	115.05	110.45
38	14	306	KC1	CAB-C3B-C4B	3.71	133.69	124.82
37	9	313	A86	C41-C32-C31	-3.71	107.15	110.47
30	9	309	CLA	O2D-CGD-CBD	3.71	117.72	111.23
38	10	306	KC1	O2D-CGD-O1D	-3.71	116.62	123.85
30	4	301	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
30	A	814	CLA	CHD-C1D-ND	-3.71	119.58	124.80
38	2	312	KC1	C4B-C3B-C2B	-3.71	103.60	106.81
30	2	308	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
38	9	311	KC1	C1C-C2C-C3C	-3.71	103.08	106.98
30	B	834	CLA	C3D-C4D-ND	3.71	116.01	109.99
30	2u	202	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
30	B	818	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
30	5	304	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
30	B	803	CLA	C3C-C4C-NC	3.70	115.18	110.43
30	11	310	CLA	C1D-CHD-C4C	-3.70	118.15	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	804	CLA	CHD-C1D-ND	-3.70	119.59	124.80
30	A	805	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
30	3	309	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
38	9	304	KC1	C2C-C1C-NC	3.70	115.03	110.45
37	10	302	A86	C12-C11-C13	3.70	122.00	116.00
39	4	316	DD6	C12-C11-C13	-3.70	112.44	118.09
30	B	814	CLA	C4A-NA-C1A	-3.70	104.99	106.68
30	5	303	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
37	10	315	A86	C4-C3-C2	-3.70	115.95	123.52
30	7	311	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
30	12	302	CLA	O2A-CGA-CBA	3.70	123.11	111.83
30	F	202	CLA	C3B-C4B-NB	3.70	113.83	110.53
30	B	815	CLA	C4A-NA-C1A	-3.70	104.99	106.68
35	15	301	LMT	C1B-O5B-C5B	3.70	120.94	113.72
30	9	303	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
30	A	806	CLA	C3B-C4B-NB	3.70	113.83	110.53
38	6	308	KC1	C1D-CHD-C4C	-3.70	117.56	126.25
38	13	305	KC1	C2A-C1A-NA	3.69	115.26	109.34
39	3	313	DD6	C35-C36-C31	-3.69	112.81	120.50
30	16	310	CLA	CED-O2D-CGD	3.69	124.29	115.92
39	3	312	DD6	C25-C24-C1	-3.69	116.24	126.36
38	14	311	KC1	C2C-C1C-NC	3.69	115.02	110.45
30	L	202	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
30	12	302	CLA	C3C-C4C-NC	3.69	115.16	110.43
30	A	808	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
38	9	311	KC1	CAA-CBA-CGA	-3.69	108.28	127.05
30	1	301	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
30	A	824	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
37	14	320	A86	C3-C4-C5	3.69	131.06	123.52
30	A	813	CLA	CHD-C1D-ND	-3.69	119.61	124.80
30	B	811	CLA	CMA-C3A-C2A	-3.69	99.73	113.98
30	2	309	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
38	13	311	KC1	C1D-CHD-C4C	-3.69	117.58	126.25
38	12	305	KC1	C1A-NA-C4A	-3.69	105.00	106.68
37	14	314	A86	C40-C32-C31	-3.69	107.17	110.47
38	2	306	KC1	C2C-C1C-NC	3.68	115.01	110.45
30	1	303	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
30	B	831	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
37	8	315	A86	C26-C25-C24	-3.68	112.53	123.20
30	A	817	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
38	3	308	KC1	C4B-C3B-C2B	-3.68	103.62	106.81
38	2	312	KC1	C1D-CHD-C4C	-3.68	117.59	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	8	313	KC1	C4C-C3C-C2C	-3.68	101.53	106.89
30	2	305	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
30	A	831	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
30	A	834	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
37	11	316	A86	C3-C4-C5	-3.68	115.99	123.52
30	A	808	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
38	8	312	KC1	C2C-C1C-NC	3.68	115.00	110.45
30	A	831	CLA	C4A-NA-C1A	-3.68	105.00	106.68
38	3	304	KC1	C1D-CHD-C4C	-3.68	117.60	126.25
37	14	320	A86	C41-C32-C31	-3.68	107.18	110.47
39	8	316	DD6	C12-C11-C13	-3.68	112.47	118.09
38	9	311	KC1	CAA-C2A-C1A	-3.68	108.53	124.64
30	A	803	CLA	CHB-C4A-NA	3.68	129.71	124.40
30	12	310	CLA	C3C-C4C-NC	3.68	115.14	110.43
30	13	302	CLA	C3C-C4C-NC	3.68	115.14	110.43
30	B	828	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
30	6	310	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
38	5	312	KC1	C1C-C2C-C3C	-3.67	103.12	106.98
30	A	811	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
30	B	823	CLA	C3C-C4C-NC	3.67	115.14	110.43
30	12	302	CLA	CHD-C1D-ND	-3.67	119.63	124.80
30	9	303	CLA	CAC-C3C-C4C	3.67	129.57	124.79
30	9	309	CLA	C3B-C4B-NB	3.67	113.81	110.53
30	B	822	CLA	O2A-CGA-CBA	3.67	123.03	111.83
30	B	833	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
38	14	311	KC1	C1C-C2C-C3C	-3.67	103.12	106.98
30	16	306	CLA	C3C-C4C-NC	3.67	115.13	110.43
30	13	302	CLA	CHD-C1D-ND	-3.67	119.64	124.80
30	15	307	CLA	C3C-C4C-NC	3.67	115.13	110.43
30	11	304	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
30	2u	202	CLA	CMB-C2B-C1B	3.67	131.01	125.42
38	2	306	KC1	CAA-CBA-CGA	-3.67	108.39	127.05
38	5	312	KC1	C1D-CHD-C4C	-3.67	117.62	126.25
30	4	305	CLA	CMB-C2B-C1B	3.67	131.00	125.42
30	A	828	CLA	C2C-C1C-NC	3.67	113.83	109.98
37	4	314	A86	C7-C6-C5	-3.67	116.87	122.82
30	7	311	CLA	CHD-C1D-ND	-3.67	119.64	124.80
30	5	309	CLA	C4A-NA-C1A	-3.67	105.01	106.68
38	3	311	KC1	C1A-NA-C4A	-3.67	105.01	106.68
30	8	305	CLA	CHD-C1D-ND	-3.67	119.64	124.80
30	B	803	CLA	CAA-C2A-C3A	-3.67	103.09	113.00
30	12	308	CLA	C3C-C4C-NC	3.67	115.13	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	305	CLA	CAA-C2A-C3A	-3.67	103.09	113.00
30	12	312	CLA	C4A-NA-C1A	-3.66	105.01	106.68
38	12	313	KC1	C1D-CHD-C4C	-3.66	117.63	126.25
30	8	303	CLA	CHD-C1D-ND	-3.66	119.64	124.80
38	11	311	KC1	C1C-C2C-C3C	-3.66	103.13	106.98
38	6	313	KC1	C1D-CHD-C4C	-3.66	117.63	126.25
38	13	312	KC1	C4B-C3B-C2B	-3.66	103.64	106.81
30	A	823	CLA	C1D-CHD-C4C	-3.66	118.23	126.02
30	1	303	CLA	C3C-C4C-NC	3.66	115.12	110.43
30	6	307	CLA	CHD-C1D-ND	-3.66	119.65	124.80
38	8	311	KC1	C4B-C3B-C2B	-3.66	103.64	106.81
38	9	312	KC1	C1D-CHD-C4C	-3.66	117.64	126.25
30	15	305	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
30	13	304	CLA	C3B-C4B-NB	3.66	113.80	110.53
30	B	812	CLA	CHD-C1D-ND	-3.66	119.65	124.80
30	7	303	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
38	8	306	KC1	C1D-CHD-C4C	-3.66	117.64	126.25
37	8	315	A86	C36-C31-C32	-3.66	116.06	119.70
30	8	304	CLA	C3C-C4C-NC	3.66	115.12	110.43
38	11	312	KC1	C1D-CHD-C4C	-3.66	117.64	126.25
38	10	312	KC1	C1C-C2C-C3C	-3.66	103.13	106.98
30	A	836	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
37	2	302	A86	C9-C8-C6	-3.66	116.33	126.36
30	6	307	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
30	10	307	CLA	CHD-C1D-ND	-3.66	119.66	124.80
30	A	804	CLA	CAA-C2A-C3A	-3.65	103.12	113.00
37	11	316	A86	C25-C24-C1	-3.65	116.34	126.36
30	B	828	CLA	CAC-C3C-C4C	3.65	129.54	124.79
38	11	305	KC1	CBA-CAA-C2A	-3.65	110.79	125.45
38	8	307	KC1	C1D-CHD-C4C	-3.65	117.66	126.25
30	A	841	CLA	C1D-CHD-C4C	-3.65	118.25	126.02
30	A	802	CLA	C4B-C3B-C2B	-3.65	102.76	107.30
30	B	829	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
30	B	815	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
30	B	834	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
30	5	307	CLA	C3D-C4D-ND	3.65	115.92	109.99
30	A	832	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
30	2	301	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
38	16	304	KC1	C1C-C2C-C3C	-3.65	103.14	106.98
38	13	308	KC1	C1D-CHD-C4C	-3.65	117.67	126.25
30	B	830	CLA	C1-O2A-CGA	3.65	125.48	116.65
30	B	826	CLA	C1C-C2C-C3C	-3.65	103.14	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	309	CLA	O2D-CGD-CBD	3.65	117.61	111.23
39	7	318	DD6	O1-C20-C21	-3.65	110.97	115.05
38	8	314	KC1	C1D-CHD-C4C	-3.65	117.67	126.25
30	7	303	CLA	O2A-CGA-CBA	3.65	122.95	111.83
38	16	304	KC1	C4B-C3B-C2B	-3.65	103.65	106.81
30	B	806	CLA	O2D-CGD-CBD	3.64	117.60	111.23
38	3	311	KC1	C1C-C2C-C3C	-3.64	103.15	106.98
30	15	308	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
39	12	315	DD6	C35-C36-C31	-3.64	112.92	120.50
30	7	304	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
37	15	323	A86	C9-C10-C11	-3.64	116.35	126.64
30	A	802	CLA	CAC-C3C-C4C	3.64	129.53	124.79
30	10	308	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
30	2	308	CLA	C1-C2-C3	-3.64	120.23	126.20
38	6	312	KC1	C2C-C1C-NC	3.64	114.95	110.45
30	B	814	CLA	C3B-C4B-NB	3.64	113.78	110.53
37	5	301	A86	C4-C3-C2	-3.64	116.07	123.52
38	8	307	KC1	C1C-C2C-C3C	-3.64	103.15	106.98
30	12	308	CLA	C4A-NA-C1A	-3.64	105.02	106.68
39	12	315	DD6	C21-C20-C15	-3.64	116.31	122.30
30	B	836	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
30	16	302	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
30	16	305	CLA	CHD-C1D-ND	-3.64	119.68	124.80
30	2	313	CLA	C1C-C2C-C3C	-3.64	103.16	106.98
37	7	316	A86	C36-C31-C32	-3.63	116.09	119.70
38	4	310	KC1	CAA-CBA-CGA	-3.63	108.57	127.05
30	B	823	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
30	A	834	CLA	C3C-C4C-NC	3.63	115.08	110.43
30	A	836	CLA	CHD-C1D-ND	-3.63	119.69	124.80
30	14	313	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
38	12	311	KC1	C1C-C2C-C3C	-3.63	103.16	106.98
30	A	832	CLA	C4A-NA-C1A	-3.63	105.02	106.68
30	11	310	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
37	2u	203	A86	C4-C3-C2	-3.63	116.10	123.52
30	4	309	CLA	CAA-C2A-C3A	-3.63	103.20	113.00
30	B	826	CLA	C4A-NA-C1A	-3.63	105.02	106.68
30	1	301	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
39	4	313	DD6	C35-C36-C31	-3.63	112.95	120.50
38	12	313	KC1	CAA-CBA-CGA	-3.63	108.61	127.05
30	9	301	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
30	7	311	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
30	B	837	CLA	C3C-C4C-NC	3.62	115.07	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	305	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
30	16	310	CLA	C3C-C4C-NC	3.62	115.07	110.43
38	14	306	KC1	CBA-CAA-C2A	-3.62	110.92	125.45
30	A	827	CLA	CHD-C4C-NC	3.62	129.84	124.23
39	12	317	DD6	C21-C20-C15	-3.62	116.34	122.30
30	B	821	CLA	CHD-C1D-ND	-3.62	119.71	124.80
30	A	838	CLA	C3B-C4B-NB	3.62	113.76	110.53
38	16	304	KC1	C1D-CHD-C4C	-3.62	117.74	126.25
38	14	306	KC1	C4C-C3C-C2C	-3.62	101.63	106.89
30	3	301	CLA	C4-C3-C5	3.62	121.50	115.23
30	B	808	CLA	C3B-C4B-NB	3.62	113.76	110.53
30	B	822	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
30	14	305	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
37	15	320	A86	C35-C34-C33	3.61	116.38	109.89
30	B	812	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
38	4	310	KC1	C1C-C2C-C3C	-3.61	103.18	106.98
30	A	825	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
30	12	304	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
30	7	307	CLA	C4A-NA-C1A	-3.61	105.03	106.68
30	A	807	CLA	C3C-C4C-NC	3.61	115.06	110.43
30	A	839	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
30	9	307	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
30	14	303	CLA	CAA-C2A-C3A	-3.61	103.25	113.00
30	A	815	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
30	B	832	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
30	A	809	CLA	CAC-C3C-C4C	3.61	129.48	124.79
39	7	302	DD6	C15-C14-C13	-3.61	118.37	125.99
30	5	304	CLA	C1D-CHD-C4C	-3.61	118.36	126.02
30	3	307	CLA	C4A-NA-C1A	-3.61	105.03	106.68
30	4	301	CLA	C4A-NA-C1A	-3.61	105.03	106.68
39	7	314	DD6	C7-C6-C8	-3.61	112.58	118.09
30	15	308	CLA	CHD-C1D-ND	-3.60	119.73	124.80
30	3	302	CLA	C3C-C4C-NC	3.60	115.05	110.43
30	A	810	CLA	O2A-CGA-CBA	3.60	122.83	111.83
30	12	321	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
30	9	305	CLA	C3C-C4C-NC	3.60	115.05	110.43
30	B	805	CLA	C1D-CHD-C4C	-3.60	118.36	126.02
30	L	203	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
30	B	829	CLA	CMB-C2B-C1B	3.60	130.90	125.42
37	6	320	A86	C40-C32-C31	-3.60	107.25	110.47
30	B	804	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
30	8	304	CLA	CHD-C1D-ND	-3.60	119.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	809	CLA	C4A-NA-C1A	-3.60	105.04	106.68
30	8	301	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
30	6	306	CLA	C3C-C4C-NC	3.60	115.04	110.43
30	4	301	CLA	C1D-CHD-C4C	-3.60	118.38	126.02
38	8	306	KC1	C4B-C3B-C2B	-3.60	103.70	106.81
30	A	805	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
30	15	311	CLA	C4A-NA-C1A	-3.59	105.04	106.68
30	B	808	CLA	O2A-CGA-CBA	3.59	122.79	111.83
30	15	309	CLA	O2D-CGD-CBD	3.59	117.51	111.23
30	A	814	CLA	C4A-NA-C1A	-3.59	105.04	106.68
30	B	807	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
30	6	307	CLA	CAA-C2A-C3A	-3.59	103.29	113.00
38	9	304	KC1	C1D-CHD-C4C	-3.59	117.80	126.25
30	15	304	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
30	A	821	CLA	C3C-C4C-NC	3.59	115.03	110.43
30	9	306	CLA	C4A-NA-C1A	-3.59	105.04	106.68
38	8	312	KC1	C1A-NA-C4A	-3.59	105.04	106.68
30	4	302	CLA	C1-C2-C3	-3.59	120.32	126.20
30	14	304	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
30	A	843	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
38	8	310	KC1	C4C-C3C-C2C	-3.59	101.67	106.89
30	B	802	CLA	CAC-C3C-C4C	3.59	129.46	124.79
37	14	320	A86	C8-C6-C5	-3.58	113.37	119.01
38	14	308	KC1	C4C-C3C-C2C	-3.58	101.67	106.89
30	B	829	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
39	10	313	DD6	C14-C13-C11	3.58	131.09	125.53
30	B	823	CLA	CHD-C1D-ND	-3.58	119.76	124.80
38	11	307	KC1	C4B-C3B-C2B	-3.58	103.71	106.81
30	15	309	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
30	2	310	CLA	C3C-C4C-NC	3.58	115.02	110.43
38	6	313	KC1	C4B-C3B-C2B	-3.58	103.71	106.81
39	4	316	DD6	C35-C36-C31	-3.58	113.05	120.50
30	4	303	CLA	C3C-C4C-NC	3.58	115.01	110.43
30	B	830	CLA	CAC-C3C-C4C	3.58	129.44	124.79
38	9	310	KC1	C1C-C2C-C3C	-3.58	103.22	106.98
30	11	309	CLA	O2A-CGA-CBA	3.58	122.74	111.83
30	A	822	CLA	C1D-CHD-C4C	-3.58	118.42	126.02
38	13	311	KC1	CAA-CBA-CGA	-3.57	108.88	127.05
30	9	308	CLA	C3C-C4C-NC	3.57	115.01	110.43
30	7	303	CLA	CHD-C1D-ND	-3.57	119.78	124.80
30	15	306	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
38	12	305	KC1	C4B-C3B-C2B	-3.57	103.72	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	313	A86	C8-C6-C5	3.57	124.62	119.01
30	2	310	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
38	7	313	KC1	C1C-C2C-C3C	-3.57	103.22	106.98
30	3	305	CLA	C3C-C4C-NC	3.57	115.00	110.43
30	9	302	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
30	B	851	CLA	CAC-C3C-C4C	3.57	129.43	124.79
30	A	830	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
30	B	822	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
30	10	309	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
38	9	311	KC1	C2C-C1C-NC	3.56	114.86	110.45
30	4	302	CLA	C4A-NA-C1A	-3.56	105.05	106.68
30	4	304	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
30	B	835	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
30	B	803	CLA	C2C-C1C-NC	3.56	113.72	109.98
30	14	312	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
30	16	302	CLA	C3C-C4C-NC	3.56	114.99	110.43
37	14	319	A86	C34-O4-C38	-3.56	111.56	117.85
37	3	314	A86	C23-C16-C17	-3.56	102.71	108.97
30	12	308	CLA	CHD-C1D-ND	-3.56	119.80	124.80
30	5	304	CLA	O2A-CGA-CBA	3.56	122.68	111.83
37	2	302	A86	C12-C11-C13	3.56	121.77	116.00
30	3	306	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
30	B	834	CLA	CHD-C1D-ND	-3.56	119.80	124.80
39	15	319	DD6	C23-C16-C15	3.56	119.65	110.05
30	8	308	CLA	C1-C2-C3	-3.56	120.37	126.20
38	8	312	KC1	C4B-C3B-C2B	-3.56	103.73	106.81
38	13	306	KC1	CAC-C3C-C4C	3.56	129.42	124.79
30	A	833	CLA	C4A-NA-C1A	-3.56	105.06	106.68
30	B	828	CLA	C3C-C4C-NC	3.55	114.98	110.43
30	2	304	CLA	C3B-C4B-NB	3.55	113.70	110.53
30	9	306	CLA	C3B-C4B-NB	3.55	113.70	110.53
30	B	827	CLA	C1C-C2C-C3C	-3.55	103.24	106.98
30	10	309	CLA	C3C-C4C-NC	3.55	114.98	110.43
38	6	313	KC1	CAA-C2A-C1A	-3.55	109.08	124.64
38	1	306	KC1	CAC-C3C-C4C	3.55	129.41	124.79
30	A	835	CLA	CAA-C2A-C3A	-3.55	103.40	113.00
30	A	804	CLA	C3C-C4C-NC	3.55	114.98	110.43
30	15	308	CLA	C4C-C3C-C2C	-3.55	101.72	106.89
39	5	314	DD6	C15-C14-C13	-3.55	118.49	125.99
30	B	814	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
30	14	310	CLA	C4A-NA-C1A	-3.55	105.06	106.68
30	6	317	CLA	CAA-C2A-C3A	-3.55	103.41	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	833	CLA	C3C-C4C-NC	3.55	114.97	110.43
30	A	810	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
30	B	816	CLA	C3B-C4B-NB	3.55	113.70	110.53
30	1	307	CLA	C3B-C4B-NB	3.55	113.70	110.53
38	5	310	KC1	C1C-C2C-C3C	-3.55	103.25	106.98
30	B	812	CLA	CAC-C3C-C4C	3.55	129.41	124.79
30	A	840	CLA	C3C-C4C-NC	3.55	114.97	110.43
30	A	821	CLA	C3B-C2B-C1B	-3.55	102.99	107.17
39	6	321	DD6	C33-C32-C31	3.55	116.47	109.49
39	3	312	DD6	O1-C20-C21	-3.54	111.09	115.05
30	A	816	CLA	C3C-C4C-NC	3.54	114.97	110.43
30	A	809	CLA	C3B-C4B-NB	3.54	113.69	110.53
38	6	312	KC1	C1D-CHD-C4C	-3.54	117.92	126.25
30	5	311	CLA	C3C-C4C-NC	3.54	114.97	110.43
38	4	307	KC1	C1D-CHD-C4C	-3.54	117.92	126.25
36	F	205	LMG	O6-C1-O1	-3.54	101.68	110.04
38	13	312	KC1	C1D-CHD-C4C	-3.54	117.92	126.25
33	2u	201	BCR	C15-C16-C17	-3.54	116.28	123.52
30	6	315	CLA	C4A-NA-C1A	-3.54	105.06	106.68
30	B	811	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
30	5	304	CLA	C3C-C4C-NC	3.54	114.96	110.43
30	16	309	CLA	C3B-C4B-NB	3.54	113.69	110.53
30	7	311	CLA	CAC-C3C-C4C	3.54	129.39	124.79
30	A	824	CLA	CMA-C3A-C2A	-3.54	100.31	113.98
37	10	302	A86	C3-C2-C1	-3.54	122.32	127.28
30	2	307	CLA	C3C-C4C-NC	3.53	114.96	110.43
30	16	303	CLA	C3C-C4C-NC	3.53	114.96	110.43
30	A	812	CLA	C4-C3-C5	3.53	121.36	115.23
30	4	306	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
30	8	301	CLA	CHD-C1D-ND	-3.53	119.83	124.80
38	4	310	KC1	C2C-C1C-NC	3.53	114.82	110.45
30	B	813	CLA	C1D-CHD-C4C	-3.53	118.51	126.02
30	B	801	CLA	C1-C2-C3	-3.53	120.41	126.20
30	6	306	CLA	C1-O2A-CGA	3.53	125.20	116.65
38	8	314	KC1	C1C-C2C-C3C	-3.53	103.27	106.98
37	10	301	A86	C21-C20-C15	-3.53	111.95	123.35
30	7	309	CLA	C4A-NA-C1A	-3.53	105.07	106.68
30	A	843	CLA	C2B-C1B-NB	3.53	113.99	110.33
30	5	303	CLA	C3C-C4C-NC	3.53	114.95	110.43
30	2	307	CLA	CHD-C1D-ND	-3.53	119.84	124.80
30	15	302	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
30	A	820	CLA	C1D-CHD-C4C	-3.53	118.53	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	310	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
30	A	822	CLA	C3C-C4C-NC	3.53	114.95	110.43
30	B	802	CLA	C4C-C3C-C2C	-3.52	101.76	106.89
30	9	309	CLA	C4B-C3B-C2B	-3.52	102.92	107.30
30	B	826	CLA	CAA-C2A-C3A	-3.52	103.48	113.00
30	12	307	CLA	CAA-C2A-C3A	-3.52	103.48	113.00
37	8	318	A86	C35-C34-C33	3.52	116.21	109.89
30	A	830	CLA	C1-C2-C3	-3.52	120.43	126.20
30	16	301	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
30	2	313	CLA	C3C-C4C-NC	3.52	114.94	110.43
30	A	815	CLA	CHC-C1C-C2C	-3.52	116.94	126.95
30	15	305	CLA	C3B-C4B-NB	3.52	113.67	110.53
30	B	804	CLA	C3C-C4C-NC	3.52	114.94	110.43
30	16	310	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
38	14	311	KC1	CMB-C2B-C1B	3.52	130.93	124.73
30	A	816	CLA	CMB-C2B-C1B	3.52	130.78	125.42
30	A	841	CLA	C3C-C4C-NC	3.52	114.94	110.43
30	B	835	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
38	11	305	KC1	C1D-CHD-C4C	-3.52	117.97	126.25
38	5	306	KC1	CHD-C1D-ND	-3.52	118.77	124.05
30	B	815	CLA	CAC-C3C-C4C	3.52	129.37	124.79
38	7	313	KC1	C1D-CHD-C4C	-3.52	117.98	126.25
30	7	310	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
39	7	317	DD6	C35-C36-C31	-3.52	113.18	120.50
38	9	311	KC1	C1D-CHD-C4C	-3.52	117.98	126.25
37	10	317	A86	C36-C31-C32	-3.52	116.21	119.70
30	A	829	CLA	C3C-C4C-NC	3.52	114.93	110.43
30	B	829	CLA	CAA-C2A-C3A	-3.52	103.50	113.00
30	5	302	CLA	C3C-C4C-NC	3.52	114.93	110.43
30	11	306	CLA	C3C-C4C-NC	3.51	114.93	110.43
30	B	817	CLA	C2C-C1C-NC	3.51	113.67	109.98
38	1	308	KC1	C1D-CHD-C4C	-3.51	117.99	126.25
30	9	309	CLA	C3C-C4C-NC	3.51	114.93	110.43
38	14	308	KC1	C1C-C2C-C3C	-3.51	103.29	106.98
30	7	312	CLA	C3B-C4B-NB	3.51	113.67	110.53
30	B	830	CLA	C4C-C3C-C2C	-3.51	101.78	106.89
37	4	315	A86	C4-C3-C2	-3.51	116.34	123.52
30	3	301	CLA	C3B-C4B-NB	3.51	113.66	110.53
30	A	810	CLA	C3C-C4C-NC	3.51	114.92	110.43
30	F	203	CLA	C3C-C4C-NC	3.51	114.92	110.43
37	7	315	A86	C26-C25-C24	-3.51	113.04	123.20
38	1	306	KC1	C1D-CHD-C4C	-3.51	118.00	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	310	CLA	C4A-NA-C1A	-3.51	105.08	106.68
38	11	305	KC1	CAA-CBA-CGA	-3.51	109.22	127.05
30	A	832	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
30	13	301	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
38	12	311	KC1	C1D-CHD-C4C	-3.51	118.00	126.25
38	8	306	KC1	CHD-C1D-ND	-3.51	118.79	124.05
38	10	306	KC1	CAA-CBA-CGA	-3.51	109.22	127.05
30	7	307	CLA	C3C-C4C-NC	3.50	114.92	110.43
30	A	826	CLA	CHD-C1D-ND	-3.50	119.87	124.80
30	A	803	CLA	C3C-C4C-NC	3.50	114.92	110.43
30	2	301	CLA	CHC-C1C-C2C	-3.50	116.99	126.95
37	7	316	A86	C25-C26-C27	-3.50	122.36	127.28
30	F	202	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
38	2	312	KC1	C1A-NA-C4A	-3.50	105.08	106.68
30	A	815	CLA	C4B-C3B-C2B	-3.50	102.95	107.30
38	8	314	KC1	CBA-CAA-C2A	-3.50	111.40	125.45
30	2	311	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
30	A	806	CLA	CAA-CBA-CGA	-3.50	103.27	113.21
37	15	322	A86	C24-C1-C2	3.50	124.52	119.01
39	16	313	DD6	C23-C16-C17	-3.50	102.82	108.97
38	13	310	KC1	CHD-C1D-ND	-3.50	118.80	124.05
37	14	315	A86	C25-C26-C27	-3.50	122.37	127.28
38	5	306	KC1	C1C-C2C-C3C	-3.50	103.30	106.98
38	8	312	KC1	C1C-C2C-C3C	-3.50	103.30	106.98
30	9	305	CLA	CBA-CAA-C2A	3.50	124.20	113.79
30	9	307	CLA	C4A-NA-C1A	-3.50	105.08	106.68
30	B	828	CLA	C3D-C2D-C1D	-3.50	101.06	105.83
38	8	312	KC1	C1D-CHD-C4C	-3.50	118.02	126.25
30	B	815	CLA	C3C-C4C-NC	3.50	114.91	110.43
38	10	312	KC1	CHD-C1D-ND	-3.50	118.80	124.05
30	8	303	CLA	C3C-C4C-NC	3.50	114.91	110.43
30	3	309	CLA	CAA-C2A-C3A	-3.50	103.55	113.00
39	7	314	DD6	C22-C16-C15	3.49	119.48	110.05
30	6	316	CLA	C3C-C4C-NC	3.49	114.91	110.43
37	10	301	A86	C3-C2-C1	-3.49	122.38	127.28
30	B	823	CLA	CAC-C3C-C4C	3.49	129.34	124.79
30	16	309	CLA	C3C-C4C-NC	3.49	114.90	110.43
30	10	311	CLA	C3C-C4C-NC	3.49	114.90	110.43
30	15	311	CLA	C3C-C4C-NC	3.49	114.90	110.43
30	1	304	CLA	CMC-C2C-C1C	3.49	130.49	125.03
38	5	312	KC1	CAA-CBA-CGA	-3.49	109.30	127.05
30	7	309	CLA	CMB-C2B-C1B	3.49	130.73	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	13	305	KC1	C1A-NA-C4A	-3.49	105.09	106.68
30	14	304	CLA	C3C-C4C-NC	3.49	114.90	110.43
30	A	807	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
30	16	303	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
30	7	306	CLA	CAC-C3C-C4C	3.49	129.32	124.79
30	B	809	CLA	C3C-C4C-NC	3.49	114.89	110.43
30	A	809	CLA	C4A-NA-C1A	-3.49	105.09	106.68
30	1	307	CLA	C3C-C4C-NC	3.48	114.89	110.43
30	A	820	CLA	CBA-CAA-C2A	3.48	124.16	113.79
37	14	317	A86	C4-C3-C2	-3.48	116.39	123.52
30	14	305	CLA	C3C-C4C-NC	3.48	114.89	110.43
30	16	305	CLA	C3C-C4C-NC	3.48	114.89	110.43
30	2	301	CLA	C3B-C4B-NB	3.48	113.64	110.53
30	14	307	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
38	11	312	KC1	CAC-C3C-C4C	3.48	129.32	124.79
30	9	302	CLA	C4A-NA-C1A	-3.48	105.09	106.68
30	B	801	CLA	CHD-C1D-ND	-3.48	119.90	124.80
30	4	302	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
38	2	306	KC1	C1D-CHD-C4C	-3.48	118.07	126.25
30	7	305	CLA	C3C-C4C-NC	3.48	114.89	110.43
30	14	310	CLA	C3C-C4C-NC	3.48	114.89	110.43
30	B	826	CLA	C3B-C4B-NB	3.48	113.63	110.53
30	5	311	CLA	C1-O2A-CGA	3.48	125.07	116.65
30	9	308	CLA	C1-C2-C3	-3.48	120.50	126.20
30	A	803	CLA	C4A-NA-C1A	-3.48	105.09	106.68
38	4	307	KC1	C1A-NA-C4A	-3.48	105.09	106.68
30	5	307	CLA	CHD-C1D-ND	-3.48	119.91	124.80
30	8	305	CLA	C3B-C4B-NB	3.47	113.63	110.53
30	B	821	CLA	C4B-C3B-C2B	-3.47	102.98	107.30
37	11	301	A86	C40-C32-C31	-3.47	107.36	110.47
30	15	308	CLA	O2A-CGA-CBA	3.47	124.97	114.00
30	12	306	CLA	CHD-C1D-ND	-3.47	119.92	124.80
30	6	314	CLA	CAA-C2A-C3A	-3.47	103.61	113.00
38	12	309	KC1	C4B-C3B-C2B	-3.47	103.80	106.81
39	12	315	DD6	C25-C24-C1	-3.47	116.84	126.36
38	4	308	KC1	CMA-C3A-C2A	-3.47	120.03	128.43
38	3	311	KC1	CHD-C1D-ND	-3.47	118.84	124.05
30	B	816	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
30	11	309	CLA	C3B-C4B-NB	3.47	113.63	110.53
37	10	301	A86	C22-C16-C17	-3.47	102.87	108.97
30	B	805	CLA	CHB-C4A-NA	3.47	129.40	124.40
30	B	822	CLA	CMB-C2B-C1B	3.47	130.70	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	825	CLA	C3B-C4B-NB	3.47	113.62	110.53
30	B	809	CLA	C2B-C1B-NB	3.47	113.92	110.33
37	12	314	A86	C41-C32-C31	-3.46	107.37	110.47
30	2	309	CLA	C3C-C4C-NC	3.46	114.87	110.43
30	B	809	CLA	CHD-C1D-ND	-3.46	119.93	124.80
38	5	305	KC1	CAA-CBA-CGA	-3.46	109.44	127.05
30	10	308	CLA	CAC-C3C-C4C	3.46	129.30	124.79
37	14	316	A86	C12-C11-C13	3.46	121.61	116.00
30	7	309	CLA	C3B-C4B-NB	3.46	113.62	110.53
39	5	313	DD6	C35-C36-C31	-3.46	113.30	120.50
30	2	308	CLA	C3C-C4C-NC	3.46	114.86	110.43
30	14	312	CLA	C3C-C4C-NC	3.46	114.86	110.43
30	16	301	CLA	C4A-NA-C1A	-3.46	105.10	106.68
33	I	101	BCR	C31-C1-C6	3.46	115.67	110.24
38	5	306	KC1	CAA-CBA-CGA	-3.46	109.47	127.05
38	12	305	KC1	C1D-CHD-C4C	-3.46	118.12	126.25
30	13	309	CLA	CAA-C2A-C3A	-3.46	103.66	113.00
39	13	314	DD6	O1-C15-C14	-3.46	106.98	116.88
30	B	829	CLA	C3C-C4C-NC	3.46	114.86	110.43
30	A	821	CLA	C3B-C4B-NB	3.45	113.61	110.53
37	11	316	A86	C3-C2-C1	-3.45	122.43	127.28
30	12	321	CLA	C3B-C4B-NB	3.45	113.61	110.53
30	B	812	CLA	C3C-C4C-NC	3.45	114.85	110.43
30	8	302	CLA	C3C-C4C-NC	3.45	114.85	110.43
30	A	834	CLA	CMB-C2B-C1B	3.45	130.68	125.42
30	1	307	CLA	C4A-NA-C1A	-3.45	105.10	106.68
30	15	303	CLA	O2A-CGA-CBA	3.45	122.36	111.83
38	8	310	KC1	C4B-C3B-C2B	-3.45	103.82	106.81
38	4	307	KC1	CBA-CAA-C2A	-3.45	111.60	125.45
30	6	315	CLA	C3C-C4C-NC	3.45	114.85	110.43
30	L	202	CLA	C3B-C4B-NB	3.45	113.61	110.53
30	B	816	CLA	C4A-NA-C1A	-3.45	105.11	106.68
30	A	814	CLA	C3C-C4C-NC	3.45	114.85	110.43
30	15	310	CLA	C3C-C4C-NC	3.45	114.85	110.43
30	B	824	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
30	3	306	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
30	11	304	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
38	7	313	KC1	CAA-CBA-CGA	-3.45	109.51	127.05
30	12	306	CLA	C3C-C4C-NC	3.45	114.85	110.43
30	12	307	CLA	C4B-C3B-C2B	-3.45	103.02	107.30
30	7	303	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
30	2	311	CLA	C1-C2-C3	-3.45	120.55	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	2	314	KC1	C4B-C3B-C2B	-3.45	103.83	106.81
38	14	308	KC1	C1D-CHD-C4C	-3.45	118.14	126.25
38	9	310	KC1	C2C-C1C-NC	3.45	114.72	110.45
37	7	319	A86	C4-C5-C6	-3.45	122.44	127.28
37	15	321	A86	C41-C32-C31	-3.45	107.39	110.47
37	8	315	A86	C24-C1-C2	-3.45	113.59	119.01
30	4	304	CLA	C3C-C4C-NC	3.45	114.84	110.43
30	2	304	CLA	C3C-C4C-NC	3.44	114.84	110.43
30	A	814	CLA	C3B-C4B-NB	3.44	113.61	110.53
30	B	838	CLA	CHC-C1C-C2C	-3.44	117.16	126.95
37	4	314	A86	C35-C34-C33	3.44	116.07	109.89
30	B	818	CLA	C1-C2-C3	-3.44	120.55	126.20
30	5	302	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
30	A	843	CLA	C4A-NA-C1A	-3.44	105.11	106.68
30	A	842	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
30	10	305	CLA	C3C-C4C-NC	3.44	114.84	110.43
30	6	305	CLA	C3B-C4B-NB	3.44	113.60	110.53
30	A	819	CLA	C4C-C3C-C2C	-3.44	101.88	106.89
38	8	314	KC1	C4B-C3B-C2B	-3.44	103.83	106.81
38	12	313	KC1	C4B-C3B-C2B	-3.44	103.83	106.81
30	3	310	CLA	C3B-C4B-NB	3.44	113.60	110.53
30	9	301	CLA	C4B-C3B-C2B	-3.44	103.03	107.30
38	11	307	KC1	CHD-C1D-ND	-3.44	118.89	124.05
37	2	319	A86	C41-C32-C31	-3.44	107.40	110.47
30	8	301	CLA	CMC-C2C-C1C	3.44	130.40	125.03
30	A	817	CLA	C4A-NA-C1A	-3.43	105.11	106.68
30	A	836	CLA	C3C-C4C-NC	3.43	114.83	110.43
30	1	305	CLA	C3B-C4B-NB	3.43	113.60	110.53
38	10	312	KC1	C1D-CHD-C4C	-3.43	118.17	126.25
30	B	819	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
30	A	832	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
30	16	306	CLA	C4B-C3B-C2B	-3.43	103.03	107.30
30	A	833	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
30	16	306	CLA	CHD-C1D-ND	-3.43	119.97	124.80
30	B	837	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
30	14	302	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
38	10	312	KC1	CBA-CAA-C2A	-3.43	111.69	125.45
30	2	303	CLA	CHB-C4A-NA	3.43	129.35	124.40
38	5	306	KC1	C2C-C1C-NC	3.43	114.69	110.45
38	7	313	KC1	CHD-C1D-ND	-3.43	118.91	124.05
30	14	313	CLA	CAA-C2A-C3A	-3.43	103.73	113.00
39	3	313	DD6	C13-C11-C10	-3.43	113.62	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	13	305	KC1	C1D-CHD-C4C	-3.43	118.19	126.25
30	A	806	CLA	C3C-C4C-NC	3.43	114.82	110.43
30	A	826	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
30	9	303	CLA	C3B-C4B-NB	3.43	113.59	110.53
30	12	321	CLA	O2D-CGD-CBD	3.43	117.22	111.23
30	11	309	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
30	A	811	CLA	C3B-C4B-NB	3.42	113.59	110.53
30	B	801	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
30	5	307	CLA	C4B-C3B-C2B	-3.42	103.05	107.30
30	A	828	CLA	CHD-C4C-NC	3.42	129.54	124.23
38	3	304	KC1	CBA-CAA-C2A	-3.42	111.72	125.45
30	A	816	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
38	3	311	KC1	C1D-CHD-C4C	-3.42	118.20	126.25
38	11	307	KC1	C1A-NA-C4A	-3.42	105.12	106.68
37	15	322	A86	C-C1-C2	-3.42	117.28	122.82
30	A	806	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
30	A	833	CLA	C3C-C4C-NC	3.42	114.81	110.43
30	A	839	CLA	C3C-C4C-NC	3.42	114.81	110.43
30	7	310	CLA	C3C-C4C-NC	3.42	114.81	110.43
30	15	308	CLA	CMB-C2B-C1B	3.42	130.63	125.42
38	9	304	KC1	C4B-C3B-C2B	-3.42	103.85	106.81
30	10	303	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
30	6	310	CLA	C4B-C3B-C2B	-3.42	103.05	107.30
38	9	311	KC1	C4B-C3B-C2B	-3.42	103.85	106.81
37	16	312	A86	C10-C9-C8	3.42	133.10	123.20
30	8	302	CLA	C3B-C4B-NB	3.42	113.58	110.53
30	A	820	CLA	CAC-C3C-C4C	3.42	129.24	124.79
38	13	312	KC1	CAA-CBA-CGA	-3.41	109.69	127.05
37	8	315	A86	C3-C4-C5	-3.41	116.53	123.52
30	L	203	CLA	C3C-C4C-NC	3.41	114.80	110.43
38	5	305	KC1	C4B-C3B-C2B	-3.41	103.85	106.81
38	11	307	KC1	CAA-CBA-CGA	-3.41	109.69	127.05
38	2	306	KC1	CHD-C1D-ND	-3.41	118.93	124.05
38	5	305	KC1	C1D-CHD-C4C	-3.41	118.22	126.25
30	5	304	CLA	C3B-C4B-NB	3.41	113.58	110.53
30	7	309	CLA	C3C-C4C-NC	3.41	114.80	110.43
39	10	313	DD6	C7-C6-C8	-3.41	112.88	118.09
30	8	303	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
30	15	311	CLA	C3B-C4B-NB	3.41	113.57	110.53
30	15	302	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
39	10	314	DD6	C19-C18-C17	3.41	117.17	110.79
30	B	808	CLA	C3C-C4C-NC	3.41	114.80	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	310	CLA	CMB-C2B-C1B	3.41	130.61	125.42
30	6	316	CLA	C1-C2-C3	-3.41	120.61	126.20
37	1	309	A86	C35-C34-C33	3.41	116.01	109.89
30	L	202	CLA	C1D-CHD-C4C	-3.41	118.78	126.02
30	16	307	CLA	C3C-C4C-NC	3.41	114.79	110.43
30	B	809	CLA	C3B-C4B-NB	3.41	113.57	110.53
38	16	311	KC1	CHD-C1D-ND	-3.40	118.94	124.05
38	5	306	KC1	C1D-CHD-C4C	-3.40	118.24	126.25
38	8	311	KC1	C1C-C2C-C3C	-3.40	103.40	106.98
38	2	314	KC1	C1D-CHD-C4C	-3.40	118.24	126.25
39	10	313	DD6	O1-C20-C21	-3.40	111.24	115.05
30	B	807	CLA	C3B-C4B-NB	3.40	113.57	110.53
30	B	827	CLA	C3B-C4B-NB	3.40	113.57	110.53
38	7	308	KC1	CBA-CAA-C2A	-3.40	111.79	125.45
38	3	308	KC1	CAC-C3C-C4C	3.40	129.22	124.79
37	8	315	A86	C4-C3-C2	-3.40	116.56	123.52
30	B	803	CLA	C1-C2-C3	-3.40	120.62	126.20
30	B	812	CLA	C3B-C4B-NB	3.40	113.57	110.53
30	16	305	CLA	C3B-C4B-NB	3.40	113.57	110.53
30	A	837	CLA	C3C-C4C-NC	3.40	114.79	110.43
39	10	313	DD6	C3-C4-C5	-3.40	116.56	123.52
30	B	816	CLA	C3C-C4C-NC	3.40	114.78	110.43
39	4	313	DD6	C25-C24-C1	-3.40	117.04	126.36
39	5	313	DD6	C15-C14-C13	-3.40	118.81	125.99
30	A	843	CLA	C4B-C3B-C2B	-3.40	103.08	107.30
30	2	303	CLA	CAC-C3C-C4C	3.40	129.21	124.79
38	6	312	KC1	CHD-C1D-ND	-3.40	118.95	124.05
38	8	307	KC1	CHD-C1D-ND	-3.40	118.95	124.05
30	12	321	CLA	C4B-C3B-C2B	-3.40	103.08	107.30
30	9	305	CLA	C3B-C4B-NB	3.40	113.56	110.53
30	A	803	CLA	CAA-C2A-C3A	-3.40	103.82	113.00
38	11	305	KC1	CHD-C1D-ND	-3.40	118.95	124.05
30	9	301	CLA	C3C-C4C-NC	3.40	114.78	110.43
30	13	304	CLA	C3C-C4C-NC	3.39	114.78	110.43
30	6	309	CLA	C3C-C4C-NC	3.39	114.78	110.43
30	15	304	CLA	C1-O2A-CGA	3.39	124.86	116.65
30	6	306	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
30	8	304	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
30	6	310	CLA	C3B-C4B-NB	3.39	113.56	110.53
30	9	302	CLA	C3C-C4C-NC	3.39	114.77	110.43
30	A	811	CLA	C3C-C4C-NC	3.39	114.77	110.43
30	7	311	CLA	C3C-C4C-NC	3.39	114.77	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	813	CLA	C3B-C4B-NB	3.39	113.56	110.53
39	3	312	DD6	C15-C14-C13	-3.39	118.83	125.99
30	2	311	CLA	C3C-C4C-NC	3.39	114.77	110.43
39	7	317	DD6	C37-C36-C35	-3.39	108.19	114.42
30	8	308	CLA	O2A-CGA-CBA	3.39	122.17	111.83
37	9	313	A86	C35-C34-C33	3.39	115.97	109.89
30	7	306	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
37	1	309	A86	C36-C31-C32	-3.39	116.33	119.70
30	6	316	CLA	C1C-C2C-C3C	-3.39	103.42	106.98
30	2	305	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
30	B	838	CLA	C4-C3-C5	3.39	121.11	115.23
30	15	313	CLA	C3C-C4C-NC	3.39	114.77	110.43
30	B	824	CLA	C3C-C4C-NC	3.38	114.77	110.43
30	B	801	CLA	C3B-C4B-NB	3.38	113.55	110.53
30	1	305	CLA	C3C-C4C-NC	3.38	114.77	110.43
30	13	309	CLA	C3B-C4B-NB	3.38	113.55	110.53
39	3	312	DD6	C21-C20-C15	-3.38	116.74	122.30
30	B	817	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
37	11	315	A86	C9-C10-C11	-3.38	117.08	126.64
30	B	806	CLA	CAA-C2A-C3A	-3.38	103.87	113.00
30	A	809	CLA	C3C-C4C-NC	3.38	114.76	110.43
30	B	838	CLA	C3C-C4C-NC	3.38	114.76	110.43
30	A	828	CLA	C3B-C4B-NB	3.38	113.55	110.53
38	12	309	KC1	C2A-C1A-NA	3.38	114.75	109.34
38	4	310	KC1	CHD-C1D-ND	-3.38	118.98	124.05
30	15	305	CLA	C3C-C4C-NC	3.38	114.76	110.43
38	2	314	KC1	CHD-C1D-ND	-3.38	118.98	124.05
30	14	307	CLA	C4C-C3C-C2C	-3.38	101.98	106.89
30	8	303	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
38	9	304	KC1	CAA-CBA-CGA	-3.38	109.88	127.05
30	15	314	CLA	CMB-C2B-C1B	3.38	130.56	125.42
30	A	828	CLA	CHD-C1D-ND	-3.38	120.05	124.80
30	A	805	CLA	C3C-C4C-NC	3.37	114.75	110.43
30	10	307	CLA	C1C-C2C-C3C	-3.37	103.43	106.98
30	A	826	CLA	CAC-C3C-C4C	3.37	129.18	124.79
38	8	314	KC1	CGD-CBD-CAD	-3.37	99.92	110.85
39	4	313	DD6	C37-C36-C35	-3.37	108.22	114.42
30	B	825	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
30	4	302	CLA	C3C-C4C-NC	3.37	114.75	110.43
30	B	805	CLA	C3C-C4C-NC	3.37	114.75	110.43
38	9	304	KC1	CBA-CAA-C2A	-3.37	111.92	125.45
30	A	817	CLA	C3B-C4B-NB	3.37	113.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	304	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
30	3	309	CLA	C3C-C4C-NC	3.37	114.75	110.43
30	8	308	CLA	C3C-C4C-NC	3.37	114.75	110.43
30	A	820	CLA	C3B-C4B-NB	3.37	113.54	110.53
30	B	813	CLA	CAC-C3C-C4C	3.37	129.17	124.79
30	12	302	CLA	CAA-C2A-C1A	-3.37	100.94	111.97
30	4	305	CLA	C3C-C4C-NC	3.37	114.75	110.43
38	8	307	KC1	C2C-C1C-NC	3.37	114.62	110.45
38	8	307	KC1	CBA-CAA-C2A	-3.37	111.94	125.45
39	1	310	DD6	C37-C36-C35	-3.37	108.23	114.42
38	10	312	KC1	CAA-CBA-CGA	-3.37	109.93	127.05
30	B	831	CLA	C3C-C4C-NC	3.36	114.74	110.43
30	16	308	CLA	C3C-C4C-NC	3.36	114.74	110.43
37	13	313	A86	C25-C26-C27	3.36	131.99	127.28
38	8	311	KC1	CHD-C1D-ND	-3.36	119.00	124.05
39	2	316	DD6	C35-C36-C31	-3.36	113.50	120.50
30	15	305	CLA	CAC-C3C-C4C	3.36	129.16	124.79
37	1	309	A86	C26-C25-C24	-3.36	113.46	123.20
30	B	802	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
37	15	321	A86	C10-C9-C8	-3.36	113.46	123.20
30	13	301	CLA	CAC-C3C-C4C	3.36	129.16	124.79
30	A	843	CLA	C3C-C4C-NC	3.36	114.73	110.43
38	14	311	KC1	C4B-C3B-C2B	-3.36	103.90	106.81
30	B	824	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
38	13	311	KC1	CHD-C1D-ND	-3.36	119.01	124.05
30	B	806	CLA	CHD-C4C-NC	3.36	129.44	124.23
37	5	316	A86	C12-C11-C13	3.36	121.44	116.00
30	3	307	CLA	C3B-C4B-NB	3.36	113.53	110.53
30	13	303	CLA	C3B-C4B-NB	3.36	113.53	110.53
30	B	809	CLA	C3B-C2B-C1B	-3.36	103.21	107.17
30	A	836	CLA	CAC-C3C-C4C	3.35	129.16	124.79
30	L	202	CLA	C3C-C4C-NC	3.35	114.73	110.43
38	2	306	KC1	CBA-CAA-C2A	-3.35	111.99	125.45
38	9	304	KC1	CAC-C3C-C4C	3.35	129.15	124.79
30	B	801	CLA	CMA-C3A-C4A	-3.35	102.76	111.77
30	B	806	CLA	C3C-C4C-NC	3.35	114.73	110.43
30	8	304	CLA	O2A-CGA-CBA	3.35	122.06	111.83
30	9	302	CLA	CAC-C3C-C4C	3.35	129.15	124.79
30	4	303	CLA	C1D-CHD-C4C	-3.35	118.89	126.02
30	A	835	CLA	C3C-C4C-NC	3.35	114.72	110.43
30	B	831	CLA	C3B-C4B-NB	3.35	113.52	110.53
30	12	304	CLA	C3B-C4B-NB	3.35	113.52	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	6	320	A86	C36-C31-C32	-3.35	116.37	119.70
30	4	303	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
30	A	822	CLA	C4B-C3B-C2B	-3.35	103.14	107.30
30	2	308	CLA	CMC-C2C-C1C	3.35	130.26	125.03
30	A	821	CLA	O2A-CGA-CBA	3.35	122.04	111.83
38	13	306	KC1	C2C-C1C-NC	3.35	114.59	110.45
30	2	301	CLA	C4B-C3B-C2B	-3.35	103.14	107.30
30	A	837	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
30	8	309	CLA	C3B-C4B-NB	3.34	113.52	110.53
30	14	309	CLA	C3B-C4B-NB	3.34	113.52	110.53
39	6	318	DD6	C25-C24-C1	-3.34	117.19	126.36
38	3	304	KC1	CHD-C1D-ND	-3.34	119.03	124.05
38	1	306	KC1	CAA-CBA-CGA	-3.34	110.04	127.05
39	9	314	DD6	O1-C15-C14	-3.34	107.30	116.88
30	B	811	CLA	C3B-C4B-NB	3.34	113.52	110.53
30	15	312	CLA	C3B-C4B-NB	3.34	113.52	110.53
30	1	301	CLA	C3C-C4C-NC	3.34	114.71	110.43
30	A	831	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
30	1	302	CLA	CAA-C2A-C3A	-3.34	103.97	113.00
30	B	818	CLA	C3B-C4B-NB	3.34	113.51	110.53
30	12	302	CLA	C3B-C4B-NB	3.34	113.51	110.53
30	B	839	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
30	7	306	CLA	C3B-C4B-NB	3.34	113.51	110.53
38	12	305	KC1	CHD-C1D-ND	-3.34	119.04	124.05
38	14	306	KC1	C2C-C1C-NC	3.34	114.58	110.45
30	A	804	CLA	C4B-C3B-C2B	-3.34	103.15	107.30
30	4	309	CLA	C3B-C4B-NB	3.34	113.51	110.53
30	12	312	CLA	CAA-C2A-C3A	-3.34	103.98	113.00
30	B	812	CLA	C4A-NA-C1A	-3.34	105.16	106.68
30	1	304	CLA	CAC-C3C-C4C	3.33	129.13	124.79
30	B	819	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
38	10	312	KC1	C2C-C1C-NC	3.33	114.58	110.45
30	A	820	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
30	B	802	CLA	O2A-CGA-CBA	3.33	122.00	111.83
30	A	836	CLA	C3B-C4B-NB	3.33	113.51	110.53
30	12	307	CLA	CHD-C1D-ND	-3.33	120.11	124.80
30	4	311	CLA	CBC-CAC-C3C	-3.33	103.39	112.42
38	14	306	KC1	C1D-CHD-C4C	-3.33	118.41	126.25
30	1	304	CLA	CHD-C1D-ND	-3.33	120.11	124.80
38	8	311	KC1	C1D-CHD-C4C	-3.33	118.41	126.25
38	6	308	KC1	C2C-C1C-NC	3.33	114.57	110.45
30	13	307	CLA	C4B-C3B-C2B	-3.33	103.16	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	303	CLA	C3C-C4C-NC	3.33	114.70	110.43
37	9	315	A86	C-C1-C24	3.33	123.17	118.09
30	A	811	CLA	C4A-NA-C1A	-3.33	105.16	106.68
30	B	805	CLA	CAC-C3C-C4C	3.33	129.12	124.79
38	7	313	KC1	C2C-C1C-NC	3.33	114.57	110.45
30	16	308	CLA	C3B-C4B-NB	3.33	113.50	110.53
30	A	842	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
30	8	305	CLA	C1C-C2C-C3C	-3.32	103.48	106.98
30	12	306	CLA	C3B-C4B-NB	3.32	113.50	110.53
30	3	306	CLA	C3C-C4C-NC	3.32	114.69	110.43
37	16	312	A86	C40-C32-C31	-3.32	107.50	110.47
39	6	318	DD6	C19-C18-C17	3.32	117.01	110.79
30	B	834	CLA	C4C-C3C-C2C	-3.32	102.05	106.89
38	6	312	KC1	CAA-CBA-CGA	-3.32	110.15	127.05
30	B	839	CLA	CHD-C4C-NC	3.32	129.38	124.23
30	A	824	CLA	C4B-C3B-C2B	-3.32	103.17	107.30
37	15	321	A86	C34-O4-C38	-3.32	111.98	117.85
30	3	301	CLA	C3C-C4C-NC	3.32	114.69	110.43
30	15	312	CLA	CBC-CAC-C3C	-3.32	103.42	112.42
38	8	307	KC1	CMB-C2B-C1B	3.32	130.58	124.73
38	8	306	KC1	C1A-NA-C4A	-3.32	105.16	106.68
30	B	814	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
30	F	201	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
30	15	304	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
39	13	314	DD6	C37-C36-C35	-3.32	108.32	114.42
31	B	840	PQN	C11-C12-C13	-3.32	121.11	126.83
30	3	307	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
38	9	312	KC1	CHD-C1D-ND	-3.32	119.07	124.05
30	A	830	CLA	CMC-C2C-C1C	3.32	130.22	125.03
30	5	308	CLA	C3C-C4C-NC	3.32	114.68	110.43
30	14	309	CLA	C3C-C4C-NC	3.32	114.68	110.43
30	B	810	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
38	13	308	KC1	CAA-CBA-CGA	-3.32	110.18	127.05
30	A	831	CLA	CAC-C3C-C4C	3.32	129.11	124.79
30	B	835	CLA	C3C-C4C-NC	3.32	114.68	110.43
30	2	305	CLA	C3C-C4C-NC	3.32	114.68	110.43
30	A	820	CLA	C1-C2-C3	-3.32	120.76	126.20
30	16	308	CLA	CAC-C3C-C4C	3.32	129.10	124.79
30	A	831	CLA	CHD-C1D-ND	-3.32	120.14	124.80
30	5	309	CLA	C3B-C4B-NB	3.31	113.49	110.53
30	A	818	CLA	CMC-C2C-C1C	3.31	130.21	125.03
34	B	848	LHG	O8-C23-C24	3.31	121.20	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	303	CLA	CBA-CAA-C2A	3.31	123.65	113.79
38	12	311	KC1	CAC-C3C-C4C	3.31	129.10	124.79
30	5	309	CLA	C3C-C4C-NC	3.31	114.67	110.43
30	14	313	CLA	C3C-C4C-NC	3.31	114.67	110.43
30	B	827	CLA	CAC-C3C-C4C	3.31	129.10	124.79
30	15	309	CLA	C3B-C4B-NB	3.31	113.48	110.53
30	A	841	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
30	9	301	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
30	9	306	CLA	CHC-C1C-C2C	-3.31	117.54	126.95
30	B	826	CLA	C4C-C3C-C2C	-3.31	102.08	106.89
37	11	314	A86	C10-C9-C8	-3.31	113.62	123.20
30	B	809	CLA	CAC-C3C-C4C	3.31	129.09	124.79
30	2	308	CLA	C1C-C2C-C3C	-3.30	103.50	106.98
30	B	823	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
30	B	811	CLA	CHD-C1D-ND	-3.30	120.15	124.80
38	14	311	KC1	CAA-CBA-CGA	-3.30	110.25	127.05
38	8	306	KC1	CAA-CBA-CGA	-3.30	110.25	127.05
30	B	813	CLA	O2A-CGA-CBA	3.30	121.90	111.83
30	A	803	CLA	C1D-CHD-C4C	-3.30	119.00	126.02
38	11	311	KC1	CHD-C1D-ND	-3.30	119.10	124.05
38	13	305	KC1	CAC-C3C-C4C	3.30	129.08	124.79
30	14	309	CLA	CHC-C1C-C2C	-3.30	117.57	126.95
30	A	821	CLA	C4A-NA-C1A	-3.30	105.17	106.68
38	3	311	KC1	CAA-CBA-CGA	-3.30	110.28	127.05
30	6	317	CLA	C3C-C4C-NC	3.30	114.66	110.43
30	16	306	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
38	6	308	KC1	CAA-CBA-CGA	-3.30	110.28	127.05
30	10	308	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
30	12	312	CLA	C3C-C4C-NC	3.29	114.65	110.43
38	4	310	KC1	C1D-CHD-C4C	-3.29	118.50	126.25
39	13	314	DD6	C35-C36-C31	-3.29	113.64	120.50
30	A	818	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
30	F	202	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
30	11	304	CLA	C3C-C4C-NC	3.29	114.65	110.43
30	15	309	CLA	C3C-C4C-NC	3.29	114.65	110.43
30	5	302	CLA	C1-C2-C3	-3.29	120.80	126.20
37	15	315	A86	C25-C24-C1	3.29	135.39	126.36
30	A	815	CLA	O2A-CGA-CBA	3.29	121.88	111.83
30	8	309	CLA	C3C-C4C-NC	3.29	114.65	110.43
30	A	829	CLA	C3B-C4B-NB	3.29	113.47	110.53
30	6	315	CLA	C3B-C4B-NB	3.29	113.47	110.53
39	12	317	DD6	C15-C14-C13	3.29	132.96	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	320	A86	C21-C20-C15	-3.29	112.72	123.35
38	13	312	KC1	CHD-C1D-ND	-3.29	119.11	124.05
30	15	307	CLA	C4B-C3B-C2B	-3.29	103.21	107.30
30	2	311	CLA	C4A-NA-C1A	-3.29	105.18	106.68
39	6	321	DD6	C21-C20-C19	-3.29	110.54	114.24
30	15	307	CLA	C3B-C4B-NB	3.29	113.47	110.53
30	15	302	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
30	A	808	CLA	C4A-NA-C1A	-3.29	105.18	106.68
37	2u	203	A86	C4-C5-C6	-3.29	122.67	127.28
38	2	314	KC1	CAA-CBA-CGA	-3.29	110.33	127.05
38	13	306	KC1	C4C-C3C-C2C	-3.29	102.11	106.89
30	3	306	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
30	A	804	CLA	C4C-C3C-C2C	-3.29	102.11	106.89
30	B	825	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
30	14	307	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
30	B	835	CLA	CAA-C2A-C3A	-3.29	104.12	113.00
38	12	311	KC1	CHD-C1D-ND	-3.29	119.12	124.05
30	3	303	CLA	C3C-C4C-NC	3.28	114.64	110.43
30	4	311	CLA	C3B-C4B-NB	3.28	113.46	110.53
30	15	303	CLA	C4-C3-C5	3.28	120.93	115.23
39	10	313	DD6	C35-C36-C31	-3.28	113.67	120.50
30	B	809	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
30	9	309	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
30	1	302	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
38	12	305	KC1	CBA-CAA-C2A	-3.28	112.28	125.45
30	4	306	CLA	C3C-C4C-NC	3.28	114.63	110.43
38	8	313	KC1	CAA-C2A-C1A	-3.28	110.26	124.64
38	8	312	KC1	CHD-C1D-ND	-3.28	119.13	124.05
30	4	305	CLA	C1D-CHD-C4C	-3.28	119.05	126.02
30	A	840	CLA	O2A-CGA-CBA	3.28	121.83	111.83
30	2	305	CLA	C3B-C4B-NB	3.28	113.46	110.53
30	A	831	CLA	CMA-C3A-C2A	-3.28	101.31	113.98
30	15	302	CLA	C3C-C4C-NC	3.28	114.63	110.43
30	B	834	CLA	C3B-C4B-NB	3.28	113.46	110.53
39	11	313	DD6	C37-C36-C35	-3.28	108.39	114.42
30	16	301	CLA	CHD-C4C-NC	3.28	129.31	124.23
30	9	302	CLA	C3B-C4B-NB	3.28	113.45	110.53
35	9	317	LMT	C1'-C2'-C3'	3.28	116.90	110.01
37	10	317	A86	C40-C32-C31	-3.28	107.54	110.47
30	2	303	CLA	CMB-C2B-C1B	3.28	130.41	125.42
30	B	810	CLA	C1-C2-C3	-3.27	120.83	126.20
30	B	815	CLA	CHC-C1C-C2C	-3.27	117.65	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	11	315	A86	C36-C31-C32	-3.27	116.45	119.70
37	4	315	A86	C10-C9-C8	-3.27	113.72	123.20
39	6	321	DD6	C37-C36-C35	-3.27	108.40	114.42
39	2	316	DD6	C10-C9-C8	-3.27	113.72	123.20
38	16	311	KC1	C4B-C3B-C2B	-3.27	103.98	106.81
30	14	310	CLA	C3B-C4B-NB	3.27	113.45	110.53
38	6	308	KC1	C1C-C2C-C3C	-3.27	103.54	106.98
30	9	308	CLA	CAC-C3C-C4C	3.27	129.04	124.79
30	B	816	CLA	CMB-C2B-C1B	3.27	130.40	125.42
37	5	301	A86	C35-C34-C33	3.27	115.76	109.89
30	A	829	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
30	16	310	CLA	CGD-CBD-CAD	-3.27	100.26	110.85
39	10	313	DD6	C15-C14-C13	3.27	132.90	125.99
31	A	845	PQN	C14-C13-C15	3.27	120.90	115.23
30	J	101	CLA	C3C-C4C-NC	3.27	114.62	110.43
30	3	305	CLA	C3B-C4B-NB	3.27	113.45	110.53
38	8	311	KC1	CAA-CBA-CGA	-3.27	110.43	127.05
30	3	305	CLA	O2D-CGD-CBD	3.27	116.94	111.23
30	13	303	CLA	CAC-C3C-C4C	3.27	129.04	124.79
38	10	310	KC1	CAA-CBA-CGA	-3.27	110.44	127.05
30	B	804	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
30	11	308	CLA	C3C-C4C-NC	3.27	114.61	110.43
30	5	303	CLA	O2D-CGD-CBD	3.27	116.94	111.23
30	7	312	CLA	CHC-C1C-C2C	-3.27	117.67	126.95
30	15	302	CLA	O2A-CGA-CBA	3.26	121.79	111.83
30	10	304	CLA	C4B-C3B-C2B	-3.26	103.24	107.30
30	6	316	CLA	CAC-C3C-C4C	3.26	129.04	124.79
30	9	308	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
37	9	315	A86	C41-C32-C31	-3.26	107.55	110.47
30	5	308	CLA	C3B-C4B-NB	3.26	113.44	110.53
30	B	851	CLA	C3C-C4C-NC	3.26	114.61	110.43
30	A	806	CLA	C4A-NA-C1A	-3.26	105.19	106.68
30	3	303	CLA	C4A-NA-C1A	-3.26	105.19	106.68
30	A	805	CLA	CMC-C2C-C1C	3.26	130.13	125.03
30	B	814	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
30	5	304	CLA	C1-O2A-CGA	3.26	124.54	116.65
30	16	307	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
30	15	303	CLA	C3B-C4B-NB	3.26	113.44	110.53
30	8	305	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
38	8	310	KC1	CHD-C4C-NC	3.26	129.22	124.31
30	16	303	CLA	C1-C2-C3	-3.26	120.86	126.20
30	A	844	CLA	C3C-C4C-NC	3.26	114.60	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	309	CLA	CAC-C3C-C4C	3.25	129.02	124.79
30	4	303	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
38	11	307	KC1	C1D-CHD-C4C	-3.25	118.60	126.25
30	B	832	CLA	C3C-C4C-NC	3.25	114.60	110.43
30	B	818	CLA	CMC-C2C-C1C	3.25	130.12	125.03
37	14	316	A86	C10-C9-C8	-3.25	113.78	123.20
37	2	318	A86	C12-C11-C13	3.25	121.27	116.00
30	4	306	CLA	C4A-NA-C1A	-3.25	105.20	106.68
39	2	315	DD6	C10-C9-C8	3.25	132.62	123.20
30	15	306	CLA	CHC-C1C-C2C	-3.25	117.71	126.95
38	5	306	KC1	C4B-C3B-C2B	-3.25	104.00	106.81
30	B	825	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
30	6	305	CLA	C3C-C4C-NC	3.25	114.59	110.43
38	7	308	KC1	CAA-CBA-CGA	-3.25	110.53	127.05
38	10	310	KC1	CHD-C1D-ND	-3.25	119.17	124.05
30	13	301	CLA	CMC-C2C-C1C	3.25	130.11	125.03
30	B	821	CLA	C3C-C4C-NC	3.25	114.59	110.43
30	B	807	CLA	CAC-C3C-C4C	3.25	129.02	124.79
30	16	302	CLA	C3B-C4B-NB	3.25	113.43	110.53
30	A	838	CLA	C1-C2-C3	-3.25	120.88	126.20
30	6	307	CLA	CHC-C1C-C2C	-3.25	117.72	126.95
38	8	306	KC1	CMB-C2B-C1B	3.25	130.44	124.73
30	6	307	CLA	C3C-C4C-NC	3.24	114.59	110.43
30	7	304	CLA	C4B-C3B-C2B	-3.24	103.27	107.30
37	16	312	A86	C4-C3-C2	-3.24	116.88	123.52
30	1	305	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
30	16	308	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
38	8	310	KC1	C1A-NA-C4A	-3.24	105.20	106.68
30	8	309	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
39	12	317	DD6	C37-C36-C35	-3.24	108.46	114.42
30	A	818	CLA	CHD-C4C-NC	3.24	129.26	124.23
30	A	820	CLA	C3C-C4C-NC	3.24	114.58	110.43
39	15	319	DD6	O1-C20-C21	-3.24	111.42	115.05
30	B	823	CLA	C3B-C4B-NB	3.24	113.42	110.53
37	2u	205	A86	C21-C20-C15	-3.24	112.89	123.35
30	5	303	CLA	C4-C3-C5	3.24	120.85	115.23
38	3	308	KC1	CAA-CBA-CGA	-3.24	110.57	127.05
37	15	321	A86	C4-C3-C2	-3.24	116.89	123.52
30	4	303	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
37	15	315	A86	C8-C6-C5	-3.24	113.91	119.01
38	6	311	KC1	CAA-CBA-CGA	-3.24	110.58	127.05
30	4	311	CLA	CHC-C1C-C2C	-3.24	117.74	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	308	CLA	C3B-C4B-NB	3.24	113.42	110.53
30	1	301	CLA	C3B-C4B-NB	3.24	113.42	110.53
30	A	815	CLA	C3C-C4C-NC	3.24	114.58	110.43
30	12	310	CLA	CMB-C2B-C1B	3.24	130.35	125.42
39	8	317	DD6	C35-C36-C31	-3.24	113.76	120.50
30	1	302	CLA	C3C-C4C-NC	3.24	114.58	110.43
39	3	313	DD6	C37-C36-C35	-3.24	108.47	114.42
30	B	808	CLA	CBA-CAA-C2A	3.24	123.42	113.79
39	2	317	DD6	C3-C4-C5	-3.23	116.90	123.52
38	9	311	KC1	CHD-C1D-ND	-3.23	119.20	124.05
38	7	313	KC1	CMB-C2B-C1B	3.23	130.42	124.73
37	14	315	A86	C41-C32-C31	-3.23	107.58	110.47
30	13	301	CLA	CMB-C2B-C1B	3.23	130.34	125.42
30	14	303	CLA	C3C-C4C-NC	3.23	114.57	110.43
38	6	308	KC1	C4C-C3C-C2C	-3.23	102.19	106.89
38	1	306	KC1	CBA-CAA-C2A	-3.23	112.49	125.45
38	16	311	KC1	CAA-CBA-CGA	-3.23	110.63	127.05
37	15	321	A86	C40-C32-C31	-3.23	107.58	110.47
38	8	311	KC1	C4C-C3C-C2C	-3.23	102.19	106.89
37	14	320	A86	C-C1-C2	-3.23	117.59	122.82
30	A	821	CLA	CHC-C1C-C2C	-3.23	117.77	126.95
38	3	304	KC1	O2D-CGD-O1D	-3.23	117.56	123.85
30	A	835	CLA	CMB-C2B-C1B	3.23	130.33	125.42
30	A	830	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
30	A	840	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
30	A	825	CLA	CMB-C2B-C1B	3.23	130.33	125.42
30	11	308	CLA	CAA-C2A-C3A	-3.23	104.28	113.00
30	7	307	CLA	CHD-C4C-NC	3.22	129.23	124.23
30	A	816	CLA	CHC-C1C-C2C	-3.22	117.78	126.95
30	7	309	CLA	CHC-C1C-C2C	-3.22	117.79	126.95
30	7	312	CLA	C3C-C4C-NC	3.22	114.56	110.43
30	10	303	CLA	C3C-C4C-NC	3.22	114.56	110.43
38	6	311	KC1	CHD-C1D-ND	-3.22	119.22	124.05
38	5	305	KC1	CHD-C1D-ND	-3.22	119.22	124.05
30	13	307	CLA	C3C-C4C-NC	3.22	114.56	110.43
30	1	307	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
30	6	317	CLA	C3B-C4B-NB	3.22	113.41	110.53
37	11	316	A86	C12-C11-C13	3.22	121.22	116.00
37	5	316	A86	C40-C32-C31	-3.22	107.59	110.47
30	A	807	CLA	C1-C2-C3	-3.22	120.92	126.20
30	6	310	CLA	C3C-C4C-NC	3.22	114.56	110.43
30	16	305	CLA	C4B-C3B-C2B	-3.22	103.30	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	304	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
30	10	305	CLA	C3B-C4B-NB	3.22	113.40	110.53
30	13	302	CLA	C3B-C4B-NB	3.22	113.40	110.53
30	A	806	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
30	4	302	CLA	C3B-C4B-NB	3.22	113.40	110.53
30	9	307	CLA	C4-C3-C5	3.22	120.81	115.23
30	7	306	CLA	C4A-NA-C1A	-3.22	105.21	106.68
30	3	303	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
30	15	303	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
30	A	810	CLA	O2D-CGD-CBD	3.22	116.85	111.23
38	2	312	KC1	CAC-C3C-C4C	3.22	128.97	124.79
30	A	803	CLA	C1C-C2C-C3C	-3.22	103.60	106.98
39	1	310	DD6	C35-C36-C31	-3.22	113.81	120.50
30	10	311	CLA	C3B-C4B-NB	3.21	113.40	110.53
38	12	313	KC1	CHD-C4C-NC	3.21	129.15	124.31
30	16	305	CLA	C1-C2-C3	-3.21	121.56	126.76
37	4	312	A86	C25-C26-C27	-3.21	122.77	127.28
30	A	835	CLA	C3B-C4B-NB	3.21	113.40	110.53
30	B	813	CLA	C3B-C4B-NB	3.21	113.40	110.53
37	11	315	A86	C21-C20-C15	-3.21	112.98	123.35
30	A	814	CLA	CHC-C1C-C2C	-3.21	117.82	126.95
30	6	314	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
30	7	306	CLA	C1-C2-C3	-3.21	120.94	126.20
39	7	302	DD6	C19-C18-C17	3.21	116.80	110.79
30	B	827	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
30	4	301	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
30	B	806	CLA	C4-C3-C5	3.21	120.80	115.23
30	15	313	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
30	B	830	CLA	C1D-CHD-C4C	-3.21	119.20	126.02
30	A	830	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
38	8	314	KC1	CHD-C1D-ND	-3.21	119.24	124.05
30	2	307	CLA	CMA-C3A-C4A	-3.21	103.16	111.77
30	3	303	CLA	C3B-C4B-NB	3.21	113.39	110.53
38	9	311	KC1	CBA-CAA-C2A	-3.21	112.58	125.45
30	11	309	CLA	C3C-C4C-NC	3.21	114.54	110.43
30	15	306	CLA	CAA-C2A-C3A	-3.21	104.34	113.00
30	14	302	CLA	C4-C3-C5	3.21	120.79	115.23
30	6	314	CLA	CAC-C3C-C4C	3.20	128.96	124.79
30	10	311	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
30	A	837	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
30	10	307	CLA	CMB-C2B-C1B	3.20	130.30	125.42
30	B	804	CLA	C3B-C4B-NB	3.20	113.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	301	CLA	C4A-NA-C1A	-3.20	105.22	106.68
37	1	309	A86	C8-C6-C5	3.20	124.05	119.01
30	15	307	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
30	B	824	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
38	9	310	KC1	CHD-C1D-ND	-3.20	119.25	124.05
38	13	308	KC1	CHD-C1D-ND	-3.20	119.25	124.05
30	B	831	CLA	CAA-C2A-C3A	-3.20	104.35	113.00
30	2	303	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
30	3	301	CLA	O2A-CGA-CBA	3.20	121.59	111.83
30	A	837	CLA	CAC-C3C-C4C	3.20	128.95	124.79
30	B	807	CLA	CMC-C2C-C1C	3.20	130.03	125.03
30	10	304	CLA	C3B-C4B-NB	3.20	113.39	110.53
38	5	306	KC1	CBA-CAA-C2A	-3.20	112.62	125.45
30	A	809	CLA	CMC-C2C-C1C	3.20	130.03	125.03
38	8	312	KC1	C4C-C3C-C2C	-3.20	102.24	106.89
38	2	306	KC1	C4B-C3B-C2B	-3.20	104.04	106.81
30	B	807	CLA	CMB-C2B-C1B	3.20	130.29	125.42
37	11	316	A86	C10-C9-C8	-3.20	113.94	123.20
38	16	311	KC1	C2A-C1A-NA	3.20	114.46	109.34
30	10	309	CLA	CAC-C3C-C4C	3.19	128.95	124.79
30	16	309	CLA	CAA-C2A-C3A	-3.19	104.37	113.00
30	2	303	CLA	O2A-CGA-CBA	3.19	121.57	111.83
30	7	306	CLA	CHD-C1D-ND	-3.19	120.31	124.80
30	A	826	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
37	15	315	A86	C7-C6-C8	3.19	122.97	118.09
30	B	803	CLA	O2A-CGA-CBA	3.19	121.57	111.83
39	10	313	DD6	C37-C36-C35	-3.19	108.55	114.42
38	8	314	KC1	CAC-C3C-C4C	3.19	128.94	124.79
39	15	319	DD6	C25-C24-C1	-3.19	117.61	126.36
30	B	810	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
30	2	309	CLA	CAC-C3C-C4C	3.19	128.94	124.79
30	6	309	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
30	15	306	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
30	9	301	CLA	C4A-NA-C1A	-3.19	105.22	106.68
30	14	302	CLA	CAC-C3C-C4C	3.19	128.94	124.79
30	4	309	CLA	C3C-C4C-NC	3.19	114.52	110.43
30	A	816	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
30	A	836	CLA	CHC-C1C-C2C	-3.19	117.89	126.95
30	12	312	CLA	C3B-C4B-NB	3.19	113.38	110.53
38	12	309	KC1	CHD-C1D-ND	-3.19	119.27	124.05
38	10	312	KC1	CHD-C4C-NC	3.19	129.11	124.31
30	A	813	CLA	O2A-CGA-CBA	3.19	121.55	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	820	CLA	CHC-C1C-C2C	-3.19	117.89	126.95
30	5	303	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
38	12	309	KC1	C1A-NA-C4A	-3.18	105.23	106.68
30	10	307	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
37	10	315	A86	C12-C11-C13	3.18	121.16	116.00
30	12	308	CLA	C4B-C3B-C2B	-3.18	103.34	107.30
30	10	309	CLA	C3B-C4B-NB	3.18	113.37	110.53
30	6	304	CLA	C1-C2-C3	-3.18	120.98	126.20
30	B	808	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
38	8	314	KC1	CAA-CBA-CGA	-3.18	110.87	127.05
30	4	311	CLA	C3C-C4C-NC	3.18	114.51	110.43
38	9	304	KC1	CHD-C1D-ND	-3.18	119.28	124.05
30	9	301	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
30	B	815	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
30	B	834	CLA	O2A-CGA-CBA	3.18	121.53	111.83
30	4	309	CLA	O2A-CGA-CBA	3.18	121.53	111.83
37	7	316	A86	C12-C11-C13	3.18	121.16	116.00
30	16	306	CLA	C1C-C2C-C3C	-3.18	103.64	106.98
39	8	316	DD6	C37-C36-C35	-3.18	108.57	114.42
30	11	309	CLA	CAC-C3C-C4C	3.18	128.93	124.79
30	6	310	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
38	16	304	KC1	CHD-C1D-ND	-3.18	119.28	124.05
30	A	816	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
30	B	802	CLA	C4-C3-C5	3.18	120.74	115.23
39	7	318	DD6	C19-C18-C17	3.18	116.73	110.79
30	4	305	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
30	A	831	CLA	CHC-C1C-C2C	-3.18	117.92	126.95
30	A	842	CLA	C4C-C3C-C2C	-3.18	102.27	106.89
38	8	313	KC1	C4B-C3B-C2B	-3.17	104.06	106.81
37	7	319	A86	C-C1-C2	-3.17	117.67	122.82
30	9	303	CLA	CHD-C4C-NC	3.17	129.15	124.23
37	4	317	A86	C21-C20-C15	-3.17	113.11	123.35
30	B	839	CLA	O2A-CGA-CBA	3.17	121.51	111.83
37	14	319	A86	C12-C11-C10	-3.17	115.96	123.67
30	7	309	CLA	CAC-C3C-C4C	3.17	128.92	124.79
30	A	842	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
39	9	314	DD6	C35-C36-C31	-3.17	113.90	120.50
30	A	811	CLA	CHC-C1C-C2C	-3.17	117.93	126.95
30	14	313	CLA	CHD-C4C-NC	3.17	129.15	124.23
30	11	306	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
30	7	304	CLA	C3C-C4C-NC	3.17	114.49	110.43
30	2	310	CLA	C4B-C3B-C2B	-3.17	103.36	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	312	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
39	16	313	DD6	C22-C16-C15	3.17	118.60	110.05
30	12	306	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
30	B	851	CLA	O2A-CGA-CBA	3.17	121.50	111.83
37	4	315	A86	C3-C2-C1	-3.17	122.83	127.28
34	5	317	LHG	O8-C23-C24	3.17	120.76	111.15
30	A	803	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
30	F	201	CLA	CHD-C1D-ND	-3.17	120.34	124.80
30	11	306	CLA	C1-C2-C3	-3.17	121.01	126.20
37	7	316	A86	C9-C8-C6	-3.17	117.68	126.36
30	14	310	CLA	C1-C2-C3	-3.17	121.64	126.76
39	3	312	DD6	C37-C36-C35	-3.17	108.60	114.42
30	A	810	CLA	CAC-C3C-C4C	3.17	128.91	124.79
30	15	314	CLA	CAC-C3C-C4C	3.17	128.91	124.79
30	1	301	CLA	CHC-C1C-C2C	-3.17	117.95	126.95
37	14	316	A86	C22-C16-C17	-3.17	103.41	108.97
37	10	316	A86	C-C1-C24	3.17	122.92	118.09
38	9	312	KC1	CAA-CBA-CGA	-3.16	110.96	127.05
30	B	825	CLA	O2A-CGA-CBA	3.16	121.48	111.83
30	12	307	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
37	14	315	A86	C24-C1-C2	-3.16	114.03	119.01
30	16	302	CLA	C1-C2-C3	-3.16	121.02	126.20
30	B	827	CLA	CHD-C1D-ND	-3.16	120.35	124.80
30	11	309	CLA	CHC-C1C-C2C	-3.16	117.96	126.95
39	2	317	DD6	C23-C16-C15	3.16	118.58	110.05
38	9	304	KC1	CAA-C2A-C1A	-3.16	110.79	124.64
30	16	305	CLA	CHC-C1C-C2C	-3.16	117.97	126.95
30	A	838	CLA	O2A-CGA-CBA	3.16	121.46	111.83
38	12	313	KC1	CHD-C1D-ND	-3.16	119.31	124.05
30	A	808	CLA	C4B-C3B-C2B	-3.16	103.38	107.30
37	9	313	A86	C9-C8-C6	-3.16	117.71	126.36
38	8	310	KC1	C2C-C1C-NC	3.16	114.36	110.45
30	A	804	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
30	B	830	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
30	16	302	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
30	A	811	CLA	C1-C2-C3	-3.15	121.03	126.20
30	14	309	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
30	A	810	CLA	CMB-C2B-C1B	3.15	130.22	125.42
30	A	807	CLA	CHD-C4C-NC	3.15	129.12	124.23
38	4	308	KC1	CHD-C1D-ND	-3.15	119.32	124.05
38	13	310	KC1	C4B-C3B-C2B	-3.15	104.08	106.81
30	11	310	CLA	C3C-C4C-NC	3.15	114.47	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	831	CLA	C4-C3-C5	3.15	120.70	115.23
37	4	314	A86	C25-C24-C1	-3.15	117.72	126.36
30	A	810	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
38	4	307	KC1	CAC-C3C-C4C	3.15	128.89	124.79
30	A	809	CLA	O2A-CGA-CBA	3.15	121.44	111.83
30	B	839	CLA	CMC-C2C-C1C	3.15	129.96	125.03
30	A	838	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
39	16	313	DD6	C35-C36-C31	-3.15	113.95	120.50
37	14	320	A86	C4-C5-C6	3.15	131.69	127.28
30	A	815	CLA	CAC-C3C-C4C	3.15	128.88	124.79
30	14	303	CLA	CAC-C3C-C4C	3.15	128.88	124.79
37	16	312	A86	C24-C1-C2	3.15	123.96	119.01
30	9	302	CLA	O2A-CGA-CBA	3.15	121.43	111.83
38	5	310	KC1	C4C-C3C-C2C	-3.15	102.31	106.89
30	A	826	CLA	CHC-C1C-C2C	-3.14	118.01	126.95
30	3	310	CLA	CHC-C1C-C2C	-3.14	118.01	126.95
30	7	304	CLA	CHC-C1C-C2C	-3.14	118.01	126.95
30	8	309	CLA	C4B-C3B-C2B	-3.14	103.39	107.30
33	F	204	BCR	C2-C1-C6	3.14	115.00	110.44
30	A	812	CLA	C3B-C4B-NB	3.14	113.34	110.53
30	A	844	CLA	C3B-C4B-NB	3.14	113.34	110.53
30	F	203	CLA	C3B-C4B-NB	3.14	113.34	110.53
30	13	301	CLA	C3B-C4B-NB	3.14	113.34	110.53
30	B	816	CLA	CHD-C4C-NC	3.14	129.10	124.23
38	4	307	KC1	O2D-CGD-O1D	-3.14	117.73	123.85
38	14	306	KC1	CHD-C1D-ND	-3.14	119.33	124.05
37	14	320	A86	C24-C1-C2	3.14	123.95	119.01
38	5	306	KC1	CAA-C2A-C1A	-3.14	110.88	124.64
30	11	310	CLA	CAC-C3C-C4C	3.14	128.87	124.79
30	A	826	CLA	C4A-NA-C1A	-3.14	105.25	106.68
30	5	307	CLA	C4A-NA-C1A	-3.14	105.25	106.68
30	10	308	CLA	O2A-CGA-CBA	3.14	121.41	111.83
30	10	311	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
30	15	304	CLA	C3B-C4B-NB	3.14	113.33	110.53
30	16	307	CLA	C3B-C4B-NB	3.14	113.33	110.53
30	B	801	CLA	CHD-C4C-NC	3.14	129.10	124.23
30	4	302	CLA	CHD-C4C-NC	3.14	129.10	124.23
30	8	305	CLA	CHD-C4C-NC	3.14	129.10	124.23
30	15	302	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
30	B	812	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
30	B	801	CLA	C4A-NA-C1A	-3.14	105.25	106.68
39	9	314	DD6	C25-C24-C1	-3.14	117.76	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	841	CLA	O2A-CGA-CBA	3.14	121.40	111.83
30	13	303	CLA	C3C-C4C-NC	3.14	114.45	110.43
30	16	310	CLA	C3B-C4B-NB	3.14	113.33	110.53
30	5	308	CLA	CAC-C3C-C4C	3.14	128.87	124.79
30	A	825	CLA	CHC-C1C-C2C	-3.13	118.04	126.95
30	A	828	CLA	C1-C2-C3	-3.13	121.06	126.20
37	14	319	A86	C3-C4-C5	-3.13	117.11	123.52
30	7	303	CLA	CMC-C2C-C1C	3.13	129.93	125.03
30	A	843	CLA	CHC-C1C-C2C	-3.13	118.04	126.95
30	2	301	CLA	C3C-C4C-NC	3.13	114.44	110.43
30	12	304	CLA	C3C-C4C-NC	3.13	114.44	110.43
30	B	831	CLA	C4-C3-C5	3.13	120.66	115.23
30	A	825	CLA	C3C-C4C-NC	3.13	114.44	110.43
30	2	310	CLA	CAC-C3C-C4C	3.13	128.86	124.79
30	8	305	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
30	12	312	CLA	C1-C2-C3	-3.13	121.07	126.20
30	B	808	CLA	O2A-CGA-O1A	-3.13	115.80	123.63
30	7	306	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
30	12	321	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
38	8	310	KC1	CMB-C2B-C1B	3.13	130.24	124.73
30	B	826	CLA	C1-C2-C3	-3.13	121.07	126.20
30	10	311	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
37	8	315	A86	C33-C32-C31	3.13	112.25	109.21
30	12	321	CLA	C3C-C4C-NC	3.13	114.44	110.43
30	B	818	CLA	CHD-C4C-NC	3.13	129.08	124.23
38	13	305	KC1	CHD-C1D-ND	-3.13	119.36	124.05
30	B	805	CLA	CHC-C1C-C2C	-3.13	118.07	126.95
30	1	304	CLA	CHD-C4C-NC	3.13	129.08	124.23
30	2	308	CLA	CAC-C3C-C4C	3.13	128.86	124.79
30	16	305	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
30	5	302	CLA	CHD-C4C-NC	3.12	129.07	124.23
38	11	312	KC1	CHD-C1D-ND	-3.12	119.36	124.05
30	2	308	CLA	CHD-C4C-NC	3.12	129.07	124.23
38	2	314	KC1	CED-O2D-CGD	3.12	123.00	115.92
30	A	830	CLA	O2A-CGA-CBA	3.12	121.36	111.83
30	14	303	CLA	C3B-C4B-NB	3.12	113.32	110.53
30	A	836	CLA	C4-C3-C5	3.12	120.65	115.23
38	4	308	KC1	CAC-C3C-C4C	3.12	128.85	124.79
30	15	311	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
30	3	301	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
38	4	307	KC1	CHD-C1D-ND	-3.12	119.37	124.05
30	A	813	CLA	C4C-C3C-C2C	-3.12	102.35	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	2	306	KC1	CAA-C2A-C1A	-3.12	110.97	124.64
38	1	306	KC1	CHD-C1D-ND	-3.12	119.37	124.05
30	2	311	CLA	CAC-C3C-C4C	3.12	128.85	124.79
30	16	303	CLA	CMB-C2B-C1B	3.12	130.17	125.42
30	B	818	CLA	C3C-C4C-NC	3.12	114.42	110.43
30	13	303	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
30	14	305	CLA	CHB-C4A-NA	3.12	128.90	124.40
30	8	302	CLA	CAA-C2A-C3A	-3.12	104.58	113.00
30	2	301	CLA	CAA-C2A-C3A	-3.12	104.58	113.00
30	B	821	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
30	2	307	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
38	6	313	KC1	CBA-CAA-C2A	-3.12	112.95	125.45
30	14	305	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
30	9	309	CLA	CAA-C2A-C3A	-3.11	104.58	113.00
30	15	310	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
33	B	841	BCR	C20-C21-C22	-3.11	122.91	127.28
30	14	313	CLA	C3B-C4B-NB	3.11	113.31	110.53
38	8	307	KC1	CHD-C4C-NC	3.11	129.00	124.31
30	7	303	CLA	C4C-C3C-C2C	-3.11	102.36	106.89
30	B	819	CLA	CHC-C1C-C2C	-3.11	118.10	126.95
30	11	310	CLA	C3B-C4B-NB	3.11	113.31	110.53
30	B	833	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
30	A	802	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
30	13	309	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
30	15	313	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
30	6	316	CLA	C4C-C3C-C2C	-3.11	102.36	106.89
30	B	815	CLA	CMB-C2B-C1B	3.11	130.16	125.42
39	10	313	DD6	O1-C15-C14	-3.11	107.97	116.88
30	A	837	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
30	A	829	CLA	CAC-C3C-C4C	3.11	128.84	124.79
30	A	829	CLA	C4C-C3C-C2C	-3.11	102.36	106.89
38	3	304	KC1	CAA-CBA-CGA	-3.11	111.24	127.05
30	1	305	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
37	9	315	A86	C35-C34-C33	3.11	115.47	109.89
39	11	313	DD6	C15-C14-C13	-3.11	119.42	125.99
30	B	822	CLA	C3C-C4C-NC	3.11	114.41	110.43
37	1	309	A86	C12-C11-C10	-3.11	116.12	123.67
30	15	313	CLA	C3B-C4B-NB	3.11	113.30	110.53
38	5	306	KC1	CAC-C3C-C4C	3.11	128.83	124.79
30	11	310	CLA	CHC-C1C-C2C	-3.11	118.12	126.95
30	A	832	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
30	B	833	CLA	C4-C3-C5	3.11	120.62	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	815	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
39	6	319	DD6	C19-C18-C17	3.10	116.60	110.79
37	2	319	A86	C40-C32-C31	-3.10	107.69	110.47
30	8	304	CLA	C4-C3-C5	3.10	120.62	115.23
37	4	312	A86	C12-C11-C13	3.10	121.03	116.00
30	B	814	CLA	CHD-C1D-ND	-3.10	120.44	124.80
30	B	851	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
39	8	316	DD6	C25-C24-C1	-3.10	117.86	126.36
30	7	306	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
30	3	303	CLA	CHC-C1C-C2C	-3.10	118.13	126.95
30	B	803	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
33	J	103	BCR	C27-C26-C25	3.10	126.89	122.70
37	7	316	A86	C7-C6-C8	3.10	122.82	118.09
34	2	320	LHG	O8-C23-C24	3.10	120.56	111.15
30	B	816	CLA	CAC-C3C-C4C	3.10	128.82	124.79
37	7	315	A86	C21-C20-C15	-3.10	113.35	123.35
39	7	318	DD6	C37-C36-C35	-3.10	108.73	114.42
37	11	315	A86	C26-C25-C24	-3.10	114.23	123.20
37	7	319	A86	C8-C6-C5	3.10	123.88	119.01
30	6	314	CLA	C3C-C4C-NC	3.10	114.40	110.43
30	6	307	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
30	1	305	CLA	CAC-C3C-C4C	3.10	128.82	124.79
38	8	306	KC1	CBC-CAC-C3C	-3.09	104.03	112.42
30	15	303	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
38	1	306	KC1	CAB-C3B-C4B	3.09	132.21	124.82
30	2	303	CLA	C3B-C4B-NB	3.09	113.29	110.53
30	B	804	CLA	CMC-C2C-C1C	3.09	129.87	125.03
39	7	302	DD6	C37-C36-C35	-3.09	108.73	114.42
37	5	316	A86	C21-C20-C15	-3.09	113.36	123.35
30	5	311	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
30	B	828	CLA	CHC-C1C-C2C	-3.09	118.16	126.95
30	B	822	CLA	CMA-C3A-C4A	-3.09	103.46	111.77
30	8	302	CLA	CBC-CAC-C3C	-3.09	104.04	112.42
30	B	838	CLA	O2A-CGA-CBA	3.09	121.26	111.83
30	A	826	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
38	9	312	KC1	CAC-C3C-C4C	3.09	128.81	124.79
30	A	829	CLA	C1-C2-C3	-3.09	121.13	126.20
30	B	804	CLA	O2A-CGA-CBA	3.09	121.26	111.83
30	B	828	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
38	3	311	KC1	C4C-C3C-C2C	-3.09	102.39	106.89
38	8	313	KC1	CBA-CAA-C2A	-3.09	113.06	125.45
30	3	307	CLA	C4B-C3B-C2B	-3.09	103.46	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	836	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
30	7	310	CLA	CMB-C2B-C1B	3.09	130.12	125.42
30	1	302	CLA	C3B-C4B-NB	3.09	113.29	110.53
30	12	307	CLA	CHD-C4C-NC	3.09	129.02	124.23
30	11	308	CLA	CHC-C1C-C2C	-3.09	118.18	126.95
30	B	802	CLA	C3B-C4B-NB	3.09	113.28	110.53
30	9	302	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
30	B	823	CLA	CHC-C1C-C2C	-3.09	118.18	126.95
30	A	842	CLA	O2A-CGA-CBA	3.09	121.24	111.83
30	8	301	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
30	B	818	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
30	14	303	CLA	CHC-C1C-C2C	-3.08	118.18	126.95
38	11	311	KC1	CAC-C3C-C4C	3.08	128.80	124.79
38	8	314	KC1	C4C-C3C-C2C	-3.08	102.40	106.89
33	A	849	BCR	C27-C26-C25	3.08	126.87	122.70
30	11	306	CLA	CAC-C3C-C4C	3.08	128.80	124.79
30	9	302	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
30	10	303	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
30	1	307	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
38	9	310	KC1	CAA-CBA-CGA	-3.08	111.39	127.05
30	B	808	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
30	1	302	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
38	16	304	KC1	C4C-C3C-C2C	-3.08	102.41	106.89
30	7	303	CLA	CAA-C2A-C3A	-3.08	104.68	113.00
30	A	822	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
30	12	312	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
30	14	304	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
30	B	831	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
30	16	309	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
30	A	808	CLA	C3B-C4B-NB	3.08	113.28	110.53
30	2	310	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
30	3	307	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
30	13	307	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
39	3	313	DD6	C25-C24-C1	-3.08	117.93	126.36
30	12	303	CLA	C4B-C3B-C2B	-3.08	103.48	107.30
30	12	302	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
37	4	317	A86	C25-C24-C1	-3.07	117.93	126.36
38	8	311	KC1	CAC-C3C-C4C	3.07	128.79	124.79
37	9	313	A86	C36-C31-C32	-3.07	116.65	119.70
39	7	302	DD6	C14-C13-C11	3.07	130.30	125.53
30	B	833	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
30	1	302	CLA	O2D-CGD-O1D	-3.07	117.87	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	309	CLA	CAC-C3C-C4C	3.07	128.79	124.79
30	13	303	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
39	5	314	DD6	C33-C32-C31	3.07	115.54	109.49
37	12	316	A86	C9-C10-C11	-3.07	117.96	126.64
30	15	310	CLA	CAC-C3C-C4C	3.07	128.79	124.79
38	2	312	KC1	C4C-C3C-C2C	-3.07	102.42	106.89
30	14	304	CLA	C3B-C4B-NB	3.07	113.27	110.53
30	13	301	CLA	CHD-C4C-NC	3.07	128.99	124.23
30	12	307	CLA	CMC-C2C-C1C	3.07	129.83	125.03
30	B	819	CLA	C3D-C2D-C1D	-3.07	101.64	105.83
38	14	311	KC1	CMC-C2C-C1C	3.07	129.83	125.03
30	11	309	CLA	C1-C2-C3	-3.07	121.17	126.20
30	3	302	CLA	CHD-C4C-NC	3.07	128.99	124.23
38	8	311	KC1	CBA-CAA-C2A	-3.07	113.14	125.45
38	16	311	KC1	C1A-NA-C4A	-3.07	105.28	106.68
30	9	308	CLA	CMC-C2C-C1C	3.07	129.83	125.03
30	15	308	CLA	C1C-C2C-C3C	-3.07	103.75	106.98
30	7	307	CLA	C1C-C2C-C3C	-3.07	103.75	106.98
30	7	304	CLA	C4-C3-C5	3.07	120.55	115.23
30	10	303	CLA	CHD-C4C-NC	3.07	128.99	124.23
30	16	306	CLA	C1-C2-C3	-3.07	121.17	126.20
37	15	322	A86	C3-C4-C5	3.07	129.79	123.52
38	13	305	KC1	C4C-C3C-C2C	-3.07	102.43	106.89
30	7	311	CLA	C4B-C3B-C2B	-3.06	103.49	107.30
30	L	203	CLA	C4B-C3B-C2B	-3.06	103.49	107.30
30	B	832	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
30	12	303	CLA	C4C-C3C-C2C	-3.06	102.43	106.89
30	B	804	CLA	CAC-C3C-C4C	3.06	128.78	124.79
30	7	305	CLA	CAA-C2A-C3A	-3.06	104.72	113.00
30	12	306	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
37	2u	203	A86	C12-C11-C10	-3.06	116.23	123.67
38	14	311	KC1	CHD-C4C-NC	3.06	128.92	124.31
30	15	304	CLA	CHC-C1C-C2C	-3.06	118.25	126.95
35	9	317	LMT	C2'-C3'-C4'	3.06	116.63	109.68
30	16	307	CLA	CHC-C1C-C2C	-3.06	118.25	126.95
30	B	832	CLA	C3B-C4B-NB	3.06	113.26	110.53
30	14	305	CLA	C3B-C4B-NB	3.06	113.26	110.53
30	7	307	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
30	4	302	CLA	CAC-C3C-C4C	3.06	128.77	124.79
38	5	310	KC1	CHD-C1D-ND	-3.06	119.46	124.05
30	15	310	CLA	CHC-C1C-C2C	-3.06	118.25	126.95
30	16	303	CLA	CHD-C4C-NC	3.06	128.97	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	314	A86	C4-C3-C2	-3.06	117.26	123.52
38	8	307	KC1	C4B-C3B-C2B	-3.06	104.16	106.81
30	15	314	CLA	C3B-C4B-NB	3.06	113.26	110.53
30	16	303	CLA	C3B-C4B-NB	3.06	113.26	110.53
30	10	304	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
30	5	309	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
30	14	302	CLA	C3C-C4C-NC	3.06	114.35	110.43
30	6	304	CLA	C3C-C4C-NC	3.06	114.35	110.43
30	10	304	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
38	2	306	KC1	CAC-C3C-C4C	3.06	128.77	124.79
30	B	808	CLA	CMB-C2B-C1B	3.06	130.07	125.42
30	B	814	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
30	A	833	CLA	C3B-C4B-NB	3.06	113.26	110.53
37	11	301	A86	C12-C11-C10	-3.06	116.24	123.67
30	A	817	CLA	C3C-C4C-NC	3.06	114.34	110.43
30	A	840	CLA	C4B-C3B-C2B	-3.05	103.50	107.30
30	A	841	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
30	9	307	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
38	16	304	KC1	CAA-CBA-CGA	-3.05	111.52	127.05
30	6	306	CLA	C3B-C4B-NB	3.05	113.25	110.53
30	1	302	CLA	CHD-C4C-NC	3.05	128.96	124.23
38	5	305	KC1	CMB-C2B-C1B	3.05	130.10	124.73
30	A	807	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
30	A	824	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
30	2	307	CLA	C3B-C4B-NB	3.05	113.25	110.53
30	12	303	CLA	CHC-C1C-C2C	-3.05	118.28	126.95
30	B	817	CLA	CHD-C4C-NC	3.05	128.96	124.23
30	10	308	CLA	C3C-C4C-NC	3.05	114.34	110.43
37	4	317	A86	C4-C5-C6	-3.05	123.00	127.28
30	6	304	CLA	CHD-C4C-NC	3.05	128.96	124.23
30	10	303	CLA	C3B-C4B-NB	3.05	113.25	110.53
30	7	309	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
30	B	827	CLA	C1-C2-C3	-3.05	121.20	126.20
30	B	832	CLA	CMA-C3A-C2A	-3.05	102.19	113.98
30	2u	202	CLA	CHD-C4C-NC	3.05	128.96	124.23
38	5	310	KC1	CAA-CBA-CGA	-3.05	111.54	127.05
30	9	301	CLA	C1C-C2C-C3C	-3.05	103.77	106.98
30	B	805	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
37	3	314	A86	C36-C31-C32	-3.05	116.67	119.70
30	B	801	CLA	CAC-C3C-C4C	3.05	128.76	124.79
30	8	301	CLA	CAC-C3C-C4C	3.05	128.76	124.79
38	1	306	KC1	CAA-C2A-C1A	-3.05	111.28	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	309	KC1	CHD-C4C-NC	3.05	128.90	124.31
30	9	307	CLA	CHD-C4C-NC	3.05	128.96	124.23
30	14	304	CLA	CAC-C3C-C4C	3.05	128.75	124.79
37	15	316	A86	C21-C20-C15	-3.05	113.52	123.35
38	11	312	KC1	CBA-CAA-C2A	-3.05	113.23	125.45
30	15	309	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
30	11	304	CLA	C1-C2-C3	-3.05	121.21	126.20
30	A	812	CLA	CMB-C2B-C1B	3.05	130.06	125.42
30	A	833	CLA	CAA-C2A-C3A	-3.05	104.77	113.00
30	6	315	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
38	8	311	KC1	C1A-NA-C4A	-3.04	105.29	106.68
30	2	303	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
30	A	821	CLA	CHD-C1D-ND	-3.04	120.52	124.80
30	5	303	CLA	C3B-C4B-NB	3.04	113.25	110.53
30	B	803	CLA	CHB-C4A-NA	3.04	128.79	124.40
30	A	808	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
30	A	817	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
30	12	302	CLA	C4-C3-C5	3.04	120.50	115.23
30	A	840	CLA	CHD-C4C-NC	3.04	128.94	124.23
30	2	311	CLA	O2A-CGA-CBA	3.04	121.10	111.83
30	B	837	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
30	10	309	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
30	B	820	CLA	CHD-C4C-NC	3.04	128.94	124.23
30	16	309	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
38	10	310	KC1	CAC-C3C-C4C	3.04	128.74	124.79
30	A	811	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
30	3	305	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
30	5	309	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
30	6	304	CLA	CMC-C2C-C1C	3.04	129.78	125.03
30	7	307	CLA	CAC-C3C-C4C	3.04	128.74	124.79
30	11	309	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
30	8	301	CLA	C3B-C4B-NB	3.04	113.24	110.53
30	A	832	CLA	O2A-CGA-CBA	3.04	121.10	111.83
30	B	831	CLA	CMB-C2B-C1B	3.04	130.04	125.42
30	4	311	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
34	6	322	LHG	O8-C23-C24	3.04	120.37	111.15
38	6	313	KC1	CHD-C1D-ND	-3.04	119.49	124.05
30	8	302	CLA	CHD-C4C-NC	3.04	128.94	124.23
30	14	305	CLA	C1-C2-C3	-3.04	121.85	126.76
30	14	302	CLA	CHD-C4C-NC	3.04	128.94	124.23
38	9	310	KC1	C4B-C3B-C2B	-3.04	104.18	106.81
30	8	303	CLA	CHC-C1C-C2C	-3.04	118.32	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	306	CLA	C1-O2A-CGA	3.04	124.00	116.65
30	B	818	CLA	O2A-CGA-CBA	3.03	121.09	111.83
37	4	312	A86	C26-C25-C24	-3.03	114.41	123.20
30	4	309	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
30	A	808	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
30	16	306	CLA	C3B-C4B-NB	3.03	113.24	110.53
30	10	311	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
30	5	308	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
30	B	814	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
38	7	313	KC1	CHD-C4C-NC	3.03	128.88	124.31
30	A	812	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
30	A	814	CLA	C1-O2A-CGA	3.03	123.98	116.65
30	A	844	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
37	8	315	A86	C-C1-C24	3.03	122.72	118.09
30	2	305	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
30	7	305	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
30	A	835	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
38	11	305	KC1	CAA-C2A-C1A	-3.03	111.37	124.64
30	A	802	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
30	15	312	CLA	CHD-C4C-NC	3.03	128.93	124.23
37	14	319	A86	C10-C9-C8	-3.03	114.43	123.20
30	B	835	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
38	6	312	KC1	CBA-CAA-C2A	-3.03	113.31	125.45
30	6	306	CLA	C4C-C3C-C2C	-3.03	102.49	106.89
30	4	311	CLA	O2A-CGA-CBA	3.03	121.06	111.83
35	15	301	LMT	O1B-C4'-C3'	3.03	114.92	107.23
39	6	321	DD6	C15-C14-C13	-3.03	119.59	125.99
30	9	301	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
30	13	307	CLA	CAC-C3C-C4C	3.03	128.73	124.79
30	A	829	CLA	CHD-C4C-NC	3.03	128.92	124.23
30	16	303	CLA	CBA-CAA-C2A	3.03	122.80	113.79
29	A	801	CL0	O2D-CGD-O1D	-3.02	117.96	123.85
30	16	309	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
39	6	318	DD6	C35-C36-C31	-3.02	114.20	120.50
38	13	310	KC1	CBA-CAA-C2A	-3.02	113.31	125.45
37	12	314	A86	C10-C9-C8	-3.02	114.44	123.20
39	8	317	DD6	C10-C9-C8	-3.02	114.44	123.20
30	1	303	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
30	A	834	CLA	C3B-C4B-NB	3.02	113.23	110.53
30	3	302	CLA	C3B-C4B-NB	3.02	113.23	110.53
30	16	307	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
30	B	838	CLA	CAA-C2A-C3A	-3.02	104.83	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	307	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
30	2	309	CLA	C3B-C4B-NB	3.02	113.23	110.53
30	15	305	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
30	15	302	CLA	CAC-C3C-C4C	3.02	128.72	124.79
30	A	839	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
30	14	312	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
30	A	823	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
30	A	837	CLA	C3B-C4B-NB	3.02	113.23	110.53
30	5	308	CLA	O2A-CGA-CBA	3.02	121.04	111.83
30	A	833	CLA	C1-C2-C3	-3.02	121.25	126.20
37	2u	205	A86	C12-C11-C10	-3.02	116.33	123.67
39	13	314	DD6	C21-C20-C15	-3.02	117.33	122.30
38	9	312	KC1	C4C-C3C-C2C	-3.02	102.50	106.89
30	9	302	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
37	14	318	A86	C25-C24-C1	-3.02	118.09	126.36
37	14	315	A86	C26-C25-C24	-3.02	114.46	123.20
37	7	316	A86	C3-C4-C5	-3.02	117.35	123.52
30	11	306	CLA	CHD-C4C-NC	3.02	128.91	124.23
30	A	819	CLA	C1C-C2C-C3C	-3.02	103.81	106.98
30	A	818	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
30	15	306	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
38	14	306	KC1	CAA-CBA-CGA	-3.02	111.72	127.05
37	7	319	A86	C3-C4-C5	-3.02	117.35	123.52
30	F	203	CLA	CHD-C4C-NC	3.01	128.91	124.23
30	8	308	CLA	CHD-C4C-NC	3.01	128.91	124.23
30	A	839	CLA	C4C-C3C-C2C	-3.01	102.50	106.89
30	15	307	CLA	C1-C2-C3	-3.01	121.89	126.76
30	9	308	CLA	C4C-C3C-C2C	-3.01	102.50	106.89
30	4	306	CLA	CHD-C4C-NC	3.01	128.90	124.23
30	6	306	CLA	CHD-C4C-NC	3.01	128.90	124.23
30	10	308	CLA	CAA-C2A-C3A	-3.01	104.86	113.00
30	15	305	CLA	CAA-C2A-C3A	-3.01	104.86	113.00
38	9	312	KC1	CMB-C2B-C1B	3.01	130.03	124.73
30	4	303	CLA	C3B-C4B-NB	3.01	113.22	110.53
30	14	310	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
37	4	312	A86	C3-C2-C1	-3.01	123.06	127.28
30	B	826	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
30	A	820	CLA	C2A-C3A-C4A	-3.01	97.01	101.87
30	B	827	CLA	CMB-C2B-C1B	3.01	130.00	125.42
30	6	316	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
30	12	308	CLA	CAA-C2A-C3A	-3.01	104.87	113.00
30	6	304	CLA	C4B-C3B-C2B	-3.01	103.56	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	303	CLA	C1-C2-C3	-3.01	121.27	126.20
30	3	301	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
30	B	831	CLA	CHD-C4C-NC	3.01	128.90	124.23
37	5	315	A86	C3-C2-C1	-3.01	123.06	127.28
39	2	315	DD6	C21-C20-C15	-3.01	117.35	122.30
38	5	305	KC1	CAC-C3C-C4C	3.01	128.70	124.79
30	A	825	CLA	O2A-CGA-CBA	3.01	121.00	111.83
30	B	802	CLA	CMC-C2C-C1C	3.01	129.73	125.03
33	A	849	BCR	C15-C14-C13	-3.01	123.06	127.28
30	1	303	CLA	CHD-C4C-NC	3.01	128.89	124.23
30	11	309	CLA	C4C-C3C-C2C	-3.01	102.52	106.89
30	B	830	CLA	C6-C7-C8	-3.00	105.98	115.97
39	3	316	DD6	O1-C20-C21	-3.00	111.69	115.05
30	13	304	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
30	6	317	CLA	CHC-C1C-C2C	-3.00	118.41	126.95
30	A	842	CLA	C1-C2-C3	-3.00	121.28	126.20
30	B	833	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
30	11	306	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
30	9	309	CLA	O2A-CGA-CBA	3.00	120.99	111.83
30	B	815	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
38	10	306	KC1	CBA-CAA-C2A	-3.00	113.41	125.45
30	A	823	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
30	B	812	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
38	6	308	KC1	CHD-C4C-NC	3.00	128.83	124.31
33	A	849	BCR	C40-C30-C25	3.00	114.95	110.24
30	8	303	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
30	B	804	CLA	C4A-NA-C1A	-3.00	105.31	106.68
30	B	808	CLA	C4A-NA-C1A	-3.00	105.31	106.68
30	14	312	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
30	4	301	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
30	A	842	CLA	CHD-C4C-NC	3.00	128.88	124.23
37	9	316	A86	C21-C20-C15	-3.00	113.67	123.35
39	10	314	DD6	C35-C36-C31	-3.00	114.26	120.50
30	A	821	CLA	CAC-C3C-C4C	3.00	128.69	124.79
37	2	319	A86	C10-C9-C8	-3.00	114.51	123.20
30	10	311	CLA	CHD-C4C-NC	3.00	128.88	124.23
38	8	312	KC1	CMB-C2B-C1B	3.00	130.01	124.73
30	16	310	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
30	B	825	CLA	CAA-C2A-C3A	-3.00	104.90	113.00
38	1	308	KC1	C4C-C3C-C2C	-3.00	102.53	106.89
30	A	802	CLA	CHB-C1B-C2B	-3.00	118.72	127.43
37	8	318	A86	C12-C11-C13	3.00	120.86	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	301	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
30	12	308	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
30	A	822	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
30	6	314	CLA	C4-C3-C5	3.00	120.43	115.23
30	A	806	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
30	A	811	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
30	A	817	CLA	CBC-CAC-C3C	-3.00	104.30	112.42
30	2u	202	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
30	2	309	CLA	CAA-C2A-C3A	-3.00	104.91	113.00
30	B	823	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
30	7	305	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
37	5	301	A86	C26-C25-C24	-2.99	114.52	123.20
30	B	802	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
30	3	310	CLA	C3C-C4C-NC	2.99	114.27	110.43
30	3	305	CLA	CHD-C4C-NC	2.99	128.87	124.23
30	4	303	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
30	13	304	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
30	A	819	CLA	CHD-C4C-NC	2.99	128.87	124.23
30	2u	202	CLA	C3B-C4B-NB	2.99	113.20	110.53
30	7	311	CLA	C3B-C4B-NB	2.99	113.20	110.53
30	A	828	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
30	8	305	CLA	C4A-NA-C1A	-2.99	105.31	106.68
38	11	312	KC1	CMB-C2B-C1B	2.99	130.00	124.73
30	B	802	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
30	12	306	CLA	CBC-CAC-C3C	-2.99	104.31	112.42
30	B	839	CLA	CMB-C2B-C1B	2.99	129.97	125.42
30	B	832	CLA	CHB-C4A-NA	2.99	128.72	124.40
38	2	314	KC1	C4C-C3C-C2C	-2.99	102.54	106.89
39	6	319	DD6	C33-C32-C31	2.99	115.38	109.49
30	A	834	CLA	CAA-C2A-C3A	-2.99	104.92	113.00
30	F	202	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
30	3	303	CLA	C1-C2-C3	-2.99	121.30	126.20
30	B	835	CLA	O2A-CGA-CBA	2.99	120.95	111.83
30	14	304	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
30	B	820	CLA	C1C-C2C-C3C	-2.99	103.84	106.98
37	4	317	A86	C10-C9-C8	-2.99	114.54	123.20
37	11	315	A86	C4-C3-C2	-2.99	117.40	123.52
30	B	832	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
30	12	306	CLA	C1-C2-C3	-2.99	121.30	126.20
39	5	314	DD6	C21-C20-C15	-2.99	117.39	122.30
33	B	845	BCR	C27-C26-C25	2.99	126.74	122.70
30	5	307	CLA	CMC-C2C-C1C	2.99	129.70	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	808	CLA	CBC-CAC-C3C	-2.99	104.32	112.42
30	B	836	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
38	13	306	KC1	C1C-C2C-C3C	-2.99	103.84	106.98
38	4	308	KC1	C2A-C1A-NA	2.99	114.13	109.34
30	B	834	CLA	CHD-C4C-NC	2.99	128.86	124.23
30	J	101	CLA	CHC-C1C-C2C	-2.99	118.46	126.95
30	9	307	CLA	C3B-C4B-NB	2.99	113.19	110.53
30	B	807	CLA	CAA-C2A-C3A	-2.99	104.93	113.00
38	8	313	KC1	CHD-C4C-NC	2.99	128.81	124.31
30	10	311	CLA	CAC-C3C-C4C	2.98	128.67	124.79
38	2	312	KC1	CBA-CAA-C2A	-2.98	113.47	125.45
39	2	315	DD6	C3-C4-C5	-2.98	117.41	123.52
30	A	819	CLA	C1-C2-C3	-2.98	121.31	126.20
30	6	305	CLA	O2A-CGA-CBA	2.98	120.93	111.83
30	15	311	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
30	F	201	CLA	C1-C2-C3	-2.98	121.31	126.20
37	2u	205	A86	C40-C32-C31	-2.98	107.80	110.47
30	5	304	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
30	2	305	CLA	C1-C2-C3	-2.98	121.31	126.20
30	13	301	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
38	1	308	KC1	CHD-C1D-ND	-2.98	119.58	124.05
37	14	301	A86	C10-C9-C8	-2.98	114.56	123.20
30	6	305	CLA	C1-C2-C3	-2.98	121.31	126.20
30	12	302	CLA	CAC-C3C-C4C	2.98	128.67	124.79
30	1	301	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
30	12	306	CLA	C4A-NA-C1A	-2.98	105.32	106.68
30	16	310	CLA	CMB-C2B-C1B	2.98	129.96	125.42
30	A	805	CLA	CBC-CAC-C3C	-2.98	104.34	112.42
30	4	301	CLA	CAA-C2A-C3A	-2.98	104.95	113.00
30	L	203	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
30	2	307	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
38	7	308	KC1	C4C-C3C-C2C	-2.98	102.56	106.89
37	7	319	A86	C7-C6-C5	-2.98	117.99	122.82
30	15	302	CLA	CHD-C4C-NC	2.98	128.85	124.23
30	15	312	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
30	4	304	CLA	CHD-C4C-NC	2.98	128.85	124.23
30	A	804	CLA	C3B-C4B-NB	2.98	113.19	110.53
30	12	308	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
38	14	311	KC1	C4C-C3C-C2C	-2.98	102.56	106.89
30	8	305	CLA	OBD-CAD-C3D	-2.98	121.46	128.42
30	10	305	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
30	2	310	CLA	C4C-C3C-C2C	-2.98	102.56	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	2	306	KC1	O2D-CGD-O1D	-2.98	118.06	123.85
30	A	817	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
30	3	305	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
30	16	303	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
37	16	314	A86	C35-C34-C33	2.97	115.23	109.89
30	12	306	CLA	CAA-C2A-C3A	-2.97	104.96	113.00
30	14	309	CLA	CAC-C3C-C4C	2.97	128.66	124.79
30	16	307	CLA	CAC-C3C-C4C	2.97	128.66	124.79
38	2	312	KC1	CHD-C1D-ND	-2.97	119.59	124.05
30	A	823	CLA	CHD-C4C-NC	2.97	128.84	124.23
38	8	314	KC1	CHB-C4A-NA	2.97	128.84	124.23
30	B	816	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
30	B	829	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
30	6	314	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
30	B	831	CLA	O1D-CGD-CBD	-2.97	118.65	124.52
30	14	303	CLA	C1-C2-C3	-2.97	121.33	126.20
30	9	302	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
38	16	311	KC1	C4C-C3C-C2C	-2.97	102.56	106.89
30	A	804	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
37	15	315	A86	C4-C5-C6	2.97	131.45	127.28
39	15	318	DD6	C33-C32-C31	2.97	115.34	109.49
30	A	805	CLA	CHD-C4C-NC	2.97	128.84	124.23
37	15	315	A86	C21-C20-C15	-2.97	113.76	123.35
30	A	813	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
30	5	307	CLA	CHD-C4C-NC	2.97	128.84	124.23
30	B	835	CLA	CHD-C4C-NC	2.97	128.84	124.23
30	12	312	CLA	CHD-C4C-NC	2.97	128.84	124.23
36	7	320	LMG	C1-C2-C3	-2.97	103.76	110.01
30	A	818	CLA	C1-C2-C3	-2.97	121.33	126.20
30	12	306	CLA	CHB-C4A-NA	2.97	128.69	124.40
30	J	101	CLA	CAC-C3C-C4C	2.97	128.65	124.79
30	A	832	CLA	CAC-C3C-C4C	2.97	128.65	124.79
30	B	811	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
30	B	820	CLA	CAC-C3C-C2C	2.97	133.01	127.56
30	10	309	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
30	9	306	CLA	CAC-C3C-C4C	2.97	128.65	124.79
30	F	201	CLA	O2A-CGA-CBA	2.97	120.88	111.83
37	12	314	A86	C26-C25-C24	-2.96	114.61	123.20
30	B	801	CLA	C1C-C2C-C3C	-2.96	103.86	106.98
30	2	313	CLA	CHC-C1C-C2C	-2.96	118.52	126.95
30	B	851	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
30	14	312	CLA	C4C-C3C-C2C	-2.96	102.58	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	304	CLA	CAC-C3C-C4C	2.96	128.65	124.79
30	15	308	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
30	B	836	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
30	8	304	CLA	C3B-C4B-NB	2.96	113.17	110.53
30	12	302	CLA	C1-C2-C3	-2.96	121.34	126.20
30	6	317	CLA	CHD-C4C-NC	2.96	128.82	124.23
30	A	836	CLA	O2A-CGA-CBA	2.96	120.86	111.83
30	A	810	CLA	C1-C2-C3	-2.96	121.35	126.20
38	12	305	KC1	CAC-C3C-C4C	2.96	128.64	124.79
30	A	833	CLA	CMB-C2B-C1B	2.96	129.93	125.42
30	L	203	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
30	B	805	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
38	10	312	KC1	CAA-C2A-C1A	-2.96	111.67	124.64
30	16	302	CLA	CHD-C4C-NC	2.96	128.82	124.23
30	6	316	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
30	10	308	CLA	CHD-C4C-NC	2.96	128.82	124.23
30	L	203	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
30	6	307	CLA	CAC-C3C-C4C	2.96	128.64	124.79
30	4	302	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
30	A	824	CLA	CHD-C4C-NC	2.96	128.82	124.23
30	9	305	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
30	12	321	CLA	CAC-C3C-C4C	2.96	128.64	124.79
38	3	311	KC1	CAC-C3C-C4C	2.96	128.64	124.79
30	11	310	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
38	9	310	KC1	C4C-C3C-C2C	-2.96	102.59	106.89
30	6	306	CLA	C4A-NA-C1A	-2.96	105.33	106.68
30	8	304	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
30	B	835	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
38	10	310	KC1	C4C-C3C-C2C	-2.96	102.59	106.89
30	12	302	CLA	CMC-C2C-C1C	2.96	129.65	125.03
30	7	307	CLA	O2A-CGA-CBA	2.96	120.85	111.83
30	A	824	CLA	C3B-C4B-NB	2.96	113.17	110.53
30	5	311	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
38	11	311	KC1	C4C-C3C-C2C	-2.96	102.59	106.89
30	2	313	CLA	CAC-C3C-C4C	2.95	128.63	124.79
30	A	824	CLA	O2A-CGA-CBA	2.95	120.84	111.83
38	4	307	KC1	CAA-CBA-CGA	-2.95	112.03	127.05
30	B	818	CLA	CHC-C1C-C2C	-2.95	118.55	126.95
30	10	307	CLA	CAC-C3C-C4C	2.95	128.63	124.79
30	2	304	CLA	CHC-C1C-C2C	-2.95	118.55	126.95
30	A	808	CLA	CAC-C3C-C4C	2.95	128.63	124.79
30	13	307	CLA	O2D-CGD-O1D	-2.95	118.10	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	304	CLA	C3B-C4B-NB	2.95	113.17	110.53
38	5	306	KC1	C4C-C3C-C2C	-2.95	102.59	106.89
37	2	319	A86	C21-C20-C15	-2.95	113.82	123.35
30	B	837	CLA	C1-C2-C3	-2.95	121.36	126.20
30	A	836	CLA	CAA-C2A-C3A	-2.95	105.03	113.00
37	2u	203	A86	C36-C31-C32	-2.95	116.77	119.70
38	13	311	KC1	CHD-C4C-NC	2.95	128.75	124.31
30	6	310	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
30	A	809	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
30	9	305	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
30	15	303	CLA	CAA-C2A-C3A	-2.95	105.03	113.00
30	A	835	CLA	C1-C2-C3	-2.95	121.36	126.20
30	6	315	CLA	CHD-C4C-NC	2.95	128.80	124.23
30	12	304	CLA	CHD-C4C-NC	2.95	128.80	124.23
30	10	303	CLA	CBC-CAC-C3C	-2.95	104.43	112.42
38	5	310	KC1	CAC-C3C-C4C	2.95	128.63	124.79
30	A	814	CLA	CHB-C4A-NA	2.95	128.65	124.40
30	B	824	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
30	14	302	CLA	O2A-CGA-CBA	2.95	120.82	111.83
30	A	818	CLA	O2A-CGA-CBA	2.95	120.82	111.83
37	14	314	A86	C12-C11-C10	-2.95	116.51	123.67
30	B	834	CLA	C1-C2-C3	-2.95	121.37	126.20
30	A	834	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
30	A	835	CLA	O2A-CGA-CBA	2.95	120.82	111.83
35	9	317	LMT	O5'-C1'-C2'	2.95	116.42	110.37
38	8	306	KC1	CHD-C4C-NC	2.95	128.75	124.31
38	13	306	KC1	CHD-C4C-NC	2.95	128.75	124.31
30	2	309	CLA	CHC-C1C-C2C	-2.95	118.58	126.95
38	9	304	KC1	CHD-C4C-NC	2.95	128.75	124.31
33	A	850	BCR	C24-C23-C22	-2.95	121.88	126.23
30	16	308	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
30	10	311	CLA	CHC-C1C-C2C	-2.94	118.58	126.95
30	12	304	CLA	C1-C2-C3	-2.94	121.37	126.20
30	12	312	CLA	CBC-CAC-C3C	-2.94	104.44	112.42
30	B	832	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
30	5	311	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
30	3	305	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
30	A	840	CLA	C3B-C4B-NB	2.94	113.16	110.53
30	2	311	CLA	C3B-C4B-NB	2.94	113.16	110.53
30	3	306	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
30	8	309	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
30	9	308	CLA	CHD-C4C-NC	2.94	128.79	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	307	CLA	CMC-C2C-C1C	2.94	129.63	125.03
30	1	304	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
30	A	840	CLA	CMB-C2B-C1B	2.94	129.90	125.42
30	13	302	CLA	CHD-C4C-NC	2.94	128.79	124.23
30	6	309	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
30	3	310	CLA	CHD-C4C-NC	2.94	128.79	124.23
30	B	811	CLA	C1-C2-C3	-2.94	121.38	126.20
37	15	320	A86	C36-C31-C32	-2.94	116.78	119.70
39	6	303	DD6	O1-C20-C21	-2.94	111.76	115.05
33	M	101	BCR	C15-C16-C17	-2.94	117.50	123.52
30	A	812	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
30	B	822	CLA	CAC-C3C-C4C	2.94	128.61	124.79
30	16	302	CLA	CAC-C3C-C4C	2.94	128.61	124.79
39	5	314	DD6	C10-C9-C8	-2.94	114.68	123.20
30	A	833	CLA	C4-C3-C5	2.94	120.33	115.23
30	7	311	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
30	B	839	CLA	C1-C2-C3	-2.94	121.38	126.20
30	B	831	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
30	3	306	CLA	C1-C2-C3	-2.94	121.39	126.20
39	15	318	DD6	C25-C24-C1	-2.94	118.31	126.36
30	A	819	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
30	4	311	CLA	CAC-C3C-C4C	2.94	128.61	124.79
38	8	313	KC1	C2C-C1C-NC	2.94	114.08	110.45
30	A	807	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
30	B	807	CLA	CMA-C3A-C2A	-2.94	102.63	113.98
30	A	834	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
39	15	318	DD6	C14-C13-C11	-2.94	120.97	125.53
30	2	313	CLA	C3B-C4B-NB	2.94	113.15	110.53
30	3	309	CLA	CHD-C4C-NC	2.94	128.78	124.23
30	13	307	CLA	C3B-C4B-NB	2.93	113.15	110.53
30	16	302	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
38	6	313	KC1	CHD-C4C-NC	2.93	128.73	124.31
30	16	301	CLA	C3B-C4B-NB	2.93	113.15	110.53
30	13	309	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
30	16	308	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
30	A	838	CLA	CHD-C4C-NC	2.93	128.78	124.23
30	1	301	CLA	CAC-C3C-C4C	2.93	128.61	124.79
30	A	833	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
38	13	310	KC1	C4C-C3C-C2C	-2.93	102.62	106.89
38	12	313	KC1	CMB-C2B-C1B	2.93	129.89	124.73
30	A	823	CLA	C3C-C4C-NC	2.93	114.19	110.43
38	12	311	KC1	C4C-C3C-C2C	-2.93	102.62	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	304	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
37	4	315	A86	C34-O4-C38	-2.93	112.67	117.85
30	B	815	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
30	A	804	CLA	CHD-C4C-NC	2.93	128.78	124.23
30	16	310	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
30	12	307	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
38	13	310	KC1	CMB-C2B-C1B	2.93	129.89	124.73
30	B	816	CLA	C4-C3-C5	2.93	120.31	115.23
30	9	307	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
36	8	320	LMG	O6-C1-O1	-2.93	103.12	110.04
30	5	303	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
37	14	314	A86	C21-C20-C15	-2.93	113.90	123.35
38	5	305	KC1	CBA-CAA-C2A	-2.93	113.70	125.45
30	15	313	CLA	CHD-C4C-NC	2.93	128.77	124.23
30	4	306	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
30	16	302	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
30	A	841	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
36	8	320	LMG	O7-C10-O9	-2.93	116.86	123.70
30	A	811	CLA	CHD-C4C-NC	2.93	128.77	124.23
30	B	811	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
30	13	302	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
30	B	828	CLA	CMD-C2D-C3D	-2.93	120.98	127.69
30	13	303	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
30	A	815	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
30	12	302	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
30	A	828	CLA	C4-C3-C5	2.93	120.31	115.23
30	B	836	CLA	O2A-CGA-CBA	2.93	120.75	111.83
30	B	829	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
30	2	303	CLA	C3C-C4C-NC	2.92	114.18	110.43
38	8	312	KC1	CBA-CAA-C2A	-2.92	113.72	125.45
30	8	309	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
30	A	825	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
30	2u	202	CLA	CAC-C3C-C4C	2.92	128.59	124.79
30	12	310	CLA	C3B-C4B-NB	2.92	113.14	110.53
30	10	309	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
30	12	321	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
37	7	315	A86	C41-C32-C31	-2.92	107.86	110.47
37	7	319	A86	C21-C20-C15	-2.92	113.92	123.35
30	A	802	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
30	12	303	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
30	A	832	CLA	CHC-C1C-C2C	-2.92	118.65	126.95
30	1	302	CLA	CBC-CAC-C3C	-2.92	104.51	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	6	312	KC1	CHD-C4C-NC	2.92	128.71	124.31
30	7	305	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
30	9	305	CLA	CHD-C4C-NC	2.92	128.75	124.23
30	4	302	CLA	CBC-CAC-C3C	-2.92	104.51	112.42
30	A	832	CLA	C3B-C4B-NB	2.92	113.13	110.53
30	4	309	CLA	C1-C2-C3	-2.92	121.42	126.20
30	3	305	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
30	A	821	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
30	A	811	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
30	4	304	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
30	12	321	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
30	B	813	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
38	14	311	KC1	CHD-C1D-ND	-2.92	119.68	124.05
30	B	827	CLA	CHC-C1C-C2C	-2.91	118.66	126.95
30	6	307	CLA	C3B-C4B-NB	2.91	113.13	110.53
39	5	313	DD6	C21-C20-C15	-2.91	117.50	122.30
30	2	307	CLA	C1-C2-C3	-2.91	121.42	126.20
30	2	313	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
30	7	312	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
30	B	851	CLA	CMB-C2B-C1B	2.91	129.85	125.42
30	11	304	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
38	16	304	KC1	CAC-C3C-C4C	2.91	128.58	124.79
37	14	314	A86	C7-C6-C5	-2.91	118.10	122.82
30	A	810	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
38	1	306	KC1	C4C-C3C-C2C	-2.91	102.65	106.89
30	B	836	CLA	C3B-C4B-NB	2.91	113.13	110.53
30	9	306	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
30	15	312	CLA	C3C-C4C-NC	2.91	114.16	110.43
30	5	303	CLA	CMB-C2B-C1B	2.91	129.85	125.42
30	A	810	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
37	14	319	A86	C25-C24-C1	-2.91	118.38	126.36
30	A	835	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
30	3	307	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
30	B	802	CLA	CHA-C1A-NA	-2.91	119.80	126.39
30	B	824	CLA	CHC-C1C-C2C	-2.91	118.68	126.95
37	4	317	A86	C19-C18-C17	-2.91	105.35	110.79
38	6	313	KC1	C4C-C3C-C2C	-2.91	102.66	106.89
30	A	834	CLA	CHD-C4C-NC	2.91	128.74	124.23
38	13	306	KC1	CHD-C1D-ND	-2.91	119.69	124.05
38	4	310	KC1	C4B-C3B-C2B	-2.91	104.29	106.81
30	6	306	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
30	A	806	CLA	CHC-C1C-C2C	-2.91	118.69	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2u	202	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
37	2	302	A86	C22-C16-C17	-2.91	103.86	108.97
30	15	314	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
36	3	317	LMG	O6-C5-C4	2.91	114.94	109.70
30	3	306	CLA	C4-C3-C5	2.91	120.27	115.23
30	B	820	CLA	C3B-C4B-NB	2.91	113.12	110.53
30	16	303	CLA	O2A-CGA-CBA	2.91	120.69	111.83
30	A	817	CLA	CHD-C4C-NC	2.91	128.74	124.23
30	2	304	CLA	CHD-C4C-NC	2.91	128.74	124.23
38	12	313	KC1	O2D-CGD-O1D	-2.91	118.19	123.85
30	14	313	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
38	4	308	KC1	CAA-CBA-CGA	-2.90	112.28	127.05
30	15	305	CLA	C4C-C3C-C2C	-2.90	102.66	106.89
38	4	308	KC1	CBC-CAC-C3C	-2.90	104.55	112.42
30	B	851	CLA	CHD-C4C-NC	2.90	128.73	124.23
30	7	310	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
30	13	302	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
30	B	805	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
37	15	315	A86	C10-C9-C8	2.90	131.61	123.20
30	13	302	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
37	4	314	A86	C40-C32-C31	-2.90	107.87	110.47
30	A	821	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
30	2	307	CLA	O2A-CGA-CBA	2.90	120.69	111.83
38	8	312	KC1	CAC-C3C-C4C	2.90	128.57	124.79
30	B	816	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
37	11	314	A86	C26-C25-C24	-2.90	114.79	123.20
38	9	310	KC1	O2D-CGD-O1D	-2.90	118.20	123.85
30	B	816	CLA	O2A-CGA-CBA	2.90	120.68	111.83
30	6	317	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
30	7	311	CLA	C1-C2-C3	-2.90	121.44	126.20
30	6	307	CLA	O2A-CGA-CBA	2.90	120.68	111.83
30	9	309	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
30	15	310	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
37	9	316	A86	C4-C3-C2	-2.90	117.58	123.52
37	3	314	A86	C25-C24-C1	-2.90	118.41	126.36
30	9	305	CLA	C1-C2-C3	-2.90	121.45	126.20
30	1	305	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
30	12	304	CLA	CAC-C3C-C4C	2.90	128.56	124.79
38	13	305	KC1	O2D-CGD-O1D	-2.90	118.20	123.85
30	A	819	CLA	CAC-C3C-C4C	2.90	128.56	124.79
30	6	305	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
30	B	806	CLA	CMB-C2B-C1B	2.90	129.83	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	304	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
39	6	319	DD6	C37-C36-C35	-2.90	109.09	114.42
30	6	315	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
30	A	838	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
37	10	316	A86	C26-C25-C24	-2.90	114.81	123.20
30	B	831	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
30	6	305	CLA	CAC-C3C-C4C	2.90	128.56	124.79
30	F	203	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
38	13	308	KC1	O2D-CGD-O1D	-2.90	118.21	123.85
30	3	303	CLA	CHD-C4C-NC	2.90	128.72	124.23
37	15	315	A86	C36-C31-C32	-2.90	116.82	119.70
38	12	313	KC1	C1A-C2A-C3A	2.90	109.94	107.28
30	5	307	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
30	L	203	CLA	CHD-C4C-NC	2.90	128.72	124.23
30	5	303	CLA	CHD-C4C-NC	2.90	128.72	124.23
30	7	305	CLA	CHD-C4C-NC	2.90	128.72	124.23
38	4	310	KC1	CAC-C3C-C4C	2.90	128.56	124.79
30	A	803	CLA	C1-C2-C3	-2.89	121.45	126.20
30	A	803	CLA	CMB-C2B-C3B	2.89	133.36	126.55
30	15	302	CLA	CMC-C2C-C1C	2.89	129.56	125.03
30	2	309	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
30	B	807	CLA	C1-C2-C3	-2.89	121.46	126.20
30	B	808	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
30	1	307	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
37	10	316	A86	C24-C1-C2	-2.89	114.46	119.01
30	B	804	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
30	8	303	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
30	9	301	CLA	C1-C2-C3	-2.89	121.46	126.20
38	13	308	KC1	CHD-C4C-NC	2.89	128.66	124.31
30	A	844	CLA	CAC-C3C-C4C	2.89	128.55	124.79
38	10	306	KC1	C4C-C3C-C2C	-2.89	102.69	106.89
38	7	308	KC1	CHD-C4C-NC	2.89	128.66	124.31
30	13	301	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
30	7	311	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
30	10	305	CLA	CAC-C3C-C4C	2.89	128.55	124.79
34	A	853	LHG	O8-C23-C24	2.89	119.92	111.15
30	6	314	CLA	CHD-C4C-NC	2.89	128.71	124.23
30	5	308	CLA	CHD-C4C-NC	2.89	128.71	124.23
30	4	306	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
37	11	314	A86	C12-C11-C13	2.89	120.68	116.00
33	L	204	BCR	C15-C16-C17	-2.89	117.61	123.52
30	5	311	CLA	CHC-C1C-C2C	-2.89	118.75	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	309	CLA	C3B-C4B-NB	2.89	113.11	110.53
30	6	305	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
30	F	202	CLA	CAC-C3C-C4C	2.89	128.54	124.79
30	11	308	CLA	CHB-C4A-NA	2.89	128.56	124.40
37	12	316	A86	C3-C4-C5	-2.88	117.62	123.52
30	A	812	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	L	202	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	15	309	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	A	828	CLA	C4A-NA-C1A	-2.88	105.36	106.68
30	B	836	CLA	CHC-C1C-C2C	-2.88	118.75	126.95
37	7	319	A86	C40-C32-C31	-2.88	107.89	110.47
30	14	304	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	2	303	CLA	CMD-C2D-C1D	2.88	129.81	124.73
30	A	816	CLA	C4-C3-C5	2.88	120.23	115.23
30	8	301	CLA	CHD-C4C-NC	2.88	128.70	124.23
37	2	302	A86	C21-C20-C15	-2.88	114.04	123.35
30	12	312	CLA	CAC-C3C-C4C	2.88	128.54	124.79
37	14	315	A86	C4-C3-C2	-2.88	117.62	123.52
30	A	839	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	4	309	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	A	838	CLA	CHC-C1C-C2C	-2.88	118.75	126.95
38	8	314	KC1	CHD-C4C-NC	2.88	128.65	124.31
30	10	304	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
30	14	303	CLA	CHD-C4C-NC	2.88	128.70	124.23
30	9	305	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
30	A	835	CLA	CHD-C4C-NC	2.88	128.70	124.23
30	2	305	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	1	301	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	14	302	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
38	6	312	KC1	C4C-C3C-C2C	-2.88	102.70	106.89
30	15	303	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
38	7	313	KC1	C4B-C3B-C2B	-2.88	104.32	106.81
30	10	303	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
30	14	305	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
37	2u	205	A86	C19-C18-C17	-2.88	105.41	110.79
30	3	309	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
30	B	808	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
30	B	817	CLA	O2A-CGA-CBA	2.88	120.61	111.83
30	B	806	CLA	CMC-C2C-C1C	2.88	129.53	125.03
37	6	320	A86	C12-C11-C13	2.88	120.67	116.00
30	B	820	CLA	C4A-NA-C1A	-2.88	105.37	106.68
30	9	308	CLA	CBA-CAA-C2A	2.88	122.35	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	802	CLA	CMC-C2C-C1C	2.88	129.53	125.03
30	3	305	CLA	C4-C3-C5	2.88	120.22	115.23
38	7	308	KC1	CHD-C1D-ND	-2.88	119.73	124.05
30	A	839	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
30	B	807	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
30	4	306	CLA	C3B-C4B-NB	2.88	113.10	110.53
30	13	309	CLA	CMB-C2B-C1B	2.88	129.80	125.42
30	5	303	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
30	A	839	CLA	O2A-CGA-CBA	2.88	120.60	111.83
30	B	824	CLA	CMB-C2B-C1B	2.88	129.80	125.42
39	6	319	DD6	C25-C24-C1	-2.88	118.48	126.36
30	B	804	CLA	CHD-C4C-NC	2.88	128.69	124.23
38	14	308	KC1	CMB-C2B-C1B	2.88	129.79	124.73
38	3	304	KC1	C4C-C3C-C2C	-2.88	102.71	106.89
30	12	306	CLA	CAC-C3C-C4C	2.88	128.53	124.79
30	7	310	CLA	CHD-C4C-NC	2.87	128.69	124.23
37	10	301	A86	C10-C9-C8	-2.87	114.87	123.20
30	6	307	CLA	C4-C3-C5	2.87	120.22	115.23
30	9	302	CLA	O1D-CGD-CBD	-2.87	118.85	124.52
39	15	319	DD6	C21-C20-C19	-2.87	111.01	114.24
37	5	316	A86	C26-C25-C24	-2.87	114.87	123.20
30	A	841	CLA	CAC-C3C-C4C	2.87	128.53	124.79
30	7	307	CLA	C3B-C4B-NB	2.87	113.09	110.53
37	11	314	A86	C4-C3-C2	-2.87	117.64	123.52
30	3	306	CLA	CAC-C3C-C4C	2.87	128.53	124.79
30	13	307	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
30	B	822	CLA	C3B-C4B-NB	2.87	113.09	110.53
37	12	314	A86	C9-C10-C11	-2.87	118.52	126.64
30	15	304	CLA	CED-O2D-CGD	2.87	122.43	115.92
30	6	309	CLA	CHD-C4C-NC	2.87	128.68	124.23
30	B	825	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
30	B	834	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
30	6	304	CLA	CBA-CAA-C2A	2.87	122.33	113.79
30	A	843	CLA	CAC-C3C-C4C	2.87	128.53	124.79
38	13	310	KC1	CMC-C2C-C1C	2.87	129.52	125.03
30	A	836	CLA	CMB-C2B-C1B	2.87	129.79	125.42
30	B	835	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
38	13	312	KC1	CHD-C4C-NC	2.87	128.63	124.31
30	B	811	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
30	16	301	CLA	CMC-C2C-C1C	2.87	129.52	125.03
30	4	303	CLA	C1-C2-C3	-2.87	121.50	126.20
30	15	307	CLA	C4C-C3C-C2C	-2.87	102.72	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	806	CLA	CBC-CAC-C3C	-2.87	104.64	112.42
38	10	306	KC1	CHD-C1D-ND	-2.87	119.75	124.05
30	2	307	CLA	CMA-C3A-C2A	-2.87	102.89	113.98
33	A	848	BCR	C27-C26-C25	2.87	126.58	122.70
30	3	302	CLA	CAA-C2A-C3A	-2.87	105.25	113.00
30	2	308	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
30	B	824	CLA	O2A-CGA-CBA	2.87	120.58	111.83
30	16	305	CLA	C4A-NA-C1A	-2.87	105.37	106.68
30	14	310	CLA	CAC-C3C-C4C	2.87	128.52	124.79
30	B	819	CLA	C1-C2-C3	-2.87	121.50	126.20
30	B	832	CLA	CMA-C3A-C4A	-2.87	104.07	111.77
39	8	317	DD6	C12-C11-C13	-2.87	113.71	118.09
37	8	315	A86	C25-C26-C27	-2.87	123.26	127.28
30	A	805	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
37	16	312	A86	C21-C20-C15	-2.87	114.10	123.35
30	12	302	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
30	B	836	CLA	CMB-C2B-C1B	2.87	129.78	125.42
30	B	822	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
37	4	314	A86	C23-C16-C17	-2.86	103.93	108.97
38	9	311	KC1	O2D-CGD-O1D	-2.86	118.27	123.85
30	3	307	CLA	C1-C2-C3	-2.86	121.50	126.20
30	B	810	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
39	13	314	DD6	C25-C24-C1	-2.86	118.51	126.36
30	16	306	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
30	12	310	CLA	O2A-CGA-CBA	2.86	120.56	111.83
30	A	836	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
30	16	307	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
30	A	816	CLA	CAC-C3C-C4C	2.86	128.51	124.79
30	A	822	CLA	C3B-C4B-NB	2.86	113.08	110.53
37	15	316	A86	C3-C4-C5	-2.86	117.66	123.52
33	B	841	BCR	C27-C26-C25	2.86	126.57	122.70
30	5	302	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
39	12	317	DD6	C22-C16-C15	2.86	117.77	110.05
30	5	308	CLA	C4-C3-C5	2.86	120.19	115.23
30	10	305	CLA	CHD-C4C-NC	2.86	128.67	124.23
38	12	309	KC1	CAA-CBA-CGA	-2.86	112.50	127.05
30	A	842	CLA	C4-C3-C5	2.86	120.19	115.23
30	14	307	CLA	C1-C2-C3	-2.86	121.51	126.20
30	12	308	CLA	CAC-C3C-C4C	2.86	128.51	124.79
30	15	309	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
37	8	318	A86	C3-C4-C5	2.86	129.37	123.52
33	L	204	BCR	C15-C14-C13	-2.86	123.27	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	5	312	KC1	CMC-C2C-C1C	2.86	129.50	125.03
30	A	844	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
30	16	301	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
30	16	302	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
30	J	101	CLA	CHD-C4C-NC	2.86	128.66	124.23
30	3	309	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
30	A	809	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
30	3	301	CLA	CHD-C4C-NC	2.86	128.66	124.23
30	12	306	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	12	312	CLA	O2A-CGA-CBA	2.86	120.55	111.83
30	16	309	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
30	2	304	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
30	4	301	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
30	15	304	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
30	B	822	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
38	9	311	KC1	CHD-C4C-NC	2.86	128.61	124.31
30	5	304	CLA	CHB-C4A-NA	2.86	128.52	124.40
30	7	303	CLA	CHD-C4C-NC	2.86	128.66	124.23
30	5	304	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
38	6	308	KC1	C4B-C3B-C2B	-2.86	104.34	106.81
30	B	835	CLA	C3B-C4B-NB	2.86	113.08	110.53
30	A	840	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
39	15	319	DD6	C14-C13-C11	-2.86	121.10	125.53
30	B	839	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
38	4	310	KC1	C4C-C3C-C2C	-2.86	102.73	106.89
38	11	305	KC1	CAC-C3C-C4C	2.86	128.51	124.79
30	12	310	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
30	14	312	CLA	C3B-C4B-NB	2.86	113.08	110.53
38	12	313	KC1	CMC-C2C-C1C	2.86	129.50	125.03
37	15	316	A86	C25-C24-C1	-2.85	118.53	126.36
37	8	318	A86	C36-C31-C32	-2.85	116.86	119.70
30	A	818	CLA	CMB-C2B-C1B	2.85	129.76	125.42
30	12	310	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
30	3	306	CLA	O2A-CGA-CBA	2.85	120.54	111.83
38	5	312	KC1	C4C-C3C-C2C	-2.85	102.74	106.89
30	3	302	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
30	B	817	CLA	CAC-C3C-C4C	2.85	128.50	124.79
30	11	304	CLA	CHD-C4C-NC	2.85	128.66	124.23
30	2	308	CLA	O2A-CGA-CBA	2.85	120.53	111.83
30	B	825	CLA	C1-C2-C3	-2.85	121.52	126.20
30	7	305	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	15	313	CLA	C4C-C3C-C2C	-2.85	102.74	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	815	CLA	CAA-C2A-C3A	-2.85	105.29	113.00
30	A	813	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
30	2	301	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	11	308	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
30	A	844	CLA	CHB-C4A-NA	2.85	128.51	124.40
30	11	304	CLA	CAC-C3C-C4C	2.85	128.50	124.79
38	11	305	KC1	CHD-C4C-NC	2.85	128.60	124.31
30	B	818	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
30	6	305	CLA	CHD-C4C-NC	2.85	128.65	124.23
33	B	841	BCR	C15-C16-C17	-2.85	117.69	123.52
30	B	837	CLA	O2A-CGA-CBA	2.85	120.52	111.83
30	B	839	CLA	O1D-CGD-CBD	-2.85	118.90	124.52
30	A	824	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
30	12	321	CLA	CHD-C4C-NC	2.85	128.65	124.23
30	15	311	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
30	10	308	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
30	13	309	CLA	CAC-C3C-C4C	2.85	128.49	124.79
30	B	827	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
30	5	307	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
29	A	801	CL0	O2A-CGA-CBA	2.85	120.51	111.83
37	15	320	A86	C25-C24-C1	-2.85	118.56	126.36
30	A	840	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
30	A	838	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
30	2	311	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
37	13	313	A86	C25-C24-C1	-2.85	118.56	126.36
38	9	304	KC1	CMB-C2B-C1B	2.84	129.74	124.73
37	16	314	A86	C3-C4-C5	-2.84	117.70	123.52
30	6	307	CLA	C1-C2-C3	-2.84	121.54	126.20
30	10	303	CLA	CAC-C3C-C4C	2.84	128.49	124.79
30	A	820	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
38	12	313	KC1	C4C-C3C-C2C	-2.84	102.75	106.89
30	5	304	CLA	CHD-C4C-NC	2.84	128.64	124.23
30	F	202	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
30	3	301	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
30	6	304	CLA	O2A-CGA-CBA	2.84	120.51	111.83
38	5	305	KC1	C4C-C3C-C2C	-2.84	102.75	106.89
30	2	304	CLA	CAC-C3C-C4C	2.84	128.49	124.79
30	6	315	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
39	6	318	DD6	C9-C8-C6	-2.84	118.57	126.36
30	L	202	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
30	B	821	CLA	CAC-C3C-C4C	2.84	128.49	124.79
30	B	806	CLA	CHC-C1C-C2C	-2.84	118.87	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	843	CLA	CMA-C3A-C2A	-2.84	103.00	113.98
30	A	813	CLA	CHD-C4C-NC	2.84	128.64	124.23
38	8	307	KC1	C4C-C3C-C2C	-2.84	102.76	106.89
30	1	305	CLA	O2A-CGA-CBA	2.84	120.50	111.83
39	2	316	DD6	C37-C36-C35	-2.84	109.20	114.42
30	10	305	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
30	3	301	CLA	CBC-CAC-C3C	-2.84	104.72	112.42
30	5	311	CLA	C4-C3-C5	2.84	120.16	115.23
30	14	313	CLA	CMB-C2B-C1B	2.84	129.74	125.42
30	8	304	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
30	A	840	CLA	CMC-C2C-C1C	2.84	129.47	125.03
30	5	303	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
30	B	816	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
30	3	302	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
30	7	312	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
30	9	303	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
30	A	837	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
30	A	813	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
30	4	305	CLA	C4-C3-C5	2.83	120.15	115.23
30	14	313	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
39	8	317	DD6	C15-C14-C13	-2.83	120.00	125.99
38	6	311	KC1	C4C-C3C-C2C	-2.83	102.77	106.89
30	5	309	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
39	2	317	DD6	C19-C18-C17	2.83	116.09	110.79
30	4	302	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
38	13	312	KC1	CAC-C3C-C4C	2.83	128.47	124.79
30	A	818	CLA	CAC-C3C-C4C	2.83	128.47	124.79
30	13	302	CLA	CAC-C3C-C4C	2.83	128.47	124.79
30	B	824	CLA	C3B-C4B-NB	2.83	113.06	110.53
33	F	204	BCR	C27-C26-C25	2.83	126.53	122.70
30	B	807	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
30	15	314	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
38	12	305	KC1	C4C-C3C-C2C	-2.83	102.77	106.89
37	13	315	A86	C12-C11-C10	-2.83	116.79	123.67
30	A	810	CLA	C4A-NA-C1A	-2.83	105.39	106.68
30	8	302	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
30	B	825	CLA	CHD-C4C-NC	2.83	128.62	124.23
30	B	837	CLA	CHD-C4C-NC	2.83	128.62	124.23
30	B	826	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
30	16	306	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
30	16	301	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
30	A	833	CLA	CHC-C1C-C2C	-2.83	118.91	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	309	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
30	12	310	CLA	CHD-C4C-NC	2.83	128.62	124.23
39	5	314	DD6	C25-C24-C1	-2.83	118.61	126.36
38	6	308	KC1	CHD-C1D-ND	-2.83	119.81	124.05
30	4	304	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
30	15	314	CLA	CMC-C2C-C1C	2.83	129.45	125.03
30	3	306	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
30	14	309	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
30	A	809	CLA	CHD-C4C-NC	2.83	128.61	124.23
30	16	310	CLA	CHD-C4C-NC	2.83	128.61	124.23
30	8	301	CLA	CHB-C4A-NA	2.83	128.48	124.40
30	5	302	CLA	CAC-C3C-C4C	2.83	128.47	124.79
38	9	310	KC1	CAC-C3C-C4C	2.83	128.47	124.79
30	9	303	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
30	A	816	CLA	CHD-C4C-NC	2.82	128.61	124.23
30	A	839	CLA	CHD-C4C-NC	2.82	128.61	124.23
30	A	830	CLA	CAC-C3C-C4C	2.82	128.47	124.79
30	B	824	CLA	CAC-C3C-C4C	2.82	128.47	124.79
30	4	306	CLA	CAC-C3C-C4C	2.82	128.47	124.79
30	4	302	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
30	A	828	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
30	8	302	CLA	C4-C3-C5	2.82	120.13	115.23
30	B	826	CLA	O1D-CGD-CBD	-2.82	118.95	124.52
30	8	304	CLA	CHD-C4C-NC	2.82	128.61	124.23
30	15	313	CLA	O2A-CGA-CBA	2.82	120.44	111.83
30	9	307	CLA	CMB-C2B-C1B	2.82	129.72	125.42
38	11	305	KC1	C4C-C3C-C2C	-2.82	102.78	106.89
30	A	839	CLA	CAC-C3C-C4C	2.82	128.46	124.79
30	13	307	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
30	2	311	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
30	4	309	CLA	CAC-C3C-C4C	2.82	128.46	124.79
38	8	313	KC1	CAC-C3C-C4C	2.82	128.46	124.79
30	7	305	CLA	CHB-C4A-NA	2.82	128.47	124.40
37	12	314	A86	C21-C20-C15	-2.82	114.24	123.35
30	11	306	CLA	CMC-C2C-C1C	2.82	129.44	125.03
30	5	304	CLA	CMB-C2B-C1B	2.82	129.72	125.42
30	4	305	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
30	16	301	CLA	CAC-C3C-C4C	2.82	128.46	124.79
30	12	308	CLA	CHD-C4C-NC	2.82	128.60	124.23
37	12	314	A86	C-C1-C24	2.82	122.40	118.09
30	10	309	CLA	O2A-CGA-CBA	2.82	120.43	111.83
37	13	315	A86	C35-C34-C33	2.82	114.95	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	303	CLA	O2A-CGA-CBA	2.82	120.43	111.83
37	9	315	A86	C36-C31-C32	-2.82	116.90	119.70
30	6	306	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
30	4	306	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
30	9	302	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
30	F	203	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
30	13	307	CLA	O2A-CGA-CBA	2.82	120.43	111.83
30	5	308	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
38	13	308	KC1	C4C-C3C-C2C	-2.82	102.79	106.89
37	15	316	A86	C34-O4-C38	-2.82	112.87	117.85
30	12	312	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
30	10	308	CLA	C3B-C4B-NB	2.82	113.04	110.53
30	A	839	CLA	C3B-C4B-NB	2.82	113.04	110.53
30	6	307	CLA	C4C-C3C-C2C	-2.81	102.79	106.89
38	13	308	KC1	CAC-C3C-C4C	2.81	128.45	124.79
37	16	314	A86	C21-C20-C15	-2.81	114.27	123.35
30	1	302	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
30	B	828	CLA	CMB-C2B-C3B	2.81	133.17	126.55
30	A	805	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
33	B	844	BCR	C15-C14-C13	-2.81	123.33	127.28
30	15	313	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
30	B	814	CLA	CHD-C4C-NC	2.81	128.59	124.23
30	12	321	CLA	O2A-CGA-CBA	2.81	120.41	111.83
30	B	838	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
30	3	303	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
37	9	313	A86	C7-C6-C8	2.81	122.39	118.09
37	5	315	A86	C10-C9-C8	-2.81	115.05	123.20
38	8	310	KC1	CHD-C1D-ND	-2.81	119.83	124.05
30	2	310	CLA	CHD-C4C-NC	2.81	128.59	124.23
30	5	309	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
34	A	852	LHG	O8-C23-C24	2.81	120.41	111.83
30	2	303	CLA	C3D-C2D-C1D	-2.81	101.99	105.83
39	8	317	DD6	C25-C24-C1	-2.81	118.65	126.36
30	2	304	CLA	O2A-CGA-CBA	2.81	120.41	111.83
30	2	305	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
38	9	311	KC1	C4C-C3C-C2C	-2.81	102.80	106.89
30	A	815	CLA	C1-C2-C3	-2.81	121.59	126.20
30	B	830	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
38	9	310	KC1	CHD-C4C-NC	2.81	128.54	124.31
30	12	308	CLA	O2A-CGA-CBA	2.81	120.40	111.83
30	B	819	CLA	CHD-C1D-ND	-2.81	120.85	124.80
30	2	309	CLA	C4B-C3B-C2B	-2.81	103.81	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	305	CLA	C4-C3-C5	2.81	120.11	115.23
30	11	310	CLA	C1-C2-C3	-2.81	121.59	126.20
30	B	837	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
30	B	851	CLA	C4-C3-C5	2.81	120.10	115.23
37	11	314	A86	C35-C34-C33	2.81	114.93	109.89
37	2u	203	A86	C40-C32-C31	-2.81	107.96	110.47
30	B	829	CLA	C4-C3-C5	2.81	120.10	115.23
38	3	308	KC1	CHD-C1D-ND	-2.81	119.84	124.05
30	9	308	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
30	14	313	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
30	12	306	CLA	C4C-C3C-C2C	-2.81	102.81	106.89
30	13	302	CLA	CMB-C2B-C1B	2.81	129.69	125.42
30	B	823	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
30	2	307	CLA	CHB-C4A-NA	2.81	128.45	124.40
38	14	306	KC1	CMC-C2C-C1C	2.81	129.42	125.03
30	7	304	CLA	CHD-C4C-NC	2.81	128.58	124.23
30	12	303	CLA	CHD-C4C-NC	2.81	128.58	124.23
38	8	314	KC1	CMB-C2B-C1B	2.80	129.67	124.73
30	14	310	CLA	CHB-C4A-NA	2.80	128.45	124.40
30	6	304	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
30	2	307	CLA	CBC-CAC-C3C	-2.80	104.82	112.42
30	5	302	CLA	CBC-CAC-C3C	-2.80	104.82	112.42
39	11	313	DD6	C19-C18-C17	2.80	116.03	110.79
30	15	311	CLA	CHD-C4C-NC	2.80	128.58	124.23
30	L	202	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
30	14	310	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
30	11	310	CLA	O2A-CGA-CBA	2.80	120.38	111.83
30	A	844	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
30	15	302	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
38	8	310	KC1	CAC-C3C-C4C	2.80	128.44	124.79
30	A	808	CLA	O2A-CGA-CBA	2.80	120.38	111.83
37	14	319	A86	C21-C20-C15	-2.80	114.31	123.35
30	A	818	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
30	3	305	CLA	CAC-C3C-C4C	2.80	128.43	124.79
30	A	810	CLA	CAA-CBA-CGA	-2.80	105.26	113.21
30	15	309	CLA	CAC-C3C-C4C	2.80	128.43	124.79
30	16	305	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
38	11	311	KC1	CAA-CBA-CGA	-2.80	112.81	127.05
38	4	308	KC1	CHD-C4C-NC	2.80	128.53	124.31
38	13	310	KC1	CAC-C3C-C4C	2.80	128.43	124.79
30	10	307	CLA	C1-C2-C3	-2.80	121.61	126.20
30	A	808	CLA	CHD-C4C-NC	2.80	128.57	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	838	CLA	CHD-C4C-NC	2.80	128.57	124.23
30	B	827	CLA	O2A-CGA-CBA	2.80	120.37	111.83
30	12	302	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
30	14	303	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
30	B	818	CLA	CAC-C3C-C4C	2.80	128.43	124.79
30	B	808	CLA	CHD-C4C-NC	2.80	128.57	124.23
30	15	307	CLA	CAC-C3C-C4C	2.80	128.43	124.79
30	A	828	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
30	8	302	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
39	5	313	DD6	C25-C24-C1	-2.80	118.69	126.36
38	5	312	KC1	CBA-CAA-C2A	-2.80	114.23	125.45
30	F	203	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
30	F	203	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
30	A	841	CLA	CHD-C4C-NC	2.80	128.57	124.23
30	B	819	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
30	5	308	CLA	CMC-C2C-C1C	2.80	129.40	125.03
30	A	842	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
39	13	314	DD6	C9-C8-C6	-2.80	118.70	126.36
38	14	311	KC1	CAC-C3C-C4C	2.80	128.43	124.79
30	11	304	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
39	2	316	DD6	C3-C4-C5	-2.80	117.80	123.52
30	4	305	CLA	CHD-C4C-NC	2.79	128.56	124.23
30	7	305	CLA	O1D-CGD-CBD	-2.79	119.01	124.52
30	2	303	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
30	B	825	CLA	C3B-C4B-NB	2.79	113.02	110.53
30	11	308	CLA	C3B-C4B-NB	2.79	113.02	110.53
33	A	851	BCR	C15-C16-C17	-2.79	117.81	123.52
30	8	308	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
30	A	808	CLA	CMC-C2C-C1C	2.79	129.40	125.03
30	2u	202	CLA	C1-C2-C3	-2.79	121.62	126.20
30	10	307	CLA	CHD-C4C-NC	2.79	128.56	124.23
30	B	834	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	A	827	CLA	CMB-C2B-C1B	2.79	129.67	125.42
30	14	312	CLA	CAC-C3C-C4C	2.79	128.42	124.79
30	4	305	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
30	A	805	CLA	C3B-C4B-NB	2.79	113.02	110.53
30	11	308	CLA	CHD-C4C-NC	2.79	128.56	124.23
30	13	303	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
30	B	810	CLA	C3B-C4B-NB	2.79	113.02	110.53
39	12	315	DD6	O1-C20-C21	-2.79	111.93	115.05
30	A	844	CLA	CHD-C4C-NC	2.79	128.55	124.23
30	16	305	CLA	CHB-C4A-NA	2.79	128.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	15	318	DD6	C32-C33-C34	2.79	119.71	113.59
30	5	307	CLA	CAC-C3C-C4C	2.79	128.41	124.79
30	6	309	CLA	CBC-CAC-C3C	-2.79	104.87	112.42
30	L	202	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	A	833	CLA	CHD-C4C-NC	2.79	128.55	124.23
38	6	313	KC1	CMB-C2B-C1B	2.79	129.63	124.73
30	11	304	CLA	C4-C3-C5	2.79	120.06	115.23
33	B	843	BCR	C15-C16-C17	-2.79	117.82	123.52
36	B	847	LMG	O1-C7-C8	-2.79	104.04	110.82
30	4	303	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
38	9	310	KC1	CMB-C2B-C1B	2.78	129.63	124.73
30	13	307	CLA	CHD-C4C-NC	2.78	128.55	124.23
30	10	307	CLA	CHC-C1C-C2C	-2.78	119.03	126.95
30	15	313	CLA	C4-C3-C5	2.78	120.06	115.23
30	B	814	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
30	9	308	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
38	13	311	KC1	C4C-C3C-C2C	-2.78	102.84	106.89
30	A	843	CLA	CBC-CAC-C3C	-2.78	104.88	112.42
39	6	318	DD6	C37-C36-C35	-2.78	109.30	114.42
30	B	810	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
30	9	305	CLA	CAC-C3C-C4C	2.78	128.41	124.79
30	5	308	CLA	CBC-CAC-C3C	-2.78	104.88	112.42
30	B	801	CLA	CMC-C2C-C1C	2.78	129.38	125.03
30	5	309	CLA	CHD-C4C-NC	2.78	128.54	124.23
30	4	304	CLA	CMB-C2B-C1B	2.78	129.65	125.42
30	9	301	CLA	O1D-CGD-CBD	-2.78	119.03	124.52
30	B	804	CLA	C1-C2-C3	-2.78	121.64	126.20
39	16	313	DD6	C23-C16-C15	-2.78	102.54	110.05
30	6	315	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
39	15	318	DD6	C19-C18-C17	2.78	115.99	110.79
30	12	302	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
39	2	317	DD6	C37-C36-C35	-2.78	109.31	114.42
30	B	826	CLA	CAC-C3C-C4C	2.78	128.41	124.79
30	B	835	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
30	A	802	CLA	CHA-C1A-NA	-2.78	120.10	126.39
37	9	315	A86	C9-C8-C6	-2.78	118.74	126.36
37	16	312	A86	C35-C34-C33	2.78	114.88	109.89
38	5	310	KC1	CHD-C4C-NC	2.78	128.49	124.31
30	12	304	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
30	12	308	CLA	C1-C2-C3	-2.78	121.65	126.20
31	B	840	PQN	C11-C3-C2	-2.78	120.13	124.89
30	1	303	CLA	CHC-C1C-C2C	-2.78	119.06	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	8	307	KC1	CAA-CBA-CGA	-2.78	112.93	127.05
33	A	847	BCR	C27-C26-C25	2.78	126.45	122.70
30	A	825	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
30	4	305	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
29	A	801	CL0	CGD-CBD-CAD	-2.78	101.86	110.85
30	A	832	CLA	C1-C2-C3	-2.78	122.27	126.76
38	4	308	KC1	C4C-C3C-C2C	-2.78	102.85	106.89
30	6	309	CLA	C4C-C3C-C2C	-2.77	102.85	106.89
30	A	843	CLA	CHD-C4C-NC	2.77	128.53	124.23
30	B	833	CLA	CHD-C4C-NC	2.77	128.53	124.23
37	11	301	A86	C21-C20-C15	-2.77	114.40	123.35
37	14	318	A86	C4-C3-C2	-2.77	117.85	123.52
38	2	306	KC1	CHD-C4C-NC	2.77	128.49	124.31
38	11	311	KC1	CHD-C4C-NC	2.77	128.49	124.31
30	5	307	CLA	C1-C2-C3	-2.77	121.66	126.20
30	7	312	CLA	CAC-C3C-C4C	2.77	128.40	124.79
30	B	823	CLA	CHD-C4C-NC	2.77	128.53	124.23
38	3	308	KC1	C4C-C3C-C2C	-2.77	102.86	106.89
37	4	315	A86	C21-C20-C15	-2.77	114.41	123.35
30	A	812	CLA	CAC-C3C-C4C	2.77	128.39	124.79
30	F	201	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
30	A	827	CLA	C1-C2-C3	-2.77	121.66	126.20
30	A	828	CLA	O2A-CGA-CBA	2.77	120.28	111.83
33	A	851	BCR	C24-C23-C22	-2.77	122.14	126.23
30	2	313	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
30	B	810	CLA	CHD-C4C-NC	2.77	128.52	124.23
30	4	304	CLA	CAC-C3C-C4C	2.77	128.39	124.79
30	F	202	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
30	B	807	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
36	2u	204	LMG	O6-C1-O1	-2.77	103.50	110.04
30	6	316	CLA	C3B-C4B-NB	2.77	113.00	110.53
30	A	844	CLA	CMA-C3A-C2A	-2.77	103.29	113.98
30	16	305	CLA	CHD-C4C-NC	2.77	128.52	124.23
30	B	818	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
30	2	304	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
30	A	827	CLA	C4C-C3C-C2C	-2.77	102.87	106.89
30	8	304	CLA	C1-C2-C3	-2.77	121.67	126.20
30	1	307	CLA	CAC-C3C-C4C	2.77	128.39	124.79
30	2	309	CLA	CHD-C4C-NC	2.77	128.52	124.23
30	B	821	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
30	B	851	CLA	C3B-C4B-NB	2.76	113.00	110.53
30	B	832	CLA	CHD-C4C-NC	2.76	128.52	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	314	A86	C-C1-C2	-2.76	118.34	122.82
38	5	306	KC1	CHD-C4C-NC	2.76	128.47	124.31
38	14	308	KC1	CAA-CBA-CGA	-2.76	113.00	127.05
30	7	311	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
39	2	316	DD6	C25-C24-C1	-2.76	118.79	126.36
30	A	804	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
37	7	319	A86	C23-C16-C17	-2.76	104.11	108.97
38	9	311	KC1	CAC-C3C-C4C	2.76	128.38	124.79
38	8	307	KC1	CBC-CAC-C3C	-2.76	104.93	112.42
30	A	829	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
39	6	303	DD6	C19-C18-C17	2.76	115.95	110.79
30	7	311	CLA	O2A-CGA-CBA	2.76	120.25	111.83
30	12	302	CLA	CHD-C4C-NC	2.76	128.51	124.23
30	4	305	CLA	O2A-CGA-CBA	2.76	120.25	111.83
30	5	304	CLA	CAC-C3C-C4C	2.76	128.38	124.79
30	7	309	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
38	7	313	KC1	C4C-C3C-C2C	-2.76	102.87	106.89
30	A	830	CLA	CHD-C4C-NC	2.76	128.51	124.23
30	B	804	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
38	11	312	KC1	C1A-NA-C4A	-2.76	105.42	106.68
30	7	305	CLA	C1-C2-C3	-2.76	121.68	126.20
30	4	311	CLA	C1-C2-C3	-2.76	122.30	126.76
30	B	803	CLA	CHD-C4C-NC	2.76	128.51	124.23
30	4	311	CLA	CHD-C4C-NC	2.76	128.51	124.23
38	9	304	KC1	C4C-C3C-C2C	-2.76	102.88	106.89
30	2	313	CLA	CHD-C4C-NC	2.76	128.51	124.23
30	3	303	CLA	CMB-C2B-C1B	2.76	129.62	125.42
30	10	304	CLA	CHD-C4C-NC	2.76	128.51	124.23
30	B	804	CLA	CHC-C1C-C2C	-2.76	119.12	126.95
38	3	304	KC1	CAC-C3C-C4C	2.76	128.38	124.79
37	7	316	A86	C40-C32-C31	-2.76	108.01	110.47
30	11	310	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
30	15	308	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
30	10	308	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
30	B	803	CLA	CMB-C2B-C1B	2.75	129.61	125.42
30	1	301	CLA	CMB-C2B-C1B	2.75	129.61	125.42
30	14	307	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
36	8	319	LMG	O6-C1-O1	-2.75	103.54	110.04
30	B	832	CLA	CAC-C3C-C4C	2.75	128.37	124.79
37	8	318	A86	C26-C25-C24	-2.75	115.22	123.20
30	A	841	CLA	C1-C2-C3	-2.75	121.69	126.20
30	6	310	CLA	C1-C2-C3	-2.75	121.69	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	309	CLA	CHD-C4C-NC	2.75	128.50	124.23
30	A	825	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
39	13	314	DD6	C23-C16-C17	-2.75	104.13	108.97
30	B	851	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
30	4	305	CLA	CAC-C3C-C4C	2.75	128.37	124.79
30	5	303	CLA	CAC-C3C-C4C	2.75	128.37	124.79
37	15	315	A86	C-C1-C2	-2.75	118.36	122.82
30	B	821	CLA	CHD-C4C-NC	2.75	128.50	124.23
30	14	312	CLA	CHD-C4C-NC	2.75	128.50	124.23
37	10	301	A86	O-C13-C11	-2.75	115.12	121.04
30	B	801	CLA	CHB-C4A-NA	2.75	128.37	124.40
33	A	847	BCR	C15-C14-C13	-2.75	123.42	127.28
38	14	308	KC1	O2D-CGD-O1D	-2.75	118.50	123.85
30	2	311	CLA	CHD-C4C-NC	2.75	128.49	124.23
30	12	302	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
30	A	814	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
30	2	311	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
30	B	817	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
37	3	315	A86	C9-C10-C11	-2.75	118.87	126.64
38	7	313	KC1	CAC-C3C-C4C	2.75	128.36	124.79
30	B	811	CLA	CHD-C4C-NC	2.75	128.49	124.23
37	10	317	A86	C21-C20-C15	-2.75	114.49	123.35
30	B	823	CLA	O1D-CGD-CBD	-2.74	119.10	124.52
30	8	302	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
38	12	309	KC1	C4C-C3C-C2C	-2.74	102.90	106.89
30	3	310	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
29	A	801	CL0	C4C-C3C-C2C	-2.74	102.53	113.37
30	13	304	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
36	8	321	LMG	O2-C2-C1	-2.74	103.54	110.08
38	4	310	KC1	CHD-C4C-NC	2.74	128.44	124.31
30	15	313	CLA	CAC-C3C-C4C	2.74	128.36	124.79
37	14	318	A86	C12-C11-C13	2.74	120.45	116.00
30	8	303	CLA	CHD-C4C-NC	2.74	128.49	124.23
30	2u	202	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
30	5	302	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
30	15	308	CLA	O2A-CGA-O1A	-2.74	116.28	123.33
30	A	816	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
37	9	313	A86	C25-C26-C27	-2.74	123.43	127.28
30	B	810	CLA	CAC-C3C-C4C	2.74	128.36	124.79
38	10	306	KC1	CAC-C3C-C4C	2.74	128.36	124.79
39	4	313	DD6	C9-C8-C6	-2.74	118.85	126.36
30	3	302	CLA	C1-C2-C3	-2.74	121.71	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	307	CLA	C1-C2-C3	-2.74	121.71	126.20
30	B	851	CLA	CMC-C2C-C1C	2.74	129.31	125.03
30	7	304	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
30	15	312	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
39	2	316	DD6	C33-C32-C31	2.74	114.89	109.49
30	B	833	CLA	CAC-C3C-C4C	2.74	128.35	124.79
37	6	320	A86	C-C1-C24	2.74	122.27	118.09
30	13	301	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
30	A	840	CLA	CAC-C3C-C4C	2.74	128.35	124.79
30	10	309	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
37	7	316	A86	C-C1-C24	2.74	122.27	118.09
30	3	305	CLA	O2A-CGA-CBA	2.74	120.18	111.83
30	L	202	CLA	CHB-C4A-NA	2.74	128.35	124.40
38	11	312	KC1	C4C-C3C-C2C	-2.74	102.91	106.89
30	A	803	CLA	C4B-C3B-C2B	-2.74	103.90	107.30
37	16	312	A86	C9-C8-C6	2.73	133.86	126.36
33	I	101	BCR	C29-C30-C25	2.73	114.41	110.44
30	3	305	CLA	CHB-C4A-NA	2.73	128.35	124.40
30	8	301	CLA	O2A-CGA-CBA	2.73	120.17	111.83
30	9	308	CLA	C4-C3-C5	2.73	119.97	115.23
30	B	804	CLA	CHB-C4A-NA	2.73	128.34	124.40
30	7	303	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
30	B	810	CLA	CMC-C2C-C1C	2.73	129.30	125.03
30	B	806	CLA	C3B-C4B-NB	2.73	112.97	110.53
38	10	306	KC1	CHD-C4C-NC	2.73	128.43	124.31
30	B	804	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
30	A	805	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	A	811	CLA	CAC-C3C-C4C	2.73	128.34	124.79
38	3	304	KC1	CHD-C4C-NC	2.73	128.43	124.31
38	9	311	KC1	O1D-CGD-CBD	-2.73	119.13	124.52
30	A	841	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
30	4	305	CLA	CHB-C4A-NA	2.73	128.34	124.40
30	B	810	CLA	CMB-C2B-C1B	2.73	129.58	125.42
30	B	830	CLA	CMB-C2B-C1B	2.73	129.58	125.42
30	15	305	CLA	CMB-C2B-C1B	2.73	129.58	125.42
30	A	841	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
30	9	306	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
30	9	308	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
38	12	311	KC1	CHD-C4C-NC	2.73	128.42	124.31
30	1	302	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	6	304	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	13	303	CLA	O2D-CGD-O1D	-2.73	118.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	305	CLA	CMB-C2B-C1B	2.73	129.57	125.42
30	16	305	CLA	CBC-CAC-C3C	-2.73	105.02	112.42
30	8	305	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	2	305	CLA	CHD-C4C-NC	2.73	128.46	124.23
38	7	313	KC1	CBC-CAC-C3C	-2.73	105.02	112.42
30	7	303	CLA	CMB-C2B-C1B	2.73	129.57	125.42
33	A	849	BCR	C30-C25-C26	-2.73	118.91	122.64
37	9	316	A86	C41-C32-C31	-2.73	108.03	110.47
30	14	304	CLA	CHD-C4C-NC	2.73	128.46	124.23
30	4	309	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
30	10	304	CLA	C1-C2-C3	-2.73	121.73	126.20
30	8	305	CLA	CBC-CAC-C3C	-2.73	105.03	112.42
30	A	804	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	15	311	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	A	825	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
30	6	309	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
37	1	309	A86	C21-C20-C15	-2.73	114.55	123.35
30	12	303	CLA	C4-C3-C5	2.73	119.96	115.23
30	A	829	CLA	O2A-CGA-CBA	2.73	120.15	111.83
30	7	310	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
37	15	315	A86	C22-C16-C17	-2.73	104.18	108.97
30	A	805	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
38	13	312	KC1	C4C-C3C-C2C	-2.73	102.92	106.89
30	4	302	CLA	CMB-C2B-C1B	2.73	129.57	125.42
30	6	314	CLA	C1-C2-C3	-2.73	121.73	126.20
30	9	305	CLA	O2A-CGA-CBA	2.73	120.15	111.83
30	A	817	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	14	302	CLA	C3B-C4B-NB	2.73	112.96	110.53
30	4	309	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
30	2	307	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
30	16	305	CLA	CAC-C3C-C4C	2.72	128.34	124.79
30	7	312	CLA	CHD-C4C-NC	2.72	128.46	124.23
30	14	310	CLA	C4B-C3B-C2B	-2.72	103.91	107.30
30	12	304	CLA	O2A-CGA-O1A	-2.72	116.81	123.63
30	6	309	CLA	C3B-C4B-NB	2.72	112.96	110.53
30	15	309	CLA	CHD-C4C-NC	2.72	128.46	124.23
30	6	305	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
38	3	304	KC1	O1D-CGD-CBD	-2.72	119.15	124.52
30	6	305	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
38	5	305	KC1	CHD-C4C-NC	2.72	128.41	124.31
30	1	301	CLA	CHD-C4C-NC	2.72	128.45	124.23
30	A	812	CLA	O2D-CGD-O1D	-2.72	118.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	318	DD6	C33-C32-C31	2.72	114.85	109.49
30	L	202	CLA	CMB-C2B-C1B	2.72	129.56	125.42
30	1	303	CLA	C3B-C4B-NB	2.72	112.96	110.53
30	3	303	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
30	A	806	CLA	O2A-CGA-CBA	2.72	120.13	111.83
38	2	306	KC1	C4C-C3C-C2C	-2.72	102.93	106.89
30	13	303	CLA	CHD-C4C-NC	2.72	128.45	124.23
30	5	309	CLA	CMB-C2B-C1B	2.72	129.56	125.42
38	9	311	KC1	CBC-CAC-C3C	-2.72	105.05	112.42
30	3	303	CLA	CAC-C3C-C4C	2.72	128.33	124.79
39	7	317	DD6	C19-C18-C17	2.72	115.87	110.79
30	11	304	CLA	O2A-CGA-CBA	2.72	120.12	111.83
30	A	803	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
38	10	312	KC1	C4C-C3C-C2C	-2.72	102.94	106.89
30	A	817	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
38	8	311	KC1	CMB-C2B-C1B	2.72	129.51	124.73
30	B	826	CLA	O2A-CGA-CBA	2.72	120.12	111.83
30	12	310	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
30	7	310	CLA	C4-C3-C5	2.72	119.94	115.23
30	10	309	CLA	C4-C3-C5	2.72	119.94	115.23
30	12	312	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
30	14	302	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
36	3	317	LMG	C4-C3-C2	-2.72	106.06	110.83
30	A	826	CLA	O1D-CGD-CBD	-2.72	119.16	124.52
30	1	303	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
35	11	318	LMT	O1B-C4'-C3'	2.72	114.13	107.23
37	5	301	A86	C21-C20-C15	-2.72	114.58	123.35
36	5	318	LMG	O6-C1-O1	-2.72	103.63	110.04
30	A	839	CLA	C1-C2-C3	-2.72	121.75	126.20
38	10	312	KC1	CAC-C3C-C4C	2.71	128.32	124.79
30	5	308	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
30	14	303	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
30	B	801	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
30	J	101	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
30	15	310	CLA	CHD-C4C-NC	2.71	128.44	124.23
30	B	821	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
30	A	824	CLA	C4-C3-C5	2.71	119.32	116.13
30	A	834	CLA	CBC-CAC-C3C	-2.71	105.07	112.42
30	A	827	CLA	C4-C3-C5	2.71	119.93	115.23
30	16	302	CLA	CMB-C2B-C1B	2.71	129.55	125.42
30	A	841	CLA	CED-O2D-CGD	2.71	122.06	115.92
30	4	302	CLA	CMC-C2C-C1C	2.71	129.27	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	4	316	DD6	C23-C16-C17	-2.71	104.20	108.97
30	15	309	CLA	O2A-CGA-CBA	2.71	120.10	111.83
30	A	830	CLA	CAA-C2A-C3A	-2.71	105.67	113.00
33	J	102	BCR	C11-C10-C9	-2.71	123.48	127.28
38	10	306	KC1	O1D-CGD-CBD	-2.71	119.17	124.52
30	16	305	CLA	O2A-CGA-CBA	2.71	120.10	111.83
30	B	814	CLA	C1-C2-C3	-2.71	121.76	126.20
30	16	303	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
30	2	304	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
38	5	312	KC1	CHD-C1D-ND	-2.71	119.99	124.05
30	B	809	CLA	CMC-C2C-C1C	2.71	129.27	125.03
30	2	304	CLA	C1-C2-C3	-2.71	121.76	126.20
30	14	303	CLA	CHB-C4A-NA	2.71	128.31	124.40
30	A	836	CLA	CHB-C4A-NA	2.71	128.31	124.40
33	L	205	BCR	C15-C16-C17	-2.71	117.98	123.52
30	10	307	CLA	CMC-C2C-C1C	2.71	129.26	125.03
30	14	304	CLA	CMB-C2B-C1B	2.71	129.54	125.42
39	4	316	DD6	C26-C25-C24	-2.71	115.36	123.20
30	14	302	CLA	CMC-C2C-C1C	2.71	129.26	125.03
39	5	314	DD6	C37-C36-C35	-2.71	109.44	114.42
30	A	805	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
30	11	310	CLA	C4B-C3B-C2B	-2.71	103.94	107.30
33	F	204	BCR	C40-C30-C25	2.71	114.48	110.24
30	A	832	CLA	CBC-CAC-C3C	-2.71	105.09	112.42
39	6	319	DD6	O1-C20-C21	-2.71	112.03	115.05
30	F	201	CLA	CHD-C4C-NC	2.70	128.43	124.23
30	12	306	CLA	CHD-C4C-NC	2.70	128.43	124.23
30	B	801	CLA	CBC-CAC-C3C	-2.70	105.09	112.42
30	13	304	CLA	CAA-C2A-C3A	-2.70	105.69	113.00
30	3	310	CLA	CAC-C3C-C4C	2.70	128.31	124.79
30	B	812	CLA	C1-O2A-CGA	2.70	123.20	116.65
30	10	305	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
30	1	307	CLA	O2A-CGA-CBA	2.70	120.08	111.83
30	L	202	CLA	CHD-C4C-NC	2.70	128.42	124.23
30	B	808	CLA	CHB-C4A-NA	2.70	128.30	124.40
30	13	309	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
30	A	815	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
30	7	306	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
30	A	830	CLA	CHD-C1D-ND	-2.70	121.00	124.80
33	A	848	BCR	C40-C30-C25	2.70	114.48	110.24
30	A	840	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
30	13	304	CLA	CHD-C4C-NC	2.70	128.42	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	12	317	DD6	C3-C4-C5	-2.70	117.99	123.52
37	14	319	A86	C40-C32-C31	-2.70	108.06	110.47
30	12	307	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
30	A	842	CLA	C3B-C4B-NB	2.70	112.94	110.53
30	B	813	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
30	15	305	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
37	15	321	A86	C7-C6-C8	2.70	122.21	118.09
30	F	201	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
30	A	806	CLA	CHD-C4C-NC	2.70	128.42	124.23
30	2	301	CLA	CMB-C2B-C1B	2.70	129.53	125.42
30	16	310	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
30	B	803	CLA	C3B-C4B-NB	2.70	112.94	110.53
38	13	310	KC1	CAA-CBA-CGA	-2.70	113.33	127.05
30	6	310	CLA	O2A-CGA-CBA	2.70	120.06	111.83
30	B	811	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
37	5	301	A86	C12-C11-C13	2.70	120.37	116.00
30	B	816	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
30	A	818	CLA	C3B-C4B-NB	2.70	112.94	110.53
30	3	306	CLA	CHD-C4C-NC	2.70	128.41	124.23
30	14	305	CLA	CAC-C3C-C4C	2.70	128.30	124.79
38	8	313	KC1	CHD-C1D-ND	-2.70	120.01	124.05
38	10	306	KC1	CMB-C2B-C1B	2.70	129.47	124.73
39	11	313	DD6	C9-C8-C6	-2.69	118.97	126.36
38	13	306	KC1	CAA-CBA-CGA	-2.69	113.35	127.05
30	B	839	CLA	CBC-CAC-C3C	-2.69	105.11	112.42
30	14	302	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
37	15	320	A86	C21-C20-C15	-2.69	114.65	123.35
30	B	828	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
39	7	314	DD6	C10-C9-C8	-2.69	115.39	123.20
38	12	313	KC1	CBA-CAA-C2A	-2.69	114.64	125.45
30	8	308	CLA	CMC-C2C-C1C	2.69	129.24	125.03
30	12	307	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
39	4	316	DD6	C21-C20-C15	-2.69	117.87	122.30
30	B	804	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
30	13	304	CLA	CAC-C3C-C4C	2.69	128.29	124.79
37	4	314	A86	C21-C20-C15	-2.69	114.66	123.35
30	15	311	CLA	CMB-C2B-C1B	2.69	129.52	125.42
33	A	850	BCR	C27-C26-C25	2.69	126.34	122.70
30	A	806	CLA	C4-C3-C5	2.69	119.90	115.23
38	9	304	KC1	CBC-CAC-C3C	-2.69	105.12	112.42
37	13	313	A86	C21-C20-C15	-2.69	114.66	123.35
30	A	843	CLA	C4C-C3C-C2C	-2.69	102.97	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	303	CLA	CMB-C2B-C1B	2.69	129.52	125.42
30	16	309	CLA	CHD-C4C-NC	2.69	128.41	124.23
30	B	807	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
39	8	317	DD6	C21-C20-C15	-2.69	117.87	122.30
30	A	844	CLA	CMB-C2B-C1B	2.69	129.52	125.42
37	14	314	A86	C7-C6-C8	-2.69	113.98	118.09
30	15	302	CLA	CHB-C1B-C2B	-2.69	119.61	127.43
33	B	846	BCR	C27-C26-C25	2.69	126.34	122.70
30	B	807	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
30	16	307	CLA	CHD-C4C-NC	2.69	128.40	124.23
38	5	312	KC1	CHD-C4C-NC	2.69	128.36	124.31
30	15	307	CLA	CBC-CAC-C3C	-2.69	105.13	112.42
30	A	802	CLA	C4-C3-C5	2.69	119.90	115.23
30	B	827	CLA	CMA-C3A-C2A	-2.69	103.58	113.98
30	A	836	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
30	2u	202	CLA	CBC-CAC-C3C	-2.69	105.13	112.42
30	6	309	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
30	B	835	CLA	CBA-CAA-C2A	2.69	121.79	113.79
36	B	847	LMG	O6-C1-O1	-2.69	103.69	110.04
37	13	315	A86	C25-C24-C1	-2.69	118.99	126.36
39	7	317	DD6	O1-C20-C21	-2.69	112.05	115.05
33	B	845	BCR	C20-C21-C22	-2.69	123.51	127.28
30	13	301	CLA	CHB-C4A-NA	2.69	128.28	124.40
30	6	314	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
38	2	314	KC1	CBA-CAA-C2A	-2.69	114.67	125.45
30	B	837	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
30	11	304	CLA	C3B-C4B-NB	2.69	112.93	110.53
30	13	303	CLA	C1-C2-C3	-2.68	121.80	126.20
33	J	102	BCR	C27-C26-C25	2.68	126.33	122.70
30	7	309	CLA	CHD-C4C-NC	2.68	128.39	124.23
30	8	304	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
30	A	809	CLA	C4C-C3C-C2C	-2.68	102.98	106.89
36	3	317	LMG	C1-O6-C5	2.68	118.96	113.72
37	10	315	A86	C21-C20-C15	-2.68	114.69	123.35
30	14	302	CLA	CMB-C2B-C1B	2.68	129.50	125.42
30	A	832	CLA	CMC-C2C-C1C	2.68	129.23	125.03
37	12	314	A86	C12-C11-C13	2.68	120.35	116.00
30	B	820	CLA	CMB-C2B-C1B	2.68	129.50	125.42
30	14	305	CLA	CHD-C4C-NC	2.68	128.39	124.23
39	6	321	DD6	C40-C32-C31	-2.68	105.71	110.52
30	B	813	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
30	13	302	CLA	C4-C3-C5	2.68	119.88	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	309	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
30	B	801	CLA	C4-C3-C5	2.68	119.88	115.23
30	8	308	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
30	16	310	CLA	CAC-C3C-C4C	2.68	128.28	124.79
30	B	829	CLA	CHB-C4A-NA	2.68	128.27	124.40
30	A	835	CLA	CAC-C3C-C4C	2.68	128.28	124.79
30	A	824	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
30	L	202	CLA	C1-C2-C3	-2.68	121.81	126.20
30	4	301	CLA	C3B-C4B-NB	2.68	112.92	110.53
37	5	315	A86	C21-C20-C15	-2.68	114.70	123.35
30	B	837	CLA	CAC-C3C-C4C	2.68	128.27	124.79
39	12	317	DD6	C23-C16-C17	-2.68	104.26	108.97
30	F	202	CLA	CHD-C4C-NC	2.68	128.38	124.23
30	A	803	CLA	C3B-C4B-NB	2.68	112.92	110.53
30	1	305	CLA	C4-C3-C5	2.68	119.87	115.23
30	2u	202	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
30	3	303	CLA	CHB-C4A-NA	2.68	128.26	124.40
30	9	306	CLA	CMB-C2B-C1B	2.67	129.49	125.42
30	15	314	CLA	CAA-C2A-C3A	-2.67	105.77	113.00
37	2u	203	A86	C21-C20-C15	-2.67	114.72	123.35
36	3	317	LMG	O6-C1-O1	-2.67	103.72	110.04
30	A	805	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
38	2	306	KC1	CMB-C2B-C1B	2.67	129.44	124.73
30	13	303	CLA	CMB-C2B-C1B	2.67	129.49	125.42
38	4	307	KC1	C4C-C3C-C2C	-2.67	103.00	106.89
37	15	322	A86	C4-C5-C6	-2.67	123.53	127.28
37	3	315	A86	C21-C20-C15	-2.67	114.72	123.35
30	J	101	CLA	C3B-C4B-NB	2.67	112.92	110.53
30	A	805	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
38	8	306	KC1	C4C-C3C-C2C	-2.67	103.00	106.89
30	B	836	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
38	4	310	KC1	CMB-C2B-C1B	2.67	129.43	124.73
30	2u	202	CLA	CMC-C2C-C1C	2.67	129.21	125.03
30	6	315	CLA	CMB-C2B-C1B	2.67	129.49	125.42
30	4	301	CLA	CHD-C4C-NC	2.67	128.37	124.23
30	15	308	CLA	CAA-CBA-CGA	2.67	119.61	112.49
30	10	307	CLA	CHB-C4A-NA	2.67	128.25	124.40
30	7	304	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
30	9	309	CLA	CHD-C4C-NC	2.67	128.37	124.23
30	11	304	CLA	CMB-C2B-C1B	2.67	129.48	125.42
30	11	306	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
30	A	823	CLA	O2D-CGD-O1D	-2.67	118.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	816	CLA	CMC-C2C-C1C	2.67	129.20	125.03
30	6	316	CLA	O2A-CGA-CBA	2.67	119.97	111.83
30	5	304	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
30	B	829	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
30	B	829	CLA	CHD-C4C-NC	2.67	128.37	124.23
30	14	307	CLA	C3B-C4B-NB	2.67	112.91	110.53
33	L	204	BCR	C27-C26-C25	2.67	126.31	122.70
37	14	317	A86	C34-O4-C38	-2.67	113.14	117.85
30	B	805	CLA	C4-C3-C5	2.67	119.86	115.23
30	A	832	CLA	CHD-C4C-NC	2.67	128.37	124.23
33	M	101	BCR	C27-C26-C25	2.67	126.31	122.70
37	4	312	A86	C21-C20-C15	-2.67	114.75	123.35
39	2	316	DD6	C21-C20-C15	-2.66	117.92	122.30
37	5	315	A86	C4-C3-C2	-2.66	118.07	123.52
37	14	314	A86	C34-O4-C38	-2.66	113.14	117.85
30	B	833	CLA	C3B-C4B-NB	2.66	112.91	110.53
37	6	320	A86	C35-C34-C33	2.66	114.67	109.89
30	9	307	CLA	CHB-C4A-NA	2.66	128.24	124.40
29	A	801	CL0	C1-C2-C3	-2.66	121.83	126.20
30	8	303	CLA	C1-C2-C3	-2.66	121.83	126.20
30	A	821	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
30	2	311	CLA	CMC-C2C-C1C	2.66	129.19	125.03
30	1	304	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
30	3	301	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
39	15	319	DD6	C19-C18-C17	2.66	115.77	110.79
30	A	809	CLA	CBA-CAA-C2A	2.66	121.71	113.79
35	7	301	LMT	O1B-C4'-C3'	2.66	114.00	107.23
38	8	312	KC1	CAA-CBA-CGA	-2.66	113.52	127.05
30	B	819	CLA	CHB-C4A-NA	2.66	128.24	124.40
37	12	314	A86	C24-C1-C2	-2.66	114.82	119.01
30	B	831	CLA	C1-C2-C3	-2.66	121.84	126.20
30	3	303	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
30	2	303	CLA	CMC-C2C-C1C	2.66	129.19	125.03
37	14	317	A86	C9-C10-C11	-2.66	119.12	126.64
30	2	301	CLA	CMC-C2C-C1C	2.66	129.19	125.03
30	A	803	CLA	CAC-C3C-C4C	2.66	128.25	124.79
30	A	830	CLA	C4-C3-C5	2.66	119.84	115.23
30	B	835	CLA	CMB-C2B-C1B	2.66	129.46	125.42
30	15	303	CLA	CAC-C3C-C4C	2.66	128.25	124.79
30	A	808	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
30	16	309	CLA	CAC-C3C-C4C	2.66	128.25	124.79
30	6	317	CLA	C4C-C3C-C2C	-2.65	103.03	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	11	314	A86	C21-C20-C15	-2.65	114.78	123.35
30	5	302	CLA	C3B-C4B-NB	2.65	112.90	110.53
30	A	807	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
30	6	314	CLA	CMB-C2B-C1B	2.65	129.46	125.42
38	8	314	KC1	O1D-CGD-CBD	-2.65	119.28	124.52
30	L	203	CLA	CAC-C3C-C4C	2.65	128.24	124.79
30	5	308	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
34	9	318	LHG	O8-C23-C24	2.65	119.93	111.83
30	2	311	CLA	CMB-C2B-C1B	2.65	129.46	125.42
30	2	305	CLA	CAC-C3C-C4C	2.65	128.24	124.79
30	15	306	CLA	CAC-C3C-C4C	2.65	128.24	124.79
30	B	831	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
30	2	308	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
37	1	309	A86	C34-O4-C38	-2.65	113.16	117.85
30	1	307	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
37	14	301	A86	C21-C20-C15	-2.65	114.79	123.35
30	1	304	CLA	CMB-C2B-C1B	2.65	129.46	125.42
30	A	841	CLA	CMC-C2C-C1C	2.65	129.18	125.03
38	13	310	KC1	CHD-C4C-NC	2.65	128.30	124.31
30	14	305	CLA	CMB-C2B-C1B	2.65	129.45	125.42
38	10	312	KC1	CMC-C2C-C1C	2.65	129.18	125.03
33	A	851	BCR	C27-C26-C25	2.65	126.28	122.70
38	6	308	KC1	CMC-C2C-C1C	2.65	129.17	125.03
30	6	304	CLA	C3B-C4B-NB	2.65	112.89	110.53
30	B	810	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
39	3	316	DD6	C9-C8-C6	-2.65	119.10	126.36
38	8	310	KC1	CBA-CAA-C2A	-2.65	114.82	125.45
30	6	310	CLA	C4C-C3C-C2C	-2.65	103.04	106.89
30	5	302	CLA	CMC-C2C-C1C	2.65	129.17	125.03
38	7	313	KC1	CHB-C4A-NA	2.65	128.34	124.23
30	15	312	CLA	CMD-C2D-C3D	-2.65	121.62	127.69
37	7	315	A86	C36-C31-C32	-2.65	117.07	119.70
30	14	310	CLA	CHD-C4C-NC	2.65	128.34	124.23
30	14	304	CLA	CAA-C2A-C3A	-2.65	105.85	113.00
30	A	808	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
30	10	309	CLA	CHD-C4C-NC	2.65	128.33	124.23
37	15	317	A86	C10-C9-C8	-2.65	115.53	123.20
30	14	307	CLA	C1-O2A-CGA	2.65	123.05	116.65
30	B	830	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
30	B	806	CLA	C4B-C3B-C2B	-2.64	104.01	107.30
30	14	313	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
30	A	803	CLA	O2D-CGD-O1D	-2.64	118.70	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	305	KC1	CHD-C4C-NC	2.64	128.29	124.31
30	7	307	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
37	8	315	A86	C21-C20-C15	-2.64	114.82	123.35
30	B	817	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
30	12	306	CLA	CMB-C2B-C1B	2.64	129.44	125.42
30	13	309	CLA	CHD-C4C-NC	2.64	128.33	124.23
30	2	313	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
30	1	307	CLA	CHD-C4C-NC	2.64	128.33	124.23
30	5	311	CLA	CHD-C4C-NC	2.64	128.33	124.23
30	2	304	CLA	CMC-C2C-C1C	2.64	129.16	125.03
33	B	841	BCR	C7-C8-C9	-2.64	122.33	126.23
37	10	302	A86	C21-C20-C15	-2.64	114.83	123.35
38	2	314	KC1	CHD-C4C-NC	2.64	128.28	124.31
30	13	302	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
30	4	306	CLA	O2A-CGA-CBA	2.64	119.88	111.83
30	A	834	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
37	15	317	A86	C12-C11-C13	2.64	120.28	116.00
30	4	306	CLA	CMC-C2C-C1C	2.64	129.16	125.03
30	6	309	CLA	CMC-C2C-C1C	2.64	129.16	125.03
30	8	303	CLA	CAC-C3C-C4C	2.64	128.22	124.79
37	15	323	A86	C4-C3-C2	2.64	128.91	123.52
30	8	304	CLA	CMB-C2B-C1B	2.64	129.43	125.42
30	A	807	CLA	O2A-CGA-O1A	-2.64	117.04	123.63
30	12	304	CLA	CBC-CAC-C3C	-2.64	105.28	112.42
30	B	823	CLA	CMC-C2C-C1C	2.64	129.15	125.03
30	A	822	CLA	CAC-C3C-C4C	2.63	128.22	124.79
30	B	811	CLA	CAA-C2A-C3A	-2.63	105.88	113.00
30	10	305	CLA	C1-O2A-CGA	2.63	123.03	116.65
30	15	303	CLA	CHD-C4C-NC	2.63	128.31	124.23
39	6	318	DD6	O1-C20-C21	-2.63	112.11	115.05
30	10	304	CLA	CAC-C3C-C4C	2.63	128.22	124.79
38	4	307	KC1	CMB-C2B-C1B	2.63	129.37	124.73
37	10	316	A86	C21-C20-C15	-2.63	114.85	123.35
30	8	305	CLA	O2A-CGA-CBA	2.63	119.86	111.83
30	A	811	CLA	CHB-C4A-NA	2.63	128.20	124.40
30	6	315	CLA	CAC-C3C-C4C	2.63	128.21	124.79
30	12	312	CLA	CMB-C2B-C1B	2.63	129.43	125.42
30	2	309	CLA	C1-O2A-CGA	2.63	123.02	116.65
37	9	315	A86	C8-C6-C5	-2.63	114.87	119.01
30	A	825	CLA	C1-C2-C3	-2.63	121.89	126.20
39	7	302	DD6	C25-C24-C1	-2.63	119.15	126.36
30	B	809	CLA	C4C-C3C-C2C	-2.63	103.06	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	829	CLA	CAC-C3C-C4C	2.63	128.21	124.79
30	A	822	CLA	CHD-C4C-NC	2.63	128.31	124.23
30	A	805	CLA	C1-C2-C3	-2.63	121.89	126.20
30	15	305	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
30	2	307	CLA	CAC-C3C-C4C	2.63	128.21	124.79
30	B	809	CLA	CHD-C4C-NC	2.63	128.30	124.23
30	B	830	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
30	B	810	CLA	CHC-C1C-C2C	-2.63	119.49	126.95
38	11	307	KC1	CMC-C2C-C1C	2.63	129.14	125.03
30	A	825	CLA	CHB-C4A-NA	2.63	128.19	124.40
30	9	302	CLA	CHB-C4A-NA	2.63	128.19	124.40
30	A	804	CLA	O2A-CGA-CBA	2.63	119.84	111.83
30	9	308	CLA	O2A-CGA-CBA	2.62	119.84	111.83
30	B	836	CLA	CHD-C4C-NC	2.62	128.30	124.23
30	11	308	CLA	CMB-C2B-C1B	2.62	129.41	125.42
30	B	826	CLA	CHD-C4C-NC	2.62	128.30	124.23
38	3	311	KC1	CHB-C4A-NA	2.62	128.30	124.23
30	B	806	CLA	C4C-C3C-C2C	-2.62	103.07	106.89
30	9	303	CLA	C4C-C3C-C2C	-2.62	103.07	106.89
30	8	305	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
30	A	839	CLA	CMB-C2B-C1B	2.62	129.41	125.42
30	16	310	CLA	CBC-CAC-C3C	-2.62	105.31	112.42
30	B	828	CLA	C1-C2-C3	-2.62	121.90	126.20
30	15	309	CLA	C4-C3-C5	2.62	119.78	115.23
30	B	805	CLA	O2A-CGA-CBA	2.62	119.83	111.83
30	B	820	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
33	A	850	BCR	C3-C4-C5	-2.62	109.38	114.06
30	10	303	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
33	2u	201	BCR	C29-C30-C25	2.62	114.25	110.44
30	16	308	CLA	CHD-C4C-NC	2.62	128.29	124.23
30	A	842	CLA	CMC-C2C-C1C	2.62	129.13	125.03
30	12	310	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
30	A	808	CLA	CHB-C4A-NA	2.62	128.18	124.40
30	5	309	CLA	CHB-C4A-NA	2.62	128.18	124.40
30	13	301	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
30	A	842	CLA	CAC-C3C-C4C	2.62	128.20	124.79
30	12	302	CLA	CHB-C4A-NA	2.62	128.18	124.40
30	16	303	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
30	10	308	CLA	CMC-C2C-C1C	2.62	129.12	125.03
30	6	306	CLA	CMB-C2B-C1B	2.62	129.41	125.42
30	2	303	CLA	CAA-C2A-C1A	-2.62	103.40	111.97
30	B	825	CLA	CHC-C1C-C2C	-2.62	119.51	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	9	310	KC1	CMC-C2C-C1C	2.62	129.12	125.03
30	13	302	CLA	C1-O2A-CGA	2.62	122.98	116.65
33	B	844	BCR	C27-C26-C25	2.62	126.24	122.70
30	15	309	CLA	C1-C2-C3	-2.62	121.91	126.20
38	3	308	KC1	CHD-C4C-NC	2.62	128.25	124.31
37	4	312	A86	C4-C3-C2	-2.62	118.17	123.52
30	A	830	CLA	CMA-C3A-C2A	-2.62	103.87	113.98
30	A	802	CLA	O2A-CGA-CBA	2.62	119.81	111.83
37	8	318	A86	C12-C11-C10	-2.61	117.31	123.67
37	2	318	A86	C-C1-C24	2.61	122.08	118.09
37	7	315	A86	C4-C5-C6	-2.61	123.61	127.28
39	13	314	DD6	C19-C18-C17	2.61	115.68	110.79
30	4	306	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
30	7	307	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
30	A	836	CLA	CBC-CAC-C3C	-2.61	105.33	112.42
30	14	303	CLA	CMB-C2B-C1B	2.61	129.40	125.42
37	11	301	A86	C25-C24-C1	-2.61	119.20	126.36
30	B	801	CLA	O2A-CGA-CBA	2.61	119.80	111.83
30	A	828	CLA	OBD-CAD-C3D	-2.61	122.31	128.42
35	B	850	LMT	C1'-C2'-C3'	2.61	115.50	110.01
37	4	315	A86	C-C1-C24	2.61	122.08	118.09
30	14	307	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
37	13	313	A86	C7-C6-C5	-2.61	118.59	122.82
36	6	301	LMG	O7-C10-O9	-2.61	117.60	123.70
30	15	302	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
30	9	307	CLA	CAC-C3C-C4C	2.61	128.19	124.79
30	3	307	CLA	CMB-C2B-C1B	2.61	129.39	125.42
30	A	820	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
39	11	313	DD6	C25-C24-C1	-2.61	119.21	126.36
38	6	311	KC1	CAC-C3C-C4C	2.61	128.19	124.79
30	10	303	CLA	CMB-C2B-C1B	2.61	129.39	125.42
30	A	838	CLA	CMB-C2B-C3B	2.61	132.69	126.55
37	5	301	A86	C3-C2-C1	-2.61	123.62	127.28
39	2	315	DD6	C30-C29-C27	-2.61	167.37	176.23
38	4	307	KC1	CHD-C4C-NC	2.61	128.24	124.31
30	8	309	CLA	CAC-C3C-C4C	2.61	128.18	124.79
38	13	311	KC1	CAC-C3C-C4C	2.61	128.18	124.79
37	15	317	A86	C3-C4-C5	-2.61	118.18	123.52
30	A	807	CLA	C3B-C4B-NB	2.61	112.86	110.53
30	5	309	CLA	C1-C2-C3	-2.61	121.92	126.20
30	4	306	CLA	CAA-CBA-CGA	-2.61	105.81	113.21
30	B	828	CLA	C1-O2A-CGA	2.61	122.96	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	12	309	KC1	CBC-CAC-C3C	-2.61	105.36	112.42
30	A	832	CLA	CMB-C2B-C1B	2.61	129.39	125.42
30	A	823	CLA	CMC-C2C-C1C	2.61	129.10	125.03
39	2	315	DD6	C37-C36-C35	-2.60	109.63	114.42
30	3	306	CLA	CHB-C1B-C2B	-2.60	119.86	127.43
30	5	302	CLA	CBA-CAA-C2A	2.60	121.54	113.79
30	11	306	CLA	CMB-C2B-C1B	2.60	129.38	125.42
30	8	305	CLA	CAA-C2A-C3A	-2.60	105.96	113.00
30	15	304	CLA	CMB-C2B-C1B	2.60	129.38	125.42
38	14	306	KC1	O2D-CGD-O1D	-2.60	118.78	123.85
30	A	827	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
30	15	312	CLA	C2A-C3A-C4A	-2.60	97.67	101.87
30	2	308	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
38	12	305	KC1	CAA-CBA-CGA	-2.60	113.82	127.05
37	4	317	A86	C7-C6-C8	2.60	122.06	118.09
30	A	818	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
30	3	305	CLA	C1-C2-C3	-2.60	121.93	126.20
30	B	835	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
30	4	311	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
30	A	829	CLA	CHB-C4A-NA	2.60	128.15	124.40
30	2	310	CLA	CBC-CAC-C3C	-2.60	105.37	112.42
38	6	308	KC1	CAC-C3C-C4C	2.60	128.17	124.79
30	A	827	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
30	5	309	CLA	O2A-CGA-CBA	2.60	119.76	111.83
30	14	310	CLA	CMB-C2B-C1B	2.60	129.38	125.42
30	6	310	CLA	CHB-C4A-NA	2.60	128.15	124.40
30	B	804	CLA	C4-C3-C5	2.60	119.74	115.23
30	6	310	CLA	CHD-C4C-NC	2.60	128.26	124.23
30	B	821	CLA	C4-C3-C2	-2.60	116.96	123.63
30	B	834	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
30	15	308	CLA	CHB-C4A-NA	2.60	128.15	124.40
39	13	314	DD6	C22-C16-C15	2.59	117.05	110.05
38	2	314	KC1	CAC-C3C-C4C	2.59	128.16	124.79
38	13	311	KC1	CBC-CAC-C3C	-2.59	105.39	112.42
38	11	307	KC1	O2D-CGD-O1D	-2.59	118.80	123.85
39	9	314	DD6	C21-C20-C15	-2.59	118.03	122.30
30	A	841	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
38	13	312	KC1	CBA-CAA-C2A	-2.59	115.04	125.45
30	6	317	CLA	CHB-C4A-NA	2.59	128.14	124.40
30	B	824	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
38	11	307	KC1	CMB-C2B-C1B	2.59	129.29	124.73
30	3	310	CLA	CAA-C2A-C3A	-2.59	105.99	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	310	CLA	CMC-C2C-C1C	2.59	129.09	125.03
30	B	812	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
30	3	309	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
30	A	807	CLA	CMB-C2B-C1B	2.59	129.37	125.42
30	B	803	CLA	CAA-CBA-CGA	-2.59	105.85	113.21
30	11	308	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
30	6	310	CLA	CAC-C3C-C4C	2.59	128.16	124.79
30	8	301	CLA	CBA-CAA-C2A	2.59	121.50	113.79
30	1	305	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
38	6	311	KC1	O2D-CGD-O1D	-2.59	118.81	123.85
30	15	304	CLA	C4-C3-C5	2.59	119.72	115.23
38	13	311	KC1	CMB-C2B-C1B	2.59	129.29	124.73
38	16	311	KC1	CHD-C4C-NC	2.59	128.21	124.31
30	A	805	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
30	14	307	CLA	O2A-CGA-CBA	2.59	119.73	111.83
30	8	305	CLA	CMC-C2C-C1C	2.59	129.08	125.03
33	L	201	BCR	C16-C15-C14	-2.59	118.22	123.52
30	A	834	CLA	O2A-CGA-CBA	2.59	119.72	111.83
30	1	304	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
30	6	315	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
30	7	310	CLA	CHB-C4A-NA	2.59	128.13	124.40
30	8	308	CLA	CHB-C4A-NA	2.59	128.13	124.40
37	4	314	A86	C12-C11-C13	2.59	120.19	116.00
38	3	311	KC1	CMB-C2B-C1B	2.59	129.28	124.73
30	A	832	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
30	2u	202	CLA	O2A-CGA-CBA	2.59	119.72	111.83
30	A	841	CLA	CHB-C1B-C2B	-2.59	119.92	127.43
37	14	314	A86	C3-C4-C5	2.59	128.81	123.52
30	B	817	CLA	CHC-C1C-C2C	-2.59	119.60	126.95
30	5	304	CLA	CMC-C2C-C1C	2.59	129.08	125.03
30	6	314	CLA	CMC-C2C-C1C	2.59	129.08	125.03
30	11	310	CLA	CHD-C4C-NC	2.59	128.24	124.23
30	11	309	CLA	O1D-CGD-CBD	-2.59	119.42	124.52
30	9	307	CLA	C1-C2-C3	-2.58	121.96	126.20
38	1	308	KC1	CHD-C4C-NC	2.58	128.20	124.31
30	8	308	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
30	5	308	CLA	CHB-C4A-NA	2.58	128.13	124.40
36	A	856	LMG	O6-C1-O1	-2.58	103.94	110.04
30	9	307	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
30	B	802	CLA	C1-C2-C3	-2.58	121.96	126.20
30	B	832	CLA	C1-C2-C3	-2.58	121.96	126.20
30	6	306	CLA	CAC-C3C-C4C	2.58	128.15	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	307	CLA	C3B-C4B-NB	2.58	112.84	110.53
30	8	305	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
30	16	308	CLA	CMB-C2B-C1B	2.58	129.35	125.42
30	A	824	CLA	CAC-C3C-C4C	2.58	128.15	124.79
30	A	829	CLA	CMC-C2C-C1C	2.58	129.07	125.03
30	B	801	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
34	B	848	LHG	C11-C10-C9	-2.58	101.32	114.37
30	B	839	CLA	CHA-C1A-NA	-2.58	120.55	126.39
30	7	307	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	B	803	CLA	CED-O2D-CGD	2.58	121.77	115.92
30	3	307	CLA	O2A-CGA-CBA	2.58	119.70	111.83
30	A	814	CLA	CHD-C4C-NC	2.58	128.23	124.23
30	6	315	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
30	2	308	CLA	CED-O2D-CGD	2.58	121.77	115.92
30	7	307	CLA	CMB-C2B-C1B	2.58	129.35	125.42
30	B	835	CLA	C1-C2-C3	-2.58	121.97	126.20
30	14	313	CLA	CAC-C3C-C4C	2.58	128.15	124.79
30	1	301	CLA	CHB-C4A-NA	2.58	128.12	124.40
38	8	312	KC1	CHD-C4C-NC	2.58	128.19	124.31
30	A	839	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
30	A	816	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
39	10	314	DD6	C25-C24-C1	-2.58	119.30	126.36
30	A	830	CLA	CHC-C1C-C2C	-2.58	119.63	126.95
30	A	813	CLA	C1-C2-C3	-2.58	121.98	126.20
30	15	307	CLA	CHD-C4C-NC	2.58	128.23	124.23
35	A	854	LMT	C1B-C2B-C3B	2.58	115.43	110.01
38	6	308	KC1	CMB-C2B-C1B	2.58	129.26	124.73
30	2	313	CLA	CMB-C2B-C1B	2.58	129.34	125.42
30	A	822	CLA	C1-C2-C3	-2.58	121.98	126.20
30	15	306	CLA	CMB-C2B-C1B	2.58	129.34	125.42
38	6	311	KC1	CMB-C2B-C1B	2.57	129.26	124.73
30	B	821	CLA	CAA-C2A-C3A	-2.57	106.04	113.00
37	15	315	A86	C9-C8-C6	2.57	133.42	126.36
37	4	312	A86	C35-C34-C33	2.57	114.51	109.89
33	A	847	BCR	C11-C10-C9	-2.57	123.67	127.28
30	4	305	CLA	CMC-C2C-C1C	2.57	129.05	125.03
30	9	309	CLA	CBC-CAC-C3C	-2.57	105.45	112.42
30	A	819	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
30	6	304	CLA	CMB-C2B-C1B	2.57	129.34	125.42
38	6	308	KC1	O2D-CGD-O1D	-2.57	118.84	123.85
38	6	312	KC1	CMB-C2B-C1B	2.57	129.26	124.73
30	B	832	CLA	C4B-C3B-C2B	-2.57	104.10	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	844	BCR	C40-C30-C25	2.57	114.28	110.24
30	10	308	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
30	A	841	CLA	C3B-C4B-NB	2.57	112.83	110.53
39	16	313	DD6	C10-C9-C8	-2.57	115.75	123.20
30	1	302	CLA	CMB-C2B-C1B	2.57	129.33	125.42
30	A	828	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
38	3	311	KC1	O2D-CGD-O1D	-2.57	118.85	123.85
30	12	310	CLA	C1-C2-C3	-2.57	121.99	126.20
30	A	836	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
30	A	819	CLA	O2A-CGA-CBA	2.57	119.67	111.83
30	A	820	CLA	CAA-C2A-C3A	-2.57	106.06	113.00
30	A	816	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	9	306	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	4	304	CLA	CAA-C2A-C3A	-2.57	106.06	113.00
30	8	302	CLA	O2A-CGA-CBA	2.57	119.66	111.83
39	11	313	DD6	O1-C20-C21	-2.57	112.18	115.05
30	B	813	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
30	9	305	CLA	CMC-C2C-C1C	2.57	129.04	125.03
38	8	314	KC1	C1A-NA-C4A	-2.57	105.51	106.68
38	13	312	KC1	CMB-C2B-C1B	2.57	129.25	124.73
30	4	301	CLA	CHB-C4A-NA	2.57	128.10	124.40
30	A	814	CLA	C4-C3-C5	2.57	119.68	115.23
38	6	312	KC1	CAC-C3C-C4C	2.57	128.13	124.79
39	1	310	DD6	C25-C24-C1	-2.57	119.33	126.36
29	A	801	CL0	C1C-CHC-C4B	2.57	125.25	116.07
30	A	842	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
30	B	817	CLA	CMC-C2C-C1C	2.57	129.04	125.03
30	B	815	CLA	CHB-C4A-NA	2.57	128.10	124.40
30	2	313	CLA	CAA-C2A-C3A	-2.57	106.07	113.00
30	B	814	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	16	301	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	B	822	CLA	CBC-CAC-C3C	-2.56	105.47	112.42
30	5	303	CLA	CBC-CAC-C3C	-2.56	105.47	112.42
30	10	303	CLA	CHB-C4A-NA	2.56	128.10	124.40
39	6	303	DD6	C25-C24-C1	-2.56	119.33	126.36
30	15	304	CLA	CHB-C4A-NA	2.56	128.10	124.40
37	16	314	A86	C7-C6-C8	2.56	122.00	118.09
37	9	315	A86	C21-C20-C15	-2.56	115.08	123.35
37	14	317	A86	C35-C34-C33	2.56	114.49	109.89
30	B	821	CLA	O2A-CGA-CBA	2.56	119.65	111.83
38	16	311	KC1	O2D-CGD-O1D	-2.56	118.86	123.85
30	16	302	CLA	C4-C3-C5	2.56	119.67	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	802	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
30	3	310	CLA	CMC-C2C-C1C	2.56	129.03	125.03
38	11	307	KC1	C4C-C3C-C2C	-2.56	103.17	106.89
30	14	312	CLA	CMB-C2B-C1B	2.56	129.31	125.42
30	A	836	CLA	CMA-C3A-C2A	-2.56	104.09	113.98
30	B	851	CLA	CED-O2D-CGD	2.56	121.72	115.92
30	A	814	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
30	A	803	CLA	CHB-C1B-C2B	-2.56	120.00	127.43
37	10	302	A86	C23-C16-C17	-2.56	104.47	108.97
30	5	311	CLA	CMB-C2B-C1B	2.56	129.31	125.42
30	12	304	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
30	5	311	CLA	CAC-C3C-C4C	2.56	128.12	124.79
38	9	311	KC1	CMB-C2B-C1B	2.56	129.23	124.73
38	12	311	KC1	CHB-C4A-NA	2.56	128.20	124.23
33	L	204	BCR	C1-C6-C5	-2.56	119.14	122.64
30	2	309	CLA	O2A-CGA-CBA	2.56	119.63	111.83
30	A	823	CLA	CAC-C3C-C4C	2.56	128.12	124.79
30	2	309	CLA	C1-C2-C3	-2.56	122.01	126.20
30	14	309	CLA	CMB-C2B-C1B	2.56	129.31	125.42
30	B	811	CLA	C4-C3-C5	2.56	119.66	115.23
39	1	310	DD6	C4-C3-C2	-2.56	118.29	123.52
30	3	306	CLA	CHB-C4A-NA	2.56	128.09	124.40
30	A	843	CLA	CMC-C2C-C1C	2.56	129.03	125.03
30	B	837	CLA	C4-C3-C5	2.56	119.66	115.23
38	13	306	KC1	CBA-CAA-C2A	-2.55	115.20	125.45
30	B	802	CLA	CHB-C1B-C2B	-2.55	120.01	127.43
30	B	836	CLA	CAC-C3C-C4C	2.55	128.11	124.79
30	J	101	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
30	14	305	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
38	3	311	KC1	CHD-C4C-NC	2.55	128.16	124.31
30	A	828	CLA	CHB-C4A-NA	2.55	128.09	124.40
30	7	306	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
30	7	311	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
30	5	309	CLA	C4-C3-C5	2.55	119.66	115.23
30	A	804	CLA	C1-C2-C3	-2.55	122.02	126.20
30	16	309	CLA	CMB-C2B-C1B	2.55	129.31	125.42
30	A	829	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
30	14	313	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
38	6	311	KC1	CHD-C4C-NC	2.55	128.15	124.31
30	15	310	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
38	9	312	KC1	CHD-C4C-NC	2.55	128.15	124.31
30	2	309	CLA	CHB-C4A-NA	2.55	128.08	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	311	CLA	CHD-C4C-NC	2.55	128.18	124.23
38	8	313	KC1	C1C-C2C-C3C	-2.55	104.30	106.98
30	13	304	CLA	CMB-C2B-C1B	2.55	129.30	125.42
30	14	302	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
30	8	309	CLA	CHD-C4C-NC	2.55	128.18	124.23
30	A	803	CLA	C1-O2A-CGA	2.55	122.82	116.65
39	7	314	DD6	C3-C4-C5	-2.55	118.31	123.52
38	8	307	KC1	O2D-CGD-O1D	-2.55	118.89	123.85
37	3	314	A86	C21-C20-C15	-2.55	115.13	123.35
30	B	830	CLA	O2A-CGA-CBA	2.55	119.60	111.83
30	A	837	CLA	CHD-C4C-NC	2.55	128.18	124.23
30	4	306	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
30	6	307	CLA	CHD-C4C-NC	2.55	128.18	124.23
30	8	309	CLA	CHB-C4A-NA	2.55	128.07	124.40
33	B	846	BCR	C10-C11-C12	-2.55	115.82	123.20
39	7	317	DD6	C21-C20-C19	-2.55	111.38	114.24
38	11	312	KC1	CHD-C4C-NC	2.54	128.14	124.31
30	A	823	CLA	C4A-NA-C1A	-2.54	105.52	106.68
37	5	301	A86	C9-C10-C11	-2.54	119.45	126.64
30	A	833	CLA	CHB-C4A-NA	2.54	128.07	124.40
30	6	317	CLA	CBC-CAC-C3C	-2.54	105.53	112.42
30	A	818	CLA	CHB-C4A-NA	2.54	128.07	124.40
37	7	316	A86	C19-C18-C17	-2.54	106.03	110.79
39	7	302	DD6	O1-C20-C21	-2.54	112.21	115.05
30	A	820	CLA	CHB-C1B-C2B	-2.54	120.05	127.43
38	14	306	KC1	O1D-CGD-CBD	-2.54	119.50	124.52
30	14	312	CLA	C4B-C3B-C2B	-2.54	104.14	107.30
30	A	805	CLA	CHB-C4A-NA	2.54	128.07	124.40
30	15	304	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
30	A	824	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
30	B	802	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
37	11	316	A86	C21-C20-C15	-2.54	115.15	123.35
30	8	302	CLA	CMB-C2B-C3B	2.54	132.53	126.55
38	12	311	KC1	CAA-CBA-CGA	-2.54	114.13	127.05
30	12	312	CLA	CMC-C2C-C1C	2.54	129.00	125.03
30	11	309	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
30	7	310	CLA	C1-C2-C3	-2.54	122.03	126.20
30	A	831	CLA	O2A-CGA-CBA	2.54	119.58	111.83
30	4	301	CLA	CMB-C2B-C1B	2.54	129.28	125.42
30	1	307	CLA	CHB-C4A-NA	2.54	128.06	124.40
30	B	825	CLA	OBD-CAD-C3D	-2.54	122.48	128.42
38	7	308	KC1	CAA-C2A-C1A	-2.54	113.52	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	305	CLA	CMC-C2C-C1C	2.54	129.00	125.03
30	9	309	CLA	CAC-C3C-C4C	2.54	128.09	124.79
30	1	307	CLA	C4-C3-C5	2.54	119.63	115.23
30	A	817	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
30	B	837	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
30	6	317	CLA	CMB-C2B-C1B	2.54	129.28	125.42
30	15	302	CLA	C3B-C4B-NB	2.54	112.79	110.53
30	F	201	CLA	CMB-C2B-C1B	2.54	129.28	125.42
30	4	306	CLA	CMB-C2B-C1B	2.54	129.28	125.42
38	11	312	KC1	CHB-C4A-NA	2.54	128.16	124.23
30	7	303	CLA	C4B-C3B-C2B	-2.54	104.15	107.30
30	3	306	CLA	CBC-CAC-C3C	-2.54	105.55	112.42
38	4	307	KC1	CBC-CAC-C3C	-2.54	105.55	112.42
30	B	851	CLA	CAA-CBA-CGA	-2.54	106.01	113.21
38	14	306	KC1	CAA-C2A-C1A	-2.53	113.53	124.64
30	5	307	CLA	O2A-CGA-CBA	2.53	119.56	111.83
30	B	827	CLA	CMC-C2C-C1C	2.53	129.00	125.03
29	A	801	CL0	CMC-C2C-C1C	2.53	129.29	124.73
38	8	313	KC1	CED-O2D-CGD	2.53	121.66	115.92
35	A	854	LMT	O1B-C4'-C3'	2.53	113.67	107.23
38	16	304	KC1	O2D-CGD-O1D	-2.53	118.92	123.85
30	11	310	CLA	CMB-C2B-C1B	2.53	129.28	125.42
30	15	308	CLA	C4B-C3B-C2B	-2.53	104.15	107.30
38	4	308	KC1	CHB-C4A-NA	2.53	128.16	124.23
30	15	303	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
38	13	305	KC1	CHD-C4C-NC	2.53	128.12	124.31
30	B	809	CLA	O2A-CGA-CBA	2.53	119.55	111.83
30	J	101	CLA	CMC-C2C-C1C	2.53	128.99	125.03
30	B	812	CLA	CHD-C4C-NC	2.53	128.16	124.23
30	12	321	CLA	C1-C2-C3	-2.53	122.05	126.20
30	A	814	CLA	CMB-C2B-C1B	2.53	129.27	125.42
30	A	839	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
30	4	304	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
30	B	813	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
37	14	320	A86	C40-C32-C31	-2.53	108.21	110.47
30	B	824	CLA	CHB-C4A-NA	2.53	128.05	124.40
30	9	303	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
30	7	303	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
30	3	303	CLA	C4-C3-C5	2.53	119.62	115.23
30	14	303	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
30	F	202	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
37	8	315	A86	C7-C6-C8	2.53	121.95	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	308	CLA	C3B-C4B-NB	2.53	112.79	110.53
30	A	841	CLA	CHB-C4A-NA	2.53	128.05	124.40
30	8	308	CLA	CMB-C2B-C1B	2.53	129.27	125.42
30	6	317	CLA	CAC-C3C-C4C	2.53	128.08	124.79
38	12	305	KC1	CMB-C2B-C1B	2.53	129.18	124.73
30	B	820	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
37	16	314	A86	C12-C11-C13	2.53	120.10	116.00
30	5	303	CLA	O2A-CGA-CBA	2.53	119.54	111.83
30	B	807	CLA	CHD-C4C-NC	2.53	128.15	124.23
30	A	804	CLA	CMA-C3A-C4A	-2.53	104.98	111.77
30	12	308	CLA	C4-C3-C5	2.53	119.61	115.23
30	7	310	CLA	C3B-C4B-NB	2.53	112.78	110.53
30	15	313	CLA	CBC-CAC-C3C	-2.53	105.57	112.42
30	14	309	CLA	CHD-C4C-NC	2.53	128.15	124.23
38	13	308	KC1	CMB-C2B-C1B	2.53	129.18	124.73
38	12	311	KC1	CBC-CAC-C3C	-2.52	105.58	112.42
30	B	831	CLA	O2A-CGA-CBA	2.52	119.53	111.83
30	4	303	CLA	O2A-CGA-CBA	2.52	119.53	111.83
37	15	322	A86	C23-C16-C17	-2.52	104.53	108.97
38	16	304	KC1	CMB-C2B-C1B	2.52	129.17	124.73
30	8	303	CLA	O2A-CGA-CBA	2.52	119.53	111.83
30	A	832	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	2	305	CLA	C1-O2A-CGA	2.52	122.76	116.65
37	13	315	A86	C21-C20-C15	-2.52	115.21	123.35
37	10	301	A86	C7-C6-C8	2.52	121.94	118.09
30	7	311	CLA	CMC-C2C-C1C	2.52	128.97	125.03
39	7	317	DD6	C3-C4-C5	-2.52	118.36	123.52
36	B	847	LMG	C40-C39-C38	-2.52	101.63	114.37
30	5	303	CLA	CMC-C2C-C1C	2.52	128.97	125.03
38	2	312	KC1	CMB-C2B-C1B	2.52	129.16	124.73
30	2	301	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	4	311	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	9	305	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	8	301	CLA	CMA-C3A-C2A	-2.52	104.24	113.98
37	3	315	A86	C9-C8-C6	-2.52	119.46	126.36
30	8	309	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
30	10	307	CLA	O2A-CGA-CBA	2.52	119.51	111.83
30	B	803	CLA	CHC-C1C-NC	2.52	128.10	124.31
30	15	313	CLA	C1-C2-C3	-2.52	122.07	126.20
30	2	304	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
30	B	822	CLA	CHD-C4C-NC	2.52	128.14	124.23
30	5	302	CLA	C4B-C3B-C2B	-2.52	104.17	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	306	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
30	F	203	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
30	B	806	CLA	O2A-CGA-CBA	2.52	119.51	111.83
30	6	310	CLA	C4-C3-C5	2.52	119.60	115.23
38	8	310	KC1	C1C-C2C-C3C	-2.52	104.33	106.98
30	B	822	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
30	13	302	CLA	CMC-C2C-C1C	2.52	128.97	125.03
30	A	815	CLA	CHB-C4A-NA	2.52	128.03	124.40
38	5	310	KC1	O2D-CGD-O1D	-2.52	118.95	123.85
37	2u	205	A86	C41-C32-C31	-2.52	108.22	110.47
30	3	302	CLA	CMC-C2C-C1C	2.51	128.96	125.03
33	L	201	BCR	C27-C26-C25	2.51	126.10	122.70
30	B	811	CLA	O2A-CGA-CBA	2.51	119.50	111.83
31	B	840	PQN	C2M-C2-C3	-2.51	120.32	124.45
33	M	101	BCR	C15-C14-C13	-2.51	123.75	127.28
30	B	830	CLA	CHB-C4A-NA	2.51	128.03	124.40
38	12	309	KC1	CAC-C3C-C4C	2.51	128.06	124.79
38	11	307	KC1	CHD-C4C-NC	2.51	128.09	124.31
30	3	306	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
38	1	308	KC1	O2D-CGD-O1D	-2.51	118.96	123.85
33	2u	201	BCR	C28-C27-C26	-2.51	109.58	114.06
34	2	320	LHG	C11-C10-C9	-2.51	101.67	114.37
38	13	312	KC1	CBC-CAC-C3C	-2.51	105.61	112.42
30	1	305	CLA	CHD-C4C-NC	2.51	128.12	124.23
30	15	306	CLA	CHD-C4C-NC	2.51	128.12	124.23
37	12	314	A86	C25-C26-C27	-2.51	123.76	127.28
30	15	314	CLA	CHD-C4C-NC	2.51	128.12	124.23
30	1	303	CLA	C4-C3-C5	2.51	119.58	115.23
37	12	316	A86	C36-C31-C32	-2.51	117.21	119.70
30	15	306	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
30	14	303	CLA	CMC-C2C-C1C	2.51	128.96	125.03
30	3	302	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
30	8	304	CLA	C1-O2A-CGA	2.51	122.72	116.65
30	14	303	CLA	CBA-CAA-C2A	2.51	121.26	113.79
30	B	806	CLA	C1-C2-C3	-2.51	122.09	126.20
33	B	842	BCR	C29-C30-C25	2.51	114.08	110.44
37	14	316	A86	C21-C20-C15	-2.51	115.26	123.35
38	13	305	KC1	CMB-C2B-C1B	2.51	129.14	124.73
30	9	308	CLA	C4B-C3B-C2B	-2.51	104.19	107.30
33	A	847	BCR	C7-C8-C9	-2.51	122.53	126.23
30	A	843	CLA	C4-C3-C5	2.51	119.58	115.23
30	B	819	CLA	CAA-C2A-C3A	-2.50	106.23	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	203	CLA	CMB-C2B-C1B	2.50	129.23	125.42
30	2	307	CLA	CHD-C4C-NC	2.50	128.12	124.23
30	2	304	CLA	CBC-CAC-C3C	-2.50	105.63	112.42
30	11	304	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	B	837	CLA	CMC-C2C-C1C	2.50	128.95	125.03
30	6	304	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
30	5	302	CLA	CMA-C3A-C2A	-2.50	104.31	113.98
37	15	317	A86	C21-C20-C15	-2.50	115.27	123.35
30	9	302	CLA	CHD-C4C-NC	2.50	128.11	124.23
30	2	309	CLA	C4-C3-C5	2.50	119.57	115.23
37	16	312	A86	C7-C6-C5	-2.50	118.76	122.82
30	15	309	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	B	808	CLA	C4-C3-C5	2.50	119.57	115.23
30	7	305	CLA	O2A-CGA-CBA	2.50	119.46	111.83
37	11	316	A86	C-C1-C24	2.50	121.91	118.09
30	A	813	CLA	CAC-C3C-C4C	2.50	128.04	124.79
30	11	308	CLA	CAC-C3C-C4C	2.50	128.04	124.79
30	12	310	CLA	CAC-C3C-C4C	2.50	128.04	124.79
30	L	202	CLA	C4A-NA-C1A	-2.50	105.54	106.68
30	A	804	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
30	16	310	CLA	O1D-CGD-CBD	2.50	129.45	124.52
30	6	309	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
30	11	309	CLA	CHD-C4C-NC	2.50	128.11	124.23
38	3	308	KC1	O2D-CGD-O1D	-2.50	118.98	123.85
38	2	312	KC1	CHD-C4C-NC	2.50	128.07	124.31
30	9	306	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
30	9	306	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
37	15	321	A86	C-C1-C24	2.50	121.91	118.09
30	A	828	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
30	9	303	CLA	C1-C2-C3	-2.50	122.10	126.20
30	2	309	CLA	CMB-C2B-C1B	2.50	129.22	125.42
30	B	817	CLA	C1-C2-C3	-2.50	122.11	126.20
30	1	304	CLA	C4-C3-C5	2.50	119.56	115.23
30	4	306	CLA	CHB-C4A-NA	2.50	128.00	124.40
30	B	823	CLA	CMB-C2B-C1B	2.50	129.22	125.42
37	15	323	A86	C21-C20-C15	-2.50	115.29	123.35
30	16	301	CLA	C4-C3-C5	2.50	119.56	115.23
30	6	307	CLA	CMA-C3A-C4A	-2.50	105.06	111.77
30	3	305	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
36	8	319	LMG	O3-C3-C2	-2.50	104.49	110.38
30	A	826	CLA	CHD-C4C-NC	2.50	128.10	124.23
30	B	818	CLA	CMB-C2B-C1B	2.50	129.22	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	304	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
30	B	827	CLA	CHD-C4C-NC	2.50	128.10	124.23
30	A	833	CLA	CAC-C3C-C4C	2.49	128.04	124.79
30	A	834	CLA	C1-C2-C3	-2.49	122.11	126.20
30	6	306	CLA	CHB-C4A-NA	2.49	128.00	124.40
30	A	826	CLA	CMC-C2C-C1C	2.49	128.93	125.03
30	A	820	CLA	CHD-C4C-NC	2.49	128.10	124.23
36	F	205	LMG	O7-C10-O9	-2.49	117.88	123.70
38	1	308	KC1	CAC-C3C-C4C	2.49	128.03	124.79
39	10	313	DD6	C19-C18-C17	2.49	115.45	110.79
30	A	819	CLA	CMC-C2C-C1C	2.49	128.93	125.03
30	2	309	CLA	CMC-C2C-C1C	2.49	128.93	125.03
37	5	316	A86	C3-C4-C5	-2.49	118.42	123.52
38	8	306	KC1	CHB-C4A-NA	2.49	128.09	124.23
37	4	314	A86	C24-C1-C2	2.49	122.93	119.01
30	15	313	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
30	A	844	CLA	C4-C3-C5	2.49	119.55	115.23
37	14	314	A86	C23-C16-C17	-2.49	104.59	108.97
30	A	823	CLA	O2A-CGA-CBA	2.49	119.43	111.83
30	A	843	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
38	4	308	KC1	CHC-C4B-C3B	-2.49	121.01	125.21
30	10	304	CLA	O2A-CGA-CBA	2.49	119.42	111.83
37	9	316	A86	C9-C10-C11	-2.49	119.60	126.64
37	14	314	A86	C25-C24-C1	-2.49	119.54	126.36
38	9	304	KC1	CMC-C2C-C1C	2.49	128.92	125.03
30	B	805	CLA	CHD-C4C-NC	2.49	128.09	124.23
37	14	318	A86	C21-C20-C15	-2.49	115.32	123.35
30	7	306	CLA	CMC-C2C-C1C	2.49	128.92	125.03
30	15	308	CLA	C3B-C4B-NB	2.49	112.75	110.53
30	15	305	CLA	CHD-C4C-NC	2.49	128.09	124.23
30	A	806	CLA	CBC-CAC-C3C	-2.49	105.68	112.42
39	12	317	DD6	C19-C18-C17	2.49	115.44	110.79
37	4	312	A86	C10-C9-C8	-2.49	116.00	123.20
30	B	826	CLA	CMB-C2B-C1B	2.49	129.21	125.42
30	4	304	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
30	15	304	CLA	O2A-CGA-CBA	2.49	119.42	111.83
30	6	314	CLA	C4C-C3C-C2C	-2.49	103.27	106.89
38	2	306	KC1	O1D-CGD-CBD	-2.49	119.61	124.52
38	1	306	KC1	CHD-C4C-NC	2.49	128.06	124.31
30	2	307	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
30	5	304	CLA	C4-C3-C5	2.49	119.54	115.23
30	A	823	CLA	O1D-CGD-CBD	-2.49	119.62	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	310	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
30	14	302	CLA	CHB-C4A-NA	2.48	127.99	124.40
30	4	304	CLA	CBC-CAC-C3C	-2.48	105.68	112.42
30	1	301	CLA	O2A-CGA-CBA	2.48	119.41	111.83
38	12	309	KC1	CHB-C4A-NA	2.48	128.08	124.23
30	1	307	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
29	A	801	CL0	C4-C3-C5	2.48	119.54	115.23
38	2	314	KC1	CAA-C2A-C1A	-2.48	113.76	124.64
30	8	304	CLA	CBA-CAA-C2A	2.48	121.18	113.79
30	A	815	CLA	CHD-C4C-NC	2.48	128.08	124.23
30	14	303	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
30	12	303	CLA	O2A-CGA-CBA	2.48	119.40	111.83
30	14	310	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
30	2	304	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
30	5	302	CLA	CMB-C2B-C1B	2.48	129.20	125.42
38	10	312	KC1	CBC-CAC-C3C	-2.48	105.69	112.42
30	3	302	CLA	CMB-C2B-C1B	2.48	129.19	125.42
38	12	305	KC1	O2D-CGD-O1D	-2.48	119.02	123.85
30	A	818	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
30	16	302	CLA	CMC-C2C-C1C	2.48	128.91	125.03
30	2	305	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
30	10	304	CLA	CMB-C2B-C1B	2.48	129.19	125.42
37	5	301	A86	C25-C26-C27	-2.48	123.81	127.28
39	5	314	DD6	C4-C3-C2	-2.48	118.45	123.52
30	A	810	CLA	CHD-C4C-NC	2.48	128.07	124.23
30	4	302	CLA	CBA-CAA-C2A	2.48	121.16	113.79
30	7	310	CLA	O2A-CGA-CBA	2.48	119.38	111.83
30	1	303	CLA	CHB-C4A-NA	2.48	127.97	124.40
30	15	302	CLA	C1-C2-C3	-2.47	122.14	126.20
30	B	812	CLA	O2A-CGA-CBA	2.47	119.38	111.83
30	B	815	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
38	11	305	KC1	CMB-C2B-C1B	2.47	129.09	124.73
38	13	305	KC1	CAA-CBA-CGA	-2.47	114.47	127.05
30	14	302	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
30	16	307	CLA	CMB-C2B-C1B	2.47	129.18	125.42
38	10	310	KC1	CHD-C4C-NC	2.47	128.03	124.31
30	A	819	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
30	15	307	CLA	CMB-C2B-C1B	2.47	129.18	125.42
30	4	304	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
30	14	305	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
30	A	841	CLA	C4-C3-C5	2.47	119.52	115.23
37	2	319	A86	C9-C10-C11	-2.47	119.66	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	307	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
30	B	806	CLA	CAC-C3C-C4C	2.47	128.00	124.79
39	3	316	DD6	C14-C13-C11	-2.47	121.70	125.53
30	A	834	CLA	CMA-C3A-C2A	-2.47	104.43	113.98
30	6	316	CLA	CHB-C4A-NA	2.47	127.96	124.40
30	7	304	CLA	CAC-C3C-C4C	2.47	128.00	124.79
30	L	203	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
30	10	308	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
30	A	816	CLA	C4A-NA-C1A	-2.47	105.55	106.68
33	B	844	BCR	C2-C1-C6	2.47	114.02	110.44
30	8	309	CLA	O2A-CGA-CBA	2.47	119.36	111.83
37	16	314	A86	C10-C9-C8	-2.47	116.05	123.20
30	B	817	CLA	CHB-C4A-NA	2.47	127.96	124.40
30	13	304	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
39	3	313	DD6	C15-C14-C13	-2.47	120.78	125.99
36	B	847	LMG	C38-C37-C36	-2.47	101.90	114.37
30	A	837	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
38	4	310	KC1	CHB-C4A-NA	2.47	128.06	124.23
33	A	849	BCR	C15-C16-C17	-2.47	118.47	123.52
30	B	826	CLA	C4-C3-C5	2.47	119.51	115.23
39	10	313	DD6	C25-C24-C1	-2.46	119.61	126.36
30	A	814	CLA	CHC-C1C-NC	2.46	128.02	124.31
39	7	314	DD6	C26-C25-C24	-2.46	116.06	123.20
37	13	313	A86	C4-C3-C2	-2.46	118.48	123.52
30	A	803	CLA	C4-C3-C5	2.46	119.50	115.23
30	2	301	CLA	CHD-C4C-NC	2.46	128.05	124.23
30	A	834	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
30	7	306	CLA	O2A-CGA-CBA	2.46	119.34	111.83
37	14	316	A86	C4-C3-C2	-2.46	118.48	123.52
30	F	201	CLA	CMC-C2C-C1C	2.46	128.88	125.03
30	16	308	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
30	L	202	CLA	O2A-CGA-CBA	2.46	119.34	111.83
30	A	809	CLA	CHB-C4A-NA	2.46	127.95	124.40
30	B	825	CLA	CAC-C3C-C4C	2.46	127.99	124.79
30	2	303	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
39	10	314	DD6	C23-C16-C22	-2.46	103.79	107.37
30	4	309	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
38	13	305	KC1	CHB-C4A-NA	2.46	128.05	124.23
30	9	308	CLA	CAA-C2A-C1A	2.46	120.04	111.97
30	A	833	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
30	1	302	CLA	C1-C2-C3	-2.46	122.17	126.20
30	1	307	CLA	C1-C2-C3	-2.46	122.17	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	307	CLA	CMB-C2B-C1B	2.46	129.16	125.42
38	12	311	KC1	CAA-C2A-C1A	-2.46	113.87	124.64
30	9	308	CLA	C3B-C4B-NB	2.46	112.72	110.53
39	6	319	DD6	C9-C8-C6	-2.46	119.62	126.36
30	14	310	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
30	10	307	CLA	C4-C3-C5	2.46	119.50	115.23
30	B	833	CLA	O2A-CGA-CBA	2.46	119.33	111.83
37	11	301	A86	C3-C4-C5	-2.46	118.49	123.52
30	A	804	CLA	C4-C3-C5	2.46	119.49	115.23
30	A	802	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
30	5	302	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
30	A	832	CLA	C4B-C3B-C2B	-2.46	104.25	107.30
30	A	822	CLA	CHB-C4A-NA	2.46	127.94	124.40
30	7	306	CLA	CHB-C4A-NA	2.46	127.94	124.40
30	B	823	CLA	CHA-C1A-NA	-2.45	120.83	126.39
30	6	314	CLA	O2A-CGA-CBA	2.45	119.32	111.83
30	10	305	CLA	C4B-C3B-C2B	-2.45	104.25	107.30
34	6	322	LHG	C11-C10-C9	-2.45	101.96	114.37
30	A	834	CLA	C4-C3-C5	2.45	119.49	115.23
33	F	204	BCR	C30-C25-C26	-2.45	119.28	122.64
37	10	317	A86	C23-C16-C17	-2.45	104.66	108.97
37	4	315	A86	C7-C6-C8	2.45	121.83	118.09
30	10	308	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	12	302	CLA	CMB-C2B-C1B	2.45	129.15	125.42
30	5	309	CLA	CMC-C2C-C1C	2.45	128.87	125.03
38	13	305	KC1	CAA-C2A-C1A	-2.45	113.90	124.64
30	8	308	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
30	3	306	CLA	CMC-C2C-C1C	2.45	128.86	125.03
33	B	846	BCR	C16-C15-C14	-2.45	118.51	123.52
37	6	320	A86	C9-C10-C11	-2.45	119.71	126.64
30	11	310	CLA	C4-C3-C5	2.45	119.48	115.23
30	9	306	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
30	12	310	CLA	C4-C3-C5	2.45	119.48	115.23
38	3	304	KC1	CHB-C4A-NA	2.45	128.03	124.23
30	5	302	CLA	O2A-CGA-CBA	2.45	119.30	111.83
30	B	804	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
38	11	305	KC1	CBC-CAC-C3C	-2.45	105.79	112.42
30	8	303	CLA	CBC-CAC-C3C	-2.45	105.79	112.42
30	B	817	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
39	15	319	DD6	C33-C32-C31	2.45	114.31	109.49
30	A	819	CLA	C3B-C4B-NB	2.45	112.71	110.53
30	A	819	CLA	CHB-C4A-NA	2.45	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	2	317	DD6	C14-C13-C11	-2.45	121.74	125.53
39	5	314	DD6	C41-C32-C31	-2.45	106.14	110.52
37	5	316	A86	C29-C30-C31	-2.44	174.78	177.66
30	15	307	CLA	CHB-C4A-NA	2.44	127.93	124.40
30	A	803	CLA	O2A-CGA-CBA	2.44	119.29	111.83
30	3	307	CLA	CHB-C4A-NA	2.44	127.93	124.40
38	3	311	KC1	CBA-CAA-C2A	-2.44	115.64	125.45
30	6	304	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
30	6	316	CLA	CHD-C4C-NC	2.44	128.02	124.23
38	5	305	KC1	CHB-C4A-NA	2.44	128.02	124.23
38	12	311	KC1	CBA-CAA-C2A	-2.44	115.65	125.45
30	B	810	CLA	C4-C3-C5	2.44	119.47	115.23
37	1	309	A86	C24-C1-C2	-2.44	115.17	119.01
30	A	802	CLA	CMB-C2B-C3B	2.44	132.29	126.55
30	F	203	CLA	CMC-C2C-C1C	2.44	128.85	125.03
30	5	308	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
33	M	101	BCR	C40-C30-C25	2.44	114.07	110.24
36	8	319	LMG	C38-C37-C36	-2.44	102.04	114.37
30	B	838	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
30	10	307	CLA	C3B-C4B-NB	2.44	112.71	110.53
37	5	301	A86	C10-C9-C8	-2.44	116.14	123.20
30	B	816	CLA	C1-C2-C3	-2.44	122.20	126.20
30	B	825	CLA	C4-C3-C5	2.44	119.46	115.23
37	10	316	A86	O-C13-C11	-2.44	115.79	121.04
30	B	819	CLA	CAC-C3C-C4C	2.44	127.96	124.79
30	2	301	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
36	B	849	LMG	C38-C37-C36	-2.44	102.05	114.37
30	11	304	CLA	CMC-C2C-C1C	2.44	128.84	125.03
30	12	310	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
30	7	303	CLA	CAC-C3C-C4C	2.44	127.96	124.79
30	A	817	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
30	B	811	CLA	CMC-C2C-C1C	2.43	128.84	125.03
30	15	308	CLA	CAA-C2A-C1A	2.43	119.95	111.97
30	A	810	CLA	CBC-CAC-C3C	-2.43	105.82	112.42
30	3	305	CLA	CMB-C2B-C1B	2.43	129.12	125.42
30	4	304	CLA	C1-C2-C3	-2.43	122.21	126.20
30	3	309	CLA	CAC-C3C-C4C	2.43	127.95	124.79
30	A	823	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
30	B	807	CLA	CHB-C4A-NA	2.43	127.91	124.40
30	B	838	CLA	CHB-C4A-NA	2.43	127.91	124.40
30	2	303	CLA	C1-O2A-CGA	2.43	122.53	116.65
30	B	835	CLA	CHB-C4A-NA	2.43	127.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	8	311	KC1	CHB-C4A-NA	2.43	128.00	124.23
30	A	815	CLA	CBC-CAC-C3C	-2.43	105.83	112.42
30	9	307	CLA	CMC-C2C-C1C	2.43	128.83	125.03
38	12	313	KC1	CAC-C3C-C4C	2.43	127.95	124.79
37	5	315	A86	C7-C6-C8	2.43	121.80	118.09
39	7	318	DD6	C9-C8-C6	-2.43	119.70	126.36
30	A	839	CLA	CBC-CAC-C3C	-2.43	105.83	112.42
30	7	304	CLA	C1-C2-C3	-2.43	122.22	126.20
30	4	311	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
30	6	309	CLA	C4-C3-C5	2.43	119.44	115.23
30	B	814	CLA	CBC-CAC-C3C	-2.43	105.84	112.42
30	12	308	CLA	CMB-C2B-C1B	2.43	129.12	125.42
38	16	304	KC1	CHB-C4A-NA	2.43	128.00	124.23
38	4	310	KC1	CBA-CAA-C2A	-2.43	115.71	125.45
30	J	101	CLA	CHB-C4A-NA	2.43	127.90	124.40
30	B	819	CLA	CED-O2D-CGD	2.43	121.42	115.92
30	4	305	CLA	CBC-CAC-C3C	-2.43	105.84	112.42
30	11	304	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
39	16	313	DD6	C25-C24-C1	-2.43	119.71	126.36
33	B	844	BCR	C3-C4-C5	-2.43	109.73	114.06
30	3	303	CLA	CBC-CAC-C3C	-2.43	105.84	112.42
38	8	311	KC1	CHD-C4C-NC	2.42	127.96	124.31
30	A	835	CLA	CHB-C4A-NA	2.42	127.90	124.40
30	B	832	CLA	CBC-CAC-C3C	-2.42	105.85	112.42
30	4	301	CLA	CAC-C3C-C4C	2.42	127.94	124.79
30	A	836	CLA	CHD-C4C-NC	2.42	127.99	124.23
30	A	823	CLA	CHB-C4A-NA	2.42	127.90	124.40
30	13	307	CLA	CBC-CAC-C3C	-2.42	105.85	112.42
30	12	303	CLA	C1-C2-C3	-2.42	122.23	126.20
30	B	827	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
36	8	320	LMG	O3-C3-C2	-2.42	104.67	110.38
30	B	830	CLA	C3B-C4B-NB	2.42	112.69	110.53
37	15	323	A86	C3-C2-C1	2.42	130.67	127.28
30	L	202	CLA	CAC-C3C-C4C	2.42	127.94	124.79
30	A	828	CLA	CMB-C2B-C1B	2.42	129.10	125.42
30	14	310	CLA	O2A-CGA-CBA	2.42	119.21	111.83
30	A	813	CLA	C4-C3-C5	2.42	119.43	115.23
38	5	306	KC1	O2D-CGD-O1D	-2.42	119.14	123.85
38	8	313	KC1	CMB-C2B-C1B	2.42	128.99	124.73
30	B	836	CLA	CMC-C2C-C1C	2.42	128.81	125.03
38	13	311	KC1	CMC-C2C-C1C	2.42	128.81	125.03
37	5	301	A86	C-C1-C24	2.42	121.78	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	806	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
30	A	823	CLA	CBC-CAC-C3C	-2.42	105.86	112.42
30	J	101	CLA	CMB-C2B-C1B	2.42	129.10	125.42
38	7	308	KC1	CAC-C3C-C4C	2.42	127.94	124.79
30	15	302	CLA	CGD-CBD-CAD	-2.42	103.02	110.85
30	7	304	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
30	4	305	CLA	C1-C2-C3	-2.42	122.24	126.20
30	7	303	CLA	C4-C3-C2	-2.42	117.42	123.63
37	14	318	A86	C9-C10-C11	-2.42	119.81	126.64
30	B	823	CLA	O2A-CGA-CBA	2.42	119.20	111.83
37	12	316	A86	C21-C20-C15	-2.42	115.55	123.35
30	11	306	CLA	CHB-C4A-NA	2.41	127.89	124.40
30	11	308	CLA	C4-C3-C5	2.41	119.42	115.23
30	12	308	CLA	CMC-C2C-C1C	2.41	128.81	125.03
38	5	306	KC1	CHB-C4A-NA	2.41	127.97	124.23
33	A	850	BCR	C15-C14-C13	-2.41	123.89	127.28
31	B	840	PQN	C17-C16-C15	-2.41	106.83	113.26
30	1	304	CLA	C3B-C4B-NB	2.41	112.69	110.53
30	4	311	CLA	CMB-C2B-C1B	2.41	129.09	125.42
39	4	316	DD6	C10-C9-C8	-2.41	116.21	123.20
30	2	313	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	8	305	CLA	CMB-C2B-C3B	2.41	132.22	126.55
33	I	101	BCR	C1-C6-C5	-2.41	119.34	122.64
30	B	832	CLA	C4-C3-C5	2.41	119.42	115.23
30	6	315	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	15	314	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	B	806	CLA	CED-O2D-CGD	2.41	121.39	115.92
30	9	309	CLA	CED-O2D-CGD	2.41	121.38	115.92
30	4	304	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	A	813	CLA	CAA-C2A-C3A	-2.41	106.49	113.00
37	7	316	A86	C10-C9-C8	-2.41	116.22	123.20
30	10	303	CLA	O2A-CGA-CBA	2.41	119.18	111.83
30	A	827	CLA	CMC-C2C-C1C	2.41	128.80	125.03
30	3	302	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
37	2u	205	A86	C23-C16-C17	-2.41	104.74	108.97
30	1	304	CLA	C1-C2-C3	-2.41	122.25	126.20
30	8	301	CLA	C4B-C3B-C2B	-2.41	104.31	107.30
37	10	316	A86	C7-C6-C8	2.41	121.77	118.09
37	1	309	A86	C3-C4-C5	2.41	128.44	123.52
38	12	311	KC1	O2D-CGD-O1D	-2.41	119.16	123.85
30	4	309	CLA	C4-C3-C5	2.41	119.41	115.23
30	A	804	CLA	CMB-C2B-C1B	2.41	129.08	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2u	202	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
30	B	803	CLA	CBC-CAC-C3C	-2.41	105.90	112.42
30	7	306	CLA	CMB-C2B-C1B	2.41	129.08	125.42
30	B	814	CLA	CAC-C3C-C4C	2.41	127.92	124.79
30	15	304	CLA	CAC-C3C-C4C	2.41	127.92	124.79
30	6	305	CLA	CBC-CAC-C3C	-2.40	105.90	112.42
30	B	813	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
30	4	311	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
38	8	307	KC1	CAA-C2A-C1A	-2.40	114.11	124.64
30	B	811	CLA	CAC-C3C-C4C	2.40	127.92	124.79
30	4	306	CLA	C4-C3-C5	2.40	119.40	115.23
38	10	306	KC1	CHB-C4A-NA	2.40	127.96	124.23
39	9	314	DD6	C4-C3-C2	-2.40	118.60	123.52
39	12	317	DD6	O1-C15-C14	-2.40	109.99	116.88
30	16	302	CLA	CBC-CAC-C3C	-2.40	105.90	112.42
37	7	316	A86	C24-C1-C2	-2.40	115.23	119.01
30	3	306	CLA	C4B-C3B-C2B	-2.40	104.31	107.30
30	3	309	CLA	CMB-C2B-C1B	2.40	129.08	125.42
30	9	303	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
30	A	821	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
36	8	321	LMG	O3-C3-C2	-2.40	104.71	110.38
30	A	803	CLA	CHD-C4C-NC	2.40	127.96	124.23
30	15	314	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
30	3	310	CLA	CHB-C4A-NA	2.40	127.87	124.40
30	10	303	CLA	CBA-CAA-C2A	2.40	120.94	113.79
38	14	306	KC1	C1C-C2C-C3C	-2.40	104.45	106.98
30	14	310	CLA	CMC-C2C-C1C	2.40	128.79	125.03
30	6	315	CLA	CMC-C2C-C1C	2.40	128.79	125.03
38	12	309	KC1	O2D-CGD-O1D	-2.40	119.17	123.85
30	3	306	CLA	C3B-C4B-NB	2.40	112.67	110.53
38	8	307	KC1	CHB-C4A-NA	2.40	127.95	124.23
30	A	813	CLA	CHB-C4A-NA	2.40	127.86	124.40
35	11	317	LMT	C1-O1'-C1'	-2.40	109.58	113.68
38	13	310	KC1	CHB-C1B-NB	-2.40	121.43	124.80
37	10	302	A86	C3-C4-C5	-2.40	118.61	123.52
36	14	321	LMG	O6-C1-O1	-2.40	104.38	110.04
30	16	303	CLA	CHB-C4A-NA	2.40	127.86	124.40
38	5	312	KC1	CAA-C2A-C1A	-2.40	114.13	124.64
30	3	301	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
30	3	301	CLA	CHB-C4A-NA	2.40	127.86	124.40
39	6	321	DD6	O1-C20-C21	-2.40	112.37	115.05
30	8	301	CLA	CBC-CAC-C3C	-2.40	105.92	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	312	A86	C9-C10-C11	-2.40	119.87	126.64
30	B	829	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
30	12	310	CLA	CBC-CAC-C3C	-2.40	105.93	112.42
30	A	826	CLA	O2A-CGA-CBA	2.40	119.14	111.83
36	8	321	LMG	O1-C1-C2	-2.39	104.64	108.27
37	10	315	A86	C22-C16-C17	-2.39	104.76	108.97
30	13	309	CLA	CHB-C4A-NA	2.39	127.86	124.40
30	A	802	CLA	C1-C2-C3	-2.39	122.27	126.20
37	8	318	A86	C4-C5-C6	2.39	130.64	127.28
37	8	318	A86	C21-C20-C15	-2.39	115.62	123.35
38	5	312	KC1	O2D-CGD-O1D	-2.39	119.19	123.85
30	5	311	CLA	O2A-CGA-CBA	2.39	119.13	111.83
30	B	829	CLA	C3B-C4B-NB	2.39	112.67	110.53
30	9	306	CLA	CHD-C4C-NC	2.39	127.94	124.23
30	5	303	CLA	CHB-C4A-NA	2.39	127.85	124.40
36	A	856	LMG	O2-C2-C1	-2.39	104.38	110.08
38	10	310	KC1	CAA-C2A-C1A	-2.39	114.16	124.64
30	B	851	CLA	C1-C2-C3	-2.39	122.28	126.20
30	A	825	CLA	CHD-C4C-NC	2.39	127.94	124.23
37	13	313	A86	C36-C31-C32	-2.39	117.32	119.70
37	11	316	A86	C40-C32-C31	-2.39	108.33	110.47
37	16	312	A86	C-C1-C2	-2.39	118.94	122.82
39	4	313	DD6	C33-C32-C31	2.39	114.20	109.49
30	3	301	CLA	CAC-C3C-C4C	2.39	127.90	124.79
30	A	822	CLA	CED-O2D-CGD	2.39	121.34	115.92
30	11	308	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
30	12	304	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
33	B	846	BCR	C15-C16-C17	-2.39	118.63	123.52
30	6	317	CLA	CMC-C2C-C1C	2.39	128.77	125.03
37	7	315	A86	C19-C18-C17	2.39	115.26	110.79
37	7	315	A86	C4-C3-C2	-2.39	118.64	123.52
38	16	304	KC1	CHD-C4C-NC	2.39	127.91	124.31
30	15	304	CLA	CHD-C4C-NC	2.39	127.93	124.23
30	A	806	CLA	CHB-C4A-NA	2.39	127.84	124.40
38	5	310	KC1	CAB-C3B-C4B	2.39	130.52	124.82
30	1	305	CLA	CHB-C4A-NA	2.39	127.84	124.40
38	2	306	KC1	CBC-CAC-C3C	-2.39	105.95	112.42
37	2	318	A86	C10-C9-C8	-2.39	116.29	123.20
30	A	812	CLA	CHD-C4C-NC	2.39	127.93	124.23
30	5	304	CLA	C4A-NA-C1A	-2.38	105.59	106.68
35	A	855	LMT	C1B-O1B-C4'	-2.38	112.33	117.98
38	6	308	KC1	CHB-C4A-NA	2.38	127.93	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	311	CLA	CMB-C2B-C1B	2.38	129.05	125.42
30	13	307	CLA	C4-C3-C5	2.38	119.37	115.23
30	6	306	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
38	1	306	KC1	CMB-C2B-C1B	2.38	128.93	124.73
30	A	827	CLA	C3B-C4B-NB	2.38	112.66	110.53
30	B	837	CLA	C3B-C4B-NB	2.38	112.66	110.53
30	B	812	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
30	3	305	CLA	CMC-C2C-C1C	2.38	128.76	125.03
37	10	302	A86	C40-C32-C31	-2.38	108.34	110.47
30	A	844	CLA	C1-C2-C3	-2.38	122.29	126.20
30	B	812	CLA	CHB-C4A-NA	2.38	127.84	124.40
30	B	818	CLA	C4C-C3C-C2C	-2.38	103.42	106.89
30	15	312	CLA	CAC-C3C-C4C	2.38	127.89	124.79
38	4	310	KC1	O2D-CGD-O1D	-2.38	119.21	123.85
38	12	311	KC1	CMB-C2B-C1B	2.38	128.92	124.73
30	4	306	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
38	13	310	KC1	CBC-CAC-C3C	-2.38	105.97	112.42
37	14	315	A86	C40-C32-C31	-2.38	108.34	110.47
30	B	819	CLA	CHD-C4C-NC	2.38	127.92	124.23
30	1	303	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
38	14	306	KC1	CHC-C4B-NB	-2.38	121.45	124.80
30	B	834	CLA	CHA-C1A-NA	-2.38	121.00	126.39
33	A	850	BCR	C11-C10-C9	-2.38	123.94	127.28
38	10	310	KC1	O2D-CGD-O1D	-2.38	119.22	123.85
30	7	312	CLA	CMB-C2B-C1B	2.38	129.04	125.42
33	L	205	BCR	C15-C14-C13	-2.38	123.94	127.28
30	A	823	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
30	13	309	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
30	2	311	CLA	CHB-C4A-NA	2.38	127.83	124.40
30	A	808	CLA	C4-C3-C5	2.38	118.93	116.13
30	2	304	CLA	CHB-C4A-NA	2.38	127.83	124.40
35	15	301	LMT	C4B-C3B-C2B	2.38	115.00	110.83
38	4	308	KC1	C1A-NA-C4A	-2.38	105.59	106.68
30	B	812	CLA	CMC-C2C-C1C	2.38	128.75	125.03
30	3	302	CLA	CAC-C3C-C4C	2.38	127.88	124.79
30	A	820	CLA	O2A-CGA-CBA	2.37	119.08	111.83
30	12	307	CLA	CMA-C3A-C2A	-2.37	104.80	113.98
33	A	850	BCR	C15-C16-C17	-2.37	118.66	123.52
38	12	309	KC1	CMB-C2B-C1B	2.37	128.91	124.73
30	2	310	CLA	O2A-CGA-CBA	2.37	119.07	111.83
30	10	308	CLA	C1-C2-C3	-2.37	122.31	126.20
38	2	306	KC1	CMC-C2C-C1C	2.37	128.74	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	303	CLA	CHB-C4A-NA	2.37	127.83	124.40
30	A	831	CLA	CMB-C2B-C3B	2.37	132.13	126.55
38	6	313	KC1	CAC-C3C-C4C	2.37	127.88	124.79
30	B	811	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	4	305	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
30	A	814	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
30	A	821	CLA	CHD-C4C-NC	2.37	127.91	124.23
30	B	824	CLA	CHD-C4C-NC	2.37	127.91	124.23
30	B	833	CLA	CMB-C2B-C1B	2.37	129.03	125.42
30	13	303	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
30	8	302	CLA	C1-C2-C3	-2.37	122.31	126.20
30	3	301	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
30	B	822	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	B	814	CLA	O2A-CGA-CBA	2.37	119.06	111.83
37	15	320	A86	C3-C2-C1	-2.37	123.95	127.28
30	B	833	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
30	1	305	CLA	C1-C2-C3	-2.37	122.31	126.20
37	4	315	A86	C35-C34-C33	2.37	114.14	109.89
30	12	321	CLA	C4-C3-C5	2.37	119.34	115.23
38	8	311	KC1	O1D-CGD-CBD	-2.37	119.85	124.52
37	7	319	A86	C4-C3-C2	-2.37	118.67	123.52
37	15	320	A86	C10-C9-C8	2.37	130.06	123.20
30	B	822	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
30	16	301	CLA	CBC-CAC-C3C	-2.37	106.00	112.42
39	7	318	DD6	C14-C13-C11	-2.37	121.86	125.53
30	4	301	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
30	A	834	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
33	B	844	BCR	C11-C10-C9	-2.37	123.96	127.28
30	A	825	CLA	CMC-C2C-C1C	2.37	128.73	125.03
30	8	308	CLA	CAC-C3C-C4C	2.37	127.87	124.79
30	7	309	CLA	CHB-C4A-NA	2.37	127.81	124.40
39	4	316	DD6	C23-C16-C15	2.36	116.43	110.05
30	A	843	CLA	O2A-CGA-CBA	2.36	119.05	111.83
30	F	203	CLA	CBC-CAC-C3C	-2.36	106.01	112.42
37	15	320	A86	C23-C16-C17	-2.36	104.81	108.97
33	A	848	BCR	C30-C25-C26	-2.36	119.41	122.64
39	9	314	DD6	C10-C9-C8	-2.36	116.35	123.20
30	B	813	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	A	822	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
30	A	831	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
37	8	318	A86	C22-C16-C17	-2.36	104.82	108.97
30	7	307	CLA	C1-O2A-CGA	2.36	122.37	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	304	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
30	1	301	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
38	10	310	KC1	CAB-C3B-C4B	2.36	130.46	124.82
37	5	301	A86	C34-O4-C38	-2.36	113.67	117.85
30	11	309	CLA	CHB-C4A-NA	2.36	127.81	124.40
38	10	306	KC1	CMC-C2C-C1C	2.36	128.72	125.03
30	14	313	CLA	CMA-C3A-C2A	-2.36	104.85	113.98
30	A	828	CLA	CAC-C3C-C2C	2.36	131.90	127.56
30	3	302	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
30	A	830	CLA	C3B-C4B-NB	2.36	112.64	110.53
30	15	314	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
33	2u	201	BCR	C15-C14-C13	-2.36	123.97	127.28
37	2	319	A86	C12-C11-C13	2.36	119.83	116.00
30	5	309	CLA	CBC-CAC-C3C	-2.36	106.03	112.42
38	11	307	KC1	CAA-C2A-C1A	-2.36	114.31	124.64
30	2	308	CLA	CHB-C4A-NA	2.36	127.80	124.40
30	14	309	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
30	12	304	CLA	CHB-C4A-NA	2.36	127.80	124.40
30	4	304	CLA	CMC-C2C-C1C	2.36	128.72	125.03
30	A	809	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
30	7	312	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
38	12	305	KC1	CHB-C4A-NA	2.36	127.89	124.23
30	A	824	CLA	CMC-C2C-C1C	2.36	128.72	125.03
37	12	316	A86	O-C13-C11	-2.36	115.97	121.04
39	3	316	DD6	C41-C32-C31	-2.36	106.30	110.52
37	14	317	A86	C10-C9-C8	-2.36	116.38	123.20
37	2	319	A86	C23-C16-C17	-2.35	104.83	108.97
30	A	822	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
38	2	306	KC1	CHB-C4A-NA	2.35	127.88	124.23
33	F	204	BCR	C31-C1-C6	2.35	113.93	110.24
30	11	309	CLA	CMA-C3A-C2A	-2.35	104.88	113.98
30	A	833	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
30	12	303	CLA	CAC-C3C-C4C	2.35	127.85	124.79
30	A	827	CLA	CAC-C3C-C2C	2.35	131.88	127.56
30	4	301	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
39	13	314	DD6	C12-C11-C13	-2.35	114.50	118.09
30	11	308	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
30	B	809	CLA	C4-C3-C5	2.35	119.31	115.23
30	13	301	CLA	CBA-CAA-C2A	2.35	120.79	113.79
30	9	302	CLA	CMB-C2B-C1B	2.35	129.00	125.42
38	3	304	KC1	CMB-C2B-C1B	2.35	128.87	124.73
33	L	201	BCR	C3-C4-C5	-2.35	109.86	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	303	CLA	CMB-C2B-C1B	2.35	129.00	125.42
30	A	809	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
30	B	808	CLA	C1-C2-C3	-2.35	122.35	126.20
30	2	310	CLA	CMC-C2C-C1C	2.35	128.71	125.03
30	B	807	CLA	O2A-CGA-CBA	2.35	119.00	111.83
39	10	313	DD6	C22-C16-C17	-2.35	104.84	108.97
30	14	305	CLA	O2A-CGA-CBA	2.35	119.00	111.83
30	A	805	CLA	O2A-CGA-CBA	2.35	118.99	111.83
30	A	834	CLA	CAC-C3C-C4C	2.35	127.84	124.79
30	10	307	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
30	3	301	CLA	CMC-C2C-C1C	2.35	128.70	125.03
30	15	305	CLA	CMC-C2C-C1C	2.35	128.70	125.03
30	B	813	CLA	CMB-C2B-C1B	2.35	128.99	125.42
30	16	306	CLA	CMC-C2C-C1C	2.35	128.70	125.03
30	3	310	CLA	C4C-C3C-C2C	-2.35	103.48	106.89
37	2	319	A86	C3-C4-C5	-2.35	118.72	123.52
30	A	837	CLA	CMC-C2C-C1C	2.35	128.70	125.03
36	B	847	LMG	O3-C3-C2	-2.35	104.85	110.38
33	B	845	BCR	C30-C25-C26	-2.35	119.43	122.64
30	14	302	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
30	7	303	CLA	C6-C5-C3	-2.35	107.75	113.47
30	B	839	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
30	6	307	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
30	B	839	CLA	CHB-C1B-C2B	-2.34	120.62	127.43
30	9	303	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
30	16	309	CLA	CHB-C4A-NA	2.34	127.78	124.40
38	2	312	KC1	CHB-C4A-NA	2.34	127.86	124.23
30	2u	202	CLA	C1-O2A-CGA	2.34	122.32	116.65
30	B	808	CLA	CAC-C3C-C4C	2.34	127.84	124.79
38	3	308	KC1	O1D-CGD-CBD	-2.34	119.90	124.52
30	8	302	CLA	CMC-C2C-C1C	2.34	128.69	125.03
37	10	301	A86	C26-C25-C24	2.34	129.99	123.20
37	16	314	A86	C34-O4-C38	-2.34	113.71	117.85
33	J	103	BCR	C15-C14-C13	-2.34	124.00	127.28
30	A	831	CLA	CHB-C4A-NA	2.34	127.78	124.40
30	15	305	CLA	CHB-C4A-NA	2.34	127.78	124.40
30	15	310	CLA	CHB-C4A-NA	2.34	127.78	124.40
29	A	801	CL0	C3D-C4D-ND	2.34	116.69	112.94
30	A	818	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
31	A	845	PQN	C11-C12-C13	-2.34	122.80	126.83
30	3	310	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
30	A	808	CLA	CMB-C2B-C1B	2.34	128.98	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	309	CLA	CMB-C2B-C1B	2.34	128.98	125.42
38	3	308	KC1	CMC-C2C-C1C	2.34	128.69	125.03
36	8	321	LMG	O6-C1-O1	-2.34	104.52	110.04
30	A	803	CLA	CMA-C3A-C2A	-2.34	104.94	113.98
38	13	308	KC1	CBC-CAC-C3C	-2.34	106.08	112.42
30	2	303	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
33	I	101	BCR	C15-C16-C17	-2.34	118.73	123.52
37	2	318	A86	C21-C20-C15	-2.34	115.80	123.35
30	A	822	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
38	4	308	KC1	O2D-CGD-O1D	-2.34	119.30	123.85
38	13	310	KC1	O2D-CGD-O1D	-2.34	119.30	123.85
38	9	311	KC1	CMC-C2C-C1C	2.34	128.69	125.03
30	2	308	CLA	C3B-C4B-NB	2.34	112.62	110.53
33	2u	201	BCR	C33-C5-C6	-2.34	121.94	124.48
36	B	847	LMG	C42-C41-C40	-2.34	102.56	114.37
30	5	309	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
30	3	309	CLA	CMC-C2C-C1C	2.34	128.68	125.03
37	9	313	A86	C-C1-C24	2.34	121.66	118.09
38	16	311	KC1	CMB-C2B-C1B	2.33	128.84	124.73
30	7	310	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
30	14	309	CLA	CBC-CAC-C3C	-2.33	106.09	112.42
30	10	309	CLA	CMB-C2B-C1B	2.33	128.97	125.42
37	2	318	A86	C26-C25-C24	2.33	129.96	123.20
35	6	302	LMT	O5'-C5'-C4'	2.33	114.55	109.72
38	8	307	KC1	CAC-C3C-C4C	2.33	127.83	124.79
30	1	305	CLA	CMB-C2B-C1B	2.33	128.97	125.42
30	8	301	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
38	2	314	KC1	CHB-C4A-NA	2.33	127.85	124.23
30	11	308	CLA	CHB-C1B-C2B	-2.33	120.65	127.43
30	15	311	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
30	A	835	CLA	CBB-CAB-C3B	-2.33	115.87	127.53
30	B	839	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
30	10	308	CLA	CMB-C2B-C1B	2.33	128.97	125.42
30	15	311	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
30	16	306	CLA	CHD-C4C-NC	2.33	127.85	124.23
33	A	851	BCR	C10-C11-C12	-2.33	116.44	123.20
38	1	308	KC1	CED-O2D-CGD	2.33	121.20	115.92
38	13	311	KC1	O2D-CGD-O1D	-2.33	119.31	123.85
30	B	829	CLA	C1-C2-C3	-2.33	122.38	126.20
30	B	809	CLA	CMB-C2B-C1B	2.33	128.97	125.42
39	10	314	DD6	O1-C20-C21	-2.33	112.44	115.05
30	5	304	CLA	CAA-C2A-C3A	-2.33	106.70	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	311	CLA	CBC-CAC-C3C	-2.33	106.11	112.42
30	5	303	CLA	CED-O2D-CGD	2.33	121.20	115.92
30	A	812	CLA	CMC-C2C-C1C	2.33	128.67	125.03
30	2u	202	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
30	A	816	CLA	C1-O2A-CGA	2.33	122.29	116.65
30	B	834	CLA	CMB-C2B-C3B	2.33	132.03	126.55
30	16	303	CLA	CAC-C3C-C4C	2.33	127.82	124.79
37	11	301	A86	C4-C3-C2	-2.33	118.76	123.52
37	15	322	A86	O-C13-C14	-2.33	116.99	121.76
37	3	315	A86	C35-C34-C33	2.33	114.07	109.89
30	15	306	CLA	CHB-C4A-NA	2.33	127.76	124.40
38	7	308	KC1	CMB-C2B-C1B	2.33	128.82	124.73
30	B	813	CLA	CHD-C4C-NC	2.33	127.84	124.23
30	13	309	CLA	CED-O2D-CGD	2.33	121.19	115.92
30	6	316	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
30	15	314	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
30	7	311	CLA	CMB-C2B-C1B	2.32	128.96	125.42
30	A	826	CLA	CHB-C4A-NA	2.32	127.75	124.40
35	9	317	LMT	C1B-O1B-C4'	-2.32	112.47	117.98
30	A	836	CLA	CED-O2D-CGD	2.32	121.19	115.92
30	A	806	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
30	2	301	CLA	C4-C3-C5	2.32	119.26	115.23
36	6	301	LMG	O6-C1-O1	-2.32	104.55	110.04
33	B	843	BCR	C27-C26-C25	2.32	125.84	122.70
36	B	847	LMG	O2-C2-C1	-2.32	104.54	110.08
38	12	309	KC1	CMC-C2C-C1C	2.32	128.67	125.03
38	11	312	KC1	CAA-CBA-CGA	-2.32	115.23	127.05
34	A	853	LHG	C11-C10-C9	-2.32	102.62	114.37
30	12	321	CLA	CMB-C2B-C1B	2.32	128.96	125.42
37	15	322	A86	C12-C11-C13	2.32	119.77	116.00
30	13	307	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	J	101	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
38	1	306	KC1	O2D-CGD-O1D	-2.32	119.33	123.85
30	10	305	CLA	O2A-CGA-CBA	2.32	118.92	111.83
39	13	314	DD6	C4-C3-C2	-2.32	118.77	123.52
37	3	315	A86	C34-O4-C38	-2.32	113.75	117.85
36	2u	204	LMG	O3-C3-C2	-2.32	104.90	110.38
33	B	841	BCR	C30-C25-C26	-2.32	119.46	122.64
30	9	303	CLA	C4-C3-C5	2.32	119.26	115.23
38	11	305	KC1	O2D-CGD-O1D	-2.32	119.33	123.85
30	5	311	CLA	CHB-C4A-NA	2.32	127.75	124.40
37	2u	203	A86	O4-C38-O5	-2.32	118.51	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	844	CLA	CED-O2D-CGD	2.32	121.18	115.92
30	10	307	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
30	A	807	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
30	A	837	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	14	312	CLA	CHB-C4A-NA	2.32	127.75	124.40
37	3	315	A86	C-C1-C24	2.32	121.63	118.09
30	15	313	CLA	CHB-C4A-NA	2.32	127.75	124.40
33	L	205	BCR	C7-C8-C9	-2.32	122.81	126.23
30	10	304	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
30	B	816	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
30	A	821	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	4	302	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	A	805	CLA	CHB-C1B-C2B	-2.32	120.70	127.43
30	9	307	CLA	O2A-CGA-CBA	2.32	118.90	111.83
30	B	818	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
30	4	311	CLA	CMC-C2C-C1C	2.32	128.66	125.03
39	8	317	DD6	C4-C3-C2	-2.32	118.78	123.52
30	A	818	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
30	B	806	CLA	CHB-C4A-NA	2.32	127.74	124.40
30	9	309	CLA	C4-C3-C5	2.32	119.25	115.23
34	5	317	LHG	C11-C10-C9	-2.32	102.66	114.37
30	2	308	CLA	CBA-CAA-C2A	2.32	120.68	113.79
30	12	306	CLA	CMC-C2C-C1C	2.32	128.65	125.03
30	A	807	CLA	CHB-C4A-NA	2.32	127.74	124.40
39	1	310	DD6	C15-C14-C13	-2.32	121.10	125.99
37	14	316	A86	C3-C4-C5	-2.32	118.78	123.52
39	7	317	DD6	C23-C16-C17	-2.31	104.90	108.97
30	9	309	CLA	C1-C2-C3	-2.31	122.41	126.20
30	B	823	CLA	CHB-C4A-NA	2.31	127.74	124.40
30	4	309	CLA	CHB-C4A-NA	2.31	127.74	124.40
38	4	307	KC1	CAA-C2A-C1A	-2.31	114.51	124.64
37	16	314	A86	C26-C25-C24	-2.31	116.50	123.20
30	B	822	CLA	CED-O2D-CGD	2.31	121.16	115.92
30	A	819	CLA	CBA-CAA-C2A	2.31	120.67	113.79
38	13	312	KC1	CHB-C4A-NA	2.31	127.82	124.23
30	B	816	CLA	CHB-C4A-NA	2.31	127.74	124.40
30	7	312	CLA	CHB-C4A-NA	2.31	127.74	124.40
30	10	305	CLA	CMC-C2C-C1C	2.31	128.65	125.03
30	15	302	CLA	C4-C3-C5	2.31	119.24	115.23
30	6	305	CLA	CHB-C4A-NA	2.31	127.73	124.40
30	12	306	CLA	O2A-CGA-CBA	2.31	118.88	111.83
38	14	308	KC1	CAC-C3C-C4C	2.31	127.80	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	L	201	BCR	C16-C17-C18	-2.31	124.04	127.28
30	B	818	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
30	A	826	CLA	CHA-C1A-NA	-2.31	121.16	126.39
37	15	323	A86	C36-C31-C32	-2.31	117.40	119.70
30	A	834	CLA	CHB-C4A-NA	2.31	127.73	124.40
30	15	303	CLA	CMC-C2C-C1C	2.31	128.64	125.03
30	15	312	CLA	C4C-C3C-C2C	-2.31	103.53	106.89
38	5	310	KC1	O1D-CGD-CBD	-2.31	119.96	124.52
30	7	303	CLA	C6-C7-C8	-2.31	108.29	115.97
30	B	830	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
38	9	310	KC1	CHB-C4A-NA	2.31	127.81	124.23
35	7	321	LMT	C1B-O1B-C4'	-2.31	112.51	117.98
30	15	308	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
30	14	309	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
30	B	851	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
30	8	302	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
30	7	310	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
30	A	827	CLA	O2A-CGA-CBA	2.31	118.87	111.83
30	A	806	CLA	CMB-C2B-C3B	2.31	131.98	126.55
37	10	317	A86	C12-C11-C10	-2.31	118.06	123.67
30	12	302	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
38	4	307	KC1	CHB-C1B-NB	-2.31	121.56	124.80
38	14	308	KC1	O2A-CGA-O1A	-2.31	118.01	122.70
30	F	202	CLA	CMC-C2C-C1C	2.31	128.64	125.03
30	A	829	CLA	CHB-C1B-C2B	-2.30	120.74	127.43
30	A	830	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
37	6	320	A86	C3-C2-C1	-2.30	124.05	127.28
30	1	307	CLA	CMC-C2C-C1C	2.30	128.63	125.03
38	5	305	KC1	O2D-CGD-O1D	-2.30	119.36	123.85
36	5	318	LMG	O1-C7-C8	-2.30	105.21	110.82
30	A	803	CLA	CMC-C2C-C1C	2.30	128.63	125.03
30	L	202	CLA	CAA-C2A-C3A	-2.30	106.77	113.00
36	8	320	LMG	O2-C2-C1	-2.30	104.59	110.08
30	7	309	CLA	O2A-CGA-CBA	2.30	118.86	111.83
30	7	306	CLA	C4-C3-C5	2.30	119.23	115.23
33	B	841	BCR	C15-C14-C13	-2.30	124.05	127.28
37	15	317	A86	C-C1-C24	2.30	121.61	118.09
30	7	305	CLA	CAC-C3C-C4C	2.30	127.78	124.79
38	8	310	KC1	C3D-C2D-C1D	-2.30	99.05	106.40
30	B	851	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
30	A	830	CLA	CHB-C1B-C2B	-2.30	120.75	127.43
38	7	313	KC1	CMC-C2C-C1C	2.30	128.63	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	849	BCR	C16-C17-C18	-2.30	124.05	127.28
38	8	311	KC1	CAA-C2A-C1A	-2.30	114.56	124.64
31	A	845	PQN	C11-C3-C2	-2.30	120.95	124.89
33	2u	201	BCR	C7-C8-C9	-2.30	122.83	126.23
38	9	304	KC1	O2D-CGD-O1D	-2.30	119.37	123.85
38	10	310	KC1	CHC-C4B-NB	-2.30	121.57	124.80
37	2u	203	A86	C3-C4-C5	-2.30	118.81	123.52
30	A	827	CLA	CBC-CAC-C3C	-2.30	106.19	112.42
37	14	318	A86	C10-C9-C8	-2.30	116.54	123.20
30	B	809	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
37	14	301	A86	C25-C24-C1	-2.30	120.06	126.36
37	10	301	A86	C25-C24-C1	2.30	132.66	126.36
37	7	316	A86	C34-O4-C38	-2.30	113.79	117.85
38	5	306	KC1	CMB-C2B-C1B	2.30	128.77	124.73
36	14	321	LMG	O3-C3-C2	-2.30	104.96	110.38
37	11	315	A86	C-C1-C24	2.30	121.60	118.09
38	5	312	KC1	CBC-CAC-C3C	-2.30	106.19	112.42
33	A	849	BCR	C38-C26-C27	-2.30	108.70	113.60
38	2	312	KC1	CMC-C2C-C1C	2.30	128.62	125.03
30	14	302	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
30	2u	202	CLA	CHB-C4A-NA	2.30	127.71	124.40
30	3	302	CLA	O2A-CGA-CBA	2.30	118.84	111.83
30	13	309	CLA	CMC-C2C-C1C	2.30	128.62	125.03
38	6	312	KC1	CMC-C2C-C1C	2.30	128.62	125.03
30	B	803	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
30	16	305	CLA	CMC-C2C-C1C	2.29	128.62	125.03
38	12	313	KC1	C3D-C2D-C1D	-2.29	99.07	106.40
39	6	303	DD6	C4-C3-C2	-2.29	118.82	123.52
30	A	814	CLA	C1-C2-C3	-2.29	122.44	126.20
33	L	205	BCR	C27-C26-C25	2.29	125.80	122.70
38	9	312	KC1	CBA-CAA-C2A	-2.29	116.25	125.45
30	1	303	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
30	1	307	CLA	O1D-CGD-CBD	-2.29	119.99	124.52
30	1	302	CLA	CMC-C2C-C1C	2.29	128.62	125.03
30	16	303	CLA	CMC-C2C-C1C	2.29	128.62	125.03
34	9	318	LHG	C11-C10-C9	-2.29	102.78	114.37
37	14	315	A86	C-C1-C24	2.29	121.59	118.09
30	2	310	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
37	9	315	A86	C7-C6-C8	2.29	121.59	118.09
30	13	302	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
30	B	815	CLA	CHD-C4C-NC	2.29	127.78	124.23
39	16	313	DD6	C3-C4-C5	-2.29	118.83	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	308	CLA	C1-C2-C3	-2.29	122.44	126.20
37	3	314	A86	C7-C6-C5	-2.29	119.10	122.82
38	9	312	KC1	CHB-C4A-NA	2.29	127.78	124.23
30	A	844	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
30	A	842	CLA	CMA-C3A-C2A	-2.29	105.12	113.98
37	10	315	A86	C7-C6-C8	2.29	121.59	118.09
30	9	305	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
30	1	303	CLA	CMB-C2B-C1B	2.29	128.91	125.42
30	14	307	CLA	CMC-C2C-C1C	2.29	128.61	125.03
30	B	807	CLA	C4-C3-C5	2.29	119.20	115.23
30	B	839	CLA	C4-C3-C5	2.29	119.20	115.23
38	16	311	KC1	CHB-C1B-NB	-2.29	121.58	124.80
30	15	305	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
30	14	302	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
37	2	318	A86	C3-C4-C5	-2.29	118.84	123.52
37	14	316	A86	C25-C24-C1	-2.29	120.09	126.36
30	A	838	CLA	C4-C3-C5	2.29	118.82	116.13
30	14	309	CLA	CHB-C4A-NA	2.29	127.70	124.40
30	A	840	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
30	A	827	CLA	OBD-CAD-C3D	-2.29	123.07	128.42
38	11	305	KC1	CMC-C2C-C1C	2.29	128.61	125.03
33	A	850	BCR	C16-C15-C14	-2.29	118.84	123.52
38	14	308	KC1	CHB-C4A-NA	2.29	127.78	124.23
30	14	304	CLA	CMC-C2C-C1C	2.28	128.60	125.03
30	F	202	CLA	CHA-C1A-NA	-2.28	121.22	126.39
38	13	312	KC1	CMC-C2C-C1C	2.28	128.60	125.03
30	8	301	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
36	14	321	LMG	O2-C2-C1	-2.28	104.64	110.08
38	11	311	KC1	O2D-CGD-O1D	-2.28	119.41	123.85
30	8	303	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
30	8	309	CLA	CMB-C2B-C1B	2.28	128.89	125.42
38	6	311	KC1	CHB-C4A-NA	2.28	127.77	124.23
33	B	843	BCR	C11-C10-C9	-2.28	124.08	127.28
30	B	805	CLA	CBA-CAA-C2A	2.28	120.58	113.79
38	8	314	KC1	CMC-C2C-C1C	2.28	128.60	125.03
30	12	308	CLA	CHB-C4A-NA	2.28	127.69	124.40
30	B	833	CLA	CHA-C1A-NA	-2.28	121.23	126.39
30	A	809	CLA	C4-C3-C5	2.28	119.19	115.23
37	11	315	A86	C35-C34-C33	2.28	113.98	109.89
30	A	840	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
30	12	312	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
30	7	305	CLA	OBD-CAD-C3D	-2.28	123.09	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	303	CLA	CHD-C4C-NC	2.28	127.77	124.23
30	7	309	CLA	CBC-CAC-C3C	-2.28	106.24	112.42
30	B	837	CLA	CHB-C4A-NA	2.28	127.69	124.40
38	5	305	KC1	CMC-C2C-C1C	2.28	128.59	125.03
30	9	301	CLA	CHD-C4C-NC	2.28	127.76	124.23
30	A	838	CLA	CHA-C1A-NA	-2.28	121.23	126.39
38	13	306	KC1	C3D-C2D-C1D	-2.28	99.13	106.40
30	A	809	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
37	16	314	A86	C9-C10-C11	-2.28	120.20	126.64
30	14	312	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
30	2	305	CLA	CHB-C4A-NA	2.28	127.69	124.40
30	7	306	CLA	CHD-C4C-NC	2.28	127.76	124.23
30	4	303	CLA	CMC-C2C-C1C	2.28	128.59	125.03
38	12	311	KC1	C3D-C2D-C1D	-2.28	99.13	106.40
30	13	303	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
30	B	832	CLA	O2A-CGA-CBA	2.28	118.77	111.83
39	7	317	DD6	C14-C13-C11	-2.28	122.00	125.53
38	10	306	KC1	CBC-CAC-C3C	-2.28	106.25	112.42
30	11	309	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
30	A	815	CLA	C4-C3-C5	2.28	119.18	115.23
30	16	308	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
38	8	314	KC1	C3D-C2D-C1D	-2.27	99.14	106.40
37	5	316	A86	C10-C9-C8	-2.27	116.61	123.20
30	15	312	CLA	CHB-C1B-C2B	-2.27	120.83	127.43
30	6	316	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
30	11	310	CLA	CHB-C4A-NA	2.27	127.68	124.40
30	6	316	CLA	CED-O2D-CGD	2.27	121.07	115.92
30	7	310	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
30	4	303	CLA	CHD-C4C-NC	2.27	127.76	124.23
30	B	819	CLA	CMB-C2B-C1B	2.27	128.88	125.42
30	13	301	CLA	O2A-CGA-CBA	2.27	118.77	111.83
39	8	316	DD6	C33-C32-C31	2.27	113.97	109.49
30	6	304	CLA	CHB-C4A-NA	2.27	127.68	124.40
30	B	822	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
30	13	303	CLA	CBA-CAA-C2A	2.27	120.55	113.79
30	9	302	CLA	CBC-CAC-C3C	-2.27	106.26	112.42
36	7	320	LMG	O1-C7-C8	-2.27	105.29	110.82
30	F	201	CLA	C4-C3-C5	2.27	119.17	115.23
30	15	303	CLA	CBC-CAC-C3C	-2.27	106.26	112.42
38	4	307	KC1	CHB-C4A-NA	2.27	127.75	124.23
35	1	311	LMT	O1B-C4'-C3'	2.27	113.00	107.23
30	15	302	CLA	C11-C12-C13	-2.27	108.42	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	301	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
38	13	306	KC1	O1D-CGD-CBD	-2.27	120.04	124.52
38	1	308	KC1	CHB-C4A-NA	2.27	127.75	124.23
37	10	316	A86	C19-C18-C17	-2.27	106.55	110.79
30	3	307	CLA	CHA-C1A-NA	-2.27	121.25	126.39
30	B	838	CLA	CMB-C2B-C1B	2.27	128.87	125.42
30	B	851	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
30	13	303	CLA	C4-C3-C5	2.27	119.17	115.23
38	5	310	KC1	CBC-CAC-C3C	-2.27	106.27	112.42
30	B	838	CLA	C1-C2-C3	-2.27	122.48	126.20
30	11	309	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
30	12	304	CLA	CMB-C2B-C1B	2.27	128.87	125.42
30	A	807	CLA	CHA-C1A-NA	-2.27	121.26	126.39
30	A	816	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
30	11	308	CLA	C1-C2-C3	-2.27	122.48	126.20
30	B	817	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
30	11	306	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
33	J	103	BCR	C15-C16-C17	-2.27	118.88	123.52
39	3	312	DD6	C3-C4-C5	-2.27	118.88	123.52
30	14	303	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
30	11	306	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
38	11	311	KC1	CMC-C2C-C1C	2.27	128.57	125.03
30	A	833	CLA	CED-O2D-CGD	2.27	121.05	115.92
30	16	302	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
38	6	313	KC1	O2D-CGD-O1D	-2.27	119.44	123.85
37	15	316	A86	O-C13-C11	-2.26	116.16	121.04
37	14	320	A86	C7-C6-C8	2.26	121.55	118.09
30	16	310	CLA	CMC-C2C-C1C	2.26	128.57	125.03
38	12	309	KC1	O1D-CGD-CBD	-2.26	120.05	124.52
30	B	829	CLA	CBC-CAC-C3C	-2.26	106.28	112.42
37	14	301	A86	C34-O4-C38	-2.26	113.85	117.85
30	3	309	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
30	16	301	CLA	CMB-C2B-C1B	2.26	128.87	125.42
38	8	310	KC1	O2D-CGD-O1D	-2.26	119.44	123.85
30	13	303	CLA	CMC-C2C-C1C	2.26	128.57	125.03
38	1	308	KC1	CBC-CAC-C3C	-2.26	106.29	112.42
30	A	812	CLA	CHB-C4A-NA	2.26	127.67	124.40
30	9	308	CLA	CBC-CAC-C3C	-2.26	106.29	112.42
30	10	311	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
30	16	309	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
33	B	842	BCR	C28-C27-C26	-2.26	110.03	114.06
30	16	307	CLA	CMC-C2C-C1C	2.26	128.57	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	309	CLA	CMB-C2B-C1B	2.26	128.86	125.42
30	9	302	CLA	CMC-C2C-C1C	2.26	128.56	125.03
30	B	820	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
30	16	310	CLA	CHB-C4A-NA	2.26	127.66	124.40
30	7	306	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
38	11	312	KC1	CBC-CAC-C3C	-2.26	106.30	112.42
38	8	312	KC1	CMC-C2C-C1C	2.26	128.56	125.03
39	8	317	DD6	C3-C4-C5	-2.26	118.90	123.52
38	14	311	KC1	CBC-CAC-C3C	-2.26	106.30	112.42
30	A	842	CLA	CMB-C2B-C1B	2.26	128.86	125.42
30	12	312	CLA	CHB-C4A-NA	2.26	127.66	124.40
30	B	832	CLA	CMB-C2B-C1B	2.26	128.86	125.42
30	A	806	CLA	C1-C2-C3	-2.26	122.50	126.20
37	11	315	A86	C12-C11-C13	2.26	119.66	116.00
30	3	302	CLA	CMA-C3A-C2A	-2.26	105.26	113.98
30	A	810	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
30	5	307	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
30	10	309	CLA	CHB-C4A-NA	2.26	127.66	124.40
30	A	839	CLA	CBA-CAA-C2A	2.26	120.50	113.79
30	16	303	CLA	C4-C3-C5	2.26	119.14	115.23
30	2	303	CLA	CBC-CAC-C3C	-2.26	106.31	112.42
36	A	856	LMG	O3-C3-C2	-2.25	105.06	110.38
30	B	809	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
30	16	307	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
37	7	316	A86	C21-C20-C15	-2.25	116.07	123.35
37	3	314	A86	C9-C8-C6	-2.25	120.18	126.36
30	7	310	CLA	CMC-C2C-C1C	2.25	128.56	125.03
33	J	102	BCR	C30-C25-C26	-2.25	119.56	122.64
39	6	303	DD6	C15-C14-C13	-2.25	121.23	125.99
30	4	303	CLA	C4-C3-C5	2.25	119.14	115.23
30	F	203	CLA	CHB-C4A-NA	2.25	127.65	124.40
38	7	313	KC1	CBA-CAA-C2A	-2.25	116.41	125.45
30	13	303	CLA	O2A-CGA-CBA	2.25	118.70	111.83
30	B	819	CLA	O2A-CGA-CBA	2.25	118.70	111.83
37	2u	203	A86	C41-C32-C31	-2.25	108.46	110.47
30	15	311	CLA	CHB-C4A-NA	2.25	127.65	124.40
30	14	302	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
33	L	204	BCR	C20-C21-C22	-2.25	124.12	127.28
30	F	202	CLA	C1-C2-C3	-2.25	122.51	126.20
30	B	825	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
30	F	202	CLA	C4-C3-C5	2.25	119.13	115.23
30	2	308	CLA	CHB-C1B-C2B	-2.25	120.90	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	9	316	A86	C19-C18-C17	2.25	115.00	110.79
30	2	305	CLA	CMB-C2B-C1B	2.25	128.84	125.42
30	6	310	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
30	4	305	CLA	C3B-C4B-NB	2.25	112.54	110.53
30	B	812	CLA	CMB-C2B-C3B	2.25	131.84	126.55
30	7	312	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
30	14	303	CLA	C4-C3-C5	2.25	119.13	115.23
38	8	310	KC1	CHB-C4A-NA	2.25	127.72	124.23
30	A	820	CLA	CBC-CAC-C3C	-2.25	106.33	112.42
37	11	314	A86	C7-C6-C5	-2.25	119.17	122.82
33	A	847	BCR	C15-C16-C17	-2.25	118.92	123.52
30	11	306	CLA	C3B-C4B-NB	2.25	112.54	110.53
39	6	321	DD6	C23-C16-C17	-2.25	105.02	108.97
30	A	811	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
30	12	307	CLA	CHB-C4A-NA	2.25	127.64	124.40
30	14	304	CLA	O2D-CGD-O1D	-2.25	119.48	123.85
30	B	821	CLA	O2A-C1-C2	2.25	116.75	108.11
38	14	308	KC1	O1D-CGD-CBD	-2.25	120.09	124.52
30	A	810	CLA	CED-O2D-CGD	2.25	121.01	115.92
30	A	808	CLA	C1-C2-C3	-2.25	122.52	126.20
30	15	307	CLA	O2D-CGD-O1D	-2.25	119.48	123.85
30	B	823	CLA	C1-O2A-CGA	2.24	122.08	116.65
38	12	311	KC1	O1D-CGD-CBD	-2.24	120.09	124.52
30	A	831	CLA	C1-C2-C3	-2.24	122.52	126.20
38	5	305	KC1	CAA-C2A-C1A	-2.24	114.81	124.64
39	12	315	DD6	C33-C32-C31	2.24	113.91	109.49
30	12	310	CLA	CHB-C4A-NA	2.24	127.64	124.40
30	6	306	CLA	CMC-C2C-C1C	2.24	128.54	125.03
30	14	303	CLA	O2A-CGA-CBA	2.24	118.67	111.83
37	3	315	A86	C3-C2-C1	-2.24	124.14	127.28
37	15	323	A86	C24-C1-C2	-2.24	115.48	119.01
30	10	305	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
38	3	308	KC1	CHB-C4A-NA	2.24	127.71	124.23
30	B	821	CLA	CHB-C1B-C2B	-2.24	120.92	127.43
38	11	311	KC1	CBC-CAC-C3C	-2.24	106.35	112.42
38	9	310	KC1	CAA-C2A-C1A	-2.24	114.83	124.64
30	4	301	CLA	O2A-CGA-CBA	2.24	118.66	111.83
30	15	313	CLA	CMB-C2B-C1B	2.24	128.83	125.42
30	B	803	CLA	C4B-C3B-C2B	-2.24	104.52	107.30
30	2	313	CLA	CMC-C2C-C1C	2.24	128.53	125.03
30	B	814	CLA	C4-C3-C5	2.24	119.11	115.23
30	16	308	CLA	CHB-C4A-NA	2.24	127.63	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	321	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
30	L	202	CLA	CMC-C2C-C1C	2.24	128.53	125.03
38	13	306	KC1	CMC-C2C-C1C	2.24	128.53	125.03
30	A	831	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
30	B	834	CLA	CMC-C2C-C1C	2.24	128.53	125.03
30	12	308	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
35	8	322	LMT	C2'-C3'-C4'	2.24	114.76	109.68
30	B	828	CLA	C4-C3-C5	2.24	119.11	115.23
30	B	822	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
30	A	841	CLA	CMB-C2B-C3B	2.24	131.81	126.55
30	A	819	CLA	CHA-C1A-NA	-2.24	121.33	126.39
39	5	313	DD6	C10-C9-C8	-2.24	116.72	123.20
30	A	822	CLA	C1-O2A-CGA	2.24	122.06	116.65
30	L	203	CLA	CHB-C4A-NA	2.24	127.63	124.40
30	B	817	CLA	C4-C3-C5	2.24	119.11	115.23
30	A	815	CLA	CHA-C1A-NA	-2.23	121.33	126.39
39	8	316	DD6	C40-C32-C31	-2.23	106.52	110.52
30	B	810	CLA	O2A-CGA-CBA	2.23	118.64	111.83
30	16	302	CLA	CED-O2D-CGD	2.23	120.98	115.92
30	A	844	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
30	14	313	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
30	14	305	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
33	A	849	BCR	C11-C10-C9	-2.23	124.15	127.28
30	9	301	CLA	O2A-CGA-CBA	2.23	118.64	111.83
30	A	835	CLA	C4B-C3B-C2B	-2.23	104.53	107.30
30	7	309	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
38	14	306	KC1	CHB-C1B-C2B	-2.23	120.84	125.49
38	13	312	KC1	O2D-CGD-O1D	-2.23	119.50	123.85
30	15	312	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
30	12	321	CLA	CHB-C4A-NA	2.23	127.62	124.40
39	15	319	DD6	C9-C8-C6	-2.23	120.25	126.36
30	14	302	CLA	C4-C3-C2	-2.23	117.90	123.63
30	7	311	CLA	CHB-C4A-NA	2.23	127.62	124.40
38	5	312	KC1	CHB-C4A-NA	2.23	127.69	124.23
30	B	820	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
30	A	837	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
37	4	314	A86	C36-C31-C32	-2.23	117.48	119.70
37	13	313	A86	C3-C2-C1	-2.23	124.15	127.28
38	8	311	KC1	C3D-C2D-C1D	-2.23	99.28	106.40
36	2u	204	LMG	O2-C2-C1	-2.23	104.76	110.08
30	F	201	CLA	C11-C10-C8	-2.23	108.56	115.97
30	1	305	CLA	O2D-CGD-O1D	-2.23	119.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	301	CLA	CBA-CAA-C2A	2.23	120.42	113.79
38	11	305	KC1	C3D-C2D-C1D	-2.23	99.28	106.40
33	B	845	BCR	C16-C15-C14	-2.23	118.96	123.52
38	6	308	KC1	C3D-C2D-C1D	-2.23	99.29	106.40
30	B	827	CLA	CBC-CAC-C3C	-2.23	106.38	112.42
38	8	312	KC1	C3D-C2D-C1D	-2.23	99.29	106.40
38	12	313	KC1	CHB-C1B-NB	-2.23	121.67	124.80
38	11	311	KC1	CHB-C4A-NA	2.23	127.68	124.23
30	A	836	CLA	CMC-C2C-C1C	2.23	128.51	125.03
30	3	307	CLA	C1-O2A-CGA	2.22	122.04	116.65
30	A	802	CLA	CHD-C4C-NC	2.22	127.68	124.23
30	8	304	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
30	B	825	CLA	CHB-C4A-NA	2.22	127.61	124.40
30	15	312	CLA	CHB-C4A-NA	2.22	127.61	124.40
30	7	309	CLA	CMC-C2C-C1C	2.22	128.51	125.03
30	13	307	CLA	CMC-C2C-C1C	2.22	128.51	125.03
30	A	830	CLA	CED-O2D-CGD	2.22	120.96	115.92
30	8	308	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
37	14	314	A86	C35-C34-C33	2.22	113.88	109.89
39	6	321	DD6	C3-C4-C5	-2.22	118.97	123.52
30	A	827	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
30	B	803	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
38	13	306	KC1	CHB-C4A-NA	2.22	127.68	124.23
30	12	307	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
36	B	849	LMG	C1-C2-C3	-2.22	105.33	110.01
37	8	315	A86	C8-C6-C5	-2.22	115.51	119.01
30	B	813	CLA	CHA-C1A-NA	-2.22	121.36	126.39
30	1	302	CLA	O2A-CGA-CBA	2.22	118.61	111.83
39	7	314	DD6	C23-C16-C22	-2.22	104.14	107.37
37	8	318	A86	O-C13-C11	-2.22	116.26	121.04
37	15	320	A86	C4-C3-C2	2.22	128.06	123.52
30	7	304	CLA	O2A-CGA-CBA	2.22	118.61	111.83
30	9	301	CLA	CHB-C4A-NA	2.22	127.61	124.40
38	14	311	KC1	CHB-C4A-NA	2.22	127.68	124.23
33	B	843	BCR	C24-C23-C22	-2.22	122.95	126.23
30	10	305	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
30	15	312	CLA	CMC-C2C-C1C	2.22	128.50	125.03
33	B	843	BCR	C40-C30-C25	2.22	113.72	110.24
30	4	303	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
30	B	828	CLA	CBC-CAC-C3C	-2.22	106.41	112.42
30	B	835	CLA	CAC-C3C-C4C	2.22	127.68	124.79
38	8	313	KC1	C3D-C2D-C1D	-2.22	99.32	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	814	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
38	8	306	KC1	CAC-C3C-C4C	2.22	127.67	124.79
30	A	838	CLA	CMC-C2C-C1C	2.22	128.50	125.03
30	11	308	CLA	C1-O2A-CGA	2.22	122.02	116.65
36	3	317	LMG	O3-C3-C2	-2.22	105.15	110.38
38	7	308	KC1	C3D-C2D-C1D	-2.22	99.32	106.40
30	3	302	CLA	C4-C3-C5	2.22	119.08	115.23
30	B	851	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
37	14	315	A86	C21-C20-C15	-2.22	116.19	123.35
38	10	312	KC1	O2D-CGD-O1D	-2.22	119.53	123.85
38	5	306	KC1	CMC-C2C-C1C	2.22	128.50	125.03
35	A	854	LMT	O3'-C3'-C2'	-2.22	105.15	110.38
30	6	314	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
30	B	810	CLA	CHB-C4A-NA	2.21	127.60	124.40
30	6	307	CLA	CHB-C4A-NA	2.21	127.60	124.40
30	B	805	CLA	CMB-C2B-C1B	2.21	128.79	125.42
30	B	811	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
30	8	308	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
30	11	310	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
38	11	307	KC1	CHB-C4A-NA	2.21	127.66	124.23
33	B	842	BCR	C30-C25-C26	-2.21	119.61	122.64
37	8	315	A86	O4-C38-O5	-2.21	118.72	122.99
30	9	301	CLA	CMB-C2B-C3B	2.21	131.75	126.55
30	1	303	CLA	CHB-C1B-C2B	-2.21	121.00	127.43
30	6	305	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
30	B	808	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
38	12	313	KC1	CBC-CAC-C3C	-2.21	106.42	112.42
30	B	831	CLA	C1-O2A-CGA	2.21	122.00	116.65
38	8	310	KC1	CHC-C1C-NC	2.21	127.66	124.23
35	11	302	LMT	C1B-O1B-C4'	-2.21	112.74	117.98
30	A	835	CLA	CHB-C1B-C2B	-2.21	121.01	127.43
30	15	304	CLA	CHB-C1B-C2B	-2.21	121.01	127.43
30	A	838	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
37	7	316	A86	C23-C16-C22	-2.21	104.16	107.37
39	5	314	DD6	C23-C16-C15	2.21	116.01	110.05
30	10	309	CLA	CED-O2D-CGD	2.21	120.93	115.92
30	A	829	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
30	5	308	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
30	9	308	CLA	CHA-C1A-NA	-2.21	121.39	126.39
37	11	315	A86	C22-C16-C17	-2.21	105.09	108.97
38	7	313	KC1	C3D-C2D-C1D	-2.21	99.35	106.40
30	12	307	CLA	CMA-C3A-C4A	-2.21	105.84	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	308	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
33	F	204	BCR	C16-C15-C14	-2.21	119.00	123.52
30	4	311	CLA	C5-C3-C4	2.21	119.67	114.59
30	6	304	CLA	CMA-C3A-C2A	-2.21	105.45	113.98
38	13	305	KC1	CAB-C3B-C4B	2.21	130.09	124.82
30	A	840	CLA	CHA-C1A-NA	-2.21	121.39	126.39
39	3	316	DD6	C3-C4-C5	-2.21	119.00	123.52
30	3	307	CLA	C4-C3-C5	2.21	119.06	115.23
30	12	304	CLA	CMC-C2C-C1C	2.21	128.48	125.03
30	3	305	CLA	CHA-C1A-NA	-2.21	121.40	126.39
30	9	305	CLA	CMB-C2B-C1B	2.21	128.78	125.42
37	5	315	A86	C34-O4-C38	-2.21	113.95	117.85
30	B	811	CLA	CBC-CAC-C3C	-2.21	106.44	112.42
30	14	309	CLA	CHA-C1A-NA	-2.20	121.40	126.39
37	8	318	A86	C7-C6-C5	2.20	126.39	122.82
37	5	316	A86	C7-C6-C8	2.20	121.46	118.09
30	8	305	CLA	C11-C10-C8	-2.20	108.64	115.97
38	11	312	KC1	C3D-C2D-C1D	-2.20	99.36	106.40
37	13	315	A86	C3-C4-C5	-2.20	119.01	123.52
30	6	309	CLA	CBA-CAA-C2A	2.20	120.35	113.79
30	B	830	CLA	CHA-C1A-NA	-2.20	121.40	126.39
30	A	805	CLA	CMB-C2B-C3B	2.20	131.73	126.55
30	7	305	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
30	11	308	CLA	O2A-CGA-CBA	2.20	118.55	111.83
39	6	319	DD6	C23-C16-C22	-2.20	104.17	107.37
30	10	309	CLA	CMC-C2C-C1C	2.20	128.48	125.03
39	8	317	DD6	C33-C32-C31	2.20	113.83	109.49
30	B	812	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
33	B	843	BCR	C15-C14-C13	-2.20	124.19	127.28
30	15	310	CLA	CMB-C2B-C3B	2.20	131.73	126.55
30	A	815	CLA	CHC-C1C-NC	2.20	127.63	124.31
36	7	320	LMG	O8-C28-O10	-2.20	118.12	123.63
30	1	303	CLA	CMC-C2C-C1C	2.20	128.47	125.03
30	2	308	CLA	CBC-CAC-C3C	-2.20	106.45	112.42
30	7	310	CLA	CBA-CAA-C2A	2.20	120.34	113.79
30	4	309	CLA	CMC-C2C-C1C	2.20	128.47	125.03
30	A	831	CLA	CBC-CAC-C3C	-2.20	106.45	112.42
30	6	317	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
30	11	306	CLA	CHB-C1B-C2B	-2.20	121.04	127.43
30	14	305	CLA	CHB-C1B-C2B	-2.20	121.04	127.43
30	B	821	CLA	CHB-C4A-NA	2.20	127.57	124.40
30	B	801	CLA	O1D-CGD-CBD	-2.20	120.18	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	813	CLA	C1-C2-C3	-2.20	122.59	126.20
38	12	313	KC1	CGD-CBD-CAD	-2.20	103.73	110.85
30	B	830	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
30	13	302	CLA	CHB-C4A-NA	2.20	127.57	124.40
30	15	312	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
30	B	821	CLA	C4-C3-C5	2.20	119.04	115.23
38	16	311	KC1	CHB-C4A-NA	2.20	127.64	124.23
38	13	306	KC1	O2D-CGD-O1D	-2.20	119.57	123.85
30	B	819	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
37	16	312	A86	C22-C16-C17	-2.20	105.11	108.97
30	A	844	CLA	CMC-C2C-C1C	2.20	128.47	125.03
30	14	313	CLA	CMC-C2C-C1C	2.20	128.47	125.03
30	5	302	CLA	CHB-C4A-NA	2.20	127.57	124.40
30	A	835	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
37	11	314	A86	C-C1-C24	2.20	121.44	118.09
30	6	309	CLA	C1-C2-C3	-2.20	122.60	126.20
38	2	312	KC1	CAA-C2A-C1A	-2.20	115.02	124.64
30	B	819	CLA	C11-C10-C8	-2.20	108.67	115.97
39	10	314	DD6	C10-C9-C8	-2.19	116.84	123.20
38	12	311	KC1	CAB-C3B-C4B	2.19	130.06	124.82
30	B	818	CLA	C2A-C3A-C4A	-2.19	98.32	101.87
30	13	307	CLA	CHB-C1B-C2B	-2.19	121.06	127.43
30	1	303	CLA	O2A-CGA-CBA	2.19	118.52	111.83
39	8	317	DD6	C23-C16-C17	-2.19	105.11	108.97
30	6	304	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
30	B	803	CLA	CAC-C3C-C4C	2.19	127.64	124.79
30	2	313	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
37	11	314	A86	C8-C6-C5	2.19	122.46	119.01
30	16	306	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
38	13	311	KC1	C3D-C2D-C1D	-2.19	99.40	106.40
30	6	314	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
36	7	320	LMG	O3-C3-C2	-2.19	105.21	110.38
30	B	809	CLA	C1-C2-C3	-2.19	122.61	126.20
30	5	303	CLA	C1-O2A-CGA	2.19	121.95	116.65
30	16	301	CLA	C4-C3-C2	-2.19	118.00	123.63
38	14	306	KC1	CMB-C2B-C1B	2.19	128.59	124.73
30	15	302	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
30	9	305	CLA	C4-C3-C5	2.19	119.03	115.23
30	5	311	CLA	C1-C2-C3	-2.19	122.61	126.20
30	7	309	CLA	C1-C2-C3	-2.19	122.61	126.20
33	J	103	BCR	C33-C5-C6	-2.19	122.10	124.48
37	14	315	A86	C3-C4-C5	-2.19	119.04	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	6	313	KC1	CHB-C4A-NA	2.19	127.62	124.23
38	11	311	KC1	CMB-C2B-C1B	2.19	128.58	124.73
30	F	202	CLA	C1-O2A-CGA	2.19	121.94	116.65
39	7	318	DD6	C4-C3-C2	-2.19	119.04	123.52
37	1	309	A86	C-C1-C24	2.19	121.43	118.09
30	B	826	CLA	CHA-C1A-NA	-2.19	121.44	126.39
39	3	313	DD6	O1-C20-C21	-2.19	112.61	115.05
36	5	318	LMG	O2-C2-C1	-2.19	104.87	110.08
38	8	306	KC1	C3D-C2D-C1D	-2.19	99.42	106.40
30	A	811	CLA	O2A-CGA-CBA	2.19	118.50	111.83
30	11	306	CLA	O2A-CGA-CBA	2.19	118.50	111.83
38	13	308	KC1	O1D-CGD-CBD	-2.19	120.21	124.52
38	6	312	KC1	C3D-C2D-C1D	-2.18	99.42	106.40
30	B	823	CLA	C1-C2-C3	-2.18	122.62	126.20
38	11	307	KC1	C3D-C2D-C1D	-2.18	99.42	106.40
37	15	315	A86	C9-C10-C11	-2.18	120.46	126.64
38	5	310	KC1	CHB-C4A-NA	2.18	127.62	124.23
39	7	302	DD6	C23-C16-C22	-2.18	104.20	107.37
30	B	801	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
30	10	305	CLA	CHB-C4A-NA	2.18	127.55	124.40
38	4	308	KC1	C3D-C2D-C1D	-2.18	99.43	106.40
30	B	834	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
30	A	819	CLA	C4-C3-C5	2.18	119.02	115.23
38	11	305	KC1	CHB-C4A-NA	2.18	127.62	124.23
30	A	834	CLA	CMC-C2C-C1C	2.18	128.44	125.03
36	F	205	LMG	O3-C3-C2	-2.18	105.23	110.38
30	2	311	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
37	9	315	A86	C12-C11-C13	2.18	119.54	116.00
30	B	802	CLA	CHD-C4C-NC	2.18	127.61	124.23
30	B	835	CLA	C4-C3-C5	2.18	119.02	115.23
30	A	842	CLA	CHB-C4A-NA	2.18	127.55	124.40
37	8	315	A86	C3-C2-C1	-2.18	124.22	127.28
30	8	308	CLA	CBC-CAC-C3C	-2.18	106.51	112.42
30	2	309	CLA	CED-O2D-CGD	2.18	120.86	115.92
37	10	317	A86	C34-O4-C38	-2.18	113.99	117.85
30	6	307	CLA	CMB-C2B-C1B	2.18	128.74	125.42
30	A	810	CLA	CHB-C4A-NA	2.18	127.55	124.40
38	7	313	KC1	O2D-CGD-O1D	-2.18	119.61	123.85
30	6	310	CLA	CBC-CAC-C3C	-2.18	106.51	112.42
30	12	312	CLA	C4-C3-C5	2.18	119.01	115.23
30	16	307	CLA	CHB-C4A-NA	2.18	127.55	124.40
34	A	852	LHG	C20-C19-C18	-2.18	103.35	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	2u	203	A86	C-C1-C2	-2.18	119.29	122.82
34	B	848	LHG	O8-C23-O10	-2.18	118.18	123.63
38	13	310	KC1	CHB-C4A-NA	2.18	127.61	124.23
33	J	103	BCR	C10-C11-C12	-2.18	116.89	123.20
30	16	305	CLA	C5-C3-C4	2.18	119.60	114.59
33	2u	201	BCR	C10-C11-C12	-2.18	116.89	123.20
37	2	318	A86	C4-C3-C2	-2.18	119.06	123.52
38	6	312	KC1	CAB-C3B-C4B	2.18	130.02	124.82
37	15	315	A86	C12-C11-C10	-2.18	118.38	123.67
30	A	837	CLA	CAA-C2A-C3A	-2.18	107.12	113.00
30	2u	202	CLA	CAA-C2A-C3A	-2.18	107.12	113.00
30	3	306	CLA	C2A-C3A-C4A	-2.18	98.35	101.87
30	5	307	CLA	CBA-CAA-C2A	2.18	120.27	113.79
30	13	301	CLA	CBC-CAC-C3C	-2.18	106.52	112.42
38	4	310	KC1	CBC-CAC-C3C	-2.18	106.52	112.42
38	13	312	KC1	C3D-C2D-C1D	-2.18	99.45	106.40
30	1	304	CLA	CHB-C4A-NA	2.18	127.54	124.40
34	A	852	LHG	C27-C26-C25	-2.18	103.37	114.37
38	9	312	KC1	CAA-C2A-C1A	-2.18	115.11	124.64
30	B	834	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
30	16	306	CLA	O2D-CGD-O1D	-2.17	119.61	123.85
38	3	304	KC1	CAA-C2A-C1A	-2.17	115.12	124.64
30	16	309	CLA	CMC-C2C-C1C	2.17	128.43	125.03
37	15	315	A86	C26-C25-C24	2.17	129.50	123.20
37	14	316	A86	C7-C6-C8	2.17	121.41	118.09
30	10	308	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
30	10	311	CLA	CMC-C2C-C1C	2.17	128.43	125.03
30	A	825	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
30	B	826	CLA	CHB-C4A-NA	2.17	127.53	124.40
37	14	317	A86	C21-C20-C15	-2.17	116.34	123.35
30	15	307	CLA	C5-C3-C4	2.17	119.58	114.59
37	15	315	A86	O-C13-C14	-2.17	117.31	121.76
38	13	308	KC1	CHB-C4A-NA	2.17	127.59	124.23
38	11	312	KC1	CED-O2D-CGD	2.17	120.83	115.92
30	7	310	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
30	B	823	CLA	C4-C3-C5	2.17	118.99	115.23
37	2	318	A86	C34-O4-C38	-2.17	114.02	117.85
30	15	309	CLA	CBC-CAC-C3C	-2.17	106.55	112.42
30	B	812	CLA	C4-C3-C5	2.17	118.99	115.23
30	A	844	CLA	O2A-CGA-CBA	2.17	118.44	111.83
37	6	320	A86	O1-C15-C20	-2.17	57.61	59.45
30	B	826	CLA	CMC-C2C-C1C	2.17	128.42	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	313	CLA	CMC-C2C-C1C	2.17	128.42	125.03
36	5	318	LMG	O3-C3-C2	-2.17	105.27	110.38
37	14	315	A86	C8-C6-C5	2.16	122.41	119.01
30	7	303	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
30	1	302	CLA	CHB-C4A-NA	2.16	127.52	124.40
33	A	850	BCR	C20-C21-C22	-2.16	124.24	127.28
30	12	303	CLA	CHA-C1A-NA	-2.16	121.49	126.39
30	B	833	CLA	CMC-C2C-C1C	2.16	128.41	125.03
30	B	818	CLA	CHA-C1A-NA	-2.16	121.49	126.39
36	5	318	LMG	O1-C1-C2	-2.16	104.99	108.27
38	8	314	KC1	CHB-C1B-NB	-2.16	121.76	124.80
30	4	306	CLA	C1-C2-C3	-2.16	122.65	126.20
30	6	304	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
30	A	830	CLA	CMB-C2B-C1B	2.16	128.71	125.42
30	7	307	CLA	C6-C7-C8	-2.16	108.78	115.97
30	12	304	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
36	8	319	LMG	O1-C1-C2	-2.16	104.99	108.27
38	1	306	KC1	CMC-C2C-C1C	2.16	128.41	125.03
30	F	201	CLA	C3B-C4B-NB	2.16	112.46	110.53
30	12	303	CLA	CED-O2D-CGD	2.16	120.82	115.92
38	12	305	KC1	C3D-C2D-C1D	-2.16	99.50	106.40
30	A	839	CLA	C4-C3-C5	2.16	118.98	115.23
30	6	309	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
30	B	804	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
37	15	321	A86	C21-C20-C15	-2.16	116.38	123.35
30	A	830	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
36	8	320	LMG	O1-C1-C2	-2.16	104.99	108.27
38	12	311	KC1	O2A-CGA-O1A	-2.16	118.30	122.70
37	14	301	A86	C4-C3-C2	-2.16	119.10	123.52
37	15	316	A86	C19-C18-C17	2.16	114.83	110.79
30	J	101	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
30	2	308	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
30	16	306	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
30	A	836	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
30	15	311	CLA	CMC-C2C-C1C	2.16	128.41	125.03
38	2	314	KC1	C3D-C2D-C1D	-2.16	99.51	106.40
30	4	304	CLA	CAA-CBA-CGA	2.16	119.33	113.21
30	A	811	CLA	CMC-C2C-C1C	2.16	128.40	125.03
36	F	205	LMG	C9-C8-C7	-2.16	106.76	111.78
38	5	306	KC1	C3D-C2D-C1D	-2.16	99.51	106.40
36	3	317	LMG	C9-C8-C7	-2.16	106.76	111.78
30	13	304	CLA	CMC-C2C-C1C	2.16	128.40	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	307	CLA	CBC-CAC-C3C	-2.16	106.58	112.42
30	2	313	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
30	7	309	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
30	A	810	CLA	CAA-C2A-C1A	2.15	119.04	111.97
30	2	305	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
38	13	305	KC1	CMC-C2C-C1C	2.15	128.40	125.03
30	B	811	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
30	8	302	CLA	CHB-C4A-NA	2.15	127.51	124.40
30	15	305	CLA	O2A-CGA-CBA	2.15	120.81	114.00
30	B	825	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
30	13	302	CLA	CED-O2D-CGD	2.15	120.80	115.92
30	3	309	CLA	CHB-C4A-NA	2.15	127.51	124.40
30	A	822	CLA	O2A-CGA-CBA	2.15	118.40	111.83
39	15	318	DD6	C3-C4-C5	-2.15	119.11	123.52
30	5	303	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
30	2	310	CLA	CHA-C1A-NA	-2.15	121.52	126.39
30	7	312	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
37	2	318	A86	C7-C6-C8	2.15	121.37	118.09
38	6	311	KC1	C3D-C2D-C1D	-2.15	99.53	106.40
38	5	310	KC1	CMB-C2B-C1B	2.15	128.51	124.73
38	5	306	KC1	CBC-CAC-C3C	-2.15	106.59	112.42
38	1	306	KC1	C3D-C2D-C1D	-2.15	99.53	106.40
37	15	321	A86	C8-C6-C5	-2.15	115.63	119.01
30	11	304	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
30	A	835	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
30	15	308	CLA	CHA-C1A-NA	-2.15	121.53	126.39
30	F	201	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
38	13	308	KC1	C3D-C2D-C1D	-2.15	99.54	106.40
37	11	315	A86	C10-C9-C8	-2.15	116.97	123.20
37	2	319	A86	C4-C3-C2	-2.15	119.12	123.52
30	5	307	CLA	CHA-C1A-NA	-2.15	121.53	126.39
36	6	301	LMG	O3-C3-C2	-2.15	105.31	110.38
30	2	309	CLA	CBC-CAC-C3C	-2.15	106.60	112.42
33	F	204	BCR	C38-C26-C27	-2.15	109.02	113.60
38	11	311	KC1	C3D-C2D-C1D	-2.15	99.54	106.40
30	9	308	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
33	J	102	BCR	C33-C5-C6	-2.15	122.14	124.48
30	11	310	CLA	CED-O2D-CGD	2.15	120.78	115.92
30	B	831	CLA	CHB-C4A-NA	2.15	127.50	124.40
39	6	321	DD6	C25-C24-C1	-2.15	120.48	126.36
30	B	802	CLA	CGD-CBD-CAD	-2.15	103.90	110.85
30	5	311	CLA	CBC-CAC-C3C	-2.15	106.60	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	10	316	A86	C34-O4-C38	-2.15	114.06	117.85
30	A	807	CLA	CMC-C2C-C1C	2.15	128.39	125.03
30	3	305	CLA	CED-O2D-CGD	2.14	120.78	115.92
30	B	833	CLA	CHB-C4A-NA	2.14	127.50	124.40
38	12	309	KC1	C3D-C2D-C1D	-2.14	99.55	106.40
33	B	844	BCR	C24-C23-C22	-2.14	123.06	126.23
38	11	307	KC1	CBC-CAC-C3C	-2.14	106.61	112.42
38	2	312	KC1	C3D-C2D-C1D	-2.14	99.55	106.40
38	8	307	KC1	C3D-C2D-C1D	-2.14	99.55	106.40
30	B	828	CLA	CHB-C4A-NA	2.14	127.49	124.40
30	12	303	CLA	CMB-C2B-C3B	2.14	131.59	126.55
39	6	319	DD6	C15-C14-C13	-2.14	121.46	125.99
37	14	301	A86	C7-C6-C8	2.14	121.36	118.09
30	B	829	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
30	F	201	CLA	CAC-C3C-C4C	2.14	127.58	124.79
35	1	311	LMT	O3'-C3'-C2'	-2.14	105.33	110.38
30	3	302	CLA	CHB-C4A-NA	2.14	127.49	124.40
37	4	317	A86	C8-C6-C5	-2.14	115.64	119.01
39	2	316	DD6	C22-C16-C17	-2.14	105.21	108.97
30	A	823	CLA	CMB-C2B-C1B	2.14	128.68	125.42
36	B	847	LMG	O7-C10-O9	-2.14	118.70	123.70
30	F	203	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
36	7	320	LMG	O7-C10-O9	-2.14	118.70	123.70
30	A	843	CLA	CHB-C4A-NA	2.14	127.49	124.40
30	13	304	CLA	CHB-C4A-NA	2.14	127.49	124.40
30	12	321	CLA	CHA-C1A-NA	-2.14	121.55	126.39
30	A	832	CLA	C5-C3-C4	2.14	119.51	114.59
38	9	304	KC1	CHB-C4A-NA	2.14	127.55	124.23
30	9	303	CLA	CHB-C4A-NA	2.14	127.48	124.40
30	1	304	CLA	O2A-CGA-CBA	2.14	118.35	111.83
38	4	308	KC1	CHC-C1C-NC	2.14	127.55	124.23
30	4	302	CLA	O2A-CGA-CBA	2.14	118.35	111.83
30	13	304	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
30	B	824	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
38	13	305	KC1	CBC-CAC-C3C	-2.14	106.63	112.42
37	14	314	A86	C26-C25-C24	-2.13	117.01	123.20
30	14	307	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
30	A	807	CLA	CAC-C3C-C4C	2.13	127.57	124.79
30	16	306	CLA	CHB-C4A-NA	2.13	127.48	124.40
30	A	829	CLA	C4-C3-C5	2.13	118.93	115.23
30	15	307	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
30	4	301	CLA	CHB-C1B-C2B	-2.13	121.23	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	10	307	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
30	A	807	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
33	A	851	BCR	C15-C14-C13	-2.13	124.29	127.28
38	1	306	KC1	CHB-C4A-NA	2.13	127.54	124.23
30	A	830	CLA	CHB-C4A-NA	2.13	127.48	124.40
30	8	303	CLA	CHB-C4A-NA	2.13	127.48	124.40
37	10	315	A86	C36-C31-C32	-2.13	117.58	119.70
30	10	307	CLA	CHA-C1A-NA	-2.13	121.56	126.39
38	10	312	KC1	C3D-C2D-C1D	-2.13	99.59	106.40
30	A	804	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
30	B	825	CLA	CMC-C2C-C1C	2.13	128.36	125.03
38	10	310	KC1	C3D-C2D-C1D	-2.13	99.60	106.40
30	15	307	CLA	CMC-C2C-C1C	2.13	128.36	125.03
30	B	836	CLA	CHB-C4A-NA	2.13	127.47	124.40
37	12	316	A86	C7-C6-C5	-2.13	119.36	122.82
37	2u	205	A86	O4-C38-O5	-2.13	118.88	122.99
34	9	318	LHG	C27-C26-C25	-2.13	103.60	114.37
30	B	818	CLA	CAA-C2A-C1A	-2.13	105.00	111.97
30	B	831	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
30	A	819	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
38	12	305	KC1	O2A-CGA-O1A	-2.13	118.36	122.70
39	10	314	DD6	C14-C13-C11	2.13	128.83	125.53
38	2	306	KC1	C3D-C2D-C1D	-2.13	99.60	106.40
38	1	306	KC1	CHC-C4B-NB	-2.13	121.81	124.80
30	B	838	CLA	CHA-C1A-NA	-2.13	121.57	126.39
30	7	305	CLA	C4-C3-C5	2.13	118.92	115.23
38	9	311	KC1	CHB-C4A-NA	2.13	127.53	124.23
30	15	308	CLA	CMC-C2C-C1C	2.13	128.36	125.03
34	A	852	LHG	C11-C10-C9	-2.13	103.62	114.37
30	A	804	CLA	CHB-C4A-NA	2.13	127.47	124.40
30	2	303	CLA	CED-O2D-CGD	2.13	120.74	115.92
30	A	814	CLA	CHA-C1A-NA	-2.13	121.58	126.39
38	6	313	KC1	C3D-C2D-C1D	-2.13	99.61	106.40
30	6	314	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
39	8	316	DD6	C4-C3-C2	-2.12	119.17	123.52
30	4	309	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
30	A	807	CLA	C4-C3-C5	2.12	118.92	115.23
30	B	813	CLA	C7-C6-C5	-2.12	107.60	113.26
38	3	304	KC1	C3D-C2D-C1D	-2.12	99.62	106.40
30	7	303	CLA	C3B-C4B-NB	2.12	112.43	110.53
30	10	303	CLA	O2D-CGD-O1D	-2.12	119.71	123.85
30	A	841	CLA	O2D-CGD-O1D	-2.12	119.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	310	CLA	CHB-C4A-NA	2.12	127.46	124.40
30	B	822	CLA	C1-C2-C3	-2.12	122.72	126.20
30	A	818	CLA	C4-C3-C5	2.12	118.91	115.23
37	9	315	A86	C26-C25-C24	2.12	129.35	123.20
30	9	305	CLA	CGD-CBD-CAD	-2.12	103.98	110.85
38	8	310	KC1	O1D-CGD-CBD	-2.12	120.33	124.52
30	B	832	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
30	10	311	CLA	CHB-C4A-NA	2.12	127.46	124.40
30	2	303	CLA	C2A-C3A-C4A	-2.12	98.44	101.87
30	7	312	CLA	CHA-C1A-NA	-2.12	121.59	126.39
33	B	842	BCR	C27-C26-C25	2.12	125.57	122.70
38	6	313	KC1	CMC-C2C-C1C	2.12	128.35	125.03
38	13	310	KC1	C3D-C2D-C1D	-2.12	99.63	106.40
30	A	840	CLA	CHB-C4A-NA	2.12	127.46	124.40
30	B	830	CLA	CMC-C2C-C1C	2.12	128.34	125.03
30	A	837	CLA	CMB-C2B-C1B	2.12	128.65	125.42
38	9	310	KC1	C3D-C2D-C1D	-2.12	99.63	106.40
30	3	305	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
38	10	310	KC1	CHB-C1B-C2B	-2.12	121.08	125.49
30	4	306	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
30	14	307	CLA	CHA-C1A-NA	-2.12	121.60	126.39
30	A	839	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
38	4	310	KC1	CMC-C2C-C1C	2.12	128.34	125.03
30	14	307	CLA	CED-O2D-CGD	2.12	120.72	115.92
30	A	832	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
30	11	306	CLA	CGD-CBD-CAD	-2.12	103.99	110.85
39	8	316	DD6	C9-C8-C6	-2.12	120.56	126.36
37	2	302	A86	C28-C27-C26	-2.12	119.39	122.82
37	3	314	A86	C8-C6-C5	2.11	122.33	119.01
30	B	828	CLA	CHD-C4C-NC	2.11	127.51	124.23
30	B	837	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
33	2u	201	BCR	C21-C20-C19	-2.11	117.08	123.20
30	9	306	CLA	CGD-CBD-CAD	-2.11	104.01	110.85
38	6	311	KC1	CBC-CAC-C3C	-2.11	106.70	112.42
30	16	308	CLA	CHA-C1A-NA	-2.11	121.61	126.39
30	B	835	CLA	CMC-C2C-C1C	2.11	128.33	125.03
37	5	315	A86	C22-C16-C17	-2.11	105.26	108.97
30	7	307	CLA	C4-C3-C5	2.11	118.89	115.23
30	9	309	CLA	CHB-C4A-NA	2.11	127.44	124.40
30	6	309	CLA	C2A-C3A-C4A	-2.11	98.46	101.87
30	4	304	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
30	B	835	CLA	CBC-CAC-C3C	-2.11	106.70	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	303	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
30	B	810	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
37	12	316	A86	C25-C24-C1	-2.11	120.58	126.36
30	B	811	CLA	C16-C15-C13	-2.11	108.96	115.97
38	5	310	KC1	C3D-C2D-C1D	-2.11	99.67	106.40
30	B	819	CLA	CMA-C3A-C4A	-2.11	106.11	111.77
30	A	813	CLA	CMB-C2B-C3B	2.11	131.51	126.55
30	6	309	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
38	13	311	KC1	CAB-C3B-C4B	2.11	129.85	124.82
36	8	319	LMG	O2-C2-C1	-2.11	105.06	110.08
30	1	304	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
30	A	820	CLA	C1-O2A-CGA	2.11	121.75	116.65
30	2	301	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
30	B	816	CLA	CBA-CAA-C2A	2.11	120.06	113.79
30	14	302	CLA	C1-O2A-CGA	2.11	121.75	116.65
39	7	318	DD6	C23-C16-C17	-2.11	105.27	108.97
38	8	312	KC1	O2A-CGA-O1A	-2.10	118.41	122.70
30	8	303	CLA	C4-C3-C5	2.10	118.88	115.23
38	9	304	KC1	C3D-C2D-C1D	-2.10	99.68	106.40
38	6	312	KC1	CHB-C4A-NA	2.10	127.49	124.23
38	6	312	KC1	O2D-CGD-O1D	-2.10	119.75	123.85
30	14	304	CLA	CHB-C4A-NA	2.10	127.43	124.40
37	7	319	A86	O-C13-C11	-2.10	116.52	121.04
30	B	851	CLA	CHB-C4A-NA	2.10	127.43	124.40
30	6	317	CLA	C1-C2-C3	-2.10	122.75	126.20
30	12	321	CLA	CED-O2D-CGD	2.10	120.68	115.92
30	15	303	CLA	CHA-C1A-NA	-2.10	121.64	126.39
37	4	312	A86	C23-C16-C17	-2.10	105.28	108.97
37	11	316	A86	O4-C38-O5	-2.10	118.94	122.99
37	7	319	A86	C3-C2-C1	-2.10	124.33	127.28
30	16	303	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
30	9	307	CLA	CHA-C1A-NA	-2.10	121.64	126.39
30	7	306	CLA	CHA-C1A-NA	-2.10	121.64	126.39
30	15	313	CLA	CGD-CBD-CAD	-2.10	104.05	110.85
30	15	310	CLA	CMC-C2C-C1C	2.10	128.31	125.03
30	7	311	CLA	CBC-CAC-C3C	-2.10	106.74	112.42
30	B	824	CLA	CAA-C2A-C1A	-2.10	105.10	111.97
37	16	312	A86	C41-C32-C31	-2.10	108.60	110.47
38	16	311	KC1	C3D-C2D-C1D	-2.10	99.71	106.40
30	6	317	CLA	C4-C3-C5	2.10	118.87	115.23
38	12	305	KC1	CMC-C2C-C1C	2.10	128.31	125.03
38	9	312	KC1	C3D-C2D-C1D	-2.09	99.71	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B	850	LMT	C2'-C3'-C4'	2.09	114.43	109.68
30	A	816	CLA	O2A-CGA-CBA	2.09	118.22	111.83
38	3	304	KC1	CMC-C2C-C1C	2.09	128.31	125.03
30	F	202	CLA	O2A-CGA-CBA	2.09	118.22	111.83
30	12	303	CLA	CHB-C4A-NA	2.09	127.42	124.40
38	12	311	KC1	CMC-C2C-C1C	2.09	128.30	125.03
30	11	309	CLA	C4-C3-C5	2.09	118.86	115.23
31	A	845	PQN	C17-C16-C15	-2.09	107.69	113.26
37	11	315	A86	C9-C8-C6	-2.09	120.63	126.36
30	13	302	CLA	O2A-CGA-CBA	2.09	118.21	111.83
30	B	805	CLA	CHA-C1A-NA	-2.09	121.66	126.39
37	4	312	A86	C40-C32-C31	-2.09	108.60	110.47
30	B	836	CLA	CHA-C1A-NA	-2.09	121.66	126.39
30	A	844	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
35	6	302	LMT	C1B-O1B-C4'	-2.09	113.03	117.98
30	B	819	CLA	C3B-C4B-NB	2.09	112.39	110.53
37	2	302	A86	C36-C31-C32	-2.09	117.62	119.70
30	11	306	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
30	A	809	CLA	C1-O2A-CGA	2.09	121.71	116.65
30	6	316	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
30	5	307	CLA	CHB-C4A-NA	2.09	127.41	124.40
38	2	314	KC1	CMB-C2B-C1B	2.09	128.40	124.73
33	B	842	BCR	C7-C8-C9	-2.09	123.15	126.23
38	7	308	KC1	CHB-C4A-NA	2.09	127.47	124.23
33	B	841	BCR	C11-C10-C9	-2.09	124.35	127.28
37	14	318	A86	C7-C6-C5	-2.09	119.44	122.82
30	B	832	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
30	B	801	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
36	F	205	LMG	C3-C4-C5	-2.09	106.45	110.23
38	6	308	KC1	CBC-CAC-C3C	-2.09	106.76	112.42
38	6	312	KC1	CAA-C2A-C1A	-2.09	115.50	124.64
30	11	310	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
37	14	319	A86	C7-C6-C5	-2.08	119.44	122.82
30	B	833	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
30	B	805	CLA	C11-C10-C8	-2.08	109.04	115.97
30	A	809	CLA	C1-C2-C3	-2.08	122.78	126.20
38	4	310	KC1	C3D-C2D-C1D	-2.08	99.74	106.40
37	4	314	A86	C9-C10-C11	-2.08	120.75	126.64
38	8	307	KC1	CMC-C2C-C1C	2.08	128.29	125.03
37	5	315	A86	C36-C31-C32	-2.08	117.63	119.70
37	15	320	A86	C9-C8-C6	2.08	132.07	126.36
38	5	305	KC1	C3D-C2D-C1D	-2.08	99.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	1	309	A86	C7-C6-C5	-2.08	119.44	122.82
38	3	311	KC1	C3D-C2D-C1D	-2.08	99.75	106.40
38	10	310	KC1	CMB-C2B-C1B	2.08	128.39	124.73
38	11	312	KC1	CMC-C2C-C1C	2.08	128.29	125.03
30	A	826	CLA	C4-C3-C5	2.08	118.84	115.23
37	11	301	A86	C22-C16-C17	-2.08	105.31	108.97
38	13	305	KC1	C3D-C2D-C1D	-2.08	99.76	106.40
37	14	315	A86	C22-C16-C17	-2.08	105.31	108.97
37	10	302	A86	C28-C27-C26	-2.08	119.45	122.82
38	9	311	KC1	C3D-C2D-C1D	-2.08	99.76	106.40
39	4	313	DD6	C4-C3-C2	-2.08	119.26	123.52
30	8	305	CLA	CHB-C4A-NA	2.08	127.40	124.40
30	14	312	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
30	16	301	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
30	A	838	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
30	B	837	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
30	3	305	CLA	CBA-CAA-C2A	2.08	119.97	113.79
30	9	309	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
39	9	314	DD6	C19-C18-C17	2.08	114.67	110.79
30	10	311	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
30	B	819	CLA	C4-C3-C5	2.08	118.83	115.23
30	3	302	CLA	CHA-C1A-NA	-2.07	121.69	126.39
33	B	845	BCR	C24-C23-C22	-2.07	123.17	126.23
39	2	315	DD6	C9-C8-C6	2.07	132.05	126.36
30	9	308	CLA	CHB-C4A-NA	2.07	127.39	124.40
30	10	305	CLA	C1-C2-C3	-2.07	122.80	126.20
30	A	842	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
30	B	829	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
30	16	306	CLA	C4-C3-C5	2.07	118.83	115.23
30	10	304	CLA	C4-C3-C5	2.07	118.83	115.23
37	9	316	A86	C40-C32-C31	-2.07	108.62	110.47
38	6	311	KC1	CMC-C2C-C1C	2.07	128.27	125.03
30	15	303	CLA	CHB-C4A-NA	2.07	127.39	124.40
30	8	309	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
30	11	304	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
30	7	303	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
38	2	314	KC1	CBC-CAC-C3C	-2.07	106.80	112.42
30	B	819	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
30	A	817	CLA	CHB-C4A-NA	2.07	127.39	124.40
37	14	316	A86	C34-O4-C38	-2.07	114.19	117.85
30	A	825	CLA	C4-C3-C5	2.07	118.82	115.23
38	9	312	KC1	CED-O2D-CGD	2.07	120.61	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	309	CLA	CMB-C2B-C3B	2.07	131.42	126.55
30	A	811	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
30	8	304	CLA	C2A-C3A-C4A	-2.07	98.53	101.87
30	A	803	CLA	CGD-CBD-CAD	2.07	117.55	110.85
30	A	806	CLA	CHC-C1C-NC	2.07	127.43	124.31
30	16	303	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
30	14	310	CLA	C5-C3-C4	2.07	119.35	114.59
30	F	201	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
39	6	303	DD6	C37-C36-C35	-2.07	110.62	114.42
30	A	839	CLA	CHB-C4A-NA	2.07	127.39	124.40
37	4	312	A86	C3-C4-C5	-2.07	119.29	123.52
30	B	813	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
30	15	314	CLA	CBB-CAB-C3B	-2.07	117.19	127.53
38	6	311	KC1	O1D-CGD-CBD	-2.07	120.44	124.52
36	8	321	LMG	O1-C7-C8	-2.07	105.79	110.82
30	1	305	CLA	CBC-CAC-C3C	-2.07	106.82	112.42
30	A	839	CLA	CMC-C2C-C1C	2.07	128.26	125.03
38	7	308	KC1	O2D-CGD-O1D	-2.07	119.83	123.85
37	7	315	A86	O-C13-C11	-2.07	116.59	121.04
33	M	101	BCR	C30-C25-C26	-2.07	119.81	122.64
30	2	307	CLA	C4-C3-C5	2.07	118.81	115.23
30	6	306	CLA	CBC-CAC-C3C	-2.07	106.82	112.42
33	A	847	BCR	C33-C5-C6	-2.07	122.23	124.48
30	15	310	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
30	1	303	CLA	CAC-C3C-C4C	2.07	127.48	124.79
37	13	313	A86	C-C1-C24	2.07	121.24	118.09
30	A	810	CLA	CMC-C2C-C1C	2.07	128.26	125.03
38	14	311	KC1	C3D-C2D-C1D	-2.06	99.80	106.40
33	M	101	BCR	C33-C5-C6	-2.06	122.23	124.48
30	B	830	CLA	CHD-C4C-NC	2.06	127.43	124.23
30	1	304	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
39	13	314	DD6	C33-C32-C31	2.06	113.56	109.49
30	6	316	CLA	CMB-C2B-C3B	2.06	131.40	126.55
30	11	306	CLA	CHA-C1A-NA	-2.06	121.72	126.39
36	8	321	LMG	O7-C10-O9	-2.06	118.88	123.70
30	9	307	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
30	L	202	CLA	C4-C3-C5	2.06	118.81	115.23
30	14	313	CLA	CGD-CBD-CAD	-2.06	104.17	110.85
38	14	308	KC1	CHD-C1D-ND	-2.06	120.96	124.05
36	6	301	LMG	O2-C2-C1	-2.06	105.16	110.08
30	6	305	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
38	10	310	KC1	CHB-C4A-NA	2.06	127.43	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	11	315	A86	C7-C6-C8	2.06	121.24	118.09
30	12	308	CLA	CED-O2D-CGD	2.06	120.59	115.92
37	14	317	A86	C12-C11-C10	-2.06	118.66	123.67
30	A	813	CLA	C6-C7-C8	-2.06	109.12	115.97
39	8	316	DD6	C22-C16-C15	2.06	115.61	110.05
30	A	802	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
38	8	311	KC1	CED-O2D-CGD	2.06	120.59	115.92
30	9	305	CLA	CAA-C2A-C1A	2.06	118.72	111.97
30	12	302	CLA	C11-C12-C13	-2.06	109.12	115.97
38	8	313	KC1	CHB-C4A-NA	2.06	127.42	124.23
30	6	307	CLA	CBB-CAB-C3B	-2.06	117.24	127.53
30	6	317	CLA	CHA-C1A-NA	-2.06	121.73	126.39
33	L	205	BCR	C33-C5-C6	-2.06	122.24	124.48
33	A	851	BCR	C8-C7-C6	-2.06	121.50	127.00
39	2	316	DD6	C34-C35-C36	-2.06	107.06	112.18
30	6	307	CLA	CBA-CAA-C2A	-2.06	107.67	113.79
39	11	313	DD6	C23-C16-C17	-2.06	105.35	108.97
30	5	307	CLA	C2A-C3A-C4A	-2.06	98.55	101.87
30	9	303	CLA	CMB-C2B-C3B	2.06	131.39	126.55
30	B	830	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
30	15	303	CLA	CHC-C4B-NB	-2.06	120.97	124.05
37	15	320	A86	C7-C6-C5	-2.06	119.49	122.82
30	A	827	CLA	CHB-C4A-NA	2.06	127.37	124.40
30	A	828	CLA	C6-C5-C3	-2.06	108.46	113.47
38	14	306	KC1	C3D-C2D-C1D	-2.05	99.84	106.40
37	10	302	A86	C-C1-C24	2.05	121.23	118.09
30	10	304	CLA	CMC-C2C-C1C	2.05	128.25	125.03
30	16	302	CLA	O2A-CGA-CBA	2.05	118.10	111.83
30	11	310	CLA	CBC-CAC-C3C	-2.05	106.85	112.42
30	9	308	CLA	CMB-C2B-C1B	2.05	128.55	125.42
37	9	313	A86	C19-C18-C17	-2.05	106.95	110.79
35	9	317	LMT	C1'-O5'-C5'	2.05	117.73	113.72
30	A	833	CLA	CMC-C2C-C1C	2.05	128.24	125.03
30	A	829	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
30	2	303	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
30	3	307	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
30	2	304	CLA	CHA-C1A-NA	-2.05	121.74	126.39
30	A	821	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
30	3	303	CLA	CMC-C2C-C1C	2.05	128.24	125.03
30	7	311	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
30	12	307	CLA	CMB-C2B-C3B	2.05	131.38	126.55
39	4	313	DD6	C23-C16-C17	-2.05	105.36	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	839	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
30	3	301	CLA	C1-C2-C3	-2.05	122.84	126.20
39	12	315	DD6	C3-C4-C5	-2.05	119.32	123.52
39	7	317	DD6	C25-C24-C1	-2.05	120.74	126.36
30	16	306	CLA	CAA-C2A-C1A	2.05	118.69	111.97
30	14	305	CLA	CMC-C2C-C1C	2.05	128.24	125.03
35	B	850	LMT	O3'-C3'-C2'	-2.05	105.54	110.38
36	B	849	LMG	O3-C3-C2	-2.05	105.55	110.38
30	5	307	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
30	A	814	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
30	3	306	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
37	2	319	A86	C29-C30-C31	-2.05	175.24	177.66
30	4	311	CLA	CHA-C1A-NA	-2.05	121.75	126.39
37	8	318	A86	C34-O4-C38	-2.05	114.23	117.85
38	13	312	KC1	O1D-CGD-CBD	-2.05	120.48	124.52
30	3	307	CLA	CAC-C3C-C4C	2.05	127.45	124.79
30	A	821	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
30	A	813	CLA	C1-O2A-CGA	2.05	121.61	116.65
30	F	203	CLA	O2A-CGA-CBA	2.05	120.47	114.00
37	14	318	A86	C-C1-C24	2.05	121.22	118.09
38	13	306	KC1	O2A-CGA-O1A	-2.05	118.53	122.70
30	B	833	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
36	2u	204	LMG	C6-C5-C4	-2.05	107.99	113.02
30	B	824	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
30	A	842	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
30	5	304	CLA	C2A-C3A-C4A	-2.05	98.56	101.87
30	A	812	CLA	O2A-CGA-CBA	2.05	118.07	111.83
37	9	316	A86	C3-C2-C1	-2.05	124.41	127.28
38	8	306	KC1	CHB-C1B-NB	-2.05	121.92	124.80
30	A	831	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
30	5	308	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
30	14	312	CLA	CED-O2D-CGD	2.04	120.55	115.92
38	9	310	KC1	O2A-CGA-O1A	-2.04	118.54	122.70
37	11	301	A86	C8-C6-C5	-2.04	115.80	119.01
38	10	312	KC1	CHB-C4A-NA	2.04	127.40	124.23
38	2	312	KC1	CED-O2D-CGD	2.04	120.55	115.92
30	B	824	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
35	B	852	LMT	C1'-C2'-C3'	2.04	114.31	110.01
38	12	305	KC1	CBC-CAC-C3C	-2.04	106.88	112.42
30	3	310	CLA	CED-O2D-CGD	2.04	120.55	115.92
30	13	307	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
30	B	834	CLA	CAA-C2A-C3A	-2.04	107.48	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	314	A86	C41-C32-C31	-2.04	108.64	110.47
33	I	101	BCR	C30-C25-C26	-2.04	119.85	122.64
39	2	317	DD6	C25-C24-C1	-2.04	120.77	126.36
38	11	312	KC1	O1D-CGD-CBD	-2.04	120.49	124.52
30	A	810	CLA	CHA-C1A-NA	-2.04	121.77	126.39
30	8	308	CLA	CHA-C1A-NA	-2.04	121.77	126.39
38	13	305	KC1	O1D-CGD-CBD	-2.04	120.49	124.52
38	1	308	KC1	C3D-C2D-C1D	-2.04	99.88	106.40
30	A	828	CLA	CAC-C3C-C4C	2.04	127.44	124.79
38	3	304	KC1	CBC-CAC-C3C	-2.04	106.89	112.42
30	B	827	CLA	CBA-CAA-C2A	2.04	119.86	113.79
30	A	805	CLA	CHA-C1A-NA	-2.04	121.78	126.39
30	7	312	CLA	O2A-CGA-CBA	2.04	119.83	112.14
30	6	314	CLA	CHA-C1A-NA	-2.04	121.78	126.39
30	4	304	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
30	10	309	CLA	C1-C2-C3	-2.03	122.86	126.20
30	F	203	CLA	CAC-C3C-C4C	2.03	127.44	124.79
30	16	301	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
37	9	316	A86	C12-C11-C13	2.03	119.30	116.00
30	A	842	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
38	8	312	KC1	CHB-C4A-NA	2.03	127.39	124.23
30	A	836	CLA	C1-C2-C3	-2.03	122.86	126.20
30	14	310	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
30	6	317	CLA	C1-O2A-CGA	2.03	121.57	116.65
30	A	809	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
38	14	308	KC1	C3D-C2D-C1D	-2.03	99.91	106.40
33	L	204	BCR	C4-C5-C6	2.03	125.45	122.70
30	B	826	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
38	2	314	KC1	CGD-CBD-CAD	-2.03	104.27	110.85
30	10	305	CLA	CAA-C2A-C1A	2.03	118.63	111.97
30	A	812	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
39	6	319	DD6	C34-C35-C36	-2.03	107.12	112.18
37	15	315	A86	C19-C18-C17	-2.03	106.99	110.79
35	12	319	LMT	O1'-C1'-C2'	2.03	111.36	108.27
30	B	823	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
30	B	805	CLA	CMC-C2C-C1C	2.03	128.21	125.03
37	10	301	A86	C9-C8-C6	-2.03	120.80	126.36
37	4	315	A86	C25-C24-C1	-2.03	120.80	126.36
30	14	310	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
30	B	827	CLA	CHB-C4A-NA	2.03	127.33	124.40
30	4	303	CLA	CHA-C1A-NA	-2.03	121.80	126.39
33	B	842	BCR	C15-C16-C17	-2.03	119.37	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	312	CLA	O2A-CGA-CBA	2.03	120.41	114.00
30	B	823	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
35	A	854	LMT	C4B-C3B-C2B	2.03	114.39	110.83
36	B	849	LMG	O7-C10-O9	-2.03	118.96	123.70
38	4	307	KC1	C3D-C2D-C1D	-2.03	99.92	106.40
38	5	312	KC1	C3D-C2D-C1D	-2.03	99.92	106.40
37	4	314	A86	C3-C4-C5	-2.03	119.37	123.52
30	7	304	CLA	C6-C7-C8	-2.03	109.23	115.97
38	10	310	KC1	O1D-CGD-CBD	-2.03	120.52	124.52
37	8	318	A86	C40-C32-C31	-2.03	108.66	110.47
30	10	308	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
35	A	855	LMT	C1'-C2'-C3'	2.03	114.27	110.01
30	10	304	CLA	CHB-C4A-NA	2.03	127.32	124.40
38	7	313	KC1	O2A-CGA-O1A	-2.03	118.57	122.70
30	L	203	CLA	CMC-C2C-C1C	2.03	128.20	125.03
38	8	306	KC1	CAA-C2A-C1A	-2.03	115.77	124.64
30	J	101	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
30	B	815	CLA	CHA-C1A-NA	-2.03	121.81	126.39
33	B	846	BCR	C21-C20-C19	-2.03	117.33	123.20
38	14	308	KC1	CHD-C4C-NC	2.03	127.36	124.31
30	7	304	CLA	CHB-C4A-NA	2.02	127.32	124.40
37	14	301	A86	C3-C4-C5	-2.02	119.38	123.52
30	13	304	CLA	CED-O2D-CGD	2.02	120.51	115.92
30	10	307	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
38	3	308	KC1	CHB-C1B-NB	-2.02	121.95	124.80
30	A	834	CLA	CBB-CAB-C3B	-2.02	117.41	127.53
30	10	303	CLA	CMC-C2C-C1C	2.02	128.20	125.03
30	A	824	CLA	CBC-CAC-C3C	-2.02	106.93	112.42
37	14	314	A86	C3-C2-C1	-2.02	124.44	127.28
30	8	303	CLA	CMC-C2C-C1C	2.02	128.20	125.03
30	16	308	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
30	A	814	CLA	O2A-CGA-CBA	2.02	118.00	111.83
30	A	826	CLA	C1-O2A-CGA	2.02	121.55	116.65
39	7	318	DD6	C25-C24-C1	-2.02	120.82	126.36
30	15	305	CLA	CHA-C1A-NA	-2.02	121.81	126.39
30	1	304	CLA	CED-O2D-CGD	2.02	120.50	115.92
37	15	321	A86	C3-C4-C5	-2.02	119.38	123.52
30	7	304	CLA	CMC-C2C-C1C	2.02	128.19	125.03
30	A	811	CLA	CMB-C2B-C1B	2.02	128.50	125.42
38	11	311	KC1	O1D-CGD-CBD	-2.02	120.53	124.52
30	A	834	CLA	CHA-C1A-NA	-2.02	121.81	126.39
39	4	316	DD6	C33-C32-C31	2.02	113.47	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	11	313	DD6	C22-C16-C17	2.02	112.52	108.97
37	11	315	A86	O4-C38-O5	-2.02	119.09	122.99
30	1	305	CLA	CHA-C1A-NA	-2.02	121.81	126.39
36	7	320	LMG	O2-C2-C1	-2.02	105.26	110.08
37	10	315	A86	C9-C8-C6	-2.02	120.83	126.36
39	9	314	DD6	C33-C32-C31	2.02	113.47	109.49
30	A	827	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
30	9	306	CLA	CAA-C2A-C1A	2.02	118.59	111.97
30	A	814	CLA	C1C-C2C-C3C	-2.02	104.86	106.98
33	A	851	BCR	C2-C1-C6	2.02	113.37	110.44
30	15	302	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
30	12	307	CLA	O2A-CGA-CBA	2.02	119.76	112.14
36	2u	204	LMG	O8-C28-O10	-2.02	118.58	123.63
30	12	306	CLA	C4-C3-C5	2.02	118.73	115.23
30	14	313	CLA	O2A-CGA-CBA	2.02	119.76	112.14
35	11	302	LMT	C1-O1'-C1'	-2.02	110.23	113.68
31	B	840	PQN	C11-C3-C4	2.02	120.70	118.58
30	1	301	CLA	CHA-C1A-NA	-2.02	121.82	126.39
30	6	315	CLA	O2A-CGA-CBA	2.02	120.37	114.00
38	11	307	KC1	CHB-C1B-NB	-2.02	121.96	124.80
30	A	838	CLA	CAC-C3C-C4C	2.02	127.41	124.79
30	B	832	CLA	C1-O2A-CGA	2.02	121.53	116.65
30	3	305	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
30	6	307	CLA	CMA-C3A-C2A	-2.02	106.19	113.98
30	4	305	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
30	15	306	CLA	O2A-CGA-CBA	2.02	120.37	114.00
35	A	857	LMT	C1B-O1B-C4'	-2.02	113.20	117.98
30	B	832	CLA	CHA-C1A-NA	-2.02	121.83	126.39
30	9	305	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
30	2	303	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
39	1	310	DD6	O1-C20-C21	-2.01	112.80	115.05
30	5	302	CLA	CHA-C1A-NA	-2.01	121.83	126.39
38	4	308	KC1	CHB-C1B-NB	-2.01	121.97	124.80
30	12	302	CLA	CBA-CAA-C2A	2.01	119.78	113.79
30	6	309	CLA	CHB-C4A-NA	2.01	127.30	124.40
37	3	315	A86	C40-C32-C31	-2.01	108.67	110.47
30	6	309	CLA	O2A-C1-C2	2.01	115.85	108.11
37	4	314	A86	C19-C18-C17	2.01	114.55	110.79
30	2	303	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
30	A	815	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
30	3	303	CLA	CAA-C2A-C1A	2.01	118.57	111.97
30	B	827	CLA	CAA-C2A-C3A	-2.01	107.56	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	11	313	DD6	C4-C3-C2	-2.01	119.41	123.52
30	B	828	CLA	O2A-CGA-CBA	2.01	117.96	111.83
30	A	804	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
30	2	305	CLA	O2A-CGA-CBA	2.01	117.96	111.83
30	9	309	CLA	CHA-C1A-NA	-2.01	121.84	126.39
30	9	306	CLA	CMC-C2C-C1C	2.01	128.17	125.03
38	2	314	KC1	CMC-C2C-C1C	2.01	128.17	125.03
37	5	301	A86	C23-C16-C22	-2.01	104.45	107.37
30	A	830	CLA	CBC-CAC-C3C	-2.01	106.97	112.42
30	7	307	CLA	CBC-CAC-C3C	-2.01	106.97	112.42
33	L	201	BCR	C10-C11-C12	-2.01	117.38	123.20
30	6	305	CLA	CHA-C1A-NA	-2.01	121.84	126.39
30	A	829	CLA	CMB-C2B-C3B	2.01	131.27	126.55
30	A	843	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
35	A	855	LMT	O3'-C3'-C2'	-2.01	105.64	110.38
30	A	812	CLA	C1-O2A-CGA	2.01	121.51	116.65
30	F	201	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
38	10	306	KC1	CAA-C2A-C1A	-2.01	115.85	124.64
30	B	809	CLA	CHA-C1A-NA	-2.01	121.85	126.39
37	2	319	A86	C7-C6-C8	2.01	121.15	118.09
37	10	315	A86	C8-C6-C5	-2.01	115.86	119.01
30	7	305	CLA	CMB-C2B-C1B	2.01	128.47	125.42
30	7	305	CLA	CMC-C2C-C1C	2.00	128.17	125.03
39	3	313	DD6	C33-C32-C31	2.00	113.44	109.49
30	A	808	CLA	CBC-CAC-C3C	-2.00	106.99	112.42
30	14	302	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
37	2	318	A86	C23-C16-C17	-2.00	105.45	108.97
30	A	821	CLA	CMC-C2C-C1C	2.00	128.16	125.03
30	3	307	CLA	CHD-C4C-NC	2.00	127.34	124.23
30	B	831	CLA	CAC-C3C-C4C	2.00	127.40	124.79
30	9	301	CLA	C4-C3-C5	2.00	118.70	115.23
30	7	307	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
38	3	308	KC1	CBC-CAC-C3C	-2.00	106.99	112.42
38	14	306	KC1	CHB-C4A-NA	2.00	127.34	124.23
33	B	846	BCR	C8-C9-C10	-2.00	115.86	119.01
38	3	308	KC1	C3D-C2D-C1D	-2.00	100.00	106.40
30	4	311	CLA	CED-O2D-CGD	2.00	120.46	115.92
30	15	303	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
35	11	317	LMT	O1B-C4'-C3'	2.00	112.32	107.23
30	16	308	CLA	O2A-CGA-O1A	-2.00	118.19	123.33

All (185) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	801	CL0	ND
29	A	801	CL0	NC
29	A	801	CL0	NA
30	A	802	CLA	ND
30	A	803	CLA	ND
30	A	804	CLA	ND
30	A	805	CLA	ND
30	A	806	CLA	ND
30	A	807	CLA	ND
30	A	808	CLA	ND
30	A	809	CLA	ND
30	A	810	CLA	ND
30	A	811	CLA	ND
30	A	812	CLA	ND
30	A	813	CLA	ND
30	A	814	CLA	ND
30	A	815	CLA	ND
30	A	816	CLA	ND
30	A	820	CLA	ND
30	A	821	CLA	ND
30	A	822	CLA	ND
30	A	824	CLA	ND
30	A	825	CLA	ND
30	A	826	CLA	ND
30	A	827	CLA	ND
30	A	828	CLA	ND
30	A	829	CLA	ND
30	A	830	CLA	ND
30	A	831	CLA	ND
30	A	833	CLA	ND
30	A	834	CLA	ND
30	A	835	CLA	ND
30	A	836	CLA	ND
30	A	837	CLA	ND
30	A	838	CLA	ND
30	A	839	CLA	ND
30	A	840	CLA	ND
30	A	841	CLA	ND
30	A	842	CLA	ND
30	A	843	CLA	ND
30	A	844	CLA	ND
30	B	801	CLA	ND
30	B	802	CLA	ND

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Mol	Chain	Res	Type	Atom
30	B	803	CLA	ND
30	B	804	CLA	ND
30	B	805	CLA	ND
30	B	806	CLA	ND
30	B	807	CLA	ND
30	B	808	CLA	ND
30	B	809	CLA	ND
30	B	810	CLA	ND
30	B	811	CLA	ND
30	B	812	CLA	ND
30	B	813	CLA	ND
30	B	814	CLA	ND
30	B	815	CLA	ND
30	B	817	CLA	ND
30	B	818	CLA	ND
30	B	819	CLA	ND
30	B	821	CLA	ND
30	B	823	CLA	ND
30	B	824	CLA	ND
30	B	825	CLA	ND
30	B	826	CLA	ND
30	B	827	CLA	ND
30	B	828	CLA	ND
30	B	829	CLA	ND
30	B	830	CLA	ND
30	B	832	CLA	ND
30	B	833	CLA	ND
30	B	834	CLA	ND
30	B	835	CLA	ND
30	B	836	CLA	ND
30	B	837	CLA	ND
30	B	838	CLA	ND
30	B	839	CLA	ND
30	F	201	CLA	ND
30	F	202	CLA	ND
30	F	203	CLA	ND
30	J	101	CLA	ND
30	L	202	CLA	ND
30	L	203	CLA	ND
30	2u	202	CLA	ND
30	1	301	CLA	ND
30	1	302	CLA	ND

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Mol	Chain	Res	Type	Atom
30	1	303	CLA	ND
30	1	304	CLA	ND
30	1	305	CLA	ND
30	2	301	CLA	ND
30	2	304	CLA	ND
30	2	305	CLA	ND
30	2	307	CLA	ND
30	2	309	CLA	ND
30	2	310	CLA	ND
30	3	301	CLA	ND
30	3	302	CLA	ND
30	3	303	CLA	ND
30	3	305	CLA	ND
30	3	306	CLA	ND
30	3	307	CLA	ND
30	4	301	CLA	ND
30	4	302	CLA	ND
30	4	303	CLA	ND
30	4	304	CLA	ND
30	4	305	CLA	ND
30	4	306	CLA	ND
30	4	309	CLA	ND
30	4	311	CLA	ND
30	5	302	CLA	ND
30	5	303	CLA	ND
30	5	304	CLA	ND
30	5	307	CLA	ND
30	5	309	CLA	ND
30	5	311	CLA	ND
30	6	304	CLA	ND
30	6	305	CLA	ND
30	6	306	CLA	ND
30	6	307	CLA	ND
30	6	309	CLA	ND
30	6	310	CLA	ND
30	6	315	CLA	ND
30	6	316	CLA	ND
30	6	317	CLA	ND
30	7	303	CLA	ND
30	7	304	CLA	ND
30	7	305	CLA	ND
30	7	306	CLA	ND

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Mol	Chain	Res	Type	Atom
30	7	309	CLA	ND
30	7	311	CLA	ND
30	7	312	CLA	ND
30	8	301	CLA	ND
30	8	302	CLA	ND
30	8	304	CLA	ND
30	8	308	CLA	ND
30	9	301	CLA	ND
30	9	302	CLA	ND
30	9	305	CLA	ND
30	9	306	CLA	ND
30	9	307	CLA	ND
30	9	308	CLA	ND
30	9	309	CLA	ND
30	10	303	CLA	ND
30	10	304	CLA	ND
30	10	305	CLA	ND
30	10	307	CLA	ND
30	10	308	CLA	ND
30	10	309	CLA	ND
30	11	304	CLA	ND
30	11	306	CLA	ND
30	11	308	CLA	ND
30	11	310	CLA	ND
30	12	303	CLA	ND
30	12	304	CLA	ND
30	12	306	CLA	ND
30	12	307	CLA	ND
30	12	308	CLA	ND
30	12	312	CLA	ND
30	12	321	CLA	ND
30	13	301	CLA	ND
30	13	302	CLA	ND
30	13	307	CLA	ND
30	13	309	CLA	ND
30	14	302	CLA	ND
30	14	303	CLA	ND
30	14	304	CLA	ND
30	14	305	CLA	ND
30	14	309	CLA	ND
30	14	310	CLA	ND
30	14	313	CLA	ND

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Mol	Chain	Res	Type	Atom
30	15	303	CLA	ND
30	15	304	CLA	ND
30	15	305	CLA	ND
30	15	306	CLA	ND
30	15	307	CLA	ND
30	15	308	CLA	ND
30	15	310	CLA	ND
30	15	311	CLA	ND
30	15	312	CLA	ND
30	16	302	CLA	ND
30	16	303	CLA	ND
30	16	305	CLA	ND
30	16	306	CLA	ND
30	16	307	CLA	ND
30	16	308	CLA	ND
30	16	310	CLA	ND

All (4046) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	801	CL0	CHA-CBD-CGD-O1D
30	A	804	CLA	C3A-C2A-CAA-CBA
30	A	806	CLA	C1A-C2A-CAA-CBA
30	A	806	CLA	C3A-C2A-CAA-CBA
30	A	807	CLA	C1A-C2A-CAA-CBA
30	A	807	CLA	CBD-CGD-O2D-CED
30	A	809	CLA	C1A-C2A-CAA-CBA
30	A	809	CLA	C3A-C2A-CAA-CBA
30	A	809	CLA	CHA-CBD-CGD-O1D
30	A	809	CLA	CHA-CBD-CGD-O2D
30	A	809	CLA	C6-C7-C8-C9
30	A	812	CLA	C1A-C2A-CAA-CBA
30	A	814	CLA	C4B-C3B-CAB-CBB
30	A	816	CLA	C4B-C3B-CAB-CBB
30	A	819	CLA	C3A-C2A-CAA-CBA
30	A	820	CLA	C1A-C2A-CAA-CBA
30	A	820	CLA	C3A-C2A-CAA-CBA
30	A	827	CLA	C4B-C3B-CAB-CBB
30	A	832	CLA	C2B-C3B-CAB-CBB
30	A	832	CLA	C4B-C3B-CAB-CBB
30	A	834	CLA	C2B-C3B-CAB-CBB
30	A	834	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	A	835	CLA	C2B-C3B-CAB-CBB
30	A	835	CLA	C4B-C3B-CAB-CBB
30	A	835	CLA	CHA-CBD-CGD-O1D
30	A	835	CLA	CHA-CBD-CGD-O2D
30	A	838	CLA	C1A-C2A-CAA-CBA
30	A	841	CLA	C2B-C3B-CAB-CBB
30	A	841	CLA	C4B-C3B-CAB-CBB
30	A	843	CLA	C4B-C3B-CAB-CBB
30	A	844	CLA	CBA-CGA-O2A-C1
30	A	844	CLA	O1A-CGA-O2A-C1
30	A	844	CLA	C11-C12-C13-C14
30	B	801	CLA	CBD-CGD-O2D-CED
30	B	804	CLA	CHA-CBD-CGD-O2D
30	B	805	CLA	C3A-C2A-CAA-CBA
30	B	806	CLA	C2B-C3B-CAB-CBB
30	B	806	CLA	C4B-C3B-CAB-CBB
30	B	808	CLA	CHA-CBD-CGD-O1D
30	B	808	CLA	CHA-CBD-CGD-O2D
30	B	809	CLA	C4B-C3B-CAB-CBB
30	B	815	CLA	C2B-C3B-CAB-CBB
30	B	815	CLA	C4B-C3B-CAB-CBB
30	B	816	CLA	C1A-C2A-CAA-CBA
30	B	816	CLA	C3A-C2A-CAA-CBA
30	B	816	CLA	C4B-C3B-CAB-CBB
30	B	818	CLA	C3A-C2A-CAA-CBA
30	B	819	CLA	C2B-C3B-CAB-CBB
30	B	819	CLA	C4B-C3B-CAB-CBB
30	B	821	CLA	C2B-C3B-CAB-CBB
30	B	821	CLA	C4B-C3B-CAB-CBB
30	B	822	CLA	C2B-C3B-CAB-CBB
30	B	822	CLA	C4B-C3B-CAB-CBB
30	B	824	CLA	C2B-C3B-CAB-CBB
30	B	824	CLA	C4B-C3B-CAB-CBB
30	B	824	CLA	CHA-CBD-CGD-O1D
30	B	824	CLA	CHA-CBD-CGD-O2D
30	B	827	CLA	C1A-C2A-CAA-CBA
30	B	827	CLA	C3A-C2A-CAA-CBA
30	B	828	CLA	CHA-CBD-CGD-O1D
30	B	828	CLA	CHA-CBD-CGD-O2D
30	B	833	CLA	C1A-C2A-CAA-CBA
30	B	833	CLA	C3A-C2A-CAA-CBA
30	B	835	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	B	835	CLA	C4B-C3B-CAB-CBB
30	F	203	CLA	C1A-C2A-CAA-CBA
30	F	203	CLA	C3A-C2A-CAA-CBA
30	L	202	CLA	C2B-C3B-CAB-CBB
30	L	202	CLA	C4B-C3B-CAB-CBB
30	1	301	CLA	C1A-C2A-CAA-CBA
30	1	301	CLA	C3A-C2A-CAA-CBA
30	1	301	CLA	C2B-C3B-CAB-CBB
30	1	301	CLA	C4B-C3B-CAB-CBB
30	1	304	CLA	C1A-C2A-CAA-CBA
30	1	304	CLA	C2B-C3B-CAB-CBB
30	1	304	CLA	C4B-C3B-CAB-CBB
30	1	307	CLA	C1A-C2A-CAA-CBA
30	1	307	CLA	C3A-C2A-CAA-CBA
30	2	303	CLA	C3A-C2A-CAA-CBA
30	2	303	CLA	CBD-CGD-O2D-CED
30	2	305	CLA	C1A-C2A-CAA-CBA
30	2	308	CLA	C3A-C2A-CAA-CBA
30	2	308	CLA	C2B-C3B-CAB-CBB
30	2	308	CLA	C4B-C3B-CAB-CBB
30	2	309	CLA	CBD-CGD-O2D-CED
30	3	303	CLA	C1A-C2A-CAA-CBA
30	3	303	CLA	C3A-C2A-CAA-CBA
30	3	303	CLA	C4B-C3B-CAB-CBB
30	3	303	CLA	CHA-CBD-CGD-O1D
30	3	303	CLA	CHA-CBD-CGD-O2D
30	3	305	CLA	C1A-C2A-CAA-CBA
30	3	305	CLA	C3A-C2A-CAA-CBA
30	3	309	CLA	CHA-CBD-CGD-O1D
30	3	309	CLA	CHA-CBD-CGD-O2D
30	4	301	CLA	C2-C1-O2A-CGA
30	4	302	CLA	C1A-C2A-CAA-CBA
30	4	302	CLA	C3A-C2A-CAA-CBA
30	4	302	CLA	C4B-C3B-CAB-CBB
30	4	304	CLA	C2B-C3B-CAB-CBB
30	4	304	CLA	C4B-C3B-CAB-CBB
30	4	306	CLA	C2B-C3B-CAB-CBB
30	4	306	CLA	C4B-C3B-CAB-CBB
30	5	302	CLA	C1A-C2A-CAA-CBA
30	5	302	CLA	C3A-C2A-CAA-CBA
30	5	302	CLA	C2B-C3B-CAB-CBB
30	5	302	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	5	304	CLA	C1A-C2A-CAA-CBA
30	5	304	CLA	C3A-C2A-CAA-CBA
30	5	307	CLA	C1A-C2A-CAA-CBA
30	5	307	CLA	C3A-C2A-CAA-CBA
30	5	308	CLA	C2-C3-C5-C6
30	5	308	CLA	C4-C3-C5-C6
30	5	311	CLA	CAD-CBD-CGD-O1D
30	5	311	CLA	CAD-CBD-CGD-O2D
30	6	304	CLA	C1A-C2A-CAA-CBA
30	6	304	CLA	C3A-C2A-CAA-CBA
30	6	306	CLA	C4B-C3B-CAB-CBB
30	6	307	CLA	C4B-C3B-CAB-CBB
30	6	309	CLA	C1A-C2A-CAA-CBA
30	6	314	CLA	CHA-CBD-CGD-O1D
30	6	314	CLA	CHA-CBD-CGD-O2D
30	6	315	CLA	CAD-CBD-CGD-O2D
30	7	303	CLA	C2B-C3B-CAB-CBB
30	7	303	CLA	C4B-C3B-CAB-CBB
30	7	307	CLA	C1A-C2A-CAA-CBA
30	7	307	CLA	C3A-C2A-CAA-CBA
30	7	307	CLA	C4B-C3B-CAB-CBB
30	7	307	CLA	CBD-CGD-O2D-CED
30	7	310	CLA	C1A-C2A-CAA-CBA
30	7	310	CLA	C3A-C2A-CAA-CBA
30	8	301	CLA	C3A-C2A-CAA-CBA
30	8	302	CLA	C2-C3-C5-C6
30	8	302	CLA	C4-C3-C5-C6
30	8	304	CLA	C2B-C3B-CAB-CBB
30	8	304	CLA	C4B-C3B-CAB-CBB
30	8	304	CLA	C2-C3-C5-C6
30	8	304	CLA	C4-C3-C5-C6
30	8	305	CLA	C1A-C2A-CAA-CBA
30	8	308	CLA	CAD-CBD-CGD-O2D
30	9	305	CLA	C1A-C2A-CAA-CBA
30	9	305	CLA	CBD-CGD-O2D-CED
30	9	306	CLA	C4B-C3B-CAB-CBB
30	9	307	CLA	C1A-C2A-CAA-CBA
30	9	307	CLA	C3A-C2A-CAA-CBA
30	9	308	CLA	C1A-C2A-CAA-CBA
30	10	303	CLA	C3A-C2A-CAA-CBA
30	10	303	CLA	C2B-C3B-CAB-CBB
30	10	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	10	305	CLA	C1A-C2A-CAA-CBA
30	10	305	CLA	C2B-C3B-CAB-CBB
30	10	305	CLA	C4B-C3B-CAB-CBB
30	10	307	CLA	C1A-C2A-CAA-CBA
30	10	307	CLA	C3A-C2A-CAA-CBA
30	10	307	CLA	C4B-C3B-CAB-CBB
30	10	311	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	C2B-C3B-CAB-CBB
30	11	304	CLA	C4B-C3B-CAB-CBB
30	11	306	CLA	C1A-C2A-CAA-CBA
30	11	306	CLA	C2B-C3B-CAB-CBB
30	11	306	CLA	C4B-C3B-CAB-CBB
30	11	306	CLA	CHA-CBD-CGD-O1D
30	11	306	CLA	CHA-CBD-CGD-O2D
30	12	307	CLA	CHA-CBD-CGD-O1D
30	12	307	CLA	CHA-CBD-CGD-O2D
30	12	312	CLA	C1A-C2A-CAA-CBA
30	13	301	CLA	C3A-C2A-CAA-CBA
30	13	303	CLA	C1A-C2A-CAA-CBA
30	13	309	CLA	C1A-C2A-CAA-CBA
30	13	309	CLA	C3A-C2A-CAA-CBA
30	14	302	CLA	C4B-C3B-CAB-CBB
30	14	303	CLA	C1A-C2A-CAA-CBA
30	14	303	CLA	CHA-CBD-CGD-O2D
30	14	304	CLA	CHA-CBD-CGD-O1D
30	14	304	CLA	CHA-CBD-CGD-O2D
30	14	305	CLA	C2B-C3B-CAB-CBB
30	14	305	CLA	C4B-C3B-CAB-CBB
30	14	312	CLA	C2B-C3B-CAB-CBB
30	14	312	CLA	C4B-C3B-CAB-CBB
30	14	312	CLA	CAD-CBD-CGD-O2D
30	14	313	CLA	C1A-C2A-CAA-CBA
30	15	302	CLA	C2-C3-C5-C6
30	15	302	CLA	C4-C3-C5-C6
30	15	303	CLA	C3A-C2A-CAA-CBA
30	15	305	CLA	C2B-C3B-CAB-CBB
30	15	305	CLA	C4B-C3B-CAB-CBB
30	15	305	CLA	CHA-CBD-CGD-O1D
30	15	305	CLA	CHA-CBD-CGD-O2D
30	15	306	CLA	CHA-CBD-CGD-O1D
30	15	306	CLA	CHA-CBD-CGD-O2D
30	15	308	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	15	309	CLA	C4B-C3B-CAB-CBB
30	15	309	CLA	CBD-CGD-O2D-CED
30	15	310	CLA	CHA-CBD-CGD-O1D
30	15	310	CLA	CHA-CBD-CGD-O2D
30	15	311	CLA	C1A-C2A-CAA-CBA
30	15	312	CLA	C2B-C3B-CAB-CBB
30	15	312	CLA	C4B-C3B-CAB-CBB
30	15	313	CLA	CAD-CBD-CGD-O1D
30	15	313	CLA	CAD-CBD-CGD-O2D
30	15	313	CLA	C2-C3-C5-C6
30	15	313	CLA	C4-C3-C5-C6
30	15	314	CLA	C2B-C3B-CAB-CBB
30	15	314	CLA	C4B-C3B-CAB-CBB
30	16	301	CLA	C3A-C2A-CAA-CBA
30	16	303	CLA	C1A-C2A-CAA-CBA
30	16	303	CLA	C3A-C2A-CAA-CBA
30	16	306	CLA	C1A-C2A-CAA-CBA
30	16	306	CLA	CHA-CBD-CGD-O1D
30	16	306	CLA	CHA-CBD-CGD-O2D
30	16	307	CLA	C1A-C2A-CAA-CBA
30	16	308	CLA	C1A-C2A-CAA-CBA
30	16	309	CLA	CHA-CBD-CGD-O1D
30	16	309	CLA	CHA-CBD-CGD-O2D
30	16	310	CLA	CBD-CGD-O2D-CED
33	A	847	BCR	C7-C8-C9-C34
33	A	847	BCR	C21-C22-C23-C24
33	A	847	BCR	C37-C22-C23-C24
33	A	848	BCR	C20-C21-C22-C37
33	A	849	BCR	C7-C8-C9-C10
33	A	849	BCR	C7-C8-C9-C34
33	A	849	BCR	C16-C17-C18-C36
33	A	849	BCR	C37-C22-C23-C24
33	A	850	BCR	C20-C21-C22-C37
33	A	850	BCR	C37-C22-C23-C24
33	A	851	BCR	C20-C21-C22-C37
33	B	841	BCR	C7-C8-C9-C10
33	B	842	BCR	C21-C22-C23-C24
33	B	842	BCR	C37-C22-C23-C24
33	B	845	BCR	C7-C8-C9-C10
33	B	845	BCR	C7-C8-C9-C34
33	B	845	BCR	C21-C22-C23-C24
33	B	845	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
33	I	101	BCR	C7-C8-C9-C34
33	J	102	BCR	C20-C21-C22-C37
33	J	102	BCR	C21-C22-C23-C24
33	J	102	BCR	C37-C22-C23-C24
33	J	103	BCR	C6-C7-C8-C9
33	J	103	BCR	C20-C21-C22-C37
33	J	103	BCR	C21-C22-C23-C24
33	L	201	BCR	C7-C8-C9-C34
33	L	201	BCR	C11-C10-C9-C8
33	L	201	BCR	C20-C21-C22-C23
33	L	204	BCR	C6-C7-C8-C9
33	L	204	BCR	C37-C22-C23-C24
33	L	204	BCR	C23-C24-C25-C26
33	M	101	BCR	C7-C8-C9-C10
33	M	101	BCR	C21-C22-C23-C24
33	2u	201	BCR	C6-C7-C8-C9
33	2u	201	BCR	C10-C11-C12-C13
33	2u	201	BCR	C11-C12-C13-C14
33	2u	201	BCR	C11-C12-C13-C35
33	2u	201	BCR	C37-C22-C23-C24
34	A	852	LHG	C3-O3-P-O4
34	B	848	LHG	O1-C1-C2-C3
34	B	848	LHG	O10-C23-O8-C6
34	B	848	LHG	C24-C23-O8-C6
34	2	320	LHG	O1-C1-C2-O2
34	2	320	LHG	O1-C1-C2-C3
34	2	320	LHG	C1-C2-C3-O3
34	2	320	LHG	C3-O3-P-O4
34	2	320	LHG	C3-O3-P-O6
34	2	320	LHG	C4-O6-P-O3
34	2	320	LHG	C4-O6-P-O5
34	5	317	LHG	C3-O3-P-O6
34	6	322	LHG	C3-O3-P-O4
34	6	322	LHG	C4-O6-P-O5
34	9	318	LHG	O1-C1-C2-O2
34	9	318	LHG	O1-C1-C2-C3
34	9	318	LHG	C3-O3-P-O5
34	9	318	LHG	C4-O6-P-O3
34	9	318	LHG	C4-O6-P-O5
34	9	318	LHG	C8-C7-O7-C5
35	12	301	LMT	O5'-C1'-O1'-C1
36	A	856	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
36	B	847	LMG	C2-C1-O1-C7
36	B	849	LMG	O6-C1-O1-C7
36	F	205	LMG	C2-C1-O1-C7
36	F	205	LMG	O6-C1-O1-C7
36	2u	204	LMG	C2-C1-O1-C7
36	2u	204	LMG	C11-C10-O7-C8
36	3	317	LMG	O6-C1-O1-C7
36	6	301	LMG	O1-C7-C8-O7
36	6	301	LMG	C11-C10-O7-C8
36	8	320	LMG	O1-C7-C8-O7
37	2u	203	A86	C10-C11-C13-O
37	2u	203	A86	C12-C11-C13-O
37	2u	205	A86	C10-C11-C13-O
37	2u	205	A86	C12-C11-C13-O
37	2u	205	A86	C13-C14-C15-O1
37	1	309	A86	C10-C11-C13-O
37	1	309	A86	C12-C11-C13-O
37	2	302	A86	C11-C10-C9-C8
37	2	302	A86	C10-C11-C13-O
37	2	302	A86	C12-C11-C13-O
37	2	302	A86	C1-C2-C3-C4
37	2	318	A86	C39-C38-O4-C34
37	2	319	A86	C39-C38-O4-C34
37	2	319	A86	C5-C6-C8-C9
37	2	319	A86	C7-C6-C8-C9
37	3	314	A86	C11-C10-C9-C8
37	3	315	A86	C-C1-C24-C25
37	3	315	A86	C2-C1-C24-C25
37	3	315	A86	C13-C14-C15-C16
37	3	315	A86	C24-C25-C26-C27
37	3	315	A86	C39-C38-O4-C34
37	3	315	A86	O5-C38-O4-C34
37	3	315	A86	C5-C6-C8-C9
37	3	315	A86	C7-C6-C8-C9
37	4	312	A86	O-C13-C14-C15
37	4	312	A86	C11-C13-C14-C15
37	4	312	A86	C13-C14-C15-O1
37	4	312	A86	C39-C38-O4-C34
37	4	312	A86	O5-C38-O4-C34
37	4	314	A86	C39-C38-O4-C34
37	4	315	A86	C-C1-C24-C25
37	4	315	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
37	4	317	A86	C39-C38-O4-C34
37	4	317	A86	O5-C38-O4-C34
37	5	301	A86	C13-C14-C15-C16
37	5	301	A86	C39-C38-O4-C34
37	5	301	A86	O5-C38-O4-C34
37	5	301	A86	C5-C6-C8-C9
37	5	301	A86	C7-C6-C8-C9
37	5	315	A86	C26-C27-C29-C30
37	5	315	A86	C39-C38-O4-C34
37	5	316	A86	O-C13-C14-C15
37	5	316	A86	C26-C27-C29-C30
37	5	316	A86	C28-C27-C29-C30
37	5	316	A86	C39-C38-O4-C34
37	6	320	A86	C2-C1-C24-C25
37	6	320	A86	C26-C27-C29-C30
37	6	320	A86	C28-C27-C29-C30
37	7	315	A86	C-C1-C24-C25
37	7	315	A86	C13-C14-C15-O1
37	7	315	A86	C39-C38-O4-C34
37	7	315	A86	C5-C6-C8-C9
37	7	315	A86	C7-C6-C8-C9
37	7	316	A86	C11-C10-C9-C8
37	7	316	A86	C10-C11-C13-O
37	7	316	A86	C12-C11-C13-O
37	7	316	A86	C5-C6-C8-C9
37	7	316	A86	C7-C6-C8-C9
37	7	319	A86	C13-C14-C15-O1
37	7	319	A86	C39-C38-O4-C34
37	7	319	A86	O5-C38-O4-C34
37	8	315	A86	C-C1-C24-C25
37	8	315	A86	O-C13-C14-C15
37	8	318	A86	C-C1-C24-C25
37	8	318	A86	C3-C4-C5-C6
37	9	313	A86	C2-C1-C24-C25
37	9	313	A86	O5-C38-O4-C34
37	9	313	A86	C5-C6-C8-C9
37	9	313	A86	C7-C6-C8-C9
37	9	315	A86	C-C1-C24-C25
37	9	315	A86	C2-C1-C24-C25
37	9	315	A86	C11-C10-C9-C8
37	9	316	A86	C26-C27-C29-C30
37	9	316	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
37	9	316	A86	C39-C38-O4-C34
37	10	301	A86	C39-C38-O4-C34
37	10	302	A86	C12-C11-C13-C14
37	10	315	A86	C-C1-C24-C25
37	10	315	A86	C2-C1-C24-C25
37	10	315	A86	O-C13-C14-C15
37	10	315	A86	C11-C13-C14-C15
37	10	315	A86	C3-C4-C5-C6
37	10	316	A86	C13-C14-C15-C16
37	10	316	A86	C39-C38-O4-C34
37	10	316	A86	C5-C6-C8-C9
37	10	317	A86	C12-C11-C13-C14
37	11	301	A86	C12-C11-C13-C14
37	11	301	A86	C39-C38-O4-C34
37	11	314	A86	O-C13-C14-C15
37	11	314	A86	C11-C13-C14-C15
37	11	314	A86	C13-C14-C15-C16
37	11	314	A86	C39-C38-O4-C34
37	11	315	A86	C2-C1-C24-C25
37	11	315	A86	C26-C27-C29-C30
37	11	315	A86	C28-C27-C29-C30
37	11	315	A86	C39-C38-O4-C34
37	11	315	A86	O5-C38-O4-C34
37	11	315	A86	C5-C6-C8-C9
37	11	316	A86	C13-C14-C15-C16
37	11	316	A86	C1-C2-C3-C4
37	11	316	A86	C24-C25-C26-C27
37	11	316	A86	O5-C38-O4-C34
37	11	316	A86	C5-C6-C8-C9
37	11	316	A86	C7-C6-C8-C9
37	12	314	A86	C-C1-C24-C25
37	12	314	A86	C2-C1-C24-C25
37	12	314	A86	C13-C14-C15-C16
37	12	314	A86	C5-C6-C8-C9
37	12	314	A86	C7-C6-C8-C9
37	12	316	A86	C13-C14-C15-C16
37	12	316	A86	C13-C14-C15-O1
37	12	316	A86	C3-C4-C5-C6
37	12	316	A86	C5-C6-C8-C9
37	12	316	A86	C7-C6-C8-C9
37	13	313	A86	C-C1-C24-C25
37	13	313	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
37	13	313	A86	C12-C11-C13-C14
37	13	315	A86	C13-C14-C15-C16
37	13	315	A86	C26-C27-C29-C30
37	13	315	A86	C28-C27-C29-C30
37	13	315	A86	C39-C38-O4-C34
37	13	315	A86	O5-C38-O4-C34
37	14	301	A86	C-C1-C24-C25
37	14	301	A86	C2-C1-C24-C25
37	14	301	A86	C39-C38-O4-C34
37	14	301	A86	O5-C38-O4-C34
37	14	314	A86	C2-C1-C24-C25
37	14	314	A86	C10-C11-C13-O
37	14	314	A86	C12-C11-C13-O
37	14	315	A86	C-C1-C24-C25
37	14	315	A86	C2-C1-C24-C25
37	14	315	A86	C11-C10-C9-C8
37	14	315	A86	O-C13-C14-C15
37	14	315	A86	C11-C13-C14-C15
37	14	315	A86	C24-C25-C26-C27
37	14	316	A86	C-C1-C24-C25
37	14	316	A86	O-C13-C14-C15
37	14	316	A86	C13-C14-C15-C16
37	14	317	A86	C-C1-C24-C25
37	14	317	A86	C2-C1-C24-C25
37	14	317	A86	O-C13-C14-C15
37	14	317	A86	C11-C13-C14-C15
37	14	317	A86	C13-C14-C15-C16
37	14	317	A86	C26-C27-C29-C30
37	14	317	A86	C3-C4-C5-C6
37	14	318	A86	C-C1-C24-C25
37	14	318	A86	C2-C1-C24-C25
37	14	318	A86	O-C13-C14-C15
37	14	318	A86	C11-C13-C14-C15
37	14	318	A86	C13-C14-C15-C16
37	14	318	A86	C24-C25-C26-C27
37	14	319	A86	C10-C11-C13-O
37	14	319	A86	C12-C11-C13-O
37	14	319	A86	C1-C2-C3-C4
37	14	319	A86	C24-C25-C26-C27
37	14	320	A86	C13-C14-C15-O1
37	14	320	A86	O5-C38-O4-C34
37	14	320	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
37	15	315	A86	C39-C38-O4-C34
37	15	316	A86	C11-C10-C9-C8
37	15	316	A86	C10-C11-C13-O
37	15	316	A86	C12-C11-C13-O
37	15	316	A86	C13-C14-C15-O1
37	15	316	A86	C24-C25-C26-C27
37	15	317	A86	O-C13-C14-C15
37	15	317	A86	C11-C13-C14-C15
37	15	317	A86	C13-C14-C15-O1
37	15	320	A86	C-C1-C24-C25
37	15	320	A86	C2-C1-C24-C25
37	15	320	A86	C10-C11-C13-O
37	15	320	A86	C12-C11-C13-O
37	15	320	A86	O-C13-C14-C15
37	15	320	A86	C13-C14-C15-O1
37	15	320	A86	C24-C25-C26-C27
37	15	320	A86	C39-C38-O4-C34
37	15	320	A86	C5-C6-C8-C9
37	15	320	A86	C7-C6-C8-C9
37	15	321	A86	C-C1-C24-C25
37	15	321	A86	C2-C1-C24-C25
37	15	321	A86	C13-C14-C15-C16
37	15	321	A86	C24-C25-C26-C27
37	15	321	A86	C39-C38-O4-C34
37	15	322	A86	O-C13-C14-C15
37	15	322	A86	C11-C13-C14-C15
37	15	322	A86	C13-C14-C15-O1
37	15	322	A86	C26-C27-C29-C30
37	15	322	A86	C28-C27-C29-C30
37	15	322	A86	C39-C38-O4-C34
37	15	322	A86	C3-C4-C5-C6
37	15	322	A86	C7-C6-C8-C9
37	15	323	A86	C-C1-C24-C25
37	15	323	A86	C2-C1-C24-C25
37	15	323	A86	C13-C14-C15-O1
37	15	323	A86	C24-C25-C26-C27
37	15	323	A86	C39-C38-O4-C34
37	15	323	A86	O5-C38-O4-C34
37	16	312	A86	C13-C14-C15-O1
37	16	312	A86	C28-C27-C29-C30
37	16	314	A86	C-C1-C24-C25
37	16	314	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
37	16	314	A86	O-C13-C14-C15
37	16	314	A86	C24-C25-C26-C27
37	16	314	A86	C5-C6-C8-C9
38	1	306	KC1	C2A-CAA-CBA-CGA
38	2	306	KC1	C2B-C3B-CAB-CBB
38	2	312	KC1	C1A-C2A-CAA-CBA
38	2	314	KC1	C1A-C2A-CAA-CBA
38	2	314	KC1	C2A-CAA-CBA-CGA
38	3	308	KC1	C3A-C2A-CAA-CBA
38	3	308	KC1	C2A-CAA-CBA-CGA
38	3	308	KC1	CHA-CBD-CGD-O1D
38	3	308	KC1	CHA-CBD-CGD-O2D
38	3	311	KC1	C1A-C2A-CAA-CBA
38	3	311	KC1	C2A-CAA-CBA-CGA
38	4	307	KC1	C3A-C2A-CAA-CBA
38	4	307	KC1	C2A-CAA-CBA-CGA
38	4	308	KC1	C3A-C2A-CAA-CBA
38	4	310	KC1	C2B-C3B-CAB-CBB
38	4	310	KC1	C4B-C3B-CAB-CBB
38	5	305	KC1	C3A-C2A-CAA-CBA
38	5	305	KC1	C2B-C3B-CAB-CBB
38	5	306	KC1	CHA-CBD-CGD-O1D
38	5	306	KC1	CHA-CBD-CGD-O2D
38	5	310	KC1	C3A-C2A-CAA-CBA
38	5	310	KC1	C2A-CAA-CBA-CGA
38	5	310	KC1	CHA-CBD-CGD-O1D
38	5	310	KC1	CHA-CBD-CGD-O2D
38	5	312	KC1	C1A-C2A-CAA-CBA
38	6	308	KC1	C1A-C2A-CAA-CBA
38	6	308	KC1	C2A-CAA-CBA-CGA
38	6	311	KC1	C3A-C2A-CAA-CBA
38	6	311	KC1	C2A-CAA-CBA-CGA
38	6	311	KC1	CHA-CBD-CGD-O1D
38	6	311	KC1	CHA-CBD-CGD-O2D
38	6	312	KC1	C3A-C2A-CAA-CBA
38	6	312	KC1	CAD-CBD-CGD-O2D
38	6	313	KC1	C3A-C2A-CAA-CBA
38	7	308	KC1	C3A-C2A-CAA-CBA
38	7	308	KC1	C2A-CAA-CBA-CGA
38	7	313	KC1	C2B-C3B-CAB-CBB
38	8	306	KC1	C3A-C2A-CAA-CBA
38	8	306	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
38	8	307	KC1	C3A-C2A-CAA-CBA
38	8	307	KC1	C2B-C3B-CAB-CBB
38	8	307	KC1	C2A-CAA-CBA-CGA
38	8	310	KC1	C1A-C2A-CAA-CBA
38	8	310	KC1	C2B-C3B-CAB-CBB
38	8	310	KC1	C4B-C3B-CAB-CBB
38	8	310	KC1	CHA-CBD-CGD-O1D
38	8	310	KC1	CHA-CBD-CGD-O2D
38	8	311	KC1	C3A-C2A-CAA-CBA
38	8	312	KC1	C2B-C3B-CAB-CBB
38	8	312	KC1	C2A-CAA-CBA-CGA
38	8	313	KC1	C3A-C2A-CAA-CBA
38	8	313	KC1	C2B-C3B-CAB-CBB
38	8	314	KC1	C3A-C2A-CAA-CBA
38	9	304	KC1	C3A-C2A-CAA-CBA
38	9	304	KC1	C2A-CAA-CBA-CGA
38	9	310	KC1	C3A-C2A-CAA-CBA
38	9	310	KC1	C2A-CAA-CBA-CGA
38	9	311	KC1	C2B-C3B-CAB-CBB
38	9	311	KC1	C2A-CAA-CBA-CGA
38	9	312	KC1	C1A-C2A-CAA-CBA
38	9	312	KC1	C2A-CAA-CBA-CGA
38	10	306	KC1	C3A-C2A-CAA-CBA
38	10	306	KC1	C2A-CAA-CBA-CGA
38	10	306	KC1	CHA-CBD-CGD-O1D
38	10	306	KC1	CHA-CBD-CGD-O2D
38	10	310	KC1	C3A-C2A-CAA-CBA
38	10	310	KC1	C2A-CAA-CBA-CGA
38	10	312	KC1	C2A-CAA-CBA-CGA
38	11	305	KC1	C3A-C2A-CAA-CBA
38	11	305	KC1	C2A-CAA-CBA-CGA
38	11	307	KC1	C3A-C2A-CAA-CBA
38	11	307	KC1	C2A-CAA-CBA-CGA
38	11	307	KC1	CHA-CBD-CGD-O1D
38	11	307	KC1	CHA-CBD-CGD-O2D
38	11	311	KC1	C3A-C2A-CAA-CBA
38	11	311	KC1	C2A-CAA-CBA-CGA
38	11	311	KC1	CHA-CBD-CGD-O1D
38	11	311	KC1	CHA-CBD-CGD-O2D
38	11	312	KC1	C1A-C2A-CAA-CBA
38	11	312	KC1	C2A-CAA-CBA-CGA
38	12	305	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
38	12	309	KC1	C3A-C2A-CAA-CBA
38	12	309	KC1	C2A-CAA-CBA-CGA
38	12	309	KC1	CHA-CBD-CGD-O1D
38	12	309	KC1	CHA-CBD-CGD-O2D
38	12	311	KC1	C2A-CAA-CBA-CGA
38	12	313	KC1	C3A-C2A-CAA-CBA
38	12	313	KC1	C2A-CAA-CBA-CGA
38	13	305	KC1	C2A-CAA-CBA-CGA
38	13	305	KC1	CHA-CBD-CGD-O1D
38	13	305	KC1	CHA-CBD-CGD-O2D
38	13	306	KC1	C1A-C2A-CAA-CBA
38	13	306	KC1	C2A-CAA-CBA-CGA
38	13	306	KC1	CHA-CBD-CGD-O1D
38	13	306	KC1	CHA-CBD-CGD-O2D
38	13	308	KC1	C3A-C2A-CAA-CBA
38	13	308	KC1	C2A-CAA-CBA-CGA
38	13	308	KC1	CHA-CBD-CGD-O1D
38	13	308	KC1	CHA-CBD-CGD-O2D
38	13	310	KC1	C1A-C2A-CAA-CBA
38	13	310	KC1	C2B-C3B-CAB-CBB
38	13	310	KC1	C2A-CAA-CBA-CGA
38	13	311	KC1	C3A-C2A-CAA-CBA
38	14	306	KC1	C2A-CAA-CBA-CGA
38	14	308	KC1	C3A-C2A-CAA-CBA
38	14	308	KC1	C2A-CAA-CBA-CGA
38	14	308	KC1	CHA-CBD-CGD-O1D
38	14	308	KC1	CHA-CBD-CGD-O2D
38	14	311	KC1	C3A-C2A-CAA-CBA
38	16	304	KC1	C3A-C2A-CAA-CBA
38	16	304	KC1	C2A-CAA-CBA-CGA
38	16	311	KC1	C3A-C2A-CAA-CBA
38	16	311	KC1	C2B-C3B-CAB-CBB
38	16	311	KC1	C4B-C3B-CAB-CBB
38	16	311	KC1	C2A-CAA-CBA-CGA
39	1	310	DD6	C-C1-C2-C3
39	1	310	DD6	C-C1-C24-C25
39	1	310	DD6	C9-C10-C11-C12
39	1	310	DD6	C10-C11-C13-C14
39	1	310	DD6	C12-C11-C13-C14
39	1	310	DD6	C4-C5-C6-C7
39	1	310	DD6	C7-C6-C8-C9
39	2	315	DD6	C-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
39	2	315	DD6	C9-C10-C11-C12
39	2	315	DD6	C9-C10-C11-C13
39	2	315	DD6	C12-C11-C13-C14
39	2	315	DD6	C4-C5-C6-C7
39	2	315	DD6	C5-C6-C8-C9
39	2	315	DD6	C7-C6-C8-C9
39	2	316	DD6	C-C1-C2-C3
39	2	316	DD6	C-C1-C24-C25
39	2	316	DD6	C9-C10-C11-C13
39	2	316	DD6	C12-C11-C13-C14
39	2	316	DD6	C13-C14-C15-O1
39	2	316	DD6	C4-C5-C6-C8
39	2	316	DD6	C7-C6-C8-C9
39	2	317	DD6	C-C1-C2-C3
39	2	317	DD6	C9-C10-C11-C13
39	2	317	DD6	C13-C14-C15-C16
39	2	317	DD6	C5-C6-C8-C9
39	2	317	DD6	C7-C6-C8-C9
39	3	312	DD6	C-C1-C2-C3
39	3	312	DD6	C9-C10-C11-C12
39	3	312	DD6	C12-C11-C13-C14
39	3	312	DD6	C4-C5-C6-C7
39	3	313	DD6	C-C1-C2-C3
39	3	313	DD6	C9-C10-C11-C12
39	3	313	DD6	C4-C5-C6-C7
39	3	316	DD6	C-C1-C2-C3
39	3	316	DD6	C9-C10-C11-C12
39	3	316	DD6	C4-C5-C6-C7
39	3	316	DD6	C7-C6-C8-C9
39	4	313	DD6	C-C1-C2-C3
39	4	313	DD6	C-C1-C24-C25
39	4	313	DD6	C9-C10-C11-C12
39	4	313	DD6	C13-C14-C15-C20
39	4	313	DD6	C13-C14-C15-O1
39	4	313	DD6	C4-C5-C6-C8
39	4	313	DD6	C7-C6-C8-C9
39	4	316	DD6	C-C1-C2-C3
39	4	316	DD6	C-C1-C24-C25
39	4	316	DD6	C9-C10-C11-C12
39	4	316	DD6	C9-C10-C11-C13
39	4	316	DD6	C12-C11-C13-C14
39	4	316	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
39	4	316	DD6	C4-C5-C6-C7
39	4	316	DD6	C5-C6-C8-C9
39	4	316	DD6	C7-C6-C8-C9
39	5	313	DD6	C-C1-C2-C3
39	5	313	DD6	C-C1-C24-C25
39	5	313	DD6	C9-C10-C11-C12
39	5	313	DD6	C4-C5-C6-C7
39	5	313	DD6	C5-C6-C8-C9
39	5	314	DD6	C-C1-C2-C3
39	5	314	DD6	C-C1-C24-C25
39	5	314	DD6	C9-C10-C11-C12
39	5	314	DD6	C13-C14-C15-O1
39	5	314	DD6	C4-C5-C6-C7
39	5	314	DD6	C5-C6-C8-C9
39	6	303	DD6	C-C1-C2-C3
39	6	303	DD6	C-C1-C24-C25
39	6	303	DD6	C9-C10-C11-C13
39	6	303	DD6	C4-C5-C6-C8
39	6	303	DD6	C7-C6-C8-C9
39	6	318	DD6	C-C1-C2-C3
39	6	318	DD6	C9-C10-C11-C12
39	6	318	DD6	C11-C10-C9-C8
39	6	318	DD6	C4-C5-C6-C7
39	6	319	DD6	C-C1-C2-C3
39	6	319	DD6	C-C1-C24-C25
39	6	319	DD6	C4-C5-C6-C8
39	6	319	DD6	C7-C6-C8-C9
39	6	321	DD6	C-C1-C2-C3
39	6	321	DD6	C2-C1-C24-C25
39	6	321	DD6	C9-C10-C11-C12
39	6	321	DD6	C4-C5-C6-C8
39	6	321	DD6	C5-C6-C8-C9
39	6	321	DD6	C7-C6-C8-C9
39	7	302	DD6	C-C1-C2-C3
39	7	302	DD6	C-C1-C24-C25
39	7	302	DD6	C2-C1-C24-C25
39	7	302	DD6	C9-C10-C11-C12
39	7	302	DD6	C24-C25-C26-C27
39	7	302	DD6	C4-C5-C6-C7
39	7	302	DD6	C5-C6-C8-C9
39	7	314	DD6	C-C1-C2-C3
39	7	314	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
39	7	314	DD6	C9-C10-C11-C12
39	7	314	DD6	C10-C11-C13-C14
39	7	314	DD6	C12-C11-C13-C14
39	7	314	DD6	C4-C5-C6-C7
39	7	314	DD6	C7-C6-C8-C9
39	7	317	DD6	C-C1-C2-C3
39	7	317	DD6	C2-C1-C24-C25
39	7	317	DD6	C9-C10-C11-C12
39	7	317	DD6	C13-C14-C15-C16
39	7	317	DD6	C4-C5-C6-C8
39	7	318	DD6	C-C1-C2-C3
39	7	318	DD6	C-C1-C24-C25
39	7	318	DD6	C2-C1-C24-C25
39	7	318	DD6	C9-C10-C11-C13
39	7	318	DD6	C4-C5-C6-C7
39	7	318	DD6	C7-C6-C8-C9
39	8	316	DD6	C-C1-C2-C3
39	8	316	DD6	C9-C10-C11-C12
39	8	316	DD6	C11-C10-C9-C8
39	8	316	DD6	C12-C11-C13-C14
39	8	316	DD6	C13-C14-C15-C20
39	8	316	DD6	C13-C14-C15-O1
39	8	316	DD6	C4-C5-C6-C7
39	8	316	DD6	C5-C6-C8-C9
39	8	316	DD6	C7-C6-C8-C9
39	8	317	DD6	C-C1-C2-C3
39	8	317	DD6	C9-C10-C11-C13
39	8	317	DD6	C10-C11-C13-C14
39	8	317	DD6	C12-C11-C13-C14
39	8	317	DD6	C4-C5-C6-C7
39	8	317	DD6	C5-C6-C8-C9
39	9	314	DD6	C-C1-C2-C3
39	9	314	DD6	C-C1-C24-C25
39	9	314	DD6	C9-C10-C11-C13
39	9	314	DD6	C10-C11-C13-C14
39	9	314	DD6	C12-C11-C13-C14
39	9	314	DD6	C4-C5-C6-C7
39	10	313	DD6	C-C1-C2-C3
39	10	313	DD6	C-C1-C24-C25
39	10	313	DD6	C9-C10-C11-C13
39	10	313	DD6	C13-C14-C15-O1
39	10	313	DD6	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	10	314	DD6	C-C1-C2-C3
39	10	314	DD6	C9-C10-C11-C12
39	10	314	DD6	C4-C5-C6-C7
39	10	314	DD6	C5-C6-C8-C9
39	11	313	DD6	C-C1-C2-C3
39	11	313	DD6	C-C1-C24-C25
39	11	313	DD6	C9-C10-C11-C13
39	11	313	DD6	C4-C5-C6-C7
39	11	313	DD6	C7-C6-C8-C9
39	12	315	DD6	C-C1-C2-C3
39	12	315	DD6	C9-C10-C11-C12
39	12	315	DD6	C10-C11-C13-C14
39	12	315	DD6	C12-C11-C13-C14
39	12	315	DD6	C4-C5-C6-C7
39	12	317	DD6	C-C1-C2-C3
39	12	317	DD6	C2-C1-C24-C25
39	12	317	DD6	C9-C10-C11-C12
39	12	317	DD6	C9-C10-C11-C13
39	12	317	DD6	C12-C11-C13-C14
39	12	317	DD6	C4-C5-C6-C7
39	12	317	DD6	C5-C6-C8-C9
39	12	317	DD6	C7-C6-C8-C9
39	13	314	DD6	C-C1-C2-C3
39	13	314	DD6	C-C1-C24-C25
39	13	314	DD6	C9-C10-C11-C12
39	13	314	DD6	C12-C11-C13-C14
39	13	314	DD6	C13-C14-C15-O1
39	13	314	DD6	C3-C4-C5-C6
39	13	314	DD6	C4-C5-C6-C7
39	13	314	DD6	C7-C6-C8-C9
39	15	318	DD6	C24-C1-C2-C3
39	15	318	DD6	C-C1-C24-C25
39	15	318	DD6	C9-C10-C11-C13
39	15	318	DD6	C13-C14-C15-C16
39	15	318	DD6	C1-C2-C3-C4
39	15	318	DD6	C4-C5-C6-C7
39	15	318	DD6	C7-C6-C8-C9
39	15	319	DD6	C-C1-C2-C3
39	15	319	DD6	C2-C1-C24-C25
39	15	319	DD6	C9-C10-C11-C12
39	15	319	DD6	C13-C14-C15-C16
39	15	319	DD6	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
39	15	319	DD6	C4-C5-C6-C7
39	15	319	DD6	C5-C6-C8-C9
39	16	313	DD6	C-C1-C2-C3
39	16	313	DD6	C9-C10-C11-C13
39	16	313	DD6	C13-C14-C15-C20
39	16	313	DD6	C13-C14-C15-O1
39	16	313	DD6	C4-C5-C6-C7
39	16	313	DD6	C5-C6-C8-C9
39	16	313	DD6	C7-C6-C8-C9
30	A	807	CLA	O1D-CGD-O2D-CED
30	2	303	CLA	O1D-CGD-O2D-CED
37	4	314	A86	O5-C38-O4-C34
37	4	315	A86	C39-C38-O4-C34
37	5	315	A86	O5-C38-O4-C34
37	7	315	A86	O5-C38-O4-C34
37	10	315	A86	C39-C38-O4-C34
37	10	316	A86	O5-C38-O4-C34
37	11	301	A86	O5-C38-O4-C34
37	12	316	A86	C39-C38-O4-C34
37	14	320	A86	C39-C38-O4-C34
37	15	316	A86	C39-C38-O4-C34
37	15	317	A86	C39-C38-O4-C34
35	A	854	LMT	O5B-C1B-O1B-C4'
35	B	852	LMT	C3'-C4'-O1B-C1B
30	F	201	CLA	O1D-CGD-O2D-CED
30	7	307	CLA	O1D-CGD-O2D-CED
30	15	304	CLA	O1D-CGD-O2D-CED
30	15	314	CLA	O1D-CGD-O2D-CED
30	16	310	CLA	O1D-CGD-O2D-CED
37	2u	203	A86	C39-C38-O4-C34
37	2	318	A86	O5-C38-O4-C34
37	2	319	A86	O5-C38-O4-C34
37	5	316	A86	O5-C38-O4-C34
37	9	316	A86	O5-C38-O4-C34
37	10	301	A86	O5-C38-O4-C34
37	10	317	A86	C39-C38-O4-C34
37	11	314	A86	O5-C38-O4-C34
37	11	316	A86	C39-C38-O4-C34
37	15	315	A86	O5-C38-O4-C34
37	15	321	A86	O5-C38-O4-C34
37	15	322	A86	O5-C38-O4-C34
37	16	314	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
30	A	811	CLA	CBD-CGD-O2D-CED
30	A	829	CLA	CBD-CGD-O2D-CED
30	B	822	CLA	CBD-CGD-O2D-CED
30	F	201	CLA	CBD-CGD-O2D-CED
30	6	317	CLA	CBD-CGD-O2D-CED
30	9	309	CLA	CBD-CGD-O2D-CED
30	12	308	CLA	CBD-CGD-O2D-CED
30	14	310	CLA	CBD-CGD-O2D-CED
30	15	304	CLA	CBD-CGD-O2D-CED
30	15	314	CLA	CBD-CGD-O2D-CED
38	2	314	KC1	CBD-CGD-O2D-CED
38	5	312	KC1	CBD-CGD-O2D-CED
35	15	301	LMT	O5B-C1B-O1B-C4'
30	A	804	CLA	O1A-CGA-O2A-C1
30	B	810	CLA	O1A-CGA-O2A-C1
30	1	304	CLA	O1A-CGA-O2A-C1
30	2	303	CLA	O1A-CGA-O2A-C1
30	7	307	CLA	O1A-CGA-O2A-C1
37	9	313	A86	C39-C38-O4-C34
37	14	316	A86	C39-C38-O4-C34
37	14	317	A86	C39-C38-O4-C34
37	15	320	A86	O5-C38-O4-C34
37	10	315	A86	C35-C34-O4-C38
37	11	315	A86	C33-C34-O4-C38
38	2	314	KC1	O1D-CGD-O2D-CED
30	A	804	CLA	CBA-CGA-O2A-C1
30	1	304	CLA	CBA-CGA-O2A-C1
30	2	303	CLA	CBA-CGA-O2A-C1
30	7	307	CLA	CBA-CGA-O2A-C1
36	8	319	LMG	C29-C28-O8-C9
37	2u	203	A86	O5-C38-O4-C34
37	2u	205	A86	O5-C38-O4-C34
30	A	806	CLA	O1A-CGA-O2A-C1
30	A	809	CLA	O1A-CGA-O2A-C1
30	A	821	CLA	O1A-CGA-O2A-C1
30	A	843	CLA	O1A-CGA-O2A-C1
30	4	301	CLA	O1A-CGA-O2A-C1
30	7	306	CLA	O1A-CGA-O2A-C1
30	11	304	CLA	O1A-CGA-O2A-C1
30	12	306	CLA	O1A-CGA-O2A-C1
34	9	318	LHG	O10-C23-O8-C6
36	6	301	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
36	8	319	LMG	O10-C28-O8-C9
37	2u	205	A86	C39-C38-O4-C34
37	10	302	A86	C39-C38-O4-C34
37	10	315	A86	O5-C38-O4-C34
38	13	312	KC1	CAA-CBA-CGA-O1A
38	13	312	KC1	CAA-CBA-CGA-O2A
38	16	304	KC1	CAA-CBA-CGA-O1A
38	16	304	KC1	CAA-CBA-CGA-O2A
30	2	309	CLA	O1D-CGD-O2D-CED
30	9	305	CLA	O1D-CGD-O2D-CED
30	15	309	CLA	O1D-CGD-O2D-CED
37	15	317	A86	O5-C38-O4-C34
34	9	318	LHG	O9-C7-O7-C5
36	A	856	LMG	O9-C10-O7-C8
36	B	849	LMG	O9-C10-O7-C8
36	2u	204	LMG	O9-C10-O7-C8
37	10	302	A86	O5-C38-O4-C34
30	A	809	CLA	C3-C5-C6-C7
30	A	810	CLA	C3-C5-C6-C7
30	A	816	CLA	C3-C5-C6-C7
30	A	821	CLA	C3-C5-C6-C7
30	A	822	CLA	C3-C5-C6-C7
30	A	844	CLA	C3-C5-C6-C7
30	B	806	CLA	C3-C5-C6-C7
30	B	808	CLA	C3-C5-C6-C7
30	B	813	CLA	C3-C5-C6-C7
30	B	834	CLA	C3-C5-C6-C7
30	F	202	CLA	C3-C5-C6-C7
30	1	301	CLA	C3-C5-C6-C7
30	2	307	CLA	C3-C5-C6-C7
30	2	310	CLA	C3-C5-C6-C7
30	3	303	CLA	C3-C5-C6-C7
30	3	306	CLA	C3-C5-C6-C7
30	3	307	CLA	C3-C5-C6-C7
30	4	309	CLA	C3-C5-C6-C7
30	5	302	CLA	C3-C5-C6-C7
30	5	303	CLA	C3-C5-C6-C7
30	5	304	CLA	C3-C5-C6-C7
30	6	305	CLA	C3-C5-C6-C7
30	6	307	CLA	C3-C5-C6-C7
30	6	309	CLA	C3-C5-C6-C7
30	6	317	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	7	303	CLA	C3-C5-C6-C7
30	7	306	CLA	C3-C5-C6-C7
30	7	310	CLA	C3-C5-C6-C7
30	7	311	CLA	C3-C5-C6-C7
30	8	304	CLA	C3-C5-C6-C7
30	9	308	CLA	C3-C5-C6-C7
30	10	304	CLA	C3-C5-C6-C7
30	10	309	CLA	C3-C5-C6-C7
30	11	309	CLA	C3-C5-C6-C7
30	14	303	CLA	C3-C5-C6-C7
30	16	302	CLA	C3-C5-C6-C7
31	B	840	PQN	C13-C15-C16-C17
30	B	801	CLA	O1D-CGD-O2D-CED
30	A	806	CLA	CBA-CGA-O2A-C1
30	A	809	CLA	CBA-CGA-O2A-C1
30	A	821	CLA	CBA-CGA-O2A-C1
30	A	843	CLA	CBA-CGA-O2A-C1
30	B	810	CLA	CBA-CGA-O2A-C1
30	4	301	CLA	CBA-CGA-O2A-C1
30	5	309	CLA	CBA-CGA-O2A-C1
30	11	304	CLA	CBA-CGA-O2A-C1
36	6	301	LMG	C29-C28-O8-C9
36	7	320	LMG	C29-C28-O8-C9
30	A	820	CLA	CBD-CGD-O2D-CED
30	A	835	CLA	CBD-CGD-O2D-CED
30	1	302	CLA	CBD-CGD-O2D-CED
30	3	307	CLA	CBD-CGD-O2D-CED
30	8	301	CLA	CBD-CGD-O2D-CED
30	11	310	CLA	CBD-CGD-O2D-CED
38	5	306	KC1	CBD-CGD-O2D-CED
38	8	311	KC1	CBD-CGD-O2D-CED
38	10	306	KC1	CBD-CGD-O2D-CED
38	11	307	KC1	CBD-CGD-O2D-CED
38	13	305	KC1	CBD-CGD-O2D-CED
38	13	306	KC1	CBD-CGD-O2D-CED
37	4	315	A86	O5-C38-O4-C34
37	14	318	A86	C39-C38-O4-C34
30	14	310	CLA	O1A-CGA-O2A-C1
37	12	316	A86	O5-C38-O4-C34
30	A	821	CLA	C4-C3-C5-C6
30	A	831	CLA	C4-C3-C5-C6
30	A	833	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	A	836	CLA	C4-C3-C5-C6
30	A	842	CLA	C4-C3-C5-C6
30	B	802	CLA	C4-C3-C5-C6
30	B	806	CLA	C4-C3-C5-C6
30	B	811	CLA	C4-C3-C5-C6
30	B	821	CLA	C4-C3-C5-C6
30	B	831	CLA	C4-C3-C5-C6
30	B	833	CLA	C4-C3-C5-C6
30	2	309	CLA	C4-C3-C5-C6
30	3	301	CLA	C4-C3-C5-C6
30	3	305	CLA	C4-C3-C5-C6
30	4	305	CLA	C4-C3-C5-C6
30	6	307	CLA	C4-C3-C5-C6
30	7	304	CLA	C4-C3-C5-C6
30	10	309	CLA	C4-C3-C5-C6
30	11	304	CLA	C4-C3-C5-C6
30	15	303	CLA	C4-C3-C5-C6
30	16	303	CLA	C4-C3-C5-C6
30	A	821	CLA	C2-C3-C5-C6
30	A	833	CLA	C2-C3-C5-C6
30	A	836	CLA	C2-C3-C5-C6
30	A	842	CLA	C2-C3-C5-C6
30	B	802	CLA	C2-C3-C5-C6
30	B	806	CLA	C2-C3-C5-C6
30	B	821	CLA	C2-C3-C5-C6
30	B	831	CLA	C2-C3-C5-C6
30	B	833	CLA	C2-C3-C5-C6
30	3	301	CLA	C2-C3-C5-C6
30	4	305	CLA	C2-C3-C5-C6
30	6	307	CLA	C2-C3-C5-C6
30	7	304	CLA	C2-C3-C5-C6
30	10	309	CLA	C2-C3-C5-C6
30	15	303	CLA	C2-C3-C5-C6
30	16	303	CLA	C2-C3-C5-C6
37	15	316	A86	O5-C38-O4-C34
30	A	824	CLA	C2A-CAA-CBA-CGA
30	A	842	CLA	C2A-CAA-CBA-CGA
30	B	810	CLA	C2A-CAA-CBA-CGA
30	B	823	CLA	C2A-CAA-CBA-CGA
36	3	317	LMG	O10-C28-O8-C9
30	A	811	CLA	C3-C5-C6-C7
30	B	810	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	1	307	CLA	C3-C5-C6-C7
30	6	314	CLA	C3-C5-C6-C7
30	9	301	CLA	C3-C5-C6-C7
30	9	305	CLA	C3-C5-C6-C7
30	10	308	CLA	C3-C5-C6-C7
30	12	303	CLA	C3-C5-C6-C7
30	14	302	CLA	C3-C5-C6-C7
30	A	815	CLA	CBA-CGA-O2A-C1
30	A	820	CLA	CBA-CGA-O2A-C1
30	B	821	CLA	CBA-CGA-O2A-C1
30	7	306	CLA	CBA-CGA-O2A-C1
30	10	309	CLA	CBA-CGA-O2A-C1
30	12	306	CLA	CBA-CGA-O2A-C1
30	14	302	CLA	CBA-CGA-O2A-C1
36	2u	204	LMG	C29-C28-O8-C9
37	16	314	A86	O5-C38-O4-C34
37	2	302	A86	C39-C38-O4-C34
37	10	317	A86	O5-C38-O4-C34
37	14	317	A86	O5-C38-O4-C34
37	9	315	A86	C3-C4-C5-C6
37	10	302	A86	C3-C4-C5-C6
37	10	316	A86	C24-C25-C26-C27
37	11	314	A86	C11-C10-C9-C8
37	12	316	A86	C24-C25-C26-C27
37	14	315	A86	C3-C4-C5-C6
37	14	317	A86	C24-C25-C26-C27
37	14	318	A86	C3-C4-C5-C6
37	15	322	A86	C11-C10-C9-C8
37	15	323	A86	C1-C2-C3-C4
37	16	314	A86	C11-C10-C9-C8
39	2	317	DD6	C11-C10-C9-C8
39	4	313	DD6	C11-C10-C9-C8
39	6	321	DD6	C1-C2-C3-C4
39	9	314	DD6	C3-C4-C5-C6
39	12	317	DD6	C11-C10-C9-C8
39	13	314	DD6	C11-C10-C9-C8
39	15	318	DD6	C24-C25-C26-C27
39	15	319	DD6	C11-C10-C9-C8
30	A	815	CLA	O1A-CGA-O2A-C1
30	B	821	CLA	O1A-CGA-O2A-C1
30	14	302	CLA	O1A-CGA-O2A-C1
30	15	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	16	306	CLA	O1A-CGA-O2A-C1
36	F	205	LMG	O9-C10-O7-C8
36	F	205	LMG	C29-C28-O8-C9
36	8	320	LMG	O6-C5-C6-O5
30	B	812	CLA	C3-C5-C6-C7
30	B	821	CLA	C3-C5-C6-C7
30	B	822	CLA	C3-C5-C6-C7
30	B	823	CLA	C3-C5-C6-C7
30	B	824	CLA	C3-C5-C6-C7
30	B	832	CLA	C3-C5-C6-C7
30	2	308	CLA	C3-C5-C6-C7
30	6	310	CLA	C3-C5-C6-C7
30	8	305	CLA	C3-C5-C6-C7
30	16	303	CLA	C3-C5-C6-C7
30	15	306	CLA	CBD-CGD-O2D-CED
38	7	308	KC1	CBD-CGD-O2D-CED
34	B	848	LHG	O2-C2-C3-O3
34	2	320	LHG	O2-C2-C3-O3
30	A	829	CLA	O1D-CGD-O2D-CED
30	9	309	CLA	O1D-CGD-O2D-CED
30	A	829	CLA	CBA-CGA-O2A-C1
30	A	833	CLA	CBA-CGA-O2A-C1
30	A	836	CLA	CBA-CGA-O2A-C1
30	7	303	CLA	CBA-CGA-O2A-C1
30	12	312	CLA	CBA-CGA-O2A-C1
30	14	310	CLA	CBA-CGA-O2A-C1
34	9	318	LHG	C24-C23-O8-C6
37	14	316	A86	O5-C38-O4-C34
30	5	309	CLA	O1A-CGA-O2A-C1
30	14	310	CLA	O1D-CGD-O2D-CED
37	8	315	A86	C39-C38-O4-C34
37	8	315	A86	O5-C38-O4-C34
36	3	317	LMG	C4-C5-C6-O5
30	3	303	CLA	CBD-CGD-O2D-CED
36	B	849	LMG	C11-C10-O7-C8
36	F	205	LMG	C11-C10-O7-C8
36	8	320	LMG	C11-C10-O7-C8
36	8	321	LMG	C11-C10-O7-C8
30	A	820	CLA	O1A-CGA-O2A-C1
30	10	309	CLA	O1A-CGA-O2A-C1
35	9	317	LMT	O5B-C5B-C6B-O6B
36	F	205	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	6	317	CLA	O1D-CGD-O2D-CED
30	5	311	CLA	C3-C5-C6-C7
30	12	312	CLA	C3-C5-C6-C7
30	13	302	CLA	C3-C5-C6-C7
30	A	823	CLA	CBD-CGD-O2D-CED
30	A	825	CLA	CBD-CGD-O2D-CED
30	A	841	CLA	CBD-CGD-O2D-CED
30	13	302	CLA	CBD-CGD-O2D-CED
38	13	308	KC1	CBD-CGD-O2D-CED
30	B	816	CLA	CBA-CGA-O2A-C1
30	15	307	CLA	CBA-CGA-O2A-C1
30	16	306	CLA	CBA-CGA-O2A-C1
36	3	317	LMG	C29-C28-O8-C9
38	5	310	KC1	CAA-CBA-CGA-O1A
38	6	308	KC1	CAA-CBA-CGA-O1A
38	7	308	KC1	CAA-CBA-CGA-O2A
38	8	313	KC1	CAA-CBA-CGA-O1A
38	11	311	KC1	CAA-CBA-CGA-O1A
30	A	812	CLA	C4-C3-C5-C6
30	B	816	CLA	C4-C3-C5-C6
30	B	838	CLA	C4-C3-C5-C6
30	1	305	CLA	C4-C3-C5-C6
30	5	303	CLA	C4-C3-C5-C6
30	6	314	CLA	C4-C3-C5-C6
30	12	302	CLA	C4-C3-C5-C6
30	14	302	CLA	C4-C3-C5-C6
30	A	812	CLA	C2-C3-C5-C6
30	A	831	CLA	C2-C3-C5-C6
30	B	816	CLA	C2-C3-C5-C6
30	B	838	CLA	C2-C3-C5-C6
30	3	305	CLA	C2-C3-C5-C6
30	6	314	CLA	C2-C3-C5-C6
30	8	305	CLA	C2-C3-C5-C6
30	9	307	CLA	C2-C3-C5-C6
30	11	304	CLA	C2-C3-C5-C6
30	12	302	CLA	C2-C3-C5-C6
30	14	302	CLA	C2-C3-C5-C6
30	A	829	CLA	O1A-CGA-O2A-C1
30	A	836	CLA	O1A-CGA-O2A-C1
36	A	856	LMG	O6-C5-C6-O5
36	3	317	LMG	O6-C5-C6-O5
30	5	302	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	9	303	CLA	CBD-CGD-O2D-CED
30	7	309	CLA	C5-C6-C7-C8
36	B	847	LMG	O6-C5-C6-O5
30	A	830	CLA	C2A-CAA-CBA-CGA
30	A	832	CLA	C2A-CAA-CBA-CGA
36	F	205	LMG	O10-C28-O8-C9
30	12	308	CLA	O1D-CGD-O2D-CED
30	7	303	CLA	O1A-CGA-O2A-C1
30	12	312	CLA	O1A-CGA-O2A-C1
30	10	303	CLA	C3-C5-C6-C7
37	9	315	A86	C39-C38-O4-C34
35	A	854	LMT	O5'-C1'-O1'-C1
35	A	855	LMT	O5'-C1'-O1'-C1
35	11	303	LMT	O5'-C1'-O1'-C1
36	B	847	LMG	O6-C1-O1-C7
36	2u	204	LMG	O6-C1-O1-C7
36	7	320	LMG	O6-C1-O1-C7
30	A	805	CLA	CBA-CGA-O2A-C1
30	A	823	CLA	CBA-CGA-O2A-C1
30	12	310	CLA	CBA-CGA-O2A-C1
30	13	307	CLA	CBA-CGA-O2A-C1
30	A	810	CLA	CBD-CGD-O2D-CED
30	A	822	CLA	CBD-CGD-O2D-CED
30	B	804	CLA	CBD-CGD-O2D-CED
30	B	809	CLA	CBD-CGD-O2D-CED
30	B	831	CLA	CBD-CGD-O2D-CED
30	3	306	CLA	CBD-CGD-O2D-CED
30	5	303	CLA	CBD-CGD-O2D-CED
30	11	309	CLA	CBD-CGD-O2D-CED
30	12	321	CLA	CBD-CGD-O2D-CED
30	15	303	CLA	CBD-CGD-O2D-CED
38	8	306	KC1	CBD-CGD-O2D-CED
37	7	319	A86	C35-C34-O4-C38
35	11	303	LMT	O5B-C5B-C6B-O6B
35	15	301	LMT	O5B-C5B-C6B-O6B
38	9	310	KC1	CAA-CBA-CGA-O1A
38	10	310	KC1	CAA-CBA-CGA-O1A
38	10	310	KC1	CAA-CBA-CGA-O2A
38	11	305	KC1	CAA-CBA-CGA-O2A
38	13	305	KC1	CAA-CBA-CGA-O1A
38	14	306	KC1	CAA-CBA-CGA-O2A
30	A	833	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	12	310	CLA	O1A-CGA-O2A-C1
36	6	301	LMG	O6-C5-C6-O5
37	14	314	A86	C39-C38-O4-C34
30	B	802	CLA	CBD-CGD-O2D-CED
30	B	808	CLA	CBD-CGD-O2D-CED
30	B	838	CLA	CBD-CGD-O2D-CED
30	8	305	CLA	CBD-CGD-O2D-CED
30	13	309	CLA	CBD-CGD-O2D-CED
38	6	311	KC1	CBD-CGD-O2D-CED
30	A	811	CLA	O1D-CGD-O2D-CED
36	8	320	LMG	C4-C5-C6-O5
37	5	301	A86	C11-C10-C9-C8
37	8	315	A86	C24-C25-C26-C27
37	10	302	A86	C1-C2-C3-C4
37	10	315	A86	C11-C10-C9-C8
37	10	317	A86	C3-C4-C5-C6
37	12	314	A86	C11-C10-C9-C8
37	14	317	A86	C11-C10-C9-C8
37	15	316	A86	C3-C4-C5-C6
37	15	317	A86	C24-C25-C26-C27
39	3	316	DD6	C11-C10-C9-C8
39	4	316	DD6	C24-C25-C26-C27
39	6	319	DD6	C11-C10-C9-C8
30	B	816	CLA	O1A-CGA-O2A-C1
30	A	807	CLA	CBA-CGA-O2A-C1
30	A	811	CLA	CBA-CGA-O2A-C1
30	A	832	CLA	CBA-CGA-O2A-C1
30	B	811	CLA	CBA-CGA-O2A-C1
30	B	813	CLA	CBA-CGA-O2A-C1
30	B	818	CLA	CBA-CGA-O2A-C1
30	B	826	CLA	CBA-CGA-O2A-C1
30	B	829	CLA	CBA-CGA-O2A-C1
30	2u	202	CLA	CBA-CGA-O2A-C1
30	1	301	CLA	CBA-CGA-O2A-C1
30	1	305	CLA	CBA-CGA-O2A-C1
30	2	309	CLA	CBA-CGA-O2A-C1
30	3	301	CLA	CBA-CGA-O2A-C1
30	3	306	CLA	CBA-CGA-O2A-C1
30	3	307	CLA	CBA-CGA-O2A-C1
30	5	308	CLA	CBA-CGA-O2A-C1
30	7	311	CLA	CBA-CGA-O2A-C1
30	8	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	9	309	CLA	CBA-CGA-O2A-C1
30	11	310	CLA	CBA-CGA-O2A-C1
30	15	302	CLA	CBA-CGA-O2A-C1
30	15	304	CLA	CBA-CGA-O2A-C1
30	16	303	CLA	CBA-CGA-O2A-C1
30	5	311	CLA	CBD-CGD-O2D-CED
38	11	311	KC1	CBD-CGD-O2D-CED
30	B	822	CLA	O1D-CGD-O2D-CED
38	5	312	KC1	O1D-CGD-O2D-CED
36	F	205	LMG	C4-C5-C6-O5
30	1	305	CLA	O1A-CGA-O2A-C1
38	4	307	KC1	CAA-CBA-CGA-O1A
38	5	310	KC1	CAA-CBA-CGA-O2A
38	6	308	KC1	CAA-CBA-CGA-O2A
38	6	311	KC1	CAA-CBA-CGA-O1A
38	7	308	KC1	CAA-CBA-CGA-O1A
38	7	313	KC1	CAA-CBA-CGA-O2A
38	8	313	KC1	CAA-CBA-CGA-O2A
38	9	304	KC1	CAA-CBA-CGA-O2A
38	9	312	KC1	CAA-CBA-CGA-O1A
38	10	312	KC1	CAA-CBA-CGA-O1A
38	10	312	KC1	CAA-CBA-CGA-O2A
38	11	307	KC1	CAA-CBA-CGA-O1A
38	11	307	KC1	CAA-CBA-CGA-O2A
38	11	311	KC1	CAA-CBA-CGA-O2A
38	12	313	KC1	CAA-CBA-CGA-O2A
38	14	306	KC1	CAA-CBA-CGA-O1A
38	14	308	KC1	CAA-CBA-CGA-O1A
38	14	308	KC1	CAA-CBA-CGA-O2A
30	9	307	CLA	C4-C3-C5-C6
30	B	811	CLA	C2-C3-C5-C6
30	1	305	CLA	C2-C3-C5-C6
30	2	309	CLA	C2-C3-C5-C6
30	5	303	CLA	C2-C3-C5-C6
30	6	309	CLA	C2-C3-C5-C6
30	A	843	CLA	C3-C5-C6-C7
30	10	305	CLA	C3-C5-C6-C7
30	A	816	CLA	C14-C13-C15-C16
30	A	833	CLA	C11-C10-C8-C9
30	B	828	CLA	C11-C12-C13-C14
30	F	202	CLA	C6-C7-C8-C9
30	1	307	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	3	307	CLA	C11-C12-C13-C14
30	4	302	CLA	C11-C12-C13-C14
30	10	308	CLA	C11-C10-C8-C9
30	11	309	CLA	C11-C10-C8-C9
30	12	304	CLA	C11-C12-C13-C14
30	16	303	CLA	C11-C12-C13-C14
35	12	318	LMT	O5B-C5B-C6B-O6B
36	B	847	LMG	C4-C5-C6-O5
35	A	854	LMT	C2'-C1'-O1'-C1
35	A	855	LMT	C2'-C1'-O1'-C1
35	11	303	LMT	C2'-C1'-O1'-C1
34	A	853	LHG	O2-C2-C3-O3
30	B	813	CLA	O1A-CGA-O2A-C1
30	8	303	CLA	O1A-CGA-O2A-C1
30	15	302	CLA	O1A-CGA-O2A-C1
30	B	828	CLA	CBD-CGD-O2D-CED
30	A	835	CLA	O1D-CGD-O2D-CED
33	A	848	BCR	C11-C12-C13-C35
33	A	850	BCR	C7-C8-C9-C34
33	A	851	BCR	C37-C22-C23-C24
33	B	841	BCR	C7-C8-C9-C34
33	B	843	BCR	C7-C8-C9-C34
33	B	844	BCR	C7-C8-C9-C34
33	B	845	BCR	C11-C12-C13-C35
33	F	204	BCR	C7-C8-C9-C34
33	F	204	BCR	C37-C22-C23-C24
33	J	102	BCR	C11-C12-C13-C35
33	L	205	BCR	C7-C8-C9-C34
33	M	101	BCR	C7-C8-C9-C34
37	2u	203	A86	C7-C6-C8-C9
37	6	320	A86	C-C1-C24-C25
37	6	320	A86	C7-C6-C8-C9
37	8	318	A86	C7-C6-C8-C9
37	9	313	A86	C-C1-C24-C25
37	9	316	A86	C-C1-C24-C25
37	10	302	A86	C-C1-C24-C25
37	10	316	A86	C-C1-C24-C25
37	10	316	A86	C7-C6-C8-C9
37	11	315	A86	C-C1-C24-C25
37	11	315	A86	C7-C6-C8-C9
37	13	315	A86	C-C1-C24-C25
37	14	314	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
37	14	314	A86	C7-C6-C8-C9
37	14	317	A86	C7-C6-C8-C9
37	15	323	A86	C7-C6-C8-C9
37	16	312	A86	C7-C6-C8-C9
37	16	314	A86	C7-C6-C8-C9
39	2	315	DD6	C-C1-C24-C25
39	2	317	DD6	C-C1-C24-C25
39	3	312	DD6	C-C1-C24-C25
39	3	312	DD6	C7-C6-C8-C9
39	3	313	DD6	C-C1-C24-C25
39	3	313	DD6	C7-C6-C8-C9
39	3	316	DD6	C12-C11-C13-C14
39	4	313	DD6	C12-C11-C13-C14
39	5	313	DD6	C12-C11-C13-C14
39	5	314	DD6	C12-C11-C13-C14
39	6	318	DD6	C-C1-C24-C25
39	6	318	DD6	C7-C6-C8-C9
39	6	321	DD6	C12-C11-C13-C14
39	7	317	DD6	C7-C6-C8-C9
39	7	318	DD6	C12-C11-C13-C14
39	8	316	DD6	C-C1-C24-C25
39	8	317	DD6	C-C1-C24-C25
39	9	314	DD6	C7-C6-C8-C9
39	10	313	DD6	C12-C11-C13-C14
39	10	314	DD6	C-C1-C24-C25
39	10	314	DD6	C12-C11-C13-C14
39	10	314	DD6	C7-C6-C8-C9
39	11	313	DD6	C12-C11-C13-C14
39	12	315	DD6	C-C1-C24-C25
39	12	317	DD6	C-C1-C24-C25
39	15	318	DD6	C12-C11-C13-C14
39	15	319	DD6	C12-C11-C13-C14
39	15	319	DD6	C7-C6-C8-C9
39	16	313	DD6	C-C1-C24-C25
39	16	313	DD6	C12-C11-C13-C14
33	A	851	BCR	C21-C22-C23-C24
37	1	309	A86	C5-C6-C8-C9
37	6	320	A86	C5-C6-C8-C9
37	7	315	A86	C2-C1-C24-C25
37	8	315	A86	C2-C1-C24-C25
37	8	318	A86	C5-C6-C8-C9
37	9	316	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
37	10	302	A86	C2-C1-C24-C25
37	10	316	A86	C2-C1-C24-C25
37	13	315	A86	C2-C1-C24-C25
37	14	314	A86	C5-C6-C8-C9
37	14	316	A86	C2-C1-C24-C25
37	14	317	A86	C5-C6-C8-C9
37	15	323	A86	C5-C6-C8-C9
37	16	312	A86	C5-C6-C8-C9
39	3	313	DD6	C10-C11-C13-C14
39	3	316	DD6	C2-C1-C24-C25
39	4	313	DD6	C5-C6-C8-C9
39	6	319	DD6	C10-C11-C13-C14
39	6	319	DD6	C5-C6-C8-C9
39	7	302	DD6	C10-C11-C13-C14
39	7	318	DD6	C5-C6-C8-C9
39	8	316	DD6	C10-C11-C13-C14
39	16	313	DD6	C10-C11-C13-C14
30	4	301	CLA	C2A-CAA-CBA-CGA
30	6	314	CLA	C2A-CAA-CBA-CGA
30	8	308	CLA	C2A-CAA-CBA-CGA
30	16	310	CLA	C2A-CAA-CBA-CGA
36	B	847	LMG	C28-C29-C30-C31
37	8	318	A86	C39-C38-O4-C34
30	A	832	CLA	O1A-CGA-O2A-C1
30	3	306	CLA	O1A-CGA-O2A-C1
30	16	303	CLA	O1A-CGA-O2A-C1
30	2u	202	CLA	C3-C5-C6-C7
30	4	302	CLA	C3-C5-C6-C7
35	11	303	LMT	C4B-C5B-C6B-O6B
36	A	856	LMG	C4-C5-C6-O5
36	6	301	LMG	C4-C5-C6-O5
37	7	319	A86	C33-C34-O4-C38
37	11	315	A86	C35-C34-O4-C38
38	5	306	KC1	CAA-CBA-CGA-O1A
38	8	307	KC1	CAA-CBA-CGA-O2A
38	9	304	KC1	CAA-CBA-CGA-O1A
38	9	310	KC1	CAA-CBA-CGA-O2A
38	9	311	KC1	CAA-CBA-CGA-O1A
38	9	312	KC1	CAA-CBA-CGA-O2A
38	11	305	KC1	CAA-CBA-CGA-O1A
38	13	305	KC1	CAA-CBA-CGA-O2A
38	13	308	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
38	13	308	KC1	CAA-CBA-CGA-O2A
30	A	831	CLA	CBA-CGA-O2A-C1
30	1	307	CLA	CBA-CGA-O2A-C1
30	3	303	CLA	CBA-CGA-O2A-C1
30	8	308	CLA	CBA-CGA-O2A-C1
30	9	303	CLA	CBA-CGA-O2A-C1
30	3	306	CLA	C10-C11-C12-C13
38	10	306	KC1	O1D-CGD-O2D-CED
30	B	826	CLA	CBD-CGD-O2D-CED
30	A	811	CLA	C8-C10-C11-C12
30	A	821	CLA	C10-C11-C12-C13
30	A	822	CLA	C8-C10-C11-C12
30	A	829	CLA	C10-C11-C12-C13
30	A	844	CLA	C10-C11-C12-C13
30	B	806	CLA	C15-C16-C17-C18
30	B	838	CLA	C8-C10-C11-C12
30	8	301	CLA	C10-C11-C12-C13
30	10	303	CLA	C15-C16-C17-C18
30	14	302	CLA	C13-C15-C16-C17
35	A	854	LMT	O5B-C5B-C6B-O6B
30	9	307	CLA	C3-C5-C6-C7
30	7	311	CLA	O1A-CGA-O2A-C1
30	9	309	CLA	O1A-CGA-O2A-C1
31	A	845	PQN	C23-C25-C26-C27
30	B	810	CLA	CBD-CGD-O2D-CED
30	B	839	CLA	CBD-CGD-O2D-CED
30	12	303	CLA	CBD-CGD-O2D-CED
30	12	307	CLA	CBD-CGD-O2D-CED
30	F	202	CLA	C11-C10-C8-C7
30	15	304	CLA	C11-C12-C13-C15
38	13	305	KC1	O1D-CGD-O2D-CED
30	7	304	CLA	CBA-CGA-O2A-C1
38	4	307	KC1	CAA-CBA-CGA-O2A
38	5	306	KC1	CAA-CBA-CGA-O2A
38	6	311	KC1	CAA-CBA-CGA-O2A
38	7	313	KC1	CAA-CBA-CGA-O1A
38	8	307	KC1	CAA-CBA-CGA-O1A
38	9	311	KC1	CAA-CBA-CGA-O2A
38	12	313	KC1	CAA-CBA-CGA-O1A
30	2	305	CLA	C15-C16-C17-C18
30	3	307	CLA	O1D-CGD-O2D-CED
37	1	309	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
37	2	319	A86	C11-C10-C9-C8
37	3	315	A86	C11-C10-C9-C8
37	4	315	A86	C24-C25-C26-C27
37	7	315	A86	C11-C10-C9-C8
37	7	315	A86	C24-C25-C26-C27
37	9	313	A86	C24-C25-C26-C27
37	9	316	A86	C24-C25-C26-C27
37	10	315	A86	C1-C2-C3-C4
37	10	315	A86	C24-C25-C26-C27
37	10	317	A86	C1-C2-C3-C4
37	11	314	A86	C24-C25-C26-C27
37	11	314	A86	C3-C4-C5-C6
37	11	316	A86	C11-C10-C9-C8
37	13	315	A86	C11-C10-C9-C8
37	13	315	A86	C24-C25-C26-C27
37	13	315	A86	C3-C4-C5-C6
37	14	316	A86	C24-C25-C26-C27
37	14	318	A86	C11-C10-C9-C8
37	14	319	A86	C3-C4-C5-C6
37	15	317	A86	C11-C10-C9-C8
39	4	316	DD6	C1-C2-C3-C4
39	7	318	DD6	C24-C25-C26-C27
39	11	313	DD6	C11-C10-C9-C8
39	11	313	DD6	C3-C4-C5-C6
30	12	310	CLA	C3-C5-C6-C7
30	13	301	CLA	C3-C5-C6-C7
30	16	301	CLA	C3-C5-C6-C7
30	A	829	CLA	C8-C10-C11-C12
30	A	843	CLA	C5-C6-C7-C8
30	B	806	CLA	C10-C11-C12-C13
30	2	304	CLA	C13-C15-C16-C17
30	8	302	CLA	C13-C15-C16-C17
30	13	302	CLA	C13-C15-C16-C17
30	15	304	CLA	C8-C10-C11-C12
36	5	318	LMG	C28-C29-C30-C31
36	7	320	LMG	C28-C29-C30-C31
30	A	805	CLA	O1A-CGA-O2A-C1
30	A	823	CLA	O1A-CGA-O2A-C1
30	B	811	CLA	O1A-CGA-O2A-C1
30	2	309	CLA	O1A-CGA-O2A-C1
30	3	303	CLA	O1A-CGA-O2A-C1
30	3	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	8	308	CLA	O1A-CGA-O2A-C1
30	11	310	CLA	O1A-CGA-O2A-C1
36	7	320	LMG	O10-C28-O8-C9
30	4	306	CLA	CBD-CGD-O2D-CED
30	5	308	CLA	CBD-CGD-O2D-CED
30	A	804	CLA	C8-C10-C11-C12
30	A	815	CLA	C5-C6-C7-C8
30	B	805	CLA	C13-C15-C16-C17
30	B	809	CLA	C13-C15-C16-C17
30	B	811	CLA	C5-C6-C7-C8
30	1	307	CLA	C5-C6-C7-C8
30	2	304	CLA	C10-C11-C12-C13
30	2	307	CLA	C10-C11-C12-C13
30	6	306	CLA	C13-C15-C16-C17
30	6	309	CLA	C10-C11-C12-C13
30	7	304	CLA	C10-C11-C12-C13
30	7	310	CLA	C8-C10-C11-C12
30	11	308	CLA	C8-C10-C11-C12
30	13	307	CLA	C10-C11-C12-C13
30	14	302	CLA	C10-C11-C12-C13
30	16	302	CLA	C8-C10-C11-C12
35	A	854	LMT	C4B-C5B-C6B-O6B
30	A	802	CLA	C2A-CAA-CBA-CGA
30	A	817	CLA	C2A-CAA-CBA-CGA
30	A	825	CLA	C2A-CAA-CBA-CGA
30	B	817	CLA	C2A-CAA-CBA-CGA
30	1	307	CLA	C2A-CAA-CBA-CGA
30	2	303	CLA	C2A-CAA-CBA-CGA
30	2	313	CLA	C2A-CAA-CBA-CGA
30	4	306	CLA	C2A-CAA-CBA-CGA
30	6	317	CLA	C2A-CAA-CBA-CGA
30	7	305	CLA	C2A-CAA-CBA-CGA
30	7	312	CLA	C2A-CAA-CBA-CGA
30	15	307	CLA	C2A-CAA-CBA-CGA
30	15	314	CLA	C2A-CAA-CBA-CGA
38	3	311	KC1	CAA-CBA-CGA-O2A
30	A	812	CLA	C5-C6-C7-C8
30	A	812	CLA	C13-C15-C16-C17
30	A	834	CLA	C5-C6-C7-C8
30	A	839	CLA	C8-C10-C11-C12
30	B	809	CLA	C10-C11-C12-C13
30	B	810	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	1	302	CLA	C13-C15-C16-C17
30	1	304	CLA	C10-C11-C12-C13
30	1	305	CLA	C15-C16-C17-C18
30	2	301	CLA	C15-C16-C17-C18
30	2	303	CLA	C5-C6-C7-C8
30	2	311	CLA	C8-C10-C11-C12
30	2	311	CLA	C10-C11-C12-C13
30	5	304	CLA	C10-C11-C12-C13
30	6	306	CLA	C8-C10-C11-C12
30	8	302	CLA	C15-C16-C17-C18
30	10	305	CLA	C15-C16-C17-C18
35	B	852	LMT	O5B-C5B-C6B-O6B
37	12	316	A86	C35-C34-O4-C38
37	14	301	A86	C33-C34-O4-C38
30	A	807	CLA	O1A-CGA-O2A-C1
30	2u	202	CLA	O1A-CGA-O2A-C1
36	2u	204	LMG	O10-C28-O8-C9
30	4	303	CLA	C3-C5-C6-C7
30	14	307	CLA	C3-C5-C6-C7
36	5	318	LMG	O6-C1-O1-C7
30	A	816	CLA	C8-C10-C11-C12
30	A	826	CLA	C13-C15-C16-C17
30	A	828	CLA	C10-C11-C12-C13
30	B	813	CLA	C15-C16-C17-C18
30	B	819	CLA	C13-C15-C16-C17
30	B	851	CLA	C13-C15-C16-C17
30	3	302	CLA	C10-C11-C12-C13
30	3	303	CLA	C8-C10-C11-C12
30	4	306	CLA	C5-C6-C7-C8
30	5	307	CLA	C10-C11-C12-C13
30	5	309	CLA	C15-C16-C17-C18
30	7	303	CLA	C10-C11-C12-C13
30	7	306	CLA	C5-C6-C7-C8
30	7	307	CLA	C15-C16-C17-C18
30	11	310	CLA	C10-C11-C12-C13
30	12	312	CLA	C8-C10-C11-C12
35	11	303	LMT	O1'-C1-C2-C3
30	A	817	CLA	CBA-CGA-O2A-C1
30	B	833	CLA	CBA-CGA-O2A-C1
30	12	302	CLA	CBD-CGD-O2D-CED
30	A	811	CLA	O1A-CGA-O2A-C1
30	B	826	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	3	301	CLA	O1A-CGA-O2A-C1
30	13	307	CLA	O1A-CGA-O2A-C1
30	15	304	CLA	O1A-CGA-O2A-C1
30	14	303	CLA	C8-C10-C11-C12
30	A	803	CLA	C13-C15-C16-C17
30	1	302	CLA	C8-C10-C11-C12
30	7	307	CLA	C13-C15-C16-C17
30	12	306	CLA	C10-C11-C12-C13
30	13	302	CLA	C8-C10-C11-C12
30	15	302	CLA	C5-C6-C7-C8
30	16	301	CLA	C13-C15-C16-C17
30	1	303	CLA	C3-C5-C6-C7
30	12	304	CLA	C3-C5-C6-C7
30	1	302	CLA	O1D-CGD-O2D-CED
38	5	306	KC1	O1D-CGD-O2D-CED
38	11	307	KC1	O1D-CGD-O2D-CED
30	A	803	CLA	C10-C11-C12-C13
30	B	813	CLA	C8-C10-C11-C12
30	3	305	CLA	C8-C10-C11-C12
30	5	304	CLA	C13-C15-C16-C17
30	7	303	CLA	C8-C10-C11-C12
30	9	309	CLA	C10-C11-C12-C13
30	15	313	CLA	C5-C6-C7-C8
38	3	304	KC1	CAA-CBA-CGA-O2A
30	B	833	CLA	CBD-CGD-O2D-CED
30	6	309	CLA	C4-C3-C5-C6
30	A	831	CLA	O1A-CGA-O2A-C1
30	1	301	CLA	O1A-CGA-O2A-C1
30	7	304	CLA	O1A-CGA-O2A-C1
35	6	302	LMT	O1'-C1-C2-C3
38	8	311	KC1	O1D-CGD-O2D-CED
30	A	805	CLA	C5-C6-C7-C8
30	B	824	CLA	C13-C15-C16-C17
30	F	201	CLA	C15-C16-C17-C18
30	9	307	CLA	C15-C16-C17-C18
30	10	309	CLA	C5-C6-C7-C8
30	14	302	CLA	C15-C16-C17-C18
30	9	308	CLA	CBA-CGA-O2A-C1
30	12	308	CLA	CBA-CGA-O2A-C1
30	A	809	CLA	CBD-CGD-O2D-CED
30	15	311	CLA	CBD-CGD-O2D-CED
36	8	319	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
38	1	308	KC1	C2A-CAA-CBA-CGA
38	4	308	KC1	C2A-CAA-CBA-CGA
38	4	310	KC1	C2A-CAA-CBA-CGA
38	13	311	KC1	C2A-CAA-CBA-CGA
38	13	312	KC1	C2A-CAA-CBA-CGA
38	14	311	KC1	C2A-CAA-CBA-CGA
37	12	316	A86	C33-C34-O4-C38
30	B	829	CLA	O1A-CGA-O2A-C1
30	1	307	CLA	O1A-CGA-O2A-C1
38	13	306	KC1	O1D-CGD-O2D-CED
35	9	317	LMT	C4B-C5B-C6B-O6B
30	2u	202	CLA	C13-C15-C16-C17
30	6	309	CLA	C15-C16-C17-C18
30	12	302	CLA	C3-C5-C6-C7
37	8	318	A86	C24-C25-C26-C27
37	11	315	A86	C11-C10-C9-C8
37	11	315	A86	C24-C25-C26-C27
37	12	316	A86	C11-C10-C9-C8
37	15	317	A86	C3-C4-C5-C6
37	15	320	A86	C1-C2-C3-C4
37	15	320	A86	C3-C4-C5-C6
37	15	323	A86	C3-C4-C5-C6
39	3	316	DD6	C1-C2-C3-C4
39	7	318	DD6	C11-C10-C9-C8
30	B	807	CLA	C15-C16-C17-C18
30	1	303	CLA	C10-C11-C12-C13
31	A	845	PQN	C25-C26-C27-C28
36	6	301	LMG	O9-C10-O7-C8
30	14	312	CLA	C2A-CAA-CBA-CGA
30	16	307	CLA	C2A-CAA-CBA-CGA
30	A	813	CLA	CBA-CGA-O2A-C1
30	B	819	CLA	CBA-CGA-O2A-C1
30	B	838	CLA	CBA-CGA-O2A-C1
30	6	309	CLA	CBA-CGA-O2A-C1
30	9	302	CLA	CBA-CGA-O2A-C1
30	A	805	CLA	C8-C10-C11-C12
30	A	809	CLA	C5-C6-C7-C8
30	A	843	CLA	C13-C15-C16-C17
30	F	201	CLA	C13-C15-C16-C17
30	2	307	CLA	C13-C15-C16-C17
30	6	304	CLA	C13-C15-C16-C17
30	6	310	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	7	311	CLA	C15-C16-C17-C18
30	9	308	CLA	C5-C6-C7-C8
30	11	308	CLA	C10-C11-C12-C13
31	B	840	PQN	C23-C25-C26-C27
30	13	301	CLA	CBD-CGD-O2D-CED
38	9	311	KC1	CBD-CGD-O2D-CED
30	A	820	CLA	O1D-CGD-O2D-CED
30	3	303	CLA	O1D-CGD-O2D-CED
30	11	310	CLA	O1D-CGD-O2D-CED
36	B	849	LMG	C10-C11-C12-C13
30	A	811	CLA	C10-C11-C12-C13
30	F	202	CLA	C10-C11-C12-C13
30	2	304	CLA	C8-C10-C11-C12
30	2	308	CLA	C10-C11-C12-C13
30	5	311	CLA	C8-C10-C11-C12
30	8	303	CLA	C10-C11-C12-C13
30	9	305	CLA	C10-C11-C12-C13
30	13	302	CLA	C5-C6-C7-C8
30	13	302	CLA	C10-C11-C12-C13
37	14	318	A86	O5-C38-O4-C34
30	A	820	CLA	C8-C10-C11-C12
30	A	826	CLA	C10-C11-C12-C13
30	A	834	CLA	C15-C16-C17-C18
30	B	825	CLA	C13-C15-C16-C17
30	1	305	CLA	C13-C15-C16-C17
30	2	308	CLA	C13-C15-C16-C17
30	5	309	CLA	C8-C10-C11-C12
30	8	302	CLA	C5-C6-C7-C8
30	16	305	CLA	CBA-CGA-O2A-C1
38	2	314	KC1	CAA-CBA-CGA-O2A
38	6	313	KC1	CAA-CBA-CGA-O1A
38	8	312	KC1	CAA-CBA-CGA-O2A
38	8	314	KC1	CAA-CBA-CGA-O2A
35	16	315	LMT	C5'-C4'-O1B-C1B
30	B	832	CLA	C15-C16-C17-C18
30	16	303	CLA	C15-C16-C17-C18
36	7	320	LMG	C11-C10-O7-C8
35	15	301	LMT	C4B-C5B-C6B-O6B
38	7	308	KC1	O1D-CGD-O2D-CED
35	B	852	LMT	C2'-C1'-O1'-C1
35	9	317	LMT	C2'-C1'-O1'-C1
36	B	849	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
36	3	317	LMG	C2-C1-O1-C7
36	5	318	LMG	C2-C1-O1-C7
36	7	320	LMG	C2-C1-O1-C7
30	8	301	CLA	O1D-CGD-O2D-CED
30	B	814	CLA	CBA-CGA-O2A-C1
30	B	834	CLA	CBA-CGA-O2A-C1
30	B	833	CLA	O1A-CGA-O2A-C1
30	9	302	CLA	O1A-CGA-O2A-C1
30	13	302	CLA	O1D-CGD-O2D-CED
33	A	848	BCR	C16-C17-C18-C36
33	B	843	BCR	C20-C21-C22-C37
33	B	844	BCR	C16-C17-C18-C36
33	B	845	BCR	C11-C10-C9-C34
33	B	846	BCR	C11-C10-C9-C34
33	B	846	BCR	C20-C21-C22-C37
33	L	201	BCR	C20-C21-C22-C37
33	L	204	BCR	C20-C21-C22-C37
33	M	101	BCR	C20-C21-C22-C37
39	2	317	DD6	C9-C10-C11-C12
39	2	317	DD6	C4-C5-C6-C7
39	6	319	DD6	C9-C10-C11-C12
39	6	321	DD6	C4-C5-C6-C7
39	8	317	DD6	C9-C10-C11-C12
39	15	318	DD6	C-C1-C2-C3
38	1	306	KC1	CAA-CBA-CGA-O2A
38	3	311	KC1	CAA-CBA-CGA-O1A
38	6	313	KC1	CAA-CBA-CGA-O2A
38	13	306	KC1	CAA-CBA-CGA-O1A
38	13	306	KC1	CAA-CBA-CGA-O2A
30	B	851	CLA	CBD-CGD-O2D-CED
30	A	833	CLA	C5-C6-C7-C8
33	B	841	BCR	C37-C22-C23-C24
33	I	101	BCR	C37-C22-C23-C24
33	J	103	BCR	C37-C22-C23-C24
33	L	205	BCR	C37-C22-C23-C24
37	1	309	A86	C7-C6-C8-C9
37	2	302	A86	C-C1-C24-C25
37	2	318	A86	C-C1-C24-C25
37	4	312	A86	C7-C6-C8-C9
37	4	317	A86	C-C1-C24-C25
37	14	315	A86	C7-C6-C8-C9
37	14	318	A86	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
37	14	320	A86	C7-C6-C8-C9
37	15	315	A86	C-C1-C24-C25
37	15	316	A86	C7-C6-C8-C9
37	15	321	A86	C7-C6-C8-C9
39	2	317	DD6	C12-C11-C13-C14
39	6	303	DD6	C12-C11-C13-C14
39	7	317	DD6	C12-C11-C13-C14
39	10	313	DD6	C7-C6-C8-C9
39	12	315	DD6	C7-C6-C8-C9
39	15	319	DD6	C-C1-C24-C25
33	L	201	BCR	C7-C8-C9-C10
33	L	204	BCR	C21-C22-C23-C24
33	L	205	BCR	C7-C8-C9-C10
37	2	302	A86	C2-C1-C24-C25
37	2	318	A86	C2-C1-C24-C25
37	4	317	A86	C2-C1-C24-C25
37	8	318	A86	C2-C1-C24-C25
37	14	315	A86	C5-C6-C8-C9
37	14	318	A86	C5-C6-C8-C9
37	14	320	A86	C5-C6-C8-C9
37	15	315	A86	C2-C1-C24-C25
37	15	316	A86	C5-C6-C8-C9
37	15	322	A86	C5-C6-C8-C9
39	2	316	DD6	C5-C6-C8-C9
39	4	316	DD6	C2-C1-C24-C25
39	6	303	DD6	C5-C6-C8-C9
39	6	318	DD6	C10-C11-C13-C14
39	7	318	DD6	C10-C11-C13-C14
39	11	313	DD6	C10-C11-C13-C14
39	15	318	DD6	C2-C1-C24-C25
30	B	819	CLA	O1A-CGA-O2A-C1
30	B	838	CLA	O1A-CGA-O2A-C1
30	9	303	CLA	O1A-CGA-O2A-C1
30	A	806	CLA	C2A-CAA-CBA-CGA
30	A	812	CLA	C2A-CAA-CBA-CGA
30	A	821	CLA	C2A-CAA-CBA-CGA
30	B	802	CLA	C2A-CAA-CBA-CGA
30	B	803	CLA	C2A-CAA-CBA-CGA
30	B	830	CLA	C2A-CAA-CBA-CGA
30	B	837	CLA	C2A-CAA-CBA-CGA
30	3	301	CLA	C2A-CAA-CBA-CGA
30	7	310	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
34	A	852	LHG	O1-C1-C2-C3
34	A	853	LHG	O1-C1-C2-C3
34	5	317	LHG	O1-C1-C2-C3
34	6	322	LHG	O1-C1-C2-C3
30	B	830	CLA	CBD-CGD-O2D-CED
37	11	314	A86	C1-C2-C3-C4
39	3	312	DD6	C24-C25-C26-C27
30	B	851	CLA	C16-C17-C18-C20
30	10	308	CLA	C16-C17-C18-C19
30	10	308	CLA	C16-C17-C18-C20
30	13	301	CLA	C16-C17-C18-C19
30	16	302	CLA	C16-C17-C18-C19
30	16	302	CLA	C16-C17-C18-C20
30	15	306	CLA	O1D-CGD-O2D-CED
38	13	308	KC1	O1D-CGD-O2D-CED
30	A	817	CLA	O1A-CGA-O2A-C1
30	5	308	CLA	O1A-CGA-O2A-C1
30	A	807	CLA	C3-C5-C6-C7
30	5	304	CLA	C5-C6-C7-C8
37	2	302	A86	O5-C38-O4-C34
33	A	849	BCR	C16-C17-C18-C19
33	A	850	BCR	C20-C21-C22-C23
33	B	843	BCR	C20-C21-C22-C23
33	B	845	BCR	C12-C13-C14-C15
33	F	204	BCR	C12-C13-C14-C15
33	J	102	BCR	C20-C21-C22-C23
33	J	103	BCR	C11-C10-C9-C8
33	L	204	BCR	C11-C10-C9-C8
39	1	310	DD6	C24-C1-C2-C3
39	1	310	DD6	C9-C10-C11-C13
39	2	316	DD6	C24-C1-C2-C3
39	2	317	DD6	C4-C5-C6-C8
39	3	312	DD6	C4-C5-C6-C8
39	3	316	DD6	C9-C10-C11-C13
39	5	313	DD6	C4-C5-C6-C8
39	6	303	DD6	C24-C1-C2-C3
39	6	319	DD6	C9-C10-C11-C13
39	6	321	DD6	C9-C10-C11-C13
39	7	302	DD6	C9-C10-C11-C13
39	8	317	DD6	C24-C1-C2-C3
39	12	315	DD6	C24-C1-C2-C3
39	13	314	DD6	C4-C5-C6-C8

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Mol	Chain	Res	Type	Atoms
39	15	318	DD6	C4-C5-C6-C8
39	16	313	DD6	C4-C5-C6-C8
35	B	852	LMT	O5'-C1'-O1'-C1
38	1	306	KC1	CAA-CBA-CGA-O1A
38	3	304	KC1	CAA-CBA-CGA-O1A
38	8	314	KC1	CAA-CBA-CGA-O1A
30	10	305	CLA	C8-C10-C11-C12
30	A	841	CLA	O1D-CGD-O2D-CED
30	8	304	CLA	CBA-CGA-O2A-C1
34	2	320	LHG	C24-C23-O8-C6
35	16	315	LMT	C3'-C4'-O1B-C1B
30	B	828	CLA	C10-C11-C12-C13
30	15	309	CLA	C10-C11-C12-C13
30	6	316	CLA	C3-C5-C6-C7
36	14	321	LMG	C4-C5-C6-O5
30	A	815	CLA	C2-C1-O2A-CGA
30	1	302	CLA	C2-C1-O2A-CGA
30	B	821	CLA	C6-C7-C8-C9
30	5	302	CLA	C16-C17-C18-C19
30	B	818	CLA	O1A-CGA-O2A-C1
33	B	844	BCR	C14-C15-C16-C17
34	A	852	LHG	C10-C11-C12-C13
35	1	311	LMT	C7-C8-C9-C10
36	7	320	LMG	C31-C32-C33-C34
30	A	825	CLA	O1D-CGD-O2D-CED
30	A	828	CLA	C13-C15-C16-C17
30	A	830	CLA	C13-C15-C16-C17
30	B	806	CLA	C13-C15-C16-C17
38	2	314	KC1	CAA-CBA-CGA-O1A
38	8	312	KC1	CAA-CBA-CGA-O1A
35	12	318	LMT	C4B-C5B-C6B-O6B
36	8	320	LMG	C33-C34-C35-C36
36	14	321	LMG	O10-C28-O8-C9
30	A	823	CLA	O1D-CGD-O2D-CED
30	12	302	CLA	CBA-CGA-O2A-C1
30	13	301	CLA	CBA-CGA-O2A-C1
34	B	848	LHG	O9-C7-O7-C5
34	A	853	LHG	O1-C1-C2-O2
34	B	848	LHG	O1-C1-C2-O2
35	A	855	LMT	C2-C1-O1'-C1'
36	B	847	LMG	C29-C30-C31-C32
36	6	301	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	11	309	CLA	C8-C10-C11-C12
30	A	822	CLA	C4B-C3B-CAB-CBB
30	A	833	CLA	C4B-C3B-CAB-CBB
30	A	836	CLA	C4B-C3B-CAB-CBB
30	B	801	CLA	C4B-C3B-CAB-CBB
30	B	807	CLA	C4B-C3B-CAB-CBB
30	B	818	CLA	C4B-C3B-CAB-CBB
30	B	827	CLA	C4B-C3B-CAB-CBB
30	B	851	CLA	C4B-C3B-CAB-CBB
30	3	302	CLA	C4B-C3B-CAB-CBB
30	5	304	CLA	C4B-C3B-CAB-CBB
30	9	305	CLA	C4B-C3B-CAB-CBB
30	9	308	CLA	C4B-C3B-CAB-CBB
30	10	308	CLA	C4B-C3B-CAB-CBB
30	12	310	CLA	C4B-C3B-CAB-CBB
30	15	308	CLA	C4B-C3B-CAB-CBB
30	16	301	CLA	C4B-C3B-CAB-CBB
36	A	856	LMG	C30-C31-C32-C33
30	A	820	CLA	C16-C17-C18-C20
30	4	304	CLA	C11-C12-C13-C14
30	4	304	CLA	C11-C12-C13-C15
30	12	308	CLA	O1A-CGA-O2A-C1
30	1	301	CLA	C2A-CAA-CBA-CGA
30	5	307	CLA	C2A-CAA-CBA-CGA
30	3	307	CLA	C10-C11-C12-C13
30	5	308	CLA	C15-C16-C17-C18
36	8	320	LMG	C16-C17-C18-C19
30	6	307	CLA	C11-C10-C8-C7
30	11	304	CLA	C12-C13-C15-C16
34	A	852	LHG	C12-C13-C14-C15
34	2	320	LHG	C11-C10-C9-C8
30	A	825	CLA	C8-C10-C11-C12
30	1	301	CLA	C10-C11-C12-C13
30	2	301	CLA	C8-C10-C11-C12
30	3	303	CLA	C5-C6-C7-C8
30	7	310	CLA	C15-C16-C17-C18
30	9	308	CLA	O1A-CGA-O2A-C1
30	3	305	CLA	C3-C5-C6-C7
30	A	802	CLA	C3A-C2A-CAA-CBA
30	A	814	CLA	C3A-C2A-CAA-CBA
30	A	838	CLA	C3A-C2A-CAA-CBA
30	B	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	B	825	CLA	C3A-C2A-CAA-CBA
30	F	201	CLA	C3A-C2A-CAA-CBA
30	1	304	CLA	C3A-C2A-CAA-CBA
30	2	305	CLA	C3A-C2A-CAA-CBA
30	3	309	CLA	C3A-C2A-CAA-CBA
30	4	306	CLA	C3A-C2A-CAA-CBA
30	4	309	CLA	C3A-C2A-CAA-CBA
30	8	304	CLA	C3A-C2A-CAA-CBA
30	9	305	CLA	C3A-C2A-CAA-CBA
30	9	306	CLA	C3A-C2A-CAA-CBA
30	9	308	CLA	C3A-C2A-CAA-CBA
30	10	305	CLA	C3A-C2A-CAA-CBA
30	10	311	CLA	C3A-C2A-CAA-CBA
30	11	306	CLA	C3A-C2A-CAA-CBA
30	13	303	CLA	C3A-C2A-CAA-CBA
30	13	304	CLA	C3A-C2A-CAA-CBA
30	14	303	CLA	C3A-C2A-CAA-CBA
30	14	313	CLA	C3A-C2A-CAA-CBA
30	15	305	CLA	C3A-C2A-CAA-CBA
30	15	308	CLA	C3A-C2A-CAA-CBA
30	15	311	CLA	C3A-C2A-CAA-CBA
30	15	312	CLA	C3A-C2A-CAA-CBA
30	16	306	CLA	C3A-C2A-CAA-CBA
30	16	307	CLA	C3A-C2A-CAA-CBA
30	16	308	CLA	C3A-C2A-CAA-CBA
30	16	309	CLA	C3A-C2A-CAA-CBA
36	B	847	LMG	C37-C38-C39-C40
30	2	310	CLA	C5-C6-C7-C8
30	6	307	CLA	C10-C11-C12-C13
30	7	307	CLA	C10-C11-C12-C13
36	8	321	LMG	C28-C29-C30-C31
38	8	306	KC1	O1D-CGD-O2D-CED
36	F	205	LMG	C10-C11-C12-C13
37	7	315	A86	C1-C2-C3-C4
37	7	315	A86	C3-C4-C5-C6
37	7	316	A86	C24-C25-C26-C27
37	11	316	A86	C3-C4-C5-C6
37	14	301	A86	C24-C25-C26-C27
39	2	315	DD6	C24-C25-C26-C27
39	6	321	DD6	C11-C10-C9-C8
39	8	316	DD6	C3-C4-C5-C6
30	13	301	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	16	301	CLA	C16-C17-C18-C20
30	A	813	CLA	O1A-CGA-O2A-C1
30	B	814	CLA	O1A-CGA-O2A-C1
30	B	834	CLA	O1A-CGA-O2A-C1
30	16	305	CLA	O1A-CGA-O2A-C1
36	7	320	LMG	C11-C12-C13-C14
30	16	303	CLA	C8-C10-C11-C12
36	8	320	LMG	C30-C31-C32-C33
30	A	819	CLA	CBA-CGA-O2A-C1
30	B	805	CLA	CBA-CGA-O2A-C1
30	1	302	CLA	CBA-CGA-O2A-C1
30	15	313	CLA	CBA-CGA-O2A-C1
36	8	320	LMG	C29-C28-O8-C9
36	14	321	LMG	C7-C8-C9-O8
30	11	304	CLA	C3-C5-C6-C7
34	B	848	LHG	C7-C8-C9-C10
36	8	319	LMG	C28-C29-C30-C31
30	9	303	CLA	O1D-CGD-O2D-CED
36	B	849	LMG	C12-C13-C14-C15
36	3	317	LMG	C14-C15-C16-C17
36	8	320	LMG	C32-C33-C34-C35
36	8	319	LMG	C36-C37-C38-C39
30	A	810	CLA	O1D-CGD-O2D-CED
30	5	302	CLA	O1D-CGD-O2D-CED
30	12	321	CLA	O1D-CGD-O2D-CED
34	A	852	LHG	C25-C26-C27-C28
35	A	854	LMT	C2-C3-C4-C5
30	7	304	CLA	C16-C17-C18-C20
34	9	318	LHG	C23-C24-C25-C26
30	A	814	CLA	C2B-C3B-CAB-CBB
30	A	816	CLA	C2B-C3B-CAB-CBB
30	A	827	CLA	C2B-C3B-CAB-CBB
30	A	843	CLA	C2B-C3B-CAB-CBB
30	B	801	CLA	C2B-C3B-CAB-CBB
30	B	807	CLA	C2B-C3B-CAB-CBB
30	B	816	CLA	C2B-C3B-CAB-CBB
30	B	829	CLA	C2B-C3B-CAB-CBB
30	B	831	CLA	C2B-C3B-CAB-CBB
30	B	851	CLA	C2B-C3B-CAB-CBB
30	2	307	CLA	C2B-C3B-CAB-CBB
30	3	303	CLA	C2B-C3B-CAB-CBB
30	4	302	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	6	306	CLA	C2B-C3B-CAB-CBB
30	7	307	CLA	C2B-C3B-CAB-CBB
30	7	310	CLA	C2B-C3B-CAB-CBB
30	9	306	CLA	C2B-C3B-CAB-CBB
30	9	307	CLA	C2B-C3B-CAB-CBB
30	10	307	CLA	C2B-C3B-CAB-CBB
30	10	308	CLA	C2B-C3B-CAB-CBB
30	12	310	CLA	C2B-C3B-CAB-CBB
30	13	309	CLA	C2B-C3B-CAB-CBB
30	14	302	CLA	C2B-C3B-CAB-CBB
30	14	313	CLA	C2B-C3B-CAB-CBB
30	15	308	CLA	C2B-C3B-CAB-CBB
30	15	309	CLA	C2B-C3B-CAB-CBB
30	16	301	CLA	C2B-C3B-CAB-CBB
30	16	302	CLA	C2B-C3B-CAB-CBB
33	J	102	BCR	C1-C6-C7-C8
33	J	102	BCR	C5-C6-C7-C8
33	J	103	BCR	C23-C24-C25-C26
33	J	103	BCR	C23-C24-C25-C30
33	L	204	BCR	C23-C24-C25-C30
33	M	101	BCR	C1-C6-C7-C8
33	2u	201	BCR	C1-C6-C7-C8
33	2u	201	BCR	C5-C6-C7-C8
33	2u	201	BCR	C23-C24-C25-C30
34	A	852	LHG	C8-C7-O7-C5
30	A	825	CLA	CBA-CGA-O2A-C1
30	4	305	CLA	CBA-CGA-O2A-C1
30	B	811	CLA	C10-C11-C12-C13
30	B	829	CLA	C15-C16-C17-C18
30	10	307	CLA	C3-C5-C6-C7
34	A	852	LHG	C32-C33-C34-C35
35	A	854	LMT	C3-C4-C5-C6
30	A	813	CLA	C2A-CAA-CBA-CGA
30	A	837	CLA	C2A-CAA-CBA-CGA
30	B	829	CLA	C2A-CAA-CBA-CGA
30	1	302	CLA	C2A-CAA-CBA-CGA
30	12	302	CLA	C2A-CAA-CBA-CGA
36	8	319	LMG	C10-C11-C12-C13
36	8	320	LMG	C12-C13-C14-C15
30	8	304	CLA	O1A-CGA-O2A-C1
30	15	313	CLA	O1A-CGA-O2A-C1
34	9	318	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
36	B	849	LMG	C29-C30-C31-C32
36	8	321	LMG	O9-C10-O7-C8
30	7	306	CLA	C4-C3-C5-C6
33	L	201	BCR	C18-C19-C20-C21
30	B	821	CLA	C6-C7-C8-C10
30	5	311	CLA	CBA-CGA-O2A-C1
30	10	308	CLA	CBA-CGA-O2A-C1
36	14	321	LMG	C29-C28-O8-C9
30	12	308	CLA	C11-C12-C13-C14
36	2u	204	LMG	O6-C5-C6-O5
35	9	317	LMT	O5'-C1'-O1'-C1
36	A	856	LMG	O6-C1-O1-C7
36	3	317	LMG	C29-C30-C31-C32
36	A	856	LMG	C2-C1-O1-C7
30	A	820	CLA	C13-C15-C16-C17
30	A	834	CLA	C10-C11-C12-C13
30	9	308	CLA	C10-C11-C12-C13
35	7	321	LMT	C3-C4-C5-C6
36	B	847	LMG	C15-C16-C17-C18
34	A	852	LHG	C24-C25-C26-C27
37	9	315	A86	O5-C38-O4-C34
30	A	824	CLA	CBA-CGA-O2A-C1
30	15	309	CLA	CBA-CGA-O2A-C1
37	14	315	A86	C1-C2-C3-C4
37	15	322	A86	C24-C25-C26-C27
39	2	315	DD6	C11-C10-C9-C8
39	3	312	DD6	C11-C10-C9-C8
39	7	302	DD6	C3-C4-C5-C6
30	B	851	CLA	C16-C17-C18-C19
34	B	848	LHG	C8-C7-O7-C5
30	1	302	CLA	O1A-CGA-O2A-C1
30	A	803	CLA	C15-C16-C17-C18
36	8	319	LMG	O9-C10-O7-C8
35	8	322	LMT	C7-C8-C9-C10
35	16	315	LMT	O5'-C5'-C6'-O6'
30	13	301	CLA	O1A-CGA-O2A-C1
30	12	312	CLA	C10-C11-C12-C13
37	3	314	A86	C7-C6-C8-C9
37	10	315	A86	C7-C6-C8-C9
37	11	314	A86	C7-C6-C8-C9
37	14	319	A86	C7-C6-C8-C9
33	A	847	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	A	850	BCR	C21-C22-C23-C24
33	B	846	BCR	C21-C22-C23-C24
37	10	315	A86	C5-C6-C8-C9
37	11	314	A86	C5-C6-C8-C9
39	3	316	DD6	C5-C6-C8-C9
39	12	317	DD6	C10-C11-C13-C14
30	A	819	CLA	C2A-CAA-CBA-CGA
30	10	307	CLA	C2A-CAA-CBA-CGA
30	5	302	CLA	C16-C17-C18-C20
30	16	301	CLA	C16-C17-C18-C19
34	A	852	LHG	C13-C14-C15-C16
30	2	303	CLA	C4-C3-C5-C6
30	5	309	CLA	C4-C3-C5-C6
30	9	301	CLA	C4-C3-C5-C6
38	2	312	KC1	C2B-C3B-CAB-CBB
38	2	314	KC1	C2B-C3B-CAB-CBB
38	3	308	KC1	C2B-C3B-CAB-CBB
38	3	311	KC1	C2B-C3B-CAB-CBB
38	4	307	KC1	C2B-C3B-CAB-CBB
38	5	306	KC1	C2B-C3B-CAB-CBB
38	5	312	KC1	C2B-C3B-CAB-CBB
38	6	308	KC1	C2B-C3B-CAB-CBB
38	6	311	KC1	C2B-C3B-CAB-CBB
38	6	313	KC1	C2B-C3B-CAB-CBB
38	8	306	KC1	C2B-C3B-CAB-CBB
38	8	311	KC1	C2B-C3B-CAB-CBB
38	8	314	KC1	C2B-C3B-CAB-CBB
38	9	304	KC1	C2B-C3B-CAB-CBB
38	9	310	KC1	C2B-C3B-CAB-CBB
38	9	312	KC1	C2B-C3B-CAB-CBB
38	10	306	KC1	C2B-C3B-CAB-CBB
38	11	305	KC1	C2B-C3B-CAB-CBB
38	11	307	KC1	C2B-C3B-CAB-CBB
38	11	312	KC1	C2B-C3B-CAB-CBB
38	12	305	KC1	C2B-C3B-CAB-CBB
38	12	313	KC1	C2B-C3B-CAB-CBB
38	13	312	KC1	C2B-C3B-CAB-CBB
38	14	311	KC1	C2B-C3B-CAB-CBB
38	16	304	KC1	C2B-C3B-CAB-CBB
30	7	309	CLA	C13-C15-C16-C17
30	A	819	CLA	O1A-CGA-O2A-C1
30	4	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	6	309	CLA	O1A-CGA-O2A-C1
30	A	833	CLA	C3-C5-C6-C7
30	11	308	CLA	C3-C5-C6-C7
30	A	820	CLA	C15-C16-C17-C18
30	A	833	CLA	C8-C10-C11-C12
30	A	833	CLA	C10-C11-C12-C13
30	B	806	CLA	C5-C6-C7-C8
30	B	822	CLA	C10-C11-C12-C13
34	9	318	LHG	C11-C10-C9-C8
30	B	838	CLA	O1D-CGD-O2D-CED
35	16	315	LMT	C7-C8-C9-C10
34	A	852	LHG	C27-C28-C29-C30
34	6	322	LHG	C11-C10-C9-C8
36	B	849	LMG	C14-C15-C16-C17
30	B	833	CLA	C8-C10-C11-C12
30	10	305	CLA	C13-C15-C16-C17
38	8	311	KC1	C4B-C3B-CAB-CBB
38	8	313	KC1	C4B-C3B-CAB-CBB
35	A	854	LMT	C7-C8-C9-C10
36	B	849	LMG	C15-C16-C17-C18
35	A	855	LMT	C2-C3-C4-C5
36	B	847	LMG	C23-C24-C25-C26
35	B	852	LMT	C1-C2-C3-C4
30	B	808	CLA	C13-C15-C16-C17
30	B	809	CLA	C15-C16-C17-C18
30	B	834	CLA	C5-C6-C7-C8
30	B	834	CLA	C10-C11-C12-C13
30	8	301	CLA	C8-C10-C11-C12
30	12	312	CLA	C15-C16-C17-C18
31	A	845	PQN	C20-C21-C22-C23
30	B	809	CLA	O1D-CGD-O2D-CED
38	6	311	KC1	O1D-CGD-O2D-CED
30	8	301	CLA	C3-C5-C6-C7
36	F	205	LMG	O7-C8-C9-O8
36	8	319	LMG	O7-C8-C9-O8
36	3	317	LMG	C12-C13-C14-C15
30	A	825	CLA	O1A-CGA-O2A-C1
36	3	317	LMG	C13-C14-C15-C16
30	A	828	CLA	C15-C16-C17-C18
37	14	314	A86	O5-C38-O4-C34
38	10	310	KC1	CBD-CGD-O2D-CED
35	7	321	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
36	8	319	LMG	O6-C5-C6-O5
30	B	811	CLA	C8-C10-C11-C12
36	6	301	LMG	C12-C13-C14-C15
36	14	321	LMG	C29-C30-C31-C32
30	A	814	CLA	C4-C3-C5-C6
30	1	304	CLA	C4-C3-C5-C6
30	3	302	CLA	C4-C3-C5-C6
30	A	828	CLA	C3-C5-C6-C7
30	B	822	CLA	C2-C3-C5-C6
30	9	301	CLA	C2-C3-C5-C6
34	B	848	LHG	C1-C2-C3-O3
30	15	302	CLA	C10-C11-C12-C13
36	B	847	LMG	C16-C17-C18-C19
30	A	818	CLA	C2A-CAA-CBA-CGA
30	5	308	CLA	C2A-CAA-CBA-CGA
30	9	302	CLA	C2A-CAA-CBA-CGA
30	9	303	CLA	C2A-CAA-CBA-CGA
30	13	301	CLA	C2A-CAA-CBA-CGA
30	13	309	CLA	C2A-CAA-CBA-CGA
30	A	826	CLA	CBD-CGD-O2D-CED
30	1	301	CLA	CBD-CGD-O2D-CED
35	11	303	LMT	C7-C8-C9-C10
35	15	301	LMT	C3-C4-C5-C6
36	A	856	LMG	C12-C13-C14-C15
36	3	317	LMG	C32-C33-C34-C35
36	7	320	LMG	C33-C34-C35-C36
30	B	804	CLA	O1D-CGD-O2D-CED
30	13	309	CLA	O1D-CGD-O2D-CED
36	B	849	LMG	C30-C31-C32-C33
30	A	810	CLA	C13-C15-C16-C17
30	B	813	CLA	C10-C11-C12-C13
30	5	308	CLA	C8-C10-C11-C12
30	5	308	CLA	C13-C15-C16-C17
30	7	307	CLA	C8-C10-C11-C12
30	8	303	CLA	C13-C15-C16-C17
30	5	303	CLA	O1D-CGD-O2D-CED
30	11	309	CLA	O1D-CGD-O2D-CED
30	B	805	CLA	O1A-CGA-O2A-C1
30	B	838	CLA	C3-C5-C6-C7
30	A	804	CLA	C1A-C2A-CAA-CBA
30	A	810	CLA	C1A-C2A-CAA-CBA
30	A	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	A	819	CLA	C1A-C2A-CAA-CBA
30	A	825	CLA	C1A-C2A-CAA-CBA
30	A	833	CLA	C1A-C2A-CAA-CBA
30	A	835	CLA	C1A-C2A-CAA-CBA
30	A	840	CLA	C1A-C2A-CAA-CBA
30	A	842	CLA	C1A-C2A-CAA-CBA
30	B	805	CLA	C1A-C2A-CAA-CBA
30	B	813	CLA	C1A-C2A-CAA-CBA
30	B	814	CLA	C1A-C2A-CAA-CBA
30	B	818	CLA	C1A-C2A-CAA-CBA
30	B	826	CLA	C1A-C2A-CAA-CBA
30	B	828	CLA	C1A-C2A-CAA-CBA
30	B	829	CLA	C1A-C2A-CAA-CBA
30	B	836	CLA	C1A-C2A-CAA-CBA
30	B	838	CLA	C1A-C2A-CAA-CBA
30	B	839	CLA	C1A-C2A-CAA-CBA
30	F	201	CLA	C1A-C2A-CAA-CBA
30	2	303	CLA	C1A-C2A-CAA-CBA
30	2	308	CLA	C1A-C2A-CAA-CBA
30	3	301	CLA	C1A-C2A-CAA-CBA
30	3	306	CLA	C1A-C2A-CAA-CBA
30	3	309	CLA	C1A-C2A-CAA-CBA
30	4	305	CLA	C1A-C2A-CAA-CBA
30	4	306	CLA	C1A-C2A-CAA-CBA
30	5	308	CLA	C1A-C2A-CAA-CBA
30	5	309	CLA	C1A-C2A-CAA-CBA
30	5	311	CLA	C1A-C2A-CAA-CBA
30	6	314	CLA	C1A-C2A-CAA-CBA
30	6	317	CLA	C1A-C2A-CAA-CBA
30	7	305	CLA	C1A-C2A-CAA-CBA
30	8	301	CLA	C1A-C2A-CAA-CBA
30	8	303	CLA	C1A-C2A-CAA-CBA
30	8	304	CLA	C1A-C2A-CAA-CBA
30	9	302	CLA	C1A-C2A-CAA-CBA
30	9	303	CLA	C1A-C2A-CAA-CBA
30	9	306	CLA	C1A-C2A-CAA-CBA
30	9	309	CLA	C1A-C2A-CAA-CBA
30	10	303	CLA	C1A-C2A-CAA-CBA
30	10	308	CLA	C1A-C2A-CAA-CBA
30	10	309	CLA	C1A-C2A-CAA-CBA
30	11	309	CLA	C1A-C2A-CAA-CBA
30	11	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	12	308	CLA	C1A-C2A-CAA-CBA
30	12	310	CLA	C1A-C2A-CAA-CBA
30	13	301	CLA	C1A-C2A-CAA-CBA
30	13	304	CLA	C1A-C2A-CAA-CBA
30	13	307	CLA	C1A-C2A-CAA-CBA
30	14	305	CLA	C1A-C2A-CAA-CBA
30	14	312	CLA	C1A-C2A-CAA-CBA
30	15	302	CLA	C1A-C2A-CAA-CBA
30	15	303	CLA	C1A-C2A-CAA-CBA
30	15	305	CLA	C1A-C2A-CAA-CBA
30	15	307	CLA	C1A-C2A-CAA-CBA
30	15	309	CLA	C1A-C2A-CAA-CBA
30	15	312	CLA	C1A-C2A-CAA-CBA
30	15	314	CLA	C1A-C2A-CAA-CBA
30	16	301	CLA	C1A-C2A-CAA-CBA
30	16	309	CLA	C1A-C2A-CAA-CBA
30	16	310	CLA	C1A-C2A-CAA-CBA
30	B	831	CLA	O1D-CGD-O2D-CED
30	1	307	CLA	C15-C16-C17-C18
30	6	305	CLA	C13-C15-C16-C17
30	12	302	CLA	C15-C16-C17-C18
37	8	318	A86	O5-C38-O4-C34
35	B	852	LMT	C6-C7-C8-C9
30	L	202	CLA	C10-C11-C12-C13
30	9	308	CLA	C13-C15-C16-C17
30	A	804	CLA	C12-C13-C15-C16
30	A	806	CLA	C11-C12-C13-C15
30	A	816	CLA	C11-C10-C8-C7
30	A	825	CLA	C11-C10-C8-C7
30	A	835	CLA	C12-C13-C15-C16
30	A	839	CLA	C11-C12-C13-C15
30	A	841	CLA	C11-C10-C8-C7
30	A	842	CLA	C12-C13-C15-C16
30	B	811	CLA	C11-C10-C8-C7
30	B	822	CLA	C11-C12-C13-C15
30	B	835	CLA	C6-C7-C8-C10
30	1	307	CLA	C11-C10-C8-C7
30	2	301	CLA	C12-C13-C15-C16
30	2	311	CLA	C11-C12-C13-C15
30	6	304	CLA	C11-C12-C13-C15
30	7	309	CLA	C6-C7-C8-C10
30	7	311	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	8	301	CLA	C11-C12-C13-C15
30	8	303	CLA	C11-C12-C13-C15
30	11	308	CLA	C11-C12-C13-C15
30	11	308	CLA	C12-C13-C15-C16
30	12	304	CLA	C11-C10-C8-C7
30	12	312	CLA	C11-C10-C8-C7
30	15	304	CLA	C6-C7-C8-C10
30	15	304	CLA	C12-C13-C15-C16
30	16	303	CLA	C6-C7-C8-C10
30	16	303	CLA	C11-C10-C8-C7
30	B	805	CLA	C10-C11-C12-C13
30	B	826	CLA	C13-C15-C16-C17
30	5	311	CLA	O1A-CGA-O2A-C1
38	5	305	KC1	CAA-CBA-CGA-O1A
30	A	821	CLA	C8-C10-C11-C12
30	2	307	CLA	C15-C16-C17-C18
30	11	309	CLA	C10-C11-C12-C13
30	A	806	CLA	C2-C3-C5-C6
30	A	818	CLA	C2-C3-C5-C6
30	B	837	CLA	C5-C6-C7-C8
30	10	307	CLA	C15-C16-C17-C18
30	B	821	CLA	C2A-CAA-CBA-CGA
30	B	826	CLA	C2A-CAA-CBA-CGA
30	9	308	CLA	C2A-CAA-CBA-CGA
30	16	301	CLA	C2A-CAA-CBA-CGA
30	A	825	CLA	C11-C10-C8-C9
30	A	835	CLA	C14-C13-C15-C16
30	A	839	CLA	C11-C12-C13-C14
30	A	842	CLA	C14-C13-C15-C16
30	B	829	CLA	C14-C13-C15-C16
30	7	307	CLA	C11-C10-C8-C9
30	7	309	CLA	C6-C7-C8-C9
30	7	311	CLA	C6-C7-C8-C9
30	8	301	CLA	C11-C12-C13-C14
30	8	303	CLA	C11-C12-C13-C14
30	11	308	CLA	C11-C12-C13-C14
30	11	310	CLA	C14-C13-C15-C16
30	12	312	CLA	C11-C10-C8-C9
30	14	303	CLA	C11-C10-C8-C9
30	15	304	CLA	C6-C7-C8-C9
30	16	303	CLA	C6-C7-C8-C9
30	16	303	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	A	818	CLA	C5-C6-C7-C8
39	8	317	DD6	C3-C4-C5-C6
30	A	834	CLA	CBA-CGA-O2A-C1
30	5	302	CLA	CBA-CGA-O2A-C1
30	6	310	CLA	CBA-CGA-O2A-C1
30	13	303	CLA	CBA-CGA-O2A-C1
30	4	302	CLA	C13-C15-C16-C17
30	11	308	CLA	C13-C15-C16-C17
30	A	824	CLA	O1A-CGA-O2A-C1
30	15	309	CLA	O1A-CGA-O2A-C1
38	11	311	KC1	O1D-CGD-O2D-CED
30	F	202	CLA	C15-C16-C17-C18
34	B	848	LHG	C4-C5-C6-O8
36	A	856	LMG	C7-C8-C9-O8
36	6	301	LMG	C7-C8-C9-O8
36	8	320	LMG	O1-C7-C8-C9
30	A	822	CLA	O1D-CGD-O2D-CED
30	7	310	CLA	C13-C15-C16-C17
30	3	306	CLA	O1D-CGD-O2D-CED
30	15	303	CLA	O1D-CGD-O2D-CED
30	A	816	CLA	CBA-CGA-O2A-C1
30	11	306	CLA	CBA-CGA-O2A-C1
35	6	302	LMT	O5B-C5B-C6B-O6B
36	8	319	LMG	C35-C36-C37-C38
36	8	320	LMG	C13-C14-C15-C16
36	B	847	LMG	C40-C41-C42-C43
29	A	801	CL0	CHA-CBD-CGD-O2D
33	B	843	BCR	C35-C13-C14-C15
33	F	204	BCR	C35-C13-C14-C15
30	A	830	CLA	C15-C16-C17-C18
30	B	821	CLA	C5-C6-C7-C8
30	12	308	CLA	C10-C11-C12-C13
30	B	819	CLA	C3-C5-C6-C7
35	A	857	LMT	O5B-C5B-C6B-O6B
30	10	308	CLA	O1A-CGA-O2A-C1
30	12	302	CLA	O1A-CGA-O2A-C1
30	A	818	CLA	C4-C3-C5-C6
30	B	822	CLA	C4-C3-C5-C6
30	6	316	CLA	C4-C3-C5-C6
30	A	834	CLA	C2-C3-C5-C6
30	3	302	CLA	C2-C3-C5-C6
30	6	316	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	7	305	CLA	C2-C3-C5-C6
30	16	302	CLA	C2-C3-C5-C6
30	B	802	CLA	C5-C6-C7-C8
30	16	302	CLA	C10-C11-C12-C13
33	J	102	BCR	C7-C8-C9-C34
37	9	315	A86	C7-C6-C8-C9
37	11	316	A86	C-C1-C24-C25
37	14	319	A86	C-C1-C24-C25
37	16	312	A86	C-C1-C24-C25
39	6	318	DD6	C12-C11-C13-C14
38	14	308	KC1	C2C-C3C-CAC-CBC
36	B	847	LMG	C32-C33-C34-C35
36	A	856	LMG	C31-C32-C33-C34
36	B	847	LMG	C21-C22-C23-C24
33	B	841	BCR	C21-C22-C23-C24
37	2u	203	A86	C5-C6-C8-C9
37	9	315	A86	C5-C6-C8-C9
37	11	316	A86	C2-C1-C24-C25
37	14	319	A86	C2-C1-C24-C25
37	14	319	A86	C5-C6-C8-C9
37	15	317	A86	C5-C6-C8-C9
37	16	312	A86	C2-C1-C24-C25
39	2	317	DD6	C10-C11-C13-C14
39	4	316	DD6	C10-C11-C13-C14
39	7	317	DD6	C10-C11-C13-C14
39	13	314	DD6	C5-C6-C8-C9
30	6	310	CLA	O1A-CGA-O2A-C1
30	13	303	CLA	O1A-CGA-O2A-C1
30	A	826	CLA	C8-C10-C11-C12
30	1	303	CLA	C2A-CAA-CBA-CGA
36	5	318	LMG	O6-C5-C6-O5
30	7	311	CLA	C13-C15-C16-C17
36	8	320	LMG	C11-C12-C13-C14
30	1	303	CLA	CBA-CGA-O2A-C1
30	4	302	CLA	CBA-CGA-O2A-C1
30	10	303	CLA	CBA-CGA-O2A-C1
36	F	205	LMG	C7-C8-O7-C10
30	15	303	CLA	C10-C11-C12-C13
37	2	318	A86	C24-C25-C26-C27
37	5	315	A86	C24-C25-C26-C27
37	9	313	A86	C11-C10-C9-C8
37	12	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
39	3	312	DD6	C3-C4-C5-C6
39	3	313	DD6	C11-C10-C9-C8
39	16	313	DD6	C24-C25-C26-C27
33	A	850	BCR	C11-C10-C9-C8
33	B	841	BCR	C20-C21-C22-C23
33	F	204	BCR	C11-C10-C9-C8
39	1	310	DD6	C4-C5-C6-C8
39	7	302	DD6	C24-C1-C2-C3
34	A	853	LHG	C1-C2-C3-O3
30	B	813	CLA	C13-C15-C16-C17
30	B	802	CLA	O1D-CGD-O2D-CED
30	B	808	CLA	O1D-CGD-O2D-CED
30	B	828	CLA	CBA-CGA-O2A-C1
30	9	301	CLA	CBA-CGA-O2A-C1
30	11	309	CLA	CBA-CGA-O2A-C1
30	2	311	CLA	CBD-CGD-O2D-CED
30	A	834	CLA	O1A-CGA-O2A-C1
30	3	307	CLA	C2C-C3C-CAC-CBC
30	B	837	CLA	C4-C3-C5-C6
30	7	305	CLA	C4-C3-C5-C6
30	8	303	CLA	C4-C3-C5-C6
30	10	305	CLA	C4-C3-C5-C6
30	11	309	CLA	C4-C3-C5-C6
30	12	308	CLA	C4-C3-C5-C6
30	16	302	CLA	C4-C3-C5-C6
36	8	320	LMG	C29-C30-C31-C32
34	A	852	LHG	O7-C5-C6-O8
36	F	205	LMG	O1-C7-C8-O7
36	7	320	LMG	O7-C8-C9-O8
30	A	836	CLA	C6-C7-C8-C9
30	2	305	CLA	CBA-CGA-O2A-C1
30	8	309	CLA	CBA-CGA-O2A-C1
30	9	307	CLA	CBA-CGA-O2A-C1
30	B	810	CLA	O1D-CGD-O2D-CED
30	B	828	CLA	O1D-CGD-O2D-CED
30	12	304	CLA	CAA-CBA-CGA-O2A
30	3	306	CLA	C2A-CAA-CBA-CGA
30	7	303	CLA	C2A-CAA-CBA-CGA
30	A	813	CLA	C3-C5-C6-C7
30	B	831	CLA	C3-C5-C6-C7
35	11	303	LMT	C1-C2-C3-C4
30	B	833	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	5	305	KC1	CAA-CBA-CGA-O2A
30	B	838	CLA	C5-C6-C7-C8
36	8	320	LMG	O9-C10-O7-C8
34	A	852	LHG	C26-C27-C28-C29
30	A	828	CLA	CBA-CGA-O2A-C1
30	6	304	CLA	CBA-CGA-O2A-C1
30	11	308	CLA	CBA-CGA-O2A-C1
30	12	304	CLA	CBA-CGA-O2A-C1
36	14	321	LMG	O6-C5-C6-O5
35	7	301	LMT	C9-C10-C11-C12
30	10	311	CLA	CBD-CGD-O2D-CED
38	1	306	KC1	CBD-CGD-O2D-CED
38	8	307	KC1	CBD-CGD-O2D-CED
30	A	813	CLA	C10-C11-C12-C13
30	3	301	CLA	C5-C6-C7-C8
30	10	304	CLA	C10-C11-C12-C13
30	8	305	CLA	O1D-CGD-O2D-CED
37	13	313	A86	C24-C25-C26-C27
30	15	302	CLA	C16-C17-C18-C19
30	A	830	CLA	C4-C3-C5-C6
30	A	834	CLA	C4-C3-C5-C6
30	A	844	CLA	C4-C3-C5-C6
30	B	807	CLA	C4-C3-C5-C6
30	2	310	CLA	C4-C3-C5-C6
30	12	306	CLA	C4-C3-C5-C6
30	13	302	CLA	C4-C3-C5-C6
30	15	309	CLA	C4-C3-C5-C6
30	8	305	CLA	CBA-CGA-O2A-C1
35	B	852	LMT	C5-C6-C7-C8
35	7	321	LMT	C6-C7-C8-C9
35	11	303	LMT	C11-C10-C9-C8
36	B	849	LMG	C16-C17-C18-C19
34	5	317	LHG	O1-C1-C2-O2
35	11	303	LMT	C2-C1-O1'-C1'
30	A	806	CLA	C11-C12-C13-C14
30	A	807	CLA	C11-C12-C13-C14
30	A	841	CLA	C11-C10-C8-C9
30	B	802	CLA	C11-C12-C13-C14
30	B	811	CLA	C11-C10-C8-C9
30	B	813	CLA	C11-C12-C13-C14
30	B	822	CLA	C11-C12-C13-C14
30	B	828	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	835	CLA	C6-C7-C8-C9
30	L	202	CLA	C11-C12-C13-C14
30	1	307	CLA	C11-C10-C8-C9
30	2	301	CLA	C14-C13-C15-C16
30	2	304	CLA	C14-C13-C15-C16
30	2	311	CLA	C11-C12-C13-C14
30	5	307	CLA	C14-C13-C15-C16
30	6	304	CLA	C11-C12-C13-C14
30	6	314	CLA	C11-C12-C13-C14
30	8	301	CLA	C11-C10-C8-C9
30	9	308	CLA	C14-C13-C15-C16
30	10	303	CLA	C11-C10-C8-C9
30	11	310	CLA	C6-C7-C8-C9
30	12	304	CLA	C11-C10-C8-C9
30	13	303	CLA	C11-C12-C13-C14
30	14	307	CLA	C11-C10-C8-C9
30	15	302	CLA	C14-C13-C15-C16
30	15	304	CLA	C14-C13-C15-C16
31	B	840	PQN	C15-C16-C17-C18
30	A	807	CLA	C4B-C3B-CAB-CBB
30	A	810	CLA	C4B-C3B-CAB-CBB
30	A	811	CLA	C4B-C3B-CAB-CBB
30	B	803	CLA	C4B-C3B-CAB-CBB
30	B	805	CLA	C4B-C3B-CAB-CBB
30	B	813	CLA	C4B-C3B-CAB-CBB
30	B	823	CLA	C4B-C3B-CAB-CBB
30	B	826	CLA	C4B-C3B-CAB-CBB
30	B	829	CLA	C4B-C3B-CAB-CBB
30	B	831	CLA	C4B-C3B-CAB-CBB
30	B	832	CLA	C4B-C3B-CAB-CBB
30	2	305	CLA	C4B-C3B-CAB-CBB
30	2	307	CLA	C4B-C3B-CAB-CBB
30	3	301	CLA	C4B-C3B-CAB-CBB
30	4	301	CLA	C4B-C3B-CAB-CBB
30	5	308	CLA	C4B-C3B-CAB-CBB
30	6	309	CLA	C4B-C3B-CAB-CBB
30	6	316	CLA	C4B-C3B-CAB-CBB
30	7	304	CLA	C4B-C3B-CAB-CBB
30	7	310	CLA	C4B-C3B-CAB-CBB
30	9	307	CLA	C4B-C3B-CAB-CBB
30	9	309	CLA	C4B-C3B-CAB-CBB
30	12	302	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	13	301	CLA	C4B-C3B-CAB-CBB
30	13	309	CLA	C4B-C3B-CAB-CBB
30	14	310	CLA	C4B-C3B-CAB-CBB
30	14	313	CLA	C4B-C3B-CAB-CBB
30	16	302	CLA	C4B-C3B-CAB-CBB
35	11	303	LMT	C6-C7-C8-C9
30	12	303	CLA	O1D-CGD-O2D-CED
30	A	815	CLA	C10-C11-C12-C13
30	B	812	CLA	C5-C6-C7-C8
30	12	307	CLA	O1D-CGD-O2D-CED
30	L	202	CLA	CBA-CGA-O2A-C1
30	8	302	CLA	C3-C5-C6-C7
34	B	848	LHG	O6-C4-C5-C6
34	6	322	LHG	O6-C4-C5-C6
30	8	304	CLA	C10-C11-C12-C13
36	5	318	LMG	C31-C32-C33-C34
30	A	807	CLA	C11-C12-C13-C15
30	A	822	CLA	C12-C13-C15-C16
30	B	802	CLA	C11-C12-C13-C15
30	B	819	CLA	C12-C13-C15-C16
30	B	828	CLA	C6-C7-C8-C10
30	B	828	CLA	C11-C12-C13-C15
30	B	829	CLA	C12-C13-C15-C16
30	B	838	CLA	C12-C13-C15-C16
30	L	202	CLA	C11-C12-C13-C15
30	2	301	CLA	C11-C10-C8-C7
30	2	304	CLA	C12-C13-C15-C16
30	5	307	CLA	C12-C13-C15-C16
30	6	314	CLA	C11-C12-C13-C15
30	7	307	CLA	C11-C10-C8-C7
30	8	301	CLA	C11-C10-C8-C7
30	9	303	CLA	C11-C10-C8-C7
30	9	308	CLA	C12-C13-C15-C16
30	10	303	CLA	C11-C10-C8-C7
30	11	310	CLA	C12-C13-C15-C16
30	13	301	CLA	C6-C7-C8-C10
30	13	303	CLA	C11-C12-C13-C15
30	14	303	CLA	C11-C10-C8-C7
30	14	307	CLA	C11-C10-C8-C7
30	15	302	CLA	C12-C13-C15-C16
30	4	303	CLA	C5-C6-C7-C8
30	15	304	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	11	306	CLA	O1A-CGA-O2A-C1
36	8	319	LMG	C32-C33-C34-C35
30	A	806	CLA	C10-C11-C12-C13
30	A	816	CLA	C10-C11-C12-C13
30	B	817	CLA	C10-C11-C12-C13
30	A	811	CLA	C4-C3-C5-C6
30	A	820	CLA	C4-C3-C5-C6
30	1	303	CLA	C3A-C2A-CAA-CBA
30	8	308	CLA	C3A-C2A-CAA-CBA
30	11	304	CLA	C3A-C2A-CAA-CBA
30	16	306	CLA	C4-C3-C5-C6
30	7	306	CLA	C2-C3-C5-C6
34	9	318	LHG	C29-C30-C31-C32
30	A	804	CLA	C10-C11-C12-C13
30	10	307	CLA	CBA-CGA-O2A-C1
37	2	319	A86	C1-C2-C3-C4
37	4	317	A86	C24-C25-C26-C27
37	5	301	A86	C24-C25-C26-C27
37	15	321	A86	C11-C10-C9-C8
39	4	316	DD6	C3-C4-C5-C6
39	5	313	DD6	C3-C4-C5-C6
39	5	314	DD6	C24-C25-C26-C27
39	6	318	DD6	C3-C4-C5-C6
39	8	316	DD6	C24-C25-C26-C27
39	10	314	DD6	C3-C4-C5-C6
39	12	315	DD6	C24-C25-C26-C27
30	A	820	CLA	C3-C5-C6-C7
30	B	809	CLA	C3-C5-C6-C7
37	15	317	A86	C7-C6-C8-C9
30	A	816	CLA	O1A-CGA-O2A-C1
30	2	305	CLA	O1A-CGA-O2A-C1
30	F	202	CLA	C13-C15-C16-C17
39	2	317	DD6	C2-C1-C24-C25
34	A	852	LHG	C19-C20-C21-C22
30	A	830	CLA	CBA-CGA-O2A-C1
30	B	827	CLA	CBA-CGA-O2A-C1
35	8	322	LMT	C4-C5-C6-C7
36	F	205	LMG	O1-C7-C8-C9
36	3	317	LMG	C7-C8-C9-O8
36	8	319	LMG	C7-C8-C9-O8
37	2	318	A86	C12-C11-C13-O
37	7	315	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
37	10	302	A86	C12-C11-C13-O
37	11	301	A86	C12-C11-C13-O
37	13	313	A86	C12-C11-C13-O
37	16	312	A86	C12-C11-C13-O
33	L	201	BCR	C14-C15-C16-C17
30	B	833	CLA	C3-C5-C6-C7
30	6	306	CLA	C3-C5-C6-C7
30	15	307	CLA	CBD-CGD-O2D-CED
30	B	830	CLA	C13-C15-C16-C17
30	8	305	CLA	O1A-CGA-O2A-C1
30	A	806	CLA	C4-C3-C5-C6
30	A	826	CLA	C4-C3-C5-C6
30	A	839	CLA	C4-C3-C5-C6
30	B	834	CLA	C4-C3-C5-C6
30	1	303	CLA	C4-C3-C5-C6
30	7	311	CLA	C4-C3-C5-C6
30	A	844	CLA	C2-C3-C5-C6
30	B	807	CLA	C2-C3-C5-C6
30	B	834	CLA	C2-C3-C5-C6
30	B	828	CLA	O1A-CGA-O2A-C1
30	9	301	CLA	O1A-CGA-O2A-C1
30	A	836	CLA	C3-C5-C6-C7
30	12	321	CLA	C3-C5-C6-C7
30	15	311	CLA	O1D-CGD-O2D-CED
37	2	318	A86	C10-C11-C13-O
37	7	315	A86	C10-C11-C13-O
37	10	302	A86	C10-C11-C13-O
37	11	301	A86	C10-C11-C13-O
37	13	313	A86	C10-C11-C13-O
37	16	312	A86	C10-C11-C13-O
30	B	830	CLA	O1D-CGD-O2D-CED
30	A	807	CLA	C2B-C3B-CAB-CBB
30	3	310	CLA	C2B-C3B-CAB-CBB
30	13	301	CLA	C2B-C3B-CAB-CBB
30	14	310	CLA	C2B-C3B-CAB-CBB
30	16	310	CLA	C2B-C3B-CAB-CBB
33	A	847	BCR	C1-C6-C7-C8
33	A	848	BCR	C1-C6-C7-C8
33	A	849	BCR	C1-C6-C7-C8
33	A	850	BCR	C1-C6-C7-C8
33	A	850	BCR	C23-C24-C25-C30
33	A	851	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	B	841	BCR	C23-C24-C25-C30
33	B	842	BCR	C1-C6-C7-C8
33	B	843	BCR	C1-C6-C7-C8
33	B	844	BCR	C23-C24-C25-C30
33	B	846	BCR	C1-C6-C7-C8
33	J	103	BCR	C1-C6-C7-C8
33	L	205	BCR	C1-C6-C7-C8
33	2u	201	BCR	C23-C24-C25-C26
34	9	318	LHG	C9-C10-C11-C12
37	16	314	A86	C33-C34-O4-C38
30	B	807	CLA	C3-C5-C6-C7
30	16	301	CLA	C5-C6-C7-C8
30	A	810	CLA	C2A-CAA-CBA-CGA
30	10	308	CLA	C2A-CAA-CBA-CGA
30	11	309	CLA	C2A-CAA-CBA-CGA
36	B	847	LMG	O1-C7-C8-O7
36	2u	204	LMG	O1-C7-C8-O7
36	5	318	LMG	O7-C8-C9-O8
36	6	301	LMG	O7-C8-C9-O8
30	1	303	CLA	O1A-CGA-O2A-C1
30	3	303	CLA	C10-C11-C12-C13
30	A	811	CLA	C2-C3-C5-C6
30	A	814	CLA	C2-C3-C5-C6
30	A	820	CLA	C2-C3-C5-C6
30	A	839	CLA	C2-C3-C5-C6
30	12	306	CLA	C2-C3-C5-C6
30	13	302	CLA	C2-C3-C5-C6
30	16	306	CLA	C2-C3-C5-C6
36	B	849	LMG	C17-C18-C19-C20
30	A	820	CLA	C16-C17-C18-C19
30	B	819	CLA	C11-C10-C8-C9
30	B	819	CLA	C14-C13-C15-C16
30	B	830	CLA	C14-C13-C15-C16
30	1	302	CLA	C11-C10-C8-C9
30	13	301	CLA	C6-C7-C8-C9
31	A	845	PQN	C21-C22-C23-C24
30	15	313	CLA	C10-C11-C12-C13
33	A	847	BCR	C22-C23-C24-C25
33	B	842	BCR	C14-C15-C16-C17
35	B	852	LMT	C4-C5-C6-C7
30	7	304	CLA	C16-C17-C18-C19
36	B	847	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
35	A	854	LMT	C11-C10-C9-C8
36	14	321	LMG	C16-C17-C18-C19
35	1	311	LMT	C9-C10-C11-C12
30	B	826	CLA	O1D-CGD-O2D-CED
38	2	306	KC1	CAA-CBA-CGA-O2A
38	12	309	KC1	CAA-CBA-CGA-O1A
38	12	309	KC1	CAA-CBA-CGA-O2A
30	B	801	CLA	C3-C5-C6-C7
30	B	851	CLA	O1D-CGD-O2D-CED
37	2	319	A86	C3-C4-C5-C6
30	A	826	CLA	C2-C3-C5-C6
30	A	830	CLA	C2-C3-C5-C6
29	A	801	CL0	C16-C17-C18-C20
30	15	302	CLA	C16-C17-C18-C20
30	B	818	CLA	C8-C10-C11-C12
36	2u	204	LMG	C11-C12-C13-C14
33	B	842	BCR	C20-C21-C22-C37
33	B	844	BCR	C35-C13-C14-C15
33	B	844	BCR	C20-C21-C22-C37
33	L	204	BCR	C35-C13-C14-C15
33	M	101	BCR	C16-C17-C18-C36
39	2	316	DD6	C9-C10-C11-C12
39	7	317	DD6	C4-C5-C6-C7
39	7	318	DD6	C9-C10-C11-C12
30	A	828	CLA	O1A-CGA-O2A-C1
34	2	320	LHG	O10-C23-O8-C6
30	A	802	CLA	C3-C5-C6-C7
38	2	306	KC1	CAA-CBA-CGA-O1A
30	B	809	CLA	C16-C17-C18-C20
30	B	827	CLA	O1A-CGA-O2A-C1
30	13	303	CLA	C13-C15-C16-C17
37	13	313	A86	C7-C6-C8-C9
37	15	316	A86	C-C1-C24-C25
39	3	313	DD6	C12-C11-C13-C14
39	6	319	DD6	C12-C11-C13-C14
30	A	833	CLA	C11-C10-C8-C7
30	A	839	CLA	C12-C13-C15-C16
30	B	813	CLA	C11-C12-C13-C15
30	B	819	CLA	C11-C10-C8-C7
30	B	830	CLA	C12-C13-C15-C16
30	2u	202	CLA	C6-C7-C8-C10
30	2u	202	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
30	2	309	CLA	C12-C13-C15-C16
30	4	302	CLA	C12-C13-C15-C16
30	7	309	CLA	C12-C13-C15-C16
30	8	305	CLA	C12-C13-C15-C16
30	11	309	CLA	C12-C13-C15-C16
30	11	310	CLA	C6-C7-C8-C10
30	A	825	CLA	C10-C11-C12-C13
30	A	841	CLA	C3-C5-C6-C7
30	6	307	CLA	C8-C10-C11-C12
30	12	304	CLA	C10-C11-C12-C13
33	A	849	BCR	C21-C22-C23-C24
33	J	102	BCR	C7-C8-C9-C10
33	2u	201	BCR	C21-C22-C23-C24
37	13	313	A86	C5-C6-C8-C9
37	15	316	A86	C2-C1-C24-C25
37	15	321	A86	C5-C6-C8-C9
39	3	316	DD6	C10-C11-C13-C14
39	4	313	DD6	C10-C11-C13-C14
39	11	313	DD6	C5-C6-C8-C9
39	15	318	DD6	C10-C11-C13-C14
39	15	319	DD6	C10-C11-C13-C14
30	4	306	CLA	CBA-CGA-O2A-C1
30	8	309	CLA	O1A-CGA-O2A-C1
30	9	307	CLA	O1A-CGA-O2A-C1
30	10	303	CLA	O1A-CGA-O2A-C1
30	F	203	CLA	C2A-CAA-CBA-CGA
30	A	813	CLA	C4-C3-C5-C6
30	6	317	CLA	C4-C3-C5-C6
30	4	302	CLA	O1A-CGA-O2A-C1
30	11	308	CLA	O1A-CGA-O2A-C1
30	12	304	CLA	O1A-CGA-O2A-C1
38	3	304	KC1	C2B-C3B-CAB-CBB
38	12	309	KC1	C2B-C3B-CAB-CBB
38	13	308	KC1	C2B-C3B-CAB-CBB
30	2	304	CLA	C3-C5-C6-C7
36	8	319	LMG	C34-C35-C36-C37
30	15	305	CLA	CBD-CGD-O2D-CED
30	4	302	CLA	C10-C11-C12-C13
35	11	317	LMT	C3'-C4'-O1B-C1B
33	2u	201	BCR	C19-C20-C21-C22
36	8	320	LMG	C18-C19-C20-C21
30	L	202	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	5	302	CLA	O1A-CGA-O2A-C1
30	6	310	CLA	C10-C11-C12-C13
33	L	205	BCR	C12-C13-C14-C15
39	5	314	DD6	C4-C5-C6-C8
39	7	318	DD6	C4-C5-C6-C8
30	B	829	CLA	C10-C11-C12-C13
30	5	307	CLA	C15-C16-C17-C18
30	B	817	CLA	CAA-CBA-CGA-O2A
34	B	848	LHG	O6-C4-C5-O7
34	6	322	LHG	O6-C4-C5-O7
30	5	308	CLA	O1D-CGD-O2D-CED
34	9	318	LHG	C4-C5-C6-O8
36	B	847	LMG	O1-C7-C8-C9
36	8	321	LMG	C7-C8-C9-O8
30	B	808	CLA	C5-C6-C7-C8
38	1	306	KC1	C4B-C3B-CAB-CBB
38	2	306	KC1	C4B-C3B-CAB-CBB
38	2	312	KC1	C4B-C3B-CAB-CBB
38	3	304	KC1	C4B-C3B-CAB-CBB
38	5	305	KC1	C4B-C3B-CAB-CBB
38	5	306	KC1	C2A-CAA-CBA-CGA
38	6	308	KC1	C4B-C3B-CAB-CBB
38	7	313	KC1	C4B-C3B-CAB-CBB
38	8	307	KC1	C4B-C3B-CAB-CBB
38	8	312	KC1	C4B-C3B-CAB-CBB
38	9	311	KC1	C4B-C3B-CAB-CBB
38	11	305	KC1	C4B-C3B-CAB-CBB
38	12	313	KC1	C4B-C3B-CAB-CBB
38	13	310	KC1	C4B-C3B-CAB-CBB
38	14	306	KC1	C4B-C3B-CAB-CBB
38	6	312	KC1	CAA-CBA-CGA-O1A
30	A	830	CLA	O1A-CGA-O2A-C1
30	10	307	CLA	O1A-CGA-O2A-C1
36	8	320	LMG	O10-C28-O8-C9
30	13	301	CLA	O1D-CGD-O2D-CED
30	B	813	CLA	C4-C3-C5-C6
30	A	822	CLA	C2A-CAA-CBA-CGA
30	1	304	CLA	C2-C3-C5-C6
30	2	303	CLA	C2-C3-C5-C6
30	5	309	CLA	C2-C3-C5-C6
30	7	311	CLA	C2-C3-C5-C6
37	3	315	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
37	5	315	A86	C28-C27-C29-C30
37	7	315	A86	C28-C27-C29-C30
37	15	317	A86	C28-C27-C29-C30
36	5	318	LMG	C10-C11-C12-C13
36	7	320	LMG	C13-C14-C15-C16
30	A	814	CLA	C3-C5-C6-C7
30	15	302	CLA	C3-C5-C6-C7
34	9	318	LHG	O7-C5-C6-O8
36	3	317	LMG	O7-C8-C9-O8
30	F	202	CLA	C8-C10-C11-C12
30	F	202	CLA	C11-C10-C8-C9
30	4	302	CLA	C14-C13-C15-C16
30	7	303	CLA	C11-C12-C13-C14
30	7	309	CLA	C14-C13-C15-C16
30	11	309	CLA	C14-C13-C15-C16
38	14	308	KC1	C4C-C3C-CAC-CBC
35	7	321	LMT	C4-C5-C6-C7
36	A	856	LMG	O10-C28-O8-C9
35	A	854	LMT	C6-C7-C8-C9
30	15	313	CLA	C13-C15-C16-C17
37	3	315	A86	C13-C14-C15-O1
37	5	301	A86	C13-C14-C15-O1
37	5	316	A86	C13-C14-C15-O1
37	10	302	A86	C13-C14-C15-O1
37	10	316	A86	C13-C14-C15-O1
37	11	301	A86	C13-C14-C15-O1
37	11	314	A86	C13-C14-C15-O1
37	11	316	A86	C13-C14-C15-O1
37	12	314	A86	C13-C14-C15-O1
37	14	316	A86	C13-C14-C15-O1
37	14	317	A86	C13-C14-C15-O1
37	14	318	A86	C13-C14-C15-O1
37	15	321	A86	C13-C14-C15-O1
34	A	852	LHG	C7-C8-C9-C10
36	B	847	LMG	C31-C32-C33-C34
30	4	306	CLA	O1D-CGD-O2D-CED
34	6	322	LHG	C8-C7-O7-C5
30	5	304	CLA	C2-C1-O2A-CGA
30	6	306	CLA	C2-C1-O2A-CGA
39	1	310	DD6	C3-C4-C5-C6
30	15	309	CLA	C16-C17-C18-C20
38	6	312	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	15	304	CLA	C3-C5-C6-C7
30	A	829	CLA	C13-C15-C16-C17
30	A	829	CLA	C15-C16-C17-C18
30	B	803	CLA	C10-C11-C12-C13
30	4	304	CLA	C10-C11-C12-C13
30	6	317	CLA	C13-C15-C16-C17
30	A	840	CLA	CBD-CGD-O2D-CED
30	4	309	CLA	CBA-CGA-O2A-C1
36	14	321	LMG	C17-C18-C19-C20
30	3	307	CLA	C4C-C3C-CAC-CBC
30	6	304	CLA	O1A-CGA-O2A-C1
35	7	301	LMT	C7-C8-C9-C10
29	A	801	CL0	C3-C5-C6-C7
30	B	835	CLA	C3-C5-C6-C7
38	8	306	KC1	CAA-CBA-CGA-O1A
30	12	302	CLA	O1D-CGD-O2D-CED
35	1	311	LMT	O1'-C1-C2-C3
30	5	311	CLA	O1D-CGD-O2D-CED
34	A	852	LHG	O1-C1-C2-O2
30	11	309	CLA	O1A-CGA-O2A-C1
30	15	308	CLA	CBD-CGD-O2D-CED
39	7	317	DD6	C-C1-C24-C25
35	12	301	LMT	C4B-C5B-C6B-O6B
30	A	812	CLA	C4B-C3B-CAB-CBB
30	A	823	CLA	C1A-C2A-CAA-CBA
30	A	825	CLA	C4B-C3B-CAB-CBB
30	A	836	CLA	C1A-C2A-CAA-CBA
30	A	839	CLA	C4B-C3B-CAB-CBB
30	A	844	CLA	C4B-C3B-CAB-CBB
30	B	808	CLA	C4B-C3B-CAB-CBB
30	F	203	CLA	C4B-C3B-CAB-CBB
30	2u	202	CLA	C4B-C3B-CAB-CBB
30	1	303	CLA	C4B-C3B-CAB-CBB
30	1	305	CLA	C1A-C2A-CAA-CBA
30	2	309	CLA	C4B-C3B-CAB-CBB
30	2	311	CLA	C4B-C3B-CAB-CBB
30	2	313	CLA	C4B-C3B-CAB-CBB
30	3	305	CLA	C4B-C3B-CAB-CBB
30	3	306	CLA	C4B-C3B-CAB-CBB
30	3	310	CLA	C1A-C2A-CAA-CBA
30	3	310	CLA	C4B-C3B-CAB-CBB
30	4	309	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	5	303	CLA	C4B-C3B-CAB-CBB
30	5	309	CLA	C4B-C3B-CAB-CBB
30	5	311	CLA	C4B-C3B-CAB-CBB
30	6	304	CLA	C4B-C3B-CAB-CBB
30	6	315	CLA	C4B-C3B-CAB-CBB
30	6	317	CLA	C4B-C3B-CAB-CBB
30	7	309	CLA	C4B-C3B-CAB-CBB
30	7	311	CLA	C1A-C2A-CAA-CBA
30	7	311	CLA	C4B-C3B-CAB-CBB
30	7	312	CLA	C4B-C3B-CAB-CBB
30	8	309	CLA	C1A-C2A-CAA-CBA
30	10	309	CLA	C4B-C3B-CAB-CBB
30	11	304	CLA	C1A-C2A-CAA-CBA
30	11	310	CLA	C4B-C3B-CAB-CBB
30	12	312	CLA	C4B-C3B-CAB-CBB
30	13	302	CLA	C4B-C3B-CAB-CBB
30	13	303	CLA	C4B-C3B-CAB-CBB
30	13	304	CLA	C4B-C3B-CAB-CBB
30	14	303	CLA	C4B-C3B-CAB-CBB
30	14	304	CLA	C4B-C3B-CAB-CBB
30	14	307	CLA	C4B-C3B-CAB-CBB
30	15	302	CLA	C4B-C3B-CAB-CBB
30	15	306	CLA	C4B-C3B-CAB-CBB
30	16	303	CLA	C4B-C3B-CAB-CBB
30	16	308	CLA	C4B-C3B-CAB-CBB
30	16	309	CLA	C4B-C3B-CAB-CBB
30	16	310	CLA	C4B-C3B-CAB-CBB
37	2	319	A86	O-C13-C14-C15
37	4	314	A86	O-C13-C14-C15
37	5	301	A86	O-C13-C14-C15
37	8	318	A86	O-C13-C14-C15
37	9	316	A86	O-C13-C14-C15
37	10	316	A86	O-C13-C14-C15
37	12	314	A86	O-C13-C14-C15
37	12	316	A86	O-C13-C14-C15
37	15	321	A86	O-C13-C14-C15
34	6	322	LHG	C24-C23-O8-C6
36	8	320	LMG	C15-C16-C17-C18
36	3	317	LMG	C28-C29-C30-C31
30	A	803	CLA	C4-C3-C5-C6
30	A	828	CLA	C4-C3-C5-C6
30	F	202	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	A	850	BCR	C22-C23-C24-C25
30	B	837	CLA	C2-C3-C5-C6
33	A	848	BCR	C21-C22-C23-C24
39	6	318	DD6	C2-C1-C24-C25
30	10	303	CLA	C2A-CAA-CBA-CGA
36	B	847	LMG	C17-C18-C19-C20
30	16	306	CLA	CBD-CGD-O2D-CED
34	A	852	LHG	O9-C7-O7-C5
30	A	809	CLA	O1D-CGD-O2D-CED
30	A	802	CLA	C6-C7-C8-C10
30	A	820	CLA	C11-C12-C13-C15
30	B	801	CLA	C11-C10-C8-C7
30	B	851	CLA	C11-C10-C8-C7
30	F	202	CLA	C11-C12-C13-C15
30	F	202	CLA	C12-C13-C15-C16
30	3	307	CLA	C11-C12-C13-C15
30	6	310	CLA	C12-C13-C15-C16
30	6	317	CLA	C12-C13-C15-C16
30	7	310	CLA	C12-C13-C15-C16
30	9	305	CLA	C11-C12-C13-C15
30	9	309	CLA	C12-C13-C15-C16
30	11	309	CLA	C11-C10-C8-C7
30	12	302	CLA	C11-C12-C13-C15
30	13	302	CLA	C6-C7-C8-C10
35	A	857	LMT	C2-C3-C4-C5
30	A	839	CLA	C10-C11-C12-C13
36	B	847	LMG	C12-C13-C14-C15
30	A	813	CLA	O1D-CGD-O2D-CED
38	8	312	KC1	CBD-CGD-O2D-CED
30	2u	202	CLA	C5-C6-C7-C8
30	8	305	CLA	C13-C15-C16-C17
36	6	301	LMG	C11-C12-C13-C14
30	3	305	CLA	O1A-CGA-O2A-C1
30	6	305	CLA	C15-C16-C17-C18
30	A	807	CLA	C3A-C2A-CAA-CBA
30	12	304	CLA	C3A-C2A-CAA-CBA
30	11	309	CLA	C2-C3-C5-C6
30	12	308	CLA	C2-C3-C5-C6
30	6	316	CLA	O1A-CGA-O2A-C1
30	B	804	CLA	C2A-CAA-CBA-CGA
30	B	801	CLA	C11-C10-C8-C9
30	B	838	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	2u	202	CLA	C11-C12-C13-C14
30	2	309	CLA	C14-C13-C15-C16
30	6	307	CLA	C11-C10-C8-C9
30	8	305	CLA	C14-C13-C15-C16
30	15	304	CLA	C11-C12-C13-C14
30	4	306	CLA	O1A-CGA-O2A-C1
30	4	309	CLA	O1A-CGA-O2A-C1
37	3	315	A86	C3-C4-C5-C6
37	6	320	A86	C11-C10-C9-C8
37	10	317	A86	C24-C25-C26-C27
39	6	303	DD6	C11-C10-C9-C8
30	A	813	CLA	CBD-CGD-O2D-CED
30	A	823	CLA	C1-C2-C3-C4
30	4	301	CLA	C1-C2-C3-C4
37	15	317	A86	C26-C27-C29-C30
37	16	312	A86	C26-C27-C29-C30
38	1	306	KC1	C3A-C2A-CAA-CBA
38	2	306	KC1	C3A-C2A-CAA-CBA
38	3	304	KC1	C3A-C2A-CAA-CBA
38	4	310	KC1	C1A-C2A-CAA-CBA
38	5	306	KC1	C3A-C2A-CAA-CBA
38	8	312	KC1	C1A-C2A-CAA-CBA
38	8	312	KC1	C3A-C2A-CAA-CBA
38	9	311	KC1	C3A-C2A-CAA-CBA
38	10	312	KC1	C3A-C2A-CAA-CBA
38	12	305	KC1	C1A-C2A-CAA-CBA
38	12	305	KC1	C3A-C2A-CAA-CBA
38	12	313	KC1	C1A-C2A-CAA-CBA
38	13	305	KC1	C1A-C2A-CAA-CBA
38	13	310	KC1	C3A-C2A-CAA-CBA
38	14	306	KC1	C3A-C2A-CAA-CBA
30	B	816	CLA	C3-C5-C6-C7
38	9	311	KC1	O1D-CGD-O2D-CED
34	B	848	LHG	O10-C23-C24-C25
30	A	827	CLA	O1A-CGA-O2A-C1
34	B	848	LHG	O7-C5-C6-O8
36	A	856	LMG	O7-C8-C9-O8
36	8	321	LMG	O7-C8-C9-O8
36	14	321	LMG	O7-C8-C9-O8
38	8	306	KC1	CAA-CBA-CGA-O2A
30	2	311	CLA	O1D-CGD-O2D-CED
30	A	812	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	F	205	LMG	C7-C8-C9-O8
36	2u	204	LMG	O1-C7-C8-C9
36	6	301	LMG	O1-C7-C8-C9
36	8	319	LMG	O1-C7-C8-C9
30	7	305	CLA	C3-C5-C6-C7
30	A	806	CLA	CAD-CBD-CGD-O2D
30	4	304	CLA	CAD-CBD-CGD-O2D
30	4	309	CLA	CAD-CBD-CGD-O2D
30	5	304	CLA	CAD-CBD-CGD-O2D
30	7	312	CLA	CAD-CBD-CGD-O2D
30	13	304	CLA	CAD-CBD-CGD-O2D
37	4	312	A86	C13-C14-C15-C20
37	7	319	A86	C13-C14-C15-C20
37	14	320	A86	C13-C14-C15-C20
37	15	316	A86	C13-C14-C15-C20
37	15	317	A86	C13-C14-C15-C20
37	15	323	A86	C13-C14-C15-C20
38	12	311	KC1	CAD-CBD-CGD-O2D
30	B	839	CLA	O1D-CGD-O2D-CED
30	A	831	CLA	C5-C6-C7-C8
36	6	301	LMG	C10-C11-C12-C13
30	7	305	CLA	C16-C17-C18-C20
35	A	854	LMT	C5'-C4'-O1B-C1B
30	A	829	CLA	C2A-CAA-CBA-CGA
30	4	305	CLA	C2A-CAA-CBA-CGA
36	14	321	LMG	C30-C31-C32-C33
30	6	306	CLA	C5-C6-C7-C8
30	A	807	CLA	CAA-CBA-CGA-O2A
30	A	812	CLA	O1A-CGA-O2A-C1
30	A	804	CLA	CHA-CBD-CGD-O1D
30	A	804	CLA	CHA-CBD-CGD-O2D
30	A	806	CLA	CAD-CBD-CGD-O1D
30	A	826	CLA	CHA-CBD-CGD-O1D
30	A	826	CLA	CHA-CBD-CGD-O2D
30	B	804	CLA	CHA-CBD-CGD-O1D
30	B	815	CLA	CHA-CBD-CGD-O1D
30	B	815	CLA	CHA-CBD-CGD-O2D
30	B	820	CLA	CHA-CBD-CGD-O1D
30	B	820	CLA	CHA-CBD-CGD-O2D
30	B	821	CLA	CHA-CBD-CGD-O1D
30	B	834	CLA	CAD-CBD-CGD-O1D
30	F	203	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	3	306	CLA	CHA-CBD-CGD-O2D
30	4	304	CLA	CAD-CBD-CGD-O1D
30	4	309	CLA	CAD-CBD-CGD-O1D
30	5	304	CLA	CAD-CBD-CGD-O1D
30	6	315	CLA	CAD-CBD-CGD-O1D
30	7	312	CLA	CAD-CBD-CGD-O1D
30	8	305	CLA	CHA-CBD-CGD-O2D
30	8	308	CLA	CAD-CBD-CGD-O1D
30	13	304	CLA	CAD-CBD-CGD-O1D
30	14	303	CLA	CHA-CBD-CGD-O1D
30	14	312	CLA	CAD-CBD-CGD-O1D
30	15	308	CLA	CHA-CBD-CGD-O1D
30	15	308	CLA	CHA-CBD-CGD-O2D
30	15	312	CLA	CHA-CBD-CGD-O1D
30	15	312	CLA	CHA-CBD-CGD-O2D
34	A	853	LHG	C3-O3-P-O5
34	2	320	LHG	C4-O6-P-O4
34	5	317	LHG	C3-O3-P-O5
34	6	322	LHG	C4-O6-P-O3
34	6	322	LHG	C4-O6-P-O4
34	9	318	LHG	C4-O6-P-O4
37	6	320	A86	C3-C4-C5-C6
37	8	318	A86	C11-C13-C14-C15
37	9	316	A86	C10-C11-C13-C14
37	11	301	A86	C24-C25-C26-C27
37	12	314	A86	C10-C11-C13-C14
37	14	318	A86	C10-C11-C13-C14
37	15	315	A86	C11-C10-C9-C8
37	16	312	A86	C10-C11-C13-C14
38	1	306	KC1	CHA-CBD-CGD-O1D
38	1	306	KC1	CHA-CBD-CGD-O2D
38	6	312	KC1	CAD-CBD-CGD-O1D
38	9	311	KC1	CHA-CBD-CGD-O2D
38	12	311	KC1	CAD-CBD-CGD-O1D
38	14	306	KC1	CHA-CBD-CGD-O1D
38	14	306	KC1	CHA-CBD-CGD-O2D
39	5	314	DD6	C3-C4-C5-C6
39	7	302	DD6	C11-C10-C9-C8
39	7	314	DD6	C11-C10-C9-C8
39	7	314	DD6	C1-C2-C3-C4
39	10	314	DD6	C24-C25-C26-C27
39	15	319	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	10	308	CLA	CBD-CGD-O2D-CED
30	A	814	CLA	C10-C11-C12-C13
30	A	816	CLA	C4-C3-C5-C6
30	11	310	CLA	C4-C3-C5-C6
30	A	812	CLA	C2B-C3B-CAB-CBB
30	A	822	CLA	C2B-C3B-CAB-CBB
30	A	833	CLA	C2B-C3B-CAB-CBB
30	A	836	CLA	C2B-C3B-CAB-CBB
30	B	809	CLA	C2B-C3B-CAB-CBB
30	B	818	CLA	C2B-C3B-CAB-CBB
30	B	827	CLA	C2B-C3B-CAB-CBB
30	F	203	CLA	C2B-C3B-CAB-CBB
30	1	305	CLA	C2B-C3B-CAB-CBB
30	2	303	CLA	C2B-C3B-CAB-CBB
30	2	309	CLA	C2B-C3B-CAB-CBB
30	2	311	CLA	C2B-C3B-CAB-CBB
30	3	305	CLA	C2B-C3B-CAB-CBB
30	3	306	CLA	C2B-C3B-CAB-CBB
30	4	301	CLA	C2B-C3B-CAB-CBB
30	4	311	CLA	C2B-C3B-CAB-CBB
30	5	303	CLA	C2B-C3B-CAB-CBB
30	5	304	CLA	C2B-C3B-CAB-CBB
30	5	309	CLA	C2B-C3B-CAB-CBB
30	6	307	CLA	C2B-C3B-CAB-CBB
30	6	314	CLA	C2B-C3B-CAB-CBB
30	6	315	CLA	C2B-C3B-CAB-CBB
30	7	309	CLA	C2B-C3B-CAB-CBB
30	7	312	CLA	C2B-C3B-CAB-CBB
30	9	305	CLA	C2B-C3B-CAB-CBB
30	9	308	CLA	C2B-C3B-CAB-CBB
30	10	311	CLA	C2B-C3B-CAB-CBB
30	11	310	CLA	C2B-C3B-CAB-CBB
30	12	312	CLA	C2B-C3B-CAB-CBB
30	13	302	CLA	C2B-C3B-CAB-CBB
30	14	307	CLA	C2B-C3B-CAB-CBB
30	16	303	CLA	C2B-C3B-CAB-CBB
30	16	309	CLA	C2B-C3B-CAB-CBB
33	B	846	BCR	C23-C24-C25-C30
33	L	201	BCR	C23-C24-C25-C30
30	A	819	CLA	CAA-CBA-CGA-O2A
30	A	813	CLA	C2-C3-C5-C6
30	A	828	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	B	813	CLA	C2-C3-C5-C6
30	2	310	CLA	C2-C3-C5-C6
30	6	317	CLA	C2-C3-C5-C6
37	2	302	A86	C35-C34-O4-C38
33	B	843	BCR	C36-C18-C19-C20
30	15	313	CLA	C3-C5-C6-C7
37	2u	203	A86	C12-C11-C13-C14
37	5	301	A86	C12-C11-C13-C14
37	12	314	A86	C12-C11-C13-C14
37	14	316	A86	C12-C11-C13-C14
37	14	318	A86	C12-C11-C13-C14
37	16	312	A86	C12-C11-C13-C14
30	4	305	CLA	C3-C5-C6-C7
30	A	805	CLA	C11-C12-C13-C14
30	4	305	CLA	C5-C6-C7-C8
30	6	314	CLA	C13-C15-C16-C17
30	B	830	CLA	C4-C3-C5-C6
37	2u	203	A86	C6-C8-C9-C10
37	2u	205	A86	C6-C8-C9-C10
37	2	302	A86	C1-C24-C25-C26
37	4	314	A86	C6-C8-C9-C10
37	9	315	A86	C1-C24-C25-C26
37	10	301	A86	C1-C24-C25-C26
37	10	302	A86	C1-C24-C25-C26
37	10	302	A86	C6-C8-C9-C10
37	11	301	A86	C6-C8-C9-C10
37	13	313	A86	C6-C8-C9-C10
37	15	315	A86	C1-C24-C25-C26
37	15	315	A86	C6-C8-C9-C10
37	15	320	A86	C6-C8-C9-C10
37	15	323	A86	C6-C8-C9-C10
37	16	312	A86	C6-C8-C9-C10
39	2	315	DD6	C6-C8-C9-C10
39	10	313	DD6	C6-C8-C9-C10
30	5	307	CLA	C5-C6-C7-C8
36	8	320	LMG	C14-C15-C16-C17
30	1	304	CLA	CBD-CGD-O2D-CED
34	A	852	LHG	C31-C32-C33-C34
37	10	316	A86	C11-C10-C9-C8
30	B	813	CLA	C16-C17-C18-C20
30	7	305	CLA	C16-C17-C18-C19
30	9	305	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	6	309	CLA	CBD-CGD-O2D-CED
30	A	804	CLA	C11-C12-C13-C14
30	A	822	CLA	C14-C13-C15-C16
30	B	851	CLA	C11-C10-C8-C9
30	F	202	CLA	C14-C13-C15-C16
30	2	301	CLA	C11-C10-C8-C9
30	4	304	CLA	C11-C10-C8-C9
30	6	310	CLA	C14-C13-C15-C16
30	7	307	CLA	C14-C13-C15-C16
30	7	310	CLA	C14-C13-C15-C16
30	9	303	CLA	C11-C10-C8-C9
30	10	303	CLA	C14-C13-C15-C16
30	15	302	CLA	C6-C7-C8-C9
30	A	834	CLA	C11-C12-C13-C15
30	6	304	CLA	C12-C13-C15-C16
30	16	303	CLA	C11-C12-C13-C15
34	A	852	LHG	C28-C29-C30-C31
33	A	848	BCR	C20-C21-C22-C23
33	B	845	BCR	C20-C21-C22-C23
39	2	315	DD6	C24-C1-C2-C3
39	3	313	DD6	C9-C10-C11-C13
39	10	313	DD6	C24-C1-C2-C3
39	12	317	DD6	C24-C1-C2-C3
33	F	204	BCR	C6-C7-C8-C9
33	J	102	BCR	C6-C7-C8-C9
36	B	847	LMG	C18-C19-C20-C21
30	8	301	CLA	CBA-CGA-O2A-C1
30	12	302	CLA	CAA-CBA-CGA-O2A
34	B	848	LHG	C10-C11-C12-C13
38	8	312	KC1	O1D-CGD-O2D-CED
38	10	310	KC1	O1D-CGD-O2D-CED
30	A	805	CLA	C4-C3-C5-C6
30	6	305	CLA	C4-C3-C5-C6
30	10	305	CLA	C2-C3-C5-C6
30	15	309	CLA	C2-C3-C5-C6
36	14	321	LMG	C14-C15-C16-C17
35	12	301	LMT	C1-C2-C3-C4
30	A	827	CLA	CBA-CGA-O2A-C1
30	6	316	CLA	CBA-CGA-O2A-C1
30	A	816	CLA	C16-C17-C18-C19
30	B	809	CLA	C16-C17-C18-C19
30	A	816	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	15	304	CLA	C13-C15-C16-C17
36	A	856	LMG	C29-C30-C31-C32
30	B	833	CLA	C10-C11-C12-C13
30	6	307	CLA	CAA-CBA-CGA-O2A
39	6	303	DD6	C3-C4-C5-C6
30	15	309	CLA	C16-C17-C18-C19
36	14	321	LMG	C11-C10-O7-C8
30	2	307	CLA	CAA-CBA-CGA-O2A
36	7	320	LMG	O9-C10-O7-C8
30	A	821	CLA	C2-C1-O2A-CGA
30	13	302	CLA	C2-C1-O2A-CGA
36	2u	204	LMG	C28-C29-C30-C31
30	A	829	CLA	C16-C17-C18-C20
30	4	304	CLA	CAA-CBA-CGA-O2A
30	B	808	CLA	C10-C11-C12-C13
30	7	309	CLA	C3-C5-C6-C7
30	5	304	CLA	CAA-CBA-CGA-O2A
30	13	301	CLA	C8-C10-C11-C12
34	A	853	LHG	C8-C7-O7-C5
37	14	301	A86	C35-C34-O4-C38
36	14	321	LMG	C12-C13-C14-C15
36	3	317	LMG	C8-C7-O1-C1
30	1	301	CLA	C5-C6-C7-C8
30	11	304	CLA	C13-C15-C16-C17
35	11	303	LMT	C5-C6-C7-C8
30	A	809	CLA	C2A-CAA-CBA-CGA
30	3	305	CLA	C2A-CAA-CBA-CGA
33	A	847	BCR	C15-C16-C17-C18
37	5	315	A86	C11-C10-C9-C8
37	14	316	A86	C11-C10-C9-C8
37	15	317	A86	C1-C2-C3-C4
39	3	316	DD6	C24-C25-C26-C27
30	A	826	CLA	C16-C17-C18-C20
35	12	320	LMT	C5-C6-C7-C8
35	15	301	LMT	O5'-C1'-O1'-C1
30	A	803	CLA	C2-C3-C5-C6
38	1	308	KC1	C2B-C3B-CAB-CBB
38	11	311	KC1	C2B-C3B-CAB-CBB
30	A	841	CLA	C15-C16-C17-C18
36	B	849	LMG	C28-C29-C30-C31
30	15	305	CLA	O1D-CGD-O2D-CED
37	16	312	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	A	813	CLA	C6-C7-C8-C9
30	B	838	CLA	C11-C10-C8-C9
30	F	202	CLA	C11-C12-C13-C14
30	1	303	CLA	C14-C13-C15-C16
30	6	304	CLA	C14-C13-C15-C16
30	6	317	CLA	C14-C13-C15-C16
30	9	305	CLA	C11-C12-C13-C14
30	12	302	CLA	C11-C12-C13-C14
30	13	302	CLA	C6-C7-C8-C9
30	A	828	CLA	C4B-C3B-CAB-CBB
30	J	101	CLA	C4B-C3B-CAB-CBB
30	3	309	CLA	C4B-C3B-CAB-CBB
30	4	311	CLA	C4B-C3B-CAB-CBB
30	10	311	CLA	C4B-C3B-CAB-CBB
30	12	307	CLA	C4B-C3B-CAB-CBB
30	J	101	CLA	CAA-CBA-CGA-O2A
30	15	306	CLA	CAA-CBA-CGA-O2A
30	A	838	CLA	CBA-CGA-O2A-C1
30	3	305	CLA	CBA-CGA-O2A-C1
30	2	310	CLA	O1A-CGA-O2A-C1
30	B	824	CLA	C4-C3-C5-C6
30	B	826	CLA	C4-C3-C5-C6
30	12	303	CLA	C4-C3-C5-C6
30	12	312	CLA	C4-C3-C5-C6
30	A	816	CLA	C2-C3-C5-C6
30	6	305	CLA	C2-C3-C5-C6
34	A	852	LHG	O6-C4-C5-O7
33	A	848	BCR	C15-C16-C17-C18
38	2	314	KC1	C4B-C3B-CAB-CBB
38	3	308	KC1	C4B-C3B-CAB-CBB
38	3	311	KC1	C4B-C3B-CAB-CBB
38	4	307	KC1	C4B-C3B-CAB-CBB
38	5	306	KC1	C4B-C3B-CAB-CBB
38	5	312	KC1	C4B-C3B-CAB-CBB
38	6	311	KC1	C4B-C3B-CAB-CBB
38	6	313	KC1	C4B-C3B-CAB-CBB
38	8	306	KC1	C4B-C3B-CAB-CBB
38	8	314	KC1	C4B-C3B-CAB-CBB
38	9	304	KC1	C4B-C3B-CAB-CBB
38	9	310	KC1	C4B-C3B-CAB-CBB
38	9	312	KC1	C4B-C3B-CAB-CBB
38	10	306	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
38	11	307	KC1	C4B-C3B-CAB-CBB
38	11	312	KC1	C4B-C3B-CAB-CBB
38	12	305	KC1	C4B-C3B-CAB-CBB
38	12	309	KC1	C4B-C3B-CAB-CBB
38	13	308	KC1	C4B-C3B-CAB-CBB
38	13	312	KC1	C4B-C3B-CAB-CBB
38	14	311	KC1	C4B-C3B-CAB-CBB
38	16	304	KC1	C4B-C3B-CAB-CBB
35	16	315	LMT	C6-C7-C8-C9
30	10	311	CLA	O1D-CGD-O2D-CED
30	A	804	CLA	C11-C12-C13-C15
30	A	813	CLA	C6-C7-C8-C10
30	1	303	CLA	C12-C13-C15-C16
30	5	309	CLA	C11-C10-C8-C7
30	16	303	CLA	C12-C13-C15-C16
35	11	317	LMT	C5'-C4'-O1B-C1B
30	12	310	CLA	C8-C10-C11-C12
30	A	838	CLA	O1A-CGA-O2A-C1
30	2	311	CLA	O1A-CGA-O2A-C1
30	7	309	CLA	O1A-CGA-O2A-C1
36	3	317	LMG	C10-C11-C12-C13
34	A	853	LHG	C24-C23-O8-C6
29	A	801	CL0	CAA-CBA-CGA-O2A
30	A	835	CLA	C5-C6-C7-C8
30	A	837	CLA	C3A-C2A-CAA-CBA
30	B	812	CLA	C3A-C2A-CAA-CBA
30	B	851	CLA	C3A-C2A-CAA-CBA
30	4	304	CLA	C3A-C2A-CAA-CBA
30	6	307	CLA	C3A-C2A-CAA-CBA
30	14	302	CLA	C3A-C2A-CAA-CBA
30	15	304	CLA	C3A-C2A-CAA-CBA
30	B	830	CLA	C2-C3-C5-C6
30	F	202	CLA	C2-C3-C5-C6
36	6	301	LMG	C14-C15-C16-C17
30	1	304	CLA	C8-C10-C11-C12
33	L	204	BCR	C11-C10-C9-C34
37	2u	203	A86	C-C1-C2-C3
37	2u	203	A86	C4-C5-C6-C7
37	2u	205	A86	C-C1-C2-C3
37	2u	205	A86	C4-C5-C6-C7
37	3	314	A86	C-C1-C2-C3
37	4	314	A86	C-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
37	4	314	A86	C4-C5-C6-C7
37	7	319	A86	C-C1-C2-C3
37	7	319	A86	C4-C5-C6-C7
37	8	318	A86	C-C1-C2-C3
37	10	301	A86	C25-C26-C27-C28
37	11	301	A86	C-C1-C2-C3
37	11	301	A86	C4-C5-C6-C7
37	14	320	A86	C-C1-C2-C3
37	15	322	A86	C-C1-C2-C3
39	10	313	DD6	C9-C10-C11-C12
30	8	302	CLA	CBD-CGD-O2D-CED
30	A	832	CLA	C2-C1-O2A-CGA
30	A	835	CLA	C2-C1-O2A-CGA
30	6	317	CLA	C2-C1-O2A-CGA
30	7	311	CLA	C2-C1-O2A-CGA
30	15	304	CLA	C2-C1-O2A-CGA
37	3	314	A86	C24-C25-C26-C27
37	6	320	A86	C1-C2-C3-C4
37	9	315	A86	C1-C2-C3-C4
37	14	314	A86	C3-C4-C5-C6
39	9	314	DD6	C24-C25-C26-C27
30	3	302	CLA	C3-C5-C6-C7
35	A	854	LMT	C9-C10-C11-C12
36	5	318	LMG	C30-C31-C32-C33
30	13	304	CLA	CAA-CBA-CGA-O2A
30	15	306	CLA	CAA-CBA-CGA-O1A
30	B	819	CLA	C10-C11-C12-C13
30	A	810	CLA	C4-C3-C5-C6
30	2	304	CLA	C4-C3-C5-C6
30	12	310	CLA	C4-C3-C5-C6
30	14	307	CLA	C4-C3-C5-C6
30	6	306	CLA	CAA-CBA-CGA-O2A
30	11	310	CLA	C2-C3-C5-C6
30	A	803	CLA	C2A-CAA-CBA-CGA
30	B	827	CLA	C2A-CAA-CBA-CGA
30	15	302	CLA	C2A-CAA-CBA-CGA
30	J	101	CLA	CAA-CBA-CGA-O1A
30	A	825	CLA	C11-C12-C13-C14
30	A	826	CLA	O1D-CGD-O2D-CED
30	8	301	CLA	O1A-CGA-O2A-C1
36	7	320	LMG	C7-C8-C9-O8
37	3	315	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
37	4	314	A86	C12-C11-C13-O
37	12	316	A86	C12-C11-C13-O
37	15	317	A86	C12-C11-C13-O
30	9	306	CLA	CAA-CBA-CGA-O1A
30	A	805	CLA	C6-C7-C8-C9
30	3	302	CLA	C6-C7-C8-C9
30	3	305	CLA	C6-C7-C8-C9
30	5	311	CLA	C11-C10-C8-C9
35	A	854	LMT	O1'-C1-C2-C3
30	A	842	CLA	C13-C15-C16-C17
30	10	308	CLA	C15-C16-C17-C18
30	F	203	CLA	CAA-CBA-CGA-O2A
30	A	815	CLA	C13-C15-C16-C17
30	B	801	CLA	C5-C6-C7-C8
30	6	304	CLA	C10-C11-C12-C13
35	A	854	LMT	C3'-C4'-O1B-C1B
30	A	844	CLA	C16-C17-C18-C19
30	15	303	CLA	CAA-CBA-CGA-O2A
30	A	805	CLA	C2-C3-C5-C6
30	A	810	CLA	C2-C3-C5-C6
30	8	303	CLA	C2-C3-C5-C6
35	7	301	LMT	O5B-C1B-O1B-C4'
34	6	322	LHG	O1-C1-C2-O2
30	A	842	CLA	O1A-CGA-O2A-C1
30	2	305	CLA	C3-C5-C6-C7
30	9	306	CLA	CAA-CBA-CGA-O2A
30	2	308	CLA	C2A-CAA-CBA-CGA
30	8	301	CLA	C2A-CAA-CBA-CGA
30	12	304	CLA	CAA-CBA-CGA-O1A
30	16	302	CLA	C15-C16-C17-C18
38	3	308	KC1	CAA-CBA-CGA-O1A
30	A	802	CLA	C1A-C2A-CAA-CBA
30	A	814	CLA	C1A-C2A-CAA-CBA
30	A	817	CLA	C1A-C2A-CAA-CBA
30	B	820	CLA	C1A-C2A-CAA-CBA
30	B	825	CLA	C1A-C2A-CAA-CBA
30	1	303	CLA	C1A-C2A-CAA-CBA
30	4	309	CLA	C1A-C2A-CAA-CBA
30	15	310	CLA	C1A-C2A-CAA-CBA
33	A	847	BCR	C11-C10-C9-C8
33	A	849	BCR	C11-C10-C9-C8
33	B	842	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
37	2u	203	A86	C24-C1-C2-C3
37	2u	203	A86	C4-C5-C6-C8
37	2u	205	A86	C24-C1-C2-C3
37	2u	205	A86	C4-C5-C6-C8
37	3	314	A86	C24-C1-C2-C3
37	3	315	A86	C10-C11-C13-O
37	4	314	A86	C24-C1-C2-C3
37	4	314	A86	C4-C5-C6-C8
37	7	319	A86	C24-C1-C2-C3
37	7	319	A86	C4-C5-C6-C8
37	10	301	A86	C25-C26-C27-C29
37	11	301	A86	C24-C1-C2-C3
37	11	301	A86	C4-C5-C6-C8
37	12	316	A86	C10-C11-C13-O
37	13	315	A86	C10-C11-C13-O
37	14	320	A86	C24-C1-C2-C3
37	15	321	A86	C10-C11-C13-O
37	15	322	A86	C24-C1-C2-C3
37	15	323	A86	C10-C11-C13-O
39	3	312	DD6	C24-C1-C2-C3
39	5	313	DD6	C24-C1-C2-C3
35	1	311	LMT	C5-C6-C7-C8
30	A	810	CLA	C2B-C3B-CAB-CBB
30	A	817	CLA	C2B-C3B-CAB-CBB
30	A	825	CLA	C2B-C3B-CAB-CBB
30	A	828	CLA	C2B-C3B-CAB-CBB
30	A	839	CLA	C2B-C3B-CAB-CBB
30	A	844	CLA	C2B-C3B-CAB-CBB
30	B	803	CLA	C2B-C3B-CAB-CBB
30	B	805	CLA	C2B-C3B-CAB-CBB
30	B	808	CLA	C2B-C3B-CAB-CBB
30	B	823	CLA	C2B-C3B-CAB-CBB
30	J	101	CLA	C2B-C3B-CAB-CBB
30	2u	202	CLA	C2B-C3B-CAB-CBB
30	1	303	CLA	C2B-C3B-CAB-CBB
30	2	305	CLA	C2B-C3B-CAB-CBB
30	2	313	CLA	C2B-C3B-CAB-CBB
30	3	302	CLA	C2B-C3B-CAB-CBB
30	3	309	CLA	C2B-C3B-CAB-CBB
30	4	309	CLA	C2B-C3B-CAB-CBB
30	5	311	CLA	C2B-C3B-CAB-CBB
30	6	304	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	6	309	CLA	C2B-C3B-CAB-CBB
30	6	317	CLA	C2B-C3B-CAB-CBB
30	7	304	CLA	C2B-C3B-CAB-CBB
30	7	311	CLA	C2B-C3B-CAB-CBB
30	10	309	CLA	C2B-C3B-CAB-CBB
30	11	308	CLA	C2B-C3B-CAB-CBB
30	12	304	CLA	C2B-C3B-CAB-CBB
30	12	307	CLA	C2B-C3B-CAB-CBB
30	13	303	CLA	C2B-C3B-CAB-CBB
30	13	304	CLA	C2B-C3B-CAB-CBB
30	14	303	CLA	C2B-C3B-CAB-CBB
30	14	304	CLA	C2B-C3B-CAB-CBB
30	15	302	CLA	C2B-C3B-CAB-CBB
30	15	306	CLA	C2B-C3B-CAB-CBB
30	16	306	CLA	C2B-C3B-CAB-CBB
30	16	307	CLA	C2B-C3B-CAB-CBB
30	16	308	CLA	C2B-C3B-CAB-CBB
33	A	847	BCR	C5-C6-C7-C8
33	A	848	BCR	C5-C6-C7-C8
33	A	848	BCR	C23-C24-C25-C30
33	A	849	BCR	C5-C6-C7-C8
33	A	850	BCR	C5-C6-C7-C8
33	A	850	BCR	C23-C24-C25-C26
33	A	851	BCR	C5-C6-C7-C8
33	A	851	BCR	C23-C24-C25-C26
33	A	851	BCR	C23-C24-C25-C30
33	B	841	BCR	C1-C6-C7-C8
33	B	841	BCR	C5-C6-C7-C8
33	B	841	BCR	C23-C24-C25-C26
33	B	842	BCR	C5-C6-C7-C8
33	B	843	BCR	C5-C6-C7-C8
33	B	844	BCR	C1-C6-C7-C8
33	B	844	BCR	C23-C24-C25-C26
33	B	845	BCR	C1-C6-C7-C8
33	B	846	BCR	C5-C6-C7-C8
33	B	846	BCR	C23-C24-C25-C26
33	F	204	BCR	C1-C6-C7-C8
33	J	103	BCR	C5-C6-C7-C8
33	L	201	BCR	C1-C6-C7-C8
33	L	201	BCR	C23-C24-C25-C26
33	L	204	BCR	C1-C6-C7-C8
33	L	205	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	L	205	BCR	C23-C24-C25-C30
33	M	101	BCR	C5-C6-C7-C8
33	M	101	BCR	C23-C24-C25-C30
30	2	310	CLA	CBA-CGA-O2A-C1
30	2	311	CLA	CBA-CGA-O2A-C1
30	7	309	CLA	CBA-CGA-O2A-C1
36	A	856	LMG	C32-C33-C34-C35
30	2	305	CLA	C4-C3-C5-C6
30	5	307	CLA	C4-C3-C5-C6
30	B	826	CLA	C2-C3-C5-C6
30	12	310	CLA	C2-C3-C5-C6
35	11	318	LMT	O5B-C1B-O1B-C4'
30	F	203	CLA	CAA-CBA-CGA-O1A
30	15	310	CLA	CAA-CBA-CGA-O2A
34	A	852	LHG	C34-C35-C36-C37
30	A	812	CLA	C6-C7-C8-C10
30	5	302	CLA	C11-C10-C8-C7
30	15	304	CLA	C11-C10-C8-C7
31	A	845	PQN	C17-C18-C20-C21
36	2u	204	LMG	O7-C8-C9-O8
35	12	301	LMT	O1'-C1-C2-C3
30	A	816	CLA	C16-C17-C18-C20
33	B	841	BCR	C36-C18-C19-C20
33	L	201	BCR	C11-C12-C13-C35
30	11	308	CLA	C4-C3-C5-C6
30	B	828	CLA	C8-C10-C11-C12
30	B	835	CLA	C5-C6-C7-C8
30	2	304	CLA	C2-C3-C5-C6
30	5	307	CLA	C2-C3-C5-C6
30	12	303	CLA	C2-C3-C5-C6
30	12	312	CLA	C2-C3-C5-C6
30	14	307	CLA	C2-C3-C5-C6
30	12	304	CLA	C2-C1-O2A-CGA
30	B	808	CLA	C8-C10-C11-C12
37	4	312	A86	C5-C6-C8-C9
38	12	311	KC1	CAA-CBA-CGA-O1A
38	14	306	KC1	C2C-C3C-CAC-CBC
30	A	842	CLA	CBA-CGA-O2A-C1
30	A	844	CLA	C2A-CAA-CBA-CGA
30	3	310	CLA	CAA-CBA-CGA-O2A
30	13	304	CLA	CAA-CBA-CGA-O1A
30	A	812	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	A	816	CLA	C6-C7-C8-C9
33	A	849	BCR	C19-C20-C21-C22
37	10	317	A86	C11-C10-C9-C8
39	13	314	DD6	C24-C25-C26-C27
30	B	825	CLA	C5-C6-C7-C8
30	9	305	CLA	C13-C15-C16-C17
30	5	311	CLA	C10-C11-C12-C13
33	M	101	BCR	C22-C23-C24-C25
30	B	808	CLA	C4-C3-C5-C6
30	B	812	CLA	C4-C3-C5-C6
30	8	308	CLA	C4-C3-C5-C6
30	9	308	CLA	C4-C3-C5-C6
34	9	318	LHG	C5-C4-O6-P
30	B	808	CLA	C2-C3-C5-C6
30	1	303	CLA	C2-C3-C5-C6
30	8	308	CLA	C2-C3-C5-C6
30	6	314	CLA	CBD-CGD-O2D-CED
30	10	305	CLA	O1A-CGA-O2A-C1
30	A	829	CLA	C16-C17-C18-C19
30	14	312	CLA	CAA-CBA-CGA-O2A
37	10	317	A86	C35-C34-O4-C38
30	6	314	CLA	C10-C11-C12-C13
30	15	310	CLA	CAA-CBA-CGA-O1A
38	1	306	KC1	O1D-CGD-O2D-CED
30	B	822	CLA	C2A-CAA-CBA-CGA
30	9	306	CLA	C2A-CAA-CBA-CGA
30	12	304	CLA	C13-C15-C16-C17
30	14	307	CLA	C8-C10-C11-C12
30	B	829	CLA	C4-C3-C5-C6
30	4	303	CLA	C4-C3-C5-C6
30	7	309	CLA	C4-C3-C5-C6
30	13	307	CLA	C4-C3-C5-C6
39	2	317	DD6	C24-C25-C26-C27
30	14	309	CLA	CAA-CBA-CGA-O2A
30	B	826	CLA	C15-C16-C17-C18
30	B	814	CLA	CBD-CGD-O2D-CED
30	A	817	CLA	C4B-C3B-CAB-CBB
30	B	804	CLA	C4B-C3B-CAB-CBB
30	B	811	CLA	C4B-C3B-CAB-CBB
30	1	305	CLA	C4B-C3B-CAB-CBB
30	2	303	CLA	C4B-C3B-CAB-CBB
30	6	314	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	12	304	CLA	C4B-C3B-CAB-CBB
30	16	307	CLA	C4B-C3B-CAB-CBB
30	16	306	CLA	O1D-CGD-O2D-CED
38	3	308	KC1	CAA-CBA-CGA-O2A
35	12	318	LMT	C4-C5-C6-C7
30	13	309	CLA	CAA-CBA-CGA-O2A
30	15	305	CLA	CAA-CBA-CGA-O1A
30	B	832	CLA	C16-C17-C18-C20
30	B	829	CLA	C13-C15-C16-C17
33	A	847	BCR	C35-C13-C14-C15
33	B	842	BCR	C11-C10-C9-C34
33	B	845	BCR	C20-C21-C22-C37
39	4	313	DD6	C4-C5-C6-C7
39	6	319	DD6	C4-C5-C6-C7
30	2	304	CLA	C5-C6-C7-C8
30	5	302	CLA	C10-C11-C12-C13
30	B	823	CLA	C4-C3-C5-C6
30	B	825	CLA	C4-C3-C5-C6
30	B	832	CLA	C4-C3-C5-C6
30	7	303	CLA	C15-C16-C17-C18
30	15	311	CLA	CAA-CBA-CGA-O2A
36	8	320	LMG	O6-C1-O1-C7
30	15	307	CLA	O1D-CGD-O2D-CED
30	1	301	CLA	C8-C10-C11-C12
30	A	844	CLA	C11-C12-C13-C15
30	2	313	CLA	CAA-CBA-CGA-O2A
30	16	308	CLA	CAA-CBA-CGA-O2A
30	B	805	CLA	C8-C10-C11-C12
30	3	310	CLA	CAA-CBA-CGA-O1A
30	A	820	CLA	C11-C12-C13-C14
30	A	829	CLA	C14-C13-C15-C16
30	A	831	CLA	C6-C7-C8-C9
30	B	826	CLA	C6-C7-C8-C9
30	B	838	CLA	C6-C7-C8-C9
30	F	201	CLA	C6-C7-C8-C9
30	3	307	CLA	C6-C7-C8-C9
31	B	840	PQN	C21-C22-C23-C24
36	B	847	LMG	C35-C36-C37-C38
36	A	856	LMG	O8-C28-C29-C30
30	13	309	CLA	CAA-CBA-CGA-O1A
30	16	310	CLA	CAA-CBA-CGA-O2A
30	6	310	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	B	805	CLA	C2-C1-O2A-CGA
30	B	811	CLA	C2-C1-O2A-CGA
30	B	812	CLA	C2-C1-O2A-CGA
30	B	821	CLA	C2-C1-O2A-CGA
30	L	202	CLA	C2-C1-O2A-CGA
30	2	307	CLA	C2-C1-O2A-CGA
30	3	307	CLA	C2-C1-O2A-CGA
30	7	305	CLA	C2-C1-O2A-CGA
30	A	826	CLA	C16-C17-C18-C19
30	B	813	CLA	C16-C17-C18-C19
30	6	317	CLA	C10-C11-C12-C13
30	A	840	CLA	O1D-CGD-O2D-CED
30	5	307	CLA	CBA-CGA-O2A-C1
30	A	812	CLA	C3A-C2A-CAA-CBA
30	A	818	CLA	C3A-C2A-CAA-CBA
30	B	802	CLA	C3A-C2A-CAA-CBA
30	B	803	CLA	C3A-C2A-CAA-CBA
30	2u	202	CLA	C4-C3-C5-C6
30	6	306	CLA	C3A-C2A-CAA-CBA
30	6	309	CLA	C3A-C2A-CAA-CBA
30	12	312	CLA	C3A-C2A-CAA-CBA
30	15	310	CLA	C3A-C2A-CAA-CBA
30	A	837	CLA	CAA-CBA-CGA-O2A
30	14	304	CLA	CAA-CBA-CGA-O2A
38	7	308	KC1	C2B-C3B-CAB-CBB
38	14	308	KC1	C2B-C3B-CAB-CBB
30	13	307	CLA	C3-C5-C6-C7
34	B	848	LHG	C4-C5-O7-C7
34	B	848	LHG	C6-C5-O7-C7
30	14	309	CLA	CAA-CBA-CGA-O1A
30	A	830	CLA	CAA-CBA-CGA-O2A
29	A	801	CL0	C16-C17-C18-C19
30	14	312	CLA	CAA-CBA-CGA-O1A
38	8	310	KC1	CAA-CBA-CGA-O2A
30	A	837	CLA	CAA-CBA-CGA-O1A
30	15	311	CLA	CAA-CBA-CGA-O1A
30	16	310	CLA	CAA-CBA-CGA-O1A
30	B	813	CLA	C2C-C3C-CAC-CBC
30	B	808	CLA	C15-C16-C17-C18
39	7	314	DD6	C13-C14-C15-O1
39	9	314	DD6	C13-C14-C15-O1
30	2	313	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	14	304	CLA	CAA-CBA-CGA-O1A
36	8	319	LMG	C37-C38-C39-C40
38	8	307	KC1	O1D-CGD-O2D-CED
34	A	852	LHG	C4-C5-C6-O8
30	A	833	CLA	CBD-CGD-O2D-CED
30	B	831	CLA	O1A-CGA-O2A-C1
30	10	303	CLA	C8-C10-C11-C12
38	1	308	KC1	C4B-C3B-CAB-CBB
38	11	311	KC1	C4B-C3B-CAB-CBB
38	12	305	KC1	CAA-CBA-CGA-O1A
38	12	305	KC1	CAA-CBA-CGA-O2A
30	1	307	CLA	C4-C3-C5-C6
30	2	301	CLA	C2A-CAA-CBA-CGA
30	15	312	CLA	CBD-CGD-O2D-CED
39	1	310	DD6	C24-C25-C26-C27
39	4	313	DD6	C1-C2-C3-C4
37	12	316	A86	C28-C27-C29-C30
37	14	317	A86	C28-C27-C29-C30
37	15	323	A86	C28-C27-C29-C30
30	A	830	CLA	C3-C5-C6-C7
30	B	813	CLA	C4C-C3C-CAC-CBC
30	A	810	CLA	C10-C11-C12-C13
30	10	309	CLA	C10-C11-C12-C13
36	3	317	LMG	C31-C32-C33-C34
30	A	803	CLA	CBA-CGA-O2A-C1
30	10	309	CLA	CBD-CGD-O2D-CED
30	1	301	CLA	O1D-CGD-O2D-CED
30	A	802	CLA	C6-C7-C8-C9
30	A	812	CLA	C6-C7-C8-C9
30	A	816	CLA	C11-C10-C8-C9
30	A	839	CLA	C14-C13-C15-C16
30	B	826	CLA	C14-C13-C15-C16
30	2u	202	CLA	C6-C7-C8-C9
30	16	303	CLA	C14-C13-C15-C16
30	B	832	CLA	C16-C17-C18-C19
30	B	821	CLA	CAA-CBA-CGA-O2A
30	2	308	CLA	CAA-CBA-CGA-O2A
37	10	317	A86	C33-C34-O4-C38
30	16	308	CLA	CAA-CBA-CGA-O1A
38	12	311	KC1	CAA-CBA-CGA-O2A
39	4	313	DD6	C2-C1-C24-C25
37	2u	203	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
37	1	309	A86	C13-C14-C15-O1
37	8	315	A86	C13-C14-C15-O1
37	10	301	A86	C13-C14-C15-O1
37	11	315	A86	C13-C14-C15-O1
37	13	313	A86	C13-C14-C15-O1
37	13	315	A86	C13-C14-C15-O1
37	14	319	A86	C13-C14-C15-O1
37	15	315	A86	C13-C14-C15-O1
30	5	307	CLA	O1A-CGA-O2A-C1
30	B	812	CLA	C2-C3-C5-C6
30	L	202	CLA	C2A-CAA-CBA-CGA
30	A	809	CLA	C6-C7-C8-C10
30	A	812	CLA	C11-C12-C13-C15
30	A	816	CLA	C12-C13-C15-C16
30	A	826	CLA	C11-C10-C8-C7
30	A	827	CLA	C12-C13-C15-C16
30	B	825	CLA	C12-C13-C15-C16
30	B	826	CLA	C6-C7-C8-C10
30	3	302	CLA	C6-C7-C8-C10
30	3	307	CLA	C6-C7-C8-C10
30	5	304	CLA	C11-C12-C13-C15
30	5	308	CLA	C12-C13-C15-C16
30	5	311	CLA	C11-C10-C8-C7
30	8	301	CLA	C12-C13-C15-C16
30	10	308	CLA	C11-C10-C8-C7
30	12	304	CLA	C11-C12-C13-C15
30	13	302	CLA	C11-C12-C13-C15
30	B	826	CLA	C8-C10-C11-C12
30	A	811	CLA	C2B-C3B-CAB-CBB
30	A	820	CLA	C2B-C3B-CAB-CBB
30	B	813	CLA	C2B-C3B-CAB-CBB
30	B	825	CLA	C2B-C3B-CAB-CBB
30	B	826	CLA	C2B-C3B-CAB-CBB
30	B	832	CLA	C2B-C3B-CAB-CBB
30	3	301	CLA	C2B-C3B-CAB-CBB
30	5	308	CLA	C2B-C3B-CAB-CBB
30	6	316	CLA	C2B-C3B-CAB-CBB
30	9	309	CLA	C2B-C3B-CAB-CBB
30	12	302	CLA	C2B-C3B-CAB-CBB
33	B	843	BCR	C23-C24-C25-C26
33	B	844	BCR	C5-C6-C7-C8
33	B	845	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	F	204	BCR	C5-C6-C7-C8
33	I	101	BCR	C1-C6-C7-C8
33	I	101	BCR	C5-C6-C7-C8
33	L	201	BCR	C5-C6-C7-C8
33	L	204	BCR	C5-C6-C7-C8
33	L	205	BCR	C23-C24-C25-C26
33	M	101	BCR	C23-C24-C25-C26
30	A	814	CLA	CAA-CBA-CGA-O2A
30	B	813	CLA	CAA-CBA-CGA-O2A
30	A	805	CLA	C2-C1-O2A-CGA
30	A	831	CLA	C2-C1-O2A-CGA
30	4	303	CLA	C2-C1-O2A-CGA
30	5	311	CLA	C2-C1-O2A-CGA
30	6	307	CLA	C2-C1-O2A-CGA
30	6	314	CLA	C2-C1-O2A-CGA
30	9	301	CLA	C2-C1-O2A-CGA
30	9	302	CLA	C2-C1-O2A-CGA
30	12	310	CLA	C2-C1-O2A-CGA
30	16	301	CLA	C2-C1-O2A-CGA
30	9	301	CLA	C16-C17-C18-C20
39	7	314	DD6	C11-C13-C14-C15
39	10	313	DD6	C11-C13-C14-C15
39	12	317	DD6	C11-C13-C14-C15
39	13	314	DD6	C11-C13-C14-C15
39	16	313	DD6	C11-C13-C14-C15
30	11	310	CLA	CAA-CBA-CGA-O2A
36	B	847	LMG	O7-C10-C11-C12
38	8	310	KC1	CAA-CBA-CGA-O1A
30	A	841	CLA	C8-C10-C11-C12
30	2	303	CLA	CAA-CBA-CGA-O2A
34	A	853	LHG	O9-C7-O7-C5
30	B	830	CLA	CAA-CBA-CGA-O2A
30	7	312	CLA	CAA-CBA-CGA-O2A
34	A	852	LHG	O8-C23-C24-C25
30	2	305	CLA	C13-C15-C16-C17
30	15	305	CLA	CAA-CBA-CGA-O2A
30	2	304	CLA	C15-C16-C17-C18
30	4	309	CLA	C5-C6-C7-C8
30	6	317	CLA	C8-C10-C11-C12
30	10	307	CLA	CAA-CBA-CGA-O2A
35	15	301	LMT	C5'-C4'-O1B-C1B
38	16	311	KC1	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	A	826	CLA	C15-C16-C17-C18
30	A	806	CLA	CAA-CBA-CGA-O2A
30	A	828	CLA	CAA-CBA-CGA-O2A
30	B	809	CLA	CAA-CBA-CGA-O2A
30	11	306	CLA	CAA-CBA-CGA-O2A
39	11	313	DD6	C9-C10-C11-C12
30	B	838	CLA	C2A-CAA-CBA-CGA
30	B	803	CLA	CAA-CBA-CGA-O2A
30	1	303	CLA	CAA-CBA-CGA-O2A
30	A	839	CLA	C5-C6-C7-C8
30	7	311	CLA	C5-C6-C7-C8
30	10	311	CLA	CAA-CBA-CGA-O2A
30	A	828	CLA	C6-C7-C8-C9
30	A	834	CLA	C11-C12-C13-C14
30	B	813	CLA	C11-C10-C8-C9
30	B	825	CLA	C14-C13-C15-C16
30	9	307	CLA	C6-C7-C8-C9
30	9	309	CLA	C14-C13-C15-C16
35	1	311	LMT	C5'-C4'-O1B-C1B
36	B	847	LMG	C20-C21-C22-C23
30	2u	202	CLA	CAA-CBA-CGA-O2A
30	12	308	CLA	CAA-CBA-CGA-O2A
30	12	302	CLA	C5-C6-C7-C8
30	A	819	CLA	C4B-C3B-CAB-CBB
30	A	820	CLA	C4B-C3B-CAB-CBB
30	B	817	CLA	C4B-C3B-CAB-CBB
30	B	825	CLA	C4B-C3B-CAB-CBB
30	B	851	CLA	C1A-C2A-CAA-CBA
30	4	303	CLA	C4B-C3B-CAB-CBB
30	6	307	CLA	C1A-C2A-CAA-CBA
30	8	308	CLA	C4B-C3B-CAB-CBB
30	9	302	CLA	C4B-C3B-CAB-CBB
30	11	308	CLA	C4B-C3B-CAB-CBB
30	12	306	CLA	C4B-C3B-CAB-CBB
30	14	309	CLA	C1A-C2A-CAA-CBA
30	15	304	CLA	C4B-C3B-CAB-CBB
30	16	306	CLA	C4B-C3B-CAB-CBB
37	1	309	A86	O-C13-C14-C15
37	3	314	A86	O-C13-C14-C15
37	10	317	A86	O-C13-C14-C15
37	11	316	A86	O-C13-C14-C15
37	14	314	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	A	844	CLA	C15-C16-C17-C18
30	B	804	CLA	CAA-CBA-CGA-O2A
30	1	301	CLA	CAA-CBA-CGA-O2A
30	3	305	CLA	CAA-CBA-CGA-O2A
30	16	306	CLA	CAA-CBA-CGA-O2A
30	2	305	CLA	C2-C3-C5-C6
36	3	317	LMG	O1-C7-C8-O7
37	3	314	A86	C5-C6-C8-C9
39	2	316	DD6	C2-C1-C24-C25
39	2	316	DD6	C10-C11-C13-C14
39	9	314	DD6	C5-C6-C8-C9
37	2u	203	A86	C3-C4-C5-C6
39	6	321	DD6	C24-C25-C26-C27
30	2	301	CLA	C13-C15-C16-C17
30	F	202	CLA	O1A-CGA-O2A-C1
30	16	301	CLA	CBA-CGA-O2A-C1
30	15	308	CLA	CAA-CBA-CGA-O2A
30	1	307	CLA	CAA-CBA-CGA-O2A
30	16	301	CLA	CAA-CBA-CGA-O2A
36	5	318	LMG	O8-C28-C29-C30
30	A	843	CLA	C2A-CAA-CBA-CGA
30	B	807	CLA	C2A-CAA-CBA-CGA
30	B	817	CLA	CAA-CBA-CGA-O1A
30	A	833	CLA	O1D-CGD-O2D-CED
30	B	807	CLA	CAA-CBA-CGA-O2A
30	6	316	CLA	CAA-CBA-CGA-O2A
30	13	301	CLA	CAA-CBA-CGA-O2A
30	16	303	CLA	C5-C6-C7-C8
34	A	852	LHG	C33-C34-C35-C36
30	2	311	CLA	C4-C3-C5-C6
30	A	813	CLA	C2-C1-O2A-CGA
30	A	843	CLA	C2-C1-O2A-CGA
30	B	814	CLA	C2-C1-O2A-CGA
30	4	306	CLA	C2-C1-O2A-CGA
30	5	309	CLA	C2-C1-O2A-CGA
30	7	303	CLA	C2-C1-O2A-CGA
30	7	306	CLA	C2-C1-O2A-CGA
30	9	309	CLA	C2-C1-O2A-CGA
30	4	301	CLA	CAA-CBA-CGA-O2A
30	8	301	CLA	CAA-CBA-CGA-O2A
30	A	807	CLA	C12-C13-C15-C16
30	F	202	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	1	307	CLA	C11-C12-C13-C15
30	2	309	CLA	C6-C7-C8-C10
30	9	308	CLA	C2-C3-C5-C6
30	1	305	CLA	C10-C11-C12-C13
30	7	306	CLA	C16-C17-C18-C20
36	8	319	LMG	O9-C10-C11-C12
30	3	302	CLA	O1A-CGA-O2A-C1
30	B	839	CLA	CAA-CBA-CGA-O2A
30	A	809	CLA	C10-C11-C12-C13
30	A	842	CLA	C5-C6-C7-C8
30	12	303	CLA	C15-C16-C17-C18
30	6	314	CLA	O1D-CGD-O2D-CED
30	B	831	CLA	CBA-CGA-O2A-C1
37	14	320	A86	C24-C25-C26-C27
30	A	814	CLA	C2A-CAA-CBA-CGA
30	9	303	CLA	C13-C15-C16-C17
30	7	307	CLA	C16-C17-C18-C19
34	B	848	LHG	O8-C23-C24-C25
35	A	854	LMT	C4-C5-C6-C7
30	2	301	CLA	C5-C6-C7-C8
30	A	802	CLA	C4-C3-C5-C6
30	A	810	CLA	C3A-C2A-CAA-CBA
30	8	305	CLA	C3A-C2A-CAA-CBA
30	B	809	CLA	CAA-CBA-CGA-O1A
30	6	314	CLA	O1A-CGA-O2A-C1
33	A	848	BCR	C16-C17-C18-C19
39	9	314	DD6	C4-C5-C6-C8
30	11	310	CLA	CAA-CBA-CGA-O1A
30	B	851	CLA	O1A-CGA-O2A-C1
30	A	808	CLA	CAA-CBA-CGA-O2A
30	B	835	CLA	CAA-CBA-CGA-O2A
30	B	813	CLA	CAA-CBA-CGA-O1A
30	7	312	CLA	CAA-CBA-CGA-O1A
30	L	203	CLA	CAA-CBA-CGA-O1A
30	A	829	CLA	C6-C7-C8-C9
30	1	307	CLA	C11-C12-C13-C14
30	5	302	CLA	C11-C10-C8-C9
30	5	308	CLA	C14-C13-C15-C16
30	13	302	CLA	C11-C12-C13-C14
31	A	845	PQN	C19-C18-C20-C21
35	8	322	LMT	C6-C7-C8-C9
30	10	307	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	13	301	CLA	CAA-CBA-CGA-O1A
37	15	321	A86	C1-C2-C3-C4
36	2u	204	LMG	C4-C5-C6-O5
34	9	318	LHG	C10-C11-C12-C13
30	7	307	CLA	C16-C17-C18-C20
30	B	821	CLA	CAA-CBA-CGA-O1A
30	1	303	CLA	CAA-CBA-CGA-O1A
36	B	847	LMG	C24-C25-C26-C27
30	B	825	CLA	C2-C3-C5-C6
37	7	315	A86	C26-C27-C29-C30
37	12	316	A86	C26-C27-C29-C30
37	15	323	A86	C26-C27-C29-C30
38	2	312	KC1	C3A-C2A-CAA-CBA
38	2	314	KC1	C3A-C2A-CAA-CBA
38	3	311	KC1	C3A-C2A-CAA-CBA
38	5	312	KC1	C3A-C2A-CAA-CBA
38	8	310	KC1	C3A-C2A-CAA-CBA
38	11	312	KC1	C3A-C2A-CAA-CBA
38	12	309	KC1	C1A-C2A-CAA-CBA
38	13	306	KC1	C3A-C2A-CAA-CBA
38	13	312	KC1	C1A-C2A-CAA-CBA
39	7	318	DD6	C13-C14-C15-C16
30	10	311	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	CAA-CBA-CGA-O1A
30	2	303	CLA	CAA-CBA-CGA-O1A
30	11	306	CLA	CAA-CBA-CGA-O1A
30	12	308	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	O1D-CGD-O2D-CED
36	B	847	LMG	C41-C42-C43-C44
30	14	302	CLA	C8-C10-C11-C12
35	9	317	LMT	C4-C5-C6-C7
30	10	303	CLA	CAA-CBA-CGA-O2A
30	A	844	CLA	C16-C17-C18-C20
30	2u	202	CLA	C8-C10-C11-C12
37	2	318	A86	C5-C6-C8-C9
37	11	301	A86	C2-C1-C24-C25
39	6	318	DD6	C5-C6-C8-C9
30	A	806	CLA	CAA-CBA-CGA-O1A
30	A	814	CLA	CAA-CBA-CGA-O1A
30	1	301	CLA	CAA-CBA-CGA-O1A
34	A	852	LHG	O10-C23-C24-C25
30	2	307	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	B	803	CLA	CAA-CBA-CGA-O1A
30	2	308	CLA	CAA-CBA-CGA-O1A
30	6	316	CLA	CAA-CBA-CGA-O1A
30	2	301	CLA	CAA-CBA-CGA-O2A
36	8	319	LMG	O7-C10-C11-C12
36	B	849	LMG	C33-C34-C35-C36
30	15	312	CLA	O1D-CGD-O2D-CED
36	5	318	LMG	C7-C8-C9-O8
37	2	319	A86	C12-C11-C13-O
37	3	314	A86	C12-C11-C13-O
37	4	312	A86	C12-C11-C13-O
37	12	314	A86	C12-C11-C13-O
37	14	318	A86	C12-C11-C13-O
37	15	322	A86	C12-C11-C13-O
37	15	323	A86	C12-C11-C13-O
38	16	311	KC1	C2C-C3C-CAC-CBC
30	11	310	CLA	C13-C15-C16-C17
31	B	840	PQN	C18-C20-C21-C22
30	A	813	CLA	CAA-CBA-CGA-O2A
38	10	312	KC1	C2B-C3B-CAB-CBB
30	1	304	CLA	C3-C5-C6-C7
35	A	854	LMT	C4'-C5'-C6'-O6'
30	B	830	CLA	CAA-CBA-CGA-O1A
30	16	306	CLA	CAA-CBA-CGA-O1A
36	5	318	LMG	O10-C28-C29-C30
30	A	808	CLA	CAD-CBD-CGD-O2D
30	A	812	CLA	CAD-CBD-CGD-O2D
30	A	815	CLA	CAD-CBD-CGD-O2D
30	B	805	CLA	CAD-CBD-CGD-O2D
30	B	837	CLA	CAD-CBD-CGD-O2D
30	4	305	CLA	CAD-CBD-CGD-O2D
30	4	306	CLA	CAD-CBD-CGD-O2D
30	5	307	CLA	CAD-CBD-CGD-O2D
30	6	306	CLA	CAD-CBD-CGD-O2D
30	6	309	CLA	CAD-CBD-CGD-O2D
30	8	303	CLA	CAD-CBD-CGD-O2D
30	9	305	CLA	CAD-CBD-CGD-O2D
30	10	307	CLA	CAD-CBD-CGD-O2D
37	2u	205	A86	C13-C14-C15-C20
37	7	315	A86	C13-C14-C15-C20
37	15	315	A86	C13-C14-C15-C20
37	15	320	A86	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
37	16	312	A86	C13-C14-C15-C20
38	11	305	KC1	CAD-CBD-CGD-O2D
38	14	311	KC1	CAD-CBD-CGD-O2D
38	16	304	KC1	CAD-CBD-CGD-O2D
30	2	305	CLA	CAA-CBA-CGA-O2A
30	2u	202	CLA	CAA-CBA-CGA-O1A
30	15	304	CLA	C2C-C3C-CAC-CBC
30	A	809	CLA	C2-C1-O2A-CGA
30	A	810	CLA	C2-C1-O2A-CGA
30	A	818	CLA	C2-C1-O2A-CGA
30	B	829	CLA	C2-C1-O2A-CGA
30	6	309	CLA	C2-C1-O2A-CGA
30	16	306	CLA	C2-C1-O2A-CGA
30	A	828	CLA	CAA-CBA-CGA-O1A
30	3	303	CLA	CAA-CBA-CGA-O2A
30	15	304	CLA	C4C-C3C-CAC-CBC
30	A	808	CLA	CAA-CBA-CGA-O1A
30	1	307	CLA	CAA-CBA-CGA-O1A
30	16	301	CLA	CAA-CBA-CGA-O1A
36	7	320	LMG	O9-C10-C11-C12
30	F	202	CLA	CBA-CGA-O2A-C1
30	A	841	CLA	CAA-CBA-CGA-O2A
30	B	812	CLA	CAA-CBA-CGA-O2A
30	B	836	CLA	CAA-CBA-CGA-O2A
36	6	301	LMG	O7-C10-C11-C12
34	A	852	LHG	C16-C17-C18-C19
30	A	816	CLA	CAA-CBA-CGA-O2A
30	8	305	CLA	CAA-CBA-CGA-O2A
30	10	309	CLA	CAA-CBA-CGA-O2A
36	2u	204	LMG	O8-C28-C29-C30
30	6	314	CLA	CBA-CGA-O2A-C1
30	16	301	CLA	O1A-CGA-O2A-C1
30	7	303	CLA	C13-C15-C16-C17
30	B	807	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

229 monomers are involved in 407 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	8	303	CLA	2	0
30	2	310	CLA	2	0
35	11	318	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	835	CLA	4	0
30	14	302	CLA	2	0
29	A	801	CL0	3	0
30	A	837	CLA	1	0
35	11	317	LMT	2	0
30	8	302	CLA	1	0
30	L	203	CLA	2	0
30	4	305	CLA	1	0
30	B	809	CLA	6	0
30	J	101	CLA	1	0
38	3	304	KC1	1	0
38	5	312	KC1	1	0
30	7	304	CLA	1	0
35	12	320	LMT	1	0
30	A	832	CLA	1	0
30	14	305	CLA	1	0
30	14	312	CLA	1	0
36	B	849	LMG	1	0
33	A	847	BCR	2	0
30	7	309	CLA	6	0
37	5	315	A86	1	0
30	A	817	CLA	3	0
30	11	309	CLA	1	0
30	16	302	CLA	1	0
30	3	302	CLA	1	0
30	3	310	CLA	2	0
30	12	302	CLA	1	0
33	B	844	BCR	2	0
30	B	833	CLA	1	0
30	2	308	CLA	1	0
33	L	204	BCR	4	0
30	A	843	CLA	2	0
30	12	312	CLA	1	0
36	3	317	LMG	2	0
30	A	829	CLA	7	0
36	14	321	LMG	2	0
30	15	307	CLA	1	0
30	2	303	CLA	4	0
30	15	302	CLA	4	0
30	8	305	CLA	2	0
30	A	809	CLA	1	0
30	B	803	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	7	307	CLA	2	0
30	F	201	CLA	4	0
30	12	321	CLA	2	0
30	A	833	CLA	6	0
30	6	316	CLA	3	0
30	L	202	CLA	4	0
30	B	813	CLA	7	0
30	2	307	CLA	2	0
30	B	823	CLA	1	0
30	2u	202	CLA	3	0
35	7	301	LMT	1	0
39	10	313	DD6	1	0
30	9	301	CLA	1	0
30	15	309	CLA	2	0
35	A	857	LMT	1	0
30	10	303	CLA	3	0
30	A	834	CLA	2	0
30	16	309	CLA	1	0
37	14	320	A86	1	0
30	A	816	CLA	4	0
39	13	314	DD6	1	0
30	4	301	CLA	3	0
30	A	811	CLA	3	0
30	B	839	CLA	1	0
30	5	302	CLA	3	0
31	A	845	PQN	5	0
30	B	827	CLA	5	0
33	2u	201	BCR	3	0
30	B	811	CLA	4	0
30	11	306	CLA	2	0
30	4	309	CLA	1	0
30	B	831	CLA	1	0
30	8	308	CLA	1	0
33	L	201	BCR	2	0
30	F	202	CLA	3	0
30	A	819	CLA	3	0
30	3	305	CLA	1	0
30	B	819	CLA	1	0
30	B	802	CLA	2	0
30	B	808	CLA	3	0
30	B	828	CLA	4	0
30	B	824	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	817	CLA	3	0
30	11	308	CLA	2	0
38	12	309	KC1	1	0
30	11	304	CLA	3	0
30	B	805	CLA	2	0
30	9	306	CLA	2	0
30	3	301	CLA	1	0
30	A	802	CLA	2	0
39	6	319	DD6	1	0
33	A	851	BCR	2	0
30	12	308	CLA	4	0
30	11	310	CLA	4	0
30	6	306	CLA	2	0
30	5	304	CLA	2	0
30	A	824	CLA	1	0
35	12	319	LMT	1	0
30	7	311	CLA	2	0
34	5	317	LHG	1	0
30	B	825	CLA	1	0
30	5	307	CLA	2	0
30	A	805	CLA	2	0
30	A	839	CLA	4	0
30	A	806	CLA	3	0
37	8	315	A86	1	0
35	B	852	LMT	1	0
30	9	302	CLA	1	0
30	9	308	CLA	2	0
30	16	306	CLA	1	0
30	B	837	CLA	2	0
30	16	307	CLA	2	0
33	A	850	BCR	2	0
30	1	303	CLA	3	0
36	8	319	LMG	1	0
36	A	856	LMG	3	0
37	14	317	A86	1	0
30	A	835	CLA	2	0
35	A	855	LMT	1	0
30	B	820	CLA	1	0
30	B	826	CLA	5	0
30	1	302	CLA	3	0
30	2	304	CLA	1	0
33	A	849	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	828	CLA	1	0
30	A	807	CLA	1	0
33	A	848	BCR	2	0
33	B	842	BCR	1	0
30	5	303	CLA	4	0
30	A	842	CLA	3	0
30	B	818	CLA	1	0
30	4	311	CLA	2	0
30	B	836	CLA	3	0
30	2	301	CLA	1	0
30	A	820	CLA	6	0
33	B	841	BCR	1	0
30	A	803	CLA	1	0
37	9	316	A86	1	0
30	A	841	CLA	1	0
30	16	301	CLA	6	0
30	6	314	CLA	2	0
30	A	836	CLA	2	0
33	J	103	BCR	4	0
30	B	851	CLA	1	0
35	6	302	LMT	2	0
30	B	821	CLA	4	0
30	7	303	CLA	1	0
30	2	309	CLA	3	0
30	14	307	CLA	1	0
30	4	306	CLA	4	0
30	13	302	CLA	2	0
30	A	822	CLA	2	0
30	4	302	CLA	1	0
30	8	301	CLA	1	0
31	B	840	PQN	1	0
34	A	852	LHG	1	0
30	A	844	CLA	1	0
38	4	310	KC1	1	0
30	B	807	CLA	2	0
30	A	814	CLA	1	0
33	M	101	BCR	3	0
30	13	301	CLA	5	0
30	7	306	CLA	2	0
30	B	830	CLA	2	0
33	F	204	BCR	3	0
38	16	304	KC1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	806	CLA	6	0
30	15	304	CLA	2	0
30	B	804	CLA	2	0
30	B	816	CLA	2	0
30	10	309	CLA	2	0
37	4	315	A86	1	0
35	11	303	LMT	1	0
36	B	847	LMG	2	0
30	A	830	CLA	4	0
30	B	838	CLA	7	0
30	1	307	CLA	2	0
30	2	311	CLA	1	0
30	9	305	CLA	2	0
38	5	310	KC1	1	0
30	16	310	CLA	1	0
30	3	306	CLA	1	0
30	12	310	CLA	1	0
30	13	307	CLA	4	0
30	A	818	CLA	1	0
30	A	804	CLA	3	0
30	6	309	CLA	2	0
35	7	321	LMT	1	0
37	11	315	A86	1	0
33	B	843	BCR	2	0
33	J	102	BCR	3	0
30	B	812	CLA	2	0
37	7	315	A86	1	0
30	A	810	CLA	4	0
30	A	831	CLA	4	0
30	A	826	CLA	4	0
33	B	845	BCR	1	0
39	6	318	DD6	1	0
30	1	301	CLA	2	0
30	9	307	CLA	4	0
36	8	321	LMG	1	0
35	12	301	LMT	2	0
34	A	853	LHG	1	0
30	3	303	CLA	2	0
30	1	304	CLA	2	0
30	2	305	CLA	2	0
30	6	307	CLA	1	0
30	5	308	CLA	2	0

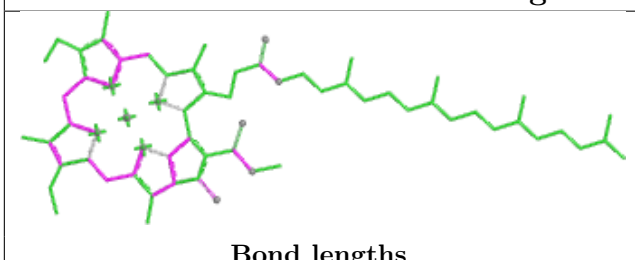
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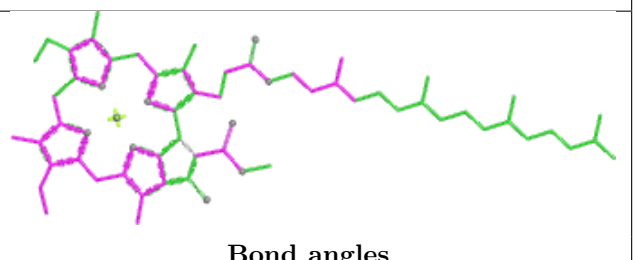
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	813	CLA	3	0
30	B	801	CLA	4	0
33	L	205	BCR	4	0
39	6	321	DD6	1	0
33	I	101	BCR	2	0
30	15	303	CLA	3	0
30	15	313	CLA	3	0
30	B	822	CLA	3	0
30	10	304	CLA	1	0
30	B	815	CLA	2	0
30	12	303	CLA	2	0
30	A	821	CLA	3	0
30	10	307	CLA	1	0
30	14	303	CLA	3	0
30	A	812	CLA	4	0
33	B	846	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.

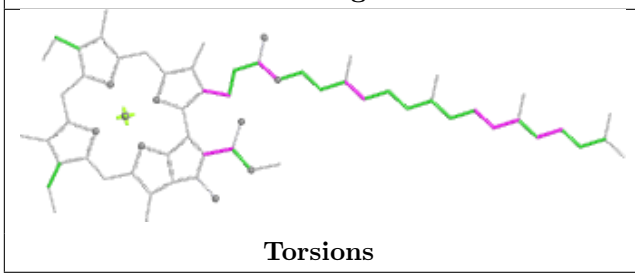
Ligand CLA 8 303



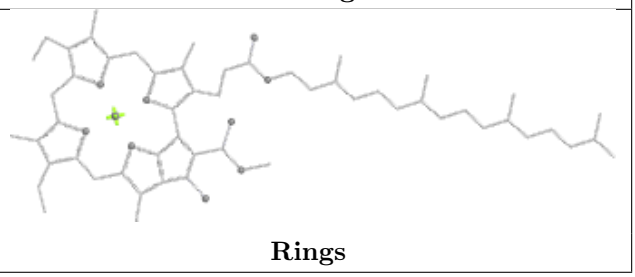
Bond lengths



Bond angles

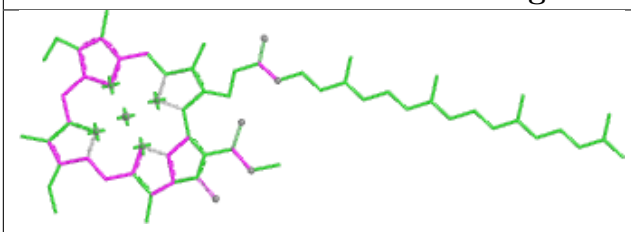


Torsions

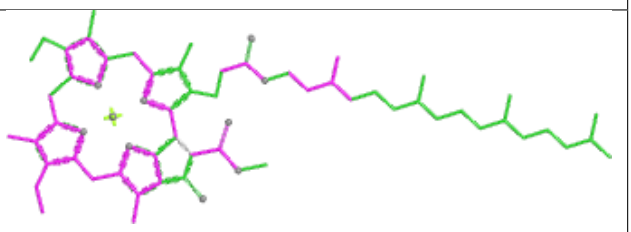


Rings

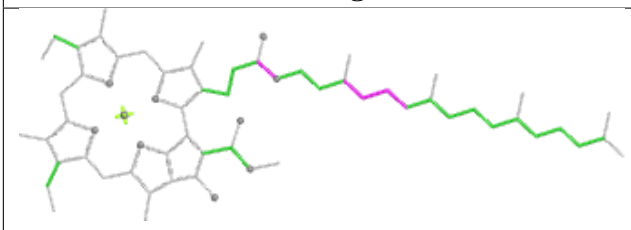
Ligand CLA 2 310



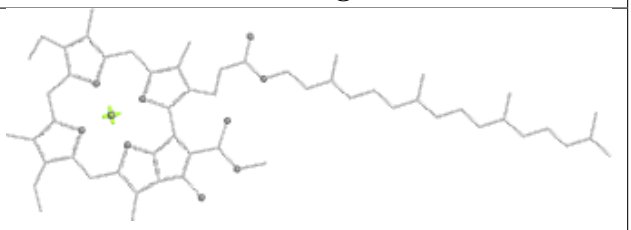
Bond lengths



Bond angles

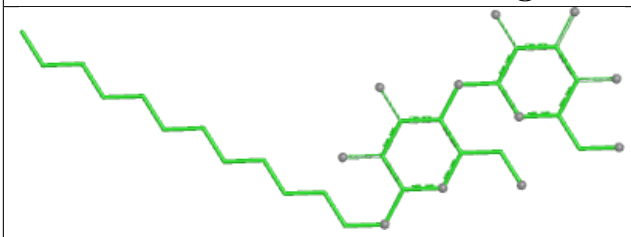


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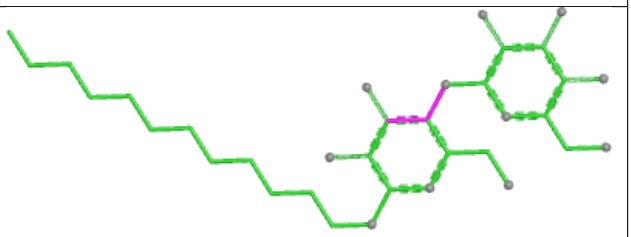


Rings

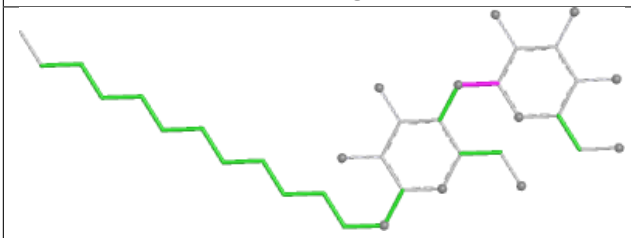
Ligand LMT 11 318



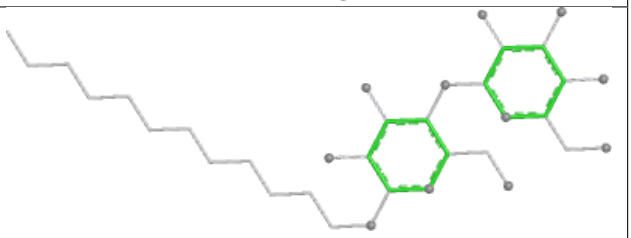
Bond lengths



Bond angles

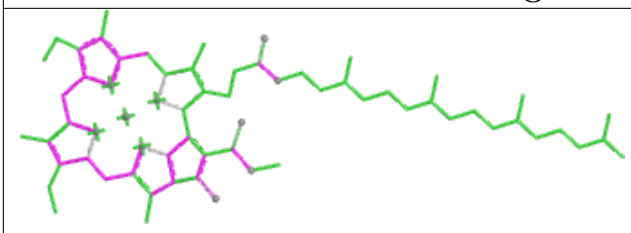


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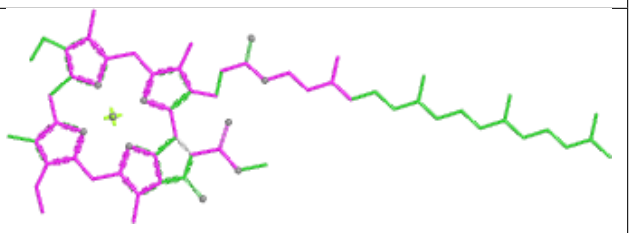


Rings

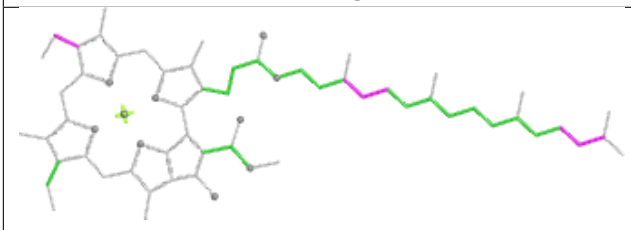
Ligand CLA B 832



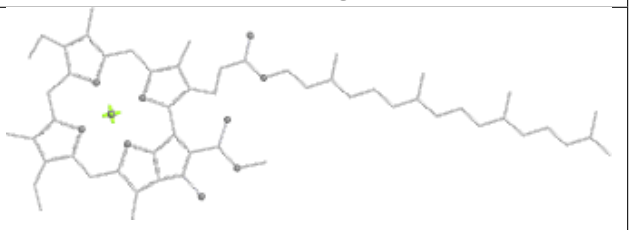
Bond lengths



Bond angles

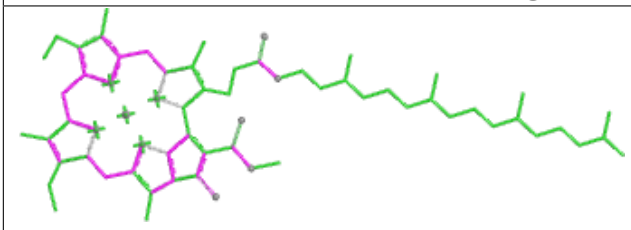


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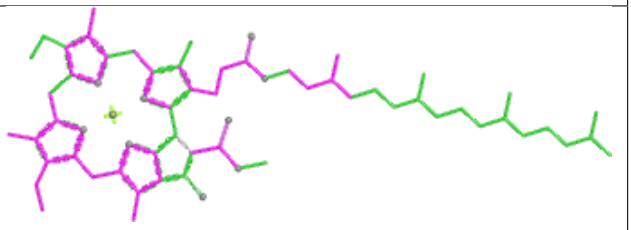


Rings

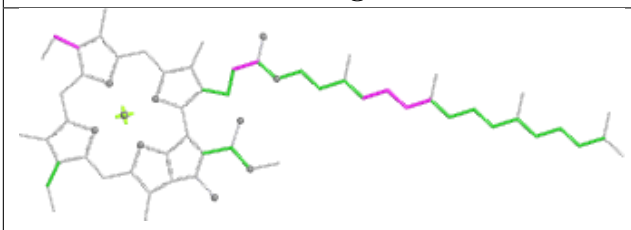
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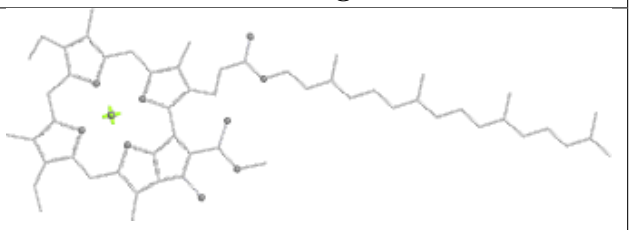
Bond lengths



Bond angles

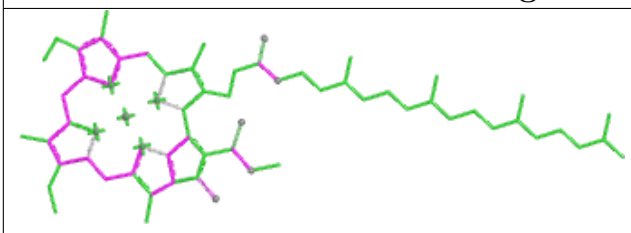


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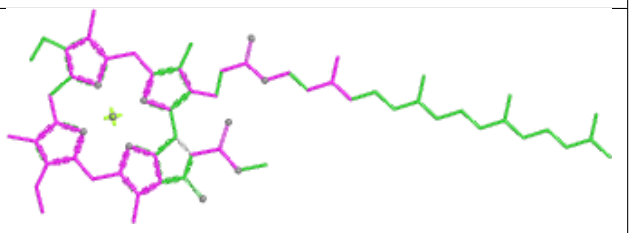


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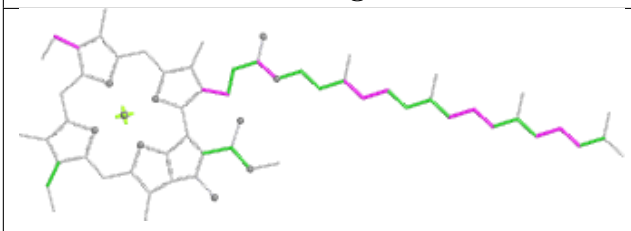
Ligand CLA 14 302



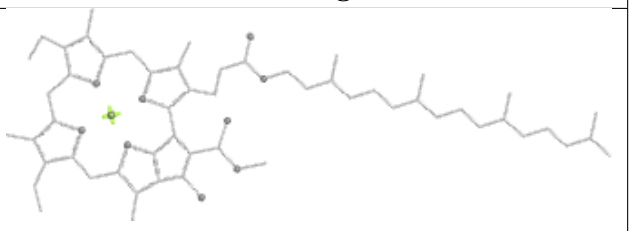
Bond lengths



Bond angles

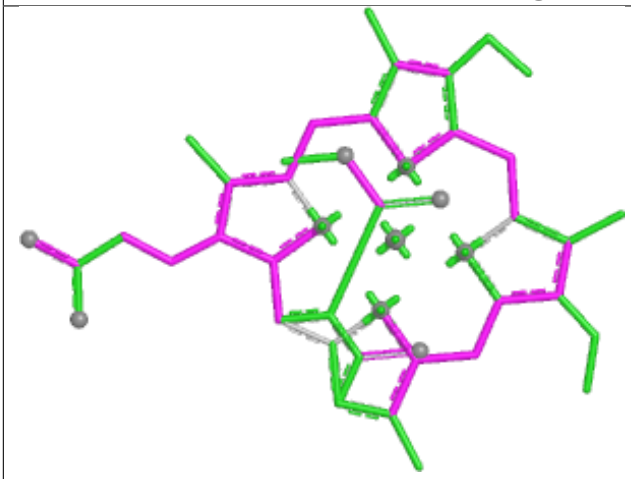


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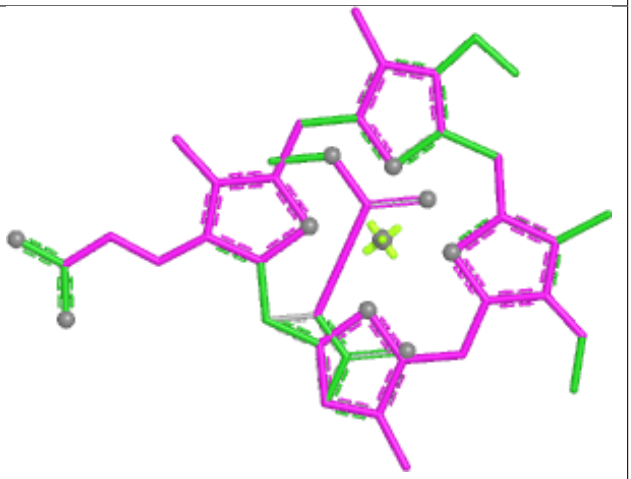


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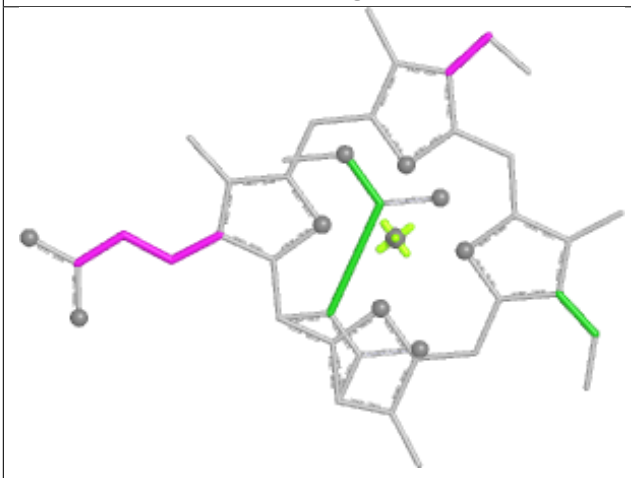
Ligand KC1 3 311



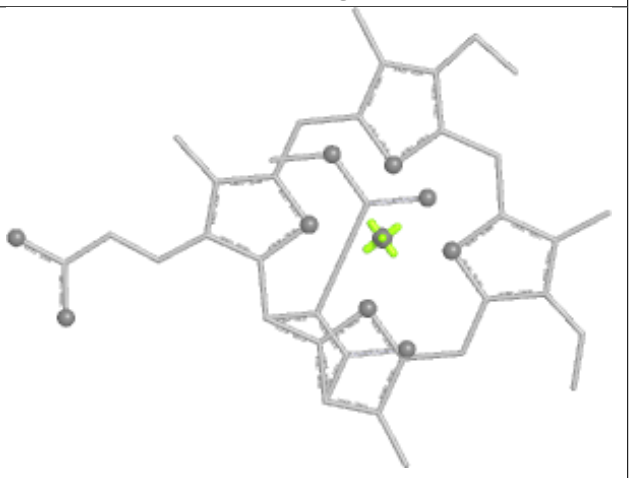
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Bond angles

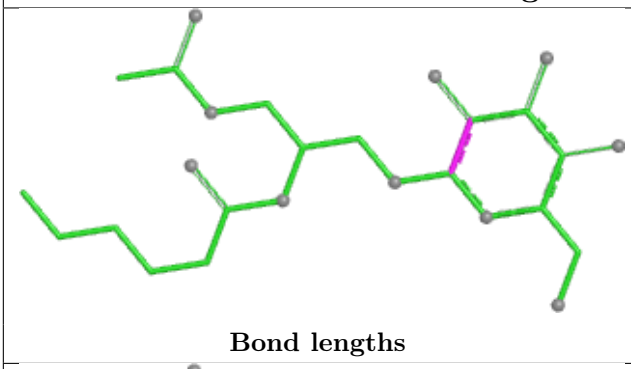


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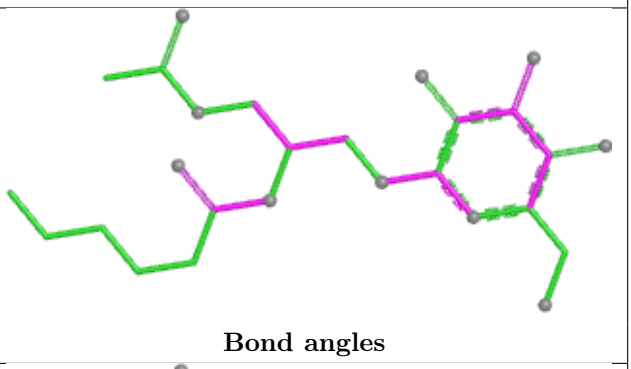


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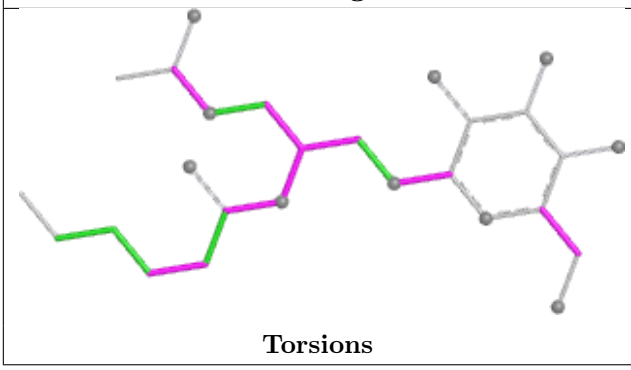
Ligand LMG F 205



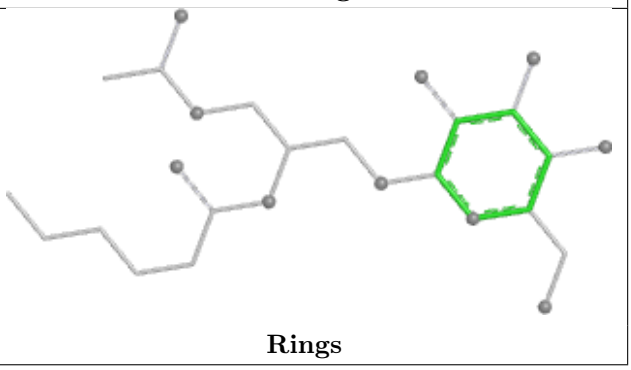
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Bond angles

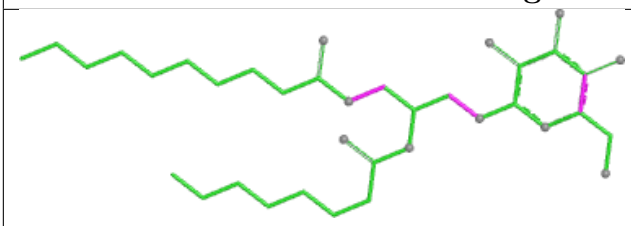


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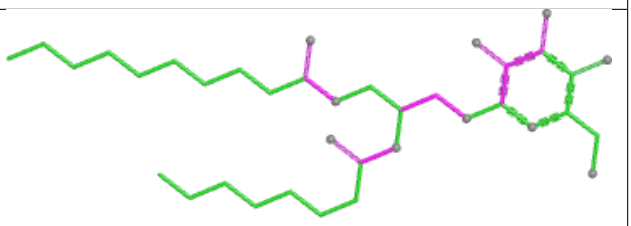


Rings

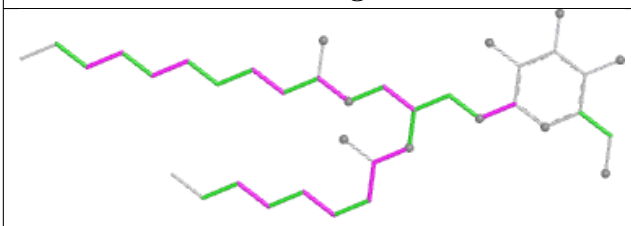
Ligand LMG 7 320



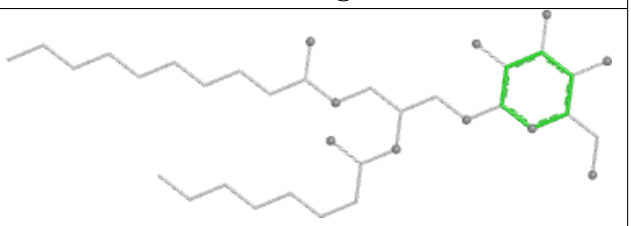
Bond lengths



Bond angles

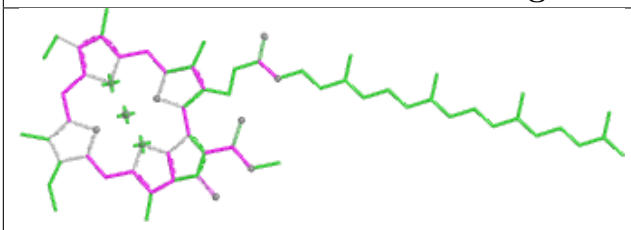


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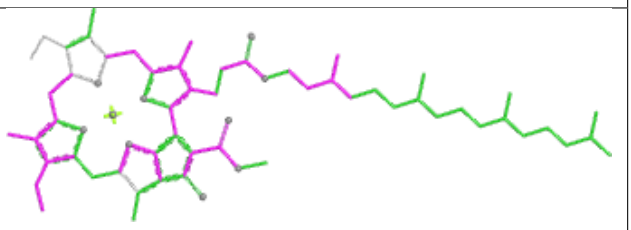


Rings

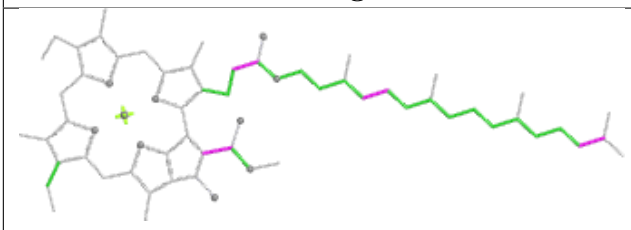
Ligand CL0 A 801



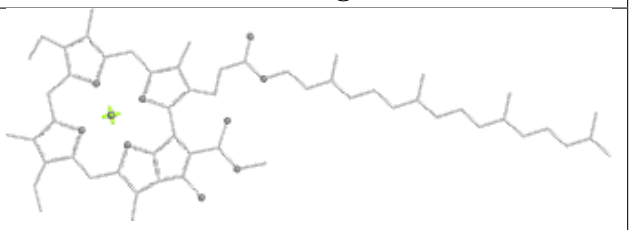
Bond lengths



Bond angles

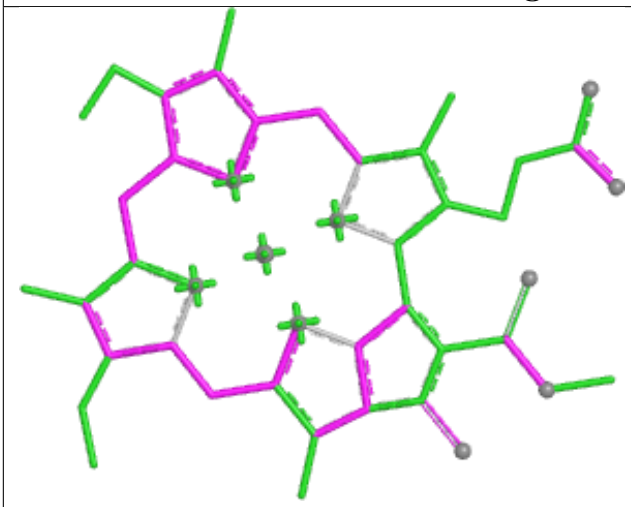


Torsions

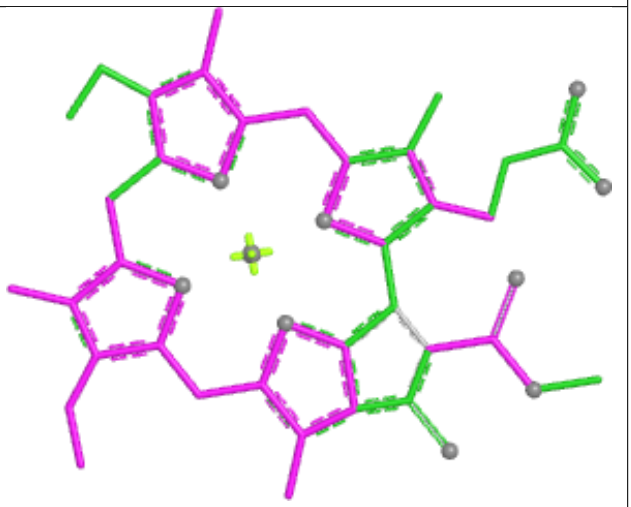


Rings

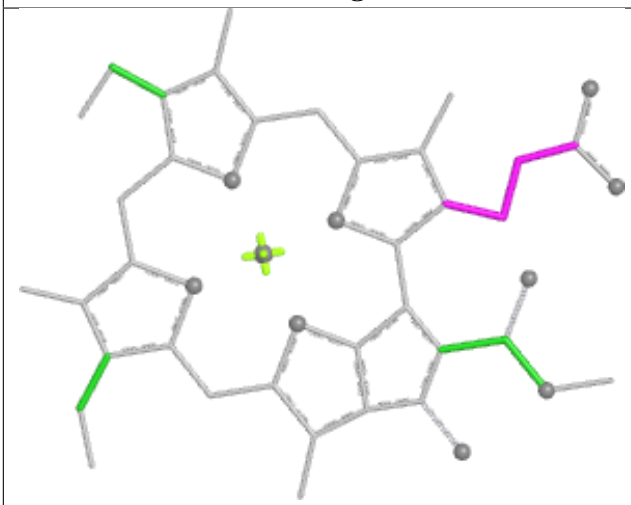
Ligand CLA A 837



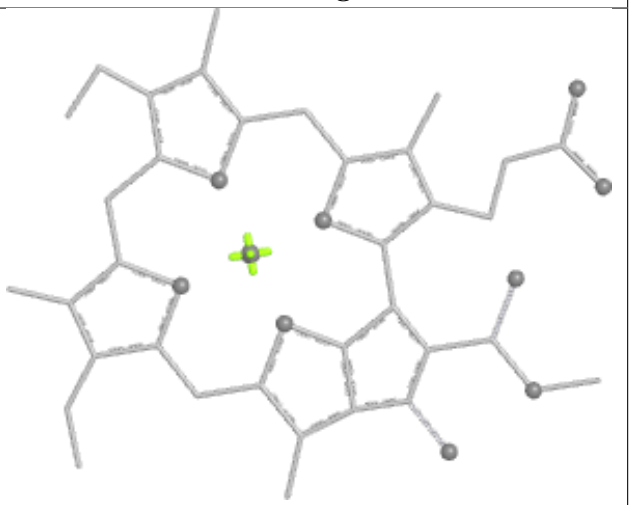
Bond lengths



Bond angles

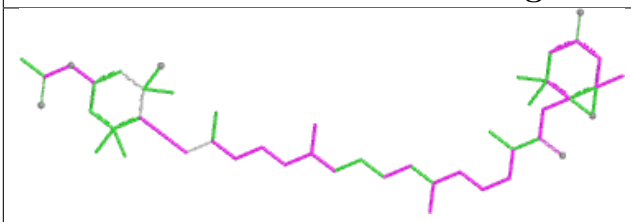


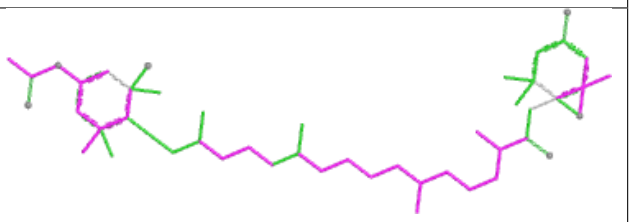
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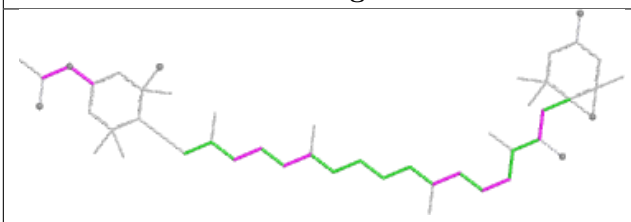


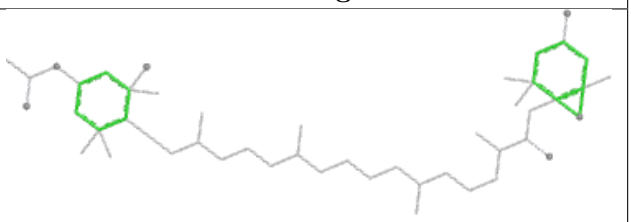
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Ligand A86 16 314

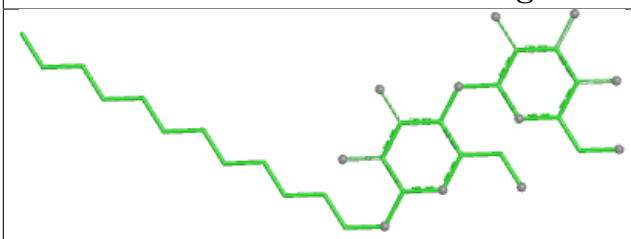

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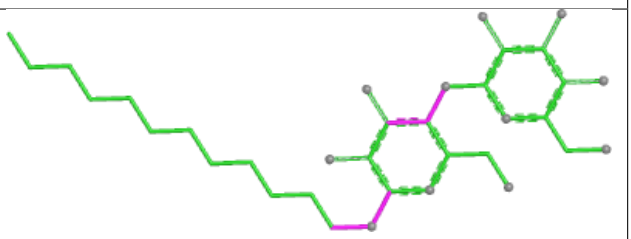

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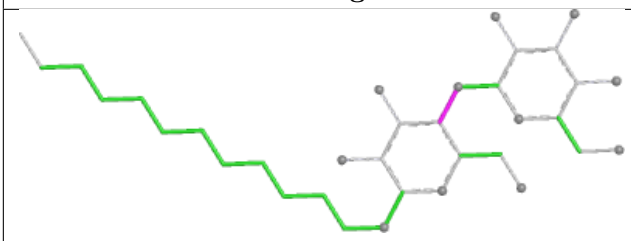

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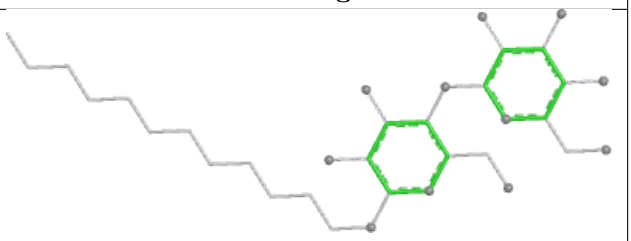

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Ligand LMT 11 317

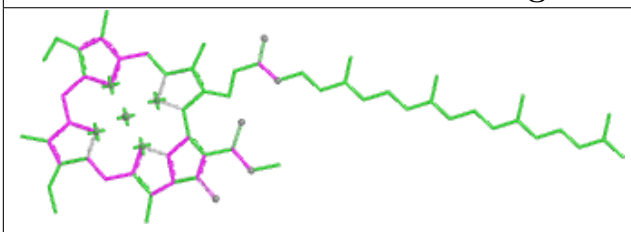

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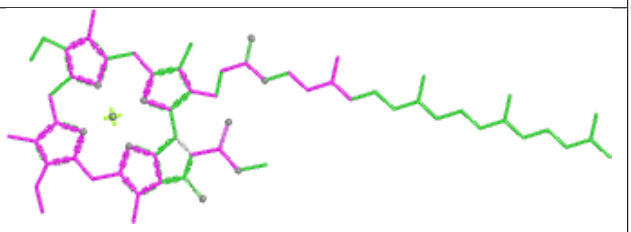

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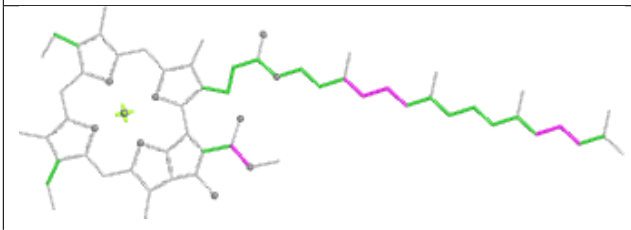

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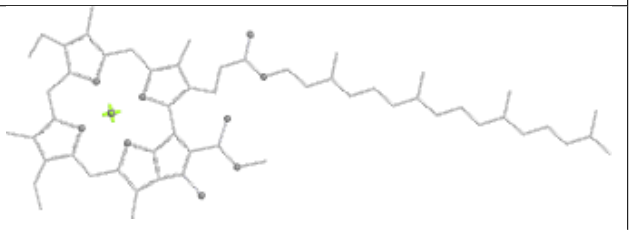

Rings

Ligand CLA 8 302

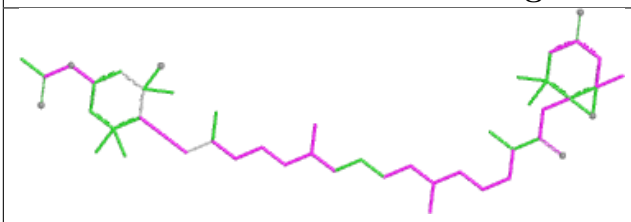

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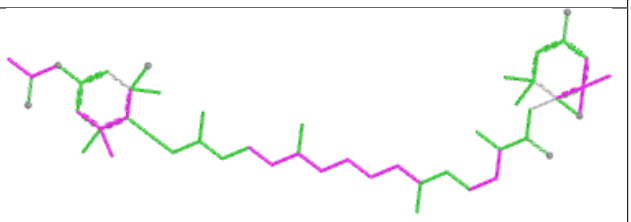

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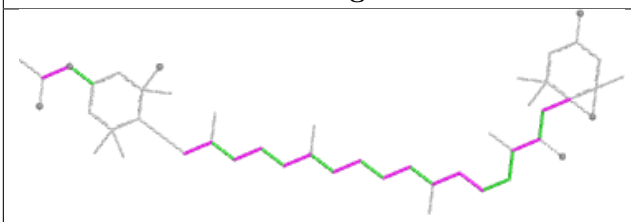
Ligand A86 15 323



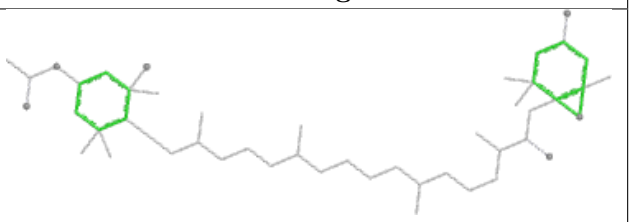
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Bond angles

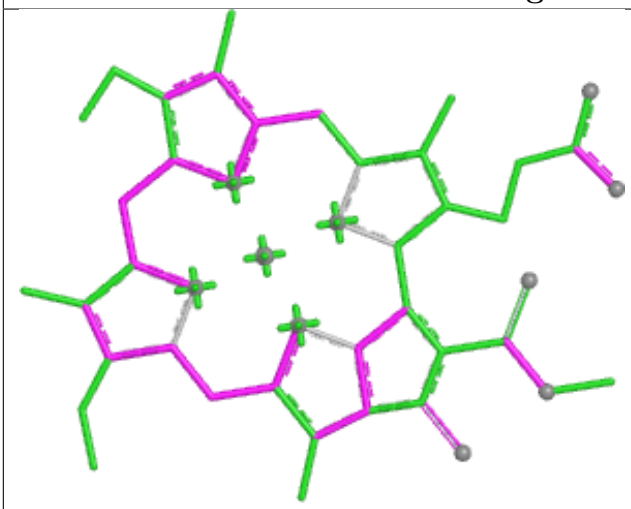


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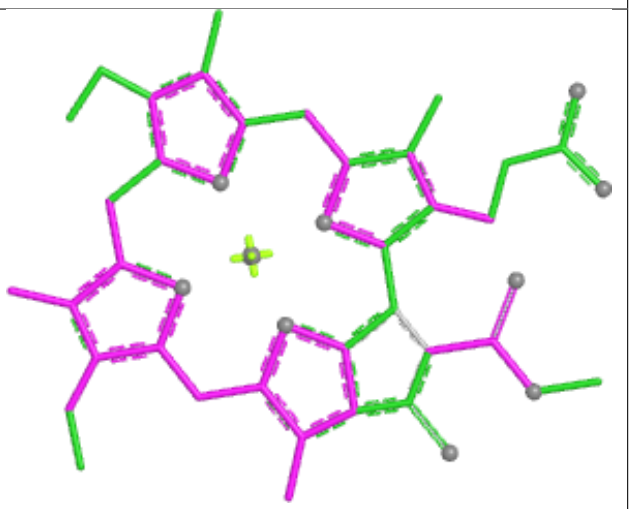


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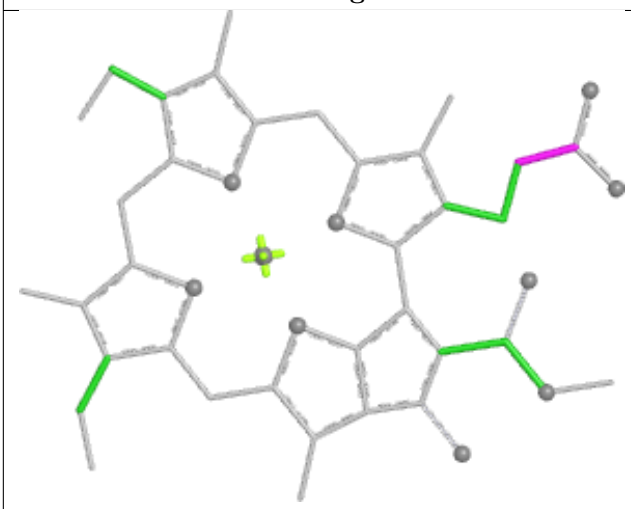
Ligand CLA L 203



Bond lengths



Bond angles

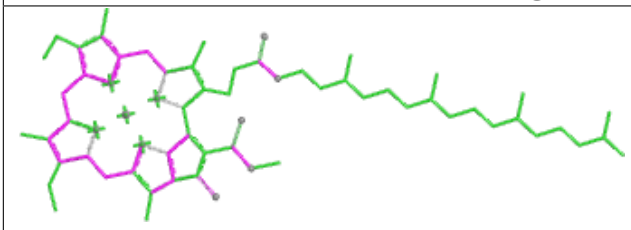


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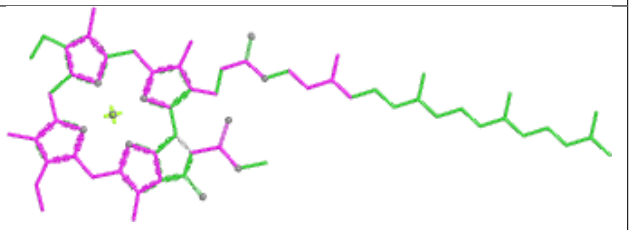


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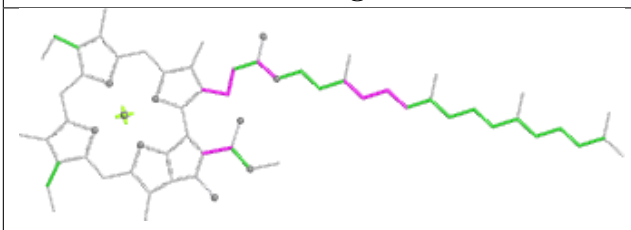
Ligand CLA 4 305



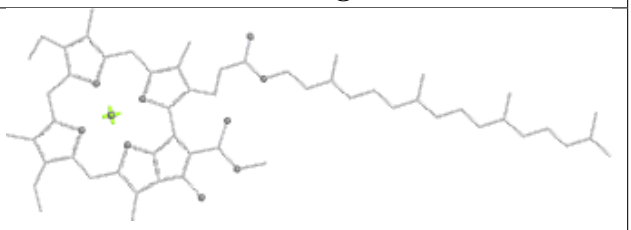
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Bond angles

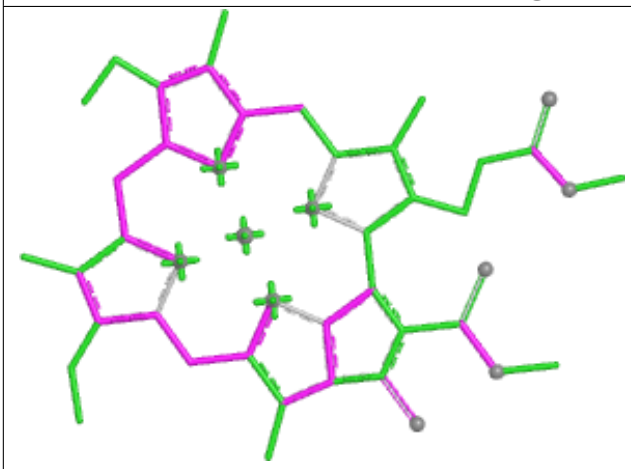


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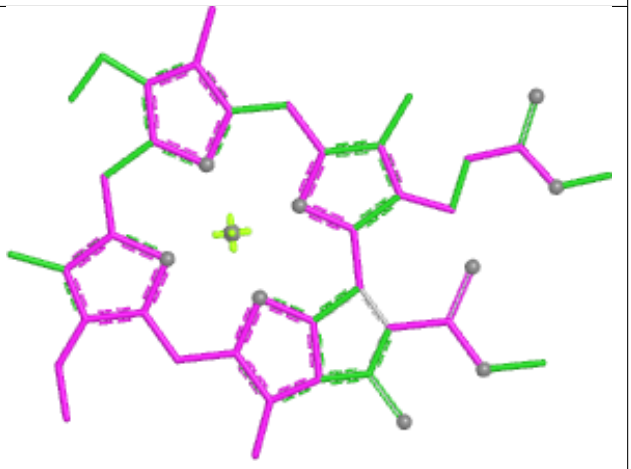


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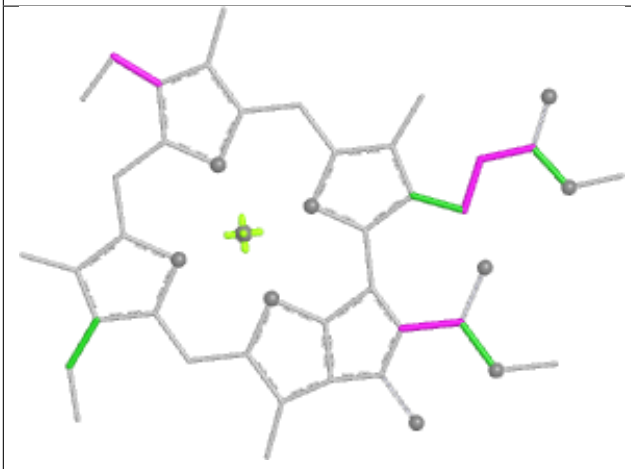
Ligand CLA 7 312



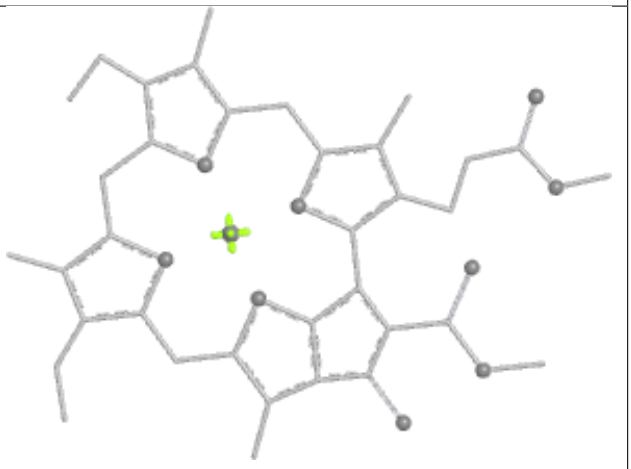
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Bond angles

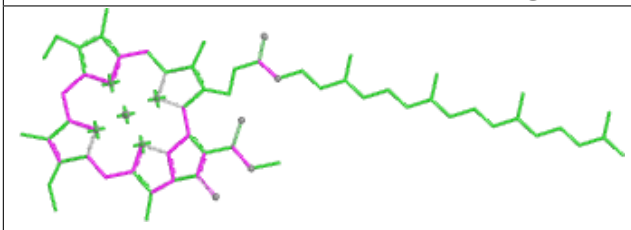


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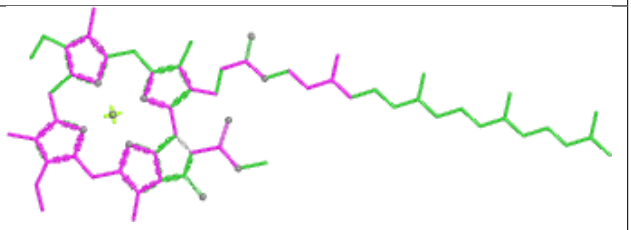


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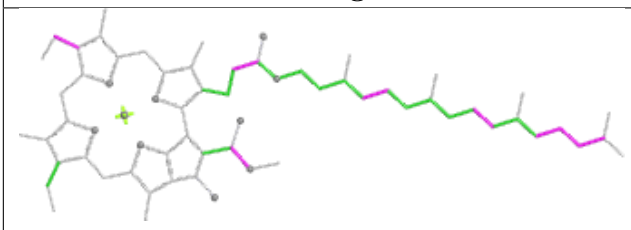
Ligand CLA B 809



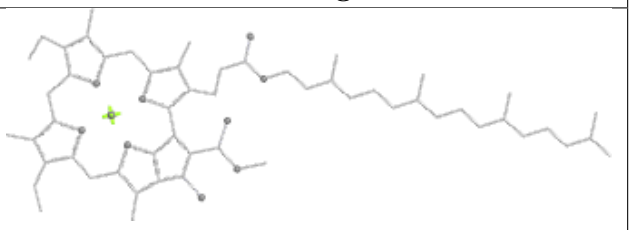
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Bond angles

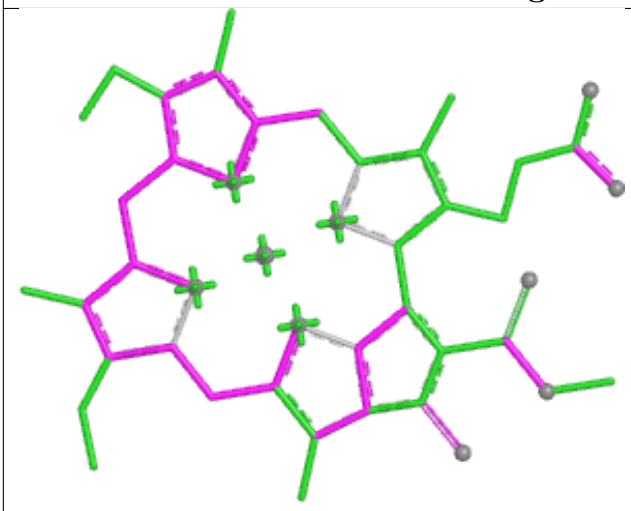


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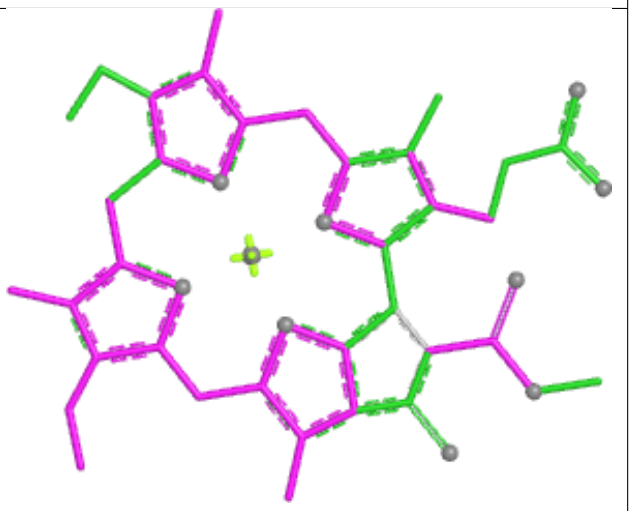


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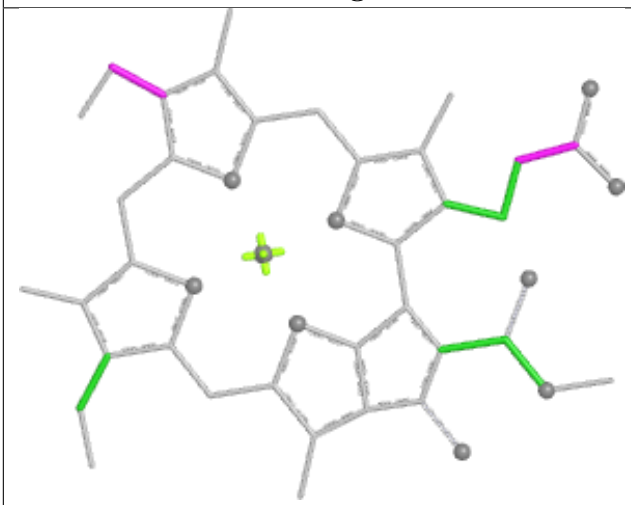
Ligand CLA J 101



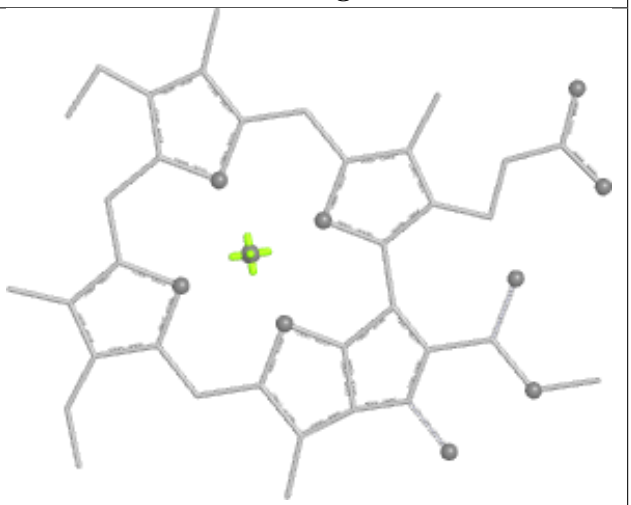
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Bond angles

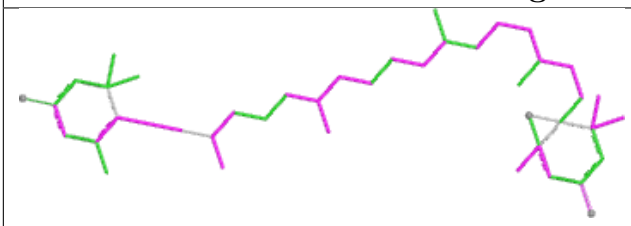


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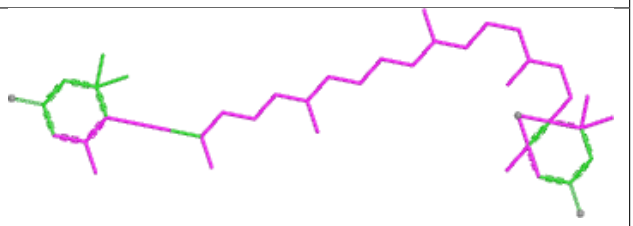


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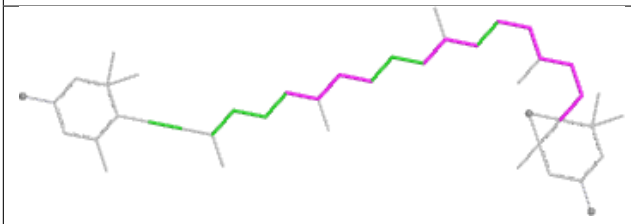
Ligand DD6 7 314



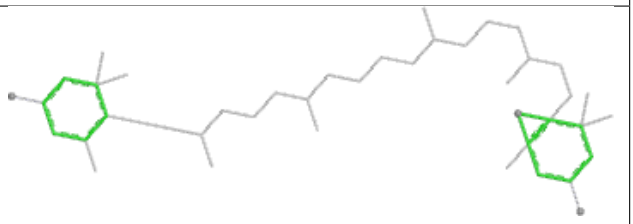
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Bond angles

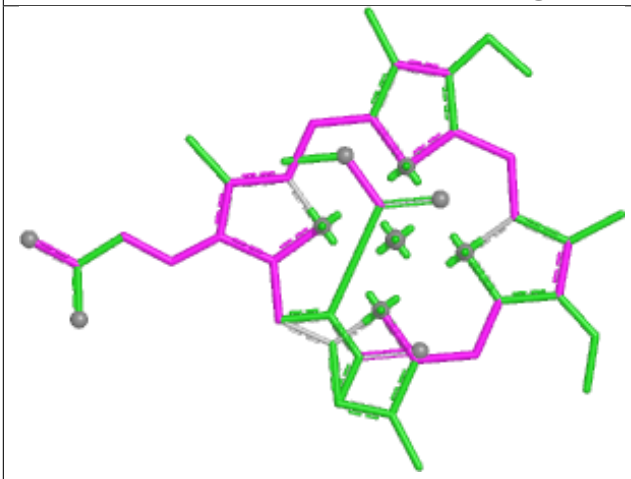


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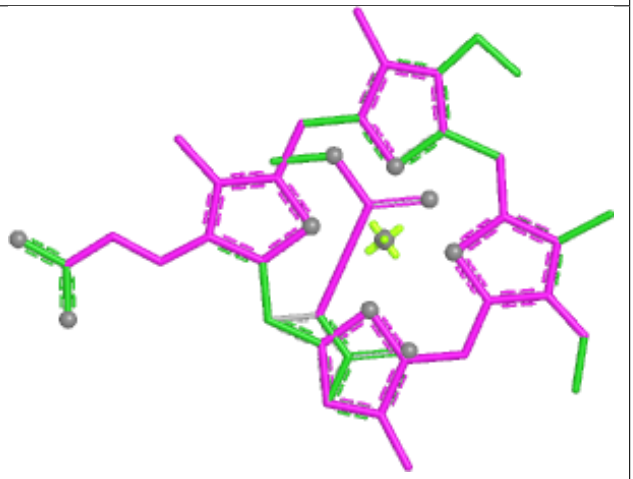


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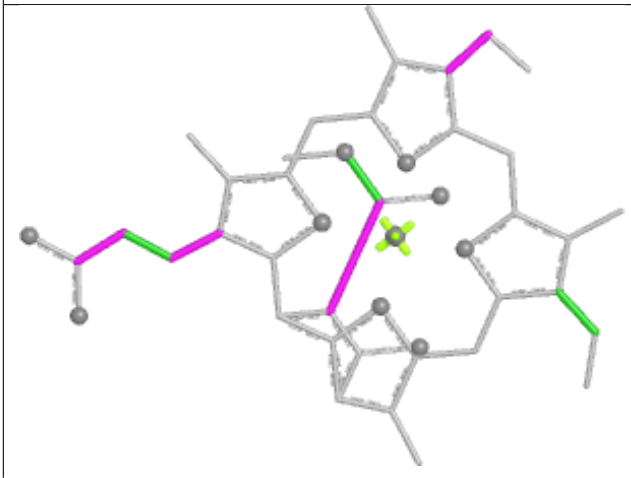
Ligand KC1 8 310



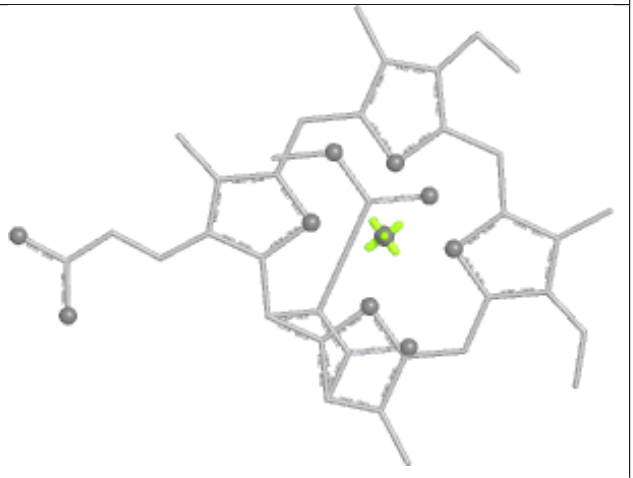
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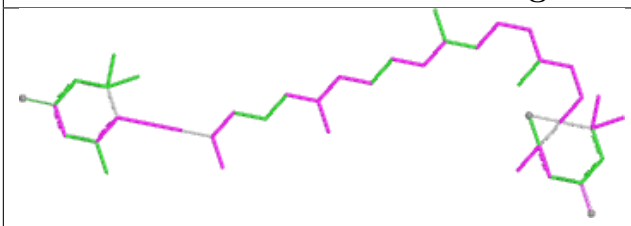


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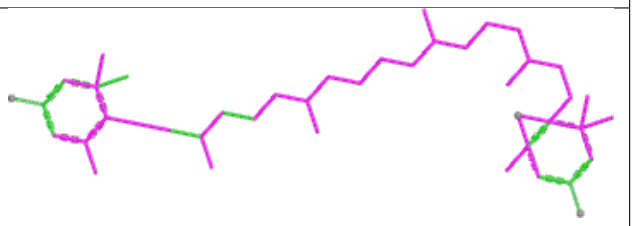


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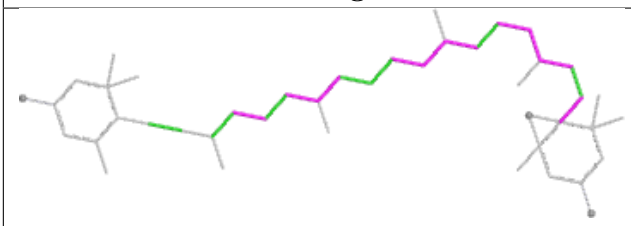
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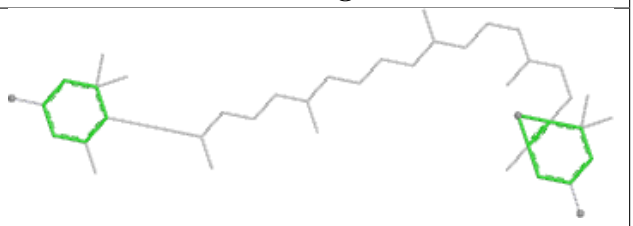
Bond lengths



Bond angles

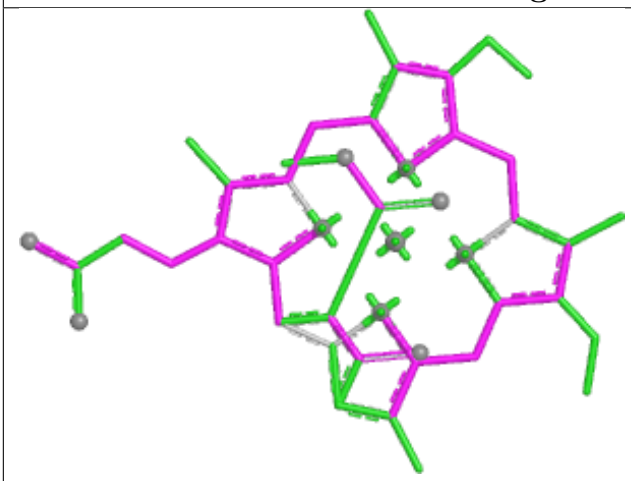


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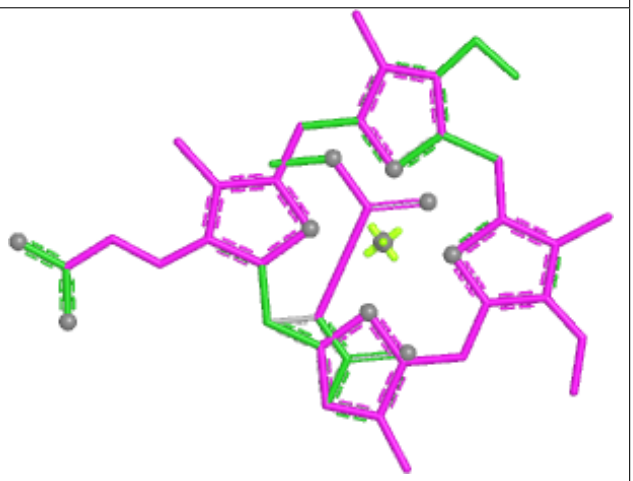


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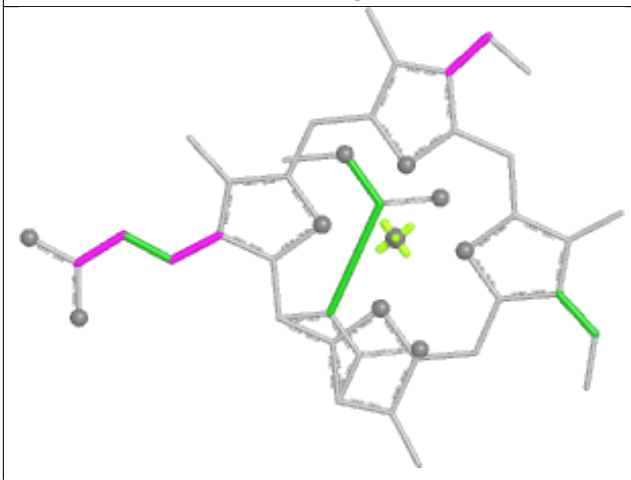
Ligand KC1 3 304



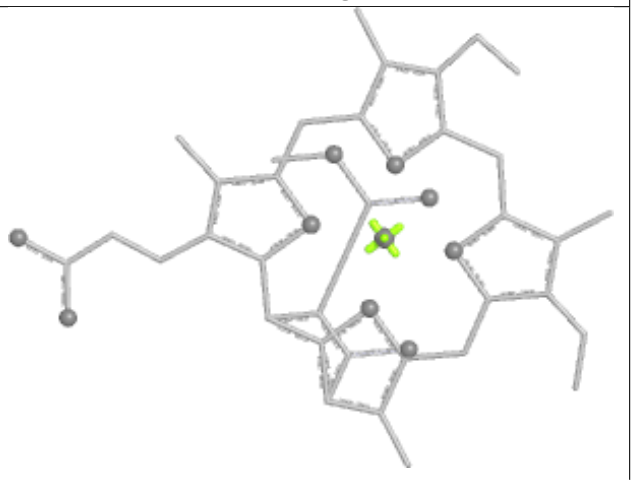
Bond lengths



Bond angles

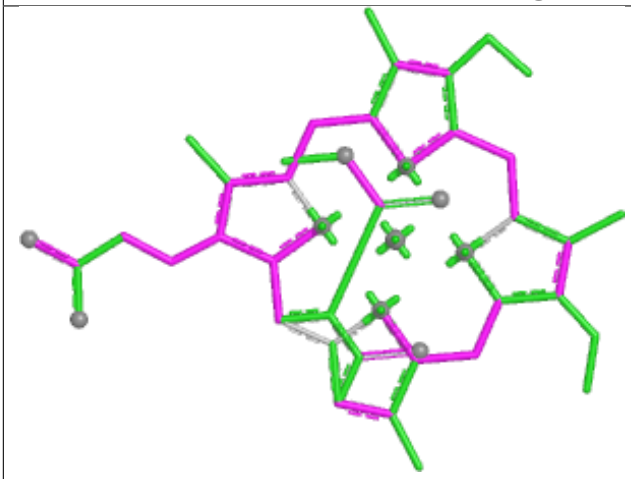


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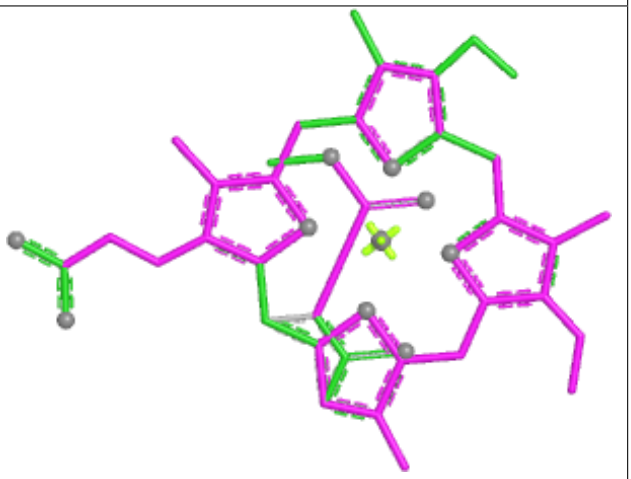


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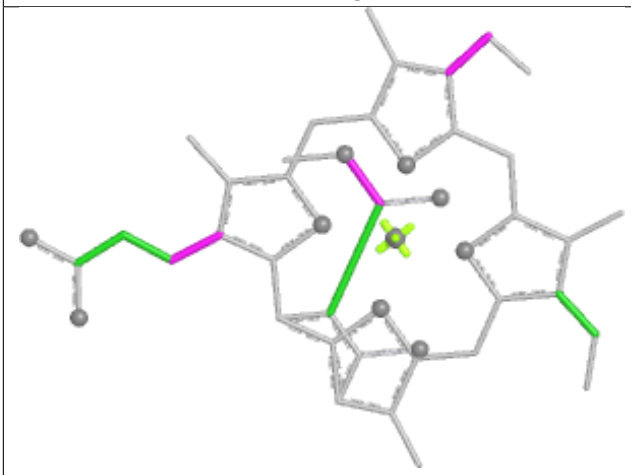
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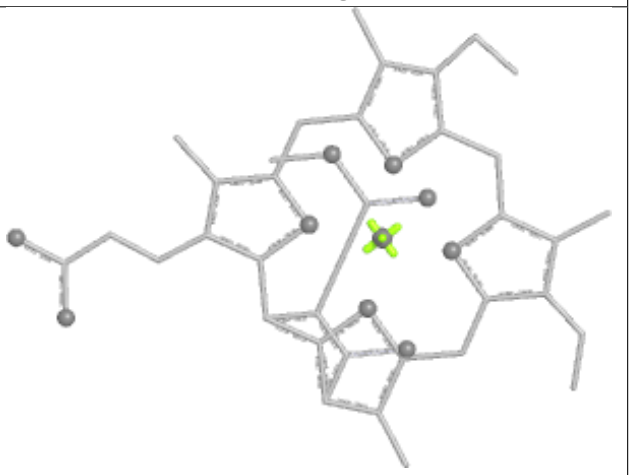
Bond lengths



Bond angles

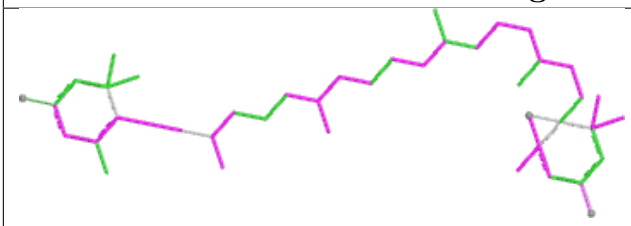


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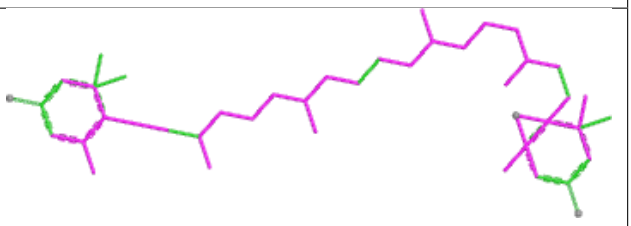


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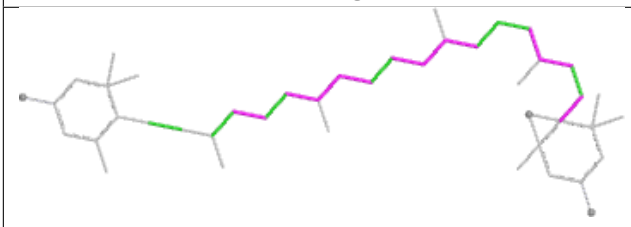
Ligand DD6 4 316



Bond lengths



Bond angles

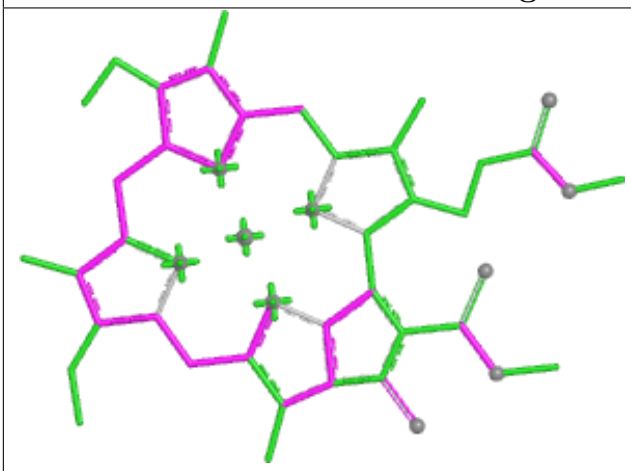


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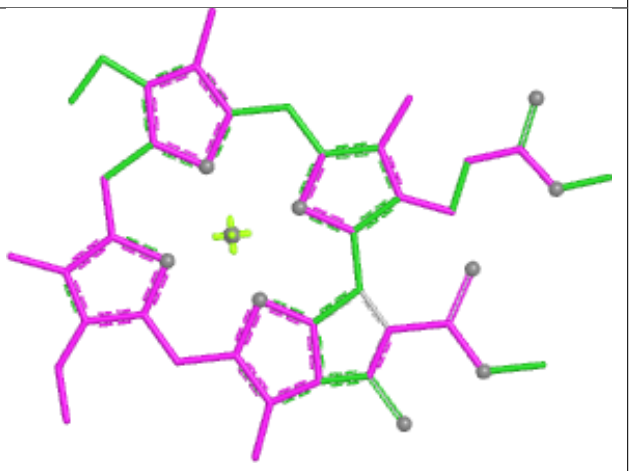


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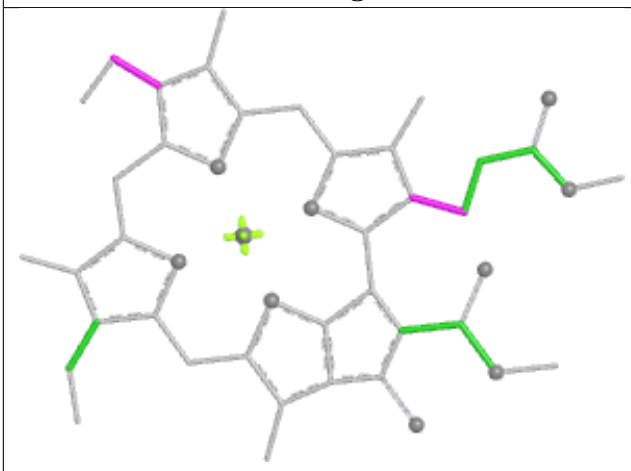
Ligand CLA 14 313



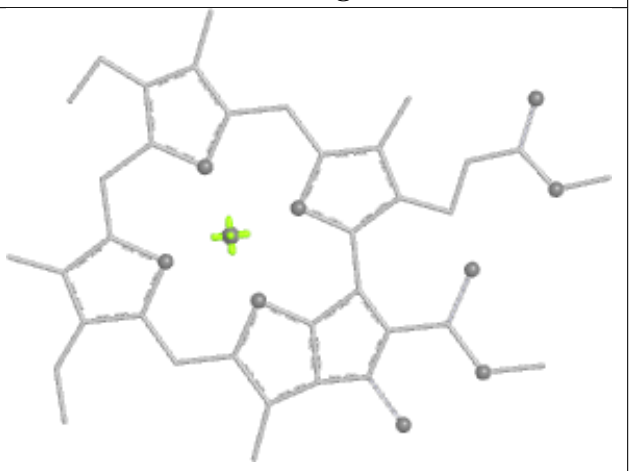
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Bond angles

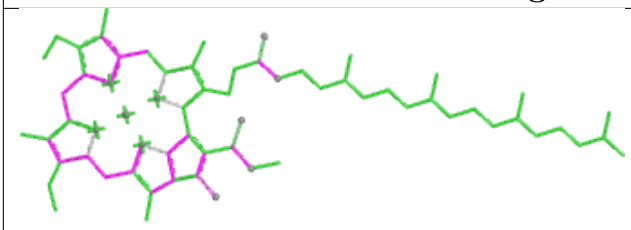


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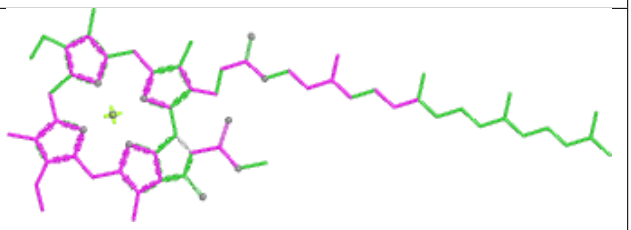


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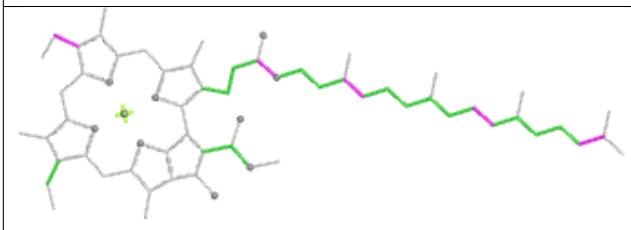
Ligand CLA 7 304



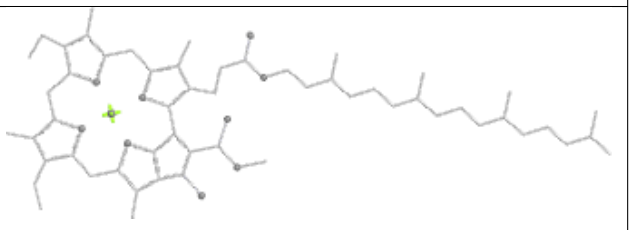
Bond lengths



Bond angles

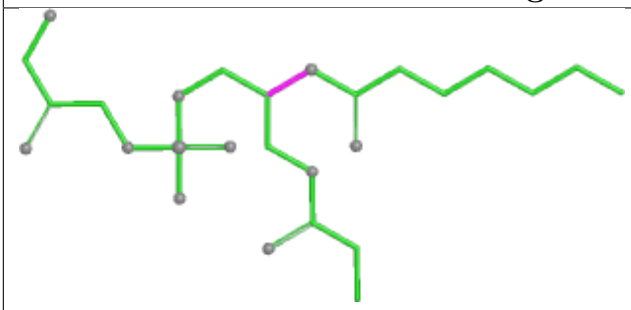


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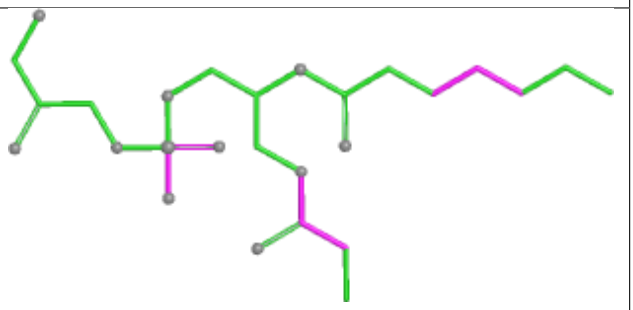


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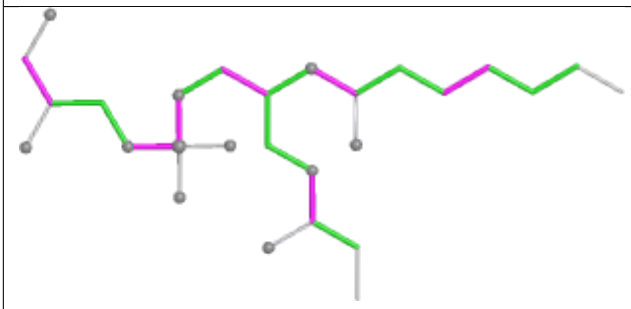
Ligand LHG 6 322



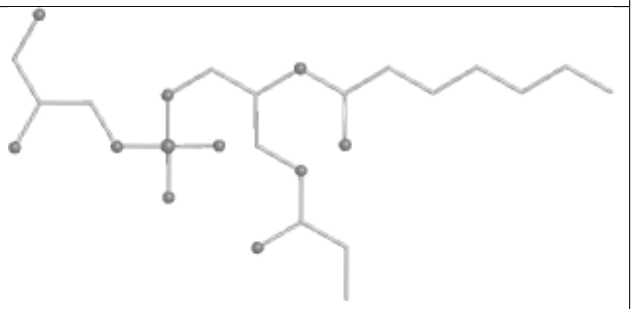
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Bond angles

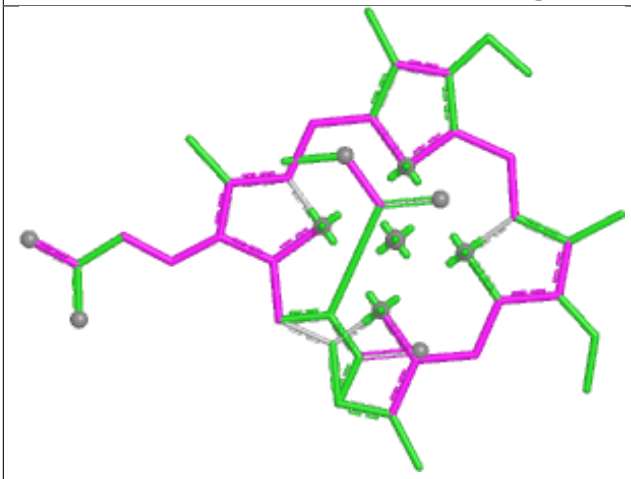


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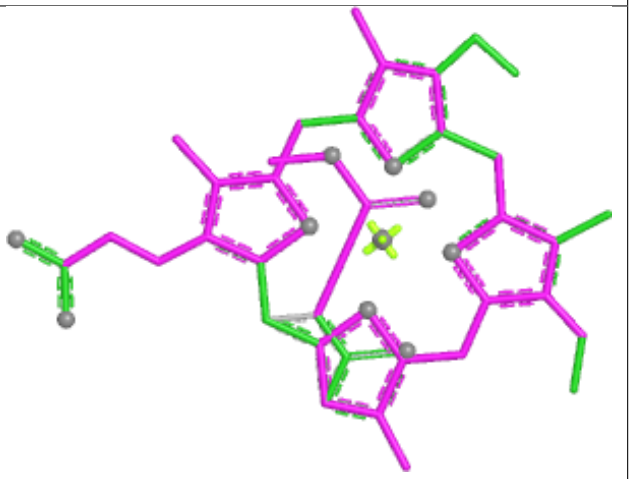


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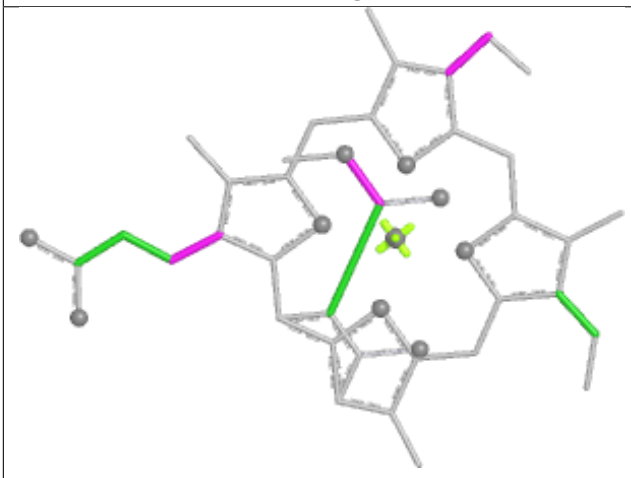
Ligand KC1 8 311



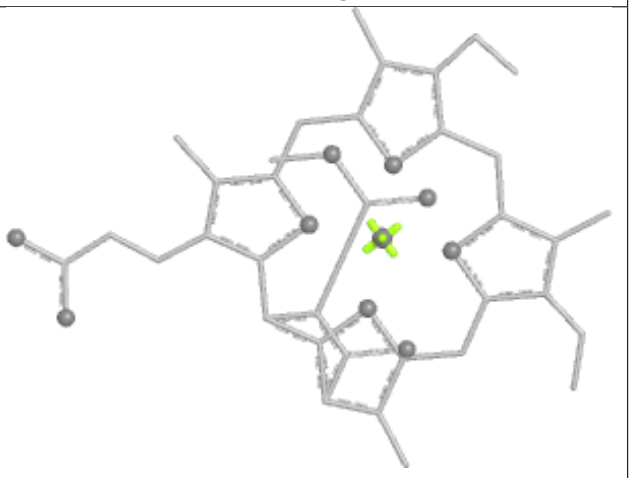
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Bond angles

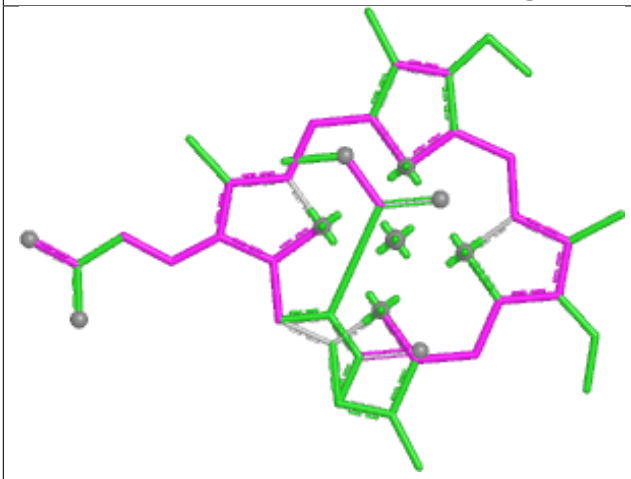


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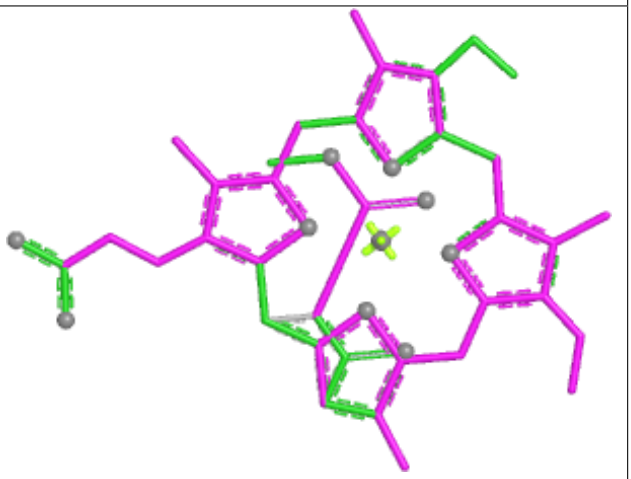


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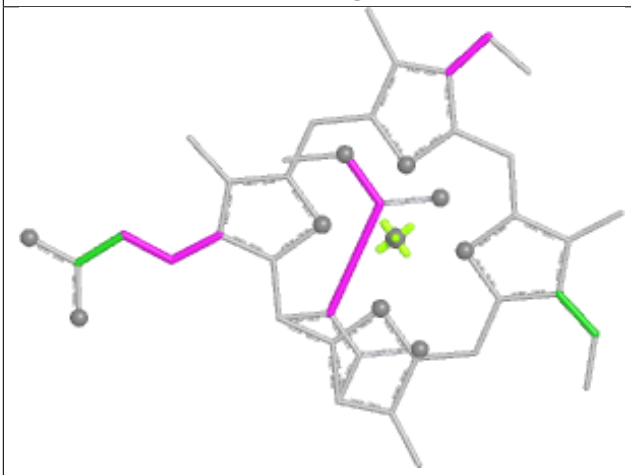
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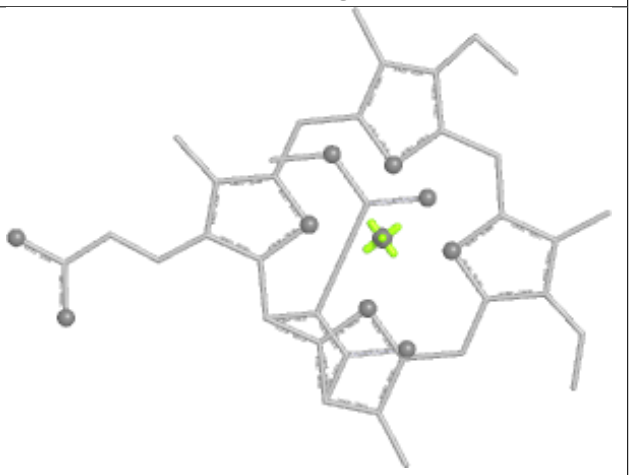
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Bond angles

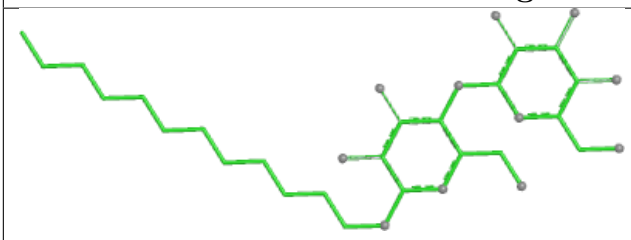


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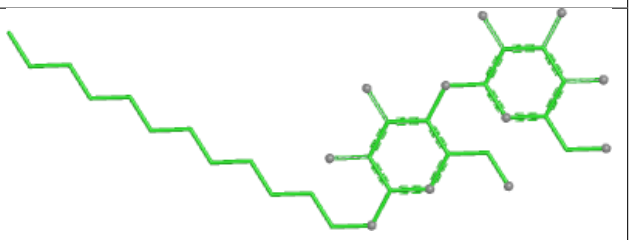


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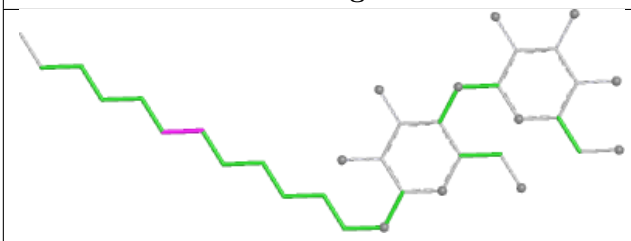
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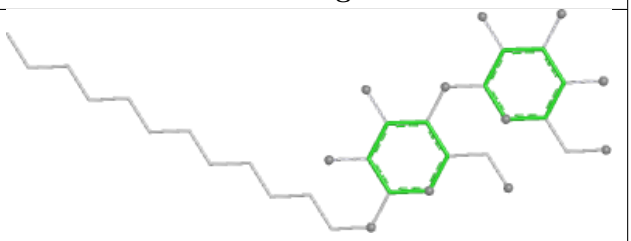
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Bond angles

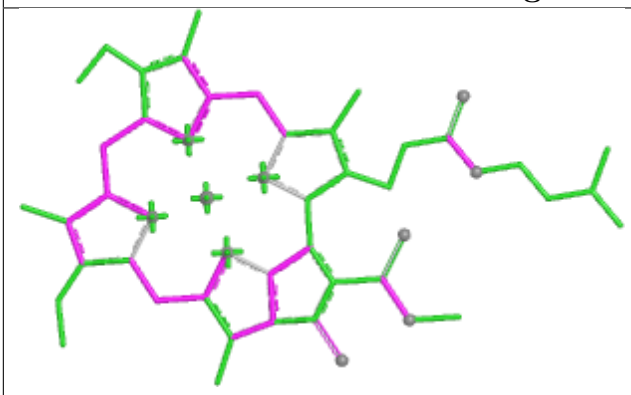


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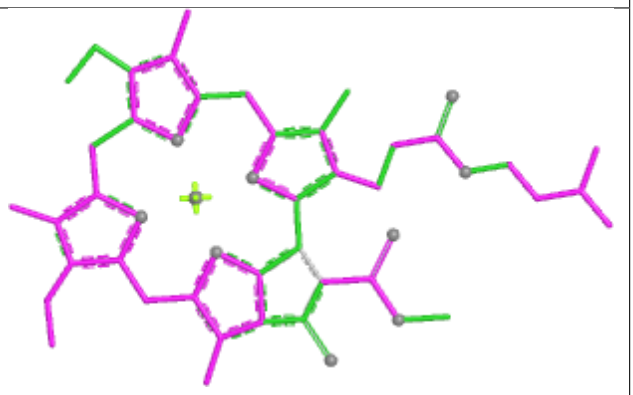


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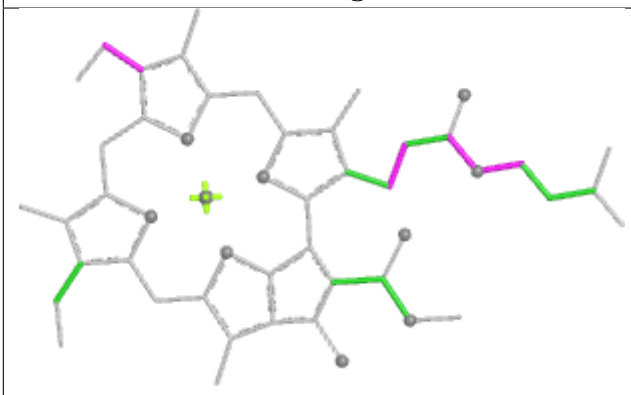
Ligand CLA A 832



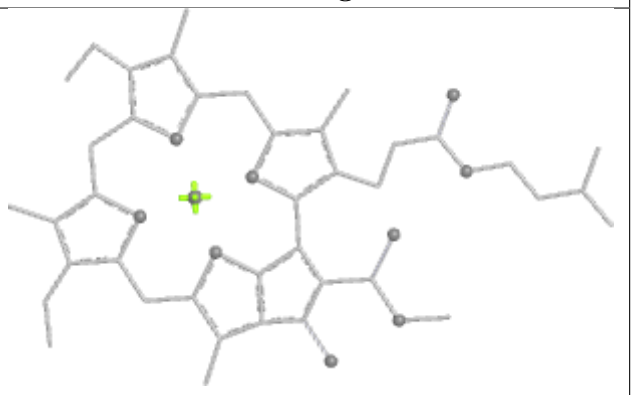
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Bond angles

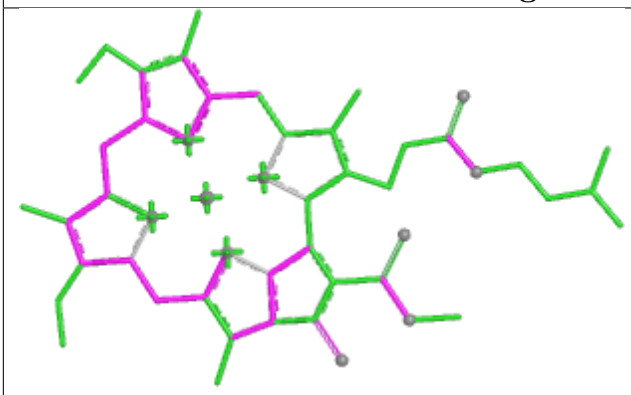


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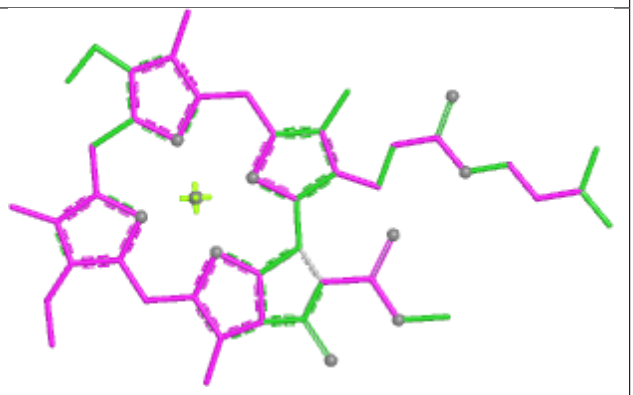


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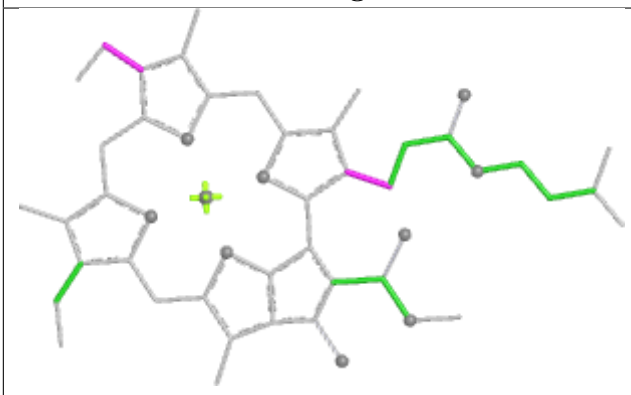
Ligand CLA 14 305



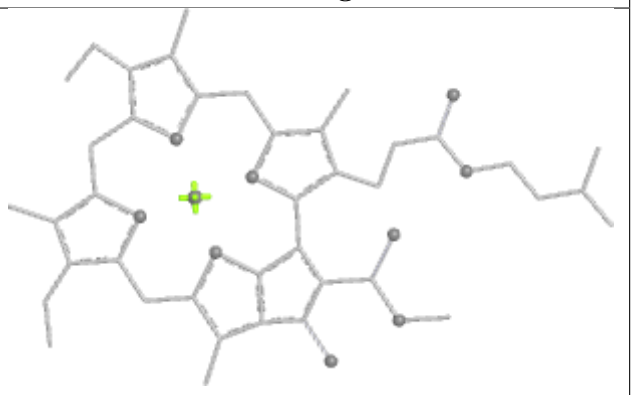
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Bond angles

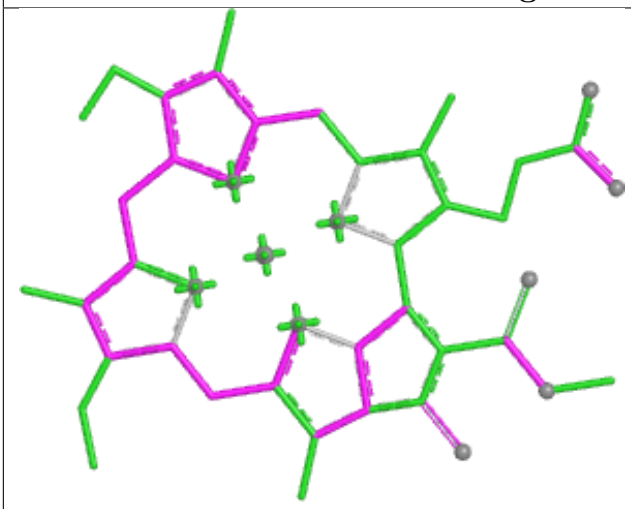


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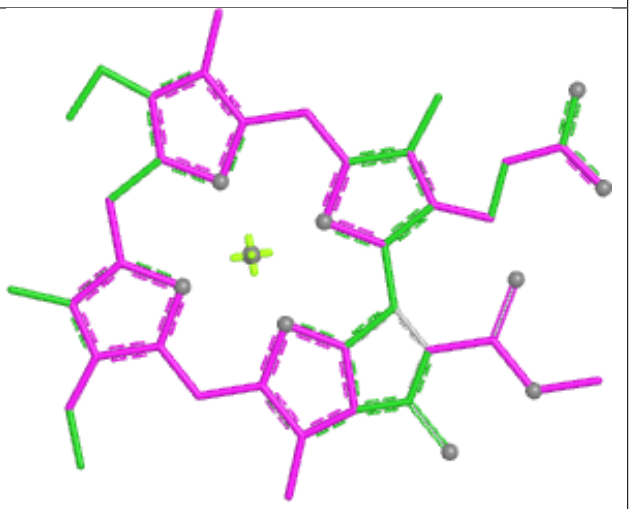


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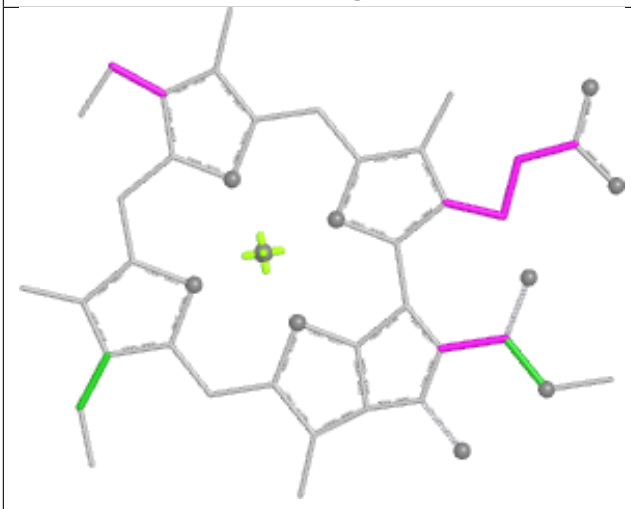
Ligand CLA 14 312



Bond lengths



Bond angles

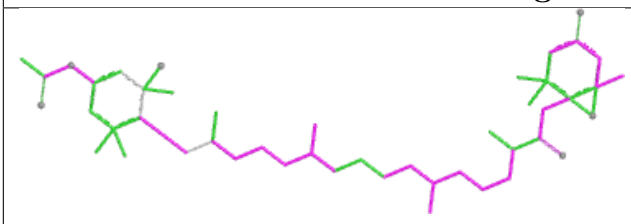


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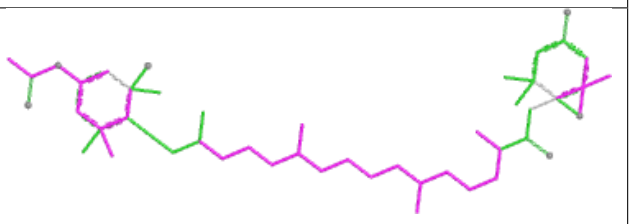


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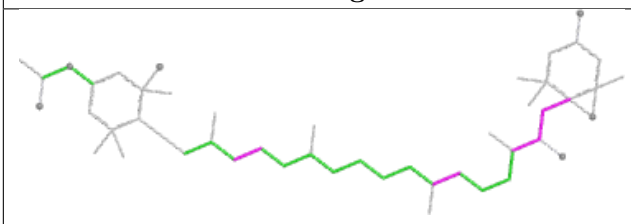
Ligand A86 1 309



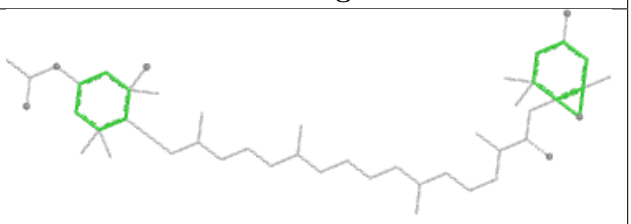
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Bond angles

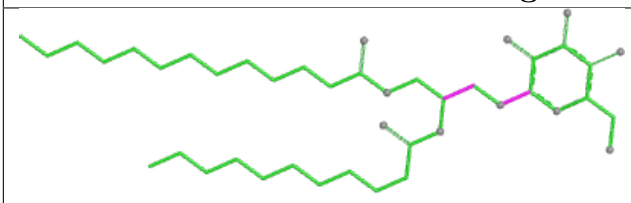


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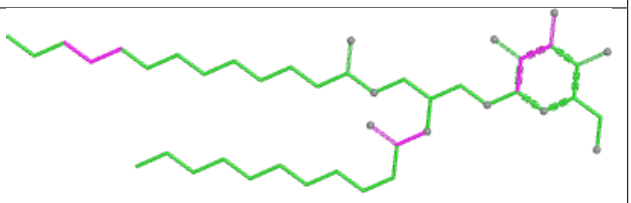


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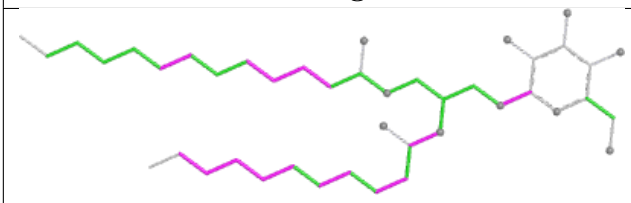
Ligand LMG B 849



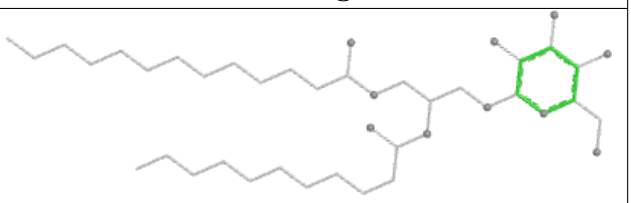
Bond lengths



Bond angles

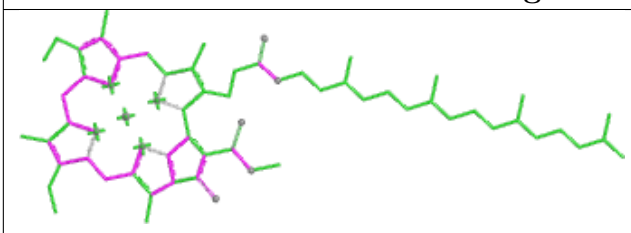


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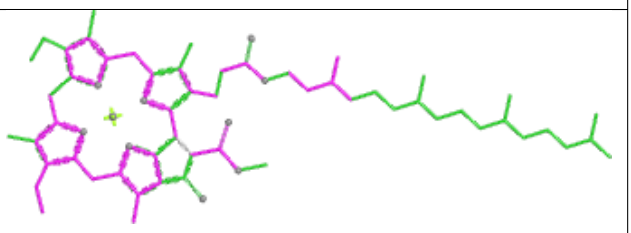


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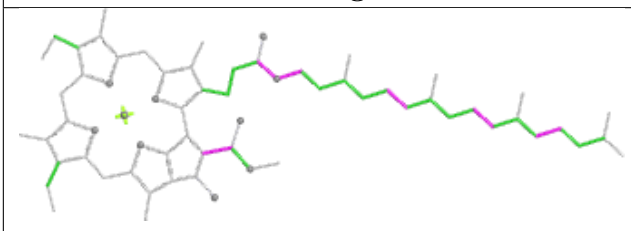
Ligand CLA A 815



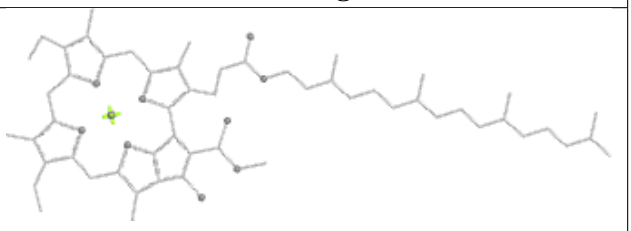
Bond lengths



Bond angles



Torsions

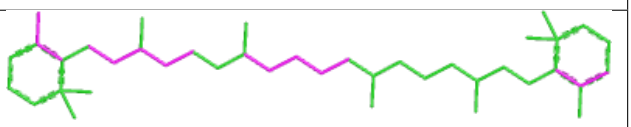


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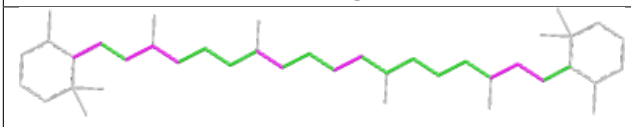
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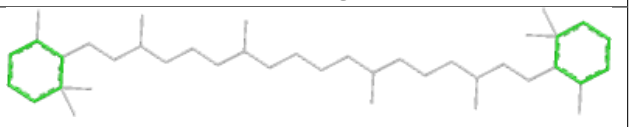
Bond lengths



Bond angles

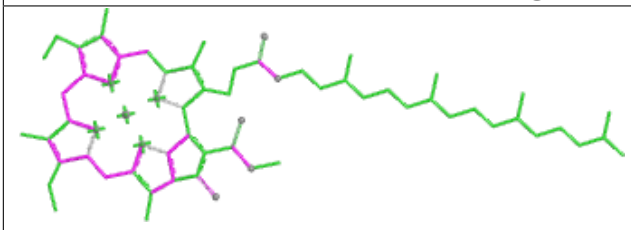


Torsions

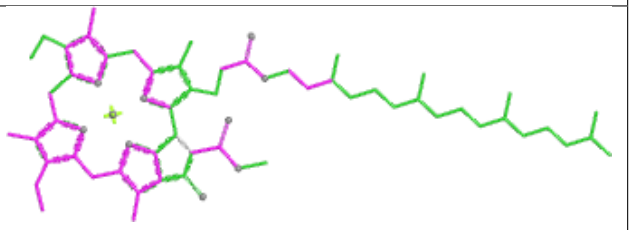


Rings

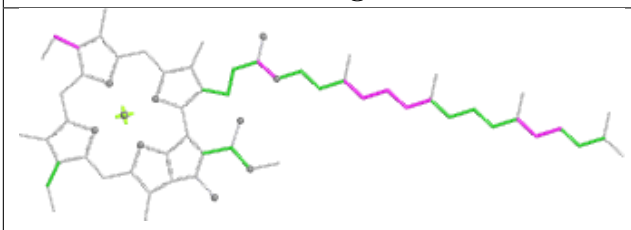
Ligand CLA 7 309



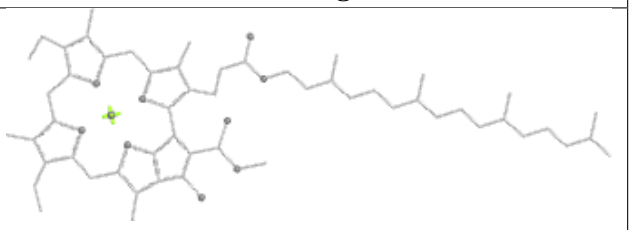
Bond lengths



Bond angles

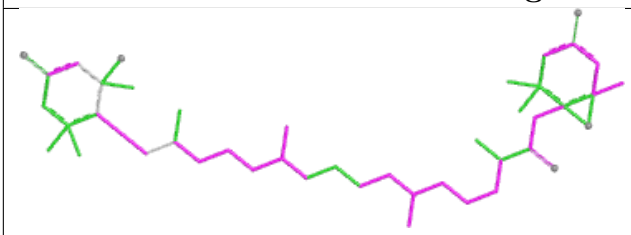


Torsions



Rings

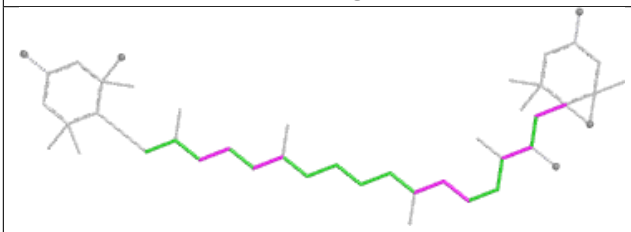
Ligand A86 13 313



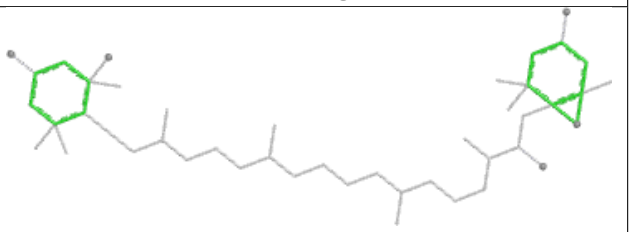
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Bond angles

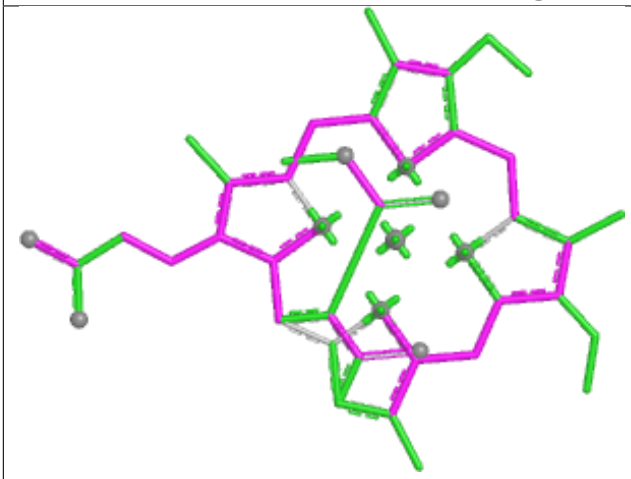


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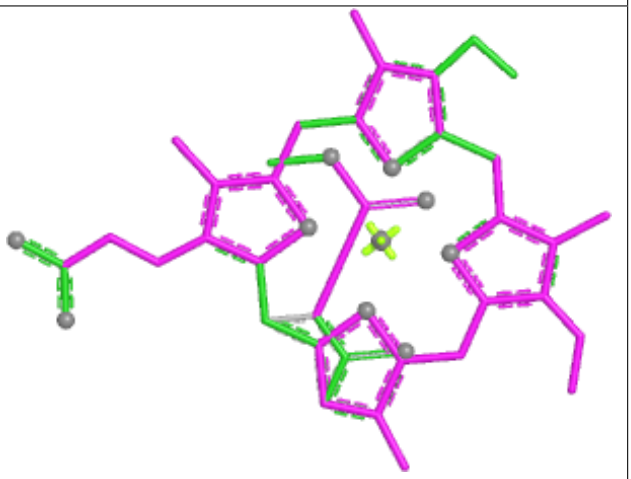


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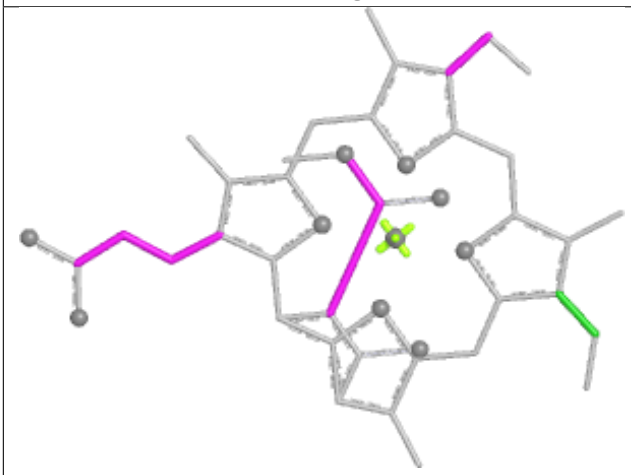
Ligand KC1 6 311



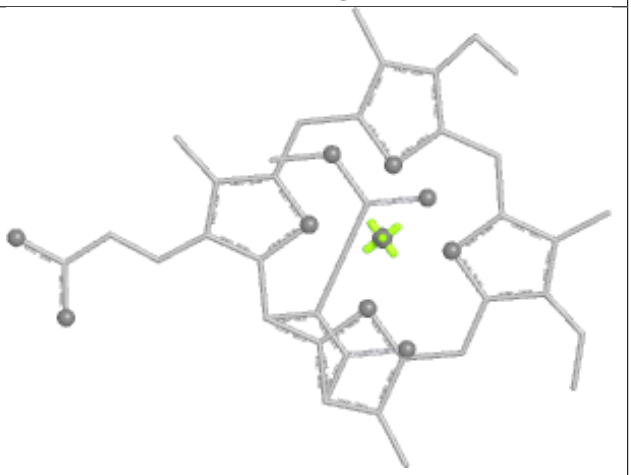
Bond lengths



Bond angles

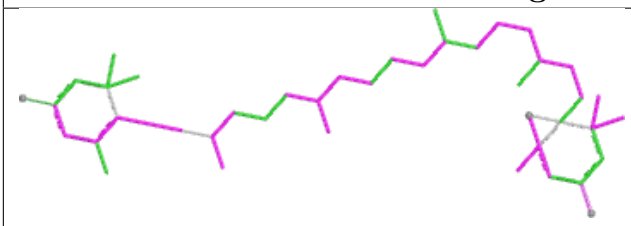


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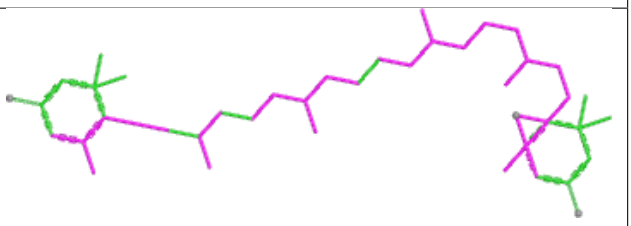


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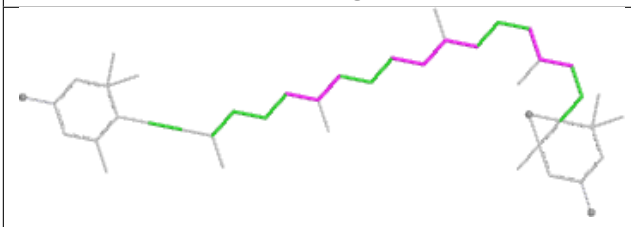
Ligand DD6 5 313



Bond lengths



Bond angles

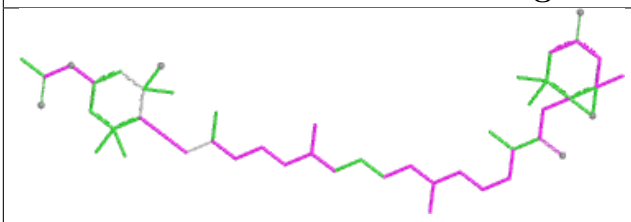


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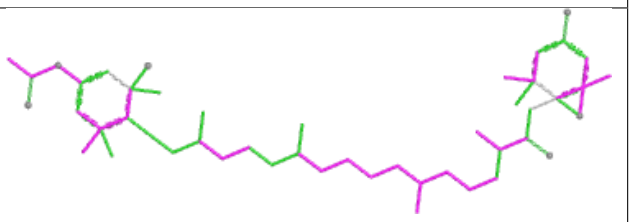


Rings

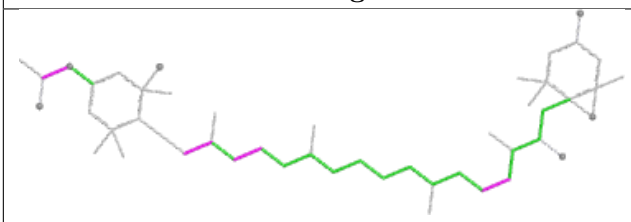
Ligand A86 5 315



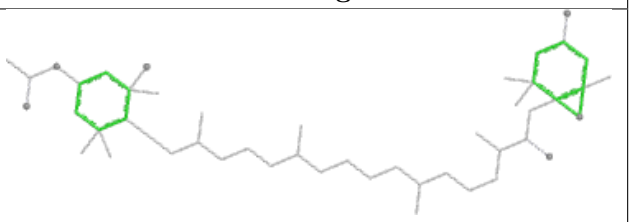
Bond lengths



Bond angles

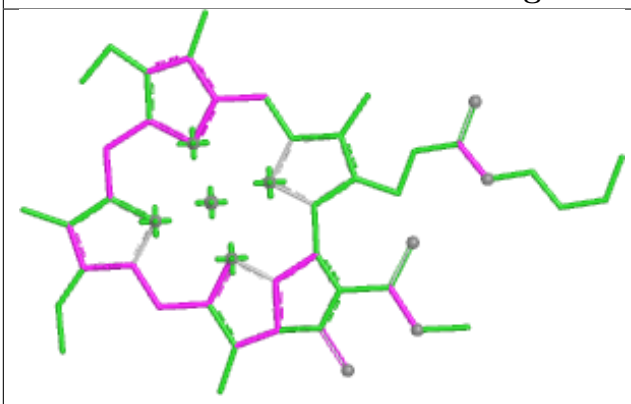


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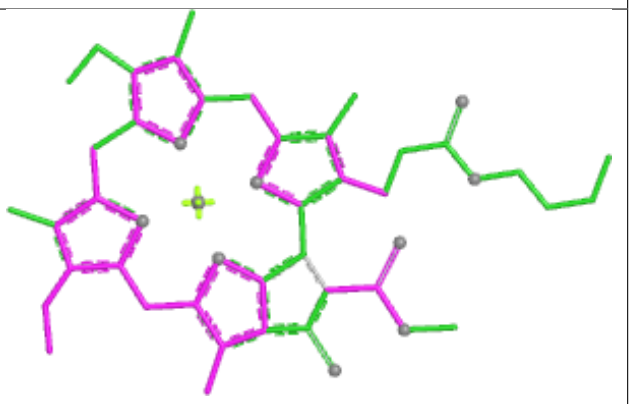


Rings

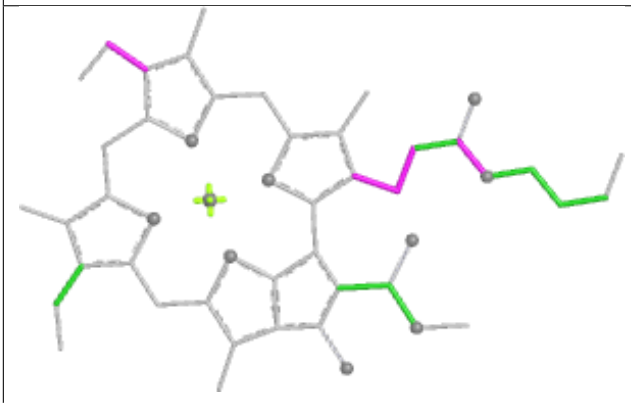
Ligand CLA A 817



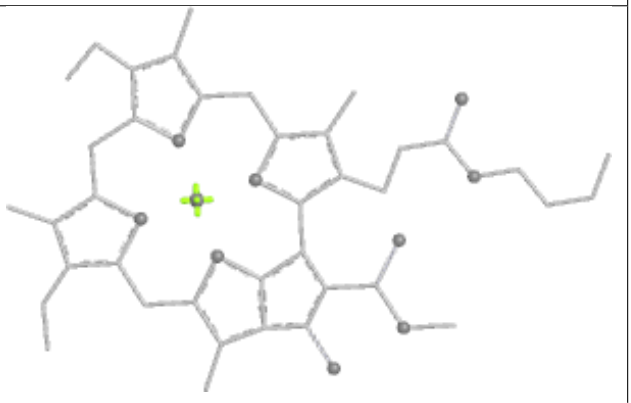
Bond lengths



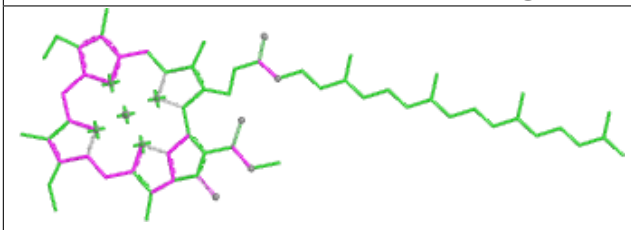
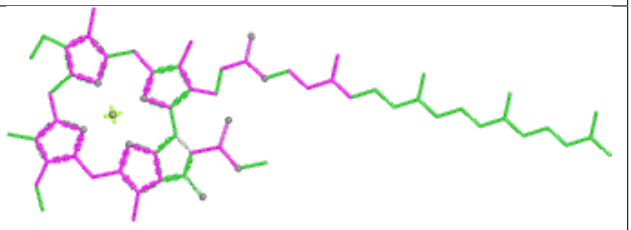
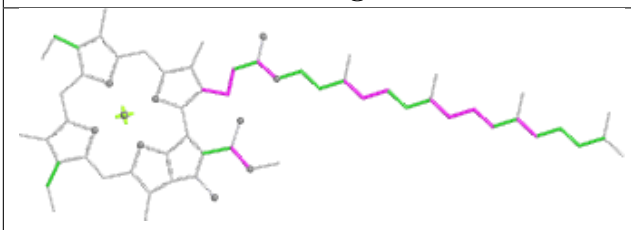
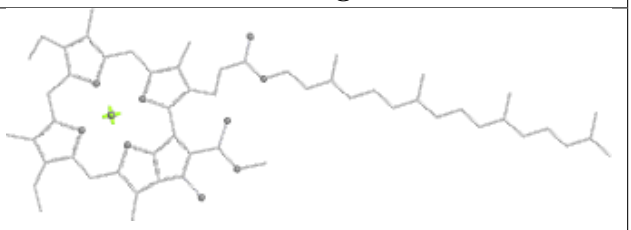
Bond angles

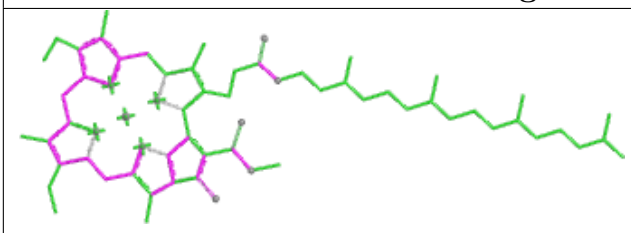
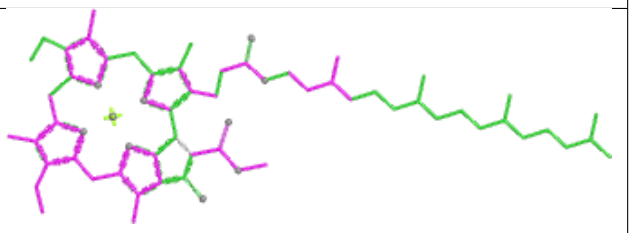
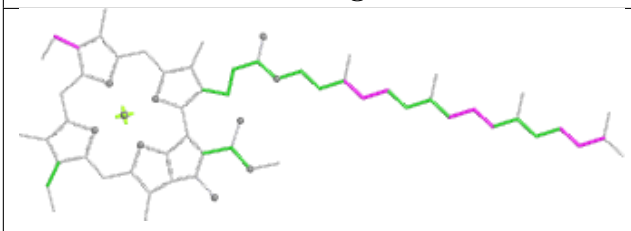
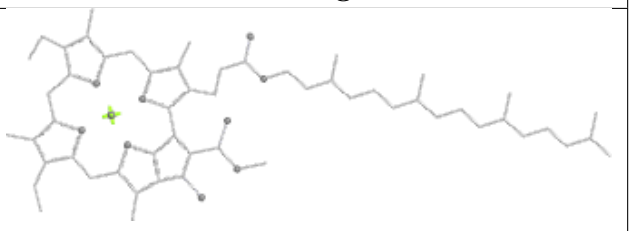


Torsions

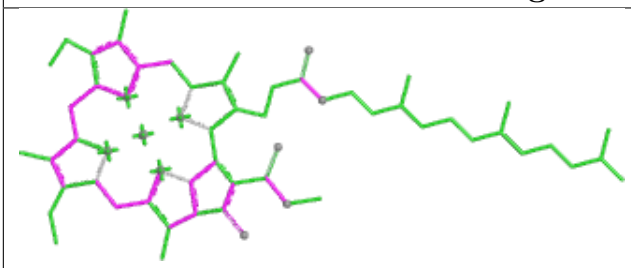


Rings

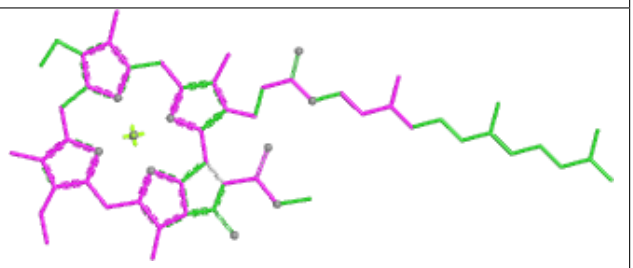
Ligand CLA 11 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 16 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

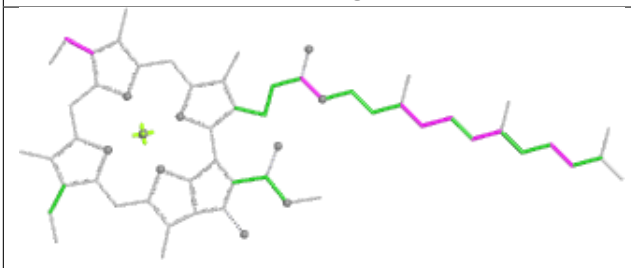
Ligand CLA 3 302



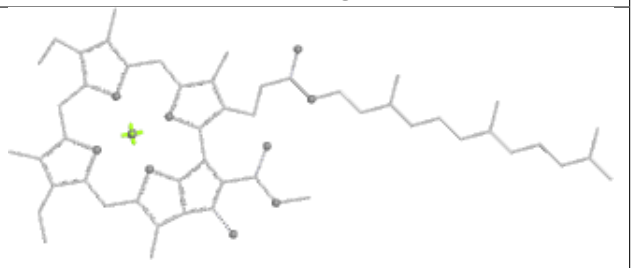
Bond lengths



Bond angles

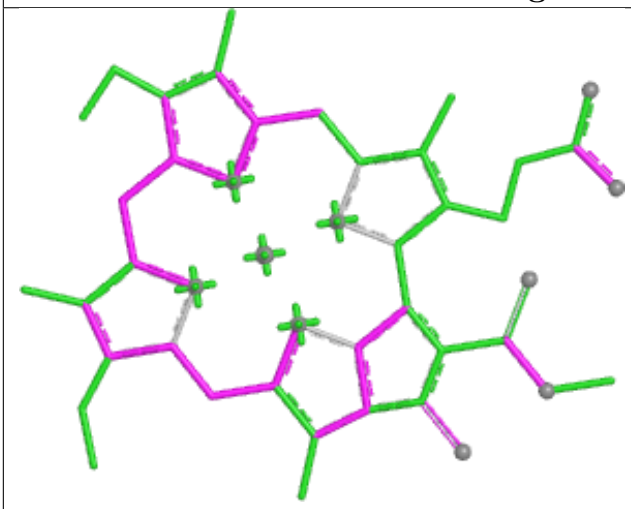


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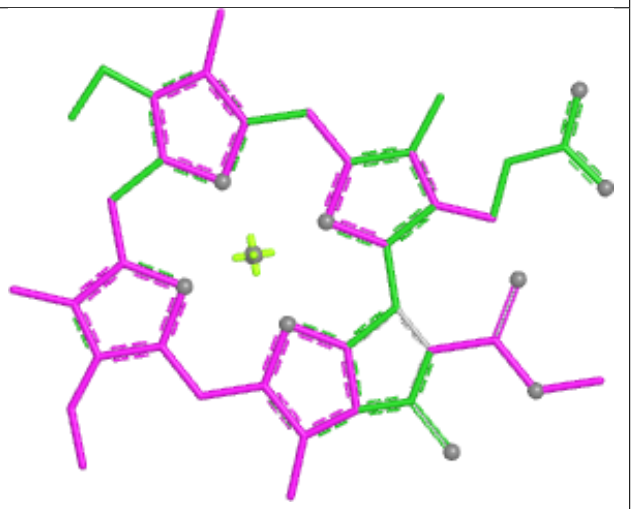


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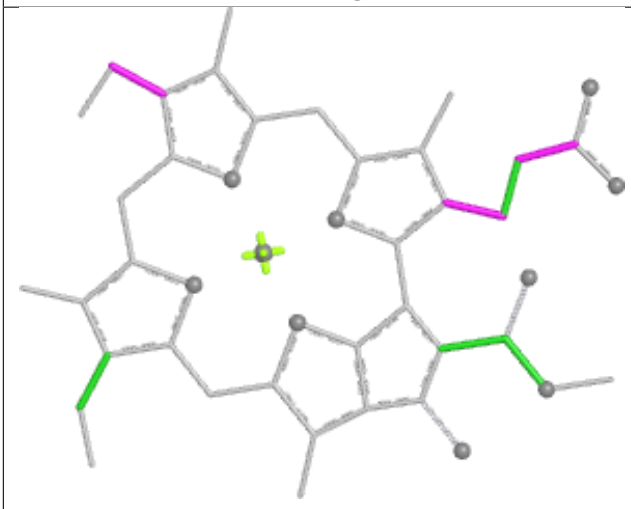
Ligand CLA 3 310



Bond lengths



Bond angles

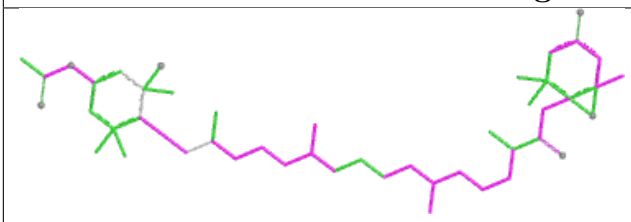


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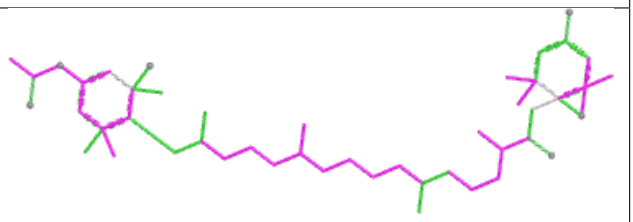


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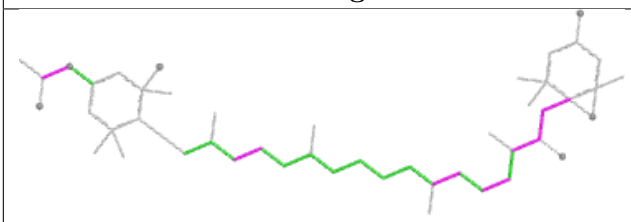
Ligand A86 5 301



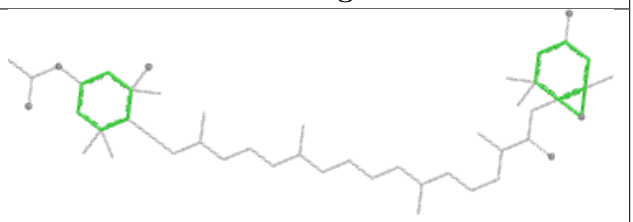
Bond lengths



Bond angles

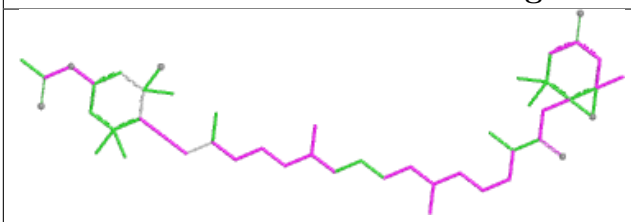


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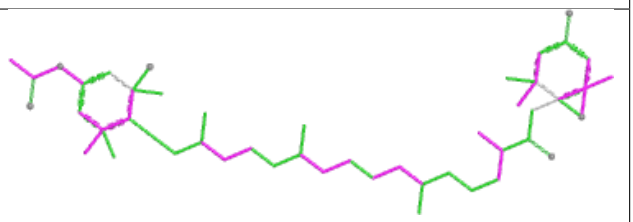


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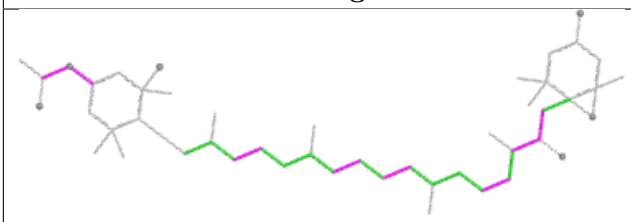
Ligand A86 10 317



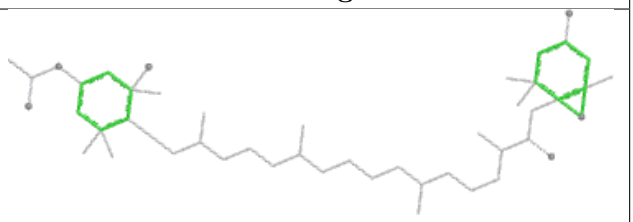
Bond lengths



Bond angles

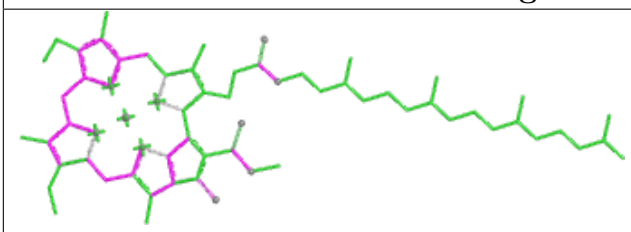


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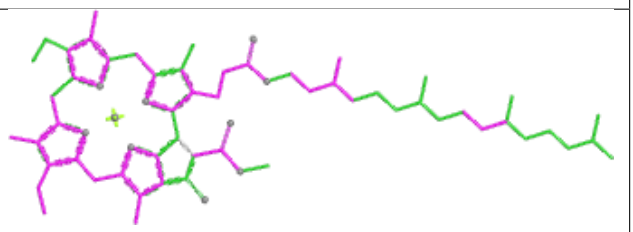


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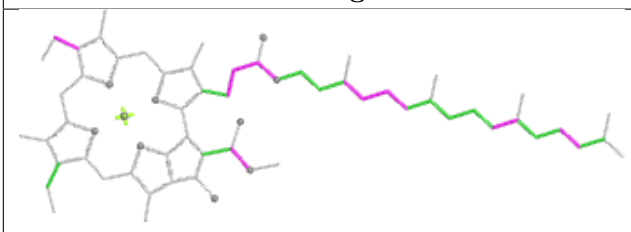
Ligand CLA 12 302



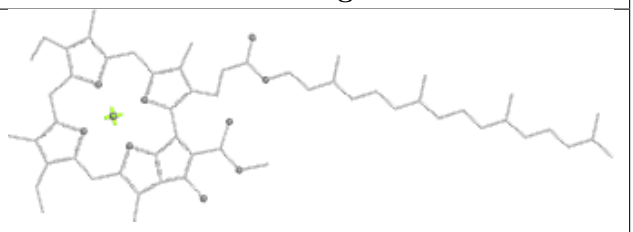
Bond lengths



Bond angles

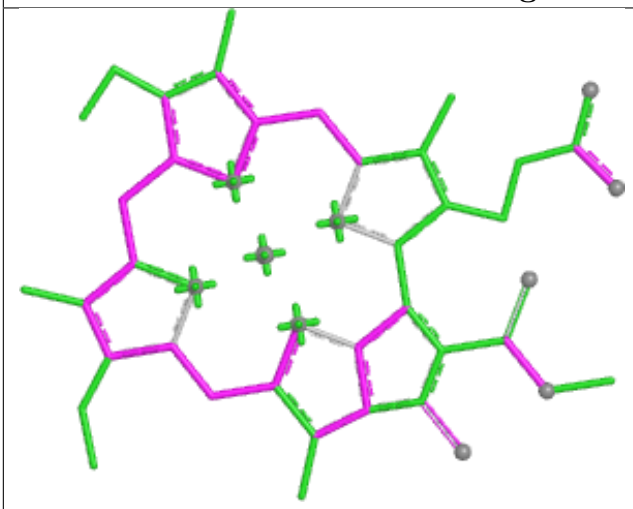


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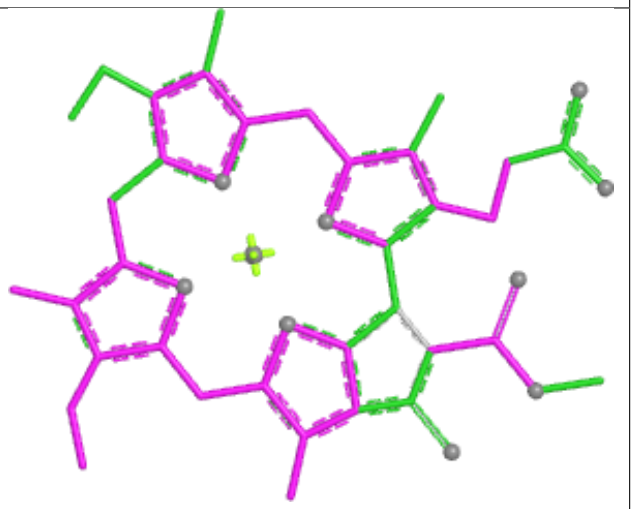


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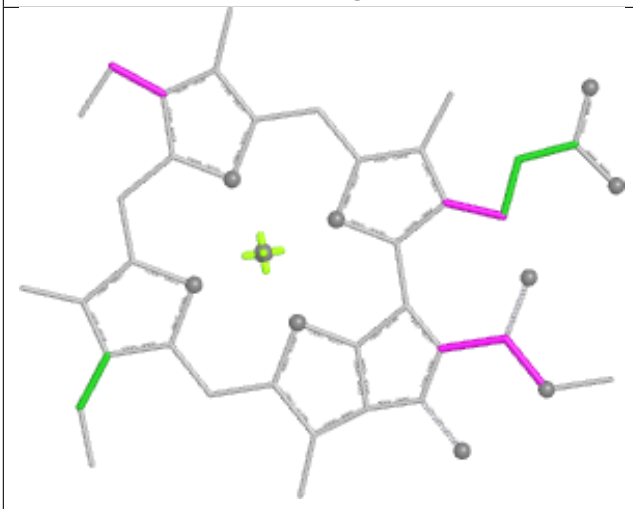
Ligand CLA 15 312



Bond lengths



Bond angles

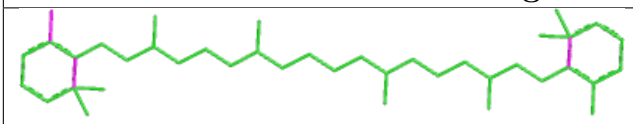


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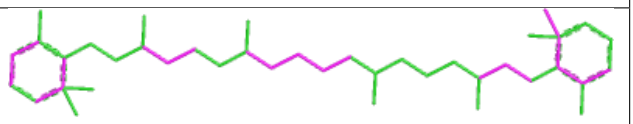


Rings

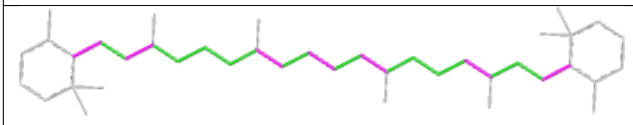
Ligand BCR B 844



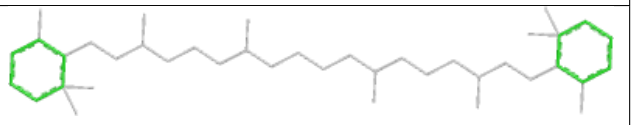
Bond lengths



Bond angles

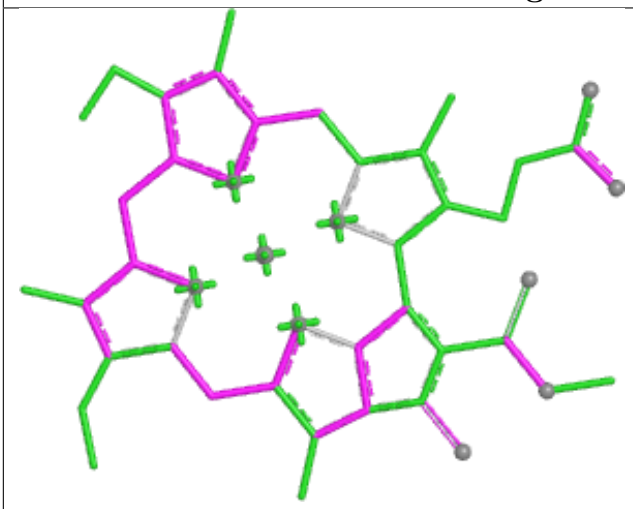


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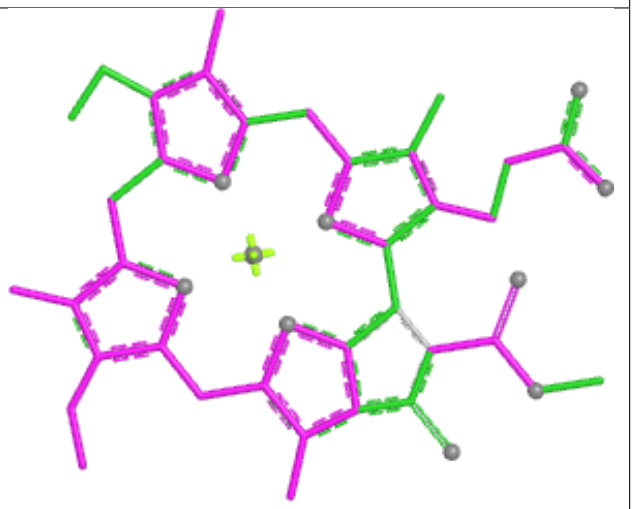


Rings

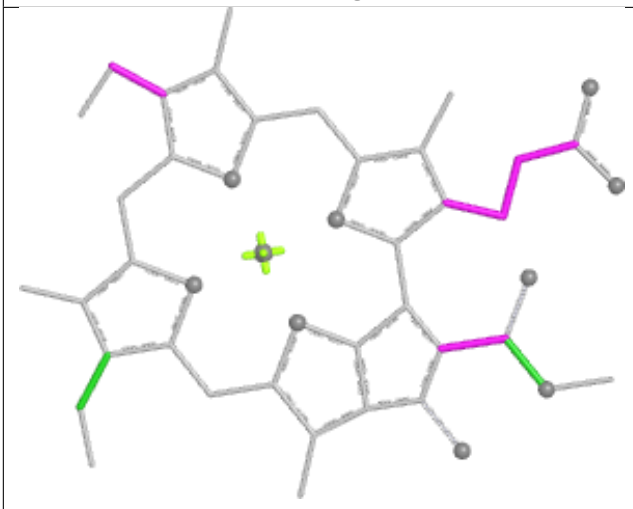
Ligand CLA F 203



Bond lengths



Bond angles

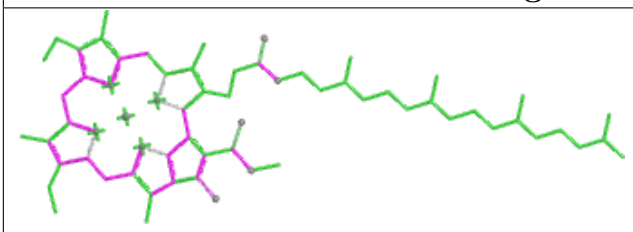


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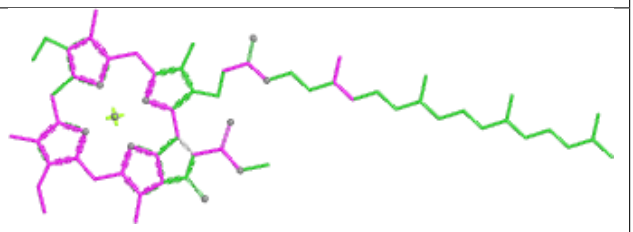


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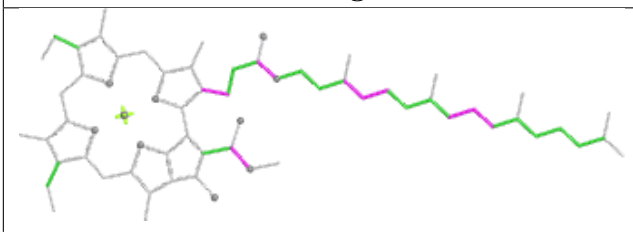
Ligand CLA B 833



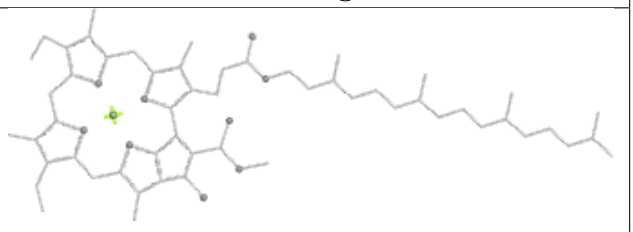
Bond lengths



Bond angles

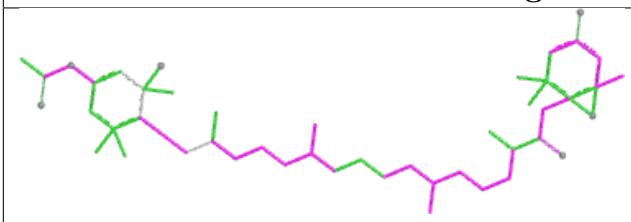


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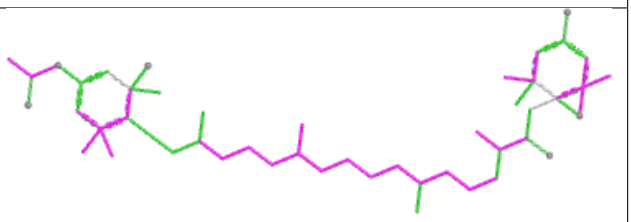


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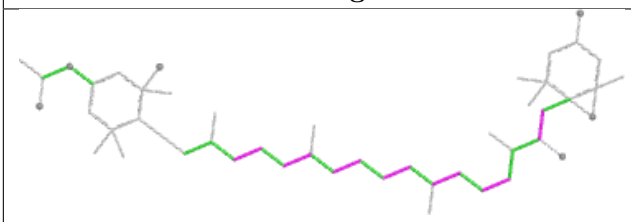
Ligand A86 14 315



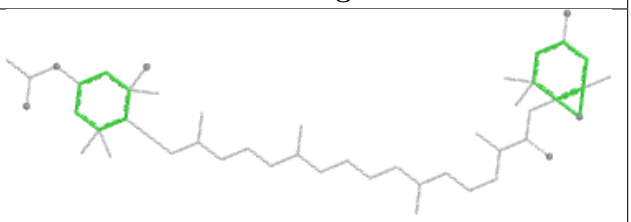
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Bond angles

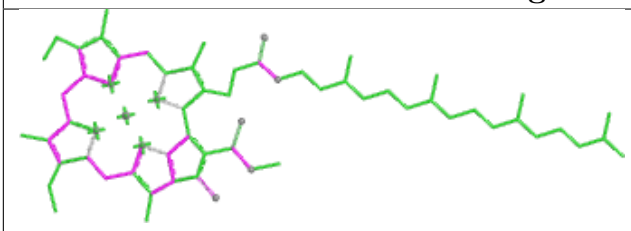


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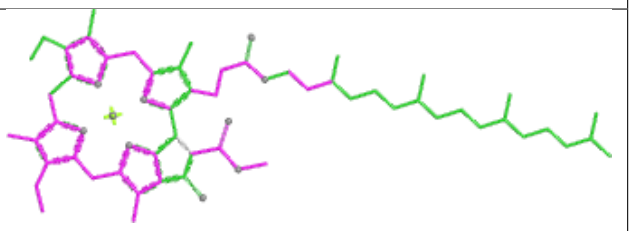


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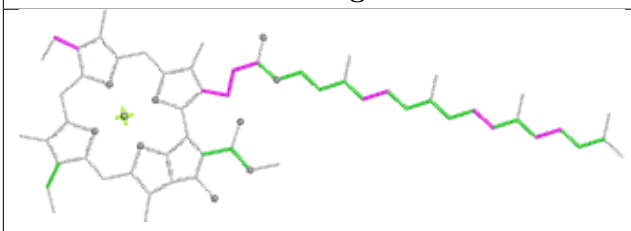
Ligand CLA 2 308



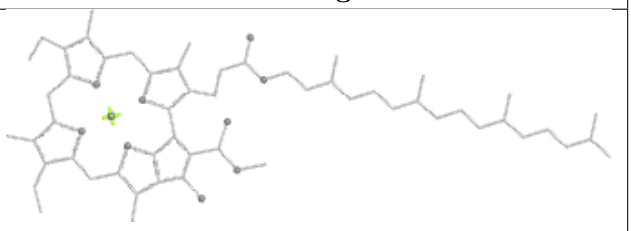
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Bond angles

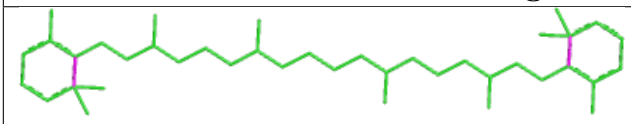


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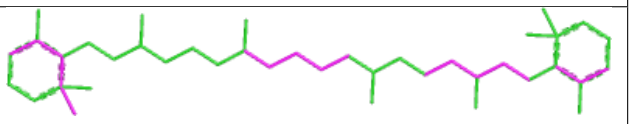


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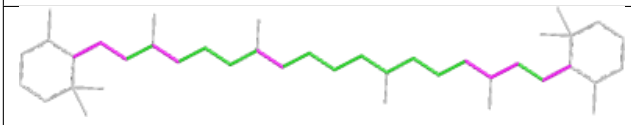
Ligand BCR L 204



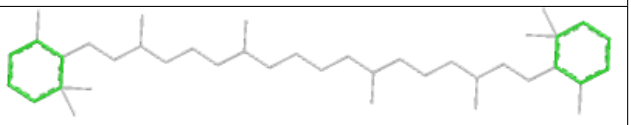
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Bond angles

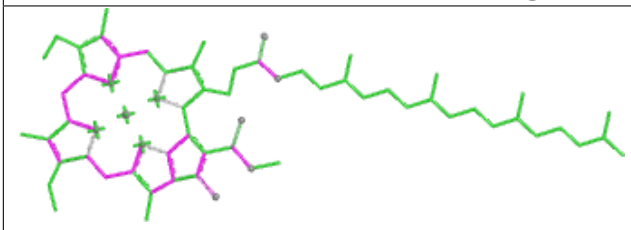


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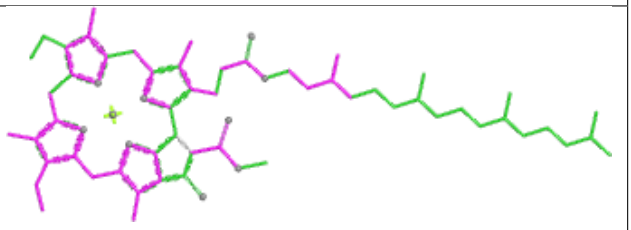


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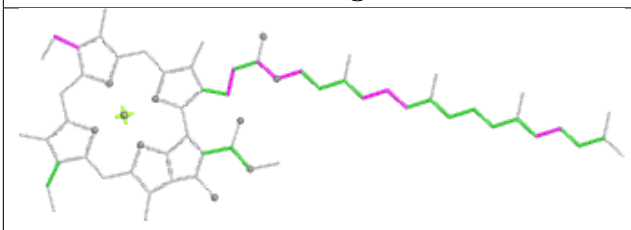
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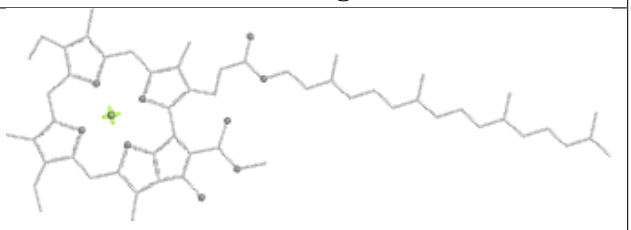
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Bond angles

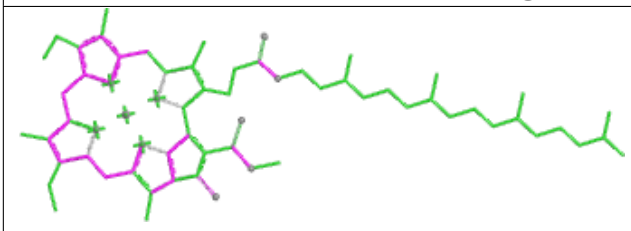


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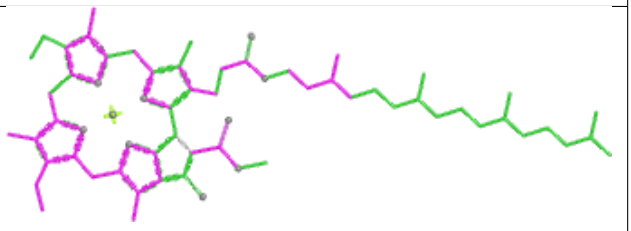


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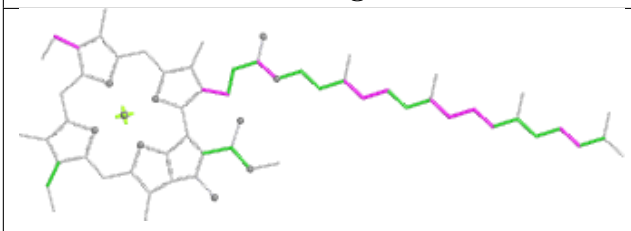
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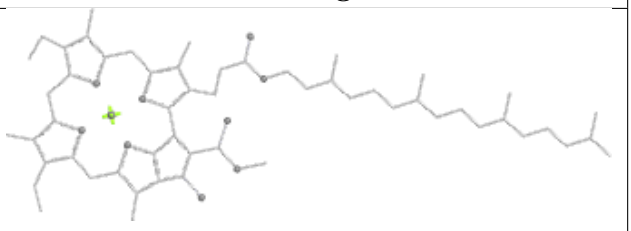
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Bond angles

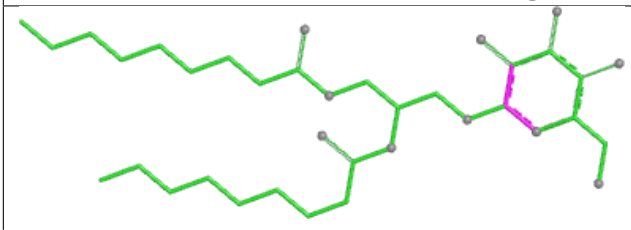


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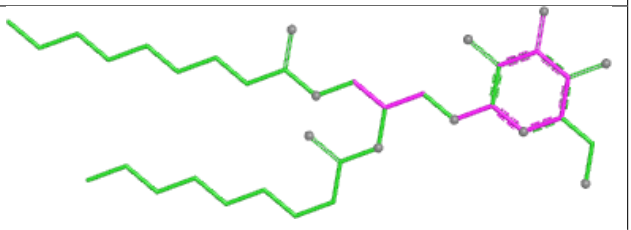


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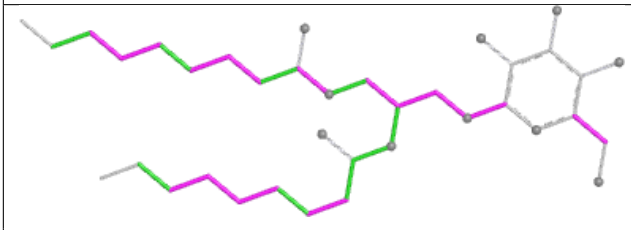
Ligand LMG 3 317



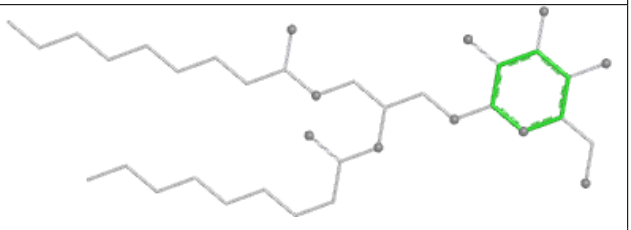
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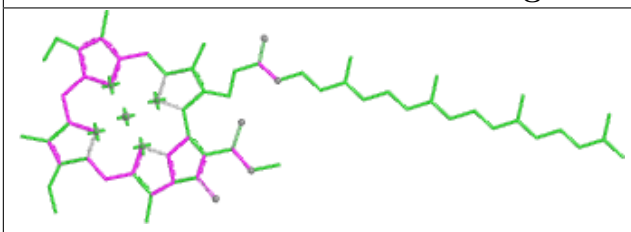


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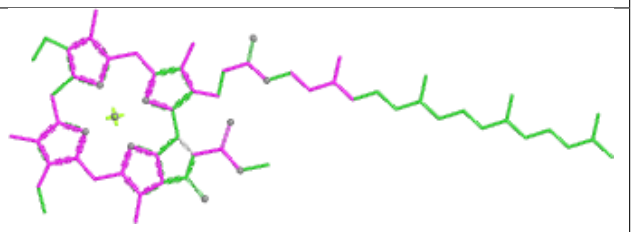


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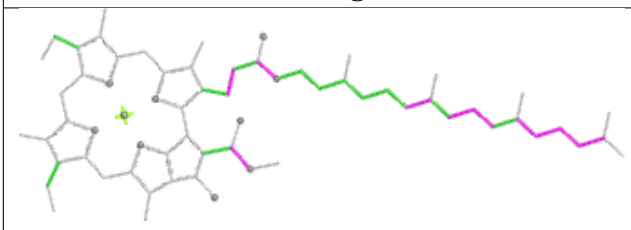
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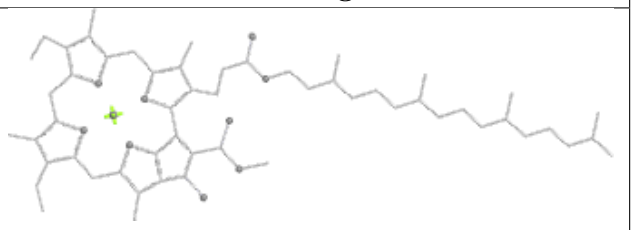
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Bond angles

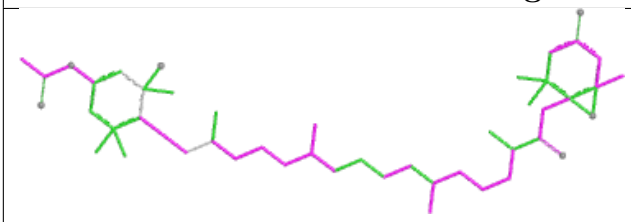


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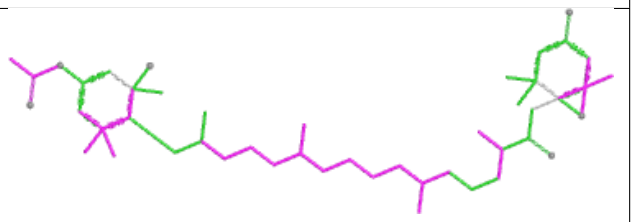


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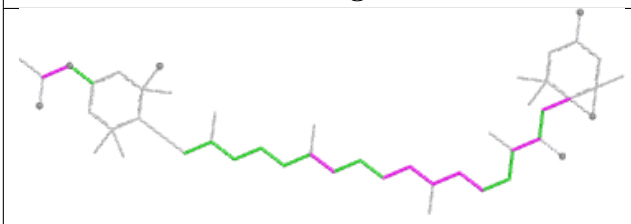
Ligand A86 2u 203



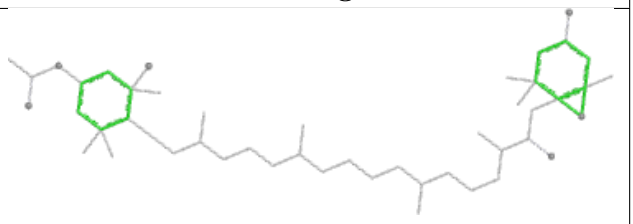
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Bond angles

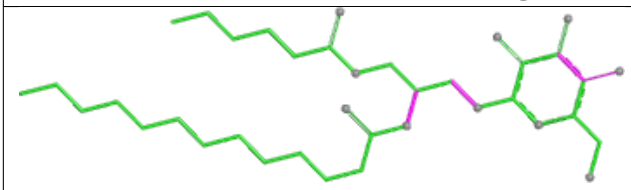


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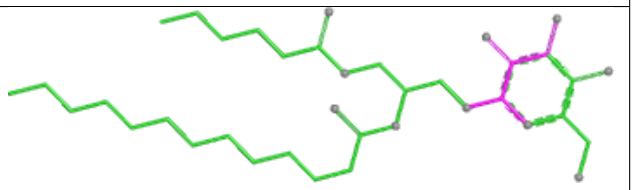


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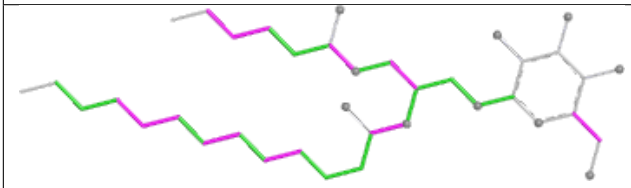
Ligand LMG 14 321



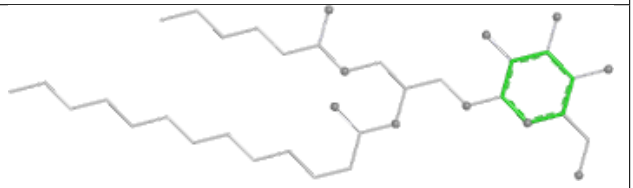
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Bond angles

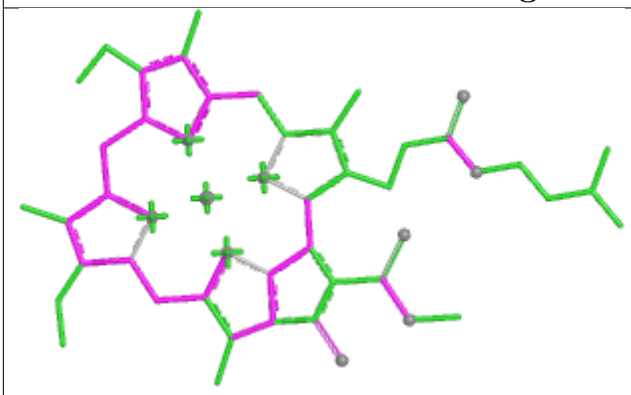


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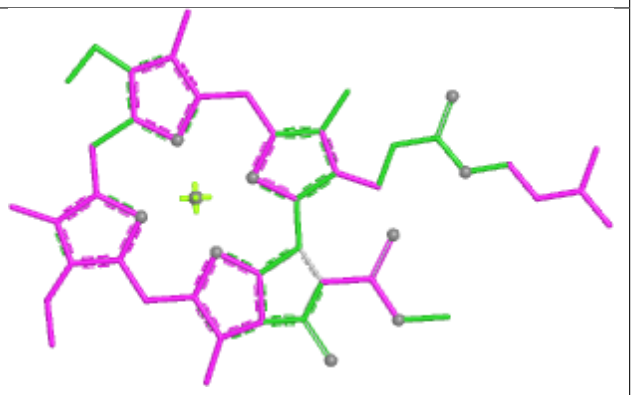


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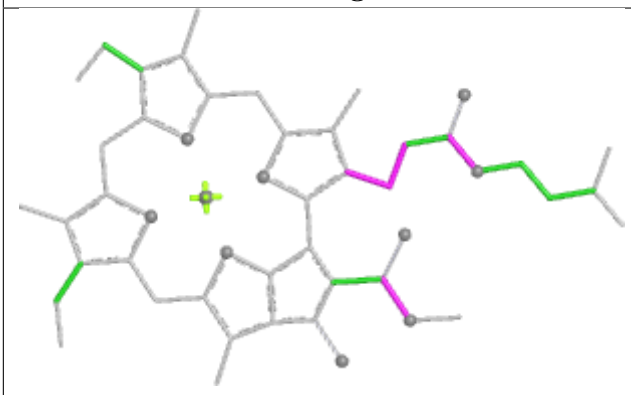
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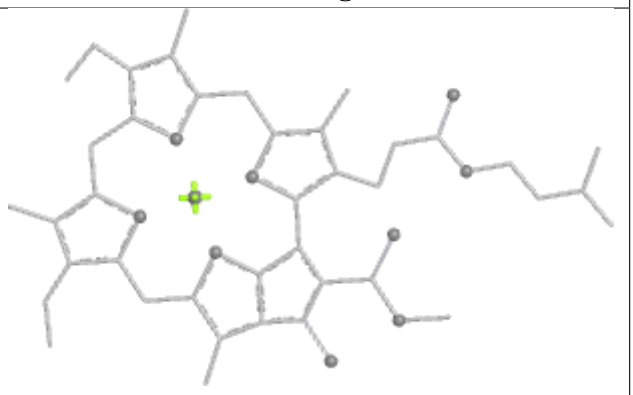
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Bond angles

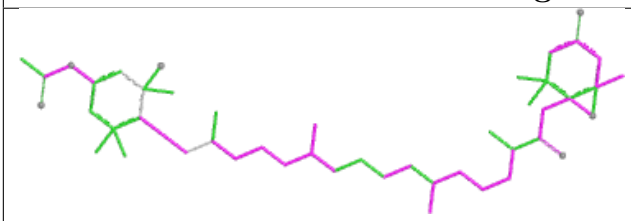


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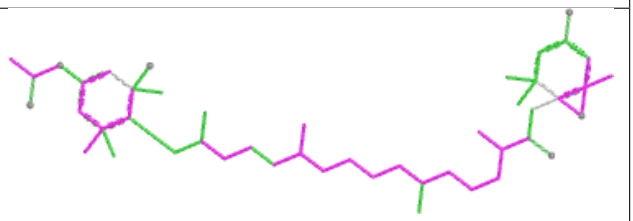


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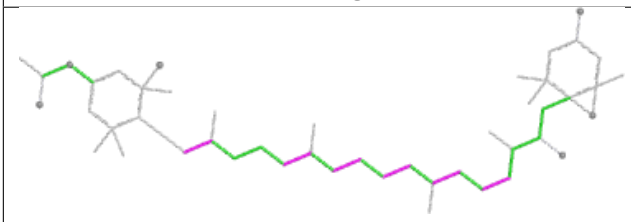
Ligand A86 6 320



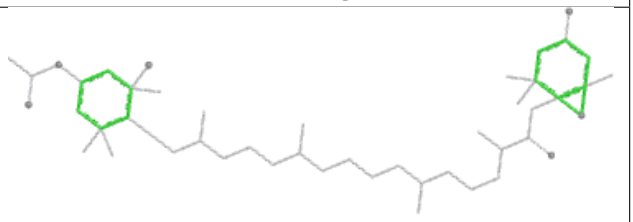
Bond lengths



Bond angles

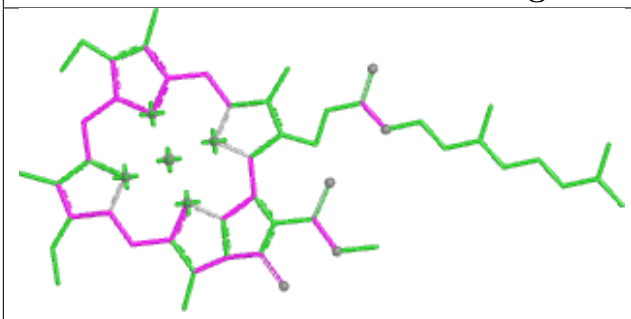


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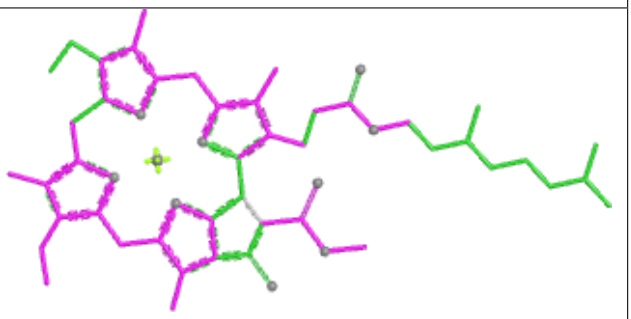


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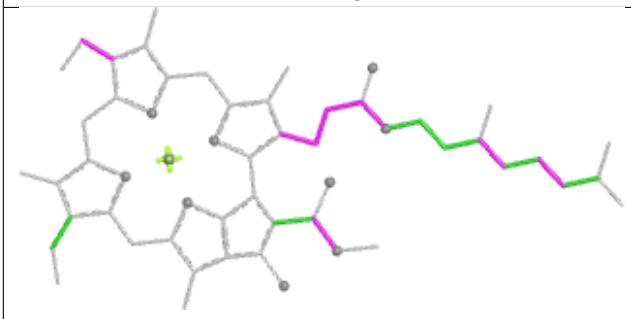
Ligand CLA 2 303



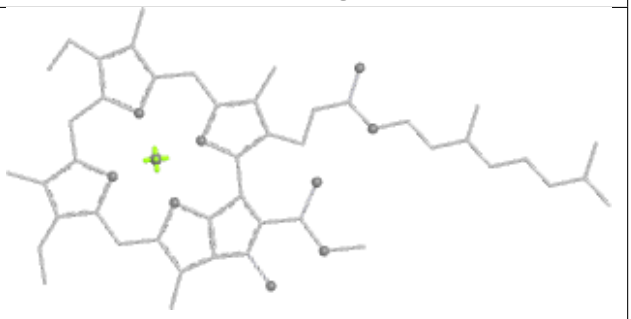
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Bond angles

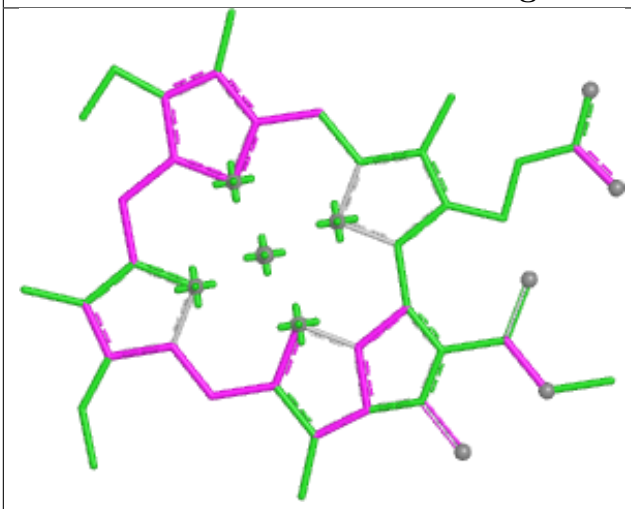


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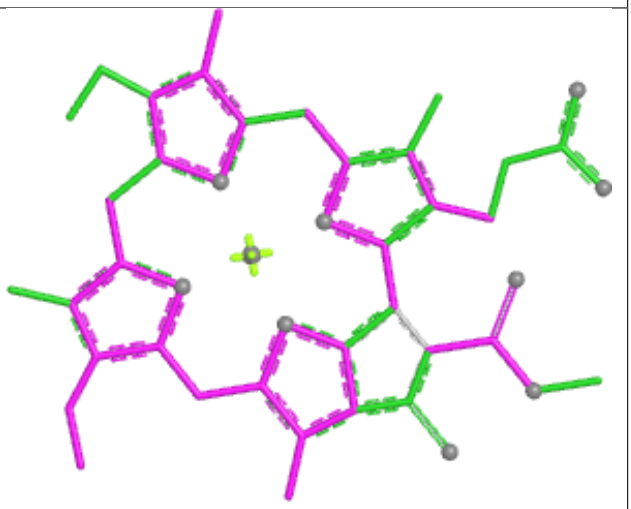


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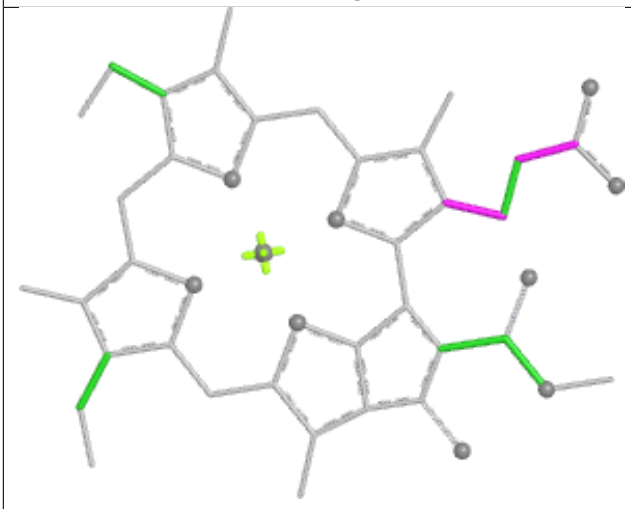
Ligand CLA 14 309



Bond lengths



Bond angles

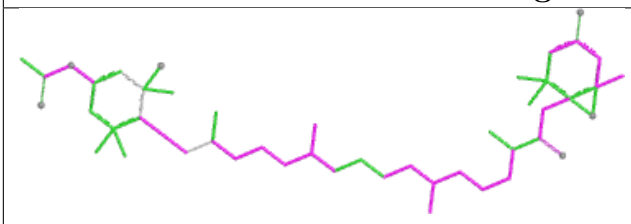


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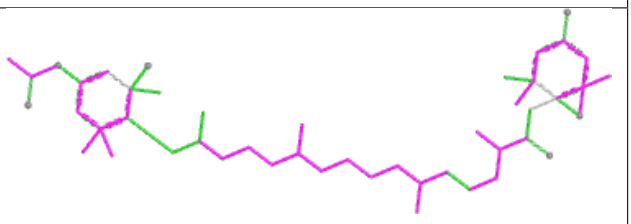


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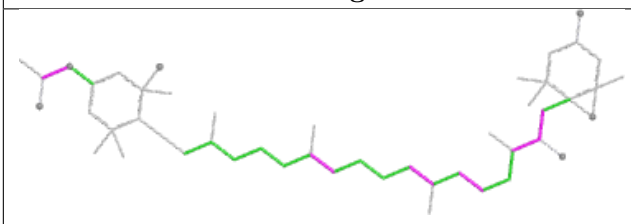
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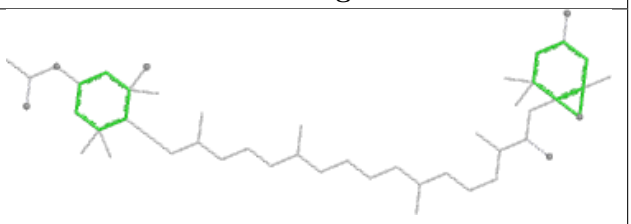
Bond lengths



Bond angles

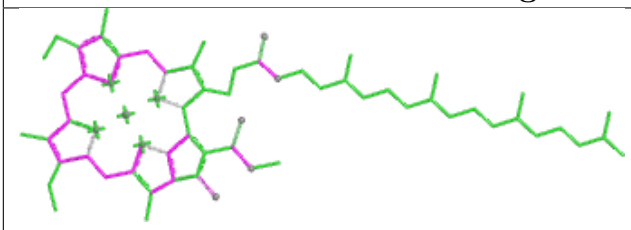


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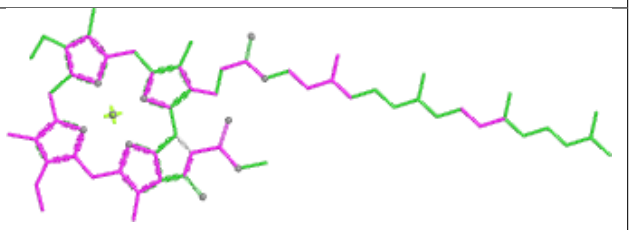


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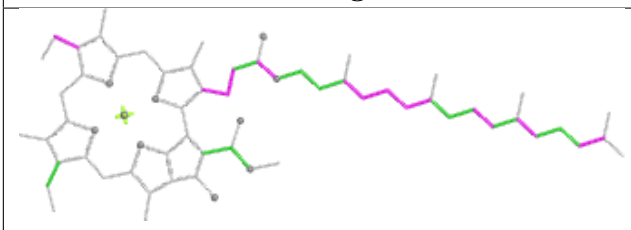
Ligand CLA 15 302



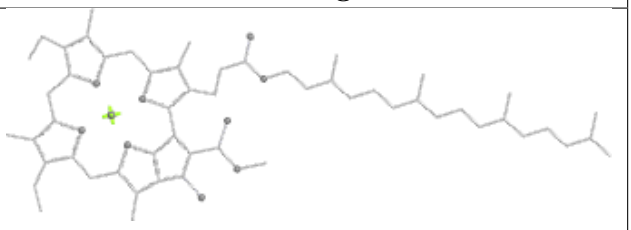
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Bond angles

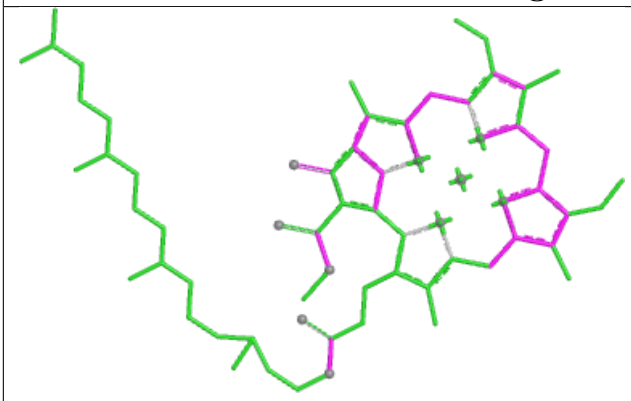


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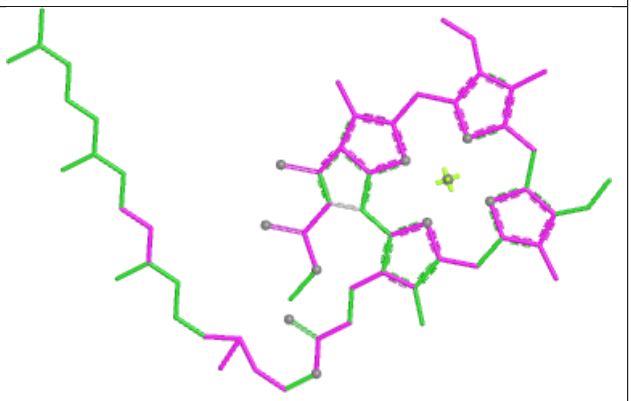


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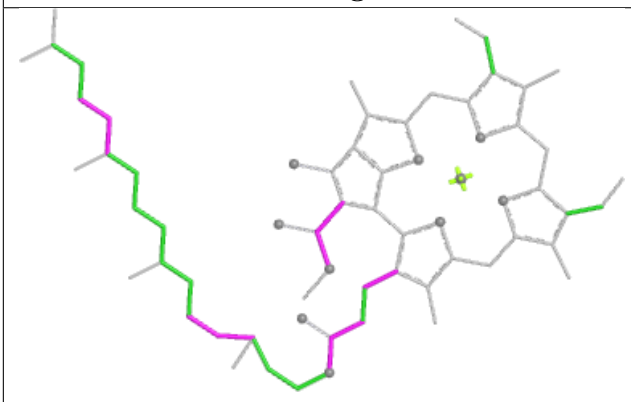
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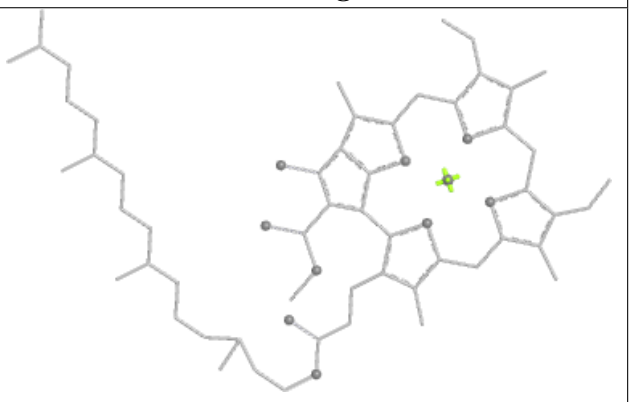
Bond lengths



Bond angles

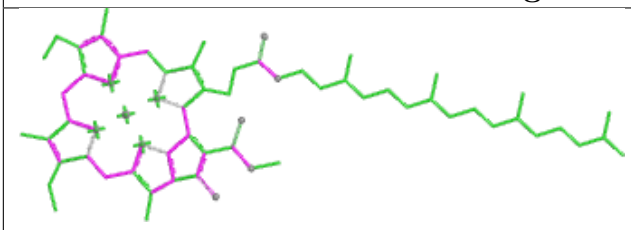


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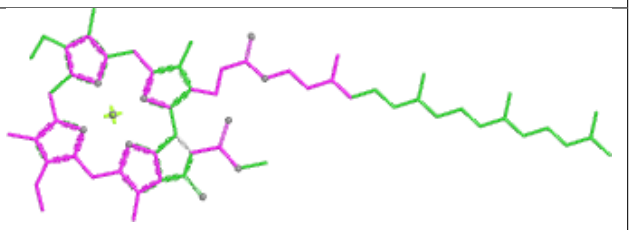


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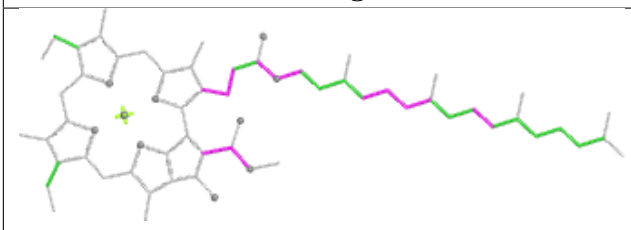
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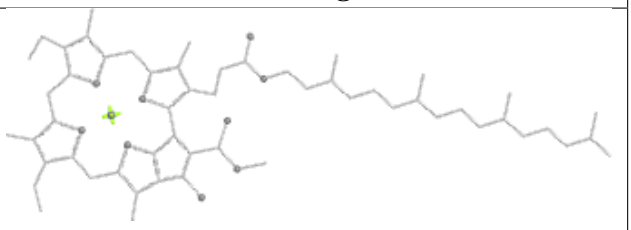
Bond lengths



Bond angles

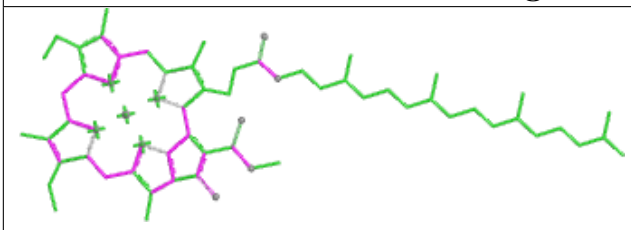


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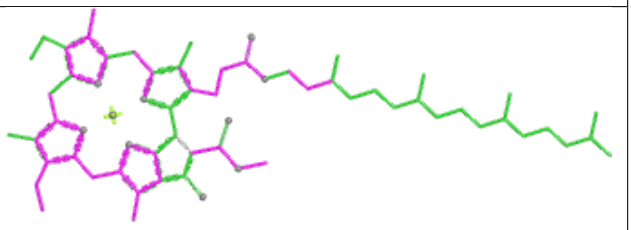


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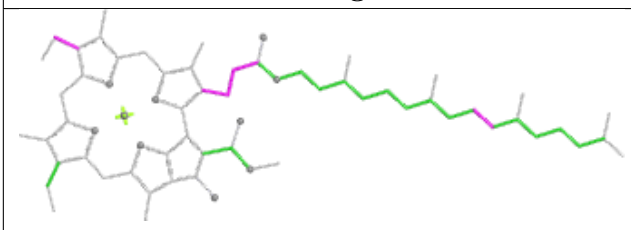
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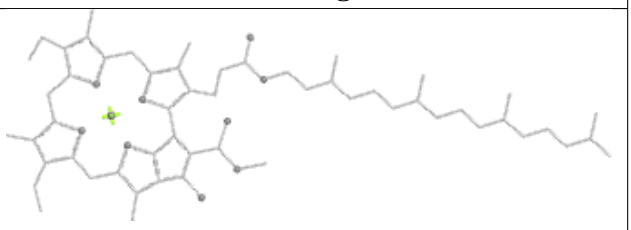
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Bond angles

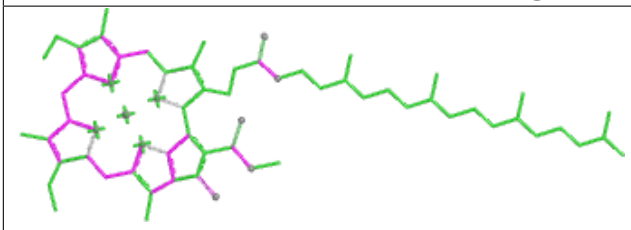


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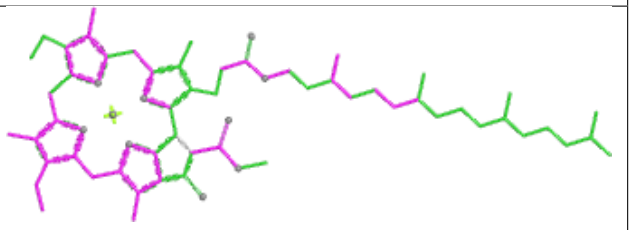


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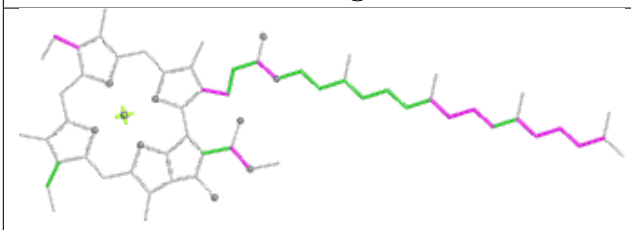
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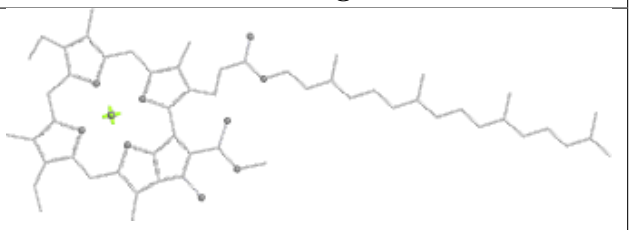
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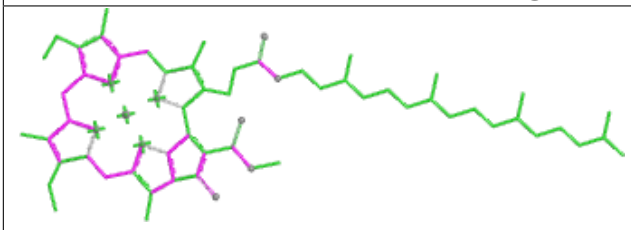


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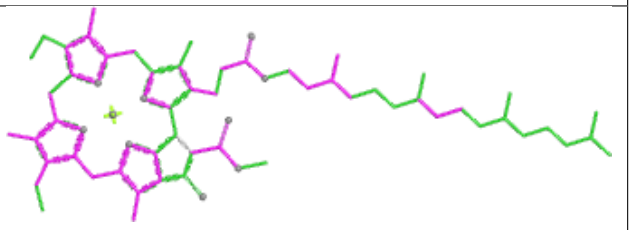


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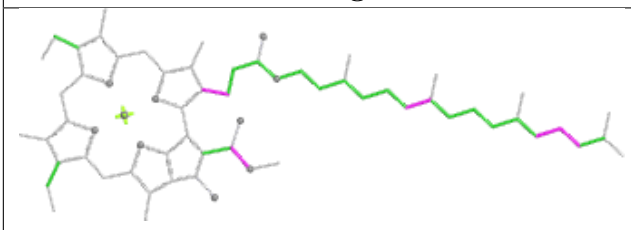
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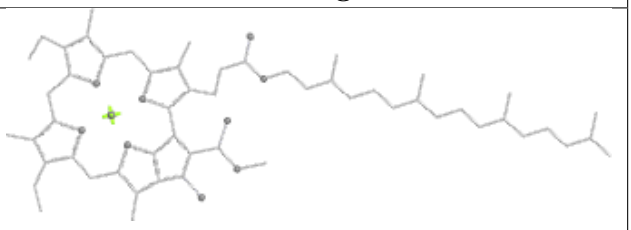
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Bond angles

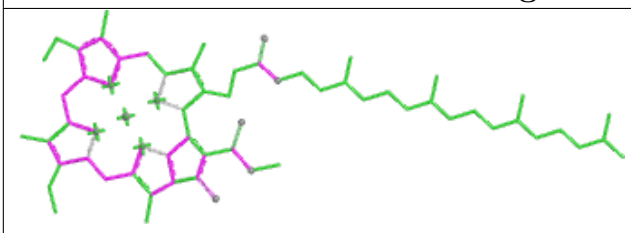


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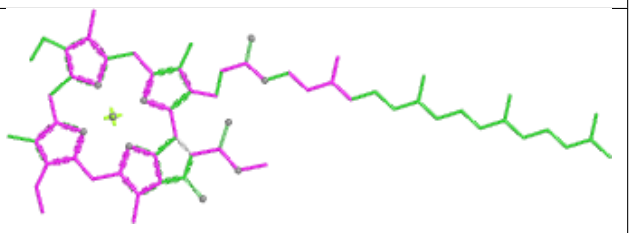


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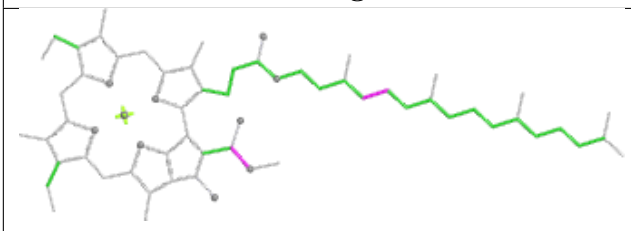
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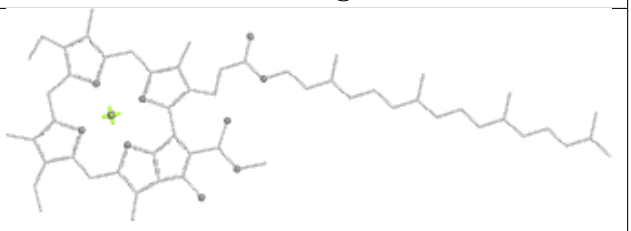
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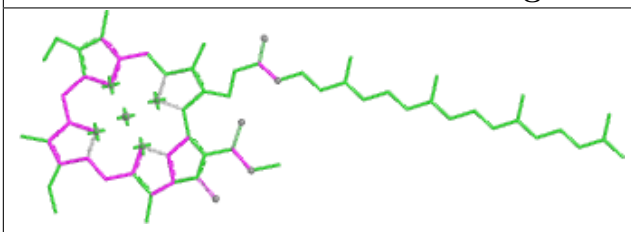


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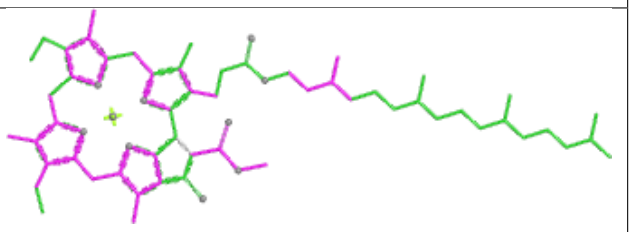


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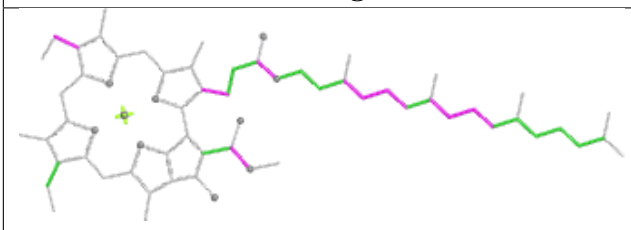
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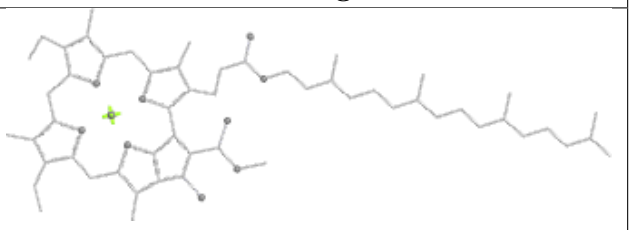
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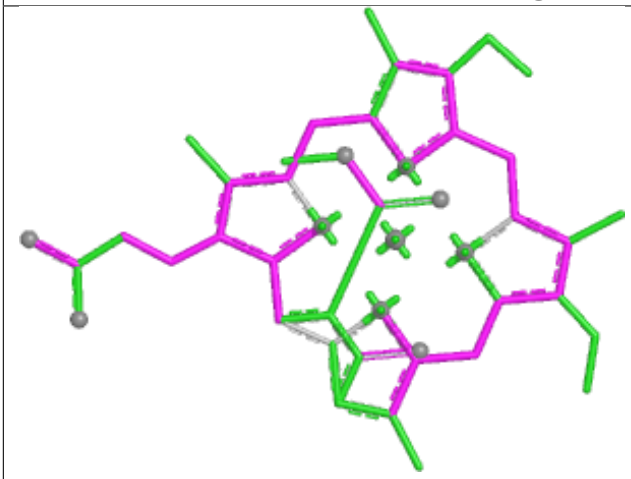


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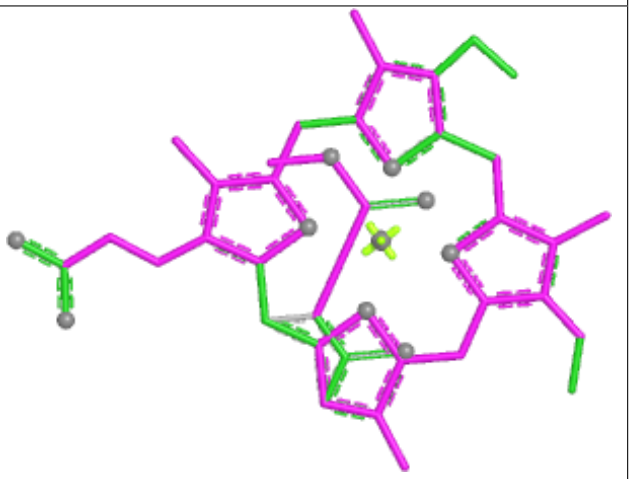


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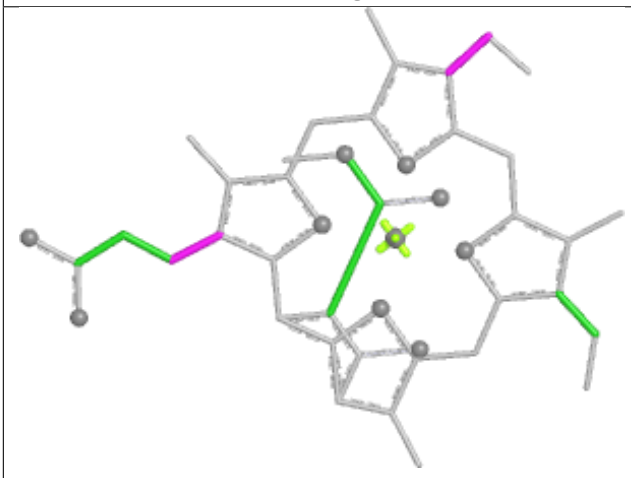
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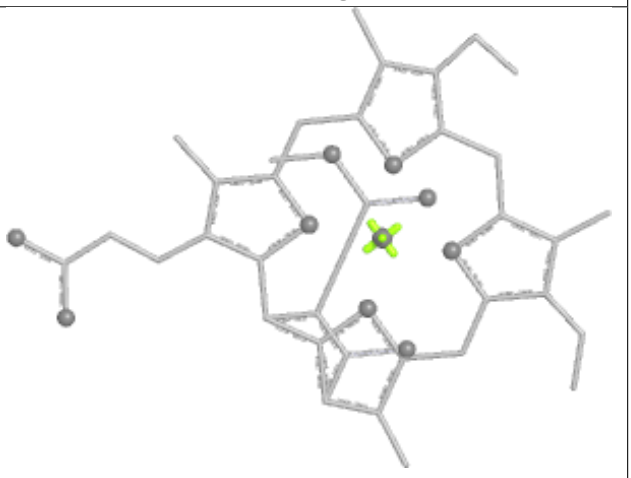
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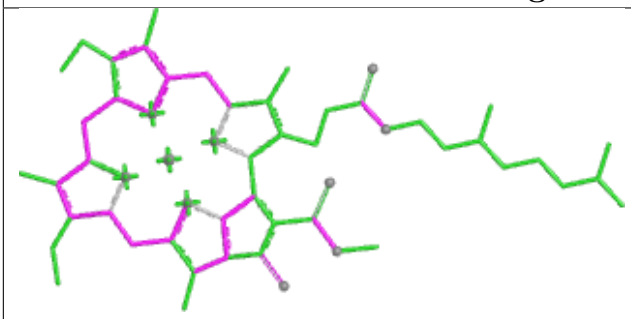


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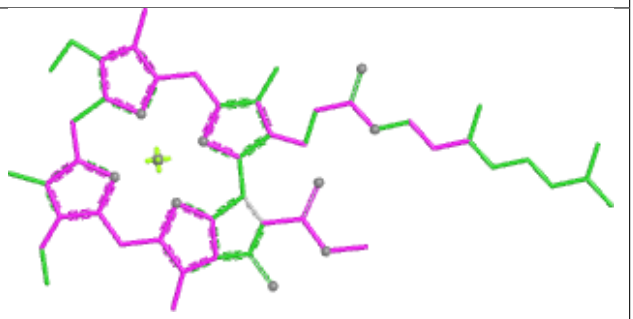


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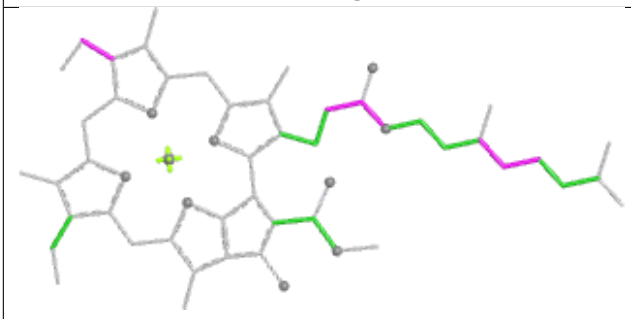
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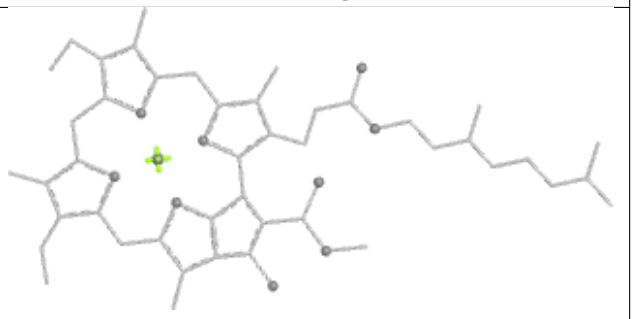
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Bond angles

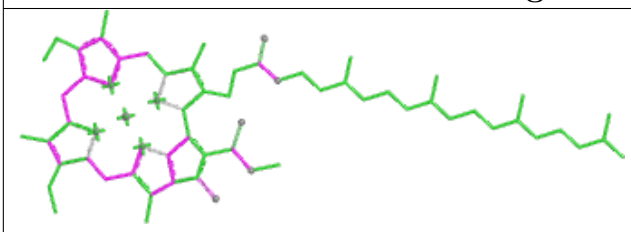


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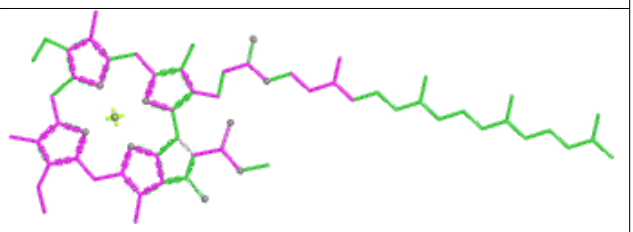


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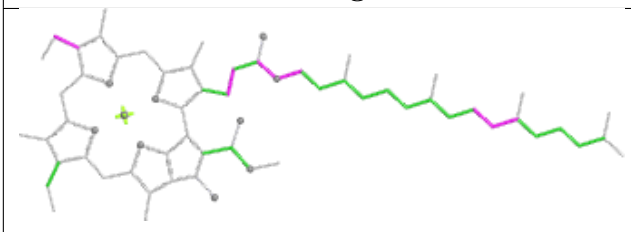
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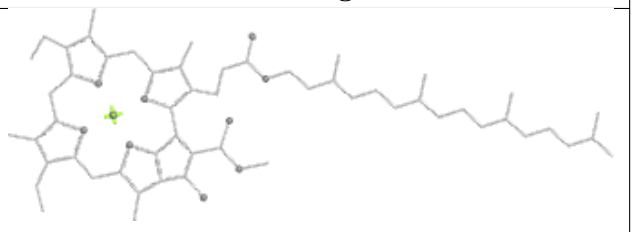
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Bond angles

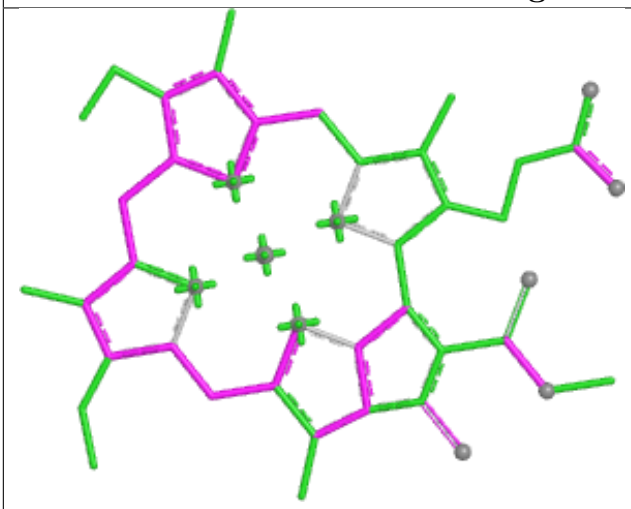


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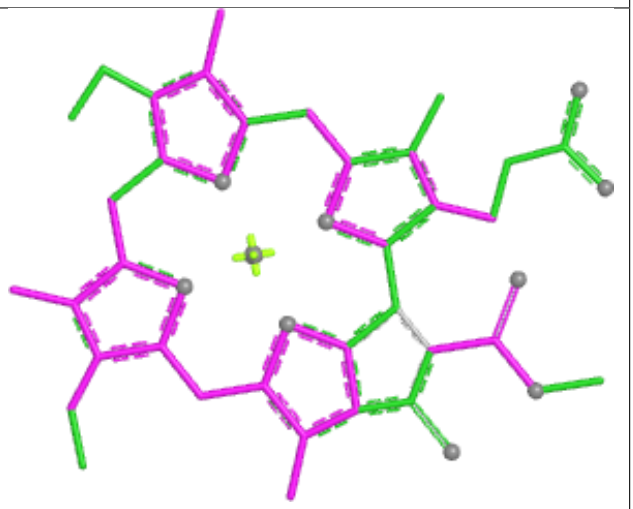


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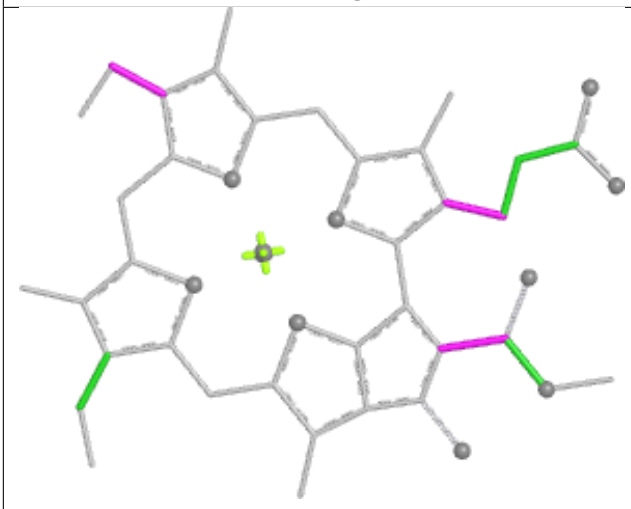
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Bond lengths



Bond angles

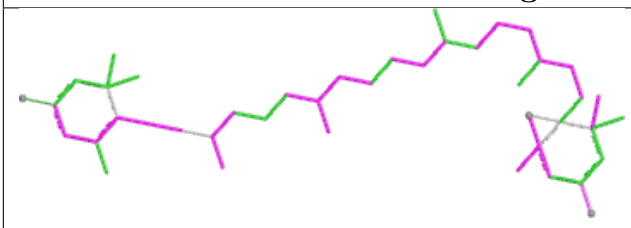


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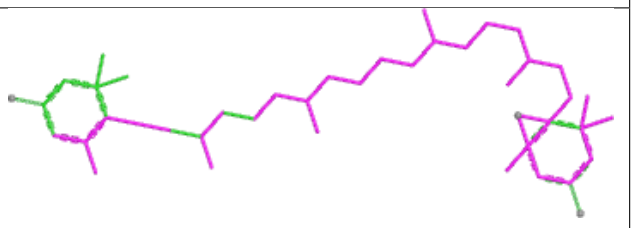


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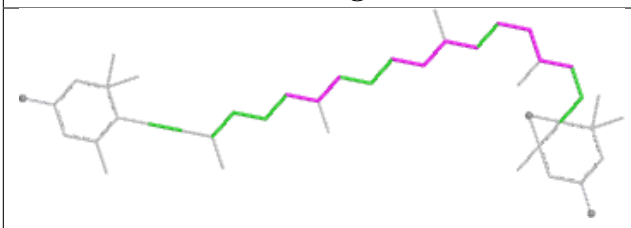
Ligand DD6 11 313



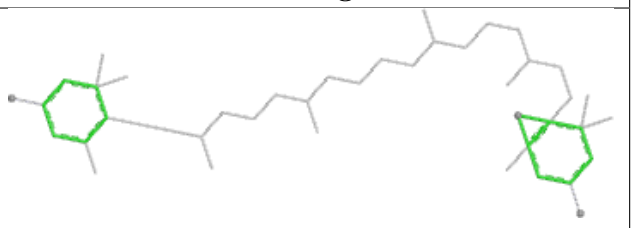
Bond lengths



Bond angles

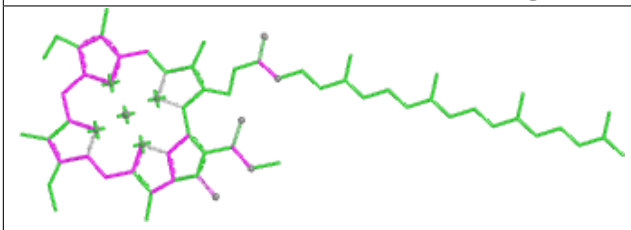


Torsions

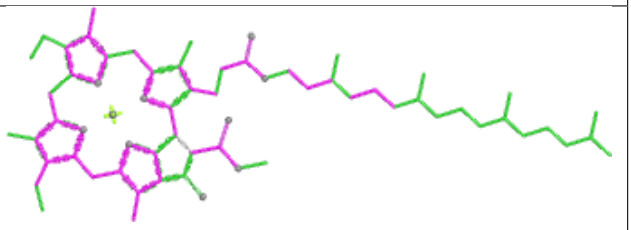


Rings

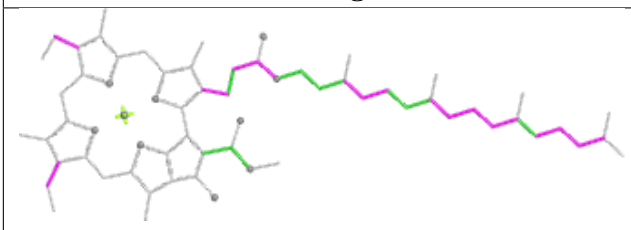
Ligand CLA B 813



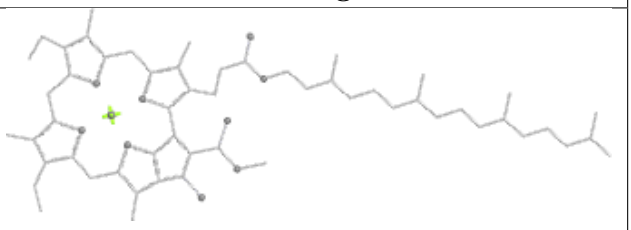
Bond lengths



Bond angles

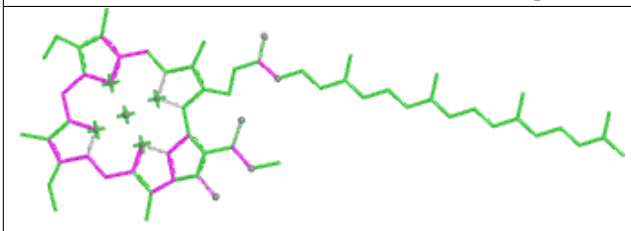


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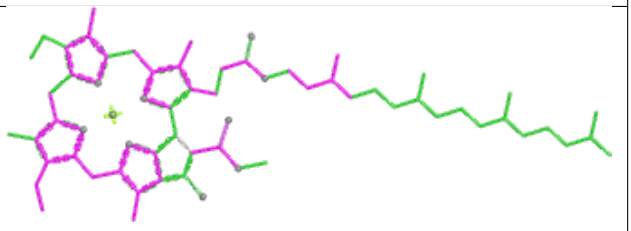


Rings

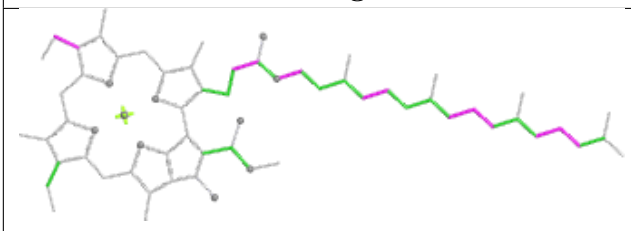
Ligand CLA 2 307



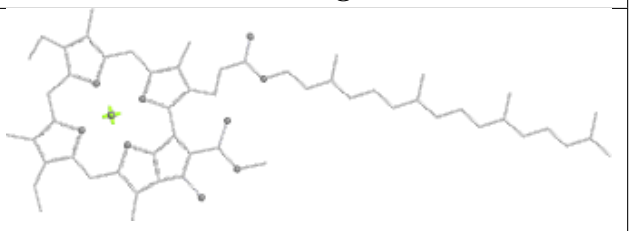
Bond lengths



Bond angles

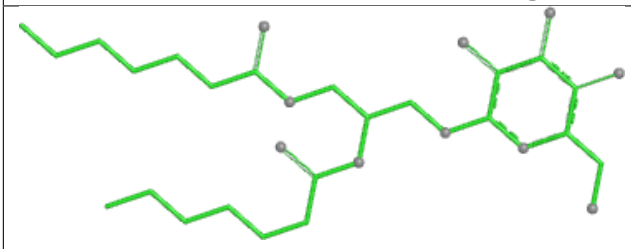


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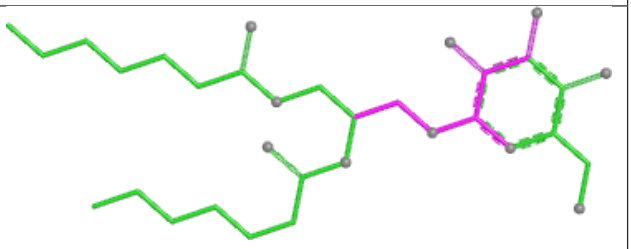


Rings

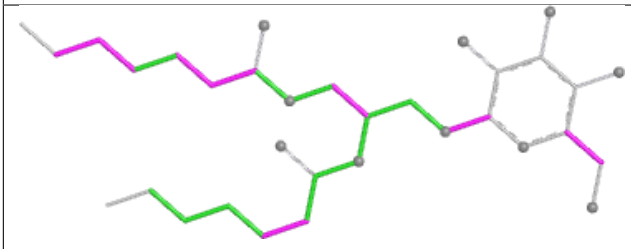
Ligand LMG 5 318



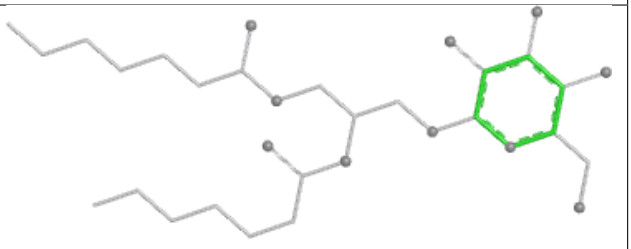
Bond lengths



Bond angles

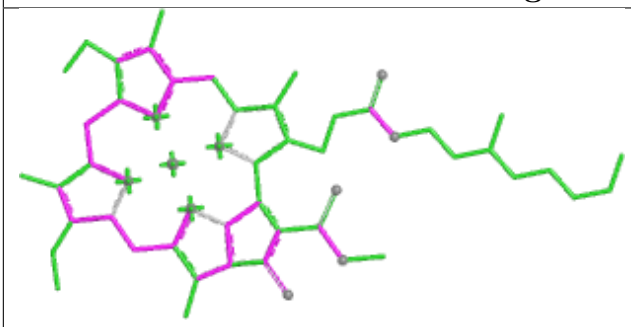


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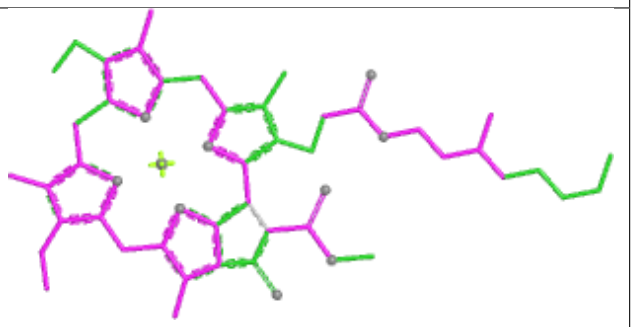


Rings

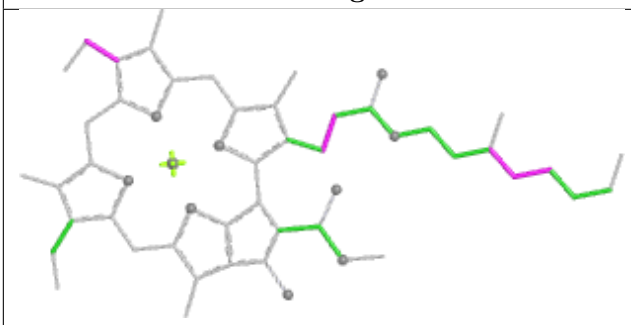
Ligand CLA B 823



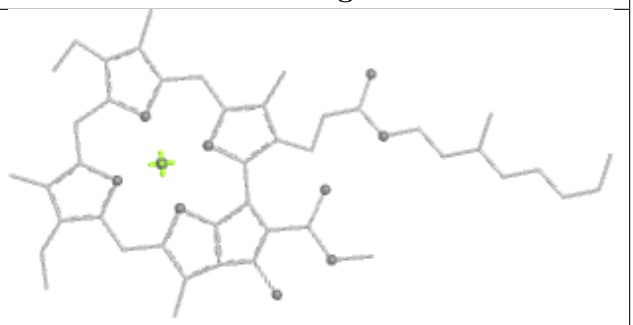
Bond lengths



Bond angles

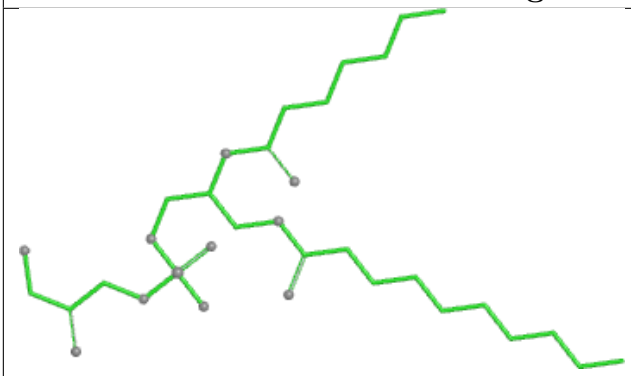


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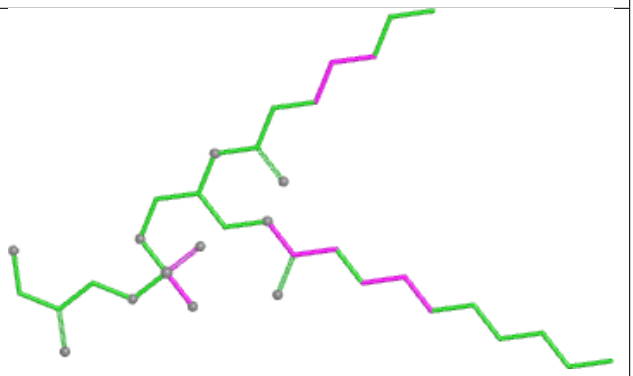


Rings

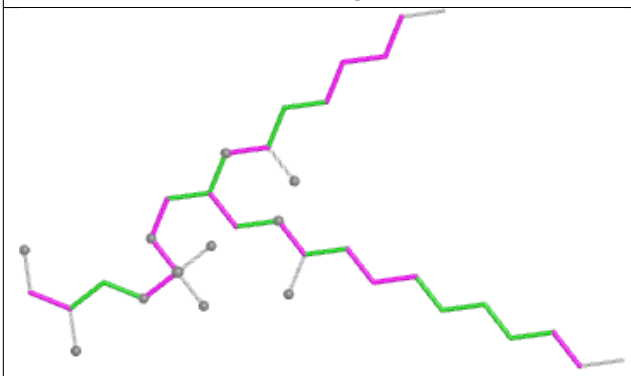
Ligand LHG 9 318



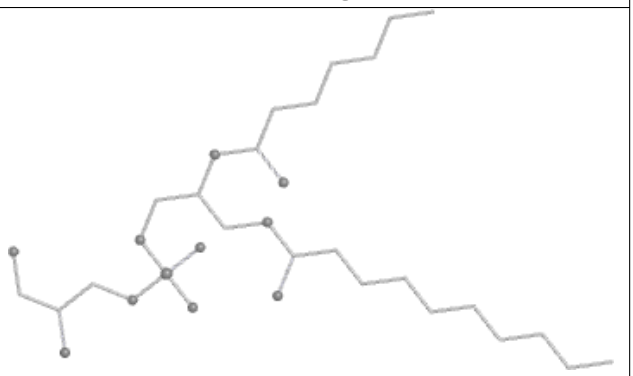
Bond lengths



Bond angles

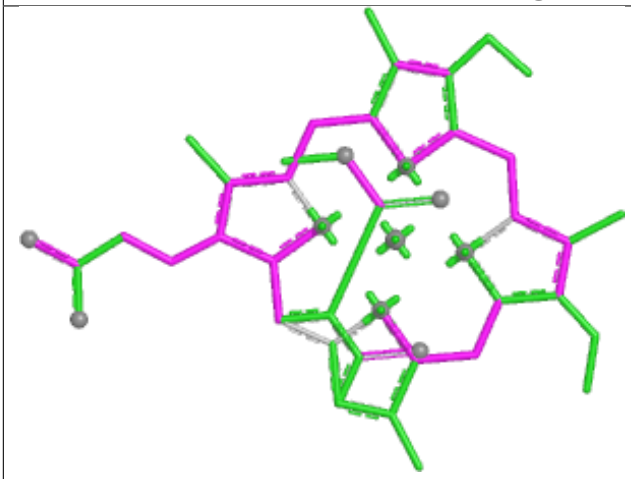


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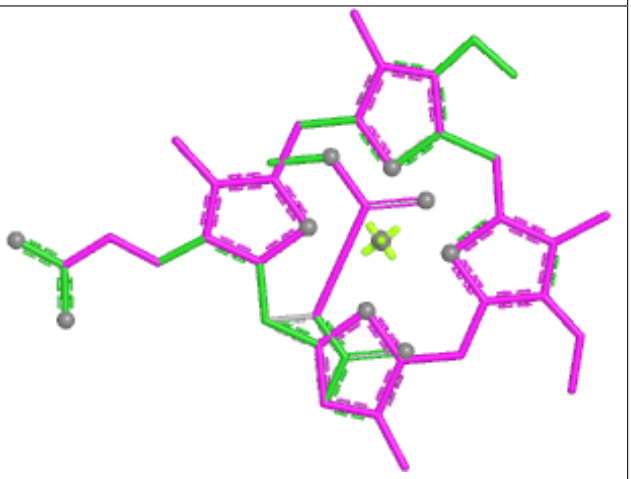


Rings

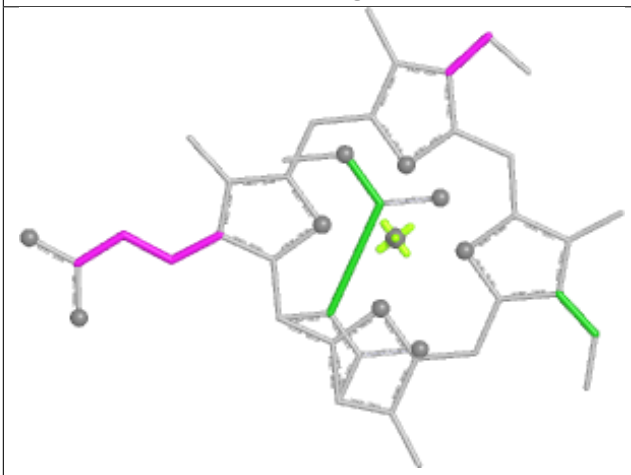
Ligand KC1 6 308



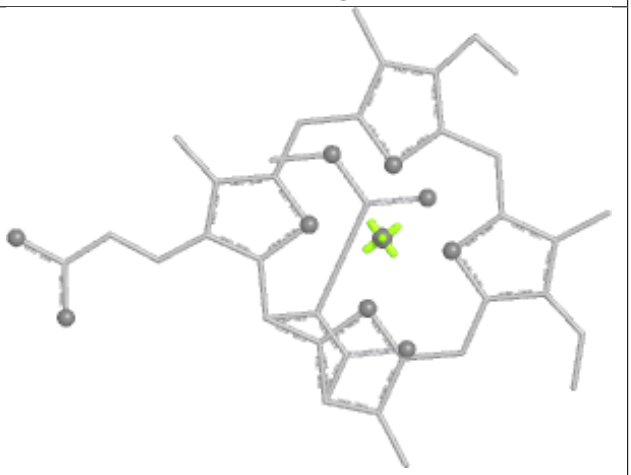
Bond lengths



Bond angles

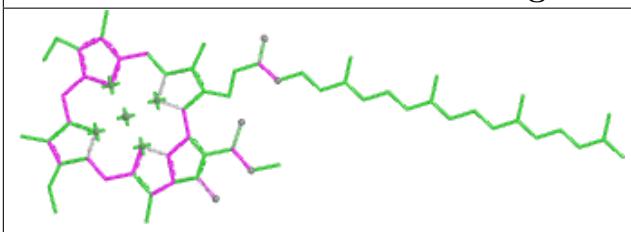


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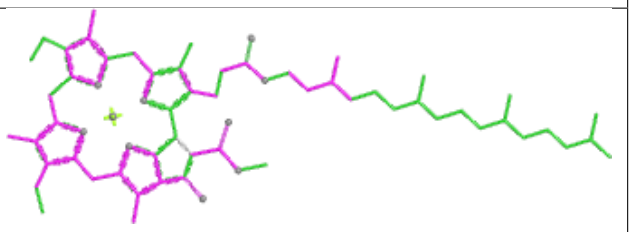


Rings

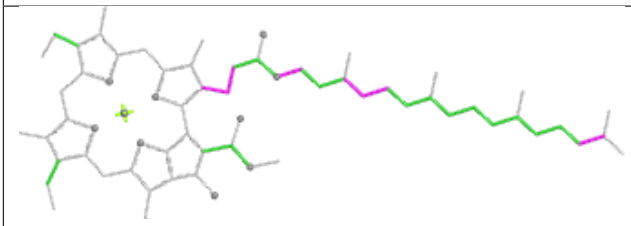
Ligand CLA 7 305



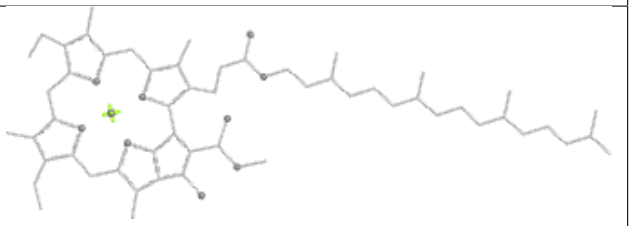
Bond lengths



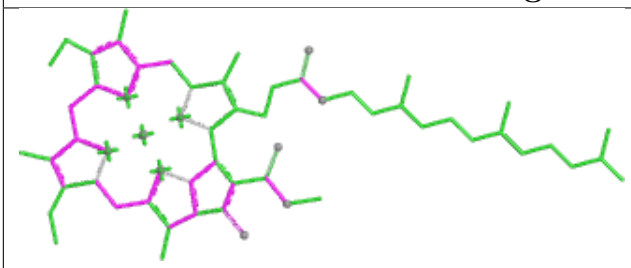
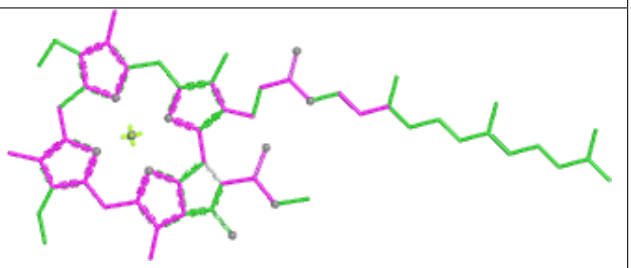
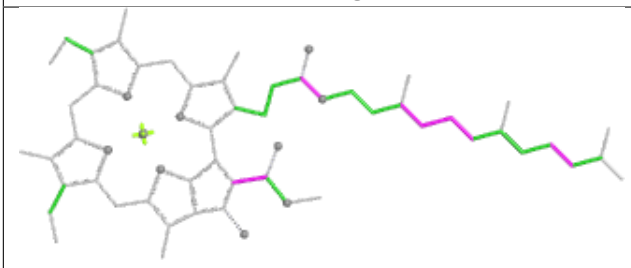
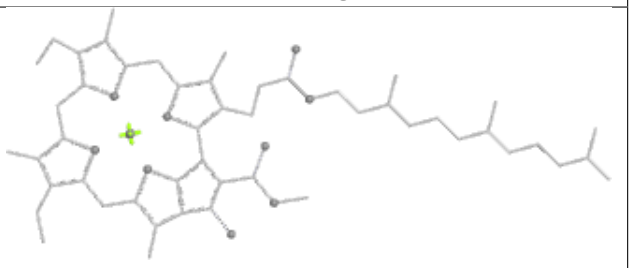
Bond angles

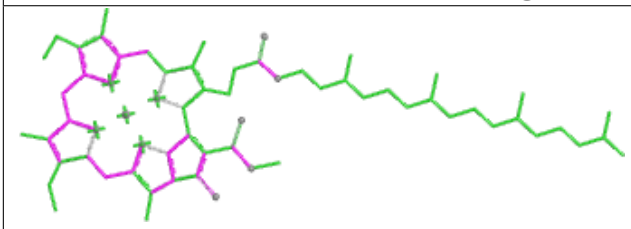
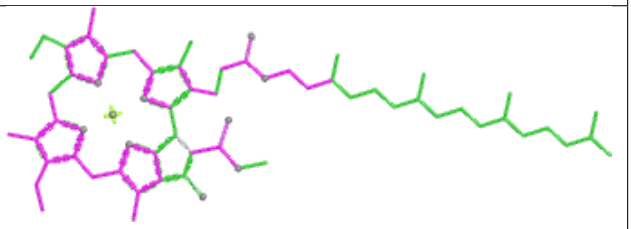
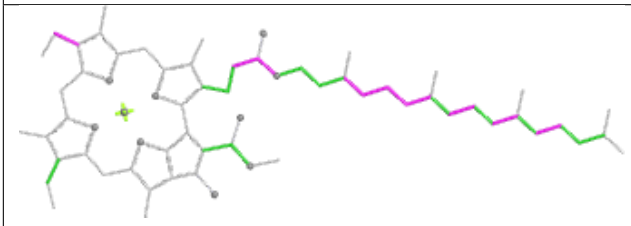
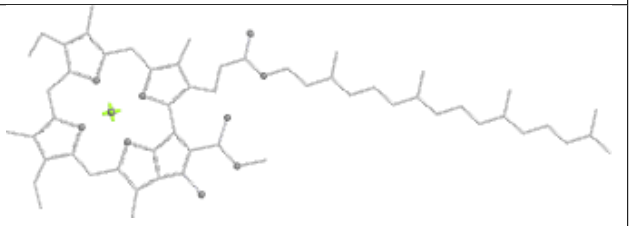


Torsions

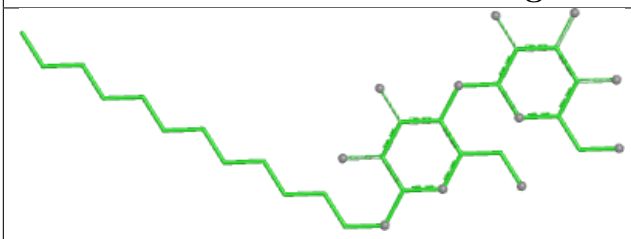


Rings

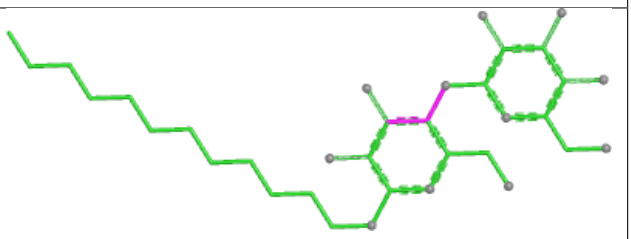
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2u 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

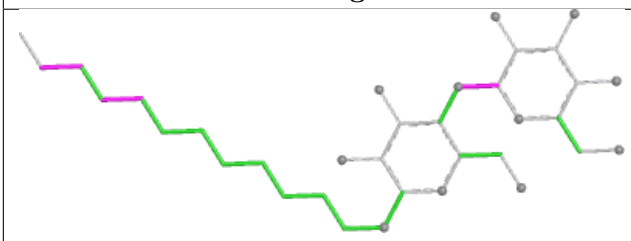
Ligand LMT 7 301



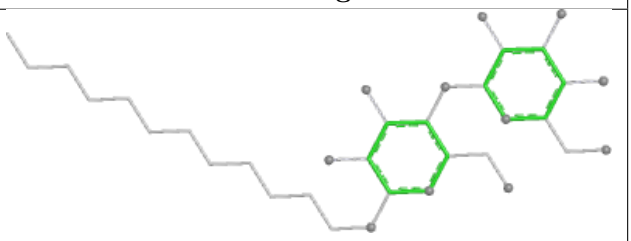
Bond lengths



Bond angles

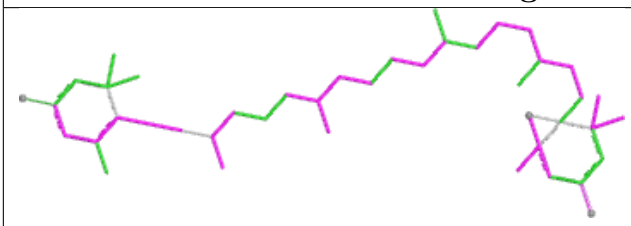


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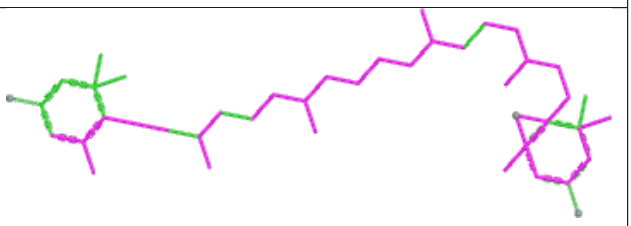


Rings

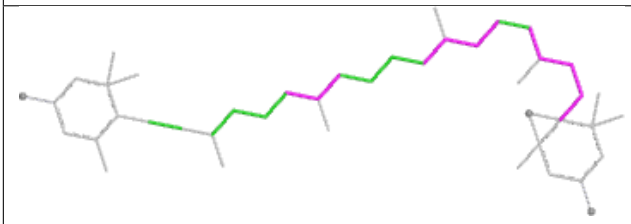
Ligand DD6 10 313



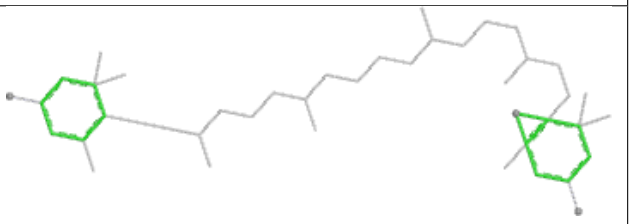
Bond lengths



Bond angles

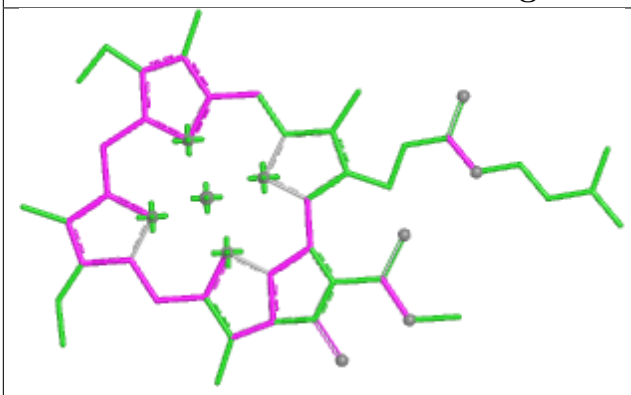


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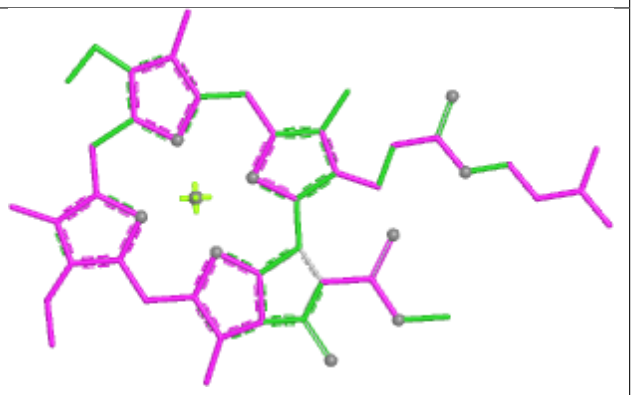


Rings

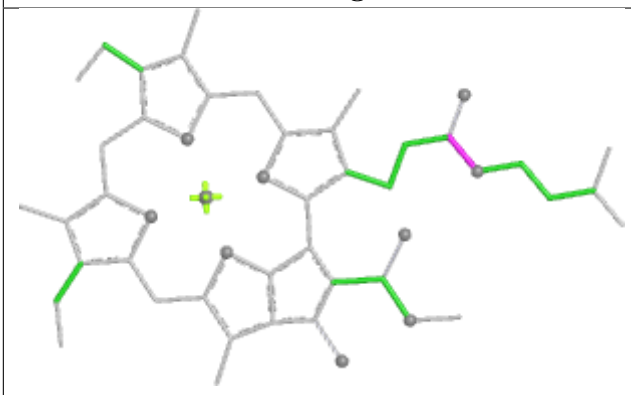
Ligand CLA 16 305



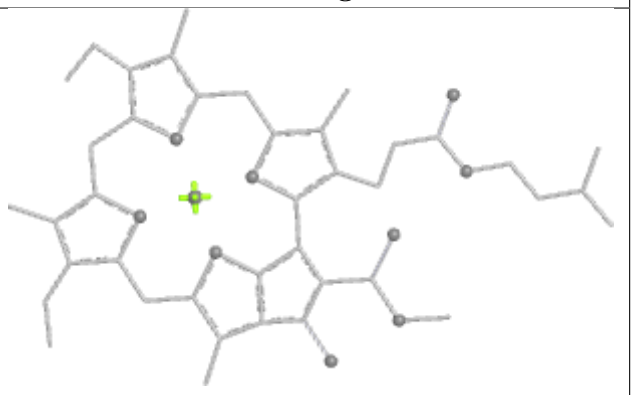
Bond lengths



Bond angles

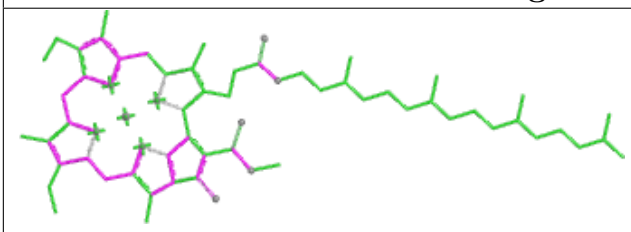


Torsions

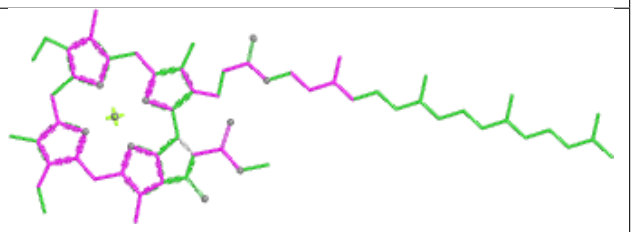


Rings

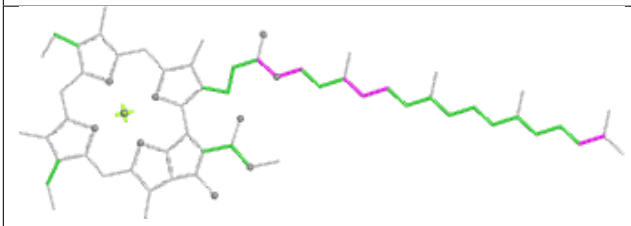
Ligand CLA 9 301



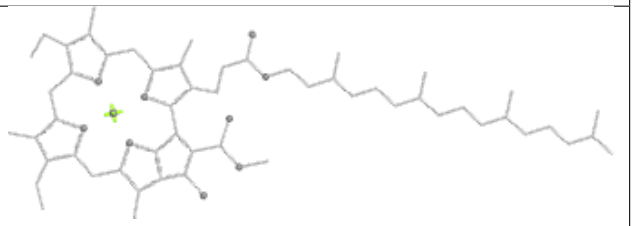
Bond lengths



Bond angles

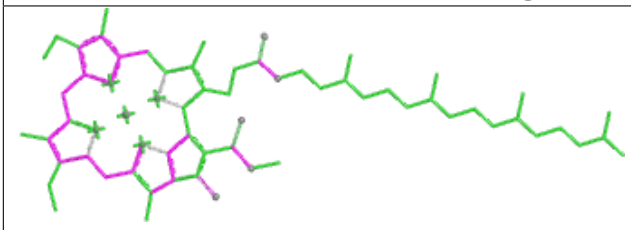


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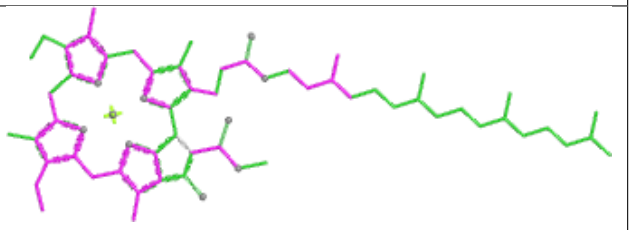


Rings

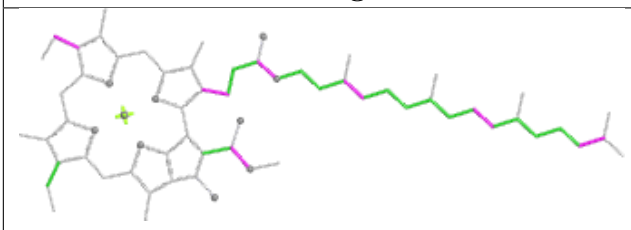
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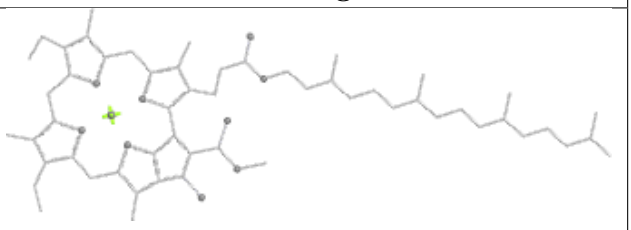
Bond lengths



Bond angles

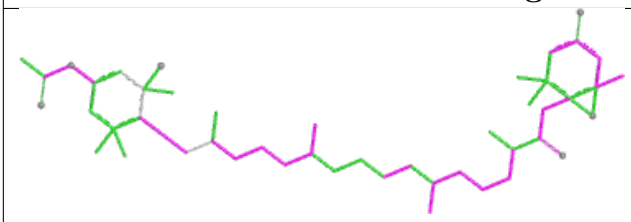


Torsions



Rings

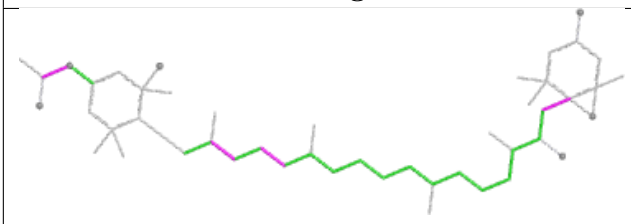
Ligand A86 10 301



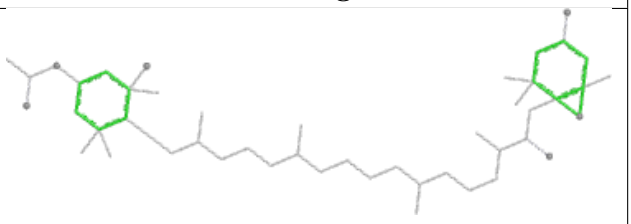
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Bond angles

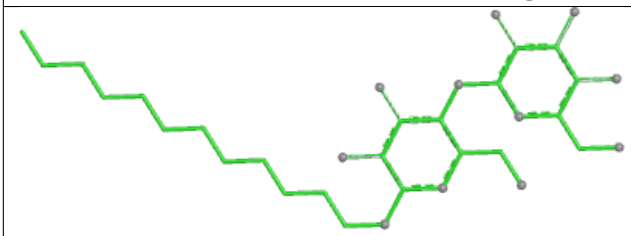


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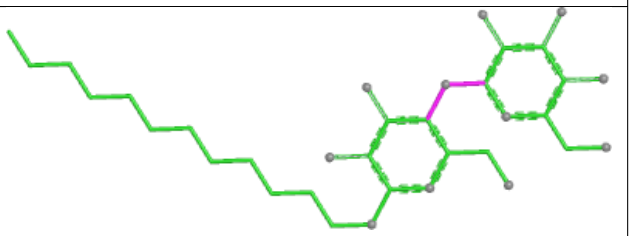


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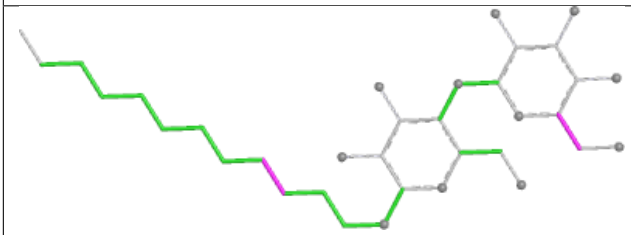
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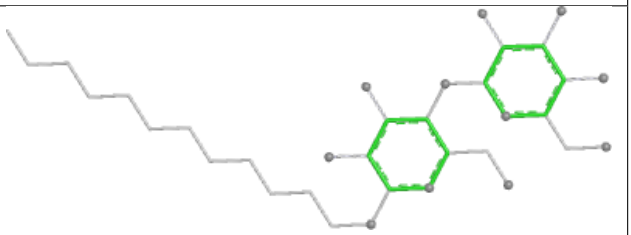
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Bond angles

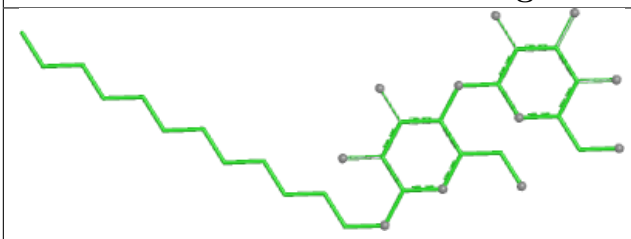


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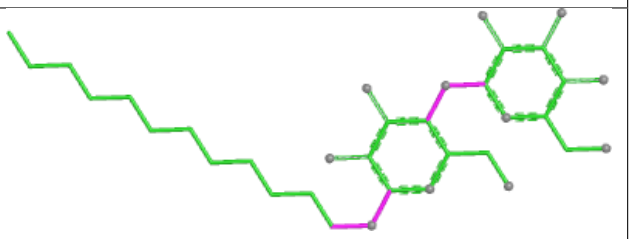


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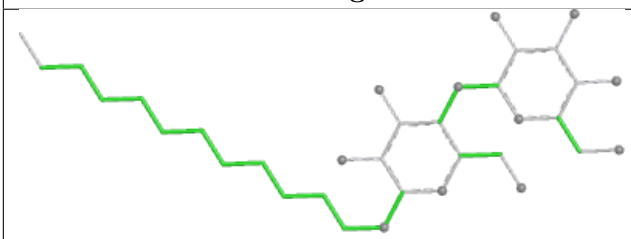
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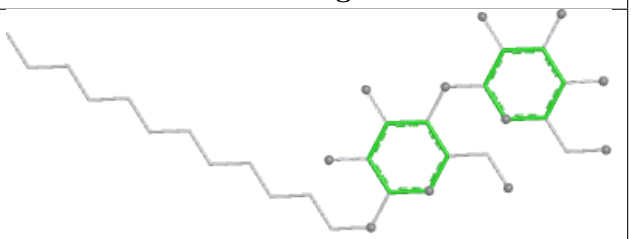
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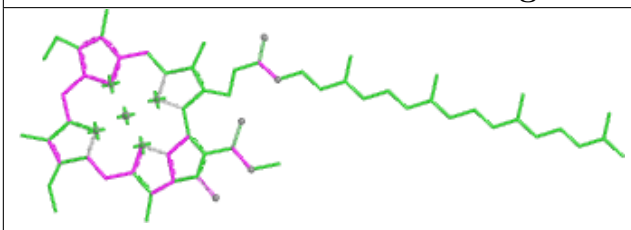


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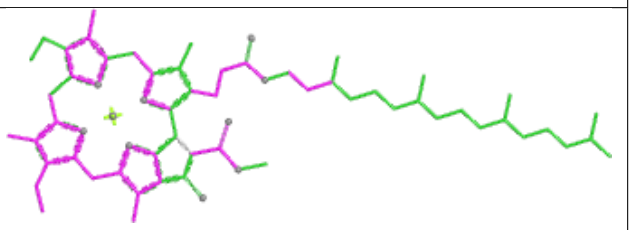


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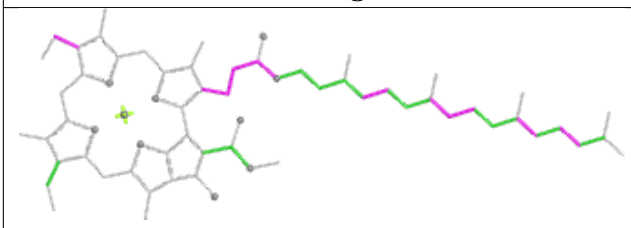
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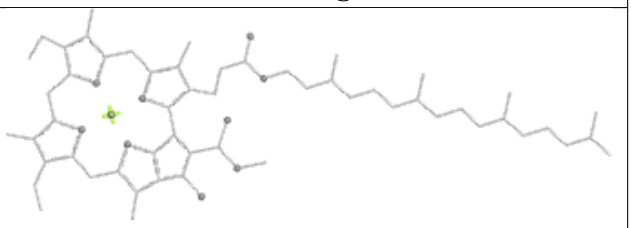
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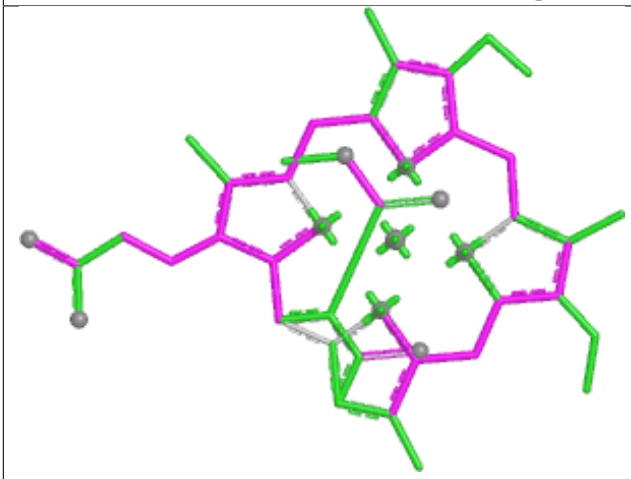


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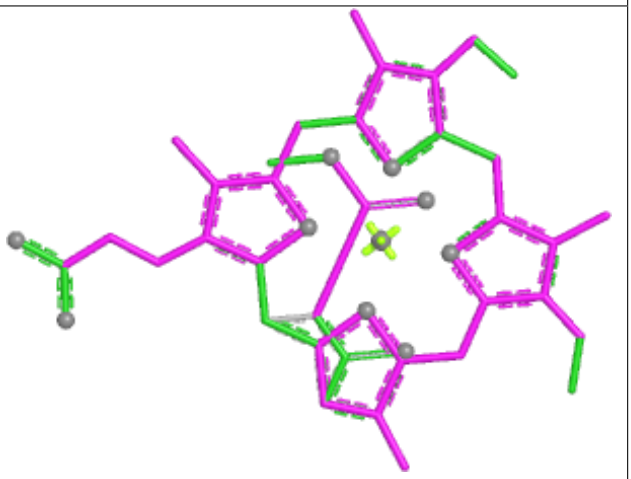


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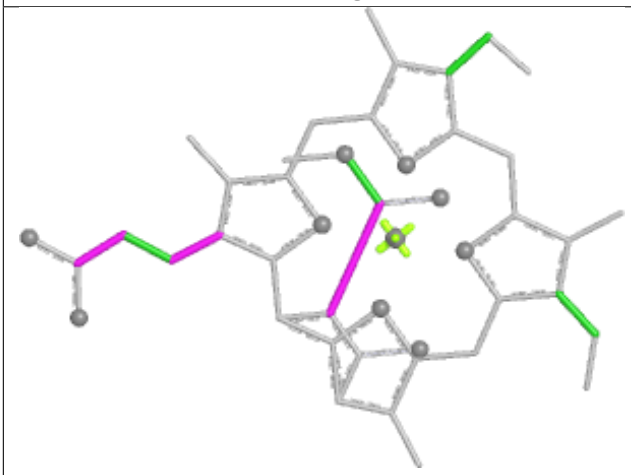
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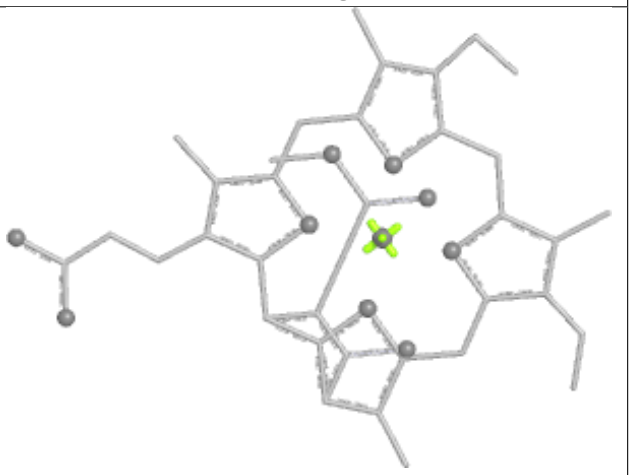
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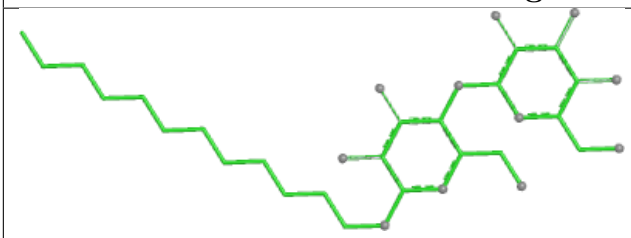


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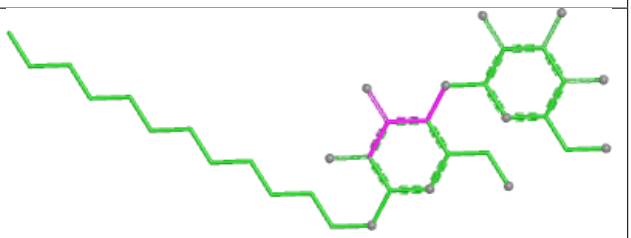


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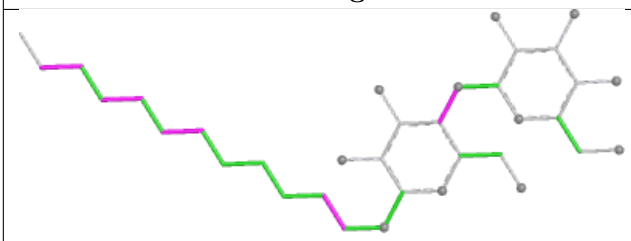
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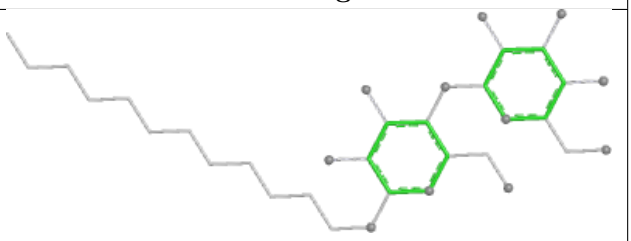
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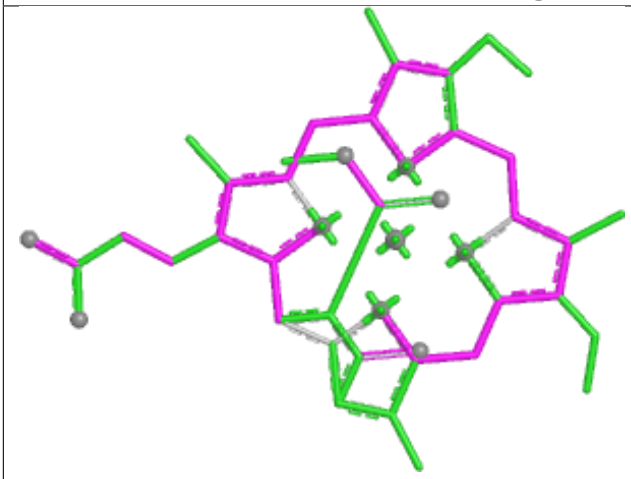


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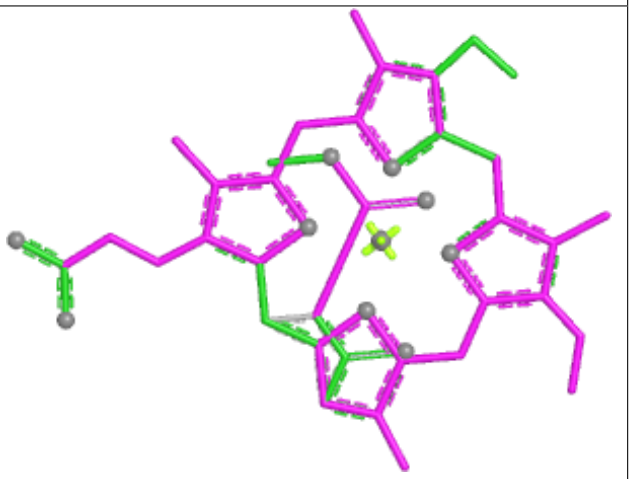


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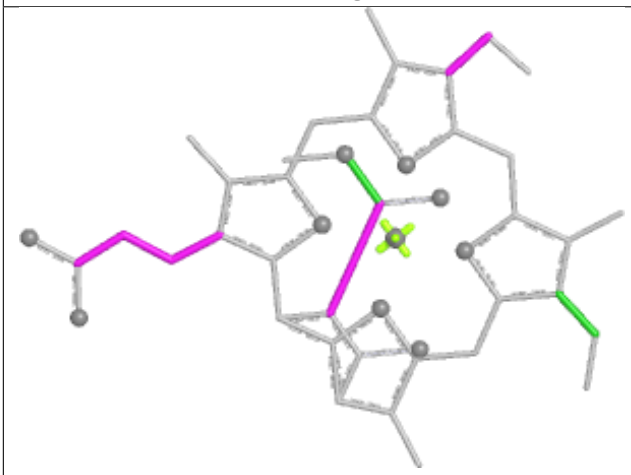
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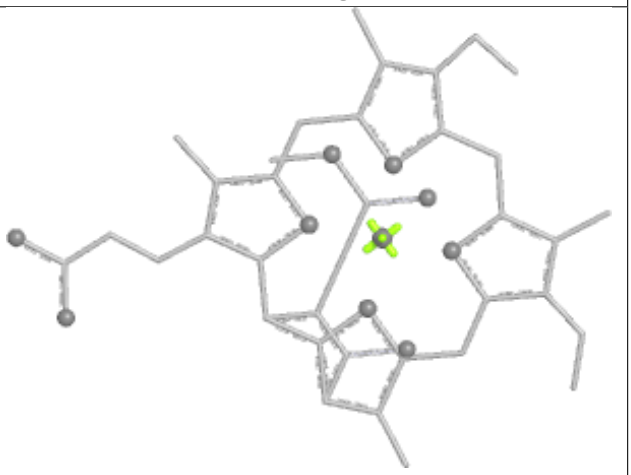
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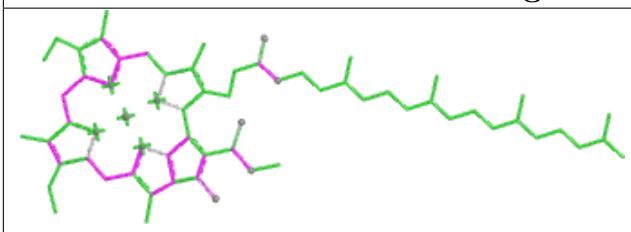


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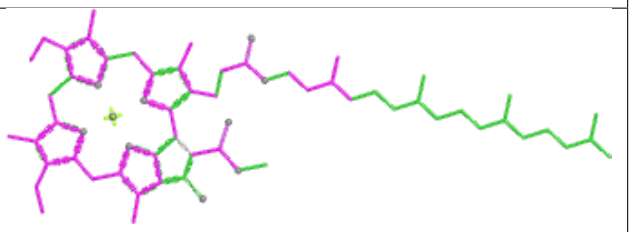


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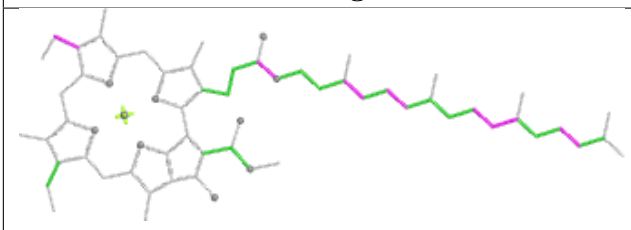
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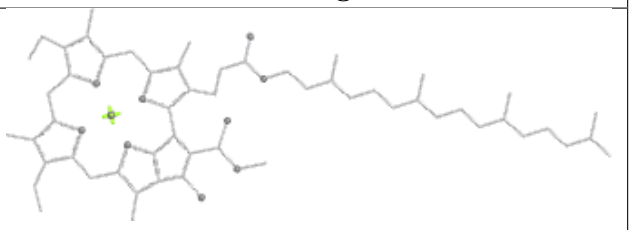
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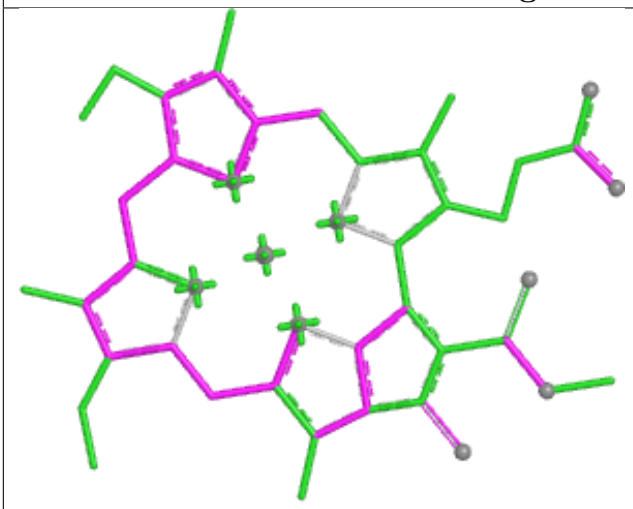


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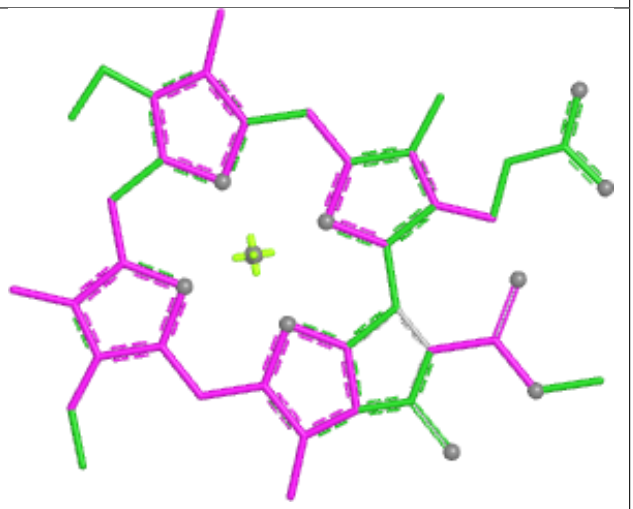


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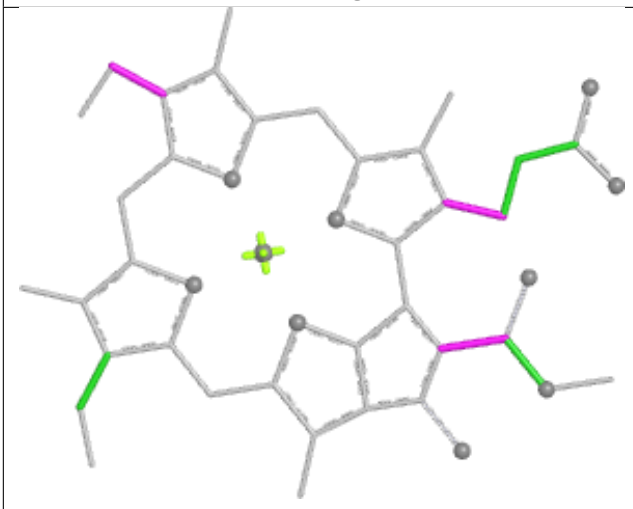
Ligand CLA 16 309



Bond lengths



Bond angles

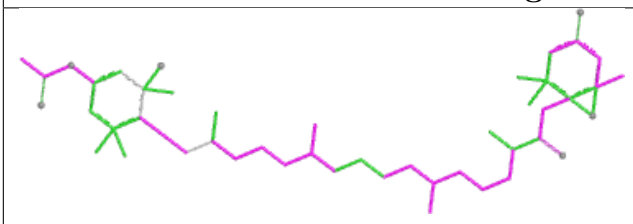


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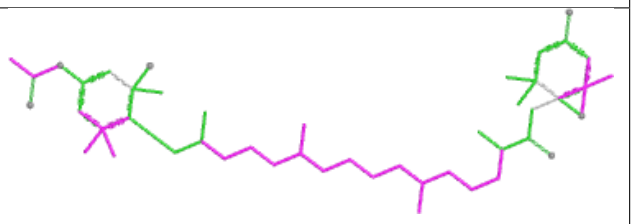


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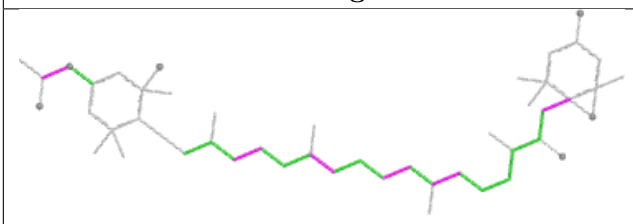
Ligand A86 14 320



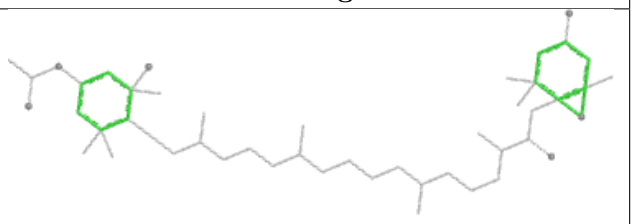
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Bond angles

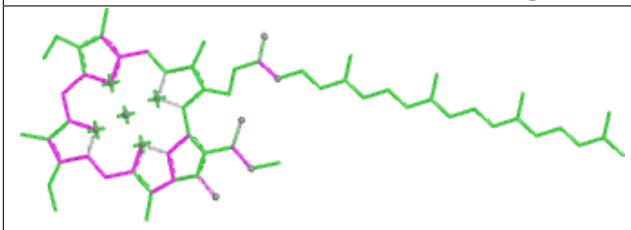


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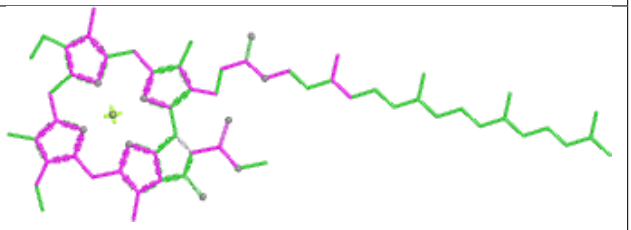


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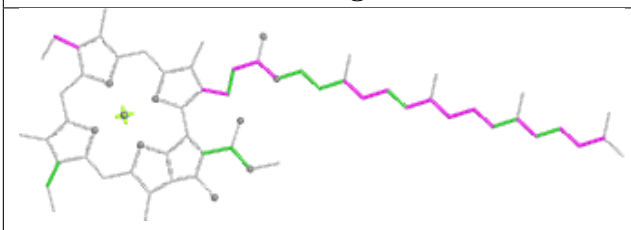
Ligand CLA A 816



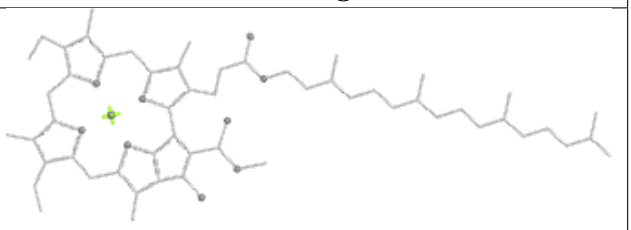
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Bond angles

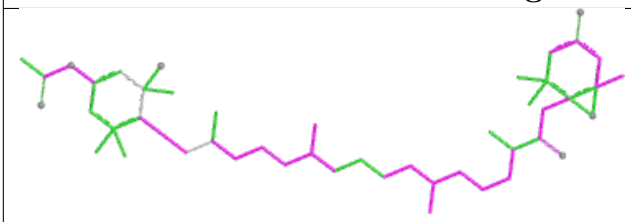


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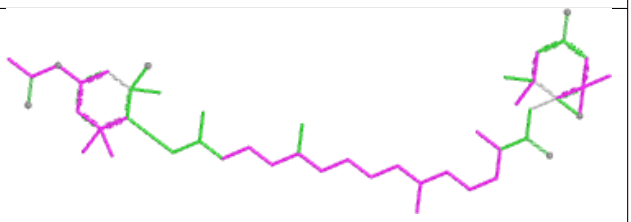


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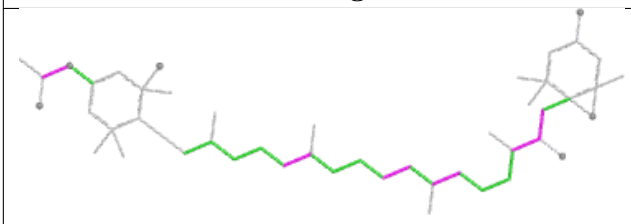
Ligand A86 14 314



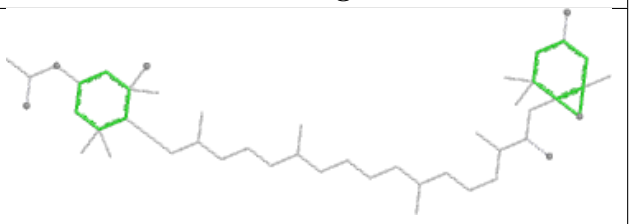
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Bond angles

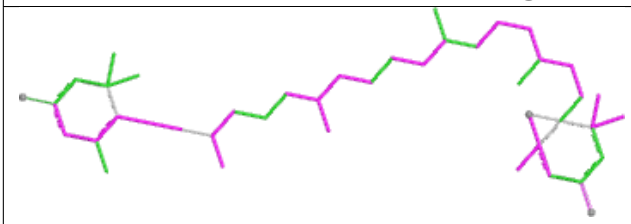


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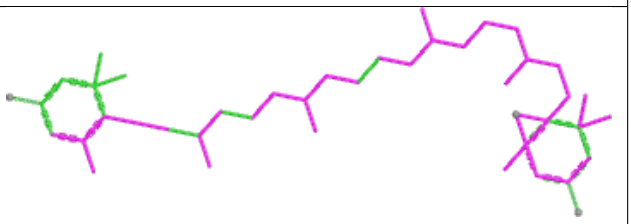


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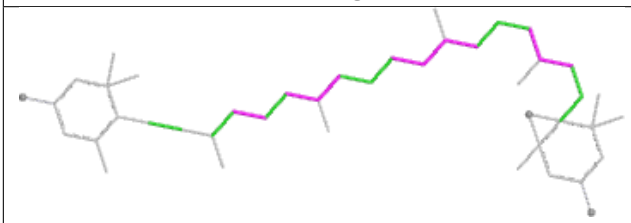
Ligand DD6 10 314



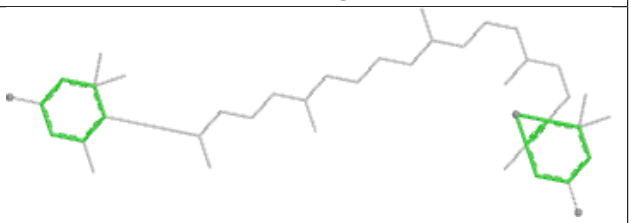
Bond lengths



Bond angles

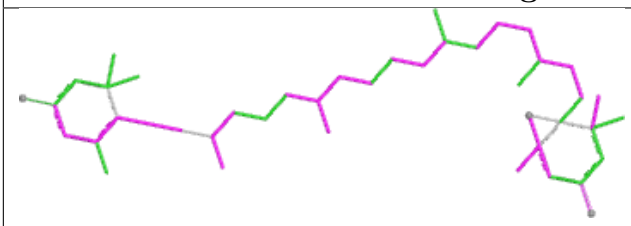


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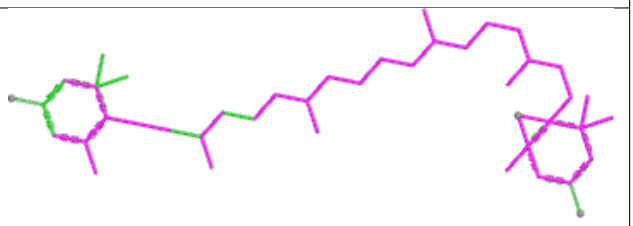


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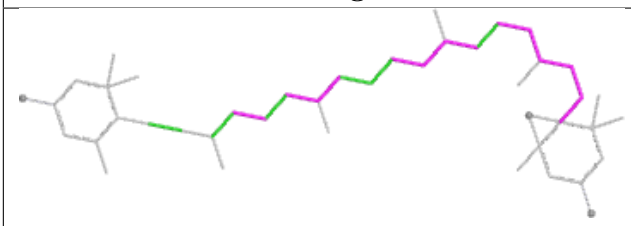
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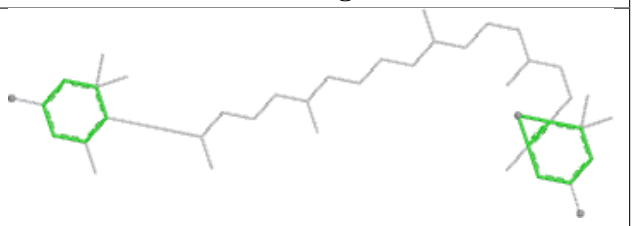
Bond lengths



Bond angles

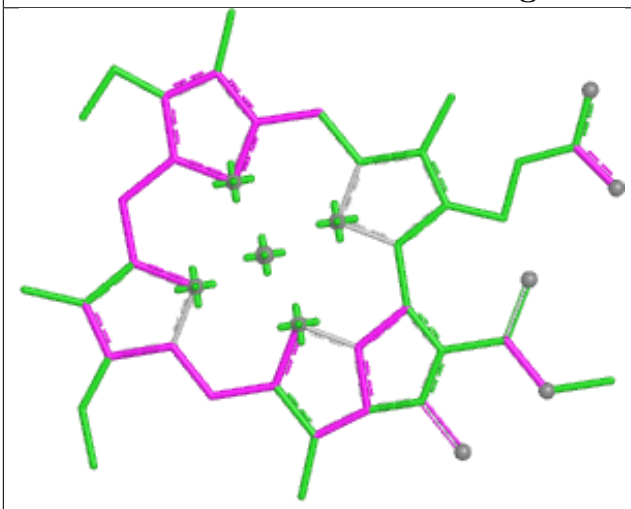


Torsions

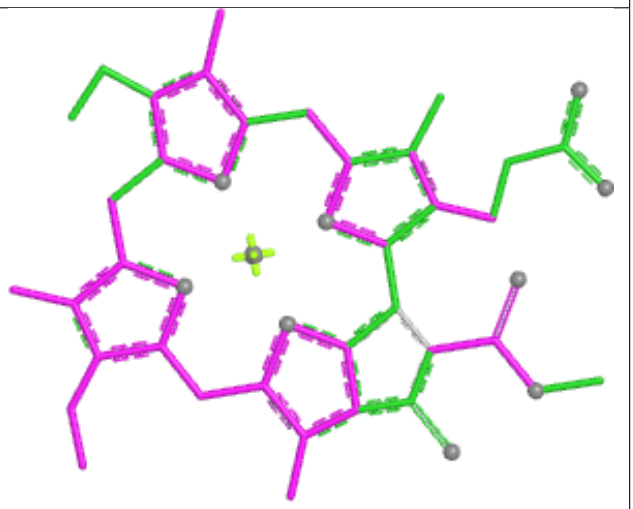


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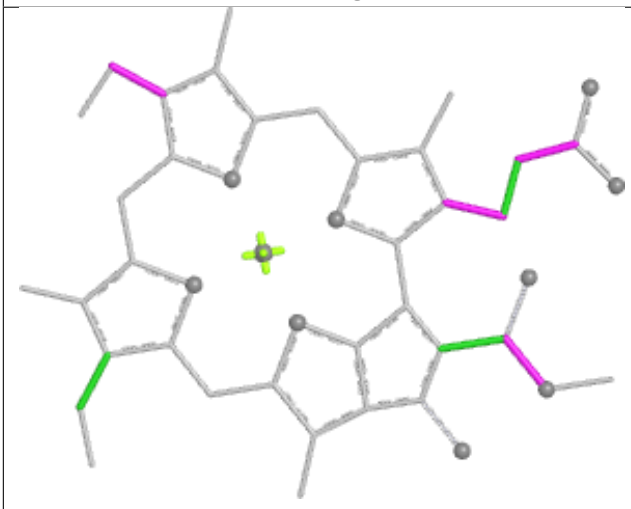
Ligand CLA 10 311



Bond lengths



Bond angles

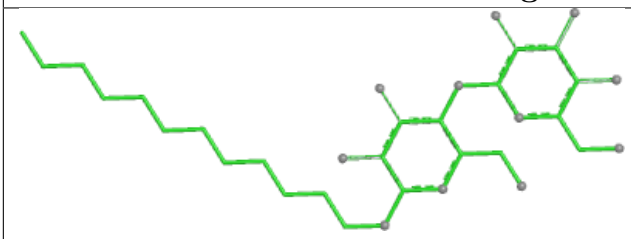


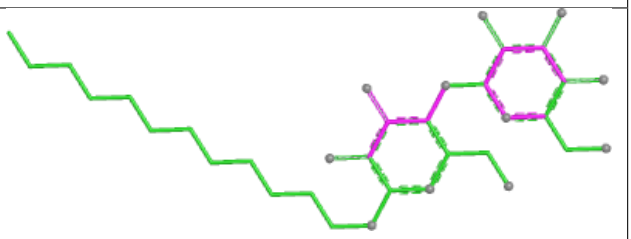
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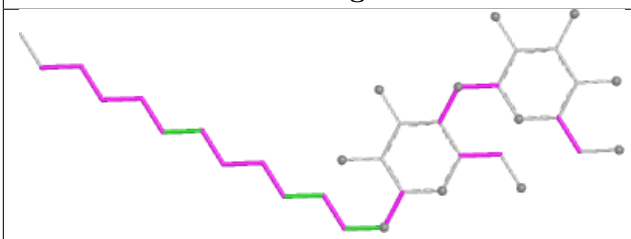


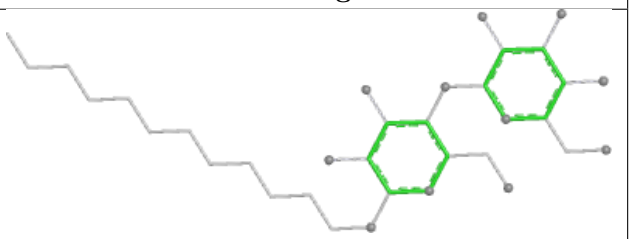
Rings

Ligand LMT A 854

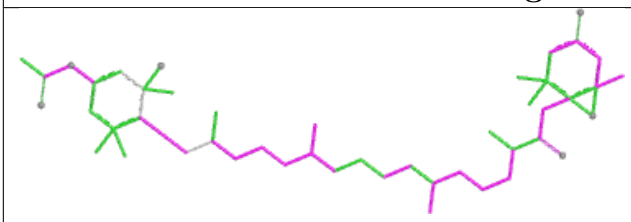

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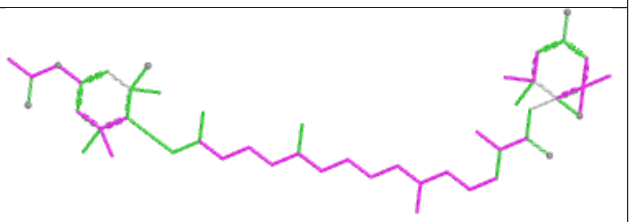

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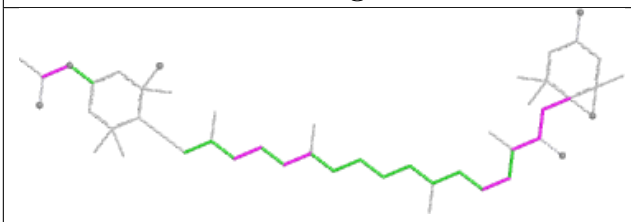

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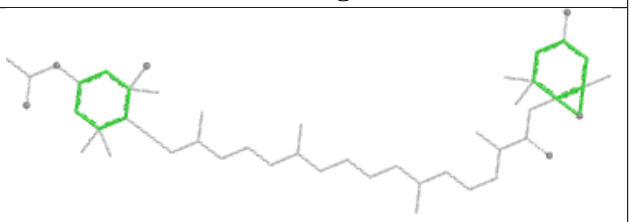

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Ligand A86 14 316

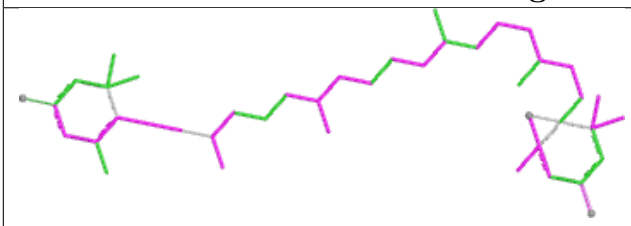

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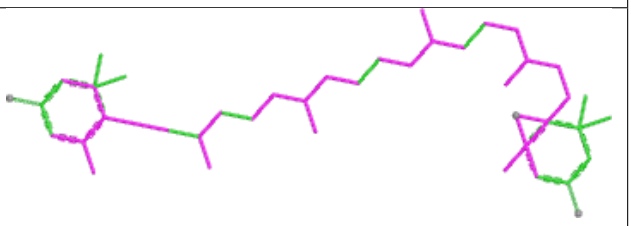

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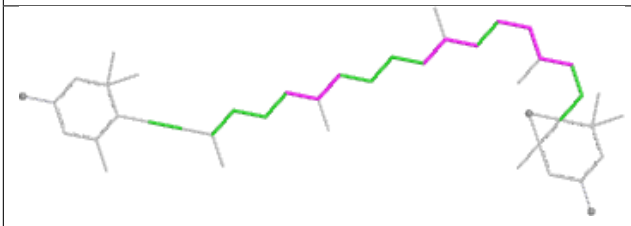

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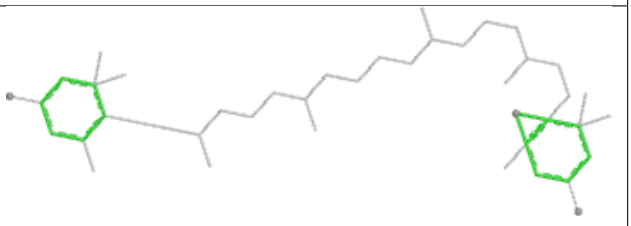

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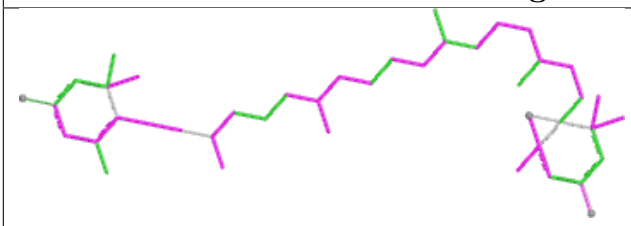

Bond lengths


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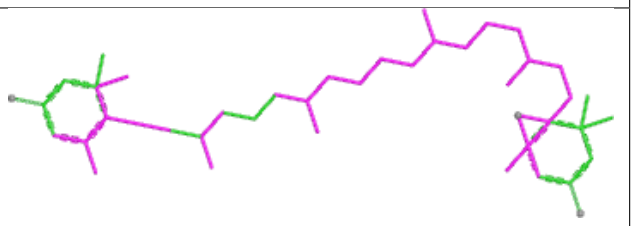

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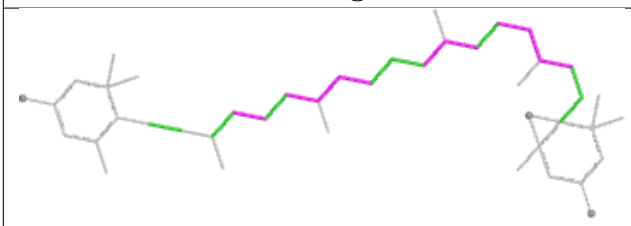
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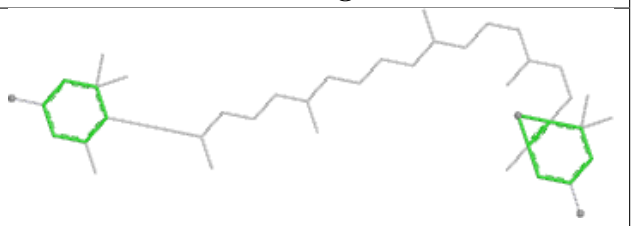
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Bond angles

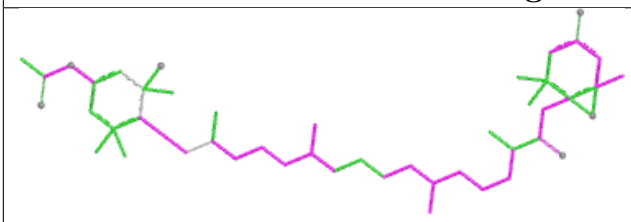


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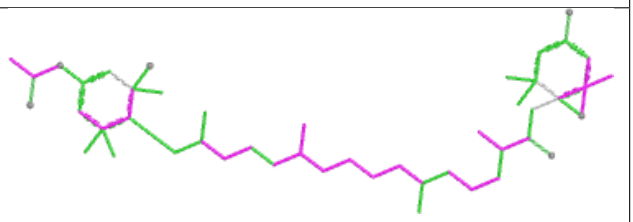


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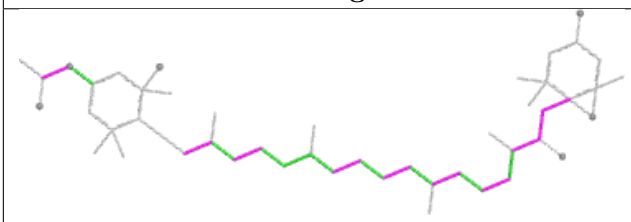
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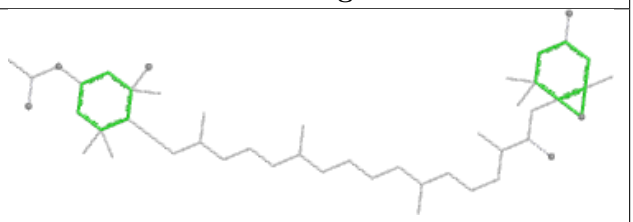
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Bond angles

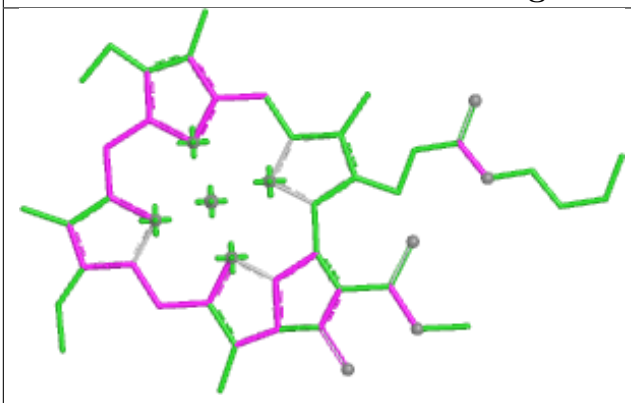


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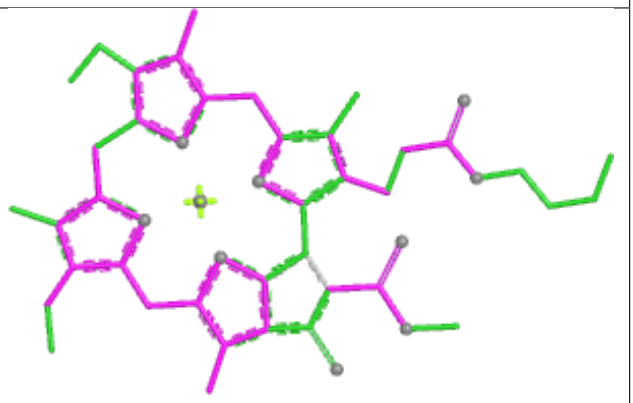


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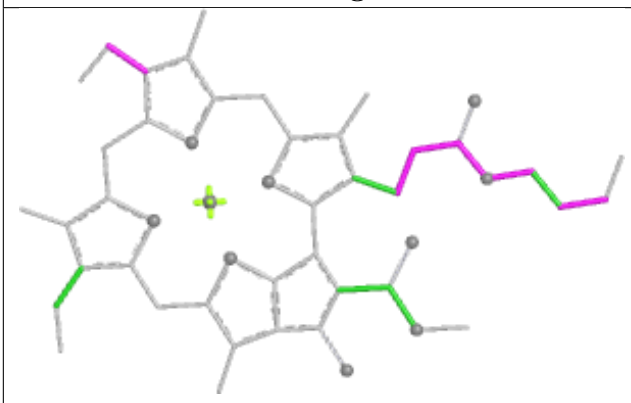
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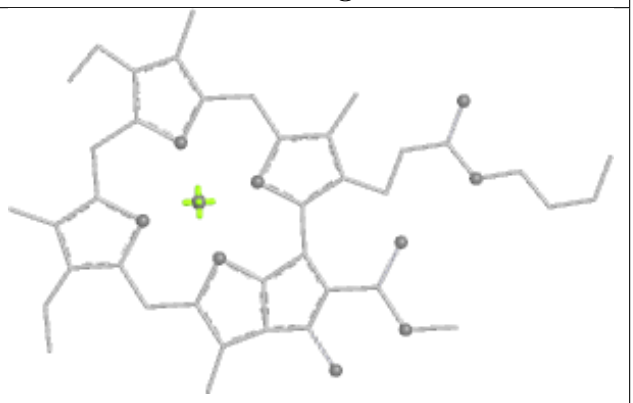
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Bond angles

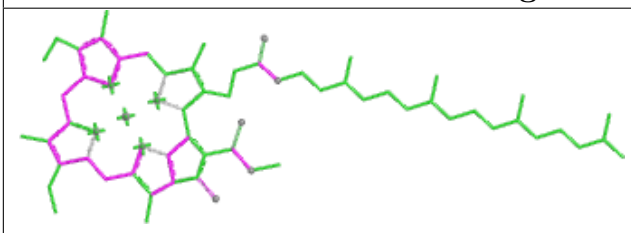


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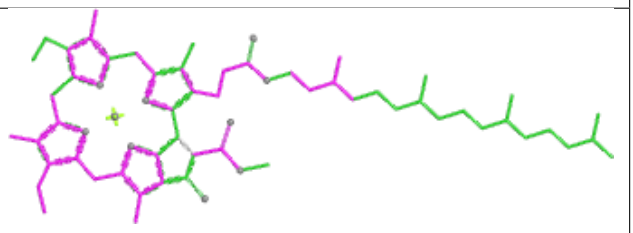


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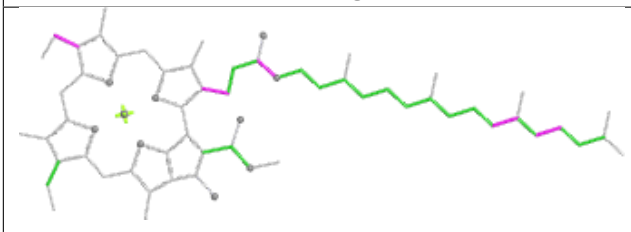
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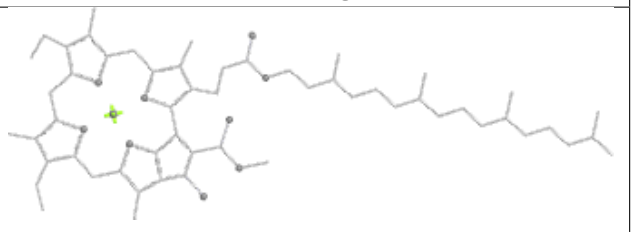
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Bond angles

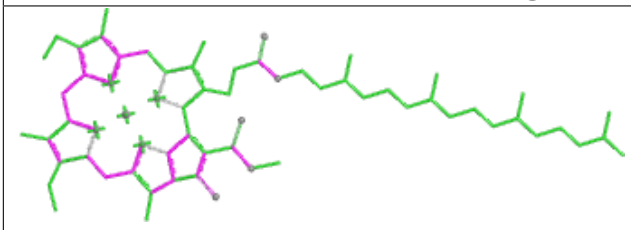


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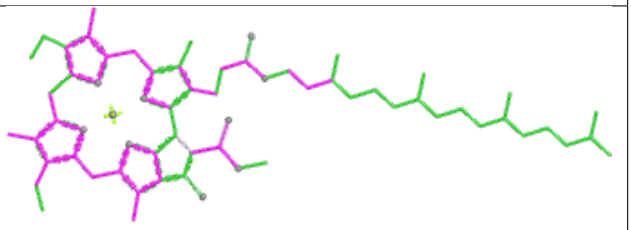


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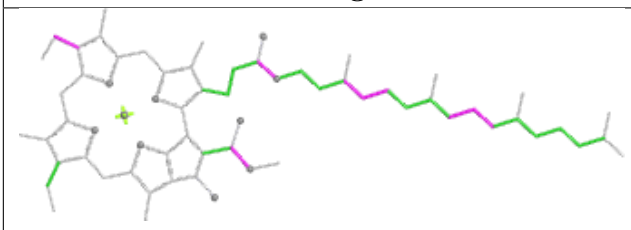
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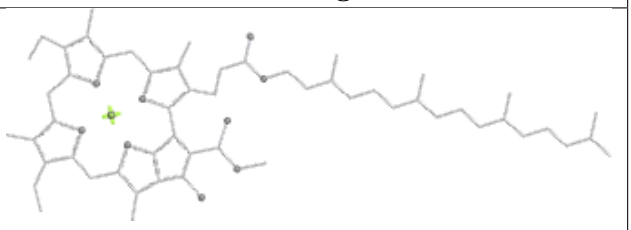
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Bond angles

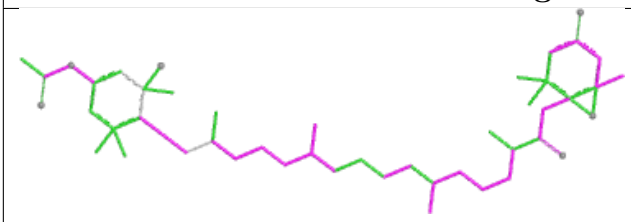


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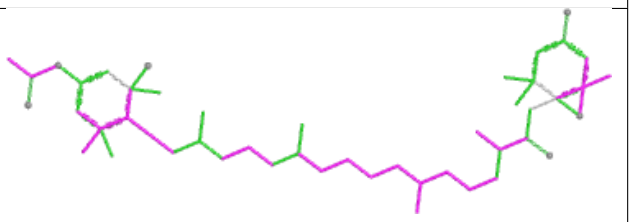


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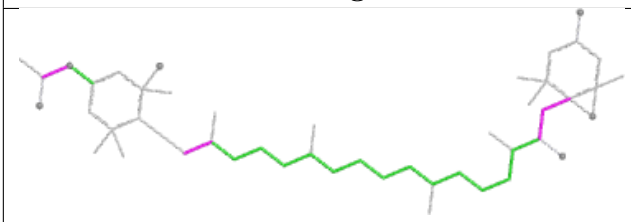
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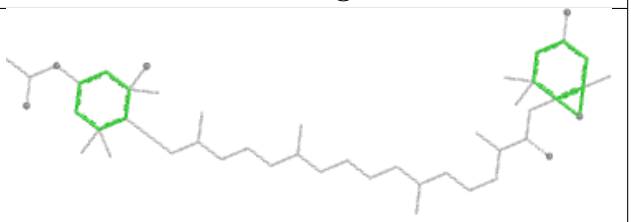
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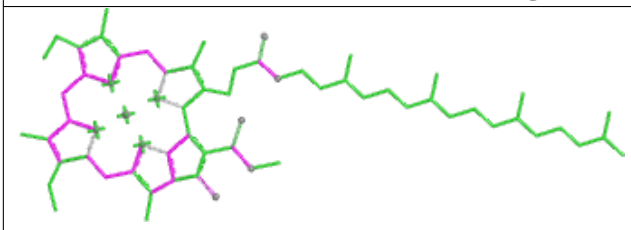


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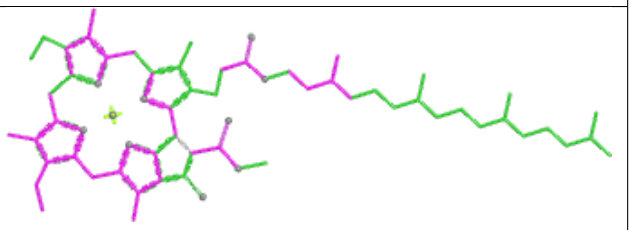


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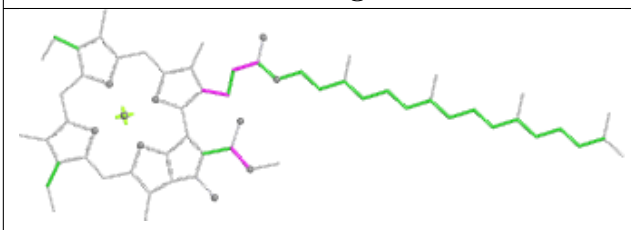
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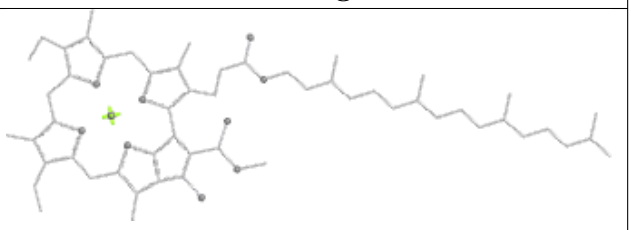
Bond lengths



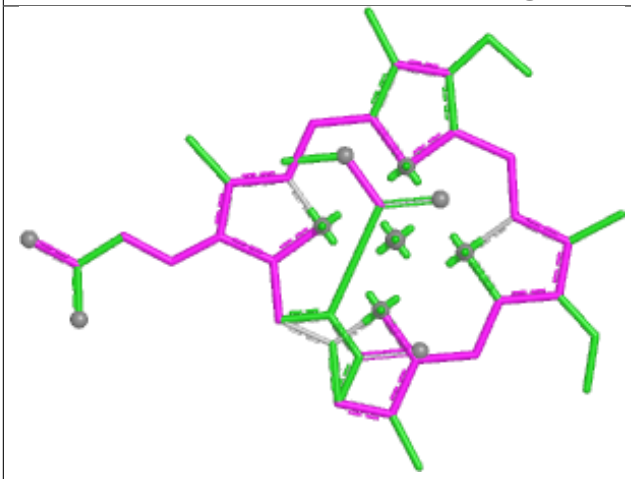
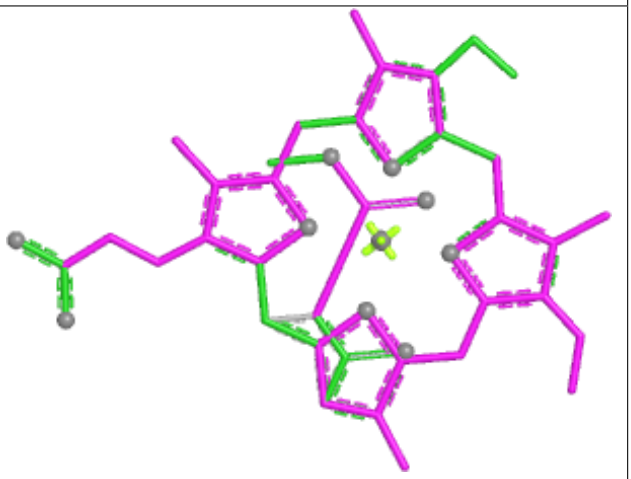
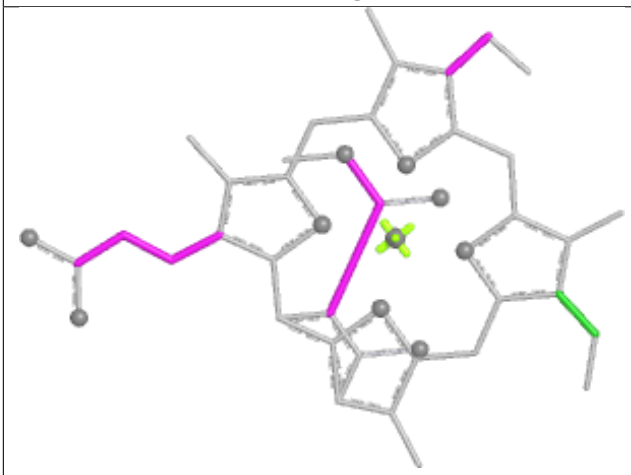
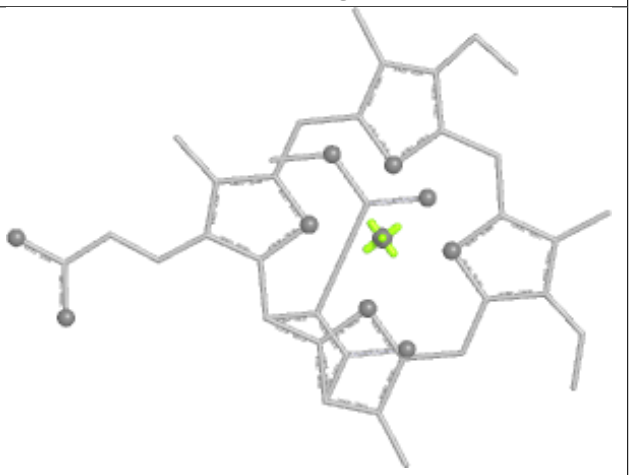
Bond angles

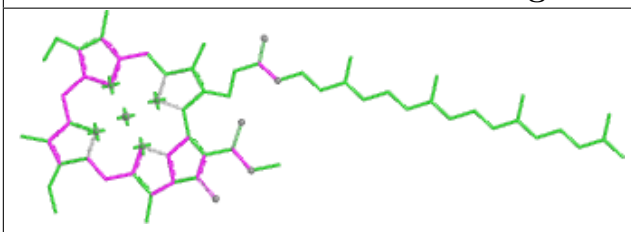
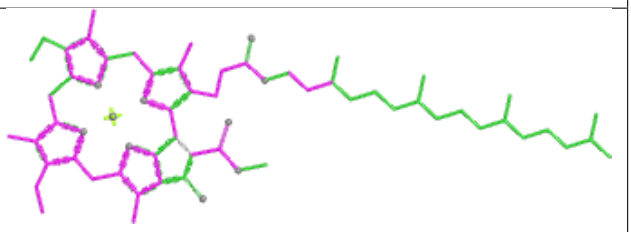
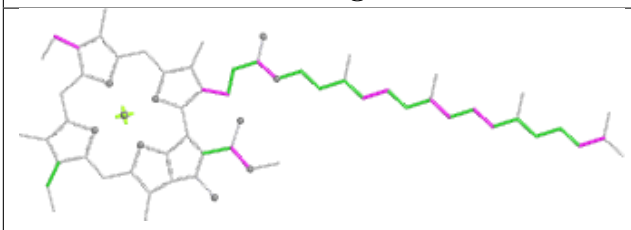
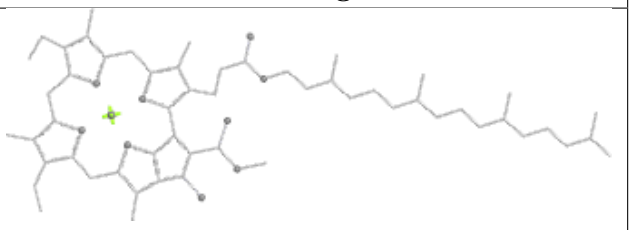


Torsions

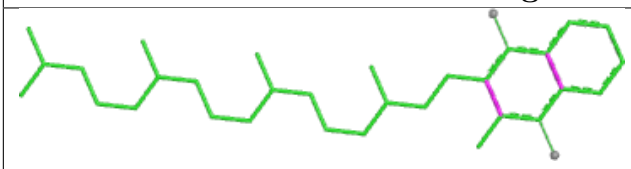


Rings

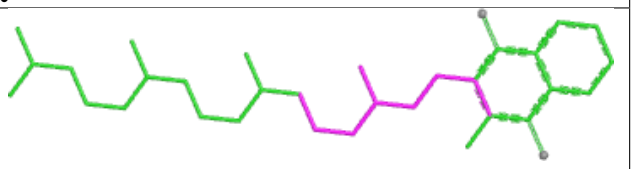
Ligand KC1 11 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

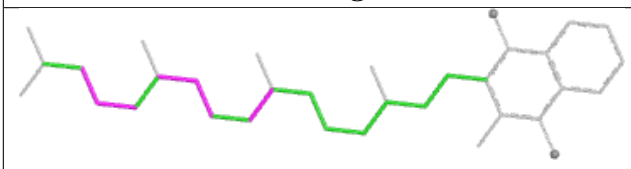
Ligand PQN A 845



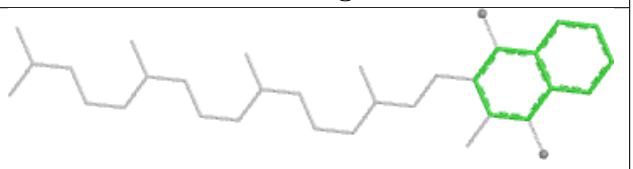
Bond lengths



Bond angles

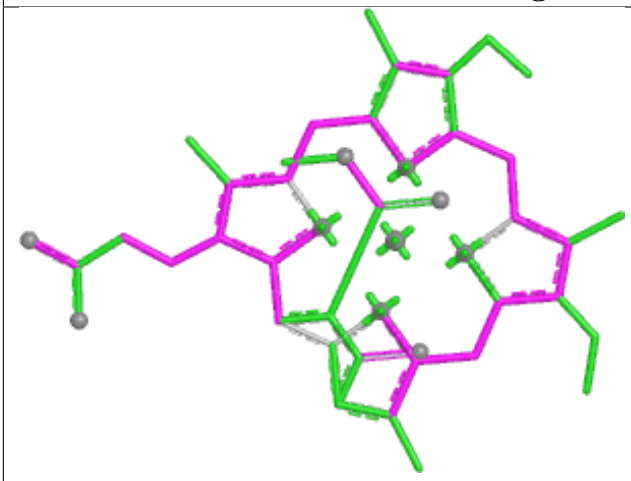


Torsions

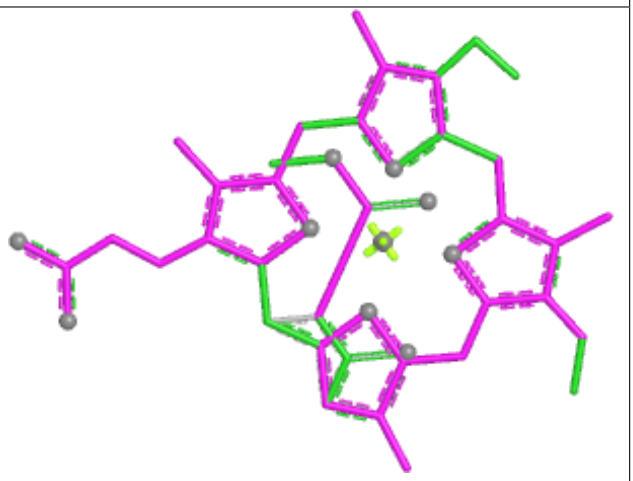


Rings

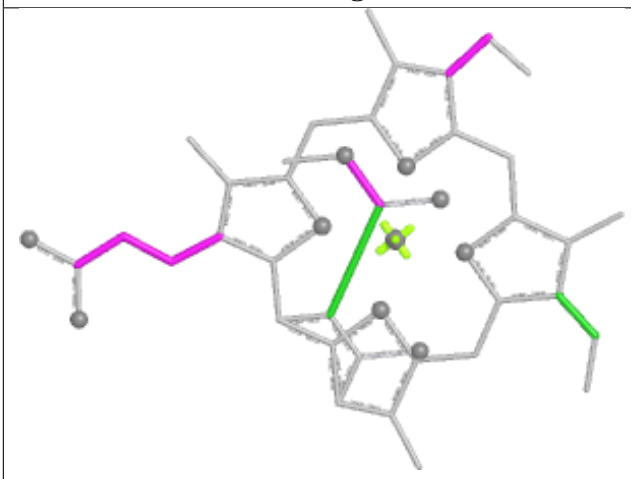
Ligand KC1 8 312



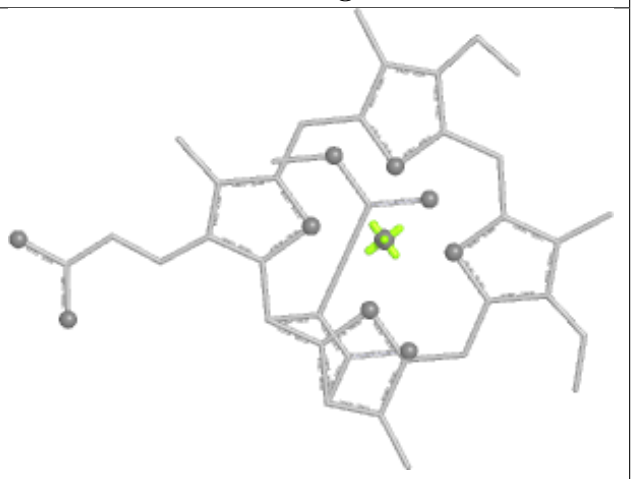
Bond lengths



Bond angles

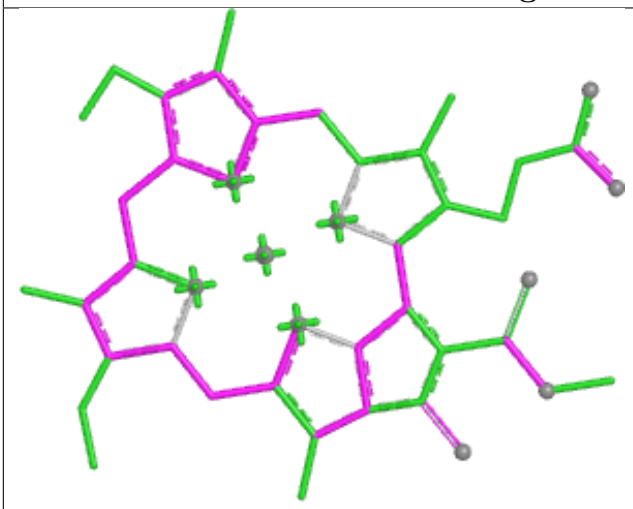


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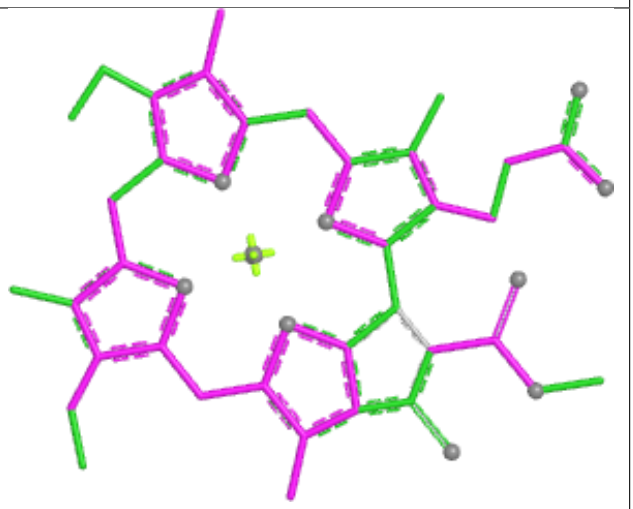


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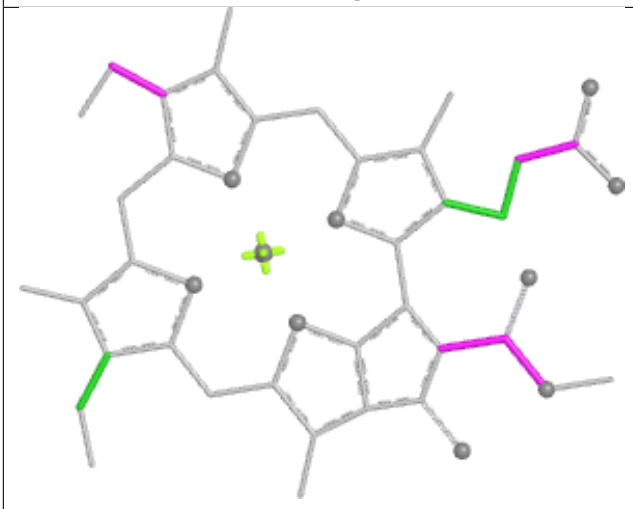
Ligand CLA 15 306



Bond lengths



Bond angles

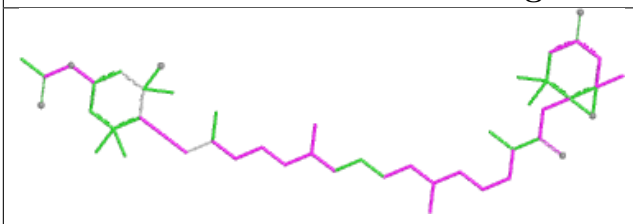


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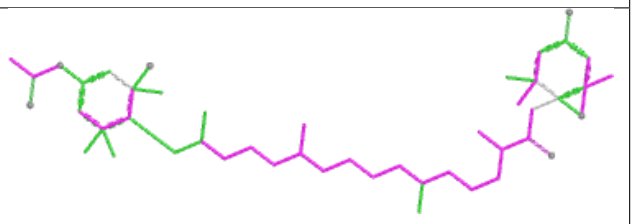


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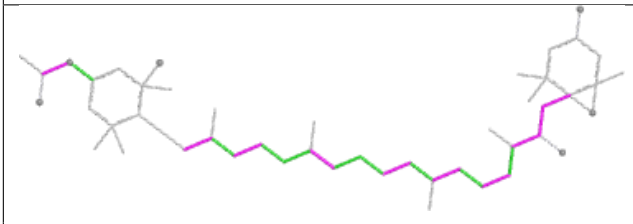
Ligand A86 15 322



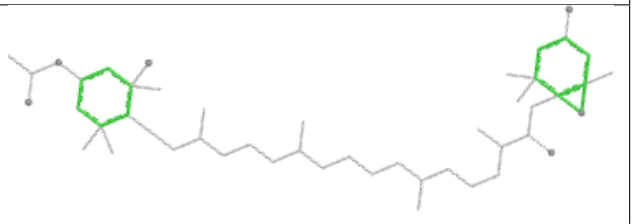
Bond lengths



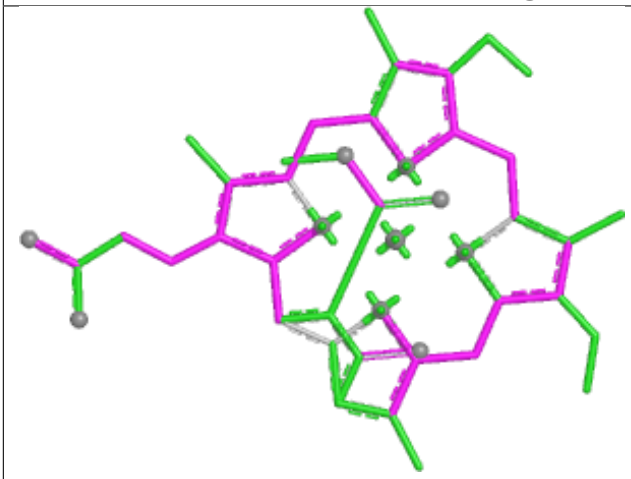
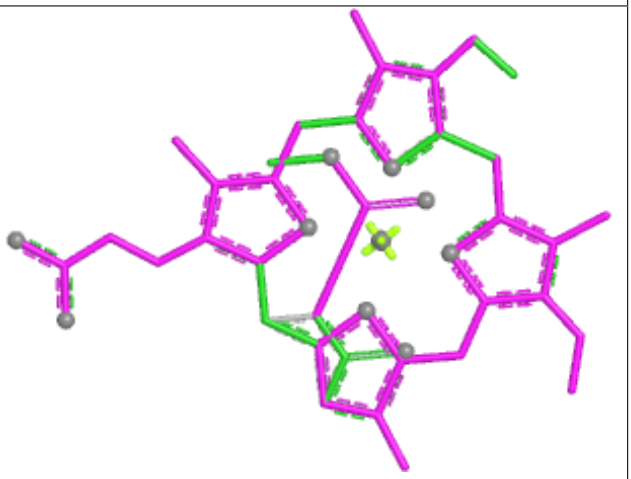
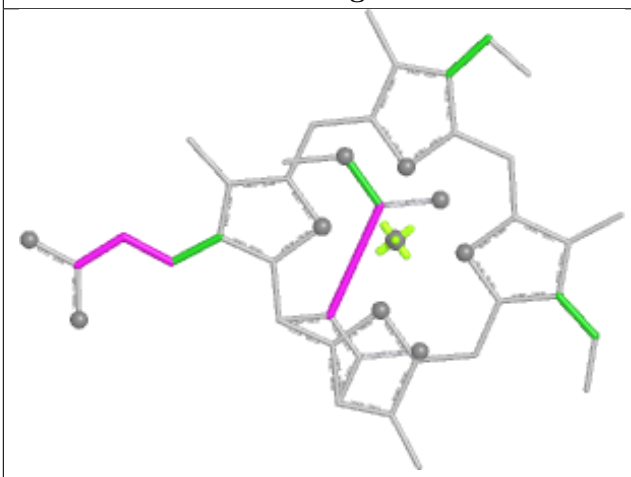
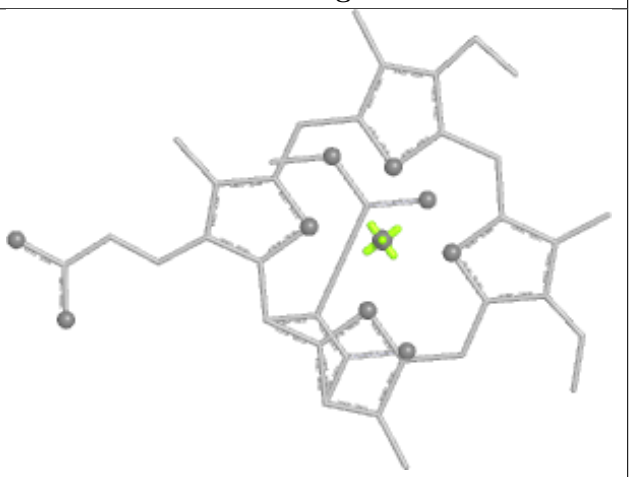
Bond angles

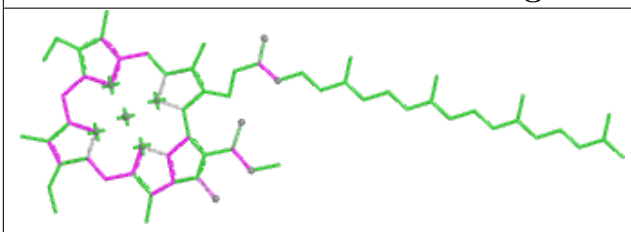
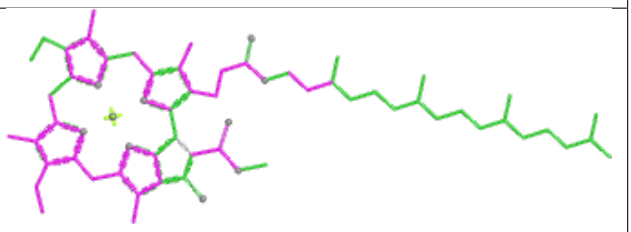
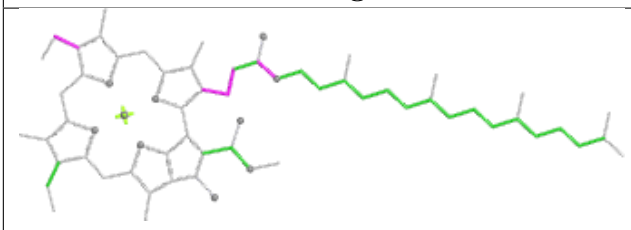
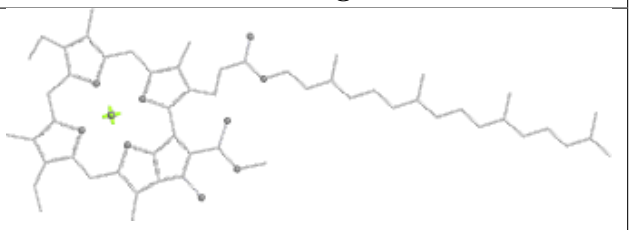


Torsions

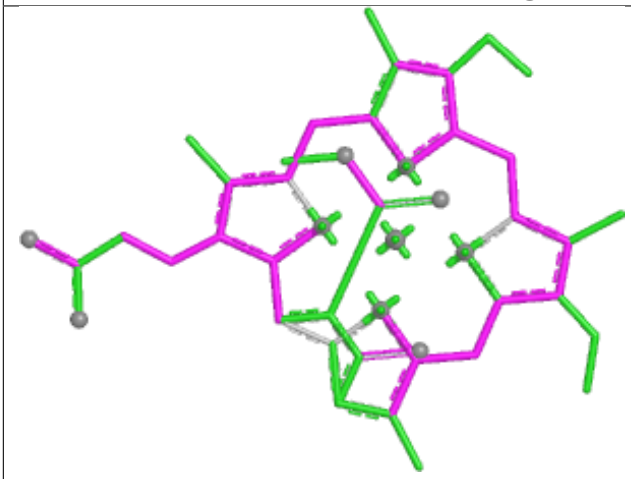


Rings

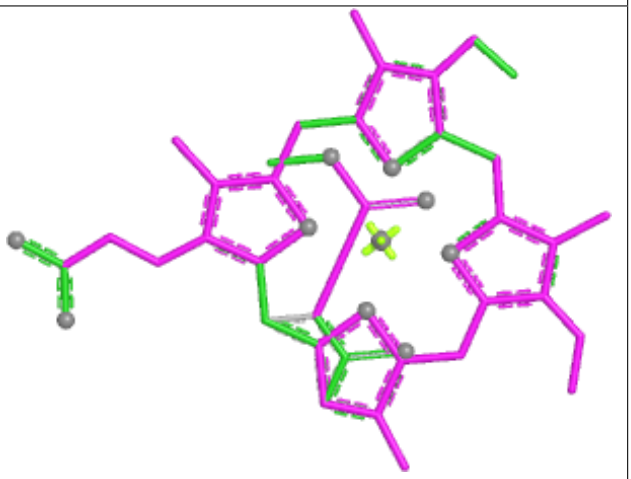
Ligand KC1 12 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

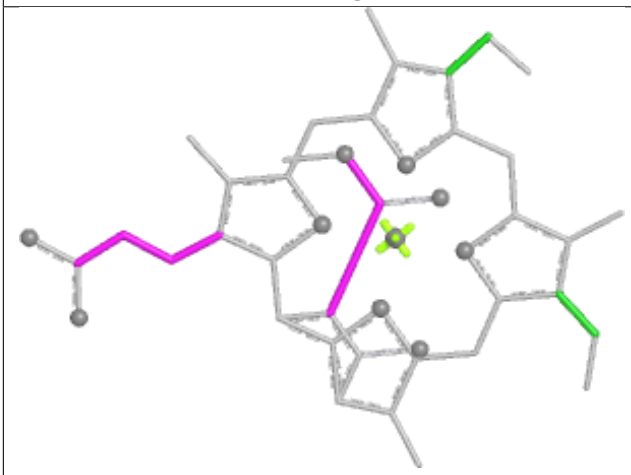
Ligand KC1 13 305



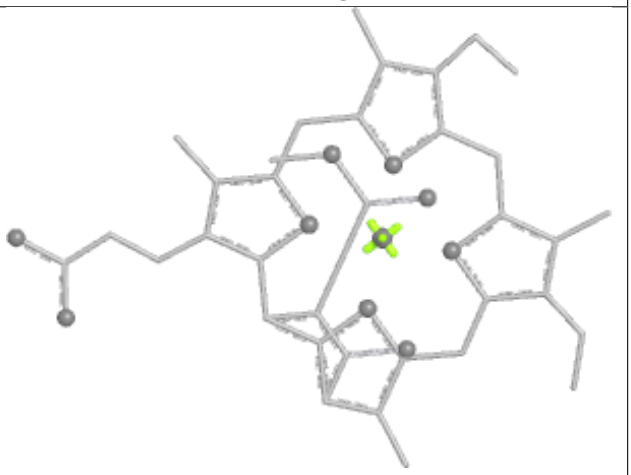
Bond lengths



Bond angles



Torsions

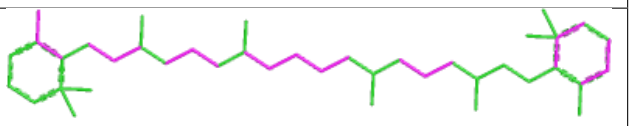


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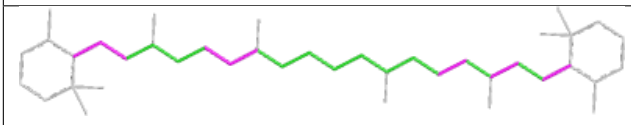
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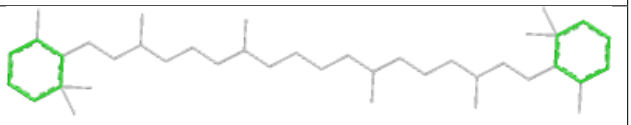
Bond lengths



Bond angles

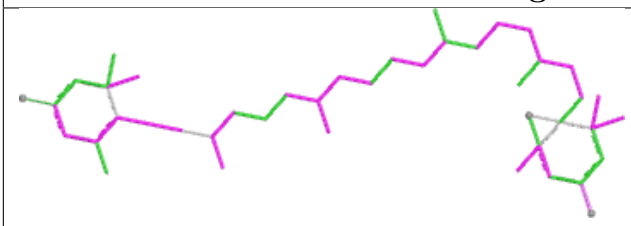


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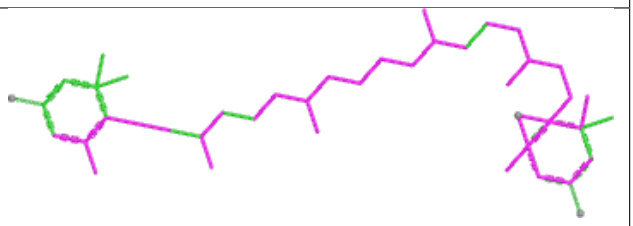


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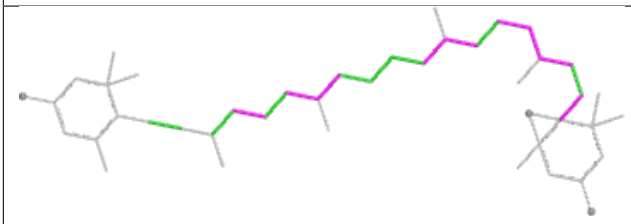
Ligand DD6 2 317



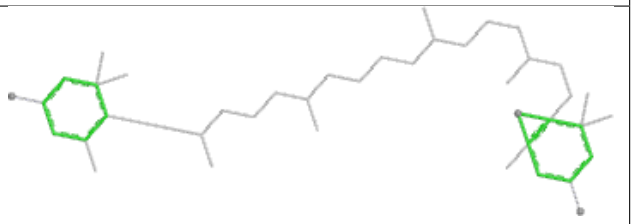
Bond lengths



Bond angles

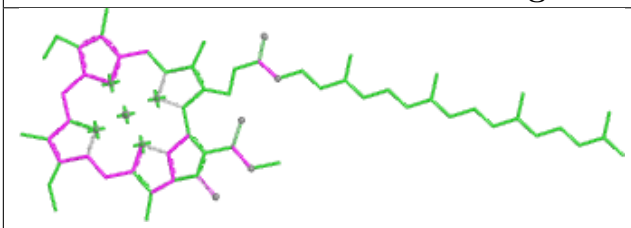


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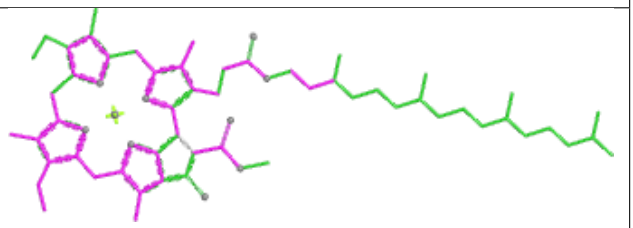


Rings

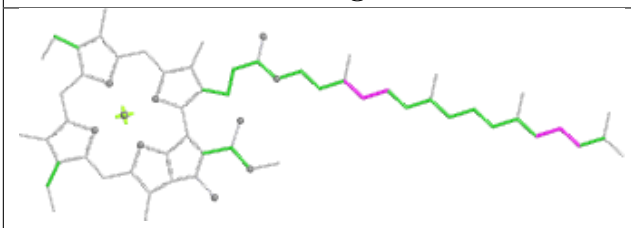
Ligand CLA 6 305



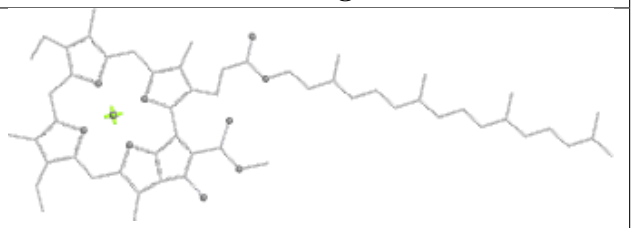
Bond lengths



Bond angles

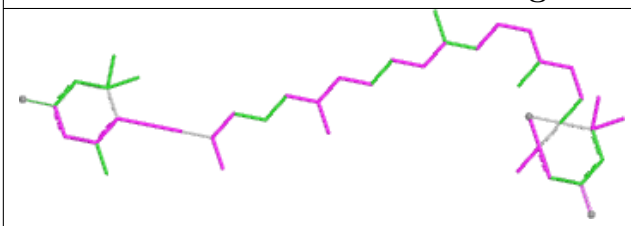


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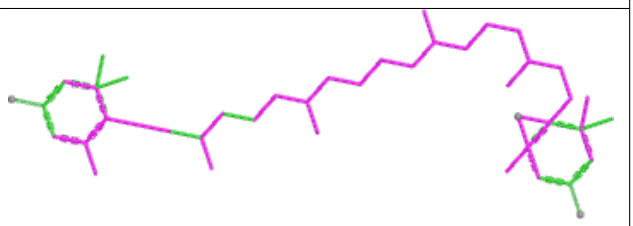


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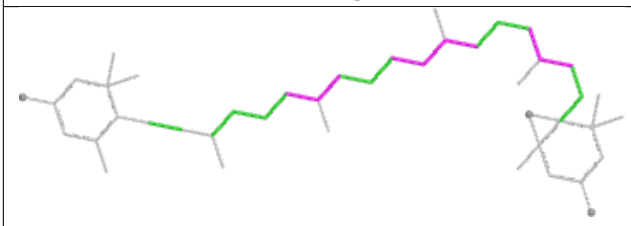
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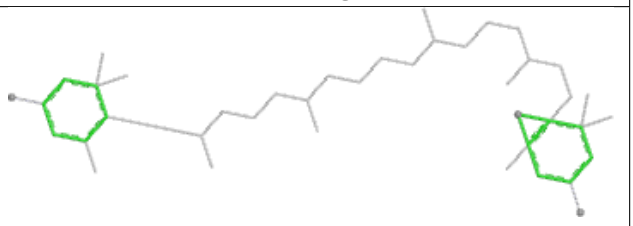
Bond lengths



Bond angles

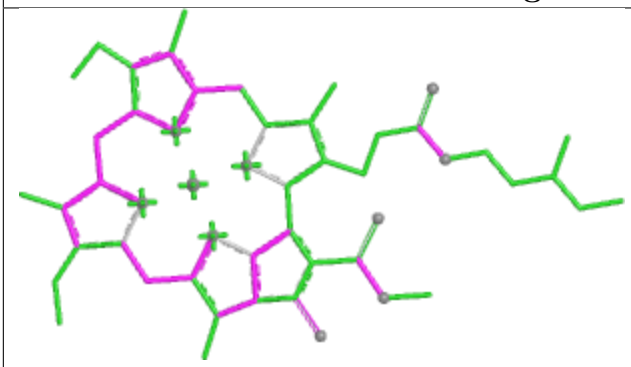


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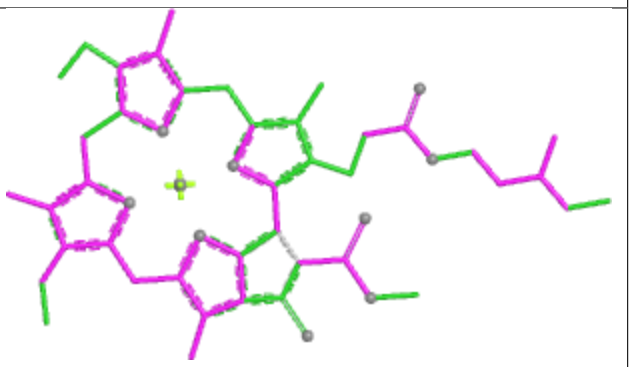


Rings

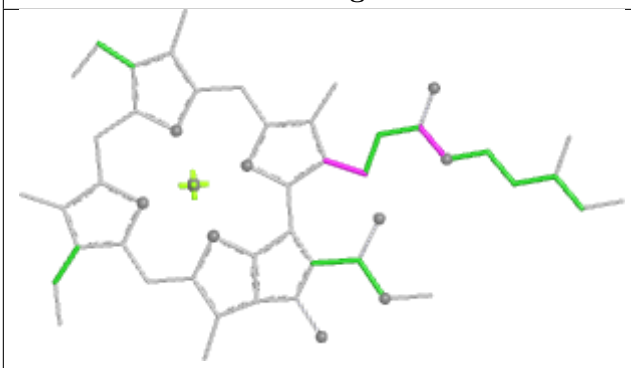
Ligand CLA A 838



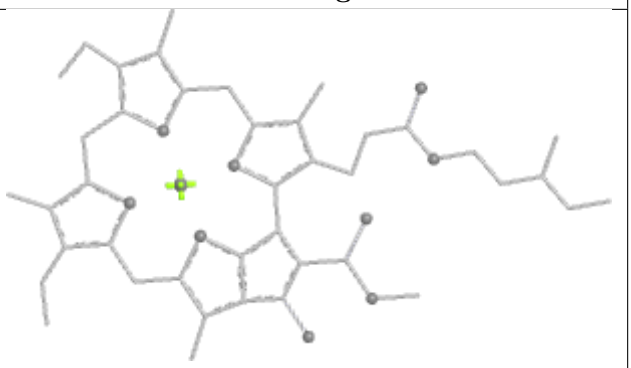
Bond lengths



Bond angles

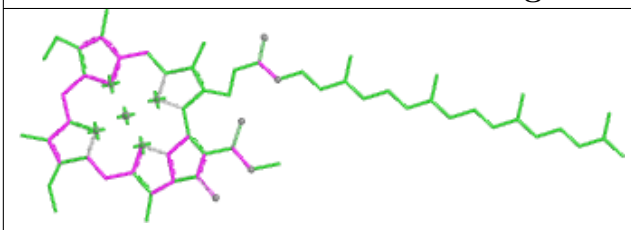


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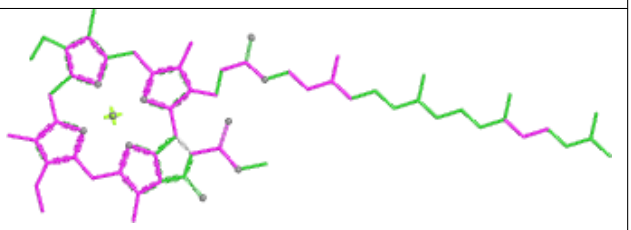


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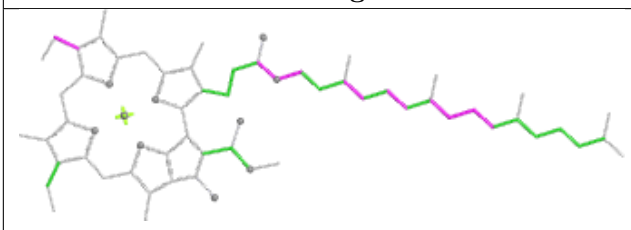
Ligand CLA B 811



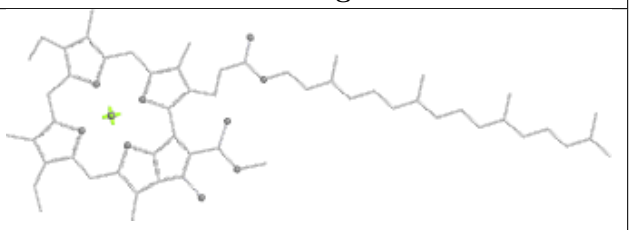
Bond lengths



Bond angles

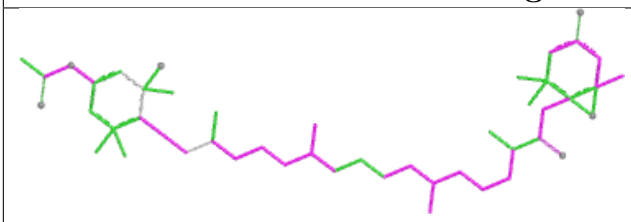


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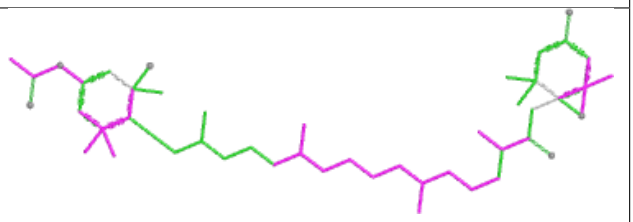


Rings

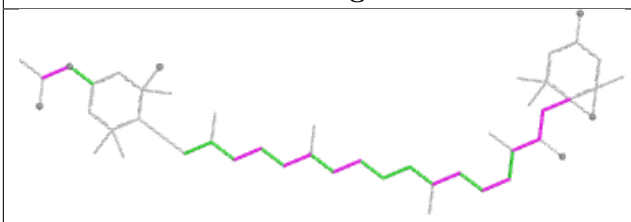
Ligand A86 15 321



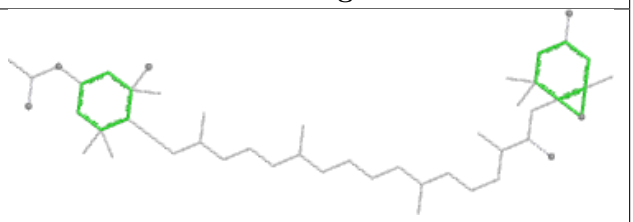
Bond lengths



Bond angles

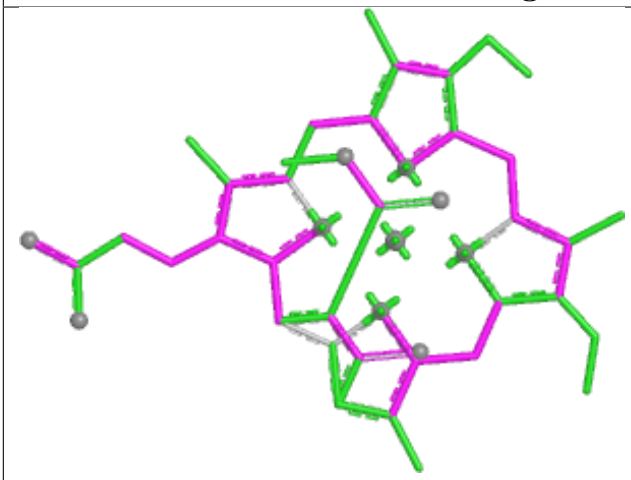


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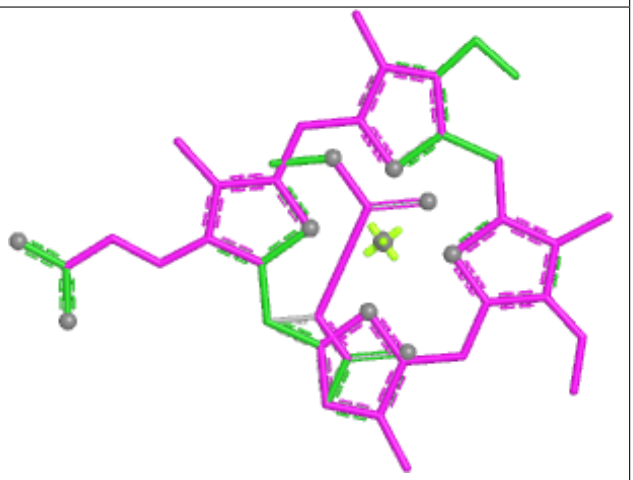


Rings

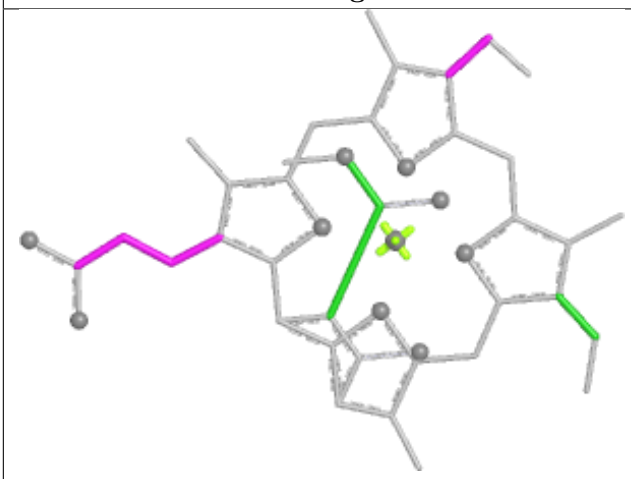
Ligand KC1 12 313



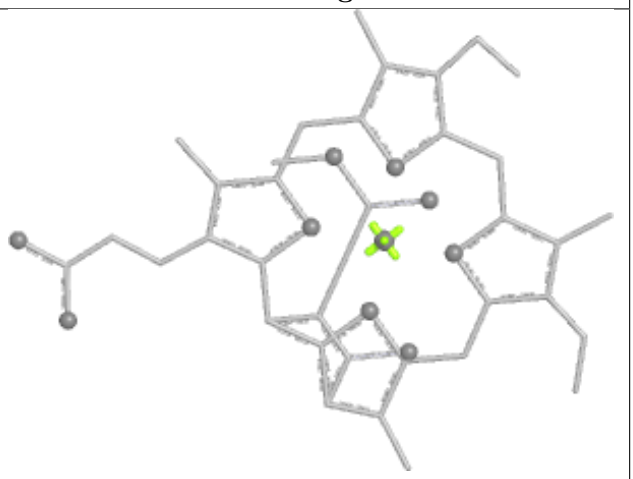
Bond lengths



Bond angles

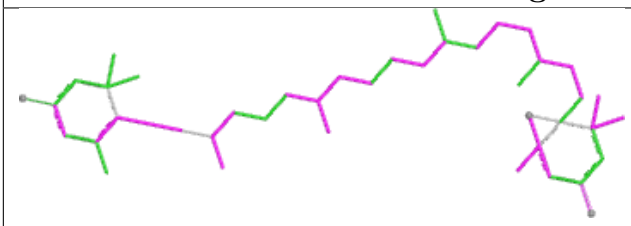


Torsions

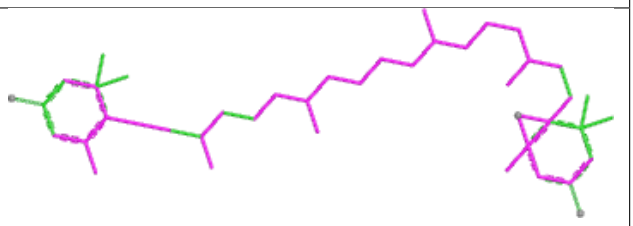


Rings

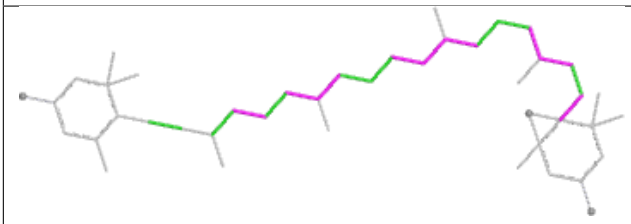
Ligand DD6 9 314



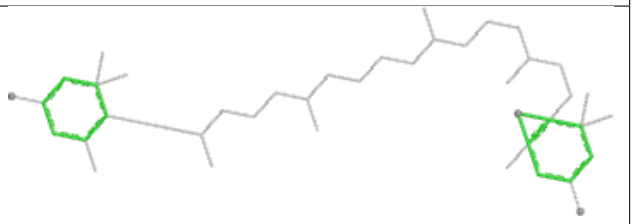
Bond lengths



Bond angles

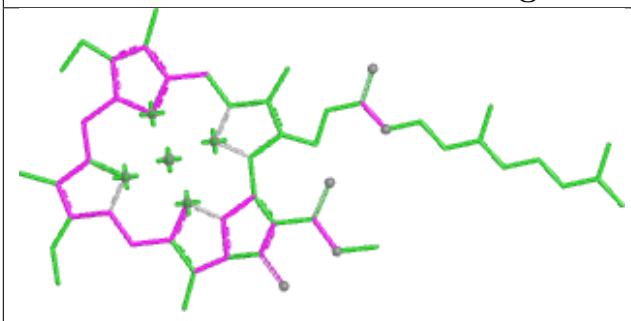


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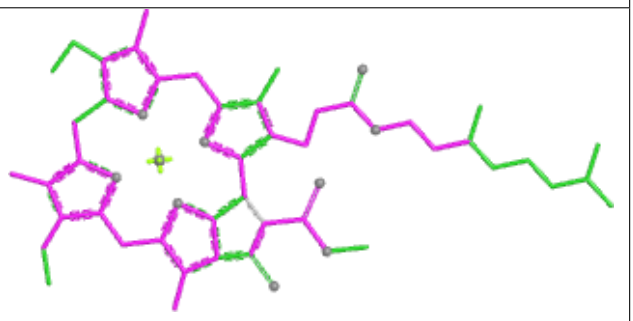


Rings

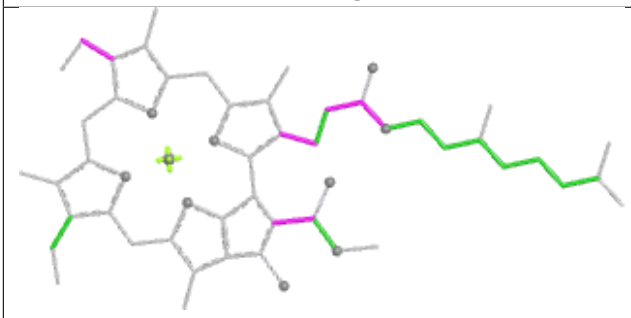
Ligand CLA 11 306



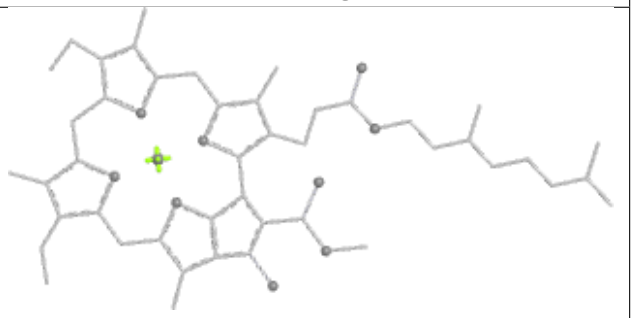
Bond lengths



Bond angles

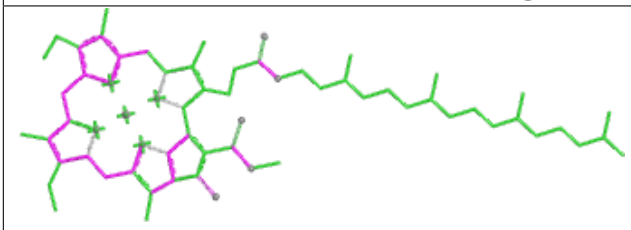


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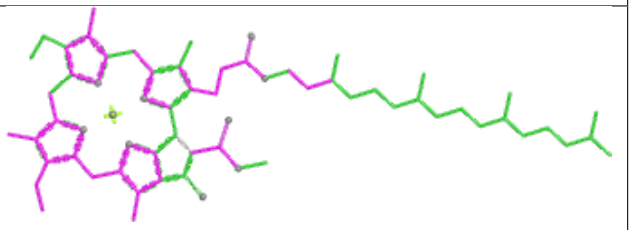


Rings

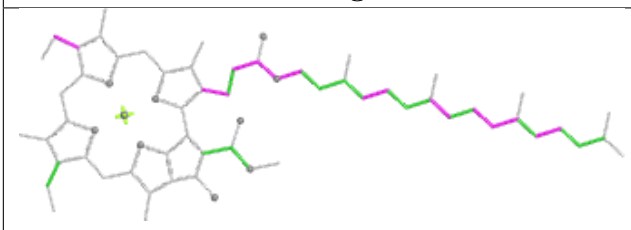
Ligand CLA 12 304



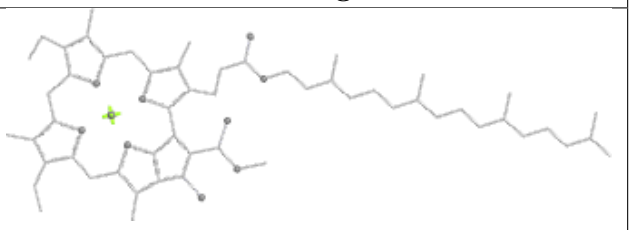
Bond lengths



Bond angles

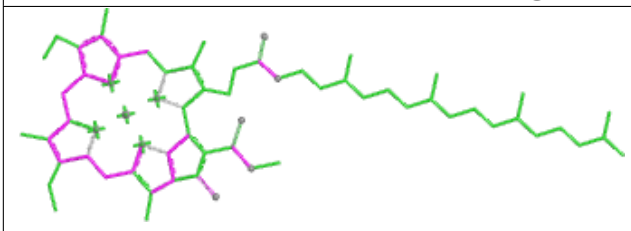


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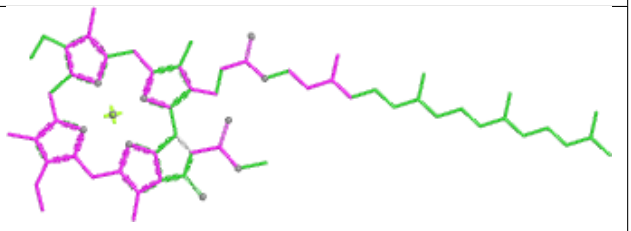


Rings

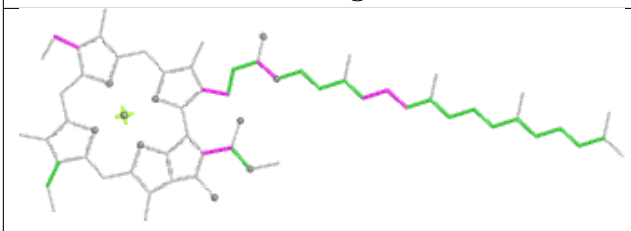
Ligand CLA 4 309



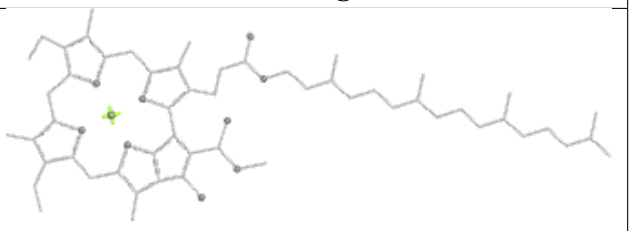
Bond lengths



Bond angles

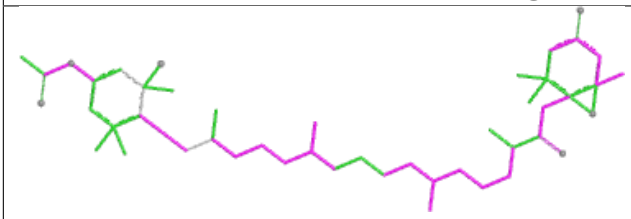


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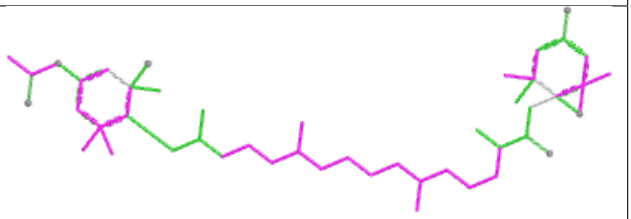


Rings

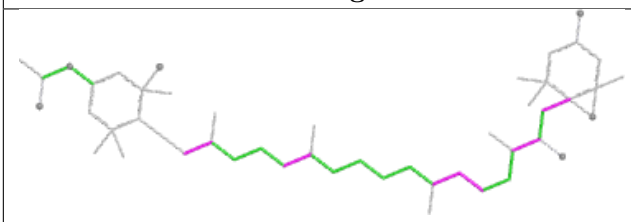
Ligand A86 16 312



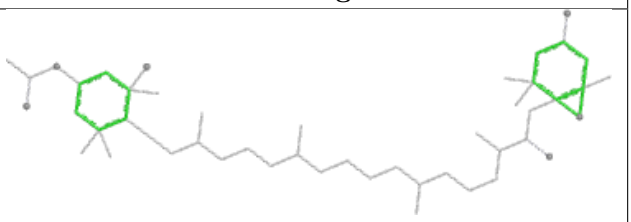
Bond lengths



Bond angles

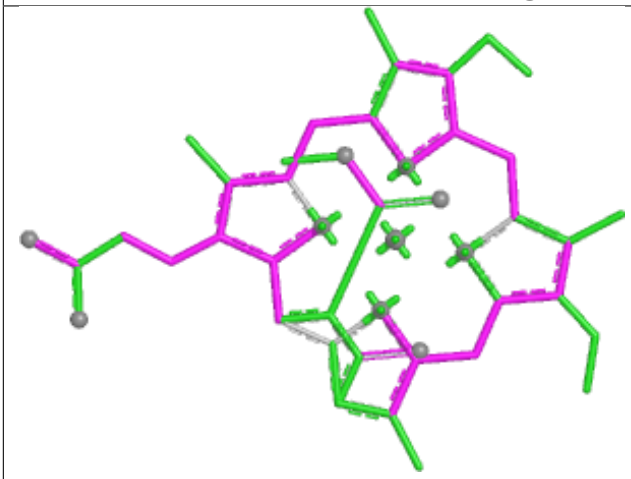


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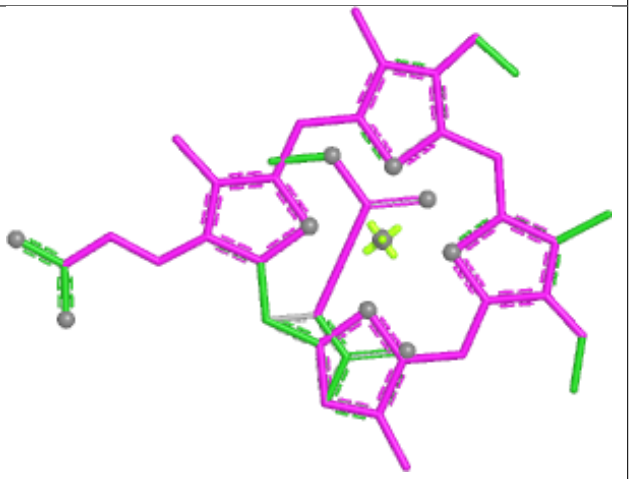


Rings

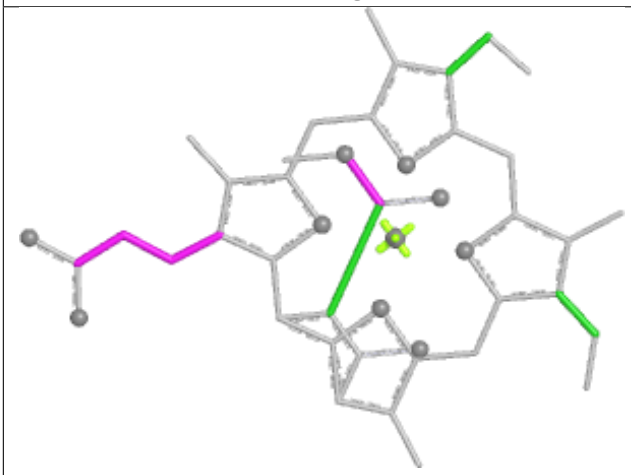
Ligand KC1 10 310



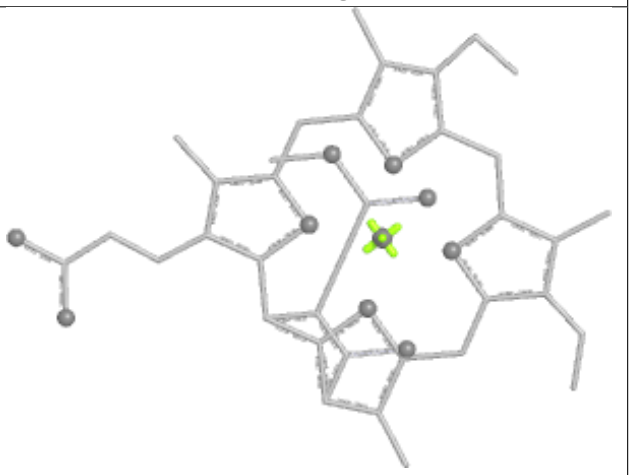
Bond lengths



Bond angles

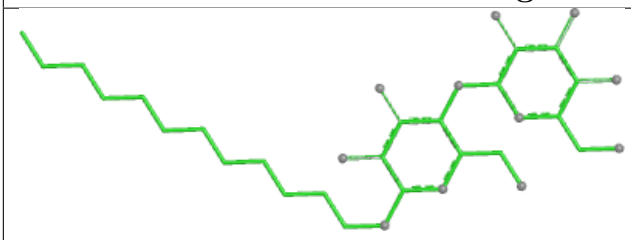


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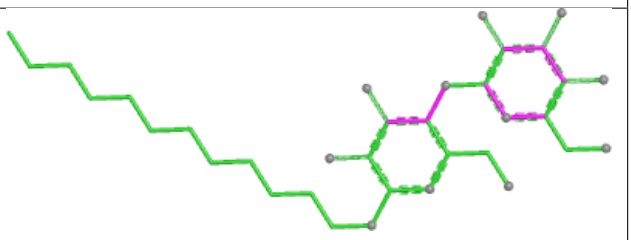


Rings

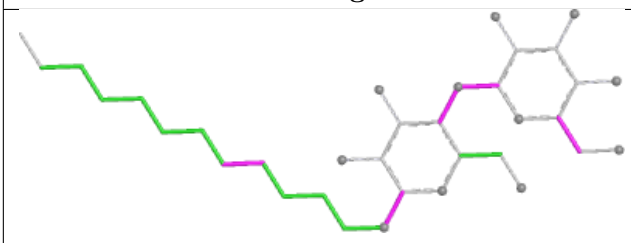
Ligand LMT 15 301



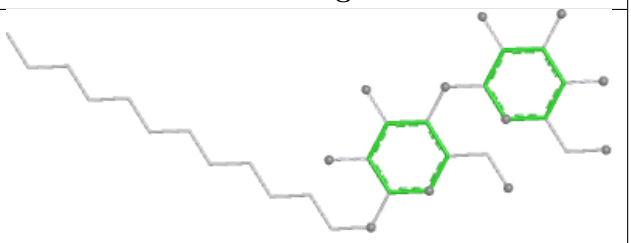
Bond lengths



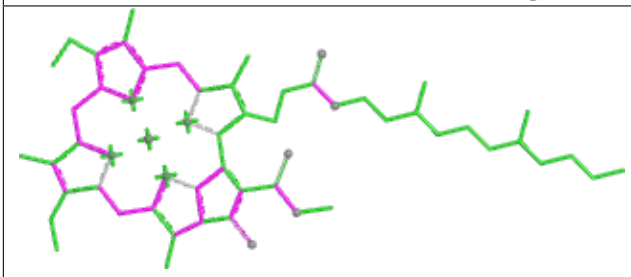
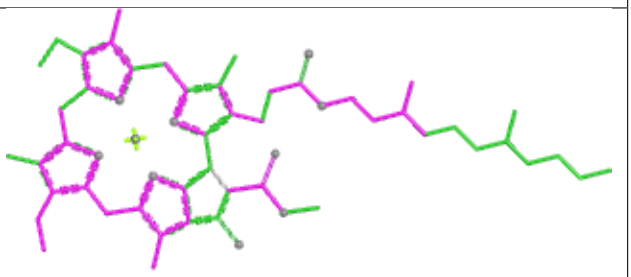
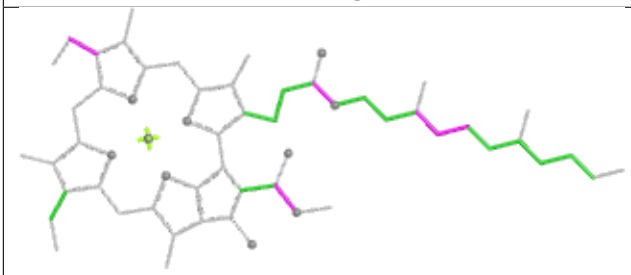
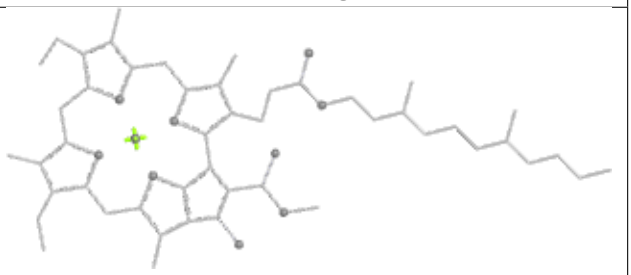
Bond angles

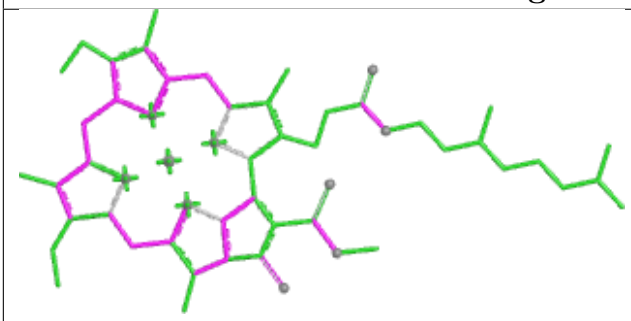
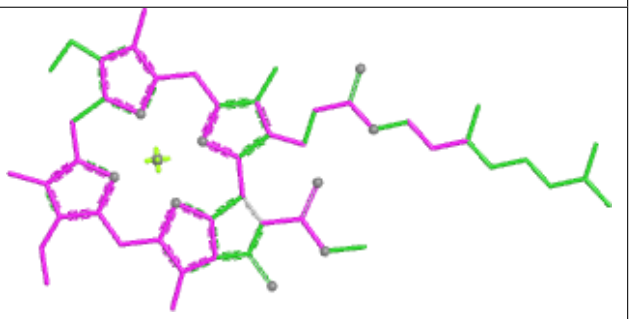
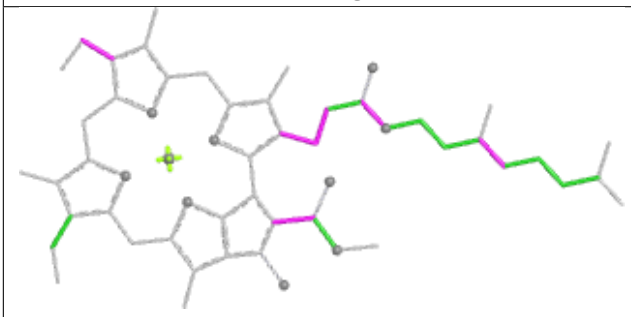
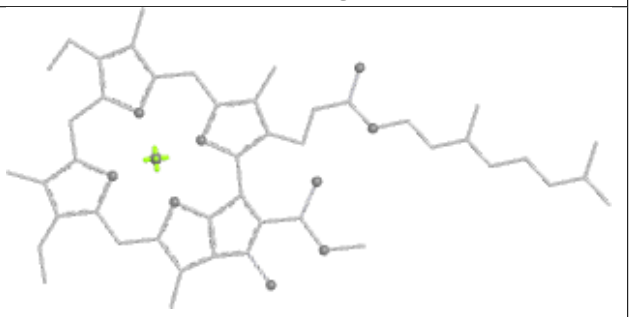


Torsions

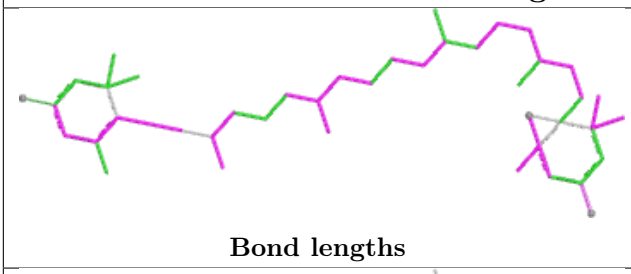


Rings

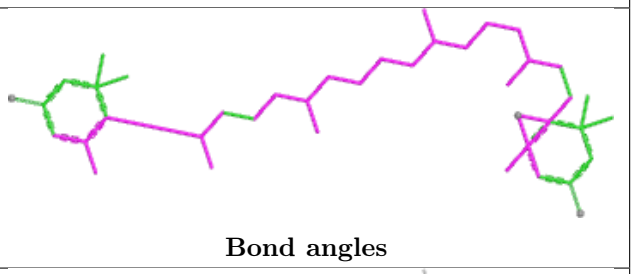
Ligand CLA B 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 8 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

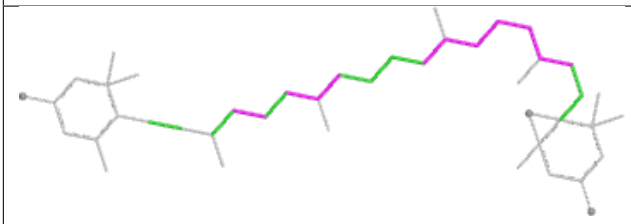
Ligand DD6 2 315



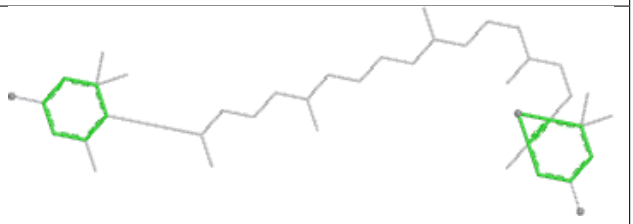
Bond lengths



Bond angles

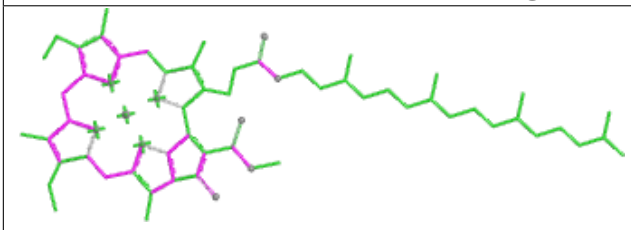


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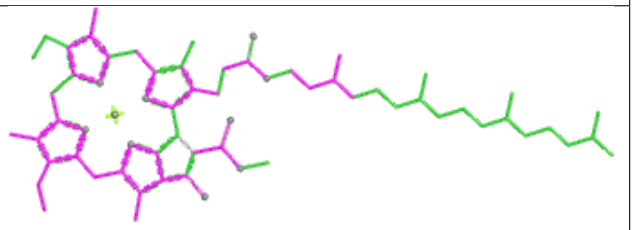


Rings

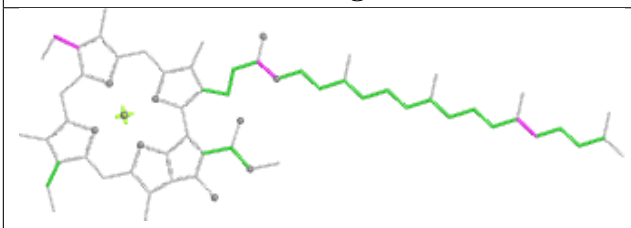
Ligand CLA A 827



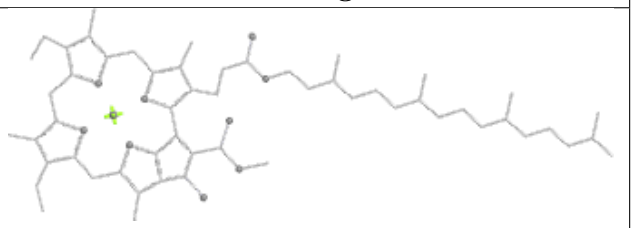
Bond lengths



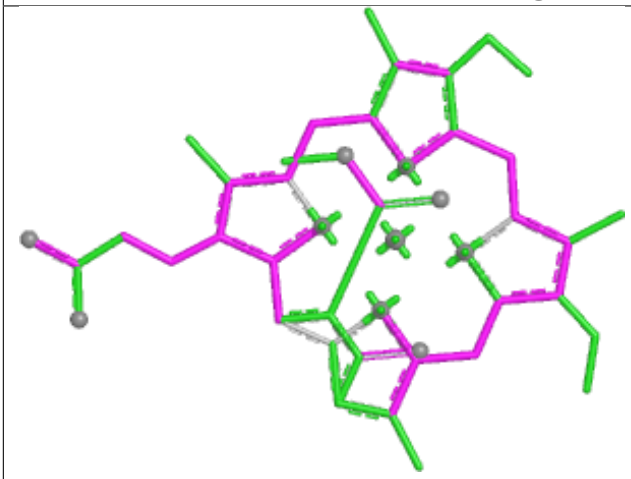
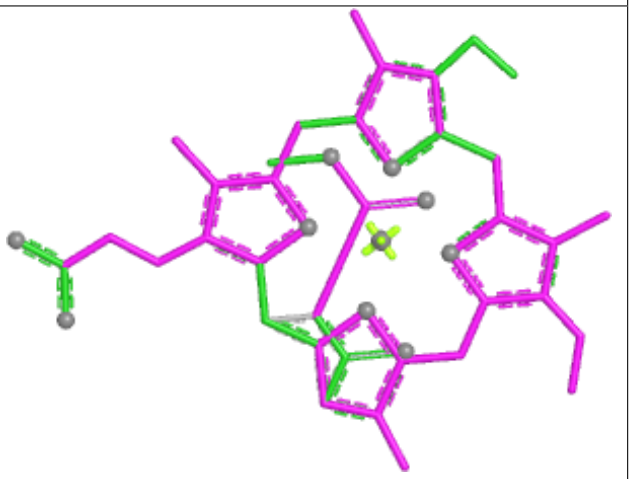
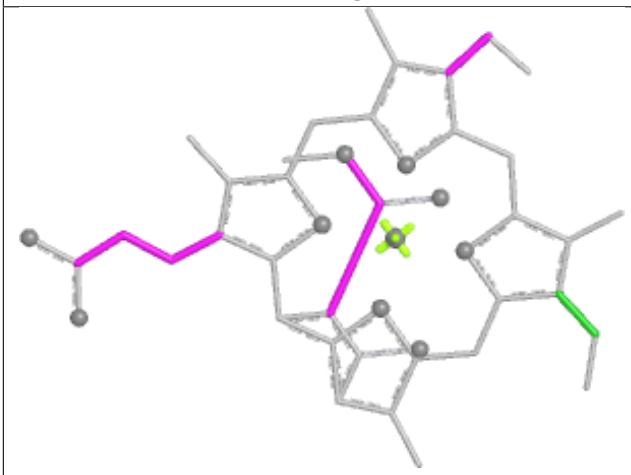
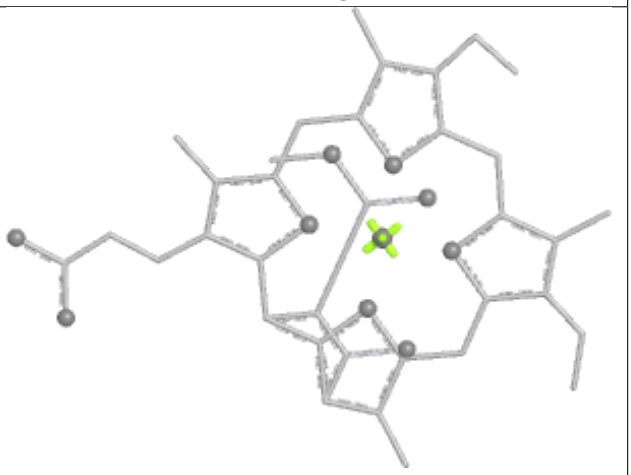
Bond angles

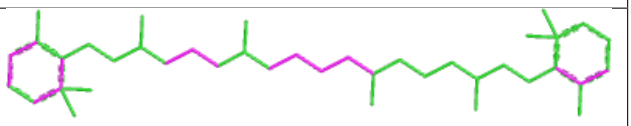
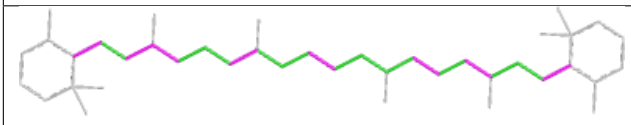
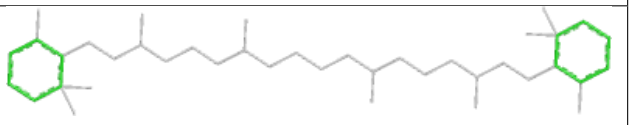


Torsions

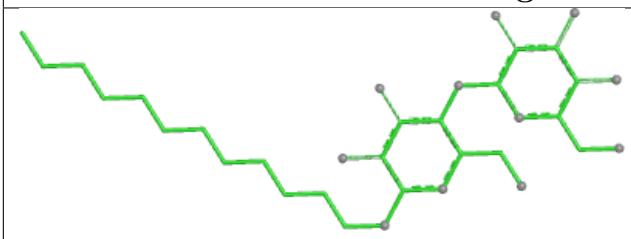


Rings

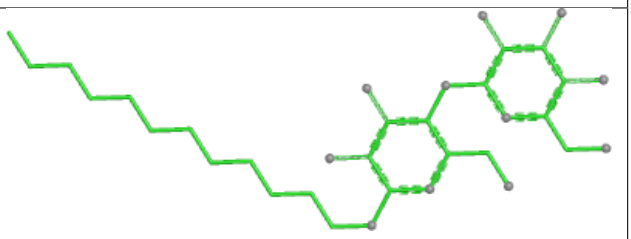
Ligand KC1 9 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR L 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

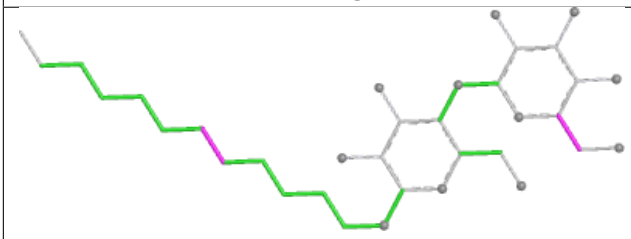
Ligand LMT 12 318



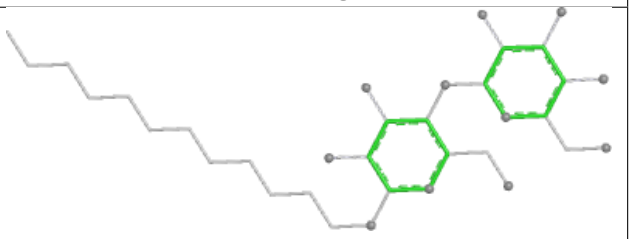
Bond lengths



Bond angles

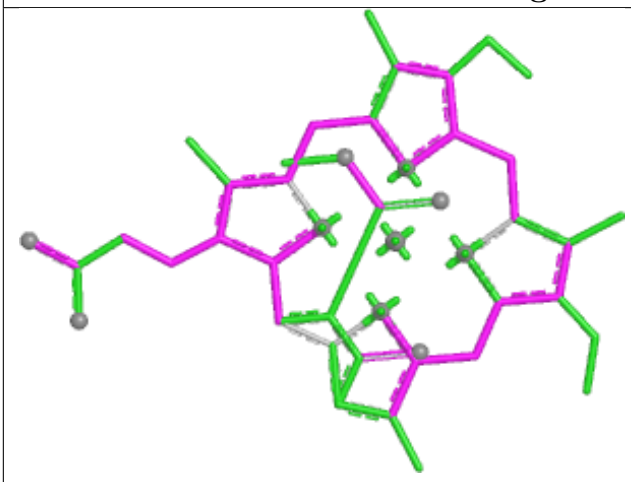


Torsions

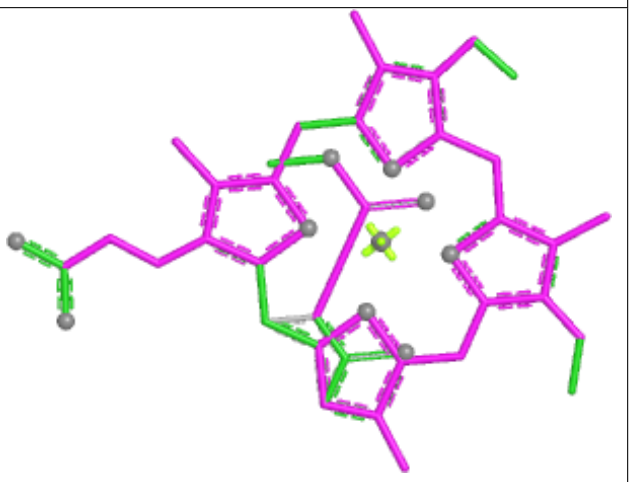


Rings

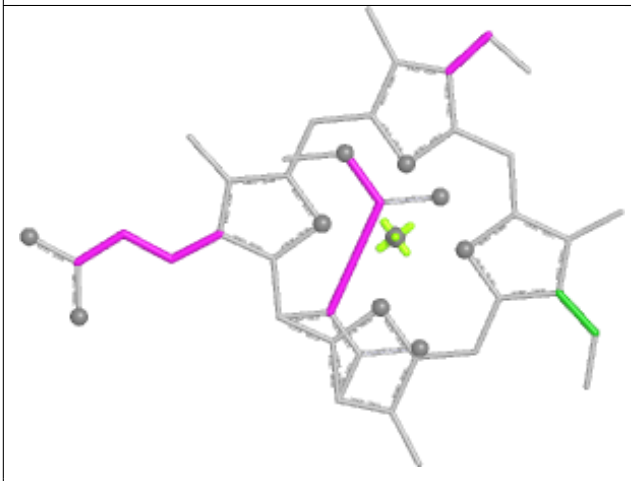
Ligand KC1 1 306



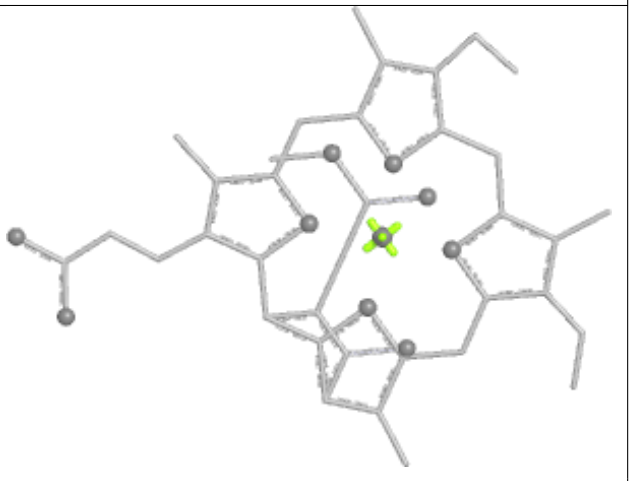
Bond lengths



Bond angles

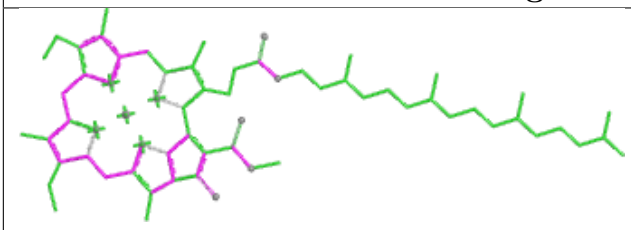


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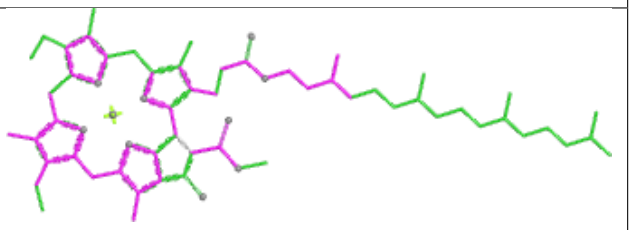


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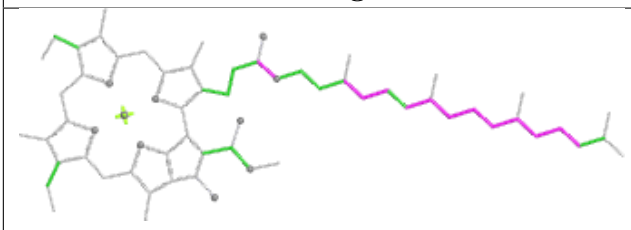
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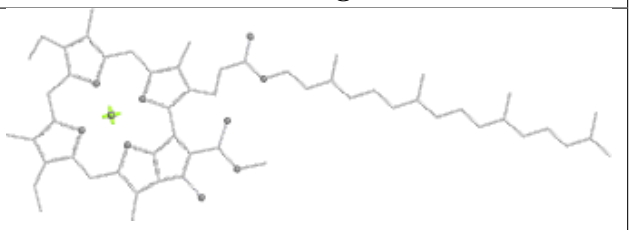
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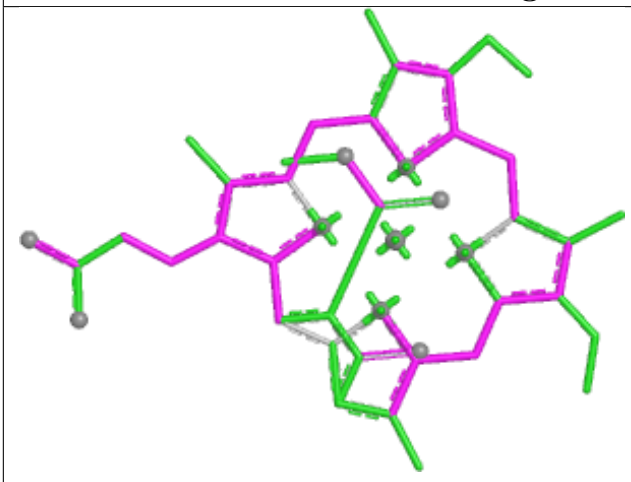


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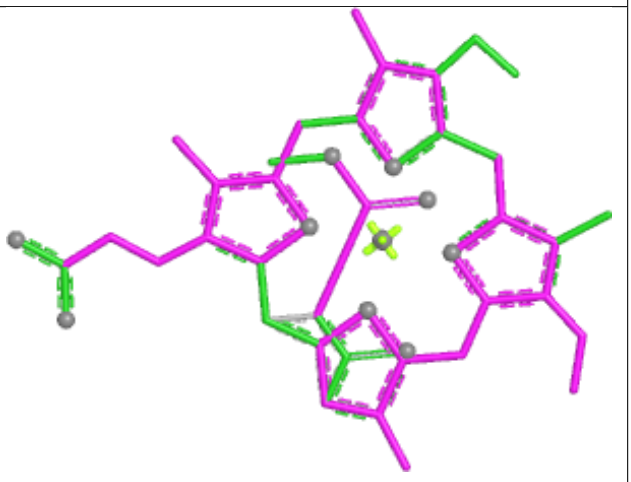


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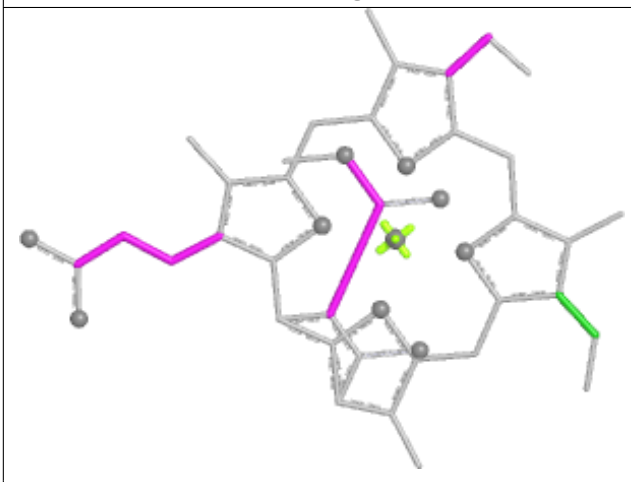
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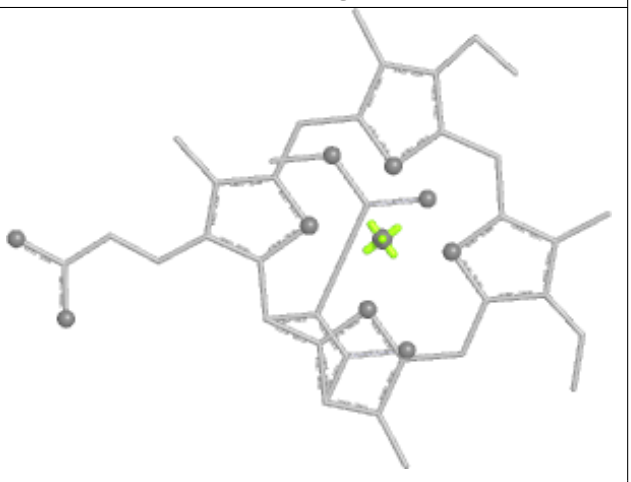
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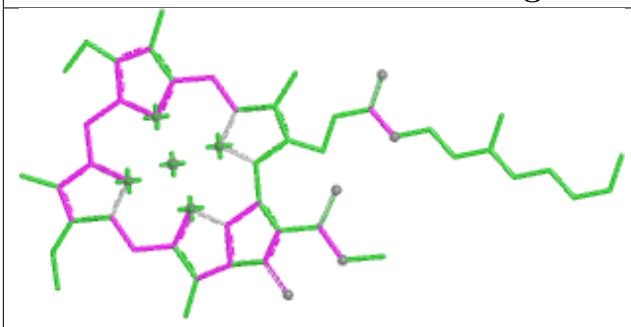


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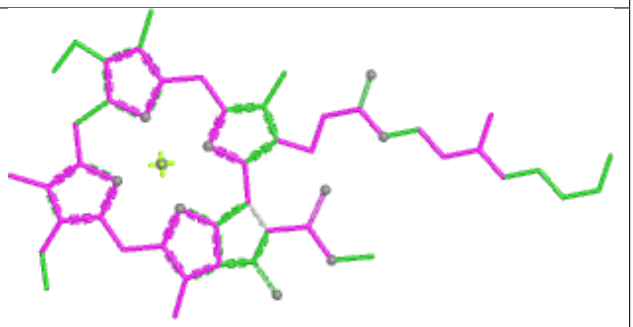


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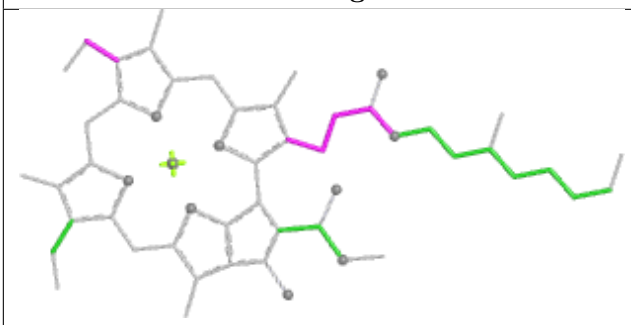
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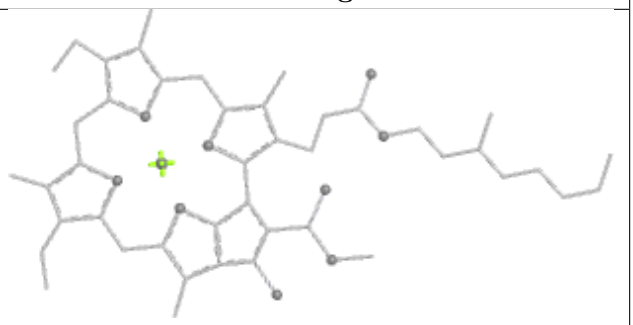
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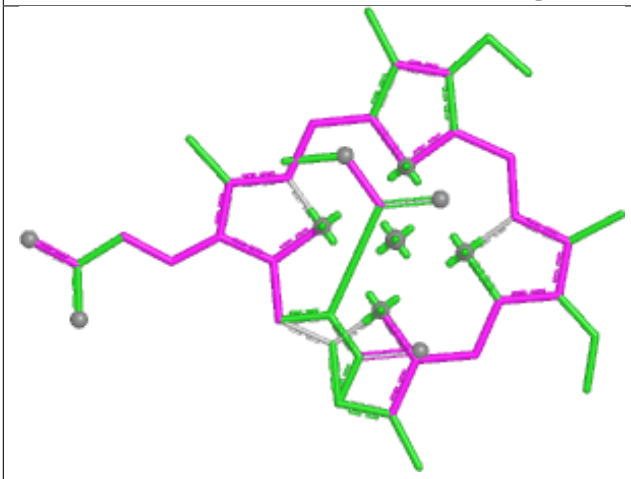


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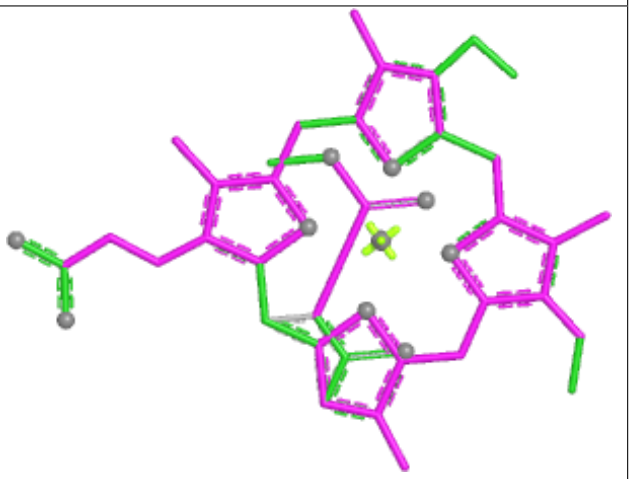


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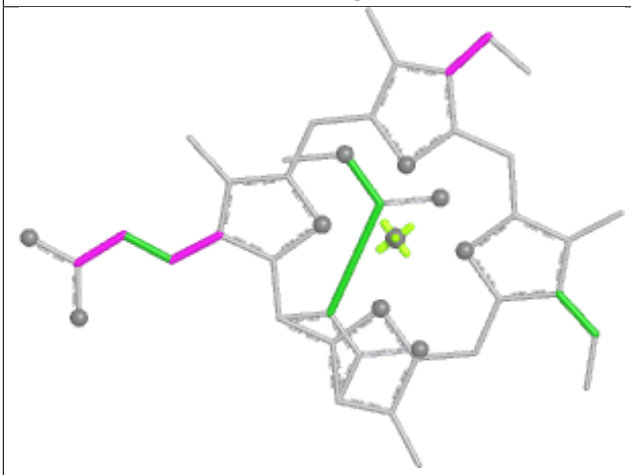
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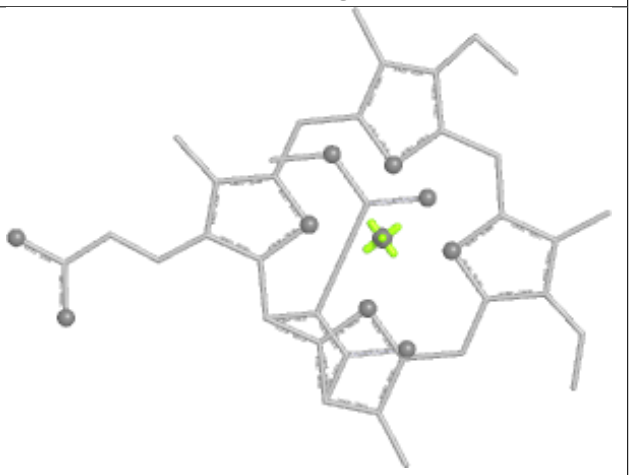
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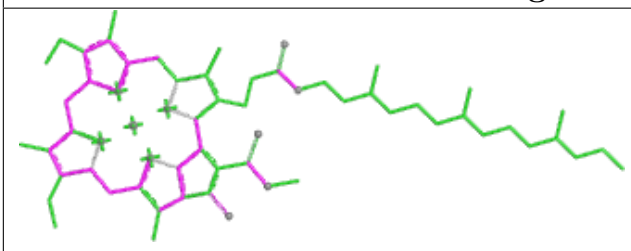


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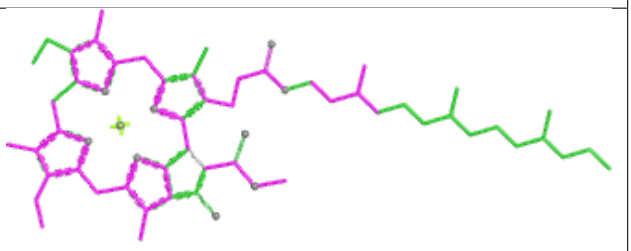


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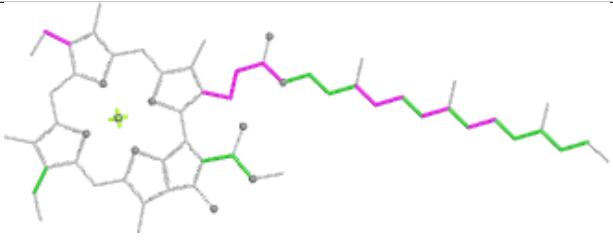
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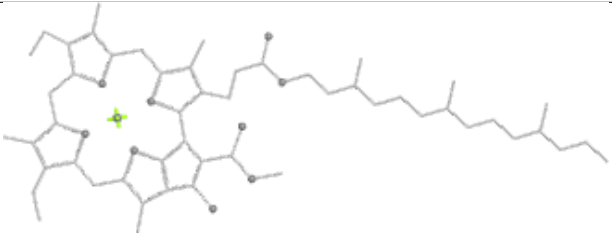
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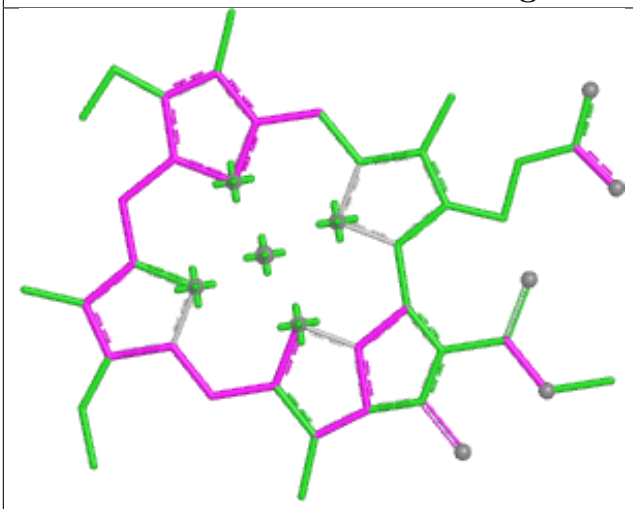


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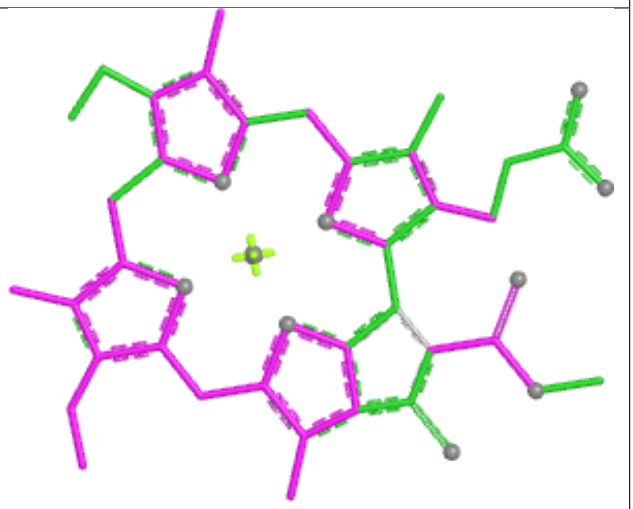


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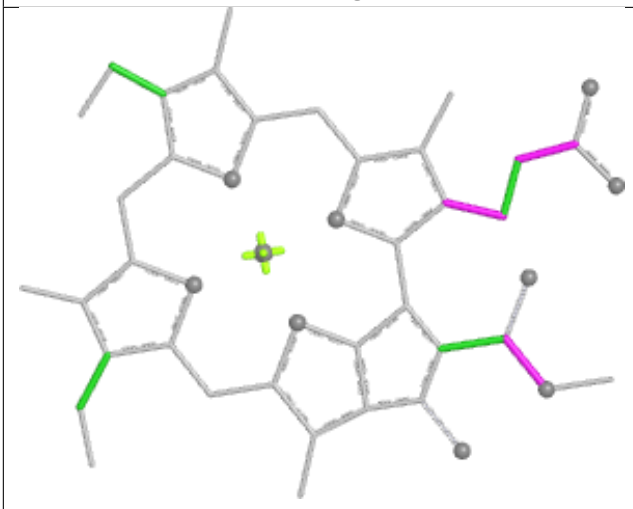
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Bond lengths



Bond angles

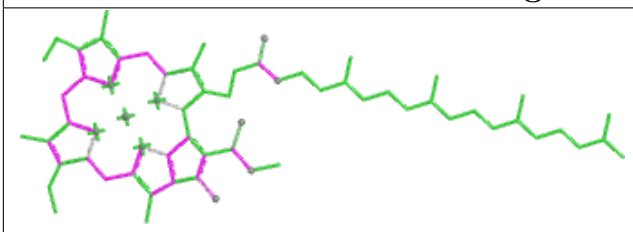


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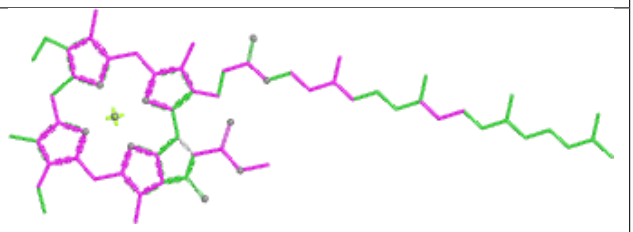


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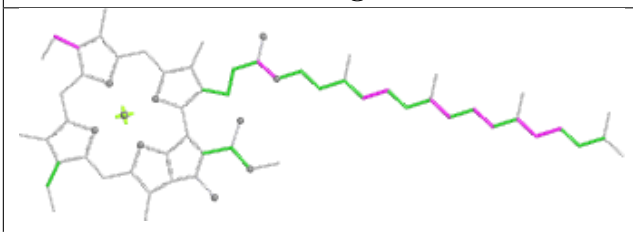
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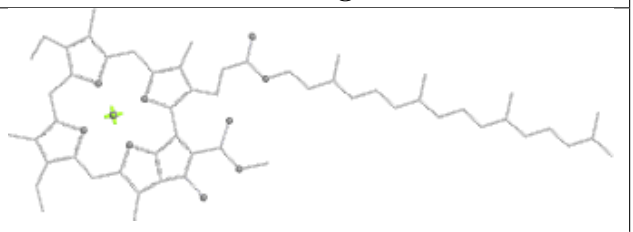
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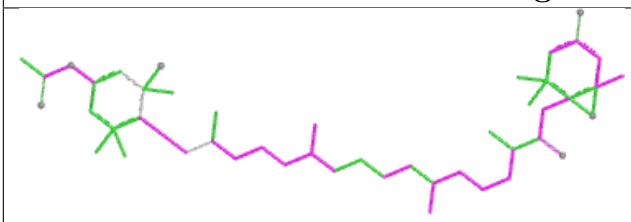


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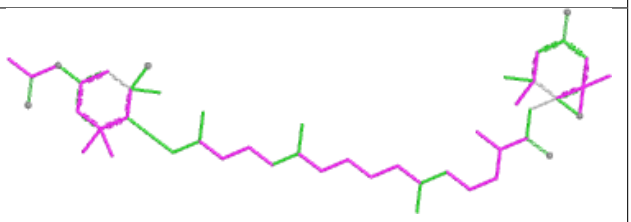


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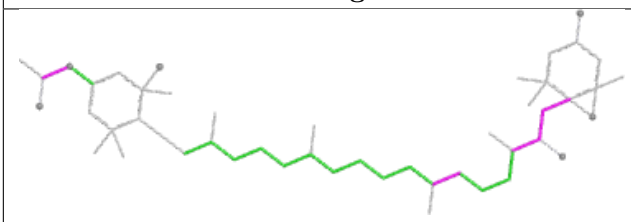
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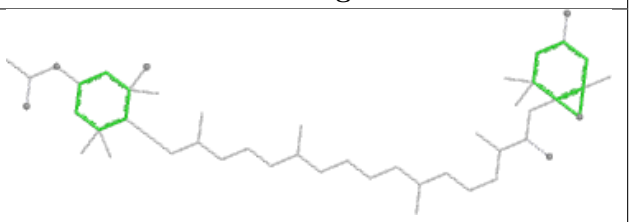
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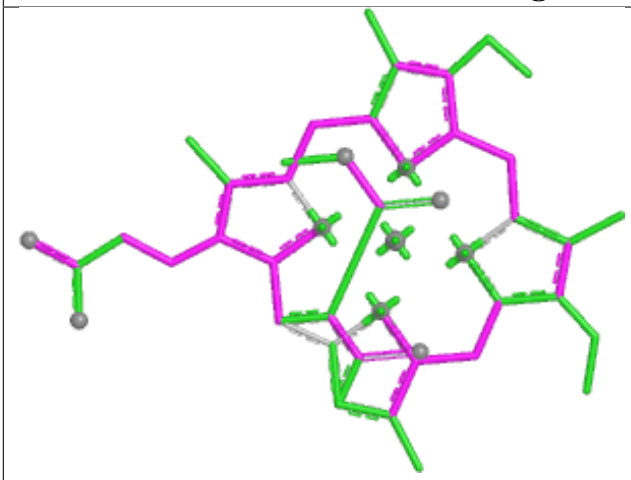


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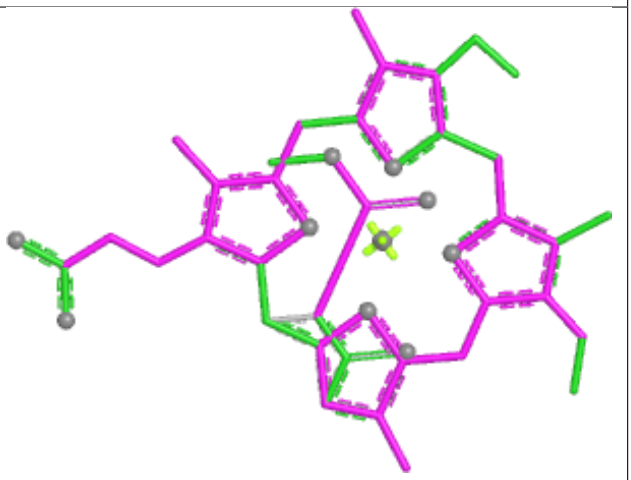


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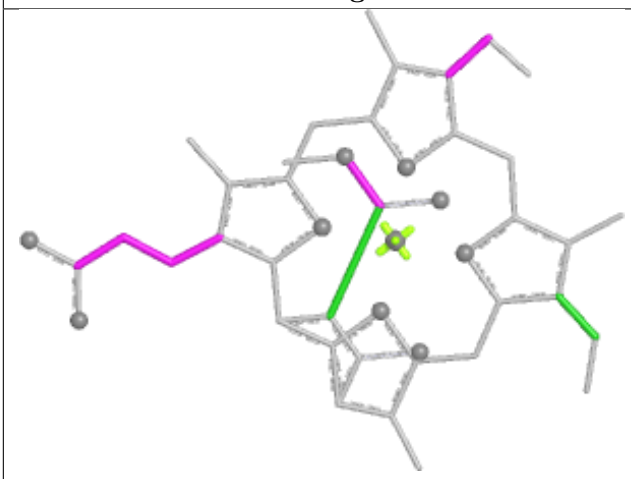
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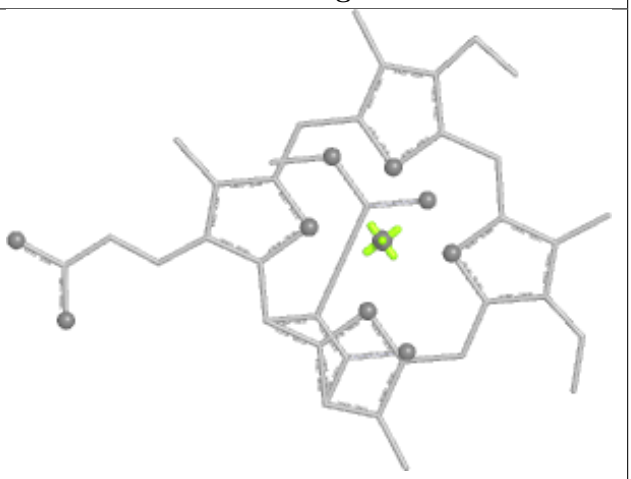
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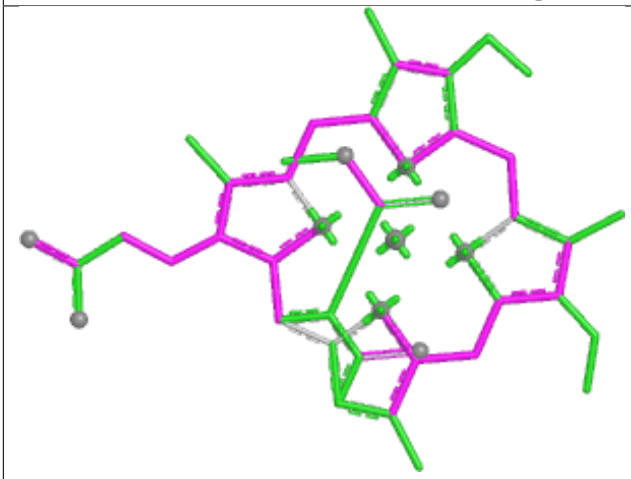


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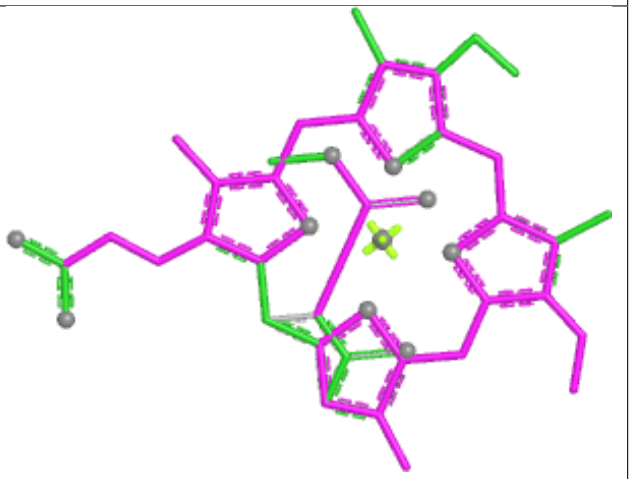


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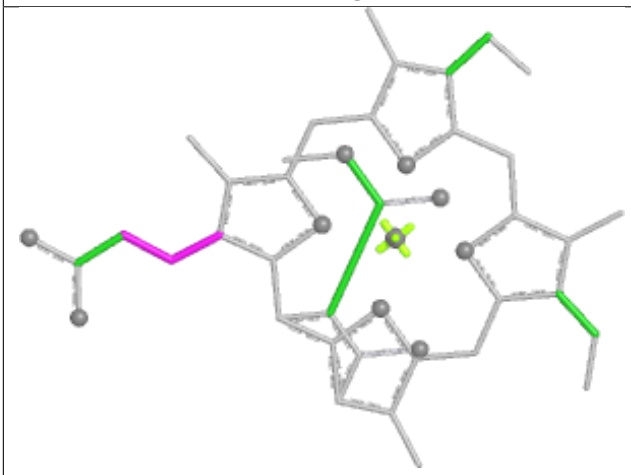
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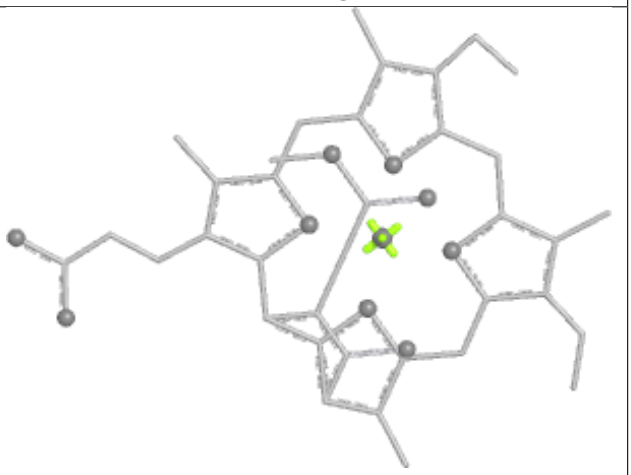
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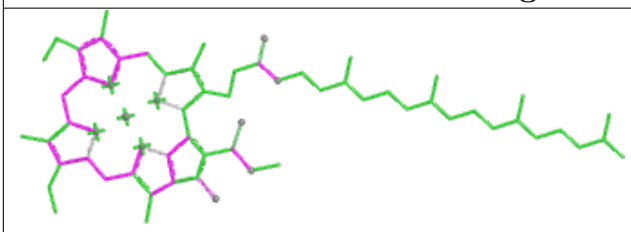


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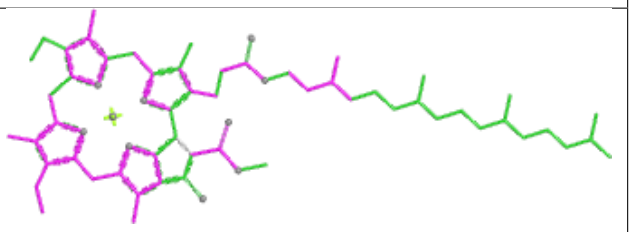


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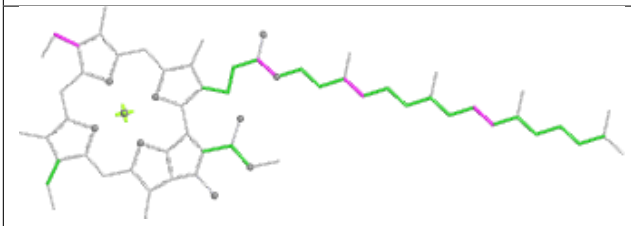
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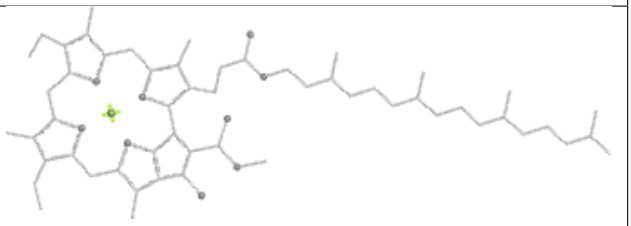
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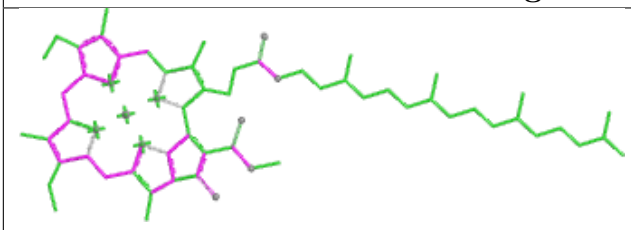


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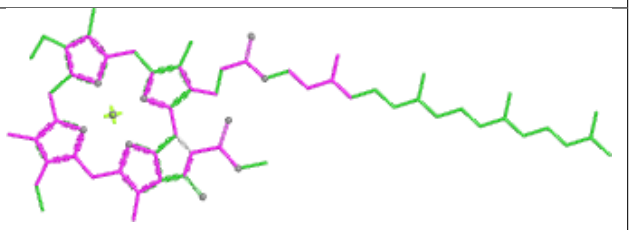


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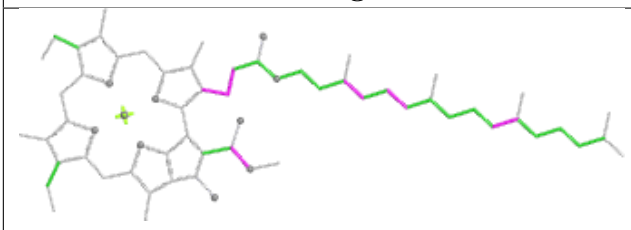
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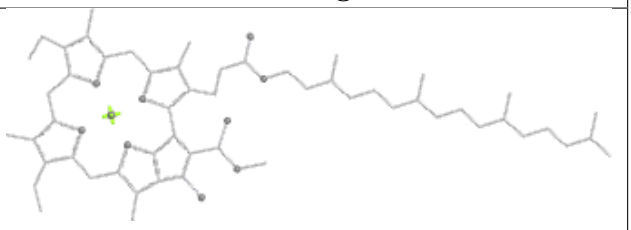
Bond lengths



Bond angles

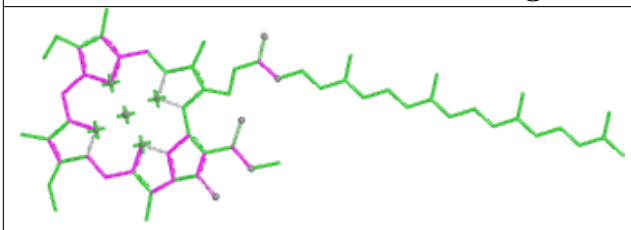


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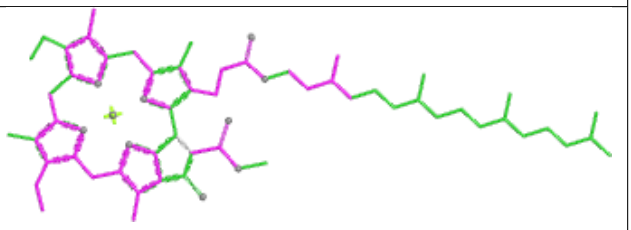


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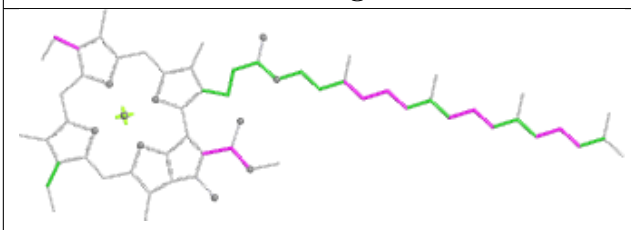
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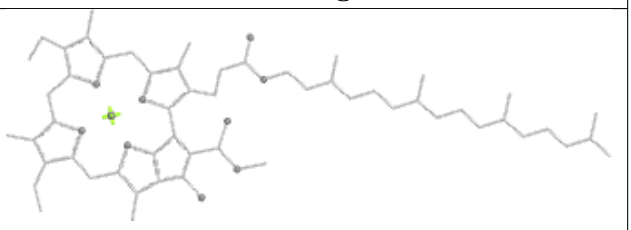
Bond lengths



Bond angles

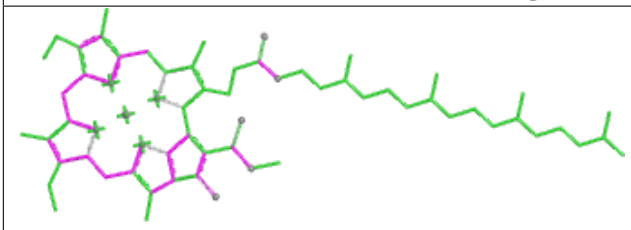


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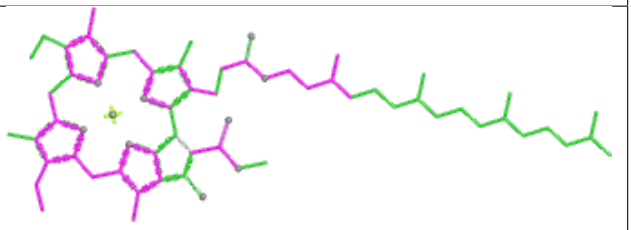


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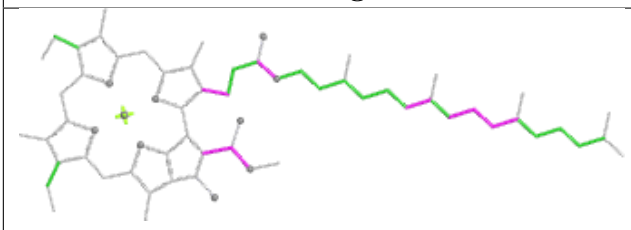
Ligand CLA B 828



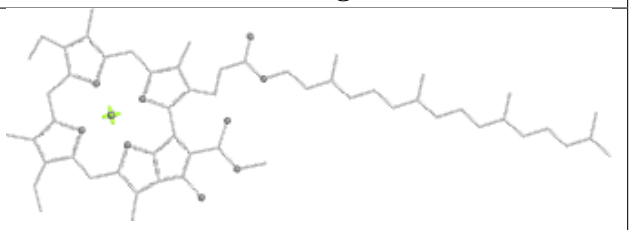
Bond lengths



Bond angles

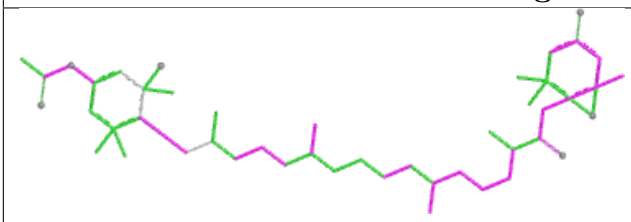


Torsions

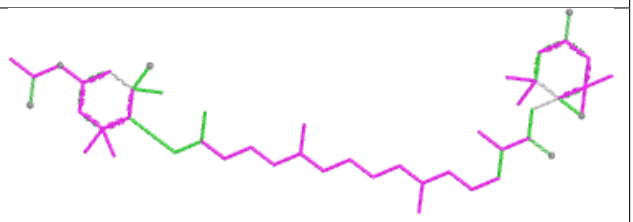


Rings

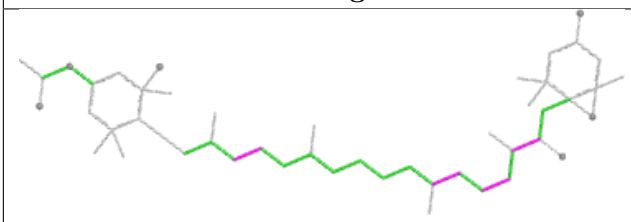
Ligand A86 7 316



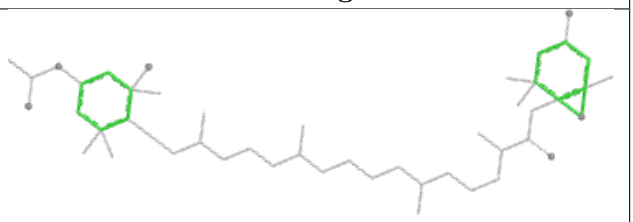
Bond lengths



Bond angles

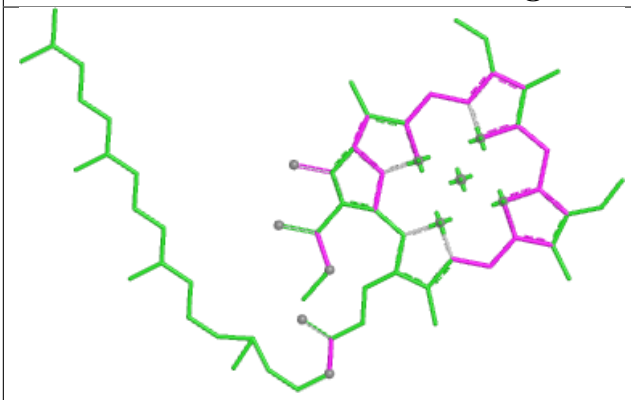


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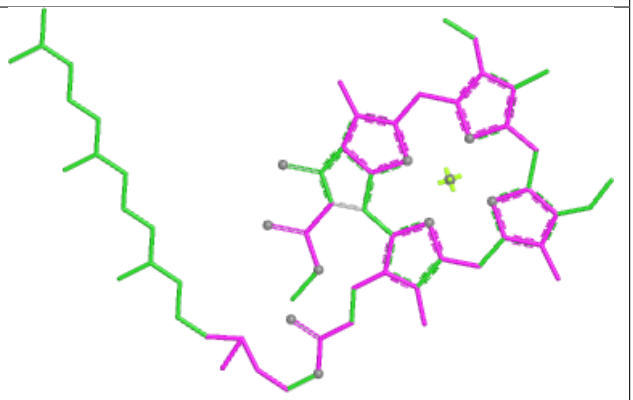


Rings

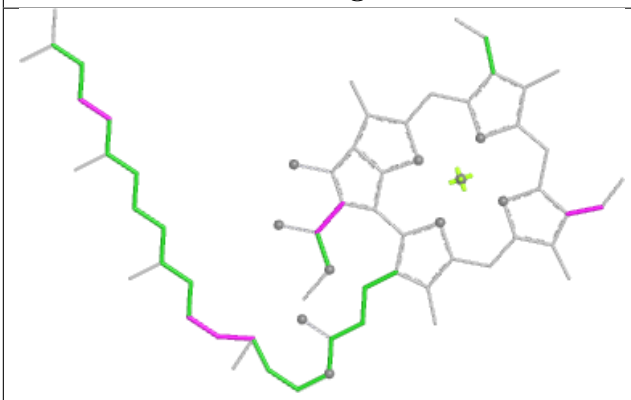
Ligand CLA B 824



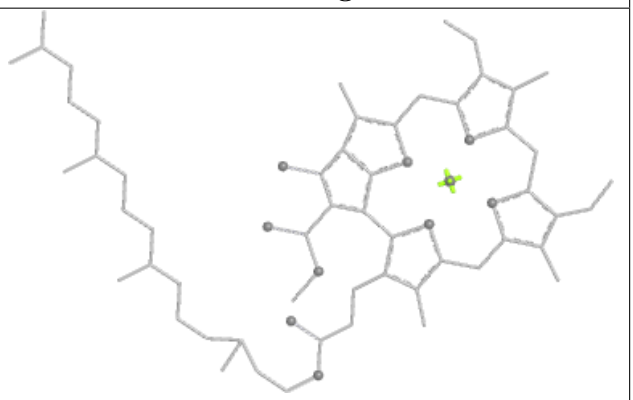
Bond lengths



Bond angles

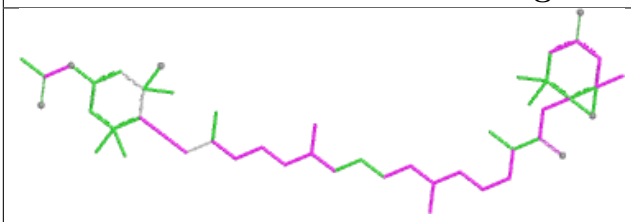


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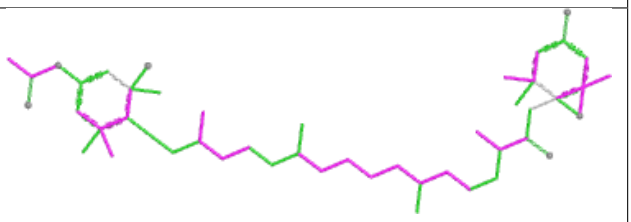


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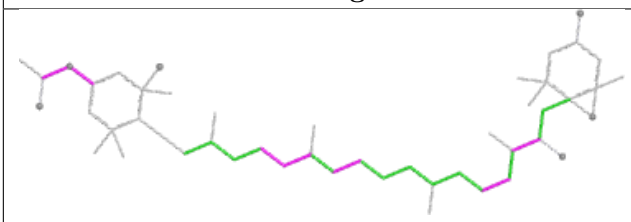
Ligand A86 2 302



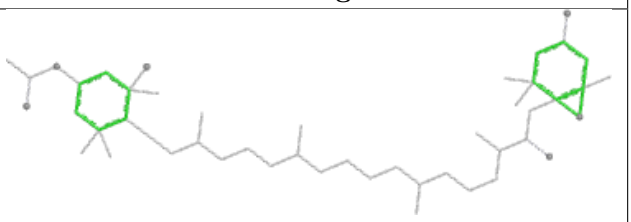
Bond lengths



Bond angles

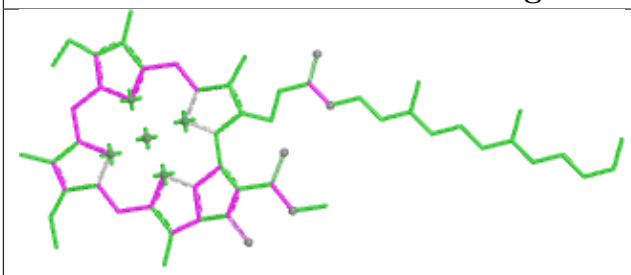


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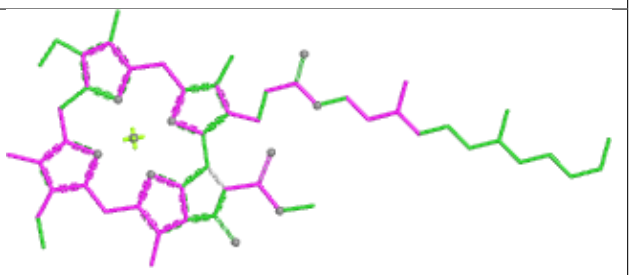


Rings

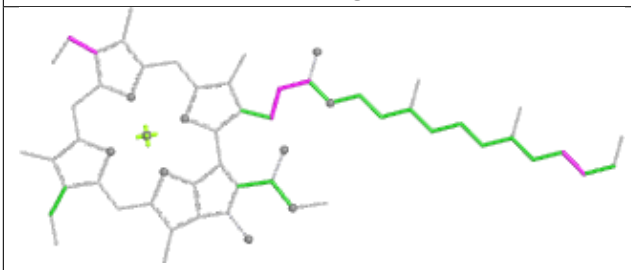
Ligand CLA B 817



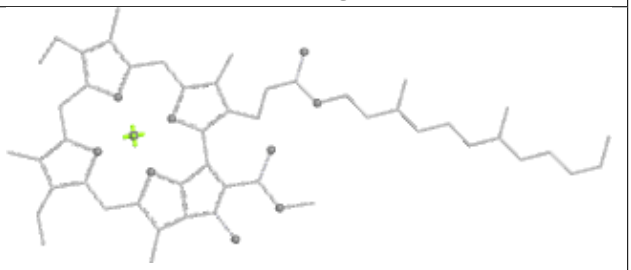
Bond lengths



Bond angles

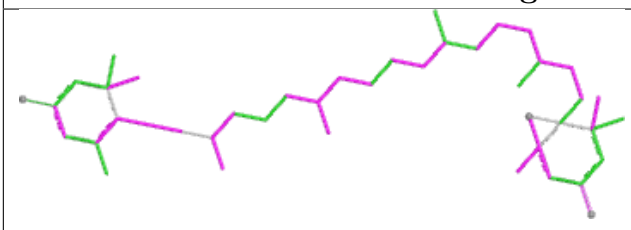


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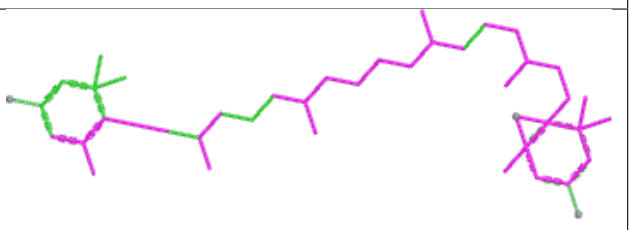


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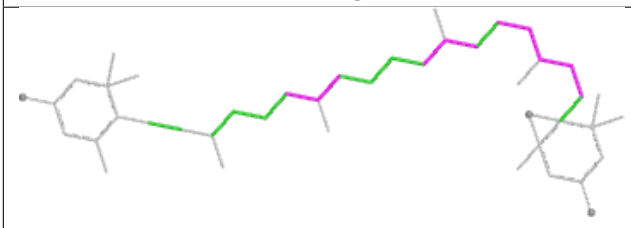
Ligand DD6 12 317



Bond lengths



Bond angles

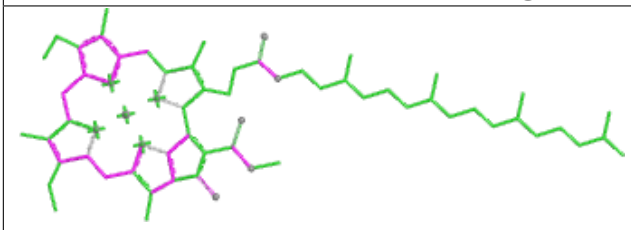


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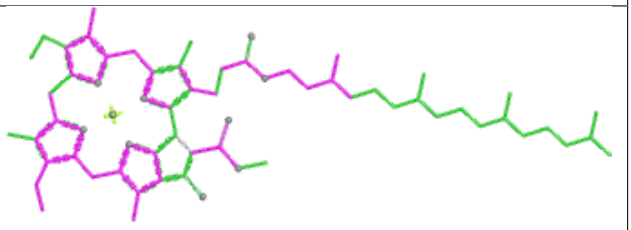


Rings

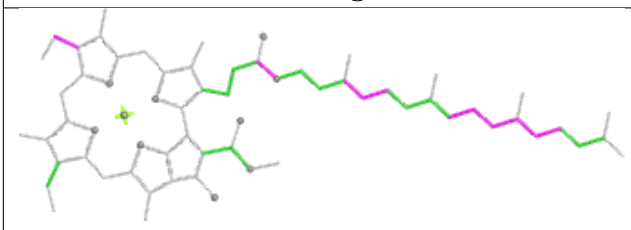
Ligand CLA 11 308



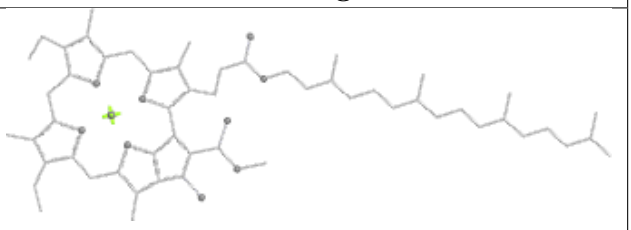
Bond lengths



Bond angles

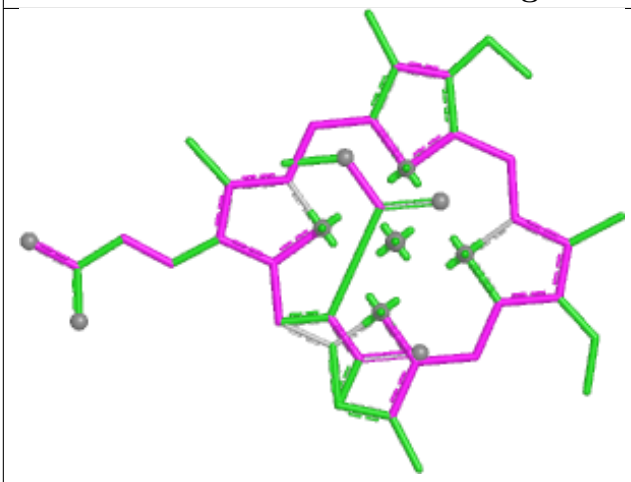


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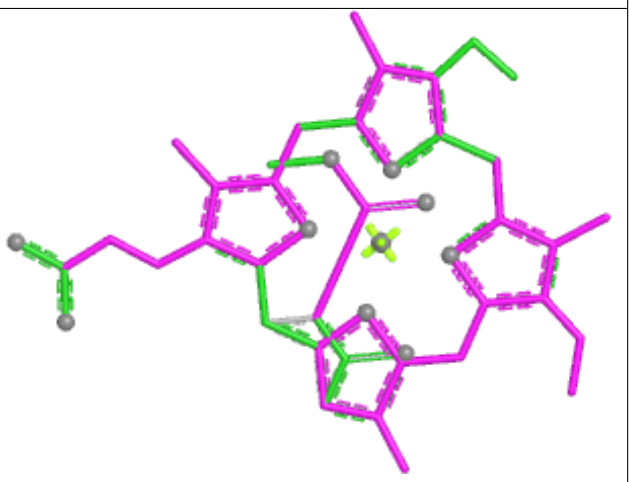


Rings

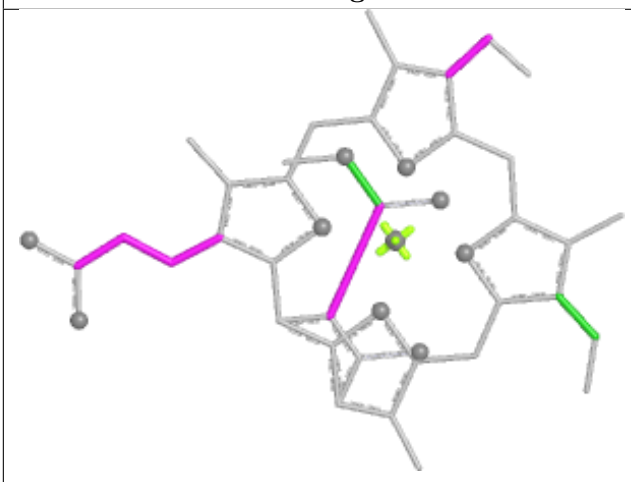
Ligand KC1 12 309



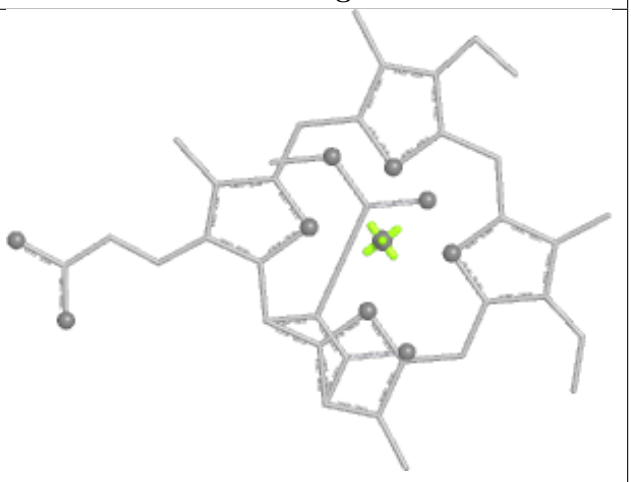
Bond lengths



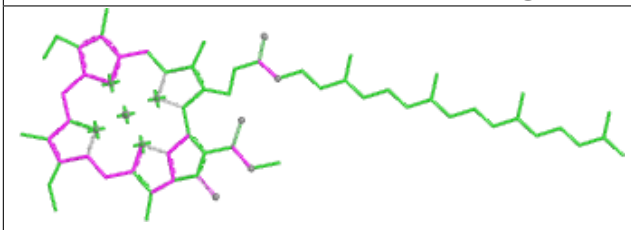
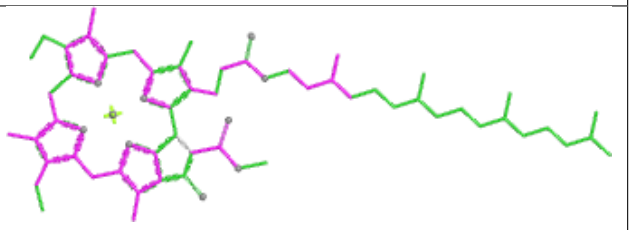
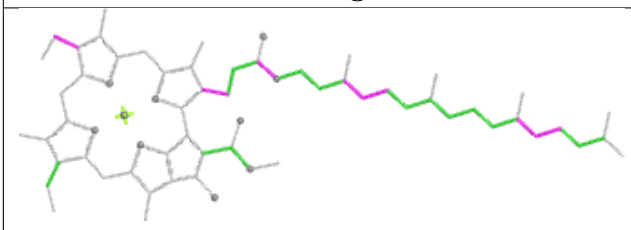
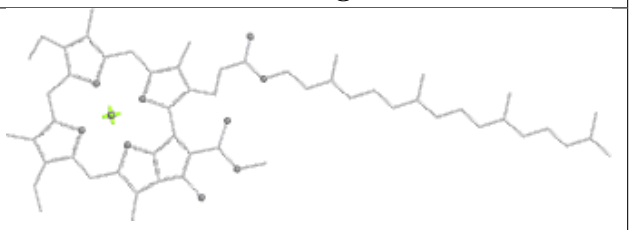
Bond angles

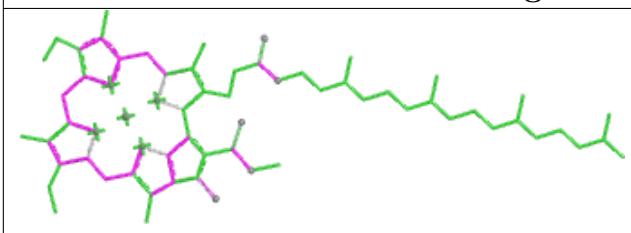
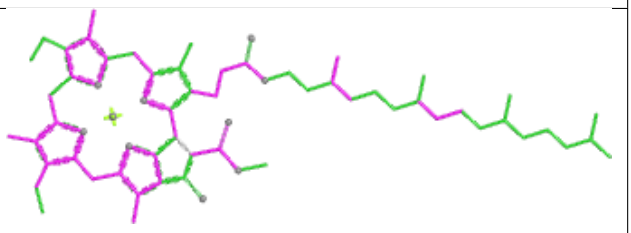
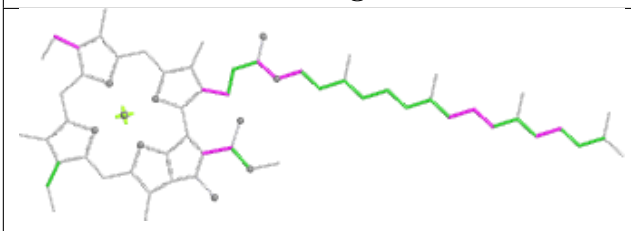
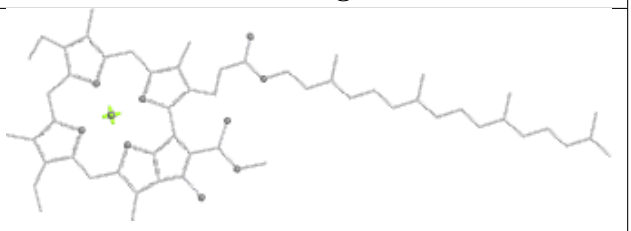


Torsions

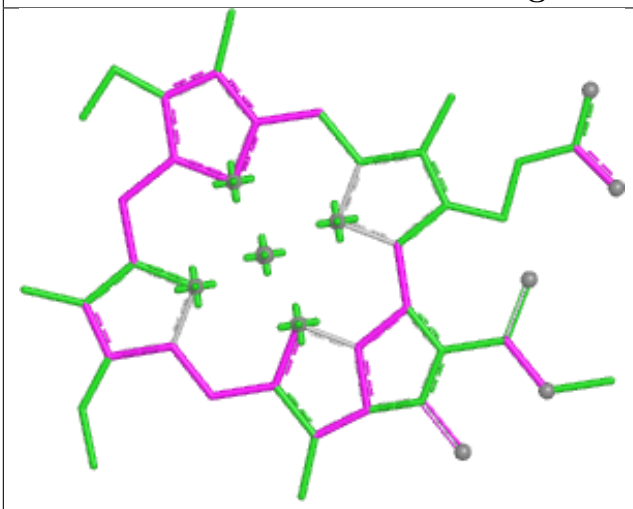


Rings

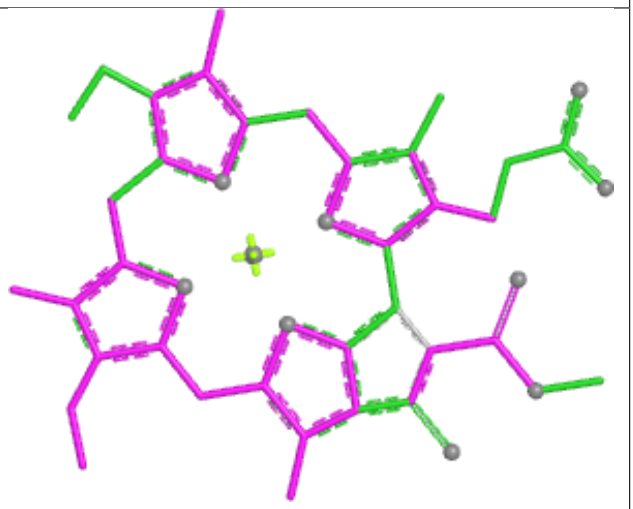
Ligand CLA 11 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

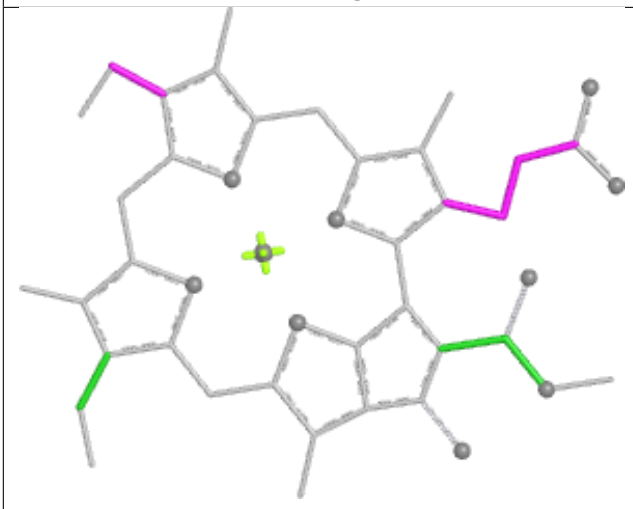
Ligand CLA 9 306



Bond lengths



Bond angles

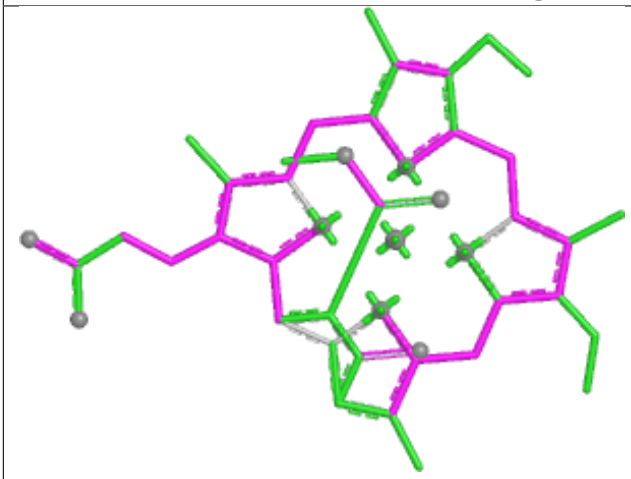


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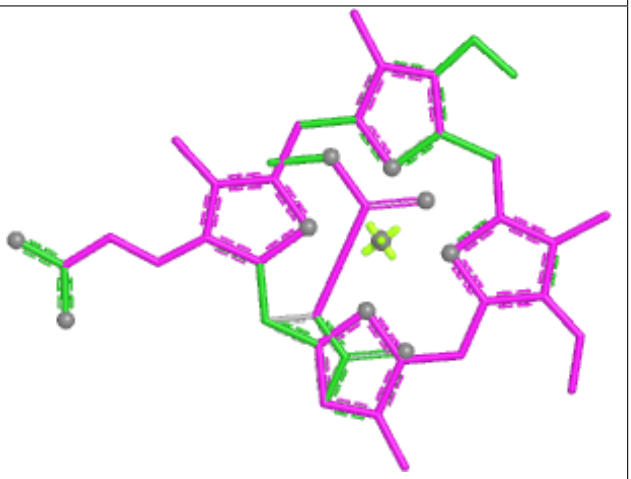


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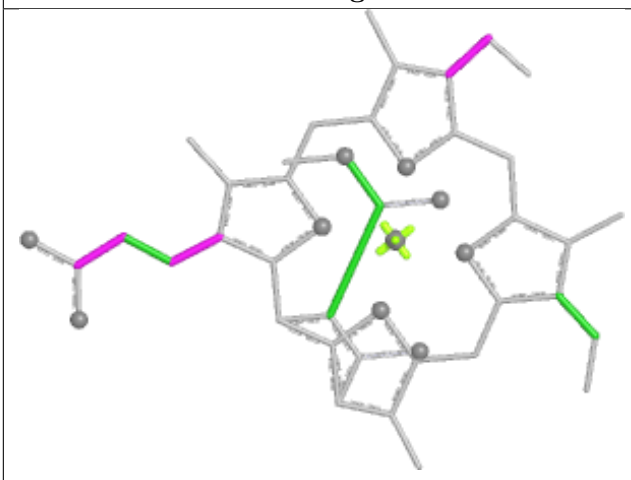
Ligand KC1 2 306



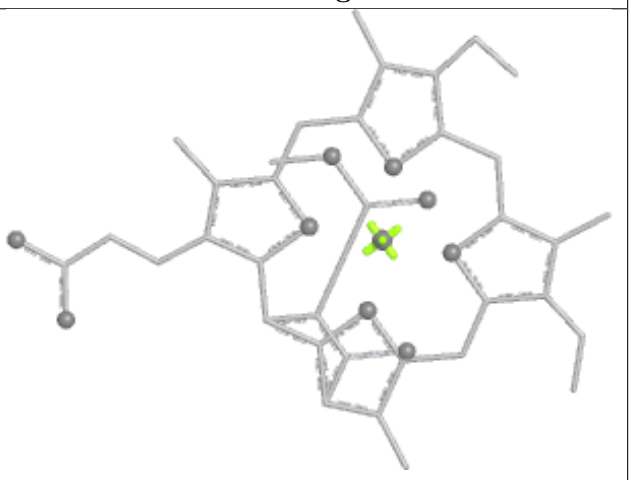
Bond lengths



Bond angles

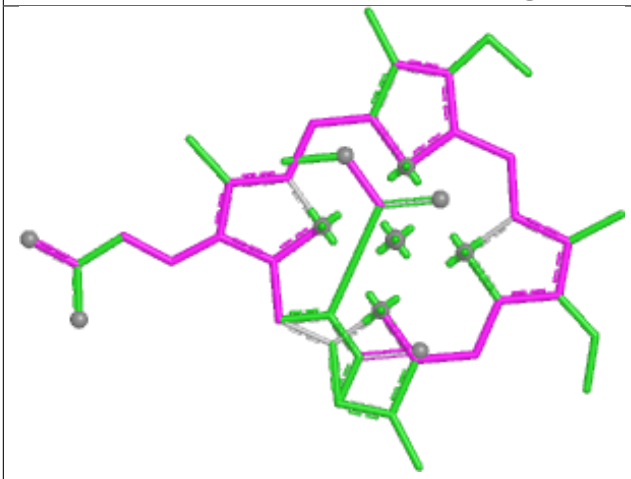


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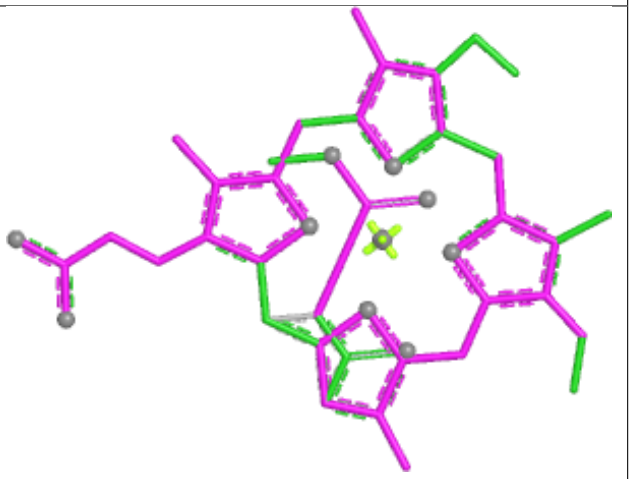


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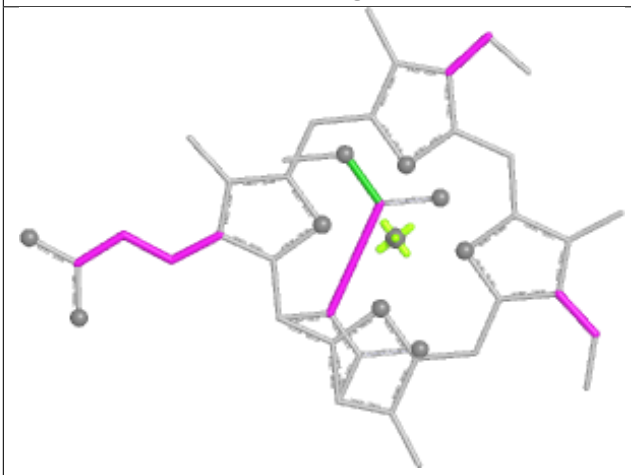
Ligand KC1 14 308



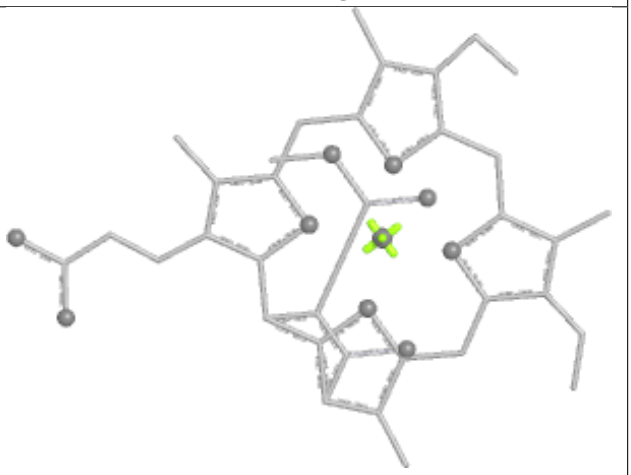
Bond lengths



Bond angles

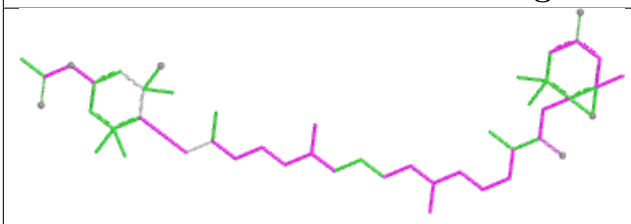


Torsions

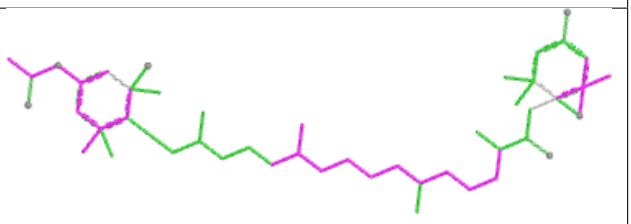


Rings

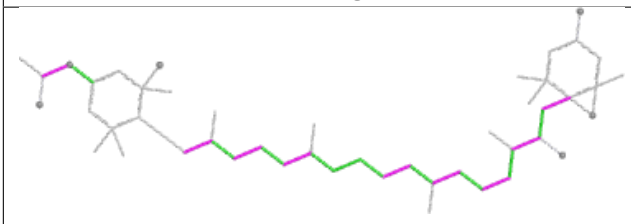
Ligand A86 3 315



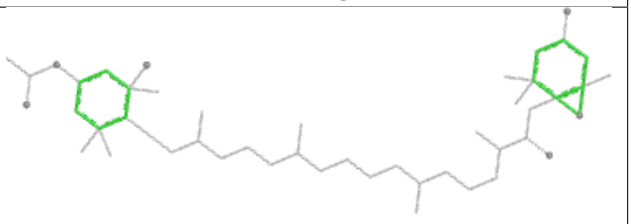
Bond lengths



Bond angles

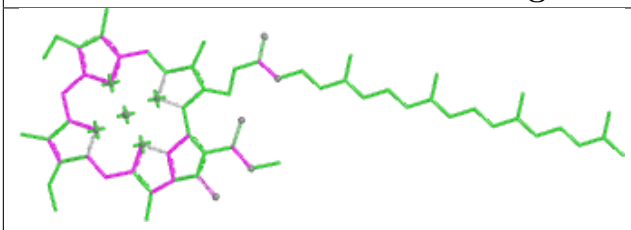


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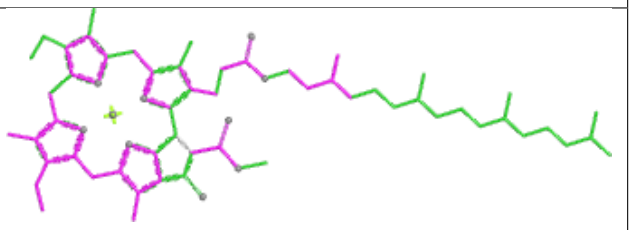


Rings

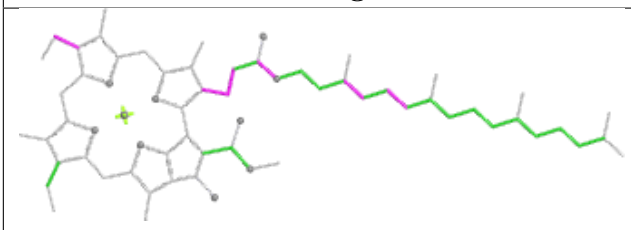
Ligand CLA 3 301



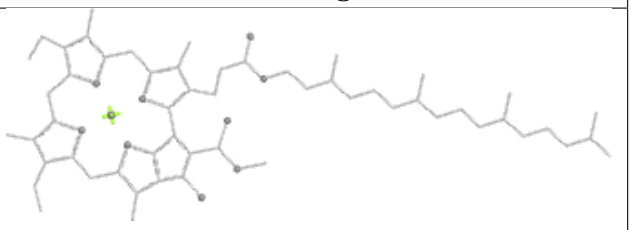
Bond lengths



Bond angles

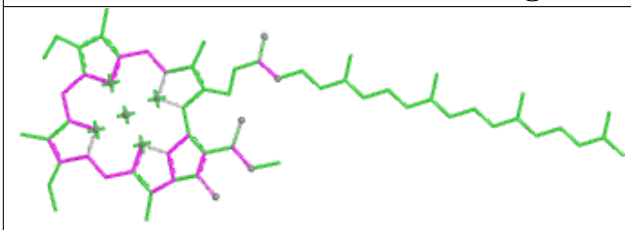


Torsions

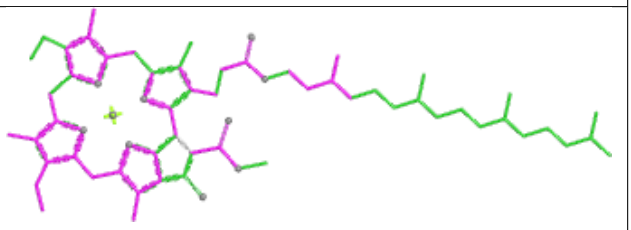


Rings

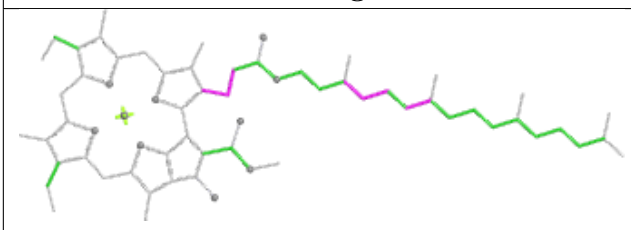
Ligand CLA A 802



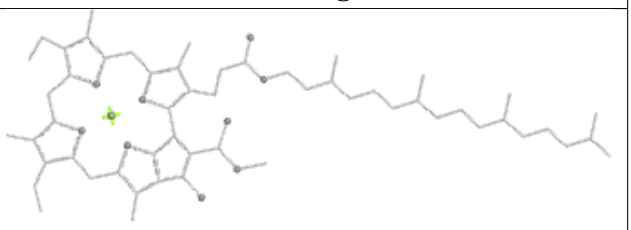
Bond lengths



Bond angles

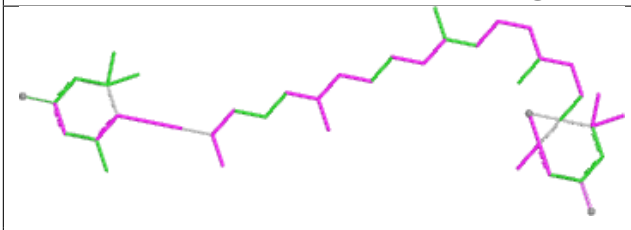


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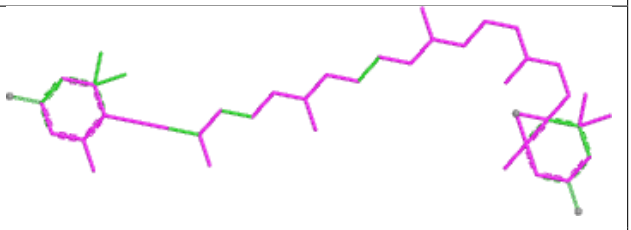


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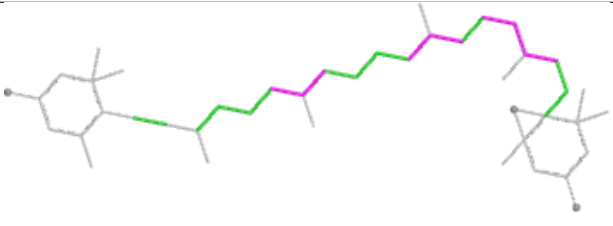
Ligand DD6 6 319



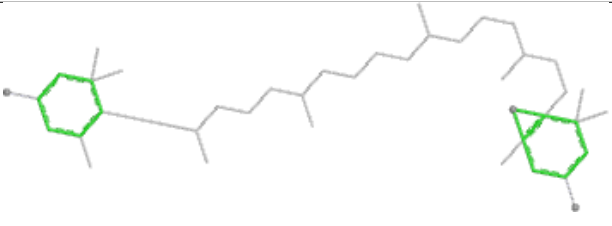
Bond lengths



Bond angles

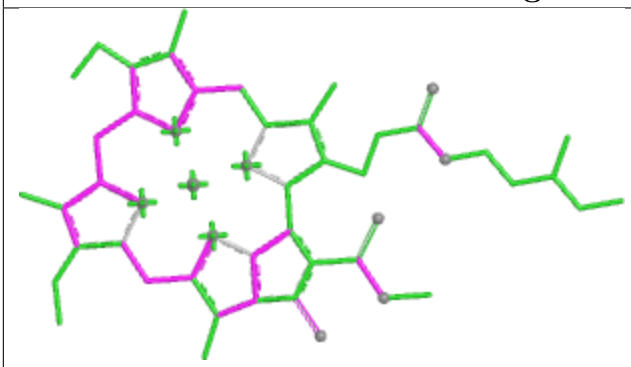


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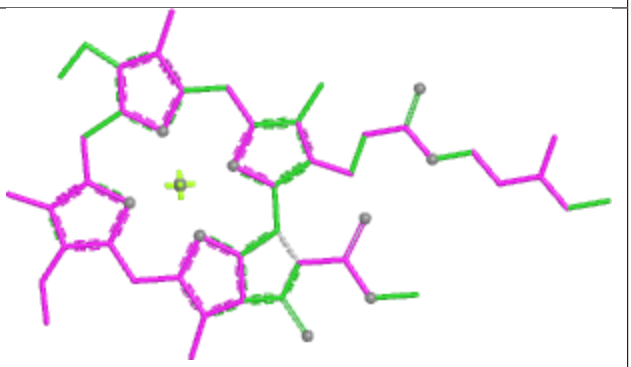


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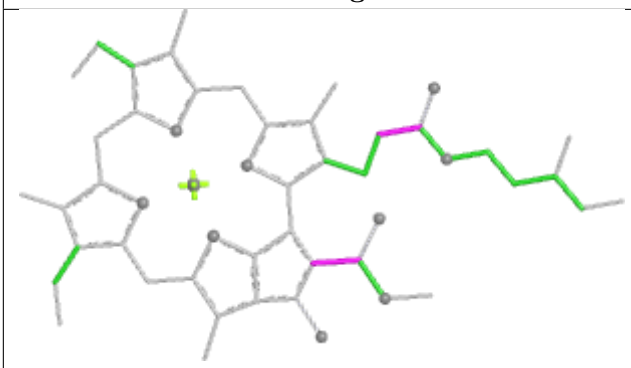
Ligand CLA A 808



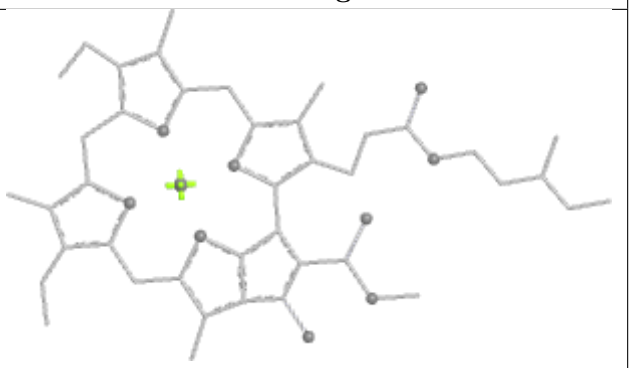
Bond lengths



Bond angles

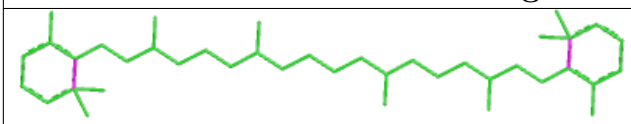


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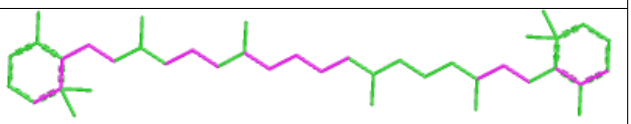


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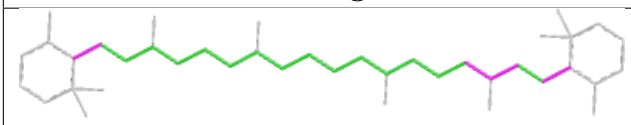
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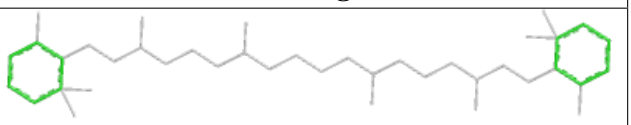
Bond lengths



Bond angles

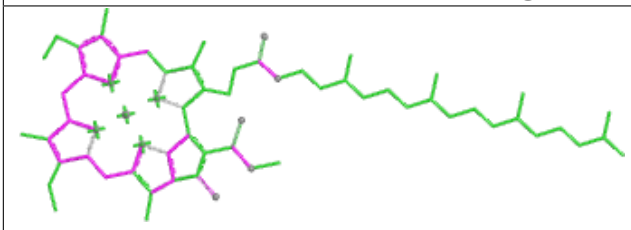


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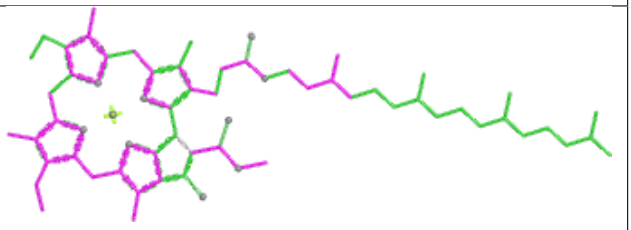


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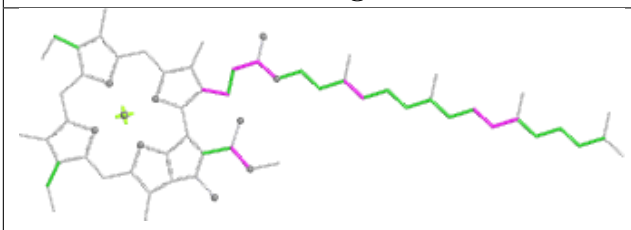
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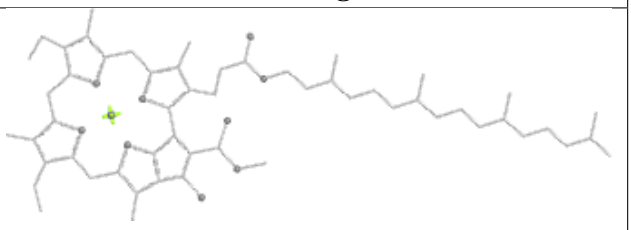
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Bond angles

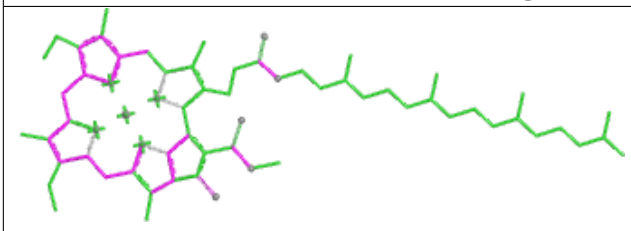


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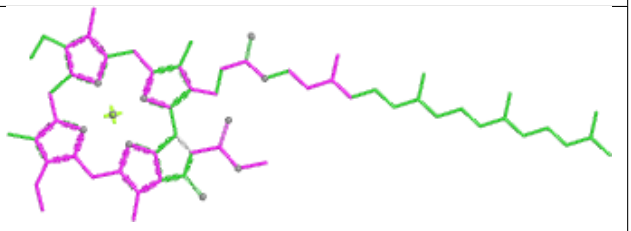


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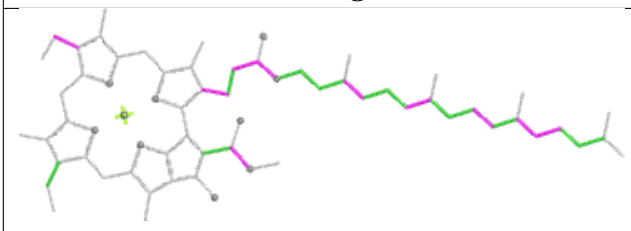
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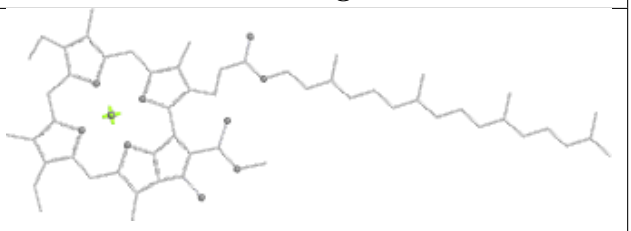
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Bond angles

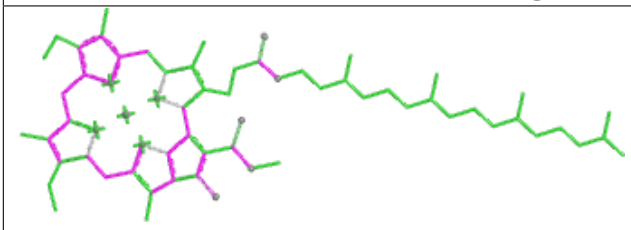


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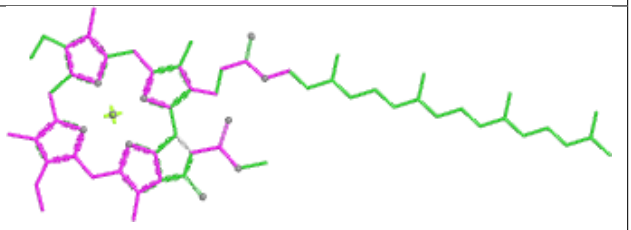


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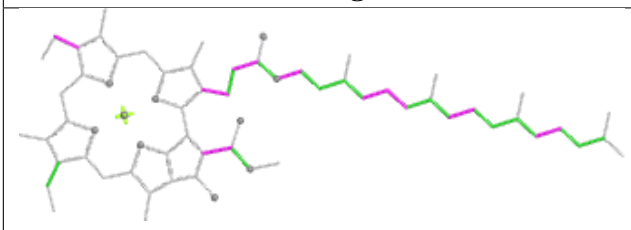
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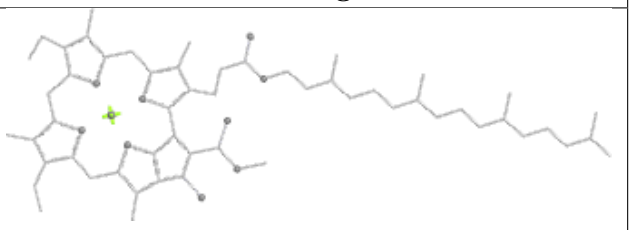
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Bond angles

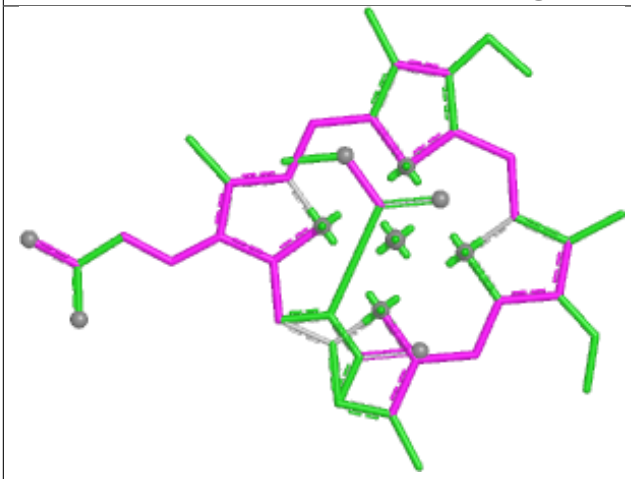


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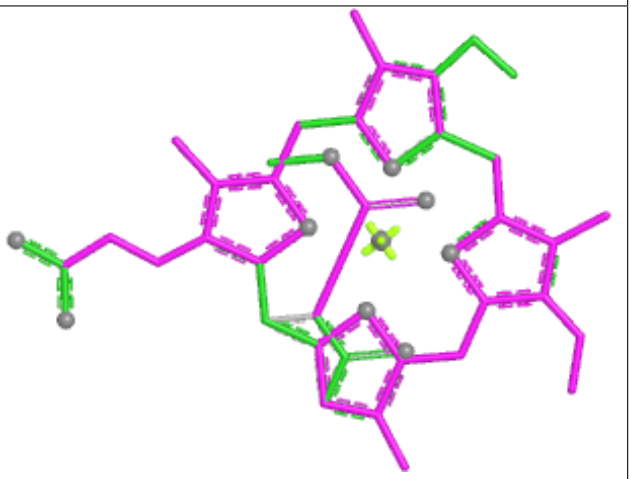


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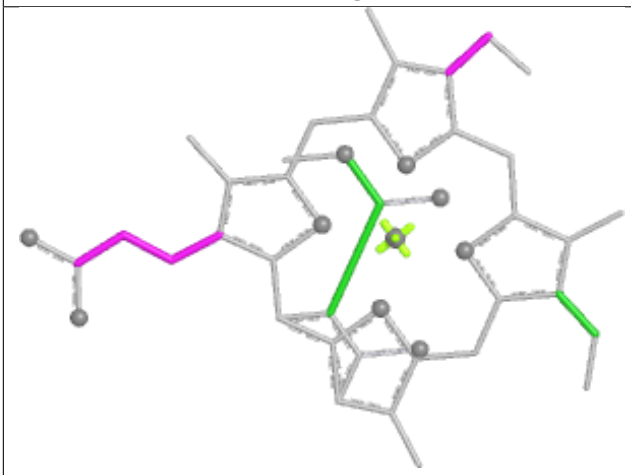
Ligand KC1 9 304



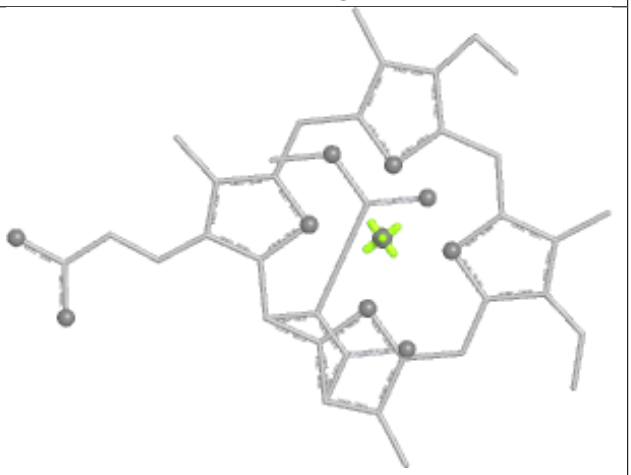
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Bond angles

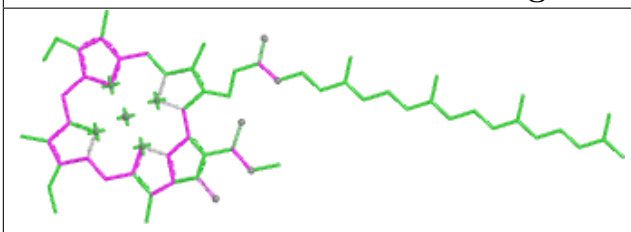


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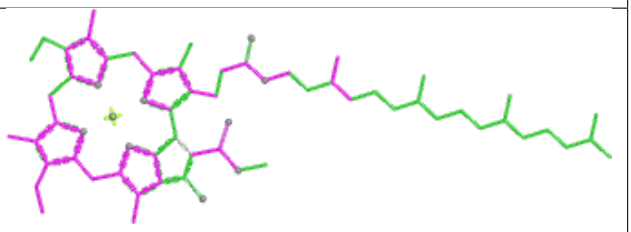


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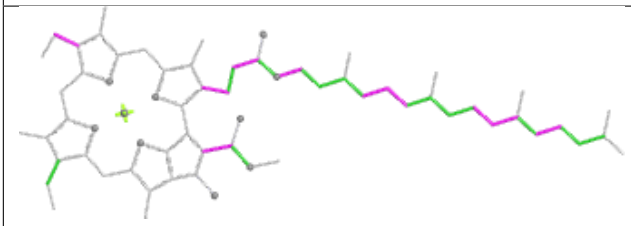
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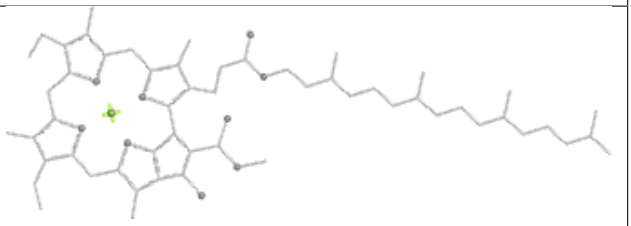
Bond lengths



Bond angles

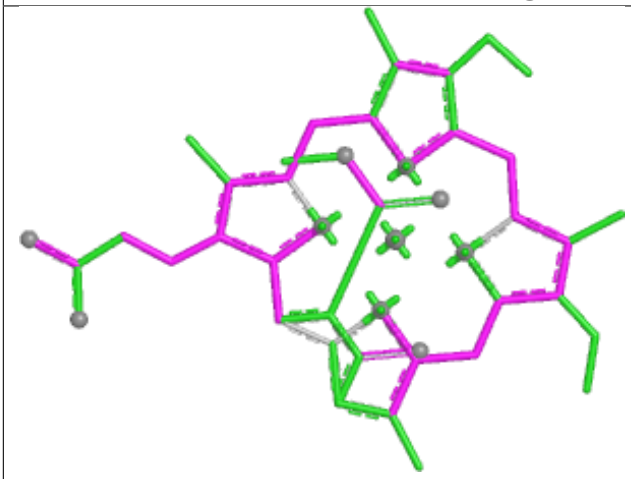


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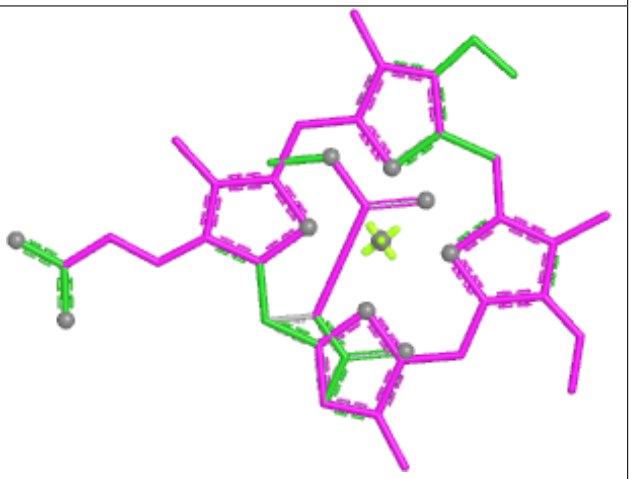


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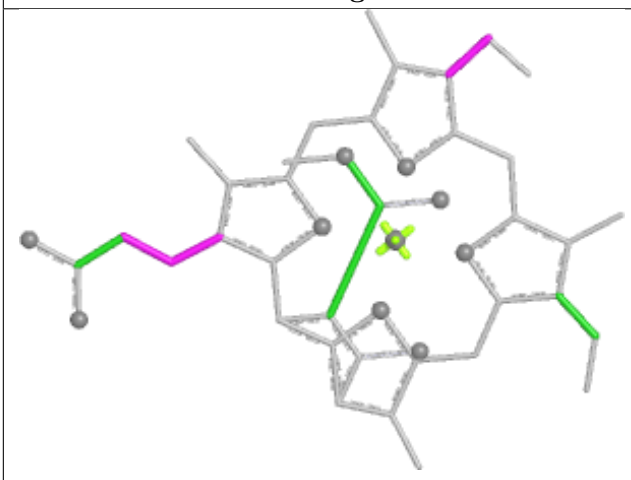
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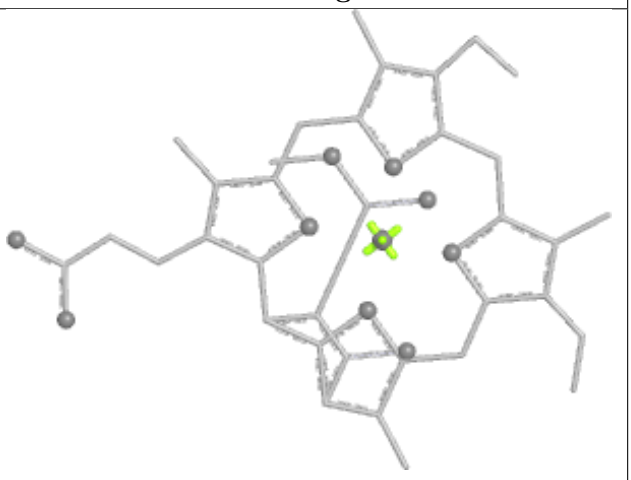
Bond lengths



Bond angles

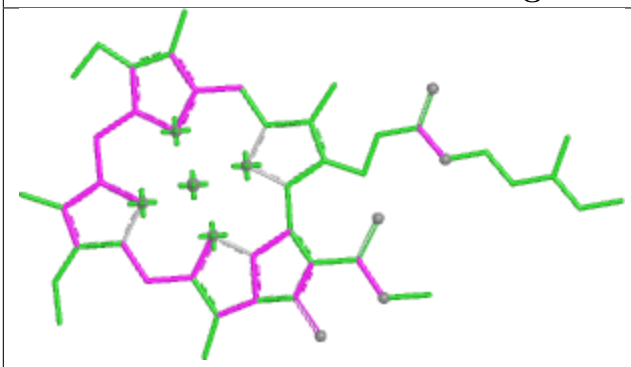


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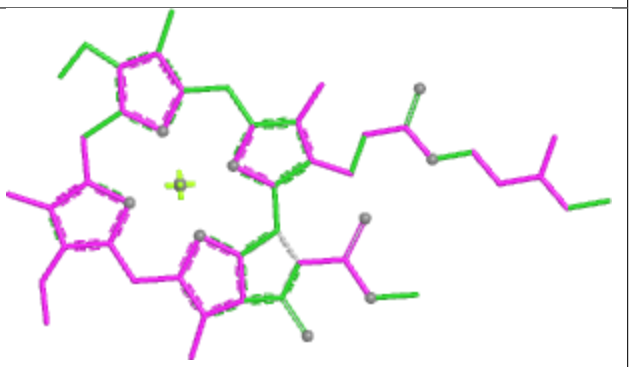


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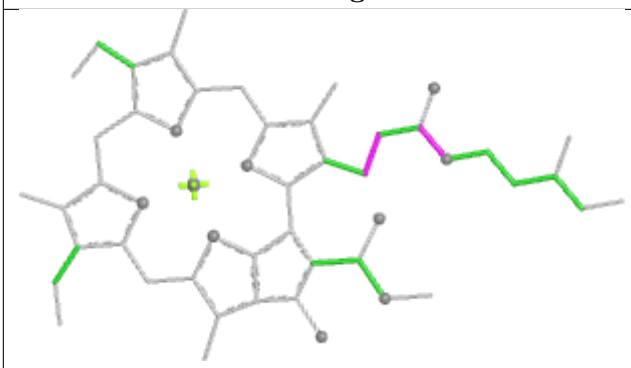
Ligand CLA A 824



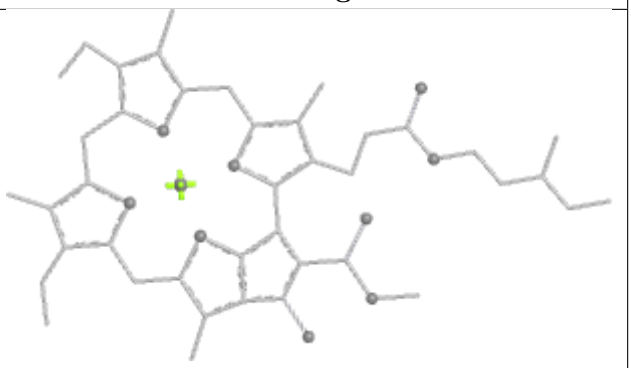
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Bond angles

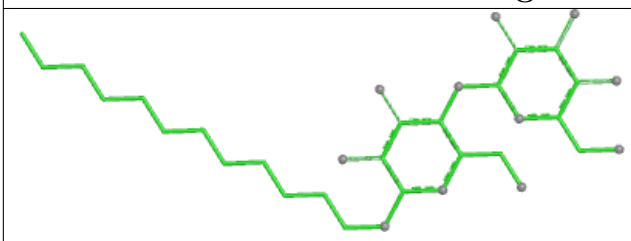


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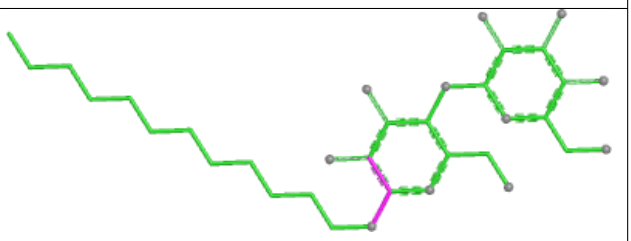


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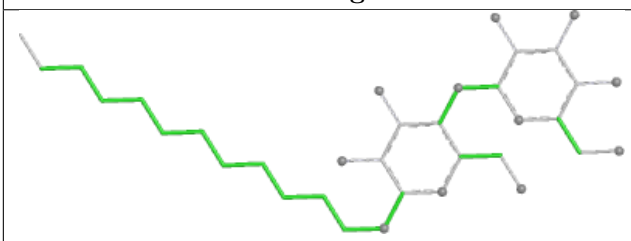
Ligand LMT 12 319



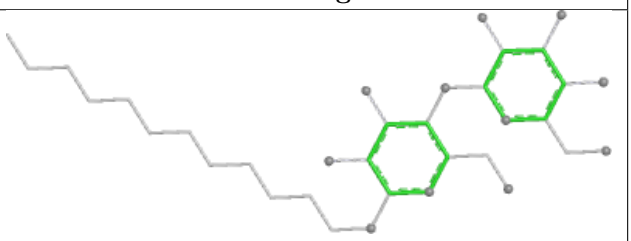
Bond lengths



Bond angles

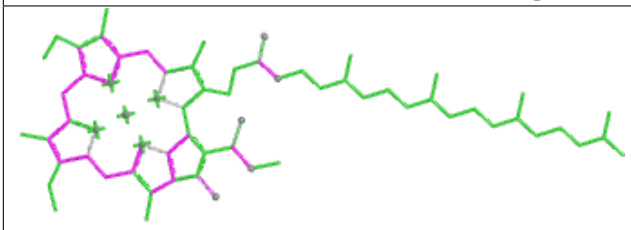


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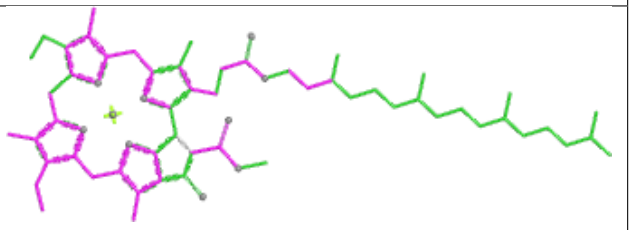


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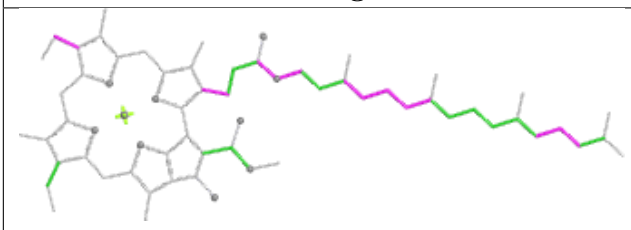
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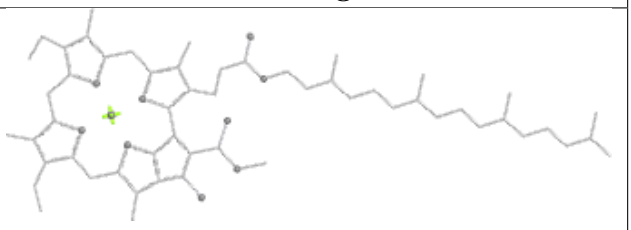
Bond lengths



Bond angles

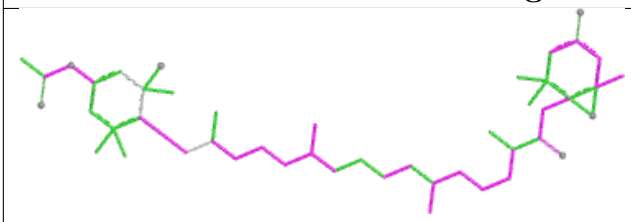


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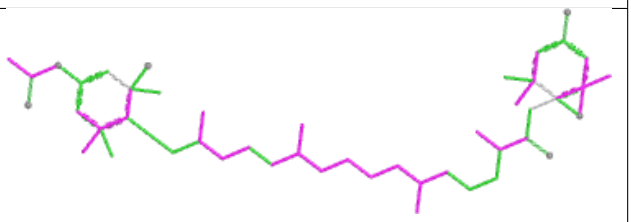


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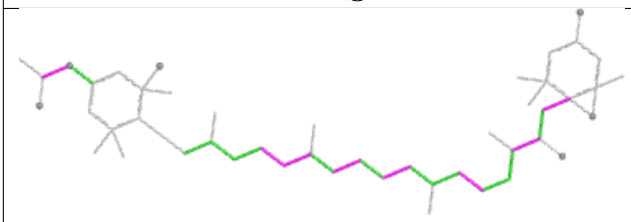
Ligand A86 10 302



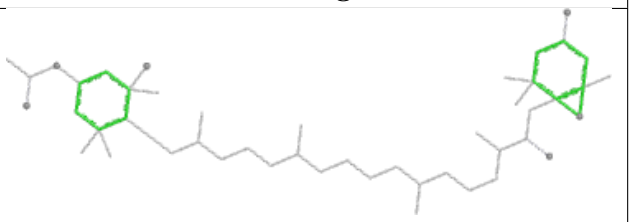
Bond lengths



Bond angles

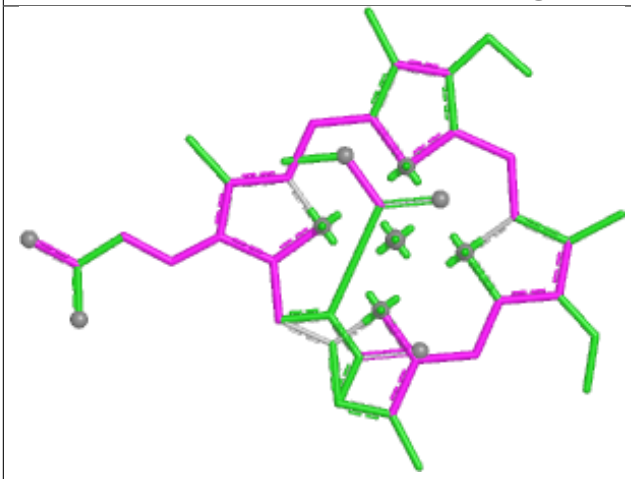


Torsions

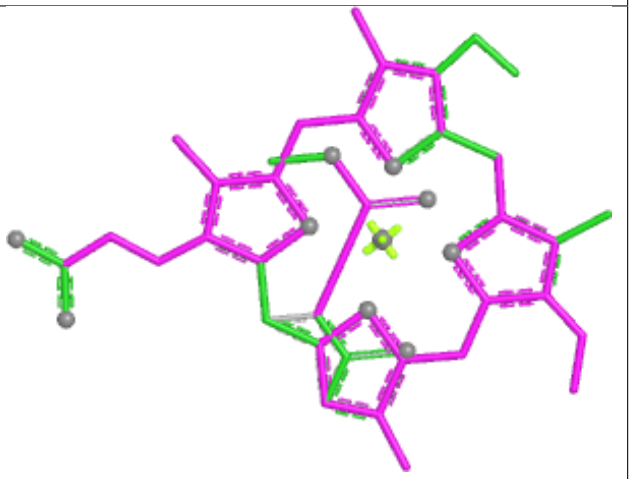


Rings

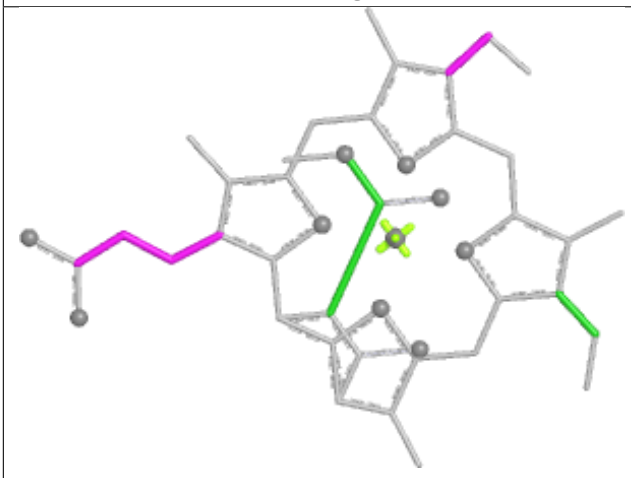
Ligand KC1 4 307



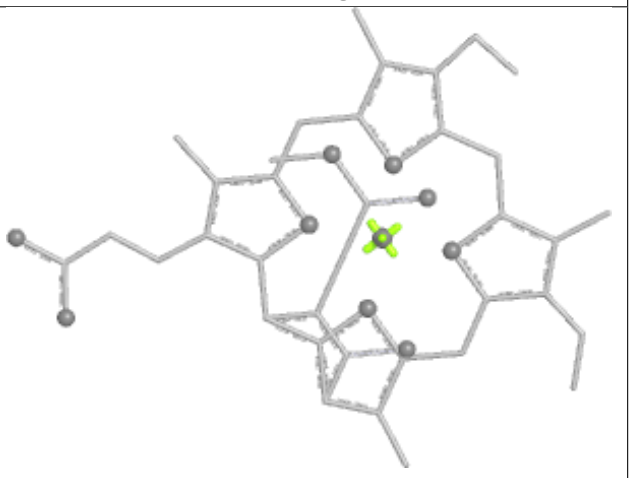
Bond lengths



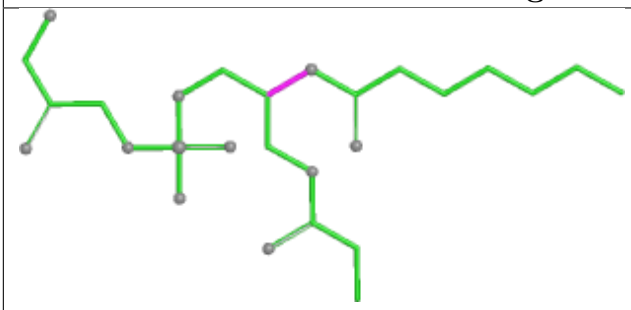
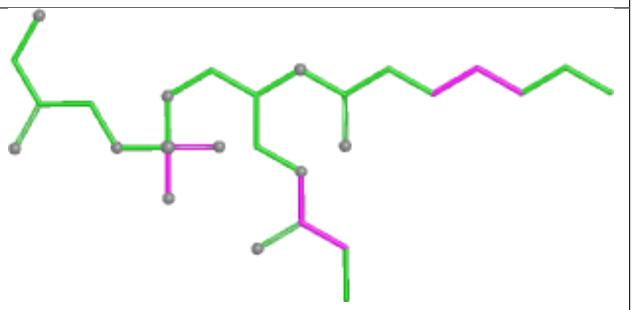
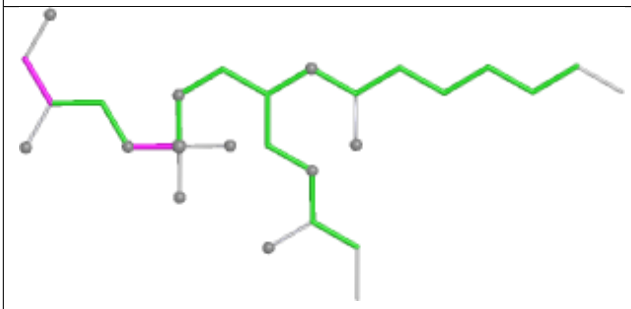
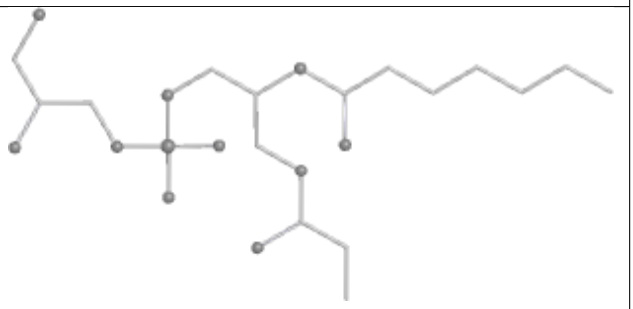
Bond angles

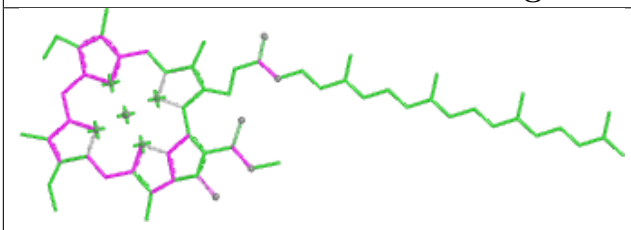
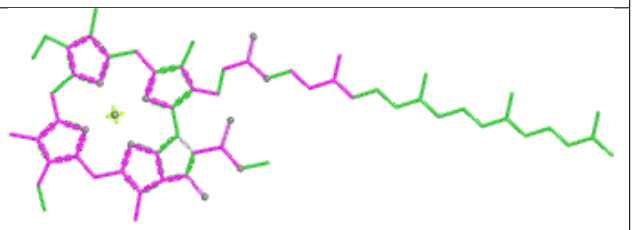
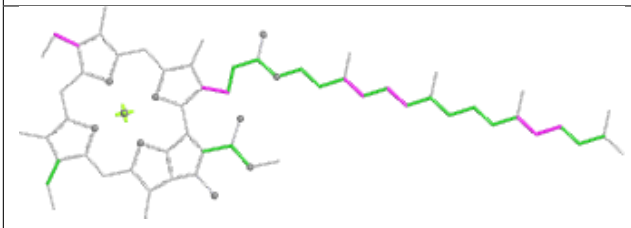
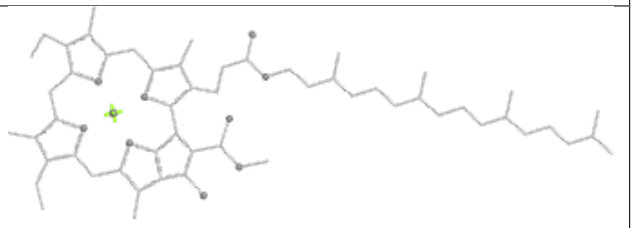


Torsions

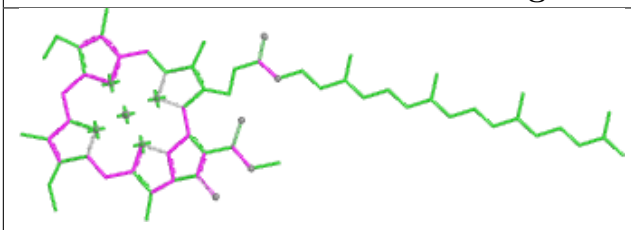


Rings

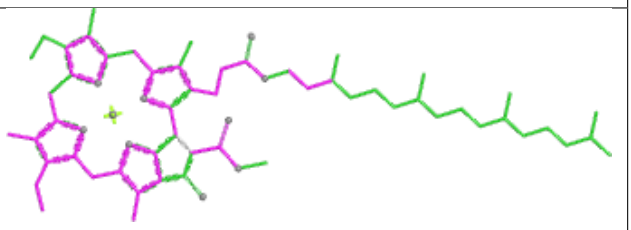
Ligand LHG 5 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

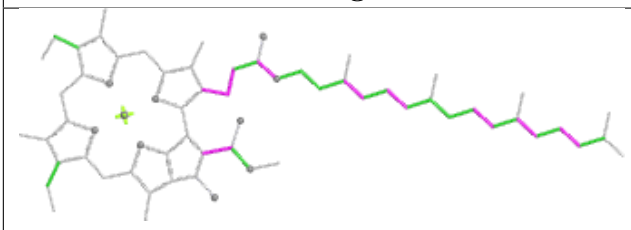
Ligand CLA 5 307



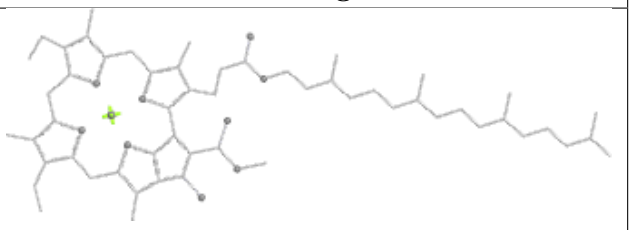
Bond lengths



Bond angles

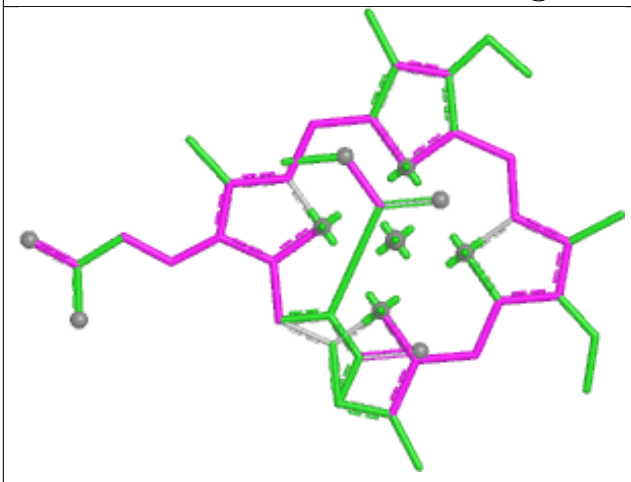


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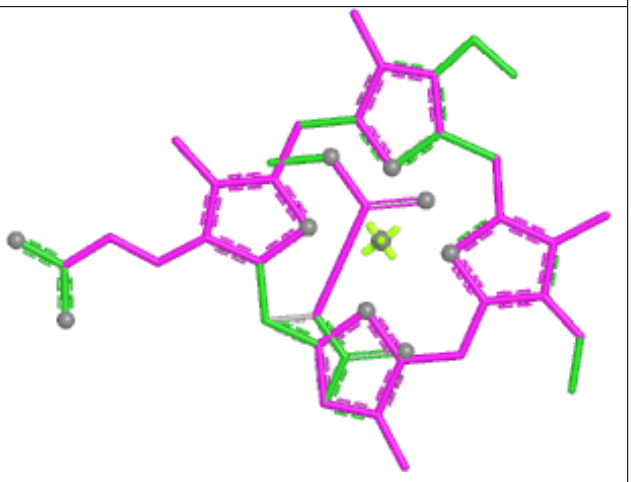


Rings

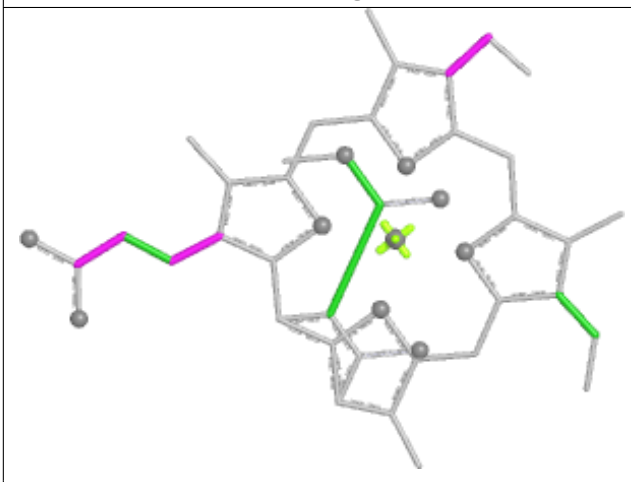
Ligand KC1 6 313



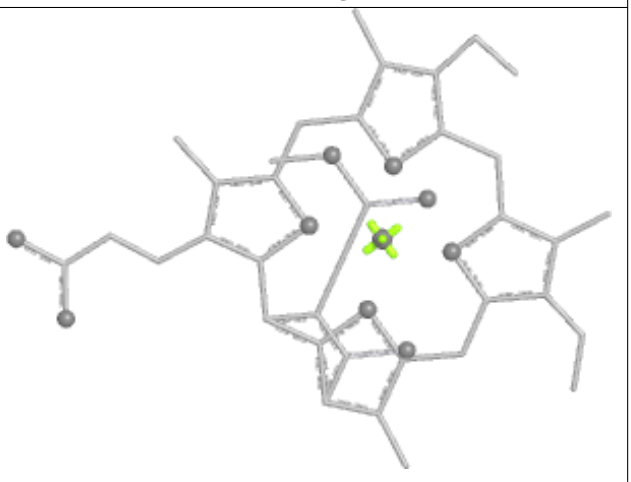
Bond lengths



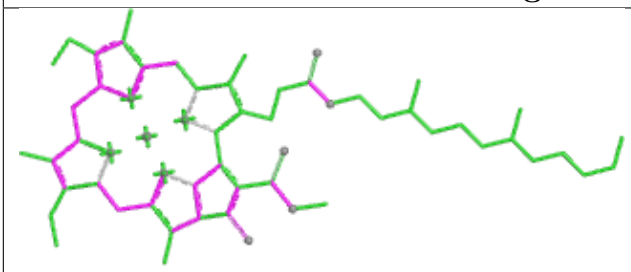
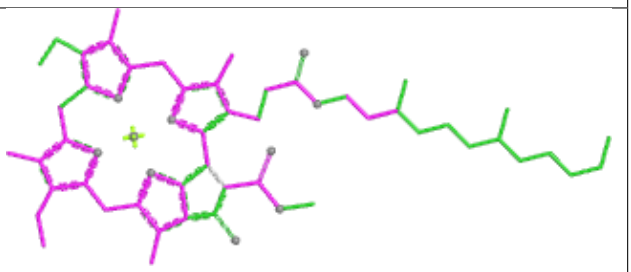
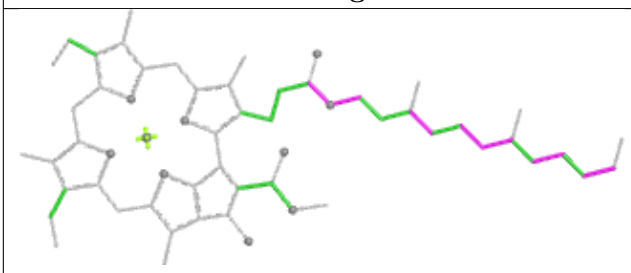
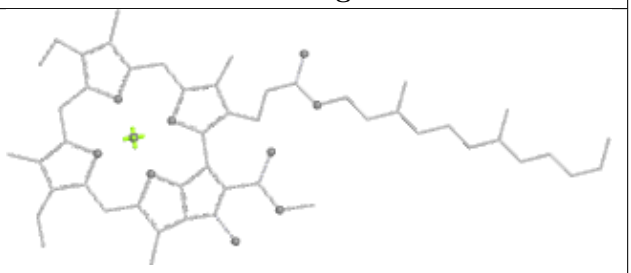
Bond angles

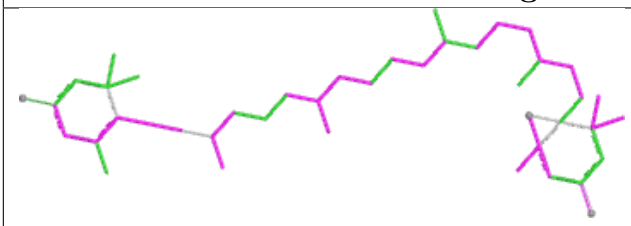
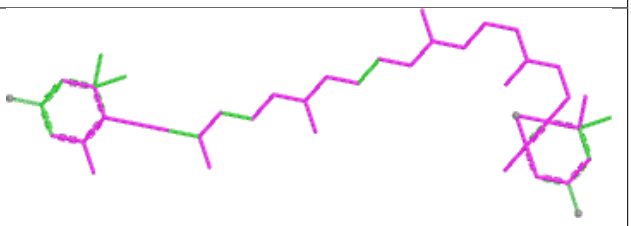
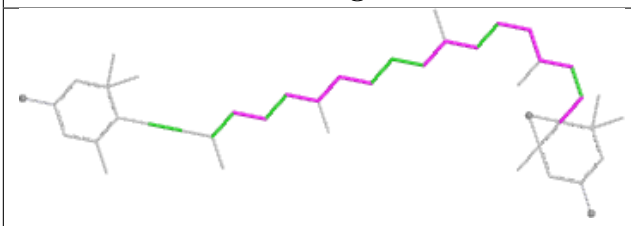
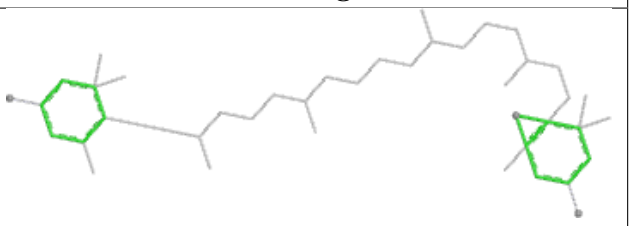


Torsions

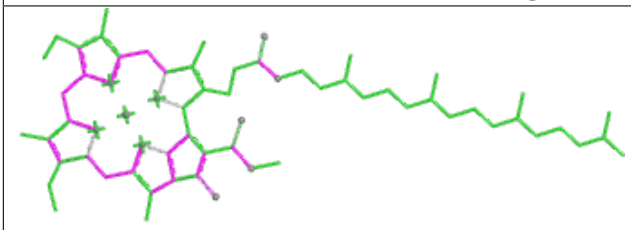


Rings

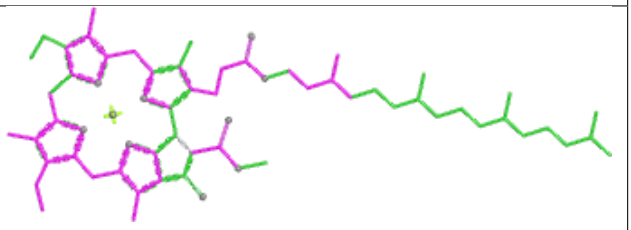
Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 15 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

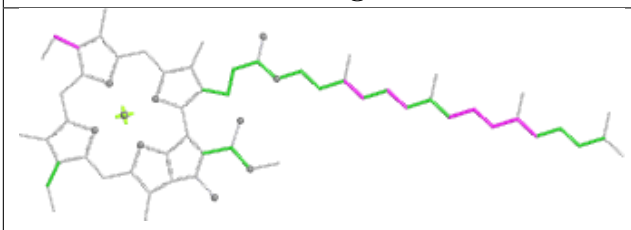
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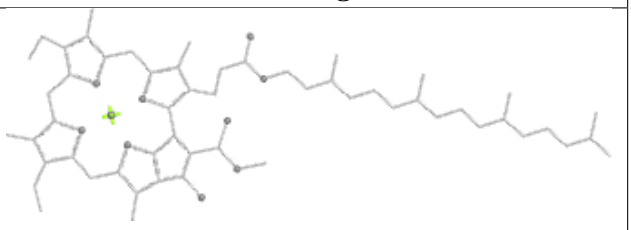
Bond lengths



Bond angles

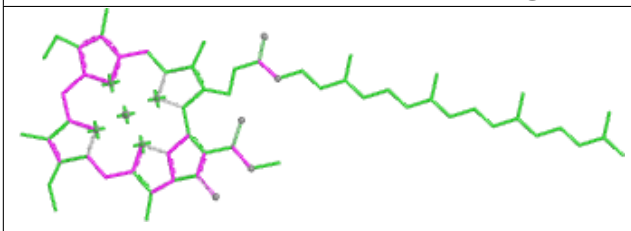


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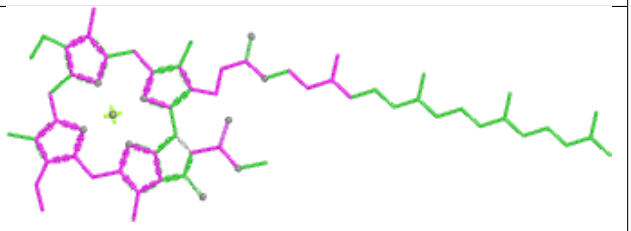


Rings

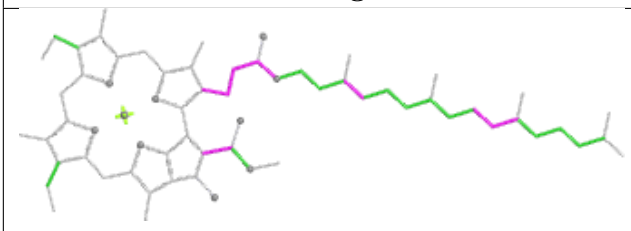
Ligand CLA A 806



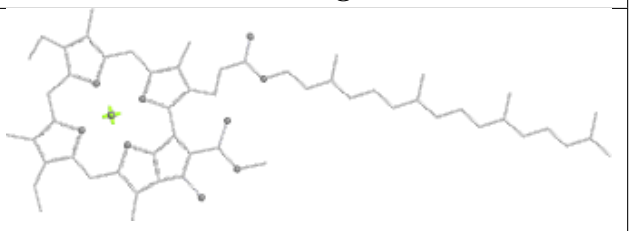
Bond lengths



Bond angles

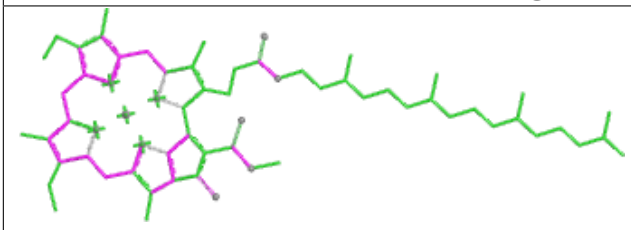


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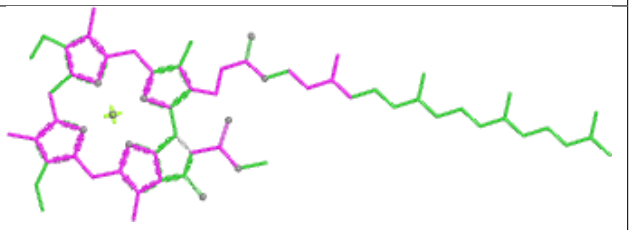


Rings

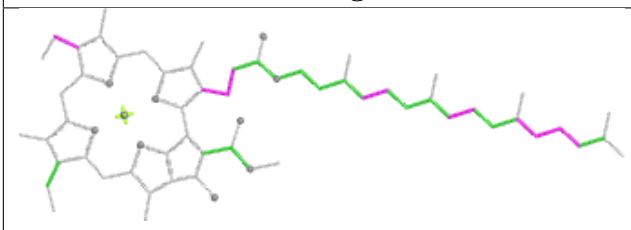
Ligand CLA 7 310



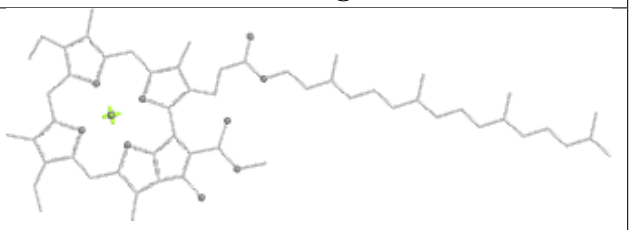
Bond lengths



Bond angles

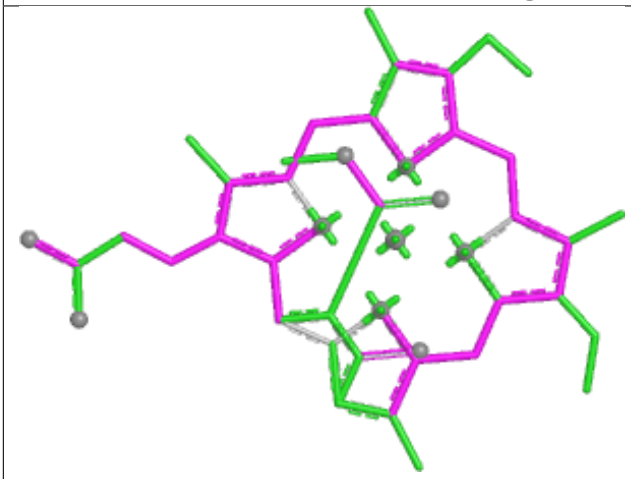


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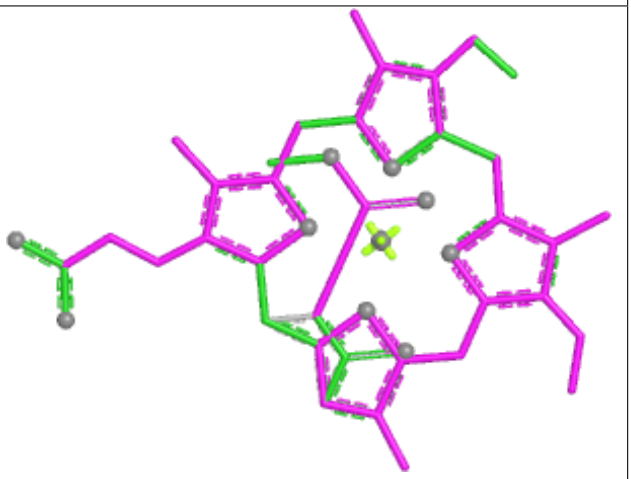


Rings

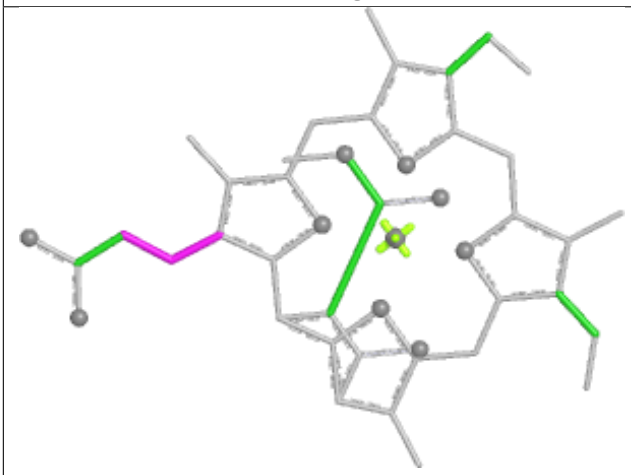
Ligand KC1 13 311



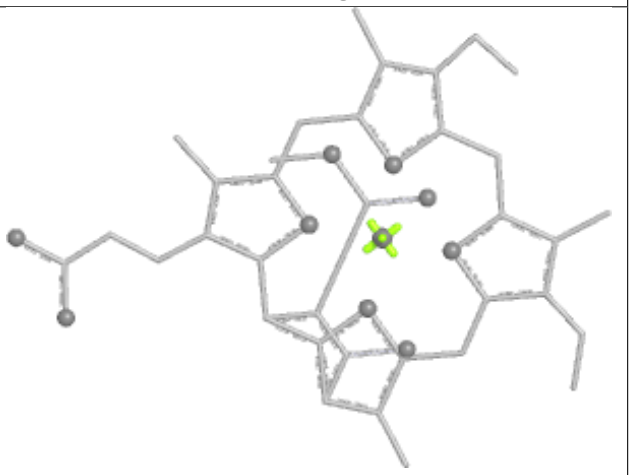
Bond lengths



Bond angles

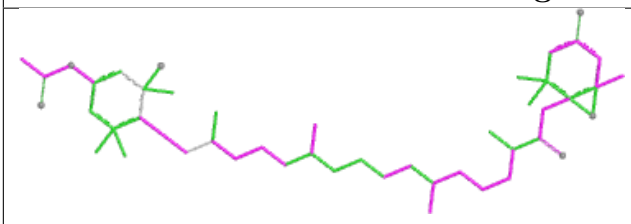


Torsions

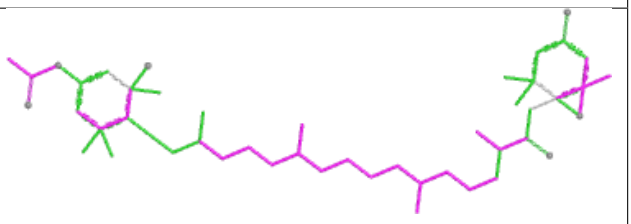


Rings

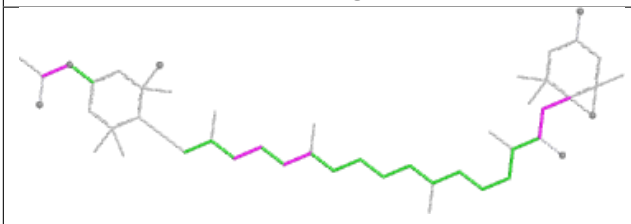
Ligand A86 8 315



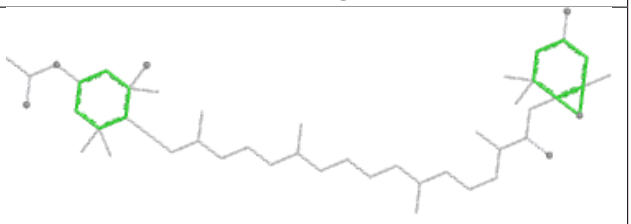
Bond lengths



Bond angles

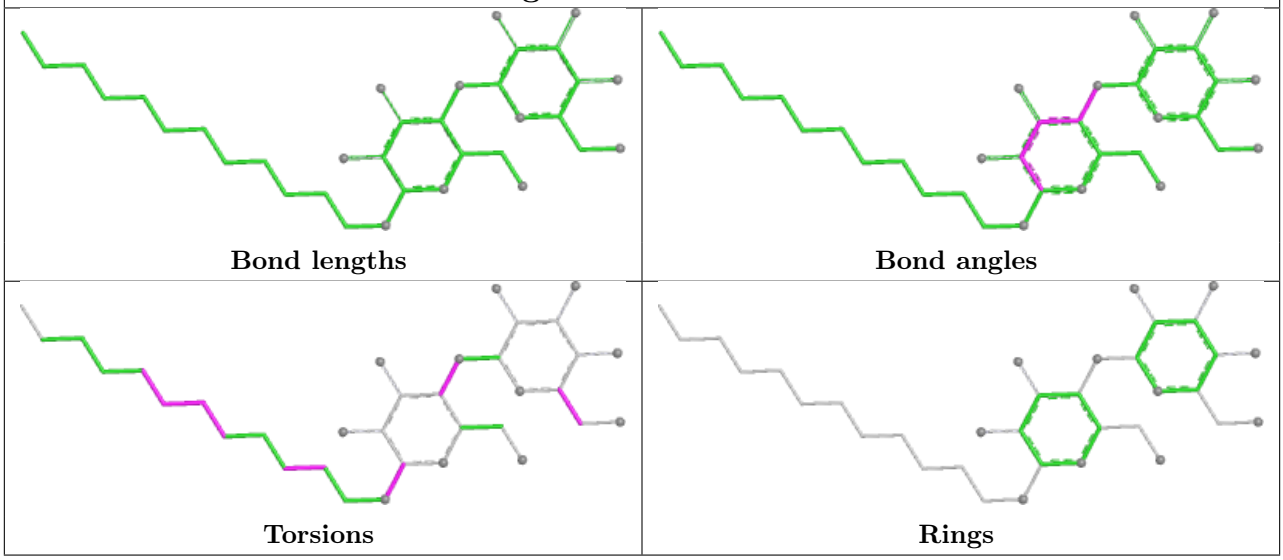


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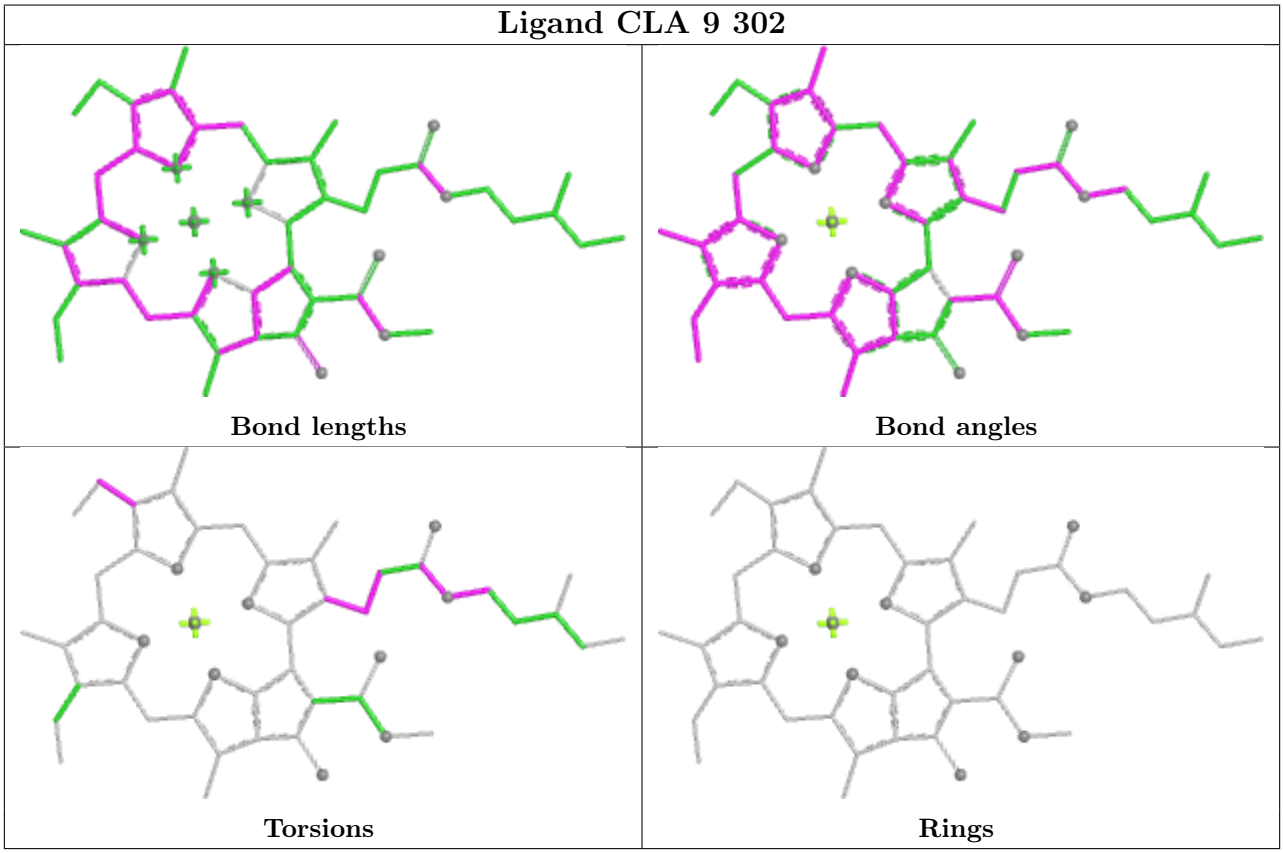


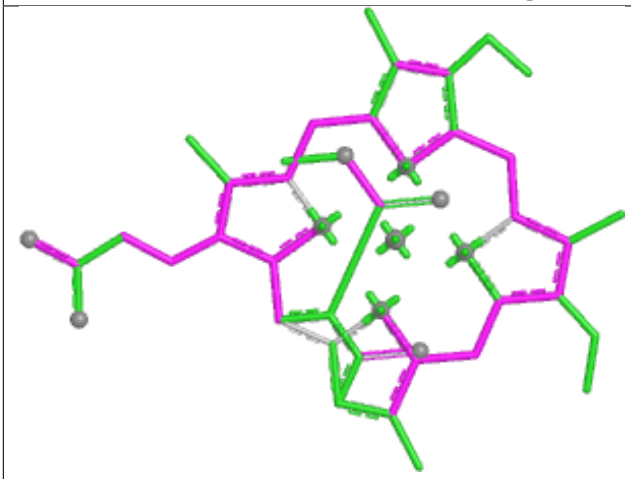
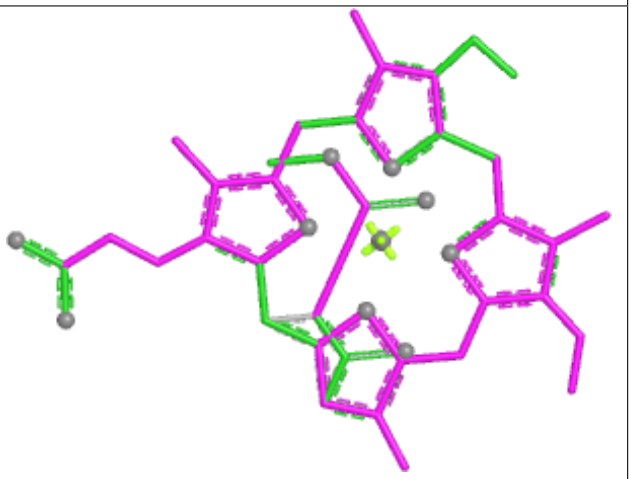
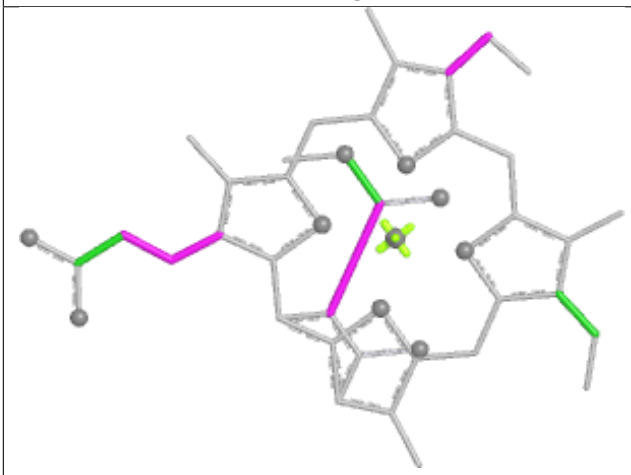
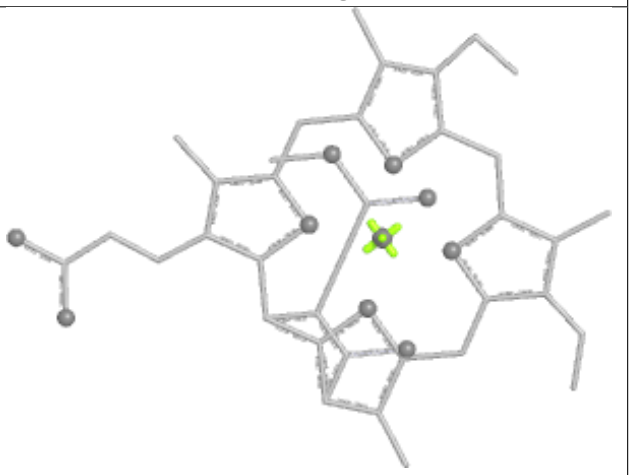
Rings

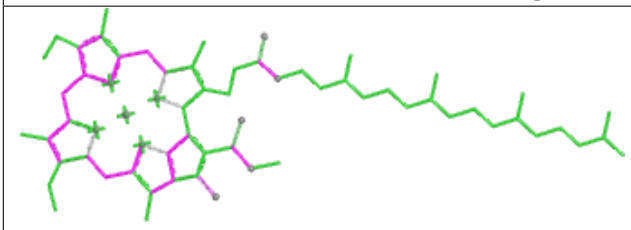
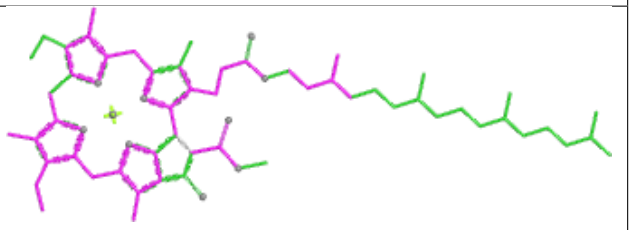
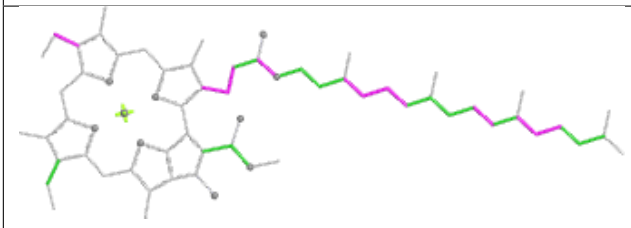
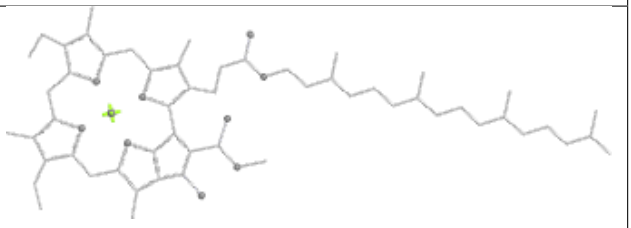
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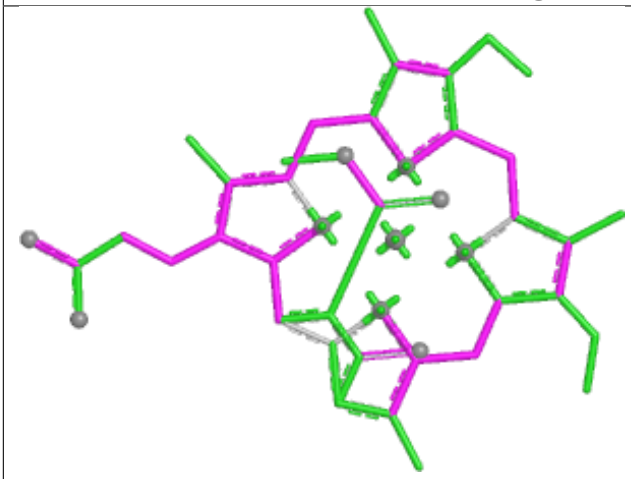
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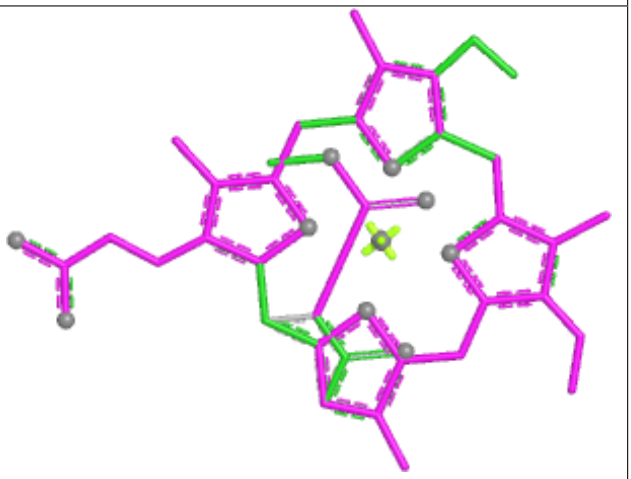
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

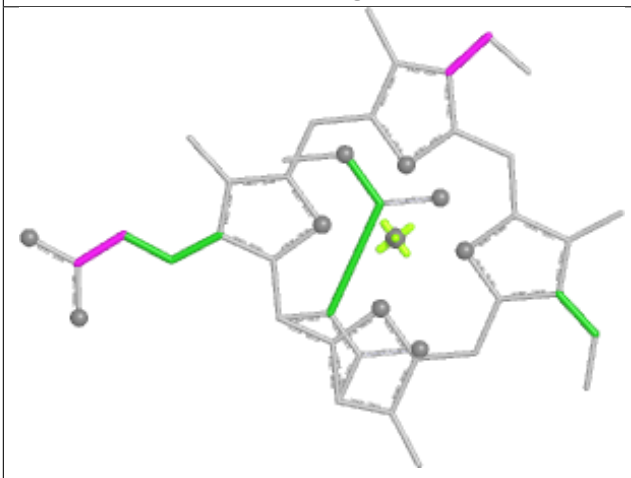
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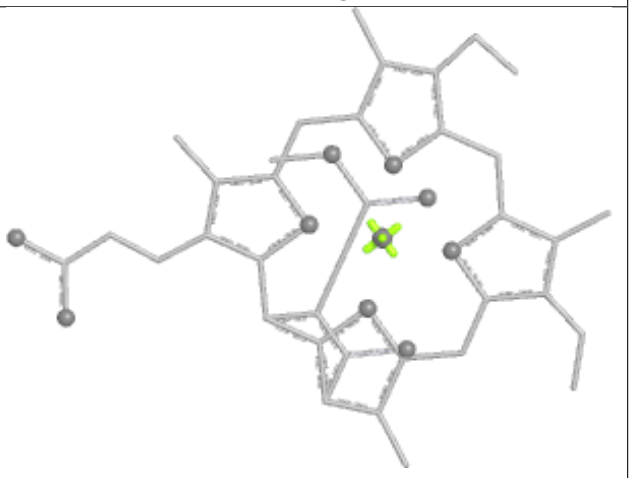
Bond lengths



Bond angles

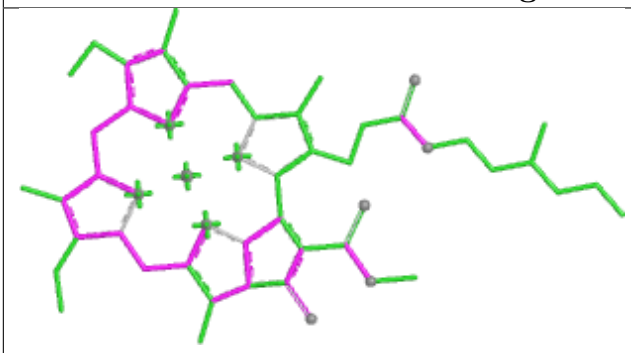


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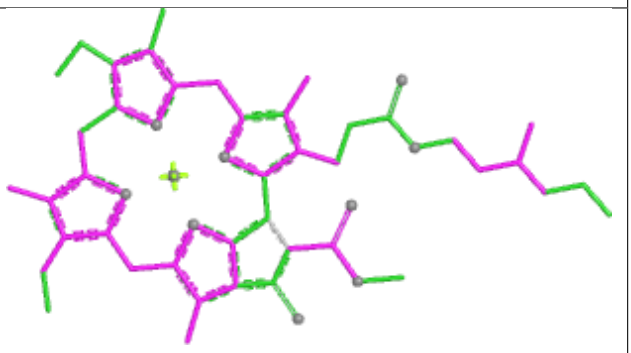


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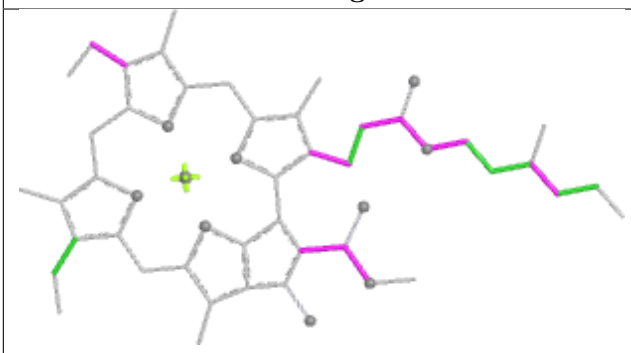
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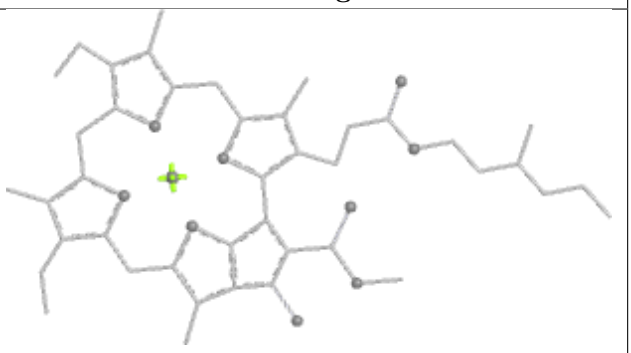
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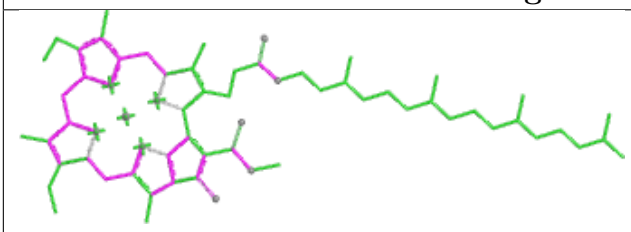


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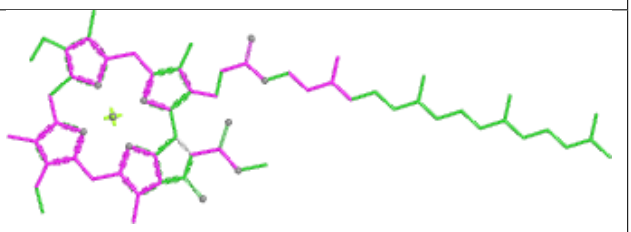


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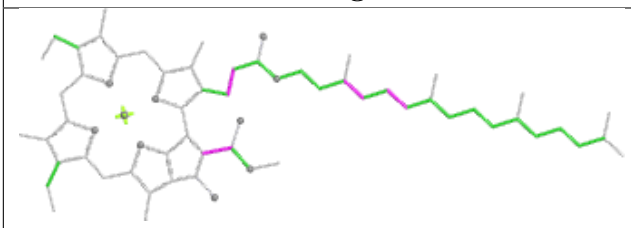
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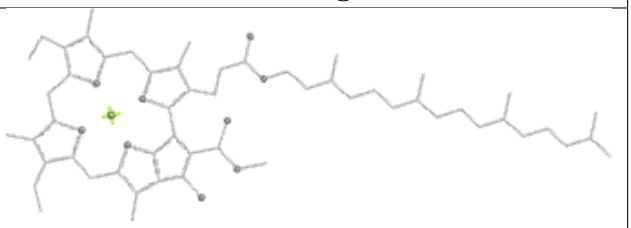
Bond lengths



Bond angles

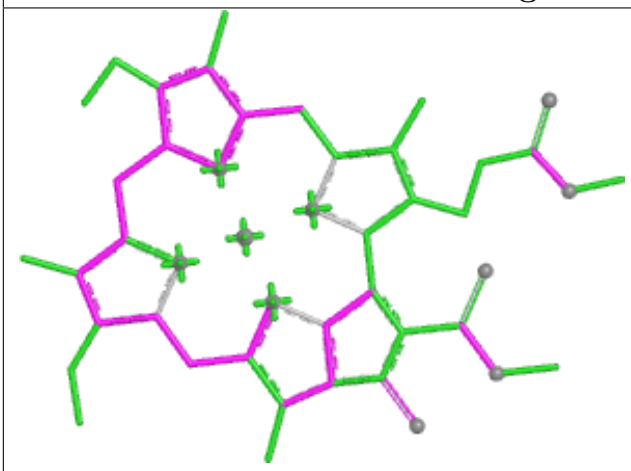


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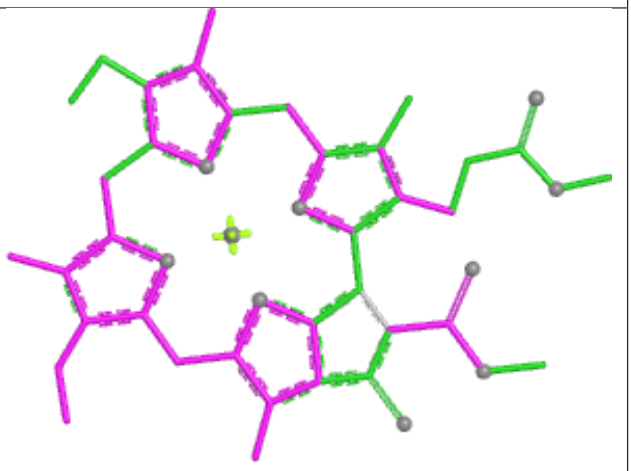


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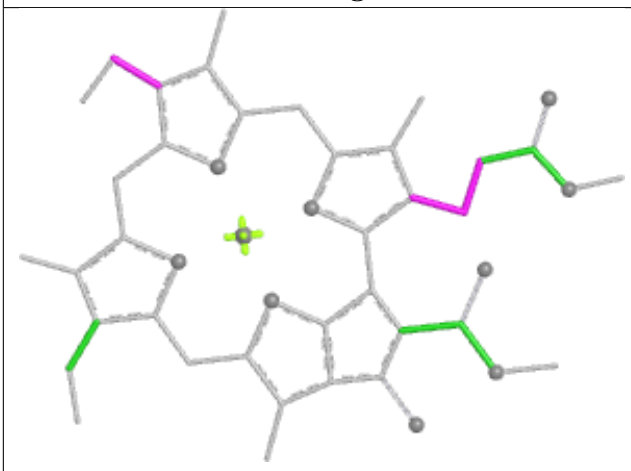
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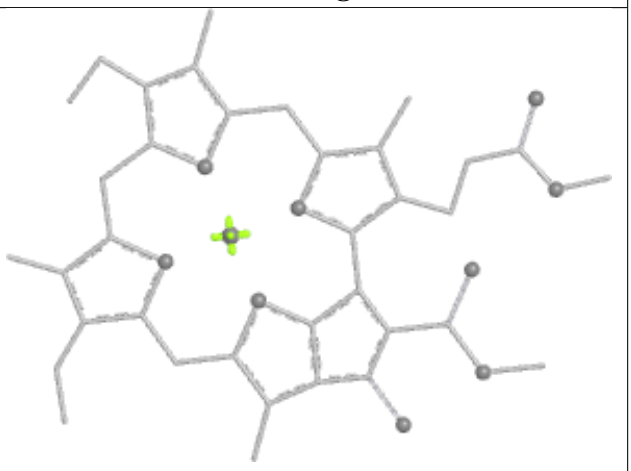
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Bond angles

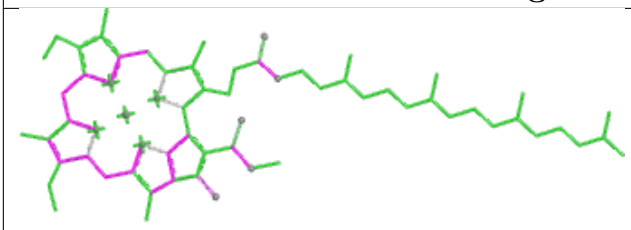


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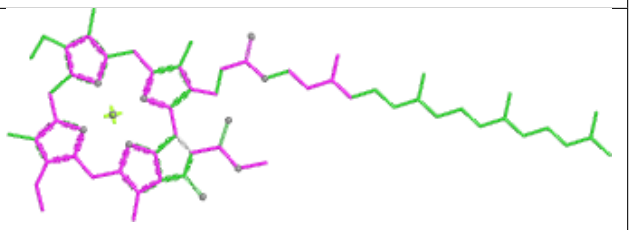


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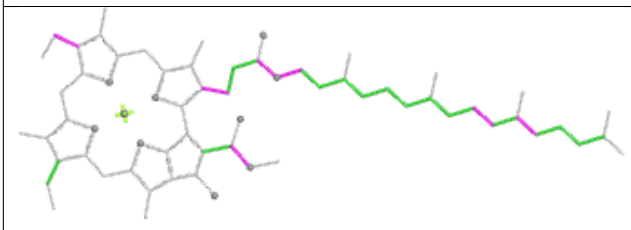
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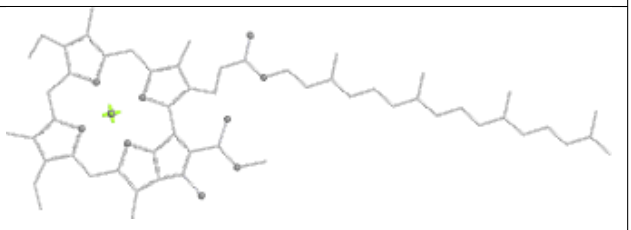
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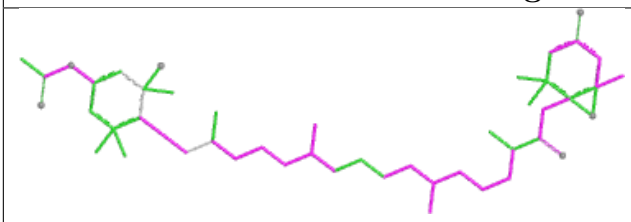


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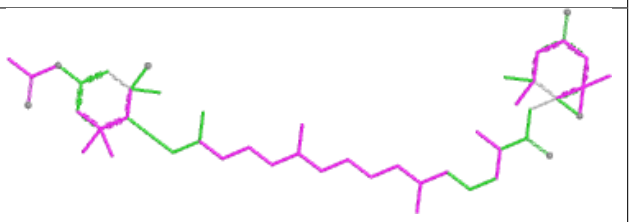


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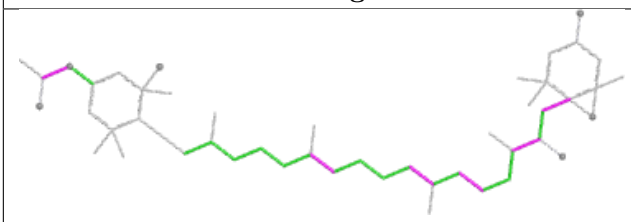
Ligand A86 2u 205



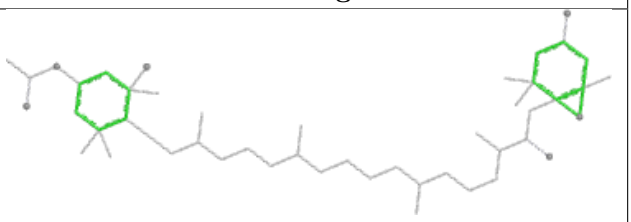
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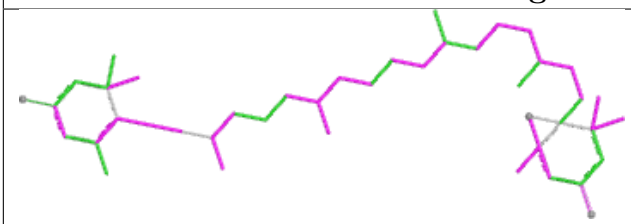


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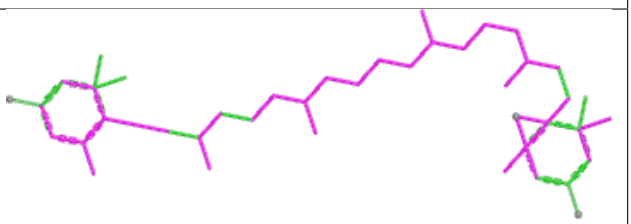


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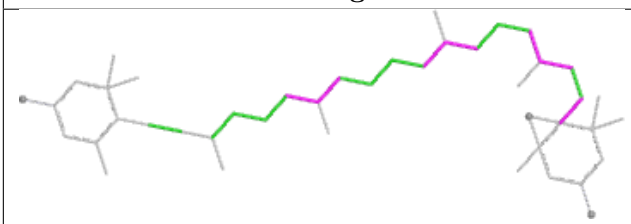
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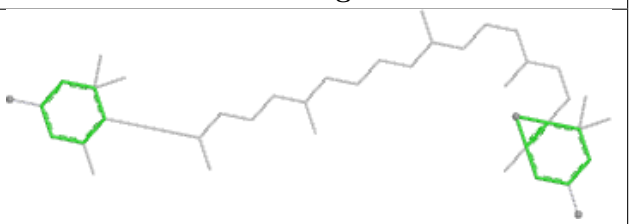
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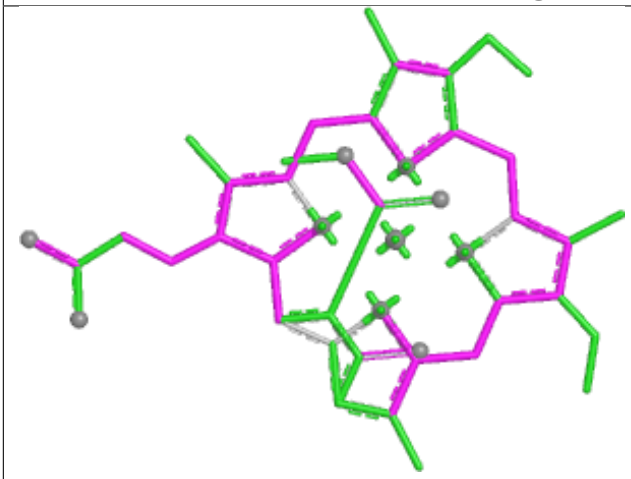


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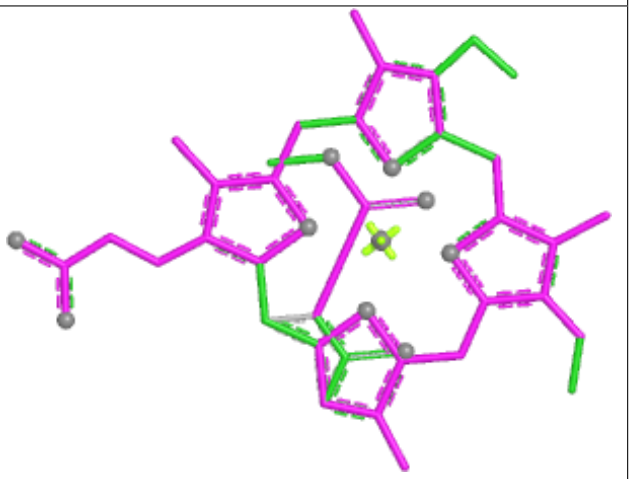


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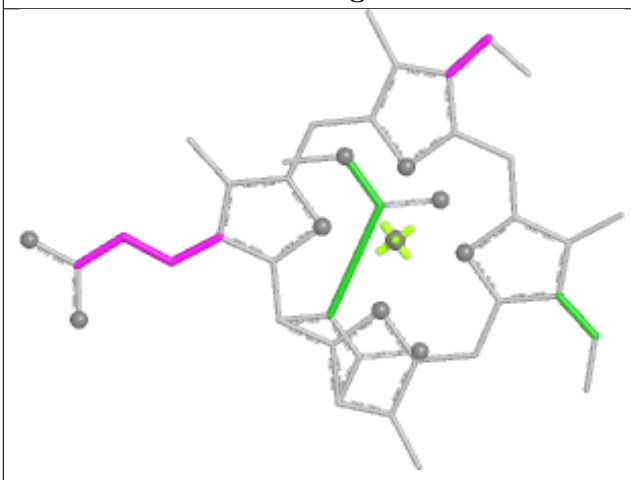
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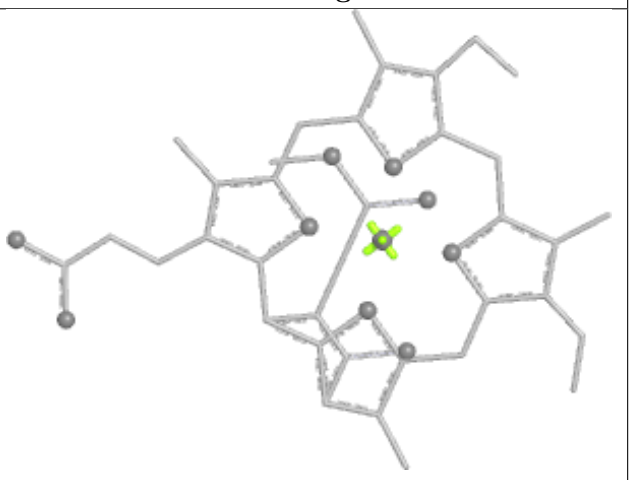
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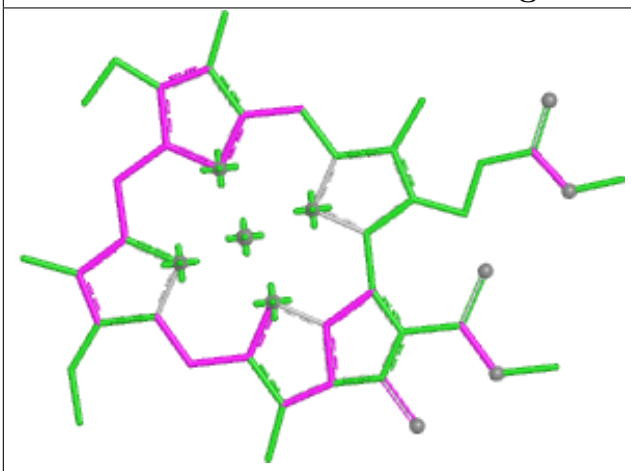


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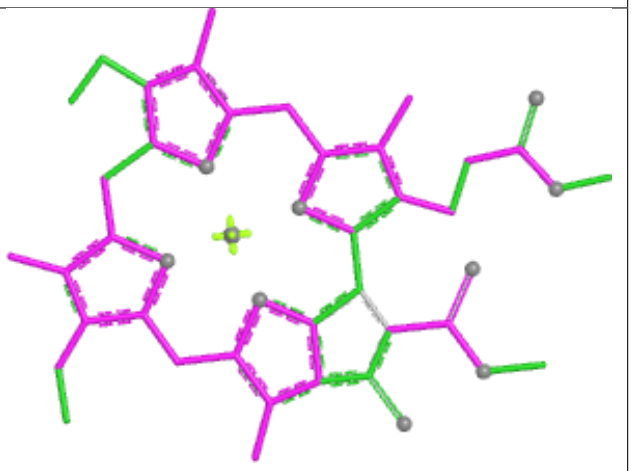


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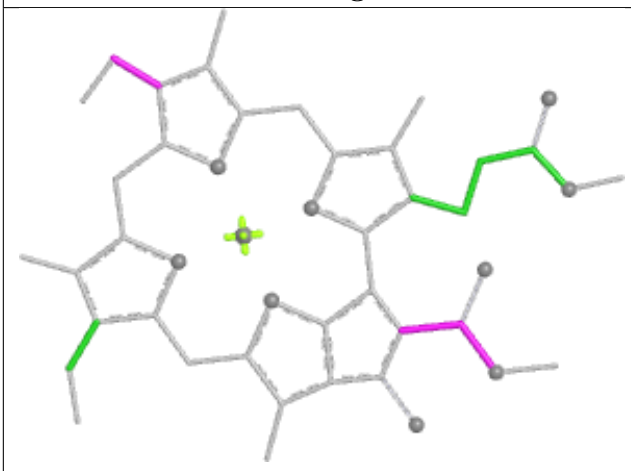
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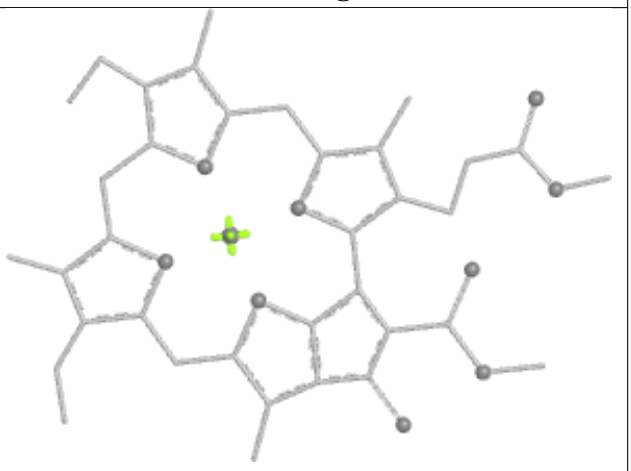
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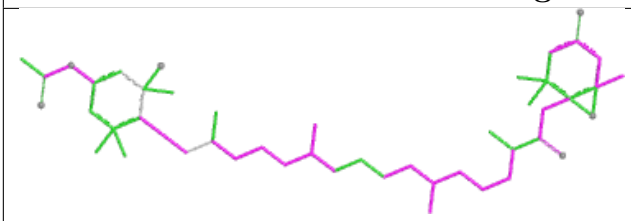


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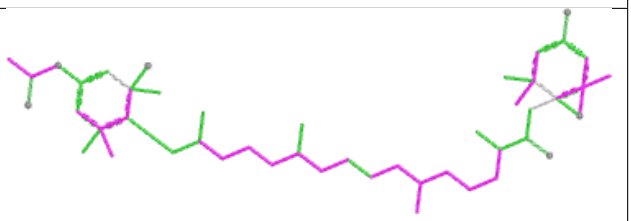


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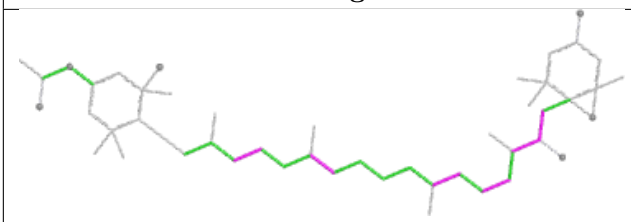
Ligand A86 3 314



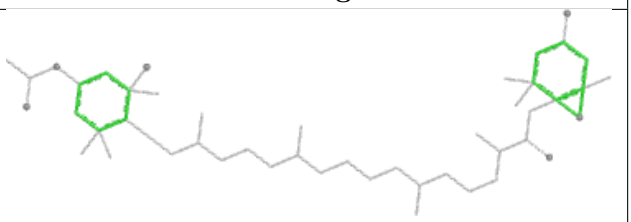
Bond lengths



Bond angles

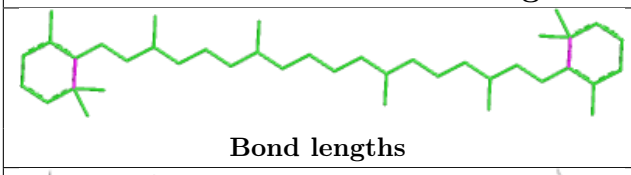


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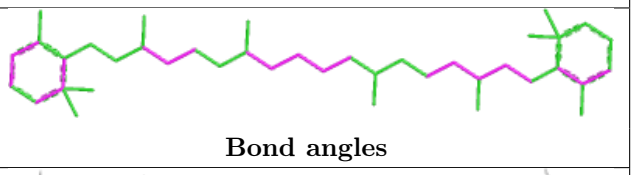


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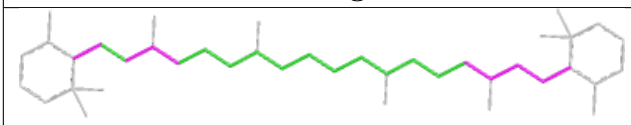
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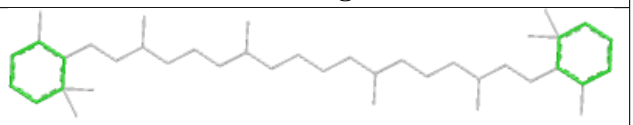
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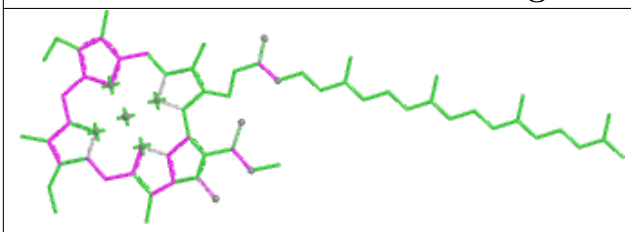


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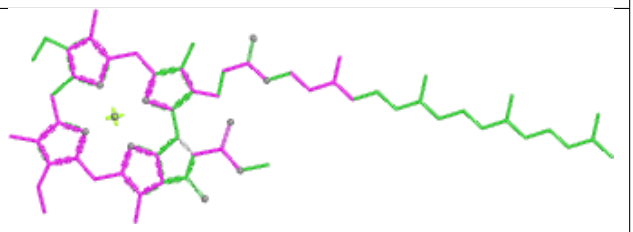


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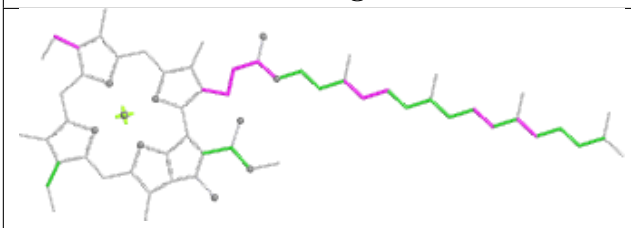
Ligand CLA 1 303



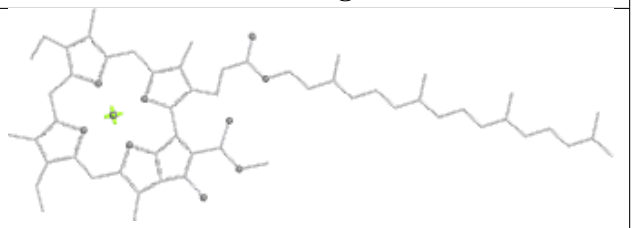
Bond lengths



Bond angles

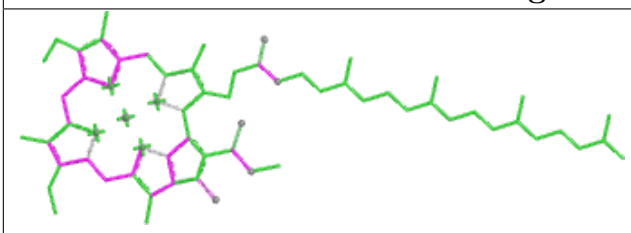


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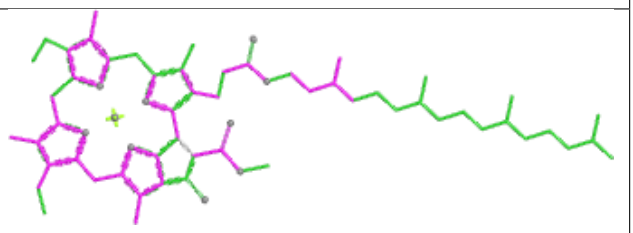


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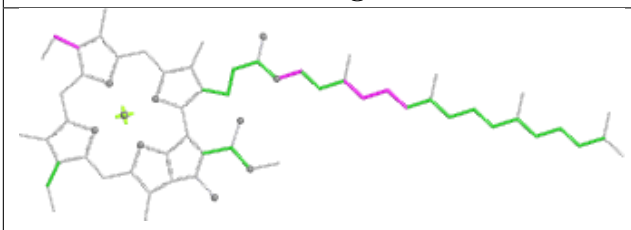
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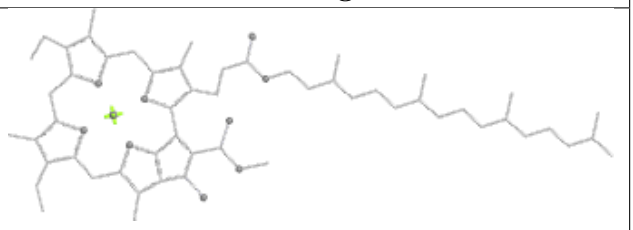
Bond lengths



Bond angles

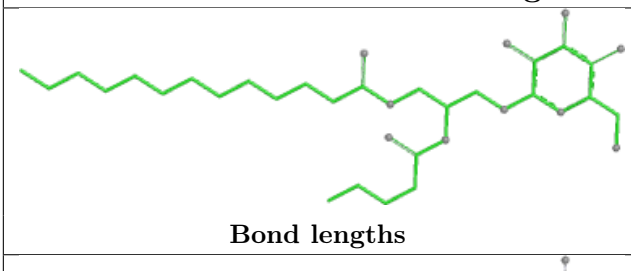


Torsions

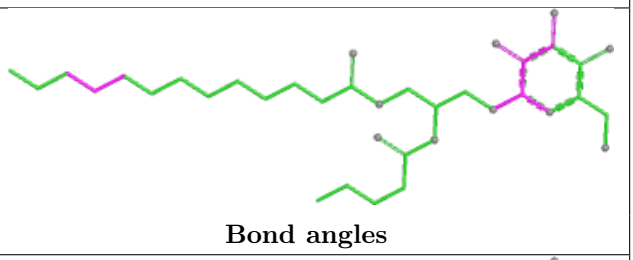


Rings

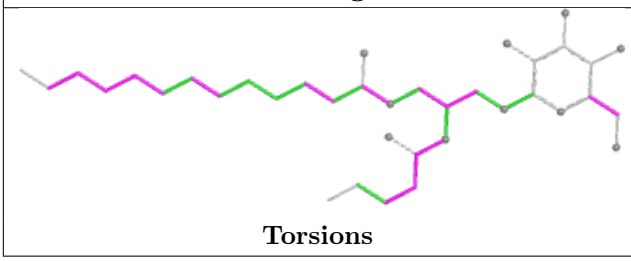
Ligand LMG 8 319



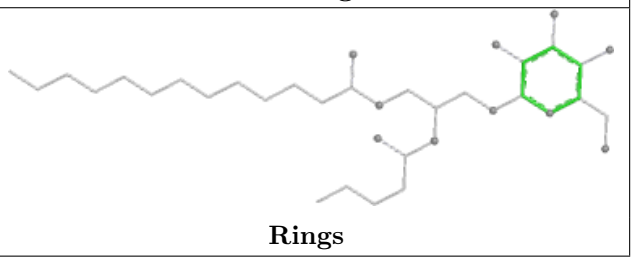
Bond lengths



Bond angles

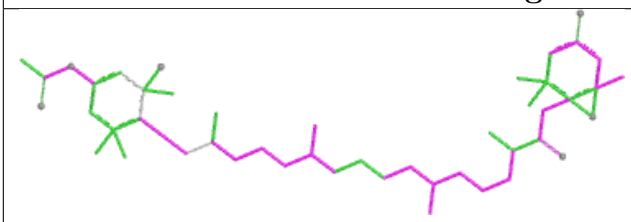


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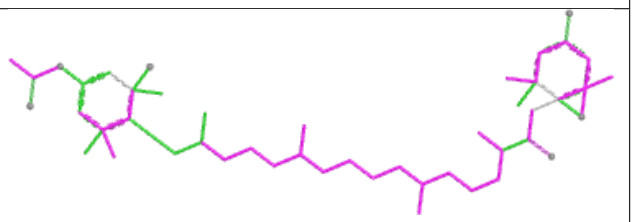


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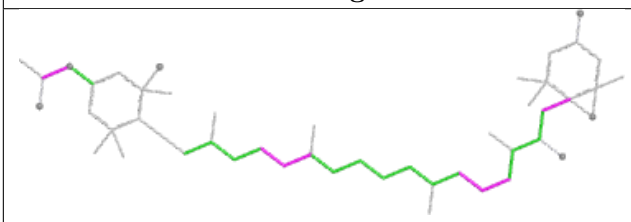
Ligand A86 15 315



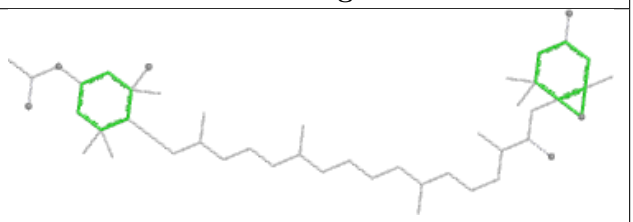
Bond lengths



Bond angles

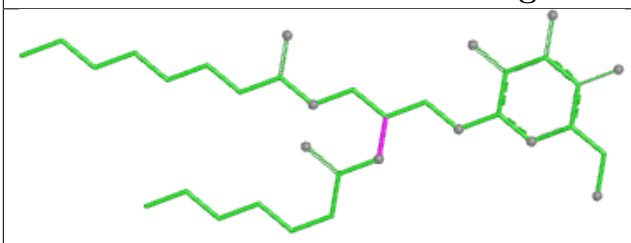


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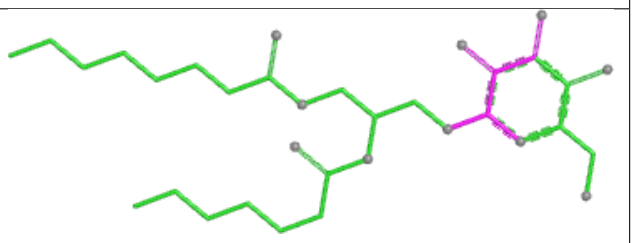


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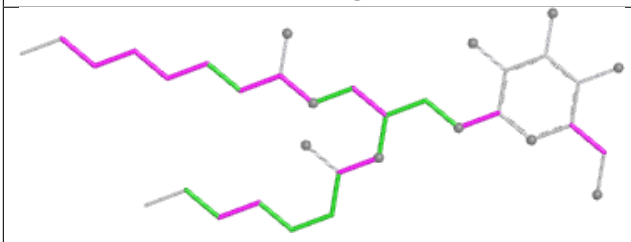
Ligand LMG A 856



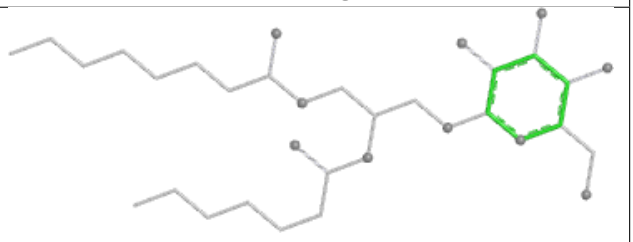
Bond lengths



Bond angles

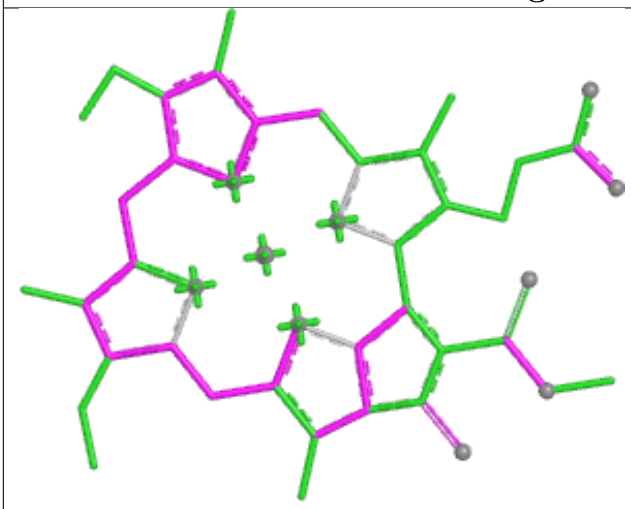


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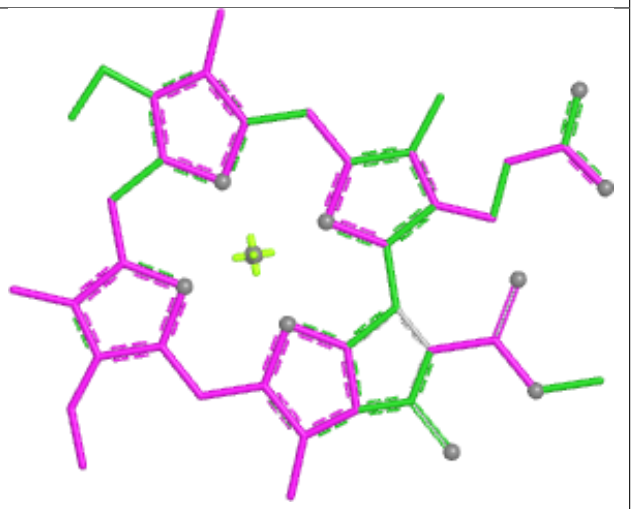


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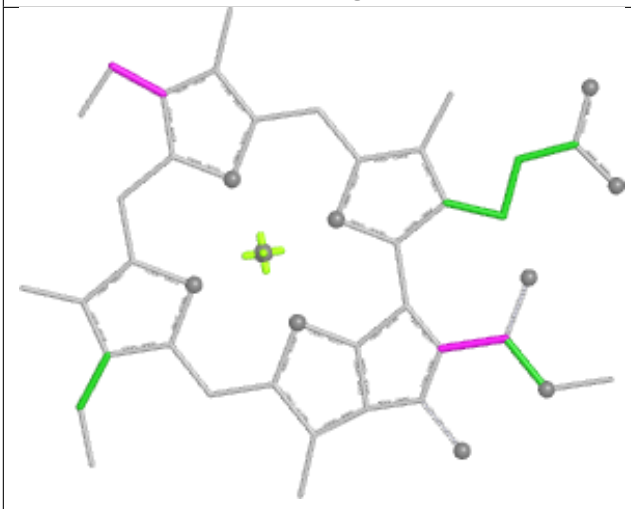
Ligand CLA 6 315



Bond lengths



Bond angles

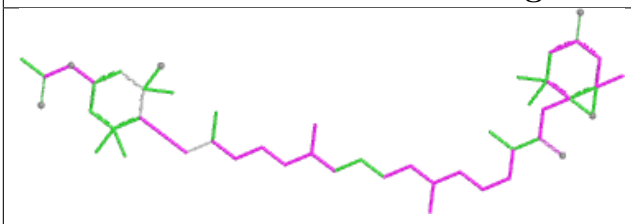


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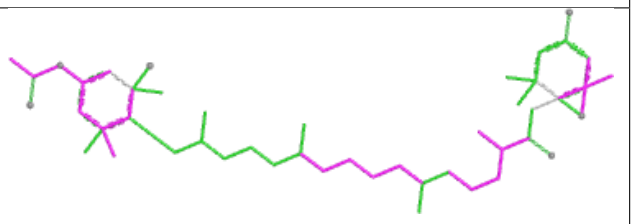


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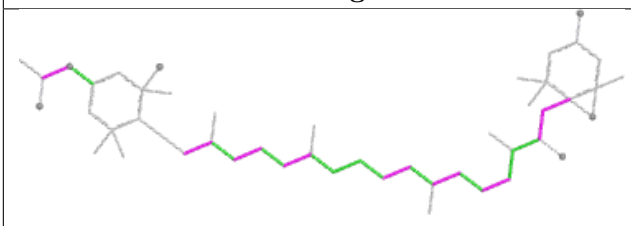
Ligand A86 14 317



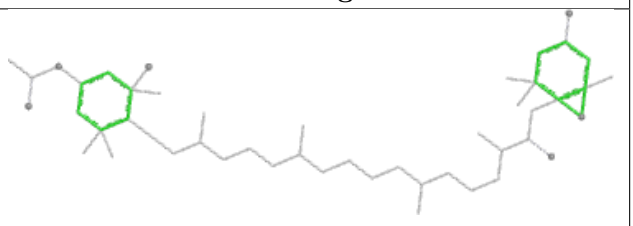
Bond lengths



Bond angles

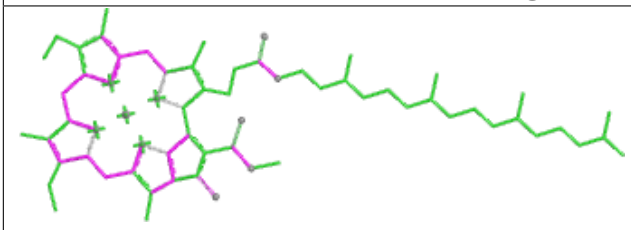


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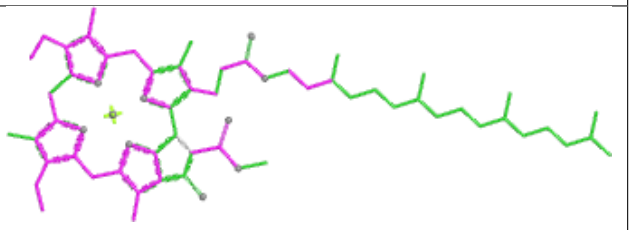


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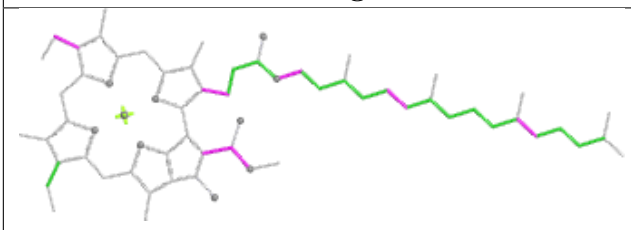
Ligand CLA A 835



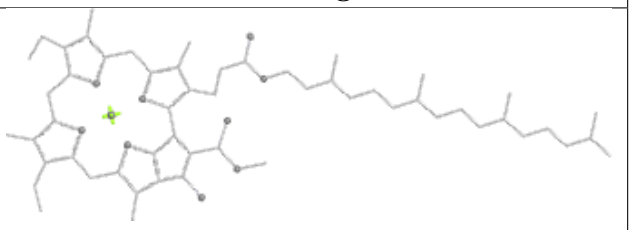
Bond lengths



Bond angles

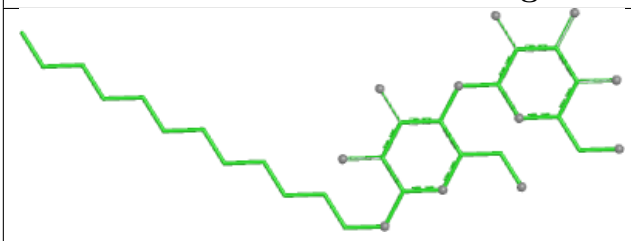


Torsions



Rings

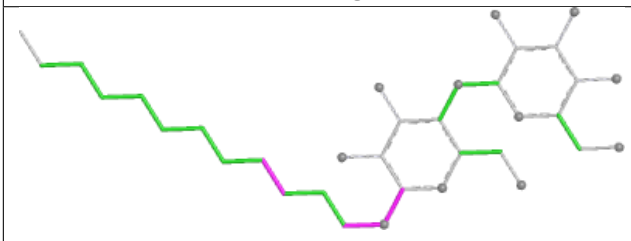
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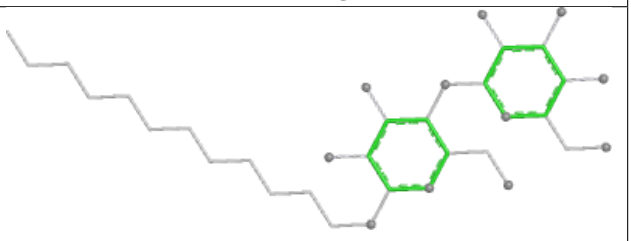
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Bond angles

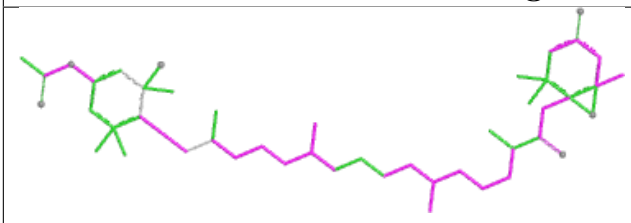


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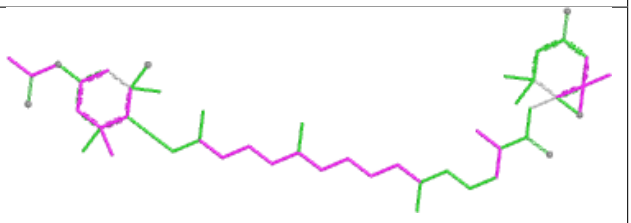


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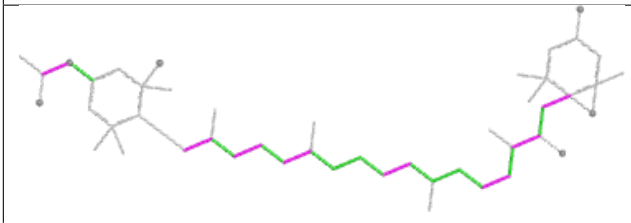
Ligand A86 13 315



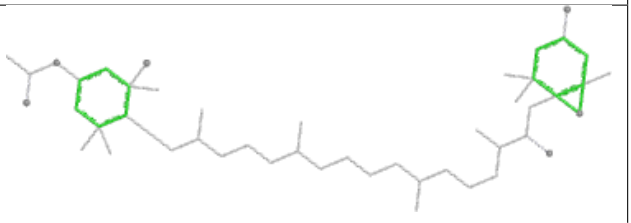
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Bond angles

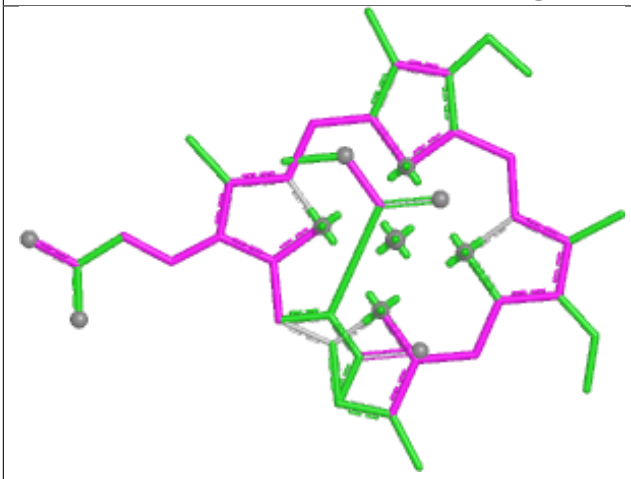


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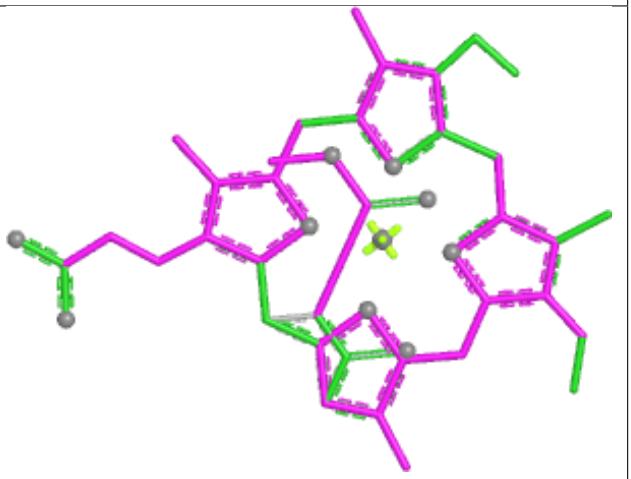


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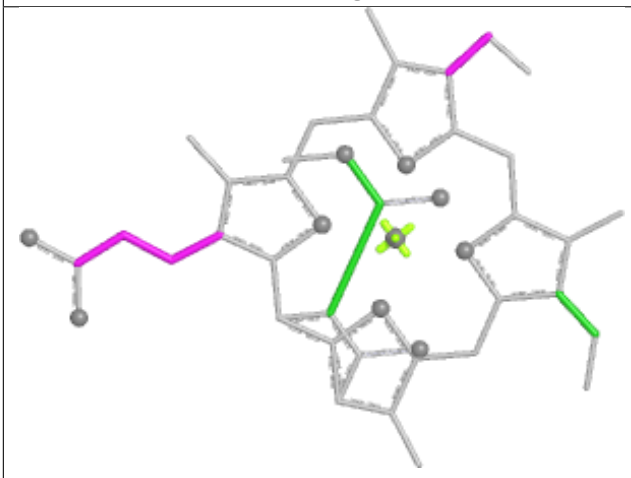
Ligand KC1 9 312



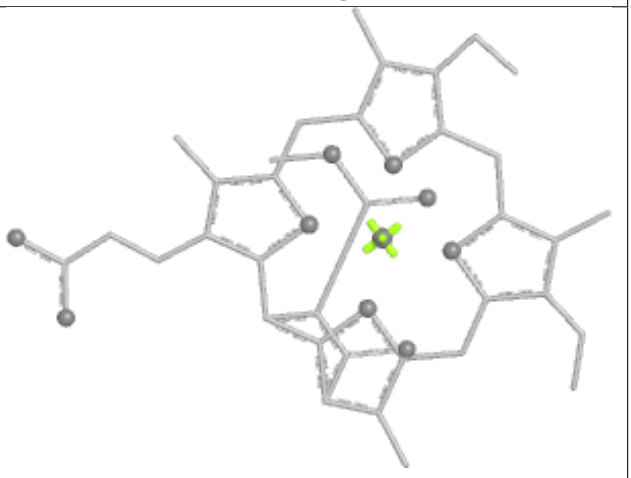
Bond lengths



Bond angles

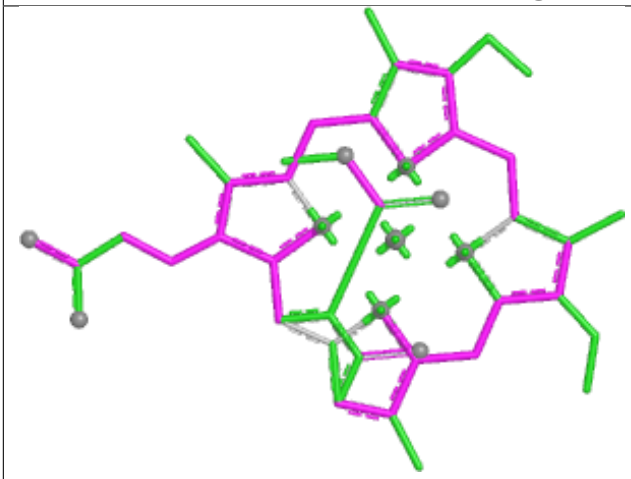


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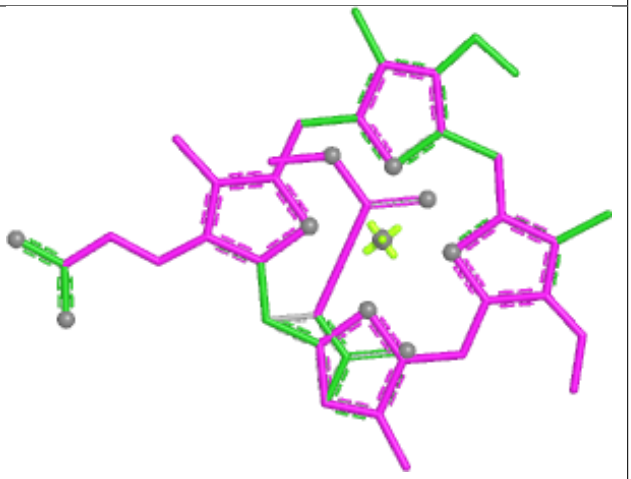


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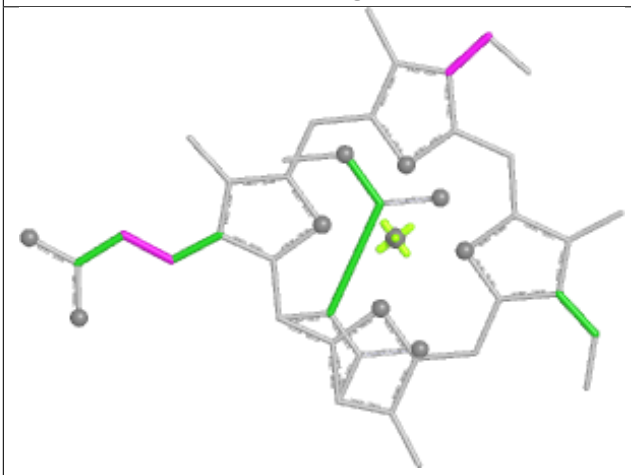
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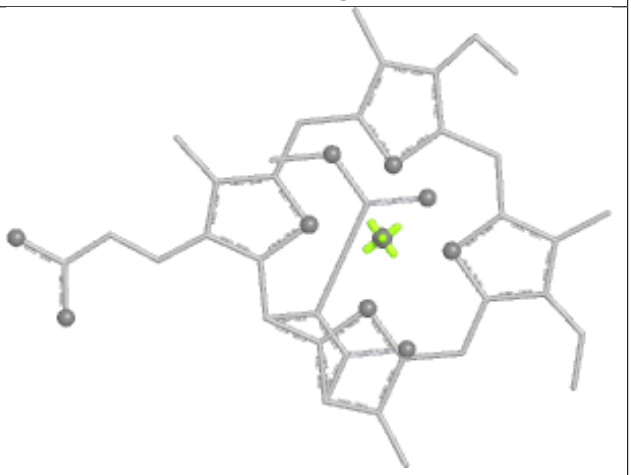
Bond lengths



Bond angles

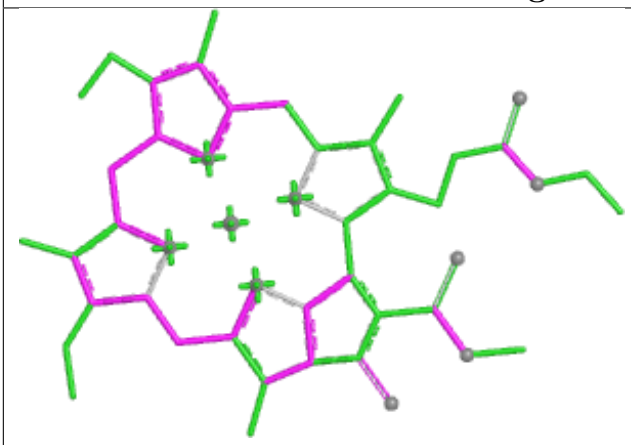


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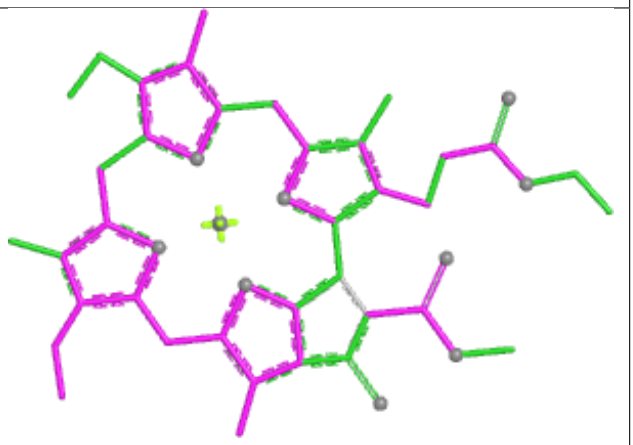


Rings

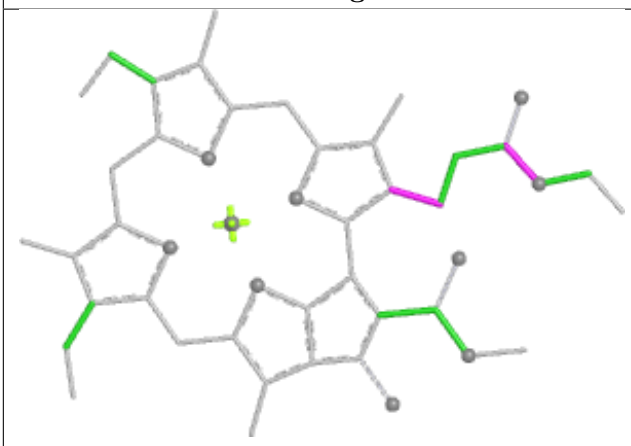
Ligand CLA 8 309



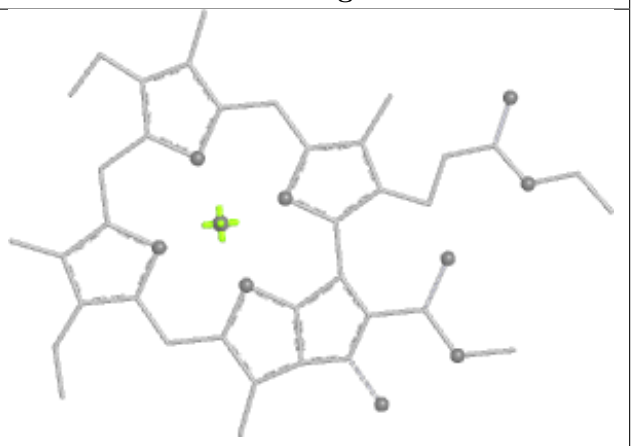
Bond lengths



Bond angles

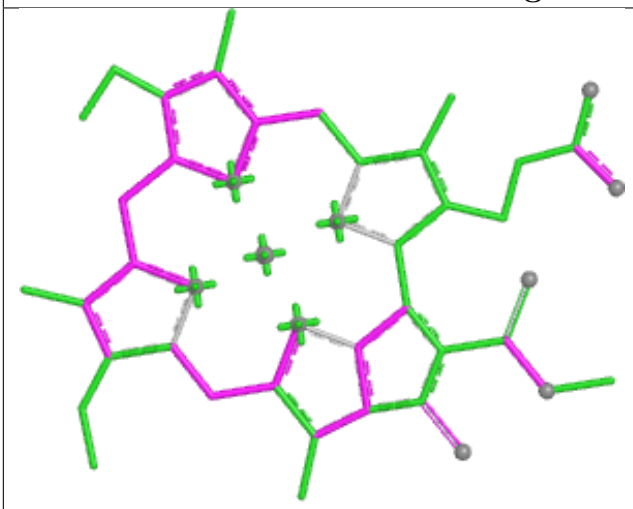


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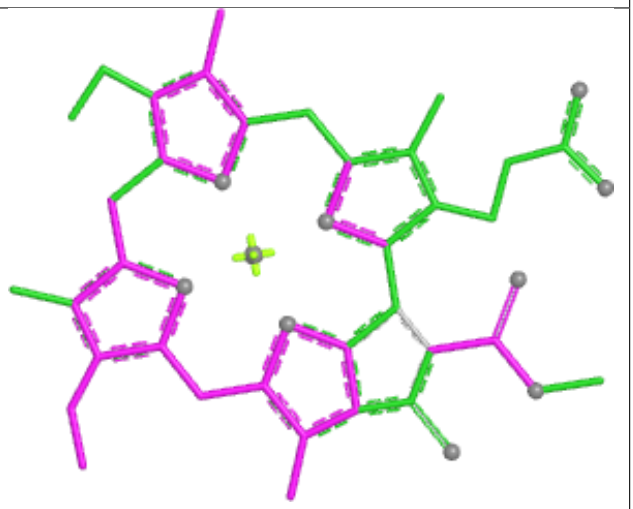


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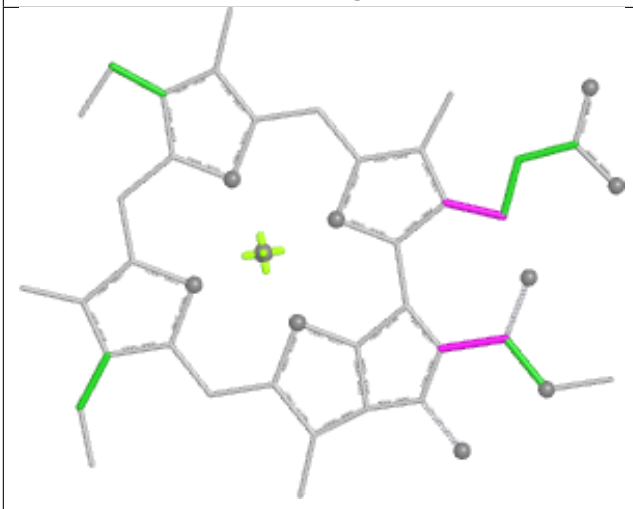
Ligand CLA B 820



Bond lengths



Bond angles

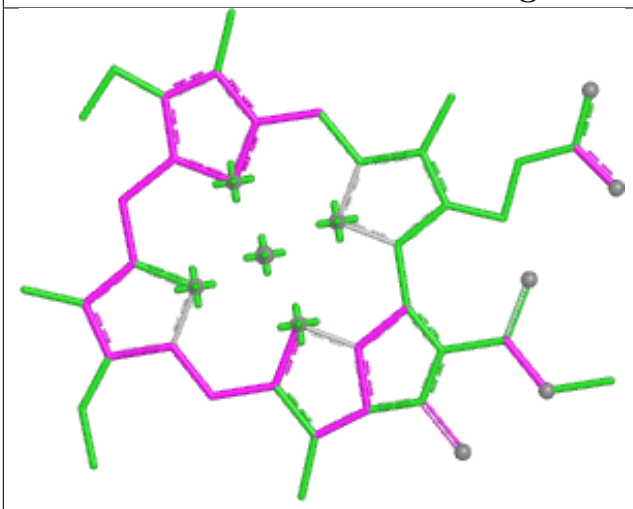


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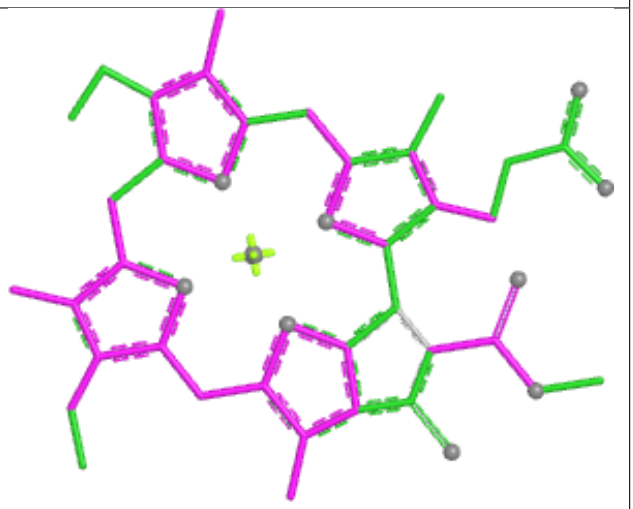


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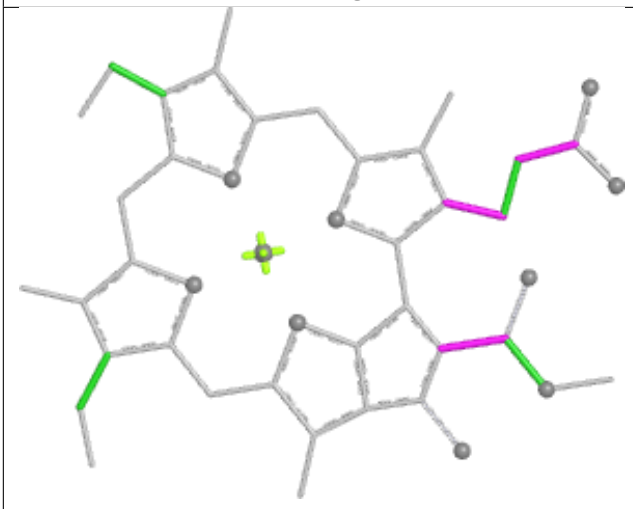
Ligand CLA 15 310



Bond lengths



Bond angles

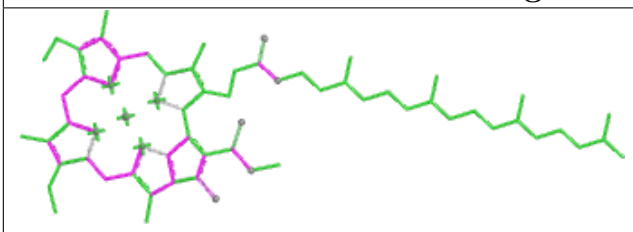


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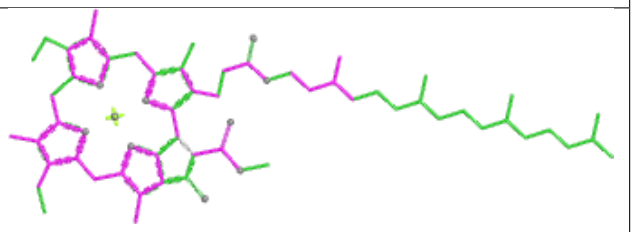


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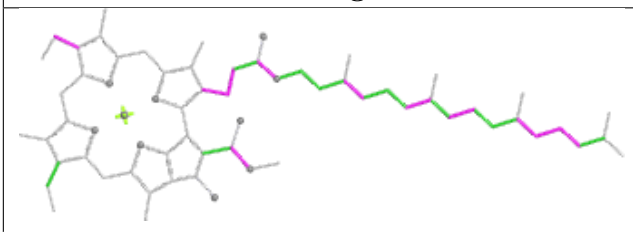
Ligand CLA B 826



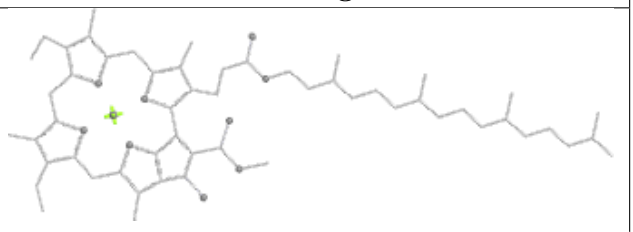
Bond lengths



Bond angles

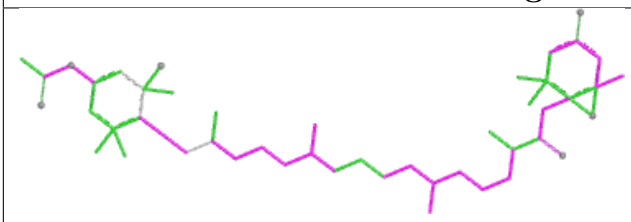


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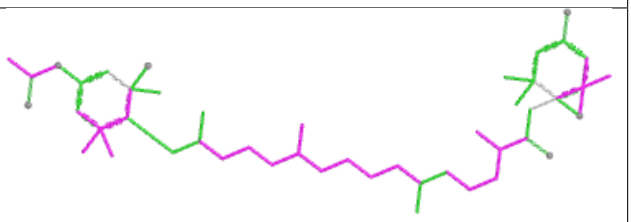


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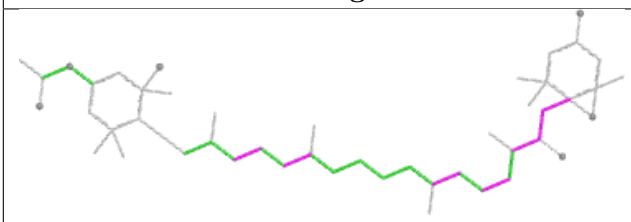
Ligand A86 12 314



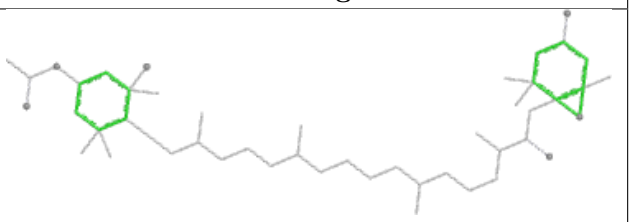
Bond lengths



Bond angles

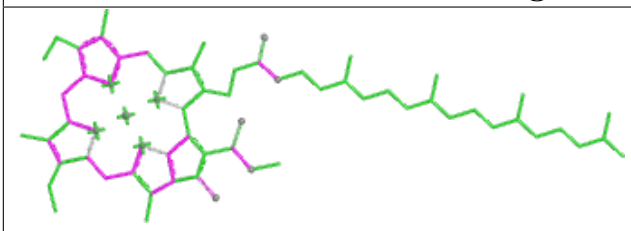


Torsions

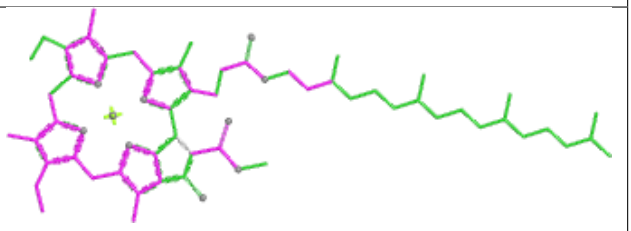


Rings

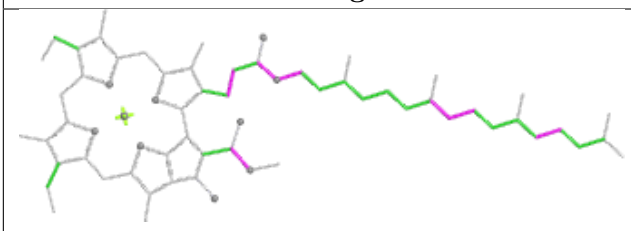
Ligand CLA 1 302



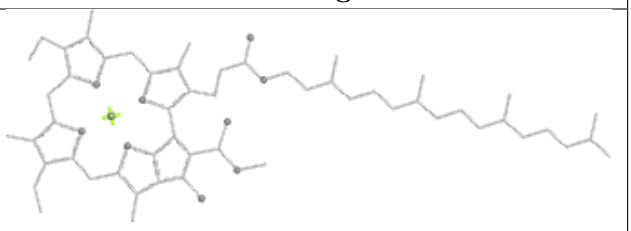
Bond lengths



Bond angles

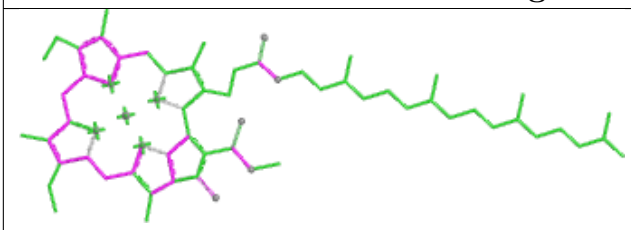


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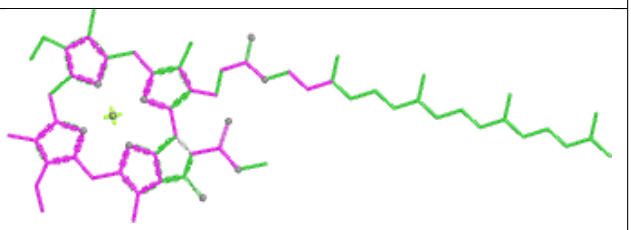


Rings

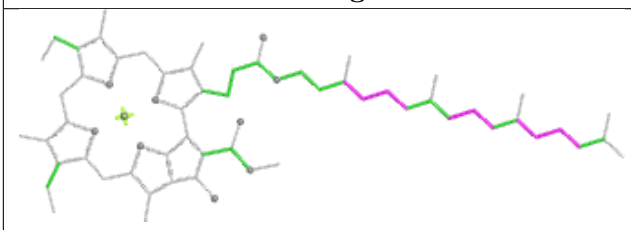
Ligand CLA 2 304



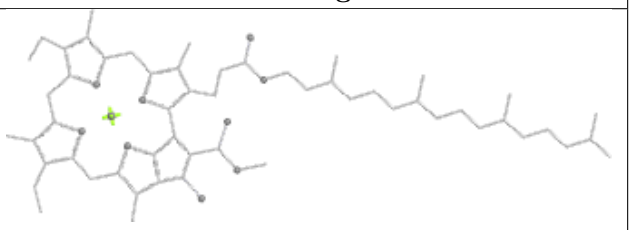
Bond lengths



Bond angles

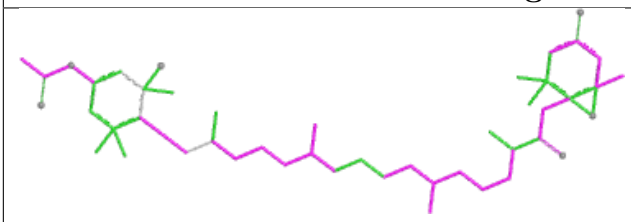


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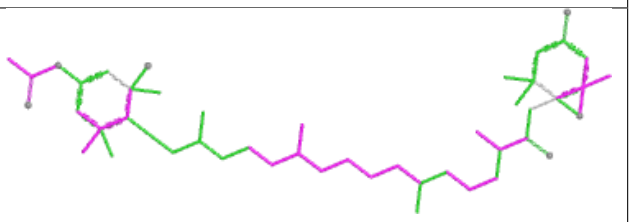


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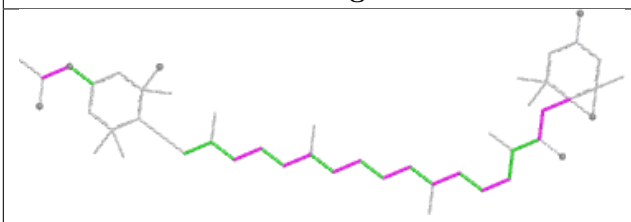
Ligand A86 11 316



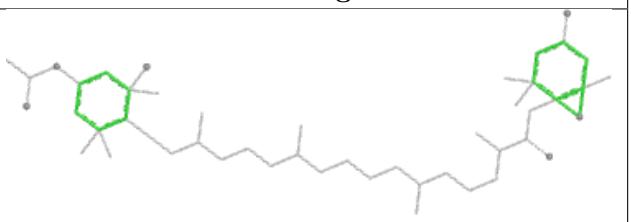
Bond lengths



Bond angles

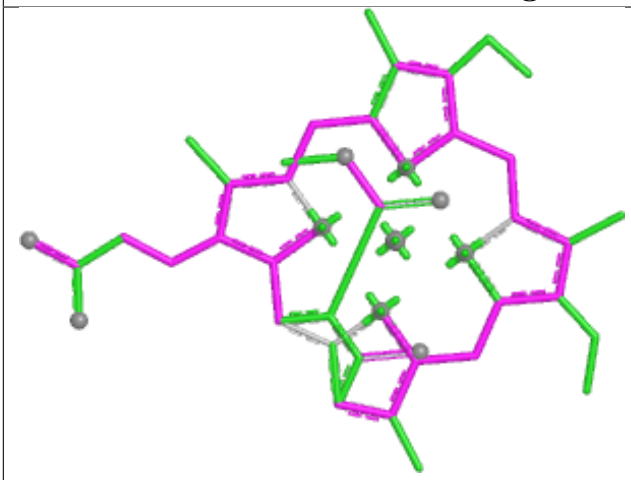


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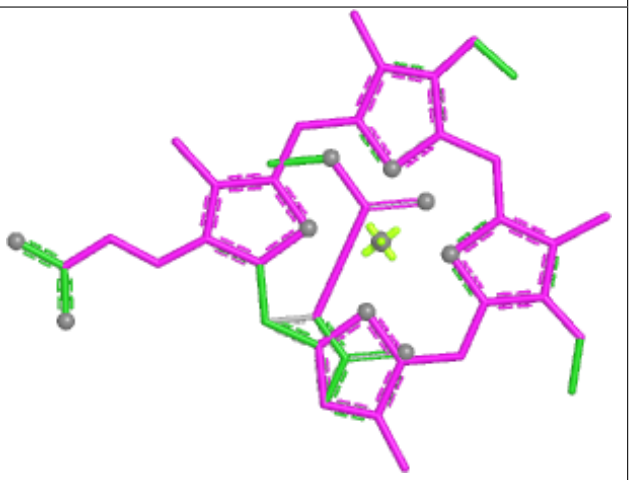


Rings

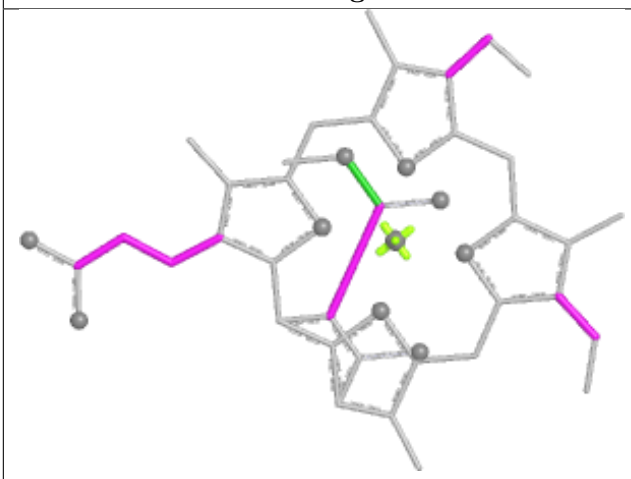
Ligand KC1 14 306



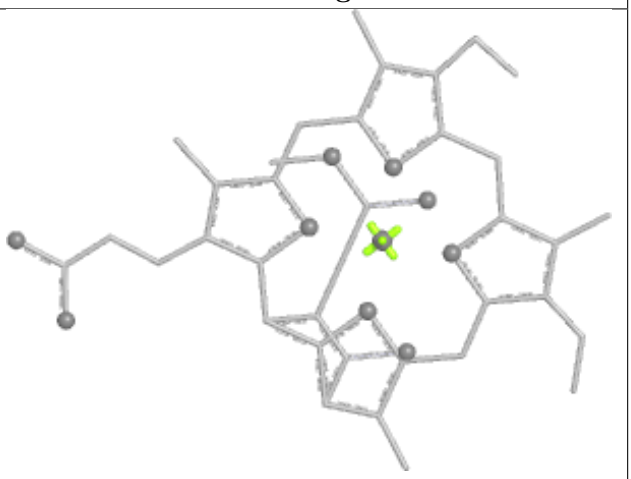
Bond lengths



Bond angles

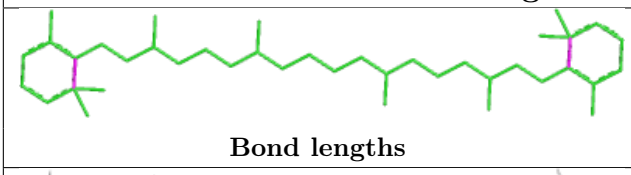


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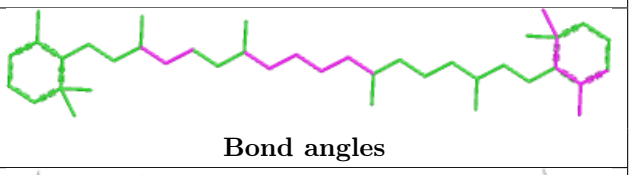


Rings

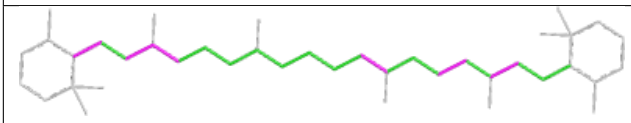
Ligand BCR A 849



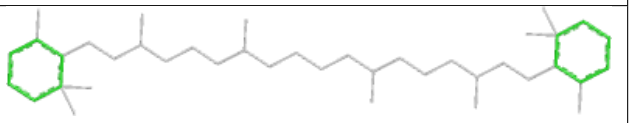
Bond lengths



Bond angles

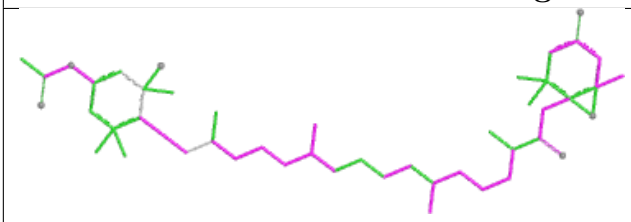


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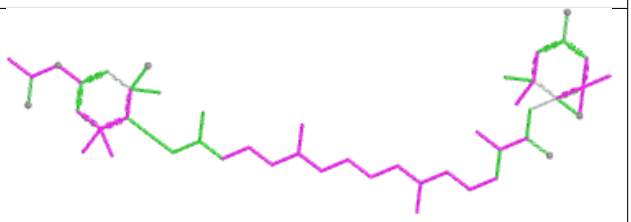


Rings

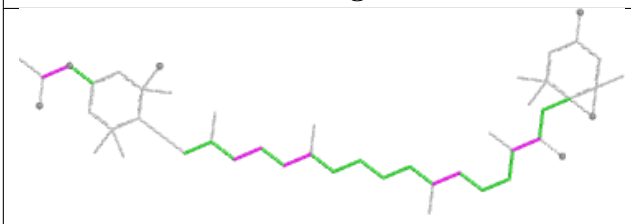
Ligand A86 2 318



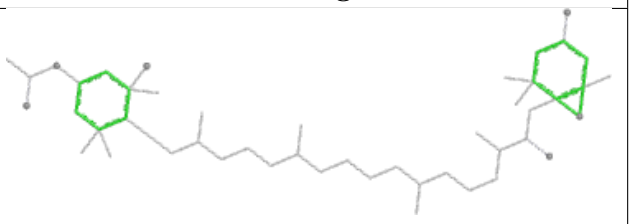
Bond lengths



Bond angles

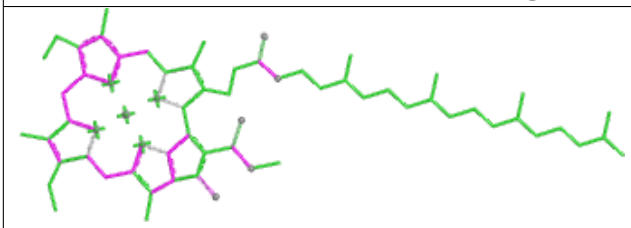


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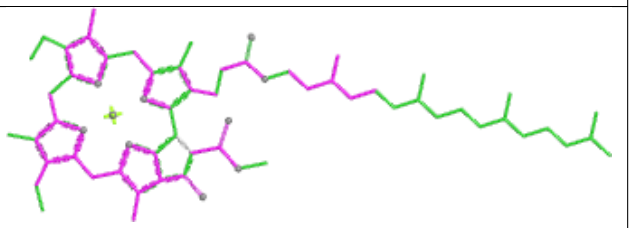


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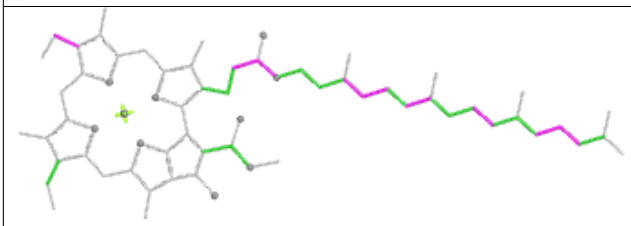
Ligand CLA A 828



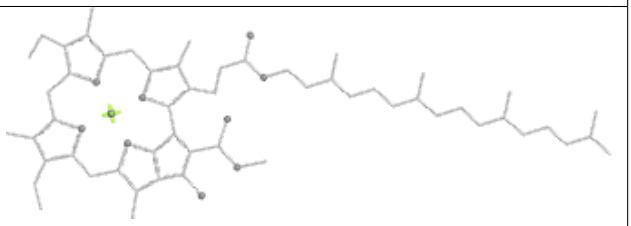
Bond lengths



Bond angles

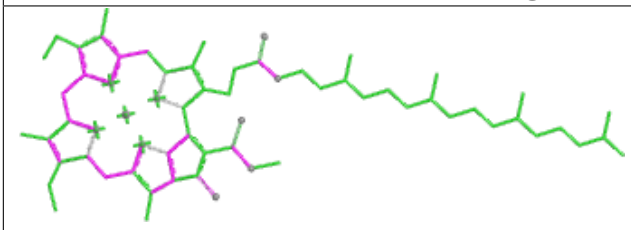


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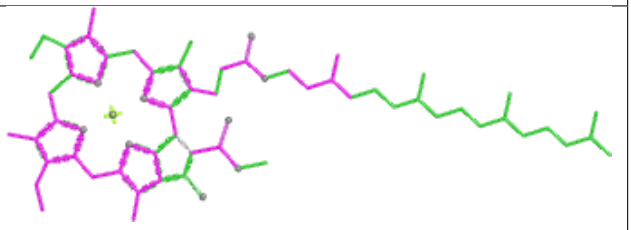


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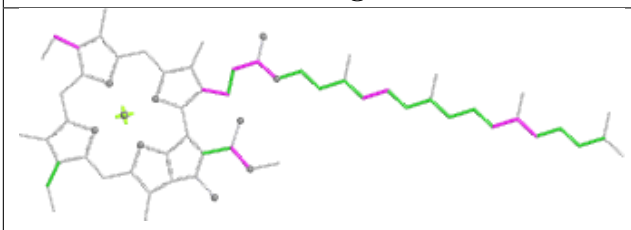
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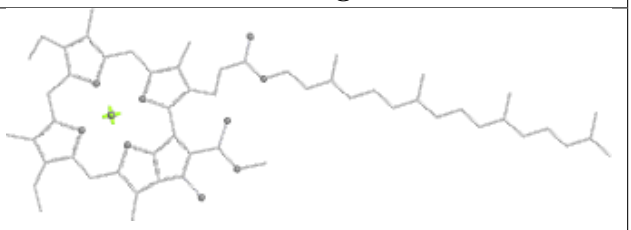
Bond lengths



Bond angles



Torsions

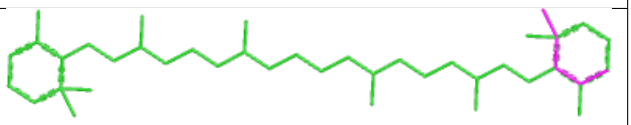


Rings

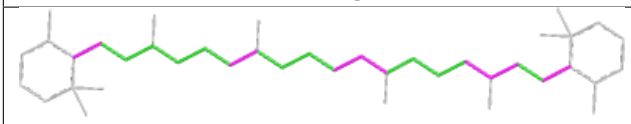
Ligand BCR A 848



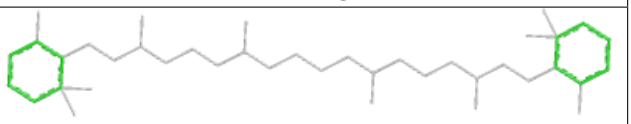
Bond lengths



Bond angles

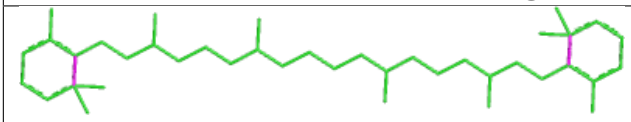


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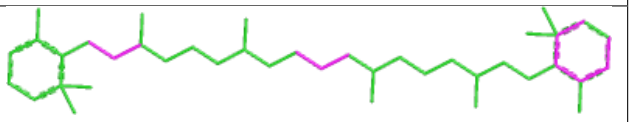


Rings

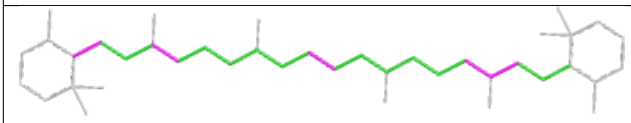
Ligand BCR B 842



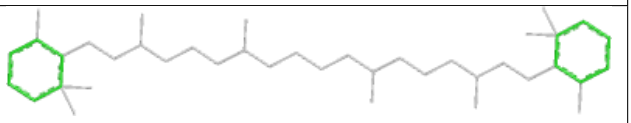
Bond lengths



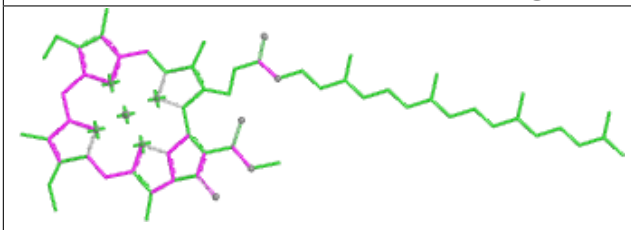
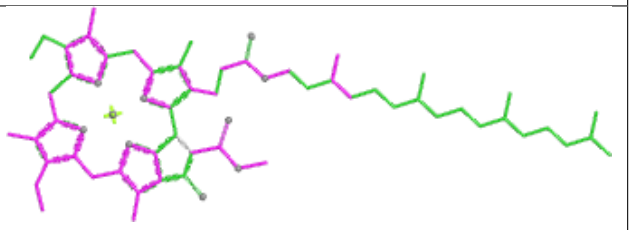
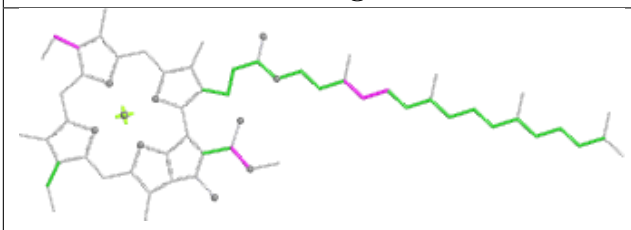
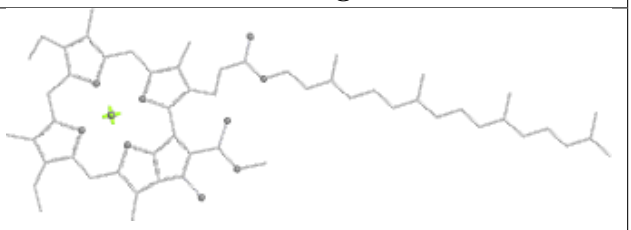
Bond angles

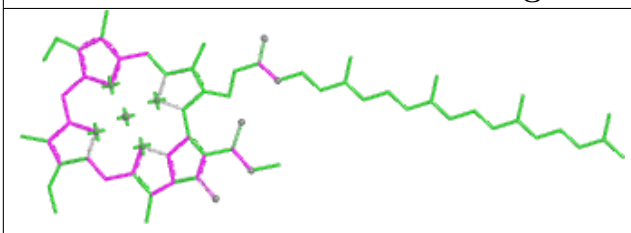
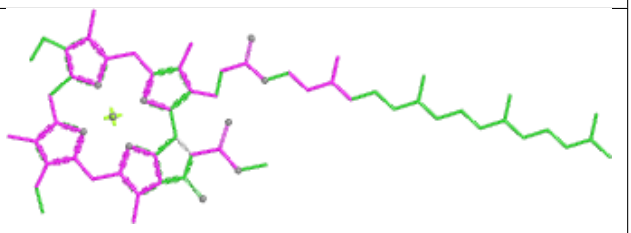
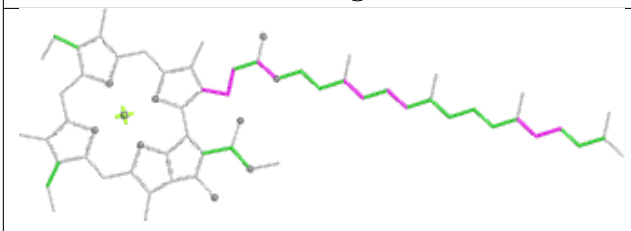
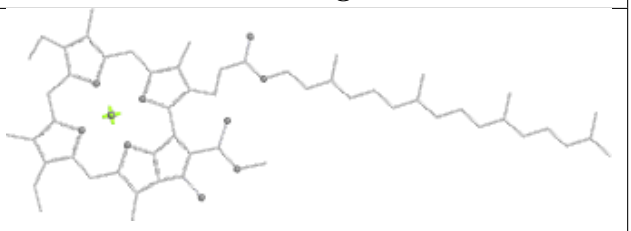


Torsions

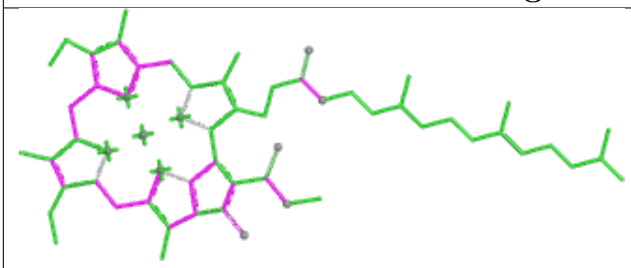


Rings

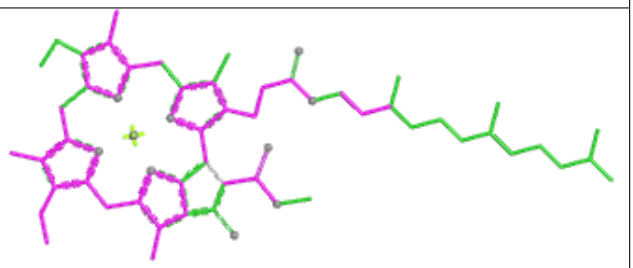
Ligand CLA 5 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

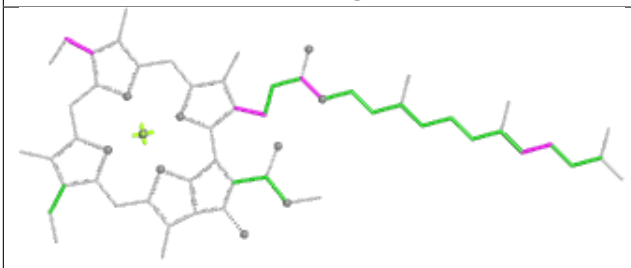
Ligand CLA B 818



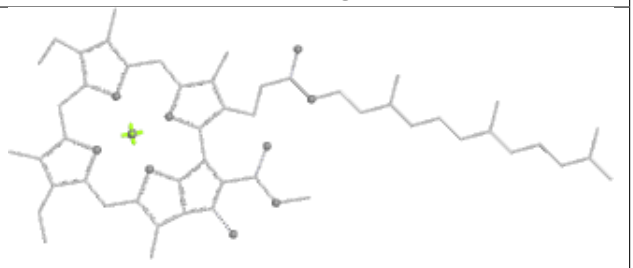
Bond lengths



Bond angles

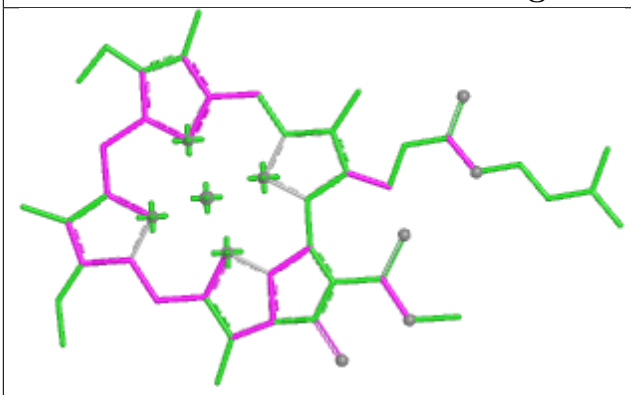


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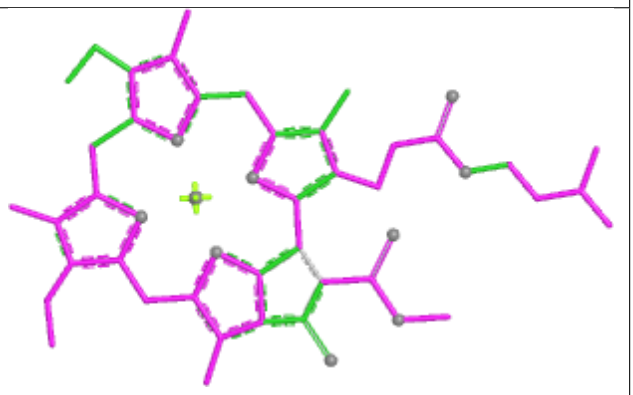


Rings

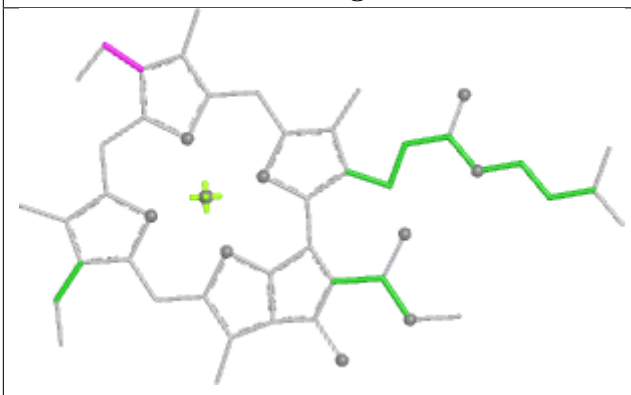
Ligand CLA 4 311



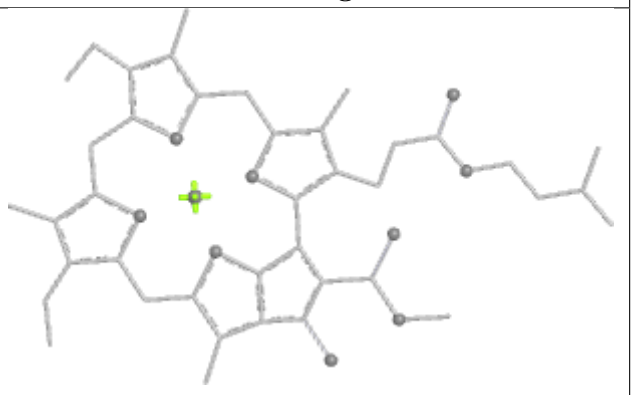
Bond lengths



Bond angles

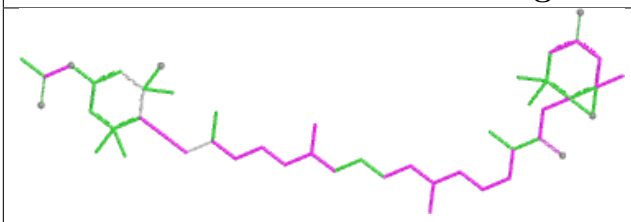


Torsions

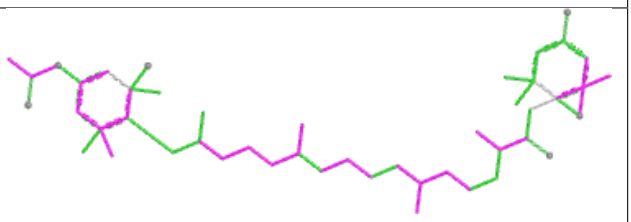


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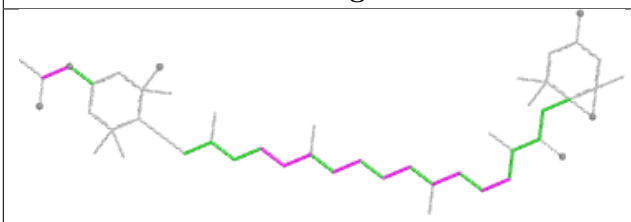
Ligand A86 9 315



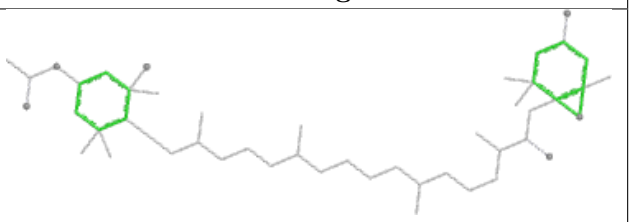
Bond lengths



Bond angles

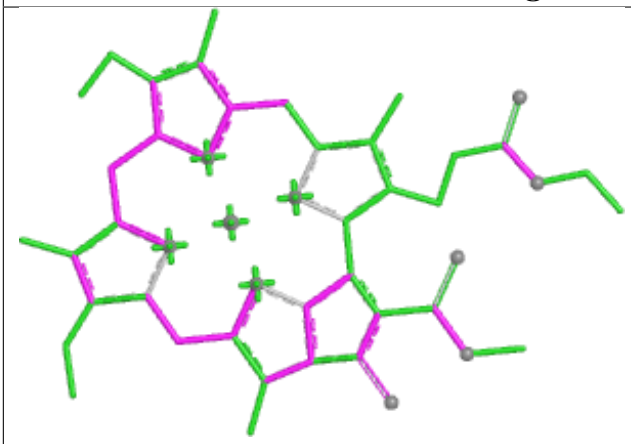


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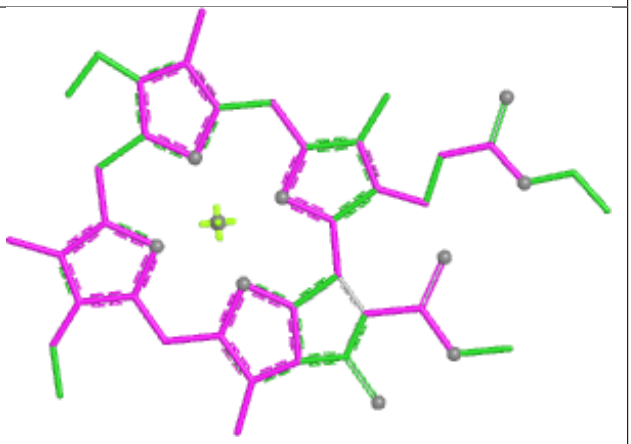


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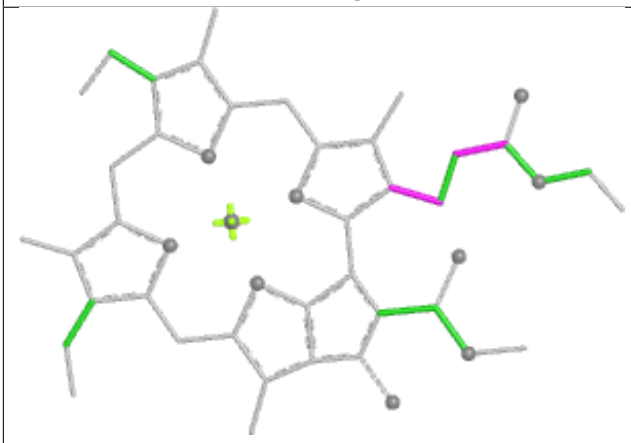
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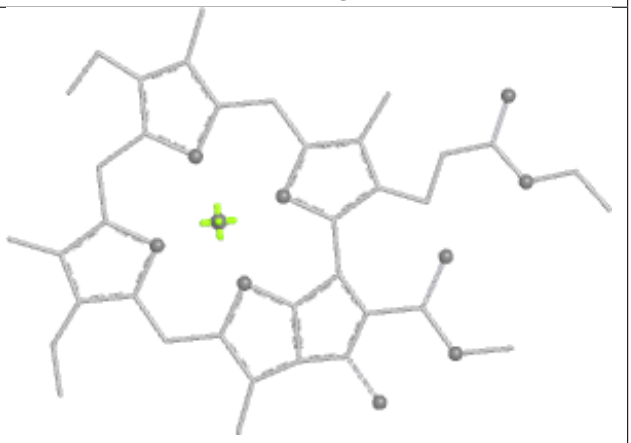
Bond lengths



Bond angles

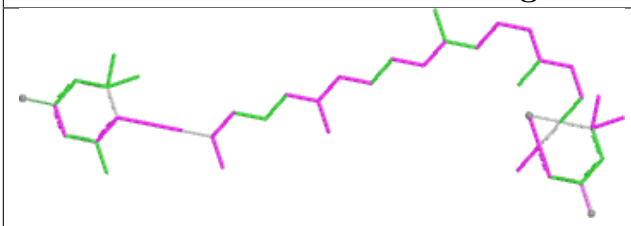


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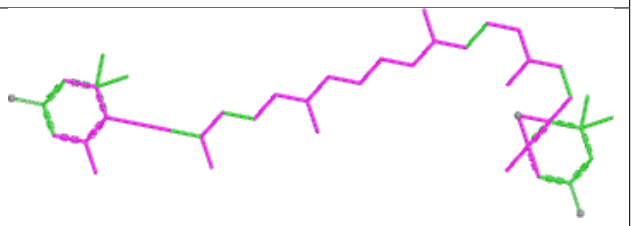


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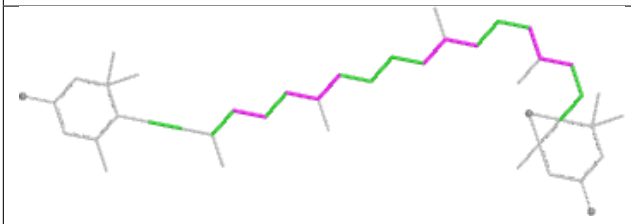
Ligand DD6 12 315



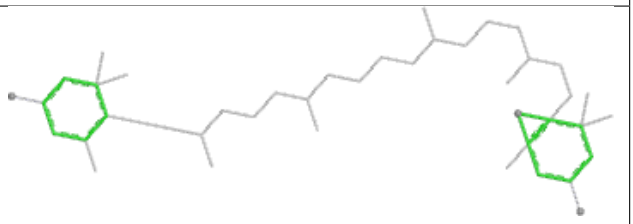
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Bond angles

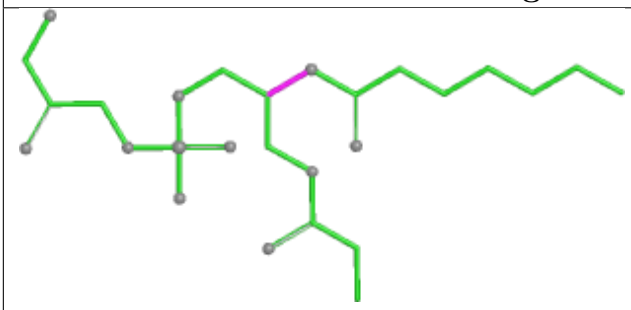


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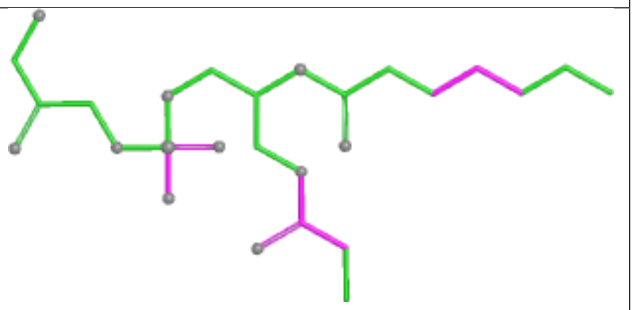


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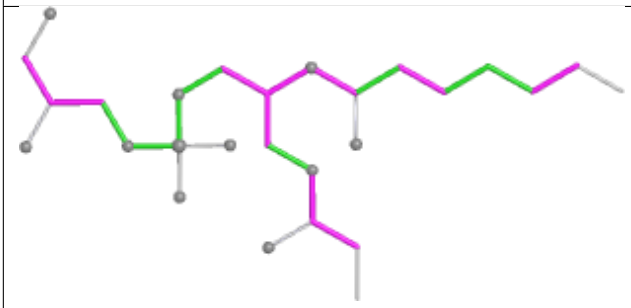
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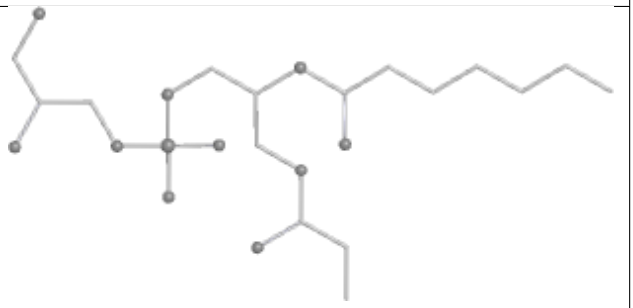
Bond lengths



Bond angles

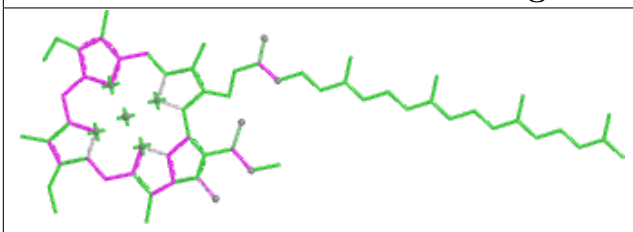


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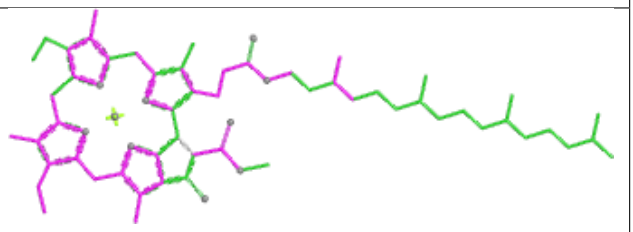


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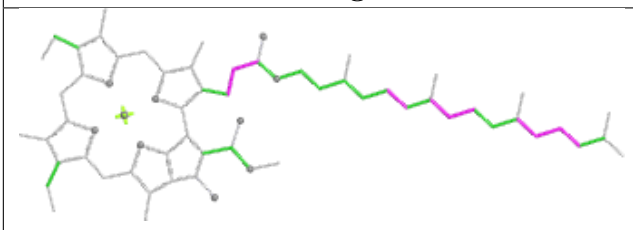
Ligand CLA 2 301



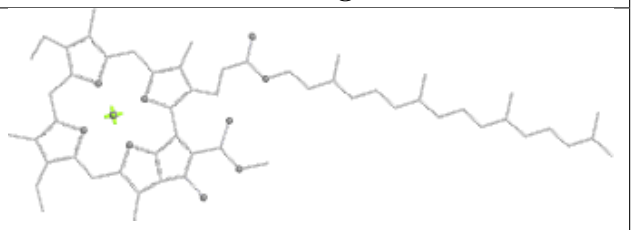
Bond lengths



Bond angles

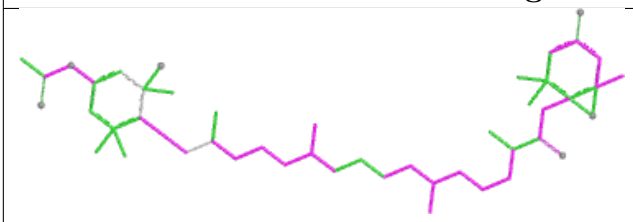


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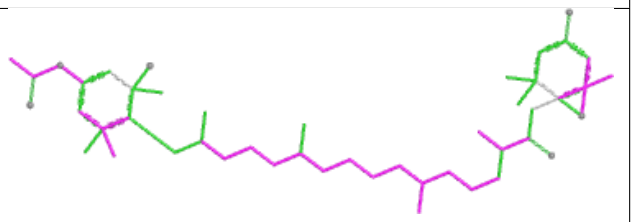


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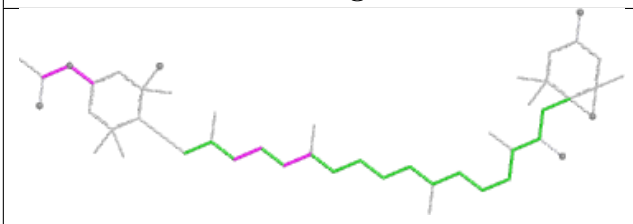
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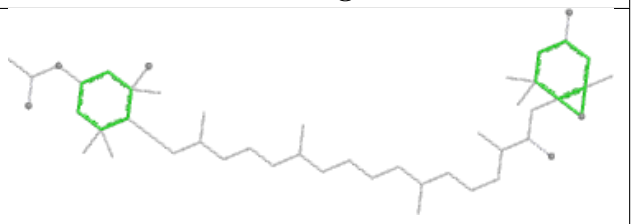
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Bond angles

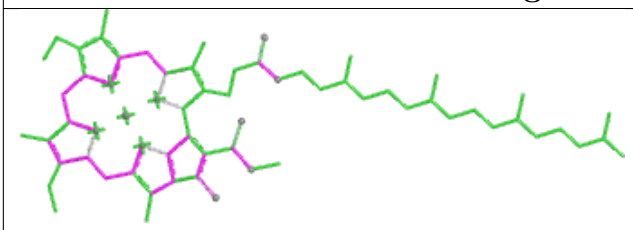


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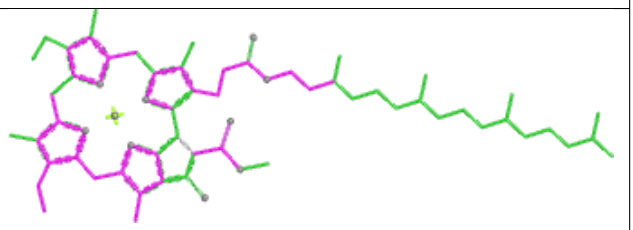


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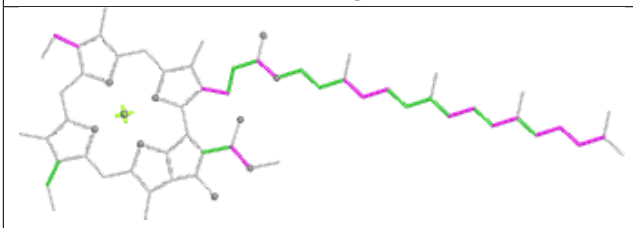
Ligand CLA A 820



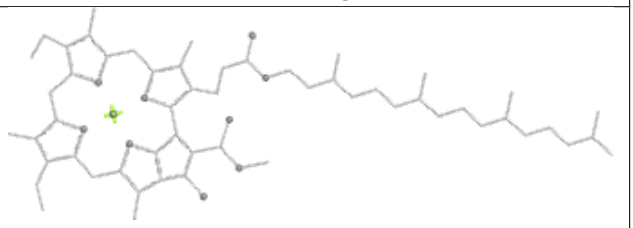
Bond lengths



Bond angles

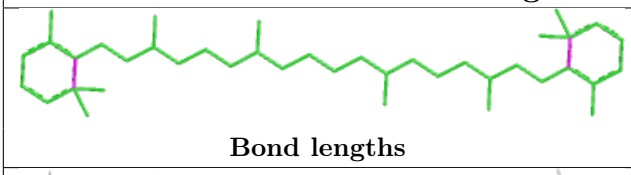


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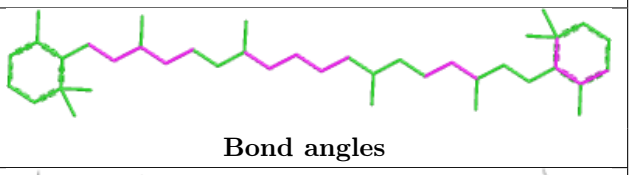


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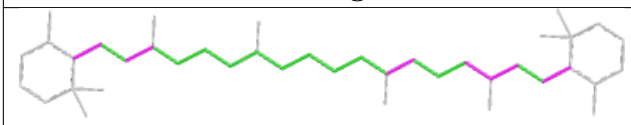
Ligand BCR B 841



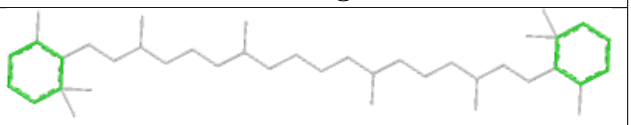
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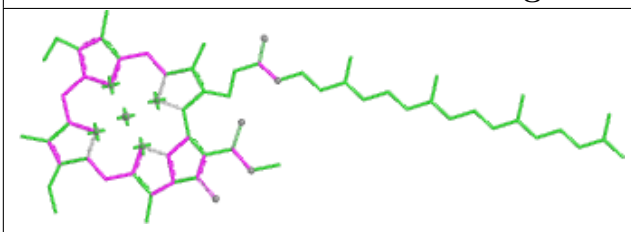


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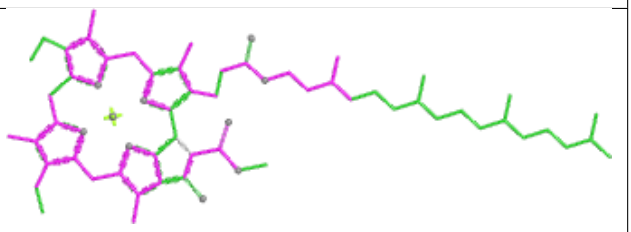


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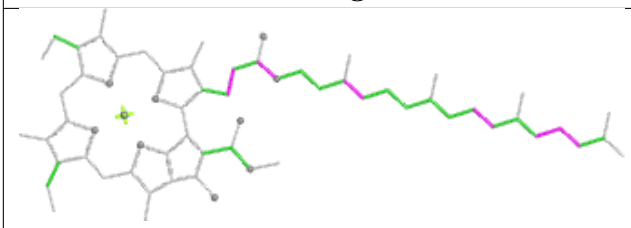
Ligand CLA A 803



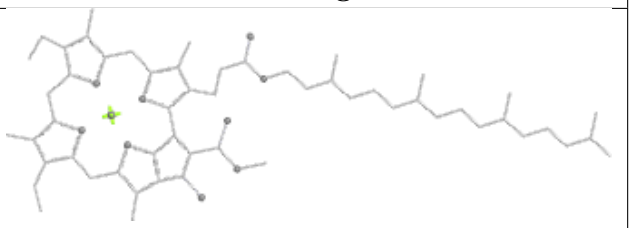
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Bond angles

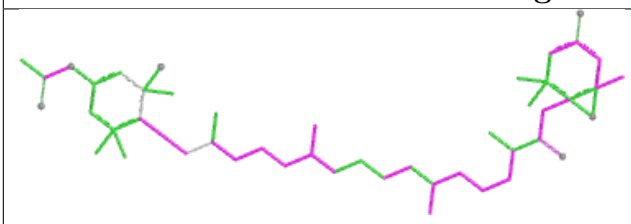


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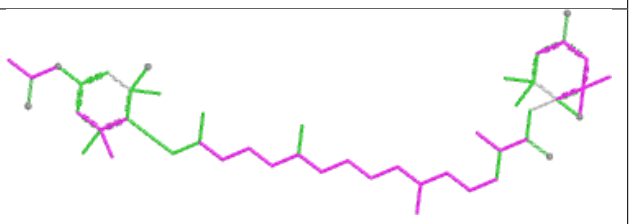


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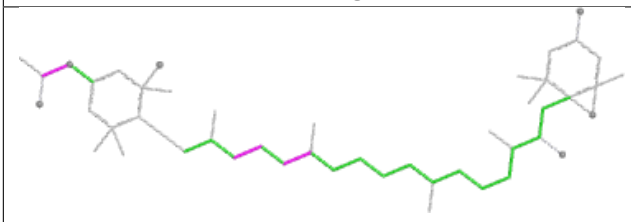
Ligand A86 4 317



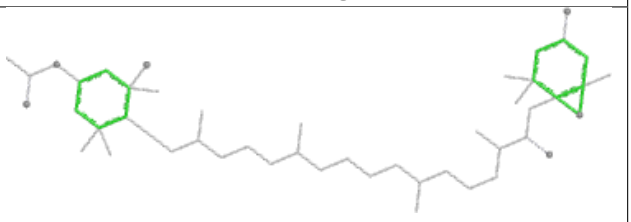
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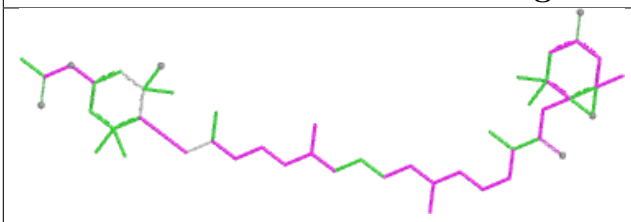


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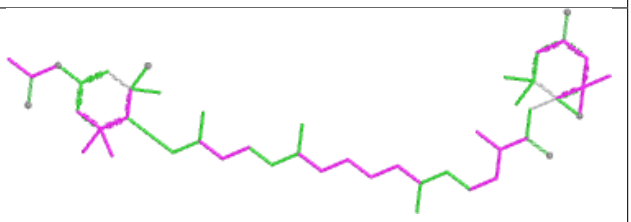


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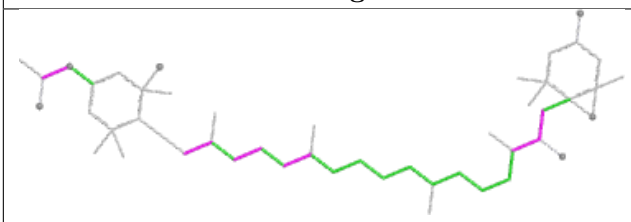
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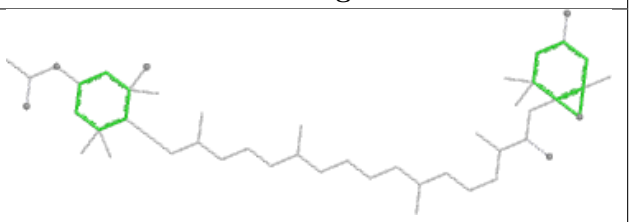
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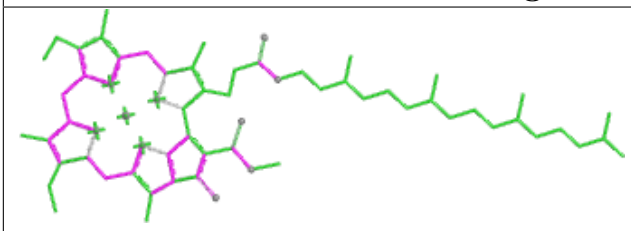


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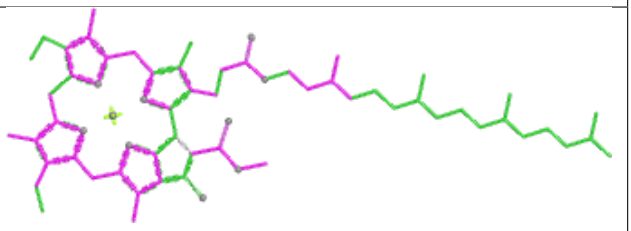


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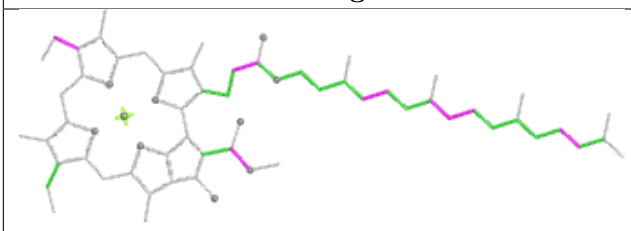
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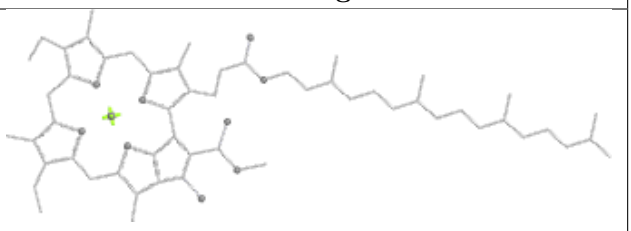
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Bond angles

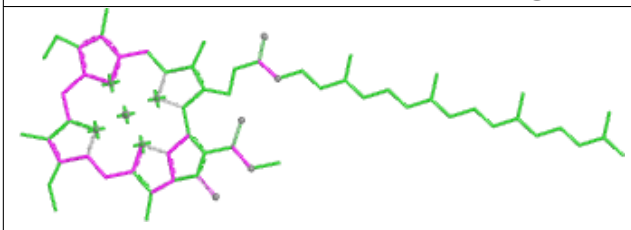


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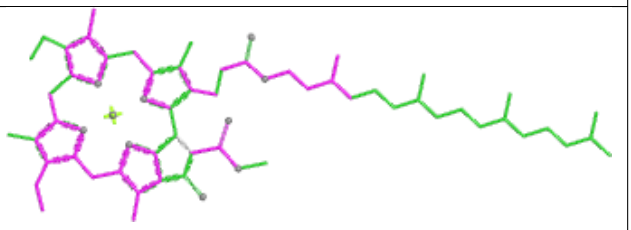


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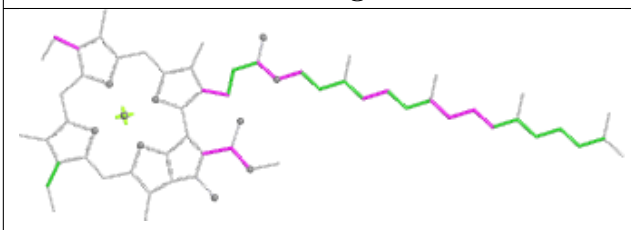
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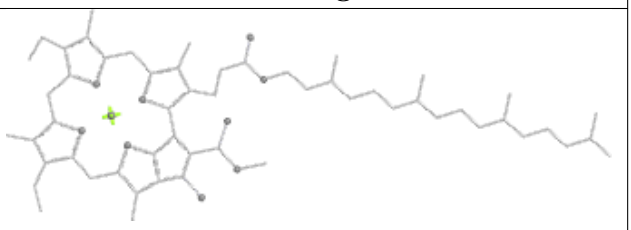
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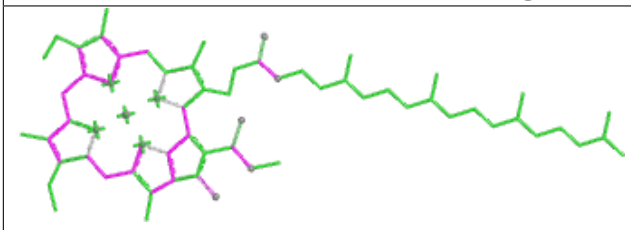
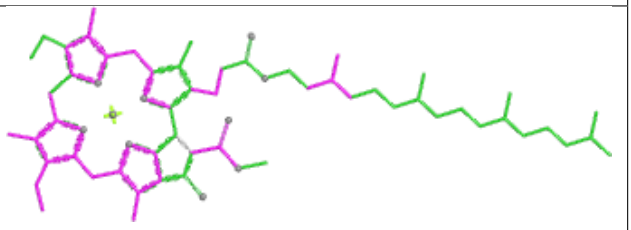
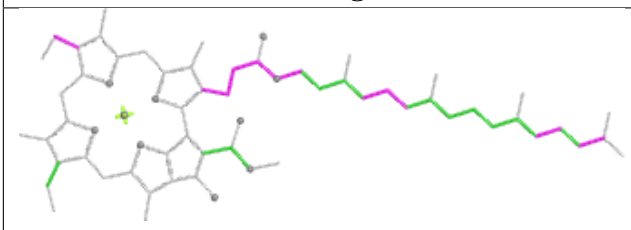
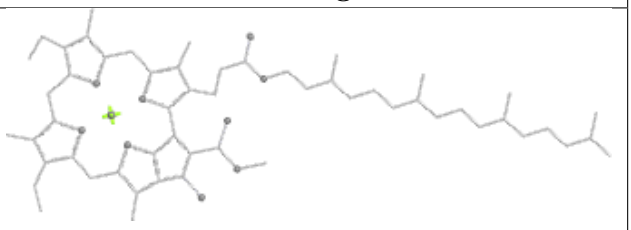
Bond angles

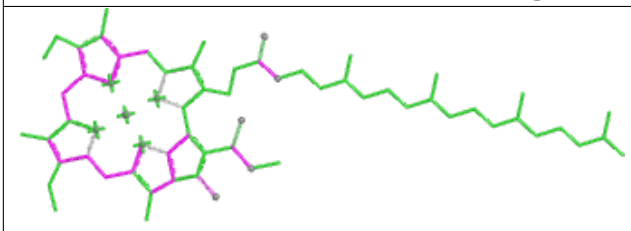
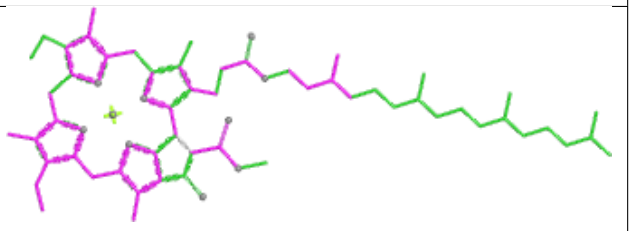
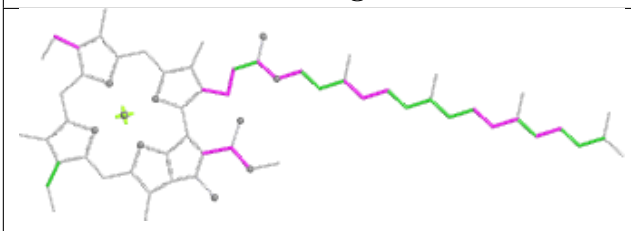
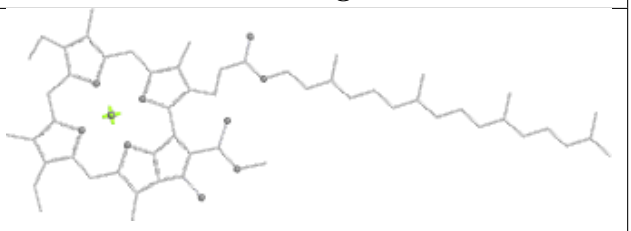


Torsions

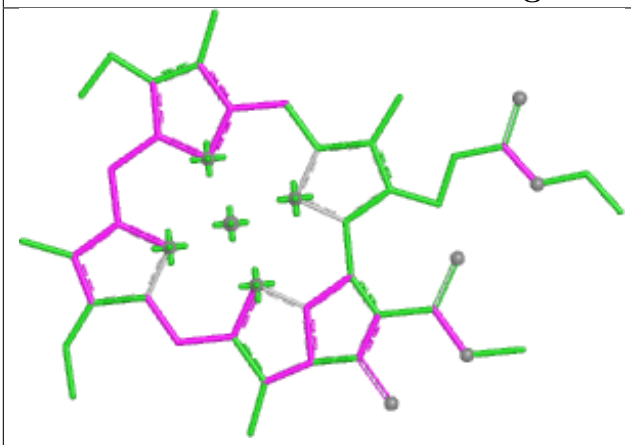


Rings

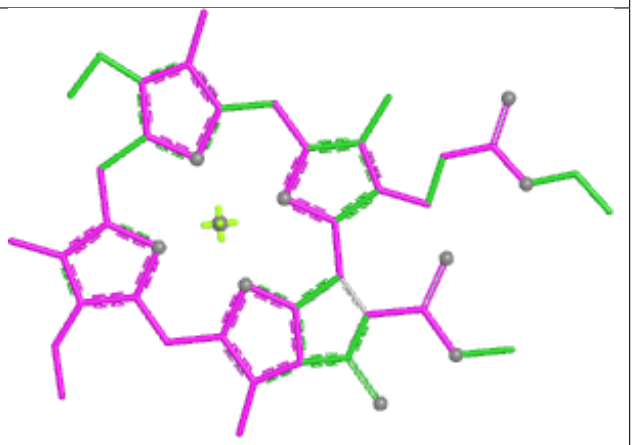
Ligand CLA 16 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

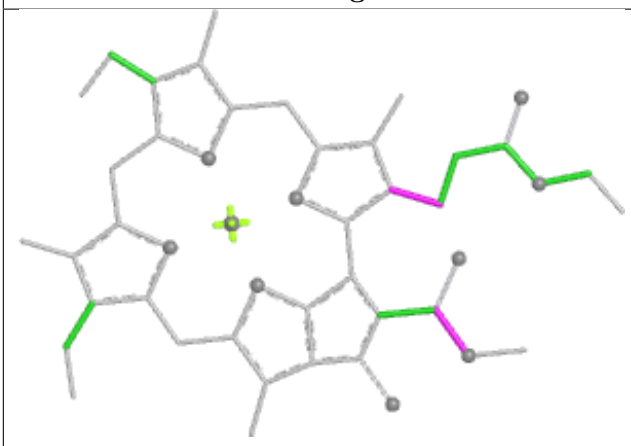
Ligand CLA A 840



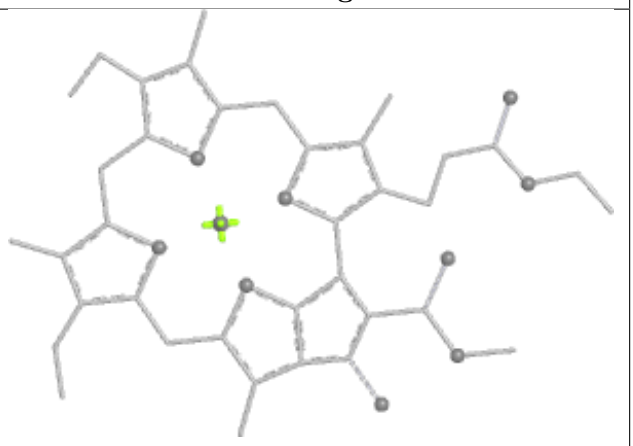
Bond lengths



Bond angles

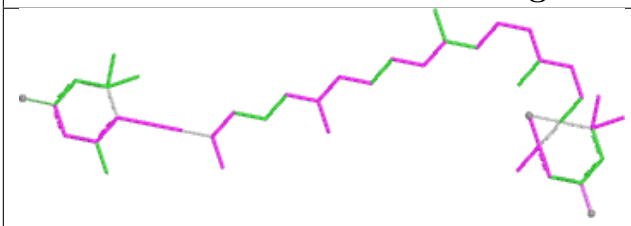


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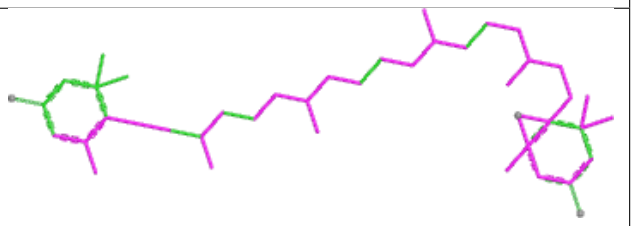


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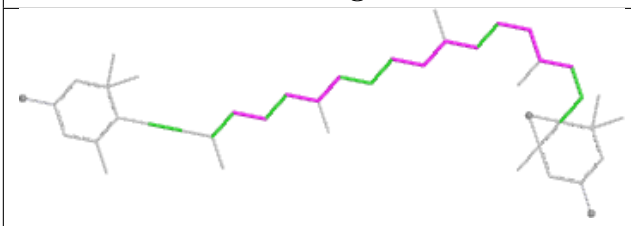
Ligand DD6 7 302



Bond lengths



Bond angles

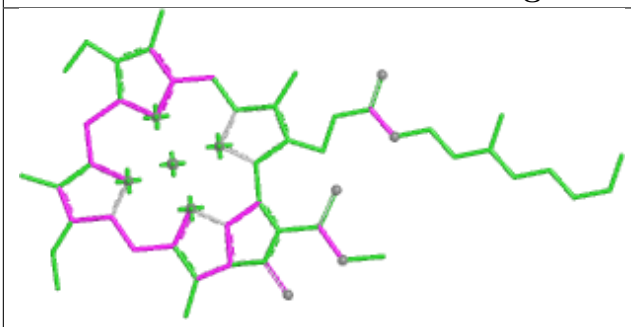


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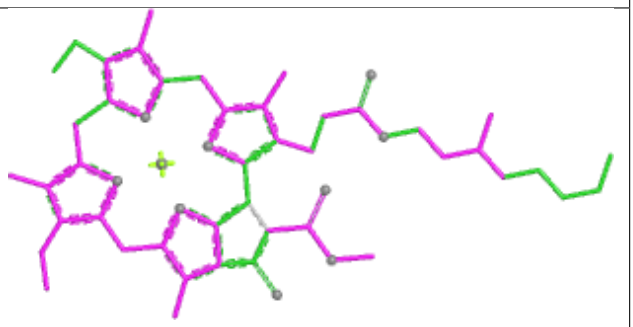


Rings

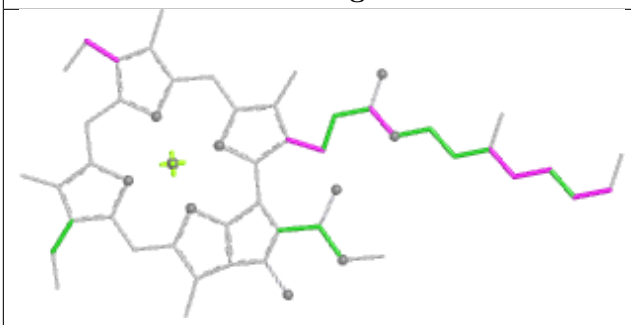
Ligand CLA A 836



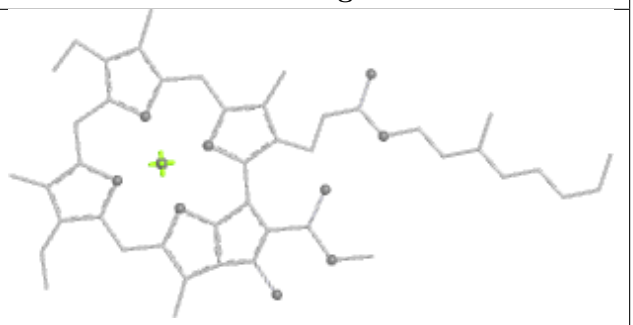
Bond lengths



Bond angles

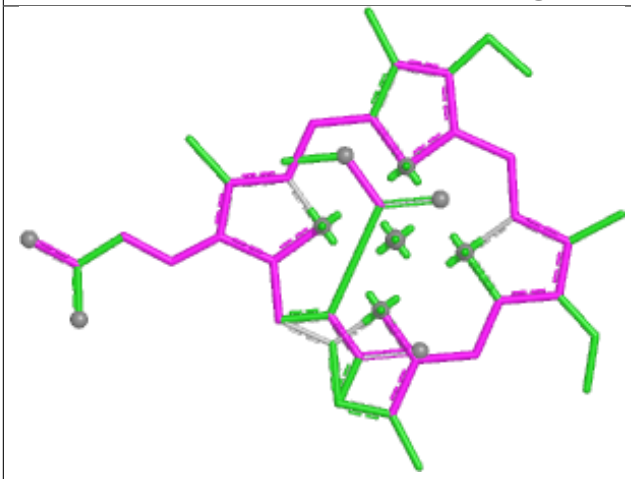


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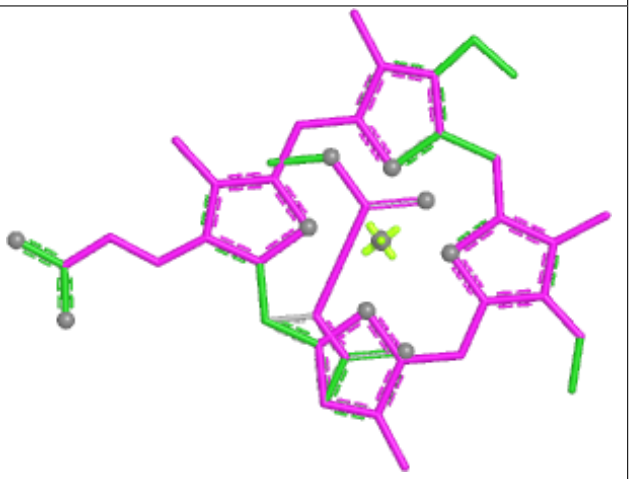


Rings

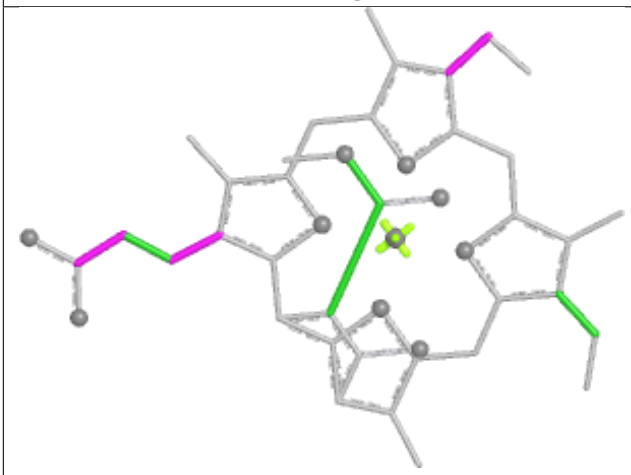
Ligand KC1 8 314



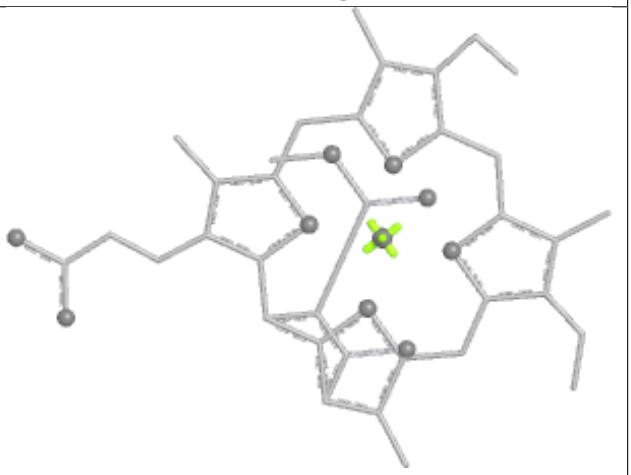
Bond lengths



Bond angles

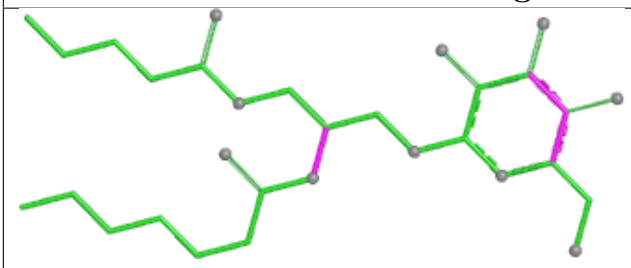


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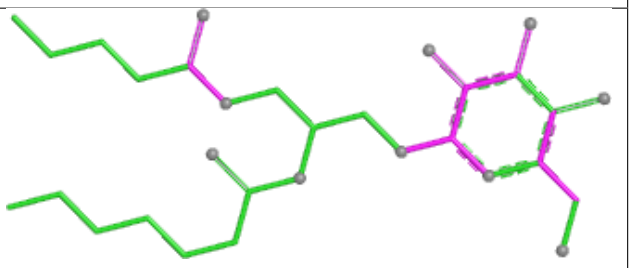


Rings

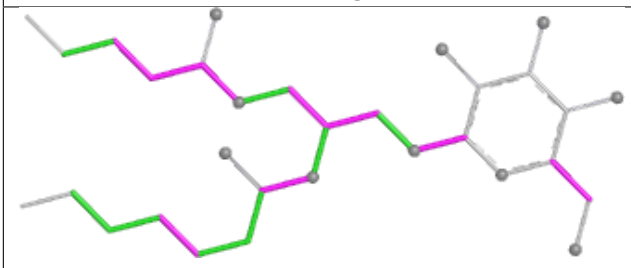
Ligand LMG 2u 204



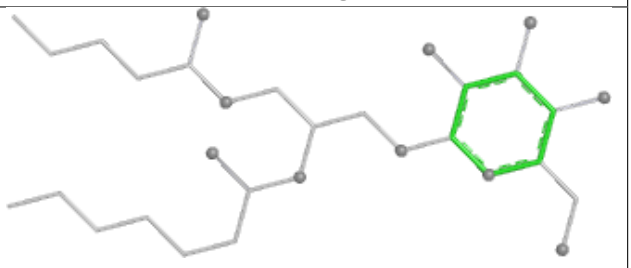
Bond lengths



Bond angles

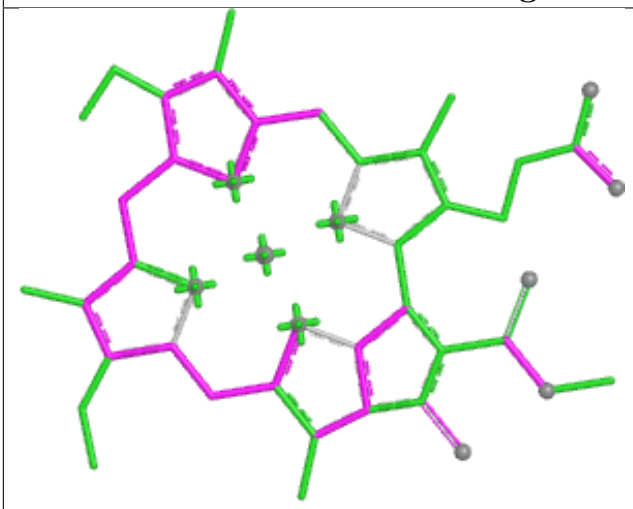


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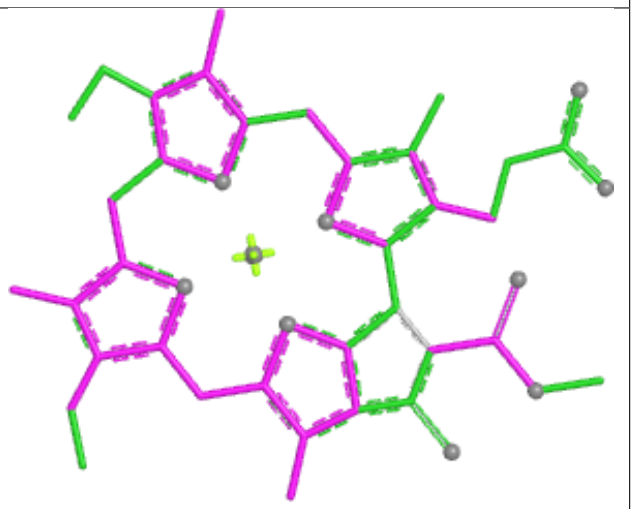


Rings

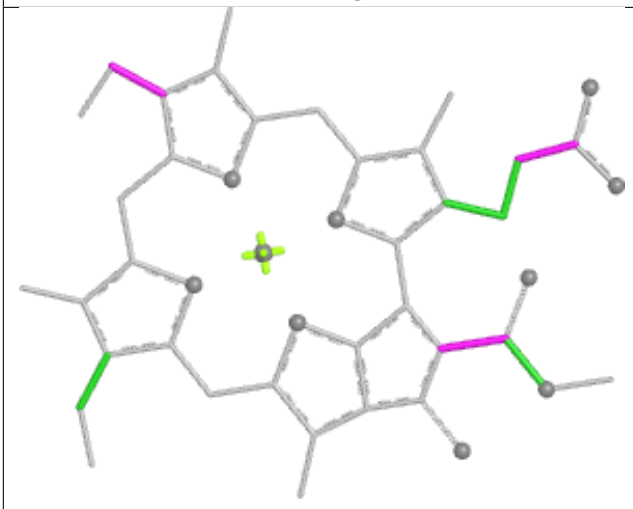
Ligand CLA 14 304



Bond lengths



Bond angles

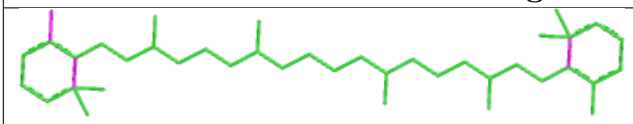


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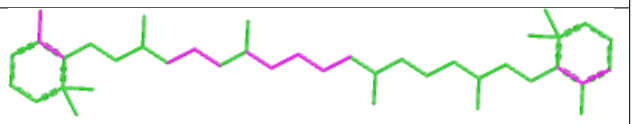


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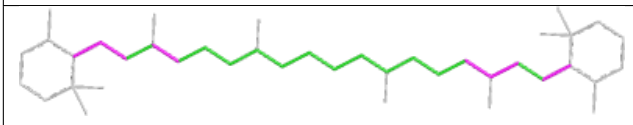
Ligand BCR J 103



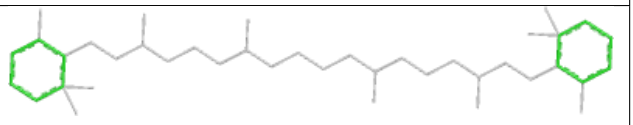
Bond lengths



Bond angles

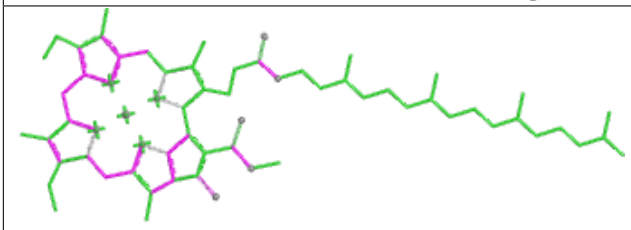


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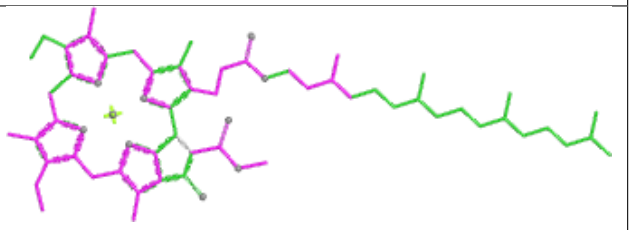


Rings

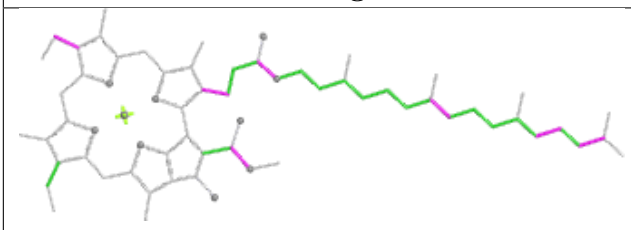
Ligand CLA B 851



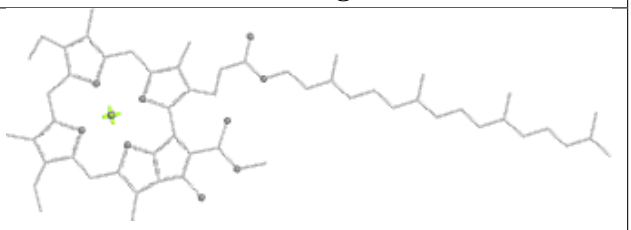
Bond lengths



Bond angles

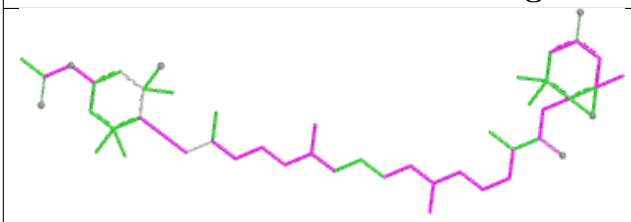


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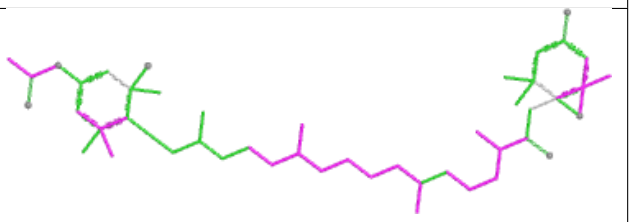


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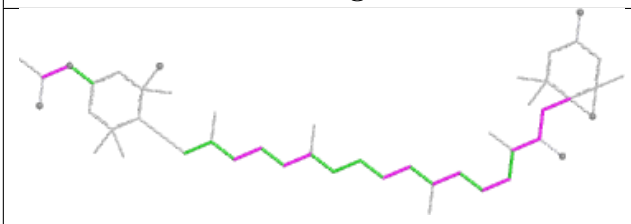
Ligand A86 14 318



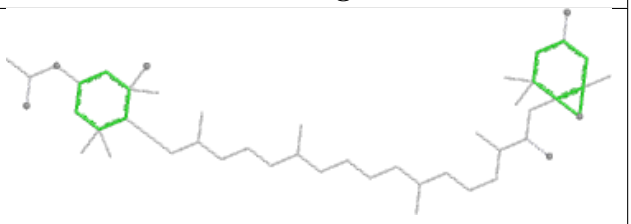
Bond lengths



Bond angles

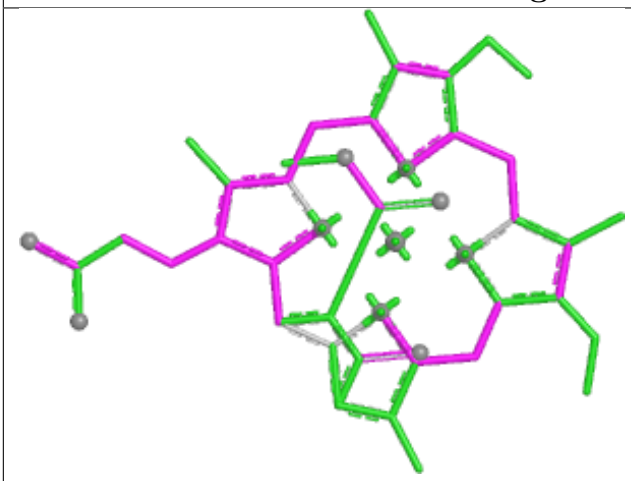


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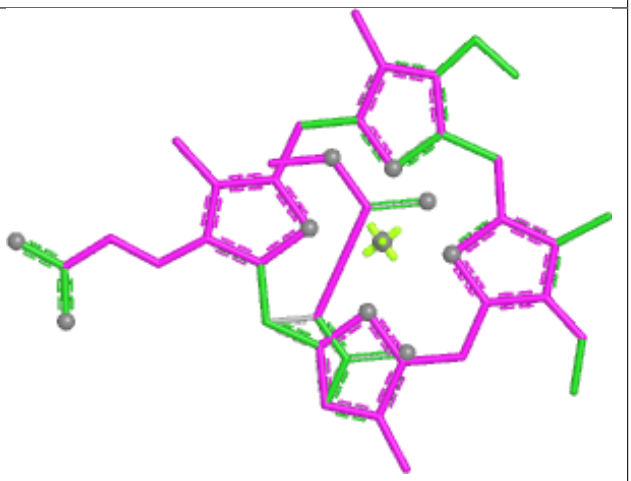


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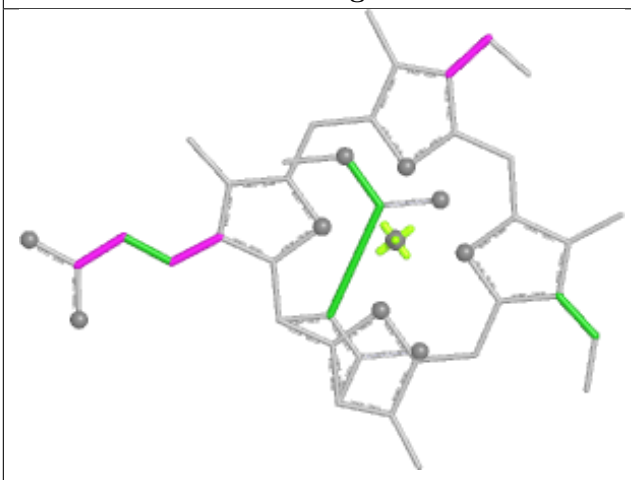
Ligand KC1 8 313



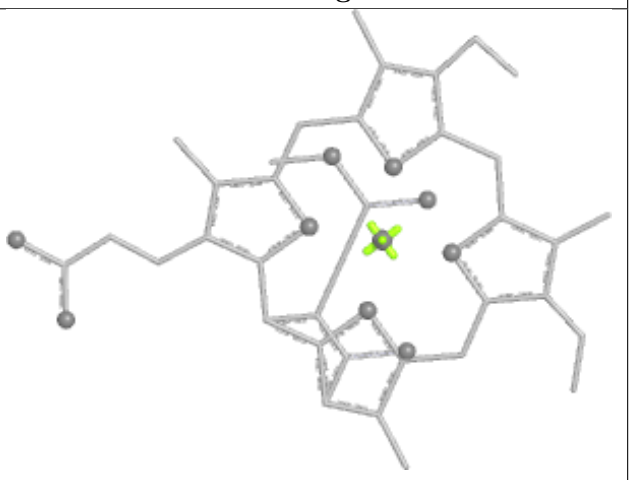
Bond lengths



Bond angles

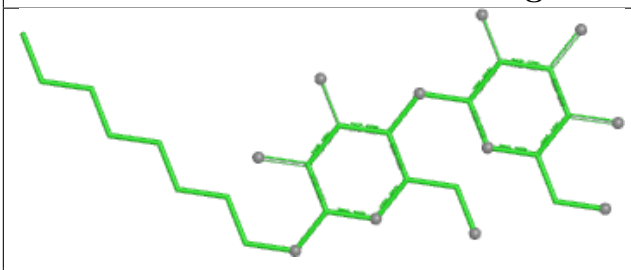


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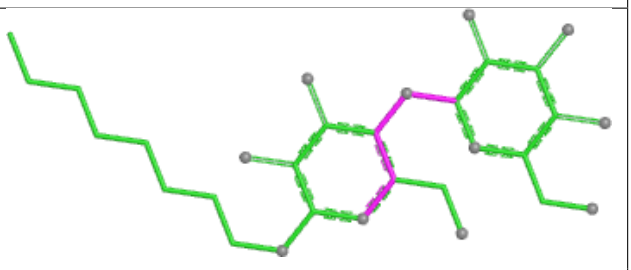


Rings

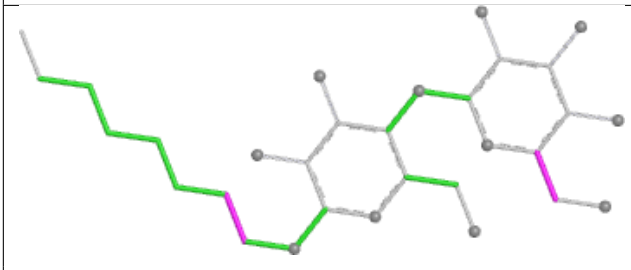
Ligand LMT 6 302



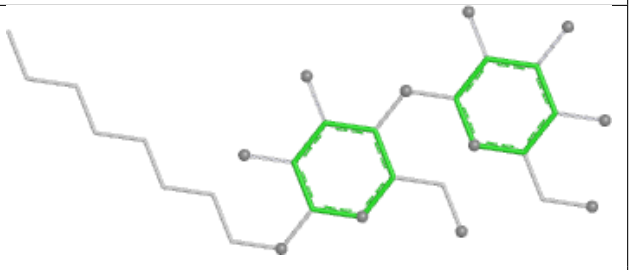
Bond lengths



Bond angles

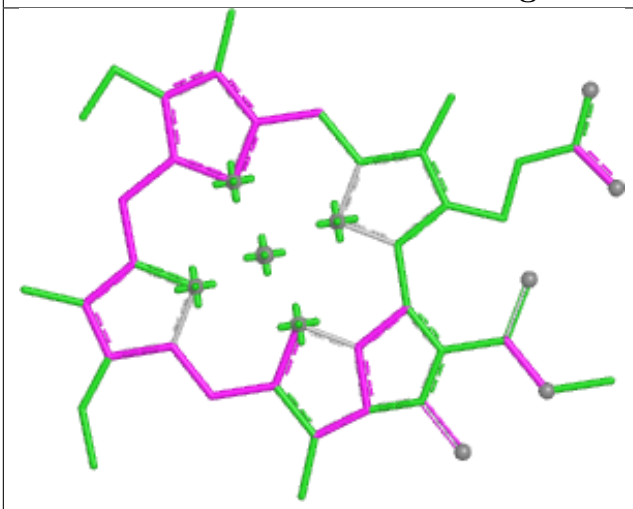


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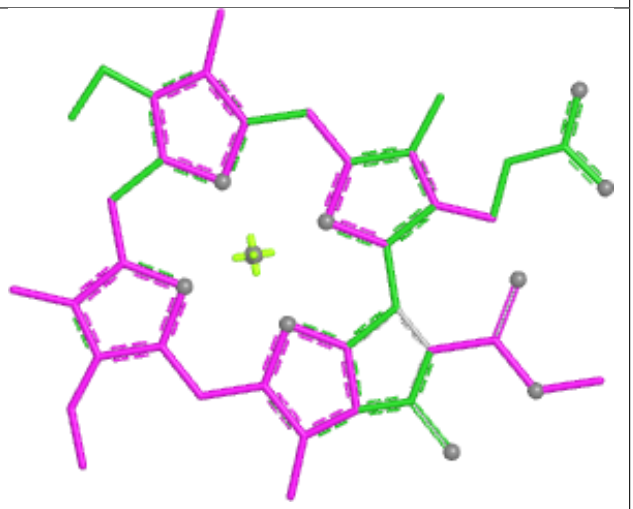


Rings

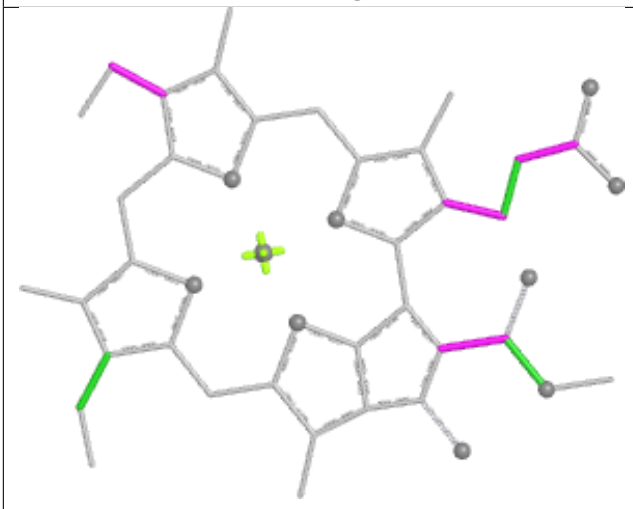
Ligand CLA 13 304



Bond lengths



Bond angles

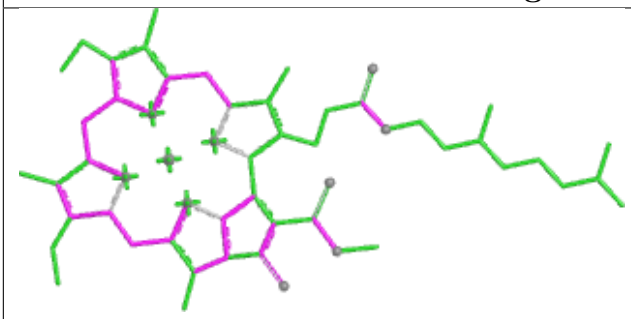


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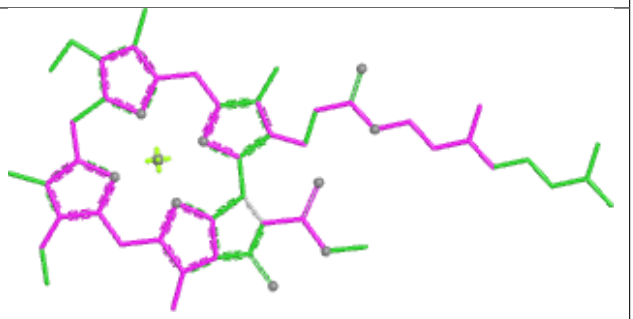


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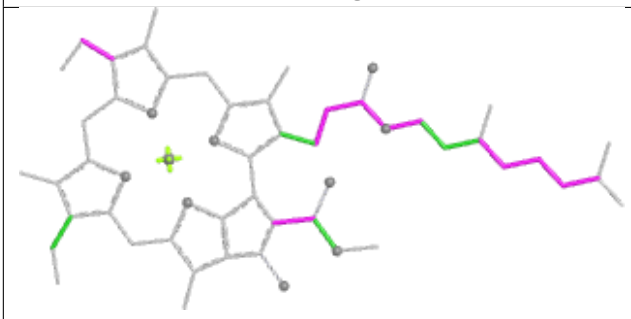
Ligand CLA B 821



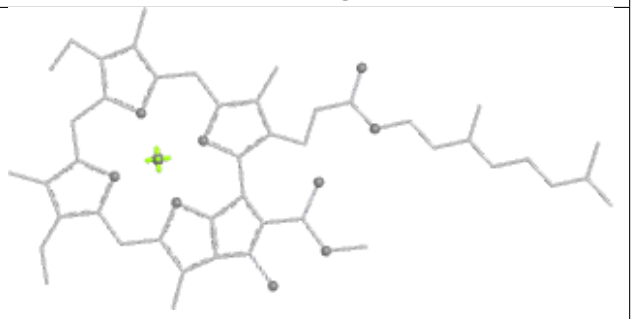
Bond lengths



Bond angles

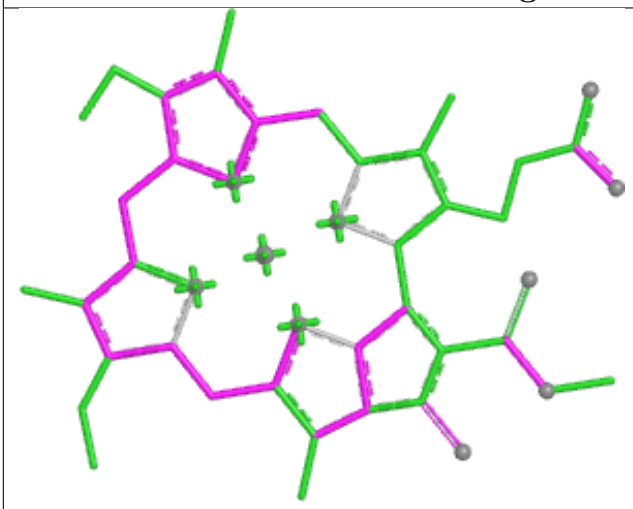


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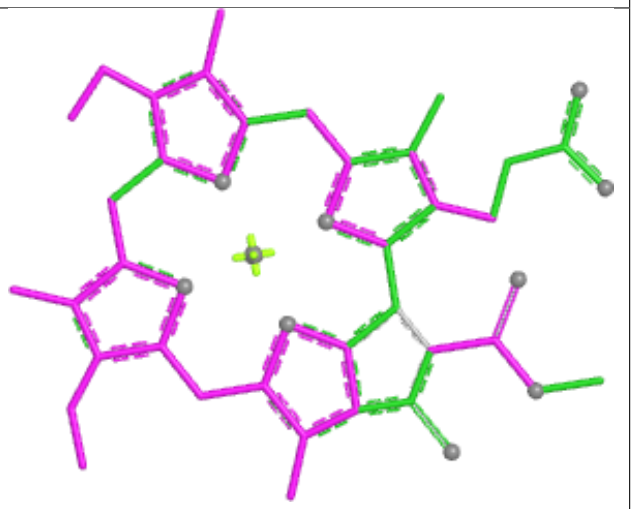


Rings

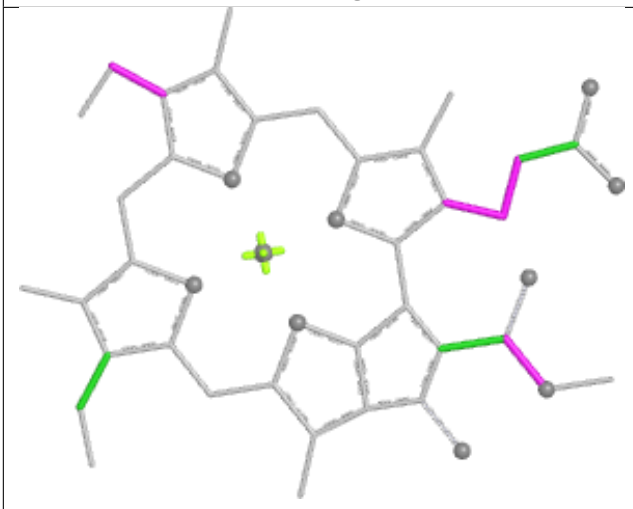
Ligand CLA 15 314



Bond lengths



Bond angles

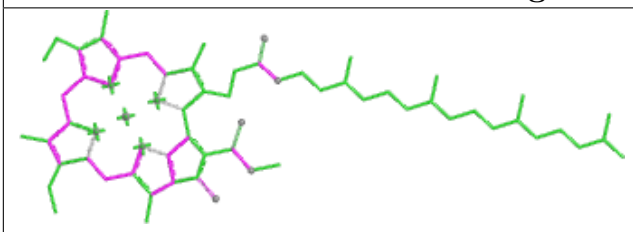


Torsions

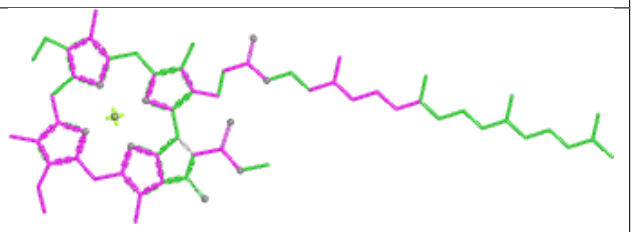


Rings

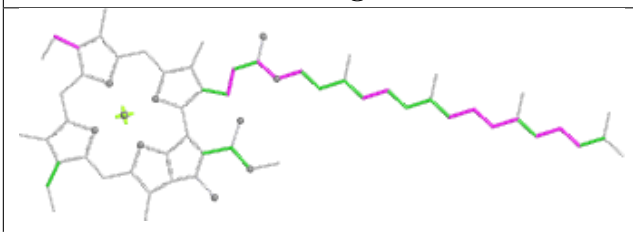
Ligand CLA 7 303



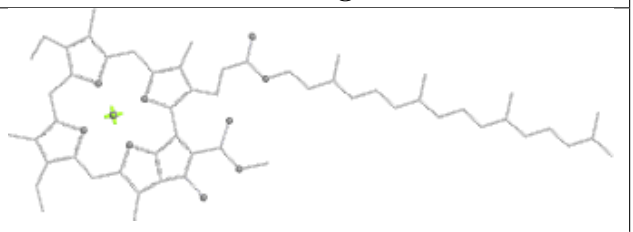
Bond lengths



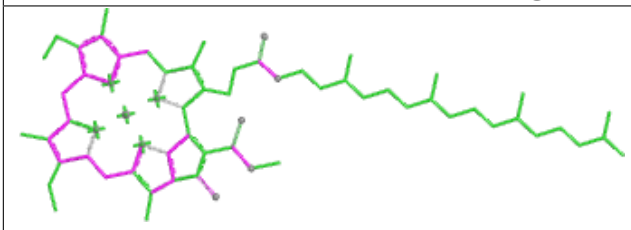
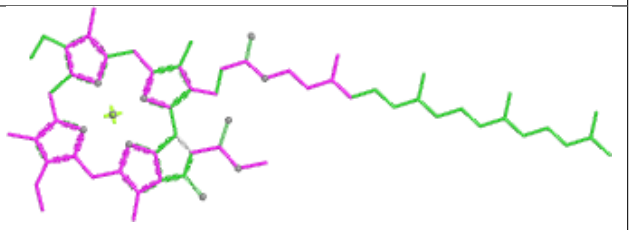
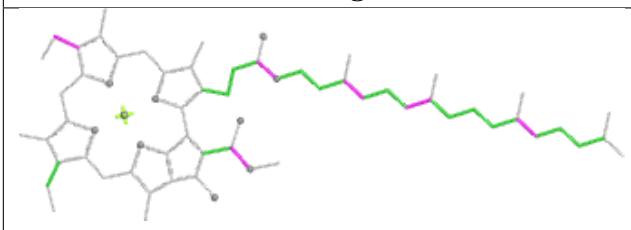
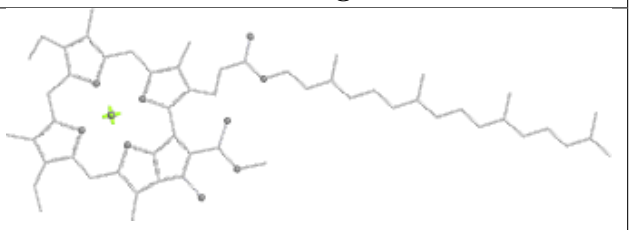
Bond angles

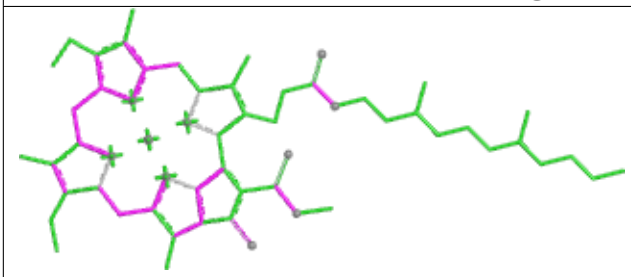
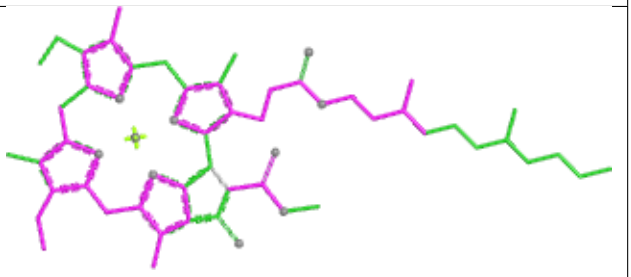
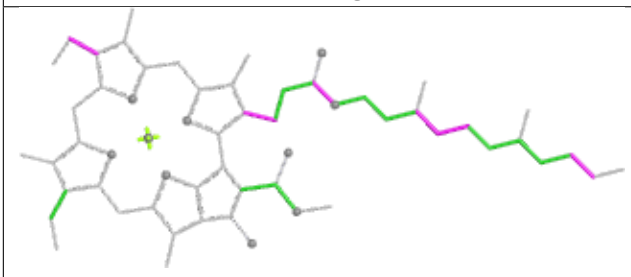
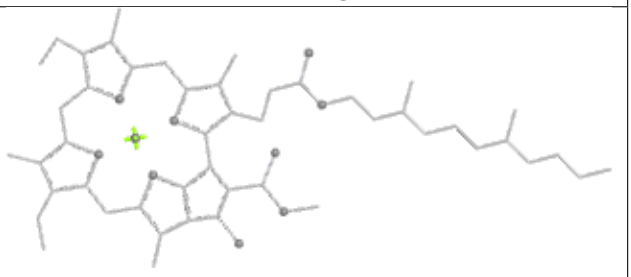


Torsions

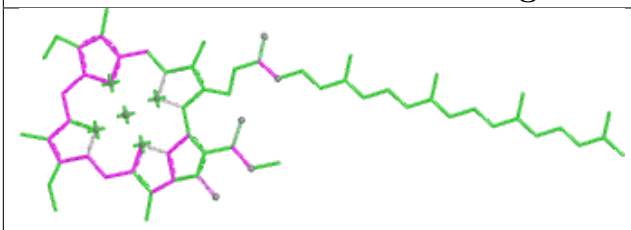


Rings

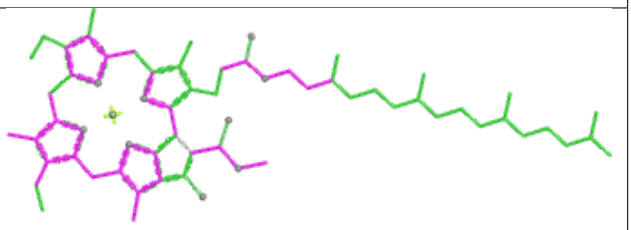
Ligand CLA 2 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

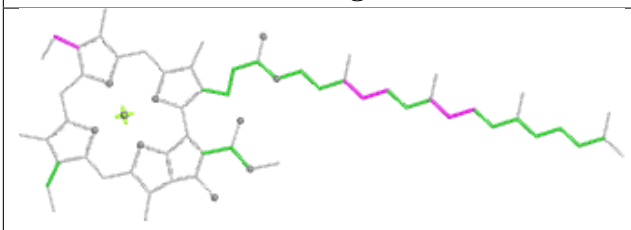
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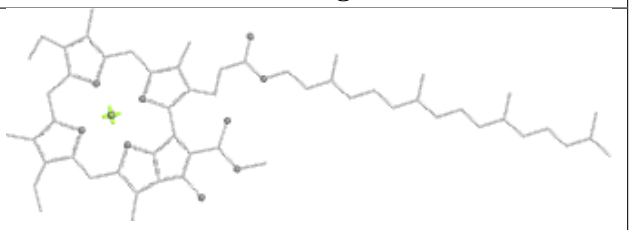
Bond lengths



Bond angles

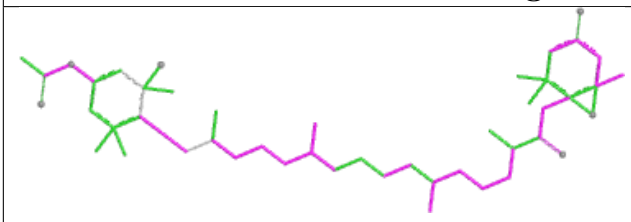


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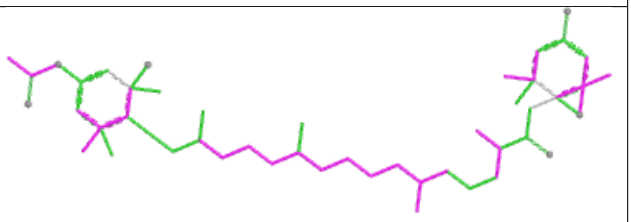


Rings

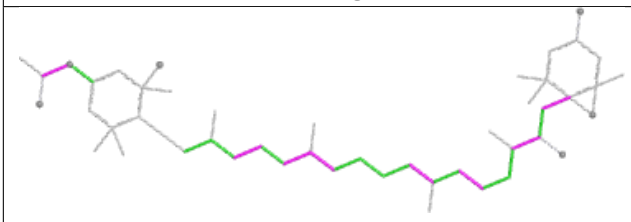
Ligand A86 11 301



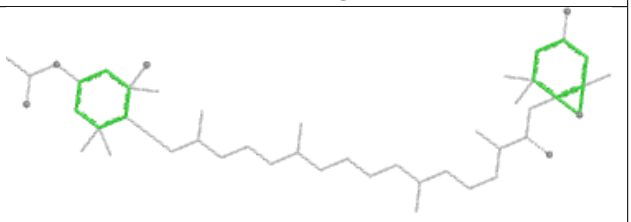
Bond lengths



Bond angles

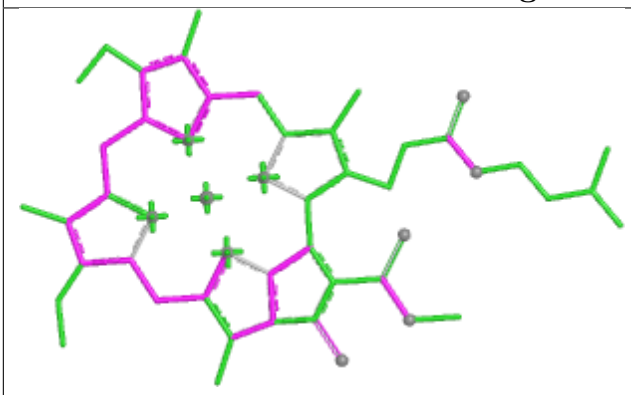


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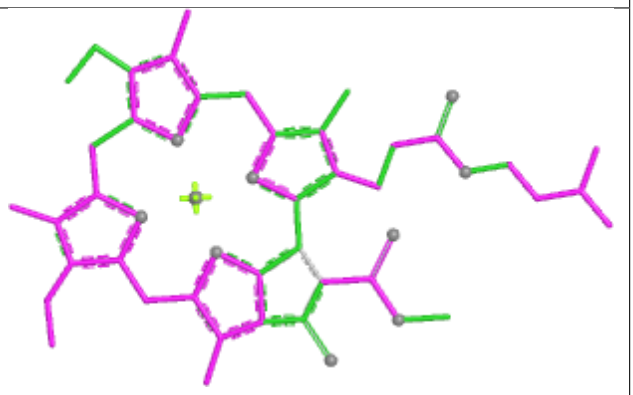


Rings

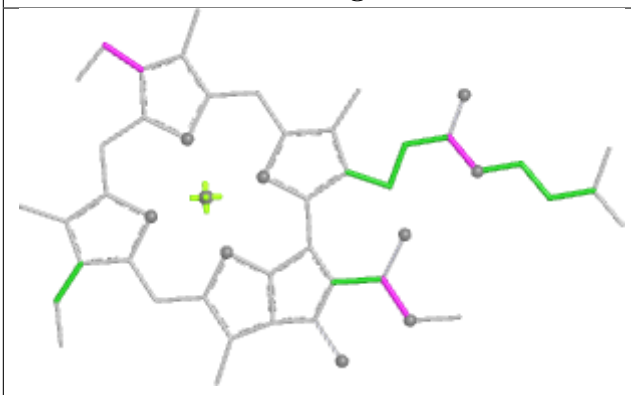
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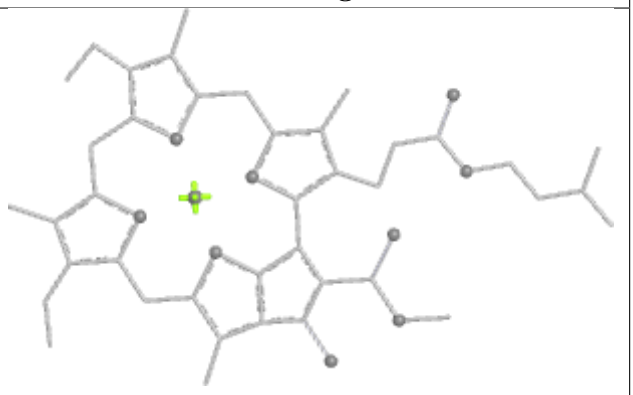
Bond lengths



Bond angles

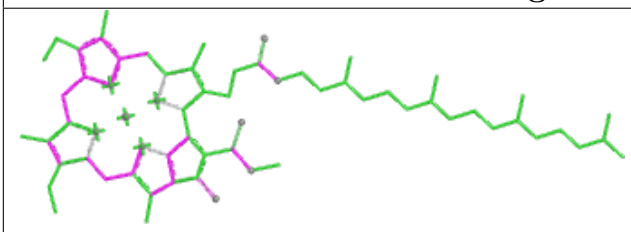


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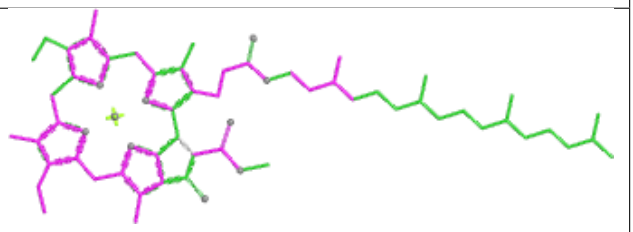


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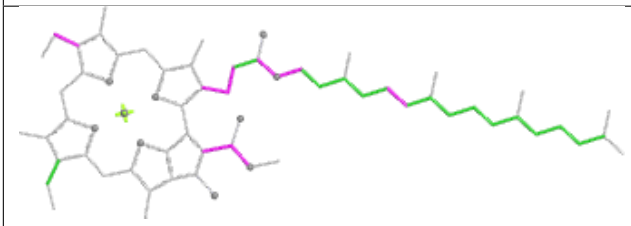
Ligand CLA 4 306



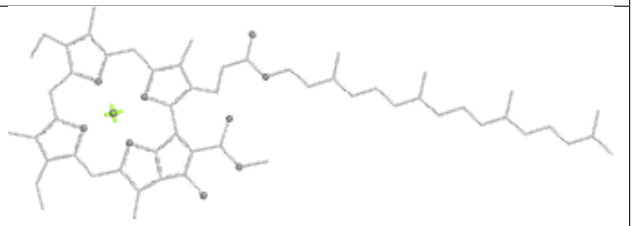
Bond lengths



Bond angles

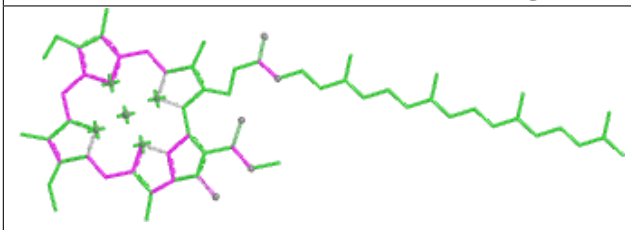


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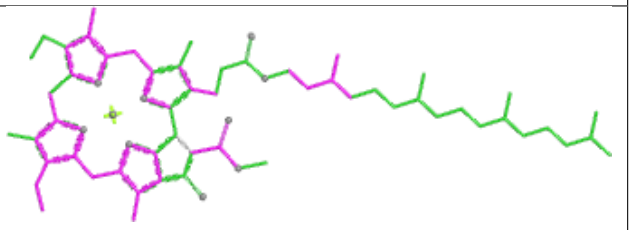


Rings

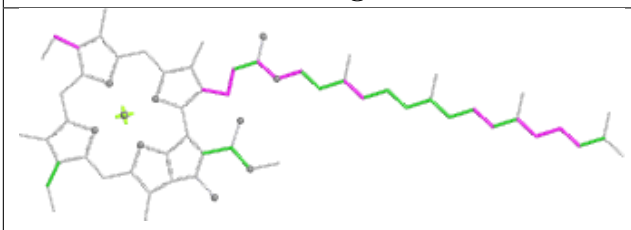
Ligand CLA B 829



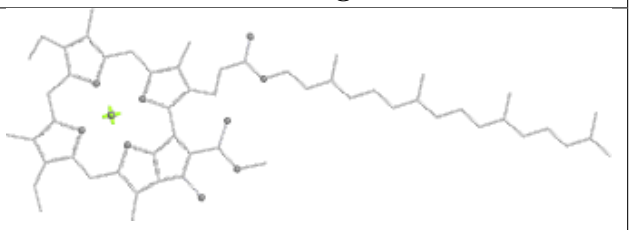
Bond lengths



Bond angles

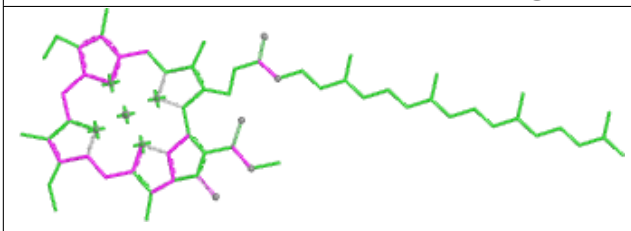


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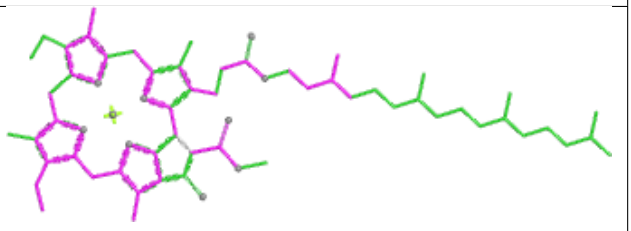


Rings

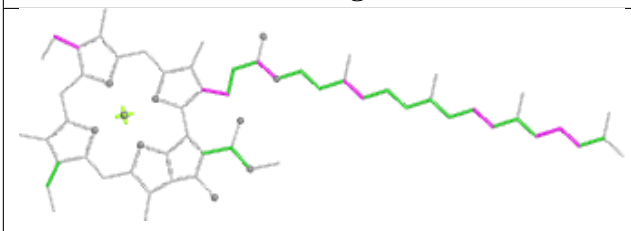
Ligand CLA 1 305



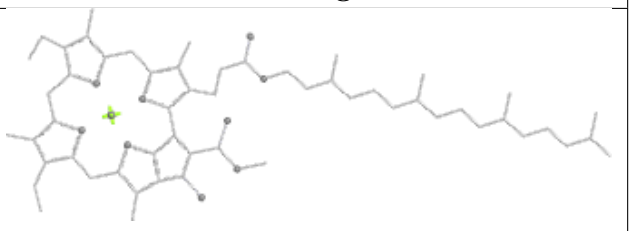
Bond lengths



Bond angles

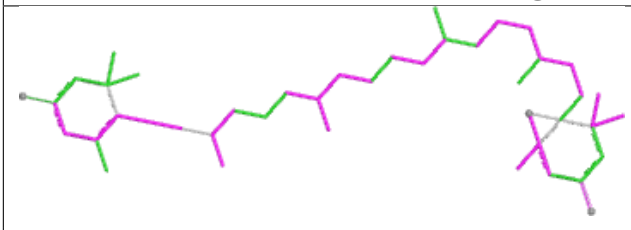


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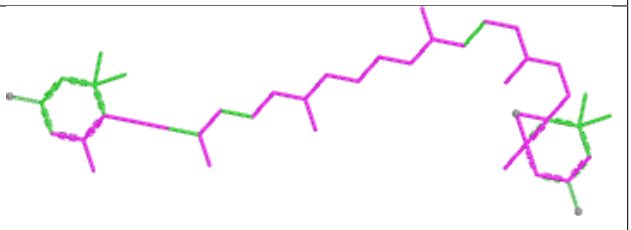


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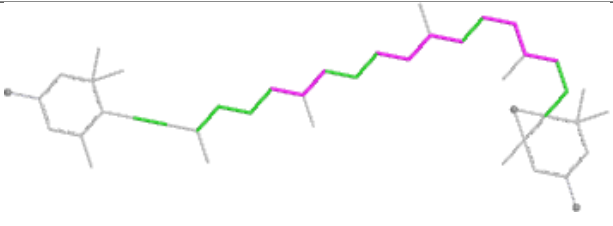
Ligand DD6 6 303



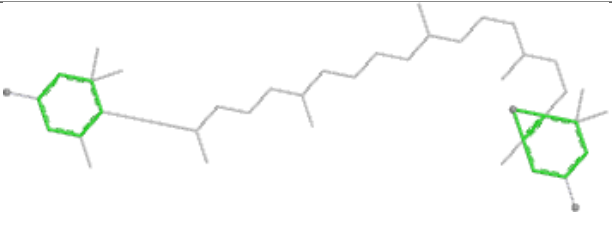
Bond lengths



Bond angles

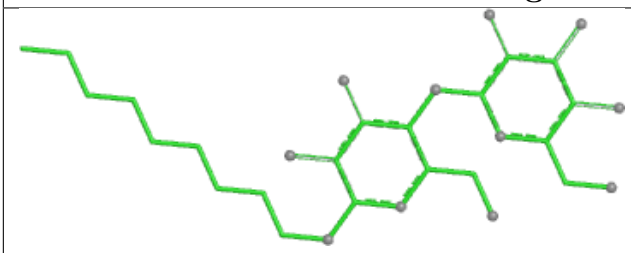


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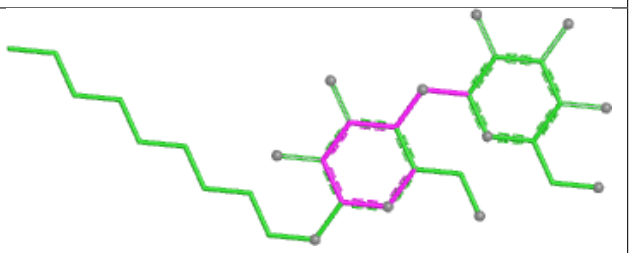


Rings

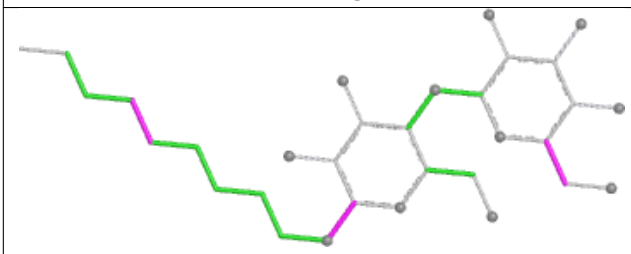
Ligand LMT 9 317



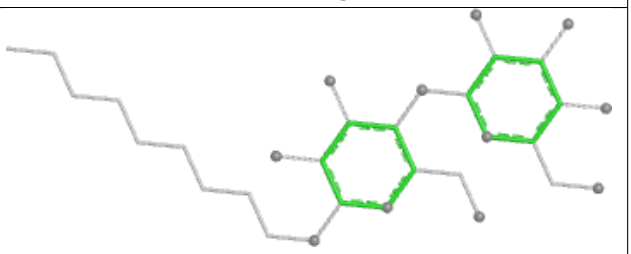
Bond lengths



Bond angles

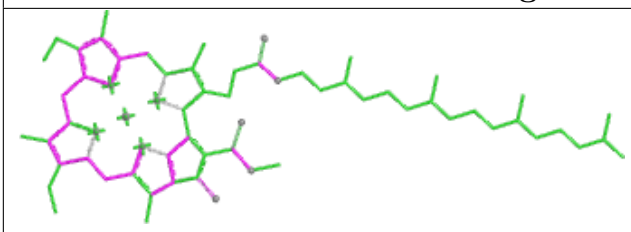


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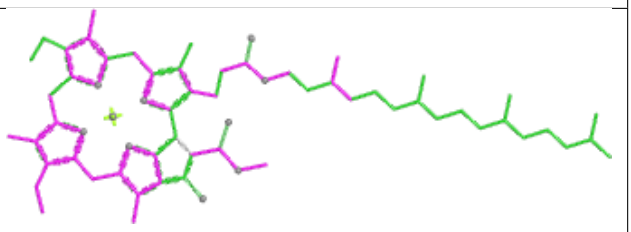


Rings

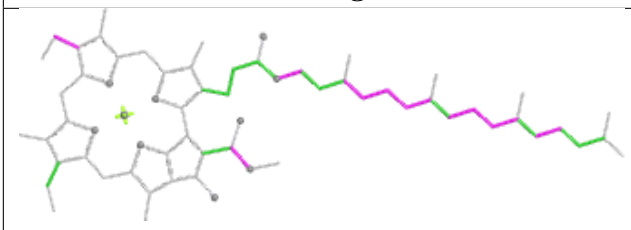
Ligand CLA 13 302



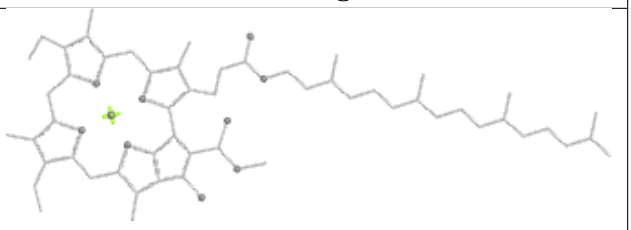
Bond lengths



Bond angles

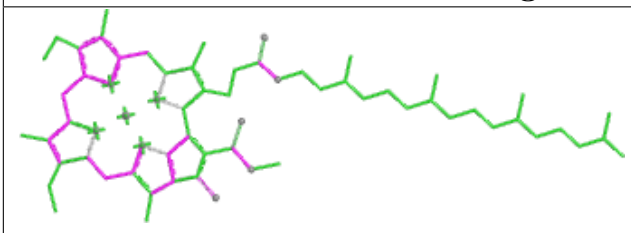


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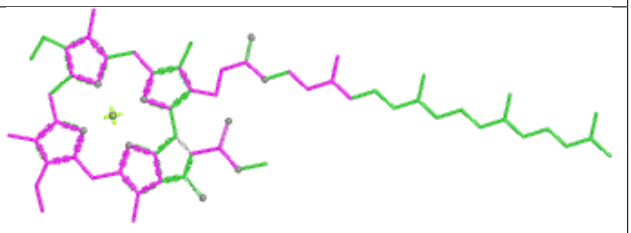


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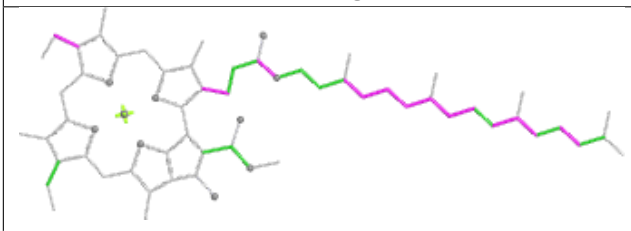
Ligand CLA 16 303



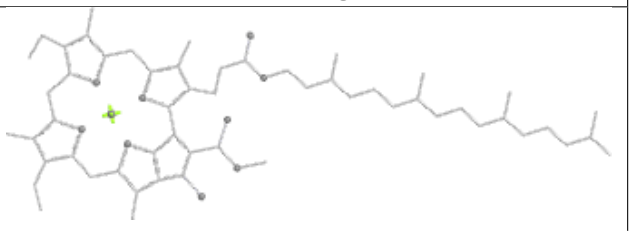
Bond lengths



Bond angles

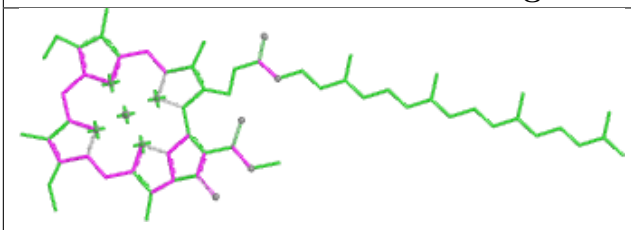


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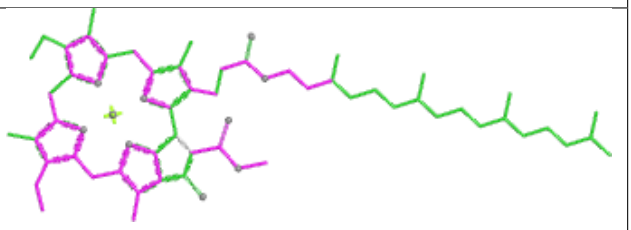


Rings

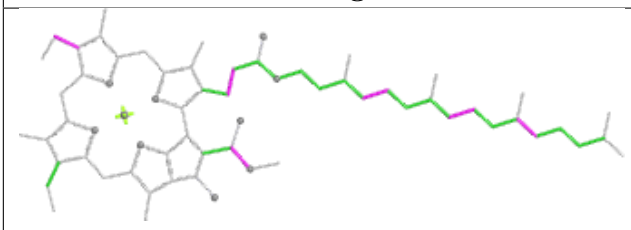
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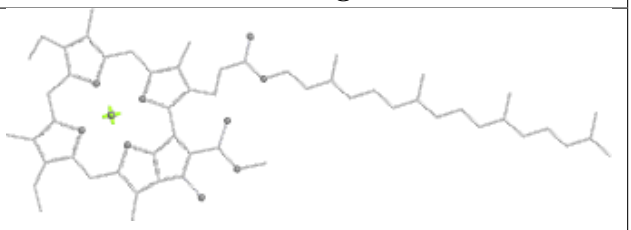
Bond lengths



Bond angles

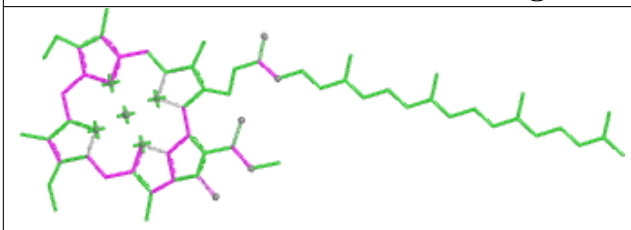


Torsions

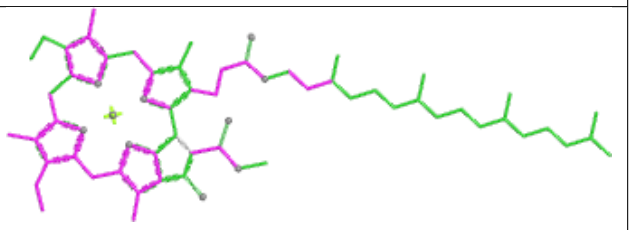


Rings

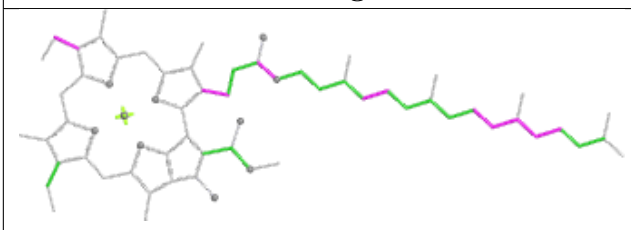
Ligand CLA 4 302



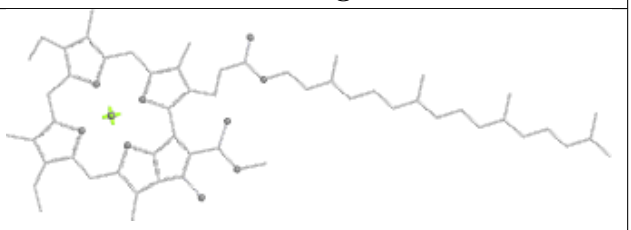
Bond lengths



Bond angles

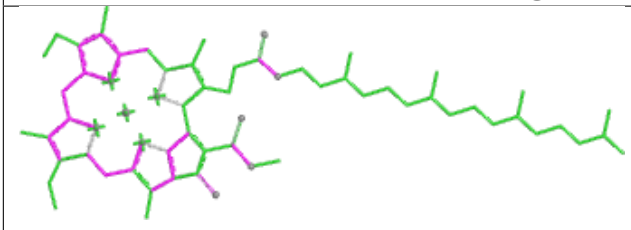


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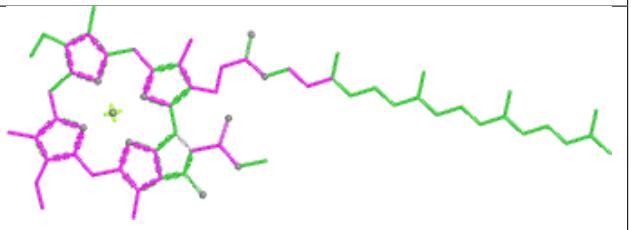


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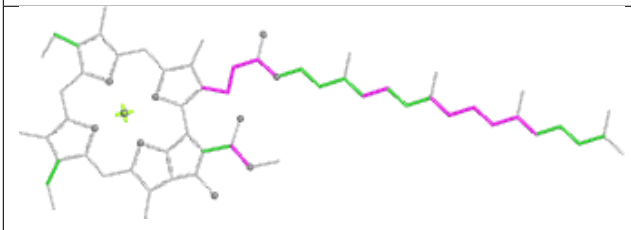
Ligand CLA 8 301



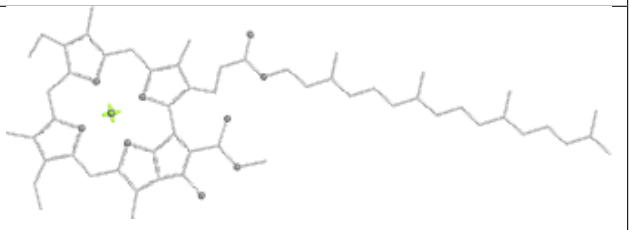
Bond lengths



Bond angles

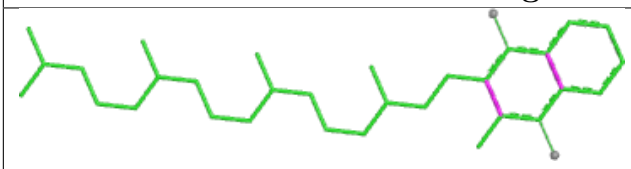


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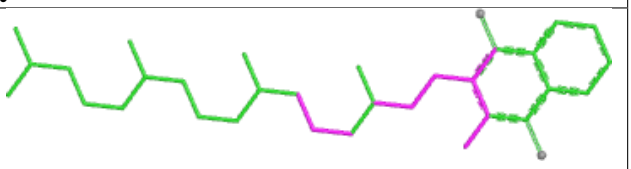


Rings

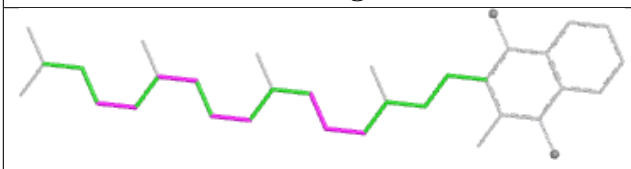
Ligand PQN B 840



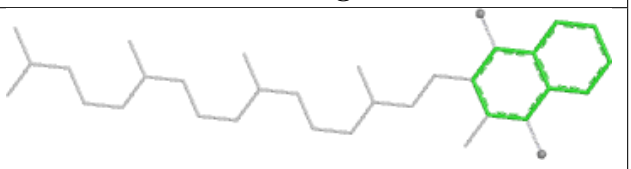
Bond lengths



Bond angles

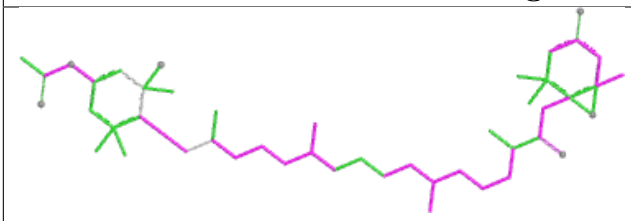


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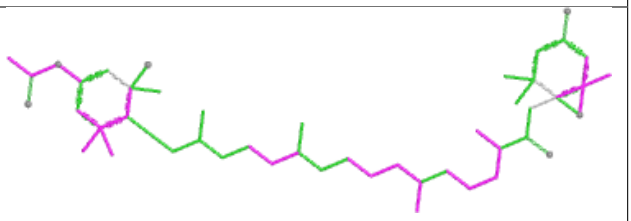


Rings

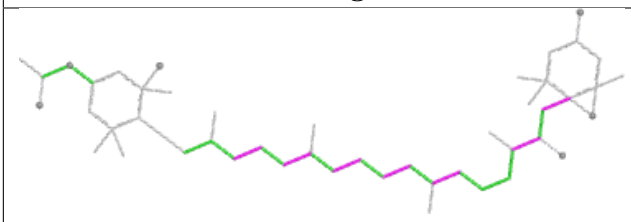
Ligand A86 14 319



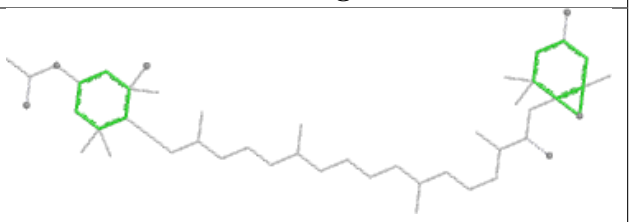
Bond lengths



Bond angles

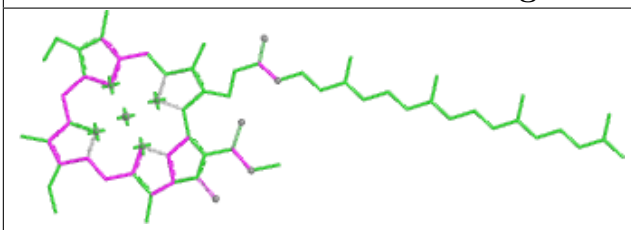


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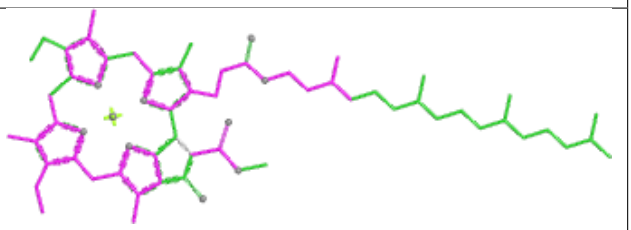


Rings

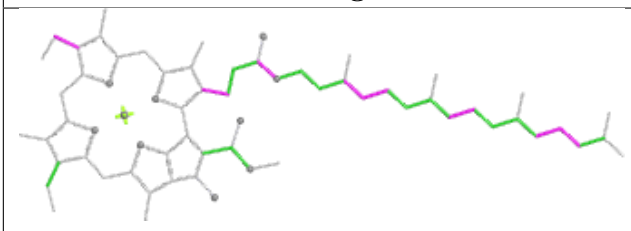
Ligand CLA 10 305



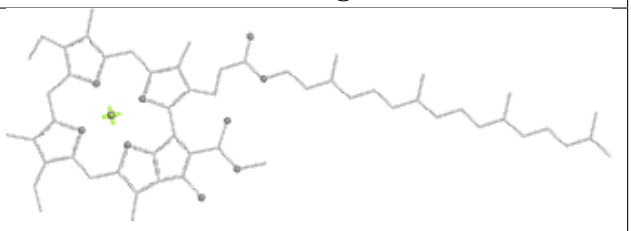
Bond lengths



Bond angles

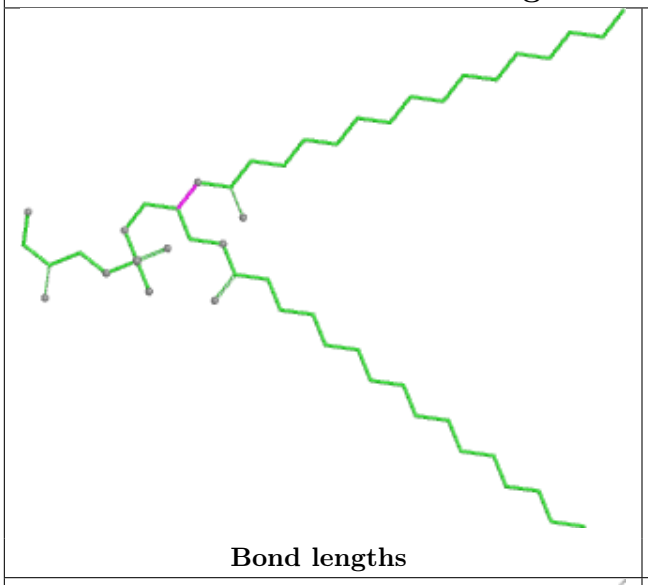


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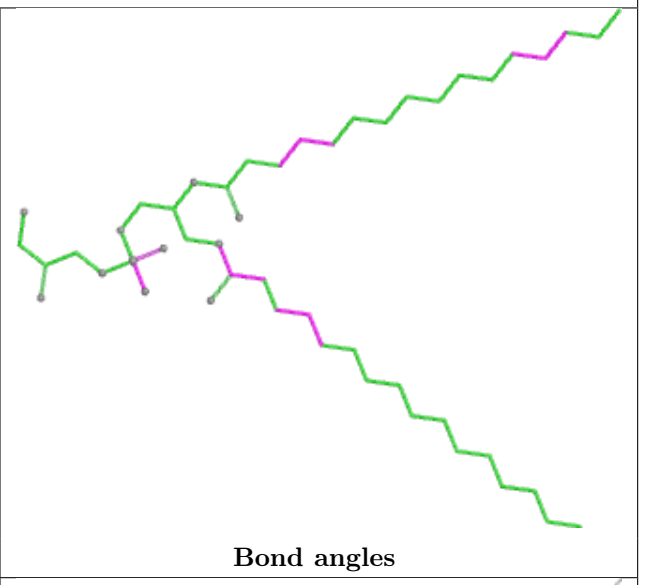


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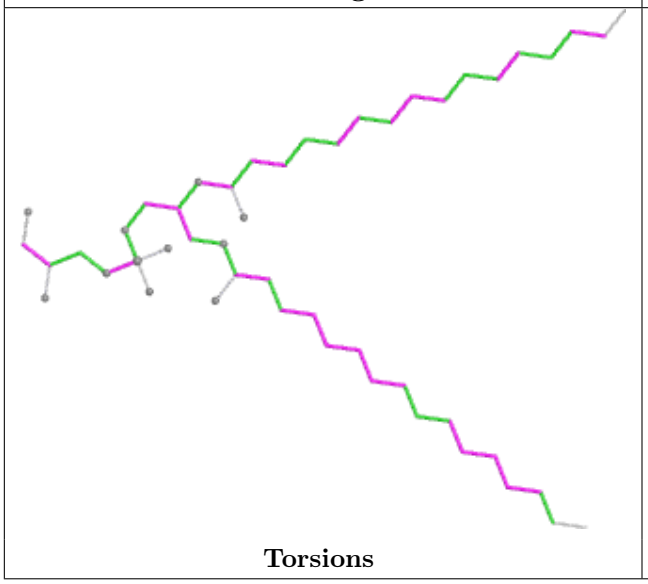
Ligand LHG A 852



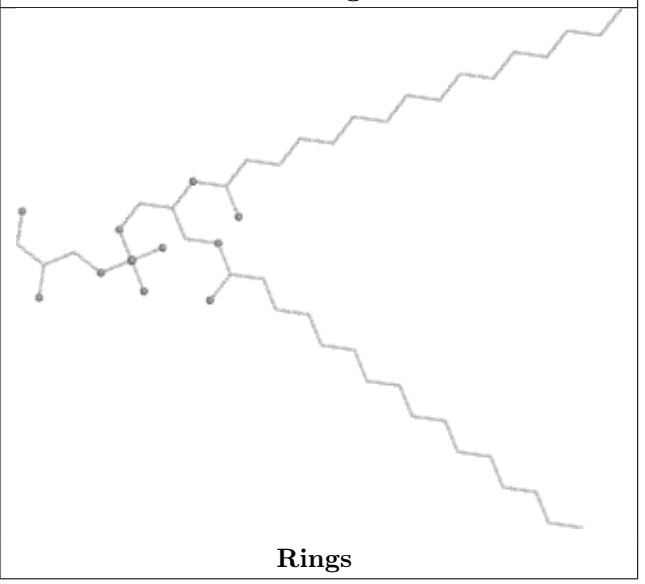
Bond lengths



Bond angles

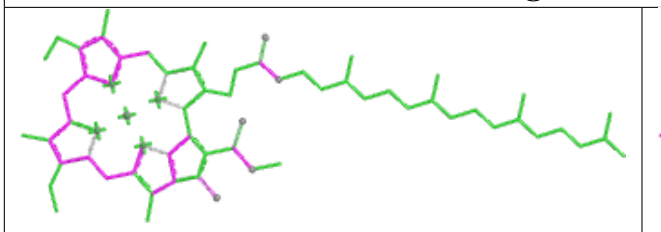


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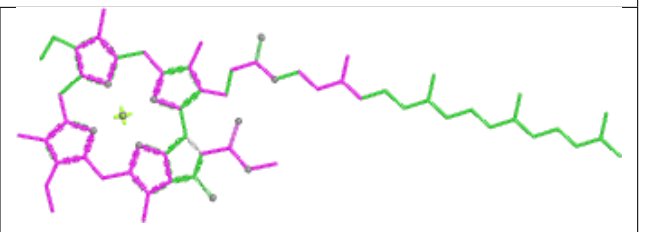


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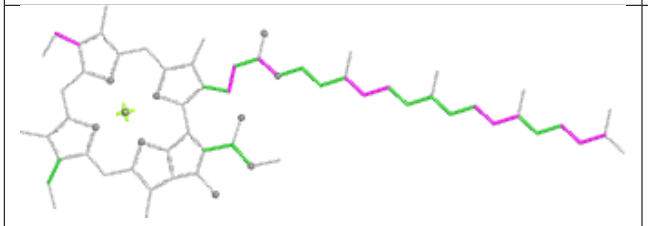
Ligand CLA A 844



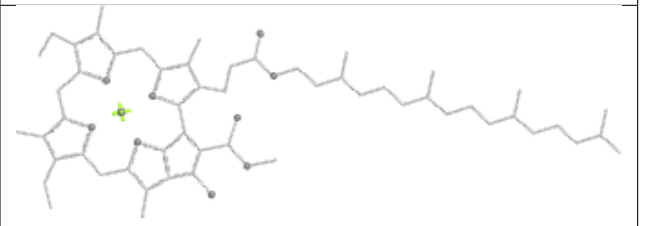
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Bond angles

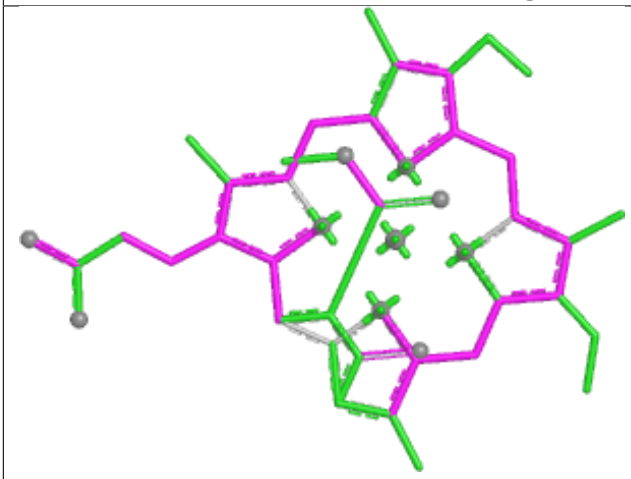


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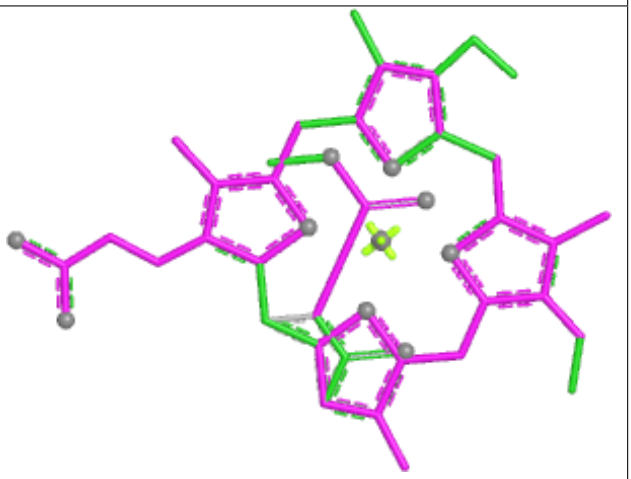


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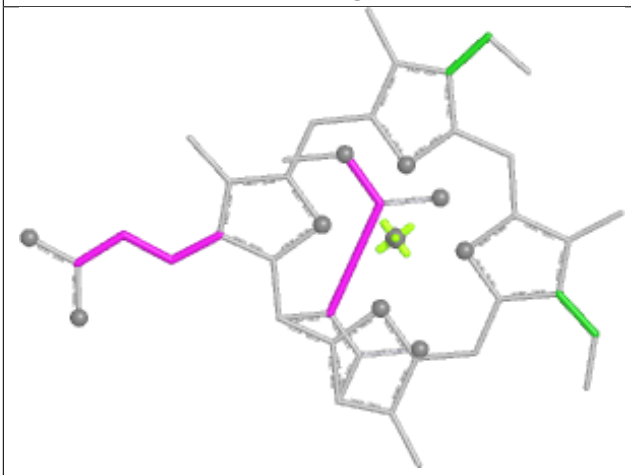
Ligand KC1 13 306



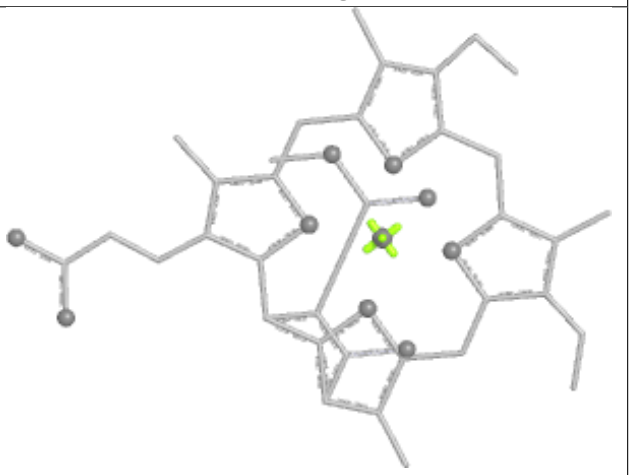
Bond lengths



Bond angles

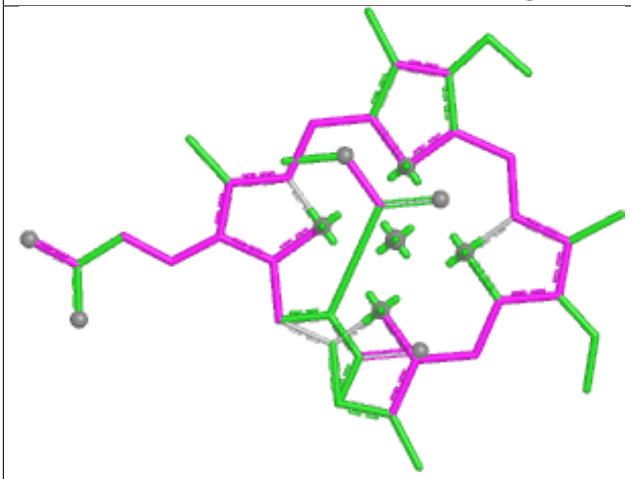


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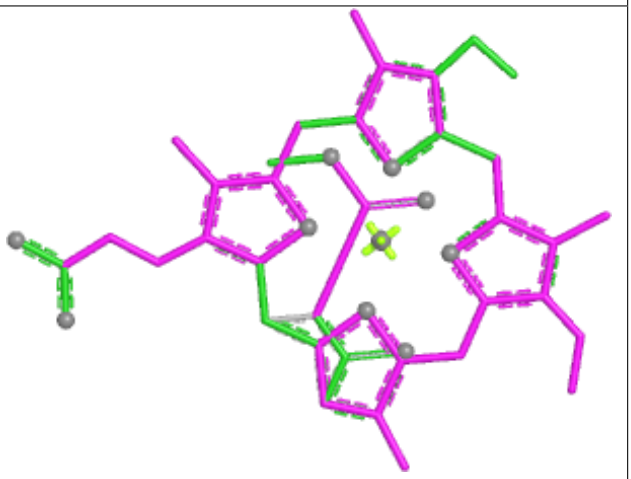


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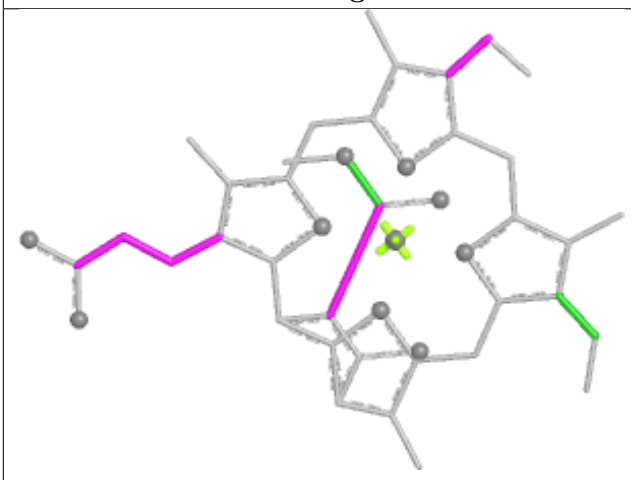
Ligand KC1 11 305



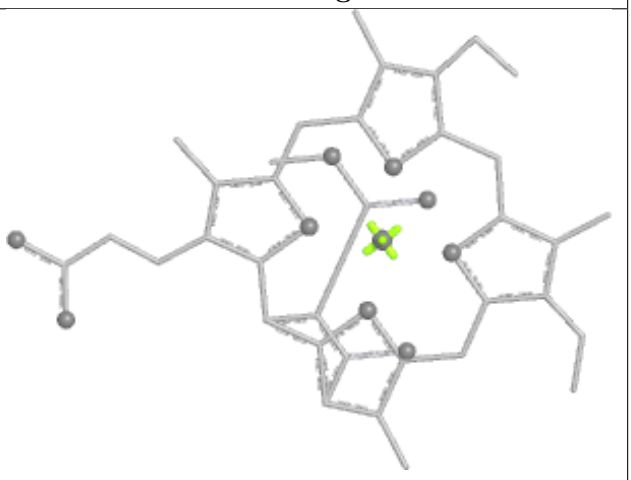
Bond lengths



Bond angles

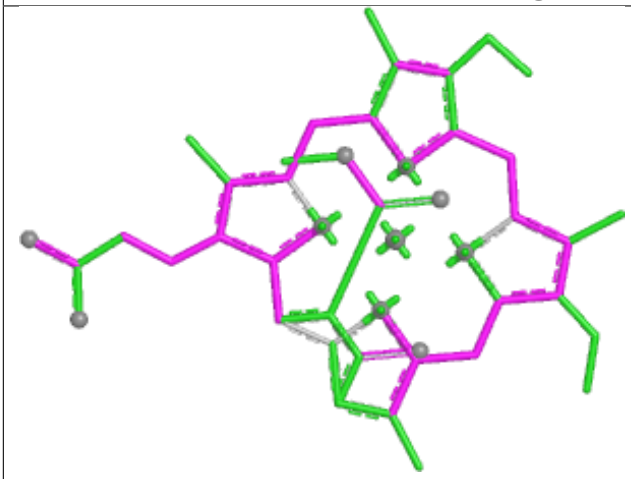


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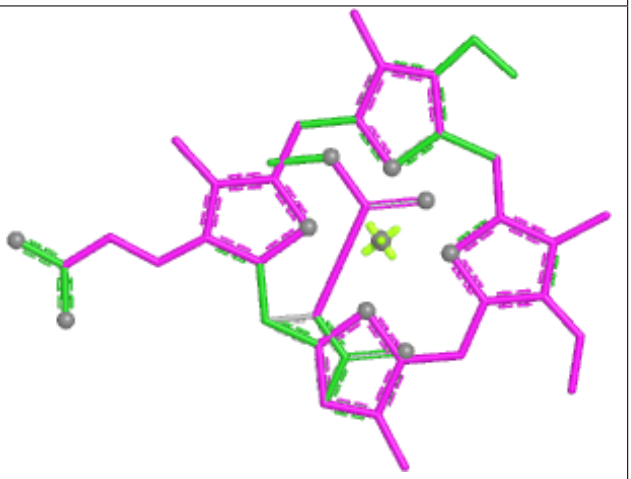


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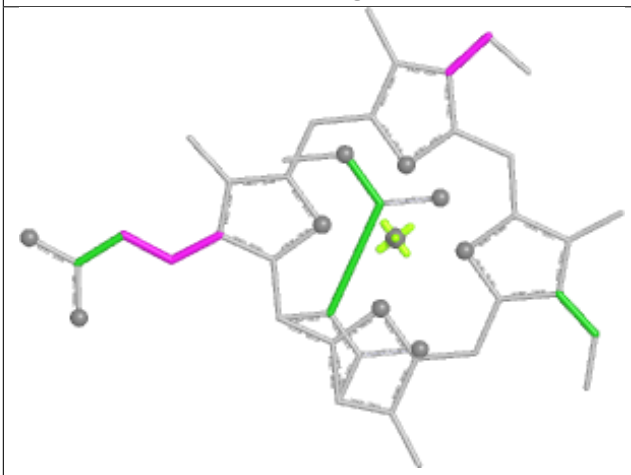
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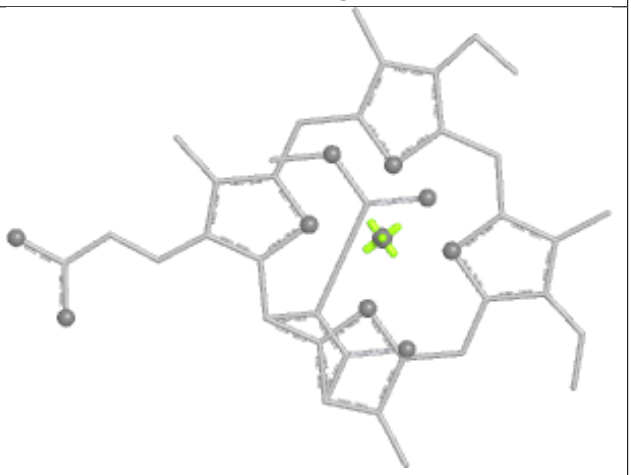
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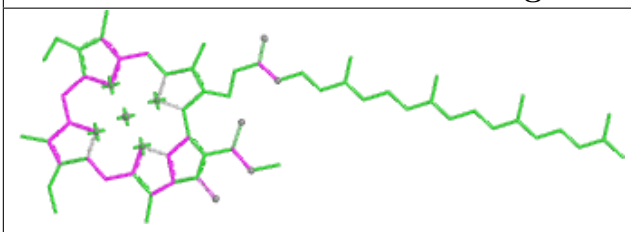


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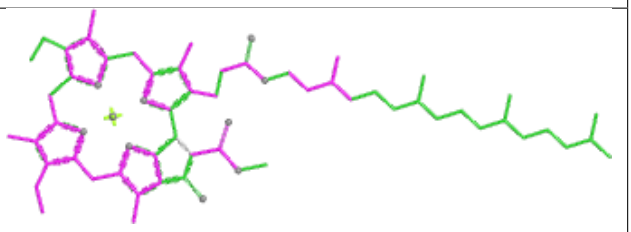


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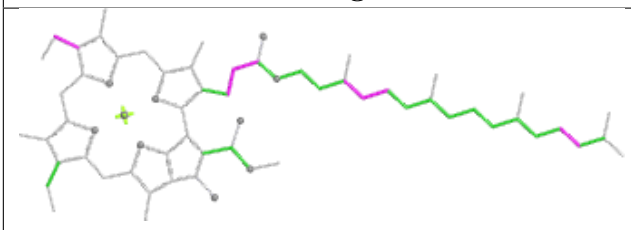
Ligand CLA B 807



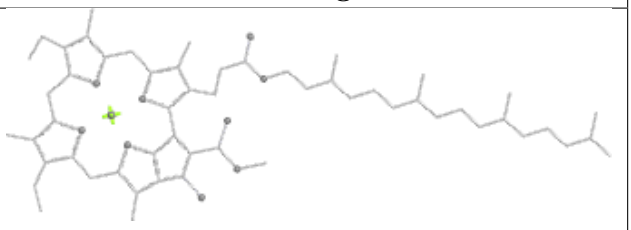
Bond lengths



Bond angles

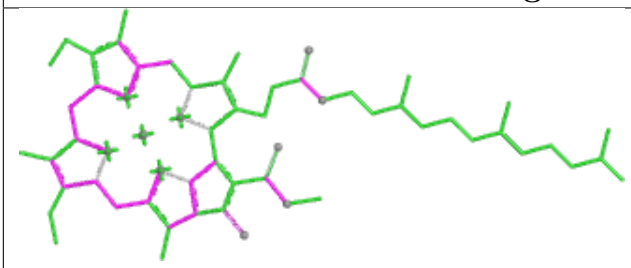


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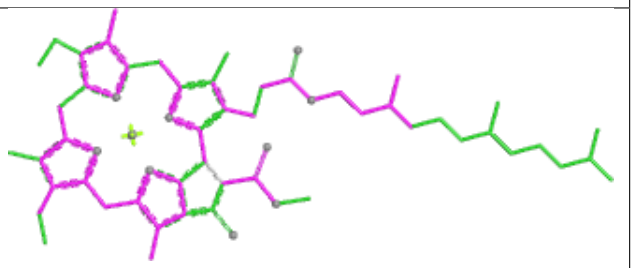


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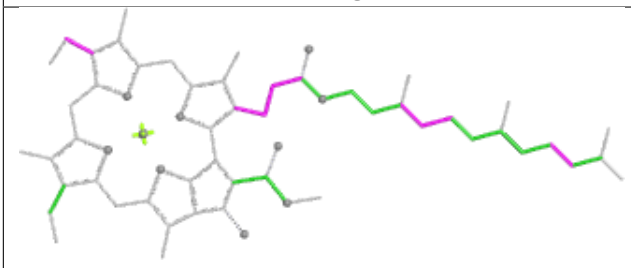
Ligand CLA A 814



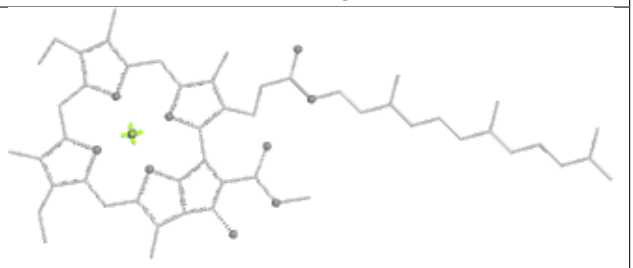
Bond lengths



Bond angles

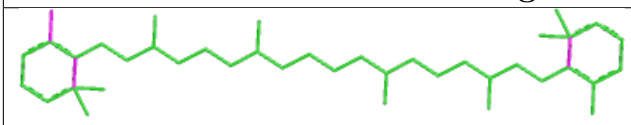


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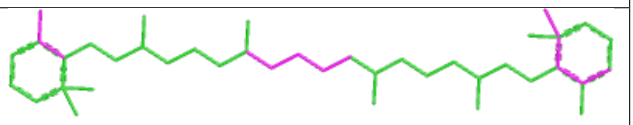


Rings

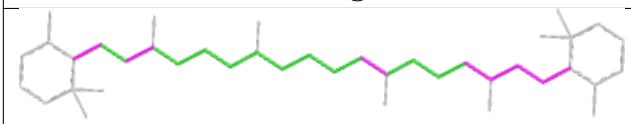
Ligand BCR M 101



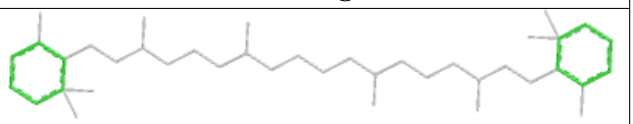
Bond lengths



Bond angles

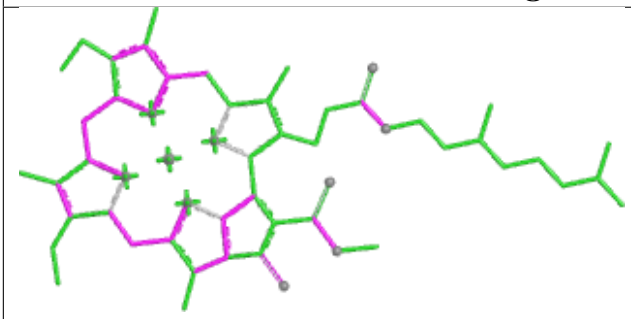


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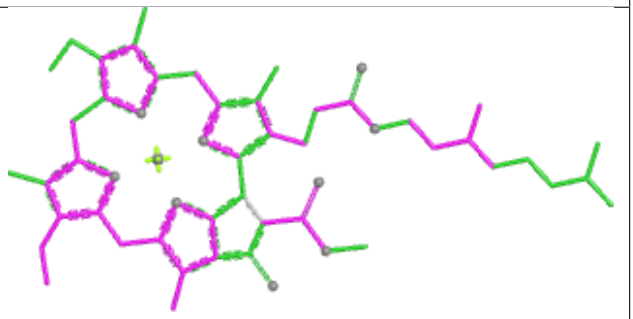


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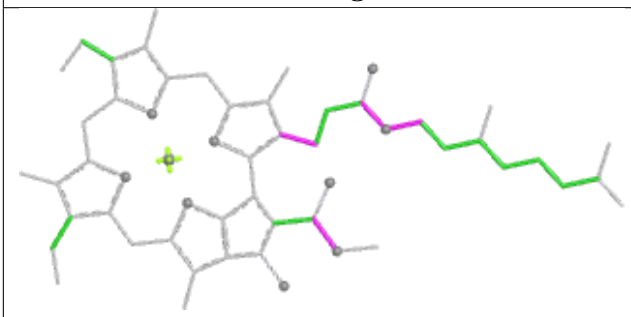
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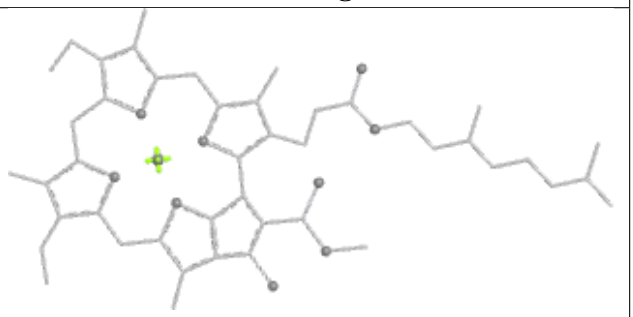
Bond lengths



Bond angles

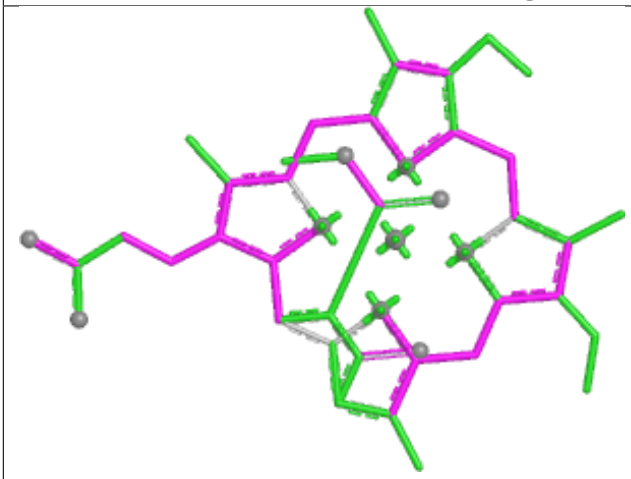


Torsions

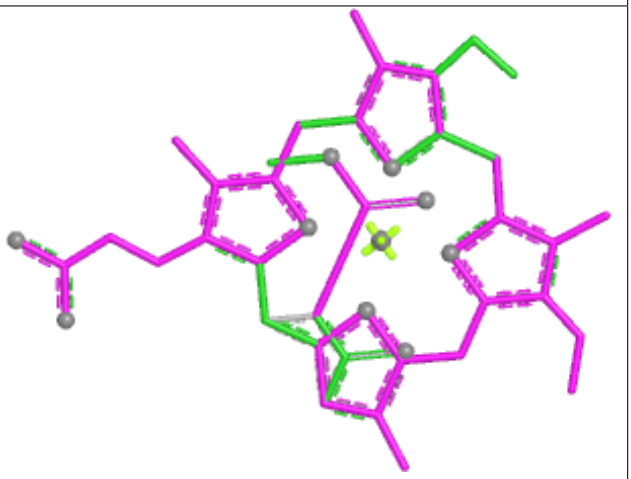


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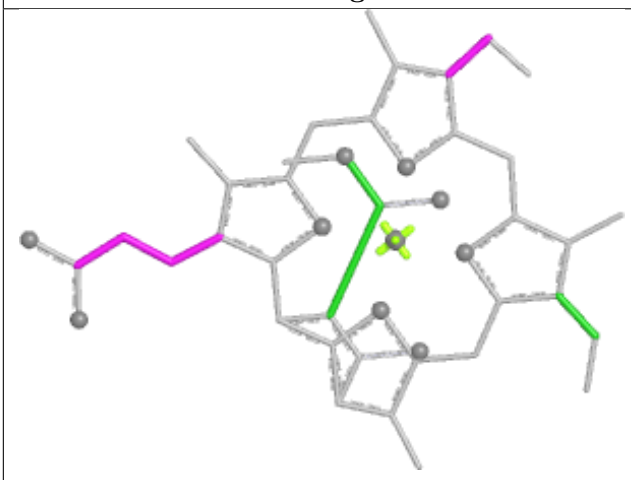
Ligand KC1 12 305



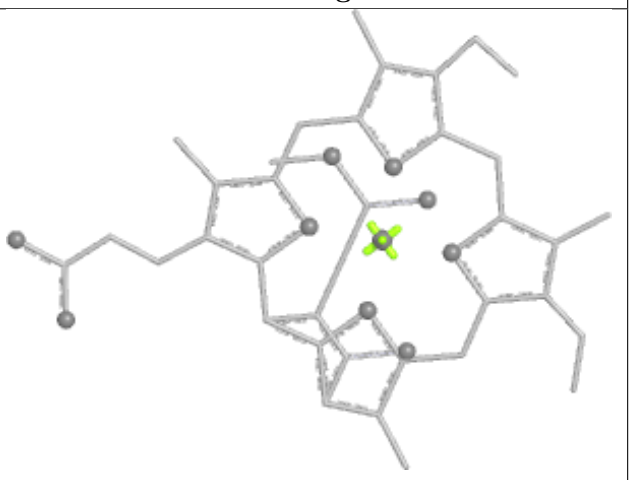
Bond lengths



Bond angles

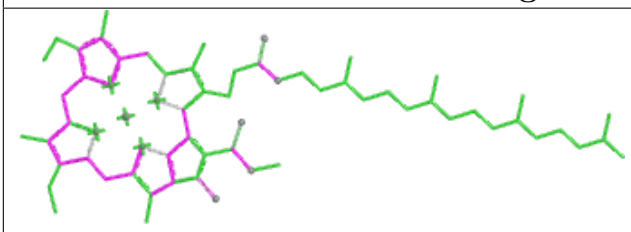


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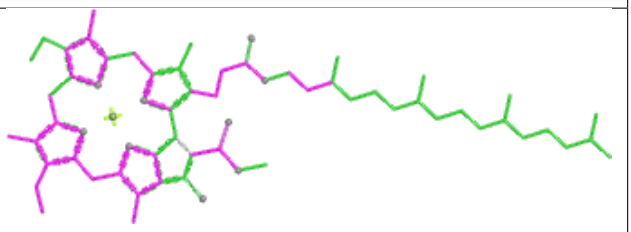


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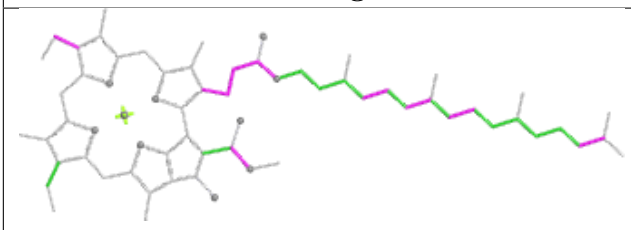
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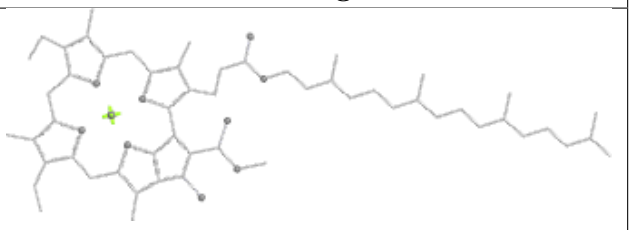
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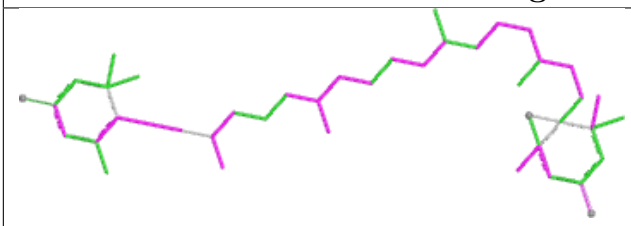


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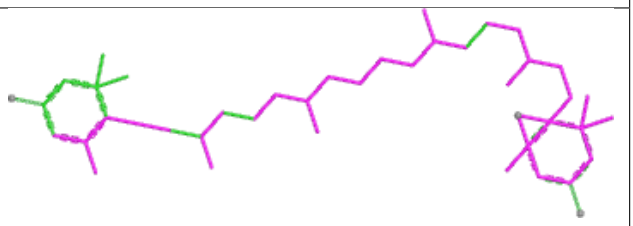


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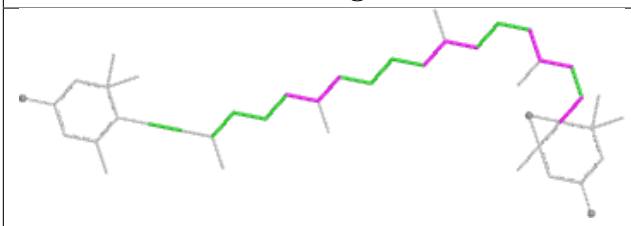
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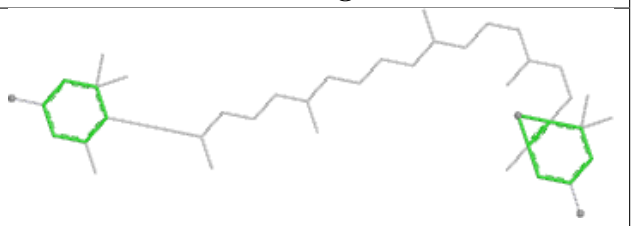
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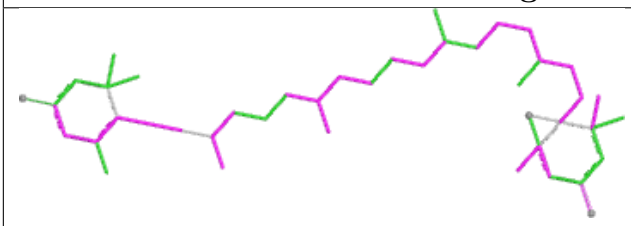


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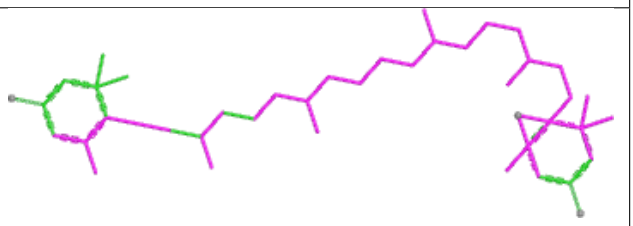


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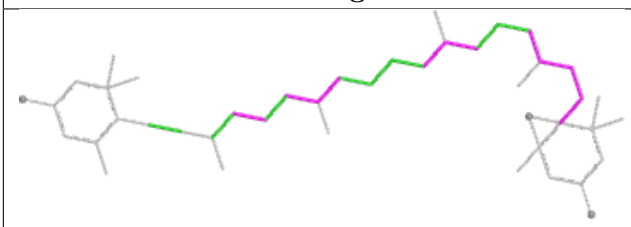
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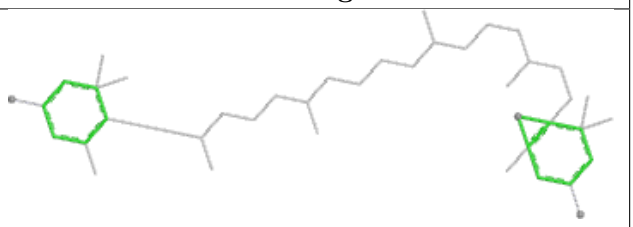
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Bond angles

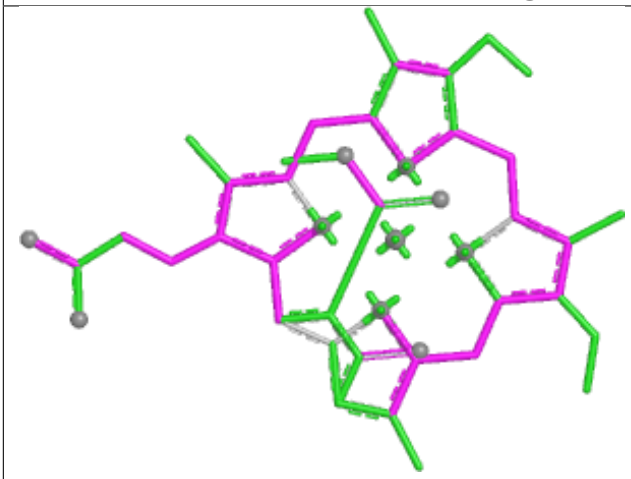


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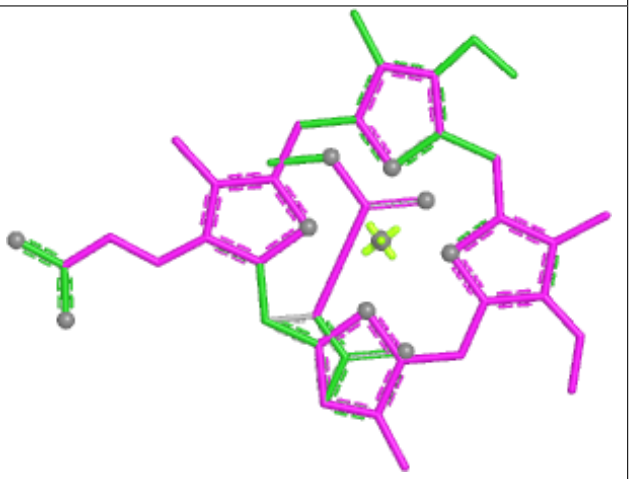


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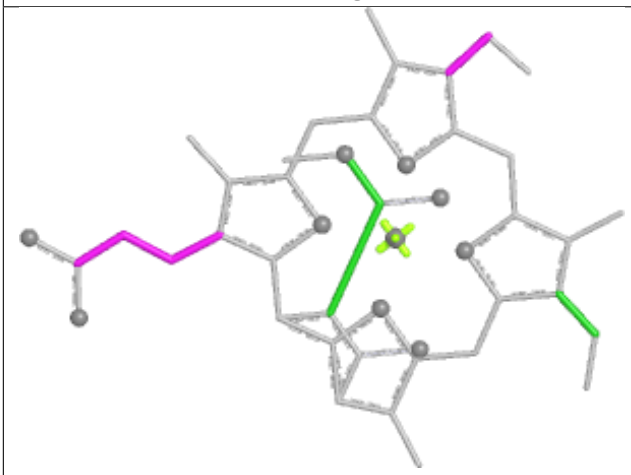
Ligand KC1 10 312



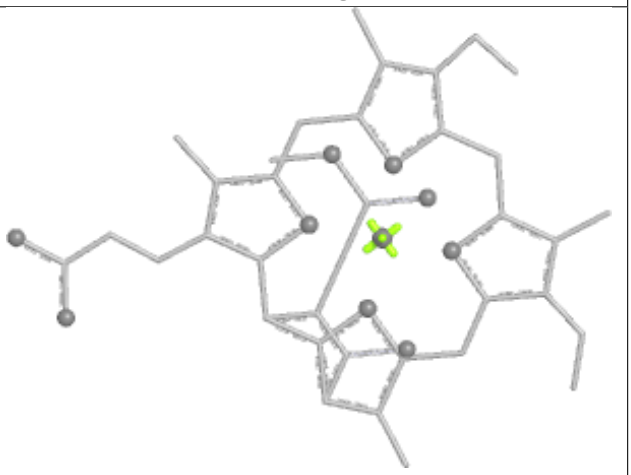
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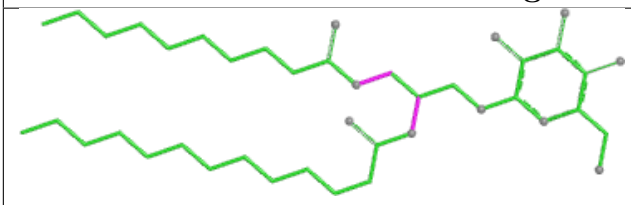


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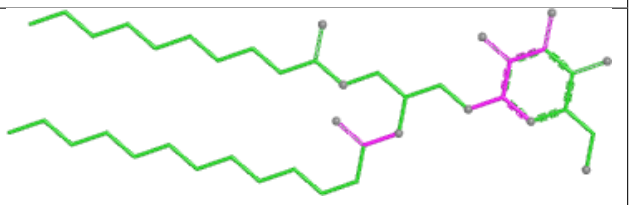


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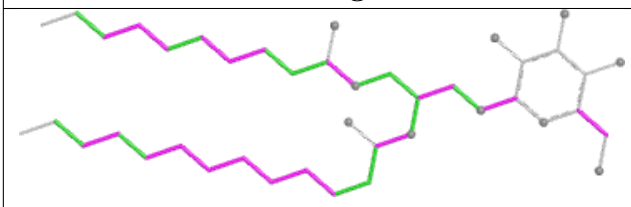
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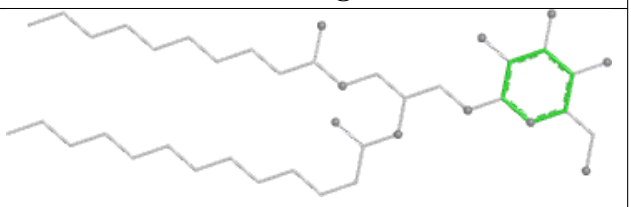
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Bond angles

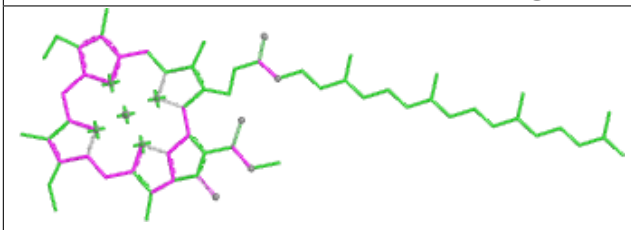


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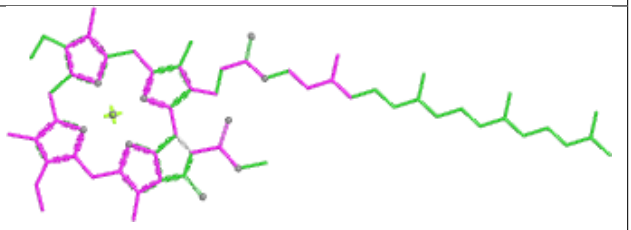


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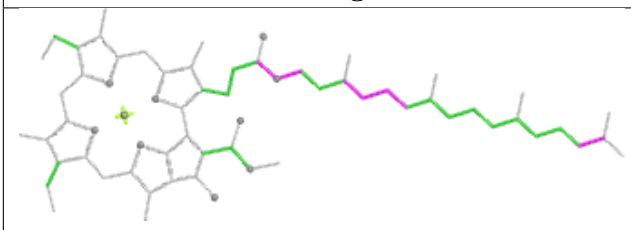
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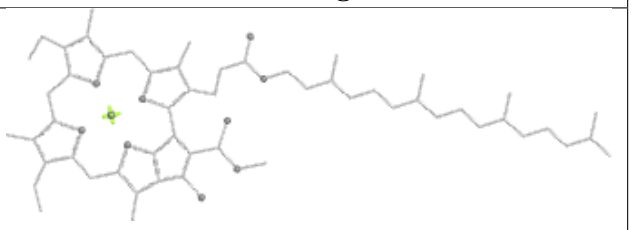
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Bond angles

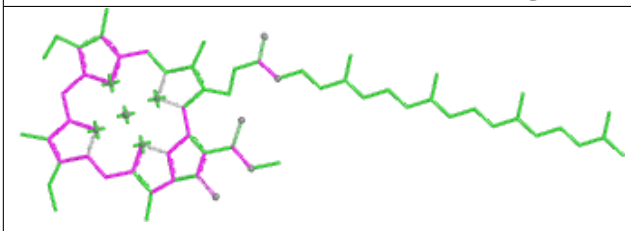


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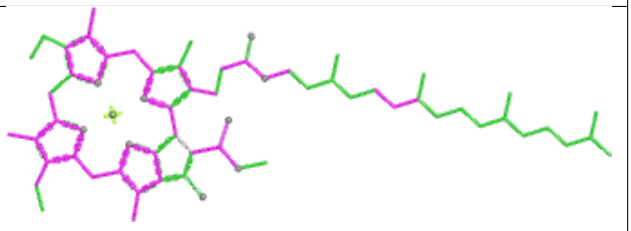


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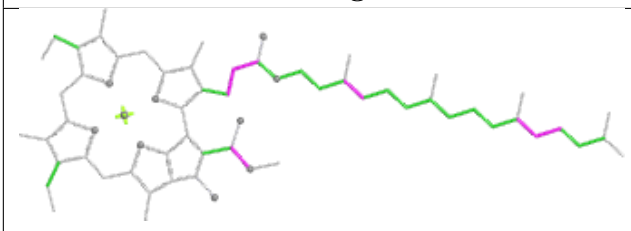
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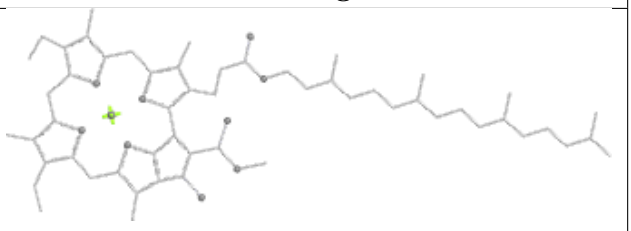
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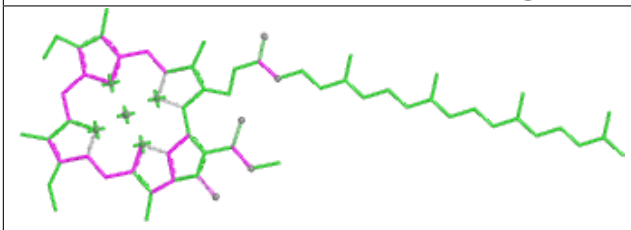


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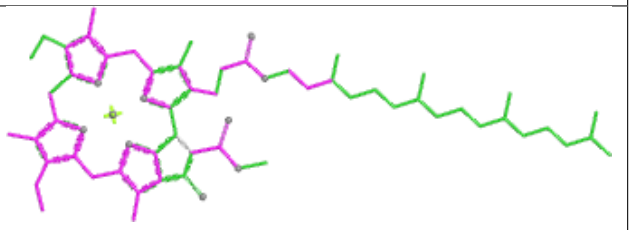


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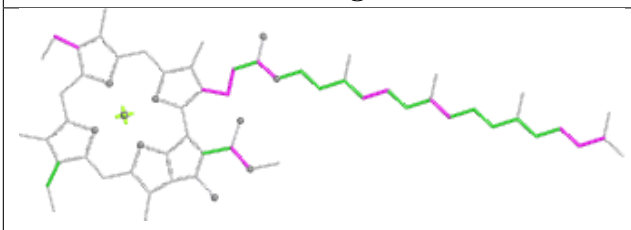
Ligand CLA 10 308



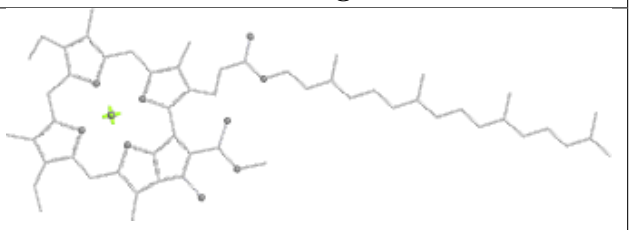
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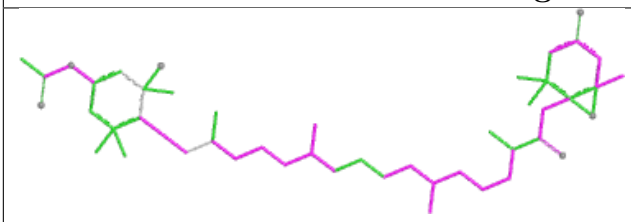


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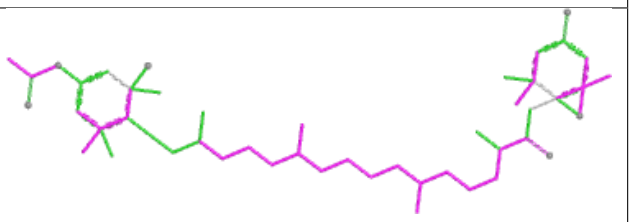


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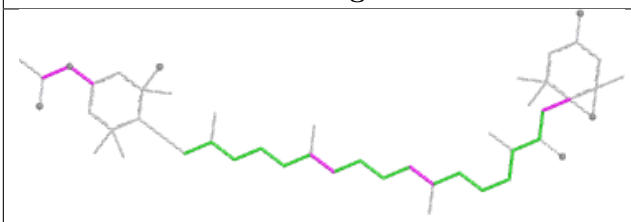
Ligand A86 7 319



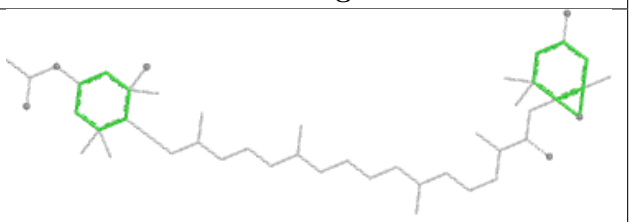
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Bond angles

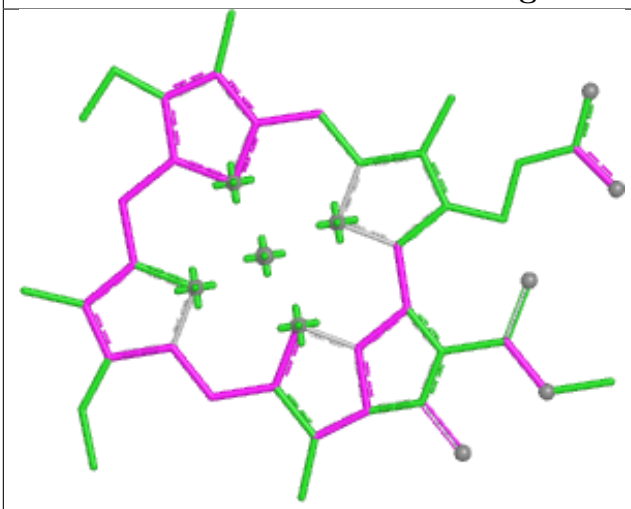


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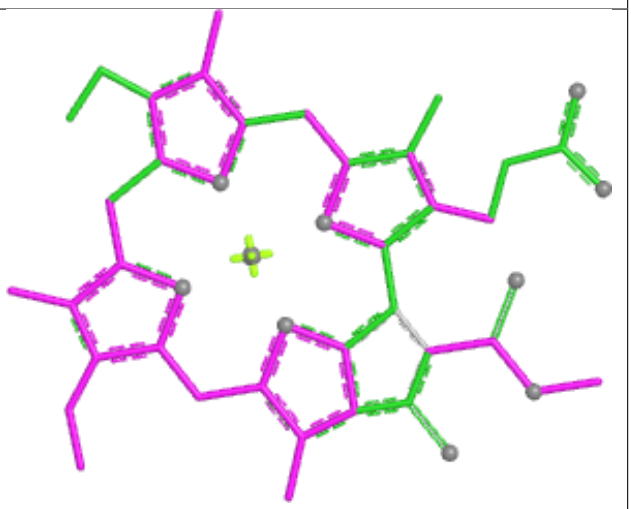


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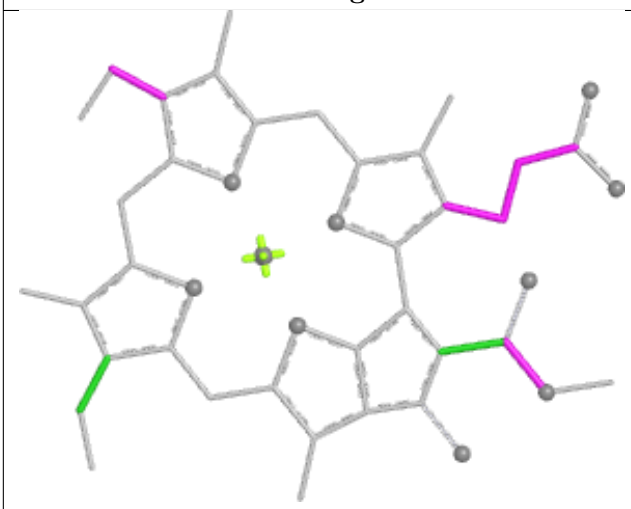
Ligand CLA 13 309



Bond lengths



Bond angles

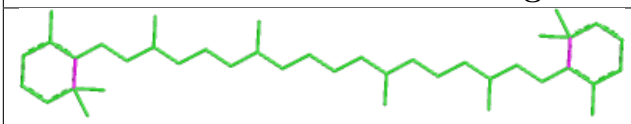


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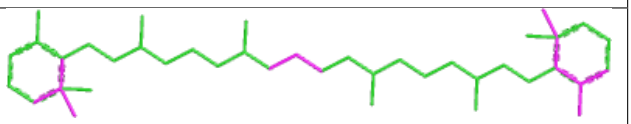


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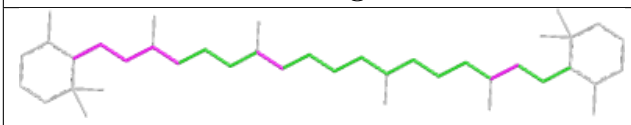
Ligand BCR F 204



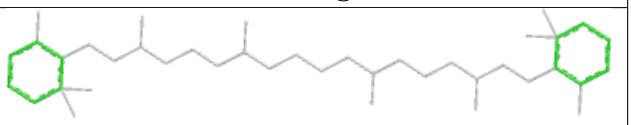
Bond lengths



Bond angles

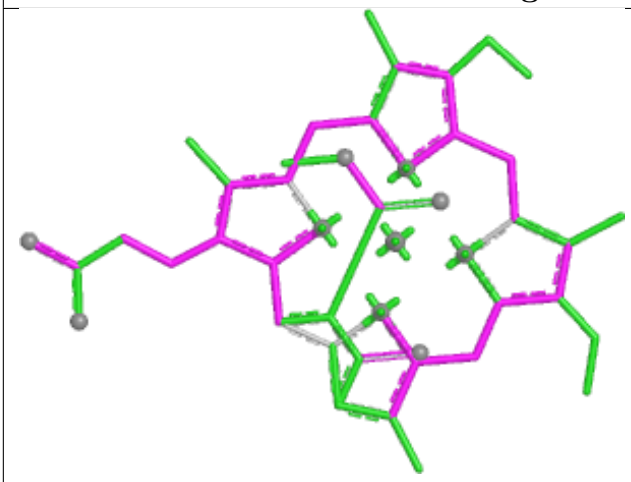


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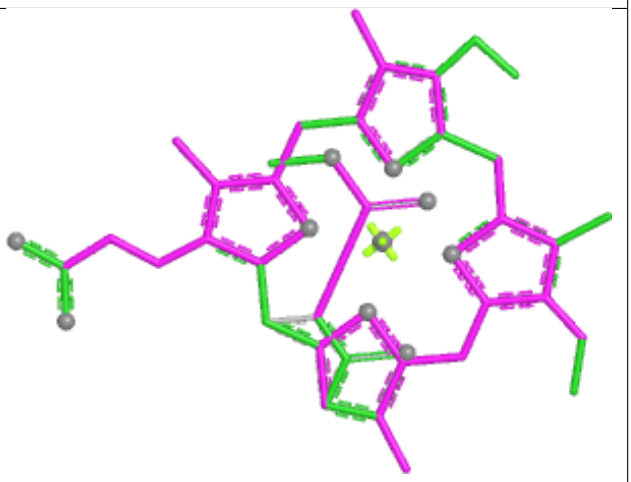


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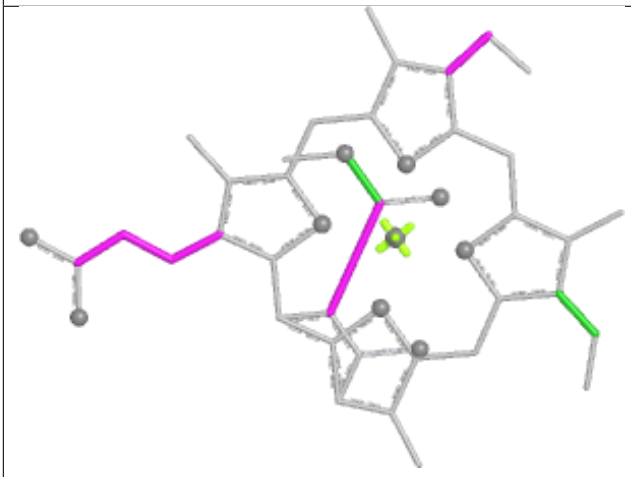
Ligand KC1 16 304



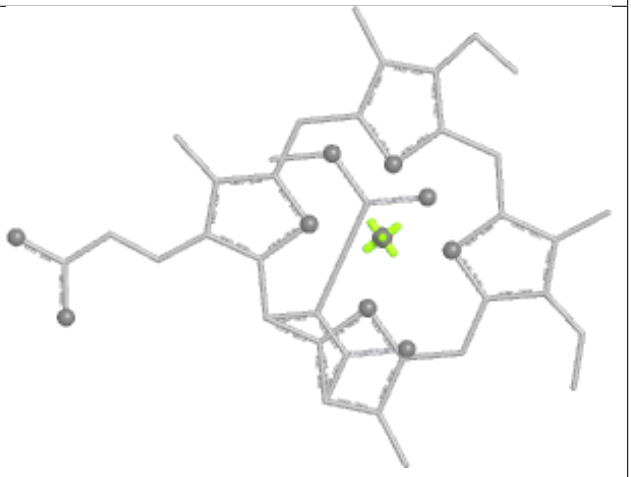
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Bond angles

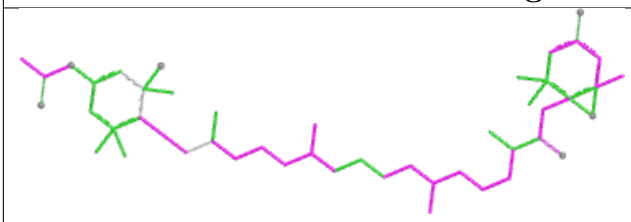


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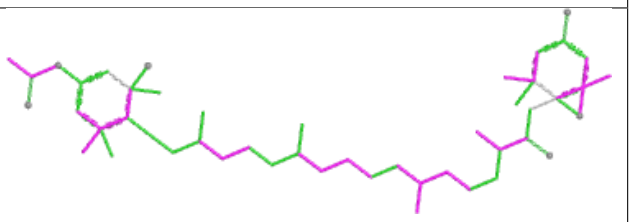


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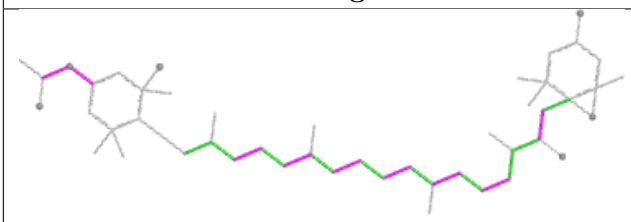
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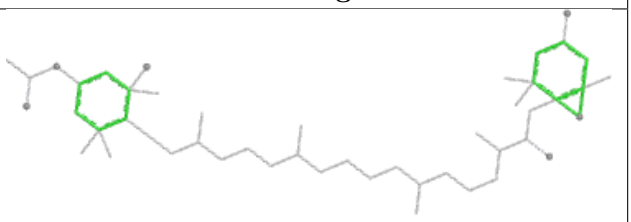
Bond lengths



Bond angles

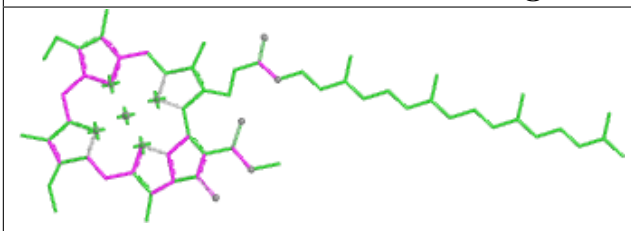


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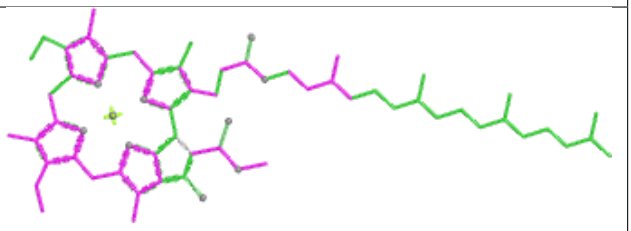


Rings

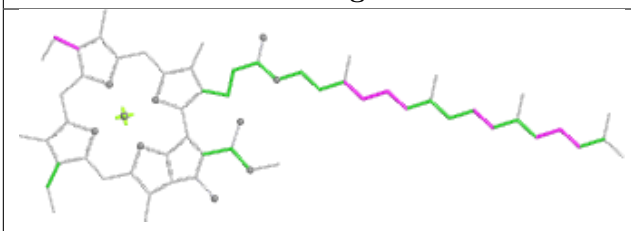
Ligand CLA B 806



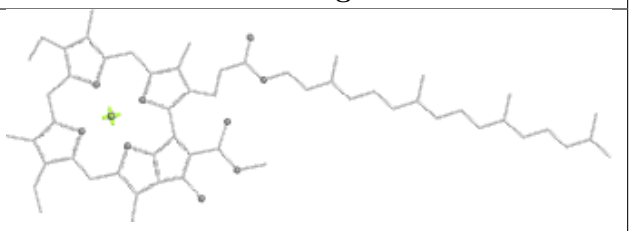
Bond lengths



Bond angles

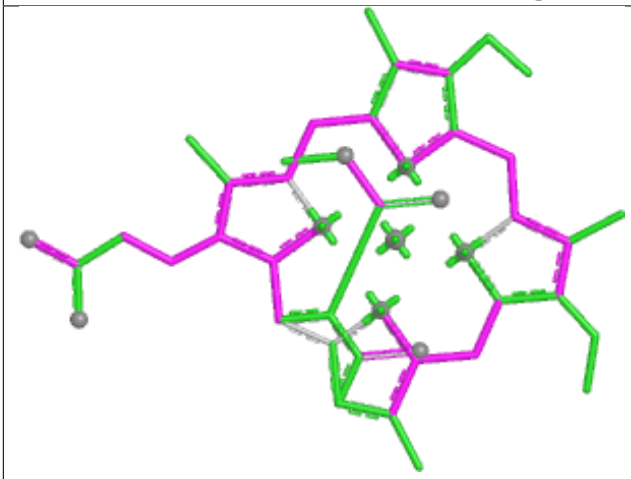


Torsions

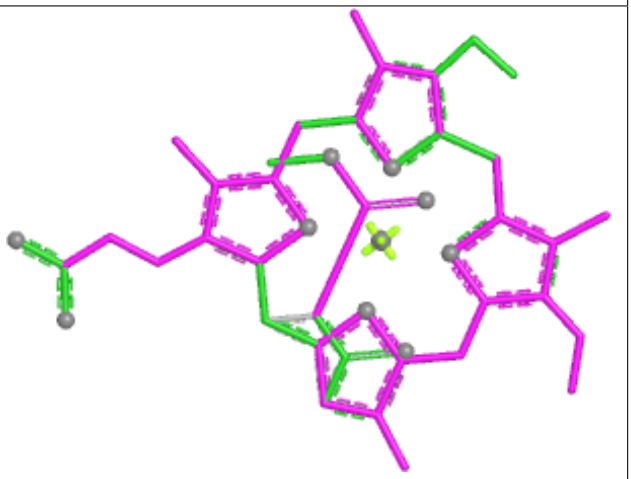


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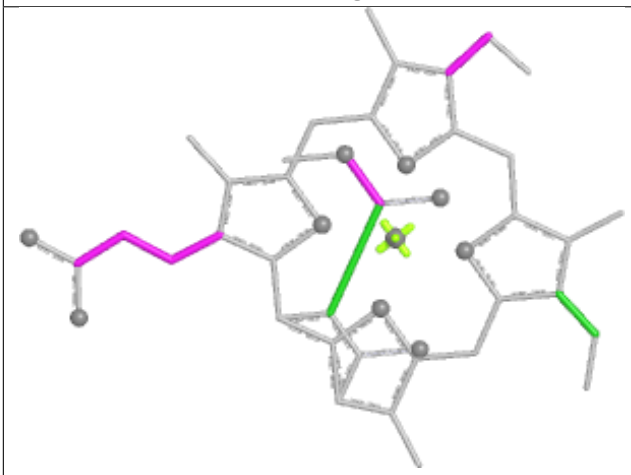
Ligand KC1 8 307



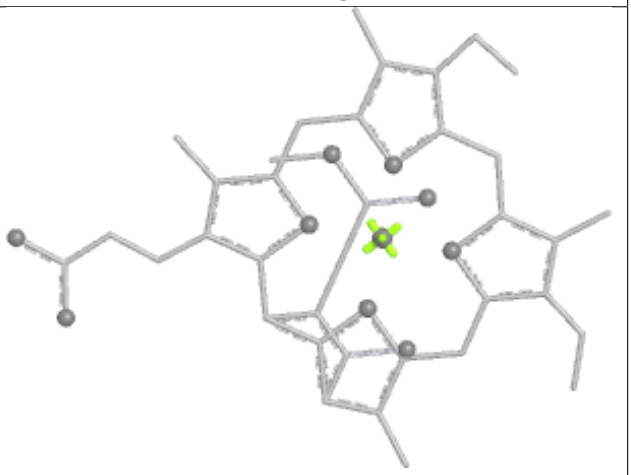
Bond lengths



Bond angles

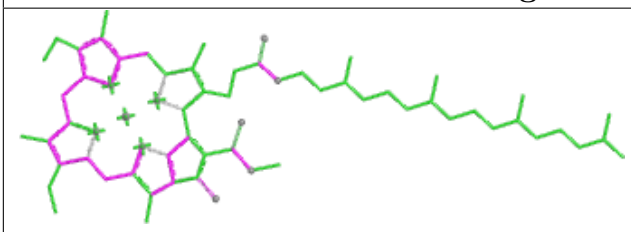


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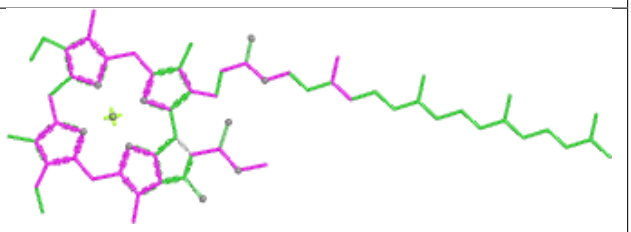


Rings

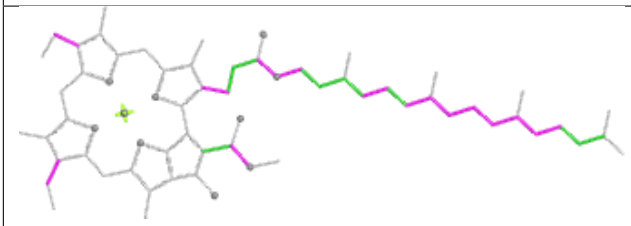
Ligand CLA 15 304



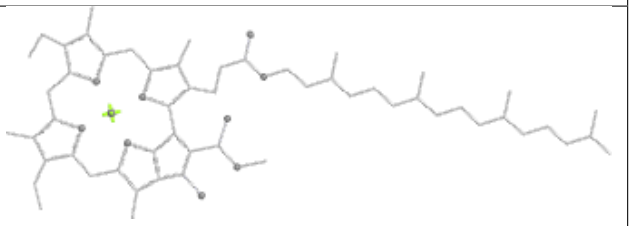
Bond lengths



Bond angles

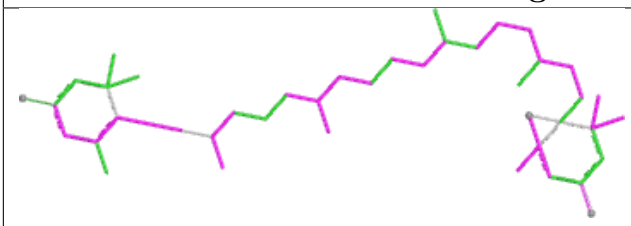


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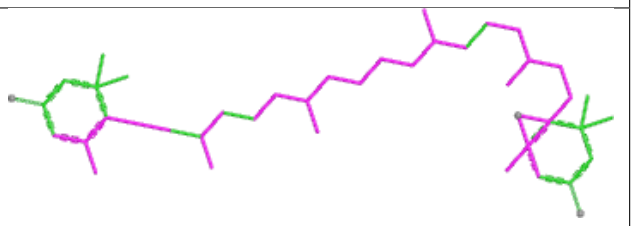


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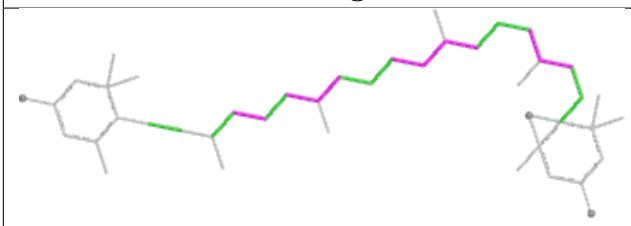
Ligand DD6 1 310



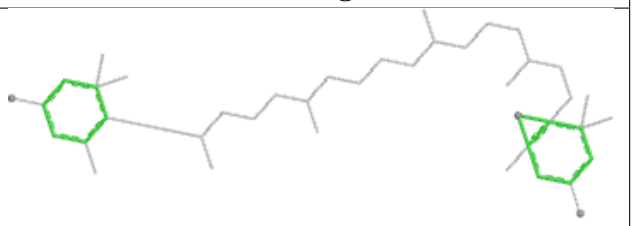
Bond lengths



Bond angles

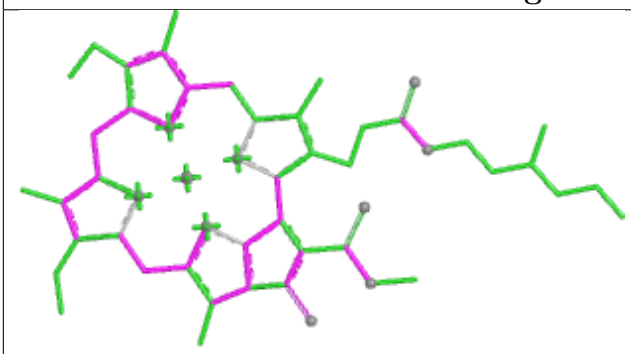


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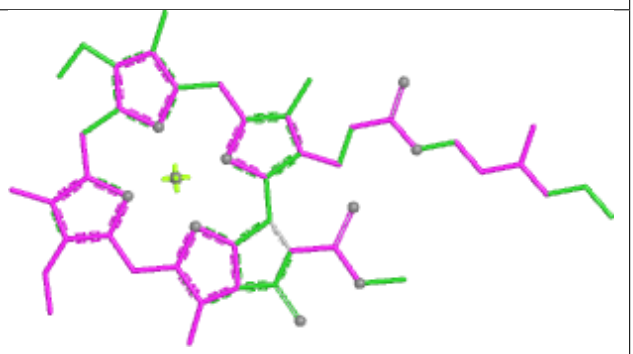


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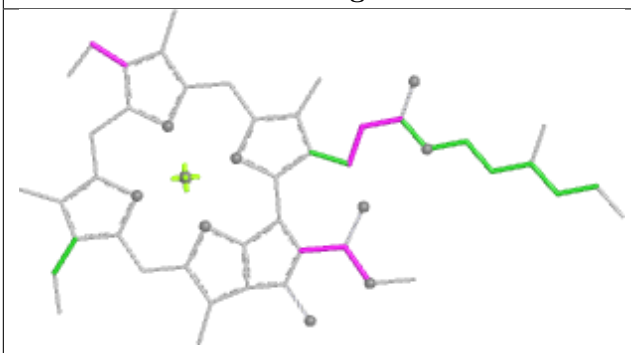
Ligand CLA B 804



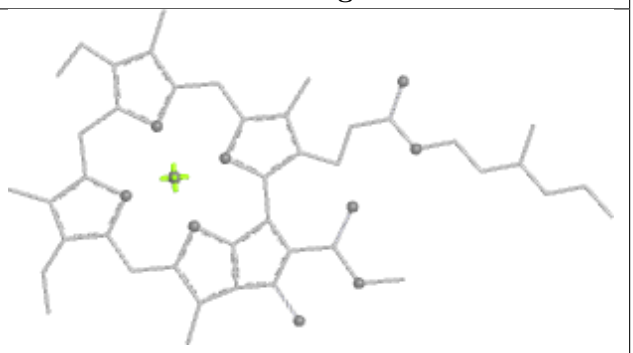
Bond lengths



Bond angles

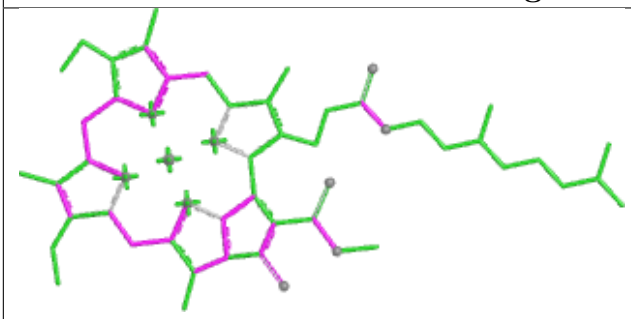


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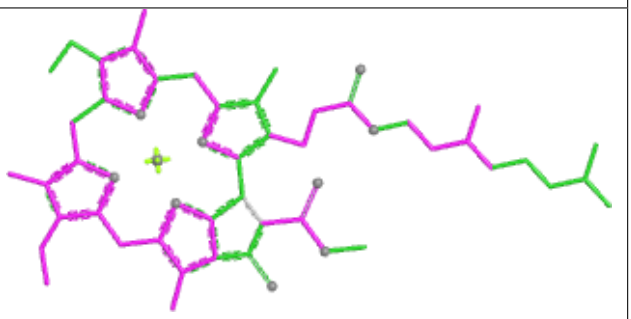


Rings

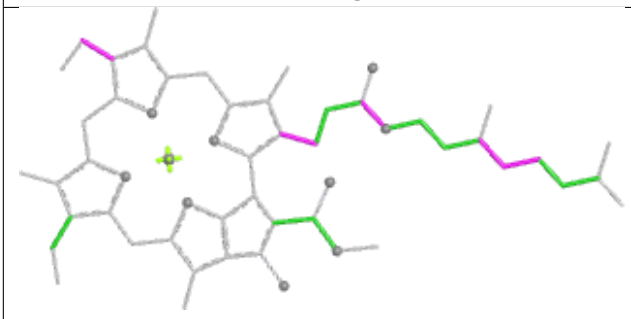
Ligand CLA B 816



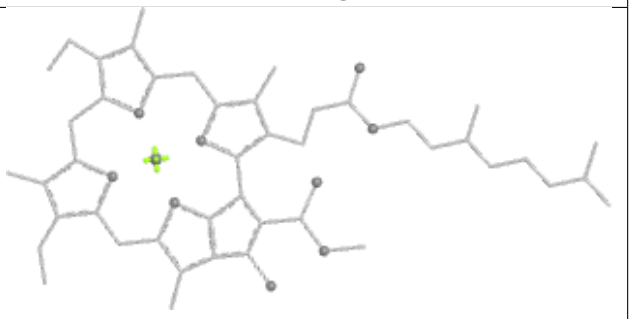
Bond lengths



Bond angles

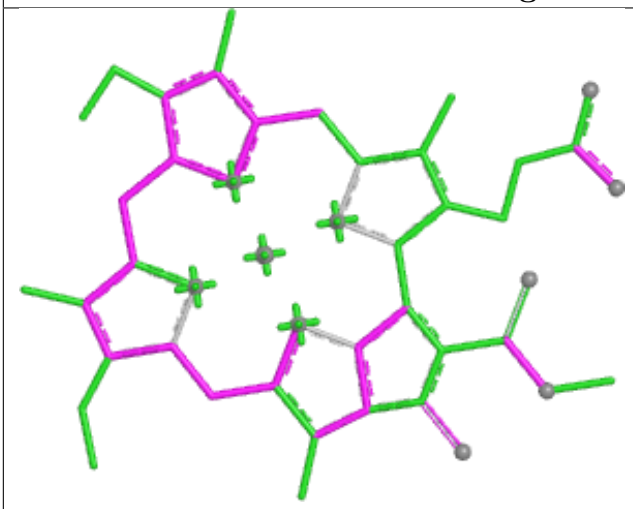


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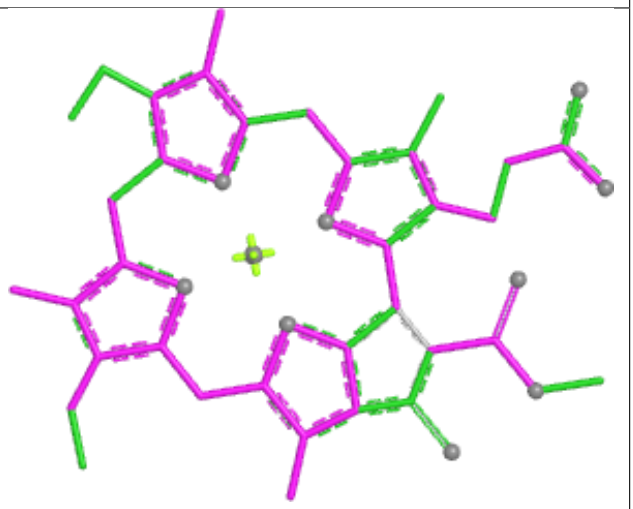


Rings

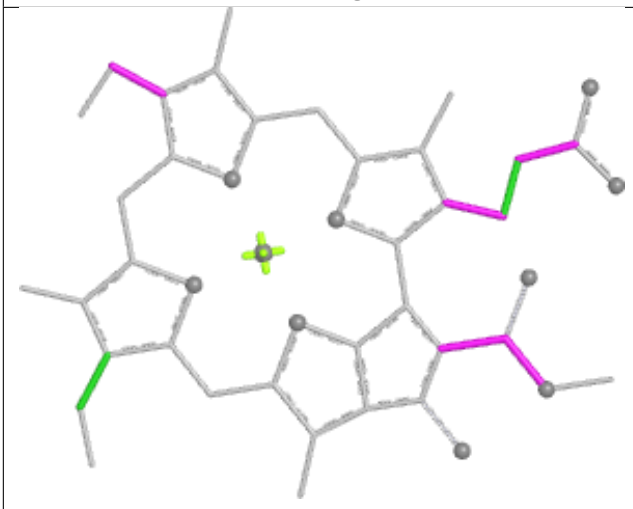
Ligand CLA 15 305



Bond lengths



Bond angles

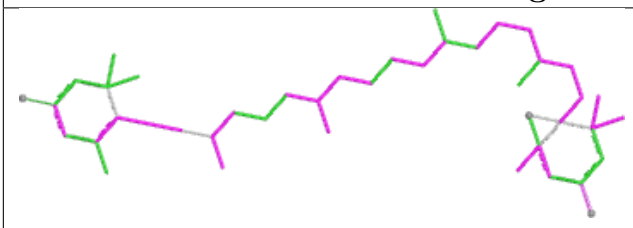


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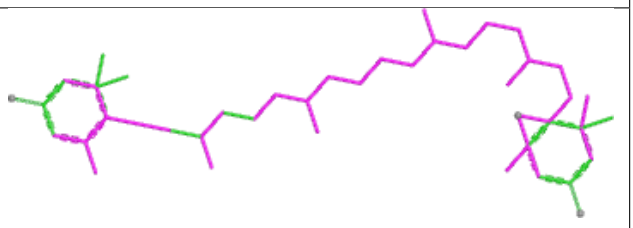


Rings

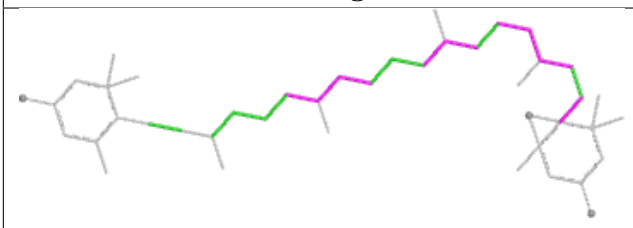
Ligand DD6 4 313



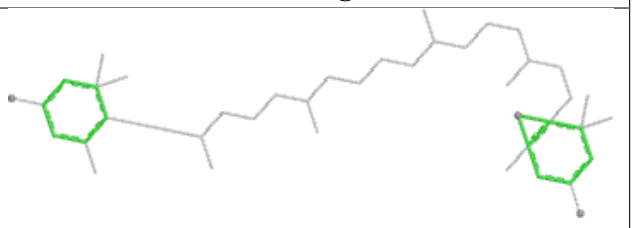
Bond lengths



Bond angles

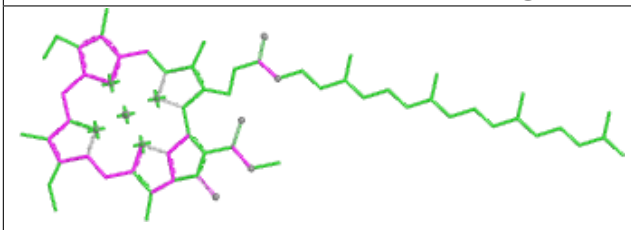


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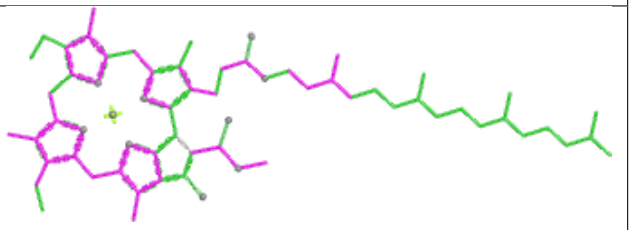


Rings

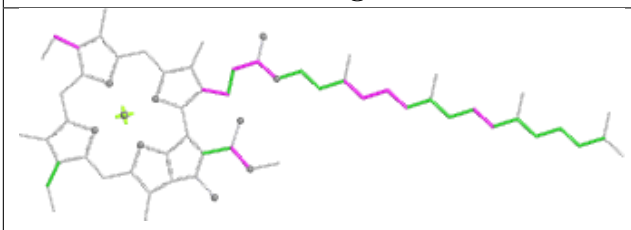
Ligand CLA 10 309



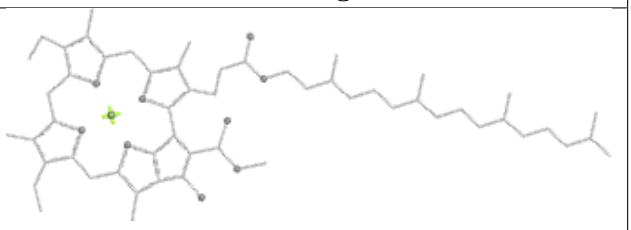
Bond lengths



Bond angles

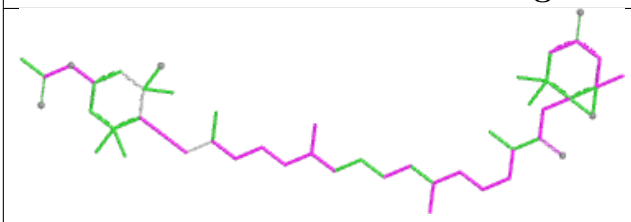


Torsions



Rings

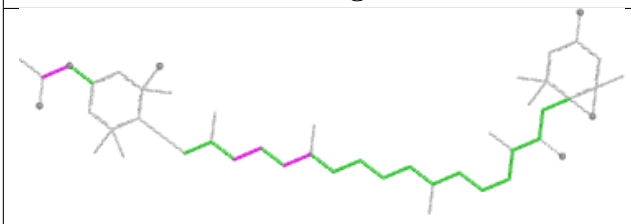
Ligand A86 4 315



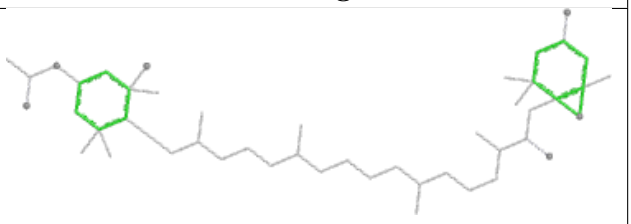
Bond lengths



Bond angles

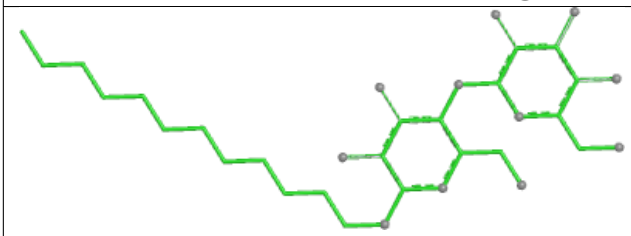


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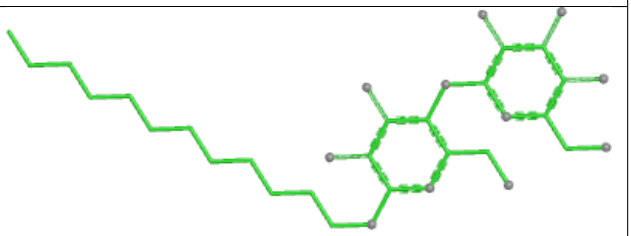


Rings

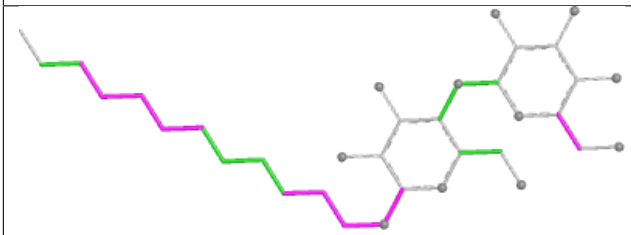
Ligand LMT 11 303



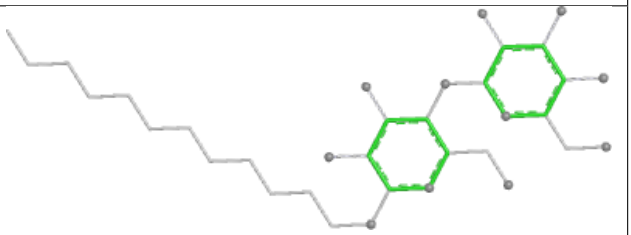
Bond lengths



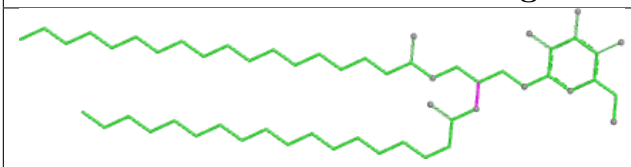
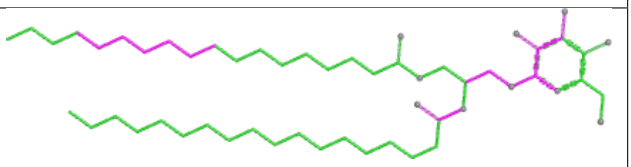
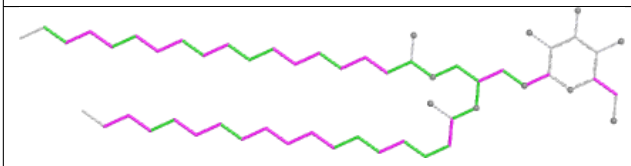
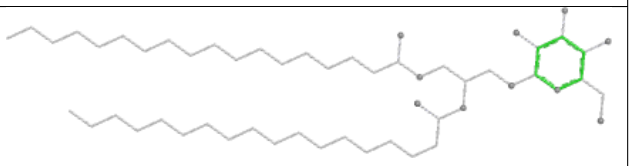
Bond angles

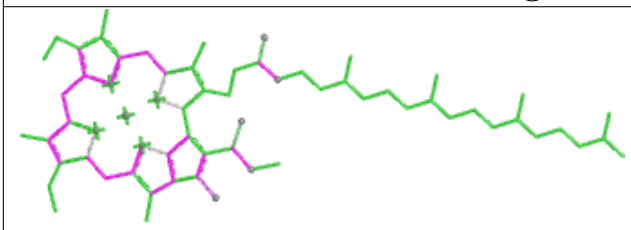
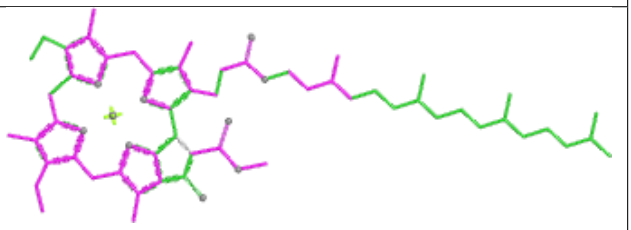
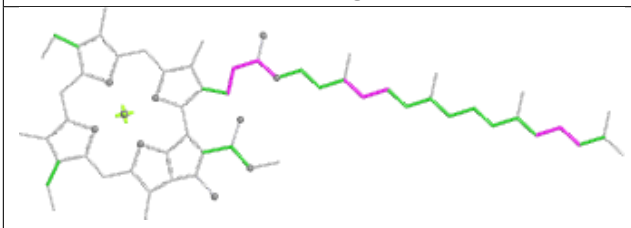
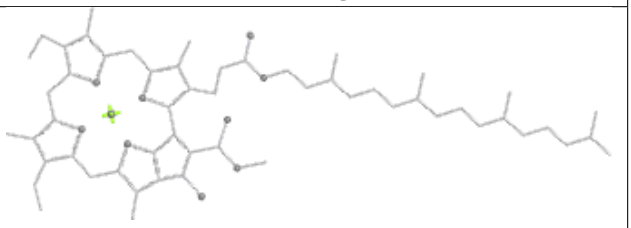


Torsions

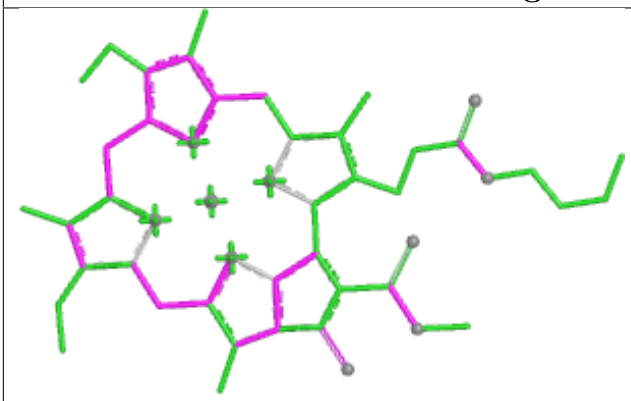


Rings

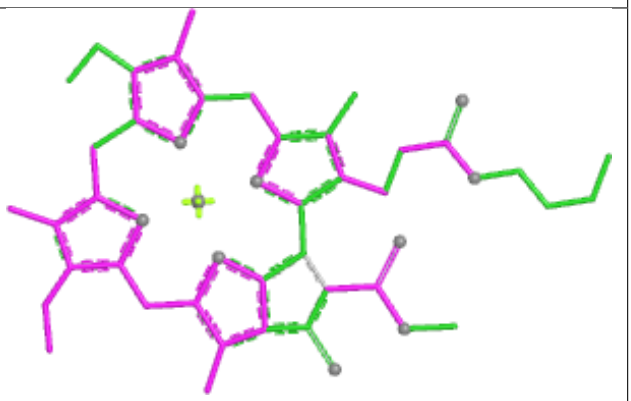
Ligand LMG B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

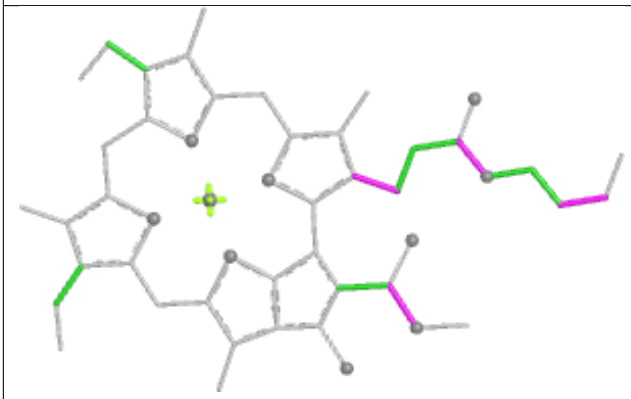
Ligand CLA A 823



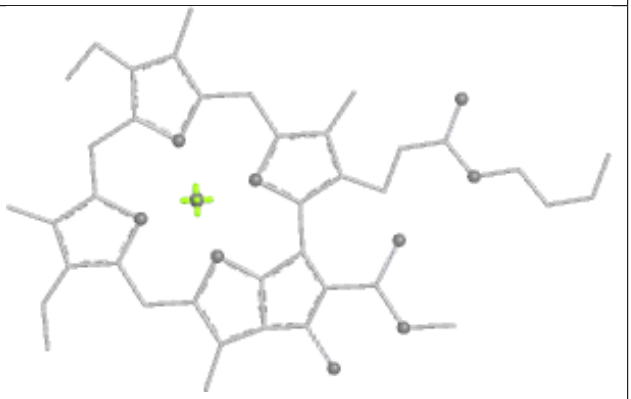
Bond lengths



Bond angles

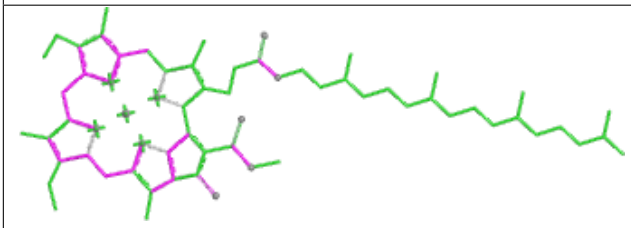


Torsions

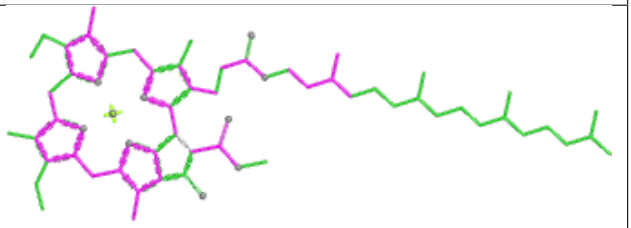


Rings

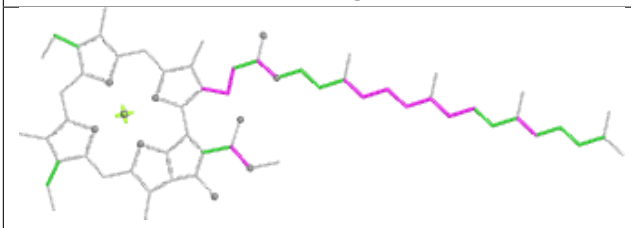
Ligand CLA B 838



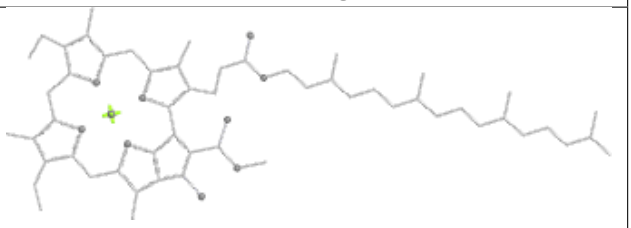
Bond lengths



Bond angles

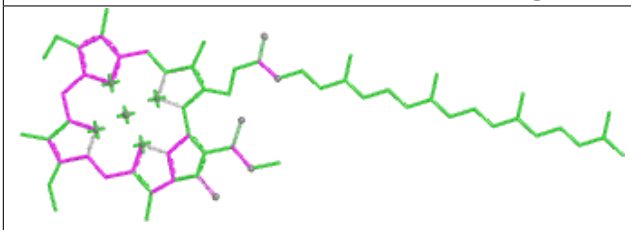


Torsions

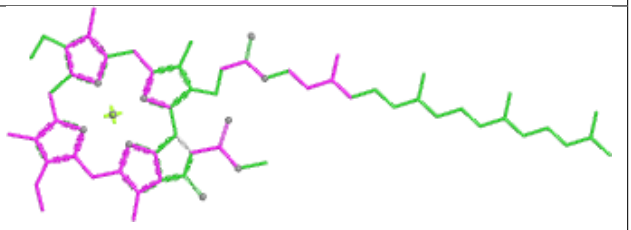


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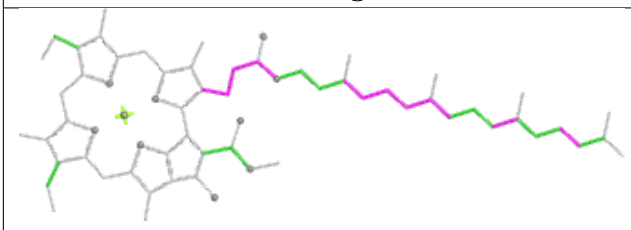
Ligand CLA 1 307



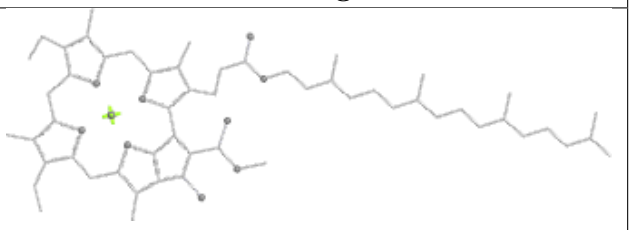
Bond lengths



Bond angles

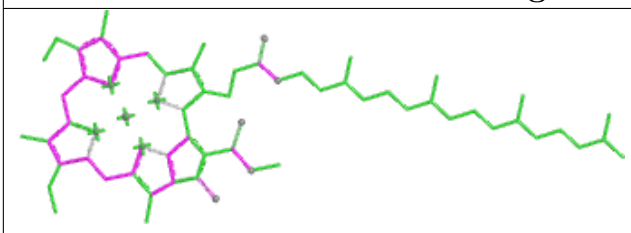


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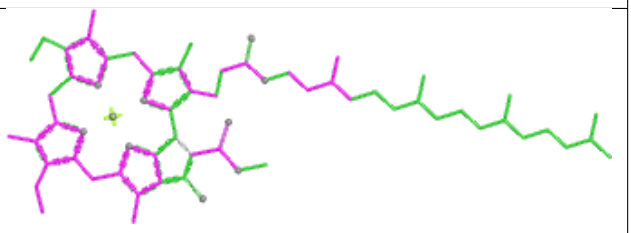


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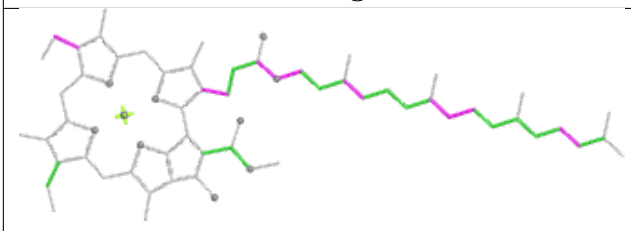
Ligand CLA 5 309



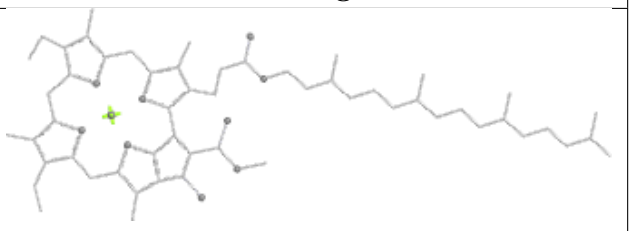
Bond lengths



Bond angles

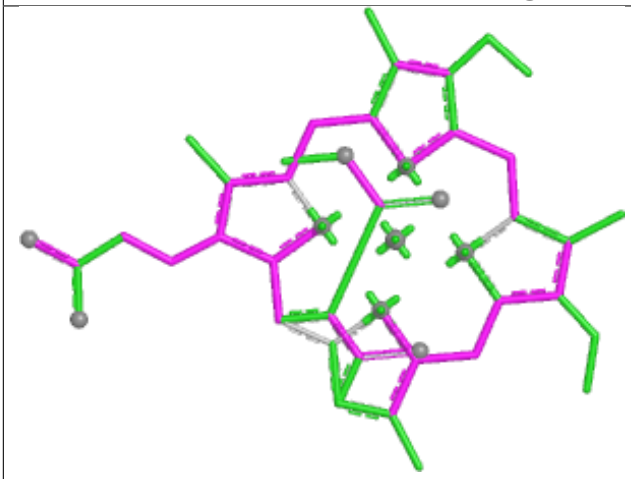


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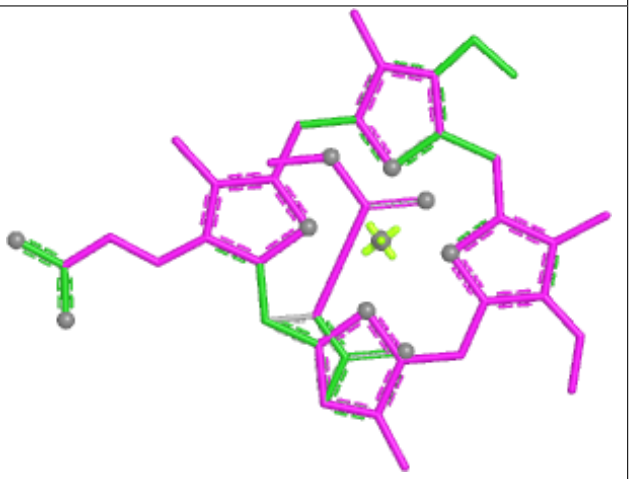


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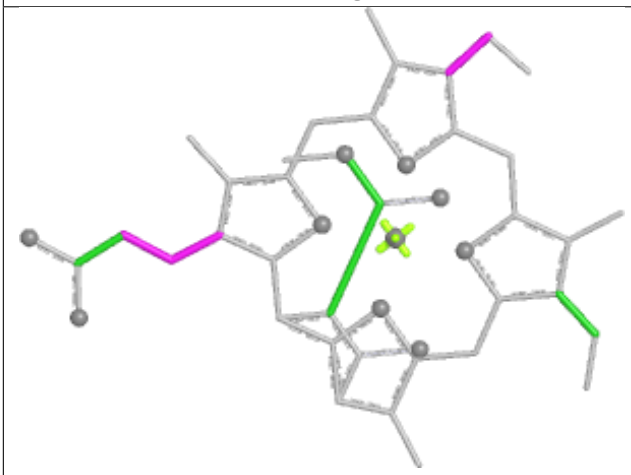
Ligand KC1 11 312



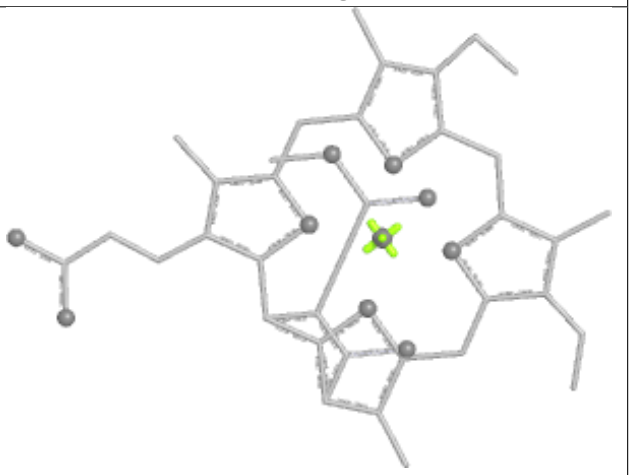
Bond lengths



Bond angles

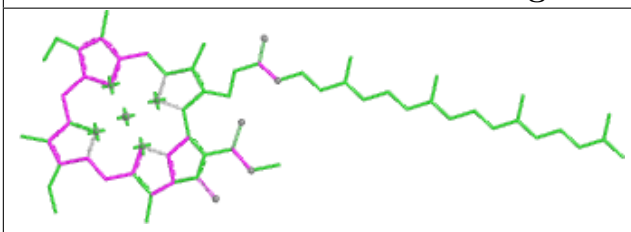


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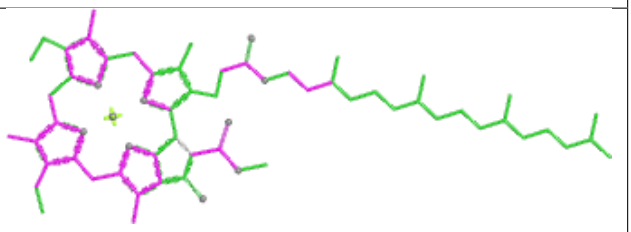


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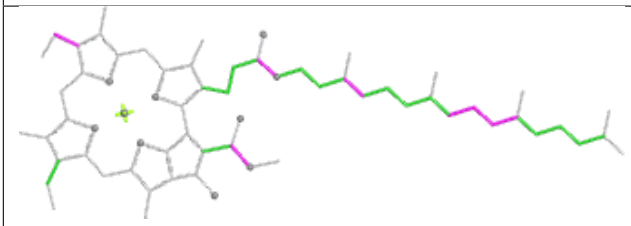
Ligand CLA 2 311



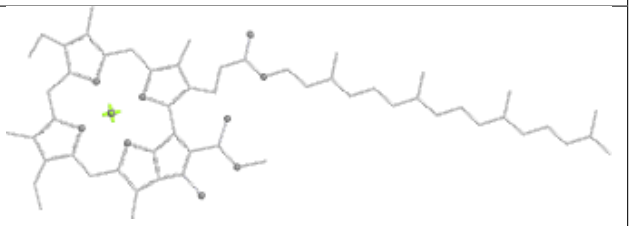
Bond lengths



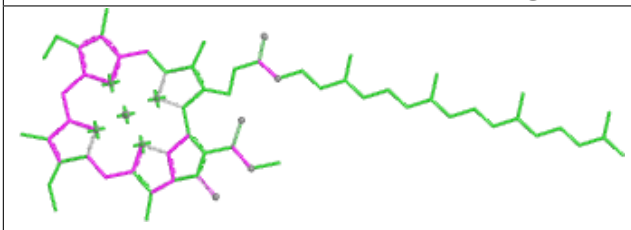
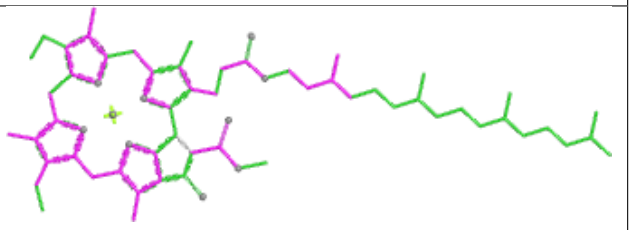
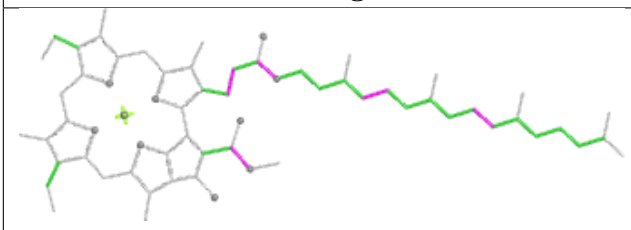
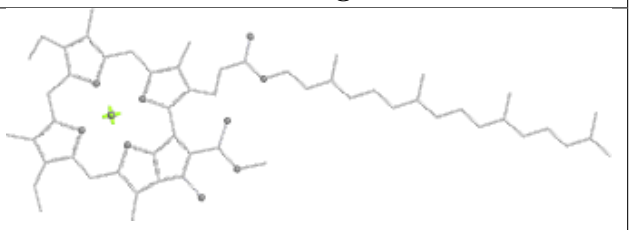
Bond angles

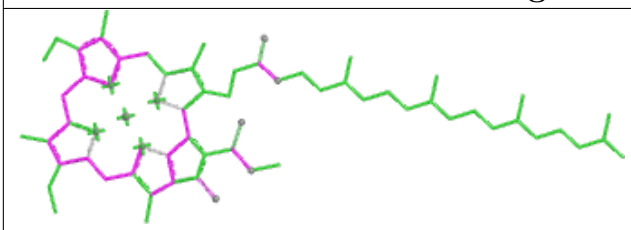
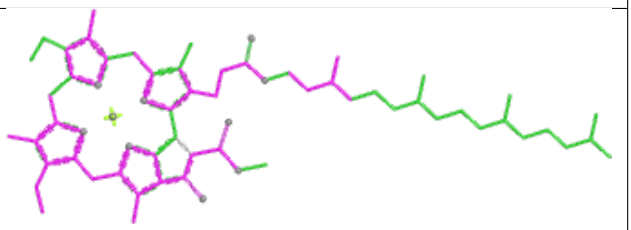
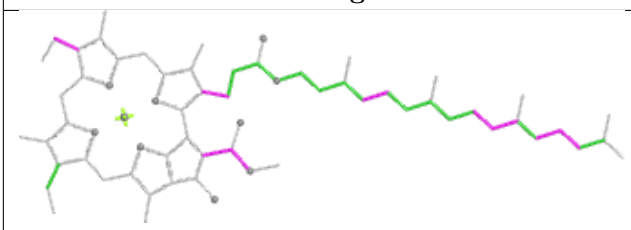
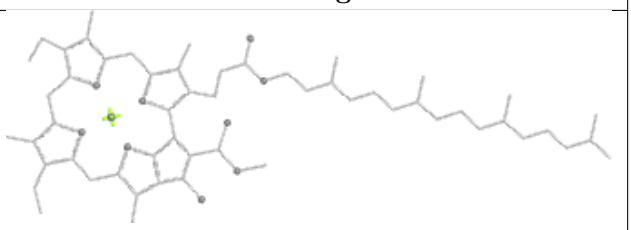


Torsions

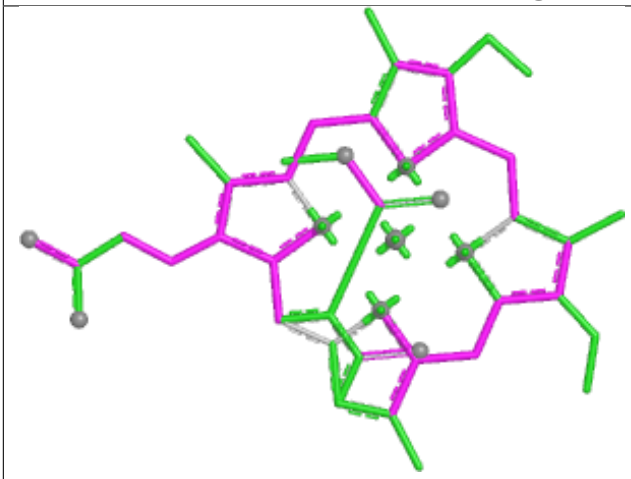


Rings

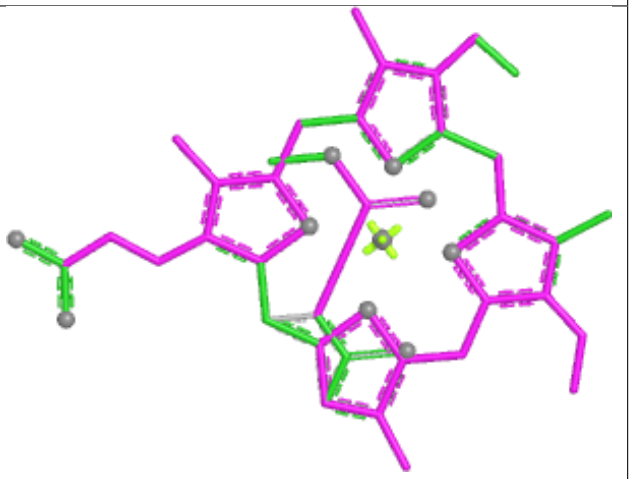
Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

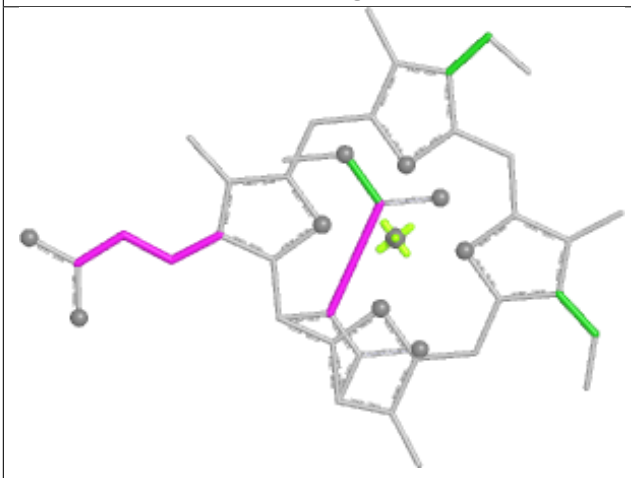
Ligand KC1 5 310



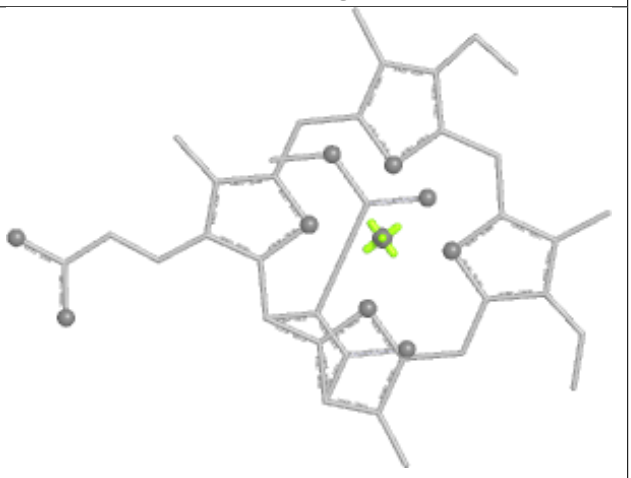
Bond lengths



Bond angles

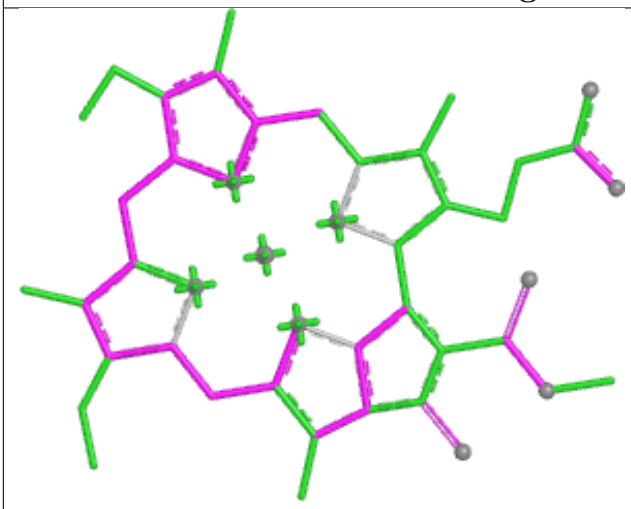


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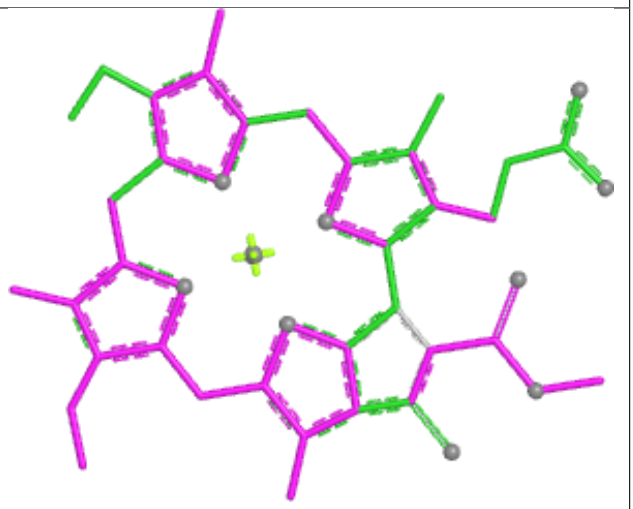


Rings

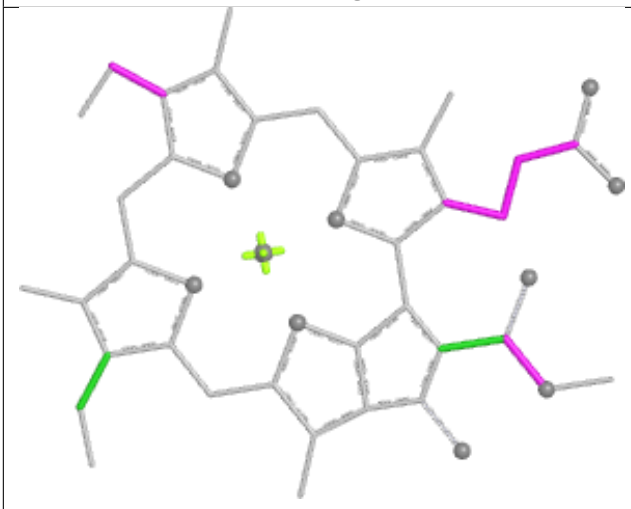
Ligand CLA 16 310



Bond lengths



Bond angles

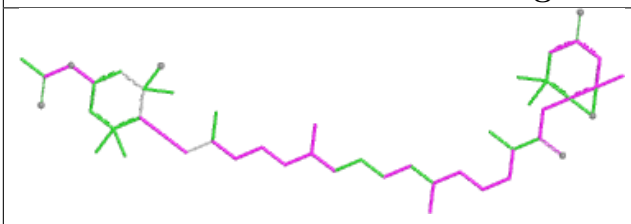


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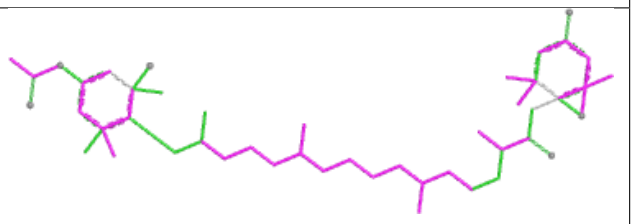


Rings

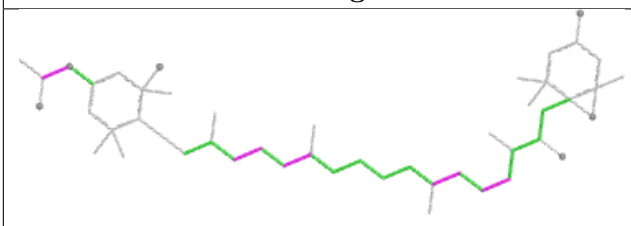
Ligand A86 9 313



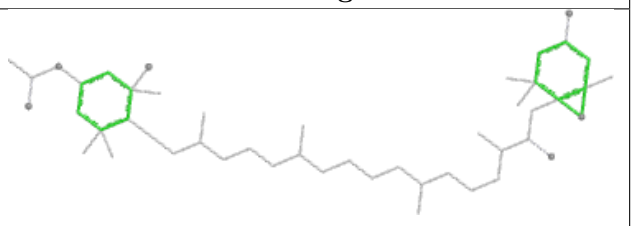
Bond lengths



Bond angles

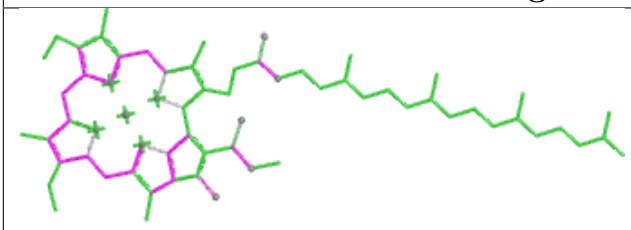


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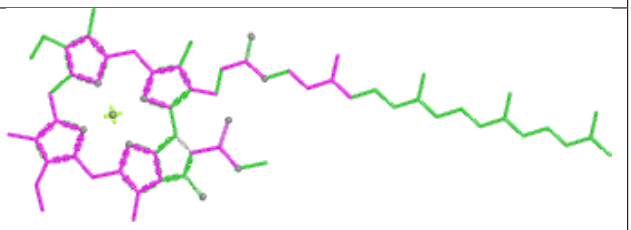


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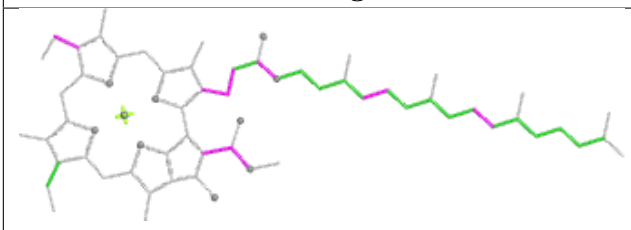
Ligand CLA 3 306



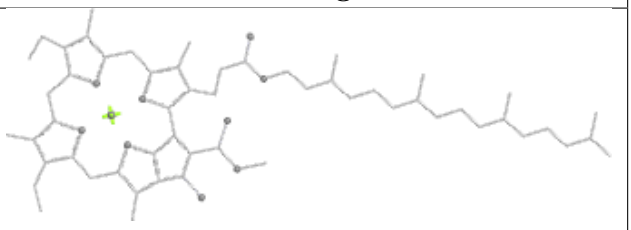
Bond lengths



Bond angles

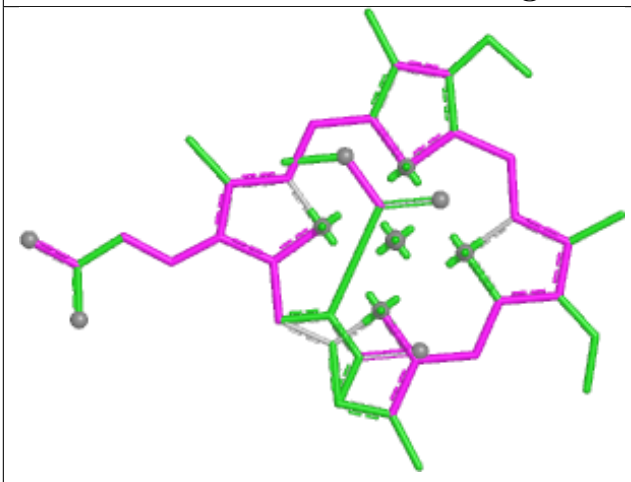


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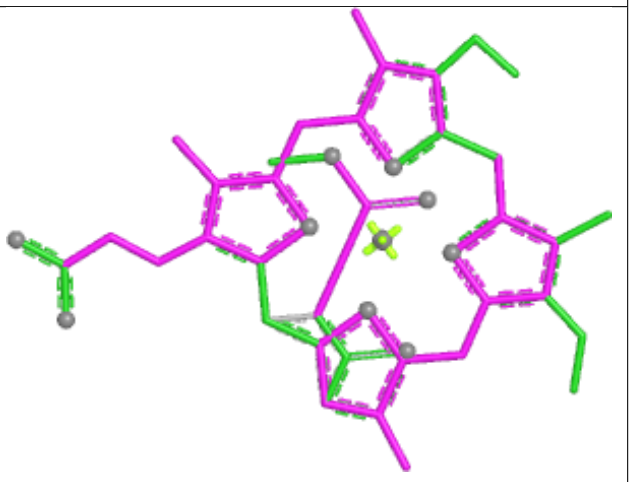


Rings

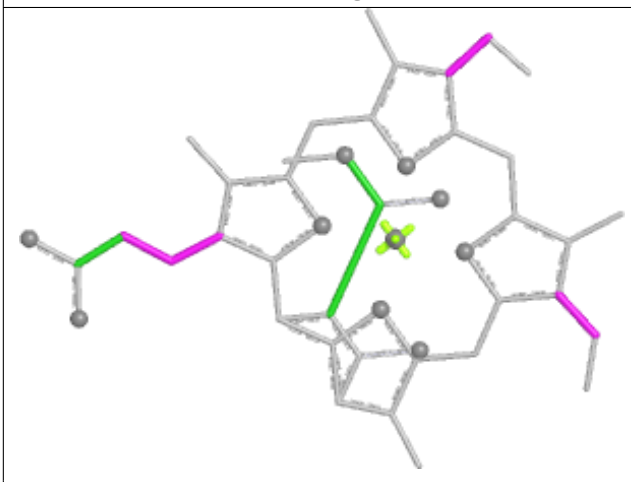
Ligand KC1 16 311



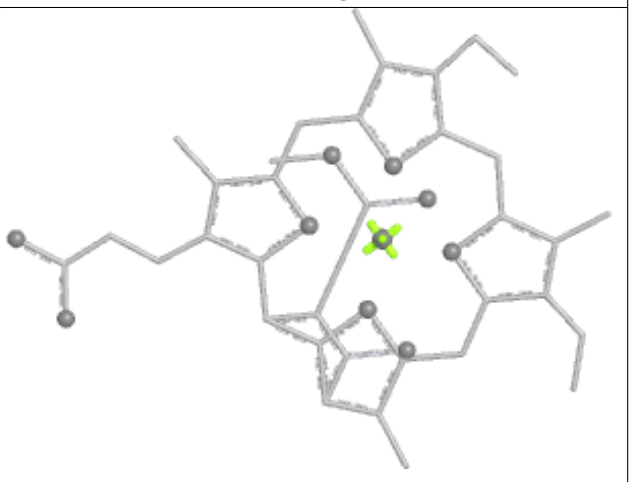
Bond lengths



Bond angles

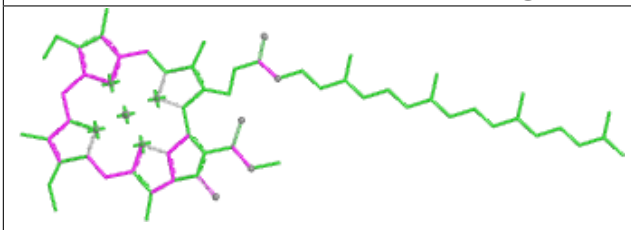


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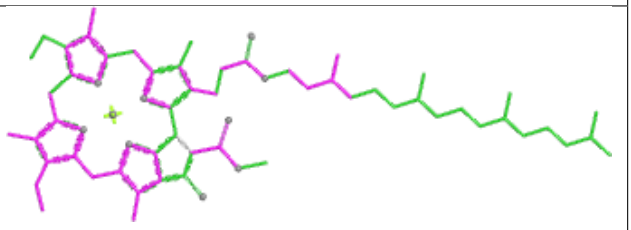


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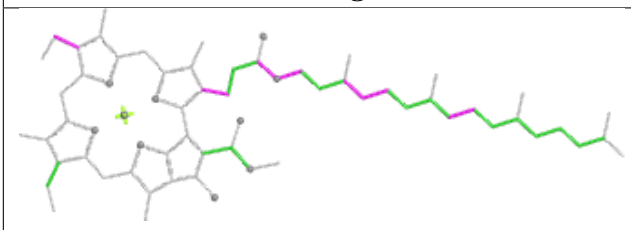
Ligand CLA 12 310



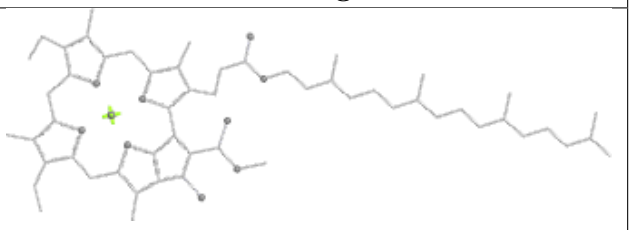
Bond lengths



Bond angles

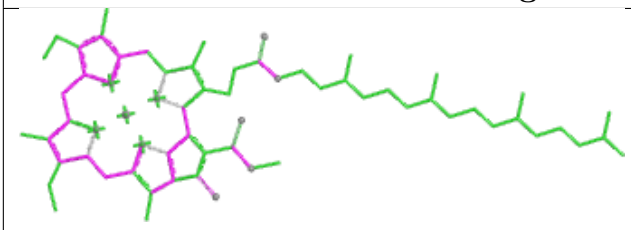


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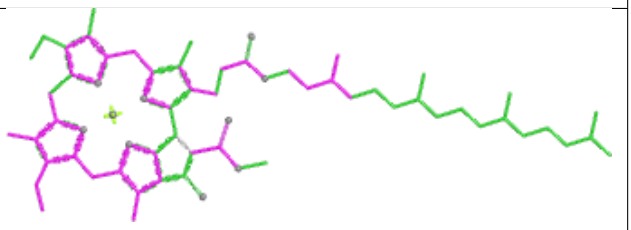


Rings

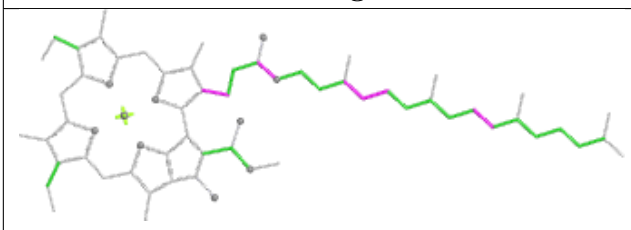
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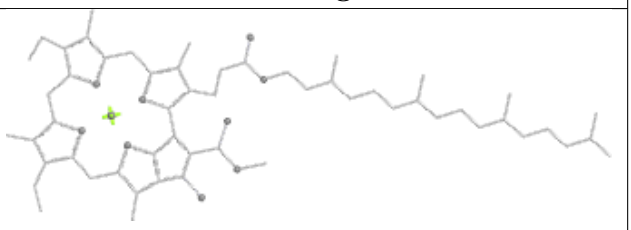
Bond lengths



Bond angles

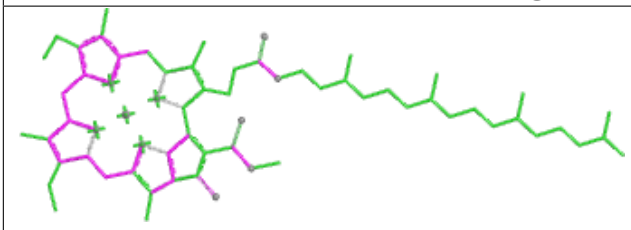


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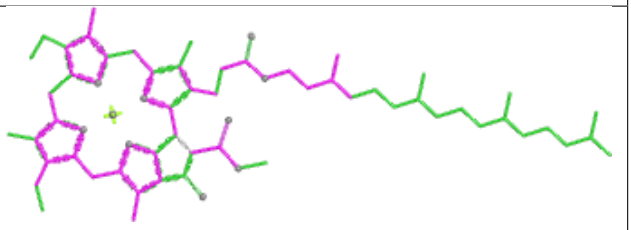


Rings

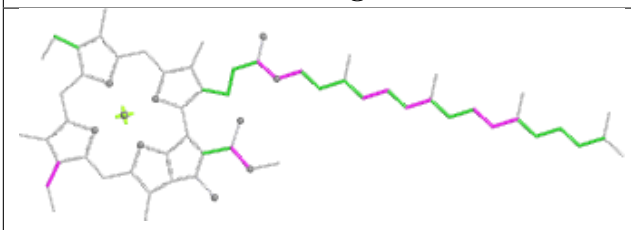
Ligand CLA 3 307



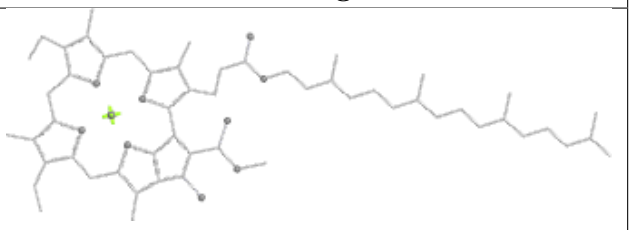
Bond lengths



Bond angles

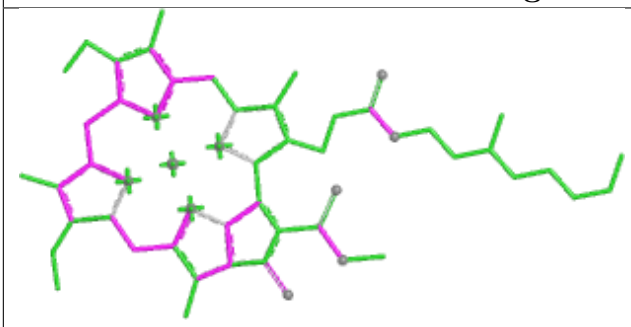


Torsions

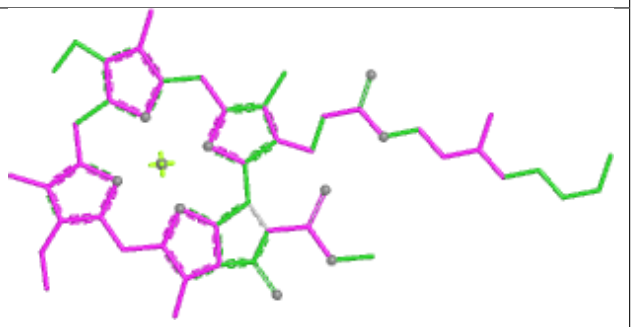


Rings

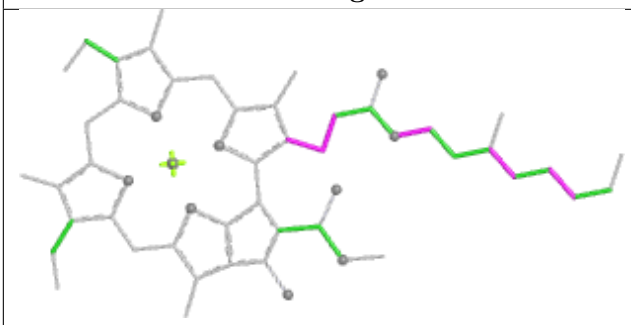
Ligand CLA A 818



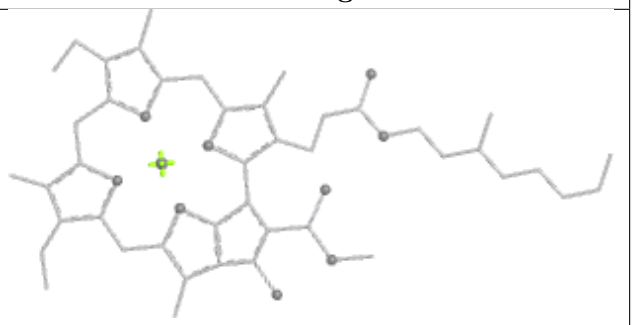
Bond lengths



Bond angles

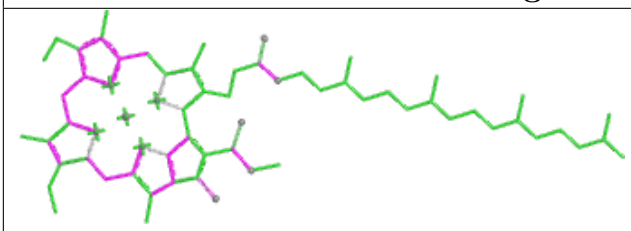


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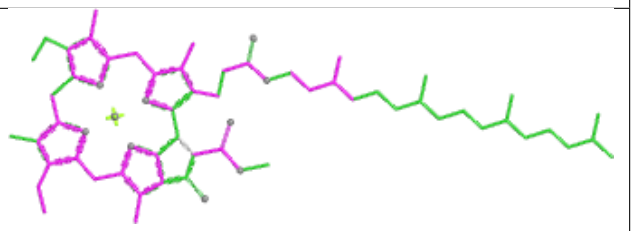


Rings

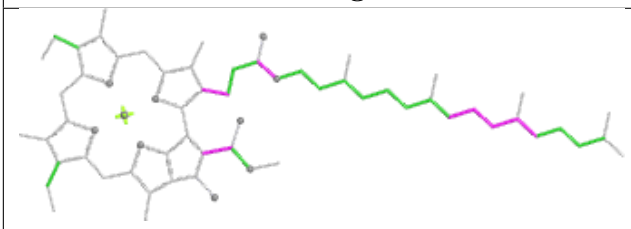
Ligand CLA A 804



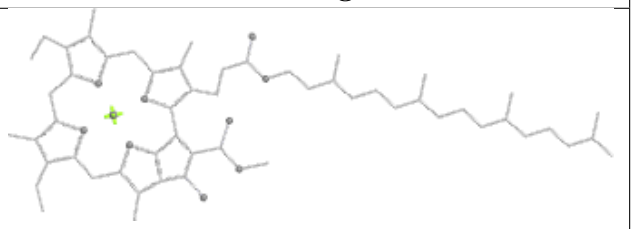
Bond lengths



Bond angles

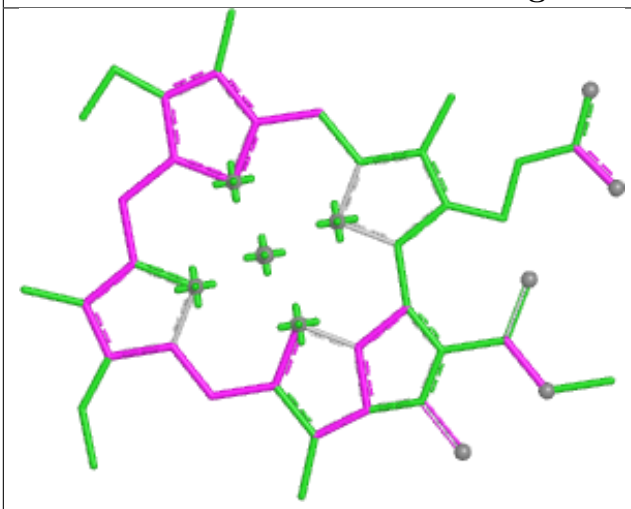


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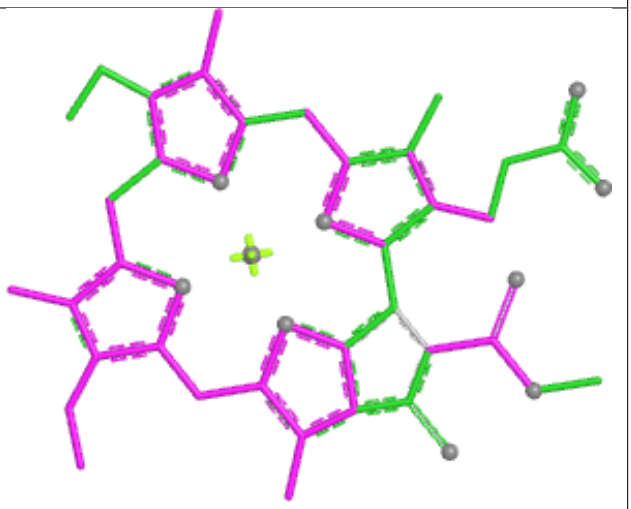


Rings

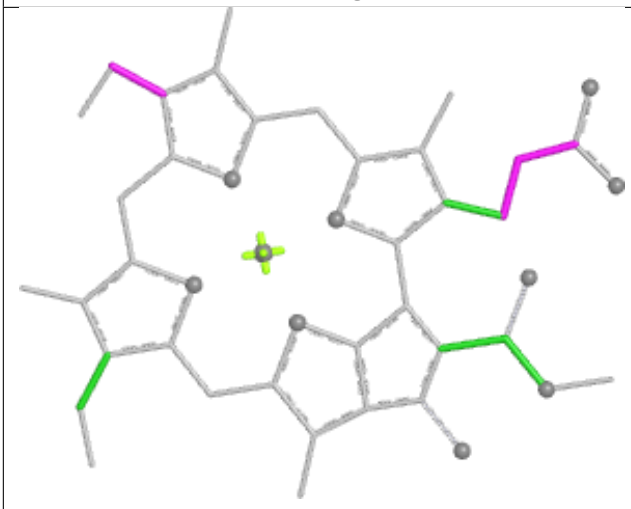
Ligand CLA 2 313



Bond lengths



Bond angles

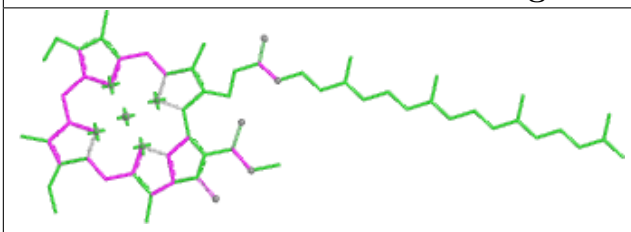


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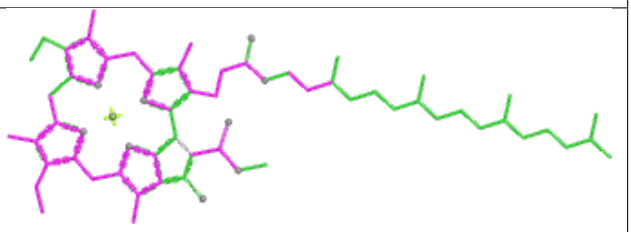


Rings

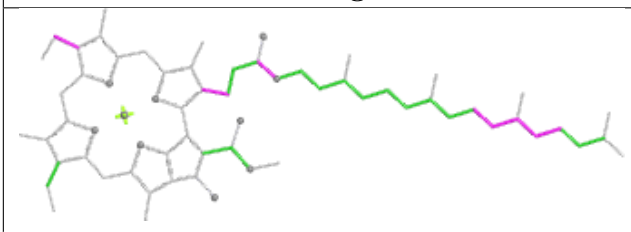
Ligand CLA 6 304



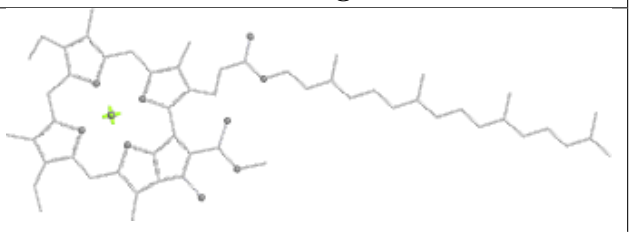
Bond lengths



Bond angles

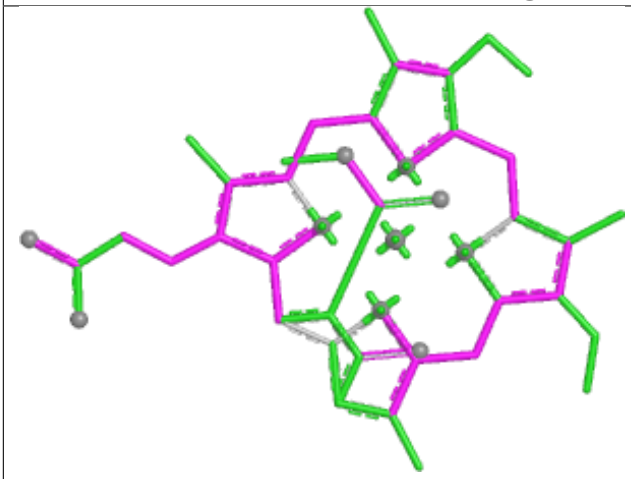


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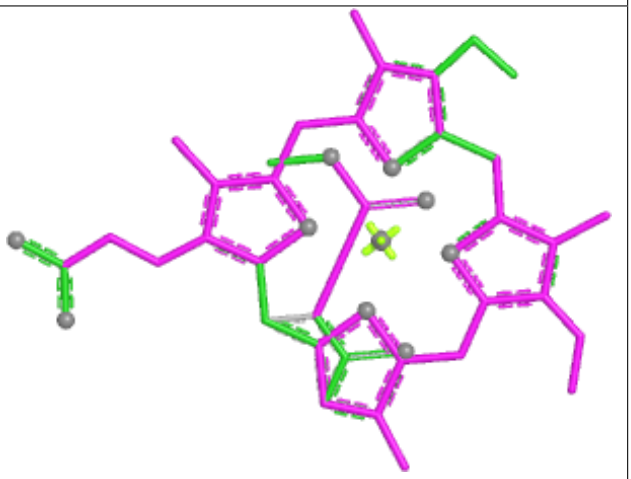


Rings

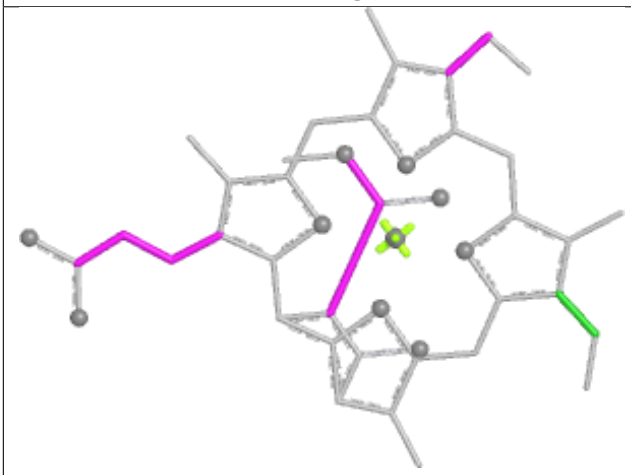
Ligand KC1 11 307



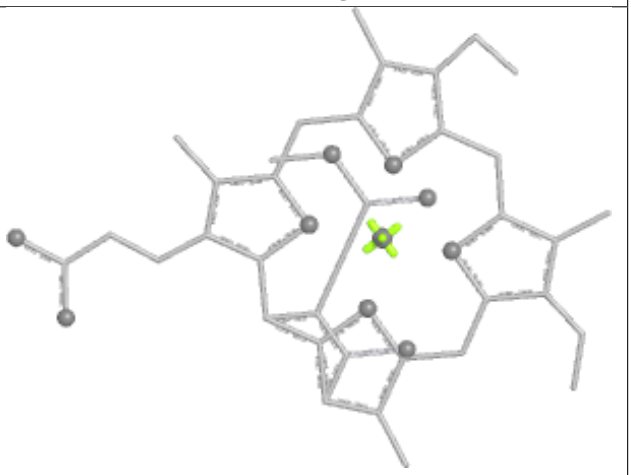
Bond lengths



Bond angles

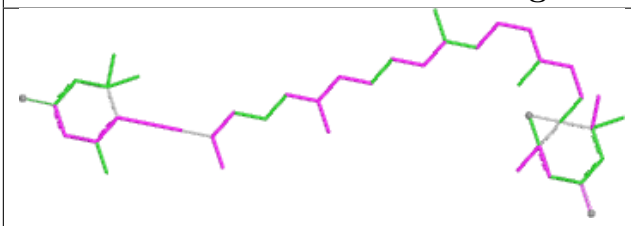


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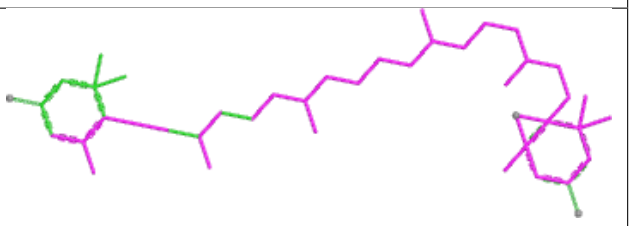


Rings

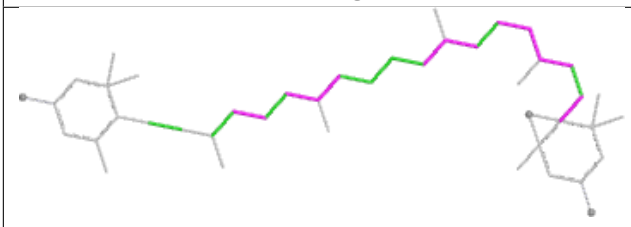
Ligand DD6 7 318



Bond lengths



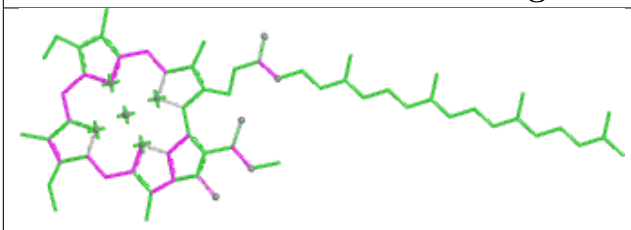
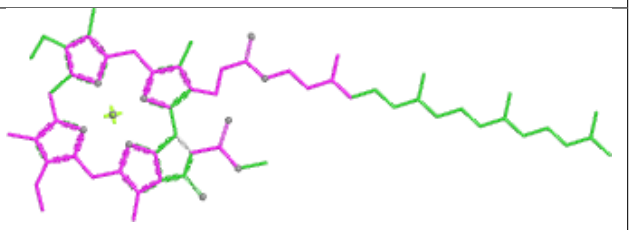
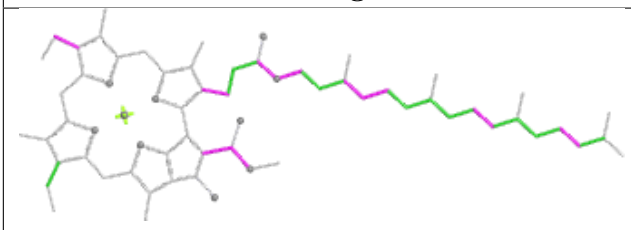
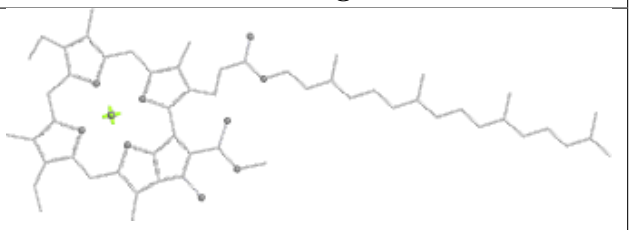
Bond angles

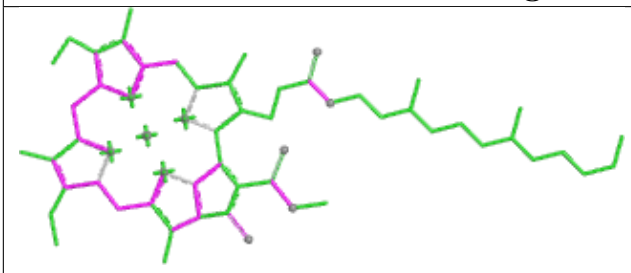
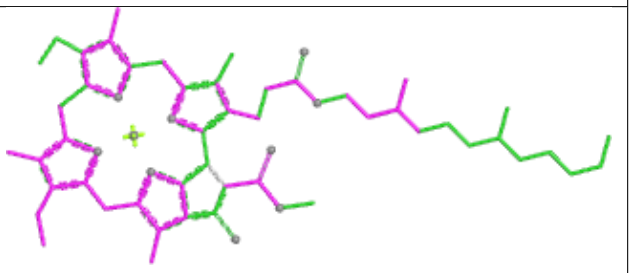
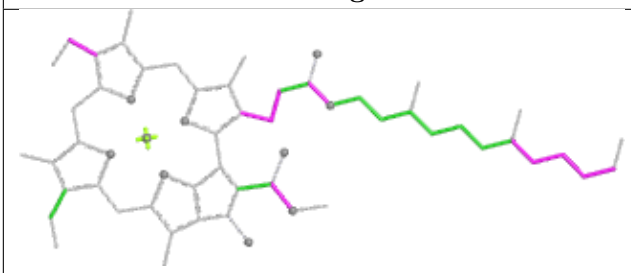
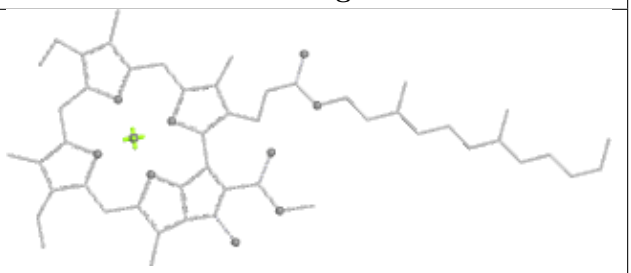


Torsions

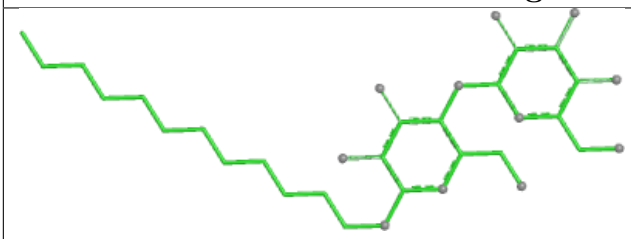


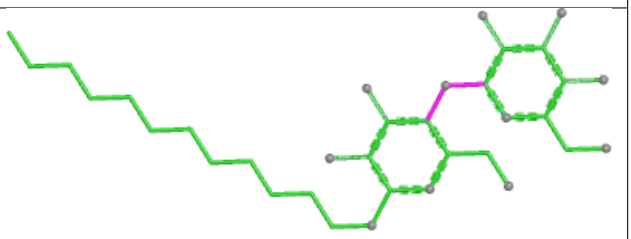
Rings

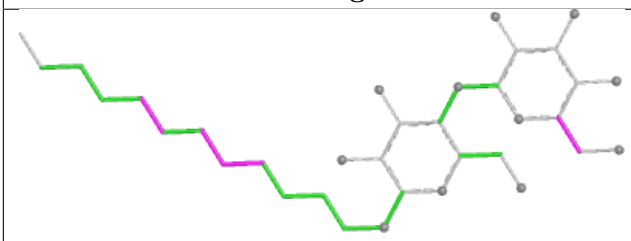
Ligand CLA 6 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

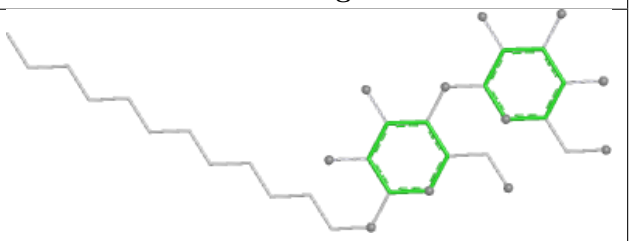
Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT 7 321

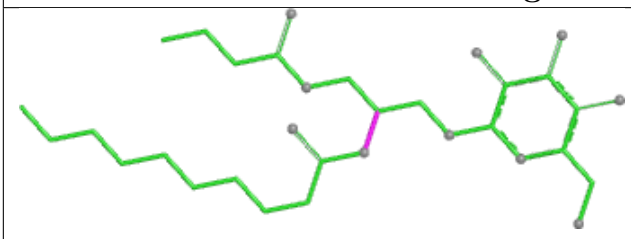

Bond lengths

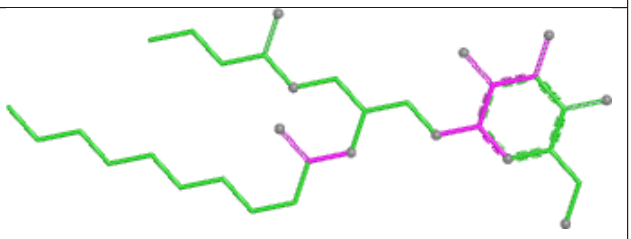

Bond angles

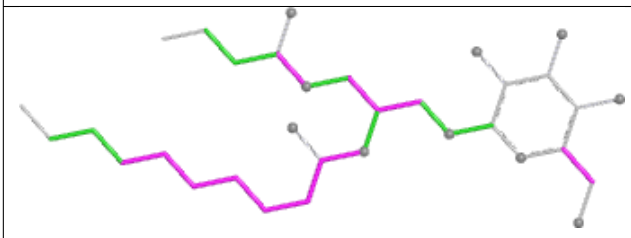

Torsions

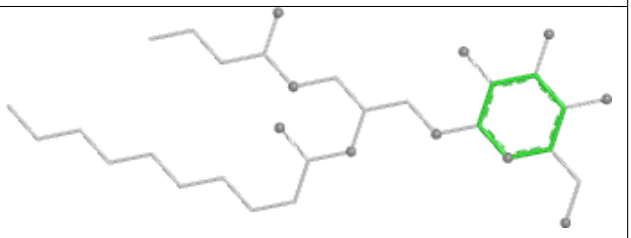

Rings

Ligand LMG 6 301

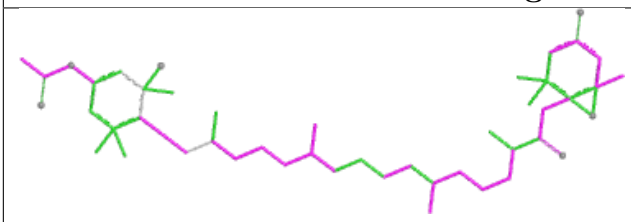

Bond lengths

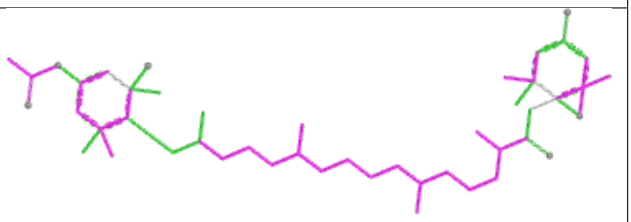

Bond angles

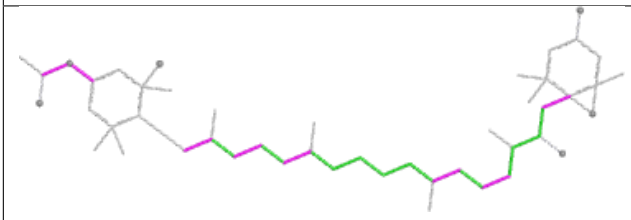

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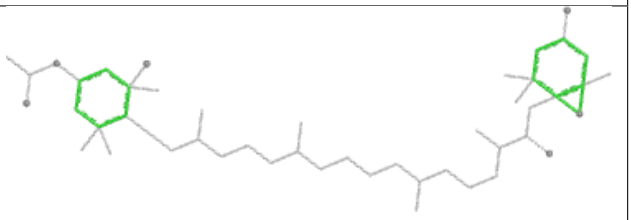

Rings

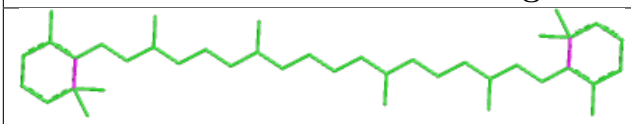
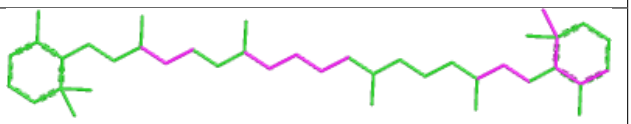
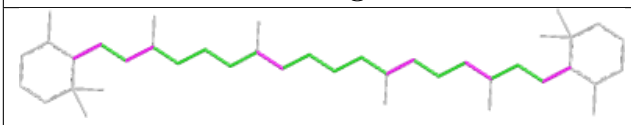
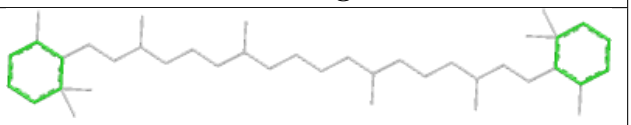
Ligand A86 11 315

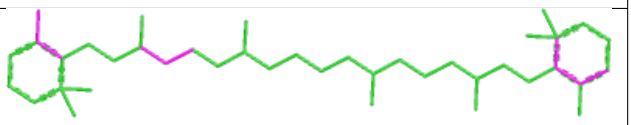
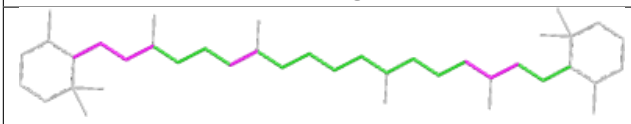
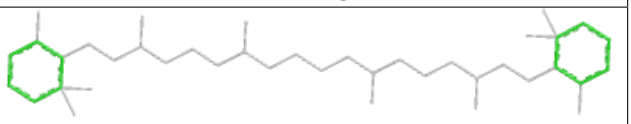

Bond lengths


Bond angles

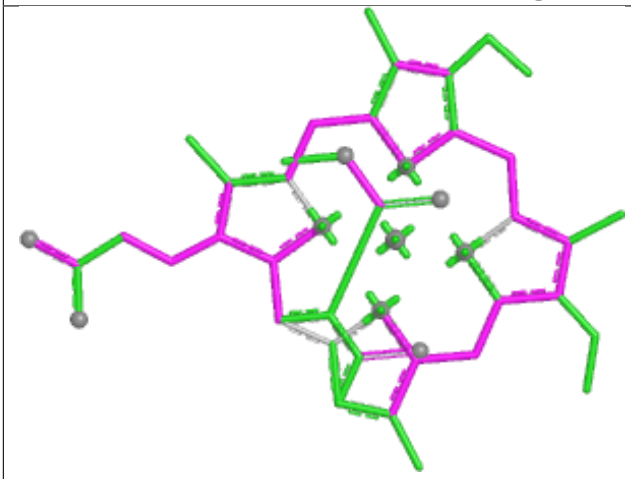

Torsions


Rings

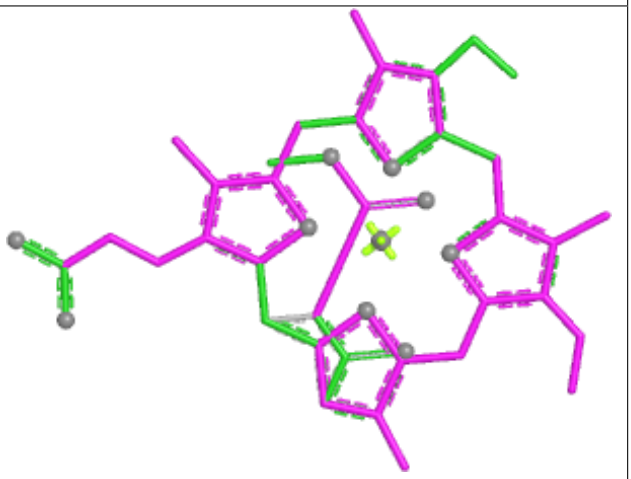
Ligand BCR B 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

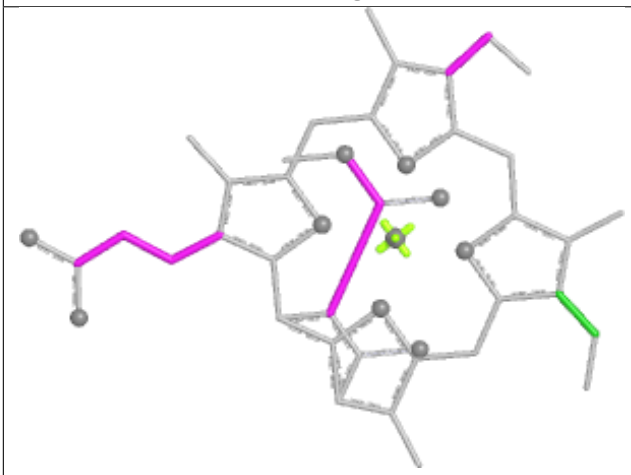
Ligand KC1 5 306



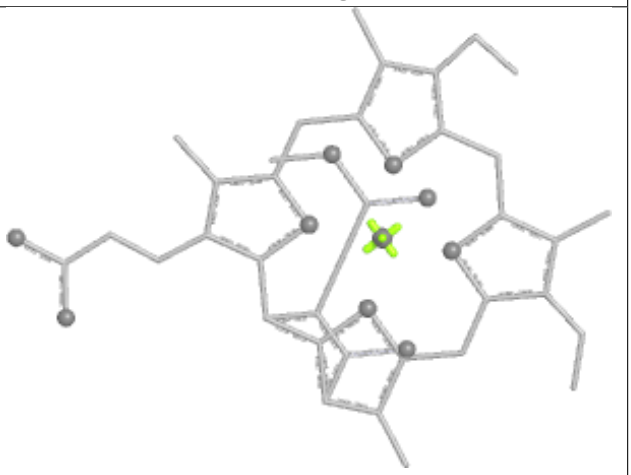
Bond lengths



Bond angles

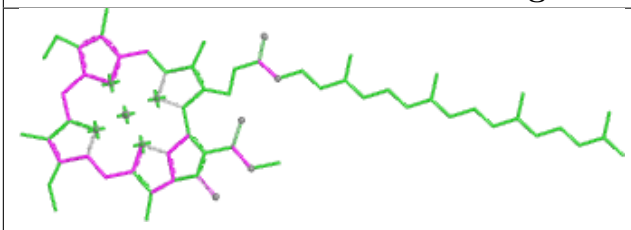


Torsions

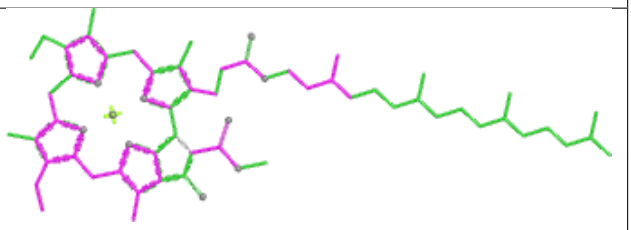


Rings

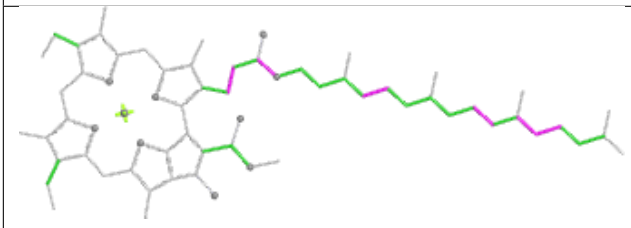
Ligand CLA 6 310



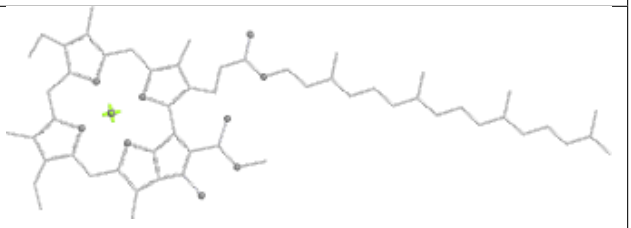
Bond lengths



Bond angles

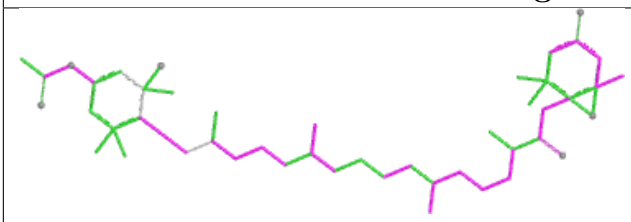


Torsions

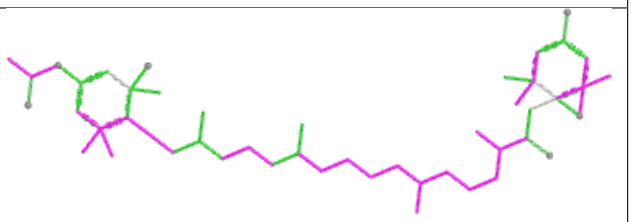


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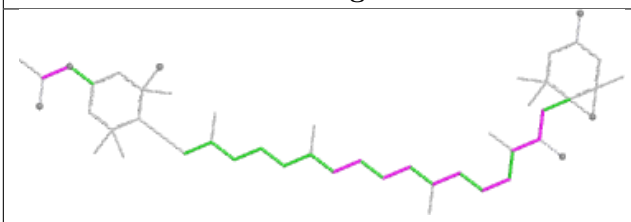
Ligand A86 2 319



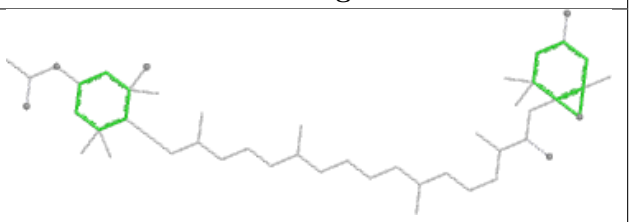
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Bond angles

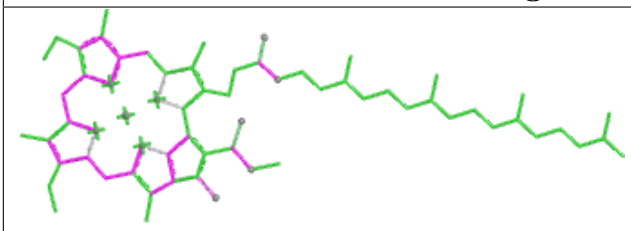


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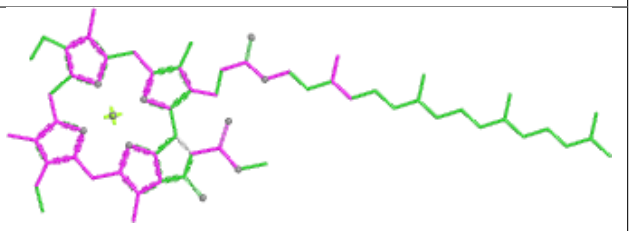


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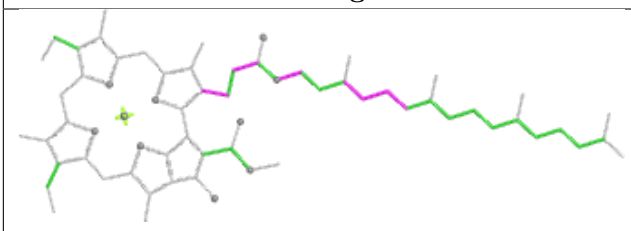
Ligand CLA B 812



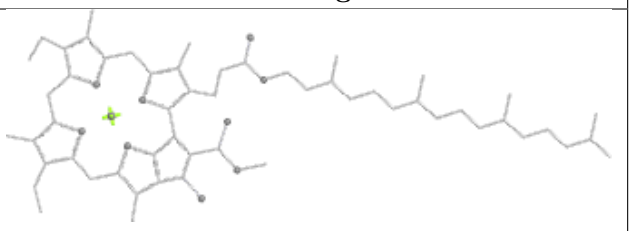
Bond lengths



Bond angles

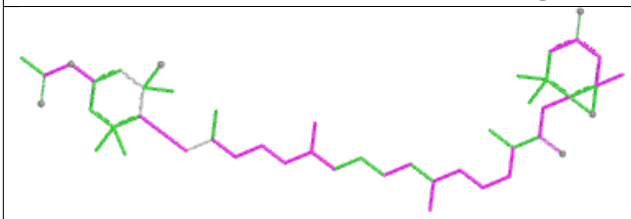


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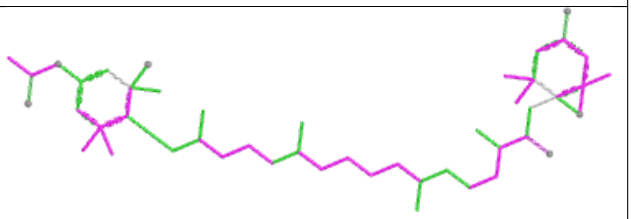


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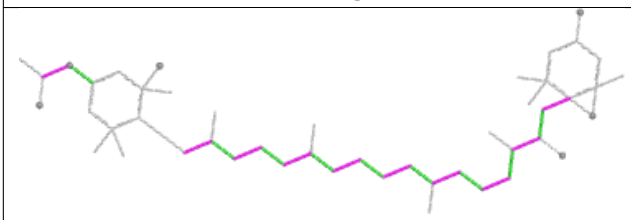
Ligand A86 7 315



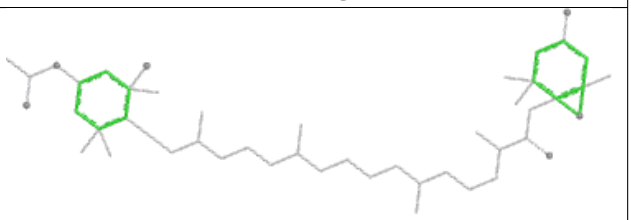
Bond lengths



Bond angles

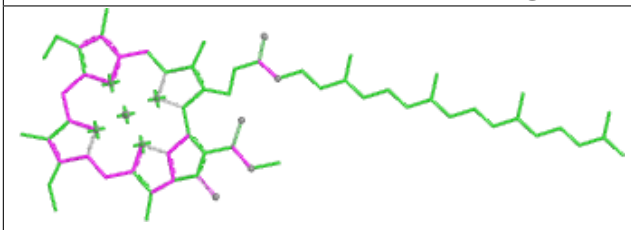


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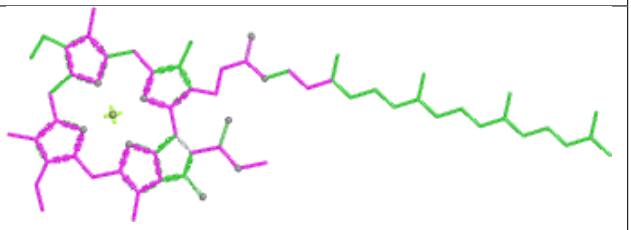


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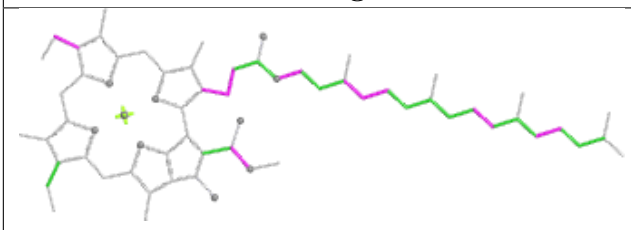
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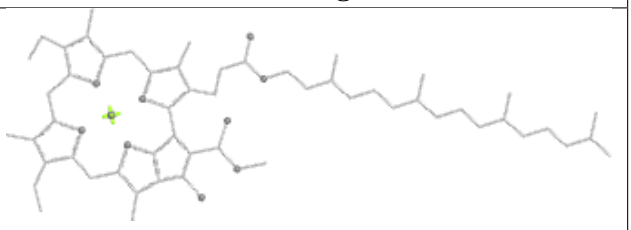
Bond lengths



Bond angles

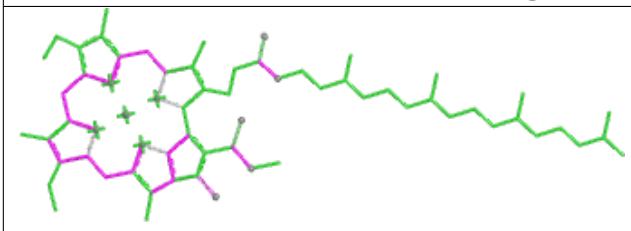


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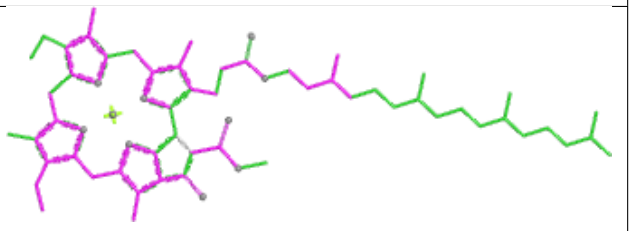


Rings

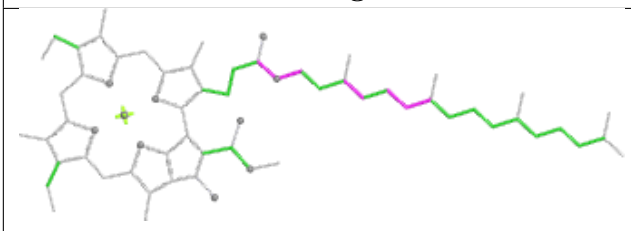
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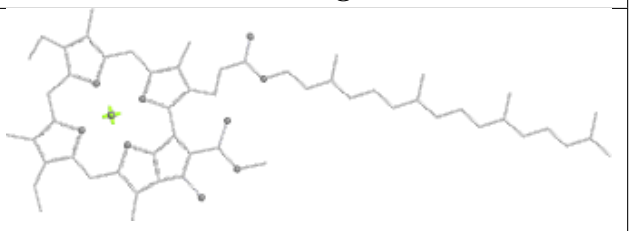
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Bond angles

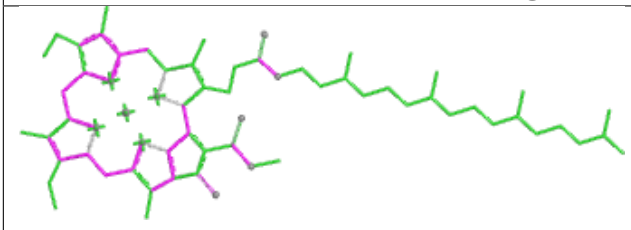


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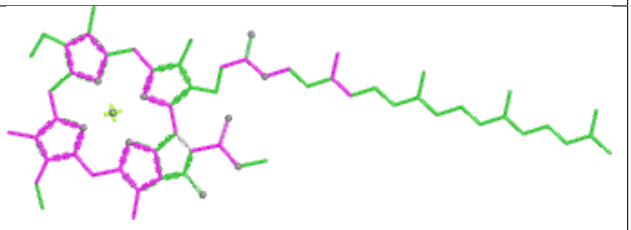


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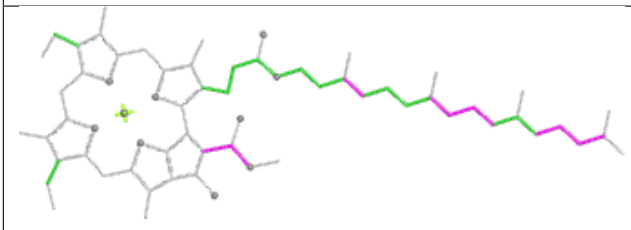
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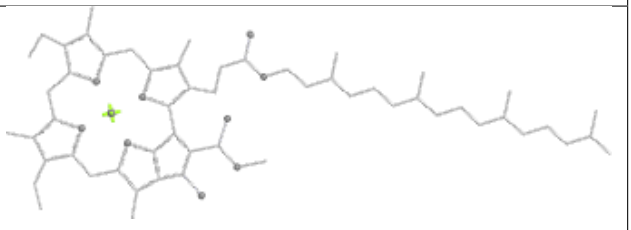
Bond lengths



Bond angles

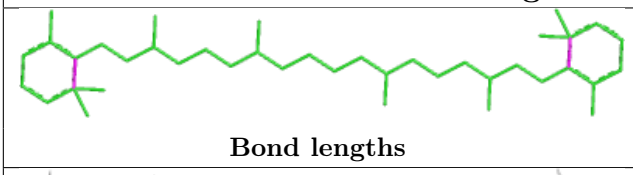


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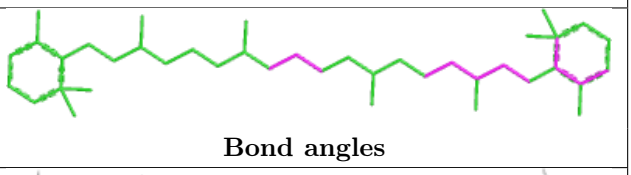


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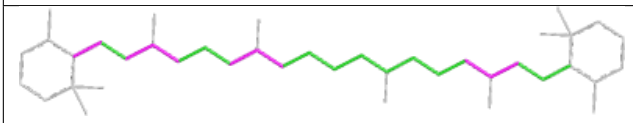
Ligand BCR B 845



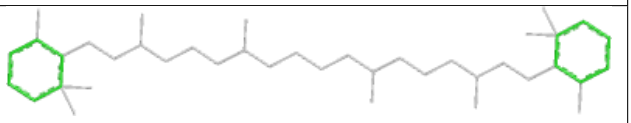
Bond lengths



Bond angles

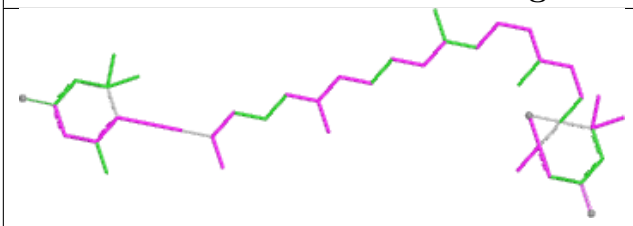


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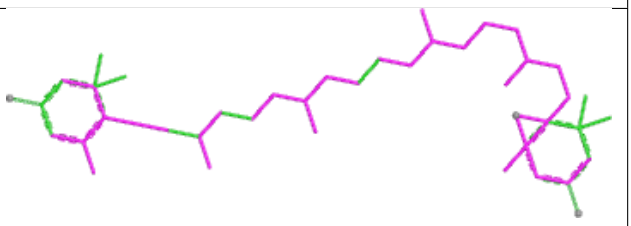


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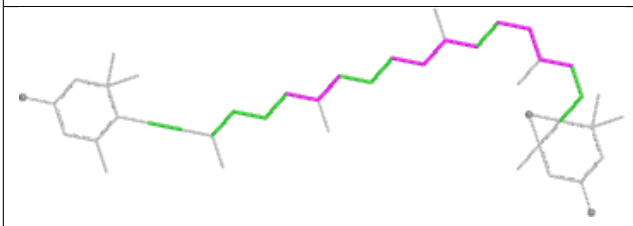
Ligand DD6 6 318



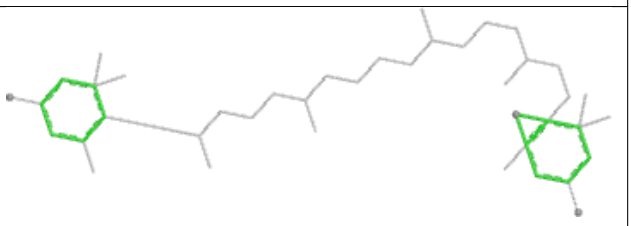
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Bond angles

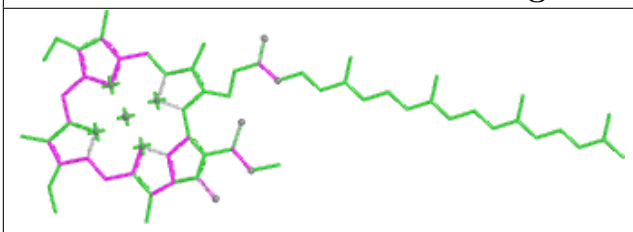


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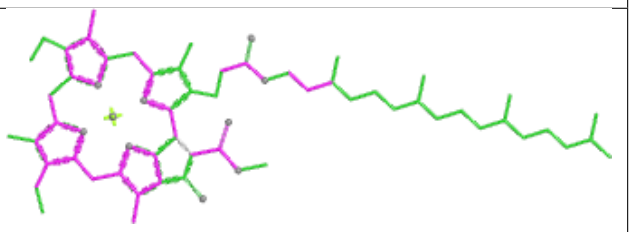


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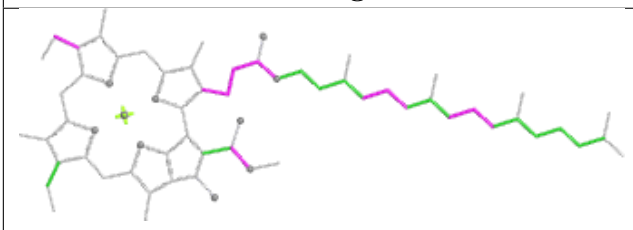
Ligand CLA 1 301



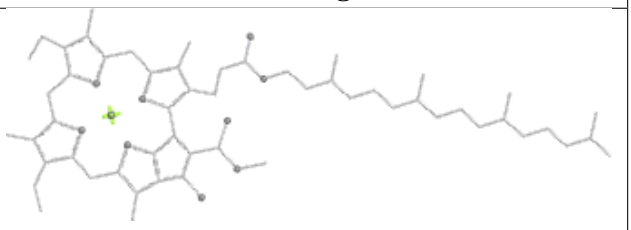
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Bond angles

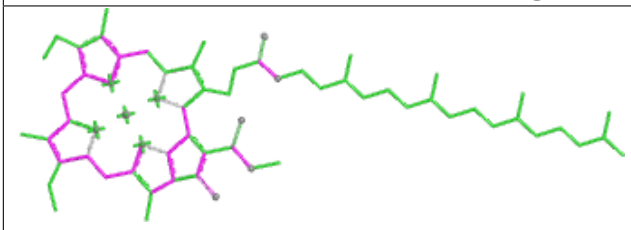


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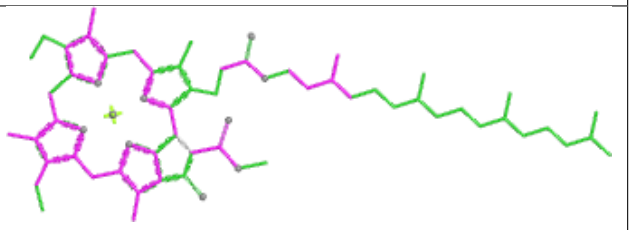


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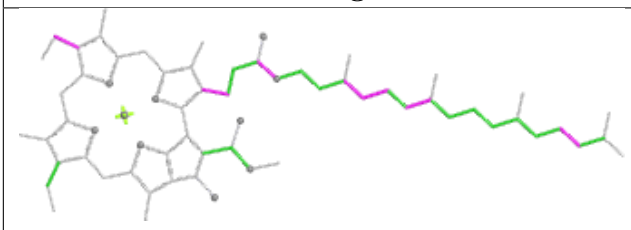
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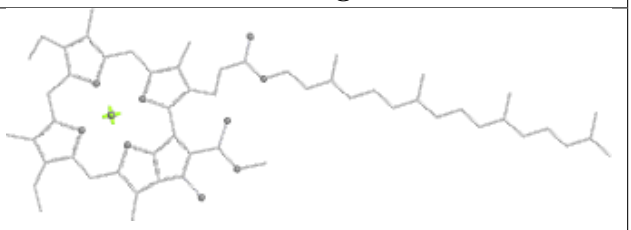
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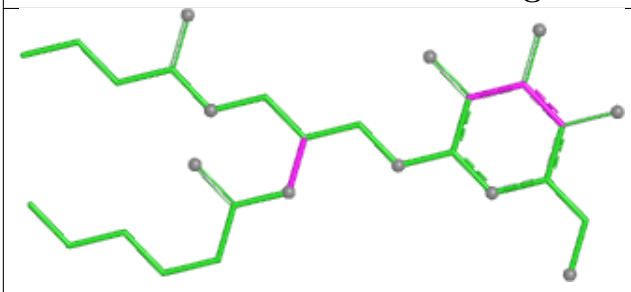


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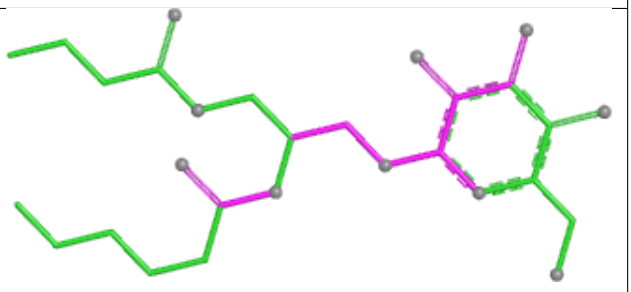


Rings

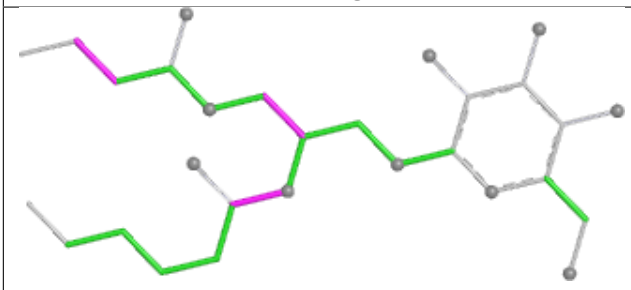
Ligand LMG 8 321



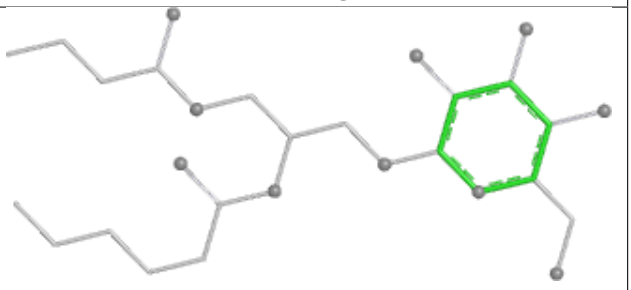
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Bond angles

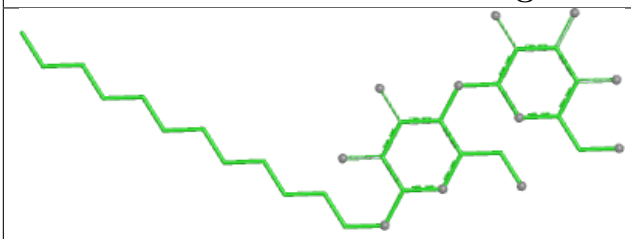


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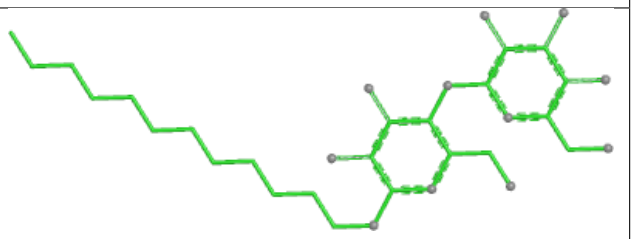


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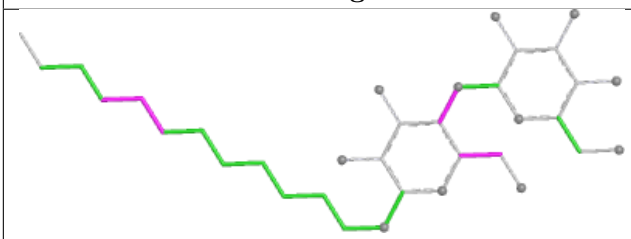
Ligand LMT 16 315



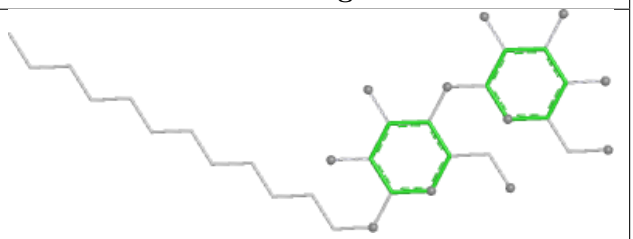
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Bond angles

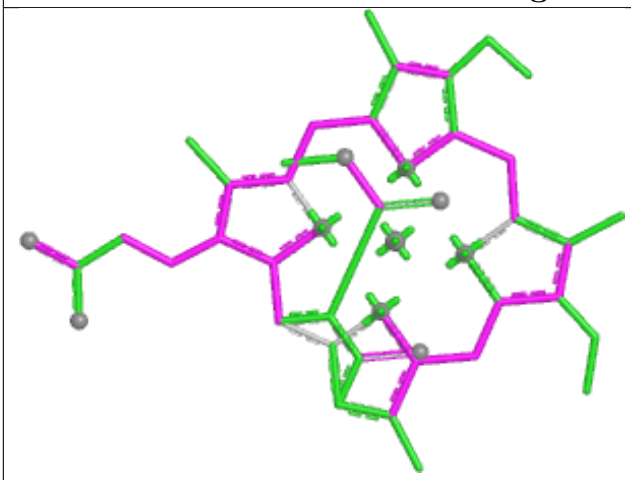


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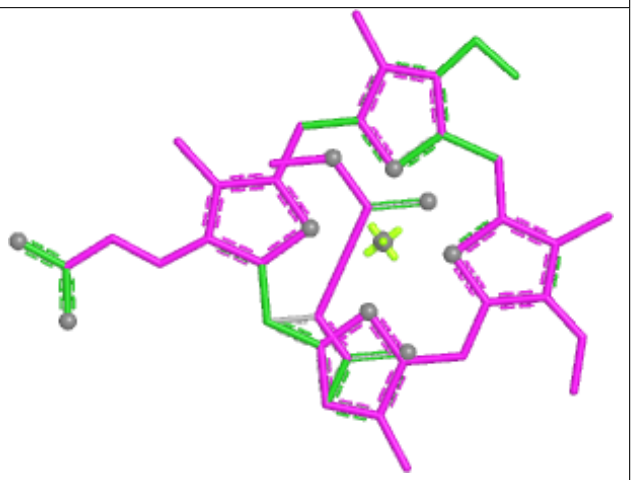


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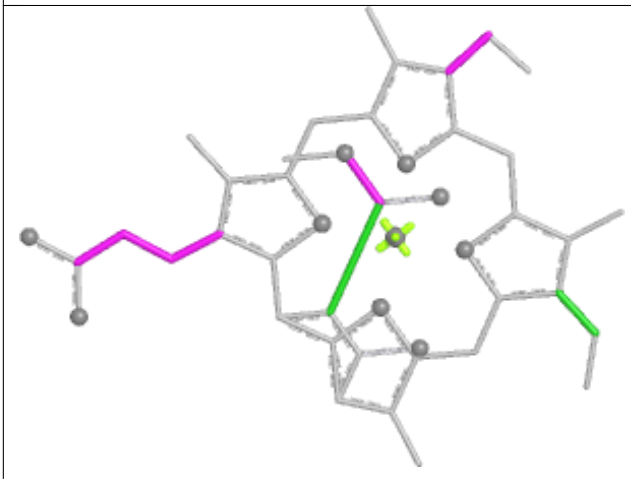
Ligand KC1 2 314



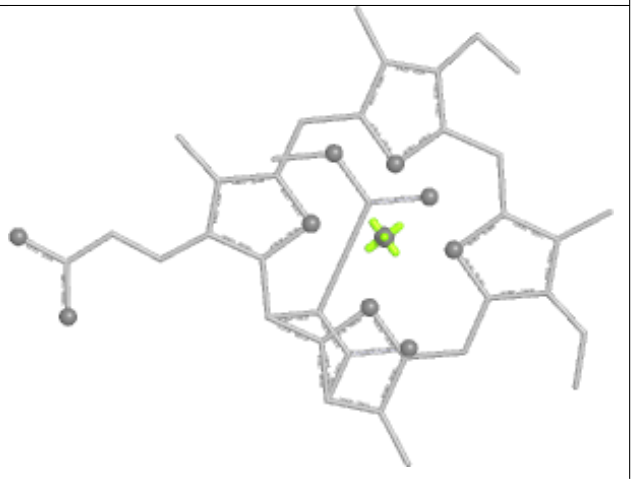
Bond lengths



Bond angles

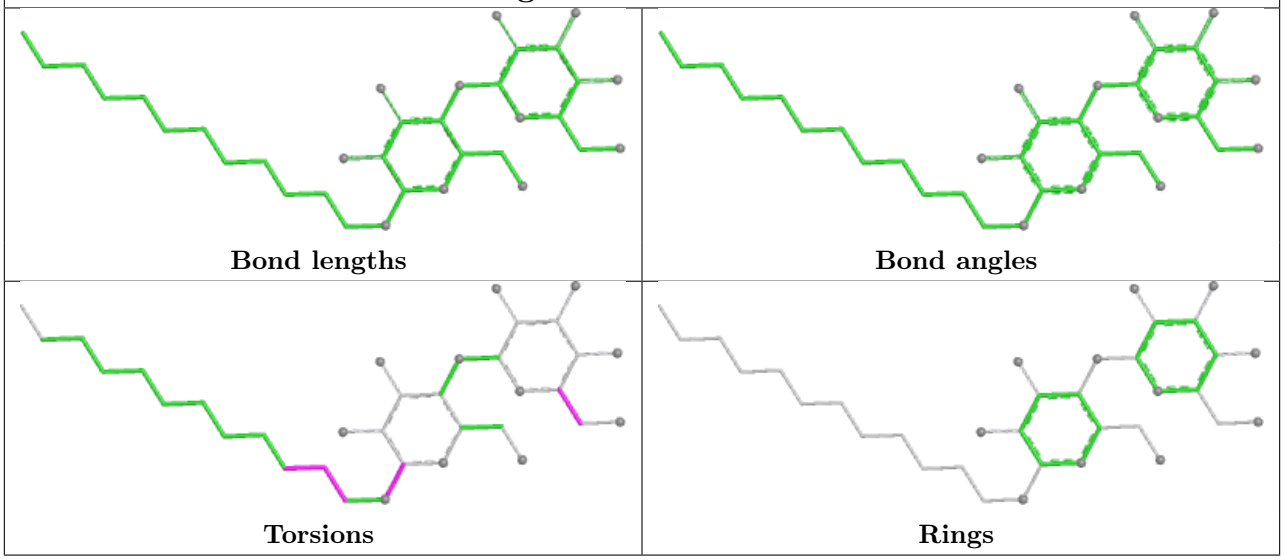


Torsions

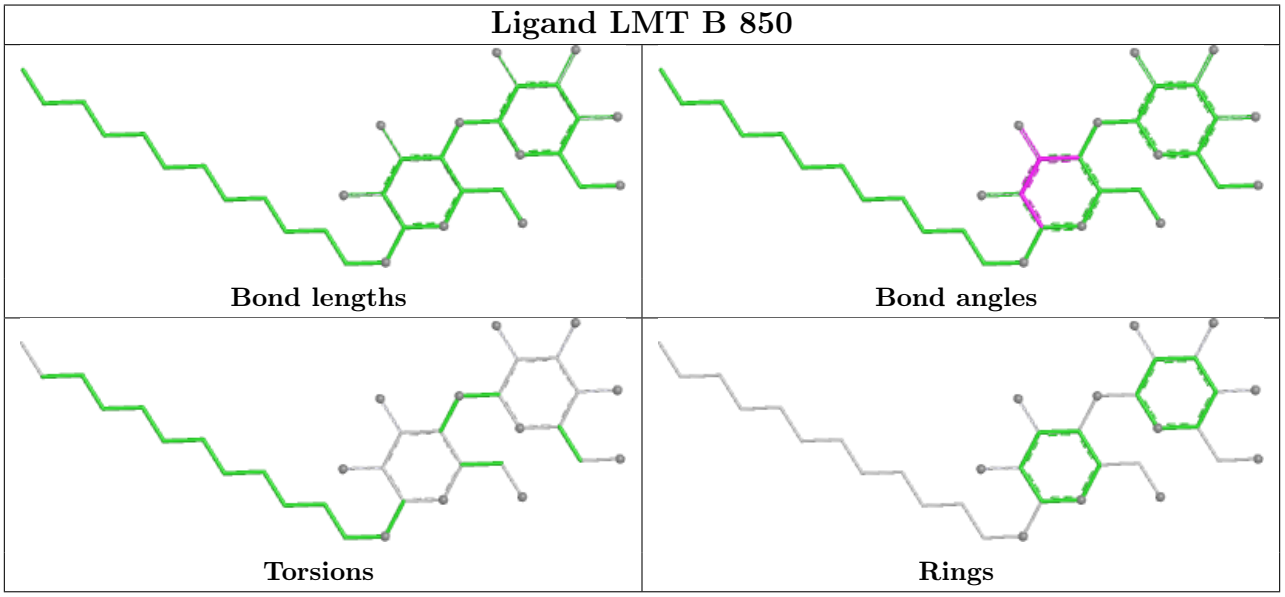


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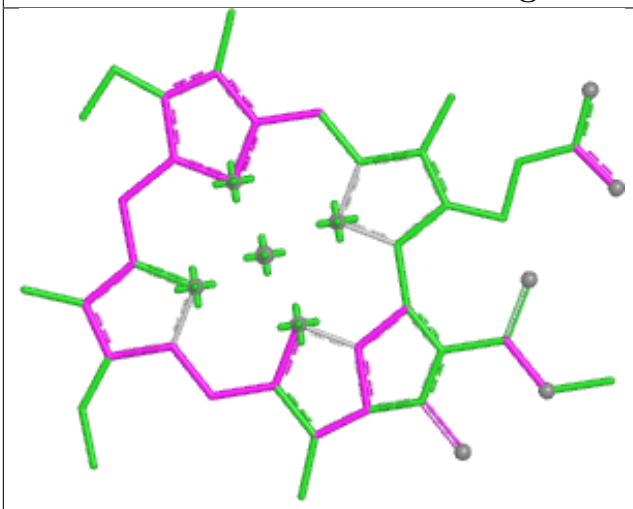
Ligand LMT 12 301



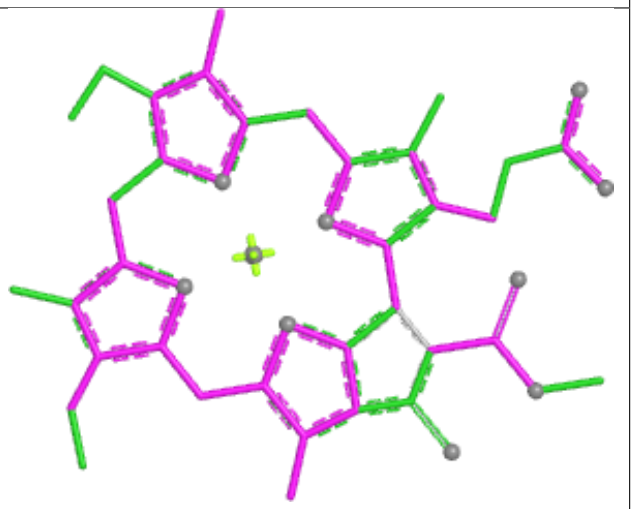
Ligand LMT B 850



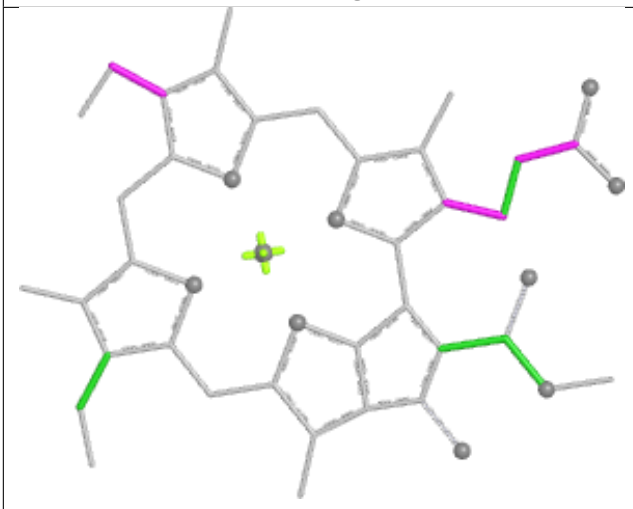
Ligand CLA 16 308



Bond lengths



Bond angles

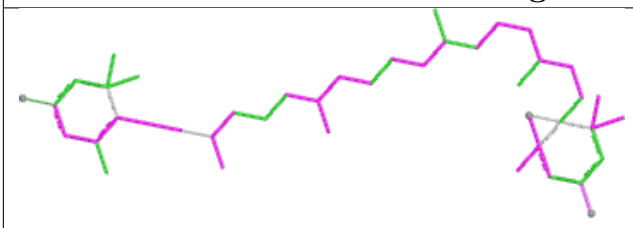


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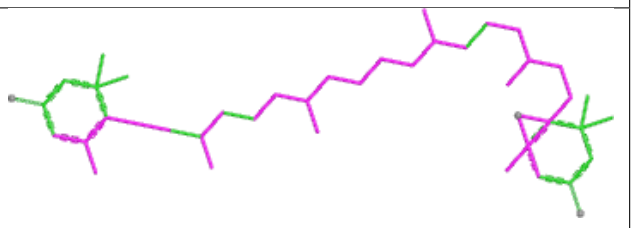


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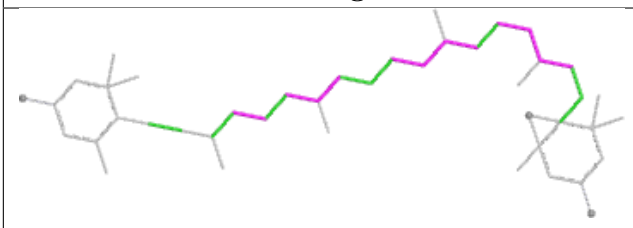
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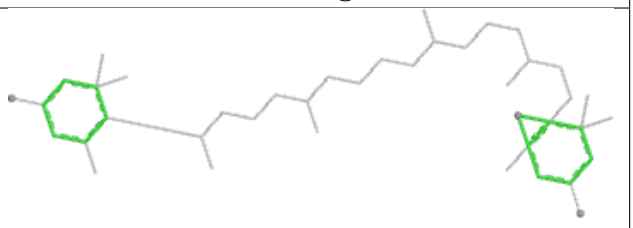
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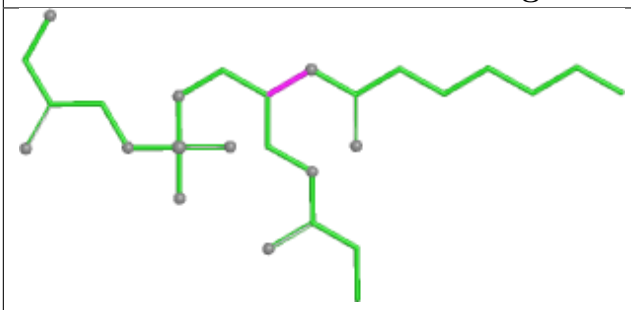
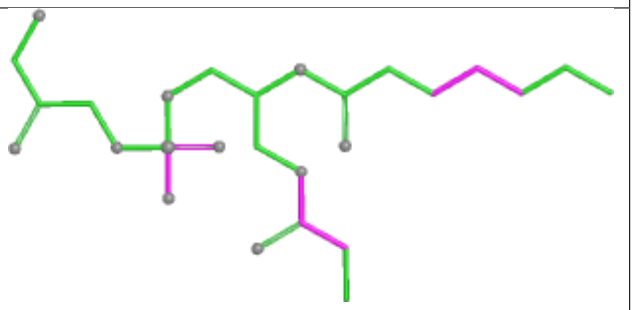
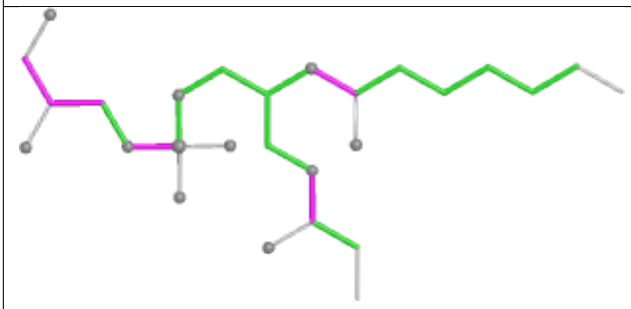
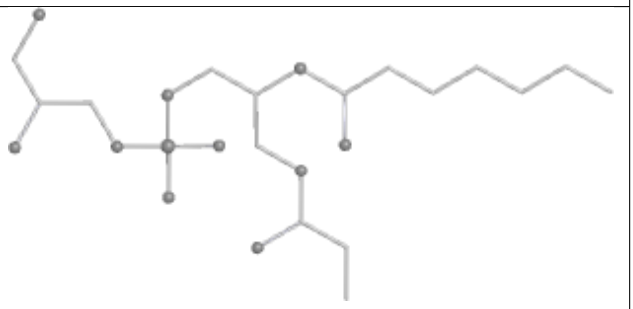
Bond angles

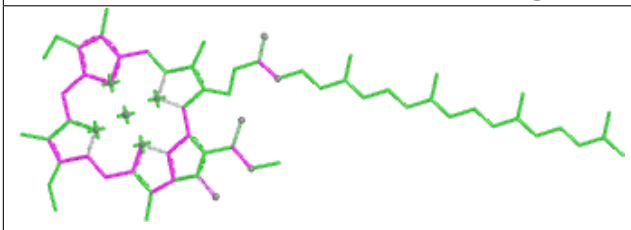
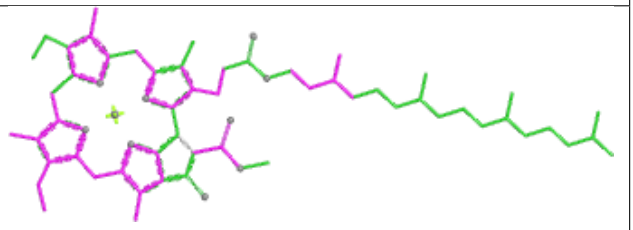
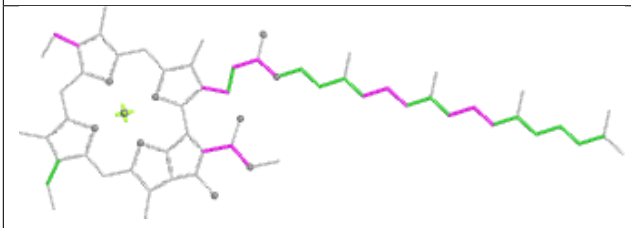
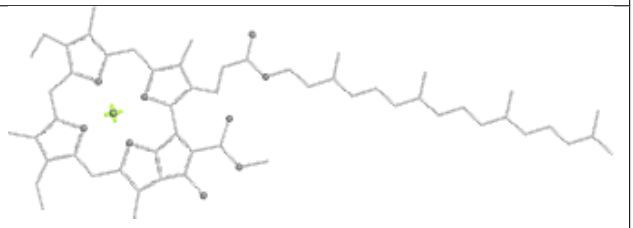


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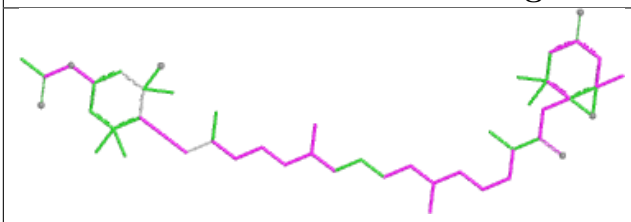


Rings

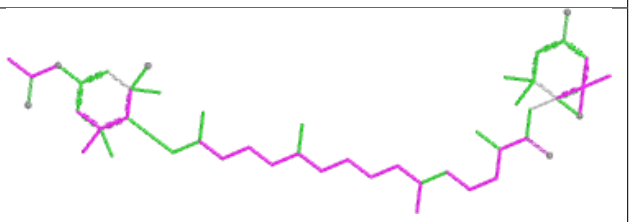
Ligand LHG A 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

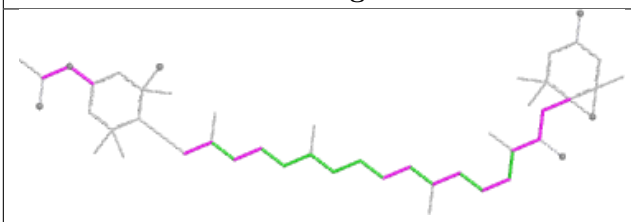
Ligand A86 12 316



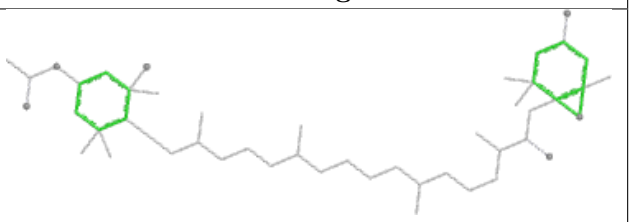
Bond lengths



Bond angles

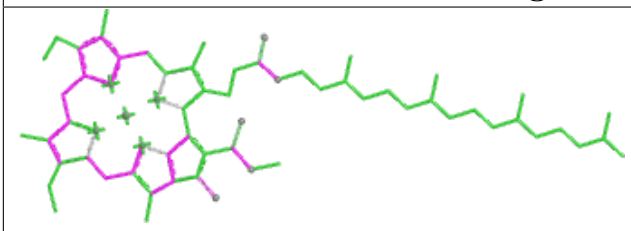


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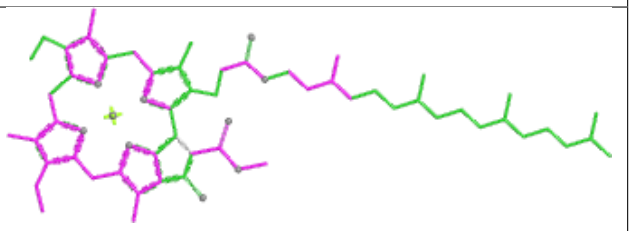


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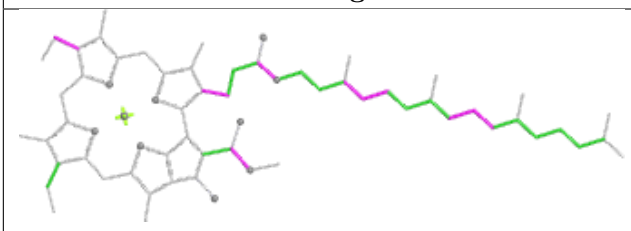
Ligand CLA 1 304



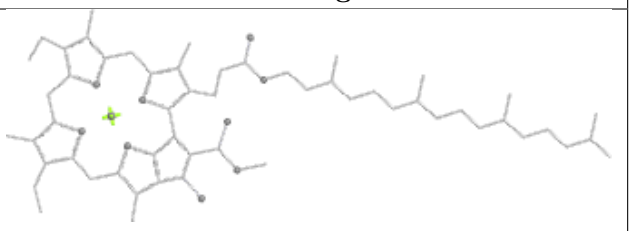
Bond lengths



Bond angles

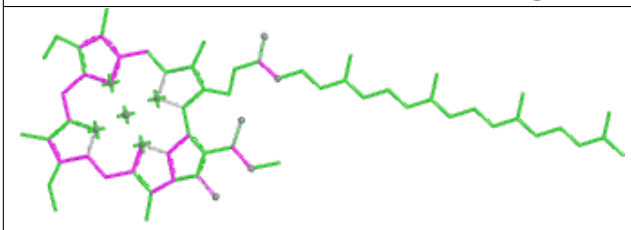


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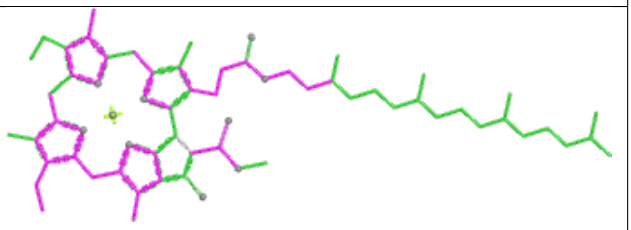


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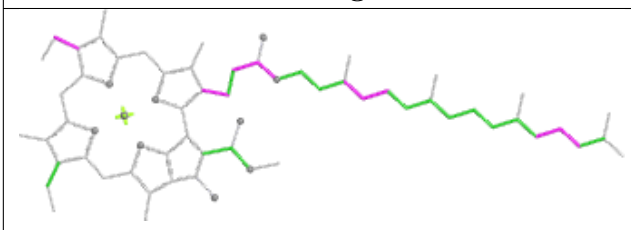
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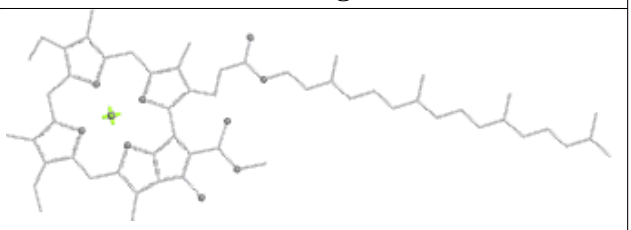
Bond lengths



Bond angles

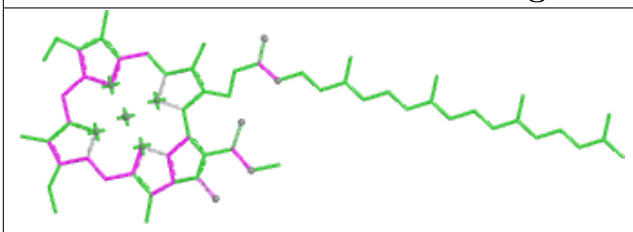


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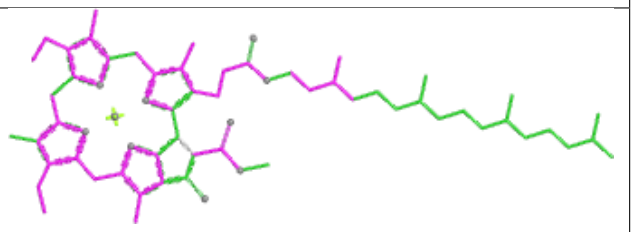


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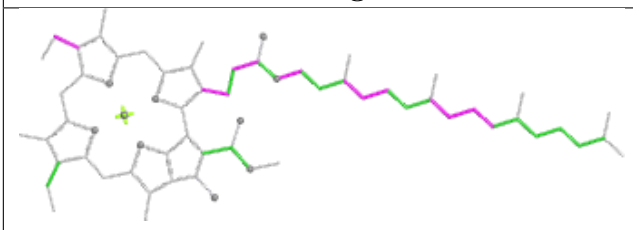
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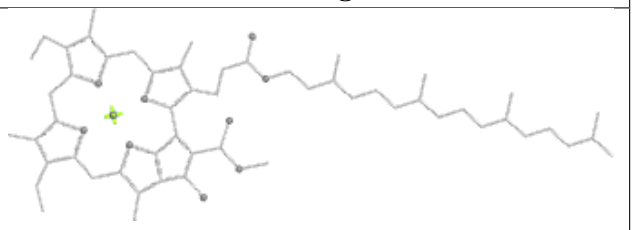
Bond lengths



Bond angles

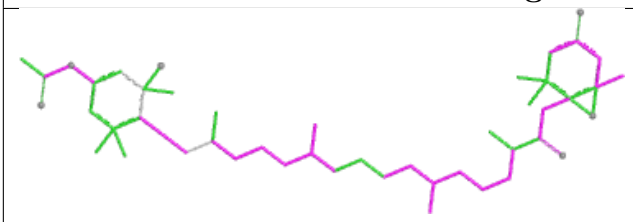


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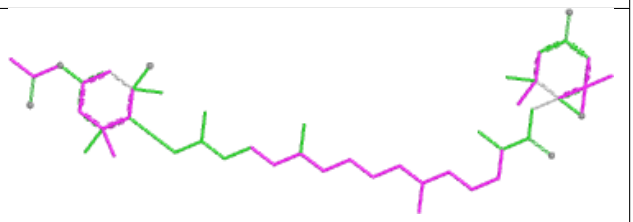


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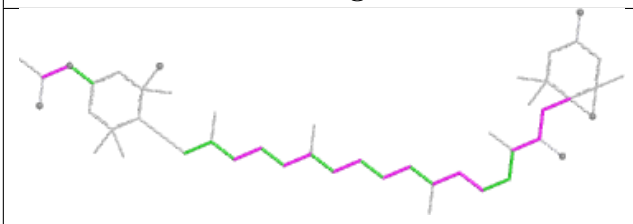
Ligand A86 15 320



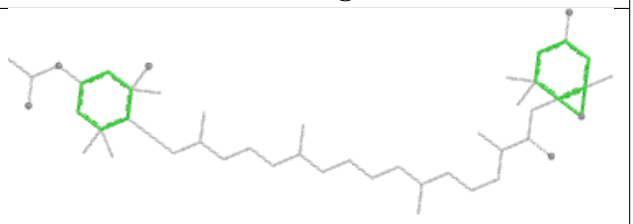
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Bond angles

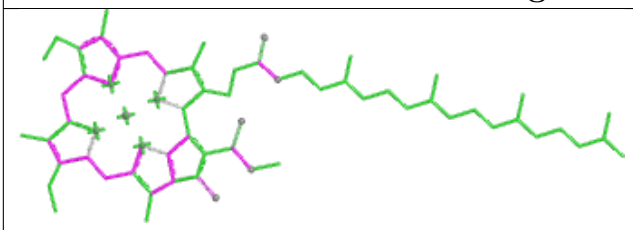


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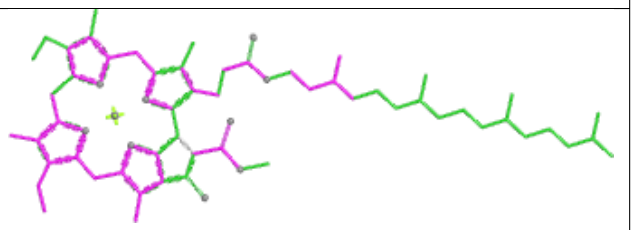


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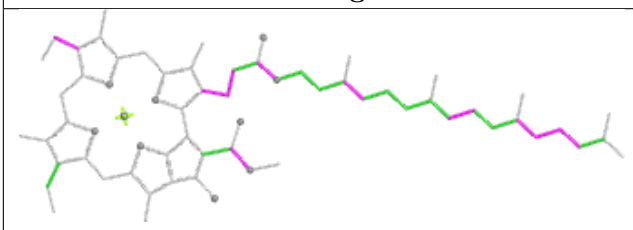
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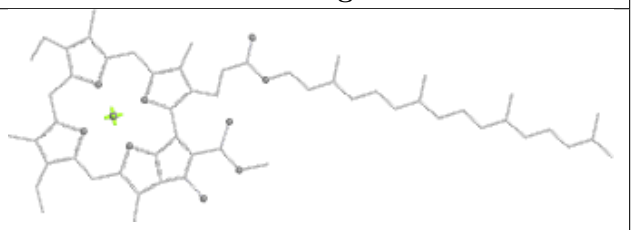
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Bond angles

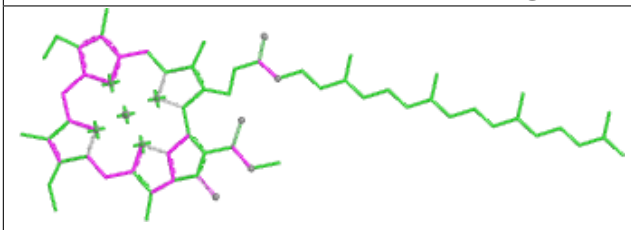


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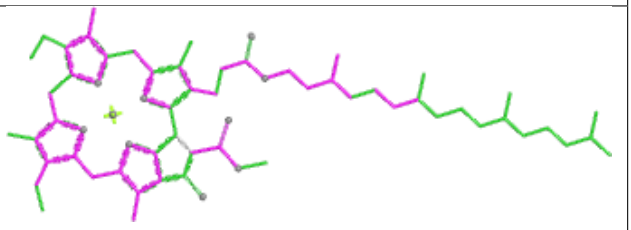


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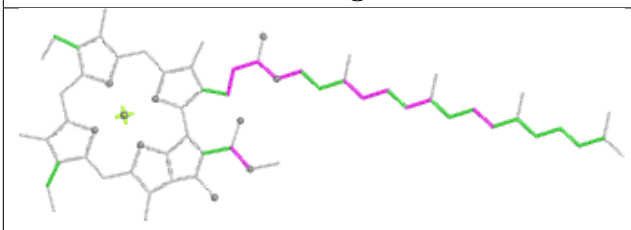
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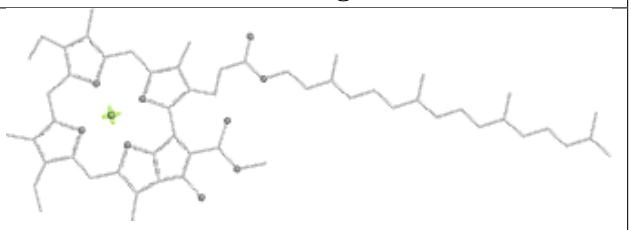
Bond lengths



Bond angles

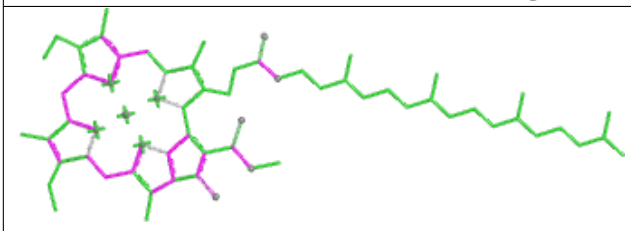


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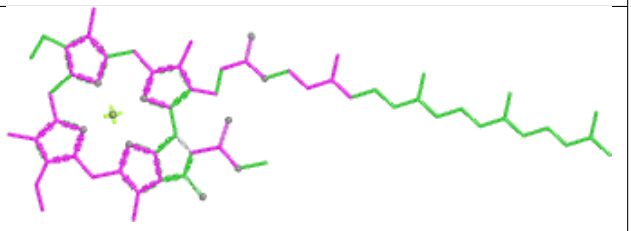


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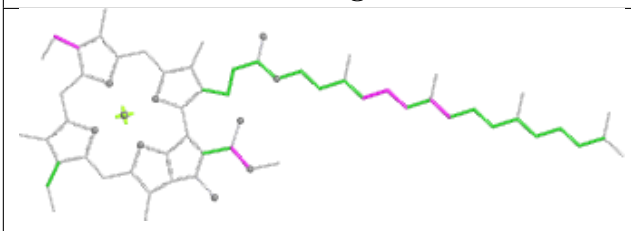
Ligand CLA B 801



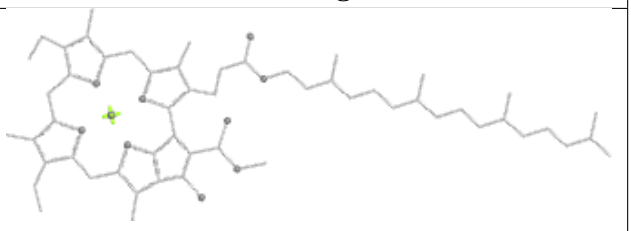
Bond lengths



Bond angles

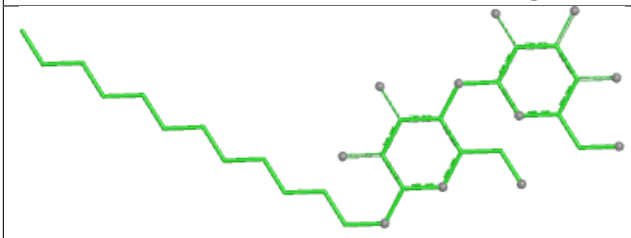


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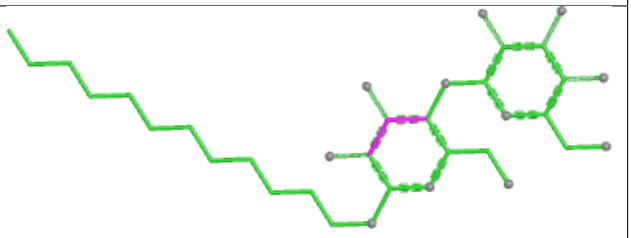


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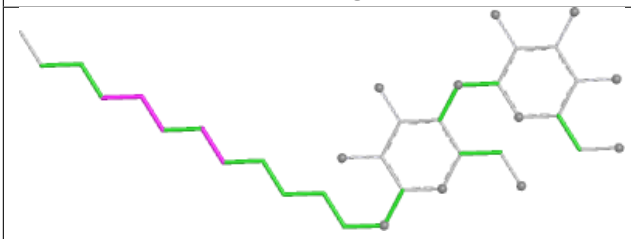
Ligand LMT 8 322



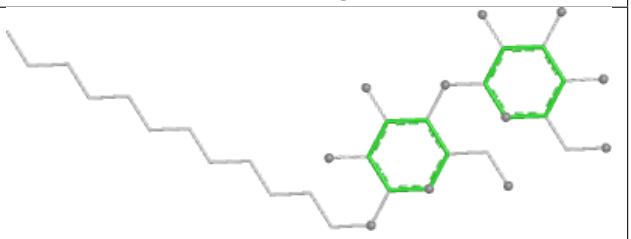
Bond lengths



Bond angles

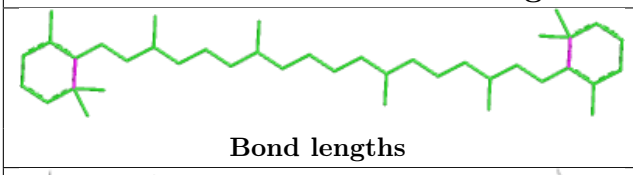


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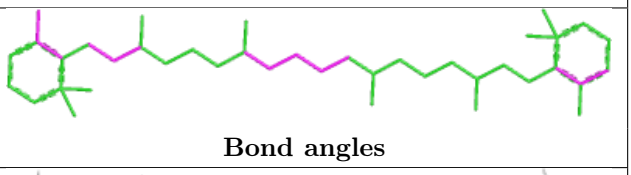


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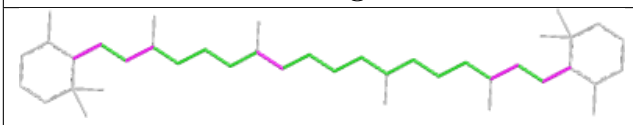
Ligand BCR L 205



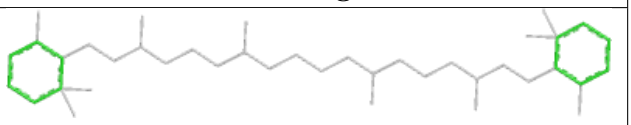
Bond lengths



Bond angles

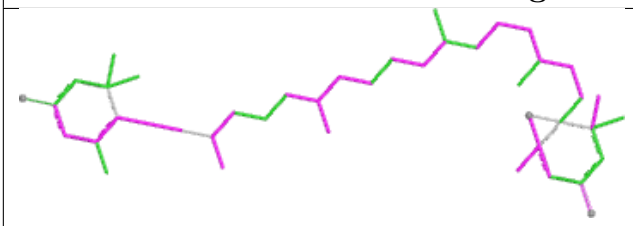


Torsions

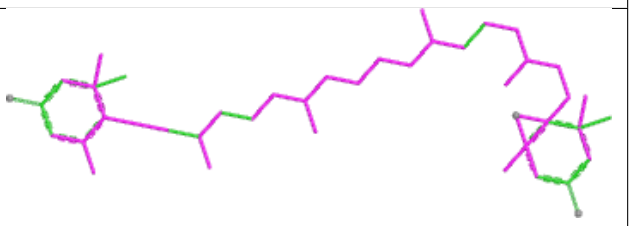


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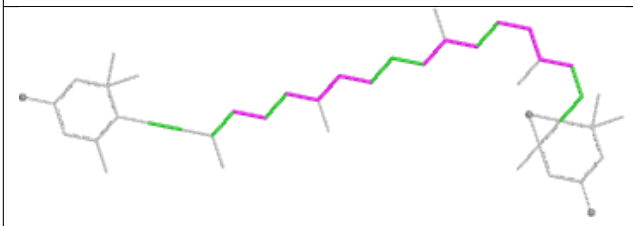
Ligand DD6 6 321



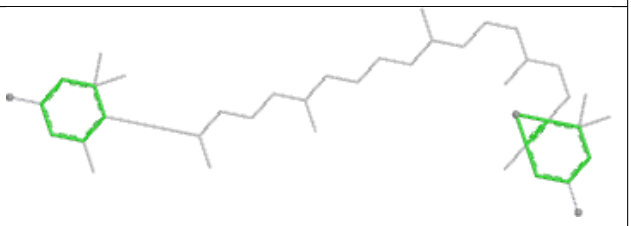
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Bond angles

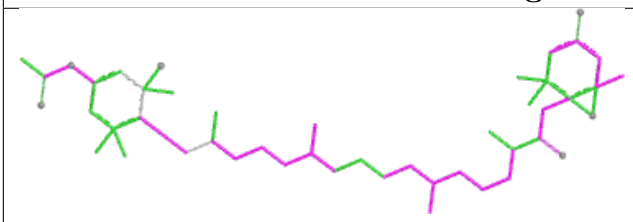


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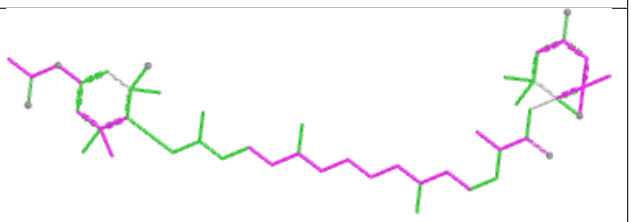


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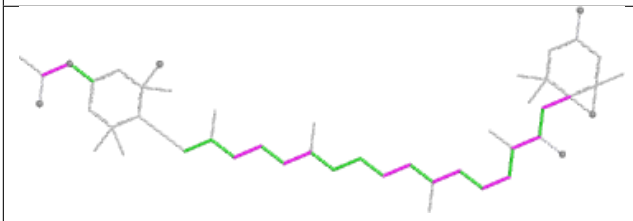
Ligand A86 15 316



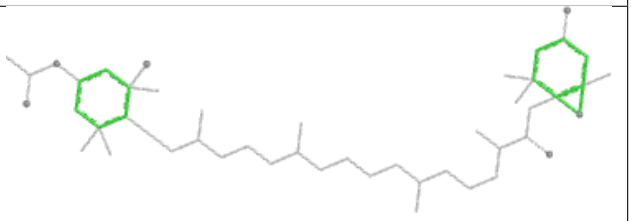
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Bond angles

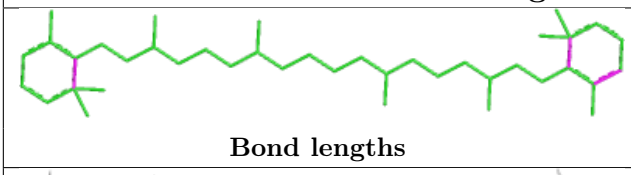


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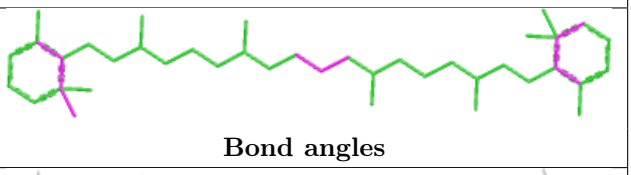


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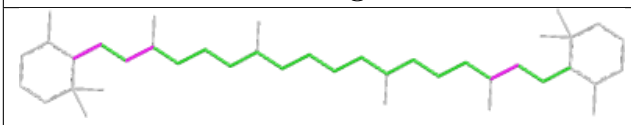
Ligand BCR I 101



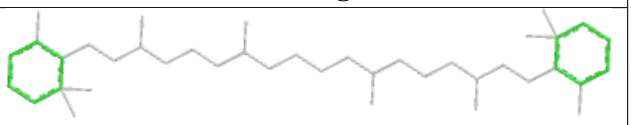
Bond lengths



Bond angles

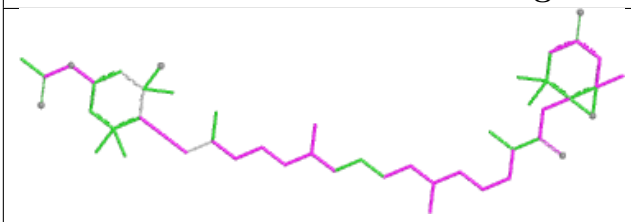


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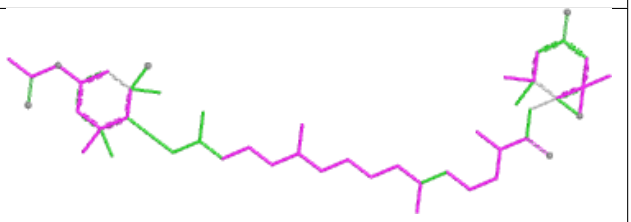


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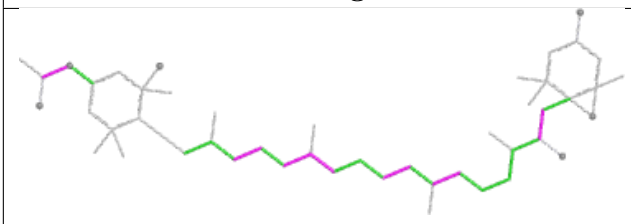
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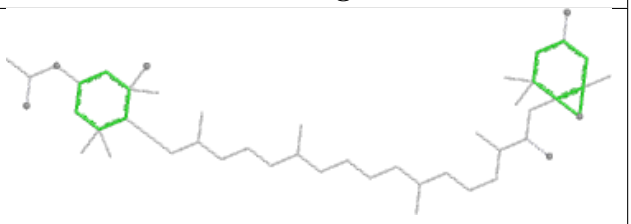
Bond lengths



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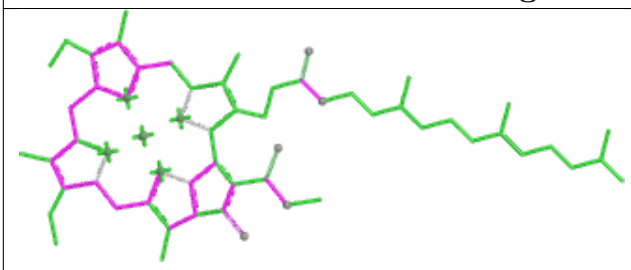


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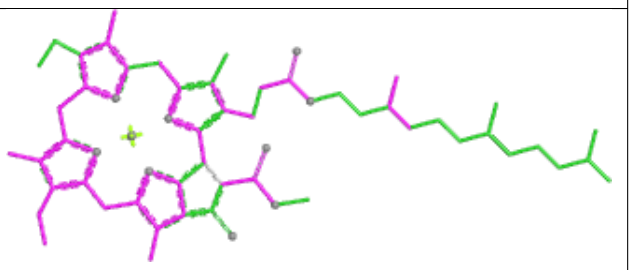


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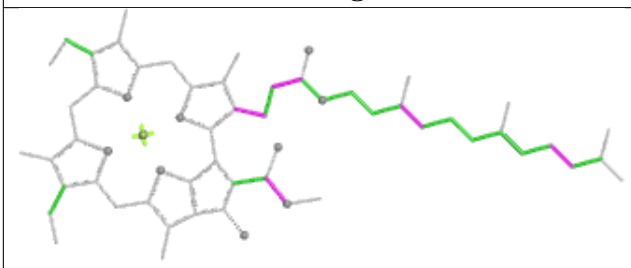
Ligand CLA 15 303



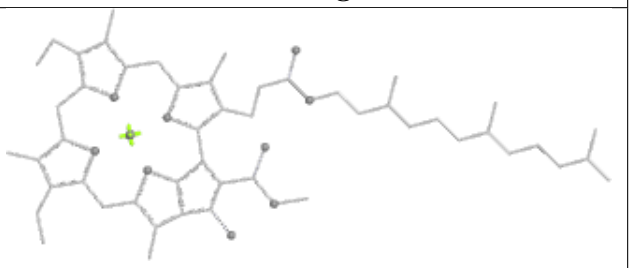
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Bond angles

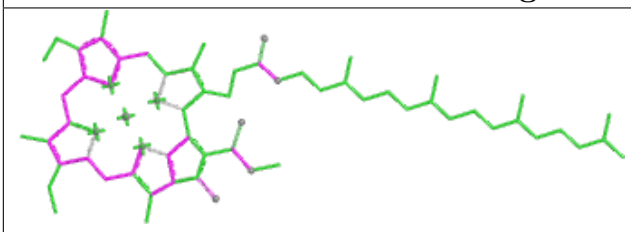


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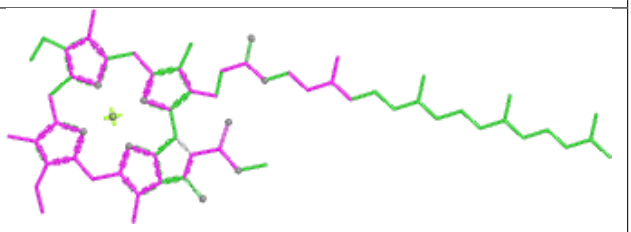


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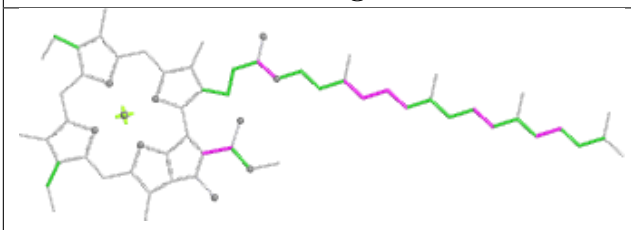
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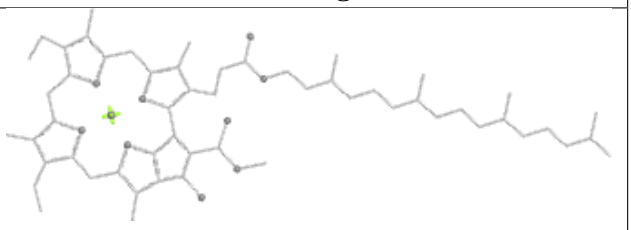
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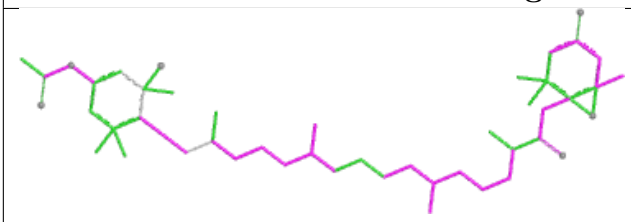


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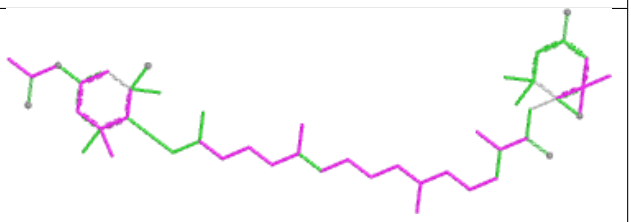


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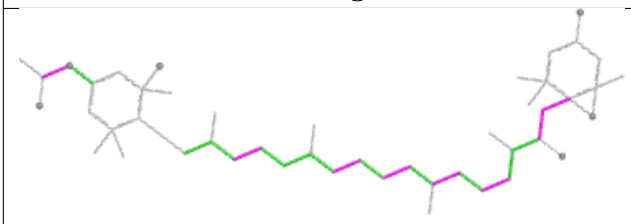
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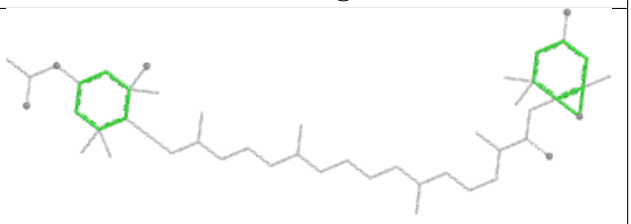
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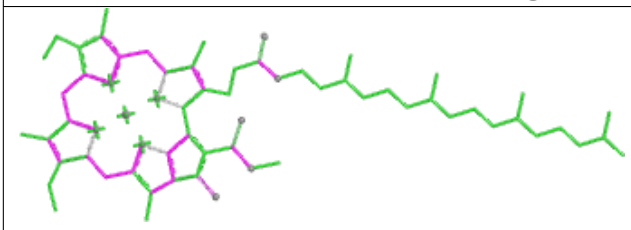


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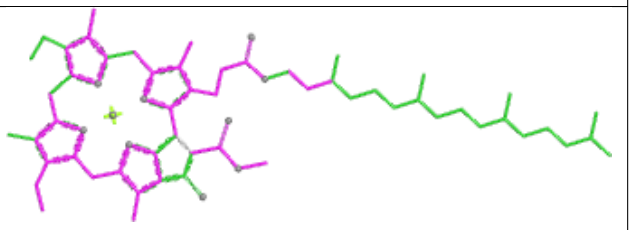


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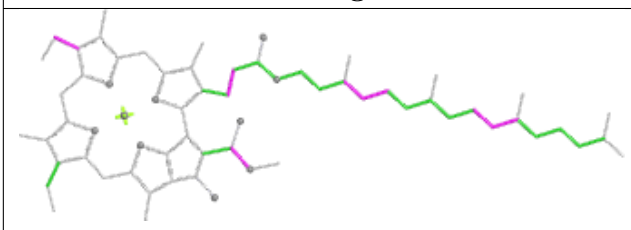
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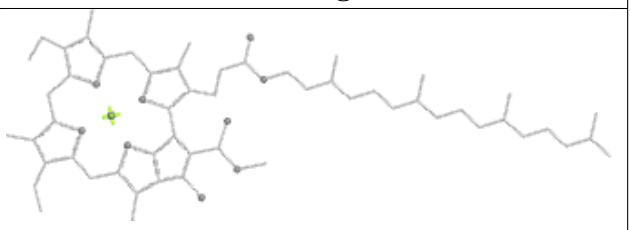
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Bond angles

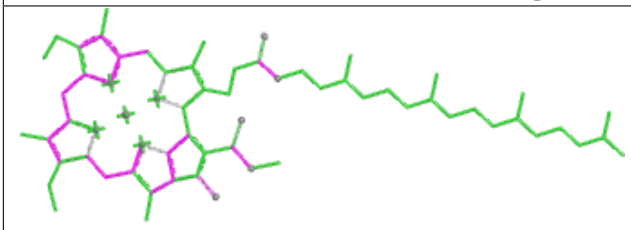


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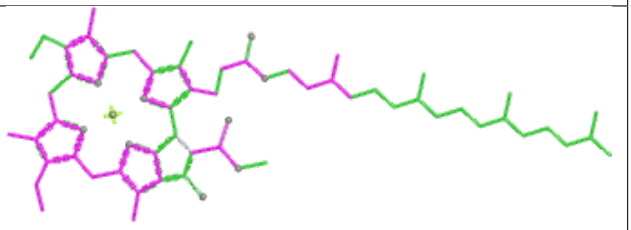


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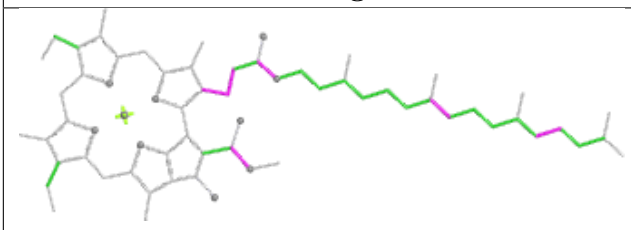
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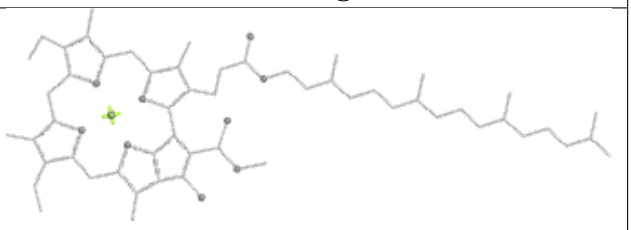
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Bond angles

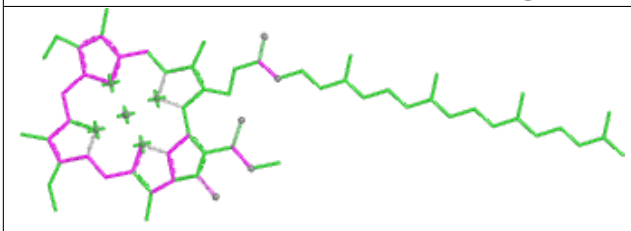


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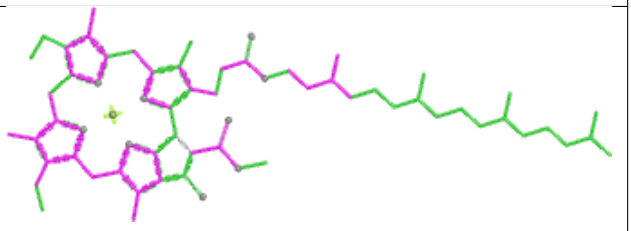


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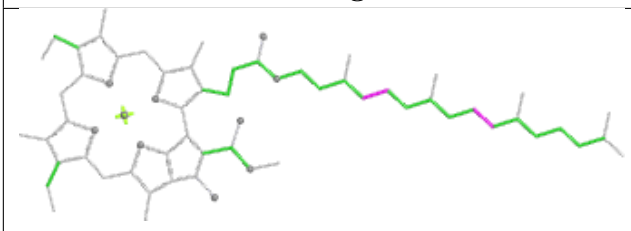
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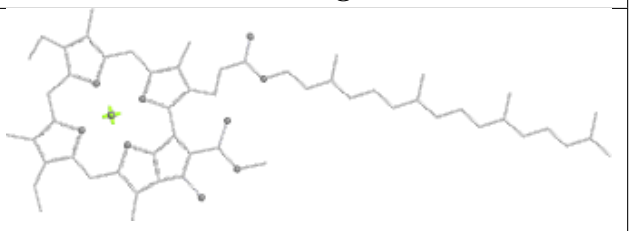
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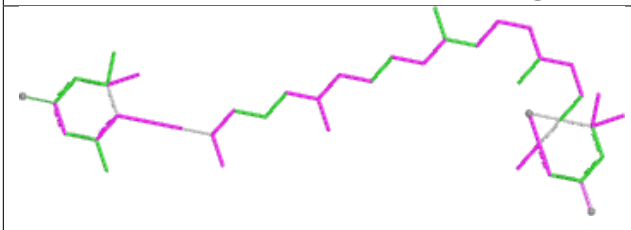


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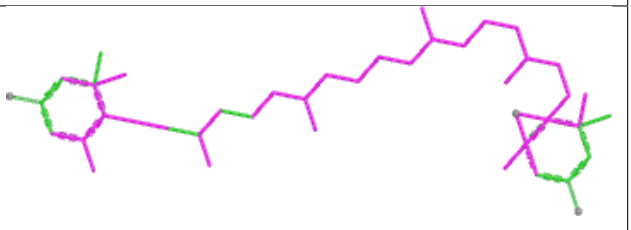


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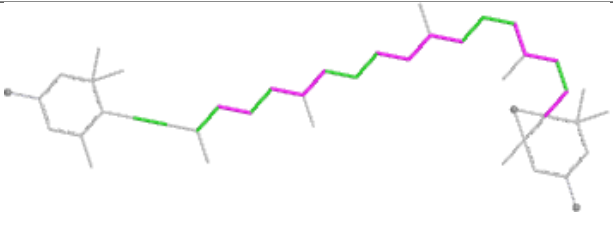
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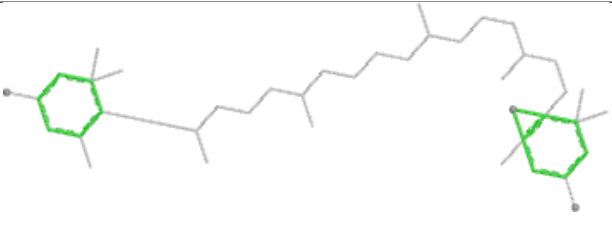
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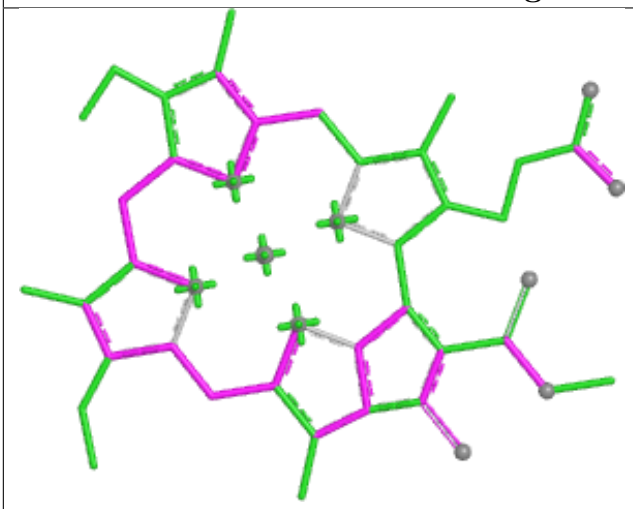


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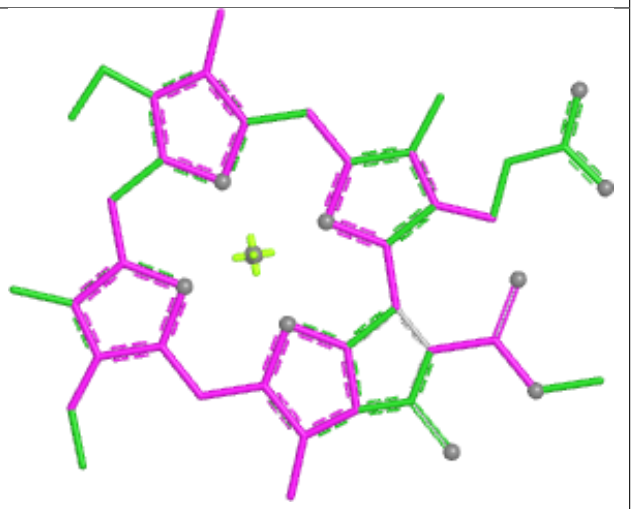


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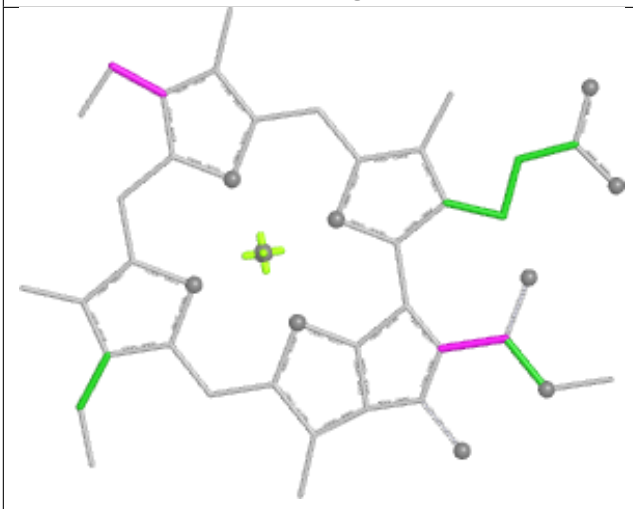
Ligand CLA B 815



Bond lengths



Bond angles

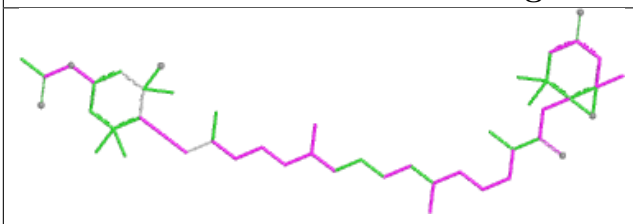


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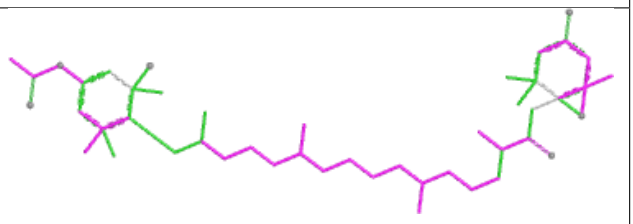


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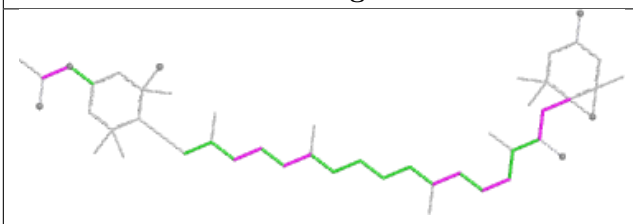
Ligand A86 10 316



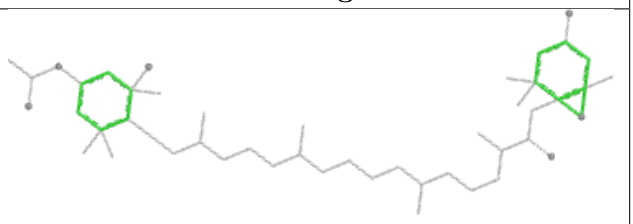
Bond lengths



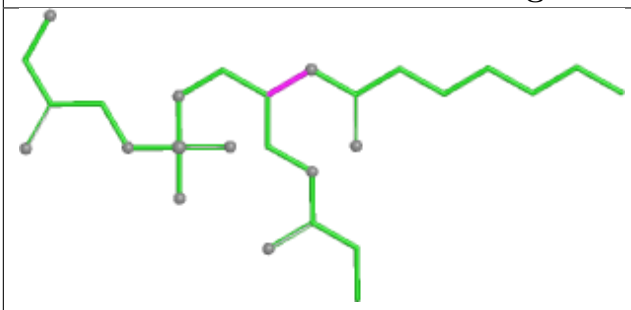
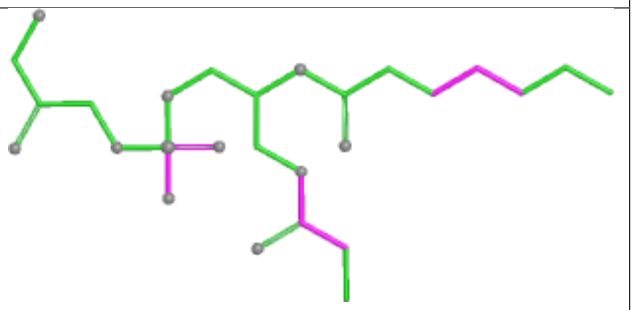
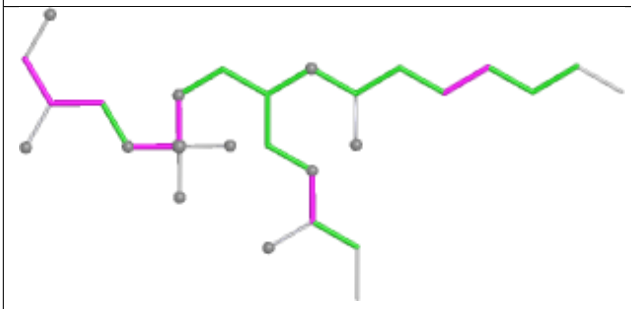
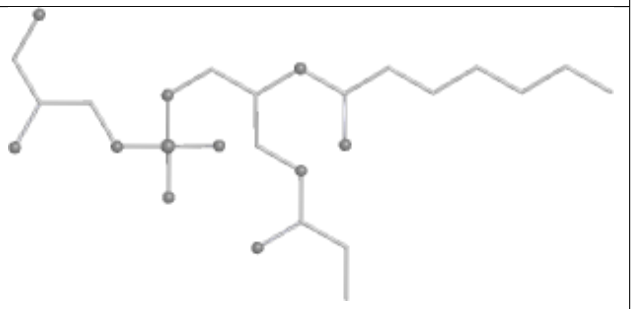
Bond angles

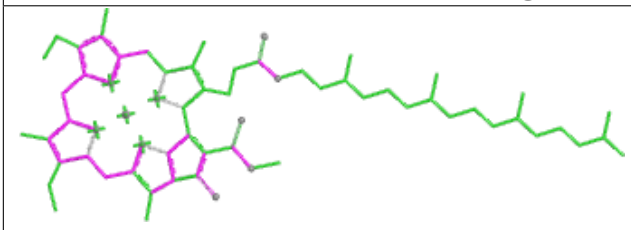
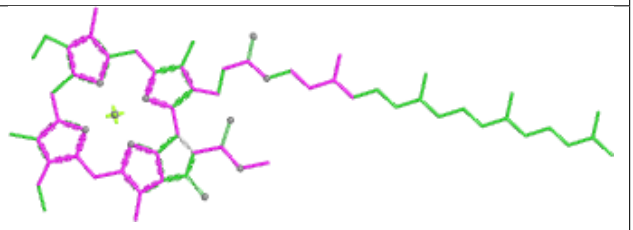
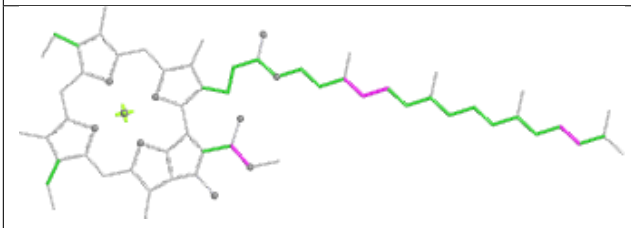
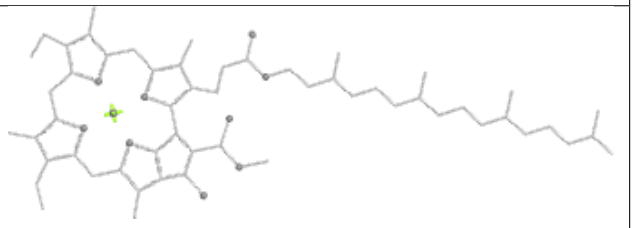


Torsions

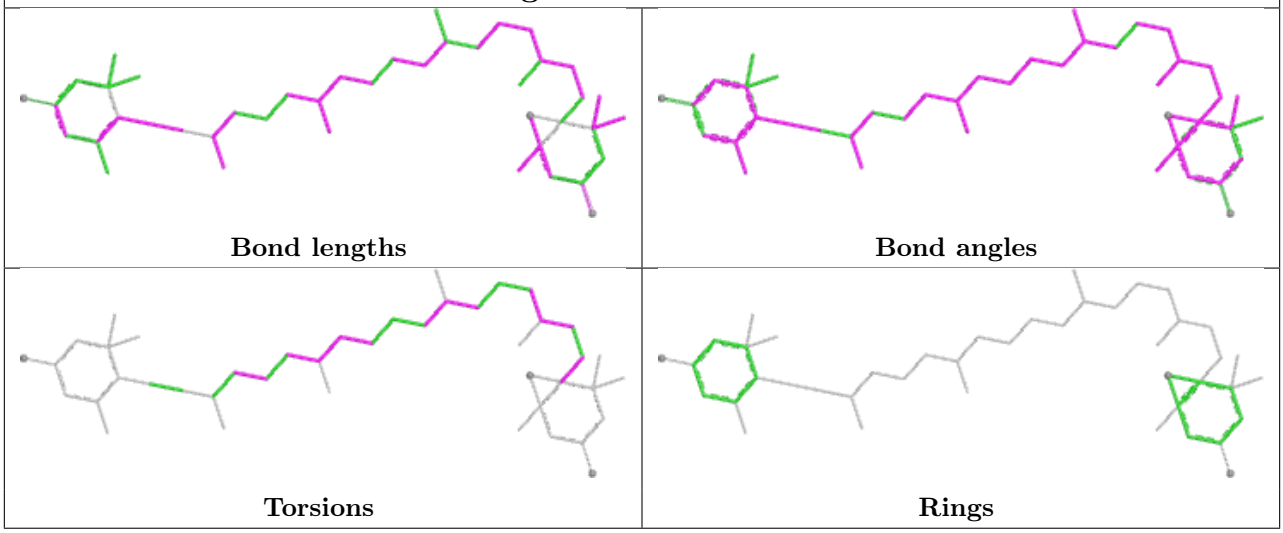


Rings

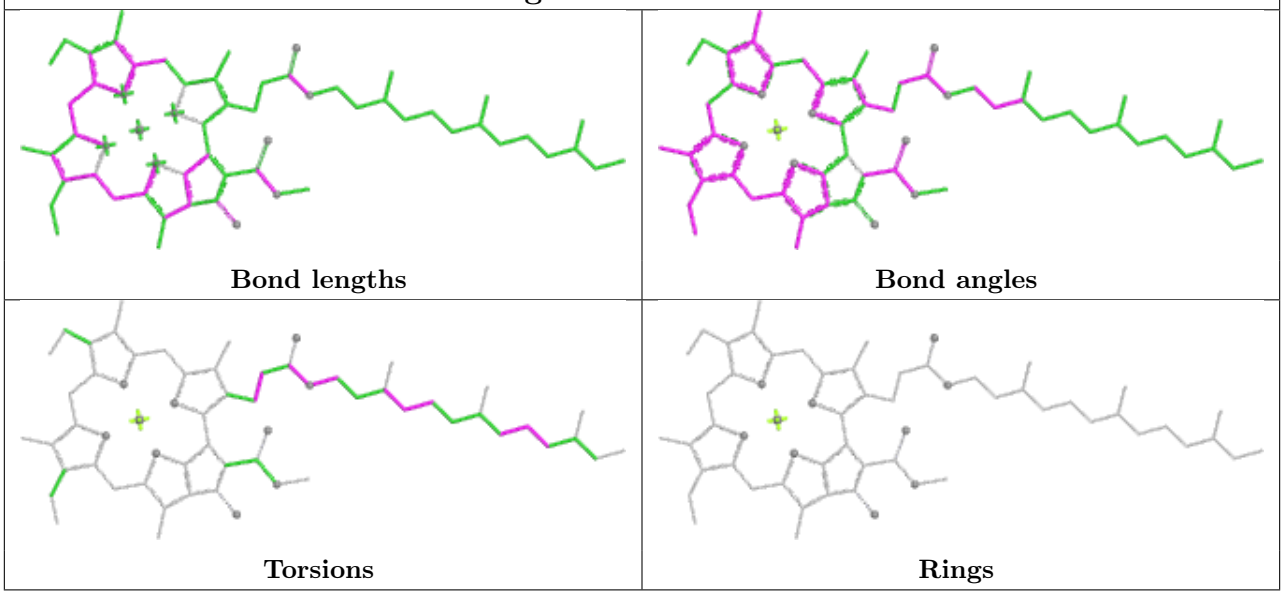
Ligand LHG 2 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 12 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

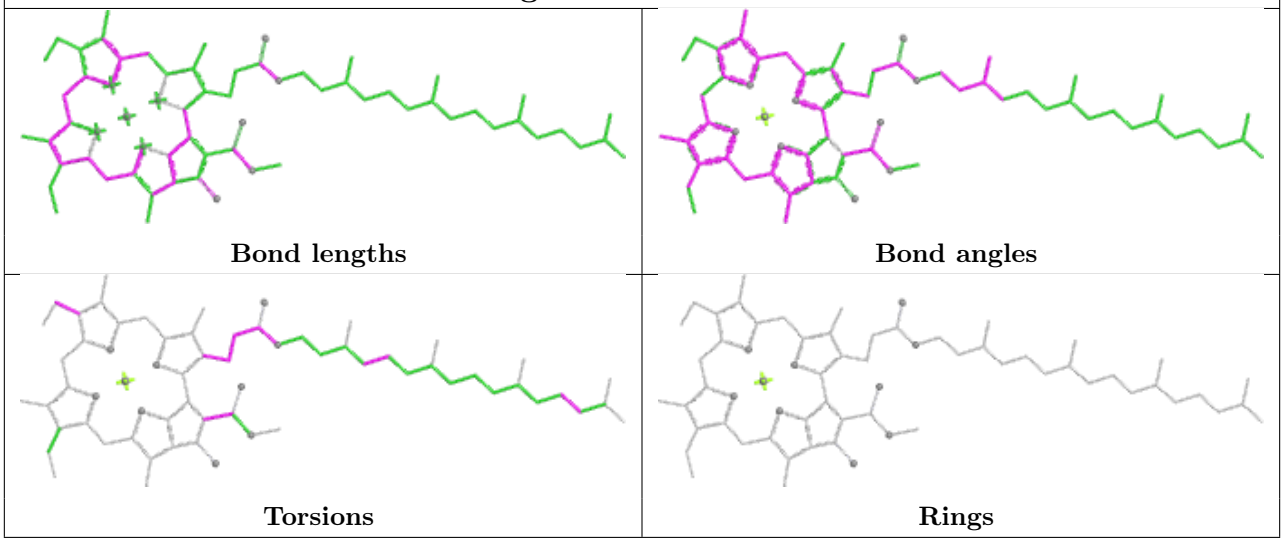
Ligand DD6 15 318



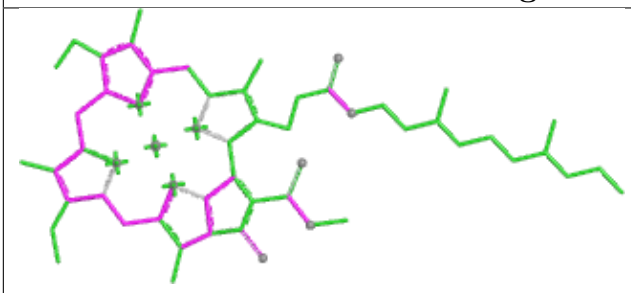
Ligand CLA A 821



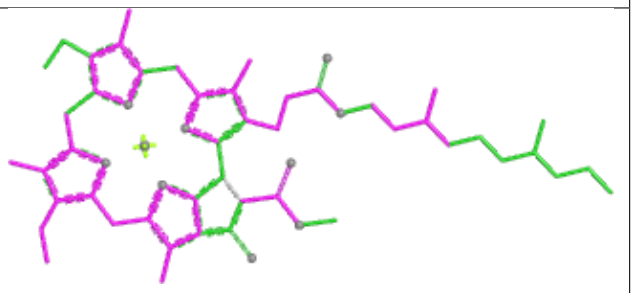
Ligand CLA 10 307



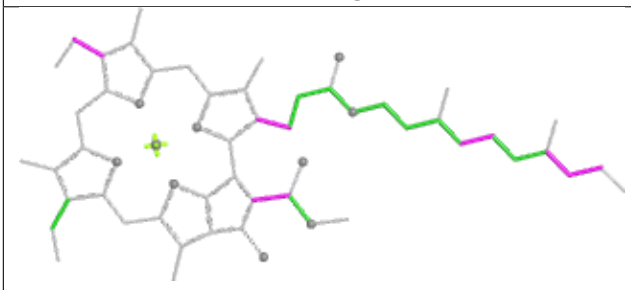
Ligand CLA 14 303



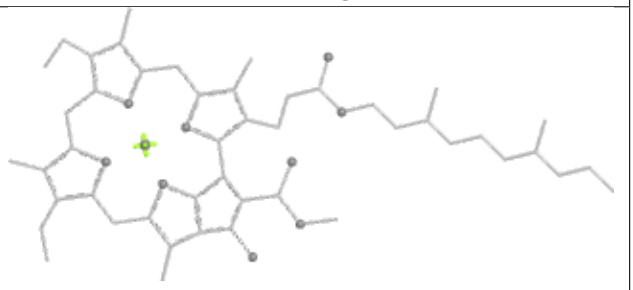
Bond lengths



Bond angles

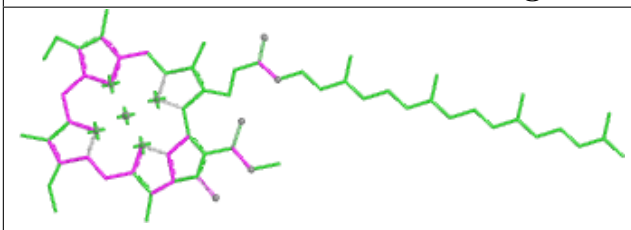


Torsions

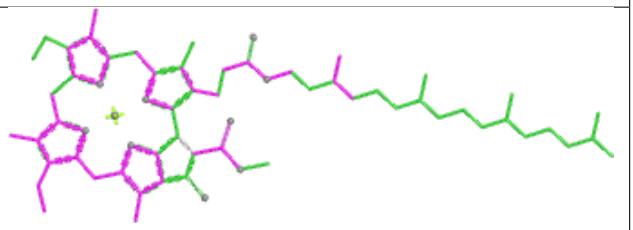


Rings

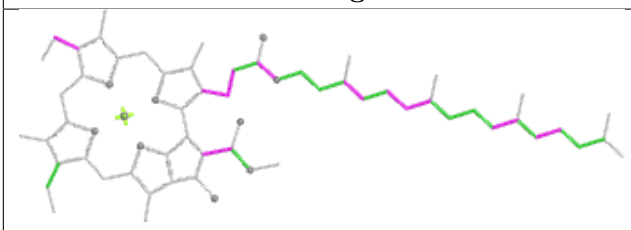
Ligand CLA A 812



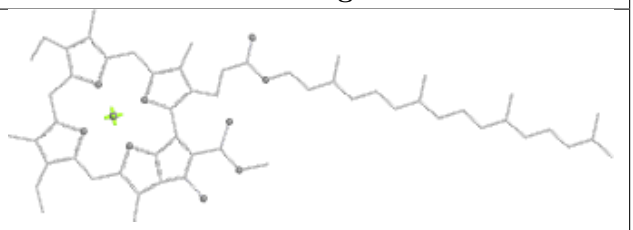
Bond lengths



Bond angles

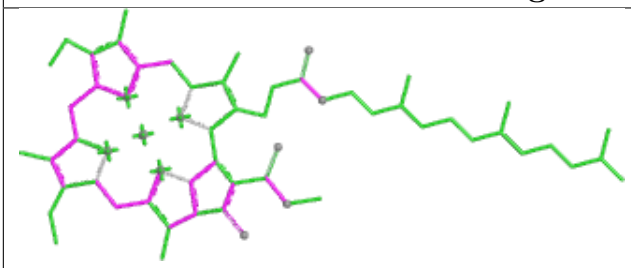


Torsions

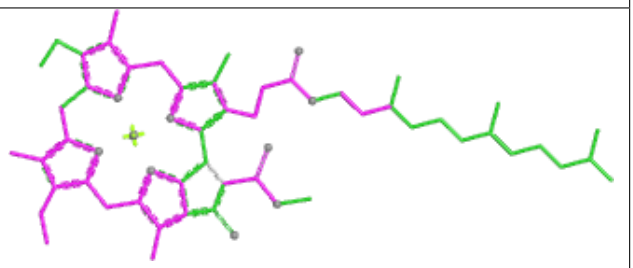


Rings

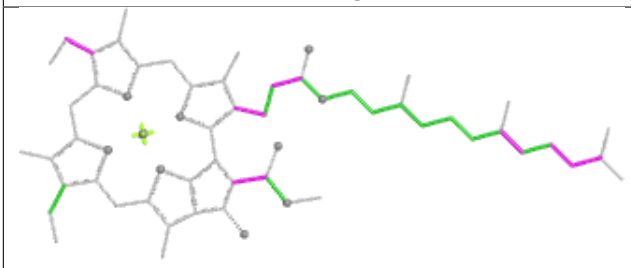
Ligand CLA 4 304



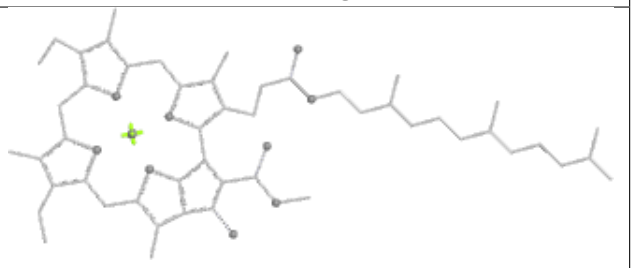
Bond lengths



Bond angles

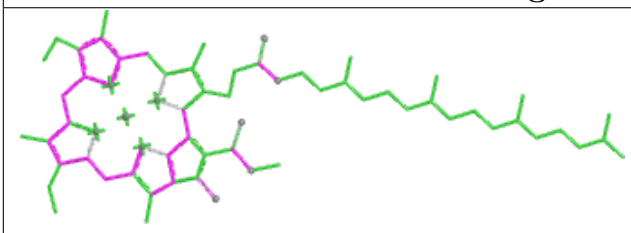


Torsions

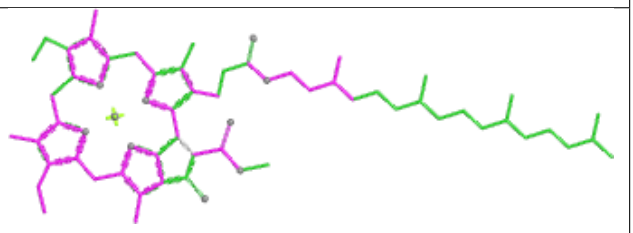


Rings

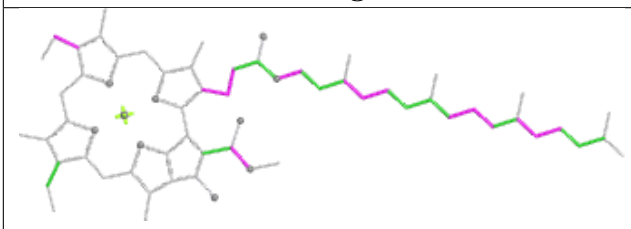
Ligand CLA 6 317



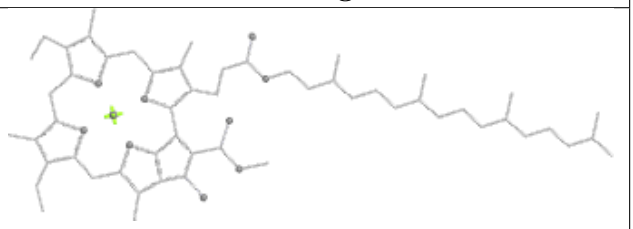
Bond lengths



Bond angles



Torsions

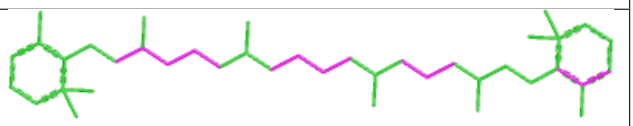


Rings

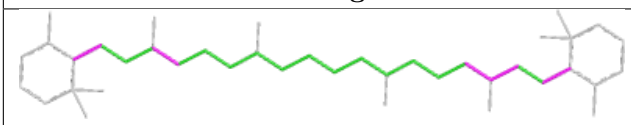
Ligand BCR B 846



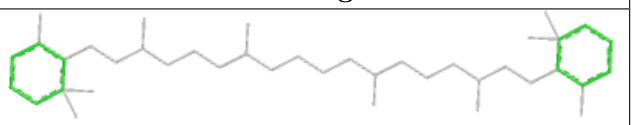
Bond lengths



Bond angles

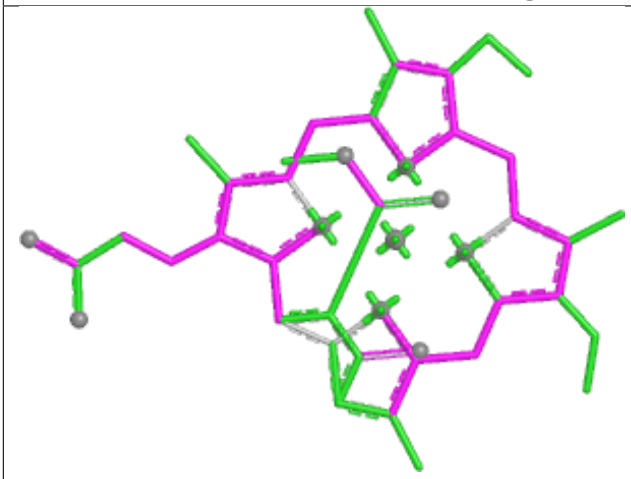


Torsions

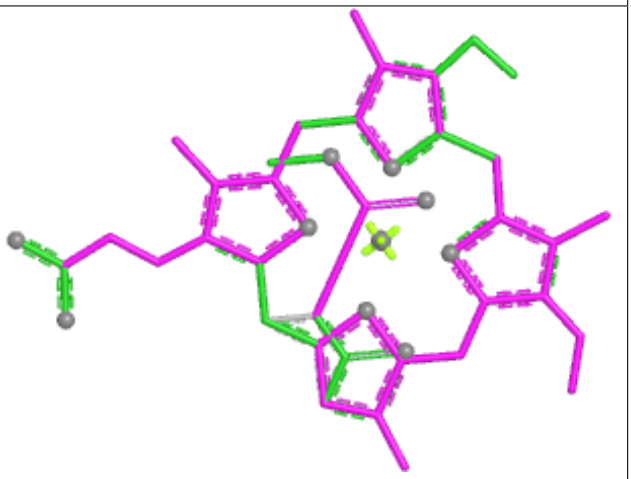


Rings

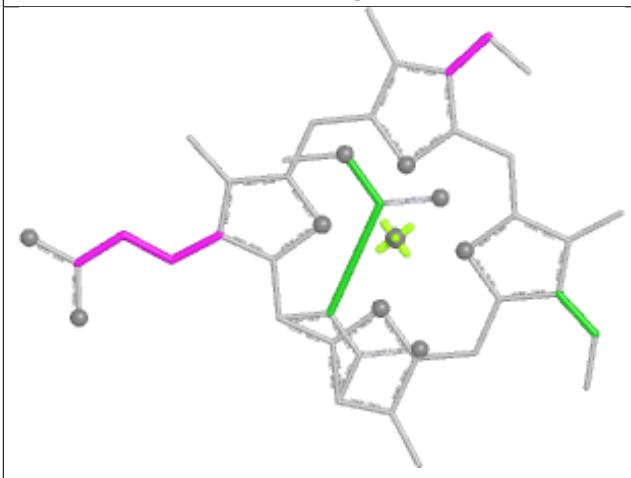
Ligand KC1 13 312



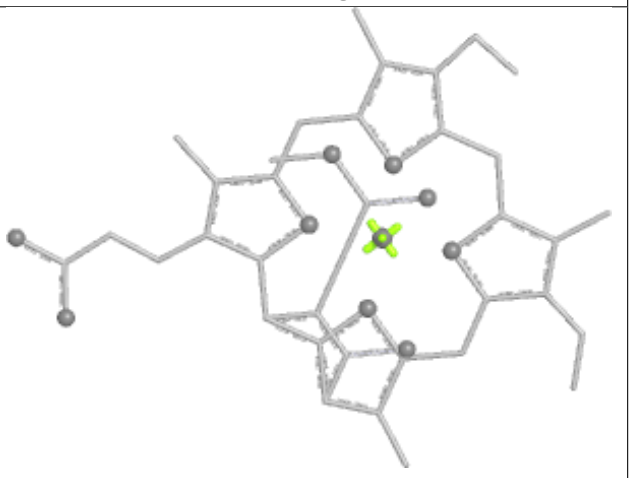
Bond lengths



Bond angles

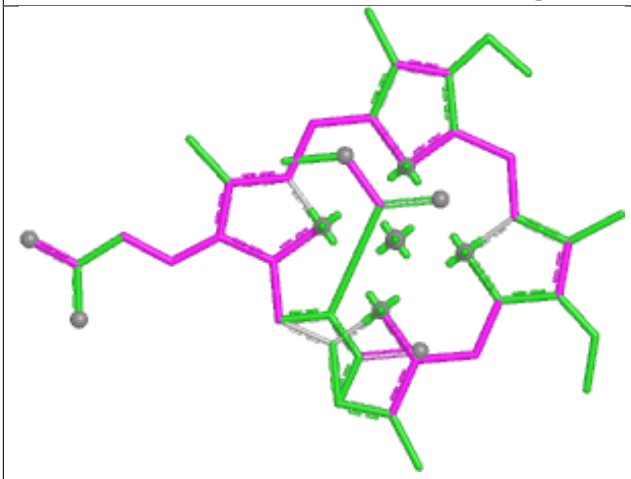


Torsions

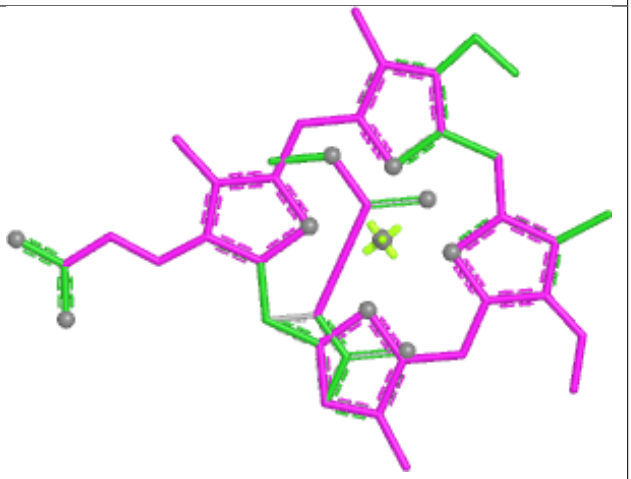


Rings

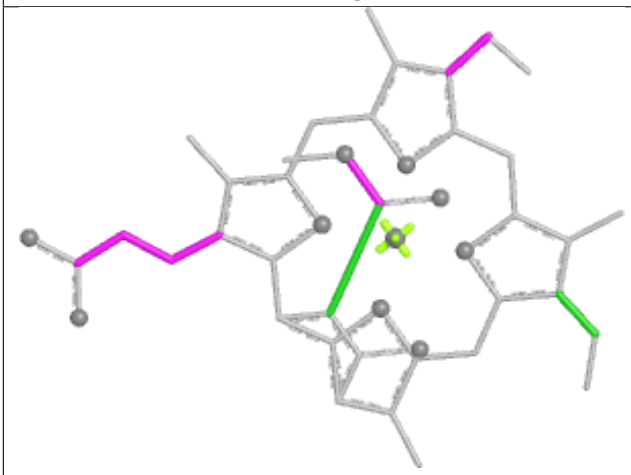
Ligand KC1 8 306



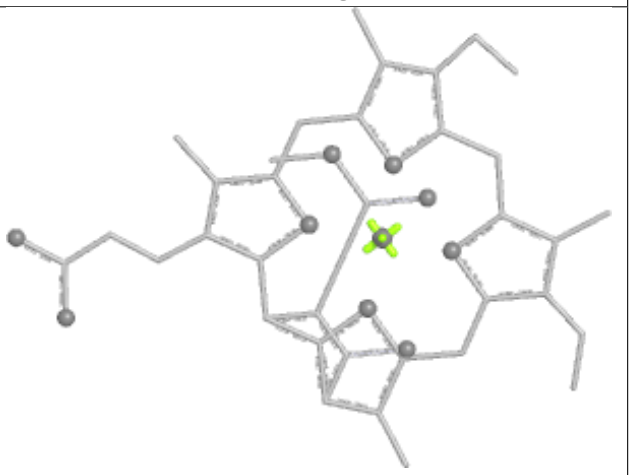
Bond lengths



Bond angles

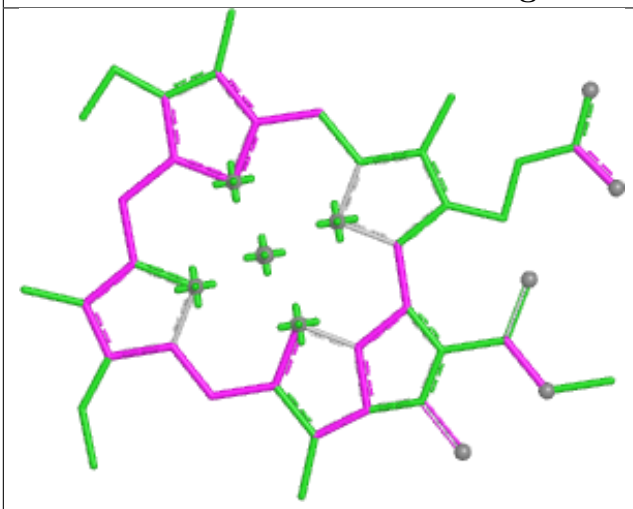


Torsions

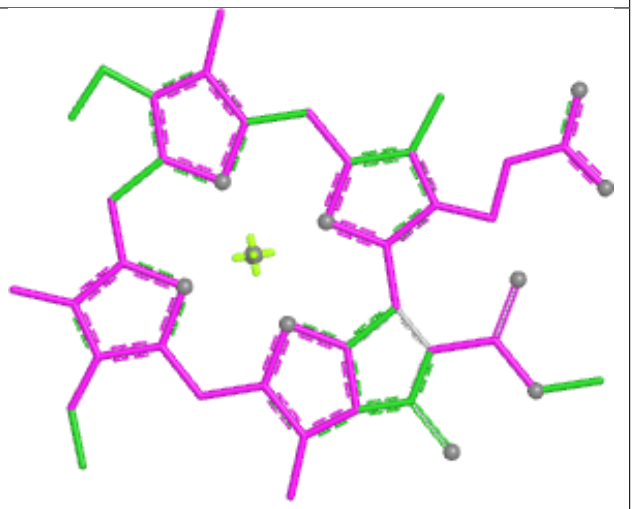


Rings

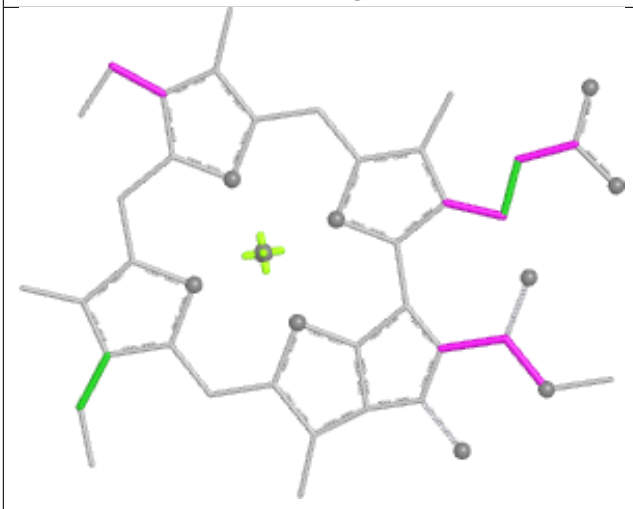
Ligand CLA 15 308



Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0835. These allow visual inspection of the internal detail of the map and identification of artifacts.

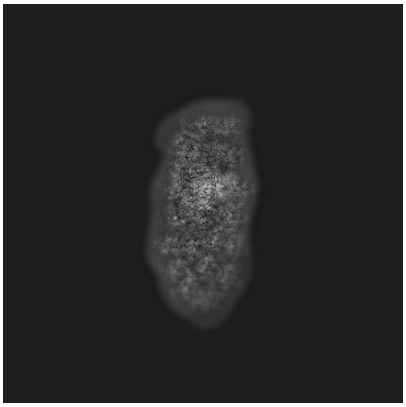
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

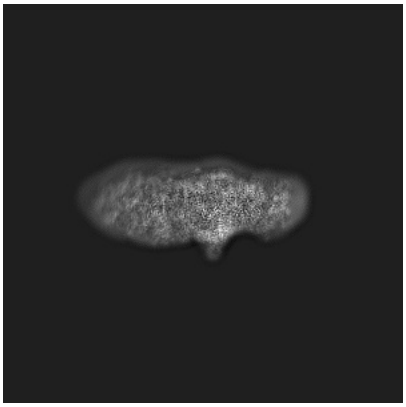
6.1.1 Primary map



X



Y



Z

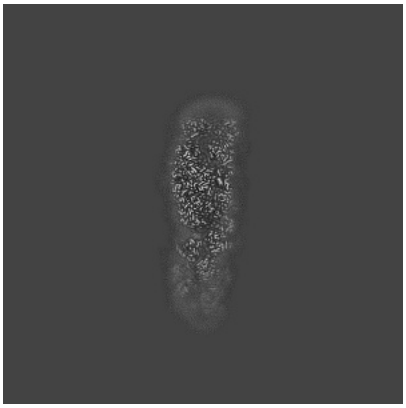
The images above show the map projected in three orthogonal directions.

6.2 Central slices

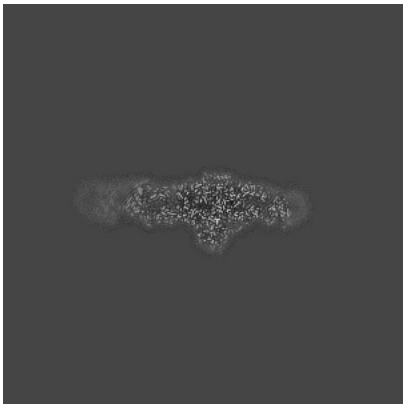
6.2.1 Primary map



X Index: 252



Y Index: 252



Z Index: 252

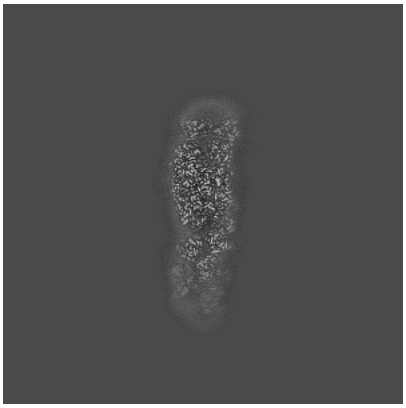
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

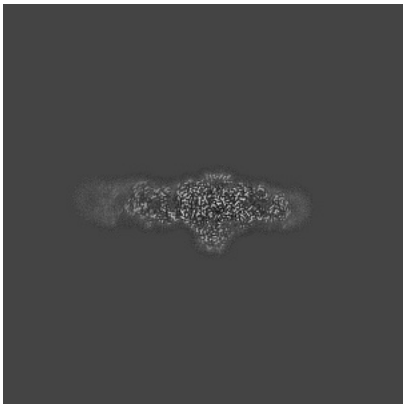
6.3.1 Primary map



X Index: 273



Y Index: 251

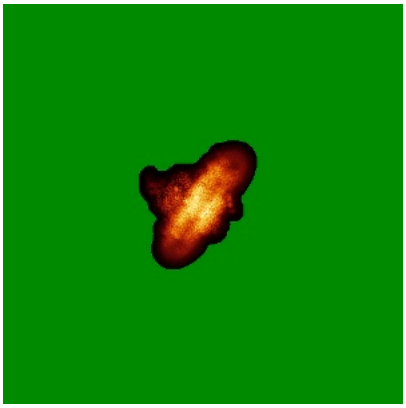


Z Index: 250

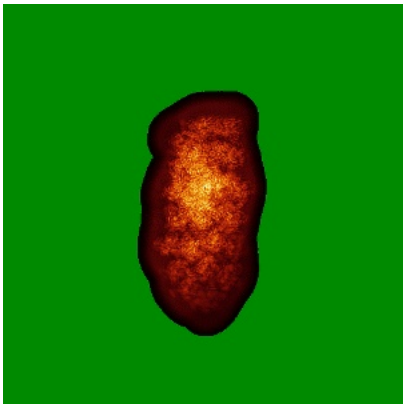
The images above show the largest variance slices of the map in three orthogonal directions.

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

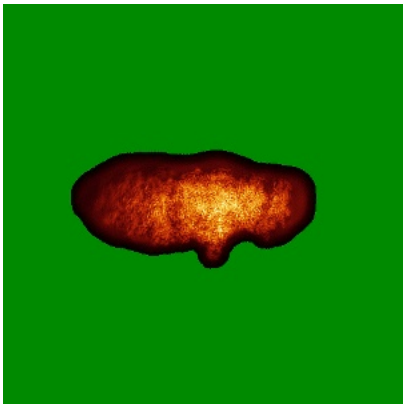
6.4.1 Primary map



X



Y

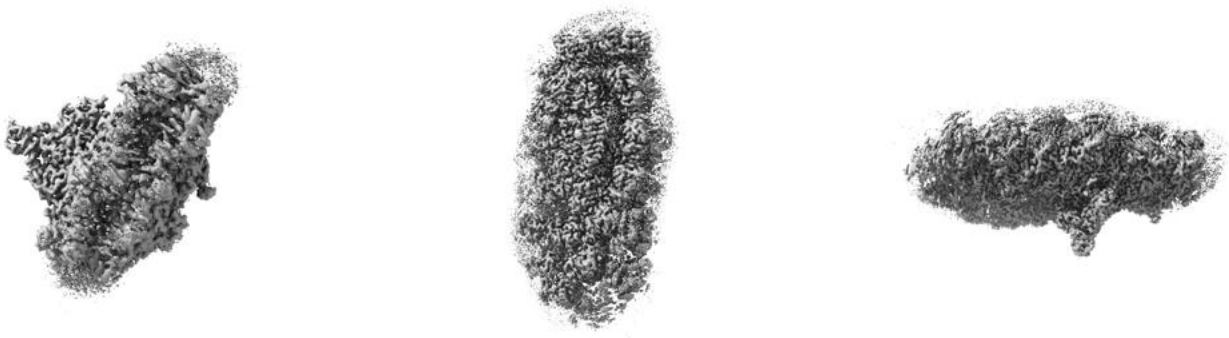


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

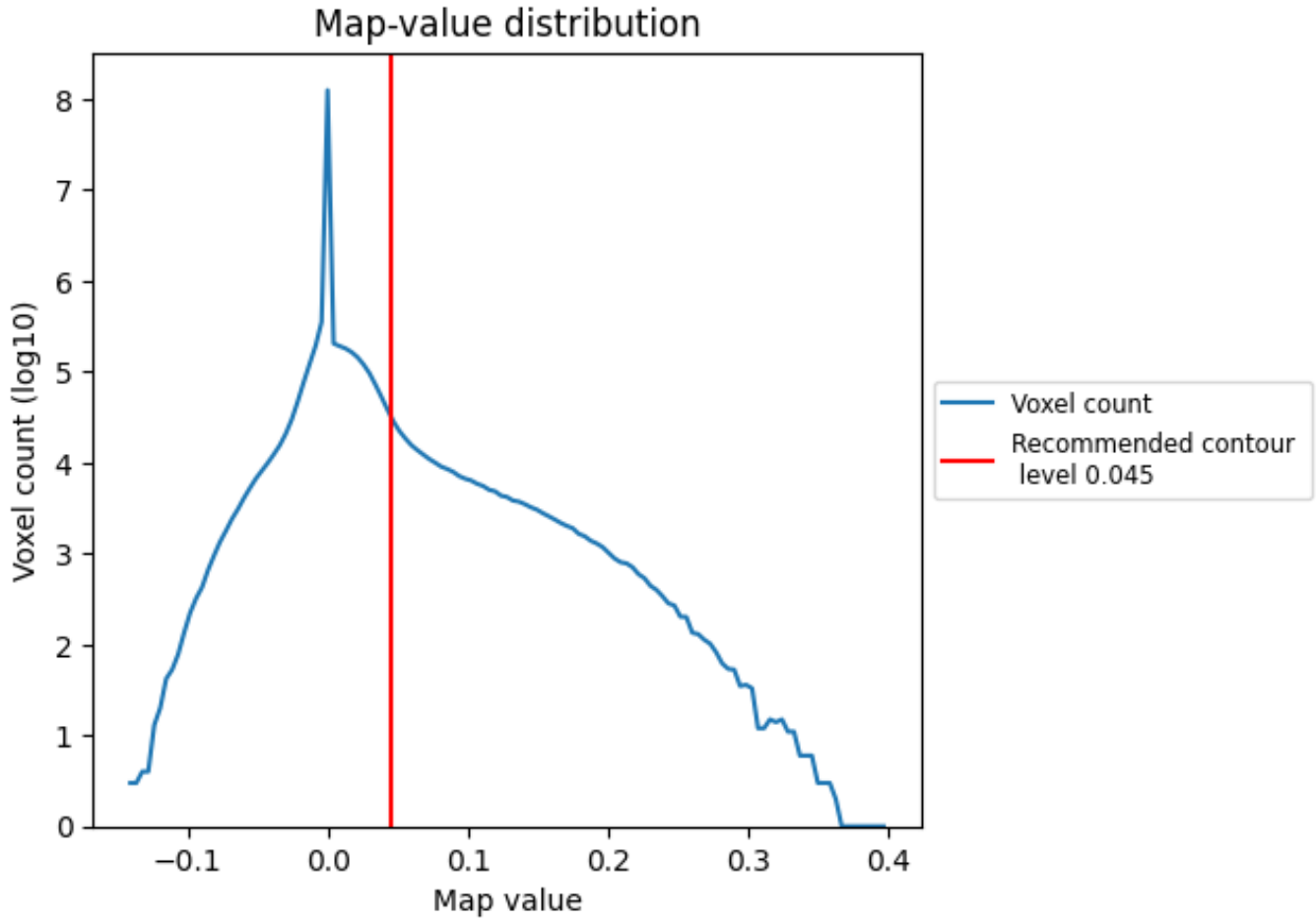
6.6 Mask visualisation (i)

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

7 Map analysis

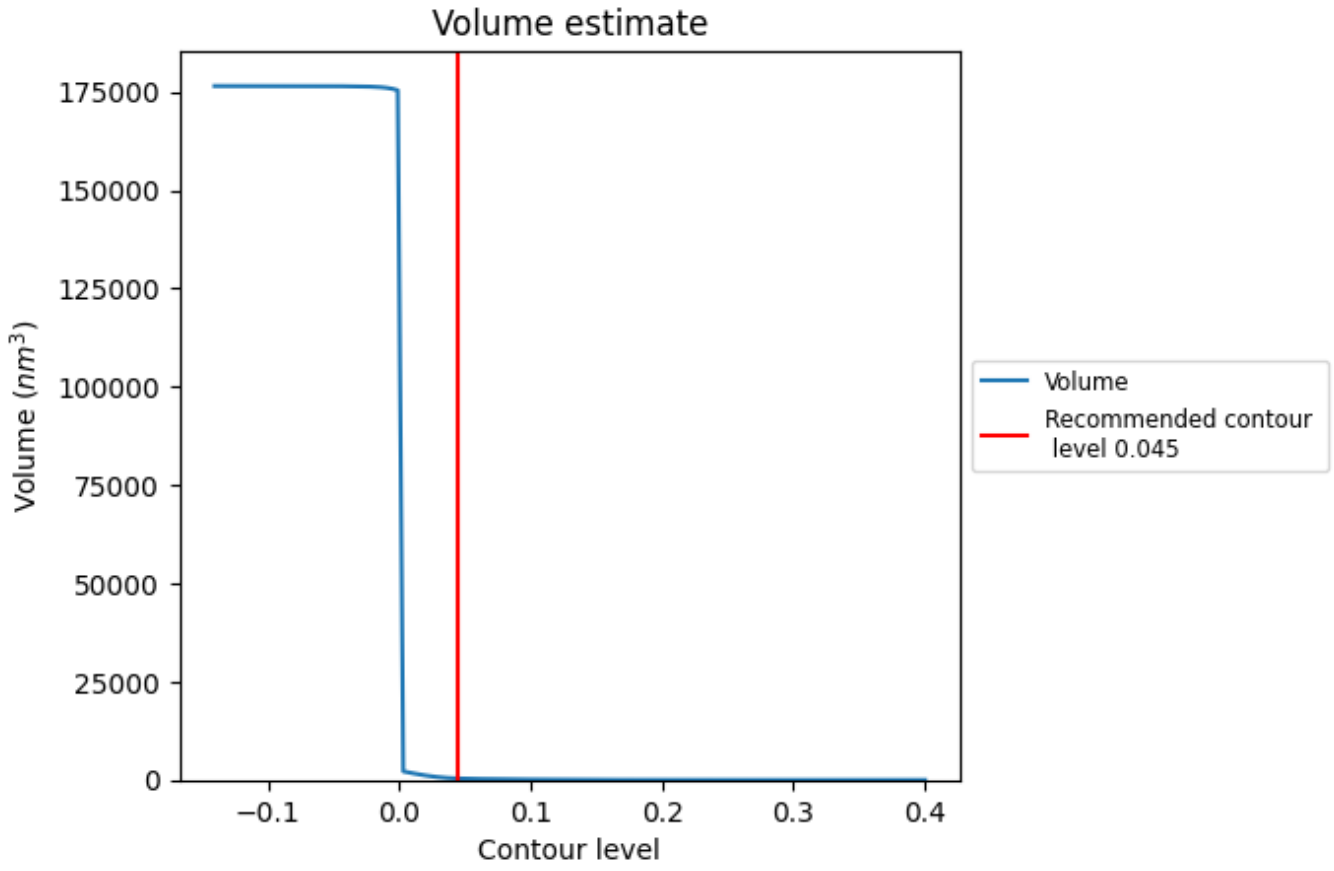
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

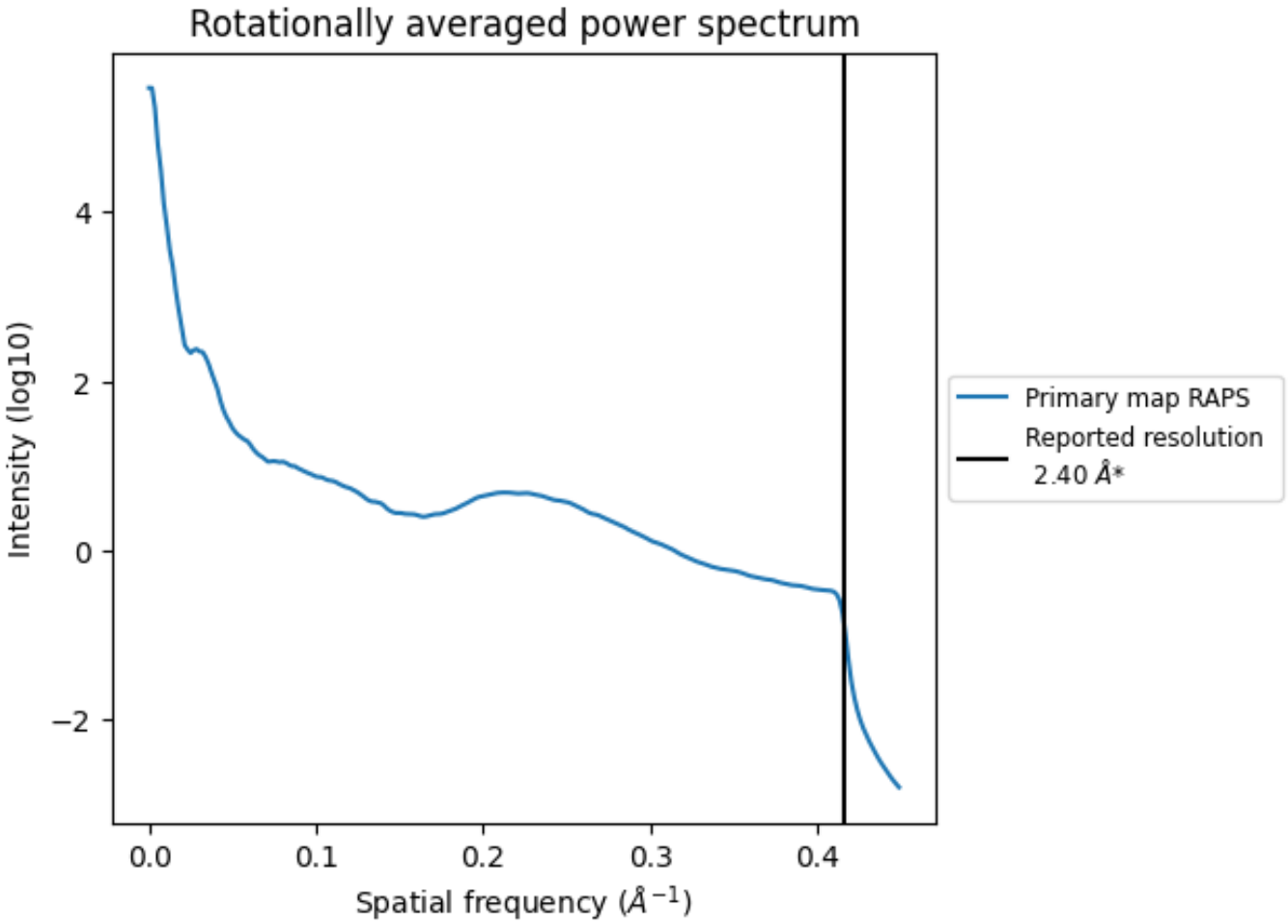
7.2 Volume estimate



The volume at the recommended contour level is 370 nm^3; this corresponds to an approximate mass of 334 kDa.

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

7.3 Rotationally averaged power spectrum (i)

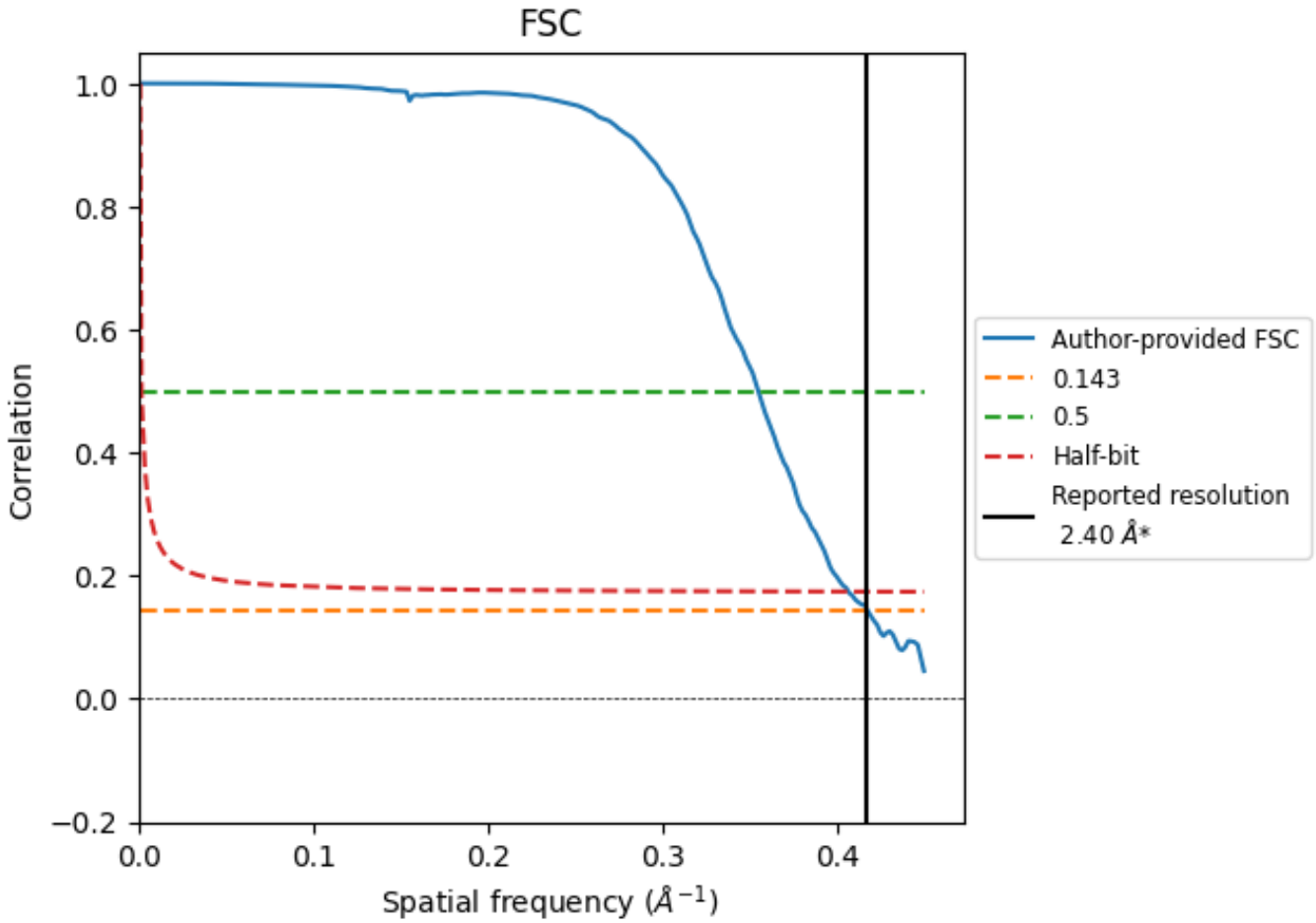


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

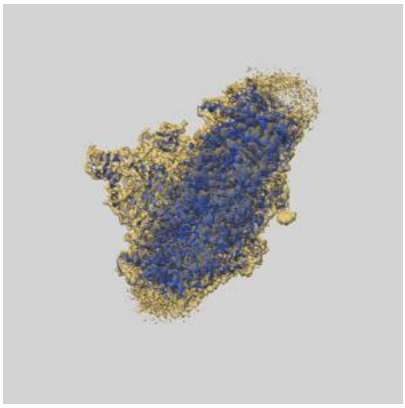
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.82	2.46
Unmasked-calculated*	-	-	-

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

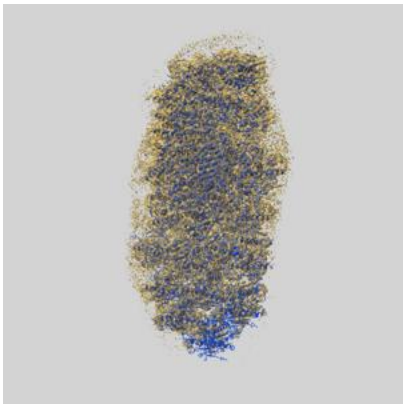
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0835 and PDB model 6L4U. Per-residue inclusion information can be found in section 3 on page 40.

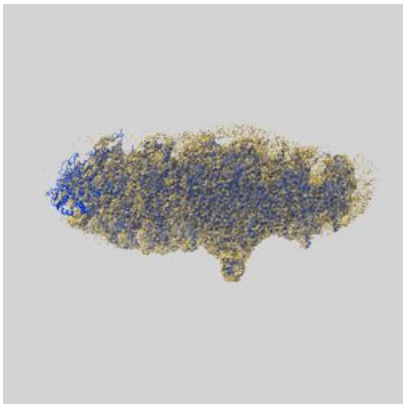
9.1 Map-model overlay



X



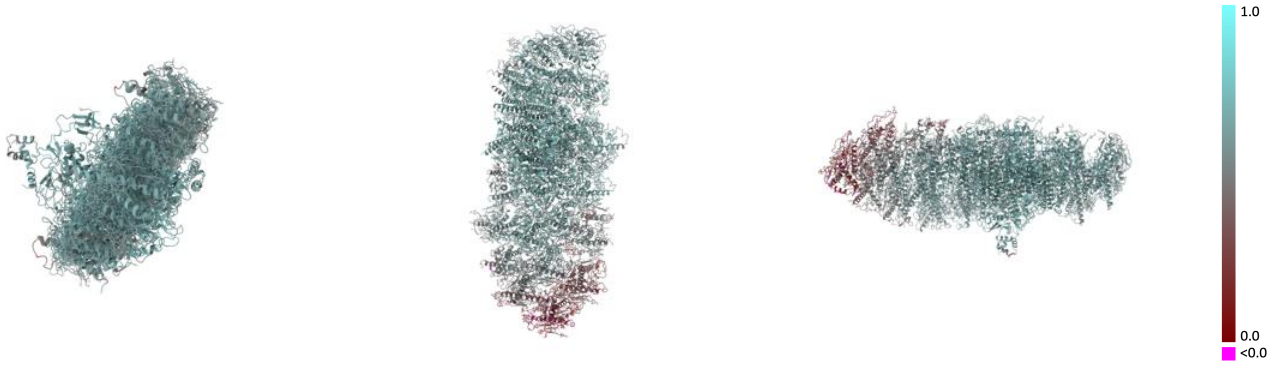
Y



Z

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

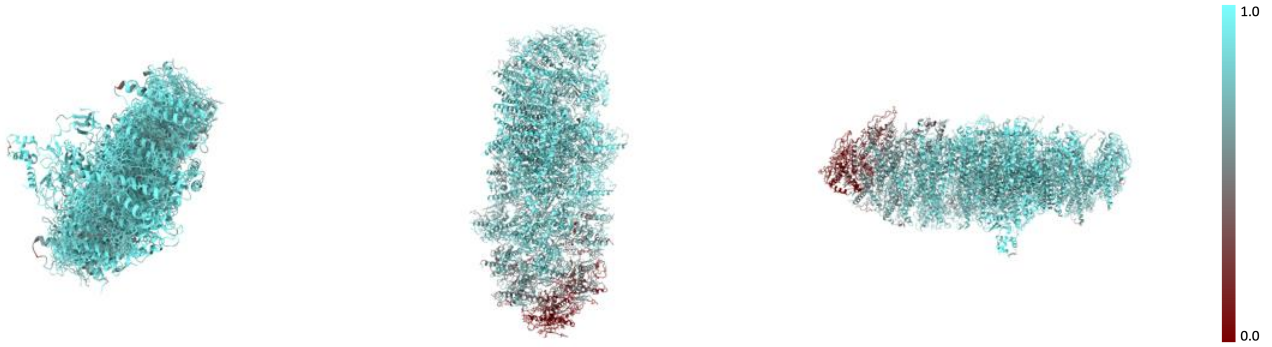
9.2 Q-score mapped to coordinate model (i)



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.

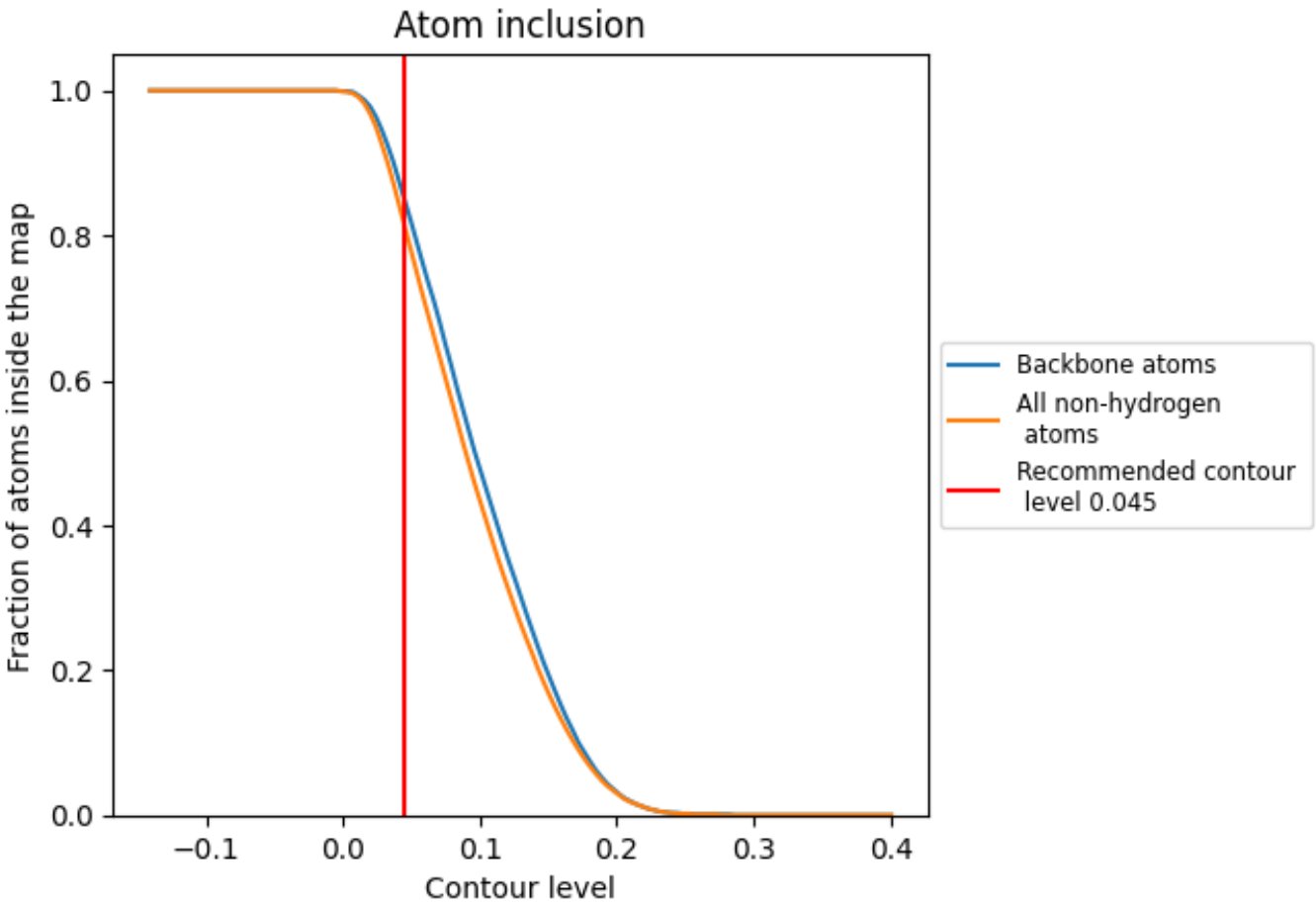
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.5870
1	0.8160	0.5890
10	0.8010	0.5590
11	0.6960	0.5050
12	0.7640	0.5640
13	0.6120	0.4800
14	0.3760	0.3440
15	0.1110	0.2110
16	0.5790	0.4140
1u	0.9010	0.5810
2	0.8680	0.6050
2u	0.9370	0.6560
3	0.8200	0.5840
4	0.8600	0.6130
5	0.8460	0.6020
6	0.8750	0.6140
7	0.8830	0.6270
8	0.9030	0.6360
9	0.8260	0.5850
A	0.9420	0.6770
B	0.9490	0.6780
C	0.9800	0.6770
D	0.9540	0.6510
E	0.9330	0.6710
F	0.9250	0.6620
I	0.9070	0.6480
J	0.9410	0.6590
L	0.9540	0.6600
M	0.9200	0.6500

