Full wwPDB EM Validation Report

Aug 7, 2026 – 12:59 AM JST

PDB ID	:	9KQP / pdb_00009kqp
EMDB ID	:	EMD-62511
Title	:	PSI-LHCI supercomplex binding with 10 Lhcas from C. subellipsoidea
Authors	:	Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on	:	2024-11-26
Resolution	:	1.92 Å(reported)
Based on initial model	:	6zzx

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

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

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

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

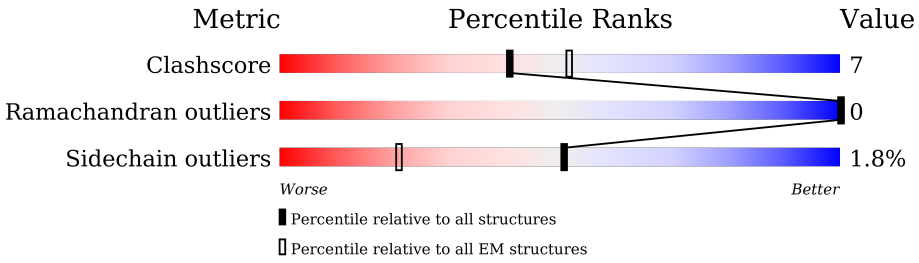
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

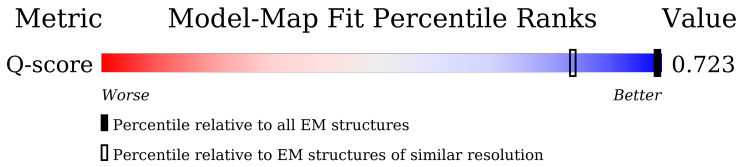
1 Overall quality at a glance

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

The reported resolution of this entry is 1.92 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	1227 (1.42 - 2.42)

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	91% 8%
2	B	734	93% 7%
3	C	81	94%
4	D	192	68% 7% 26%

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Mol	Chain	Length	Quality of chain
5	E	71	83% 15%
6	F	245	63% 33%
7	G	138	68% 6% 25%
8	H	133	7% 59% 9% 32%
9	I	36	78% 14% 8%
10	J	41	78% 17% 5%
11	K	131	49% 12% 38%
12	M	31	90% 10%
13	a	229	77% 8% 15%
13	b	229	14% 46% 9% 45%
14	3	246	73% 9% 17%
15	7	259	75% 7% 17%
16	8	255	76% 11% 13%
17	9	230	68% 11% 20%
18	L	210	61% 10% 30%
19	O	142	6% 46% 8% 45%
20	2	273	8% 59% 15% 25%
21	4	246	15% 67% 12% 22%
22	5	274	68% 15% 16%
23	6	272	10% 68% 12% 19%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	UNL	3	306	-	-	X	-
36	LUT	4	302	-	X	-	-
36	LUT	6	303	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	LUT	9	302	-	X	-	-
36	LUT	9	305	-	X	-	-
36	LUT	F	304	-	X	-	-
36	LUT	a	305	-	X	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 52991 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	740	5814	3800	992	1004	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5808	3812	985	998	13	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	596	365	103	117	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1110	711	193	203	3	0	0

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	60	490	316	83	90	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1264	805	223	234	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	103	Total	C	N	O	S	0	0
			767	488	132	146	1		

- Molecule 8 is a protein called Photosystem I reaction centre subunit VI.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	91	Total	C	N	O	0	0
			706	449	120	137		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			248	171	34	41	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	39	Total	C	N	O	S	0	0
			319	220	46	52	1		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			560	356	96	107	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			237	160	35	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
13	b	126	Total	C	N	O	S	0	0
			952	606	168	176	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	203	Total	C	N	O	S	0	0
			1580	1036	255	286	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	214	Total	C	N	O	S	0	0
			1633	1059	276	296	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	9	184	Total	C	N	O	S	0	0
			1414	915	238	258	3		

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	148	Total	C	N	O	S	0	0
			1102	723	183	194	2		

- Molecule 19 is a protein called Photosystem I PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	78	Total	C	N	O	0	0
			605	403	98	104		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic/Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	204	Total	C	N	O	S	0	0
			1606	1046	270	286	4		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4	193	Total	C	N	O	S	0	0
			1506	984	246	273	3		

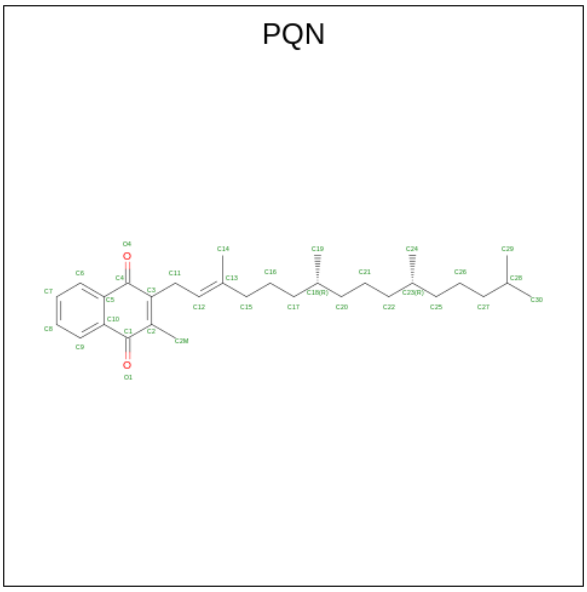
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5	229	Total	C	N	O	S	0	0
			1766	1152	303	307	4		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

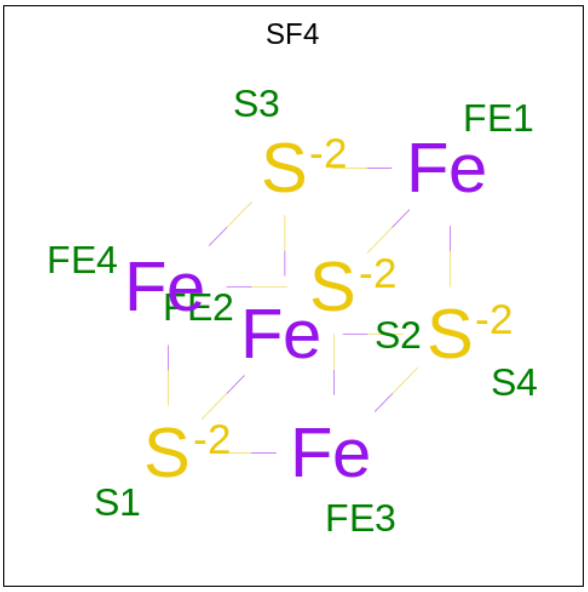
Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	219	Total	C	N	O	S	0	0
			1658	1088	276	287	7		

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



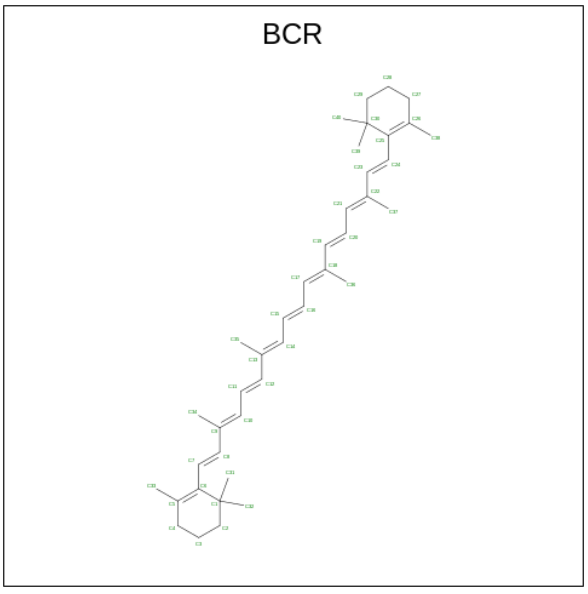
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			33	31	2	
24	B	1	Total	C	O	0
			33	31	2	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	I	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	M	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	8	1	Total C 40 40	0

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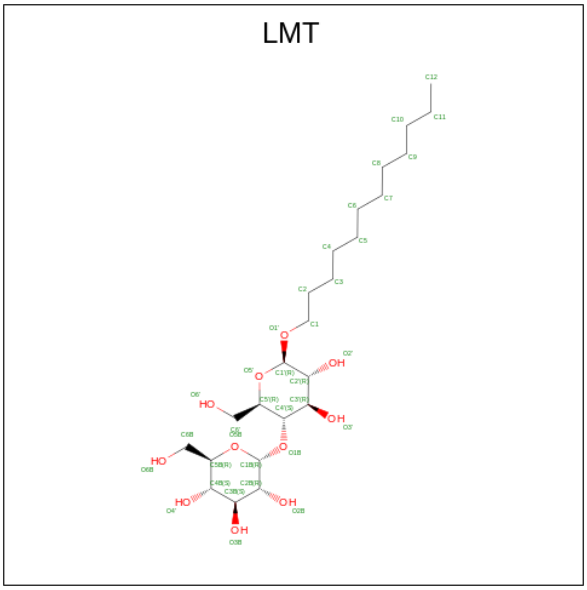
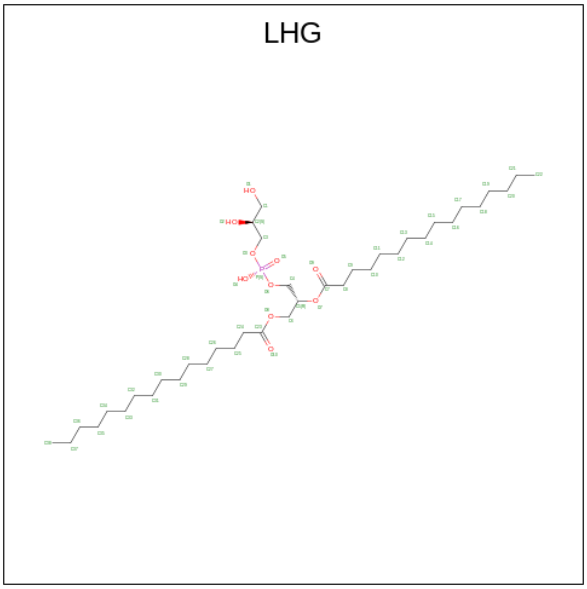
Mol	Chain	Residues	Atoms	AltConf
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	O	1	Total C 40 40	0
26	2	1	Total C 40 40	0
26	5	1	Total C 40 40	0
26	6	1	Total C 40 40	0

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O 35 24 11	0
27	A	1	Total C O 35 24 11	0
27	9	1	Total C O 35 24 11	0
27	5	1	Total C O 35 24 11	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

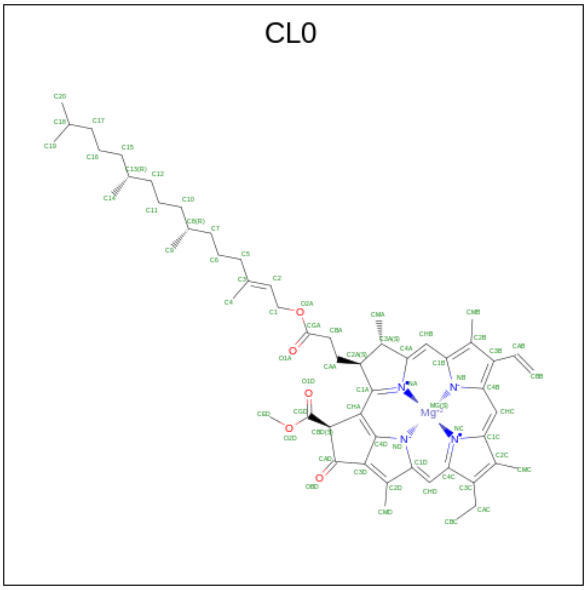


Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			32	21	10	1	
28	a	1	Total	C	O	P	0
			49	38	10	1	
28	7	1	Total	C	O	P	0
			49	38	10	1	
28	7	1	Total	C	O	P	0
			37	26	10	1	
28	8	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			35	24	10	1	
28	6	1	Total	C	O	P	0
			27	16	10	1	
28	6	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

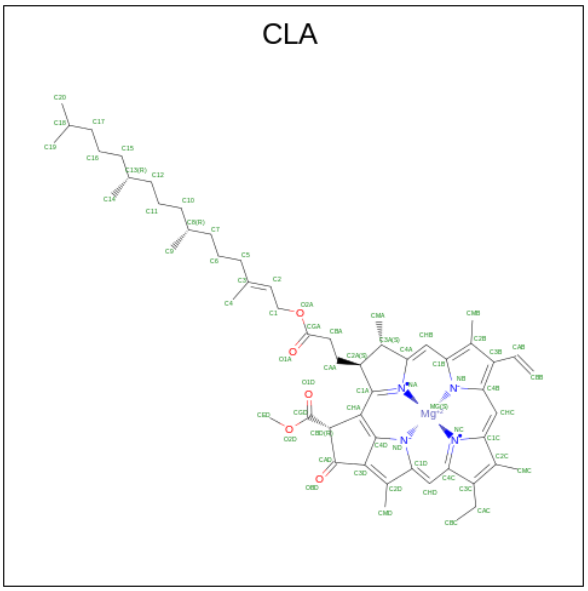
Mol	Chain	Residues	Atoms	AltConf
29	A	2	Total C 20 20	0
29	B	2	Total C 24 24	0
29	a	2	Total C 27 27	0
29	3	1	Total C 11 11	0
29	7	1	Total C 8 8	0
29	8	1	Total C 18 18	0
29	9	6	Total C 81 81	0
29	2	1	Total C 11 11	0
29	4	1	Total C 13 13	0

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
31	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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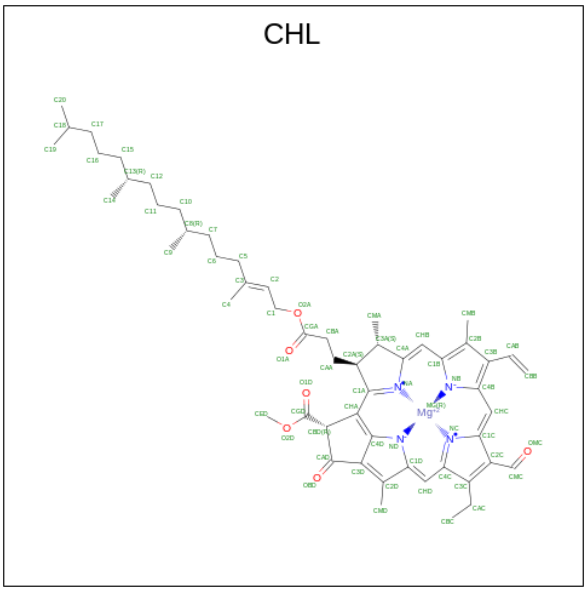
Mol	Chain	Residues	Atoms					AltConf
31	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	6	1	Total 46	C 36	Mg 1	N 4	O 5	0

- Molecule 32 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
32	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	K	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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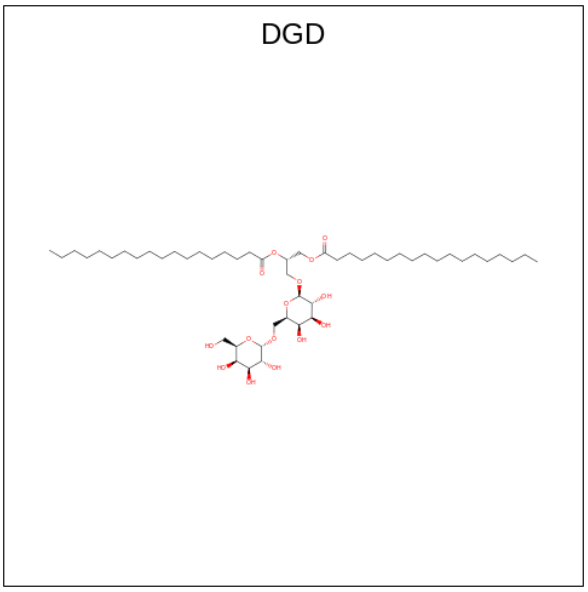
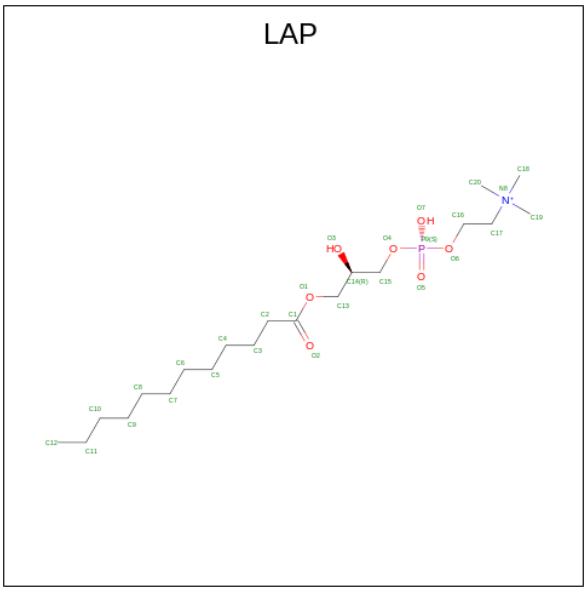
Mol	Chain	Residues	Atoms					AltConf
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



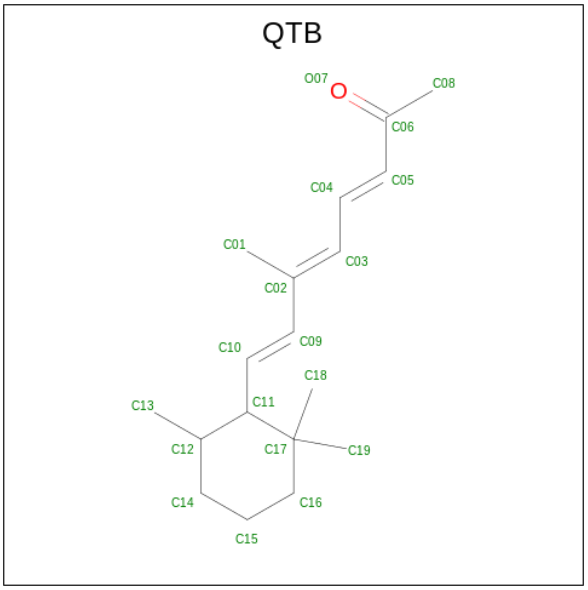
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			61	46	15	
33	7	1	Total	C	O	0
			52	37	15	

- Molecule 34 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: $C_{20}H_{43}NO_7P$) (labeled as "Ligand of Interest" by depositor).



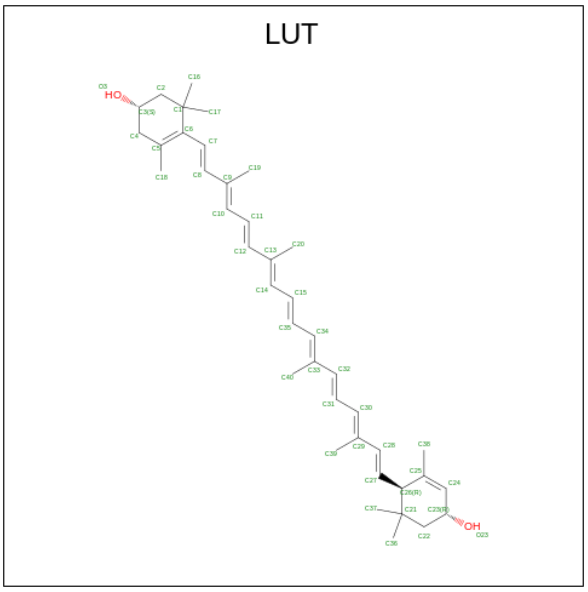
Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 35 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: $C_{18}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
35	F	1	Total C O 19 18 1	0
35	a	1	Total C O 19 18 1	0
35	7	1	Total C O 19 18 1	0
35	9	1	Total C O 19 18 1	0

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	F	1	Total	C	O	0
			42	40	2	
36	J	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	L	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	

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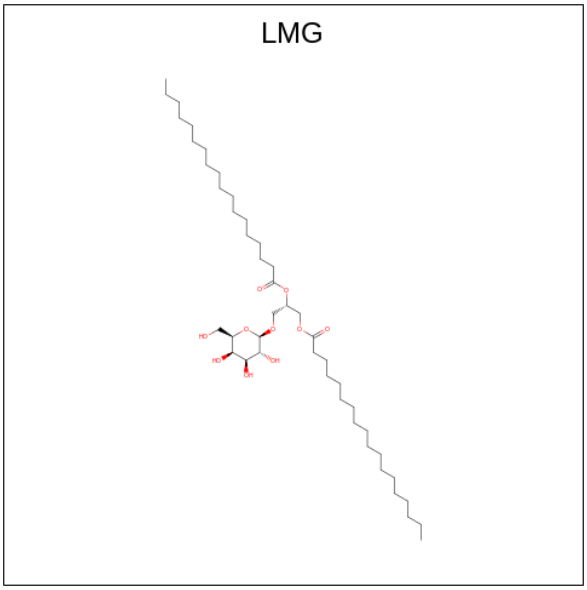
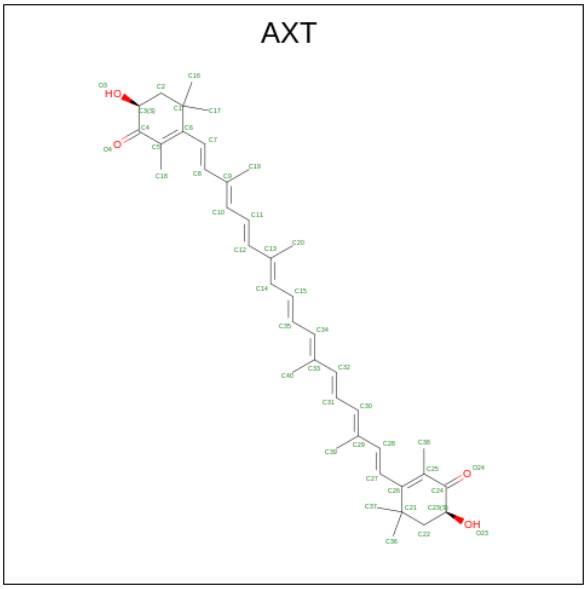
Mol	Chain	Residues	Atoms	AltConf
36	2	1	Total C O 42 40 2	0
36	4	1	Total C O 42 40 2	0
36	4	1	Total C O 42 40 2	0
36	5	1	Total C O 42 40 2	0
36	5	1	Total C O 42 40 2	0
36	6	1	Total C O 42 40 2	0
36	6	1	Total C O 42 40 2	0

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



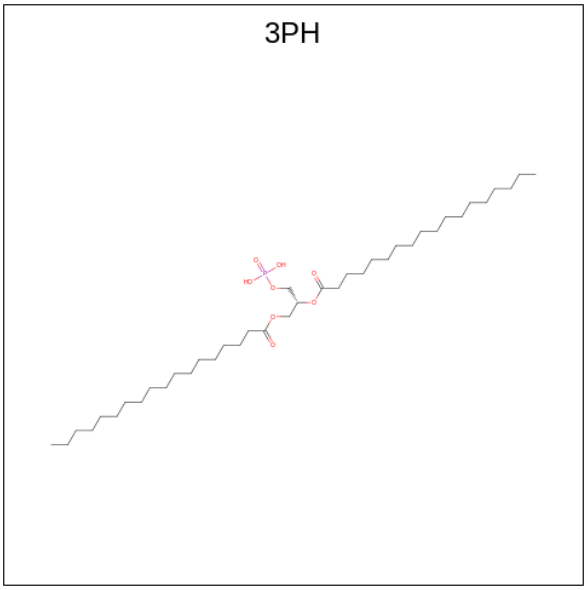
Mol	Chain	Residues	Atoms	AltConf
37	G	1	Total C O 44 34 10	0
37	J	1	Total C O 49 39 10	0
37	J	1	Total C O 29 19 10	0
37	a	1	Total C O 42 32 10	0

- Molecule 38 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



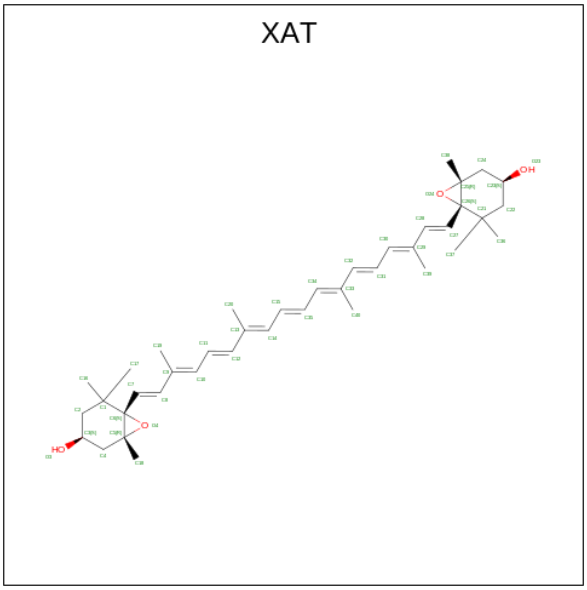
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	a	1	43	40	3	0

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



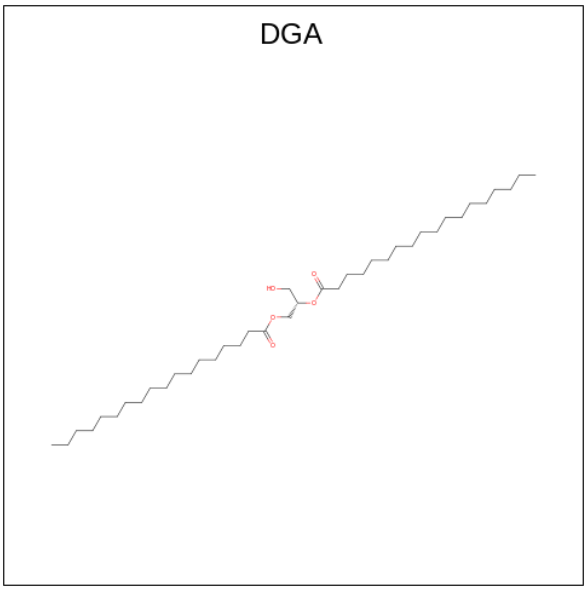
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
39	7	1	33	24	8	1	0

- Molecule 40 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



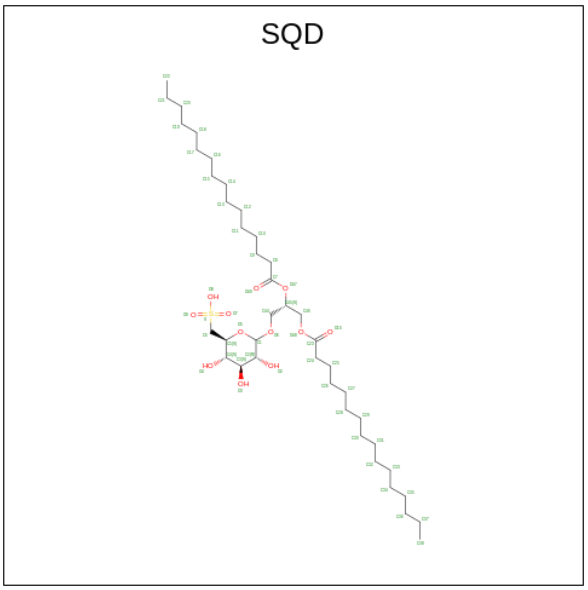
Mol	Chain	Residues	Atoms			AltConf
40	7	1	Total	C	O	0
			44	40	4	

- Molecule 41 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



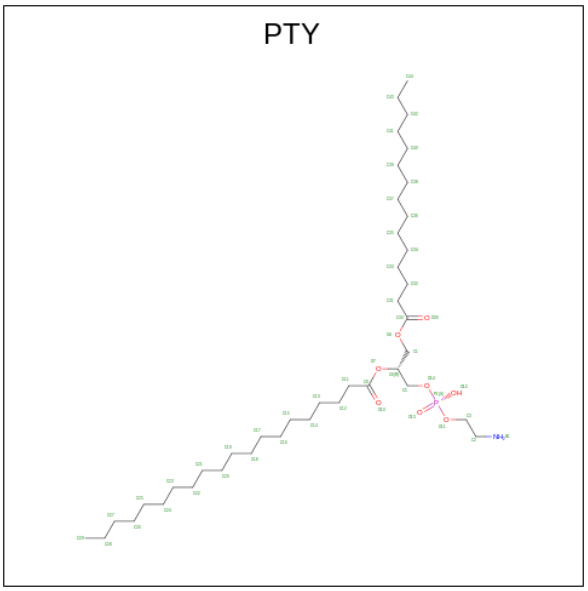
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	8	1	28	23	5	0

- Molecule 42 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
42	4	1	35	22	12	1	0

- Molecule 43 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	297	Total	O	0
			297	297	
44	B	311	Total	O	0
			311	311	
44	C	60	Total	O	0
			60	60	
44	D	53	Total	O	0
			53	53	
44	E	28	Total	O	0
			28	28	
44	F	57	Total	O	0
			57	57	
44	G	18	Total	O	0
			18	18	
44	H	6	Total	O	0
			6	6	
44	I	6	Total	O	0
			6	6	
44	J	16	Total	O	0
			16	16	
44	K	2	Total	O	0
			2	2	

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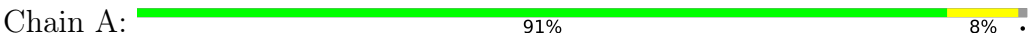
Mol	Chain	Residues	Atoms	AltConf
44	M	5	Total O 5 5	0
44	a	34	Total O 34 34	0
44	3	32	Total O 32 32	0
44	7	39	Total O 39 39	0
44	8	37	Total O 37 37	0
44	9	21	Total O 21 21	0
44	L	17	Total O 17 17	0
44	O	4	Total O 4 4	0
44	2	3	Total O 3 3	0
44	4	1	Total O 1 1	0
44	5	11	Total O 11 11	0
44	6	2	Total O 2 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.

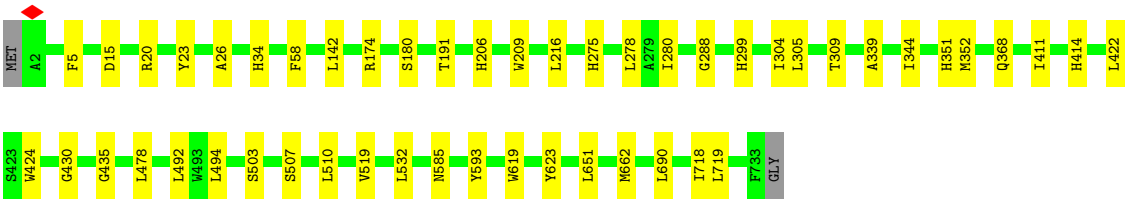
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



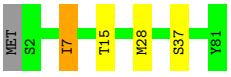
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



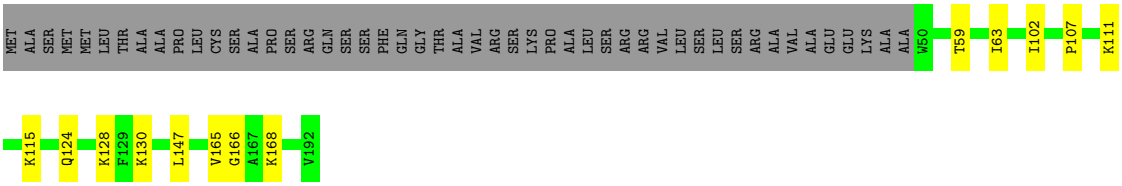
• Molecule 3: Photosystem I iron-sulfur center

Chain C:

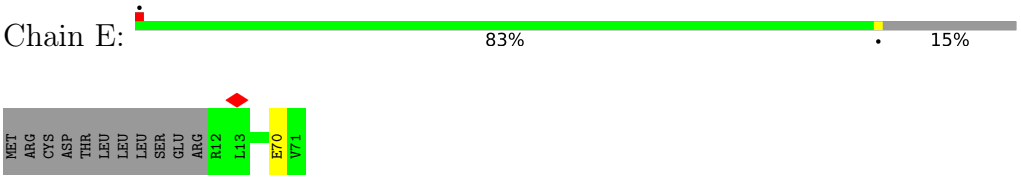


• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

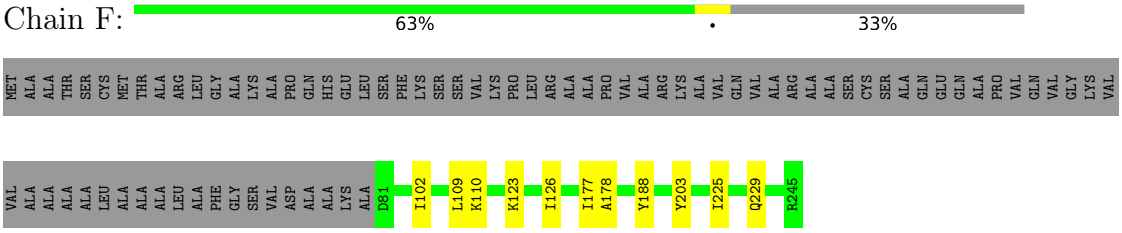
Chain D:



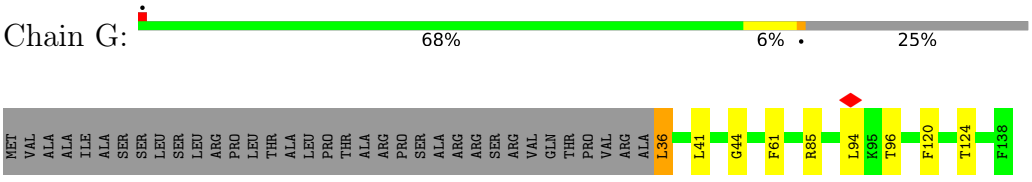
• Molecule 5: Photosystem I reaction centre subunit IV/PsaE



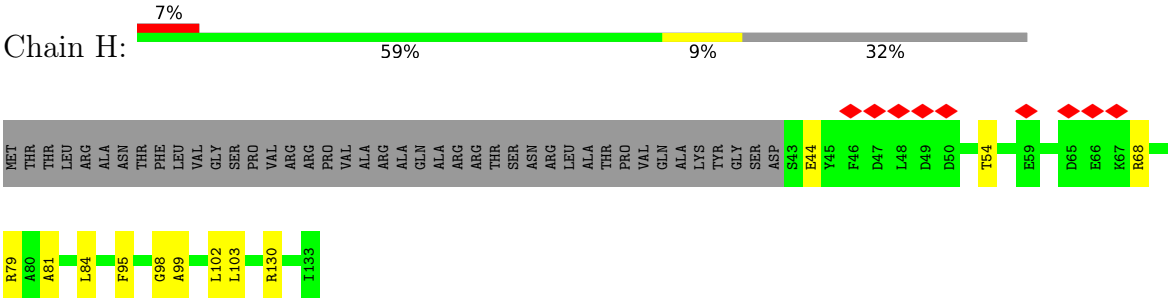
• Molecule 6: Photosystem I reaction center subunit III



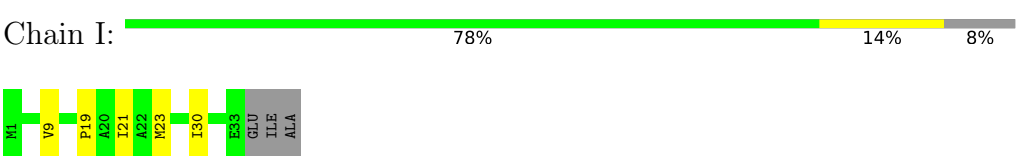
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic



• Molecule 8: Photosystem I reaction centre subunit VI

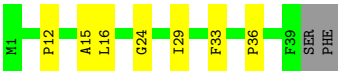


• Molecule 9: Photosystem I reaction center subunit VIII



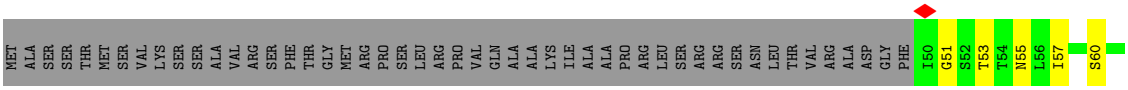
• Molecule 10: Photosystem I reaction center subunit IX

Chain J:



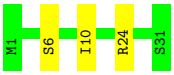
• Molecule 11: PSI-K

Chain K:



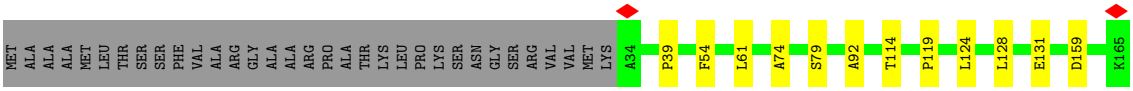
• Molecule 12: Photosystem I reaction center subunit XII

Chain M:



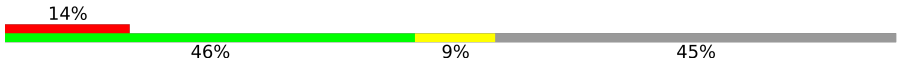
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

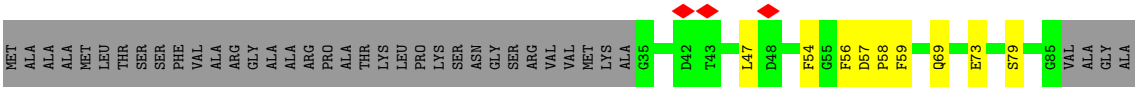
Chain a:

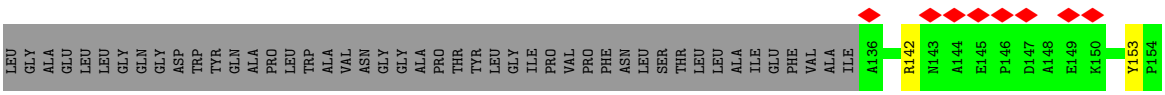


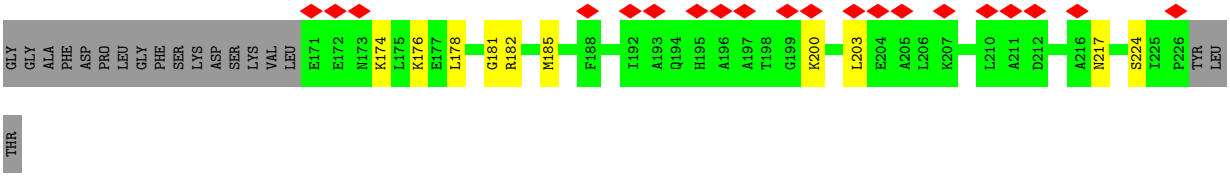
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain b:



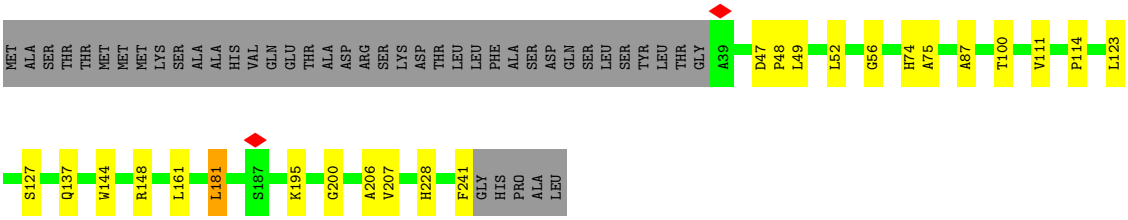






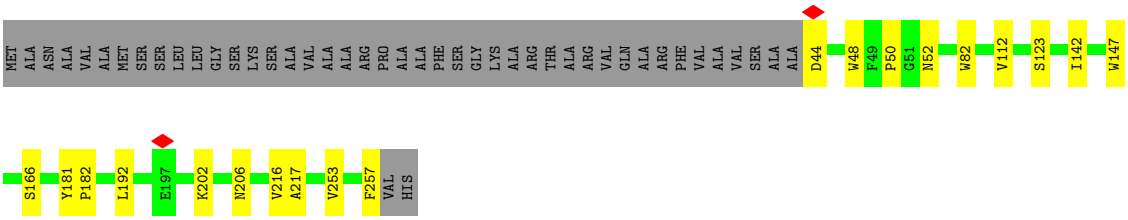
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



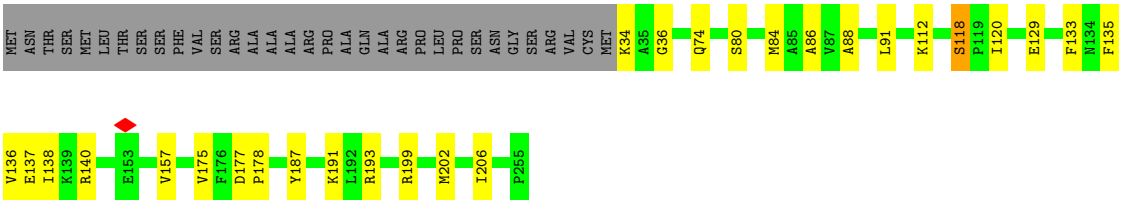
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



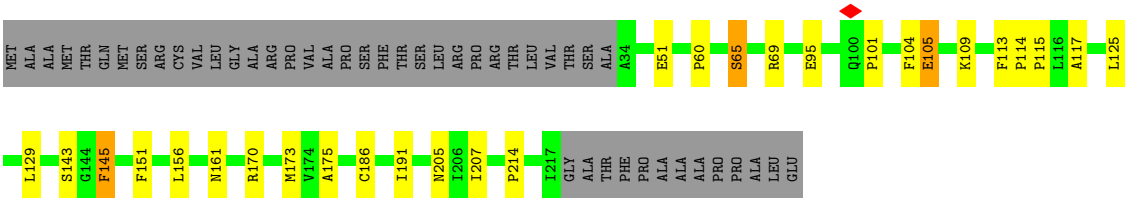
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



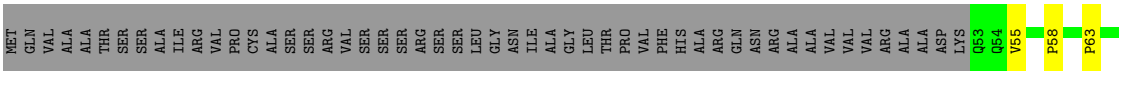
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

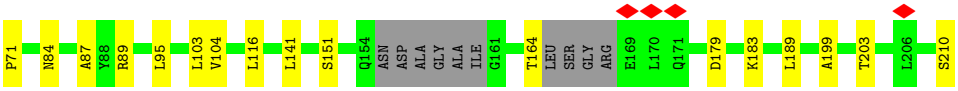
Chain 9:



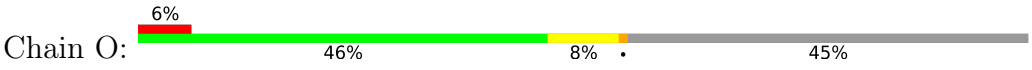
• Molecule 18: PSI subunit V

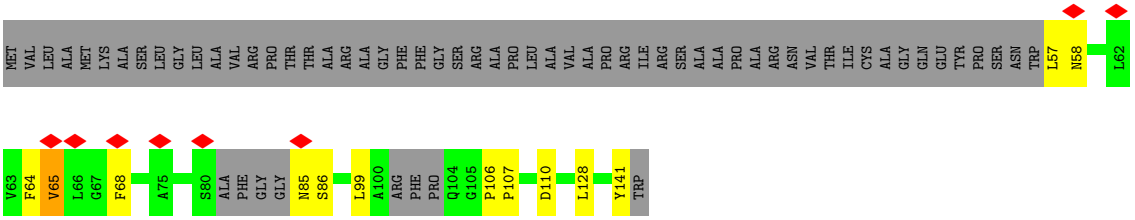
Chain L:



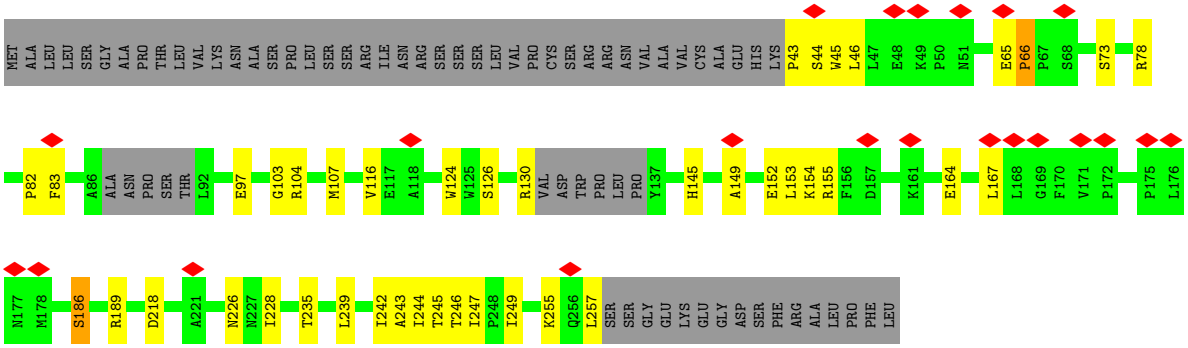


• Molecule 19: Photosystem I PsaO

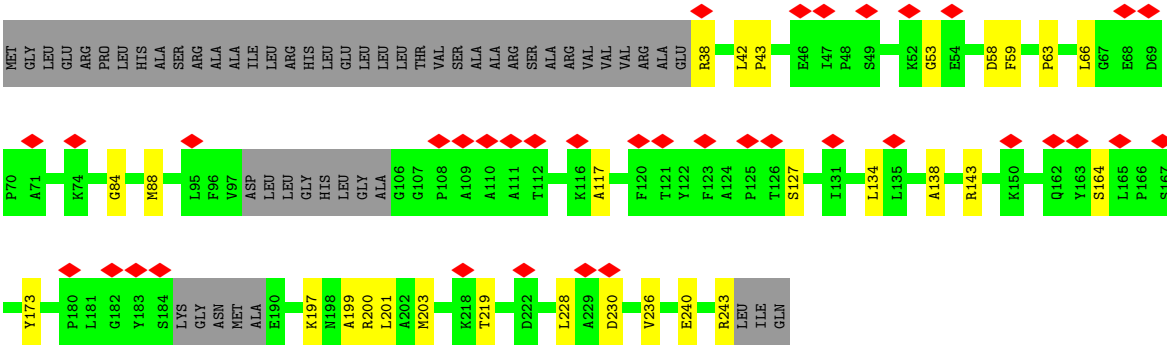




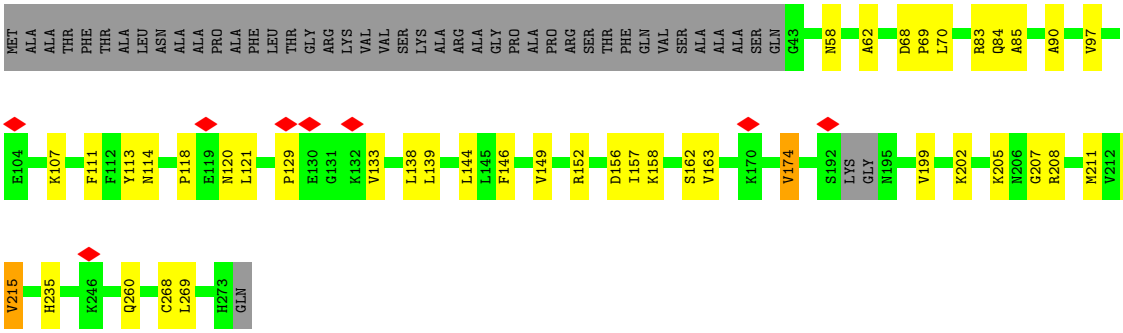
• Molecule 20: Chlorophyll a-b binding protein, chloroplastic/Lhca2



• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

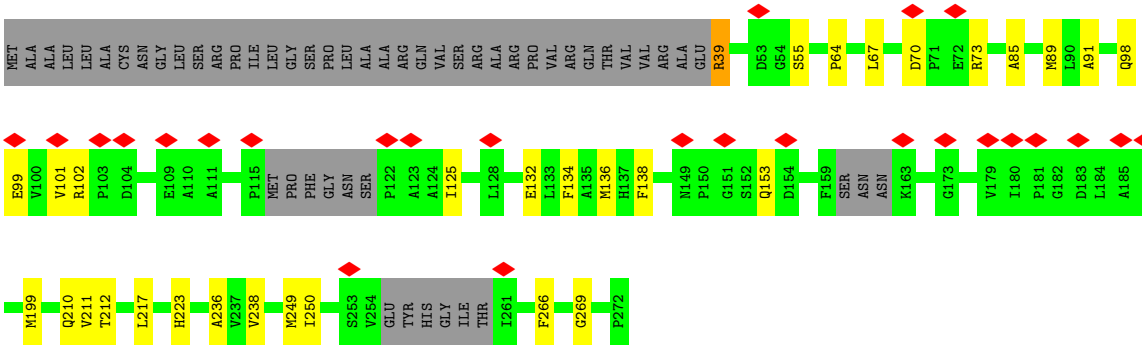


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic



• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224674	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.393	Depositor
Minimum map value	-0.655	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGA, QTB, AXT, 3PH, BCR, CHL, SF4, PTY, LAP, LMT, LHG, XAT, CL0, CLA, DGD, LMG, PQN, SQD, LUT, UNL

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	0.24	0/6012	0.45	0/8202
2	B	0.23	0/6017	0.45	0/8218
3	C	0.30	0/606	0.58	0/822
4	D	0.18	0/1136	0.37	0/1537
5	E	0.19	0/502	0.38	0/686
6	F	0.20	0/1288	0.38	0/1737
7	G	0.18	0/783	0.39	0/1063
8	H	0.18	0/722	0.42	0/972
9	I	0.28	0/254	0.51	0/347
10	J	0.20	0/330	0.41	0/452
11	K	0.18	0/568	0.42	0/773
12	M	0.21	0/240	0.34	0/325
13	a	0.20	0/1501	0.41	0/2045
13	b	0.13	0/977	0.29	0/1322
14	3	0.26	0/1629	0.47	0/2217
15	7	0.20	0/1684	0.38	0/2298
16	8	0.21	0/1752	0.39	0/2379
17	9	0.20	0/1451	0.41	0/1964
18	L	0.19	0/1129	0.42	0/1542
19	O	0.16	0/619	0.39	0/839
20	2	0.22	0/1654	0.54	1/2254 (0.0%)
21	4	0.18	0/1553	0.37	0/2113
22	5	0.21	0/1820	0.46	1/2477 (0.0%)
23	6	0.21	0/1709	0.38	0/2328
All	All	0.22	0/35936	0.43	2/48912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	6	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	66	PRO	CA-N-CD	-8.66	99.87	112.00
22	5	129	PRO	N-CD-CG	-7.27	92.30	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	6	39	ARG	Sidechain

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	5814	0	5649	45	0
2	B	5808	0	5584	38	0
3	C	596	0	573	3	0
4	D	1110	0	1131	9	0
5	E	490	0	482	0	0
6	F	1264	0	1300	9	0
7	G	767	0	749	6	0
8	H	706	0	687	12	0
9	I	248	0	269	4	0
10	J	319	0	326	7	0
11	K	560	0	583	9	0
12	M	237	0	260	2	0
13	a	1458	0	1423	17	0
13	b	952	0	917	15	0
14	3	1580	0	1546	25	0
15	7	1633	0	1579	16	0
16	8	1701	0	1683	18	0
17	9	1414	0	1405	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1102	0	1129	14	0
19	O	605	0	616	7	0
20	2	1606	0	1578	34	0
21	4	1506	0	1468	25	0
22	5	1766	0	1746	34	0
23	6	1658	0	1657	28	0
24	A	33	0	46	1	0
24	B	33	0	46	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	2	40	0	56	3	0
26	3	120	0	168	7	0
26	5	40	0	56	2	0
26	6	40	0	56	2	0
26	7	40	0	56	6	0
26	8	40	0	56	4	0
26	A	160	0	224	11	0
26	B	200	0	280	16	0
26	F	40	0	56	1	0
26	G	80	0	112	1	0
26	I	40	0	56	1	0
26	J	40	0	56	1	0
26	K	80	0	112	7	0
26	L	120	0	168	6	0
26	M	40	0	56	3	0
26	O	40	0	56	2	0
27	5	35	0	44	0	0
27	9	35	0	44	0	0
27	A	70	0	89	4	0
28	5	35	0	40	1	0
28	6	59	0	58	3	0
28	7	86	0	118	8	0
28	8	49	0	74	0	0
28	A	133	0	188	7	0
28	B	32	0	34	1	0
28	a	49	0	74	9	0
29	2	11	0	0	0	0
29	3	11	0	0	4	0
29	4	13	0	0	1	0
29	7	8	0	0	0	0
29	8	18	0	0	0	0
29	9	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	20	0	0	0	0
29	B	24	0	0	0	0
29	a	27	0	0	0	0
30	A	65	0	72	3	0
31	2	574	0	442	16	0
31	3	736	0	697	19	0
31	4	685	0	550	25	0
31	5	678	0	588	21	0
31	6	545	0	436	15	0
31	7	523	0	445	11	0
31	8	692	0	606	19	0
31	9	524	0	452	4	0
31	A	2450	0	2472	93	0
31	B	2382	0	2381	63	0
31	F	161	0	144	4	0
31	G	141	0	105	8	0
31	H	138	0	99	10	0
31	J	42	0	31	1	0
31	K	142	0	105	1	0
31	L	150	0	125	6	0
31	O	134	0	98	0	0
31	a	601	0	547	18	0
31	b	520	0	389	7	0
32	3	56	0	46	1	0
32	4	141	0	92	13	0
32	5	197	0	136	15	0
32	6	296	0	217	18	0
32	7	297	0	272	25	0
32	8	111	0	99	9	0
32	9	95	0	62	5	0
32	A	180	0	165	10	0
32	K	47	0	31	1	0
32	a	157	0	120	13	0
32	b	47	0	30	1	0
33	7	52	0	65	0	0
33	B	61	0	83	4	0
34	B	29	0	42	4	0
35	7	19	0	0	0	0
35	9	19	0	0	0	0
35	F	19	0	0	0	0
35	a	19	0	0	0	0
36	2	42	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	84	0	111	10	0
36	4	84	0	111	11	0
36	5	84	0	111	9	0
36	6	84	0	111	5	0
36	7	42	0	56	3	0
36	8	84	0	112	7	0
36	9	126	0	165	8	0
36	F	42	0	55	2	0
36	J	42	0	54	3	0
36	L	42	0	55	1	0
36	a	84	0	109	10	0
36	b	42	0	56	5	0
37	G	44	0	58	4	0
37	J	78	0	99	4	0
37	a	42	0	54	2	0
38	a	43	0	52	1	0
39	7	33	0	39	1	0
40	7	44	0	56	0	0
41	8	28	0	38	2	0
42	4	35	0	34	1	0
43	5	31	0	35	1	0
44	2	3	0	0	0	0
44	3	32	0	0	0	0
44	4	1	0	0	0	0
44	5	11	0	0	0	0
44	6	2	0	0	0	0
44	7	39	0	0	0	0
44	8	37	0	0	0	0
44	9	21	0	0	0	0
44	A	297	0	0	1	0
44	B	311	0	0	2	0
44	C	60	0	0	0	0
44	D	53	0	0	0	0
44	E	28	0	0	0	0
44	F	57	0	0	0	0
44	G	18	0	0	0	0
44	H	6	0	0	1	0
44	I	6	0	0	0	0
44	J	16	0	0	0	0
44	K	2	0	0	0	0
44	L	17	0	0	0	0
44	M	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	O	4	0	0	0	0
44	a	34	0	0	0	0
All	All	52991	0	50690	710	0

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

All (710) 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)
31:H:902:CLA:HAA1	20:2:153:LEU:HD23	1.31	1.06
14:3:241:PHE:CD2	29:3:306:UNL:C2	2.39	1.05
31:A:829:CLA:HBA2	28:7:302:LHG:H242	1.39	1.02
31:H:902:CLA:O1A	20:2:153:LEU:HD21	1.61	0.99
20:2:243:ALA:O	20:2:247:ILE:HG13	1.64	0.96
14:3:241:PHE:CE2	29:3:306:UNL:C2	2.56	0.88
26:2:302:BCR:H12C	31:2:304:CLA:HAB	1.58	0.86
1:A:241:HIS:NE2	31:A:829:CLA:HMD3	1.92	0.84
31:A:825:CLA:H2	14:3:49:LEU:HD13	1.60	0.83
36:b:301:LUT:H32	31:b:313:CLA:HAB	1.62	0.82
31:H:902:CLA:O1A	20:2:153:LEU:CD2	2.28	0.80
14:3:241:PHE:HD2	29:3:306:UNL:C2	1.93	0.77
31:H:902:CLA:CAA	20:2:153:LEU:HD23	2.14	0.75
31:2:312:CLA:HBB1	31:2:314:CLA:HBB1	1.70	0.74
1:A:350:HIS:HD2	1:A:408:HIS:HD1	1.36	0.72
26:M:101:BCR:H23C	31:2:315:CLA:HBB1	1.71	0.72
31:5:318:CLA:MG	31:5:318:CLA:ND	1.48	0.71
12:M:24:ARG:NH1	44:M:201:HOH:O	2.22	0.71
32:8:316:CHL:H92	32:8:316:CHL:H41	1.73	0.70
32:5:316:CHL:HAB	32:5:319:CHL:HBB2	1.74	0.70
31:B:834:CLA:HBB2	31:B:850:CLA:HBA2	1.74	0.69
13:b:185:MET:HB3	36:b:301:LUT:H35	1.72	0.69
36:a:305:LUT:H11	32:a:320:CHL:HHB	1.73	0.69
14:3:49:LEU:HD12	36:3:305:LUT:H222	1.72	0.69
2:B:209:TRP:HB3	34:B:851:LAP:H202	1.75	0.68
1:A:31:LYS:NZ	44:A:903:HOH:O	2.28	0.67
20:2:104:ARG:HH22	31:2:304:CLA:HED2	1.59	0.67
31:A:837:CLA:H201	31:A:837:CLA:HAB	1.77	0.66
20:2:66:PRO:HD2	20:2:66:PRO:O	1.96	0.66
23:6:210:GLN:HE22	23:6:266:PHE:H	1.41	0.66
1:A:483:PHE:HB3	31:A:850:CLA:H2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:829:CLA:CBA	28:7:302:LHG:H242	2.22	0.65
16:8:193:ARG:HG3	31:8:313:CLA:HED2	1.80	0.64
20:2:149:ALA:O	20:2:153:LEU:HG	1.98	0.64
32:5:317:CHL:HAB	32:5:322:CHL:CMC	2.28	0.64
13:b:182:ARG:HB3	31:b:313:CLA:HBC2	1.80	0.63
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.81	0.63
36:3:305:LUT:H393	31:3:319:CLA:H151	1.81	0.63
14:3:75:ALA:HB1	14:3:200:GLY:HA3	1.81	0.62
1:A:16:VAL:HG12	14:3:56:GLY:HA3	1.81	0.62
31:A:832:CLA:H141	32:A:840:CHL:H202	1.81	0.62
21:4:88:MET:CE	31:4:305:CLA:HHC	2.29	0.62
22:5:208:ARG:HH22	31:5:310:CLA:HED3	1.65	0.61
1:A:350:HIS:CD2	1:A:408:HIS:HD1	2.18	0.61
32:4:310:CHL:HAA1	32:4:317:CHL:HHD	1.83	0.61
31:A:835:CLA:HMD2	26:K:202:BCR:H24C	1.82	0.61
1:A:32:PRO:HB3	31:A:816:CLA:HAC1	1.82	0.61
31:A:851:CLA:H191	31:L:305:CLA:H93	1.81	0.61
36:b:301:LUT:H11	31:b:305:CLA:HBC3	1.82	0.61
31:A:816:CLA:HHC	31:A:816:CLA:HBB1	1.82	0.61
26:A:803:BCR:H21C	27:A:807:LMT:H123	1.83	0.61
32:a:317:CHL:HMA2	16:8:138:ILE:HD13	1.81	0.61
14:3:195:LYS:NZ	31:3:308:CLA:O1D	2.33	0.61
1:A:241:HIS:CD2	31:A:829:CLA:HMD3	2.35	0.60
20:2:242:ILE:O	20:2:246:THR:HG23	2.01	0.60
41:8:305:DGA:HG11	31:8:321:CLA:HED2	1.83	0.60
32:A:839:CHL:HMA2	32:A:840:CHL:O1D	2.01	0.60
14:3:161:LEU:HD22	26:3:302:BCR:HC32	1.83	0.60
7:G:124:THR:HG22	31:G:206:CLA:HED2	1.84	0.60
36:4:302:LUT:H392	31:4:305:CLA:HBC3	1.83	0.60
32:7:318:CHL:HMC	32:7:318:CHL:HBC2	1.84	0.60
20:2:145:HIS:HD2	31:2:314:CLA:HBB2	1.66	0.59
1:A:197:MET:HB2	31:A:826:CLA:HBC2	1.82	0.59
31:B:843:CLA:HED3	31:G:206:CLA:HMA2	1.82	0.59
26:A:806:BCR:H23C	31:A:815:CLA:H111	1.84	0.59
31:A:830:CLA:CHD	32:A:831:CHL:HBB2	2.32	0.59
31:3:309:CLA:H192	15:7:52:ASN:HD22	1.66	0.59
31:A:825:CLA:H51	31:3:319:CLA:H8	1.84	0.59
16:8:112:LYS:HB2	32:8:316:CHL:HED2	1.83	0.59
31:4:311:CLA:NB	28:6:301:LHG:O4	2.35	0.59
33:B:808:DGD:HA91	31:B:813:CLA:HBC1	1.84	0.58
13:a:39:PRO:HD2	32:a:317:CHL:HED3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:6:85:ALA:HB1	23:6:195:GLY:HA3	1.84	0.58
31:A:833:CLA:C2	14:3:48:PRO:HB2	2.33	0.58
26:7:304:BCR:H21C	32:7:320:CHL:C2	2.33	0.58
31:B:825:CLA:H12	31:G:206:CLA:HED1	1.83	0.58
15:7:181:TYR:HB3	31:7:309:CLA:HED3	1.84	0.58
23:6:210:GLN:HA	23:6:250:ILE:HD12	1.85	0.58
14:3:137:GLN:NE2	31:3:309:CLA:O1D	2.37	0.58
17:9:101:PRO:HG2	17:9:109:LYS:HD2	1.86	0.58
31:2:306:CLA:H101	31:2:306:CLA:HAB	1.84	0.58
26:B:804:BCR:HC31	37:G:202:LMG:H391	1.85	0.58
32:9:320:CHL:C1C	32:9:322:CHL:HMC	2.34	0.58
2:B:216:LEU:HD11	17:9:214:PRO:HA	1.86	0.57
36:9:303:LUT:H393	31:9:314:CLA:H121	1.87	0.57
1:A:217:GLN:HA	1:A:221:SER:HB2	1.86	0.57
31:H:903:CLA:HAC1	18:L:84:ASN:HB3	1.87	0.57
22:5:146:PHE:HA	22:5:149:VAL:HG22	1.87	0.57
15:7:257:PHE:HE1	31:7:322:CLA:HAB	1.69	0.57
21:4:138:ALA:HA	31:4:316:CLA:HBB1	1.84	0.57
26:A:804:BCR:HC8	31:A:818:CLA:H72	1.85	0.57
13:b:142:ARG:NH1	31:b:311:CLA:O1D	2.37	0.57
26:5:302:BCR:H372	32:5:316:CHL:HBB1	1.86	0.57
31:B:820:CLA:HBB2	31:B:822:CLA:HMA3	1.85	0.57
31:A:823:CLA:H12	31:A:825:CLA:H43	1.85	0.57
36:a:303:LUT:H31	31:a:309:CLA:H72	1.85	0.57
20:2:82:PRO:HD2	36:2:301:LUT:H3	1.85	0.57
32:4:310:CHL:HAA1	32:4:317:CHL:CHD	2.35	0.57
27:A:807:LMT:O3'	31:A:828:CLA:O1D	2.22	0.57
36:4:303:LUT:H193	31:4:314:CLA:HBA2	1.86	0.57
36:5:304:LUT:H363	31:5:315:CLA:H43	1.86	0.57
13:a:183:LEU:HG	36:a:303:LUT:H11	1.87	0.56
32:7:319:CHL:HBB1	32:7:319:CHL:HMB3	1.87	0.56
11:K:77:ALA:O	11:K:92:SER:OG	2.22	0.56
13:b:47:LEU:HD11	13:b:57:ASP:HB2	1.87	0.56
31:6:306:CLA:HMB2	31:6:322:CLA:C2D	2.35	0.56
31:A:853:CLA:H111	31:A:853:CLA:HAB	1.88	0.56
13:a:176:LYS:HG3	31:a:315:CLA:HED2	1.87	0.56
32:5:317:CHL:OMC	32:5:322:CHL:HMC	2.06	0.56
6:F:109:LEU:HD21	6:F:123:LYS:HZ3	1.70	0.56
10:J:24:GLY:HA3	31:J:105:CLA:HAB	1.88	0.56
19:O:65:VAL:HA	19:O:68:PHE:HB2	1.87	0.56
13:b:176:LYS:HD3	31:b:302:CLA:HED2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:H:902:CLA:HAA1	20:2:153:LEU:CD2	2.21	0.56
22:5:90:ALA:HB1	22:5:207:GLY:HA3	1.88	0.56
36:a:303:LUT:H31	31:a:309:CLA:H111	1.88	0.56
31:3:309:CLA:HBA2	32:7:317:CHL:H102	1.88	0.56
13:b:79:SER:HB2	13:b:181:GLY:HA3	1.88	0.55
22:5:114:ASN:O	22:5:120:ASN:ND2	2.39	0.55
14:3:241:PHE:CD2	29:3:306:UNL:C3	2.89	0.55
31:3:309:CLA:H111	15:7:48:TRP:HH2	1.71	0.55
15:7:192:LEU:HD21	23:6:67:LEU:HD23	1.88	0.55
21:4:59:PHE:CD2	32:4:313:CHL:HMC	2.41	0.55
20:2:65:GLU:HB3	20:2:255:LYS:HE2	1.89	0.55
31:4:312:CLA:HED2	23:6:134:PHE:HE2	1.70	0.55
23:6:102:ARG:NH1	31:6:314:CLA:OBD	2.38	0.55
22:5:69:PRO:HD2	36:5:304:LUT:H23	1.87	0.55
13:b:58:PRO:HD2	36:b:301:LUT:H23	1.88	0.55
31:B:819:CLA:H171	8:H:98:GLY:HA3	1.88	0.55
37:G:202:LMG:H121	31:a:319:CLA:HBA1	1.89	0.55
17:9:95:GLU:HB3	17:9:191:ILE:HD12	1.88	0.55
28:A:811:LHG:H161	31:A:855:CLA:HBA2	1.88	0.54
36:7:305:LUT:H181	31:7:311:CLA:HBB1	1.89	0.54
21:4:84:GLY:HA3	21:4:199:ALA:HB1	1.89	0.54
32:5:319:CHL:HED1	31:5:320:CLA:CGA	2.36	0.54
23:6:91:ALA:HB2	36:6:304:LUT:H192	1.90	0.54
17:9:173:MET:HB3	36:9:303:LUT:H402	1.89	0.54
1:A:119:TRP:HB3	36:J:103:LUT:H42	1.89	0.54
31:A:814:CLA:HHB	31:B:811:CLA:H202	1.90	0.54
2:B:424:TRP:HZ3	31:B:845:CLA:HBC2	1.71	0.54
17:9:105:GLU:HA	32:9:320:CHL:HED1	1.90	0.54
23:6:193:LYS:NZ	31:6:315:CLA:O1D	2.40	0.54
36:5:304:LUT:H382	31:5:310:CLA:H2	1.90	0.54
28:A:811:LHG:H223	31:A:819:CLA:HED3	1.88	0.54
31:A:841:CLA:H201	26:J:102:BCR:H15C	1.89	0.54
32:4:310:CHL:HMA2	32:4:317:CHL:HAC2	1.90	0.54
2:B:507:SER:HA	2:B:510:LEU:HD21	1.90	0.54
7:G:44:GLY:HA3	31:G:204:CLA:H2	1.89	0.54
36:a:305:LUT:H41	31:a:314:CLA:H2	1.88	0.54
31:A:845:CLA:H8	31:L:305:CLA:H91	1.90	0.53
28:a:306:LHG:HC42	26:8:301:BCR:HC32	1.90	0.53
31:7:311:CLA:H52	32:7:317:CHL:H92	1.89	0.53
22:5:118:PRO:HA	22:5:121:LEU:HD12	1.89	0.53
32:6:318:CHL:C4C	32:6:320:CHL:HMC	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD11	31:A:832:CLA:H51	1.90	0.53
31:B:844:CLA:H93	31:B:845:CLA:HBC1	1.91	0.53
32:8:316:CHL:H41	32:8:316:CHL:C9	2.38	0.53
28:a:306:LHG:H142	26:8:301:BCR:HC8	1.89	0.53
6:F:102:ILE:HD12	6:F:126:ILE:HG23	1.89	0.53
12:M:10:ILE:HD11	20:2:235:THR:OG1	2.09	0.53
32:a:317:CHL:HBA1	16:8:135:PHE:HA	1.90	0.53
15:7:82:TRP:CE2	32:7:319:CHL:HED3	2.44	0.53
22:5:260:GLN:HG3	26:5:302:BCR:H311	1.91	0.53
17:9:117:ALA:HB1	31:2:311:CLA:HED1	1.92	0.52
4:D:124:GLN:HG3	4:D:128:LYS:HE3	1.91	0.52
32:a:317:CHL:HBB1	32:a:317:CHL:HMB1	1.92	0.52
28:A:811:LHG:H332	31:A:819:CLA:H72	1.91	0.52
2:B:26:ALA:HA	31:B:837:CLA:H42	1.90	0.52
26:A:803:BCR:H392	26:K:202:BCR:HC8	1.92	0.52
4:D:63:ILE:HB	4:D:102:ILE:HB	1.92	0.52
36:8:302:LUT:H31	31:8:308:CLA:H112	1.91	0.52
36:5:304:LUT:H193	32:5:316:CHL:HAB	1.92	0.52
15:7:123:SER:HB2	32:7:318:CHL:HED2	1.92	0.52
32:5:316:CHL:H8	32:6:309:CHL:CED	2.40	0.52
21:4:63:PRO:HD2	36:4:303:LUT:H23	1.91	0.52
31:B:820:CLA:H201	31:B:823:CLA:H92	1.91	0.51
19:O:85:ASN:OD1	19:O:85:ASN:N	2.42	0.51
28:6:305:LHG:HC82	28:6:305:LHG:H262	1.91	0.51
32:4:310:CHL:HBC2	32:4:310:CHL:HHD	1.91	0.51
10:J:16:LEU:HD13	36:J:103:LUT:H30	1.92	0.51
17:9:145:PHE:H	17:9:151:PHE:HB2	1.76	0.51
1:A:740:TRP:NE1	31:A:841:CLA:O1A	2.38	0.51
1:A:241:HIS:CE1	31:A:829:CLA:C2D	2.94	0.51
36:8:302:LUT:H27	31:8:317:CLA:H42	1.93	0.51
1:A:322:ILE:HG21	31:A:838:CLA:HAC1	1.93	0.51
31:A:846:CLA:H102	31:B:846:CLA:H51	1.92	0.51
31:B:831:CLA:HBB2	31:B:848:CLA:H52	1.91	0.51
32:7:317:CHL:O1D	32:7:317:CHL:HAA1	2.11	0.51
3:C:7:ILE:O	4:D:168:LYS:N	2.42	0.51
31:G:206:CLA:HMC2	32:a:318:CHL:HED3	1.93	0.51
31:A:827:CLA:H62	31:A:829:CLA:CMB	2.40	0.51
22:5:97:VAL:HG11	36:5:303:LUT:H10	1.93	0.51
21:4:138:ALA:CA	31:4:316:CLA:HBB1	2.41	0.51
22:5:156:ASP:HB2	32:5:317:CHL:HAC1	1.93	0.51
31:A:845:CLA:H2	31:L:305:CLA:H43	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:HIS:ND1	31:B:850:CLA:OBD	2.43	0.50
31:5:323:CLA:HED2	32:6:317:CHL:H3A	1.92	0.50
23:6:249:MET:SD	23:6:249:MET:N	2.84	0.50
8:H:84:LEU:HD13	18:L:189:LEU:HD23	1.93	0.50
31:A:853:CLA:HAA2	31:B:839:CLA:HMB1	1.93	0.50
36:a:305:LUT:H27	31:a:321:CLA:HAB	1.93	0.50
18:L:71:PRO:HB3	19:O:57:LEU:HG	1.92	0.50
23:6:211:VAL:HG23	23:6:212:THR:HG23	1.93	0.50
31:A:836:CLA:HAB	31:A:854:CLA:HAB	1.93	0.50
4:D:59:THR:HG23	4:D:107:PRO:HB2	1.92	0.50
8:H:103:LEU:HD22	9:I:9:VAL:HG13	1.93	0.50
1:A:501:ASN:HB2	31:A:849:CLA:HED2	1.93	0.50
31:A:857:CLA:H13	18:L:141:LEU:HD21	1.94	0.50
14:3:52:LEU:HB2	31:3:319:CLA:HBA2	1.92	0.50
28:7:307:LHG:H321	31:7:311:CLA:H91	1.94	0.50
13:a:74:ALA:HB2	31:a:319:CLA:HED3	1.94	0.50
31:7:313:CLA:HAC1	32:7:318:CHL:HBB2	1.93	0.50
20:2:218:ASP:HB3	20:2:226:ASN:HD22	1.77	0.50
36:4:302:LUT:C39	31:4:305:CLA:HBC3	2.42	0.50
15:7:142:ILE:HG21	31:8:314:CLA:HMC2	1.94	0.50
26:7:304:BCR:H21C	32:7:320:CHL:H61	1.93	0.50
36:8:303:LUT:H393	31:8:310:CLA:H13	1.94	0.50
1:A:373:SER:HB2	32:A:840:CHL:HMC	1.94	0.49
26:B:804:BCR:H323	37:G:202:LMG:H361	1.94	0.49
10:J:12:PRO:HB2	36:J:103:LUT:H363	1.94	0.49
2:B:368:GLN:NE2	44:B:918:HOH:O	2.45	0.49
1:A:349:TRP:HB3	31:A:818:CLA:HAC1	1.94	0.49
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.94	0.49
31:A:814:CLA:H121	31:A:841:CLA:H151	1.94	0.49
10:J:29:ILE:HG12	37:J:101:LMG:H341	1.93	0.49
22:5:213:ALA:HB2	36:5:303:LUT:H192	1.94	0.49
31:4:314:CLA:C3D	32:4:317:CHL:HMC	2.43	0.49
23:6:70:ASP:HB2	23:6:73:ARG:HB2	1.95	0.49
1:A:119:TRP:CD2	31:A:822:CLA:HED3	2.47	0.49
31:A:828:CLA:H191	36:3:305:LUT:H8	1.94	0.49
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.94	0.49
2:B:690:LEU:HD11	18:L:87:ALA:HB1	1.94	0.49
16:8:133:PHE:HA	16:8:136:VAL:HG22	1.94	0.49
31:4:318:CLA:HAA2	31:4:318:CLA:HED2	1.94	0.49
32:A:840:CHL:HBB1	32:A:840:CHL:HMB3	1.94	0.49
2:B:339:ALA:HB2	26:B:805:BCR:H372	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:228:HIS:CD2	31:3:320:CLA:NC	2.80	0.49
1:A:68:GLU:HG3	1:A:72:LYS:HE2	1.94	0.49
7:G:85:ARG:NH1	17:9:65:SER:OG	2.44	0.49
26:7:304:BCR:C21	32:7:320:CHL:H61	2.43	0.49
31:5:318:CLA:H143	32:6:309:CHL:H2	1.94	0.49
13:a:79:SER:HB3	13:a:181:GLY:HA3	1.94	0.49
20:2:152:GLU:OE2	31:2:314:CLA:NB	2.45	0.49
23:6:64:PRO:HD2	36:6:304:LUT:H23	1.95	0.49
31:5:318:CLA:H191	31:6:308:CLA:HBC1	1.95	0.49
17:9:156:LEU:O	17:9:161:ASN:ND2	2.45	0.48
21:4:138:ALA:HB2	31:4:316:CLA:CBB	2.43	0.48
23:6:132:GLU:OE1	32:6:318:CHL:HMC	2.13	0.48
24:A:801:PQN:H202	31:F:301:CLA:HAB	1.95	0.48
31:H:901:CLA:HBB2	26:L:303:BCR:H311	1.94	0.48
32:5:317:CHL:HAA1	32:5:317:CHL:CGD	2.43	0.48
31:6:306:CLA:HBA2	31:6:306:CLA:H3A	1.45	0.48
28:A:810:LHG:H302	31:A:837:CLA:H172	1.95	0.48
30:A:813:CL0:H33	31:A:856:CLA:C1D	2.44	0.48
34:B:851:LAP:H32	17:9:104:PHE:CD2	2.49	0.48
21:4:170:GLU:HB2	21:4:173:TYR:HB2	1.95	0.48
8:H:130:ARG:NH1	44:H:1002:HOH:O	2.37	0.48
17:9:60:PRO:HD2	36:9:303:LUT:H23	1.96	0.48
32:4:313:CHL:H11	23:6:134:PHE:HD1	1.79	0.48
31:6:306:CLA:HMB2	31:6:322:CLA:C3D	2.43	0.48
31:A:829:CLA:HAB	28:7:302:LHG:H322	1.95	0.48
2:B:5:PHE:HB2	9:I:30:ILE:HA	1.95	0.48
13:a:176:LYS:HD3	31:a:310:CLA:HBA1	1.95	0.48
36:a:305:LUT:H161	36:a:305:LUT:H192	1.95	0.48
16:8:34:LYS:NZ	16:8:36:GLY:O	2.40	0.48
15:7:182:PRO:HB3	31:7:321:CLA:HBC2	1.95	0.48
16:8:80:SER:O	16:8:84:MET:HB2	2.13	0.48
2:B:305:LEU:HD11	31:B:832:CLA:HMC1	1.96	0.48
17:9:175:ALA:HB2	36:9:302:LUT:H192	1.96	0.48
20:2:66:PRO:O	20:2:66:PRO:CD	2.61	0.48
9:I:19:PRO:O	9:I:23:MET:HG3	2.14	0.48
21:4:197:LYS:HD3	28:6:301:LHG:HC61	1.96	0.48
31:4:318:CLA:HBA1	31:4:318:CLA:H3A	1.66	0.48
32:7:318:CHL:H51	32:7:318:CHL:H93	1.96	0.47
10:J:36:PRO:HB2	37:J:101:LMG:H112	1.96	0.47
20:2:103:GLY:O	20:2:107:MET:HG2	2.13	0.47
31:A:814:CLA:HBC2	2:B:585:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:819:CLA:H71	31:A:843:CLA:HBC3	1.96	0.47
31:A:848:CLA:H41	31:A:848:CLA:H61	1.62	0.47
8:H:95:PHE:CE1	9:I:21:ILE:HD11	2.49	0.47
14:3:111:VAL:HG21	36:3:305:LUT:H172	1.96	0.47
20:2:152:GLU:HA	20:2:155:ARG:HB2	1.96	0.47
36:4:303:LUT:H172	31:4:314:CLA:HHB	1.96	0.47
22:5:111:PHE:HB3	22:5:114:ASN:HB2	1.95	0.47
36:5:303:LUT:H30	31:5:307:CLA:H61	1.96	0.47
32:A:831:CHL:HBB1	32:A:831:CHL:H92	1.95	0.47
22:5:107:LYS:HB3	22:5:107:LYS:HE3	1.73	0.47
32:6:321:CHL:HBC2	32:6:321:CHL:HMC	1.96	0.47
26:A:806:BCR:H362	31:A:814:CLA:H2	1.96	0.47
31:A:827:CLA:H62	31:A:829:CLA:HMB1	1.96	0.47
11:K:113:ILE:HD11	26:K:202:BCR:H23C	1.97	0.47
32:7:318:CHL:HMB3	32:7:318:CHL:H52	1.96	0.47
13:b:69:GLN:NE2	13:b:73:GLU:OE2	2.44	0.47
36:6:303:LUT:H32	31:6:307:CLA:HMC2	1.97	0.47
1:A:241:HIS:CG	31:A:829:CLA:C1D	2.98	0.47
27:A:807:LMT:H122	26:3:303:BCR:H331	1.96	0.47
13:a:128:LEU:HD21	32:a:318:CHL:HAC2	1.96	0.47
28:a:306:LHG:H351	28:a:306:LHG:H322	1.62	0.47
21:4:38:ARG:NH2	21:4:58:ASP:OD1	2.48	0.47
21:4:117:ALA:HB1	32:4:310:CHL:HED1	1.95	0.47
22:5:139:LEU:HD21	31:5:318:CLA:H171	1.95	0.47
15:7:202:LYS:HD3	31:7:315:CLA:HED1	1.97	0.47
18:L:199:ALA:O	18:L:203:THR:HG23	2.15	0.47
23:6:210:GLN:HE22	23:6:266:PHE:N	2.12	0.47
1:A:610:PHE:O	1:A:614:MET:HG2	2.15	0.47
31:A:823:CLA:HBB2	31:A:826:CLA:HMA3	1.97	0.47
26:3:302:BCR:HC31	22:5:70:LEU:HD22	1.97	0.47
17:9:125:LEU:HD23	32:9:322:CHL:HMA2	1.96	0.47
22:5:235:HIS:CG	31:5:309:CLA:HAA2	2.49	0.47
1:A:684:MET:HB2	31:A:815:CLA:C1C	2.45	0.47
32:7:318:CHL:HBA2	32:7:318:CHL:H3A	1.69	0.47
32:8:316:CHL:H93	32:8:316:CHL:H51	1.96	0.47
13:b:54:PHE:CD2	32:b:309:CHL:HMC	2.49	0.47
22:5:138:LEU:HD12	22:5:138:LEU:HA	1.77	0.47
2:B:411:ILE:HA	2:B:414:HIS:CE1	2.50	0.46
31:a:315:CLA:HBB1	16:8:157:VAL:HG21	1.96	0.46
32:7:324:CHL:O1D	32:7:324:CHL:HAA2	2.15	0.46
31:4:305:CLA:HBC2	31:4:315:CLA:O2A	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:813:CL0:H33	31:A:856:CLA:CHD	2.45	0.46
2:B:718:ILE:HG22	31:B:835:CLA:H52	1.96	0.46
3:C:7:ILE:N	4:D:166:GLY:O	2.40	0.46
32:9:322:CHL:HAA2	32:9:322:CHL:CGD	2.45	0.46
6:F:177:ILE:HG23	31:F:306:CLA:HAA1	1.98	0.46
17:9:69:ARG:HD2	17:9:69:ARG:HA	1.63	0.46
22:5:138:LEU:HD11	32:5:319:CHL:C2D	2.45	0.46
31:6:306:CLA:HBB1	31:6:306:CLA:HMB1	1.98	0.46
31:6:306:CLA:HBB2	31:6:322:CLA:HBC3	1.98	0.46
31:A:830:CLA:H41	31:A:830:CLA:H62	1.54	0.46
31:A:835:CLA:H2	31:A:835:CLA:H62	1.70	0.46
13:a:131:GLU:OE1	32:a:318:CHL:HMC	2.16	0.46
22:5:268:CYS:HB2	43:5:306:PTY:HN12	1.80	0.46
20:2:154:LYS:HB3	20:2:154:LYS:HE3	1.77	0.46
22:5:144:LEU:HD11	31:6:316:CLA:HBD	1.97	0.46
1:A:203:ALA:HB2	1:A:309:GLY:HA3	1.98	0.46
31:A:823:CLA:HBA1	31:A:825:CLA:HMD2	1.97	0.46
2:B:719:LEU:HD23	31:B:835:CLA:H41	1.97	0.46
14:3:206:ALA:HB2	36:3:304:LUT:H192	1.96	0.46
1:A:157:LEU:HD12	31:A:829:CLA:HED3	1.97	0.46
2:B:58:PHE:HD1	2:B:142:LEU:HD22	1.81	0.46
2:B:275:HIS:HB3	31:B:850:CLA:HMB2	1.97	0.46
13:a:188:PHE:CD2	38:a:304:AXT:H12	2.51	0.46
23:6:223:HIS:CG	31:6:311:CLA:HAA2	2.51	0.46
28:A:810:LHG:H362	28:A:810:LHG:H332	1.75	0.46
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.98	0.46
1:A:199:ASN:HB3	31:A:833:CLA:HMD2	1.97	0.45
26:F:302:BCR:HC32	37:J:101:LMG:H142	1.97	0.45
11:K:75:PRO:O	11:K:109:TYR:OH	2.34	0.45
28:a:306:LHG:H262	31:a:312:CLA:HAC2	1.98	0.45
18:L:104:VAL:HG21	31:L:305:CLA:HED3	1.98	0.45
31:L:305:CLA:H92	31:L:305:CLA:H61	1.75	0.45
13:b:217:ASN:N	13:b:217:ASN:OD1	2.48	0.45
1:A:34:HIS:HE1	31:A:824:CLA:HED2	1.81	0.45
32:a:317:CHL:H91	32:a:317:CHL:H111	1.64	0.45
31:A:845:CLA:HBC2	31:A:852:CLA:HMC2	1.97	0.45
31:B:816:CLA:H102	26:I:801:BCR:HC41	1.98	0.45
22:5:84:GLN:HG3	22:5:157:ILE:HG12	1.98	0.45
22:5:207:GLY:O	22:5:211:MET:HG3	2.16	0.45
31:B:822:CLA:H92	31:B:832:CLA:H11	1.98	0.45
20:2:228:ILE:N	31:2:306:CLA:O1A	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:230:ASP:OD1	21:4:230:ASP:N	2.48	0.45
32:A:839:CHL:H3A	32:A:839:CHL:HBA2	1.63	0.45
36:a:305:LUT:H182	32:a:320:CHL:HAA1	1.98	0.45
36:6:304:LUT:H31	31:6:312:CLA:H151	1.97	0.45
32:6:309:CHL:HAA2	32:6:309:CHL:HED2	1.99	0.45
32:7:319:CHL:HBC2	32:7:320:CHL:H122	1.99	0.45
36:9:303:LUT:H31	31:9:314:CLA:H142	1.98	0.45
20:2:244:ILE:HA	20:2:247:ILE:HD12	1.98	0.45
4:D:130:LYS:HA	4:D:130:LYS:HD3	1.83	0.45
11:K:60:SER:O	11:K:64:ILE:HG13	2.17	0.45
20:2:126:SER:OG	20:2:130:ARG:NH1	2.49	0.45
32:8:319:CHL:HBB1	32:8:319:CHL:HMB3	1.97	0.45
19:O:107:PRO:HD2	19:O:110:ASP:HB2	1.98	0.45
31:A:834:CLA:H122	31:A:837:CLA:H93	1.98	0.45
26:B:804:BCR:H20C	26:B:804:BCR:H361	1.83	0.45
14:3:137:GLN:HE22	31:3:309:CLA:C1A	2.30	0.45
15:7:217:ALA:HB2	36:7:305:LUT:H192	1.99	0.45
32:7:318:CHL:H91	32:7:318:CHL:H112	1.71	0.45
18:L:103:LEU:HD22	26:L:303:BCR:H10C	1.99	0.45
31:A:833:CLA:H3A	31:A:833:CLA:HBA2	1.59	0.45
2:B:478:LEU:HD22	2:B:494:LEU:HD11	1.97	0.45
24:B:801:PQN:H241	31:B:847:CLA:HBA2	1.99	0.45
31:B:842:CLA:H143	31:B:842:CLA:H112	1.90	0.45
10:J:33:PHE:HB3	37:J:101:LMG:HC2	1.99	0.45
20:2:186:SER:OG	31:2:310:CLA:OBD	2.34	0.45
32:4:310:CHL:HBA1	31:4:319:CLA:HHB	1.99	0.45
23:6:101:VAL:HG12	23:6:102:ARG:HG2	1.98	0.45
31:A:853:CLA:H18	31:F:301:CLA:H72	1.99	0.44
21:4:143:ARG:HE	31:4:315:CLA:HMC3	1.81	0.44
22:5:215:VAL:HG11	31:5:310:CLA:H192	1.99	0.44
28:5:305:LHG:H132	28:5:305:LHG:H102	1.78	0.44
31:B:831:CLA:HAB	31:B:838:CLA:HMD2	1.99	0.44
11:K:51:GLY:H	11:K:55:ASN:HD22	1.66	0.44
22:5:174:VAL:HG23	32:5:322:CHL:HMD3	1.98	0.44
2:B:23:TYR:CE2	33:B:808:DGD:HG32	2.52	0.44
31:B:815:CLA:H93	31:B:815:CLA:H61	1.86	0.44
8:H:79:ARG:NE	31:H:902:CLA:OBD	2.38	0.44
28:a:306:LHG:H322	31:8:307:CLA:HED1	1.98	0.44
32:7:317:CHL:H41	32:7:317:CHL:H62	1.62	0.44
26:B:805:BCR:H313	31:B:842:CLA:HAB	1.98	0.44
31:B:826:CLA:H43	17:9:60:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:159:ASP:OD1	36:a:303:LUT:O23	2.33	0.44
32:7:317:CHL:H41	32:7:317:CHL:C10	2.46	0.44
16:8:177:ASP:OD1	36:8:302:LUT:O23	2.33	0.44
21:4:236:VAL:HG22	31:4:318:CLA:HBC3	1.99	0.44
26:A:804:BCR:H20C	26:A:804:BCR:H361	1.75	0.44
31:A:851:CLA:H102	31:A:851:CLA:H62	1.76	0.44
31:B:814:CLA:H112	31:B:814:CLA:HBD	2.00	0.44
13:b:178:LEU:HD23	13:b:178:LEU:HA	1.86	0.44
31:2:304:CLA:HBA2	31:2:304:CLA:H3A	1.74	0.44
23:6:98:GLN:HG2	31:6:314:CLA:HED3	1.98	0.44
28:A:809:LHG:H242	18:L:116:LEU:HD21	2.00	0.44
31:B:812:CLA:H141	31:B:819:CLA:HBC1	1.98	0.44
36:3:304:LUT:H201	36:3:304:LUT:H15	1.73	0.44
31:8:310:CLA:H152	31:8:310:CLA:H112	1.75	0.44
31:8:311:CLA:H61	31:8:311:CLA:H41	1.72	0.44
1:A:587:SER:OG	1:A:590:ASP:OD2	2.31	0.44
31:A:834:CLA:HMC3	32:A:840:CHL:H203	1.99	0.44
2:B:23:TYR:CZ	33:B:808:DGD:HG11	2.53	0.44
32:K:201:CHL:HED2	26:K:203:BCR:H391	1.99	0.44
31:a:316:CLA:H3A	31:a:316:CLA:HBA2	1.75	0.44
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.99	0.44
26:A:805:BCR:H12C	31:A:834:CLA:H71	2.00	0.44
31:B:843:CLA:HAB	31:B:843:CLA:HHC	1.78	0.44
31:G:206:CLA:HBC2	37:a:301:LMG:H132	1.98	0.44
31:8:309:CLA:HBC1	29:4:301:UNL:C13	2.48	0.44
32:8:316:CHL:H51	32:8:316:CHL:C3B	2.48	0.44
21:4:203:MET:HB3	36:4:303:LUT:H402	1.99	0.44
32:6:317:CHL:H3A	32:6:317:CHL:HBA2	1.49	0.44
31:3:313:CLA:H92	31:3:313:CLA:H62	1.90	0.44
39:7:301:3PH:H252	39:7:301:3PH:H221	1.84	0.44
36:8:302:LUT:H15	36:8:302:LUT:H201	1.79	0.44
18:L:179:ASP:O	18:L:183:LYS:HG3	2.18	0.44
31:6:313:CLA:HAB	31:6:313:CLA:HHC	1.82	0.44
26:A:806:BCR:H20C	26:A:806:BCR:H361	1.76	0.43
31:A:855:CLA:H41	31:A:855:CLA:H62	1.68	0.43
26:B:802:BCR:H282	31:B:836:CLA:ND	2.33	0.43
20:2:239:LEU:HD23	20:2:239:LEU:HA	1.87	0.43
26:B:805:BCR:H352	31:B:845:CLA:H12	1.99	0.43
31:B:840:CLA:H2	31:B:840:CLA:H62	1.74	0.43
8:H:68:ARG:HD2	18:L:89:ARG:HG3	2.00	0.43
26:K:203:BCR:H24C	26:K:203:BCR:H371	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:303:LUT:H12	31:9:315:CLA:HBC3	1.99	0.43
26:O:201:BCR:H15C	26:O:201:BCR:H351	1.90	0.43
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.99	0.43
11:K:53:THR:O	11:K:57:ILE:HD12	2.18	0.43
32:a:318:CHL:HMC	32:a:318:CHL:HBC2	2.01	0.43
20:2:44:SER:N	20:2:164:GLU:OE1	2.51	0.43
31:4:314:CLA:C4D	32:4:317:CHL:HMC	2.47	0.43
22:5:68:ASP:OD1	36:5:304:LUT:O23	2.33	0.43
31:5:310:CLA:H72	31:5:310:CLA:H111	1.80	0.43
1:A:32:PRO:HG2	6:F:203:TYR:HE2	1.82	0.43
31:A:843:CLA:H102	31:A:855:CLA:HAA1	1.99	0.43
2:B:422:LEU:HG	31:B:845:CLA:CBB	2.49	0.43
15:7:50:PRO:HD2	32:7:317:CHL:HED3	2.00	0.43
31:b:308:CLA:HBA2	31:b:308:CLA:H3A	1.75	0.43
21:4:66:LEU:HD23	21:4:66:LEU:HA	1.86	0.43
31:A:846:CLA:H51	26:B:806:BCR:H372	1.99	0.43
31:B:841:CLA:H41	31:B:841:CLA:H62	1.70	0.43
7:G:61:PHE:HE1	37:G:202:LMG:HC1	1.83	0.43
31:3:308:CLA:HED3	31:3:313:CLA:H8	2.01	0.43
16:8:118:SER:OG	16:8:120:ILE:O	2.34	0.43
31:L:305:CLA:H61	31:L:305:CLA:H2	1.86	0.43
31:A:853:CLA:H193	6:F:188:TYR:HB2	1.99	0.43
31:A:856:CLA:H122	26:B:806:BCR:H12C	2.00	0.43
26:B:802:BCR:H16C	31:B:820:CLA:H142	2.01	0.43
31:B:839:CLA:H91	31:B:839:CLA:H112	1.86	0.43
26:L:302:BCR:H15C	26:L:302:BCR:H351	1.86	0.43
23:6:236:ALA:O	32:6:309:CHL:HBB1	2.18	0.43
31:A:836:CLA:H61	31:A:836:CLA:H41	1.71	0.43
31:B:813:CLA:HBA2	31:B:813:CLA:H142	1.99	0.43
17:9:170:ARG:HA	17:9:173:MET:HE3	2.00	0.43
26:L:301:BCR:H403	26:L:301:BCR:H23C	2.00	0.43
20:2:104:ARG:HG2	31:2:304:CLA:C4C	2.49	0.43
26:3:301:BCR:H24C	26:3:301:BCR:H371	1.91	0.43
4:D:115:LYS:HE3	4:D:147:LEU:HD13	2.01	0.43
31:2:306:CLA:H41	31:2:306:CLA:H62	1.69	0.43
23:6:89:MET:SD	31:6:307:CLA:HAB	2.59	0.43
31:A:823:CLA:HMD1	31:3:311:CLA:H102	2.00	0.43
6:F:225:ILE:O	6:F:229:GLN:HG3	2.19	0.43
8:H:99:ALA:O	8:H:103:LEU:HG	2.19	0.43
36:7:305:LUT:H15	36:7:305:LUT:H201	1.79	0.43
31:b:313:CLA:H112	31:b:313:CLA:H142	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:6:195:GLY:O	23:6:199:MET:HG3	2.19	0.43
32:6:319:CHL:HMC	32:6:321:CHL:HMC	2.01	0.43
28:A:809:LHG:H241	28:A:809:LHG:H271	1.88	0.42
2:B:34:HIS:HE1	31:B:813:CLA:HED1	1.84	0.42
31:B:840:CLA:H8	6:F:178:ALA:HB1	2.00	0.42
28:a:306:LHG:H172	28:a:306:LHG:H201	1.87	0.42
31:a:319:CLA:H93	31:a:319:CLA:H111	1.84	0.42
15:7:206:ASN:ND2	31:7:315:CLA:OBD	2.41	0.42
32:7:324:CHL:H3A	32:7:324:CHL:HBA2	1.83	0.42
16:8:86:ALA:HB2	36:8:303:LUT:H192	2.01	0.42
31:8:308:CLA:H162	31:8:308:CLA:H202	1.85	0.42
36:2:301:LUT:H31	31:2:308:CLA:HAC2	2.01	0.42
1:A:274:ASP:OD1	1:A:274:ASP:N	2.51	0.42
31:A:820:CLA:HMB3	31:A:821:CLA:HHB	2.01	0.42
31:A:822:CLA:HAB	31:A:822:CLA:HHC	1.84	0.42
26:3:303:BCR:H24C	26:3:303:BCR:H371	1.79	0.42
17:9:129:LEU:HD13	36:9:305:LUT:H172	2.01	0.42
19:O:106:PRO:HA	19:O:107:PRO:HD3	1.90	0.42
1:A:150:ALA:HB2	1:A:378:PRO:HD2	2.00	0.42
26:B:802:BCR:H20C	26:B:802:BCR:H361	1.88	0.42
6:F:110:LYS:HE2	6:F:110:LYS:HB3	1.92	0.42
31:H:901:CLA:HBA1	31:H:901:CLA:H3A	1.71	0.42
31:3:311:CLA:HAB	31:3:311:CLA:HHC	1.81	0.42
32:7:318:CHL:H151	32:7:318:CHL:CMB	2.49	0.42
36:6:303:LUT:H15	36:6:303:LUT:H201	1.80	0.42
1:A:646:LEU:HD22	2:B:651:LEU:HD21	2.01	0.42
31:A:818:CLA:H172	31:A:826:CLA:H61	2.00	0.42
31:A:857:CLA:H72	31:B:846:CLA:H43	2.01	0.42
2:B:299:HIS:HB3	2:B:304:ILE:HD11	2.00	0.42
31:B:818:CLA:H93	31:B:818:CLA:H61	1.83	0.42
22:5:202:LYS:HD3	31:5:308:CLA:HBD	2.01	0.42
31:5:323:CLA:H92	31:5:323:CLA:H62	1.88	0.42
31:A:821:CLA:H93	31:A:821:CLA:H61	1.86	0.42
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.86	0.42
26:G:201:BCR:H20C	26:G:201:BCR:H361	1.87	0.42
32:7:320:CHL:HBB1	32:7:320:CHL:HMB1	2.00	0.42
22:5:85:ALA:HB2	31:5:318:CLA:HED2	2.01	0.42
32:5:322:CHL:HBA2	32:5:322:CHL:H3A	1.57	0.42
31:A:835:CLA:HBB2	31:A:836:CLA:HBC2	2.02	0.42
33:B:808:DGD:HBW2	31:B:837:CLA:H93	2.01	0.42
3:C:15:THR:HG22	3:C:28:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:54:PHE:CD1	32:a:317:CHL:HBC2	2.54	0.42
32:7:318:CHL:HBC3	32:7:320:CHL:C1C	2.49	0.42
17:9:205:ASN:HD22	17:9:207:ILE:H	1.68	0.42
23:6:125:ILE:HD11	32:6:318:CHL:HBC1	2.01	0.42
23:6:132:GLU:O	23:6:136:MET:HB2	2.19	0.42
2:B:435:GLY:HA3	31:B:841:CLA:HAB	2.01	0.42
15:7:216:VAL:HG21	28:7:307:LHG:H281	2.02	0.42
16:8:129:GLU:OE1	32:8:316:CHL:HMC	2.20	0.42
26:6:302:BCR:H402	32:6:318:CHL:HBA2	2.02	0.42
26:K:203:BCR:H20C	26:K:203:BCR:H361	1.87	0.42
13:a:124:LEU:HD11	37:a:301:LMG:H142	2.01	0.42
28:a:306:LHG:O3	28:a:306:LHG:O1	2.33	0.42
14:3:74:HIS:HD2	36:3:305:LUT:H15	1.84	0.42
14:3:87:ALA:HA	26:3:302:BCR:H272	2.01	0.42
32:8:316:CHL:H3A	32:8:316:CHL:HBA2	1.31	0.42
31:8:320:CLA:H91	31:8:320:CLA:H111	1.80	0.42
32:9:320:CHL:HMC	32:9:320:CHL:HBC2	2.02	0.42
36:4:302:LUT:H373	31:4:305:CLA:H11	2.01	0.42
22:5:158:LYS:HB2	22:5:158:LYS:HE3	1.85	0.42
34:B:851:LAP:H52	34:B:851:LAP:H82	1.30	0.42
4:D:111:LYS:HE2	8:H:44:GLU:HB3	2.02	0.42
26:M:101:BCR:H24C	26:M:101:BCR:H371	1.82	0.42
28:7:307:LHG:H311	31:7:315:CLA:HAC1	2.01	0.42
41:8:305:DGA:HA52	31:8:321:CLA:HBA2	2.02	0.42
13:b:56:PHE:HE2	36:b:301:LUT:H27	1.84	0.42
13:b:153:TYR:CZ	13:b:174:LYS:HD3	2.54	0.42
31:5:323:CLA:HBA2	31:5:323:CLA:H3A	1.76	0.42
1:A:289:LEU:HD21	1:A:374:MET:HB3	2.01	0.42
26:B:802:BCR:H15C	26:B:802:BCR:H351	1.90	0.42
26:B:803:BCR:H24C	26:B:803:BCR:H371	1.90	0.42
31:B:825:CLA:H52	7:G:120:PHE:HD1	1.85	0.42
31:B:842:CLA:H13	31:G:206:CLA:HBB1	2.01	0.42
11:K:65:PHE:HE1	31:K:206:CLA:HAB	1.84	0.42
28:a:306:LHG:H301	31:a:312:CLA:HBC1	2.02	0.42
14:3:181:LEU:HD23	36:3:304:LUT:H23	2.02	0.42
20:2:83:PHE:HD2	36:2:301:LUT:C2	2.32	0.42
22:5:113:TYR:CD1	32:5:316:CHL:HMA2	2.55	0.42
22:5:205:LYS:HE2	31:5:313:CLA:C4D	2.49	0.42
23:6:238:VAL:HB	32:6:309:CHL:C1C	2.50	0.42
31:A:814:CLA:H171	31:A:814:CLA:H13	1.78	0.41
31:B:814:CLA:H203	31:B:814:CLA:H162	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:LYS:NZ	8:H:54:THR:O	2.46	0.41
13:a:114:THR:HG22	13:a:119:PRO:HA	2.02	0.41
26:O:201:BCR:H371	26:O:201:BCR:H24C	1.77	0.41
20:2:124:TRP:HE3	36:2:301:LUT:H221	1.84	0.41
31:4:308:CLA:HAB	31:4:308:CLA:HHC	1.82	0.41
22:5:62:ALA:O	22:5:83:ARG:NH2	2.51	0.41
23:6:99:GLU:HG2	23:6:217:LEU:HD12	2.01	0.41
1:A:443:TRP:CD1	31:A:846:CLA:HED2	2.55	0.41
2:B:174:ARG:HB2	31:B:822:CLA:HBC2	2.00	0.41
28:B:807:LHG:H271	13:a:61:LEU:HD21	2.02	0.41
31:B:844:CLA:HAB	31:B:844:CLA:HHC	1.80	0.41
31:3:309:CLA:HED2	31:3:309:CLA:H11	2.02	0.41
31:8:308:CLA:HAB	31:8:308:CLA:HHC	1.87	0.41
18:L:58:PRO:HB3	18:L:63:PRO:HA	2.02	0.41
31:2:313:CLA:H2A	31:2:313:CLA:HED3	2.01	0.41
22:5:113:TYR:CD1	32:5:316:CHL:HED1	2.55	0.41
22:5:152:ARG:NH1	32:6:317:CHL:OBD	2.52	0.41
36:5:304:LUT:H10	31:5:311:CLA:HMC3	2.01	0.41
32:5:319:CHL:OBD	32:5:319:CHL:HED2	2.20	0.41
1:A:521:VAL:HG11	1:A:524:MET:HE3	2.02	0.41
31:A:815:CLA:O1A	2:B:430:GLY:HA3	2.21	0.41
31:B:834:CLA:H191	31:B:848:CLA:H152	2.02	0.41
8:H:81:ALA:HB3	18:L:95:LEU:HD11	2.01	0.41
14:3:144:TRP:CE2	14:3:148:ARG:HD2	2.56	0.41
31:3:318:CLA:H2	31:3:320:CLA:HMD2	2.03	0.41
16:8:206:ILE:HG21	31:8:310:CLA:H202	2.01	0.41
31:8:311:CLA:H52	31:8:311:CLA:H12	1.87	0.41
26:L:302:BCR:H20C	26:L:302:BCR:H361	1.86	0.41
36:L:304:LUT:H7	36:L:304:LUT:H161	1.76	0.41
36:4:302:LUT:H201	36:4:302:LUT:H15	1.77	0.41
7:G:36:LEU:HD11	7:G:41:LEU:HD13	2.03	0.41
11:K:109:TYR:CE1	26:K:202:BCR:H382	2.55	0.41
14:3:114:PRO:HG2	31:3:314:CLA:HAB	2.03	0.41
32:4:313:CHL:HBA1	23:6:138:PHE:HA	2.02	0.41
22:5:269:LEU:HD23	22:5:269:LEU:HA	1.94	0.41
1:A:441:LEU:HD21	1:A:547:VAL:HG12	2.01	0.41
31:B:817:CLA:HAB	31:B:818:CLA:HAA2	2.02	0.41
31:B:837:CLA:H52	31:B:837:CLA:H8	1.95	0.41
6:F:225:ILE:HD12	31:8:311:CLA:H43	2.02	0.41
36:F:304:LUT:H193	36:F:304:LUT:H7	1.87	0.41
14:3:47:ASP:CG	31:3:319:CLA:HBA1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:315:CHL:H61	32:3:315:CHL:H41	1.70	0.41
16:8:178:PRO:HA	13:b:59:PHE:HE1	1.86	0.41
32:8:316:CHL:H142	32:8:316:CHL:H112	1.63	0.41
26:L:303:BCR:H15C	26:L:303:BCR:H351	1.90	0.41
22:5:199:VAL:HG22	31:5:307:CLA:HHB	2.01	0.41
13:a:92:ALA:HB1	31:a:314:CLA:HED3	2.02	0.41
13:a:178:LEU:HD23	13:a:178:LEU:HA	1.92	0.41
20:2:43:PRO:HB2	20:2:46:LEU:HD12	2.02	0.41
20:2:78:ARG:CZ	20:2:189:ARG:HH21	2.33	0.41
21:4:134:LEU:HD12	21:4:134:LEU:HA	1.92	0.41
26:A:806:BCR:H24C	31:B:841:CLA:HMC1	2.03	0.41
31:A:821:CLA:HAA1	31:A:841:CLA:HED2	2.03	0.41
2:B:352:MET:HE2	2:B:352:MET:HB3	1.90	0.41
31:B:833:CLA:HED2	31:B:834:CLA:HBD	2.01	0.41
31:H:903:CLA:H3A	31:H:903:CLA:HBA2	1.83	0.41
16:8:88:ALA:HB2	36:8:302:LUT:H401	2.02	0.41
21:4:43:PRO:HB2	23:6:153:GLN:HE22	1.86	0.41
36:4:302:LUT:H11	36:4:302:LUT:H191	1.86	0.41
32:6:318:CHL:HBA2	32:6:318:CHL:H3A	1.43	0.41
1:A:671:ILE:HG12	31:A:841:CLA:H142	2.03	0.41
30:A:813:CL0:H36	30:A:813:CL0:CED	2.50	0.41
31:B:813:CLA:H162	31:B:813:CLA:H141	1.83	0.41
31:B:825:CLA:CHD	31:B:850:CLA:HBB2	2.50	0.41
31:F:301:CLA:H42	10:J:15:ALA:HA	2.02	0.41
36:a:305:LUT:H11	32:a:320:CHL:CHB	2.48	0.41
14:3:123:LEU:HG	14:3:127:SER:HB2	2.02	0.41
15:7:147:TRP:CZ2	26:7:304:BCR:HC8	2.56	0.41
17:9:114:PRO:HA	17:9:115:PRO:HD3	1.97	0.41
18:L:55:VAL:HG12	19:O:58:ASN:HB2	2.03	0.41
13:b:203:LEU:HD23	13:b:203:LEU:HA	1.87	0.41
20:2:245:THR:HA	31:2:313:CLA:HAB	2.02	0.41
21:4:243:ARG:HG2	31:4:318:CLA:HAB	2.03	0.41
26:6:302:BCR:H20C	26:6:302:BCR:H361	1.78	0.41
1:A:430:VAL:HG11	31:A:834:CLA:H193	2.01	0.41
1:A:438:VAL:HG21	1:A:556:TYR:HE1	1.85	0.41
1:A:707:LEU:HD13	36:F:304:LUT:H383	2.02	0.41
31:A:820:CLA:HAB	31:A:820:CLA:HHC	1.81	0.41
32:A:839:CHL:H43	31:A:851:CLA:HBA1	2.03	0.41
2:B:519:VAL:HG21	2:B:593:TYR:HB2	2.03	0.41
24:B:801:PQN:H141	31:B:846:CLA:HBB2	2.01	0.41
31:B:837:CLA:H72	31:B:847:CLA:HED1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:842:CLA:H72	31:B:842:CLA:H111	1.85	0.41
13:a:209:HIS:CG	31:a:311:CLA:HAA2	2.56	0.41
36:3:305:LUT:H11	36:3:305:LUT:H191	1.90	0.41
16:8:187:TYR:CZ	16:8:191:LYS:HE3	2.56	0.41
20:2:249:ILE:HD12	20:2:249:ILE:HA	1.93	0.41
26:2:302:BCR:H15C	26:2:302:BCR:H351	1.90	0.41
21:4:201:LEU:HG	36:4:302:LUT:H11	2.03	0.41
42:4:304:SQD:H91	31:4:316:CLA:HBA1	2.02	0.41
31:5:311:CLA:HED2	32:6:309:CHL:H142	2.02	0.41
32:6:319:CHL:H3A	32:6:319:CHL:HBA2	1.49	0.41
26:A:805:BCR:H10C	31:A:834:CLA:H101	2.03	0.41
31:A:837:CLA:H162	31:A:837:CLA:H121	1.78	0.41
32:A:839:CHL:H52	31:A:850:CLA:H11	2.02	0.41
2:B:619:TRP:O	2:B:623:TYR:HB3	2.21	0.41
26:B:804:BCR:H24C	26:B:804:BCR:H371	1.88	0.41
28:a:306:LHG:HC31	31:a:315:CLA:C1B	2.51	0.41
15:7:112:VAL:HG21	23:6:269:GLY:HA2	2.03	0.41
28:7:307:LHG:HC31	31:7:315:CLA:C1B	2.50	0.41
26:2:302:BCR:H11C	26:2:302:BCR:H341	1.89	0.41
21:4:240:GLU:HB3	31:4:318:CLA:C1C	2.51	0.41
1:A:403:VAL:HG11	1:A:596:LEU:HG	2.02	0.40
31:A:834:CLA:H2	31:A:834:CLA:H61	1.87	0.40
26:B:805:BCR:H24C	26:B:805:BCR:H371	1.88	0.40
11:K:70:ARG:NH2	11:K:98:ASP:OD1	2.49	0.40
31:a:309:CLA:H92	31:a:309:CLA:H62	1.94	0.40
31:3:310:CLA:H62	31:3:310:CLA:H2	1.80	0.40
26:7:304:BCR:H15C	26:7:304:BCR:H351	1.91	0.40
26:8:301:BCR:H20C	26:8:301:BCR:H361	1.91	0.40
21:4:228:LEU:HD23	21:4:228:LEU:HA	1.90	0.40
1:A:37:ARG:HD3	1:A:37:ARG:HA	1.86	0.40
31:A:845:CLA:HMB1	31:A:857:CLA:HAA2	2.01	0.40
31:G:205:CLA:HED3	31:9:313:CLA:HED2	2.03	0.40
26:M:101:BCR:H20C	26:M:101:BCR:H361	1.85	0.40
26:7:304:BCR:H20C	26:7:304:BCR:H361	1.89	0.40
26:8:301:BCR:H11C	26:8:301:BCR:H341	1.92	0.40
21:4:42:LEU:HD12	21:4:42:LEU:HA	1.84	0.40
31:4:314:CLA:CAD	32:4:317:CHL:HMC	2.50	0.40
26:B:805:BCR:H15C	26:B:805:BCR:H351	1.86	0.40
34:B:851:LAP:H51	17:9:104:PHE:HB2	2.03	0.40
14:3:207:VAL:HG11	36:3:305:LUT:H12	2.04	0.40
36:4:302:LUT:H401	36:4:302:LUT:H35	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:321:CLA:HAA1	31:4:321:CLA:H2	2.03	0.40
32:6:309:CHL:H92	32:6:309:CHL:H62	1.76	0.40
27:A:807:LMT:H81	28:7:302:LHG:H372	2.03	0.40
2:B:206:HIS:ND1	44:B:906:HOH:O	2.35	0.40
2:B:662:MET:HB2	31:B:812:CLA:C1C	2.52	0.40
31:B:816:CLA:HHB	31:B:817:CLA:HMB3	2.04	0.40
8:H:102:LEU:HA	8:H:102:LEU:HD23	1.89	0.40
31:a:313:CLA:H71	31:a:313:CLA:H112	1.81	0.40
26:3:302:BCR:H20C	26:3:302:BCR:H361	1.89	0.40
16:8:137:GLU:CD	16:8:140:ARG:HH21	2.29	0.40
20:2:45:TRP:NE1	20:2:97:GLU:OE2	2.54	0.40
32:4:310:CHL:H3A	32:4:317:CHL:C4C	2.51	0.40
1:A:326:LEU:O	1:A:338:HIS:HB2	2.21	0.40
26:A:803:BCR:H20C	26:A:803:BCR:H361	1.82	0.40
2:B:492:LEU:HD22	31:B:825:CLA:HED2	2.04	0.40
31:B:814:CLA:HBA1	31:B:814:CLA:H3A	1.90	0.40
32:7:324:CHL:H41	31:8:315:CLA:H42	2.02	0.40
16:8:199:ARG:HA	16:8:202:MET:HE3	2.03	0.40
31:8:311:CLA:HAB	31:8:311:CLA:HHC	1.90	0.40
36:9:303:LUT:H161	36:9:303:LUT:H8	2.04	0.40
19:O:85:ASN:HB2	19:O:86:SER:H	1.70	0.40
21:4:53:GLY:HA2	21:4:58:ASP:HB3	2.02	0.40
21:4:200:ARG:HA	21:4:203:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/751 (98%)	721 (98%)	17 (2%)	0	100	100
2	B	730/734 (100%)	719 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100
5	E	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
6	F	163/245 (66%)	160 (98%)	3 (2%)	0	100	100
7	G	101/138 (73%)	99 (98%)	2 (2%)	0	100	100
8	H	89/133 (67%)	87 (98%)	2 (2%)	0	100	100
9	I	31/36 (86%)	31 (100%)	0	0	100	100
10	J	37/41 (90%)	37 (100%)	0	0	100	100
11	K	79/131 (60%)	79 (100%)	0	0	100	100
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	a	193/229 (84%)	191 (99%)	2 (1%)	0	100	100
13	b	120/229 (52%)	119 (99%)	1 (1%)	0	100	100
14	3	201/246 (82%)	194 (96%)	7 (4%)	0	100	100
15	7	212/259 (82%)	209 (99%)	3 (1%)	0	100	100
16	8	220/255 (86%)	215 (98%)	5 (2%)	0	100	100
17	9	182/230 (79%)	179 (98%)	3 (2%)	0	100	100
18	L	142/210 (68%)	139 (98%)	3 (2%)	0	100	100
19	O	72/142 (51%)	71 (99%)	1 (1%)	0	100	100
20	2	198/273 (72%)	184 (93%)	14 (7%)	0	100	100
21	4	187/246 (76%)	180 (96%)	7 (4%)	0	100	100
22	5	225/274 (82%)	216 (96%)	9 (4%)	0	100	100
23	6	211/272 (78%)	206 (98%)	5 (2%)	0	100	100
All	All	4437/5449 (81%)	4336 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	603/613 (98%)	597 (99%)	6 (1%)	68	64
2	B	592/593 (100%)	588 (99%)	4 (1%)	76	73
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	21
4	D	118/156 (76%)	117 (99%)	1 (1%)	73	71
5	E	56/67 (84%)	55 (98%)	1 (2%)	51	39
6	F	131/183 (72%)	131 (100%)	0	100	100
7	G	78/106 (74%)	75 (96%)	3 (4%)	29	14
8	H	71/105 (68%)	71 (100%)	0	100	100
9	I	26/28 (93%)	26 (100%)	0	100	100
10	J	35/37 (95%)	35 (100%)	0	100	100
11	K	59/100 (59%)	55 (93%)	4 (7%)	14	4
12	M	26/26 (100%)	25 (96%)	1 (4%)	29	14
13	a	141/166 (85%)	141 (100%)	0	100	100
13	b	92/166 (55%)	90 (98%)	2 (2%)	45	32
14	3	162/197 (82%)	160 (99%)	2 (1%)	63	57
15	7	166/195 (85%)	163 (98%)	3 (2%)	51	39
16	8	175/202 (87%)	171 (98%)	4 (2%)	44	30
17	9	143/177 (81%)	136 (95%)	7 (5%)	22	8
18	L	115/161 (71%)	112 (97%)	3 (3%)	40	24
19	O	65/110 (59%)	60 (92%)	5 (8%)	12	3
20	2	166/225 (74%)	161 (97%)	5 (3%)	36	20
21	4	155/195 (80%)	152 (98%)	3 (2%)	50	37
22	5	178/208 (86%)	172 (97%)	6 (3%)	32	16
23	6	170/212 (80%)	168 (99%)	2 (1%)	63	57
All	All	3591/4297 (84%)	3527 (98%)	64 (2%)	51	39

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	14	LYS
1	A	60	ASP
1	A	118	VAL
1	A	372	TYR
1	A	584	CYS

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Mol	Chain	Res	Type
2	B	280	ILE
2	B	309	THR
2	B	344	ILE
2	B	503	SER
3	C	7	ILE
3	C	37	SER
4	D	165	VAL
5	E	70	GLU
7	G	36	LEU
7	G	94	LEU
7	G	96	THR
11	K	88	SER
11	K	96	THR
11	K	109	TYR
11	K	128	ILE
12	M	6	SER
14	3	100	THR
14	3	181	LEU
15	7	44	ASP
15	7	166	SER
15	7	253	VAL
16	8	74	GLN
16	8	91	LEU
16	8	118	SER
16	8	175	VAL
17	9	51	GLU
17	9	65	SER
17	9	105	GLU
17	9	113	PHE
17	9	143	SER
17	9	145	PHE
17	9	186	CYS
18	L	151	SER
18	L	164	THR
18	L	210	SER
19	O	64	PHE
19	O	65	VAL
19	O	99	LEU
19	O	128	LEU
19	O	141	TYR
13	b	200	LYS
13	b	224	SER

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Mol	Chain	Res	Type
20	2	73	SER
20	2	116	VAL
20	2	167	LEU
20	2	186	SER
20	2	257	LEU
21	4	127	SER
21	4	164	SER
21	4	219	THR
22	5	58	ASN
22	5	133	VAL
22	5	162	SER
22	5	163	VAL
22	5	174	VAL
22	5	215	VAL
23	6	39	ARG
23	6	55	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	217	GLN
1	A	350	HIS
1	A	637	GLN
1	A	659	GLN
2	B	235	GLN
2	B	368	GLN
2	B	633	ASN
2	B	636	ASN
4	D	91	GLN
6	F	111	GLN
8	H	118	GLN
11	K	55	ASN
13	a	102	GLN
14	3	68	GLN
15	7	78	GLN
16	8	74	GLN
17	9	135	GLN
17	9	204	ASN
17	9	205	ASN
18	L	57	GLN
18	L	182	GLN

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Mol	Chain	Res	Type
18	L	204	GLN
19	O	85	ASN
19	O	93	GLN
19	O	98	ASN
19	O	131	GLN
20	2	215	ASN
20	2	227	ASN
21	4	82	GLN
21	4	156	GLN
22	5	103	GLN
22	5	125	ASN
22	5	247	ASN
23	6	153	GLN
23	6	210	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 354 ligands modelled in this entry, 17 are unknown - leaving 337 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LHG	5	305	31	34,34,48	0.33	0	37,40,54	0.40	0
31	CLA	6	308	44	51,55,73	3.10	22 (43%)	61,91,113	2.67	23 (37%)
31	CLA	7	321	44	51,55,73	3.17	22 (43%)	61,91,113	2.72	25 (40%)
31	CLA	a	314	44	54,58,73	3.86	22 (40%)	65,95,113	2.60	26 (40%)
31	CLA	K	204	44	54,58,73	3.41	22 (40%)	65,95,113	2.60	23 (35%)
32	CHL	5	316	44	60,64,74	2.80	21 (35%)	68,102,114	2.43	26 (38%)
25	SF4	A	802	2,1	0,12,12	-	-	-		
41	DGA	8	305	-	27,27,43	0.25	0	29,29,45	0.17	0
31	CLA	9	311	17	59,63,73	4.99	22 (37%)	71,101,113	2.47	30 (42%)
31	CLA	A	838	44	69,73,73	2.65	23 (33%)	83,113,113	2.45	24 (28%)
31	CLA	B	843	44	49,53,73	2.90	21 (42%)	59,89,113	2.71	24 (40%)
26	BCR	O	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
32	CHL	6	318	44	50,54,74	3.77	22 (44%)	56,90,114	2.51	25 (44%)
31	CLA	A	820	1	59,63,73	3.00	24 (40%)	71,101,113	2.58	23 (32%)
31	CLA	5	311	22	50,54,73	2.77	21 (42%)	60,90,113	2.72	26 (43%)
32	CHL	a	318	44	52,56,74	3.03	19 (36%)	58,92,114	2.50	22 (37%)
31	CLA	3	312	44	69,73,73	2.70	21 (30%)	83,113,113	2.31	27 (32%)
33	DGD	7	308	-	53,53,67	1.05	4 (7%)	67,67,81	1.53	12 (17%)
31	CLA	3	317	44	55,59,73	3.09	21 (38%)	66,96,113	2.66	26 (39%)
31	CLA	G	204	7	54,58,73	3.13	22 (40%)	65,95,113	2.58	26 (40%)
31	CLA	b	307	-	50,54,73	5.50	23 (46%)	60,90,113	2.76	25 (41%)
31	CLA	9	321	17	60,64,73	2.59	22 (36%)	72,102,113	2.45	27 (37%)
31	CLA	A	823	1	59,63,73	3.02	20 (33%)	71,101,113	2.42	23 (32%)
31	CLA	K	205	11	50,54,73	3.19	22 (44%)	60,90,113	2.71	23 (38%)
31	CLA	7	312	15	66,70,73	2.66	24 (36%)	79,109,113	2.33	24 (30%)
36	LUT	2	301	-	42,43,43	5.53	19 (45%)	51,60,60	5.77	32 (62%)
31	CLA	a	310	13	49,53,73	3.23	22 (44%)	59,89,113	2.77	23 (38%)
31	CLA	5	308	22	50,54,73	3.76	22 (44%)	60,90,113	2.70	24 (40%)
31	CLA	A	825	1	58,62,73	2.77	24 (41%)	69,99,113	2.61	27 (39%)
31	CLA	A	845	1	60,64,73	2.59	22 (36%)	72,102,113	2.50	23 (31%)
26	BCR	2	302	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	7 (12%)
31	CLA	B	834	2	69,73,73	2.86	21 (30%)	83,113,113	2.37	27 (32%)
31	CLA	5	323	22	60,64,73	3.01	19 (31%)	72,102,113	2.56	26 (36%)
31	CLA	A	835	1	59,63,73	2.85	23 (38%)	71,101,113	2.51	22 (30%)
31	CLA	A	856	44	69,73,73	2.40	21 (30%)	83,113,113	2.32	24 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	B	823	2	59,63,73	2.68	21 (35%)	71,101,113	2.54	26 (36%)
31	CLA	2	313	20	50,54,73	3.36	20 (40%)	60,90,113	2.55	21 (35%)
31	CLA	4	318	21	49,53,73	3.74	22 (44%)	59,89,113	2.64	23 (38%)
26	BCR	K	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	6 (10%)
31	CLA	3	318	14	55,59,73	3.48	21 (38%)	66,96,113	2.60	28 (42%)
31	CLA	B	814	2	69,73,73	3.07	23 (33%)	83,113,113	2.36	24 (28%)
38	AXT	a	304	-	44,44,45	0.70	1 (2%)	55,62,64	0.91	1 (1%)
31	CLA	b	303	-	50,54,73	4.11	23 (46%)	60,90,113	2.72	24 (40%)
31	CLA	B	821	2	62,66,73	2.68	19 (30%)	74,104,113	2.42	22 (29%)
26	BCR	A	803	-	41,41,41	1.04	2 (4%)	56,56,56	1.13	3 (5%)
31	CLA	9	312	17	50,54,73	2.88	20 (40%)	60,90,113	2.68	22 (36%)
31	CLA	4	308	21	64,68,73	2.41	22 (34%)	77,107,113	2.50	27 (35%)
31	CLA	G	205	7	50,54,73	2.90	23 (46%)	60,90,113	2.66	21 (35%)
31	CLA	a	321	44	54,58,73	2.92	19 (35%)	65,95,113	2.66	30 (46%)
36	LUT	4	302	-	42,43,43	5.65	19 (45%)	51,60,60	5.74	34 (66%)
31	CLA	a	312	13	69,73,73	3.10	23 (33%)	83,113,113	2.37	24 (28%)
31	CLA	3	313	-	64,68,73	2.76	20 (31%)	77,107,113	2.50	27 (35%)
28	LHG	B	807	31	31,31,48	0.81	1 (3%)	34,37,54	1.27	4 (11%)
27	LMT	9	306	-	36,36,36	1.26	6 (16%)	47,47,47	0.95	2 (4%)
32	CHL	3	315	44	60,64,74	2.30	17 (28%)	68,102,114	2.60	25 (36%)
36	LUT	a	305	-	42,43,43	5.74	20 (47%)	51,60,60	5.70	29 (56%)
31	CLA	3	307	14	69,73,73	3.13	23 (33%)	83,113,113	2.32	27 (32%)
26	BCR	B	802	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	4 (7%)
31	CLA	b	305	13	50,54,73	3.19	25 (50%)	60,90,113	2.59	25 (41%)
35	QTB	F	303	-	19,19,19	1.31	3 (15%)	20,26,26	1.32	4 (20%)
31	CLA	7	316	15	50,54,73	3.28	22 (44%)	60,90,113	2.70	24 (40%)
31	CLA	7	313	15	47,52,73	3.09	23 (48%)	56,88,113	2.64	21 (37%)
32	CHL	A	831	1	62,66,74	2.23	19 (30%)	70,104,114	2.61	28 (40%)
36	LUT	3	305	-	42,43,43	5.47	19 (45%)	51,60,60	5.76	32 (62%)
31	CLA	5	307	22	59,63,73	3.80	22 (37%)	71,101,113	2.48	28 (39%)
31	CLA	3	311	14	69,73,73	2.78	23 (33%)	83,113,113	2.33	26 (31%)
32	CHL	8	316	44	70,74,74	2.12	20 (28%)	80,114,114	2.19	25 (31%)
31	CLA	8	317	44	54,58,73	2.83	21 (38%)	65,95,113	2.71	25 (38%)
32	CHL	5	319	-	51,55,74	3.28	19 (37%)	57,91,114	2.47	22 (38%)
35	QTB	9	304	-	19,19,19	1.29	2 (10%)	20,26,26	1.46	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	3	308	14	50,54,73	3.63	22 (44%)	60,90,113	2.71	22 (36%)
31	CLA	J	105	10	46,50,73	3.15	21 (45%)	55,85,113	2.85	23 (41%)
31	CLA	3	314	14	56,60,73	2.99	20 (35%)	67,97,113	2.49	26 (38%)
35	QTB	a	302	-	19,19,19	1.28	2 (10%)	20,26,26	1.69	4 (20%)
31	CLA	A	816	1	69,73,73	2.49	20 (28%)	83,113,113	2.26	25 (30%)
36	LUT	4	303	-	42,43,43	5.65	19 (45%)	51,60,60	5.53	31 (60%)
31	CLA	4	320	21	49,53,73	3.35	24 (48%)	59,89,113	2.66	24 (40%)
32	CHL	b	309	13	51,55,74	2.41	20 (39%)	57,91,114	2.43	23 (40%)
31	CLA	A	814	44	69,73,73	2.69	23 (33%)	83,113,113	2.33	26 (31%)
31	CLA	A	821	1	69,73,73	2.55	20 (28%)	83,113,113	2.42	26 (31%)
31	CLA	K	206	11	50,54,73	3.36	20 (40%)	60,90,113	2.62	21 (35%)
27	LMT	A	807	-	36,36,36	1.21	6 (16%)	47,47,47	1.06	3 (6%)
31	CLA	A	830	1	64,68,73	2.90	23 (35%)	77,107,113	2.49	27 (35%)
31	CLA	7	311	15	69,73,73	2.46	21 (30%)	83,113,113	2.31	24 (28%)
31	CLA	B	838	2	50,54,73	2.99	24 (48%)	60,90,113	2.58	24 (40%)
31	CLA	4	305	21	56,60,73	2.42	22 (39%)	67,97,113	4.56	35 (52%)
26	BCR	3	303	-	41,41,41	1.08	3 (7%)	56,56,56	1.25	5 (8%)
31	CLA	8	318	16	54,58,73	2.53	20 (37%)	65,95,113	2.58	25 (38%)
36	LUT	L	304	31	42,43,43	5.64	20 (47%)	51,60,60	5.75	33 (64%)
31	CLA	A	834	44	69,73,73	2.42	21 (30%)	83,113,113	2.25	23 (27%)
31	CLA	B	847	2	69,73,73	2.79	22 (31%)	83,113,113	2.32	21 (25%)
31	CLA	H	902	44	50,54,73	3.75	22 (44%)	60,90,113	2.66	24 (40%)
31	CLA	4	314	-	49,53,73	4.21	22 (44%)	59,89,113	2.77	26 (44%)
31	CLA	8	307	16	50,54,73	3.01	23 (46%)	60,90,113	2.75	23 (38%)
31	CLA	9	317	-	51,55,73	3.44	24 (47%)	61,91,113	2.65	21 (34%)
31	CLA	A	848	1	61,65,73	2.78	21 (34%)	73,103,113	2.37	23 (31%)
31	CLA	B	833	44	59,63,73	2.41	21 (35%)	71,101,113	2.43	21 (29%)
31	CLA	3	320	14	49,53,73	3.56	23 (46%)	59,89,113	2.71	23 (38%)
31	CLA	L	306	44	49,53,73	2.76	23 (46%)	59,89,113	2.66	22 (37%)
31	CLA	A	849	1	50,54,73	3.42	22 (44%)	60,90,113	2.60	23 (38%)
31	CLA	B	832	44	69,73,73	2.37	22 (31%)	83,113,113	2.49	29 (34%)
31	CLA	7	309	15	64,68,73	2.32	21 (32%)	77,107,113	2.37	26 (33%)
31	CLA	B	849	2	54,58,73	3.07	21 (38%)	65,95,113	2.56	24 (36%)
31	CLA	A	850	1	55,59,73	2.81	22 (40%)	66,96,113	2.65	26 (39%)
32	CHL	4	317	-	50,54,74	2.62	18 (36%)	56,90,114	2.48	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	8	314	44	56,60,73	2.74	21 (37%)	67,97,113	2.59	28 (41%)
31	CLA	6	322	23	50,54,73	3.10	22 (44%)	60,90,113	2.62	24 (40%)
31	CLA	4	319	-	46,50,73	4.16	22 (47%)	55,85,113	2.71	24 (43%)
32	CHL	8	319	44	49,53,74	2.62	18 (36%)	54,88,114	2.57	22 (40%)
26	BCR	M	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.16	3 (5%)
32	CHL	4	313	21	52,56,74	3.66	17 (32%)	58,92,114	2.46	26 (44%)
32	CHL	4	310	-	51,55,74	3.10	20 (39%)	57,91,114	2.43	23 (40%)
36	LUT	6	304	-	42,43,43	5.62	19 (45%)	51,60,60	5.35	31 (60%)
37	LMG	J	104	-	29,29,55	1.03	1 (3%)	37,37,63	1.19	3 (8%)
33	DGD	B	808	-	62,62,67	1.03	2 (3%)	76,76,81	1.29	5 (6%)
31	CLA	7	310	15	48,52,73	3.30	22 (45%)	58,88,113	2.78	25 (43%)
31	CLA	a	311	44	64,68,73	2.68	22 (34%)	77,107,113	2.47	28 (36%)
31	CLA	O	203	44	59,63,73	2.74	23 (38%)	71,101,113	2.53	28 (39%)
31	CLA	B	819	2	69,73,73	2.53	23 (33%)	83,113,113	2.48	29 (34%)
26	BCR	B	805	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
26	BCR	G	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
31	CLA	A	837	1	69,73,73	2.50	21 (30%)	83,113,113	2.33	24 (28%)
32	CHL	9	320	44	52,56,74	2.51	19 (36%)	58,92,114	2.40	23 (39%)
31	CLA	A	826	1	69,73,73	2.53	21 (30%)	83,113,113	2.31	25 (30%)
28	LHG	a	306	31	48,48,48	0.62	1 (2%)	51,54,54	1.23	5 (9%)
31	CLA	5	309	22	51,55,73	3.84	22 (43%)	61,91,113	2.64	24 (39%)
31	CLA	B	811	2	69,73,73	2.57	21 (30%)	83,113,113	2.42	24 (28%)
31	CLA	B	837	2	59,63,73	2.94	22 (37%)	71,101,113	2.37	25 (35%)
37	LMG	G	202	-	44,44,55	0.87	1 (2%)	52,52,63	1.30	5 (9%)
31	CLA	2	314	20	50,54,73	4.80	22 (44%)	60,90,113	2.63	25 (41%)
32	CHL	7	319	15	51,55,74	2.61	20 (39%)	57,91,114	2.82	18 (31%)
32	CHL	a	317	13	65,69,74	2.20	19 (29%)	74,108,114	2.26	29 (39%)
31	CLA	b	304	13	50,54,73	4.05	24 (48%)	60,90,113	2.60	23 (38%)
31	CLA	a	322	13	50,54,73	3.20	21 (42%)	60,90,113	2.56	23 (38%)
32	CHL	7	324	16	70,74,74	1.82	20 (28%)	80,114,114	2.20	28 (35%)
31	CLA	B	826	2	54,58,73	2.83	22 (40%)	65,95,113	2.71	25 (38%)
27	LMT	A	808	-	36,36,36	1.21	5 (13%)	47,47,47	0.99	2 (4%)
31	CLA	2	311	20	49,53,73	4.96	23 (46%)	59,89,113	2.62	22 (37%)
31	CLA	A	853	1	69,73,73	2.68	22 (31%)	83,113,113	2.34	28 (33%)
31	CLA	2	309	-	50,54,73	2.69	21 (42%)	60,90,113	2.58	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	F	302	-	41,41,41	0.98	2 (4%)	56,56,56	1.02	2 (3%)
35	QTB	7	303	-	19,19,19	1.28	2 (10%)	20,26,26	1.53	4 (20%)
31	CLA	A	847	1	69,73,73	2.60	20 (28%)	83,113,113	2.44	25 (30%)
31	CLA	2	304	20	50,54,73	3.19	23 (46%)	60,90,113	2.61	21 (35%)
31	CLA	A	822	1	59,63,73	2.66	23 (38%)	71,101,113	2.58	27 (38%)
36	LUT	9	305	-	42,43,43	5.68	19 (45%)	51,60,60	5.95	32 (62%)
31	CLA	A	844	1	54,58,73	3.12	22 (40%)	65,95,113	2.61	24 (36%)
31	CLA	7	314	44	58,62,73	2.76	21 (36%)	70,100,113	2.52	27 (38%)
31	CLA	A	817	31,1	59,63,73	2.77	21 (35%)	71,101,113	2.54	23 (32%)
32	CHL	A	840	1	70,74,74	2.23	20 (28%)	80,114,114	2.12	24 (30%)
31	CLA	B	818	2	59,63,73	2.44	19 (32%)	71,101,113	2.50	26 (36%)
26	BCR	B	804	-	41,41,41	1.03	2 (4%)	56,56,56	1.12	3 (5%)
31	CLA	A	815	-	69,73,73	2.63	21 (30%)	83,113,113	2.31	25 (30%)
31	CLA	A	819	1	69,73,73	2.32	22 (31%)	83,113,113	2.42	29 (34%)
31	CLA	A	846	1	69,73,73	2.60	22 (31%)	83,113,113	2.38	27 (32%)
26	BCR	B	806	-	41,41,41	1.04	2 (4%)	56,56,56	1.05	5 (8%)
31	CLA	B	828	44	64,68,73	2.47	21 (32%)	77,107,113	2.35	25 (32%)
31	CLA	A	832	1	69,73,73	2.30	19 (27%)	83,113,113	2.24	24 (28%)
26	BCR	8	301	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	6 (10%)
31	CLA	4	315	44	49,53,73	5.09	23 (46%)	59,89,113	2.64	23 (38%)
31	CLA	G	206	44	49,53,73	3.45	21 (42%)	59,89,113	2.61	21 (35%)
31	CLA	B	848	28	69,73,73	2.29	22 (31%)	83,113,113	2.35	24 (28%)
31	CLA	B	824	2	61,65,73	3.09	23 (37%)	73,103,113	2.52	27 (36%)
26	BCR	K	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	8 (14%)
31	CLA	b	313	13	64,68,73	3.42	22 (34%)	77,107,113	2.35	25 (32%)
36	LUT	J	103	-	42,43,43	5.66	20 (47%)	51,60,60	5.75	31 (60%)
31	CLA	2	307	20	61,65,73	2.89	22 (36%)	73,103,113	2.53	26 (35%)
31	CLA	2	305	20	49,53,73	4.13	22 (44%)	59,89,113	2.71	22 (37%)
31	CLA	A	836	1	64,68,73	2.58	22 (34%)	77,107,113	2.44	25 (32%)
32	CHL	6	319	-	51,55,74	4.63	20 (39%)	57,91,114	2.54	26 (45%)
31	CLA	4	321	21	54,58,73	3.73	22 (40%)	65,95,113	2.64	28 (43%)
31	CLA	2	310	20	49,53,73	6.63	23 (46%)	59,89,113	2.69	24 (40%)
36	LUT	7	305	-	42,43,43	5.55	20 (47%)	51,60,60	5.71	31 (60%)
31	CLA	4	316	-	51,55,73	3.33	24 (47%)	61,91,113	2.98	21 (34%)
28	LHG	7	307	31	36,36,48	0.77	1 (2%)	39,42,54	1.24	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	F	301	44	69,73,73	2.49	23 (33%)	83,113,113	2.40	28 (33%)
36	LUT	9	302	-	42,43,43	5.49	20 (47%)	51,60,60	5.76	33 (64%)
36	LUT	3	304	-	42,43,43	5.56	20 (47%)	51,60,60	5.67	33 (64%)
31	CLA	b	308	13	50,54,73	3.61	23 (46%)	60,90,113	2.57	24 (40%)
31	CLA	5	313	28	50,54,73	3.64	25 (50%)	60,90,113	2.76	21 (35%)
27	LMT	5	301	-	36,36,36	1.22	5 (13%)	47,47,47	0.96	2 (4%)
28	LHG	A	810	31	41,41,48	0.72	1 (2%)	44,47,54	1.14	4 (9%)
31	CLA	7	315	28	59,63,73	3.78	23 (38%)	70,100,113	2.53	25 (35%)
40	XAT	7	306	-	39,47,47	1.60	8 (20%)	54,74,74	1.55	9 (16%)
31	CLA	H	903	18	50,54,73	3.04	20 (40%)	60,90,113	2.56	21 (35%)
36	LUT	F	304	-	42,43,43	5.43	20 (47%)	51,60,60	6.02	35 (68%)
36	LUT	5	304	-	42,43,43	5.61	19 (45%)	51,60,60	5.48	31 (60%)
31	CLA	8	321	16	50,54,73	3.19	21 (42%)	60,90,113	2.68	20 (33%)
31	CLA	A	857	44	69,73,73	2.24	20 (28%)	83,113,113	2.42	29 (34%)
36	LUT	8	303	-	42,43,43	5.52	20 (47%)	51,60,60	5.71	34 (66%)
31	CLA	b	306	-	50,54,73	4.62	22 (44%)	60,90,113	2.63	22 (36%)
31	CLA	2	312	20	50,54,73	3.61	22 (44%)	60,90,113	2.72	24 (40%)
39	3PH	7	301	-	32,32,47	0.75	1 (3%)	36,37,52	0.73	1 (2%)
26	BCR	L	301	-	41,41,41	0.98	1 (2%)	56,56,56	1.19	5 (8%)
31	CLA	2	315	44	50,54,73	3.23	23 (46%)	60,90,113	2.70	23 (38%)
26	BCR	3	302	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
31	CLA	B	827	2	64,68,73	2.42	19 (29%)	77,107,113	2.45	25 (32%)
26	BCR	A	806	-	41,41,41	1.01	2 (4%)	56,56,56	1.10	5 (8%)
31	CLA	5	321	22	50,54,73	3.35	20 (40%)	60,90,113	2.70	25 (41%)
31	CLA	B	830	2	64,68,73	2.65	22 (34%)	77,107,113	2.32	27 (35%)
36	LUT	5	303	-	42,43,43	5.56	19 (45%)	51,60,60	5.70	33 (64%)
31	CLA	3	316	44	54,58,73	2.61	22 (40%)	65,95,113	2.55	25 (38%)
32	CHL	5	317	44	51,55,74	2.97	18 (35%)	57,91,114	2.55	21 (36%)
31	CLA	B	850	2	66,70,73	2.60	21 (31%)	79,109,113	2.30	24 (30%)
32	CHL	5	322	22	51,55,74	2.98	19 (37%)	57,91,114	2.46	23 (40%)
31	CLA	a	309	13	64,68,73	4.60	24 (37%)	77,107,113	2.47	29 (37%)
31	CLA	L	305	18	64,68,73	2.55	22 (34%)	77,107,113	2.41	24 (31%)
31	CLA	b	310	-	50,54,73	2.80	21 (42%)	60,90,113	2.60	23 (38%)
32	CHL	6	320	-	51,55,74	3.08	19 (37%)	57,91,114	2.41	21 (36%)
31	CLA	4	309	21	64,68,73	2.53	23 (35%)	77,107,113	2.49	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	SF4	C	101	3	0,12,12	-	-	-		
30	CL0	A	813	1	69,73,73	1.85	17 (24%)	83,113,113	3.26	30 (36%)
31	CLA	4	312	21	51,55,73	2.91	22 (43%)	61,91,113	2.63	25 (40%)
31	CLA	A	828	1	69,73,73	2.53	23 (33%)	83,113,113	2.38	24 (28%)
31	CLA	B	817	2	69,73,73	2.47	21 (30%)	83,113,113	2.43	25 (30%)
31	CLA	L	307	36	49,53,73	3.87	20 (40%)	59,89,113	2.67	24 (40%)
31	CLA	A	854	28	50,54,73	2.85	21 (42%)	60,90,113	2.75	21 (35%)
31	CLA	B	831	2	54,58,73	2.67	23 (42%)	65,95,113	2.60	28 (43%)
31	CLA	H	901	8	50,54,73	2.78	22 (44%)	60,90,113	2.59	25 (41%)
31	CLA	B	845	2	54,58,73	2.77	21 (38%)	65,95,113	2.66	25 (38%)
31	CLA	B	815	2	69,73,73	2.31	21 (30%)	83,113,113	2.35	25 (30%)
31	CLA	8	320	16	69,73,73	2.56	23 (33%)	83,113,113	2.28	27 (32%)
32	CHL	6	309	23	70,74,74	2.14	20 (28%)	80,114,114	2.11	25 (31%)
24	PQN	A	801	-	34,34,34	0.35	0	42,45,45	0.58	0
32	CHL	6	317	23	51,55,74	2.76	20 (39%)	57,91,114	2.41	22 (38%)
37	LMG	a	301	-	42,42,55	0.83	0	50,50,63	1.26	4 (8%)
32	CHL	6	321	23	47,51,74	3.60	18 (38%)	52,86,114	2.49	22 (42%)
31	CLA	F	305	6	50,54,73	2.88	23 (46%)	60,90,113	2.80	26 (43%)
31	CLA	6	314	23	51,55,73	4.15	22 (43%)	61,91,113	2.68	24 (39%)
31	CLA	6	315	28	50,54,73	5.69	24 (48%)	60,90,113	2.68	22 (36%)
31	CLA	5	314	22	49,53,73	3.34	23 (46%)	59,89,113	2.72	24 (40%)
31	CLA	B	813	2	69,73,73	2.73	24 (34%)	83,113,113	2.44	25 (30%)
26	BCR	J	102	-	41,41,41	0.99	2 (4%)	56,56,56	1.20	3 (5%)
31	CLA	a	315	28	59,63,73	2.56	22 (37%)	71,101,113	2.60	24 (33%)
43	PTY	5	306	-	30,30,49	0.54	0	33,35,54	0.80	1 (3%)
31	CLA	B	844	2	69,73,73	2.42	21 (30%)	83,113,113	2.36	25 (30%)
32	CHL	a	320	44	52,56,74	2.29	19 (36%)	58,92,114	2.52	22 (37%)
31	CLA	8	313	28	50,54,73	3.49	24 (48%)	60,90,113	2.70	23 (38%)
26	BCR	G	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	4 (7%)
31	CLA	2	306	20	64,68,73	3.44	24 (37%)	77,107,113	2.38	26 (33%)
31	CLA	A	855	1	69,73,73	2.75	21 (30%)	83,113,113	2.36	26 (31%)
31	CLA	O	204	-	45,49,73	3.04	22 (48%)	54,84,113	2.76	25 (46%)
26	BCR	3	301	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
31	CLA	3	309	14	69,73,73	2.32	22 (31%)	83,113,113	2.39	27 (32%)
31	CLA	B	840	2	69,73,73	2.48	24 (34%)	83,113,113	2.33	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LHG	A	809	-	41,41,48	0.72	2 (4%)	44,47,54	1.29	6 (13%)
28	LHG	8	304	31	48,48,48	0.63	1 (2%)	51,54,54	1.24	6 (11%)
36	LUT	9	303	-	42,43,43	5.55	19 (45%)	51,60,60	5.53	30 (58%)
26	BCR	6	302	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
31	CLA	b	312	13	50,54,73	5.15	22 (44%)	60,90,113	2.61	24 (40%)
31	CLA	B	841	2	59,63,73	2.67	21 (35%)	71,101,113	2.55	28 (39%)
31	CLA	6	316	23	54,58,73	4.63	23 (42%)	65,95,113	2.65	27 (41%)
31	CLA	4	311	28	50,54,73	6.47	23 (46%)	60,90,113	2.62	24 (40%)
26	BCR	B	803	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	2 (3%)
31	CLA	B	816	2	65,69,73	3.02	22 (33%)	78,108,113	2.51	26 (33%)
36	LUT	6	303	-	42,43,43	5.57	19 (45%)	51,60,60	5.78	34 (66%)
31	CLA	7	322	15	50,54,73	3.20	22 (44%)	60,90,113	2.62	22 (36%)
31	CLA	A	833	1	51,55,73	3.42	23 (45%)	61,91,113	2.78	24 (39%)
26	BCR	A	804	-	41,41,41	1.09	2 (4%)	56,56,56	1.14	4 (7%)
31	CLA	9	318	44	69,73,73	2.89	20 (28%)	83,113,113	2.30	26 (31%)
31	CLA	5	320	22	50,54,73	5.59	25 (50%)	60,90,113	2.67	26 (43%)
31	CLA	6	312	23	69,73,73	3.13	24 (34%)	83,113,113	2.34	25 (30%)
31	CLA	B	829	2	59,63,73	2.55	21 (35%)	71,101,113	2.69	25 (35%)
31	CLA	8	308	16	69,73,73	2.63	25 (36%)	83,113,113	2.35	25 (30%)
31	CLA	5	315	22	69,73,73	4.22	23 (33%)	83,113,113	4.28	28 (33%)
31	CLA	8	310	16	69,73,73	2.54	22 (31%)	83,113,113	2.40	24 (28%)
31	CLA	b	302	13	50,54,73	2.98	21 (42%)	60,90,113	2.73	25 (41%)
31	CLA	3	310	14	64,68,73	3.06	22 (34%)	77,107,113	2.46	26 (33%)
31	CLA	A	843	1	69,73,73	2.82	22 (31%)	83,113,113	2.27	24 (28%)
25	SF4	C	102	3	0,12,12	-	-	-		
31	CLA	6	306	23	50,54,73	3.30	25 (50%)	60,90,113	2.70	18 (30%)
31	CLA	5	310	22	69,73,73	2.66	23 (33%)	83,113,113	2.39	29 (34%)
31	CLA	B	839	2	64,68,73	2.57	23 (35%)	77,107,113	2.37	26 (33%)
31	CLA	B	812	-	69,73,73	2.31	22 (31%)	83,113,113	2.39	26 (31%)
36	LUT	a	303	-	42,43,43	5.61	19 (45%)	51,60,60	5.48	34 (66%)
31	CLA	B	836	2	69,73,73	2.52	21 (30%)	83,113,113	2.27	24 (28%)
26	BCR	L	302	-	41,41,41	1.04	2 (4%)	56,56,56	1.14	6 (10%)
37	LMG	J	101	-	49,49,55	0.83	3 (6%)	57,57,63	1.23	2 (3%)
32	CHL	7	317	15	61,65,74	2.45	20 (32%)	69,103,114	2.30	26 (37%)
31	CLA	9	319	17	50,54,73	5.00	21 (42%)	60,90,113	2.73	25 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	A	852	1	55,59,73	3.30	22 (40%)	66,96,113	2.68	24 (36%)
31	CLA	O	202	19	40,46,73	3.33	21 (52%)	48,80,113	2.78	22 (45%)
31	CLA	9	314	17	64,68,73	3.49	23 (35%)	77,107,113	2.44	25 (32%)
28	LHG	6	301	31	26,26,48	0.78	0	29,32,54	1.22	2 (6%)
31	CLA	A	851	1	69,73,73	2.77	22 (31%)	83,113,113	2.31	22 (26%)
31	CLA	A	827	1	59,63,73	2.84	21 (35%)	71,101,113	2.47	22 (30%)
31	CLA	8	315	16	56,60,73	2.85	23 (41%)	67,97,113	2.55	28 (41%)
31	CLA	b	311	13	50,54,73	3.86	23 (46%)	60,90,113	2.68	24 (40%)
42	SQD	4	304	-	34,35,54	1.80	7 (20%)	43,46,65	1.54	6 (13%)
31	CLA	9	313	17	49,53,73	4.51	24 (48%)	59,89,113	2.75	22 (37%)
31	CLA	B	822	2	69,73,73	2.64	22 (31%)	83,113,113	2.27	23 (27%)
31	CLA	8	311	16	59,63,73	2.87	22 (37%)	71,101,113	2.55	25 (35%)
31	CLA	9	316	17	54,58,73	2.97	22 (40%)	65,95,113	2.61	23 (35%)
26	BCR	5	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
31	CLA	a	313	13	64,68,73	2.69	24 (37%)	77,107,113	2.45	24 (31%)
31	CLA	5	312	44	54,58,73	2.81	22 (40%)	65,95,113	2.66	28 (43%)
24	PQN	B	801	-	34,34,34	0.51	0	42,45,45	0.75	1 (2%)
31	CLA	6	313	23	50,54,73	2.97	24 (48%)	60,90,113	2.79	24 (40%)
31	CLA	a	319	13	69,73,73	2.50	20 (28%)	83,113,113	2.40	26 (31%)
31	CLA	F	306	44	54,58,73	2.79	21 (38%)	65,95,113	2.60	26 (40%)
26	BCR	A	805	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
31	CLA	A	829	44	54,58,73	2.57	16 (29%)	65,95,113	3.22	26 (40%)
31	CLA	8	309	16	54,58,73	3.09	22 (40%)	65,95,113	2.74	30 (46%)
26	BCR	I	801	-	41,41,41	1.05	1 (2%)	56,56,56	1.18	4 (7%)
32	CHL	K	201	11	51,55,74	2.20	19 (37%)	57,91,114	3.20	22 (38%)
28	LHG	A	811	-	48,48,48	0.72	1 (2%)	51,54,54	1.26	5 (9%)
34	LAP	B	851	-	28,28,28	0.34	0	33,35,35	0.38	0
31	CLA	2	308	20	50,54,73	3.03	22 (44%)	60,90,113	2.72	25 (41%)
32	CHL	7	318	44	70,74,74	2.29	19 (27%)	80,114,114	2.32	25 (31%)
31	CLA	A	824	31,1	66,70,73	2.72	20 (30%)	79,109,113	2.38	26 (32%)
32	CHL	7	320	44	65,69,74	3.05	20 (30%)	74,108,114	2.28	27 (36%)
31	CLA	a	316	13	49,53,73	3.23	22 (44%)	59,89,113	2.66	26 (44%)
31	CLA	4	306	21	49,53,73	3.26	23 (46%)	59,89,113	2.67	25 (42%)
31	CLA	B	820	2	69,73,73	3.04	24 (34%)	83,113,113	2.32	25 (30%)
31	CLA	6	310	23	51,55,73	4.59	23 (45%)	61,91,113	2.68	26 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CHL	9	322	44	51,55,74	3.36	22 (43%)	57,91,114	2.45	24 (42%)
31	CLA	B	842	2	65,69,73	2.74	21 (32%)	78,108,113	2.42	29 (37%)
36	LUT	b	301	-	42,43,43	5.67	19 (45%)	51,60,60	5.69	33 (64%)
31	CLA	4	307	21	60,64,73	2.72	22 (36%)	72,102,113	2.45	29 (40%)
31	CLA	A	818	1	69,73,73	2.26	22 (31%)	83,113,113	2.35	25 (30%)
31	CLA	6	307	23	54,58,73	3.90	22 (40%)	65,95,113	2.56	27 (41%)
31	CLA	B	825	2	64,68,73	2.71	23 (35%)	77,107,113	2.46	26 (33%)
28	LHG	6	305	31	31,31,48	0.74	1 (3%)	34,37,54	1.29	4 (11%)
26	BCR	L	303	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	6 (10%)
28	LHG	7	302	-	48,48,48	0.58	0	51,54,54	1.26	5 (9%)
31	CLA	9	315	17	58,62,73	2.71	21 (36%)	69,99,113	2.62	27 (39%)
31	CLA	8	312	44	54,58,73	2.86	21 (38%)	65,95,113	2.58	25 (38%)
31	CLA	3	319	14	65,69,73	2.81	22 (33%)	78,108,113	2.47	28 (35%)
26	BCR	7	304	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	4 (7%)
31	CLA	6	311	23	59,63,73	4.05	22 (37%)	71,101,113	2.53	27 (38%)
31	CLA	B	846	44	69,73,73	2.41	21 (30%)	83,113,113	2.27	25 (30%)
31	CLA	A	842	1	69,73,73	2.83	23 (33%)	83,113,113	2.43	26 (31%)
36	LUT	8	302	-	42,43,43	5.50	19 (45%)	51,60,60	5.63	31 (60%)
31	CLA	5	318	22	69,73,73	5.34	23 (33%)	83,113,113	2.32	27 (32%)
31	CLA	A	841	1	69,73,73	2.49	21 (30%)	83,113,113	2.51	28 (33%)
31	CLA	B	835	2	61,65,73	3.04	22 (36%)	73,103,113	2.51	25 (34%)
32	CHL	A	839	44	60,64,74	2.15	19 (31%)	68,102,114	2.85	27 (39%)

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
28	LHG	5	305	31	-	24/39/39/53	-
31	CLA	6	308	44	-	7/18/94/115	-
31	CLA	7	321	44	-	7/18/94/115	-
31	CLA	a	314	44	-	6/21/97/115	-
31	CLA	K	204	44	-	5/21/97/115	-
32	CHL	5	316	44	-	14/29/105/117	-
25	SF4	A	802	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	DGA	8	305	-	-	18/29/29/45	-
31	CLA	9	311	17	-	5/27/103/115	-
31	CLA	A	838	44	-	11/39/115/115	-
31	CLA	B	843	44	-	5/15/91/115	-
26	BCR	O	201	-	-	4/29/63/63	0/2/2/2
32	CHL	6	318	44	-	11/17/93/117	-
31	CLA	A	820	1	-	4/27/103/115	-
31	CLA	5	311	22	-	5/17/93/115	-
32	CHL	a	318	44	-	6/20/96/117	-
31	CLA	3	312	44	-	9/39/115/115	-
33	DGD	7	308	-	-	14/41/81/95	0/2/2/2
31	CLA	3	317	44	-	8/23/99/115	-
31	CLA	G	204	7	-	5/21/97/115	-
31	CLA	b	307	-	-	7/17/93/115	-
31	CLA	9	321	17	-	14/29/105/115	-
31	CLA	A	823	1	-	7/27/103/115	-
31	CLA	K	205	11	-	3/17/93/115	-
31	CLA	7	312	15	-	11/36/112/115	-
36	LUT	2	301	-	-	13/29/67/67	0/2/2/2
31	CLA	a	310	13	-	7/15/91/115	-
31	CLA	5	308	22	-	4/17/93/115	-
31	CLA	A	825	1	-	2/26/102/115	-
31	CLA	A	845	1	-	7/29/105/115	-
26	BCR	2	302	-	-	7/29/63/63	0/2/2/2
31	CLA	B	834	2	-	5/39/115/115	-
31	CLA	5	323	22	-	9/29/105/115	-
31	CLA	A	835	1	-	5/27/103/115	-
31	CLA	A	856	44	-	7/39/115/115	-
31	CLA	B	823	2	-	9/27/103/115	-
31	CLA	2	313	20	-	8/17/93/115	-
31	CLA	4	318	21	-	7/15/91/115	-
26	BCR	K	203	-	-	5/29/63/63	0/2/2/2
31	CLA	3	318	14	-	9/23/99/115	-
31	CLA	B	814	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	AXT	a	304	-	-	2/29/71/75	0/2/2/2
31	CLA	b	303	-	-	5/17/93/115	-
31	CLA	B	821	2	-	4/31/107/115	-
26	BCR	A	803	-	-	5/29/63/63	0/2/2/2
31	CLA	9	312	17	-	2/17/93/115	-
31	CLA	4	308	21	-	8/33/109/115	-
31	CLA	G	205	7	-	6/17/93/115	-
31	CLA	a	321	44	-	6/21/97/115	-
36	LUT	4	302	-	-	16/29/67/67	0/2/2/2
31	CLA	a	312	13	-	13/39/115/115	-
31	CLA	3	313	-	-	12/33/109/115	-
28	LHG	B	807	31	-	7/36/36/53	-
27	LMT	9	306	-	-	10/21/61/61	0/2/2/2
32	CHL	3	315	44	-	7/29/105/117	-
36	LUT	a	305	-	-	22/29/67/67	0/2/2/2
31	CLA	3	307	14	-	10/39/115/115	-
26	BCR	B	802	-	-	5/29/63/63	0/2/2/2
31	CLA	b	305	13	-	6/17/93/115	-
35	QTB	F	303	-	-	7/11/28/28	1/1/1/1
31	CLA	7	316	15	-	5/17/93/115	-
31	CLA	7	313	15	-	4/13/89/115	-
32	CHL	A	831	1	-	13/32/108/117	-
36	LUT	3	305	-	-	13/29/67/67	0/2/2/2
31	CLA	5	307	22	-	5/27/103/115	-
31	CLA	3	311	14	-	11/39/115/115	-
32	CHL	8	316	44	-	12/41/117/117	-
31	CLA	8	317	44	-	2/21/97/115	-
32	CHL	5	319	-	-	4/19/95/117	-
35	QTB	9	304	-	-	6/11/28/28	0/1/1/1
31	CLA	3	308	14	-	5/17/93/115	-
31	CLA	J	105	10	-	6/12/88/115	-
31	CLA	3	314	14	-	9/24/100/115	-
35	QTB	a	302	-	-	5/11/28/28	0/1/1/1
31	CLA	A	816	1	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	4	303	-	-	16/29/67/67	0/2/2/2
31	CLA	4	320	21	-	9/15/91/115	-
32	CHL	b	309	13	-	12/19/95/117	-
31	CLA	A	814	44	-	10/39/115/115	-
31	CLA	A	821	1	-	12/39/115/115	-
31	CLA	K	206	11	-	7/17/93/115	-
27	LMT	A	807	-	-	6/21/61/61	0/2/2/2
31	CLA	A	830	1	-	11/33/109/115	-
31	CLA	7	311	15	-	12/39/115/115	-
31	CLA	B	838	2	-	3/17/93/115	-
31	CLA	4	305	21	-	7/24/100/115	-
26	BCR	3	303	-	-	9/29/63/63	0/2/2/2
31	CLA	8	318	16	-	2/21/97/115	-
36	LUT	L	304	31	-	15/29/67/67	0/2/2/2
31	CLA	A	834	44	-	10/39/115/115	-
31	CLA	B	847	2	-	11/39/115/115	-
31	CLA	H	902	44	-	3/17/93/115	-
31	CLA	4	314	-	-	6/15/91/115	-
31	CLA	8	307	16	-	3/17/93/115	-
31	CLA	9	317	-	-	8/18/94/115	-
31	CLA	A	848	1	-	13/30/106/115	-
31	CLA	B	833	44	-	7/27/103/115	-
31	CLA	3	320	14	-	4/15/91/115	-
31	CLA	L	306	44	-	4/15/91/115	-
31	CLA	A	849	1	-	9/17/93/115	-
31	CLA	B	832	44	-	9/39/115/115	-
31	CLA	7	309	15	-	4/33/109/115	-
31	CLA	B	849	2	-	4/21/97/115	-
31	CLA	A	850	1	-	8/23/99/115	-
32	CHL	4	317	-	-	10/17/93/117	-
31	CLA	8	314	44	-	4/24/100/115	-
31	CLA	6	322	23	-	7/17/93/115	-
31	CLA	4	319	-	-	7/12/88/115	-
32	CHL	8	319	44	-	3/16/92/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	M	101	-	-	7/29/63/63	0/2/2/2
32	CHL	4	313	21	-	10/20/96/117	-
32	CHL	4	310	-	-	6/19/95/117	-
36	LUT	6	304	-	-	16/29/67/67	0/2/2/2
37	LMG	J	104	-	-	11/24/44/70	0/1/1/1
33	DGD	B	808	-	-	22/50/90/95	0/2/2/2
31	CLA	7	310	15	-	4/13/89/115	-
31	CLA	a	311	44	-	11/33/109/115	-
31	CLA	O	203	44	-	14/27/103/115	-
31	CLA	B	819	2	-	6/39/115/115	-
26	BCR	B	805	-	-	7/29/63/63	0/2/2/2
26	BCR	G	201	-	-	8/29/63/63	0/2/2/2
31	CLA	A	837	1	-	18/39/115/115	-
32	CHL	9	320	44	-	9/20/96/117	-
31	CLA	A	826	1	-	14/39/115/115	-
28	LHG	a	306	31	-	19/53/53/53	-
31	CLA	5	309	22	-	7/18/94/115	-
31	CLA	B	811	2	-	6/39/115/115	-
31	CLA	B	837	2	-	6/27/103/115	-
37	LMG	G	202	-	-	23/39/59/70	0/1/1/1
31	CLA	2	314	20	-	2/17/93/115	-
32	CHL	7	319	15	-	1/19/95/117	-
32	CHL	a	317	13	-	15/35/111/117	-
31	CLA	b	304	13	-	5/17/93/115	-
31	CLA	a	322	13	-	7/17/93/115	-
32	CHL	7	324	16	-	14/41/117/117	-
31	CLA	B	826	2	-	9/21/97/115	-
27	LMT	A	808	-	-	6/21/61/61	0/2/2/2
31	CLA	2	311	20	-	8/15/91/115	-
31	CLA	A	853	1	-	12/39/115/115	-
31	CLA	2	309	-	-	5/17/93/115	-
26	BCR	F	302	-	-	7/29/63/63	0/2/2/2
35	QTB	7	303	-	-	10/11/28/28	1/1/1/1
31	CLA	A	847	1	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	304	20	-	11/17/93/115	-
31	CLA	A	822	1	-	9/27/103/115	-
36	LUT	9	305	-	-	18/29/67/67	0/2/2/2
31	CLA	A	844	1	-	3/21/97/115	-
31	CLA	7	314	44	-	7/25/101/115	-
31	CLA	A	817	31,1	-	6/27/103/115	-
32	CHL	A	840	1	-	13/41/117/117	-
31	CLA	B	818	2	-	5/27/103/115	-
26	BCR	B	804	-	-	5/29/63/63	0/2/2/2
31	CLA	A	815	-	-	5/39/115/115	-
31	CLA	A	819	1	-	10/39/115/115	-
31	CLA	A	846	1	-	7/39/115/115	-
26	BCR	B	806	-	-	6/29/63/63	0/2/2/2
31	CLA	B	828	44	-	4/33/109/115	-
31	CLA	A	832	1	-	6/39/115/115	-
26	BCR	8	301	-	-	6/29/63/63	0/2/2/2
31	CLA	4	315	44	-	5/15/91/115	-
31	CLA	G	206	44	-	2/15/91/115	-
31	CLA	B	848	28	-	9/39/115/115	-
31	CLA	B	824	2	-	10/30/106/115	-
26	BCR	K	202	-	-	9/29/63/63	0/2/2/2
36	LUT	J	103	-	-	16/29/67/67	0/2/2/2
31	CLA	b	313	13	-	12/33/109/115	-
31	CLA	2	307	20	-	9/30/106/115	-
31	CLA	2	305	20	-	7/15/91/115	-
31	CLA	A	836	1	-	8/33/109/115	-
32	CHL	6	319	-	-	8/19/95/117	-
31	CLA	4	321	21	-	8/21/97/115	-
31	CLA	2	310	20	-	6/15/91/115	-
36	LUT	7	305	-	-	14/29/67/67	0/2/2/2
31	CLA	4	316	-	-	6/18/94/115	-
28	LHG	7	307	31	-	21/41/41/53	-
31	CLA	F	301	44	-	9/39/115/115	-
36	LUT	9	302	-	-	17/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	3	304	-	-	13/29/67/67	0/2/2/2
31	CLA	b	308	13	-	7/17/93/115	-
31	CLA	5	313	28	-	6/17/93/115	-
27	LMT	5	301	-	-	9/21/61/61	0/2/2/2
28	LHG	A	810	31	-	18/46/46/53	-
31	CLA	7	315	28	-	8/27/103/115	-
40	XAT	7	306	-	-	4/31/93/93	0/4/4/4
31	CLA	H	903	18	-	5/17/93/115	-
36	LUT	F	304	-	-	17/29/67/67	0/2/2/2
36	LUT	5	304	-	-	16/29/67/67	0/2/2/2
31	CLA	8	321	16	-	3/17/93/115	-
31	CLA	A	857	44	-	16/39/115/115	-
36	LUT	8	303	-	-	14/29/67/67	0/2/2/2
31	CLA	b	306	-	-	7/17/93/115	-
31	CLA	2	312	20	-	6/17/93/115	-
39	3PH	7	301	-	-	15/34/34/49	-
26	BCR	L	301	-	-	9/29/63/63	0/2/2/2
31	CLA	2	315	44	-	8/17/93/115	-
26	BCR	3	302	-	-	8/29/63/63	0/2/2/2
31	CLA	B	827	2	-	9/33/109/115	-
26	BCR	A	806	-	-	7/29/63/63	0/2/2/2
31	CLA	5	321	22	-	6/17/93/115	-
31	CLA	B	830	2	-	7/33/109/115	-
36	LUT	5	303	-	-	13/29/67/67	0/2/2/2
31	CLA	3	316	44	-	4/21/97/115	-
32	CHL	5	317	44	-	6/19/95/117	-
31	CLA	B	850	2	-	8/36/112/115	-
32	CHL	5	322	22	-	5/19/95/117	-
31	CLA	a	309	13	-	6/33/109/115	-
31	CLA	L	305	18	-	10/33/109/115	-
31	CLA	b	310	-	-	6/17/93/115	-
32	CHL	6	320	-	-	11/19/95/117	-
31	CLA	4	309	21	-	12/33/109/115	-
25	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CL0	A	813	1	-	9/39/115/115	-
31	CLA	4	312	21	-	9/18/94/115	-
31	CLA	A	828	1	-	7/39/115/115	-
31	CLA	B	817	2	-	13/39/115/115	-
31	CLA	L	307	36	-	9/15/91/115	-
31	CLA	A	854	28	-	6/17/93/115	-
31	CLA	B	831	2	-	6/21/97/115	-
31	CLA	H	901	8	-	9/17/93/115	-
31	CLA	B	845	2	-	3/21/97/115	-
31	CLA	B	815	2	-	17/39/115/115	-
31	CLA	8	320	16	-	12/39/115/115	-
32	CHL	6	309	23	-	18/41/117/117	-
24	PQN	A	801	-	-	2/23/43/43	0/2/2/2
32	CHL	6	317	23	-	10/19/95/117	-
37	LMG	a	301	-	-	21/37/57/70	0/1/1/1
32	CHL	6	321	23	-	9/14/90/117	-
31	CLA	F	305	6	-	6/17/93/115	-
31	CLA	6	314	23	-	6/18/94/115	-
31	CLA	6	315	28	-	3/17/93/115	-
31	CLA	5	314	22	-	7/15/91/115	-
31	CLA	B	813	2	-	8/39/115/115	-
26	BCR	J	102	-	-	6/29/63/63	0/2/2/2
31	CLA	a	315	28	-	7/27/103/115	-
43	PTY	5	306	-	-	17/34/34/53	-
31	CLA	B	844	2	-	10/39/115/115	-
32	CHL	a	320	44	-	7/20/96/117	-
31	CLA	8	313	28	-	8/17/93/115	-
26	BCR	G	203	-	-	11/29/63/63	0/2/2/2
31	CLA	2	306	20	-	11/33/109/115	-
31	CLA	A	855	1	-	15/39/115/115	-
31	CLA	O	204	-	-	4/10/86/115	-
26	BCR	3	301	-	-	9/29/63/63	0/2/2/2
31	CLA	3	309	14	-	16/39/115/115	-
31	CLA	B	840	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	A	809	-	-	20/46/46/53	-
28	LHG	8	304	31	-	15/53/53/53	-
36	LUT	9	303	-	-	16/29/67/67	0/2/2/2
26	BCR	6	302	-	-	15/29/63/63	0/2/2/2
31	CLA	b	312	13	-	5/17/93/115	-
31	CLA	B	841	2	-	10/27/103/115	-
31	CLA	6	316	23	-	3/21/97/115	-
31	CLA	4	311	28	-	8/17/93/115	-
26	BCR	B	803	-	-	9/29/63/63	0/2/2/2
31	CLA	B	816	2	-	5/35/111/115	-
36	LUT	6	303	-	-	18/29/67/67	0/2/2/2
31	CLA	7	322	15	-	6/17/93/115	-
31	CLA	A	833	1	-	9/18/94/115	-
26	BCR	A	804	-	-	9/29/63/63	0/2/2/2
31	CLA	9	318	44	-	10/39/115/115	-
31	CLA	5	320	22	-	3/17/93/115	-
31	CLA	6	312	23	-	10/39/115/115	-
31	CLA	B	829	2	-	5/27/103/115	-
31	CLA	8	308	16	-	13/39/115/115	-
31	CLA	5	315	22	-	11/39/115/115	-
31	CLA	8	310	16	-	10/39/115/115	-
31	CLA	b	302	13	-	6/17/93/115	-
31	CLA	3	310	14	-	10/33/109/115	-
31	CLA	A	843	1	-	9/39/115/115	-
25	SF4	C	102	3	-	-	0/6/5/5
31	CLA	6	306	23	-	5/17/93/115	-
31	CLA	5	310	22	-	6/39/115/115	-
31	CLA	B	839	2	-	10/33/109/115	-
31	CLA	B	812	-	-	9/39/115/115	-
36	LUT	a	303	-	-	14/29/67/67	0/2/2/2
31	CLA	B	836	2	-	6/39/115/115	-
26	BCR	L	302	-	-	6/29/63/63	0/2/2/2
37	LMG	J	101	-	-	20/44/64/70	0/1/1/1
32	CHL	7	317	15	-	12/31/107/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	9	319	17	-	9/17/93/115	-
31	CLA	A	852	1	-	2/23/99/115	-
31	CLA	O	202	19	-	3/6/78/115	-
31	CLA	9	314	17	-	10/33/109/115	-
28	LHG	6	301	31	-	16/31/31/53	-
31	CLA	A	851	1	-	9/39/115/115	-
31	CLA	A	827	1	-	9/27/103/115	-
31	CLA	8	315	16	-	7/24/100/115	-
31	CLA	b	311	13	-	7/17/93/115	-
42	SQD	4	304	-	-	12/30/50/69	0/1/1/1
31	CLA	9	313	17	-	6/15/91/115	-
31	CLA	B	822	2	-	17/39/115/115	-
31	CLA	8	311	16	-	11/27/103/115	-
31	CLA	9	316	17	-	5/21/97/115	-
26	BCR	5	302	-	-	13/29/63/63	0/2/2/2
31	CLA	a	313	13	-	7/33/109/115	-
31	CLA	5	312	44	-	10/21/97/115	-
24	PQN	B	801	-	-	4/23/43/43	0/2/2/2
31	CLA	6	313	23	-	5/17/93/115	-
31	CLA	a	319	13	-	13/39/115/115	-
31	CLA	F	306	44	-	4/21/97/115	-
26	BCR	A	805	-	-	8/29/63/63	0/2/2/2
31	CLA	A	829	44	-	5/21/97/115	-
31	CLA	8	309	16	-	6/21/97/115	-
26	BCR	I	801	-	-	6/29/63/63	0/2/2/2
32	CHL	K	201	11	-	9/19/95/117	-
28	LHG	A	811	-	-	19/53/53/53	-
34	LAP	B	851	-	-	16/30/30/30	-
31	CLA	2	308	20	-	3/17/93/115	-
32	CHL	7	318	44	-	23/41/117/117	-
31	CLA	A	824	31,1	-	8/36/112/115	-
32	CHL	7	320	44	-	12/35/111/117	-
31	CLA	a	316	13	-	11/15/91/115	-
31	CLA	4	306	21	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	820	2	-	11/39/115/115	-
31	CLA	6	310	23	-	4/18/94/115	-
32	CHL	9	322	44	-	4/19/95/117	-
31	CLA	B	842	2	-	10/35/111/115	-
36	LUT	b	301	-	-	14/29/67/67	0/2/2/2
31	CLA	4	307	21	-	10/29/105/115	-
31	CLA	A	818	1	-	10/39/115/115	-
31	CLA	6	307	23	-	7/21/97/115	-
31	CLA	B	825	2	-	8/33/109/115	-
28	LHG	6	305	31	-	8/36/36/53	-
26	BCR	L	303	-	-	7/29/63/63	0/2/2/2
28	LHG	7	302	-	-	32/53/53/53	-
31	CLA	9	315	17	-	9/26/102/115	-
31	CLA	8	312	44	-	4/21/97/115	-
31	CLA	3	319	14	-	7/35/111/115	-
26	BCR	7	304	-	-	7/29/63/63	0/2/2/2
31	CLA	6	311	23	-	12/27/103/115	-
31	CLA	B	846	44	-	10/39/115/115	-
31	CLA	A	842	1	-	5/39/115/115	-
36	LUT	8	302	-	-	16/29/67/67	0/2/2/2
31	CLA	5	318	22	-	11/39/115/115	-
31	CLA	A	841	1	-	13/39/115/115	-
31	CLA	B	835	2	-	8/30/106/115	-
32	CHL	A	839	44	-	6/29/105/117	-

All (5939) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	310	CLA	MG-NA	30.68	2.79	2.06
31	b	307	CLA	MG-NA	29.70	2.76	2.06
31	6	315	CLA	MG-NA	29.56	2.76	2.06
31	5	318	CLA	MG-ND	-28.84	1.48	2.05
31	9	319	CLA	MG-NA	28.29	2.73	2.06
31	4	311	CLA	MG-ND	-26.69	1.52	2.05
31	5	318	CLA	MG-NB	26.39	2.58	2.05
31	2	311	CLA	MG-NA	25.66	2.67	2.06
31	4	311	CLA	MG-NA	23.77	2.62	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	320	CLA	MG-NC	23.37	2.61	2.06
31	6	314	CLA	MG-NA	22.99	2.60	2.06
31	4	311	CLA	MG-NB	22.51	2.50	2.05
31	2	305	CLA	MG-NA	22.11	2.58	2.06
31	5	315	CLA	MG-ND	-21.91	1.62	2.05
32	6	319	CHL	MG-NA	21.90	2.58	2.06
31	4	315	CLA	MG-ND	-21.88	1.62	2.05
31	9	311	CLA	MG-ND	-21.75	1.62	2.05
31	b	312	CLA	MG-NB	-21.61	1.62	2.05
31	6	316	CLA	MG-NA	21.34	2.57	2.06
31	9	311	CLA	MG-NB	21.04	2.47	2.05
31	2	310	CLA	MG-ND	20.99	2.47	2.05
31	2	314	CLA	MG-ND	-20.98	1.64	2.05
31	L	307	CLA	MG-NA	20.83	2.55	2.06
31	4	319	CLA	MG-NA	20.75	2.55	2.06
31	5	320	CLA	MG-NB	20.51	2.46	2.05
31	a	309	CLA	MG-ND	-20.29	1.65	2.05
31	2	310	CLA	MG-NB	-19.60	1.66	2.05
31	6	307	CLA	MG-NA	19.39	2.52	2.06
31	H	902	CLA	MG-NA	19.39	2.52	2.06
31	a	309	CLA	MG-NA	19.29	2.52	2.06
32	4	313	CHL	MG-NC	19.09	2.51	2.06
31	b	312	CLA	MG-ND	19.04	2.43	2.05
31	6	311	CLA	MG-NA	18.85	2.51	2.06
31	7	315	CLA	MG-NA	18.75	2.50	2.06
31	5	307	CLA	MG-ND	-18.32	1.69	2.05
31	4	315	CLA	MG-NB	18.11	2.41	2.05
31	a	314	CLA	MG-NC	17.92	2.48	2.06
32	6	321	CHL	MG-NA	17.65	2.48	2.06
31	5	315	CLA	MG-NB	17.64	2.40	2.05
31	6	310	CLA	MG-ND	17.47	2.40	2.05
31	B	834	CLA	MG-NA	17.28	2.47	2.06
36	9	305	LUT	C24-C25	17.28	1.54	1.33
31	3	320	CLA	MG-NA	17.26	2.47	2.06
31	9	313	CLA	MG-NA	17.23	2.47	2.06
31	9	318	CLA	MG-NA	17.18	2.47	2.06
31	b	303	CLA	MG-NB	-17.13	1.71	2.05
31	a	309	CLA	MG-NB	17.07	2.39	2.05
36	8	303	LUT	C24-C25	16.98	1.54	1.33
36	a	305	LUT	C24-C25	16.97	1.54	1.33
36	6	303	LUT	C24-C25	16.93	1.54	1.33
36	a	303	LUT	C24-C25	16.91	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	3	305	LUT	C24-C25	16.86	1.54	1.33
36	4	302	LUT	C24-C25	16.85	1.54	1.33
31	b	306	CLA	MG-NB	-16.81	1.72	2.05
31	5	321	CLA	MG-NC	16.81	2.46	2.06
36	J	103	LUT	C24-C25	16.80	1.54	1.33
32	6	319	CHL	MG-NC	-16.72	1.66	2.06
31	5	320	CLA	MG-ND	-16.69	1.72	2.05
36	5	303	LUT	C24-C25	16.66	1.53	1.33
36	b	301	LUT	C24-C25	16.66	1.53	1.33
36	7	305	LUT	C24-C25	16.63	1.53	1.33
31	8	313	CLA	MG-NA	16.63	2.45	2.06
36	F	304	LUT	C24-C25	16.63	1.53	1.33
31	3	308	CLA	MG-NA	16.62	2.45	2.06
31	b	306	CLA	MG-NA	16.60	2.45	2.06
31	9	311	CLA	MG-NA	16.60	2.45	2.06
36	9	302	LUT	C24-C25	16.59	1.53	1.33
36	8	302	LUT	C24-C25	16.59	1.53	1.33
36	4	303	LUT	C24-C25	16.56	1.53	1.33
36	L	304	LUT	C24-C25	16.55	1.53	1.33
31	a	312	CLA	MG-NA	16.54	2.45	2.06
36	5	304	LUT	C24-C25	16.50	1.53	1.33
31	5	323	CLA	MG-NA	16.41	2.45	2.06
36	9	303	LUT	C24-C25	16.38	1.53	1.33
31	A	852	CLA	MG-NC	16.38	2.45	2.06
36	3	304	LUT	C24-C25	16.37	1.53	1.33
31	4	314	CLA	MG-ND	-16.37	1.73	2.05
36	6	304	LUT	C24-C25	16.36	1.53	1.33
31	2	314	CLA	MG-NB	16.36	2.38	2.05
31	3	318	CLA	MG-NA	16.31	2.45	2.06
31	B	835	CLA	MG-NA	16.24	2.44	2.06
36	2	301	LUT	C24-C25	16.23	1.53	1.33
31	6	310	CLA	MG-NB	-16.22	1.73	2.05
32	5	319	CHL	MG-NC	16.19	2.44	2.06
31	6	312	CLA	MG-NA	16.11	2.44	2.06
31	K	204	CLA	MG-NC	15.99	2.44	2.06
31	7	316	CLA	MG-NA	15.73	2.43	2.06
31	b	304	CLA	MG-NB	-15.72	1.74	2.05
31	7	321	CLA	MG-NA	15.62	2.43	2.06
31	3	317	CLA	MG-NC	15.61	2.43	2.06
31	b	311	CLA	MG-NB	-15.60	1.74	2.05
31	9	313	CLA	MG-NB	-15.48	1.75	2.05
31	6	316	CLA	MG-ND	15.45	2.36	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	309	CLA	MG-NA	15.24	2.42	2.06
31	2	312	CLA	MG-NA	15.07	2.42	2.06
31	a	322	CLA	MG-NA	15.01	2.41	2.06
31	3	314	CLA	MG-NA	14.95	2.41	2.06
31	A	844	CLA	MG-NC	14.93	2.41	2.06
31	b	306	CLA	MG-ND	14.92	2.35	2.05
31	2	315	CLA	MG-NC	14.78	2.41	2.06
31	K	205	CLA	MG-NA	14.71	2.41	2.06
31	A	843	CLA	MG-NA	14.68	2.41	2.06
31	B	816	CLA	MG-NC	14.66	2.41	2.06
31	2	306	CLA	MG-ND	-14.56	1.76	2.05
31	4	320	CLA	MG-NC	14.55	2.40	2.06
31	6	311	CLA	MG-NB	-14.51	1.77	2.05
31	9	314	CLA	MG-ND	-14.48	1.77	2.05
31	4	306	CLA	MG-NA	14.47	2.40	2.06
31	3	312	CLA	MG-NA	14.44	2.40	2.06
31	3	311	CLA	MG-NA	14.42	2.40	2.06
31	3	313	CLA	MG-NA	14.27	2.40	2.06
31	a	310	CLA	MG-NA	14.22	2.40	2.06
31	6	315	CLA	MG-NB	14.10	2.33	2.05
31	A	824	CLA	MG-NA	14.09	2.39	2.06
36	4	303	LUT	C30-C29	14.08	1.54	1.35
36	b	301	LUT	C14-C13	14.01	1.54	1.35
36	a	305	LUT	C30-C29	13.99	1.54	1.35
31	4	318	CLA	MG-NB	-13.97	1.78	2.05
31	7	310	CLA	MG-NA	13.91	2.39	2.06
31	B	849	CLA	MG-NC	13.91	2.39	2.06
36	5	304	LUT	C14-C13	13.88	1.54	1.35
36	b	301	LUT	C30-C29	13.88	1.54	1.35
36	2	301	LUT	C30-C29	13.86	1.54	1.35
31	K	206	CLA	MG-NA	13.86	2.39	2.06
31	a	316	CLA	MG-NA	13.85	2.39	2.06
36	6	304	LUT	C30-C29	13.84	1.54	1.35
31	A	827	CLA	MG-NA	13.83	2.39	2.06
36	9	305	LUT	C30-C29	13.83	1.54	1.35
36	6	304	LUT	C14-C13	13.81	1.54	1.35
31	5	310	CLA	MG-NA	13.80	2.39	2.06
31	9	314	CLA	MG-NA	13.79	2.39	2.06
31	2	304	CLA	MG-NA	13.76	2.39	2.06
31	8	309	CLA	MG-NA	13.76	2.38	2.06
36	3	305	LUT	C30-C29	13.75	1.54	1.35
36	9	303	LUT	C14-C13	13.74	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	9	303	LUT	C30-C29	13.72	1.54	1.35
31	b	307	CLA	MG-NC	-13.69	1.73	2.06
31	a	321	CLA	MG-NA	13.68	2.38	2.06
36	4	302	LUT	C10-C9	13.68	1.53	1.35
36	9	305	LUT	C34-C33	13.65	1.53	1.35
36	4	303	LUT	C14-C13	13.64	1.53	1.35
32	7	320	CHL	MG-NB	-13.64	1.78	2.05
31	9	316	CLA	MG-NC	13.63	2.38	2.06
36	4	303	LUT	C10-C9	13.63	1.53	1.35
31	5	313	CLA	MG-NC	13.61	2.38	2.06
31	b	304	CLA	MG-ND	13.61	2.32	2.05
36	4	302	LUT	C30-C29	13.61	1.53	1.35
36	J	103	LUT	C30-C29	13.61	1.53	1.35
31	b	313	CLA	MG-NC	13.61	2.38	2.06
36	6	304	LUT	C10-C9	13.60	1.53	1.35
36	6	303	LUT	C30-C29	13.60	1.53	1.35
36	8	303	LUT	C14-C13	13.60	1.53	1.35
36	a	305	LUT	C10-C9	13.59	1.53	1.35
36	b	301	LUT	C34-C33	13.59	1.53	1.35
36	J	103	LUT	C10-C9	13.59	1.53	1.35
36	9	303	LUT	C10-C9	13.58	1.53	1.35
36	L	304	LUT	C30-C29	13.57	1.53	1.35
36	J	103	LUT	C14-C13	13.55	1.53	1.35
36	6	303	LUT	C14-C13	13.55	1.53	1.35
36	3	304	LUT	C10-C9	13.54	1.53	1.35
36	8	303	LUT	C10-C9	13.54	1.53	1.35
36	5	303	LUT	C14-C13	13.54	1.53	1.35
31	A	821	CLA	MG-NA	13.53	2.38	2.06
36	5	304	LUT	C10-C9	13.51	1.53	1.35
36	L	304	LUT	C10-C9	13.51	1.53	1.35
31	3	307	CLA	MG-ND	-13.50	1.79	2.05
36	a	303	LUT	C10-C9	13.49	1.53	1.35
36	a	305	LUT	C34-C33	13.49	1.53	1.35
31	A	820	CLA	MG-NC	13.48	2.38	2.06
36	9	305	LUT	C10-C9	13.48	1.53	1.35
36	a	305	LUT	C14-C13	13.46	1.53	1.35
31	9	313	CLA	MG-ND	13.45	2.32	2.05
36	5	303	LUT	C10-C9	13.45	1.53	1.35
36	5	304	LUT	C30-C29	13.45	1.53	1.35
31	A	842	CLA	MG-NA	13.43	2.38	2.06
36	8	303	LUT	C30-C29	13.42	1.53	1.35
32	6	320	CHL	MG-NA	13.42	2.38	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	303	LUT	C30-C29	13.39	1.53	1.35
36	a	303	LUT	C14-C13	13.39	1.53	1.35
36	b	301	LUT	C10-C9	13.37	1.53	1.35
31	4	321	CLA	MG-NB	-13.37	1.79	2.05
31	4	314	CLA	MG-NB	13.36	2.32	2.05
36	L	304	LUT	C14-C13	13.36	1.53	1.35
36	7	305	LUT	C30-C29	13.34	1.53	1.35
36	4	303	LUT	C34-C33	13.34	1.53	1.35
31	2	313	CLA	MG-NC	13.33	2.37	2.06
36	4	302	LUT	C14-C13	13.33	1.53	1.35
36	J	103	LUT	C34-C33	13.31	1.53	1.35
36	L	304	LUT	C34-C33	13.31	1.53	1.35
36	3	304	LUT	C5-C6	13.28	1.57	1.34
36	9	302	LUT	C34-C33	13.28	1.53	1.35
36	3	304	LUT	C14-C13	13.26	1.53	1.35
31	B	824	CLA	MG-NA	13.26	2.37	2.06
36	7	305	LUT	C5-C6	13.25	1.57	1.34
36	6	303	LUT	C10-C9	13.25	1.53	1.35
36	3	304	LUT	C30-C29	13.25	1.53	1.35
31	2	308	CLA	MG-NC	13.24	2.37	2.06
36	2	301	LUT	C14-C13	13.24	1.53	1.35
36	8	302	LUT	C14-C13	13.24	1.53	1.35
36	9	302	LUT	C30-C29	13.20	1.53	1.35
36	5	303	LUT	C30-C29	13.20	1.53	1.35
36	9	302	LUT	C10-C9	13.18	1.53	1.35
36	9	305	LUT	C14-C13	13.18	1.53	1.35
32	6	318	CHL	MG-NA	13.18	2.37	2.06
36	6	304	LUT	C34-C33	13.17	1.53	1.35
36	8	302	LUT	C34-C33	13.16	1.53	1.35
36	3	305	LUT	C14-C13	13.14	1.53	1.35
36	3	305	LUT	C10-C9	13.13	1.53	1.35
36	7	305	LUT	C10-C9	13.13	1.53	1.35
36	2	301	LUT	C10-C9	13.13	1.53	1.35
36	4	302	LUT	C34-C33	13.12	1.53	1.35
31	B	820	CLA	MG-NA	13.12	2.37	2.06
31	8	307	CLA	MG-NA	13.10	2.37	2.06
36	8	302	LUT	C10-C9	13.07	1.53	1.35
36	F	304	LUT	C30-C29	13.06	1.53	1.35
36	a	303	LUT	C34-C33	13.02	1.53	1.35
36	7	305	LUT	C14-C13	13.02	1.53	1.35
36	8	302	LUT	C30-C29	13.00	1.53	1.35
36	6	303	LUT	C34-C33	12.97	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	304	LUT	C10-C9	12.93	1.52	1.35
31	2	314	CLA	MG-NA	12.93	2.37	2.06
36	2	301	LUT	C34-C33	12.92	1.52	1.35
32	6	318	CHL	MG-ND	-12.91	1.80	2.05
31	4	316	CLA	MG-NC	12.91	2.36	2.06
31	b	313	CLA	MG-ND	-12.87	1.80	2.05
31	B	821	CLA	MG-NA	12.86	2.36	2.06
36	5	304	LUT	C34-C33	12.84	1.52	1.35
36	9	303	LUT	C34-C33	12.82	1.52	1.35
36	5	303	LUT	C34-C33	12.81	1.52	1.35
31	4	315	CLA	MG-NA	12.81	2.36	2.06
36	F	304	LUT	C14-C13	12.80	1.52	1.35
36	F	304	LUT	C34-C33	12.75	1.52	1.35
31	5	314	CLA	MG-NA	12.75	2.36	2.06
31	4	321	CLA	MG-ND	12.69	2.30	2.05
32	5	317	CHL	MG-NC	12.67	2.36	2.06
31	B	837	CLA	MG-NA	12.67	2.36	2.06
31	A	817	CLA	MG-NA	12.67	2.36	2.06
36	a	305	LUT	C5-C6	12.64	1.56	1.34
36	3	305	LUT	C34-C33	12.63	1.52	1.35
36	5	304	LUT	C5-C6	12.62	1.56	1.34
31	6	315	CLA	MG-NC	-12.62	1.76	2.06
31	2	306	CLA	MG-NB	12.61	2.30	2.05
32	5	316	CHL	MG-NB	-12.55	1.80	2.05
31	H	903	CLA	MG-NA	12.52	2.36	2.06
31	6	316	CLA	MG-NB	-12.50	1.81	2.05
31	8	317	CLA	MG-NA	12.47	2.35	2.06
31	7	312	CLA	MG-NA	12.46	2.35	2.06
31	6	310	CLA	MG-NC	12.45	2.35	2.06
31	5	307	CLA	MG-NB	12.44	2.30	2.05
36	L	304	LUT	C5-C6	12.43	1.56	1.34
36	J	103	LUT	C5-C6	12.43	1.56	1.34
32	9	322	CHL	MG-NB	-12.41	1.81	2.05
36	5	303	LUT	C5-C6	12.39	1.55	1.34
36	9	302	LUT	C5-C6	12.37	1.55	1.34
36	3	304	LUT	C34-C33	12.37	1.52	1.35
36	a	303	LUT	C5-C6	12.37	1.55	1.34
31	9	317	CLA	MG-NC	12.35	2.35	2.06
36	2	301	LUT	C5-C6	12.34	1.55	1.34
36	9	302	LUT	C14-C13	12.34	1.52	1.35
36	7	305	LUT	C34-C33	12.32	1.52	1.35
36	4	302	LUT	C5-C6	12.31	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	202	CLA	MG-NC	12.30	2.35	2.06
36	8	302	LUT	C5-C6	12.24	1.55	1.34
36	6	304	LUT	C5-C6	12.24	1.55	1.34
31	A	830	CLA	MG-NA	12.18	2.35	2.06
31	B	814	CLA	MG-NB	12.12	2.29	2.05
32	4	310	CHL	MG-NB	-12.08	1.81	2.05
31	A	815	CLA	MG-NC	12.07	2.34	2.06
31	8	320	CLA	MG-NA	12.04	2.34	2.06
36	b	301	LUT	C5-C6	12.04	1.55	1.34
36	8	303	LUT	C34-C33	12.04	1.51	1.35
31	A	814	CLA	MG-NA	12.02	2.34	2.06
31	B	830	CLA	MG-NA	12.00	2.34	2.06
36	9	305	LUT	C5-C6	11.98	1.55	1.34
31	A	849	CLA	MG-NA	11.98	2.34	2.06
32	6	317	CHL	MG-NC	11.97	2.34	2.06
31	A	828	CLA	MG-NC	11.87	2.34	2.06
31	b	305	CLA	MG-NA	11.87	2.34	2.06
31	9	315	CLA	MG-NA	11.85	2.34	2.06
32	5	322	CHL	MG-ND	-11.83	1.82	2.05
31	B	841	CLA	MG-NA	11.83	2.34	2.06
32	6	318	CHL	MG-NB	11.80	2.29	2.05
31	G	204	CLA	MG-NC	11.78	2.34	2.06
31	B	814	CLA	MG-NA	11.76	2.34	2.06
31	5	308	CLA	MG-ND	-11.76	1.82	2.05
31	F	306	CLA	MG-NA	11.76	2.34	2.06
31	A	854	CLA	MG-NA	11.70	2.34	2.06
32	a	318	CHL	MG-ND	11.69	2.29	2.05
36	F	304	LUT	C5-C6	11.67	1.54	1.34
31	5	313	CLA	MG-NA	11.67	2.34	2.06
31	5	309	CLA	MG-NB	-11.65	1.82	2.05
31	a	319	CLA	MG-NA	11.65	2.33	2.06
31	5	318	CLA	MG-NC	11.64	2.33	2.06
36	4	303	LUT	C5-C6	11.64	1.54	1.34
31	5	315	CLA	MG-NA	11.60	2.33	2.06
31	b	312	CLA	MG-NA	11.58	2.33	2.06
31	B	820	CLA	MG-NB	11.55	2.28	2.05
31	5	308	CLA	MG-NB	11.47	2.28	2.05
36	6	303	LUT	C5-C6	11.43	1.54	1.34
31	A	841	CLA	MG-NA	11.39	2.33	2.06
36	8	303	LUT	C5-C6	11.38	1.54	1.34
31	7	314	CLA	MG-NC	11.38	2.33	2.06
31	B	819	CLA	MG-NC	11.36	2.33	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	307	CLA	MG-NA	11.36	2.33	2.06
31	7	311	CLA	MG-NA	11.32	2.33	2.06
36	9	303	LUT	C5-C6	11.30	1.54	1.34
31	B	842	CLA	MG-NC	11.29	2.33	2.06
31	b	303	CLA	MG-ND	11.28	2.28	2.05
31	8	311	CLA	MG-NC	11.27	2.33	2.06
31	8	315	CLA	MG-NA	11.26	2.33	2.06
31	A	826	CLA	MG-NC	11.26	2.33	2.06
31	a	313	CLA	MG-NC	11.26	2.33	2.06
31	8	321	CLA	MG-NA	11.22	2.32	2.06
31	7	322	CLA	MG-NC	11.21	2.32	2.06
31	b	308	CLA	MG-ND	11.19	2.28	2.05
31	3	310	CLA	MG-NB	11.17	2.27	2.05
31	6	322	CLA	MG-NA	11.13	2.32	2.06
31	6	306	CLA	MG-NC	11.11	2.32	2.06
31	8	308	CLA	MG-NA	11.08	2.32	2.06
32	7	318	CHL	MG-NA	11.07	2.32	2.06
31	B	836	CLA	MG-NA	11.06	2.32	2.06
31	B	847	CLA	MG-NC	11.03	2.32	2.06
32	4	313	CHL	MG-NA	-11.02	1.80	2.06
31	6	313	CLA	MG-NC	11.01	2.32	2.06
31	3	307	CLA	MG-NA	11.01	2.32	2.06
31	b	311	CLA	MG-ND	11.00	2.27	2.05
31	7	315	CLA	MG-ND	-11.00	1.84	2.05
36	3	305	LUT	C5-C6	11.00	1.53	1.34
31	G	206	CLA	MG-ND	-10.96	1.84	2.05
31	3	310	CLA	MG-ND	-10.91	1.84	2.05
31	6	311	CLA	MG-ND	10.86	2.27	2.05
32	8	319	CHL	MG-NC	10.86	2.32	2.06
31	4	305	CLA	C1D-ND	10.86	1.51	1.37
32	a	318	CHL	MG-NB	-10.83	1.84	2.05
31	J	105	CLA	MG-NC	10.82	2.32	2.06
31	A	850	CLA	MG-NA	10.82	2.32	2.06
31	B	846	CLA	MG-NA	10.80	2.31	2.06
31	b	302	CLA	MG-NC	10.77	2.31	2.06
31	b	307	CLA	MG-NB	10.76	2.27	2.05
31	B	843	CLA	MG-NC	10.76	2.31	2.06
31	8	312	CLA	MG-NA	10.75	2.31	2.06
31	A	825	CLA	MG-NA	10.73	2.31	2.06
31	B	838	CLA	MG-NC	10.73	2.31	2.06
31	B	822	CLA	MG-NA	10.73	2.31	2.06
31	6	315	CLA	MG-ND	-10.72	1.84	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	314	CLA	MG-NA	10.63	2.31	2.06
32	7	320	CHL	MG-NA	10.61	2.31	2.06
31	A	846	CLA	MG-NC	10.60	2.31	2.06
31	G	206	CLA	MG-NA	10.60	2.31	2.06
31	a	311	CLA	MG-NA	10.58	2.31	2.06
31	A	849	CLA	MG-ND	-10.56	1.84	2.05
31	2	310	CLA	MG-NC	-10.52	1.81	2.06
31	A	848	CLA	MG-NA	10.51	2.31	2.06
31	9	314	CLA	MG-NB	10.48	2.26	2.05
31	G	205	CLA	MG-NA	10.48	2.31	2.06
32	6	321	CHL	MG-NC	-10.44	1.81	2.06
31	b	313	CLA	MG-NB	10.43	2.26	2.05
32	9	322	CHL	MG-NA	10.31	2.30	2.06
31	4	318	CLA	MG-ND	10.29	2.26	2.05
32	3	315	CHL	MG-NA	10.26	2.30	2.06
32	9	322	CHL	MG-ND	10.25	2.26	2.05
31	b	310	CLA	MG-NC	10.22	2.30	2.06
31	B	826	CLA	MG-NA	10.20	2.30	2.06
31	A	833	CLA	MG-NB	10.19	2.26	2.05
31	A	853	CLA	MG-NC	10.15	2.30	2.06
31	b	303	CLA	MG-NA	10.14	2.30	2.06
31	2	311	CLA	MG-NB	10.13	2.25	2.05
31	B	845	CLA	MG-NA	10.10	2.30	2.06
31	A	835	CLA	MG-NC	10.08	2.30	2.06
31	A	855	CLA	MG-NC	10.04	2.30	2.06
31	B	850	CLA	MG-NC	10.02	2.30	2.06
31	9	317	CLA	MG-NA	10.00	2.30	2.06
31	A	816	CLA	MG-NC	10.00	2.30	2.06
31	B	825	CLA	MG-NA	10.00	2.30	2.06
31	5	309	CLA	MG-ND	9.96	2.25	2.05
31	B	823	CLA	MG-NC	9.96	2.29	2.06
31	B	844	CLA	MG-NC	9.96	2.29	2.06
31	9	312	CLA	MG-NA	9.95	2.29	2.06
32	7	320	CHL	MG-ND	9.91	2.25	2.05
31	A	833	CLA	MG-NA	9.91	2.29	2.06
31	A	838	CLA	MG-NA	9.89	2.29	2.06
31	A	855	CLA	MG-NA	9.84	2.29	2.06
31	F	301	CLA	MG-NC	9.83	2.29	2.06
31	B	813	CLA	MG-NA	9.83	2.29	2.06
31	a	314	CLA	MG-NB	-9.81	1.86	2.05
31	3	319	CLA	MG-NC	9.81	2.29	2.06
31	9	319	CLA	MG-ND	9.80	2.25	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	308	CLA	MG-NC	9.79	2.29	2.06
31	a	314	CLA	MG-ND	9.78	2.25	2.05
31	A	823	CLA	MG-NA	9.78	2.29	2.06
32	5	316	CHL	MG-ND	9.78	2.25	2.05
31	A	851	CLA	MG-NC	9.77	2.29	2.06
31	B	827	CLA	MG-NA	9.76	2.29	2.06
32	6	309	CHL	MG-NA	9.76	2.29	2.06
31	2	306	CLA	MG-NA	9.74	2.29	2.06
31	4	314	CLA	MG-NC	9.72	2.29	2.06
31	O	203	CLA	MG-NC	9.68	2.29	2.06
31	3	307	CLA	MG-NB	9.66	2.24	2.05
31	3	319	CLA	MG-ND	9.64	2.24	2.05
31	B	839	CLA	MG-NA	9.62	2.29	2.06
31	4	312	CLA	MG-NA	9.59	2.29	2.06
31	7	315	CLA	MG-NB	9.59	2.24	2.05
31	6	307	CLA	MG-NB	-9.58	1.86	2.05
31	a	315	CLA	MG-NA	9.58	2.29	2.06
31	b	308	CLA	MG-NA	9.55	2.28	2.06
31	2	311	CLA	MG-NC	-9.52	1.83	2.06
31	A	847	CLA	MG-NC	9.51	2.28	2.06
31	A	833	CLA	MG-ND	-9.50	1.87	2.05
31	A	851	CLA	MG-NA	9.46	2.28	2.06
31	A	845	CLA	MG-NA	9.37	2.28	2.06
31	A	853	CLA	MG-ND	9.36	2.24	2.05
31	A	829	CLA	C1D-ND	9.35	1.49	1.37
31	K	206	CLA	MG-NB	-9.34	1.87	2.05
31	5	308	CLA	MG-NC	9.32	2.28	2.06
31	B	811	CLA	MG-NA	9.25	2.28	2.06
31	b	312	CLA	MG-NC	9.24	2.28	2.06
31	A	823	CLA	MG-NB	9.21	2.24	2.05
31	G	206	CLA	MG-NB	9.20	2.24	2.05
31	B	832	CLA	MG-NA	9.16	2.28	2.06
31	A	847	CLA	MG-NA	9.15	2.28	2.06
31	4	321	CLA	MG-NC	9.15	2.28	2.06
32	5	317	CHL	MG-NA	-9.15	1.84	2.06
31	A	836	CLA	MG-NA	9.02	2.27	2.06
31	a	312	CLA	MG-ND	-9.01	1.87	2.05
31	2	307	CLA	MG-ND	-9.00	1.87	2.05
31	3	318	CLA	MG-NB	9.00	2.23	2.05
31	5	307	CLA	MG-NA	8.98	2.27	2.06
31	9	319	CLA	MG-NC	-8.98	1.84	2.06
31	B	814	CLA	MG-ND	-8.96	1.88	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	819	CLA	MG-NA	8.91	2.27	2.06
31	5	312	CLA	MG-NC	8.89	2.27	2.06
31	2	312	CLA	MG-NB	-8.88	1.88	2.05
31	O	204	CLA	MG-NC	8.88	2.27	2.06
31	B	816	CLA	MG-NB	8.87	2.23	2.05
31	6	310	CLA	MG-NA	8.87	2.27	2.06
31	L	305	CLA	MG-NA	8.86	2.27	2.06
31	A	842	CLA	MG-NB	8.86	2.23	2.05
31	3	309	CLA	MG-NC	8.83	2.27	2.06
32	4	310	CHL	MG-ND	8.83	2.23	2.05
31	B	840	CLA	MG-NC	8.82	2.27	2.06
31	B	813	CLA	MG-ND	8.75	2.23	2.05
31	B	847	CLA	MG-ND	8.74	2.23	2.05
32	7	317	CHL	MG-NB	-8.70	1.88	2.05
31	b	308	CLA	MG-NC	8.69	2.26	2.06
31	B	825	CLA	MG-NC	8.69	2.26	2.06
31	B	848	CLA	MG-NA	8.68	2.26	2.06
31	A	846	CLA	MG-NA	8.65	2.26	2.06
31	7	313	CLA	MG-NA	8.64	2.26	2.06
31	A	834	CLA	MG-NA	8.64	2.26	2.06
31	5	308	CLA	MG-NA	8.64	2.26	2.06
31	A	837	CLA	MG-NC	8.58	2.26	2.06
31	A	823	CLA	MG-NC	8.56	2.26	2.06
31	A	830	CLA	MG-NC	8.51	2.26	2.06
31	6	312	CLA	MG-ND	-8.50	1.88	2.05
31	B	824	CLA	MG-NB	8.50	2.22	2.05
32	6	319	CHL	MG-ND	-8.49	1.89	2.05
31	B	847	CLA	MG-NA	8.47	2.26	2.06
31	3	310	CLA	MG-NC	8.47	2.26	2.06
31	b	308	CLA	MG-NB	-8.47	1.89	2.05
32	5	322	CHL	MG-NB	8.45	2.22	2.05
31	2	313	CLA	MG-NB	-8.44	1.89	2.05
31	8	310	CLA	MG-NA	8.44	2.26	2.06
32	5	319	CHL	MG-NA	-8.42	1.86	2.06
32	b	309	CHL	MG-NC	8.41	2.26	2.06
31	2	311	CLA	MG-ND	-8.38	1.89	2.05
31	B	822	CLA	MG-NC	8.36	2.26	2.06
31	B	813	CLA	MG-NC	8.33	2.26	2.06
31	B	817	CLA	MG-NC	8.29	2.26	2.06
31	4	309	CLA	MG-NA	8.25	2.25	2.06
31	F	305	CLA	MG-NC	8.23	2.25	2.06
31	A	837	CLA	MG-NA	8.20	2.25	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	850	CLA	MG-NA	8.19	2.25	2.06
32	A	840	CHL	MG-NA	8.19	2.25	2.06
31	4	316	CLA	MG-NA	8.17	2.25	2.06
32	A	831	CHL	MG-NC	8.15	2.25	2.06
32	4	317	CHL	MG-NC	8.13	2.25	2.06
31	B	815	CLA	MG-NC	8.12	2.25	2.06
31	6	314	CLA	MG-NC	-8.09	1.87	2.06
32	6	319	CHL	MG-NB	8.08	2.21	2.05
31	A	832	CLA	MG-NA	8.07	2.25	2.06
32	a	317	CHL	MG-NC	8.07	2.25	2.06
31	A	836	CLA	MG-NC	8.06	2.25	2.06
31	2	312	CLA	MG-ND	8.06	2.21	2.05
32	7	319	CHL	MG-ND	8.04	2.21	2.05
31	b	311	CLA	MG-NC	8.02	2.25	2.06
31	B	818	CLA	MG-NC	8.02	2.25	2.06
31	5	311	CLA	MG-NC	8.00	2.25	2.06
31	B	829	CLA	MG-NC	7.98	2.25	2.06
31	B	831	CLA	MG-NC	7.97	2.25	2.06
31	4	318	CLA	MG-NA	7.97	2.25	2.06
31	3	308	CLA	MG-ND	7.95	2.21	2.05
31	8	321	CLA	MG-ND	7.92	2.21	2.05
31	G	204	CLA	MG-NB	7.92	2.21	2.05
31	L	306	CLA	MG-NC	7.91	2.25	2.06
32	A	840	CHL	MG-NB	7.88	2.21	2.05
31	6	307	CLA	MG-ND	7.77	2.21	2.05
32	4	317	CHL	MG-ND	-7.76	1.90	2.05
31	B	840	CLA	MG-NA	7.74	2.24	2.06
32	7	317	CHL	MG-ND	7.71	2.21	2.05
31	B	811	CLA	MG-ND	7.68	2.21	2.05
31	B	829	CLA	MG-NA	7.67	2.24	2.06
31	F	305	CLA	MG-NA	7.67	2.24	2.06
31	L	305	CLA	MG-NC	7.65	2.24	2.06
31	B	837	CLA	MG-NC	7.64	2.24	2.06
31	6	306	CLA	MG-NA	7.64	2.24	2.06
31	b	304	CLA	MG-NC	7.61	2.24	2.06
31	6	312	CLA	MG-NB	7.61	2.20	2.05
31	b	305	CLA	MG-NB	7.61	2.20	2.05
31	A	838	CLA	MG-NC	7.57	2.24	2.06
31	4	319	CLA	MG-NC	-7.56	1.88	2.06
31	8	308	CLA	MG-ND	-7.54	1.90	2.05
31	A	822	CLA	MG-NC	7.50	2.24	2.06
31	5	311	CLA	MG-NA	7.49	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	314	CLA	MG-ND	7.48	2.20	2.05
31	A	851	CLA	MG-ND	7.46	2.20	2.05
31	4	321	CLA	MG-NA	7.45	2.24	2.06
32	6	320	CHL	MG-NC	-7.43	1.88	2.06
31	8	318	CLA	MG-NA	7.42	2.23	2.06
31	A	856	CLA	MG-NC	7.41	2.23	2.06
31	8	310	CLA	MG-ND	-7.41	1.91	2.05
31	B	817	CLA	MG-NB	7.39	2.20	2.05
31	B	828	CLA	MG-NC	7.36	2.23	2.06
31	H	901	CLA	MG-NA	7.35	2.23	2.06
31	3	316	CLA	MG-NA	7.34	2.23	2.06
31	A	829	CLA	MG-NC	7.34	2.23	2.06
31	7	322	CLA	MG-NB	7.33	2.20	2.05
31	7	322	CLA	MG-ND	-7.31	1.91	2.05
31	8	321	CLA	MG-NB	-7.29	1.91	2.05
31	7	313	CLA	MG-NC	7.29	2.23	2.06
31	6	308	CLA	MG-ND	-7.27	1.91	2.05
31	A	849	CLA	MG-NB	7.26	2.20	2.05
32	4	310	CHL	MG-NA	7.24	2.23	2.06
31	B	838	CLA	MG-NA	7.23	2.23	2.06
31	b	304	CLA	MG-NA	7.21	2.23	2.06
31	A	830	CLA	MG-NB	7.16	2.20	2.05
32	8	316	CHL	MG-ND	-7.14	1.91	2.05
31	3	319	CLA	MG-NB	-7.12	1.91	2.05
31	4	307	CLA	MG-NA	7.12	2.23	2.06
31	A	850	CLA	MG-NC	7.12	2.23	2.06
31	B	842	CLA	MG-ND	7.07	2.19	2.05
32	9	320	CHL	MG-NB	-7.06	1.91	2.05
31	8	311	CLA	MG-NB	7.05	2.19	2.05
31	B	820	CLA	MG-NC	7.04	2.23	2.06
31	b	302	CLA	MG-NA	7.03	2.23	2.06
31	K	204	CLA	MG-ND	-7.02	1.91	2.05
30	A	813	CL0	C1D-ND	7.02	1.46	1.37
31	4	308	CLA	MG-NC	7.02	2.22	2.06
31	A	816	CLA	MG-NB	7.00	2.19	2.05
31	G	204	CLA	MG-NA	6.98	2.22	2.06
31	A	815	CLA	MG-NA	6.98	2.22	2.06
31	A	820	CLA	MG-NA	6.97	2.22	2.06
31	4	312	CLA	MG-NC	6.97	2.22	2.06
31	2	309	CLA	MG-NC	6.94	2.22	2.06
31	B	833	CLA	MG-NC	6.90	2.22	2.06
31	B	817	CLA	MG-NA	6.89	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	318	CLA	MG-NC	6.86	2.22	2.06
31	J	105	CLA	MG-NB	-6.85	1.92	2.05
31	A	835	CLA	MG-ND	-6.82	1.92	2.05
31	B	811	CLA	MG-NC	6.81	2.22	2.06
31	4	307	CLA	MG-NC	6.80	2.22	2.06
31	A	857	CLA	MG-NC	6.79	2.22	2.06
31	9	321	CLA	MG-NC	6.73	2.22	2.06
31	4	316	CLA	C1D-ND	6.73	1.46	1.37
31	A	814	CLA	MG-NB	-6.73	1.92	2.05
31	7	309	CLA	MG-NC	6.70	2.22	2.06
31	A	838	CLA	MG-NB	-6.68	1.92	2.05
31	5	313	CLA	C4D-ND	6.68	1.46	1.37
31	A	814	CLA	MG-ND	6.64	2.19	2.05
31	A	833	CLA	MG-NC	6.64	2.22	2.06
31	A	855	CLA	MG-ND	6.63	2.18	2.05
32	7	319	CHL	MG-NC	6.63	2.22	2.06
31	b	307	CLA	MG-ND	-6.62	1.92	2.05
31	B	842	CLA	MG-NB	-6.62	1.92	2.05
32	9	320	CHL	MG-NC	6.61	2.22	2.06
31	4	309	CLA	MG-NC	6.60	2.21	2.06
31	5	314	CLA	MG-NB	-6.60	1.92	2.05
31	B	831	CLA	MG-NA	6.59	2.21	2.06
31	B	824	CLA	MG-NC	6.57	2.21	2.06
31	4	308	CLA	MG-NA	6.56	2.21	2.06
31	B	823	CLA	MG-NA	6.53	2.21	2.06
31	A	822	CLA	MG-ND	-6.53	1.92	2.05
31	4	314	CLA	MG-NA	6.53	2.21	2.06
31	9	312	CLA	MG-NC	6.52	2.21	2.06
31	A	834	CLA	MG-NB	-6.52	1.92	2.05
31	5	312	CLA	MG-NB	-6.51	1.92	2.05
31	3	318	CLA	MG-ND	-6.50	1.92	2.05
31	6	306	CLA	C4D-ND	6.49	1.46	1.37
31	3	308	CLA	MG-NB	-6.49	1.92	2.05
31	9	317	CLA	C4D-ND	6.42	1.46	1.37
31	J	105	CLA	MG-ND	6.40	2.18	2.05
32	A	839	CHL	MG-ND	6.37	2.18	2.05
31	A	818	CLA	MG-NA	6.36	2.21	2.06
31	4	307	CLA	MG-ND	-6.34	1.93	2.05
32	6	320	CHL	MG-ND	-6.34	1.93	2.05
31	B	815	CLA	MG-NA	6.31	2.21	2.06
31	a	313	CLA	MG-NB	6.29	2.18	2.05
31	B	826	CLA	MG-NC	6.29	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	303	CLA	MG-NC	6.23	2.21	2.06
31	a	312	CLA	MG-NB	6.20	2.18	2.05
31	B	819	CLA	MG-NA	6.16	2.20	2.06
31	A	832	CLA	MG-NC	6.15	2.20	2.06
31	6	313	CLA	MG-NA	6.15	2.20	2.06
31	H	901	CLA	MG-NC	6.14	2.20	2.06
31	b	311	CLA	MG-NA	6.13	2.20	2.06
32	6	317	CHL	MG-NA	-6.13	1.91	2.06
31	3	316	CLA	MG-NC	6.11	2.20	2.06
31	5	320	CLA	MG-NA	-6.10	1.91	2.06
31	B	839	CLA	MG-NB	6.09	2.17	2.05
31	O	202	CLA	C3C-C2C	6.08	1.48	1.36
31	A	848	CLA	MG-NB	-6.07	1.93	2.05
32	a	320	CHL	MG-NB	-6.06	1.93	2.05
31	A	857	CLA	MG-NA	6.05	2.20	2.06
31	4	320	CLA	MG-ND	-6.03	1.93	2.05
32	7	319	CHL	MG-NB	-6.02	1.93	2.05
31	A	845	CLA	MG-NC	6.02	2.20	2.06
31	7	313	CLA	MG-ND	-6.02	1.93	2.05
31	a	316	CLA	MG-ND	6.01	2.17	2.05
32	9	320	CHL	MG-ND	5.97	2.17	2.05
31	A	818	CLA	MG-NC	5.95	2.20	2.06
31	H	902	CLA	MG-NC	-5.90	1.92	2.06
31	3	311	CLA	MG-ND	-5.88	1.94	2.05
31	7	314	CLA	C3C-C2C	5.88	1.48	1.36
31	B	836	CLA	MG-NC	5.87	2.20	2.06
31	A	848	CLA	MG-ND	5.86	2.17	2.05
31	A	847	CLA	MG-NB	5.85	2.17	2.05
31	7	310	CLA	C3C-C2C	5.84	1.48	1.36
31	A	843	CLA	MG-ND	5.84	2.17	2.05
32	A	831	CHL	MG-ND	5.84	2.17	2.05
31	9	321	CLA	MG-NA	5.83	2.20	2.06
31	B	845	CLA	MG-NC	5.82	2.20	2.06
31	B	830	CLA	MG-NC	5.80	2.20	2.06
32	8	316	CHL	MG-NA	5.79	2.20	2.06
31	A	856	CLA	MG-NA	5.79	2.20	2.06
31	K	204	CLA	MG-NB	5.78	2.17	2.05
31	B	812	CLA	MG-NC	5.78	2.20	2.06
31	4	319	CLA	MG-NB	-5.78	1.94	2.05
31	6	322	CLA	MG-NC	5.77	2.20	2.06
31	8	311	CLA	MG-NA	5.73	2.19	2.06
31	6	308	CLA	MG-NB	5.73	2.17	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	313	CLA	MG-ND	5.71	2.17	2.05
31	B	828	CLA	MG-NA	5.67	2.19	2.06
31	b	311	CLA	C3C-C2C	5.65	1.48	1.36
31	A	820	CLA	MG-NB	5.63	2.16	2.05
31	4	319	CLA	C3C-C2C	5.62	1.48	1.36
31	B	816	CLA	MG-ND	-5.61	1.94	2.05
31	4	320	CLA	C3C-C2C	5.60	1.48	1.36
31	B	832	CLA	MG-NC	5.60	2.19	2.06
31	O	203	CLA	MG-NA	5.60	2.19	2.06
31	8	310	CLA	MG-NB	5.60	2.16	2.05
31	O	204	CLA	MG-NA	5.59	2.19	2.06
31	6	308	CLA	MG-NA	5.58	2.19	2.06
31	5	318	CLA	C3C-C2C	5.58	1.48	1.36
31	b	306	CLA	C3C-C2C	5.58	1.48	1.36
31	B	844	CLA	MG-NA	5.57	2.19	2.06
31	4	311	CLA	MG-NC	-5.56	1.93	2.06
31	9	317	CLA	C3C-C2C	5.56	1.48	1.36
31	3	310	CLA	C3C-C2C	5.56	1.48	1.36
31	2	313	CLA	C3C-C2C	5.55	1.48	1.36
31	5	313	CLA	C3C-C2C	5.55	1.48	1.36
31	9	321	CLA	MG-NB	-5.54	1.94	2.05
31	2	304	CLA	MG-NB	-5.54	1.94	2.05
31	b	313	CLA	C3C-C2C	5.52	1.48	1.36
31	7	313	CLA	MG-NB	5.52	2.16	2.05
31	a	311	CLA	MG-ND	-5.51	1.94	2.05
31	6	306	CLA	C3C-C2C	5.51	1.48	1.36
31	B	812	CLA	MG-NB	-5.50	1.94	2.05
31	O	203	CLA	MG-NB	-5.50	1.94	2.05
31	2	305	CLA	MG-NB	5.50	2.16	2.05
32	8	316	CHL	MG-NB	5.50	2.16	2.05
31	A	825	CLA	MG-NB	5.50	2.16	2.05
31	H	901	CLA	C3C-C2C	5.50	1.48	1.36
31	A	823	CLA	C3C-C2C	5.49	1.48	1.36
31	2	310	CLA	C3C-C2C	5.49	1.48	1.36
31	A	835	CLA	MG-NB	5.49	2.16	2.05
31	8	309	CLA	MG-NC	5.48	2.19	2.06
31	A	843	CLA	MG-NC	5.48	2.19	2.06
31	3	320	CLA	C3C-C2C	5.48	1.48	1.36
31	8	315	CLA	MG-NB	5.47	2.16	2.05
31	4	312	CLA	C3C-C2C	5.47	1.48	1.36
31	B	821	CLA	C3C-C2C	5.47	1.48	1.36
31	O	203	CLA	C3C-C2C	5.47	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	314	CLA	C3C-C2C	5.47	1.48	1.36
31	4	316	CLA	C3C-C2C	5.46	1.48	1.36
31	a	314	CLA	C3C-C2C	5.45	1.48	1.36
32	6	318	CHL	MG-NC	-5.45	1.93	2.06
31	4	314	CLA	C3C-C2C	5.45	1.48	1.36
32	8	319	CHL	MG-NA	-5.45	1.93	2.06
31	B	822	CLA	C3C-C2C	5.44	1.48	1.36
31	H	903	CLA	C3C-C2C	5.44	1.48	1.36
31	L	305	CLA	C3C-C2C	5.44	1.48	1.36
31	O	204	CLA	C3C-C2C	5.44	1.48	1.36
31	2	312	CLA	C3C-C2C	5.44	1.48	1.36
31	4	311	CLA	C3C-C2C	5.44	1.48	1.36
31	5	314	CLA	C3C-C2C	5.44	1.48	1.36
31	B	812	CLA	MG-NA	5.43	2.19	2.06
31	A	848	CLA	C3C-C2C	5.43	1.48	1.36
31	A	851	CLA	C3C-C2C	5.43	1.48	1.36
31	a	319	CLA	C3C-C2C	5.42	1.48	1.36
31	5	320	CLA	C3C-C2C	5.42	1.48	1.36
31	b	307	CLA	C3C-C2C	5.42	1.48	1.36
31	A	852	CLA	MG-NB	5.42	2.16	2.05
31	9	316	CLA	C3C-C2C	5.42	1.48	1.36
31	6	308	CLA	C3C-C2C	5.41	1.48	1.36
31	5	321	CLA	C3C-C2C	5.41	1.48	1.36
31	b	308	CLA	C3C-C2C	5.41	1.48	1.36
31	9	312	CLA	C3C-C2C	5.41	1.48	1.36
31	2	308	CLA	C3C-C2C	5.40	1.48	1.36
31	A	849	CLA	C3C-C2C	5.40	1.48	1.36
31	6	314	CLA	C3C-C2C	5.40	1.48	1.36
31	8	313	CLA	MG-NB	-5.40	1.95	2.05
31	7	322	CLA	C3C-C2C	5.40	1.48	1.36
31	9	318	CLA	C3C-C2C	5.40	1.48	1.36
31	2	309	CLA	C3C-C2C	5.40	1.48	1.36
31	K	205	CLA	C3C-C2C	5.40	1.48	1.36
31	2	311	CLA	C3C-C2C	5.39	1.48	1.36
31	K	206	CLA	C3C-C2C	5.39	1.48	1.36
31	8	312	CLA	C3C-C2C	5.39	1.48	1.36
31	a	322	CLA	C3C-C2C	5.38	1.48	1.36
31	9	313	CLA	C3C-C2C	5.38	1.48	1.36
31	2	305	CLA	C3C-C2C	5.38	1.48	1.36
31	3	316	CLA	C3C-C2C	5.38	1.48	1.36
31	5	308	CLA	C3C-C2C	5.37	1.48	1.36
31	b	310	CLA	C3C-C2C	5.37	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	316	CLA	C3C-C2C	5.37	1.48	1.36
31	L	307	CLA	C3C-C2C	5.37	1.48	1.36
31	A	822	CLA	MG-NB	5.37	2.16	2.05
31	A	822	CLA	MG-NA	5.36	2.19	2.06
31	3	317	CLA	C3C-C2C	5.36	1.48	1.36
31	3	313	CLA	C3C-C2C	5.36	1.48	1.36
31	A	853	CLA	MG-NA	5.36	2.19	2.06
31	b	303	CLA	CHD-C1D	5.36	1.48	1.38
31	A	828	CLA	C3C-C2C	5.35	1.48	1.36
31	a	315	CLA	C3C-C2C	5.35	1.48	1.36
31	b	304	CLA	C3C-C2C	5.35	1.48	1.36
31	B	823	CLA	C3C-C2C	5.35	1.48	1.36
31	5	315	CLA	C3C-C2C	5.35	1.48	1.36
31	8	315	CLA	C3C-C2C	5.35	1.48	1.36
31	b	303	CLA	C3C-C2C	5.35	1.48	1.36
31	5	312	CLA	C3C-C2C	5.35	1.48	1.36
31	B	831	CLA	C3C-C2C	5.34	1.48	1.36
31	4	321	CLA	C3C-C2C	5.34	1.48	1.36
31	3	309	CLA	C3C-C2C	5.34	1.48	1.36
31	H	902	CLA	C3C-C2C	5.34	1.48	1.36
31	4	309	CLA	MG-NB	5.33	2.16	2.05
31	a	321	CLA	C3C-C2C	5.33	1.48	1.36
31	b	312	CLA	C3C-C2C	5.33	1.48	1.36
31	G	205	CLA	C3C-C2C	5.33	1.48	1.36
31	4	321	CLA	O2D-CGD	5.33	1.46	1.33
31	b	305	CLA	C3C-C2C	5.33	1.48	1.36
31	b	312	CLA	CHD-C1D	5.33	1.48	1.38
31	4	306	CLA	C3C-C2C	5.33	1.48	1.36
31	4	307	CLA	C3C-C2C	5.32	1.48	1.36
31	2	314	CLA	C3C-C2C	5.32	1.48	1.36
31	A	826	CLA	C3C-C2C	5.32	1.48	1.36
31	6	322	CLA	C3C-C2C	5.32	1.48	1.36
31	5	307	CLA	C3C-C2C	5.32	1.48	1.36
31	3	320	CLA	O2D-CGD	5.32	1.46	1.33
31	2	306	CLA	C3C-C2C	5.32	1.48	1.36
31	b	305	CLA	O2D-CGD	5.32	1.46	1.33
31	A	836	CLA	C3C-C2C	5.31	1.48	1.36
31	3	308	CLA	C3C-C2C	5.31	1.48	1.36
31	O	204	CLA	O2D-CGD	5.31	1.46	1.33
31	6	311	CLA	C3C-C2C	5.31	1.48	1.36
31	2	312	CLA	O2D-CGD	5.31	1.46	1.33
31	8	314	CLA	MG-NB	-5.31	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	H	901	CLA	CHD-C1D	5.30	1.48	1.38
31	7	316	CLA	C3C-C2C	5.30	1.48	1.36
31	L	307	CLA	CHD-C1D	5.30	1.48	1.38
31	5	310	CLA	MG-NB	-5.30	1.95	2.05
31	b	306	CLA	O2D-CGD	5.30	1.46	1.33
31	7	311	CLA	C3C-C2C	5.30	1.48	1.36
31	A	835	CLA	C3C-C2C	5.30	1.48	1.36
31	2	305	CLA	O2D-CGD	5.29	1.46	1.33
31	H	902	CLA	MG-ND	-5.29	1.95	2.05
31	G	204	CLA	C3C-C2C	5.29	1.48	1.36
31	b	302	CLA	C3C-C2C	5.29	1.48	1.36
31	A	834	CLA	C3C-C2C	5.29	1.48	1.36
31	A	814	CLA	C3C-C2C	5.29	1.48	1.36
31	a	313	CLA	C3C-C2C	5.29	1.48	1.36
31	B	835	CLA	C3C-C2C	5.29	1.48	1.36
31	5	323	CLA	C3C-C2C	5.29	1.48	1.36
31	A	819	CLA	MG-NC	5.29	2.18	2.06
31	3	318	CLA	C3C-C2C	5.28	1.48	1.36
31	6	312	CLA	C3C-C2C	5.28	1.48	1.36
31	5	308	CLA	O2D-CGD	5.28	1.46	1.33
31	B	849	CLA	MG-NB	5.28	2.16	2.05
31	6	322	CLA	MG-NB	-5.28	1.95	2.05
31	A	852	CLA	C3C-C2C	5.28	1.47	1.36
31	6	313	CLA	C3C-C2C	5.28	1.47	1.36
31	6	313	CLA	O2D-CGD	5.28	1.46	1.33
31	3	314	CLA	C3C-C2C	5.28	1.47	1.36
31	3	312	CLA	C3C-C2C	5.27	1.47	1.36
31	B	842	CLA	C3C-C2C	5.27	1.47	1.36
31	5	309	CLA	C3C-C2C	5.27	1.47	1.36
31	3	312	CLA	CHD-C1D	5.27	1.48	1.38
31	6	310	CLA	C3C-C2C	5.27	1.47	1.36
31	b	307	CLA	CHD-C1D	5.27	1.48	1.38
31	9	321	CLA	C3C-C2C	5.26	1.47	1.36
31	B	819	CLA	C3C-C2C	5.26	1.47	1.36
31	B	814	CLA	C3C-C2C	5.26	1.47	1.36
31	a	310	CLA	C3C-C2C	5.26	1.47	1.36
31	9	314	CLA	C3C-C2C	5.26	1.47	1.36
31	2	306	CLA	CHD-C1D	5.26	1.48	1.38
31	5	309	CLA	CHD-C1D	5.25	1.48	1.38
31	B	837	CLA	C3C-C2C	5.25	1.47	1.36
31	b	312	CLA	O2D-CGD	5.25	1.46	1.33
31	2	313	CLA	CHD-C1D	5.25	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	H	901	CLA	O2D-CGD	5.25	1.46	1.33
31	a	309	CLA	C3C-C2C	5.25	1.47	1.36
31	4	307	CLA	MG-NB	5.25	2.16	2.05
31	9	319	CLA	C3C-C2C	5.25	1.47	1.36
31	6	316	CLA	MG-NC	-5.25	1.93	2.06
31	7	315	CLA	C3C-C2C	5.25	1.47	1.36
31	4	307	CLA	CHD-C1D	5.25	1.48	1.38
31	A	842	CLA	C3C-C2C	5.25	1.47	1.36
31	a	311	CLA	C3C-C2C	5.24	1.47	1.36
31	B	840	CLA	C3C-C2C	5.24	1.47	1.36
31	9	319	CLA	O2D-CGD	5.24	1.46	1.33
31	A	819	CLA	C3C-C2C	5.24	1.47	1.36
31	2	308	CLA	O2D-CGD	5.24	1.46	1.33
31	5	318	CLA	CHD-C1D	5.24	1.48	1.38
31	2	304	CLA	C3C-C2C	5.24	1.47	1.36
31	O	204	CLA	CHD-C1D	5.24	1.48	1.38
31	B	826	CLA	C3C-C2C	5.24	1.47	1.36
31	9	311	CLA	C3C-C2C	5.24	1.47	1.36
31	O	204	CLA	MG-NB	-5.24	1.95	2.05
31	A	856	CLA	C3C-C2C	5.23	1.47	1.36
31	B	829	CLA	C3C-C2C	5.23	1.47	1.36
31	B	828	CLA	C3C-C2C	5.23	1.47	1.36
31	L	306	CLA	C3C-C2C	5.23	1.47	1.36
31	B	824	CLA	C3C-C2C	5.23	1.47	1.36
31	G	206	CLA	C3C-C2C	5.23	1.47	1.36
31	4	318	CLA	O2D-CGD	5.23	1.46	1.33
31	6	307	CLA	CHD-C1D	5.23	1.48	1.38
31	b	308	CLA	CHD-C1D	5.23	1.48	1.38
31	8	309	CLA	C3C-C2C	5.23	1.47	1.36
31	O	202	CLA	CHD-C1D	5.23	1.48	1.38
31	A	825	CLA	C3C-C2C	5.23	1.47	1.36
31	B	843	CLA	C3C-C2C	5.22	1.47	1.36
31	8	320	CLA	CHD-C1D	5.22	1.48	1.38
31	8	313	CLA	C3C-C2C	5.22	1.47	1.36
31	B	833	CLA	C3C-C2C	5.22	1.47	1.36
31	4	308	CLA	C3C-C2C	5.22	1.47	1.36
31	K	204	CLA	C3C-C2C	5.22	1.47	1.36
31	3	311	CLA	C3C-C2C	5.21	1.47	1.36
31	4	320	CLA	O2D-CGD	5.21	1.45	1.33
31	L	307	CLA	O2D-CGD	5.21	1.45	1.33
31	A	843	CLA	C3C-C2C	5.21	1.47	1.36
31	A	855	CLA	C3C-C2C	5.21	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	311	CLA	CHD-C1D	5.21	1.48	1.38
31	a	322	CLA	CHD-C1D	5.21	1.48	1.38
31	B	846	CLA	C3C-C2C	5.21	1.47	1.36
31	6	307	CLA	C3C-C2C	5.21	1.47	1.36
31	A	853	CLA	O2D-CGD	5.21	1.45	1.33
31	9	321	CLA	CHD-C1D	5.21	1.48	1.38
31	A	833	CLA	C3C-C2C	5.21	1.47	1.36
31	B	830	CLA	C3C-C2C	5.20	1.47	1.36
31	5	308	CLA	CHD-C1D	5.20	1.48	1.38
31	5	323	CLA	O2D-CGD	5.20	1.45	1.33
31	A	827	CLA	C3C-C2C	5.20	1.47	1.36
31	8	314	CLA	O2D-CGD	5.20	1.45	1.33
31	4	315	CLA	C3C-C2C	5.20	1.47	1.36
31	b	308	CLA	O2D-CGD	5.20	1.45	1.33
31	A	844	CLA	C3C-C2C	5.20	1.47	1.36
31	6	311	CLA	CHD-C1D	5.20	1.48	1.38
31	2	307	CLA	O2D-CGD	5.19	1.45	1.33
31	A	846	CLA	C3C-C2C	5.19	1.47	1.36
31	B	818	CLA	MG-NA	5.19	2.18	2.06
31	a	316	CLA	C3C-C2C	5.19	1.47	1.36
31	6	315	CLA	C3C-C2C	5.19	1.47	1.36
31	3	313	CLA	CHD-C1D	5.19	1.48	1.38
31	J	105	CLA	C3C-C2C	5.18	1.47	1.36
31	A	821	CLA	C3C-C2C	5.18	1.47	1.36
31	8	320	CLA	C3C-C2C	5.18	1.47	1.36
31	b	310	CLA	O2D-CGD	5.18	1.45	1.33
31	A	841	CLA	MG-NC	5.18	2.18	2.06
31	B	815	CLA	O2D-CGD	5.18	1.45	1.33
31	b	303	CLA	O2D-CGD	5.18	1.45	1.33
31	B	836	CLA	C3C-C2C	5.18	1.47	1.36
31	2	307	CLA	C3C-C2C	5.18	1.47	1.36
31	4	314	CLA	CHD-C1D	5.18	1.48	1.38
31	A	835	CLA	MG-NA	5.18	2.18	2.06
31	B	839	CLA	C3C-C2C	5.17	1.47	1.36
31	5	314	CLA	O2D-CGD	5.17	1.45	1.33
31	7	313	CLA	C3C-C2C	5.17	1.47	1.36
31	A	832	CLA	C3C-C2C	5.17	1.47	1.36
31	4	319	CLA	O2D-CGD	5.17	1.45	1.33
31	A	847	CLA	C3C-C2C	5.17	1.47	1.36
31	B	820	CLA	C3C-C2C	5.17	1.47	1.36
31	6	307	CLA	O2D-CGD	5.17	1.45	1.33
31	5	312	CLA	CHD-C1D	5.17	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	203	CLA	O2D-CGD	5.16	1.45	1.33
31	5	315	CLA	CHD-C1D	5.16	1.48	1.38
31	6	316	CLA	O2D-CGD	5.16	1.45	1.33
31	7	321	CLA	C3C-C2C	5.16	1.47	1.36
31	A	841	CLA	C3C-C2C	5.16	1.47	1.36
31	5	311	CLA	C3C-C2C	5.16	1.47	1.36
31	L	306	CLA	O2D-CGD	5.16	1.45	1.33
31	8	312	CLA	MG-NB	-5.16	1.95	2.05
31	8	307	CLA	C3C-C2C	5.16	1.47	1.36
31	6	311	CLA	O2D-CGD	5.16	1.45	1.33
31	F	305	CLA	C3C-C2C	5.15	1.47	1.36
31	A	844	CLA	MG-NB	5.15	2.16	2.05
31	F	306	CLA	C3C-C2C	5.15	1.47	1.36
31	4	309	CLA	O2D-CGD	5.15	1.45	1.33
31	8	321	CLA	C3C-C2C	5.15	1.47	1.36
31	8	318	CLA	C3C-C2C	5.15	1.47	1.36
31	6	314	CLA	O2D-CGD	5.15	1.45	1.33
31	K	205	CLA	CHD-C1D	5.15	1.48	1.38
31	b	313	CLA	O2D-CGD	5.15	1.45	1.33
31	2	309	CLA	MG-NA	5.14	2.18	2.06
31	B	844	CLA	C3C-C2C	5.14	1.47	1.36
31	2	311	CLA	CHD-C1D	5.14	1.48	1.38
31	5	321	CLA	CHD-C1D	5.14	1.48	1.38
32	5	322	CHL	MG-NA	5.14	2.18	2.06
31	4	308	CLA	O2D-CGD	5.14	1.45	1.33
31	8	315	CLA	CHD-C1D	5.14	1.48	1.38
31	4	312	CLA	CHD-C1D	5.14	1.48	1.38
31	4	315	CLA	CHD-C1D	5.14	1.48	1.38
31	6	310	CLA	O2D-CGD	5.14	1.45	1.33
31	b	311	CLA	O2D-CGD	5.13	1.45	1.33
31	A	824	CLA	C3C-C2C	5.13	1.47	1.36
31	A	823	CLA	CHD-C1D	5.13	1.48	1.38
31	B	849	CLA	C3C-C2C	5.13	1.47	1.36
31	H	903	CLA	CHD-C1D	5.13	1.48	1.38
31	2	304	CLA	O2D-CGD	5.13	1.45	1.33
31	3	317	CLA	CHD-C1D	5.13	1.48	1.38
31	b	310	CLA	CHD-C1D	5.13	1.48	1.38
31	A	849	CLA	CHD-C1D	5.13	1.48	1.38
31	8	308	CLA	C3C-C2C	5.13	1.47	1.36
31	B	847	CLA	C3C-C2C	5.12	1.47	1.36
31	K	206	CLA	O2D-CGD	5.12	1.45	1.33
31	G	204	CLA	CHD-C1D	5.12	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	314	CLA	O2D-CGD	5.12	1.45	1.33
31	B	838	CLA	C3C-C2C	5.12	1.47	1.36
31	3	319	CLA	CHC-C1C	5.12	1.48	1.38
31	B	843	CLA	O2D-CGD	5.12	1.45	1.33
31	b	304	CLA	O2D-CGD	5.12	1.45	1.33
31	6	312	CLA	O2D-CGD	5.12	1.45	1.33
31	B	845	CLA	C3C-C2C	5.12	1.47	1.36
31	a	315	CLA	O2D-CGD	5.11	1.45	1.33
31	2	309	CLA	O2D-CGD	5.11	1.45	1.33
31	B	824	CLA	MG-ND	-5.11	1.95	2.05
31	5	321	CLA	O2D-CGD	5.11	1.45	1.33
31	7	310	CLA	O2D-CGD	5.11	1.45	1.33
32	a	317	CHL	MG-NB	-5.11	1.95	2.05
31	2	309	CLA	CHD-C1D	5.11	1.48	1.38
31	4	318	CLA	C3C-C2C	5.11	1.47	1.36
31	6	322	CLA	CHD-C1D	5.11	1.48	1.38
31	4	309	CLA	C3C-C2C	5.11	1.47	1.36
31	4	307	CLA	O2D-CGD	5.11	1.45	1.33
31	5	309	CLA	O2D-CGD	5.11	1.45	1.33
31	4	311	CLA	O2D-CGD	5.10	1.45	1.33
31	5	310	CLA	C3C-C2C	5.10	1.47	1.36
31	A	838	CLA	C3C-C2C	5.10	1.47	1.36
31	2	314	CLA	CHD-C1D	5.10	1.48	1.38
31	K	206	CLA	CHD-C1D	5.10	1.48	1.38
31	A	838	CLA	CHD-C1D	5.10	1.48	1.38
31	B	813	CLA	C3C-C2C	5.10	1.47	1.36
31	A	824	CLA	O2D-CGD	5.10	1.45	1.33
31	b	307	CLA	O2D-CGD	5.10	1.45	1.33
31	7	309	CLA	MG-NA	5.10	2.18	2.06
31	7	309	CLA	C3C-C2C	5.10	1.47	1.36
31	A	837	CLA	O2D-CGD	5.10	1.45	1.33
31	9	315	CLA	C3C-C2C	5.10	1.47	1.36
31	2	314	CLA	O2D-CGD	5.09	1.45	1.33
31	4	315	CLA	O2D-CGD	5.09	1.45	1.33
31	A	854	CLA	O2D-CGD	5.09	1.45	1.33
31	6	322	CLA	O2D-CGD	5.09	1.45	1.33
31	3	318	CLA	CHD-C1D	5.09	1.48	1.38
31	7	314	CLA	CHD-C1D	5.09	1.48	1.38
31	8	310	CLA	CHC-C1C	5.09	1.48	1.38
31	F	305	CLA	O2D-CGD	5.09	1.45	1.33
31	O	203	CLA	CHD-C1D	5.09	1.48	1.38
31	a	321	CLA	CHD-C1D	5.09	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	314	CLA	O2D-CGD	5.09	1.45	1.33
31	2	307	CLA	CHD-C1D	5.09	1.48	1.38
31	3	318	CLA	O2D-CGD	5.08	1.45	1.33
31	4	306	CLA	O2D-CGD	5.08	1.45	1.33
31	B	850	CLA	CHC-C1C	5.08	1.48	1.38
31	4	314	CLA	O2D-CGD	5.08	1.45	1.33
31	A	817	CLA	C3C-C2C	5.08	1.47	1.36
31	5	315	CLA	O2D-CGD	5.08	1.45	1.33
31	a	314	CLA	CHD-C1D	5.08	1.48	1.38
31	a	309	CLA	O2D-CGD	5.08	1.45	1.33
31	3	319	CLA	O2D-CGD	5.08	1.45	1.33
31	B	831	CLA	O2D-CGD	5.08	1.45	1.33
31	A	822	CLA	C3C-C2C	5.08	1.47	1.36
31	9	314	CLA	O2D-CGD	5.08	1.45	1.33
31	6	322	CLA	MG-ND	5.08	2.15	2.05
31	8	310	CLA	MG-NC	5.08	2.18	2.06
31	b	306	CLA	CHD-C1D	5.07	1.48	1.38
31	2	310	CLA	CHD-C1D	5.07	1.48	1.38
31	2	305	CLA	MG-NC	-5.07	1.94	2.06
31	a	310	CLA	O2D-CGD	5.07	1.45	1.33
31	b	311	CLA	CHD-C1D	5.07	1.48	1.38
31	7	322	CLA	O2D-CGD	5.07	1.45	1.33
31	A	845	CLA	C3C-C2C	5.07	1.47	1.36
31	8	312	CLA	O2D-CGD	5.07	1.45	1.33
31	A	820	CLA	C3C-C2C	5.07	1.47	1.36
31	7	312	CLA	C3C-C2C	5.07	1.47	1.36
31	3	307	CLA	C3C-C2C	5.07	1.47	1.36
31	6	315	CLA	O2D-CGD	5.07	1.45	1.33
31	8	315	CLA	O2D-CGD	5.07	1.45	1.33
31	a	319	CLA	CHD-C1D	5.07	1.48	1.38
31	G	205	CLA	O2D-CGD	5.07	1.45	1.33
31	4	311	CLA	CHD-C1D	5.06	1.48	1.38
31	9	315	CLA	MG-NC	5.06	2.18	2.06
31	B	838	CLA	CHD-C1D	5.06	1.48	1.38
31	a	311	CLA	MG-NC	5.06	2.18	2.06
31	2	315	CLA	C3C-C2C	5.06	1.47	1.36
31	9	319	CLA	CHD-C1D	5.06	1.48	1.38
31	7	316	CLA	CHD-C1D	5.06	1.48	1.38
31	3	313	CLA	O2D-CGD	5.06	1.45	1.33
31	B	843	CLA	CHD-C1D	5.06	1.48	1.38
31	5	311	CLA	O2D-CGD	5.06	1.45	1.33
31	3	320	CLA	CHD-C1D	5.06	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	815	CLA	C3C-C2C	5.06	1.47	1.36
31	2	312	CLA	CHD-C1D	5.06	1.48	1.38
31	8	311	CLA	C3C-C2C	5.05	1.47	1.36
31	F	301	CLA	MG-NA	5.05	2.18	2.06
31	5	318	CLA	O2D-CGD	5.05	1.45	1.33
31	L	306	CLA	CHD-C1D	5.05	1.48	1.38
31	B	817	CLA	C3C-C2C	5.05	1.47	1.36
31	9	311	CLA	CHD-C1D	5.05	1.48	1.38
31	J	105	CLA	O2D-CGD	5.05	1.45	1.33
31	9	311	CLA	O2D-CGD	5.05	1.45	1.33
31	6	312	CLA	CHD-C1D	5.05	1.48	1.38
31	A	826	CLA	MG-NA	5.05	2.18	2.06
31	9	317	CLA	O2D-CGD	5.05	1.45	1.33
31	a	316	CLA	CHD-C1D	5.05	1.48	1.38
31	b	302	CLA	CHD-C1D	5.04	1.48	1.38
31	6	314	CLA	CHD-C1D	5.04	1.48	1.38
31	5	320	CLA	CHC-C1C	5.04	1.48	1.38
31	b	304	CLA	CHC-C1C	5.04	1.48	1.38
31	9	312	CLA	O2D-CGD	5.04	1.45	1.33
31	B	815	CLA	C3C-C2C	5.04	1.47	1.36
31	B	850	CLA	O2D-CGD	5.04	1.45	1.33
31	B	816	CLA	C3C-C2C	5.04	1.47	1.36
31	3	317	CLA	O2D-CGD	5.04	1.45	1.33
31	A	849	CLA	O2D-CGD	5.04	1.45	1.33
31	A	837	CLA	C3C-C2C	5.04	1.47	1.36
31	5	312	CLA	O2D-CGD	5.04	1.45	1.33
31	5	313	CLA	O2D-CGD	5.04	1.45	1.33
31	7	315	CLA	O2D-CGD	5.03	1.45	1.33
31	2	305	CLA	CHD-C1D	5.03	1.48	1.38
31	4	312	CLA	O2D-CGD	5.03	1.45	1.33
31	A	836	CLA	CHD-C1D	5.03	1.48	1.38
31	3	307	CLA	O2D-CGD	5.03	1.45	1.33
31	K	205	CLA	O2D-CGD	5.03	1.45	1.33
31	3	309	CLA	O2D-CGD	5.03	1.45	1.33
31	b	302	CLA	O2D-CGD	5.03	1.45	1.33
31	2	313	CLA	O2D-CGD	5.03	1.45	1.33
31	7	309	CLA	O2D-CGD	5.03	1.45	1.33
32	A	839	CHL	MG-NC	5.02	2.18	2.06
31	5	320	CLA	O2D-CGD	5.02	1.45	1.33
31	4	319	CLA	CHD-C1D	5.02	1.48	1.38
31	a	312	CLA	O2D-CGD	5.02	1.45	1.33
31	8	311	CLA	CHD-C1D	5.02	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	320	CLA	CHD-C1D	5.02	1.48	1.38
31	6	313	CLA	CHD-C1D	5.02	1.48	1.38
31	3	316	CLA	CHD-C1D	5.02	1.48	1.38
31	3	311	CLA	MG-NB	5.02	2.15	2.05
31	4	318	CLA	CHD-C1D	5.02	1.48	1.38
31	B	830	CLA	O2D-CGD	5.02	1.45	1.33
31	B	850	CLA	C3C-C2C	5.01	1.47	1.36
31	A	820	CLA	O2D-CGD	5.01	1.45	1.33
31	3	314	CLA	CHD-C1D	5.01	1.48	1.38
31	8	312	CLA	CHD-C1D	5.01	1.48	1.38
31	6	306	CLA	CHC-C1C	5.01	1.48	1.38
31	2	315	CLA	O2D-CGD	5.01	1.45	1.33
31	5	314	CLA	CHD-C1D	5.01	1.48	1.38
31	A	857	CLA	O2D-CGD	5.01	1.45	1.33
31	B	834	CLA	C3C-C2C	5.01	1.47	1.36
31	3	308	CLA	CHD-C1D	5.01	1.48	1.38
31	9	318	CLA	O2D-CGD	5.01	1.45	1.33
31	A	832	CLA	CHD-C1D	5.01	1.48	1.38
31	8	309	CLA	O2D-CGD	5.01	1.45	1.33
31	G	205	CLA	CHD-C1D	5.01	1.48	1.38
31	F	301	CLA	O2D-CGD	5.00	1.45	1.33
31	B	811	CLA	C3C-C2C	5.00	1.47	1.36
31	7	312	CLA	CHC-C1C	5.00	1.48	1.38
31	9	316	CLA	O2D-CGD	5.00	1.45	1.33
31	B	821	CLA	CHD-C1D	5.00	1.48	1.38
31	5	307	CLA	O2D-CGD	5.00	1.45	1.33
31	5	320	CLA	CHD-C1D	5.00	1.48	1.38
31	8	313	CLA	O2D-CGD	5.00	1.45	1.33
31	b	313	CLA	CHC-C1C	5.00	1.48	1.38
31	a	322	CLA	O2D-CGD	5.00	1.45	1.33
31	B	828	CLA	O2D-CGD	5.00	1.45	1.33
31	7	312	CLA	O2D-CGD	5.00	1.45	1.33
31	9	313	CLA	O2D-CGD	5.00	1.45	1.33
31	9	313	CLA	CHD-C1D	5.00	1.48	1.38
31	B	838	CLA	O2D-CGD	5.00	1.45	1.33
31	B	848	CLA	C3C-C2C	5.00	1.47	1.36
31	4	306	CLA	CHD-C1D	5.00	1.48	1.38
31	A	843	CLA	CHD-C1D	4.99	1.48	1.38
31	6	310	CLA	CHD-C1D	4.99	1.48	1.38
31	8	310	CLA	O2D-CGD	4.99	1.45	1.33
31	b	305	CLA	CHD-C1D	4.99	1.48	1.38
31	O	203	CLA	CHC-C1C	4.99	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	828	CLA	O2D-CGD	4.99	1.45	1.33
31	A	850	CLA	C3C-C2C	4.99	1.47	1.36
31	3	308	CLA	O2D-CGD	4.99	1.45	1.33
31	2	306	CLA	O2D-CGD	4.98	1.45	1.33
31	5	311	CLA	CHD-C1D	4.98	1.48	1.38
31	A	835	CLA	O2D-CGD	4.98	1.45	1.33
31	F	305	CLA	CHD-C1D	4.98	1.48	1.38
31	A	853	CLA	C3C-C2C	4.98	1.47	1.36
31	A	856	CLA	MG-NB	-4.98	1.95	2.05
31	7	311	CLA	CHD-C1D	4.98	1.48	1.38
31	K	204	CLA	O2D-CGD	4.98	1.45	1.33
31	5	310	CLA	O2D-CGD	4.98	1.45	1.33
31	b	311	CLA	CHC-C1C	4.98	1.48	1.38
31	8	308	CLA	O2D-CGD	4.97	1.45	1.33
31	F	306	CLA	O2D-CGD	4.97	1.45	1.33
31	B	830	CLA	CHD-C1D	4.97	1.48	1.38
31	a	319	CLA	O2D-CGD	4.97	1.45	1.33
31	a	321	CLA	O2D-CGD	4.97	1.45	1.33
31	6	308	CLA	O2D-CGD	4.97	1.45	1.33
31	A	837	CLA	CHD-C1D	4.97	1.48	1.38
31	a	313	CLA	CHD-C1D	4.97	1.48	1.38
31	a	315	CLA	CHD-C1D	4.97	1.48	1.38
31	8	311	CLA	O2D-CGD	4.97	1.45	1.33
31	8	321	CLA	O2D-CGD	4.97	1.45	1.33
31	O	204	CLA	CHC-C1C	4.97	1.48	1.38
31	2	304	CLA	CHC-C1C	4.97	1.48	1.38
31	A	834	CLA	CHD-C1D	4.97	1.48	1.38
31	H	902	CLA	O2D-CGD	4.97	1.45	1.33
31	2	311	CLA	O2D-CGD	4.97	1.45	1.33
31	B	835	CLA	O2D-CGD	4.97	1.45	1.33
31	5	310	CLA	CHD-C1D	4.97	1.48	1.38
31	A	851	CLA	CHD-C1D	4.97	1.48	1.38
31	H	903	CLA	O2D-CGD	4.96	1.45	1.33
31	3	314	CLA	O2D-CGD	4.96	1.45	1.33
31	2	308	CLA	CHC-C1C	4.96	1.48	1.38
31	B	824	CLA	CHD-C1D	4.96	1.48	1.38
31	b	310	CLA	CHC-C1C	4.96	1.48	1.38
31	B	847	CLA	O2D-CGD	4.96	1.45	1.33
31	A	824	CLA	CHD-C1D	4.96	1.48	1.38
31	B	832	CLA	C3C-C2C	4.96	1.47	1.36
31	F	301	CLA	C3C-C2C	4.96	1.47	1.36
31	8	318	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	848	CLA	O2D-CGD	4.96	1.45	1.33
31	6	312	CLA	CHC-C1C	4.96	1.48	1.38
31	3	311	CLA	CHD-C1D	4.96	1.48	1.38
31	2	311	CLA	CHC-C1C	4.96	1.48	1.38
31	B	825	CLA	O2D-CGD	4.96	1.45	1.33
31	2	304	CLA	CHD-C1D	4.96	1.48	1.38
32	4	317	CHL	O2D-CGD	4.96	1.45	1.33
31	3	307	CLA	CHC-C1C	4.96	1.48	1.38
31	4	316	CLA	O2D-CGD	4.96	1.45	1.33
31	B	822	CLA	CHD-C1D	4.96	1.48	1.38
31	A	818	CLA	CHC-C1C	4.96	1.48	1.38
31	4	305	CLA	O2D-CGD	4.95	1.45	1.33
31	3	311	CLA	O2D-CGD	4.95	1.45	1.33
31	7	322	CLA	CHD-C1D	4.95	1.48	1.38
31	a	316	CLA	O2D-CGD	4.95	1.45	1.33
31	2	310	CLA	O2D-CGD	4.95	1.45	1.33
31	7	309	CLA	CHC-C1C	4.95	1.48	1.38
31	7	309	CLA	CHD-C1D	4.95	1.48	1.38
31	6	315	CLA	CHD-C1D	4.95	1.48	1.38
31	7	316	CLA	CHC-C1C	4.95	1.48	1.38
31	2	312	CLA	CHC-C1C	4.95	1.48	1.38
31	H	902	CLA	CHD-C1D	4.94	1.48	1.38
32	7	324	CHL	MG-NC	4.94	2.18	2.06
31	A	829	CLA	O2D-CGD	4.94	1.45	1.33
31	A	834	CLA	O2D-CGD	4.94	1.45	1.33
31	A	847	CLA	CHD-C1D	4.94	1.48	1.38
31	A	823	CLA	O2D-CGD	4.94	1.45	1.33
31	A	832	CLA	O2D-CGD	4.94	1.45	1.33
31	9	321	CLA	O2D-CGD	4.94	1.45	1.33
31	B	842	CLA	O2D-CGD	4.94	1.45	1.33
31	a	311	CLA	O2D-CGD	4.94	1.45	1.33
31	B	846	CLA	O2D-CGD	4.94	1.45	1.33
31	b	308	CLA	CHC-C1C	4.94	1.48	1.38
31	3	316	CLA	O2D-CGD	4.94	1.45	1.33
31	A	848	CLA	CHD-C1D	4.94	1.48	1.38
31	B	841	CLA	C3C-C2C	4.94	1.47	1.36
31	2	309	CLA	CHC-C1C	4.94	1.48	1.38
31	4	321	CLA	CHD-C1D	4.93	1.48	1.38
31	8	320	CLA	O2D-CGD	4.93	1.45	1.33
31	A	828	CLA	CHD-C1D	4.93	1.48	1.38
31	B	816	CLA	O2D-CGD	4.93	1.45	1.33
31	9	318	CLA	CHD-C1D	4.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	315	CLA	CHC-C1C	4.93	1.48	1.38
31	9	318	CLA	CHC-C1C	4.93	1.48	1.38
32	5	322	CHL	O2D-CGD	4.93	1.45	1.33
31	8	317	CLA	C3C-C2C	4.93	1.47	1.36
31	B	826	CLA	O2D-CGD	4.92	1.45	1.33
31	a	309	CLA	CHC-C1C	4.92	1.48	1.38
31	B	836	CLA	O2D-CGD	4.92	1.45	1.33
31	B	824	CLA	O2D-CGD	4.92	1.45	1.33
31	4	319	CLA	CHC-C1C	4.92	1.48	1.38
31	B	823	CLA	O2D-CGD	4.92	1.45	1.33
31	7	311	CLA	O2D-CGD	4.92	1.45	1.33
31	A	851	CLA	O2D-CGD	4.92	1.45	1.33
31	3	308	CLA	CHC-C1C	4.92	1.48	1.38
31	L	305	CLA	O2D-CGD	4.92	1.45	1.33
31	7	315	CLA	CHD-C1D	4.92	1.47	1.38
31	A	815	CLA	O2D-CGD	4.92	1.45	1.33
31	4	314	CLA	CHC-C1C	4.92	1.48	1.38
31	8	317	CLA	O2D-CGD	4.92	1.45	1.33
31	5	312	CLA	CHC-C1C	4.92	1.48	1.38
31	A	852	CLA	CHD-C1D	4.92	1.47	1.38
31	b	313	CLA	CHD-C1D	4.92	1.47	1.38
32	8	319	CHL	O2D-CGD	4.92	1.45	1.33
31	3	312	CLA	O2D-CGD	4.91	1.45	1.33
32	6	321	CHL	O2D-CGD	4.91	1.45	1.33
31	A	835	CLA	CHD-C1D	4.91	1.47	1.38
31	b	304	CLA	CHD-C1D	4.91	1.47	1.38
31	4	311	CLA	CHC-C1C	4.91	1.48	1.38
31	A	823	CLA	CHC-C1C	4.91	1.48	1.38
31	a	313	CLA	O2D-CGD	4.91	1.45	1.33
31	B	845	CLA	O2D-CGD	4.91	1.45	1.33
31	B	839	CLA	O2D-CGD	4.91	1.45	1.33
31	7	312	CLA	CHD-C1D	4.90	1.47	1.38
31	8	313	CLA	CHD-C1D	4.90	1.47	1.38
31	3	313	CLA	CHC-C1C	4.90	1.48	1.38
32	4	313	CHL	O2D-CGD	4.90	1.45	1.33
31	6	308	CLA	CHC-C1C	4.90	1.48	1.38
31	A	825	CLA	CHC-C1C	4.90	1.48	1.38
31	B	848	CLA	CHC-C1C	4.90	1.48	1.38
31	a	312	CLA	C3C-C2C	4.90	1.47	1.36
31	A	817	CLA	CHC-C1C	4.90	1.48	1.38
31	b	306	CLA	CHC-C1C	4.90	1.48	1.38
31	9	315	CLA	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	854	CLA	C3C-C2C	4.90	1.47	1.36
31	B	829	CLA	O2D-CGD	4.90	1.45	1.33
31	A	830	CLA	CHD-C1D	4.90	1.47	1.38
31	B	844	CLA	O2D-CGD	4.90	1.45	1.33
31	G	204	CLA	O2D-CGD	4.90	1.45	1.33
31	a	312	CLA	CHD-C1D	4.90	1.47	1.38
31	A	850	CLA	O2D-CGD	4.89	1.45	1.33
31	B	818	CLA	C3C-C2C	4.89	1.47	1.36
31	A	857	CLA	C3C-C2C	4.89	1.47	1.36
31	A	830	CLA	O2D-CGD	4.89	1.45	1.33
31	A	819	CLA	O2D-CGD	4.89	1.45	1.33
32	a	320	CHL	MG-NC	4.89	2.17	2.06
31	6	308	CLA	CHD-C1D	4.89	1.47	1.38
31	B	825	CLA	CHD-C1D	4.89	1.47	1.38
31	G	205	CLA	CHC-C1C	4.89	1.48	1.38
31	8	312	CLA	MG-NC	4.89	2.17	2.06
32	A	840	CHL	MG-NC	4.89	2.17	2.06
31	3	309	CLA	CHD-C1D	4.89	1.47	1.38
32	b	309	CHL	O2D-CGD	4.89	1.45	1.33
31	B	825	CLA	C3C-C2C	4.88	1.47	1.36
31	3	307	CLA	CHD-C1D	4.88	1.47	1.38
31	4	308	CLA	CHD-C1D	4.88	1.47	1.38
31	B	827	CLA	O2D-CGD	4.88	1.45	1.33
31	8	315	CLA	CHC-C1C	4.88	1.48	1.38
31	B	828	CLA	CHD-C1D	4.88	1.47	1.38
31	L	305	CLA	CHC-C1C	4.88	1.48	1.38
31	5	307	CLA	CHD-C1D	4.88	1.47	1.38
31	9	315	CLA	CHD-C1D	4.88	1.47	1.38
31	B	837	CLA	CHD-C1D	4.88	1.47	1.38
31	7	312	CLA	MG-NB	-4.88	1.96	2.05
31	A	852	CLA	O2D-CGD	4.88	1.45	1.33
31	8	308	CLA	CHD-C1D	4.88	1.47	1.38
31	4	306	CLA	CHC-C1C	4.88	1.48	1.38
31	B	841	CLA	O2D-CGD	4.88	1.45	1.33
31	9	312	CLA	CHD-C1D	4.88	1.47	1.38
31	A	842	CLA	O2D-CGD	4.87	1.45	1.33
31	F	306	CLA	CHD-C1D	4.87	1.47	1.38
32	6	320	CHL	O2D-CGD	4.87	1.45	1.33
31	8	314	CLA	CHD-C1D	4.87	1.47	1.38
31	a	313	CLA	MG-NA	4.87	2.17	2.06
31	A	838	CLA	O2D-CGD	4.87	1.45	1.33
31	B	827	CLA	CHD-C1D	4.87	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	813	CLA	CHC-C1C	4.87	1.48	1.38
31	B	820	CLA	O2D-CGD	4.87	1.45	1.33
31	a	312	CLA	CHC-C1C	4.87	1.48	1.38
31	4	315	CLA	MG-NC	4.87	2.17	2.06
31	A	825	CLA	O2D-CGD	4.87	1.45	1.33
31	A	833	CLA	O2D-CGD	4.87	1.45	1.33
31	B	823	CLA	CHD-C1D	4.87	1.47	1.38
31	A	855	CLA	O2D-CGD	4.87	1.45	1.33
31	8	307	CLA	O2D-CGD	4.87	1.45	1.33
31	A	844	CLA	O2D-CGD	4.87	1.45	1.33
31	A	821	CLA	O2D-CGD	4.86	1.45	1.33
31	B	844	CLA	CHC-C1C	4.86	1.48	1.38
31	5	314	CLA	CHC-C1C	4.86	1.48	1.38
31	B	819	CLA	O2D-CGD	4.86	1.45	1.33
31	9	313	CLA	CHC-C1C	4.86	1.48	1.38
31	B	839	CLA	CHD-C1D	4.86	1.47	1.38
31	5	307	CLA	CHC-C1C	4.86	1.48	1.38
31	A	827	CLA	CHD-C1D	4.86	1.47	1.38
31	6	316	CLA	CHD-C1D	4.86	1.47	1.38
31	B	811	CLA	O2D-CGD	4.86	1.45	1.33
31	8	318	CLA	CHD-C1D	4.86	1.47	1.38
31	B	828	CLA	CHC-C1C	4.86	1.48	1.38
31	6	316	CLA	CHC-C1C	4.85	1.48	1.38
31	6	306	CLA	O2D-CGD	4.85	1.45	1.33
31	A	845	CLA	CHD-C1D	4.85	1.47	1.38
31	A	816	CLA	C3C-C2C	4.85	1.47	1.36
31	a	310	CLA	CHD-C1D	4.85	1.47	1.38
31	A	837	CLA	MG-NB	4.85	2.15	2.05
31	B	848	CLA	O2D-CGD	4.85	1.45	1.33
31	A	826	CLA	CHD-C1D	4.85	1.47	1.38
31	B	813	CLA	O2D-CGD	4.85	1.45	1.33
32	7	317	CHL	O2D-CGD	4.85	1.45	1.33
31	7	316	CLA	O2D-CGD	4.85	1.45	1.33
31	7	321	CLA	O2D-CGD	4.85	1.45	1.33
32	6	317	CHL	O2D-CGD	4.85	1.45	1.33
31	G	206	CLA	CHD-C1D	4.84	1.47	1.38
31	H	901	CLA	CHC-C1C	4.84	1.48	1.38
31	8	307	CLA	CHD-C1D	4.84	1.47	1.38
31	B	833	CLA	O2D-CGD	4.84	1.45	1.33
31	5	315	CLA	CHC-C1C	4.84	1.48	1.38
31	3	320	CLA	CHC-C1C	4.84	1.48	1.38
31	3	310	CLA	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	313	CLA	CHC-C1C	4.84	1.48	1.38
31	B	814	CLA	MG-NC	4.84	2.17	2.06
31	4	312	CLA	CHC-C1C	4.84	1.48	1.38
31	A	853	CLA	CHD-C1D	4.84	1.47	1.38
31	9	314	CLA	CHD-C1D	4.84	1.47	1.38
31	2	310	CLA	CHC-C1C	4.84	1.48	1.38
31	3	310	CLA	CHD-C1D	4.84	1.47	1.38
31	A	829	CLA	C3C-C2C	4.84	1.47	1.36
31	B	829	CLA	CHD-C1D	4.83	1.47	1.38
31	A	830	CLA	C3C-C2C	4.83	1.47	1.36
31	b	307	CLA	CHC-C1C	4.83	1.48	1.38
31	B	849	CLA	MG-NA	4.83	2.17	2.06
31	A	849	CLA	CHC-C1C	4.83	1.48	1.38
31	O	202	CLA	CHC-C1C	4.83	1.48	1.38
31	A	845	CLA	O2D-CGD	4.83	1.45	1.33
31	B	840	CLA	CHC-C1C	4.83	1.48	1.38
31	B	827	CLA	C3C-C2C	4.83	1.47	1.36
31	A	817	CLA	O2D-CGD	4.83	1.45	1.33
31	L	306	CLA	CHC-C1C	4.83	1.48	1.38
31	A	847	CLA	O2D-CGD	4.83	1.45	1.33
31	a	309	CLA	CHD-C1D	4.83	1.47	1.38
31	H	902	CLA	CHC-C1C	4.83	1.48	1.38
31	4	320	CLA	CHC-C1C	4.82	1.48	1.38
31	A	852	CLA	CHC-C1C	4.82	1.48	1.38
31	a	314	CLA	CHC-C1C	4.82	1.48	1.38
31	7	321	CLA	CHD-C1D	4.82	1.47	1.38
31	8	313	CLA	CHC-C1C	4.82	1.48	1.38
31	A	842	CLA	CHC-C1C	4.82	1.48	1.38
31	7	310	CLA	CHD-C1D	4.82	1.47	1.38
31	A	835	CLA	CHC-C1C	4.81	1.48	1.38
32	6	309	CHL	O2D-CGD	4.81	1.44	1.33
31	9	312	CLA	CHC-C1C	4.81	1.48	1.38
31	B	834	CLA	O2D-CGD	4.81	1.44	1.33
31	2	306	CLA	CHC-C1C	4.81	1.48	1.38
32	9	320	CHL	O2D-CGD	4.81	1.44	1.33
31	B	820	CLA	CHC-C1C	4.81	1.48	1.38
31	5	308	CLA	CHC-C1C	4.81	1.48	1.38
31	A	833	CLA	CHD-C1D	4.81	1.47	1.38
31	B	814	CLA	O2D-CGD	4.81	1.44	1.33
31	A	836	CLA	O2D-CGD	4.80	1.44	1.33
31	B	825	CLA	CHC-C1C	4.80	1.48	1.38
31	B	832	CLA	O2D-CGD	4.80	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	322	CLA	CHC-C1C	4.80	1.48	1.38
32	a	317	CHL	O2D-CGD	4.80	1.44	1.33
31	8	308	CLA	CHC-C1C	4.80	1.48	1.38
31	B	817	CLA	O2D-CGD	4.80	1.44	1.33
32	5	319	CHL	O2D-CGD	4.80	1.44	1.33
31	8	312	CLA	CHC-C1C	4.80	1.48	1.38
31	6	315	CLA	CHC-C1C	4.80	1.48	1.38
31	6	314	CLA	CHC-C1C	4.80	1.48	1.38
31	L	307	CLA	CHC-C1C	4.80	1.48	1.38
31	9	316	CLA	CHD-C1D	4.80	1.47	1.38
31	B	822	CLA	O2D-CGD	4.79	1.44	1.33
31	6	310	CLA	CHC-C1C	4.79	1.48	1.38
32	K	201	CHL	O2D-CGD	4.79	1.44	1.33
31	A	836	CLA	CHC-C1C	4.79	1.48	1.38
31	9	319	CLA	CHC-C1C	4.79	1.48	1.38
31	3	319	CLA	C3C-C2C	4.79	1.46	1.36
31	5	310	CLA	CHC-C1C	4.79	1.48	1.38
31	a	315	CLA	CHC-C1C	4.78	1.48	1.38
31	3	317	CLA	CHC-C1C	4.78	1.48	1.38
31	B	842	CLA	CHC-C1C	4.78	1.48	1.38
31	a	316	CLA	CHC-C1C	4.78	1.48	1.38
31	B	813	CLA	CHD-C1D	4.78	1.47	1.38
31	K	204	CLA	CHD-C1D	4.78	1.47	1.38
31	F	301	CLA	MG-ND	-4.78	1.96	2.05
31	9	314	CLA	CHC-C1C	4.78	1.48	1.38
31	A	846	CLA	CHD-C1D	4.77	1.47	1.38
31	a	322	CLA	CHC-C1C	4.77	1.48	1.38
31	2	307	CLA	CHC-C1C	4.77	1.48	1.38
31	B	820	CLA	CHD-C1D	4.77	1.47	1.38
32	7	324	CHL	O2D-CGD	4.77	1.44	1.33
31	5	318	CLA	CHC-C1C	4.77	1.48	1.38
31	A	814	CLA	O2D-CGD	4.77	1.44	1.33
31	B	822	CLA	CHC-C1C	4.77	1.48	1.38
31	B	849	CLA	O2D-CGD	4.77	1.44	1.33
31	8	321	CLA	CHD-C1D	4.77	1.47	1.38
31	B	832	CLA	CHD-C1D	4.77	1.47	1.38
31	A	856	CLA	CHC-C1C	4.76	1.48	1.38
31	B	846	CLA	CHD-C1D	4.76	1.47	1.38
31	5	323	CLA	CHD-C1D	4.76	1.47	1.38
31	H	903	CLA	MG-NC	4.76	2.17	2.06
31	B	831	CLA	CHC-C1C	4.76	1.48	1.38
31	b	305	CLA	CHC-C1C	4.76	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	844	CLA	CHD-C1D	4.76	1.47	1.38
32	K	201	CHL	C3D-C4D	-4.76	1.33	1.44
31	2	315	CLA	CHD-C1D	4.76	1.47	1.38
31	9	316	CLA	CHC-C1C	4.76	1.48	1.38
31	A	827	CLA	O2D-CGD	4.76	1.44	1.33
31	B	821	CLA	O2D-CGD	4.76	1.44	1.33
31	b	312	CLA	CHC-C1C	4.75	1.48	1.38
31	B	812	CLA	O2D-CGD	4.75	1.44	1.33
31	B	839	CLA	CHC-C1C	4.75	1.48	1.38
31	A	816	CLA	CHD-C1D	4.75	1.47	1.38
31	B	826	CLA	CHD-C1D	4.75	1.47	1.38
31	B	849	CLA	CHC-C1C	4.75	1.48	1.38
31	3	309	CLA	CHC-C1C	4.75	1.48	1.38
31	7	321	CLA	CHC-C1C	4.75	1.48	1.38
31	4	307	CLA	CHC-C1C	4.75	1.48	1.38
31	A	851	CLA	CHC-C1C	4.75	1.48	1.38
31	2	308	CLA	CHD-C1D	4.75	1.47	1.38
31	A	856	CLA	O2D-CGD	4.75	1.44	1.33
31	B	833	CLA	CHD-C1D	4.75	1.47	1.38
31	B	819	CLA	CHD-C1D	4.75	1.47	1.38
31	B	847	CLA	CHD-C1D	4.75	1.47	1.38
31	7	310	CLA	MG-ND	-4.75	1.96	2.05
31	A	856	CLA	MG-ND	4.75	2.15	2.05
31	7	314	CLA	CHC-C1C	4.75	1.48	1.38
31	3	316	CLA	CHC-C1C	4.75	1.48	1.38
31	A	854	CLA	CHD-C1D	4.75	1.47	1.38
31	B	844	CLA	CHD-C1D	4.75	1.47	1.38
30	A	813	CL0	O2D-CGD	4.74	1.44	1.33
31	K	205	CLA	CHC-C1C	4.74	1.48	1.38
31	8	309	CLA	CHD-C1D	4.74	1.47	1.38
31	7	311	CLA	CHC-C1C	4.74	1.48	1.38
31	7	313	CLA	CHD-C1D	4.74	1.47	1.38
31	A	846	CLA	O2D-CGD	4.74	1.44	1.33
31	A	818	CLA	O2D-CGD	4.74	1.44	1.33
31	2	305	CLA	CHC-C1C	4.74	1.48	1.38
31	6	307	CLA	CHC-C1C	4.74	1.48	1.38
31	B	848	CLA	CHD-C1D	4.74	1.47	1.38
31	B	828	CLA	MG-ND	-4.74	1.96	2.05
31	A	824	CLA	CHC-C1C	4.74	1.48	1.38
31	5	321	CLA	CHC-C1C	4.74	1.48	1.38
31	5	313	CLA	CHC-C4B	4.74	1.50	1.39
31	B	845	CLA	CHD-C1D	4.74	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	315	CLA	MG-NC	4.74	2.17	2.06
31	4	309	CLA	CHD-C1D	4.73	1.47	1.38
31	B	832	CLA	MG-NB	-4.73	1.96	2.05
31	3	310	CLA	CHC-C1C	4.73	1.48	1.38
31	8	310	CLA	C3C-C2C	4.73	1.46	1.36
32	9	322	CHL	O2D-CGD	4.73	1.44	1.33
31	8	321	CLA	CHC-C1C	4.73	1.48	1.38
31	H	903	CLA	CHC-C1C	4.73	1.48	1.38
31	J	105	CLA	CHD-C1D	4.73	1.47	1.38
31	A	856	CLA	CHD-C1D	4.73	1.47	1.38
31	B	826	CLA	CHC-C1C	4.73	1.48	1.38
31	A	826	CLA	O2D-CGD	4.73	1.44	1.33
31	B	816	CLA	CHD-C1D	4.72	1.47	1.38
31	B	815	CLA	CHC-C1C	4.72	1.48	1.38
31	K	204	CLA	CHC-C1C	4.72	1.48	1.38
32	a	320	CHL	O2D-CGD	4.72	1.44	1.33
31	B	835	CLA	CHD-C1D	4.72	1.47	1.38
31	A	827	CLA	CHC-C1C	4.72	1.48	1.38
31	7	310	CLA	MG-NC	4.72	2.17	2.06
31	2	314	CLA	CHC-C1C	4.72	1.48	1.38
31	b	302	CLA	CHC-C1C	4.72	1.48	1.38
31	F	301	CLA	CHD-C1D	4.72	1.47	1.38
31	A	820	CLA	CHD-C1D	4.72	1.47	1.38
31	G	204	CLA	CHC-C1C	4.72	1.48	1.38
31	5	323	CLA	CHC-C1C	4.72	1.48	1.38
31	B	811	CLA	CHD-C1D	4.71	1.47	1.38
31	B	846	CLA	CHC-C1C	4.71	1.48	1.38
31	A	825	CLA	CHD-C1D	4.71	1.47	1.38
31	F	301	CLA	CHC-C1C	4.71	1.48	1.38
32	7	320	CHL	O2D-CGD	4.71	1.44	1.33
31	A	841	CLA	CHD-C1D	4.71	1.47	1.38
31	B	833	CLA	CHC-C1C	4.71	1.48	1.38
31	B	836	CLA	CHD-C1D	4.71	1.47	1.38
31	B	811	CLA	CHC-C1C	4.71	1.48	1.38
31	5	309	CLA	CHC-C1C	4.71	1.48	1.38
31	A	822	CLA	CHC-C1C	4.70	1.48	1.38
31	2	315	CLA	CHC-C1C	4.70	1.48	1.38
31	9	311	CLA	CHC-C1C	4.70	1.48	1.38
31	5	313	CLA	C3D-C4D	-4.70	1.33	1.44
31	4	318	CLA	CHC-C1C	4.70	1.48	1.38
31	2	307	CLA	MG-NB	4.70	2.15	2.05
31	B	837	CLA	O2D-CGD	4.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	818	CLA	C3C-C2C	4.70	1.46	1.36
31	A	819	CLA	CHD-C1D	4.69	1.47	1.38
31	A	837	CLA	CHC-C1C	4.69	1.48	1.38
31	3	314	CLA	CHC-C1C	4.69	1.48	1.38
31	B	814	CLA	CHC-C1C	4.69	1.48	1.38
31	A	842	CLA	CHD-C1D	4.69	1.47	1.38
31	B	849	CLA	CHD-C1D	4.69	1.47	1.38
31	B	835	CLA	CHC-C1C	4.69	1.48	1.38
31	3	318	CLA	CHC-C1C	4.69	1.48	1.38
31	A	822	CLA	CHD-C1D	4.69	1.47	1.38
31	A	816	CLA	O2D-CGD	4.69	1.44	1.33
31	A	820	CLA	CHC-C1C	4.69	1.48	1.38
31	6	306	CLA	CHB-C1B	4.68	1.49	1.39
31	8	307	CLA	CHC-C1C	4.68	1.48	1.38
31	B	837	CLA	CHC-C1C	4.68	1.48	1.38
31	a	313	CLA	CHC-C1C	4.68	1.48	1.38
31	4	321	CLA	CHC-C1C	4.68	1.48	1.38
31	G	206	CLA	CHC-C1C	4.68	1.48	1.38
31	B	834	CLA	CHC-C1C	4.68	1.48	1.38
31	A	845	CLA	CHC-C1C	4.67	1.48	1.38
31	B	818	CLA	O2D-CGD	4.67	1.44	1.33
31	A	814	CLA	CHC-C1C	4.67	1.48	1.38
32	8	316	CHL	O2D-CGD	4.67	1.44	1.33
31	A	828	CLA	CHC-C1C	4.67	1.48	1.38
31	A	818	CLA	CHD-C1D	4.67	1.47	1.38
31	6	306	CLA	CHC-C4B	4.67	1.49	1.39
31	8	313	CLA	MG-ND	4.67	2.15	2.05
31	A	834	CLA	CHC-C1C	4.67	1.48	1.38
31	B	842	CLA	CHD-C1D	4.67	1.47	1.38
31	a	321	CLA	CHC-C1C	4.67	1.48	1.38
31	9	321	CLA	CHC-C1C	4.67	1.48	1.38
31	3	312	CLA	CHC-C1C	4.67	1.48	1.38
31	B	814	CLA	CHD-C1D	4.66	1.47	1.38
31	A	822	CLA	O2D-CGD	4.66	1.44	1.33
31	A	843	CLA	O2D-CGD	4.66	1.44	1.33
31	8	314	CLA	CHC-C1C	4.66	1.48	1.38
31	B	840	CLA	CHD-C1D	4.66	1.47	1.38
31	b	303	CLA	CHC-C1C	4.66	1.48	1.38
31	A	857	CLA	CHD-C1D	4.66	1.47	1.38
31	8	310	CLA	CHD-C1D	4.65	1.47	1.38
31	A	826	CLA	CHC-C1C	4.65	1.48	1.38
31	A	817	CLA	CHD-C1D	4.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	315	CLA	MG-NB	-4.65	1.96	2.05
31	B	839	CLA	MG-NC	4.65	2.17	2.06
31	4	309	CLA	CHC-C1C	4.65	1.48	1.38
31	B	818	CLA	CHD-C1D	4.65	1.47	1.38
31	B	830	CLA	CHC-C1C	4.65	1.48	1.38
31	3	319	CLA	CHD-C1D	4.65	1.47	1.38
31	6	313	CLA	CHC-C1C	4.64	1.48	1.38
31	B	821	CLA	CHC-C1C	4.64	1.47	1.38
31	7	322	CLA	CHC-C1C	4.64	1.47	1.38
31	B	831	CLA	CHD-C1D	4.63	1.47	1.38
31	A	828	CLA	MG-NA	4.63	2.17	2.06
31	4	308	CLA	CHC-C1C	4.63	1.47	1.38
31	5	313	CLA	CHC-C1C	4.63	1.47	1.38
32	7	318	CHL	MG-ND	-4.63	1.96	2.05
31	A	848	CLA	MG-NC	4.63	2.17	2.06
31	A	855	CLA	CHC-C1C	4.62	1.47	1.38
31	A	814	CLA	CHD-C1D	4.62	1.47	1.38
31	A	853	CLA	CHC-C1C	4.62	1.47	1.38
32	6	318	CHL	O2D-CGD	4.62	1.44	1.33
31	A	821	CLA	CHD-C1D	4.61	1.47	1.38
31	O	202	CLA	O2D-CGD	4.61	1.45	1.30
31	A	821	CLA	CHC-C1C	4.61	1.47	1.38
32	7	318	CHL	O2D-CGD	4.61	1.44	1.33
31	a	319	CLA	CHC-C1C	4.61	1.47	1.38
31	9	317	CLA	CHC-C1C	4.61	1.47	1.38
31	3	311	CLA	CHC-C1C	4.61	1.47	1.38
31	A	855	CLA	CHD-C1D	4.61	1.47	1.38
32	A	839	CHL	O2D-CGD	4.61	1.44	1.33
31	B	812	CLA	C3C-C2C	4.61	1.46	1.36
31	4	316	CLA	CHD-C4C	4.61	1.49	1.39
31	B	840	CLA	O2D-CGD	4.60	1.44	1.33
32	5	317	CHL	O2D-CGD	4.60	1.44	1.33
31	7	310	CLA	CHC-C1C	4.60	1.47	1.38
31	B	823	CLA	CHC-C1C	4.60	1.47	1.38
31	B	824	CLA	CHC-C1C	4.60	1.47	1.38
31	K	206	CLA	CHC-C1C	4.59	1.47	1.38
31	7	313	CLA	CHC-C1C	4.59	1.47	1.38
32	4	317	CHL	O2A-CGA	4.59	1.46	1.30
32	K	201	CHL	C2C-C3C	4.59	1.46	1.36
31	A	815	CLA	CHC-C1C	4.59	1.47	1.38
31	a	311	CLA	CHC-C1C	4.59	1.47	1.38
31	G	205	CLA	MG-NC	4.59	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	313	CLA	O2D-CGD	4.59	1.45	1.30
31	L	307	CLA	O2A-CGA	4.58	1.46	1.30
31	8	317	CLA	CHD-C1D	4.58	1.47	1.38
31	A	846	CLA	CHC-C1C	4.58	1.47	1.38
31	8	311	CLA	CHC-C1C	4.58	1.47	1.38
32	a	318	CHL	O2D-CGD	4.57	1.44	1.33
31	B	815	CLA	CHD-C1D	4.57	1.47	1.38
31	B	816	CLA	CHC-C1C	4.57	1.47	1.38
31	8	318	CLA	CHC-C1C	4.57	1.47	1.38
31	A	848	CLA	CHC-C1C	4.57	1.47	1.38
31	A	854	CLA	CHC-C1C	4.56	1.47	1.38
31	A	815	CLA	MG-NB	4.56	2.14	2.05
42	4	304	SQD	O48-C23	4.56	1.46	1.33
31	A	838	CLA	MG-ND	4.56	2.14	2.05
32	5	316	CHL	O2A-CGA	4.56	1.46	1.33
31	B	841	CLA	CHC-C1C	4.56	1.47	1.38
31	A	819	CLA	CHC-C1C	4.56	1.47	1.38
31	b	305	CLA	MG-NC	4.56	2.17	2.06
31	8	320	CLA	CHC-C1C	4.55	1.47	1.38
31	J	105	CLA	CHC-C1C	4.55	1.47	1.38
32	5	316	CHL	O2D-CGD	4.55	1.44	1.33
32	A	840	CHL	O2D-CGD	4.54	1.44	1.33
31	B	812	CLA	CHC-C1C	4.54	1.47	1.38
31	B	838	CLA	CHC-C1C	4.54	1.47	1.38
31	5	311	CLA	CHC-C1C	4.54	1.47	1.38
31	A	850	CLA	CHC-C1C	4.54	1.47	1.38
31	F	306	CLA	CHC-C1C	4.54	1.47	1.38
31	B	850	CLA	CHD-C1D	4.54	1.47	1.38
31	9	315	CLA	CHC-C1C	4.54	1.47	1.38
31	A	857	CLA	CHC-C1C	4.53	1.47	1.38
31	F	305	CLA	CHC-C1C	4.53	1.47	1.38
31	4	314	CLA	O2A-CGA	4.53	1.46	1.30
31	G	206	CLA	O2A-CGA	4.53	1.46	1.30
31	A	850	CLA	CHD-C1D	4.52	1.47	1.38
32	6	318	CHL	O2A-CGA	4.52	1.45	1.30
31	5	314	CLA	O2A-CGA	4.52	1.45	1.30
31	6	311	CLA	CHC-C1C	4.52	1.47	1.38
31	a	310	CLA	CHC-C1C	4.52	1.47	1.38
32	4	310	CHL	O2D-CGD	4.52	1.44	1.33
31	A	825	CLA	MG-NC	4.51	2.17	2.06
31	3	320	CLA	O2A-CGA	4.51	1.45	1.30
32	7	320	CHL	O2A-CGA	4.51	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	316	CLA	O2A-CGA	4.51	1.45	1.30
31	A	830	CLA	CHC-C1C	4.50	1.47	1.38
31	A	841	CLA	O2D-CGD	4.50	1.44	1.33
31	8	309	CLA	CHC-C1C	4.50	1.47	1.38
31	B	836	CLA	CHC-C1C	4.50	1.47	1.38
31	4	318	CLA	O2A-CGA	4.50	1.45	1.30
31	8	317	CLA	CHC-C1C	4.50	1.47	1.38
31	2	305	CLA	O2A-CGA	4.50	1.45	1.30
31	7	315	CLA	CHC-C1C	4.50	1.47	1.38
31	B	837	CLA	MG-NB	4.50	2.14	2.05
31	F	306	CLA	MG-NC	4.50	2.17	2.06
31	5	318	CLA	MG-NA	4.49	2.16	2.06
31	2	311	CLA	O2A-CGA	4.49	1.45	1.30
31	6	306	CLA	MG-NB	4.49	2.14	2.05
31	4	316	CLA	CHB-C1B	4.49	1.49	1.39
31	A	851	CLA	MG-NB	-4.49	1.96	2.05
31	4	320	CLA	O2A-CGA	4.48	1.45	1.30
32	8	316	CHL	O2A-CGA	4.47	1.46	1.33
31	B	817	CLA	CHD-C1D	4.47	1.47	1.38
31	4	306	CLA	O2A-CGA	4.47	1.45	1.30
31	B	841	CLA	CHD-C1D	4.47	1.47	1.38
32	6	319	CHL	O2D-CGD	4.46	1.44	1.33
31	8	308	CLA	MG-NB	4.46	2.14	2.05
31	2	310	CLA	O2A-CGA	4.45	1.45	1.30
31	A	825	CLA	O2A-CGA	4.45	1.46	1.33
31	7	313	CLA	O2A-CGA	4.44	1.45	1.30
31	9	313	CLA	O2A-CGA	4.44	1.45	1.30
32	a	317	CHL	MG-ND	4.44	2.14	2.05
31	4	315	CLA	O2A-CGA	4.44	1.45	1.30
31	L	306	CLA	O2A-CGA	4.44	1.45	1.30
31	A	832	CLA	CHC-C1C	4.44	1.47	1.38
31	a	310	CLA	O2A-CGA	4.44	1.45	1.30
31	B	843	CLA	O2A-CGA	4.43	1.45	1.30
31	9	317	CLA	CHC-C4B	4.43	1.49	1.39
31	4	305	CLA	C3D-C4D	-4.43	1.34	1.44
31	9	321	CLA	O2A-CGA	4.42	1.46	1.33
31	G	206	CLA	O2D-CGD	4.42	1.44	1.33
31	A	833	CLA	CHC-C1C	4.41	1.47	1.38
32	A	831	CHL	O2D-CGD	4.41	1.44	1.33
32	K	201	CHL	CHC-C1C	4.41	1.47	1.38
31	4	316	CLA	C3D-C4D	-4.40	1.34	1.44
31	L	305	CLA	CHD-C1D	4.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	812	CLA	CHD-C1D	4.39	1.46	1.38
31	B	845	CLA	MG-NB	4.38	2.14	2.05
31	A	852	CLA	MG-ND	4.38	2.14	2.05
31	6	307	CLA	MG-NC	-4.38	1.95	2.06
31	A	843	CLA	CHC-C1C	4.38	1.47	1.38
31	B	843	CLA	CHC-C1C	4.38	1.47	1.38
31	A	857	CLA	O2A-CGA	4.37	1.46	1.33
31	3	309	CLA	O2A-CGA	4.37	1.46	1.33
31	A	841	CLA	CHC-C1C	4.37	1.47	1.38
32	a	318	CHL	MG-NC	4.37	2.16	2.06
31	H	903	CLA	CHB-C1B	4.37	1.49	1.39
31	A	816	CLA	CHC-C1C	4.37	1.47	1.38
31	a	311	CLA	CHB-C1B	4.37	1.49	1.39
31	9	317	CLA	C3D-C4D	-4.35	1.34	1.44
31	5	323	CLA	O2A-CGA	4.35	1.46	1.33
32	a	320	CHL	O2A-CGA	4.35	1.46	1.33
31	9	315	CLA	O2A-CGA	4.35	1.46	1.33
31	A	826	CLA	MG-ND	4.35	2.14	2.05
32	9	320	CHL	O2A-CGA	4.34	1.46	1.33
31	5	313	CLA	CHD-C1D	4.34	1.46	1.38
32	a	317	CHL	O2A-CGA	4.34	1.46	1.33
31	5	307	CLA	O2A-CGA	4.33	1.46	1.33
31	7	310	CLA	O2A-CGA	4.33	1.45	1.30
31	A	847	CLA	CHC-C1C	4.32	1.47	1.38
31	A	819	CLA	O2A-CGA	4.32	1.46	1.33
31	B	812	CLA	MG-ND	4.32	2.14	2.05
31	7	322	CLA	CHB-C1B	4.32	1.49	1.39
31	9	318	CLA	CHB-C1B	4.32	1.49	1.39
31	O	202	CLA	CHB-C1B	4.32	1.49	1.39
31	9	318	CLA	CHC-C4B	4.32	1.49	1.39
31	B	833	CLA	O2A-CGA	4.32	1.46	1.33
32	a	318	CHL	O2A-CGA	4.32	1.46	1.33
31	B	826	CLA	O2A-CGA	4.32	1.46	1.33
32	4	313	CHL	O2A-CGA	4.32	1.46	1.33
31	A	842	CLA	MG-NC	4.32	2.16	2.06
31	6	310	CLA	CHB-C1B	4.31	1.49	1.39
31	B	847	CLA	CHC-C1C	4.31	1.47	1.38
31	A	838	CLA	CHC-C1C	4.31	1.47	1.38
32	7	317	CHL	O2A-CGA	4.31	1.45	1.33
31	B	833	CLA	MG-NA	4.31	2.16	2.06
31	6	314	CLA	O2A-CGA	4.31	1.45	1.33
32	3	315	CHL	O2D-CGD	4.31	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	315	CLA	O2A-CGA	4.30	1.45	1.33
31	A	844	CLA	CHC-C1C	4.30	1.47	1.38
31	A	824	CLA	O2A-CGA	4.30	1.45	1.33
31	O	203	CLA	O2A-CGA	4.30	1.45	1.33
31	8	310	CLA	CHC-C4B	4.29	1.49	1.39
31	B	839	CLA	O2A-CGA	4.29	1.45	1.33
31	4	319	CLA	CHB-C1B	4.29	1.49	1.39
31	K	204	CLA	O2A-CGA	4.29	1.45	1.33
31	b	313	CLA	O2A-CGA	4.29	1.45	1.33
31	8	312	CLA	O2A-CGA	4.29	1.45	1.33
31	6	315	CLA	CHB-C1B	4.29	1.49	1.39
31	O	203	CLA	CHC-C4B	4.29	1.49	1.39
31	O	202	CLA	MG-NA	4.29	2.16	2.06
31	4	316	CLA	MG-NB	4.29	2.14	2.05
31	3	310	CLA	O2A-CGA	4.28	1.45	1.33
31	4	309	CLA	O2A-CGA	4.28	1.45	1.33
31	6	316	CLA	CHB-C1B	4.28	1.49	1.39
31	3	319	CLA	O2A-CGA	4.28	1.45	1.33
31	8	311	CLA	O2A-CGA	4.28	1.45	1.33
36	L	304	LUT	C8-C9	4.28	1.55	1.45
31	9	317	CLA	MG-ND	4.28	2.14	2.05
31	6	314	CLA	CHB-C1B	4.27	1.49	1.39
31	5	309	CLA	O2A-CGA	4.27	1.45	1.33
31	L	307	CLA	CHB-C1B	4.27	1.49	1.39
31	B	829	CLA	CHC-C1C	4.27	1.47	1.38
31	O	204	CLA	CHB-C1B	4.26	1.49	1.39
31	5	309	CLA	CHB-C1B	4.26	1.49	1.39
31	6	308	CLA	O2A-CGA	4.26	1.45	1.33
31	A	857	CLA	CHB-C1B	4.26	1.49	1.39
31	A	815	CLA	CHD-C1D	4.26	1.46	1.38
31	4	307	CLA	O2A-CGA	4.26	1.45	1.33
31	B	827	CLA	CHC-C1C	4.26	1.47	1.38
31	b	307	CLA	CHB-C1B	4.26	1.49	1.39
31	4	319	CLA	CHC-C4B	4.26	1.49	1.39
31	9	317	CLA	CHD-C1D	4.25	1.46	1.38
31	6	307	CLA	O2A-CGA	4.25	1.45	1.33
31	B	816	CLA	O2A-CGA	4.25	1.45	1.33
32	3	315	CHL	O2A-CGA	4.25	1.45	1.33
31	8	320	CLA	O2A-CGA	4.25	1.45	1.33
31	5	312	CLA	O2A-CGA	4.25	1.45	1.33
31	b	308	CLA	CHD-C4C	4.25	1.48	1.39
31	5	320	CLA	CHB-C1B	4.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	309	CLA	MG-NA	4.24	2.16	2.06
31	6	310	CLA	O2A-CGA	4.24	1.45	1.33
31	7	310	CLA	CHB-C1B	4.24	1.48	1.39
31	B	817	CLA	CHC-C1C	4.24	1.47	1.38
31	8	320	CLA	CHB-C1B	4.24	1.48	1.39
31	a	311	CLA	MG-NB	4.24	2.14	2.05
31	8	314	CLA	CHB-C1B	4.24	1.48	1.39
31	O	202	CLA	CHC-C4B	4.24	1.48	1.39
31	a	321	CLA	O2A-CGA	4.23	1.45	1.33
31	5	320	CLA	CHC-C4B	4.23	1.48	1.39
31	B	831	CLA	O2A-CGA	4.23	1.45	1.33
31	4	321	CLA	O2A-CGA	4.23	1.45	1.33
31	b	313	CLA	CHC-C4B	4.23	1.48	1.39
31	4	320	CLA	CHB-C1B	4.23	1.48	1.39
31	a	310	CLA	MG-NC	4.23	2.16	2.06
31	7	311	CLA	CHB-C1B	4.23	1.48	1.39
31	a	315	CLA	MG-NC	4.23	2.16	2.06
36	4	303	LUT	C8-C9	4.22	1.55	1.45
32	6	320	CHL	O2A-CGA	4.22	1.46	1.33
31	F	301	CLA	MG-NB	4.22	2.14	2.05
31	3	308	CLA	CHB-C1B	4.22	1.48	1.39
31	B	837	CLA	CHB-C1B	4.22	1.48	1.39
32	5	317	CHL	CHC-C1C	4.22	1.47	1.38
31	7	314	CLA	O2A-CGA	4.21	1.45	1.33
31	9	317	CLA	O2A-CGA	4.21	1.45	1.33
31	a	313	CLA	O2A-CGA	4.21	1.45	1.33
31	A	845	CLA	O2A-CGA	4.21	1.45	1.33
31	3	320	CLA	CHB-C1B	4.21	1.48	1.39
31	K	204	CLA	CHB-C1B	4.21	1.48	1.39
31	6	308	CLA	CHD-C4C	4.21	1.48	1.39
31	B	848	CLA	O2A-CGA	4.20	1.45	1.33
31	8	309	CLA	O2A-CGA	4.20	1.45	1.33
31	4	312	CLA	O2A-CGA	4.20	1.45	1.33
32	A	831	CHL	O2A-CGA	4.20	1.45	1.33
31	A	820	CLA	CHB-C1B	4.20	1.48	1.39
31	B	816	CLA	CHB-C1B	4.20	1.48	1.39
31	8	318	CLA	O2A-CGA	4.20	1.45	1.33
31	b	311	CLA	CHB-C1B	4.20	1.48	1.39
31	B	830	CLA	O2A-CGA	4.20	1.45	1.33
31	A	855	CLA	CHB-C1B	4.20	1.48	1.39
31	a	309	CLA	CHC-C4B	4.20	1.48	1.39
31	2	315	CLA	CHB-C1B	4.20	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	F	306	CLA	O2A-CGA	4.20	1.45	1.33
31	a	319	CLA	O2A-CGA	4.20	1.45	1.33
31	8	307	CLA	CHB-C1B	4.20	1.48	1.39
31	5	313	CLA	CHB-C1B	4.20	1.48	1.39
31	B	850	CLA	CHC-C4B	4.19	1.48	1.39
31	6	316	CLA	O2A-CGA	4.19	1.45	1.33
31	B	834	CLA	MG-ND	4.19	2.14	2.05
31	b	306	CLA	CHC-C4B	4.19	1.48	1.39
31	B	842	CLA	O2A-CGA	4.19	1.45	1.33
36	F	304	LUT	C8-C9	4.19	1.54	1.45
31	3	317	CLA	O2A-CGA	4.19	1.45	1.33
31	B	847	CLA	O2A-CGA	4.19	1.45	1.33
31	6	315	CLA	CHC-C4B	4.19	1.48	1.39
31	9	311	CLA	O2A-CGA	4.19	1.45	1.33
31	B	846	CLA	O2A-CGA	4.19	1.45	1.33
32	9	322	CHL	O2A-CGA	4.18	1.46	1.33
31	a	312	CLA	CHB-C1B	4.18	1.48	1.39
31	b	308	CLA	CHC-C4B	4.18	1.48	1.39
31	8	317	CLA	O2A-CGA	4.18	1.45	1.33
31	8	309	CLA	MG-ND	-4.18	1.97	2.05
31	a	311	CLA	O2A-CGA	4.18	1.45	1.33
31	8	312	CLA	CHB-C1B	4.18	1.48	1.39
31	A	838	CLA	CHB-C1B	4.18	1.48	1.39
31	9	317	CLA	CHB-C1B	4.18	1.48	1.39
31	2	308	CLA	CHB-C1B	4.18	1.48	1.39
31	G	205	CLA	CHC-C4B	4.18	1.48	1.39
31	B	846	CLA	MG-NC	4.18	2.16	2.06
31	3	307	CLA	O2A-CGA	4.18	1.45	1.33
31	L	307	CLA	CHC-C4B	4.18	1.48	1.39
31	3	316	CLA	O2A-CGA	4.18	1.45	1.33
31	4	307	CLA	CHB-C1B	4.18	1.48	1.39
31	A	815	CLA	O2A-CGA	4.17	1.45	1.33
31	b	312	CLA	CHB-C1B	4.17	1.48	1.39
31	B	818	CLA	O2A-CGA	4.17	1.45	1.33
32	6	309	CHL	O2A-CGA	4.17	1.45	1.33
31	F	305	CLA	MG-ND	4.17	2.14	2.05
31	5	315	CLA	O2A-CGA	4.17	1.45	1.33
36	8	302	LUT	C35-C34	4.17	1.56	1.43
31	A	828	CLA	O2A-CGA	4.17	1.45	1.33
31	3	318	CLA	O2A-CGA	4.17	1.45	1.33
31	8	314	CLA	O2A-CGA	4.17	1.45	1.33
30	A	813	CL0	C3D-C4D	-4.17	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	311	CLA	CHC-C4B	4.17	1.48	1.39
31	a	309	CLA	O2A-CGA	4.17	1.45	1.33
31	a	314	CLA	CHB-C1B	4.17	1.48	1.39
36	b	301	LUT	C35-C34	4.17	1.56	1.43
31	A	851	CLA	O2A-CGA	4.17	1.45	1.33
31	4	306	CLA	CHC-C4B	4.17	1.48	1.39
31	B	845	CLA	O2A-CGA	4.17	1.45	1.33
32	7	318	CHL	O2A-CGA	4.17	1.45	1.33
31	5	310	CLA	CHB-C1B	4.17	1.48	1.39
31	a	319	CLA	CHB-C1B	4.16	1.48	1.39
31	9	314	CLA	CHB-C1B	4.16	1.48	1.39
31	G	204	CLA	O2A-CGA	4.16	1.45	1.33
31	B	822	CLA	CHB-C1B	4.16	1.48	1.39
31	B	835	CLA	CHB-C1B	4.16	1.48	1.39
31	4	312	CLA	CHB-C1B	4.16	1.48	1.39
31	A	823	CLA	O2A-CGA	4.16	1.45	1.33
31	7	314	CLA	CHB-C1B	4.16	1.48	1.39
31	b	303	CLA	CHB-C1B	4.16	1.48	1.39
31	5	323	CLA	CHB-C1B	4.16	1.48	1.39
31	5	312	CLA	MG-NA	4.16	2.16	2.06
31	4	316	CLA	O2A-CGA	4.16	1.45	1.33
31	6	311	CLA	CHB-C1B	4.16	1.48	1.39
31	b	306	CLA	O2A-CGA	4.16	1.46	1.33
31	A	835	CLA	O2A-CGA	4.16	1.45	1.33
36	4	303	LUT	C35-C34	4.16	1.56	1.43
31	8	309	CLA	MG-NB	4.16	2.14	2.05
31	5	312	CLA	CHC-C4B	4.15	1.48	1.39
31	2	310	CLA	CHB-C1B	4.15	1.48	1.39
31	6	313	CLA	CHB-C1B	4.15	1.48	1.39
31	B	850	CLA	O2A-CGA	4.15	1.45	1.33
31	B	847	CLA	CHB-C1B	4.15	1.48	1.39
31	B	841	CLA	O2A-CGA	4.15	1.45	1.33
31	B	829	CLA	CHB-C1B	4.15	1.48	1.39
31	8	320	CLA	MG-NC	4.15	2.16	2.06
31	O	204	CLA	CHD-C4C	4.15	1.48	1.39
31	O	204	CLA	CHC-C4B	4.15	1.48	1.39
31	2	304	CLA	CHC-C4B	4.15	1.48	1.39
31	2	306	CLA	O2A-CGA	4.15	1.45	1.33
31	H	902	CLA	CHB-C1B	4.15	1.48	1.39
31	B	821	CLA	O2A-CGA	4.15	1.45	1.33
31	4	318	CLA	CHB-C1B	4.15	1.48	1.39
31	B	819	CLA	CHC-C1C	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	308	CLA	CHC-C4B	4.15	1.48	1.39
31	5	308	CLA	CHB-C1B	4.15	1.48	1.39
31	7	309	CLA	O2A-CGA	4.15	1.45	1.33
31	2	305	CLA	CHB-C1B	4.15	1.48	1.39
31	4	315	CLA	CHC-C4B	4.15	1.48	1.39
31	2	306	CLA	CHB-C1B	4.15	1.48	1.39
31	a	314	CLA	O2A-CGA	4.15	1.45	1.33
32	5	317	CHL	O2A-CGA	4.15	1.46	1.33
31	5	318	CLA	O2A-CGA	4.14	1.45	1.33
32	A	839	CHL	O2A-CGA	4.14	1.45	1.33
32	7	319	CHL	O2A-CGA	4.14	1.46	1.33
31	3	313	CLA	CHD-C4C	4.14	1.48	1.39
32	7	324	CHL	O2A-CGA	4.14	1.45	1.33
31	4	311	CLA	CHB-C1B	4.14	1.48	1.39
32	5	322	CHL	O2A-CGA	4.14	1.46	1.33
32	A	840	CHL	O2A-CGA	4.14	1.45	1.33
31	A	825	CLA	CHB-C1B	4.14	1.48	1.39
31	4	311	CLA	CHC-C4B	4.14	1.48	1.39
31	4	316	CLA	CHC-C1C	4.14	1.46	1.38
31	A	836	CLA	CHB-C1B	4.14	1.48	1.39
31	L	306	CLA	MG-NA	4.14	2.16	2.06
32	4	310	CHL	O2A-CGA	4.14	1.46	1.33
31	b	302	CLA	CHB-C1B	4.14	1.48	1.39
31	L	305	CLA	O2A-CGA	4.14	1.45	1.33
31	A	851	CLA	CHB-C1B	4.14	1.48	1.39
31	a	319	CLA	MG-NB	-4.14	1.97	2.05
31	A	837	CLA	O2A-CGA	4.14	1.45	1.33
31	B	823	CLA	CHB-C1B	4.14	1.48	1.39
31	5	314	CLA	CHB-C1B	4.14	1.48	1.39
31	9	319	CLA	CHB-C1B	4.14	1.48	1.39
31	4	320	CLA	CHC-C4B	4.14	1.48	1.39
32	7	319	CHL	CHC-C1C	4.14	1.46	1.38
31	9	313	CLA	CHC-C4B	4.14	1.48	1.39
31	A	852	CLA	MG-NA	4.14	2.16	2.06
31	A	850	CLA	O2A-CGA	4.14	1.45	1.33
31	2	312	CLA	CHC-C4B	4.14	1.48	1.39
31	9	313	CLA	CHB-C1B	4.13	1.48	1.39
31	B	825	CLA	MG-NB	4.13	2.14	2.05
31	3	320	CLA	CHC-C4B	4.13	1.48	1.39
31	b	303	CLA	CHD-C4C	4.13	1.48	1.39
31	L	305	CLA	CHB-C1B	4.13	1.48	1.39
31	7	310	CLA	CHC-C4B	4.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	304	CLA	CHB-C1B	4.13	1.48	1.39
31	B	825	CLA	CHB-C1B	4.13	1.48	1.39
31	B	845	CLA	CHC-C1C	4.13	1.46	1.38
31	2	307	CLA	O2A-CGA	4.13	1.45	1.33
31	9	316	CLA	O2A-CGA	4.13	1.45	1.33
31	A	844	CLA	O2A-CGA	4.13	1.45	1.33
31	b	304	CLA	CHC-C4B	4.13	1.48	1.39
31	B	837	CLA	O2A-CGA	4.13	1.45	1.33
31	B	840	CLA	MG-NB	4.13	2.14	2.05
31	7	315	CLA	O2A-CGA	4.12	1.45	1.33
31	A	836	CLA	O2A-CGA	4.12	1.45	1.33
31	J	105	CLA	CHB-C1B	4.12	1.48	1.39
31	3	313	CLA	CHC-C4B	4.12	1.48	1.39
31	b	310	CLA	CHB-C1B	4.12	1.48	1.39
31	2	310	CLA	CHC-C4B	4.12	1.48	1.39
31	8	308	CLA	O2A-CGA	4.12	1.45	1.33
31	4	305	CLA	O2A-CGA	4.12	1.45	1.33
31	2	314	CLA	CHB-C1B	4.12	1.48	1.39
31	B	834	CLA	CHD-C1D	4.12	1.46	1.38
31	B	820	CLA	O2A-CGA	4.12	1.45	1.33
31	B	849	CLA	O2A-CGA	4.12	1.45	1.33
31	5	310	CLA	O2A-CGA	4.12	1.45	1.33
31	A	846	CLA	CHB-C1B	4.12	1.48	1.39
31	6	312	CLA	O2A-CGA	4.12	1.45	1.33
31	A	843	CLA	O2A-CGA	4.12	1.45	1.33
31	B	823	CLA	O2A-CGA	4.11	1.45	1.33
32	b	309	CHL	O2A-CGA	4.11	1.46	1.33
31	8	309	CLA	CHB-C1B	4.11	1.48	1.39
31	7	312	CLA	O2A-CGA	4.11	1.45	1.33
31	b	304	CLA	CHB-C1B	4.11	1.48	1.39
31	b	311	CLA	CHC-C4B	4.11	1.48	1.39
31	H	901	CLA	CHB-C1B	4.11	1.48	1.39
31	F	306	CLA	CHB-C1B	4.11	1.48	1.39
31	O	203	CLA	CHB-C1B	4.11	1.48	1.39
31	A	833	CLA	O2A-CGA	4.11	1.45	1.33
31	4	312	CLA	CHC-C4B	4.11	1.48	1.39
31	B	818	CLA	CHC-C1C	4.11	1.46	1.38
31	5	321	CLA	CHB-C1B	4.11	1.48	1.39
31	A	826	CLA	O2A-CGA	4.10	1.45	1.33
31	A	820	CLA	O2A-CGA	4.10	1.45	1.33
31	8	313	CLA	CHB-C1B	4.10	1.48	1.39
31	3	311	CLA	O2A-CGA	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	855	CLA	O2A-CGA	4.10	1.45	1.33
31	G	205	CLA	CHB-C1B	4.10	1.48	1.39
31	6	308	CLA	CHB-C1B	4.10	1.48	1.39
31	8	315	CLA	CHD-C4C	4.10	1.48	1.39
32	A	840	CHL	CHC-C1C	4.10	1.46	1.38
31	B	826	CLA	CHB-C1B	4.10	1.48	1.39
31	A	829	CLA	O2A-CGA	4.10	1.45	1.33
31	3	312	CLA	O2A-CGA	4.10	1.45	1.33
31	5	308	CLA	CHC-C4B	4.10	1.48	1.39
36	5	304	LUT	C8-C9	4.10	1.54	1.45
31	A	817	CLA	O2A-CGA	4.10	1.45	1.33
31	B	826	CLA	MG-NB	4.10	2.13	2.05
31	A	829	CLA	C1B-NB	-4.09	1.32	1.37
32	6	319	CHL	O2A-CGA	4.09	1.46	1.33
31	5	312	CLA	CHB-C1B	4.09	1.48	1.39
36	J	103	LUT	C8-C9	4.09	1.54	1.45
31	B	832	CLA	O2A-CGA	4.09	1.45	1.33
31	8	309	CLA	CHC-C4B	4.09	1.48	1.39
31	9	312	CLA	CHB-C1B	4.09	1.48	1.39
31	b	308	CLA	O2A-CGA	4.09	1.46	1.33
31	H	901	CLA	CHD-C4C	4.09	1.48	1.39
31	6	307	CLA	CHD-C4C	4.09	1.48	1.39
31	A	856	CLA	O2A-CGA	4.09	1.45	1.33
31	a	309	CLA	CHB-C1B	4.09	1.48	1.39
31	9	318	CLA	O2A-CGA	4.09	1.45	1.33
31	4	314	CLA	CHD-C4C	4.09	1.48	1.39
31	8	308	CLA	CHC-C4B	4.09	1.48	1.39
31	9	314	CLA	O2A-CGA	4.09	1.45	1.33
36	a	305	LUT	C8-C9	4.09	1.54	1.45
31	A	826	CLA	CHB-C1B	4.09	1.48	1.39
31	B	827	CLA	MG-NC	4.09	2.16	2.06
31	3	307	CLA	CHC-C4B	4.09	1.48	1.39
31	A	830	CLA	O2A-CGA	4.08	1.45	1.33
31	3	307	CLA	CHB-C1B	4.08	1.48	1.39
31	8	321	CLA	CHB-C1B	4.08	1.48	1.39
31	5	315	CLA	CHB-C1B	4.08	1.48	1.39
31	8	321	CLA	O2A-CGA	4.08	1.46	1.33
31	7	315	CLA	CHB-C1B	4.08	1.48	1.39
31	6	316	CLA	CHC-C4B	4.08	1.48	1.39
31	5	318	CLA	CHD-C4C	4.08	1.48	1.39
31	B	829	CLA	O2A-CGA	4.08	1.45	1.33
31	A	825	CLA	CHC-C4B	4.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	313	CLA	O2A-CGA	4.08	1.45	1.33
31	3	314	CLA	O2A-CGA	4.08	1.45	1.33
31	A	838	CLA	O2A-CGA	4.08	1.45	1.33
31	8	313	CLA	O2A-CGA	4.08	1.46	1.33
31	b	306	CLA	CHB-C1B	4.08	1.48	1.39
31	5	314	CLA	CHC-C4B	4.08	1.48	1.39
31	A	814	CLA	CHB-C1B	4.08	1.48	1.39
31	A	834	CLA	MG-ND	4.08	2.13	2.05
31	b	308	CLA	CHB-C1B	4.08	1.48	1.39
31	4	314	CLA	CHB-C1B	4.08	1.48	1.39
31	2	309	CLA	CHC-C4B	4.08	1.48	1.39
31	B	832	CLA	CHC-C1C	4.08	1.46	1.38
31	B	815	CLA	O2A-CGA	4.08	1.45	1.33
32	7	319	CHL	O2D-CGD	4.08	1.43	1.33
31	6	307	CLA	CHC-C4B	4.07	1.48	1.39
31	A	855	CLA	MG-NB	-4.07	1.97	2.05
31	A	827	CLA	O2A-CGA	4.07	1.45	1.33
36	J	103	LUT	C35-C34	4.07	1.56	1.43
31	b	307	CLA	CHC-C4B	4.07	1.48	1.39
31	2	306	CLA	CHC-C4B	4.07	1.48	1.39
31	B	818	CLA	CHB-C1B	4.07	1.48	1.39
31	a	312	CLA	CHC-C4B	4.07	1.48	1.39
31	3	320	CLA	MG-NB	4.07	2.13	2.05
31	a	322	CLA	CHD-C4C	4.07	1.48	1.39
31	4	312	CLA	CHD-C4C	4.07	1.48	1.39
31	8	310	CLA	O2A-CGA	4.07	1.45	1.33
31	5	321	CLA	CHC-C4B	4.07	1.48	1.39
31	3	310	CLA	CHB-C1B	4.07	1.48	1.39
31	3	318	CLA	CHB-C1B	4.07	1.48	1.39
31	a	310	CLA	MG-ND	-4.07	1.97	2.05
31	B	828	CLA	CHD-C4C	4.07	1.48	1.39
31	B	813	CLA	CHC-C4B	4.07	1.48	1.39
31	6	312	CLA	CHC-C4B	4.07	1.48	1.39
31	A	852	CLA	O2A-CGA	4.07	1.45	1.33
31	L	305	CLA	CHC-C4B	4.07	1.48	1.39
31	9	316	CLA	CHB-C1B	4.06	1.48	1.39
31	3	314	CLA	CHD-C4C	4.06	1.48	1.39
31	4	305	CLA	C3C-C2C	4.06	1.45	1.36
31	A	814	CLA	CHC-C4B	4.06	1.48	1.39
31	B	819	CLA	O2A-CGA	4.06	1.45	1.33
31	G	205	CLA	O2A-CGA	4.06	1.45	1.33
31	H	902	CLA	CHC-C4B	4.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	308	CLA	O2A-CGA	4.06	1.45	1.33
31	4	321	CLA	CHB-C1B	4.06	1.48	1.39
31	2	309	CLA	CHD-C4C	4.06	1.48	1.39
31	K	205	CLA	O2A-CGA	4.06	1.45	1.33
31	7	311	CLA	MG-NC	4.06	2.15	2.06
31	A	854	CLA	O2A-CGA	4.06	1.45	1.33
31	3	317	CLA	CHC-C4B	4.06	1.48	1.39
31	2	311	CLA	CHB-C1B	4.06	1.48	1.39
31	2	312	CLA	CHB-C1B	4.06	1.48	1.39
31	6	310	CLA	CHC-C4B	4.06	1.48	1.39
31	5	315	CLA	CHD-C4C	4.06	1.48	1.39
31	b	305	CLA	O2A-CGA	4.06	1.45	1.33
31	B	833	CLA	CHB-C1B	4.05	1.48	1.39
31	a	316	CLA	CHD-C4C	4.05	1.48	1.39
31	b	310	CLA	CHC-C4B	4.05	1.48	1.39
31	B	836	CLA	O2A-CGA	4.05	1.45	1.33
31	b	302	CLA	O2A-CGA	4.05	1.45	1.33
31	b	307	CLA	O2A-CGA	4.05	1.45	1.33
31	A	816	CLA	CHB-C1B	4.05	1.48	1.39
31	a	321	CLA	CHD-C4C	4.05	1.48	1.39
31	6	315	CLA	O2A-CGA	4.05	1.45	1.33
31	A	814	CLA	O2A-CGA	4.05	1.45	1.33
31	3	313	CLA	CHB-C1B	4.05	1.48	1.39
31	6	306	CLA	CHD-C1D	4.05	1.46	1.38
32	6	317	CHL	O2A-CGA	4.05	1.45	1.33
31	A	848	CLA	O2A-CGA	4.05	1.45	1.33
31	2	309	CLA	O2A-CGA	4.05	1.45	1.33
31	3	312	CLA	CHD-C4C	4.05	1.48	1.39
31	2	311	CLA	CHD-C4C	4.05	1.48	1.39
31	K	204	CLA	MG-NA	-4.05	1.96	2.06
36	6	304	LUT	C35-C34	4.05	1.56	1.43
31	A	846	CLA	O2A-CGA	4.05	1.45	1.33
31	B	814	CLA	O2A-CGA	4.05	1.45	1.33
31	B	831	CLA	CHB-C1B	4.05	1.48	1.39
31	7	312	CLA	CHB-C1B	4.05	1.48	1.39
31	2	307	CLA	CHC-C4B	4.05	1.48	1.39
31	B	838	CLA	O2A-CGA	4.04	1.45	1.33
31	a	322	CLA	O2A-CGA	4.04	1.45	1.33
31	4	307	CLA	CHD-C4C	4.04	1.48	1.39
31	B	834	CLA	O2A-CGA	4.04	1.45	1.33
31	7	321	CLA	CHB-C1B	4.04	1.48	1.39
31	b	304	CLA	O2A-CGA	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	206	CLA	O2A-CGA	4.04	1.45	1.33
31	L	307	CLA	CHD-C4C	4.04	1.48	1.39
31	B	824	CLA	O2A-CGA	4.04	1.45	1.33
31	8	307	CLA	O2A-CGA	4.04	1.45	1.33
31	3	312	CLA	CHB-C1B	4.04	1.48	1.39
31	7	309	CLA	CHC-C4B	4.04	1.48	1.39
31	2	309	CLA	CHB-C1B	4.04	1.48	1.39
31	A	849	CLA	O2A-CGA	4.04	1.45	1.33
31	F	301	CLA	O2A-CGA	4.04	1.45	1.33
31	K	205	CLA	CHB-C1B	4.04	1.48	1.39
31	2	312	CLA	CHD-C4C	4.04	1.48	1.39
31	2	314	CLA	O2A-CGA	4.04	1.45	1.33
31	7	316	CLA	CHC-C4B	4.04	1.48	1.39
31	K	205	CLA	CHD-C4C	4.04	1.48	1.39
31	7	322	CLA	O2A-CGA	4.04	1.45	1.33
31	7	316	CLA	CHD-C4C	4.03	1.48	1.39
31	5	311	CLA	O2A-CGA	4.03	1.45	1.33
31	b	310	CLA	CHD-C4C	4.03	1.48	1.39
31	A	835	CLA	CHC-C4B	4.03	1.48	1.39
31	A	845	CLA	CHB-C1B	4.03	1.48	1.39
31	9	321	CLA	CHB-C1B	4.03	1.48	1.39
31	b	305	CLA	CHB-C1B	4.03	1.48	1.39
31	2	313	CLA	CHB-C1B	4.03	1.48	1.39
31	6	307	CLA	CHB-C1B	4.03	1.48	1.39
32	K	201	CHL	CHD-C1D	4.03	1.46	1.38
31	a	313	CLA	CHB-C1B	4.03	1.48	1.39
31	A	847	CLA	O2A-CGA	4.03	1.45	1.33
31	b	310	CLA	O2A-CGA	4.03	1.45	1.33
31	7	313	CLA	CHB-C1B	4.03	1.48	1.39
31	O	202	CLA	CHD-C4C	4.03	1.48	1.39
31	B	813	CLA	O2A-CGA	4.03	1.45	1.33
31	B	828	CLA	CHB-C1B	4.03	1.48	1.39
31	8	310	CLA	CHB-C1B	4.03	1.48	1.39
31	6	322	CLA	CHB-C1B	4.03	1.48	1.39
31	7	309	CLA	CHB-C1B	4.03	1.48	1.39
31	3	309	CLA	CHC-C4B	4.03	1.48	1.39
31	L	306	CLA	CHB-C1B	4.03	1.48	1.39
31	2	305	CLA	CHC-C4B	4.03	1.48	1.39
31	4	321	CLA	CHC-C4B	4.03	1.48	1.39
31	8	307	CLA	CHC-C4B	4.03	1.48	1.39
36	9	303	LUT	C35-C34	4.03	1.55	1.43
31	6	311	CLA	O2A-CGA	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	313	CLA	O2A-CGA	4.02	1.45	1.33
31	7	321	CLA	O2A-CGA	4.02	1.45	1.33
31	3	320	CLA	CHD-C4C	4.02	1.48	1.39
31	b	313	CLA	CHD-C4C	4.02	1.48	1.39
31	B	835	CLA	O2A-CGA	4.02	1.45	1.33
31	7	311	CLA	CHC-C4B	4.02	1.48	1.39
31	2	306	CLA	CHD-C4C	4.02	1.48	1.39
31	5	320	CLA	CHD-C4C	4.02	1.48	1.39
36	4	302	LUT	C8-C9	4.02	1.54	1.45
32	K	201	CHL	O2A-CGA	4.02	1.45	1.33
31	B	835	CLA	MG-NB	4.02	2.13	2.05
32	6	321	CHL	CHC-C1C	4.02	1.46	1.38
31	A	822	CLA	O2A-CGA	4.02	1.45	1.33
31	4	314	CLA	CHC-C4B	4.02	1.48	1.39
31	6	322	CLA	CHC-C4B	4.02	1.48	1.39
31	9	321	CLA	CHD-C4C	4.02	1.48	1.39
31	b	312	CLA	CHC-C4B	4.02	1.48	1.39
31	9	321	CLA	CHC-C4B	4.02	1.48	1.39
31	2	313	CLA	O2A-CGA	4.02	1.45	1.33
31	a	315	CLA	CHB-C1B	4.02	1.48	1.39
31	6	311	CLA	CHC-C4B	4.02	1.48	1.39
31	B	840	CLA	CHB-C1B	4.02	1.48	1.39
31	3	314	CLA	CHC-C4B	4.02	1.48	1.39
31	6	313	CLA	O2A-CGA	4.02	1.45	1.33
31	B	822	CLA	O2A-CGA	4.02	1.45	1.33
31	a	314	CLA	CHD-C4C	4.02	1.48	1.39
31	H	903	CLA	O2A-CGA	4.02	1.45	1.33
31	F	301	CLA	CHC-C4B	4.02	1.48	1.39
32	5	316	CHL	MG-NA	4.01	2.15	2.06
31	B	848	CLA	CHB-C1B	4.01	1.48	1.39
31	4	309	CLA	CHB-C1B	4.01	1.48	1.39
31	A	818	CLA	O2A-CGA	4.01	1.45	1.33
31	a	321	CLA	CHB-C1B	4.01	1.48	1.39
31	a	314	CLA	CHC-C4B	4.01	1.48	1.39
31	8	313	CLA	CHC-C4B	4.01	1.48	1.39
31	K	206	CLA	CHB-C1B	4.01	1.48	1.39
31	b	306	CLA	CHD-C4C	4.01	1.48	1.39
31	6	312	CLA	CHD-C4C	4.01	1.48	1.39
31	B	820	CLA	CHB-C1B	4.01	1.48	1.39
31	3	317	CLA	CHB-C1B	4.01	1.48	1.39
31	A	823	CLA	CHC-C4B	4.01	1.48	1.39
31	A	816	CLA	O2A-CGA	4.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	309	CLA	CHC-C4B	4.01	1.48	1.39
31	3	308	CLA	CHC-C4B	4.01	1.48	1.39
31	3	319	CLA	CHC-C4B	4.01	1.48	1.39
31	B	817	CLA	O2A-CGA	4.01	1.45	1.33
31	A	824	CLA	CHC-C4B	4.01	1.48	1.39
31	b	312	CLA	CHD-C4C	4.01	1.48	1.39
31	B	825	CLA	O2A-CGA	4.01	1.45	1.33
31	8	308	CLA	CHB-C1B	4.01	1.48	1.39
31	5	309	CLA	CHD-C4C	4.01	1.48	1.39
32	9	322	CHL	CHD-C1D	4.01	1.46	1.38
32	6	309	CHL	CHD-C1D	4.01	1.46	1.38
31	B	825	CLA	CHC-C4B	4.01	1.48	1.39
31	4	308	CLA	CHB-C1B	4.01	1.48	1.39
31	B	820	CLA	CHC-C4B	4.00	1.48	1.39
31	2	313	CLA	CHC-C4B	4.00	1.48	1.39
32	5	319	CHL	O2A-CGA	4.00	1.45	1.33
31	A	837	CLA	CHB-C1B	4.00	1.48	1.39
31	B	840	CLA	O2A-CGA	4.00	1.45	1.33
31	4	315	CLA	CHD-C4C	4.00	1.48	1.39
31	2	313	CLA	CHD-C4C	4.00	1.48	1.39
31	4	306	CLA	CHB-C1B	4.00	1.48	1.39
31	6	312	CLA	CHB-C1B	4.00	1.48	1.39
31	2	312	CLA	O2A-CGA	4.00	1.45	1.33
31	b	303	CLA	O2A-CGA	4.00	1.45	1.33
31	8	312	CLA	CHC-C4B	4.00	1.48	1.39
31	6	306	CLA	O2A-CGA	4.00	1.45	1.33
31	H	901	CLA	O2A-CGA	4.00	1.45	1.33
31	4	318	CLA	CHD-C4C	4.00	1.48	1.39
31	5	320	CLA	O2A-CGA	4.00	1.45	1.33
30	A	813	CL0	O2A-CGA	4.00	1.45	1.33
31	K	206	CLA	MG-ND	4.00	2.13	2.05
31	3	311	CLA	CHB-C1B	4.00	1.48	1.39
31	7	316	CLA	O2A-CGA	4.00	1.45	1.33
36	L	304	LUT	C35-C34	4.00	1.55	1.43
31	6	313	CLA	CHC-C4B	4.00	1.48	1.39
31	G	205	CLA	CHD-C4C	4.00	1.48	1.39
31	B	840	CLA	CHC-C4B	4.00	1.48	1.39
31	6	322	CLA	O2A-CGA	4.00	1.45	1.33
31	a	312	CLA	O2A-CGA	4.00	1.45	1.33
31	2	315	CLA	O2A-CGA	3.99	1.45	1.33
31	A	853	CLA	O2A-CGA	3.99	1.45	1.33
36	5	304	LUT	C35-C34	3.99	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	320	CLA	CHD-C4C	3.99	1.48	1.39
31	5	315	CLA	CHC-C4B	3.99	1.48	1.39
31	5	314	CLA	CHD-C4C	3.99	1.48	1.39
31	B	830	CLA	CHB-C1B	3.99	1.48	1.39
31	a	310	CLA	CHB-C1B	3.99	1.48	1.39
31	8	320	CLA	CHD-C4C	3.99	1.48	1.39
31	A	833	CLA	CHB-C1B	3.99	1.48	1.39
31	B	832	CLA	CHB-C1B	3.99	1.48	1.39
31	a	322	CLA	CHB-C1B	3.99	1.48	1.39
31	b	305	CLA	CHC-C4B	3.99	1.48	1.39
31	5	321	CLA	O2A-CGA	3.99	1.45	1.33
36	9	305	LUT	C35-C34	3.99	1.55	1.43
32	7	317	CHL	MG-NC	3.99	2.15	2.06
31	B	837	CLA	CHC-C4B	3.99	1.48	1.39
31	4	318	CLA	CHC-C4B	3.99	1.48	1.39
31	4	315	CLA	CHB-C1B	3.99	1.48	1.39
32	4	310	CHL	C2C-C3C	3.99	1.45	1.36
31	b	312	CLA	O2A-CGA	3.99	1.45	1.33
31	a	315	CLA	CHC-C4B	3.98	1.48	1.39
31	b	311	CLA	O2A-CGA	3.98	1.45	1.33
32	b	309	CHL	CHC-C1C	3.98	1.46	1.38
31	b	305	CLA	MG-ND	-3.98	1.97	2.05
31	A	855	CLA	CHC-C4B	3.98	1.48	1.39
31	A	841	CLA	O2A-CGA	3.98	1.45	1.33
31	8	315	CLA	O2A-CGA	3.98	1.45	1.33
32	a	318	CHL	CHC-C1C	3.98	1.46	1.38
31	A	835	CLA	CHB-C1B	3.98	1.48	1.39
31	b	313	CLA	CHB-C1B	3.98	1.48	1.39
31	8	311	CLA	CHB-C1B	3.98	1.48	1.39
31	A	822	CLA	CHB-C1B	3.98	1.48	1.39
31	9	312	CLA	O2A-CGA	3.98	1.45	1.33
31	K	206	CLA	CHD-C4C	3.98	1.48	1.39
36	9	303	LUT	C12-C13	3.98	1.54	1.45
31	3	309	CLA	CHB-C1B	3.98	1.48	1.39
31	B	844	CLA	O2A-CGA	3.98	1.45	1.33
31	7	314	CLA	CHD-C4C	3.98	1.48	1.39
36	a	305	LUT	C12-C13	3.98	1.54	1.45
31	7	316	CLA	CHB-C1B	3.98	1.48	1.39
31	6	316	CLA	CHD-C4C	3.98	1.48	1.39
31	4	319	CLA	CHD-C4C	3.98	1.48	1.39
31	B	846	CLA	CHB-C1B	3.98	1.48	1.39
31	K	204	CLA	CHC-C4B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	314	CLA	CHC-C4B	3.97	1.48	1.39
31	A	836	CLA	CHC-C4B	3.97	1.48	1.39
31	L	306	CLA	CHD-C4C	3.97	1.48	1.39
31	9	319	CLA	O2A-CGA	3.97	1.45	1.33
31	A	843	CLA	CHB-C1B	3.97	1.48	1.39
31	9	314	CLA	CHC-C4B	3.97	1.48	1.39
31	A	834	CLA	CHD-C4C	3.97	1.48	1.39
31	b	303	CLA	CHC-C4B	3.97	1.48	1.39
31	A	850	CLA	CHB-C1B	3.97	1.48	1.39
31	3	316	CLA	CHC-C4B	3.97	1.48	1.39
31	B	812	CLA	O2A-CGA	3.97	1.44	1.33
31	A	830	CLA	CHB-C1B	3.97	1.48	1.39
31	B	839	CLA	CHD-C4C	3.97	1.48	1.39
31	a	311	CLA	CHD-C4C	3.97	1.48	1.39
32	6	320	CHL	CHC-C1C	3.97	1.46	1.38
31	9	315	CLA	CHB-C1B	3.97	1.48	1.39
31	H	902	CLA	O2A-CGA	3.97	1.45	1.33
31	H	903	CLA	CHD-C4C	3.97	1.48	1.39
31	A	823	CLA	CHB-C1B	3.97	1.48	1.39
31	B	827	CLA	O2A-CGA	3.97	1.44	1.33
31	5	318	CLA	CHB-C1B	3.96	1.48	1.39
31	3	319	CLA	CHB-C1B	3.96	1.48	1.39
31	B	811	CLA	O2A-CGA	3.96	1.44	1.33
31	A	851	CLA	CHC-C4B	3.96	1.48	1.39
31	7	314	CLA	CHC-C4B	3.96	1.48	1.39
31	6	311	CLA	CHD-C4C	3.96	1.48	1.39
31	5	308	CLA	O2A-CGA	3.96	1.45	1.33
31	B	821	CLA	CHB-C1B	3.96	1.48	1.39
31	9	319	CLA	CHC-C4B	3.96	1.48	1.39
31	7	312	CLA	CHC-C4B	3.96	1.48	1.39
31	4	308	CLA	CHC-C4B	3.96	1.48	1.39
31	A	823	CLA	CHD-C4C	3.96	1.48	1.39
35	9	304	QTB	C03-C02	3.96	1.41	1.35
31	6	314	CLA	CHC-C4B	3.96	1.48	1.39
31	4	306	CLA	MG-NB	3.96	2.13	2.05
31	2	308	CLA	O2A-CGA	3.96	1.45	1.33
36	a	305	LUT	C35-C34	3.96	1.55	1.43
31	5	311	CLA	CHB-C1B	3.96	1.48	1.39
36	9	303	LUT	C8-C9	3.95	1.54	1.45
31	2	304	CLA	O2A-CGA	3.95	1.45	1.33
31	B	838	CLA	CHB-C1B	3.95	1.48	1.39
31	3	314	CLA	CHB-C1B	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	302	CLA	CHC-C4B	3.95	1.48	1.39
31	2	304	CLA	CHD-C4C	3.95	1.48	1.39
31	A	828	CLA	CHB-C1B	3.95	1.48	1.39
31	A	816	CLA	MG-NA	3.95	2.15	2.06
31	B	848	CLA	CHC-C4B	3.95	1.48	1.39
31	8	318	CLA	MG-NC	3.95	2.15	2.06
31	a	311	CLA	CHC-C4B	3.95	1.48	1.39
31	A	846	CLA	MG-ND	3.95	2.13	2.05
31	9	318	CLA	CHD-C4C	3.95	1.48	1.39
31	A	845	CLA	CHC-C4B	3.95	1.48	1.39
31	5	312	CLA	CHD-C4C	3.95	1.48	1.39
31	B	824	CLA	CHB-C1B	3.95	1.48	1.39
31	B	835	CLA	CHC-C4B	3.95	1.48	1.39
31	5	307	CLA	CHB-C1B	3.95	1.48	1.39
31	5	307	CLA	CHC-C4B	3.95	1.48	1.39
31	4	311	CLA	O2A-CGA	3.95	1.45	1.33
31	a	315	CLA	CHD-C4C	3.95	1.48	1.39
31	H	901	CLA	CHC-C4B	3.95	1.48	1.39
31	A	832	CLA	O2A-CGA	3.95	1.44	1.33
31	B	815	CLA	CHB-C1B	3.95	1.48	1.39
31	A	853	CLA	CHB-C1B	3.95	1.48	1.39
31	A	849	CLA	CHD-C4C	3.95	1.48	1.39
36	a	305	LUT	C28-C29	3.95	1.54	1.45
31	b	307	CLA	CHD-C4C	3.95	1.48	1.39
31	A	834	CLA	O2A-CGA	3.95	1.44	1.33
31	8	311	CLA	CHD-C4C	3.95	1.48	1.39
31	A	856	CLA	CHB-C1B	3.95	1.48	1.39
31	B	831	CLA	CHC-C4B	3.94	1.48	1.39
31	B	842	CLA	CHC-C4B	3.94	1.48	1.39
36	6	303	LUT	C35-C34	3.94	1.55	1.43
31	3	308	CLA	O2A-CGA	3.94	1.45	1.33
31	8	317	CLA	CHB-C1B	3.94	1.48	1.39
32	A	831	CHL	CHC-C1C	3.94	1.46	1.38
31	O	203	CLA	CHD-C4C	3.94	1.48	1.39
31	5	323	CLA	CHC-C4B	3.94	1.48	1.39
32	a	320	CHL	CHC-C1C	3.94	1.46	1.38
31	A	830	CLA	CHC-C4B	3.94	1.48	1.39
31	A	832	CLA	CHB-C1B	3.94	1.48	1.39
31	a	319	CLA	CHC-C4B	3.94	1.48	1.39
31	9	319	CLA	CHD-C4C	3.94	1.48	1.39
31	H	903	CLA	CHC-C4B	3.94	1.48	1.39
31	2	307	CLA	CHB-C1B	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	837	CLA	CHD-C4C	3.94	1.48	1.39
31	A	817	CLA	CHC-C4B	3.94	1.48	1.39
31	A	852	CLA	CHB-C1B	3.94	1.48	1.39
31	3	318	CLA	CHD-C4C	3.94	1.48	1.39
31	2	315	CLA	CHC-C4B	3.93	1.48	1.39
32	8	316	CHL	CHC-C1C	3.93	1.46	1.38
31	9	311	CLA	CHC-C4B	3.93	1.48	1.39
32	6	321	CHL	C2C-C3C	3.93	1.45	1.36
31	A	821	CLA	CHB-C1B	3.93	1.48	1.39
31	A	827	CLA	MG-NC	3.93	2.15	2.06
31	9	316	CLA	CHC-C4B	3.93	1.48	1.39
36	6	304	LUT	C8-C9	3.93	1.54	1.45
32	7	318	CHL	C2C-C3C	3.93	1.45	1.36
31	7	311	CLA	CHD-C4C	3.93	1.48	1.39
31	a	322	CLA	CHC-C4B	3.93	1.48	1.39
32	8	319	CHL	C2C-C3C	3.93	1.45	1.36
31	B	846	CLA	CHC-C4B	3.93	1.48	1.39
31	B	828	CLA	O2A-CGA	3.93	1.44	1.33
31	A	824	CLA	CHD-C4C	3.93	1.48	1.39
31	8	315	CLA	CHC-C4B	3.93	1.48	1.39
31	B	827	CLA	CHD-C4C	3.93	1.48	1.39
31	3	316	CLA	CHD-C4C	3.93	1.48	1.39
31	9	312	CLA	CHC-C4B	3.93	1.48	1.39
31	A	827	CLA	CHB-C1B	3.93	1.48	1.39
31	F	305	CLA	O2A-CGA	3.92	1.45	1.33
31	7	309	CLA	CHD-C4C	3.92	1.48	1.39
31	a	314	CLA	MG-NA	-3.92	1.97	2.06
31	B	827	CLA	CHB-C1B	3.92	1.48	1.39
31	7	311	CLA	O2A-CGA	3.92	1.44	1.33
32	7	318	CHL	CHC-C1C	3.92	1.46	1.38
31	F	305	CLA	CHB-C1B	3.92	1.48	1.39
31	8	318	CLA	CHB-C1B	3.92	1.48	1.39
32	A	839	CHL	CHC-C1C	3.92	1.46	1.38
32	7	324	CHL	CHC-C1C	3.92	1.46	1.38
31	A	842	CLA	CHC-C4B	3.92	1.48	1.39
31	L	306	CLA	CHC-C4B	3.92	1.48	1.39
31	b	304	CLA	CHD-C4C	3.92	1.48	1.39
31	B	821	CLA	CHC-C4B	3.92	1.48	1.39
31	8	318	CLA	CHD-C4C	3.92	1.48	1.39
31	9	313	CLA	CHD-C4C	3.92	1.48	1.39
31	A	845	CLA	CHD-C4C	3.92	1.48	1.39
31	3	310	CLA	CHD-C4C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	103	LUT	C12-C13	3.92	1.54	1.45
31	6	322	CLA	CHD-C4C	3.92	1.48	1.39
31	a	310	CLA	CHC-C4B	3.92	1.48	1.39
31	B	819	CLA	CHB-C1B	3.91	1.48	1.39
32	5	322	CHL	C2C-C3C	3.91	1.45	1.36
31	3	316	CLA	CHB-C1B	3.91	1.48	1.39
31	a	316	CLA	CHB-C1B	3.91	1.48	1.39
31	B	845	CLA	CHB-C1B	3.91	1.48	1.39
36	4	302	LUT	C35-C34	3.91	1.55	1.43
32	4	317	CHL	C2C-C3C	3.91	1.45	1.36
31	a	313	CLA	CHD-C4C	3.91	1.48	1.39
31	B	826	CLA	CHC-C4B	3.91	1.48	1.39
31	B	839	CLA	CHB-C1B	3.91	1.48	1.39
31	8	313	CLA	CHD-C4C	3.91	1.48	1.39
31	8	315	CLA	MG-NC	3.91	2.15	2.06
31	B	843	CLA	CHB-C1B	3.91	1.48	1.39
31	b	311	CLA	CHD-C4C	3.90	1.48	1.39
31	7	321	CLA	CHC-C4B	3.90	1.48	1.39
31	G	204	CLA	CHC-C4B	3.90	1.48	1.39
31	A	852	CLA	CHC-C4B	3.90	1.48	1.39
36	8	303	LUT	C8-C9	3.90	1.54	1.45
31	A	819	CLA	CHC-C4B	3.90	1.48	1.39
31	4	307	CLA	CHC-C4B	3.90	1.48	1.39
31	b	305	CLA	CHD-C4C	3.90	1.48	1.39
31	A	854	CLA	CHB-C1B	3.90	1.48	1.39
31	A	849	CLA	CHC-C4B	3.90	1.48	1.39
31	A	836	CLA	CHD-C4C	3.90	1.48	1.39
32	6	317	CHL	C2C-C3C	3.90	1.45	1.36
31	2	310	CLA	CHD-C4C	3.90	1.48	1.39
31	3	308	CLA	CHD-C4C	3.89	1.48	1.39
31	2	314	CLA	CHD-C4C	3.89	1.48	1.39
31	7	315	CLA	CHC-C4B	3.89	1.48	1.39
36	5	303	LUT	C8-C9	3.89	1.54	1.45
32	5	316	CHL	CHC-C1C	3.89	1.46	1.38
31	B	844	CLA	CHC-C4B	3.89	1.48	1.39
36	4	303	LUT	C12-C13	3.89	1.54	1.45
31	G	204	CLA	CHD-C4C	3.89	1.48	1.39
32	3	315	CHL	MG-NC	-3.89	1.97	2.06
31	B	844	CLA	CHB-C1B	3.89	1.48	1.39
31	B	841	CLA	CHB-C1B	3.89	1.48	1.39
31	8	312	CLA	CHD-C4C	3.89	1.48	1.39
31	7	313	CLA	CHC-C4B	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	310	CLA	CHC-C4B	3.89	1.48	1.39
36	9	302	LUT	C35-C34	3.89	1.55	1.43
31	A	837	CLA	CHC-C4B	3.89	1.48	1.39
31	G	206	CLA	CHB-C1B	3.89	1.48	1.39
31	9	311	CLA	CHB-C1B	3.89	1.48	1.39
31	A	832	CLA	CHD-C4C	3.88	1.48	1.39
31	B	843	CLA	MG-ND	-3.88	1.98	2.05
32	7	317	CHL	CHC-C1C	3.88	1.46	1.38
31	B	821	CLA	CHD-C4C	3.88	1.48	1.39
32	5	322	CHL	CHC-C1C	3.88	1.46	1.38
31	A	821	CLA	O2A-CGA	3.88	1.44	1.33
31	L	305	CLA	CHD-C4C	3.88	1.48	1.39
31	B	828	CLA	CHC-C4B	3.88	1.48	1.39
36	a	303	LUT	C35-C34	3.88	1.55	1.43
31	3	317	CLA	CHD-C4C	3.88	1.48	1.39
31	B	813	CLA	CHB-C1B	3.88	1.48	1.39
31	9	311	CLA	CHD-C4C	3.88	1.48	1.39
31	7	322	CLA	CHC-C4B	3.88	1.48	1.39
31	7	312	CLA	CHD-C4C	3.88	1.48	1.39
31	4	306	CLA	CHD-C4C	3.88	1.48	1.39
31	A	816	CLA	CHC-C4B	3.88	1.48	1.39
31	a	316	CLA	CHC-C4B	3.87	1.48	1.39
31	B	850	CLA	CHB-C1B	3.87	1.48	1.39
31	J	105	CLA	CHC-C4B	3.87	1.48	1.39
31	A	851	CLA	CHD-C4C	3.87	1.48	1.39
31	G	204	CLA	CHB-C1B	3.87	1.48	1.39
31	7	312	CLA	MG-ND	3.87	2.13	2.05
31	B	814	CLA	CHC-C4B	3.87	1.48	1.39
31	B	815	CLA	CHC-C4B	3.87	1.48	1.39
31	A	828	CLA	CHD-C4C	3.87	1.48	1.39
36	b	301	LUT	C15-C14	3.87	1.55	1.43
32	4	310	CHL	CHC-C1C	3.87	1.46	1.38
31	G	206	CLA	CHD-C4C	3.87	1.48	1.39
31	6	315	CLA	CHD-C4C	3.87	1.48	1.39
31	A	824	CLA	CHB-C1B	3.87	1.48	1.39
31	4	311	CLA	CHD-C4C	3.87	1.48	1.39
32	9	322	CHL	C2C-C3C	3.87	1.45	1.36
32	5	319	CHL	C2C-C3C	3.87	1.45	1.36
31	B	849	CLA	CHC-C4B	3.87	1.48	1.39
36	3	304	LUT	C8-C9	3.86	1.54	1.45
31	3	318	CLA	CHC-C4B	3.86	1.48	1.39
32	5	322	CHL	CHD-C1D	3.86	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	H	902	CLA	CHD-C4C	3.86	1.48	1.39
31	5	308	CLA	CHD-C4C	3.86	1.48	1.39
31	B	817	CLA	CHB-C1B	3.86	1.48	1.39
31	B	841	CLA	CHC-C4B	3.86	1.48	1.39
31	9	316	CLA	CHD-C4C	3.86	1.48	1.39
31	B	833	CLA	CHC-C4B	3.86	1.48	1.39
31	3	319	CLA	CHD-C4C	3.86	1.48	1.39
31	a	313	CLA	CHC-C4B	3.86	1.48	1.39
31	5	318	CLA	CHC-C4B	3.86	1.48	1.39
31	7	315	CLA	CHD-C4C	3.85	1.48	1.39
32	8	319	CHL	CHC-C1C	3.85	1.46	1.38
31	B	820	CLA	CHD-C4C	3.85	1.48	1.39
31	6	314	CLA	CHD-C4C	3.85	1.48	1.39
32	6	309	CHL	C2C-C3C	3.85	1.45	1.36
31	A	827	CLA	CHC-C4B	3.85	1.48	1.39
31	A	835	CLA	CHD-C4C	3.85	1.48	1.39
31	A	849	CLA	CHB-C1B	3.85	1.48	1.39
31	K	205	CLA	CHC-C4B	3.85	1.48	1.39
31	3	312	CLA	CHC-C4B	3.85	1.48	1.39
31	B	823	CLA	CHD-C4C	3.85	1.48	1.39
31	5	321	CLA	CHD-C4C	3.85	1.48	1.39
36	4	303	LUT	C11-C10	3.85	1.55	1.43
31	B	842	CLA	CHB-C1B	3.85	1.48	1.39
31	B	822	CLA	CHC-C4B	3.84	1.48	1.39
31	a	319	CLA	CHD-C4C	3.84	1.48	1.39
32	3	315	CHL	CHC-C1C	3.84	1.46	1.38
31	B	823	CLA	CHC-C4B	3.84	1.48	1.39
36	a	305	LUT	C31-C30	3.84	1.55	1.43
31	8	314	CLA	CHC-C4B	3.84	1.48	1.39
31	A	842	CLA	CHD-C4C	3.84	1.48	1.39
31	3	309	CLA	CHD-C4C	3.84	1.48	1.39
31	B	829	CLA	CHD-C4C	3.84	1.48	1.39
31	B	828	CLA	MG-NB	3.84	2.13	2.05
31	5	307	CLA	CHD-C4C	3.84	1.48	1.39
31	8	315	CLA	CHB-C1B	3.84	1.48	1.39
36	9	305	LUT	C32-C33	3.84	1.54	1.45
31	B	848	CLA	CHD-C4C	3.84	1.48	1.39
31	2	305	CLA	CHD-C4C	3.84	1.48	1.39
31	A	841	CLA	CHC-C4B	3.83	1.48	1.39
36	5	303	LUT	C35-C34	3.83	1.55	1.43
31	2	307	CLA	CHD-C4C	3.83	1.48	1.39
31	6	308	CLA	CHC-C4B	3.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	320	CLA	MG-NA	-3.83	1.97	2.06
36	J	103	LUT	C15-C14	3.83	1.55	1.43
31	a	321	CLA	CHC-C4B	3.83	1.48	1.39
32	6	317	CHL	CHC-C1C	3.83	1.46	1.38
32	5	319	CHL	CHC-C1C	3.83	1.46	1.38
36	b	301	LUT	C8-C9	3.83	1.54	1.45
31	8	320	CLA	CHC-C4B	3.82	1.48	1.39
31	A	819	CLA	CHB-C1B	3.82	1.48	1.39
31	5	311	CLA	CHC-C4B	3.82	1.48	1.39
31	K	204	CLA	CHD-C4C	3.82	1.48	1.39
32	6	309	CHL	CHC-C1C	3.82	1.46	1.38
31	A	828	CLA	CHC-C4B	3.82	1.48	1.39
36	6	303	LUT	C8-C9	3.82	1.54	1.45
31	A	848	CLA	CHD-C4C	3.82	1.48	1.39
31	B	826	CLA	CHD-C4C	3.82	1.48	1.39
32	4	313	CHL	CHC-C1C	3.82	1.46	1.38
31	6	313	CLA	CHD-C4C	3.82	1.48	1.39
32	b	309	CHL	C2C-C3C	3.82	1.45	1.36
31	2	312	CLA	OBD-CAD	3.82	1.29	1.22
36	2	301	LUT	C35-C34	3.81	1.55	1.43
31	F	306	CLA	CHD-C4C	3.81	1.47	1.39
31	A	842	CLA	O2A-CGA	3.81	1.44	1.33
32	4	310	CHL	CHD-C1D	3.81	1.45	1.38
31	B	830	CLA	CHC-C4B	3.81	1.48	1.39
36	4	303	LUT	C15-C14	3.81	1.55	1.43
31	A	816	CLA	CHD-C4C	3.81	1.47	1.39
31	B	819	CLA	CHD-C4C	3.81	1.47	1.39
32	6	318	CHL	CHC-C1C	3.81	1.46	1.38
31	F	306	CLA	CHC-C4B	3.81	1.48	1.39
31	A	825	CLA	CHD-C4C	3.81	1.47	1.39
31	B	824	CLA	CHD-C4C	3.81	1.47	1.39
31	B	822	CLA	MG-ND	3.81	2.13	2.05
36	4	303	LUT	C28-C29	3.81	1.54	1.45
31	4	321	CLA	CHD-C4C	3.81	1.47	1.39
31	9	315	CLA	CHC-C4B	3.81	1.47	1.39
31	4	316	CLA	CHC-C4B	3.80	1.47	1.39
31	A	817	CLA	MG-NC	3.80	2.15	2.06
31	A	852	CLA	CHD-C4C	3.80	1.47	1.39
31	3	310	CLA	CHC-C4B	3.80	1.47	1.39
32	6	319	CHL	C2C-C3C	3.80	1.44	1.36
32	7	319	CHL	C2C-C3C	3.80	1.44	1.36
31	B	825	CLA	CHD-C4C	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	844	CLA	CHD-C4C	3.80	1.47	1.39
31	B	849	CLA	CHD-C4C	3.80	1.47	1.39
32	a	317	CHL	CHC-C1C	3.80	1.46	1.38
32	A	831	CHL	C2C-C3C	3.80	1.44	1.36
31	A	844	CLA	CHB-C1B	3.80	1.47	1.39
36	9	305	LUT	C8-C9	3.80	1.54	1.45
31	A	818	CLA	CHD-C4C	3.80	1.47	1.39
32	4	313	CHL	C2C-C3C	3.80	1.44	1.36
31	A	834	CLA	CHC-C4B	3.80	1.47	1.39
32	5	319	CHL	CHD-C1D	3.80	1.45	1.38
31	A	821	CLA	CHC-C4B	3.80	1.47	1.39
31	A	821	CLA	CHD-C4C	3.80	1.47	1.39
31	8	311	CLA	CHC-C4B	3.80	1.47	1.39
31	G	206	CLA	CHC-C4B	3.79	1.47	1.39
36	9	305	LUT	C15-C14	3.79	1.55	1.43
36	6	304	LUT	C12-C13	3.79	1.54	1.45
36	4	303	LUT	C31-C30	3.79	1.55	1.43
31	B	849	CLA	CHB-C1B	3.79	1.47	1.39
31	A	829	CLA	MG-NA	3.79	2.15	2.06
36	a	303	LUT	C31-C30	3.79	1.55	1.43
31	K	206	CLA	CHC-C4B	3.79	1.47	1.39
31	A	818	CLA	C1B-NB	-3.79	1.33	1.37
32	6	320	CHL	C2C-C3C	3.79	1.44	1.36
31	A	833	CLA	CHC-C4B	3.79	1.47	1.39
31	8	314	CLA	CHD-C4C	3.79	1.47	1.39
32	a	317	CHL	C2C-C3C	3.78	1.44	1.36
31	2	311	CLA	OBD-CAD	3.78	1.29	1.22
31	b	302	CLA	CHD-C4C	3.78	1.47	1.39
31	4	319	CLA	OBD-CAD	3.78	1.29	1.22
31	A	853	CLA	CHC-C4B	3.78	1.47	1.39
31	B	843	CLA	CHD-C4C	3.78	1.47	1.39
31	3	307	CLA	CHD-C4C	3.78	1.47	1.39
31	8	308	CLA	CHD-C4C	3.78	1.47	1.39
31	A	847	CLA	CHD-C4C	3.78	1.47	1.39
31	A	815	CLA	CHB-C1B	3.78	1.47	1.39
36	4	302	LUT	C15-C14	3.78	1.55	1.43
32	6	318	CHL	CHD-C1D	3.78	1.45	1.38
31	A	856	CLA	CHD-C4C	3.77	1.47	1.39
31	6	306	CLA	CHD-C4C	3.77	1.47	1.39
36	6	303	LUT	C15-C14	3.77	1.55	1.43
31	A	846	CLA	CHC-C4B	3.77	1.47	1.39
32	7	320	CHL	CHC-C1C	3.77	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	854	CLA	CHC-C4B	3.77	1.47	1.39
31	B	842	CLA	CHD-C4C	3.77	1.47	1.39
31	B	841	CLA	MG-NB	3.77	2.13	2.05
31	7	322	CLA	CHD-C4C	3.77	1.47	1.39
31	A	827	CLA	CHD-C4C	3.77	1.47	1.39
31	A	833	CLA	CHD-C4C	3.77	1.47	1.39
31	8	321	CLA	CHD-C4C	3.77	1.47	1.39
31	A	822	CLA	CHC-C4B	3.77	1.47	1.39
31	6	310	CLA	CHD-C4C	3.77	1.47	1.39
31	A	843	CLA	CHC-C4B	3.77	1.47	1.39
31	5	311	CLA	CHD-C4C	3.77	1.47	1.39
31	4	308	CLA	CHD-C4C	3.77	1.47	1.39
31	A	842	CLA	CHB-C1B	3.77	1.47	1.39
31	A	848	CLA	CHC-C4B	3.77	1.47	1.39
31	B	836	CLA	CHB-C1B	3.76	1.47	1.39
36	8	303	LUT	C35-C34	3.76	1.55	1.43
31	B	816	CLA	CHD-C4C	3.76	1.47	1.39
31	A	826	CLA	CHC-C4B	3.76	1.47	1.39
31	4	321	CLA	OBD-CAD	3.76	1.29	1.22
32	5	317	CHL	C2C-C3C	3.76	1.44	1.36
32	9	322	CHL	CHC-C1C	3.76	1.46	1.38
36	9	305	LUT	C31-C30	3.76	1.55	1.43
31	A	817	CLA	CHD-C4C	3.76	1.47	1.39
31	A	847	CLA	CHB-C1B	3.76	1.47	1.39
31	a	309	CLA	CHD-C4C	3.76	1.47	1.39
32	5	316	CHL	CHD-C1D	3.76	1.45	1.38
31	A	820	CLA	CHC-C4B	3.76	1.47	1.39
36	6	304	LUT	C15-C14	3.76	1.55	1.43
36	9	305	LUT	C28-C29	3.76	1.54	1.45
31	B	834	CLA	CHB-C1B	3.76	1.47	1.39
31	B	830	CLA	CHD-C4C	3.76	1.47	1.39
31	A	856	CLA	CHC-C4B	3.76	1.47	1.39
31	B	834	CLA	CHC-C4B	3.75	1.47	1.39
36	4	302	LUT	C12-C13	3.75	1.54	1.45
31	9	317	CLA	CHD-C4C	3.75	1.47	1.39
31	4	309	CLA	CHD-C4C	3.75	1.47	1.39
31	A	853	CLA	CHD-C4C	3.75	1.47	1.39
31	B	814	CLA	CHB-C1B	3.75	1.47	1.39
31	A	850	CLA	CHC-C4B	3.75	1.47	1.39
31	A	830	CLA	CHD-C4C	3.75	1.47	1.39
31	B	845	CLA	CHC-C4B	3.75	1.47	1.39
31	B	839	CLA	CHC-C4B	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	313	CLA	CHD-C4C	3.75	1.47	1.39
31	B	811	CLA	CHB-C1B	3.75	1.47	1.39
36	L	304	LUT	C31-C30	3.75	1.55	1.43
31	H	901	CLA	OBD-CAD	3.75	1.28	1.22
32	9	320	CHL	CHC-C1C	3.75	1.46	1.38
31	3	311	CLA	CHC-C4B	3.74	1.47	1.39
35	7	303	QTB	C03-C02	3.74	1.40	1.35
31	5	323	CLA	CHD-C4C	3.74	1.47	1.39
31	B	845	CLA	CHD-C4C	3.74	1.47	1.39
36	2	301	LUT	C31-C30	3.74	1.55	1.43
31	a	312	CLA	CHD-C4C	3.74	1.47	1.39
36	L	304	LUT	C12-C13	3.74	1.54	1.45
31	O	204	CLA	OBD-CAD	3.74	1.28	1.22
31	B	818	CLA	MG-NB	-3.74	1.98	2.05
31	A	818	CLA	CHC-C4B	3.74	1.47	1.39
32	6	318	CHL	C2C-C3C	3.74	1.44	1.36
31	B	838	CLA	CHD-C4C	3.74	1.47	1.39
31	8	317	CLA	CHD-C4C	3.74	1.47	1.39
31	A	829	CLA	C3D-C4D	-3.74	1.35	1.44
36	J	103	LUT	C31-C30	3.74	1.55	1.43
36	5	303	LUT	C15-C14	3.73	1.55	1.43
36	4	303	LUT	C32-C33	3.73	1.54	1.45
31	B	829	CLA	CHC-C4B	3.73	1.47	1.39
31	5	320	CLA	OBD-CAD	3.73	1.28	1.22
36	a	305	LUT	C11-C10	3.73	1.55	1.43
31	B	816	CLA	CHC-C4B	3.73	1.47	1.39
32	3	315	CHL	C2C-C3C	3.73	1.44	1.36
31	A	837	CLA	CHD-C4C	3.73	1.47	1.39
31	9	312	CLA	CHD-C4C	3.73	1.47	1.39
36	9	303	LUT	C15-C14	3.73	1.55	1.43
31	8	321	CLA	CHC-C4B	3.73	1.47	1.39
36	2	301	LUT	C28-C29	3.73	1.54	1.45
32	a	318	CHL	C2C-C3C	3.73	1.44	1.36
36	6	303	LUT	C31-C30	3.73	1.55	1.43
36	a	305	LUT	C26-C27	3.73	1.55	1.50
31	7	321	CLA	CHD-C4C	3.73	1.47	1.39
31	A	834	CLA	CHB-C1B	3.73	1.47	1.39
31	A	843	CLA	CHD-C4C	3.73	1.47	1.39
31	B	833	CLA	CHD-C4C	3.73	1.47	1.39
31	A	817	CLA	CHB-C1B	3.73	1.47	1.39
31	4	309	CLA	CHC-C4B	3.72	1.47	1.39
32	a	320	CHL	CHD-C1D	3.72	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	838	CLA	CHD-C4C	3.72	1.47	1.39
31	B	824	CLA	CHC-C4B	3.72	1.47	1.39
32	b	309	CHL	CHD-C1D	3.72	1.45	1.38
32	4	313	CHL	CHD-C1D	3.72	1.45	1.38
31	2	315	CLA	CHD-C4C	3.72	1.47	1.39
31	9	314	CLA	CHD-C4C	3.72	1.47	1.39
36	4	302	LUT	C31-C30	3.72	1.55	1.43
32	6	319	CHL	CHD-C1D	3.72	1.45	1.38
31	9	316	CLA	OBD-CAD	3.72	1.28	1.22
31	8	318	CLA	CHC-C4B	3.71	1.47	1.39
36	7	305	LUT	C35-C34	3.71	1.55	1.43
36	a	305	LUT	C15-C14	3.71	1.55	1.43
31	B	840	CLA	CHD-C4C	3.71	1.47	1.39
36	8	302	LUT	C15-C14	3.71	1.54	1.43
31	B	836	CLA	CHD-C4C	3.71	1.47	1.39
35	a	302	QTB	C03-C02	3.71	1.40	1.35
31	F	305	CLA	CHC-C4B	3.71	1.47	1.39
36	b	301	LUT	C31-C30	3.71	1.54	1.43
32	K	201	CHL	CHD-C4C	3.71	1.47	1.39
32	a	320	CHL	C2C-C3C	3.71	1.44	1.36
32	6	319	CHL	CHC-C1C	3.71	1.46	1.38
31	A	841	CLA	CHB-C1B	3.70	1.47	1.39
36	3	305	LUT	C35-C34	3.70	1.54	1.43
31	F	301	CLA	CHB-C1B	3.70	1.47	1.39
31	B	813	CLA	CHD-C4C	3.70	1.47	1.39
31	7	314	CLA	MG-ND	-3.70	1.98	2.05
31	A	854	CLA	CHD-C4C	3.70	1.47	1.39
31	J	105	CLA	CHD-C4C	3.70	1.47	1.39
36	9	303	LUT	C11-C10	3.70	1.54	1.43
32	A	840	CHL	C2C-C3C	3.70	1.44	1.36
31	A	815	CLA	C1D-ND	-3.70	1.33	1.37
36	J	103	LUT	C11-C10	3.70	1.54	1.43
32	7	318	CHL	CHD-C1D	3.70	1.45	1.38
31	B	835	CLA	CHD-C4C	3.70	1.47	1.39
31	6	306	CLA	C4D-CHA	3.69	1.51	1.38
32	7	320	CHL	C2C-C3C	3.69	1.44	1.36
31	L	307	CLA	MG-NC	-3.69	1.97	2.06
31	A	857	CLA	CHC-C4B	3.69	1.47	1.39
31	3	311	CLA	CHD-C4C	3.69	1.47	1.39
32	4	317	CHL	CHC-C1C	3.69	1.46	1.38
31	B	812	CLA	CHC-C4B	3.69	1.47	1.39
36	5	304	LUT	C11-C10	3.68	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	314	CLA	OBD-CAD	3.68	1.28	1.22
31	B	819	CLA	CHC-C4B	3.68	1.47	1.39
36	b	301	LUT	C12-C13	3.68	1.53	1.45
36	7	305	LUT	C8-C9	3.68	1.53	1.45
36	a	303	LUT	C15-C14	3.68	1.54	1.43
31	A	826	CLA	CHD-C4C	3.68	1.47	1.39
31	A	846	CLA	CHD-C4C	3.68	1.47	1.39
31	B	831	CLA	CHD-C4C	3.68	1.47	1.39
36	3	304	LUT	C7-C6	3.68	1.58	1.45
31	A	848	CLA	CHB-C1B	3.68	1.47	1.39
32	7	318	CHL	MG-NB	3.68	2.13	2.05
31	8	307	CLA	CHD-C4C	3.68	1.47	1.39
36	3	305	LUT	C31-C30	3.68	1.54	1.43
36	9	305	LUT	C11-C10	3.68	1.54	1.43
31	5	310	CLA	CHD-C4C	3.67	1.47	1.39
31	F	305	CLA	CHD-C4C	3.67	1.47	1.39
31	A	838	CLA	CHC-C4B	3.67	1.47	1.39
36	L	304	LUT	C32-C33	3.67	1.53	1.45
36	3	304	LUT	C35-C34	3.67	1.54	1.43
31	A	841	CLA	CHD-C4C	3.67	1.47	1.39
31	A	844	CLA	CHC-C4B	3.67	1.47	1.39
32	5	316	CHL	C2C-C3C	3.67	1.44	1.36
31	A	818	CLA	CHB-C1B	3.66	1.47	1.39
31	B	847	CLA	CHD-C4C	3.66	1.47	1.39
31	b	303	CLA	OBD-CAD	3.66	1.28	1.22
31	B	823	CLA	MG-ND	3.66	2.13	2.05
31	2	304	CLA	OBD-CAD	3.66	1.28	1.22
31	A	820	CLA	CHD-C4C	3.66	1.47	1.39
36	L	304	LUT	C15-C14	3.66	1.54	1.43
31	6	306	CLA	MG-ND	3.66	2.13	2.05
32	7	320	CHL	CHD-C1D	3.66	1.45	1.38
31	B	812	CLA	CHD-C4C	3.66	1.47	1.39
31	9	317	CLA	MG-NB	3.66	2.13	2.05
31	5	313	CLA	CHD-C4C	3.66	1.47	1.39
31	4	306	CLA	OBD-CAD	3.66	1.28	1.22
36	4	302	LUT	C11-C10	3.66	1.54	1.43
32	6	321	CHL	CHD-C1D	3.65	1.45	1.38
36	J	103	LUT	C32-C33	3.65	1.53	1.45
32	4	317	CHL	CHD-C1D	3.65	1.45	1.38
31	4	312	CLA	OBD-CAD	3.65	1.28	1.22
36	3	304	LUT	C31-C30	3.65	1.54	1.43
31	5	314	CLA	OBD-CAD	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	103	LUT	C28-C29	3.65	1.53	1.45
31	A	841	CLA	MG-NB	3.65	2.13	2.05
31	3	320	CLA	OBD-CAD	3.65	1.28	1.22
36	2	301	LUT	C15-C14	3.65	1.54	1.43
31	B	843	CLA	OBD-CAD	3.65	1.28	1.22
36	9	302	LUT	C31-C30	3.65	1.54	1.43
31	A	844	CLA	CHD-C4C	3.65	1.47	1.39
31	B	848	CLA	MG-NB	3.65	2.13	2.05
31	8	317	CLA	CHC-C4B	3.65	1.47	1.39
36	F	304	LUT	C35-C34	3.64	1.54	1.43
36	5	304	LUT	C15-C14	3.64	1.54	1.43
31	B	822	CLA	CHD-C4C	3.64	1.47	1.39
32	8	316	CHL	C2C-C3C	3.64	1.44	1.36
31	F	301	CLA	CHD-C4C	3.64	1.47	1.39
31	a	310	CLA	MG-NB	3.64	2.13	2.05
31	2	305	CLA	OBD-CAD	3.64	1.28	1.22
31	6	316	CLA	OBD-CAD	3.64	1.28	1.22
31	H	903	CLA	OBD-CAD	3.64	1.28	1.22
36	a	303	LUT	C8-C9	3.64	1.53	1.45
31	L	307	CLA	OBD-CAD	3.64	1.28	1.22
31	b	302	CLA	OBD-CAD	3.64	1.28	1.22
31	B	818	CLA	CHD-C4C	3.64	1.47	1.39
36	5	303	LUT	C31-C30	3.64	1.54	1.43
31	G	205	CLA	OBD-CAD	3.64	1.28	1.22
36	6	303	LUT	C28-C29	3.64	1.53	1.45
31	A	857	CLA	CHD-C4C	3.64	1.47	1.39
31	b	308	CLA	OBD-CAD	3.64	1.28	1.22
31	2	308	CLA	CHD-C4C	3.64	1.47	1.39
31	3	313	CLA	OBD-CAD	3.64	1.28	1.22
36	9	305	LUT	C12-C13	3.64	1.53	1.45
31	B	841	CLA	CHD-C4C	3.63	1.47	1.39
32	7	317	CHL	C2C-C3C	3.63	1.44	1.36
36	a	303	LUT	C12-C13	3.63	1.53	1.45
31	L	306	CLA	OBD-CAD	3.63	1.28	1.22
31	3	318	CLA	OBD-CAD	3.63	1.28	1.22
31	a	316	CLA	OBD-CAD	3.63	1.28	1.22
31	B	846	CLA	C1D-ND	-3.63	1.33	1.37
31	K	206	CLA	OBD-CAD	3.63	1.28	1.22
31	A	815	CLA	CHC-C4B	3.63	1.47	1.39
31	B	811	CLA	CHC-C4B	3.63	1.47	1.39
31	B	811	CLA	CHD-C4C	3.63	1.47	1.39
36	a	303	LUT	C28-C29	3.63	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	832	CLA	CHC-C4B	3.63	1.47	1.39
31	B	838	CLA	CHC-C4B	3.63	1.47	1.39
32	a	318	CHL	CHD-C1D	3.62	1.45	1.38
36	6	303	LUT	C11-C10	3.62	1.54	1.43
31	B	820	CLA	MG-ND	-3.62	1.98	2.05
31	B	850	CLA	CHD-C4C	3.62	1.47	1.39
36	6	304	LUT	C32-C33	3.62	1.53	1.45
31	4	316	CLA	OBD-CAD	3.62	1.28	1.22
30	A	813	CL0	C3C-C2C	3.62	1.44	1.36
31	A	814	CLA	C1D-ND	-3.61	1.33	1.37
36	9	302	LUT	C8-C9	3.61	1.53	1.45
31	B	832	CLA	CHD-C4C	3.61	1.47	1.39
36	3	305	LUT	C8-C9	3.61	1.53	1.45
36	6	303	LUT	C26-C27	3.61	1.55	1.50
36	6	304	LUT	C31-C30	3.61	1.54	1.43
31	9	315	CLA	CHD-C4C	3.61	1.47	1.39
31	A	818	CLA	C1D-ND	-3.61	1.33	1.37
31	4	318	CLA	OBD-CAD	3.61	1.28	1.22
31	5	307	CLA	OBD-CAD	3.61	1.28	1.22
32	a	317	CHL	CHD-C1D	3.61	1.45	1.38
36	7	305	LUT	C31-C30	3.61	1.54	1.43
31	6	314	CLA	OBD-CAD	3.61	1.28	1.22
31	A	815	CLA	CHD-C4C	3.61	1.47	1.39
36	b	301	LUT	C28-C29	3.61	1.53	1.45
31	2	313	CLA	OBD-CAD	3.61	1.28	1.22
36	3	305	LUT	C32-C33	3.60	1.53	1.45
31	b	310	CLA	OBD-CAD	3.60	1.28	1.22
31	B	827	CLA	CHC-C4B	3.60	1.47	1.39
31	A	829	CLA	OBD-CAD	3.60	1.28	1.22
32	7	324	CHL	C2C-C3C	3.60	1.44	1.36
31	A	816	CLA	C3B-C4B	3.60	1.51	1.42
31	2	309	CLA	OBD-CAD	3.60	1.28	1.22
31	A	850	CLA	CHD-C4C	3.60	1.47	1.39
31	8	310	CLA	CHD-C4C	3.59	1.47	1.39
36	b	301	LUT	C11-C10	3.59	1.54	1.43
31	A	819	CLA	CHD-C4C	3.59	1.47	1.39
31	6	312	CLA	OBD-CAD	3.59	1.28	1.22
32	9	320	CHL	C2C-C3C	3.59	1.44	1.36
36	L	304	LUT	C26-C27	3.59	1.55	1.50
36	a	303	LUT	C32-C33	3.59	1.53	1.45
36	L	304	LUT	C11-C10	3.59	1.54	1.43
32	8	319	CHL	CHD-C1D	3.59	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	817	CLA	CHC-C4B	3.59	1.47	1.39
42	4	304	SQD	O5-C1	3.59	1.51	1.41
31	5	312	CLA	OBD-CAD	3.58	1.28	1.22
32	A	839	CHL	C2C-C3C	3.58	1.44	1.36
31	7	314	CLA	MG-NA	3.58	2.14	2.06
31	B	812	CLA	C1D-ND	-3.58	1.33	1.37
32	6	309	CHL	CHD-C4C	3.58	1.47	1.39
32	4	310	CHL	CHD-C4C	3.58	1.47	1.39
40	7	306	XAT	C10-C9	3.58	1.40	1.35
31	b	304	CLA	OBD-CAD	3.58	1.28	1.22
31	5	323	CLA	OBD-CAD	3.58	1.28	1.22
32	6	317	CHL	CHD-C1D	3.58	1.45	1.38
31	6	306	CLA	OBD-CAD	3.58	1.28	1.22
31	O	202	CLA	OBD-CAD	3.58	1.28	1.22
31	b	311	CLA	OBD-CAD	3.57	1.28	1.22
31	A	847	CLA	CHC-C4B	3.57	1.47	1.39
31	L	305	CLA	C1D-ND	-3.57	1.33	1.37
31	4	320	CLA	OBD-CAD	3.57	1.28	1.22
31	B	843	CLA	CHC-C4B	3.57	1.47	1.39
31	B	847	CLA	CHC-C4B	3.57	1.47	1.39
31	3	317	CLA	OBD-CAD	3.57	1.28	1.22
36	5	304	LUT	C31-C30	3.57	1.54	1.43
36	b	301	LUT	C26-C27	3.57	1.55	1.50
31	B	814	CLA	CHD-C4C	3.57	1.47	1.39
31	9	321	CLA	OBD-CAD	3.57	1.28	1.22
31	4	311	CLA	OBD-CAD	3.57	1.28	1.22
31	7	322	CLA	OBD-CAD	3.57	1.28	1.22
32	7	319	CHL	CHD-C1D	3.57	1.45	1.38
31	3	312	CLA	MG-ND	-3.57	1.98	2.05
32	A	831	CHL	CHD-C1D	3.57	1.45	1.38
32	9	320	CHL	CHD-C1D	3.56	1.45	1.38
31	A	814	CLA	CHD-C4C	3.56	1.47	1.39
32	4	310	CHL	OBD-CAD	3.56	1.28	1.22
35	F	303	QTB	C03-C02	3.56	1.40	1.35
36	7	305	LUT	C15-C14	3.56	1.54	1.43
31	2	315	CLA	OBD-CAD	3.56	1.28	1.22
31	A	826	CLA	OBD-CAD	3.56	1.28	1.22
31	2	307	CLA	OBD-CAD	3.56	1.28	1.22
36	8	303	LUT	C15-C14	3.56	1.54	1.43
31	2	306	CLA	OBD-CAD	3.55	1.28	1.22
32	4	313	CHL	OBD-CAD	3.55	1.28	1.22
31	4	316	CLA	CHD-C1D	3.55	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	3	304	LUT	C15-C14	3.55	1.54	1.43
36	5	304	LUT	C12-C13	3.55	1.53	1.45
36	3	305	LUT	C15-C14	3.55	1.54	1.43
32	6	320	CHL	CHD-C1D	3.55	1.45	1.38
32	5	316	CHL	C3D-C4D	-3.55	1.36	1.44
31	B	836	CLA	CHC-C4B	3.55	1.47	1.39
31	b	312	CLA	OBD-CAD	3.55	1.28	1.22
31	K	204	CLA	C3D-C2D	3.55	1.48	1.39
31	9	312	CLA	OBD-CAD	3.55	1.28	1.22
31	b	306	CLA	OBD-CAD	3.55	1.28	1.22
31	3	319	CLA	C1D-ND	-3.54	1.33	1.37
31	2	314	CLA	OBD-CAD	3.54	1.28	1.22
31	5	315	CLA	OBD-CAD	3.54	1.28	1.22
31	A	824	CLA	MG-ND	-3.54	1.98	2.05
36	6	304	LUT	C11-C10	3.54	1.54	1.43
31	B	832	CLA	CHC-C4B	3.54	1.47	1.39
31	7	316	CLA	OBD-CAD	3.54	1.28	1.22
31	B	846	CLA	CHD-C4C	3.54	1.47	1.39
36	a	305	LUT	C32-C33	3.53	1.53	1.45
31	B	844	CLA	MG-ND	3.53	2.12	2.05
31	3	310	CLA	OBD-CAD	3.53	1.28	1.22
36	L	304	LUT	C28-C29	3.53	1.53	1.45
31	8	313	CLA	MG-NC	-3.53	1.97	2.06
32	7	317	CHL	CHD-C1D	3.53	1.45	1.38
31	6	311	CLA	OBD-CAD	3.53	1.28	1.22
31	B	835	CLA	C1D-ND	-3.53	1.33	1.37
36	4	302	LUT	C23-C24	3.53	1.55	1.50
31	A	844	CLA	MG-ND	-3.53	1.98	2.05
32	A	831	CHL	CHD-C4C	3.53	1.47	1.39
36	7	305	LUT	C7-C6	3.53	1.57	1.45
31	B	841	CLA	C1D-ND	-3.53	1.33	1.37
31	B	812	CLA	CHB-C1B	3.53	1.47	1.39
31	6	322	CLA	OBD-CAD	3.53	1.28	1.22
31	A	857	CLA	C1D-ND	-3.53	1.33	1.37
31	6	310	CLA	OBD-CAD	3.53	1.28	1.22
31	a	312	CLA	OBD-CAD	3.52	1.28	1.22
31	7	315	CLA	OBD-CAD	3.52	1.28	1.22
36	F	304	LUT	C23-C24	3.52	1.55	1.50
31	9	319	CLA	OBD-CAD	3.52	1.28	1.22
36	9	303	LUT	C32-C33	3.52	1.53	1.45
32	9	322	CHL	CHD-C4C	3.52	1.47	1.39
32	K	201	CHL	OBD-CAD	3.52	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	318	CLA	MG-ND	-3.52	1.98	2.05
36	5	303	LUT	C12-C13	3.52	1.53	1.45
31	A	848	CLA	OBD-CAD	3.52	1.28	1.22
31	6	315	CLA	OBD-CAD	3.52	1.28	1.22
32	5	322	CHL	CHD-C4C	3.52	1.47	1.39
31	J	105	CLA	OBD-CAD	3.51	1.28	1.22
31	4	308	CLA	OBD-CAD	3.51	1.28	1.22
36	8	302	LUT	C31-C30	3.51	1.54	1.43
32	4	317	CHL	OBD-CAD	3.51	1.28	1.22
36	a	303	LUT	C26-C27	3.51	1.55	1.50
36	3	304	LUT	C11-C10	3.51	1.54	1.43
31	9	313	CLA	OBD-CAD	3.51	1.28	1.22
31	4	307	CLA	OBD-CAD	3.51	1.28	1.22
31	3	312	CLA	OBD-CAD	3.51	1.28	1.22
31	7	310	CLA	CHD-C4C	3.51	1.47	1.39
36	9	303	LUT	C31-C30	3.51	1.54	1.43
42	4	304	SQD	O47-C45	-3.51	1.37	1.46
31	A	841	CLA	C1D-ND	-3.51	1.33	1.37
31	B	838	CLA	MG-NB	3.51	2.12	2.05
32	7	324	CHL	CHD-C1D	3.51	1.45	1.38
31	b	307	CLA	OBD-CAD	3.51	1.28	1.22
31	8	309	CLA	CHD-C4C	3.50	1.47	1.39
31	B	839	CLA	C1D-ND	-3.50	1.33	1.37
31	F	305	CLA	OBD-CAD	3.50	1.28	1.22
36	b	301	LUT	C32-C33	3.50	1.53	1.45
31	B	815	CLA	CHD-C4C	3.50	1.47	1.39
36	4	302	LUT	C28-C29	3.50	1.53	1.45
36	6	303	LUT	C12-C13	3.50	1.53	1.45
31	2	310	CLA	OBD-CAD	3.50	1.28	1.22
31	8	309	CLA	OBD-CAD	3.50	1.28	1.22
36	a	303	LUT	C23-C24	3.50	1.55	1.50
32	3	315	CHL	CHD-C1D	3.50	1.45	1.38
31	9	314	CLA	OBD-CAD	3.50	1.28	1.22
36	9	302	LUT	C28-C29	3.50	1.53	1.45
31	b	313	CLA	OBD-CAD	3.50	1.28	1.22
31	6	313	CLA	OBD-CAD	3.50	1.28	1.22
36	9	303	LUT	C28-C29	3.50	1.53	1.45
31	5	321	CLA	OBD-CAD	3.50	1.28	1.22
36	9	302	LUT	C32-C33	3.50	1.53	1.45
31	2	311	CLA	C3D-C2D	3.49	1.48	1.39
31	5	309	CLA	OBD-CAD	3.49	1.28	1.22
31	4	305	CLA	OBD-CAD	3.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	9	305	LUT	C26-C27	3.49	1.55	1.50
31	4	306	CLA	MG-ND	-3.49	1.98	2.05
31	9	317	CLA	OBD-CAD	3.49	1.28	1.22
31	K	205	CLA	OBD-CAD	3.49	1.28	1.22
32	4	310	CHL	C3D-C4D	-3.49	1.36	1.44
31	a	315	CLA	OBD-CAD	3.49	1.28	1.22
31	6	306	CLA	C3D-C4D	-3.49	1.36	1.44
32	5	317	CHL	CHD-C1D	3.48	1.45	1.38
31	B	840	CLA	C1D-ND	-3.48	1.33	1.37
31	5	313	CLA	OBD-CAD	3.48	1.28	1.22
40	7	306	XAT	C30-C29	3.48	1.40	1.35
31	A	822	CLA	CHD-C4C	3.48	1.47	1.39
36	4	302	LUT	C32-C33	3.48	1.53	1.45
31	7	310	CLA	MG-NB	3.48	2.12	2.05
31	A	856	CLA	C1D-ND	-3.48	1.33	1.37
36	6	304	LUT	C28-C29	3.48	1.53	1.45
32	b	309	CHL	CHD-C4C	3.48	1.47	1.39
31	7	312	CLA	OBD-CAD	3.48	1.28	1.22
31	8	307	CLA	OBD-CAD	3.48	1.28	1.22
31	B	825	CLA	OBD-CAD	3.48	1.28	1.22
31	8	312	CLA	OBD-CAD	3.48	1.28	1.22
31	G	206	CLA	OBD-CAD	3.48	1.28	1.22
31	A	825	CLA	OBD-CAD	3.48	1.28	1.22
36	F	304	LUT	C15-C14	3.48	1.54	1.43
31	b	308	CLA	C3D-C2D	3.47	1.48	1.39
31	A	847	CLA	OBD-CAD	3.47	1.28	1.22
31	7	316	CLA	MG-ND	3.47	2.12	2.05
32	7	319	CHL	CHD-C4C	3.47	1.47	1.39
31	5	318	CLA	OBD-CAD	3.47	1.28	1.22
36	5	303	LUT	C11-C10	3.47	1.54	1.43
31	B	842	CLA	OBD-CAD	3.47	1.28	1.22
36	8	303	LUT	C12-C13	3.46	1.53	1.45
36	F	304	LUT	C31-C30	3.46	1.54	1.43
31	8	321	CLA	OBD-CAD	3.46	1.28	1.22
32	8	316	CHL	CHD-C1D	3.46	1.45	1.38
36	2	301	LUT	C32-C33	3.46	1.53	1.45
32	a	318	CHL	CHD-C4C	3.46	1.47	1.39
31	9	321	CLA	MG-ND	3.46	2.12	2.05
31	a	321	CLA	OBD-CAD	3.46	1.28	1.22
31	8	320	CLA	C3D-C2D	3.46	1.48	1.39
32	6	319	CHL	OBD-CAD	3.46	1.28	1.22
36	6	303	LUT	C32-C33	3.46	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	310	CLA	CHD-C4C	3.46	1.47	1.39
31	8	313	CLA	OBD-CAD	3.46	1.28	1.22
31	7	311	CLA	OBD-CAD	3.46	1.28	1.22
32	6	321	CHL	OBD-CAD	3.46	1.28	1.22
31	B	820	CLA	OBD-CAD	3.46	1.28	1.22
36	3	304	LUT	C28-C29	3.46	1.53	1.45
36	8	303	LUT	C31-C30	3.46	1.54	1.43
31	B	827	CLA	MG-ND	-3.45	1.98	2.05
31	B	817	CLA	CHD-C4C	3.45	1.47	1.39
36	8	302	LUT	C8-C9	3.45	1.53	1.45
36	4	302	LUT	C26-C27	3.45	1.55	1.50
31	A	855	CLA	CHD-C4C	3.45	1.47	1.39
31	3	309	CLA	OBD-CAD	3.45	1.28	1.22
31	6	311	CLA	C3D-C2D	3.45	1.48	1.39
32	b	309	CHL	MG-NB	3.45	2.12	2.05
31	B	850	CLA	OBD-CAD	3.45	1.28	1.22
31	4	315	CLA	OBD-CAD	3.45	1.28	1.22
31	B	811	CLA	OBD-CAD	3.45	1.28	1.22
31	K	206	CLA	C3D-C2D	3.45	1.48	1.39
36	9	302	LUT	C15-C14	3.45	1.54	1.43
31	3	314	CLA	OBD-CAD	3.45	1.28	1.22
31	8	320	CLA	OBD-CAD	3.45	1.28	1.22
36	3	304	LUT	C12-C13	3.45	1.53	1.45
31	G	204	CLA	OBD-CAD	3.45	1.28	1.22
31	2	304	CLA	MG-ND	3.44	2.12	2.05
32	5	319	CHL	CHD-C4C	3.44	1.47	1.39
36	F	304	LUT	C12-C13	3.44	1.53	1.45
36	a	303	LUT	C11-C10	3.44	1.54	1.43
36	4	303	LUT	C7-C6	3.44	1.57	1.45
36	3	305	LUT	C28-C29	3.44	1.53	1.45
36	5	304	LUT	C32-C33	3.44	1.53	1.45
32	4	317	CHL	CHD-C4C	3.44	1.47	1.39
31	B	831	CLA	C1D-ND	-3.44	1.33	1.37
32	7	318	CHL	CHD-C4C	3.44	1.47	1.39
31	9	311	CLA	OBD-CAD	3.44	1.28	1.22
31	2	306	CLA	C3D-C2D	3.43	1.48	1.39
36	7	305	LUT	C28-C29	3.43	1.53	1.45
31	2	305	CLA	MG-ND	-3.43	1.99	2.05
31	3	312	CLA	C3D-C2D	3.43	1.48	1.39
31	H	901	CLA	C3D-C2D	3.43	1.48	1.39
31	B	843	CLA	MG-NA	3.43	2.14	2.06
31	B	821	CLA	OBD-CAD	3.43	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	7	306	XAT	C14-C13	3.43	1.40	1.35
26	5	302	BCR	C30-C25	-3.43	1.49	1.53
31	B	811	CLA	C1D-ND	-3.43	1.33	1.37
32	4	313	CHL	CHD-C4C	3.43	1.47	1.39
31	2	308	CLA	MG-NA	3.43	2.14	2.06
31	a	316	CLA	C3D-C2D	3.43	1.48	1.39
31	B	826	CLA	C1D-ND	-3.43	1.33	1.37
32	3	315	CHL	CHD-C4C	3.42	1.47	1.39
31	B	818	CLA	CHC-C4B	3.42	1.47	1.39
32	5	317	CHL	CHD-C4C	3.42	1.47	1.39
31	2	315	CLA	C3D-C2D	3.42	1.48	1.39
31	A	820	CLA	OBD-CAD	3.42	1.28	1.22
31	8	317	CLA	OBD-CAD	3.42	1.28	1.22
32	b	309	CHL	OBD-CAD	3.42	1.28	1.22
31	A	833	CLA	OBD-CAD	3.42	1.28	1.22
31	3	308	CLA	OBD-CAD	3.42	1.28	1.22
31	A	834	CLA	C1D-ND	-3.42	1.33	1.37
31	K	204	CLA	C1D-ND	-3.42	1.33	1.37
36	6	303	LUT	C23-C24	3.42	1.55	1.50
31	5	308	CLA	OBD-CAD	3.42	1.28	1.22
36	5	304	LUT	C28-C29	3.41	1.53	1.45
31	3	316	CLA	OBD-CAD	3.41	1.28	1.22
31	6	307	CLA	OBD-CAD	3.41	1.28	1.22
31	A	853	CLA	C1D-ND	-3.41	1.33	1.37
31	A	850	CLA	MG-NB	3.41	2.12	2.05
31	4	311	CLA	C3D-C2D	3.41	1.48	1.39
31	L	306	CLA	C3D-C2D	3.41	1.48	1.39
31	a	309	CLA	OBD-CAD	3.41	1.28	1.22
31	4	319	CLA	C3D-C2D	3.41	1.48	1.39
36	L	304	LUT	C23-C24	3.41	1.55	1.50
31	B	824	CLA	OBD-CAD	3.41	1.28	1.22
32	6	320	CHL	OBD-CAD	3.41	1.28	1.22
31	a	314	CLA	OBD-CAD	3.41	1.28	1.22
32	3	315	CHL	C3D-C4D	-3.40	1.36	1.44
31	b	303	CLA	C3D-C2D	3.40	1.48	1.39
32	7	320	CHL	C3D-C4D	-3.40	1.36	1.44
36	8	302	LUT	C12-C13	3.40	1.53	1.45
31	A	829	CLA	CHD-C4C	3.40	1.47	1.39
31	5	307	CLA	C3D-C2D	3.40	1.48	1.39
31	A	817	CLA	C1D-ND	-3.40	1.33	1.37
31	7	310	CLA	OBD-CAD	3.40	1.28	1.22
31	O	203	CLA	OBD-CAD	3.40	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	835	CLA	C3D-C2D	3.40	1.48	1.39
31	A	846	CLA	OBD-CAD	3.40	1.28	1.22
31	8	317	CLA	C1D-ND	-3.40	1.33	1.37
31	A	834	CLA	C3D-C2D	3.40	1.48	1.39
31	2	313	CLA	C3D-C2D	3.40	1.48	1.39
31	A	844	CLA	OBD-CAD	3.40	1.28	1.22
31	a	319	CLA	OBD-CAD	3.39	1.28	1.22
36	2	301	LUT	C8-C9	3.39	1.53	1.45
31	B	813	CLA	C1D-ND	-3.39	1.33	1.37
31	J	105	CLA	C1D-ND	-3.39	1.33	1.37
31	A	829	CLA	CHD-C1D	3.39	1.45	1.38
36	8	302	LUT	C32-C33	3.39	1.53	1.45
31	4	309	CLA	OBD-CAD	3.39	1.28	1.22
31	9	311	CLA	C3D-C2D	3.39	1.48	1.39
36	3	305	LUT	C12-C13	3.39	1.53	1.45
32	6	321	CHL	CHD-C4C	3.39	1.47	1.39
31	B	819	CLA	MG-NB	3.39	2.12	2.05
31	7	321	CLA	OBD-CAD	3.39	1.28	1.22
31	b	307	CLA	C3D-C2D	3.39	1.48	1.39
31	6	314	CLA	C3D-C2D	3.39	1.48	1.39
31	5	312	CLA	C3D-C2D	3.39	1.48	1.39
31	8	310	CLA	C1D-ND	-3.39	1.33	1.37
31	B	827	CLA	OBD-CAD	3.38	1.28	1.22
36	3	304	LUT	C32-C33	3.38	1.53	1.45
31	A	842	CLA	C1D-ND	-3.38	1.33	1.37
31	L	305	CLA	OBD-CAD	3.38	1.28	1.22
31	4	320	CLA	C3D-C2D	3.38	1.48	1.39
31	3	318	CLA	C3D-C2D	3.38	1.48	1.39
31	b	311	CLA	C3D-C2D	3.38	1.48	1.39
31	A	854	CLA	OBD-CAD	3.38	1.28	1.22
32	6	319	CHL	CHD-C4C	3.38	1.46	1.39
32	6	317	CHL	OBD-CAD	3.37	1.28	1.22
31	7	315	CLA	MG-NC	-3.37	1.98	2.06
31	a	315	CLA	C3D-C2D	3.37	1.48	1.39
31	O	202	CLA	C3D-C2D	3.37	1.48	1.39
31	6	308	CLA	OBD-CAD	3.37	1.28	1.22
32	5	322	CHL	OBD-CAD	3.37	1.28	1.22
31	B	812	CLA	OBD-CAD	3.37	1.28	1.22
32	a	318	CHL	C3D-C4D	-3.37	1.36	1.44
32	6	317	CHL	CHD-C4C	3.37	1.46	1.39
31	5	308	CLA	C3D-C2D	3.37	1.48	1.39
31	B	838	CLA	OBD-CAD	3.37	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	812	CLA	C3D-C2D	3.37	1.48	1.39
31	4	307	CLA	C3D-C2D	3.37	1.48	1.39
31	6	316	CLA	C1D-ND	-3.37	1.33	1.37
32	a	318	CHL	C1D-ND	-3.37	1.33	1.37
31	3	313	CLA	C3D-C2D	3.37	1.48	1.39
31	H	903	CLA	C3D-C2D	3.36	1.48	1.39
31	5	318	CLA	C3D-C2D	3.36	1.48	1.39
31	B	830	CLA	OBD-CAD	3.36	1.28	1.22
31	7	311	CLA	C3D-C2D	3.36	1.48	1.39
31	B	841	CLA	OBD-CAD	3.36	1.28	1.22
31	8	315	CLA	OBD-CAD	3.36	1.28	1.22
31	5	311	CLA	OBD-CAD	3.36	1.28	1.22
31	B	847	CLA	C1D-ND	-3.36	1.33	1.37
31	8	307	CLA	C3D-C2D	3.36	1.48	1.39
32	5	317	CHL	C3D-C4D	-3.36	1.36	1.44
36	5	303	LUT	C32-C33	3.36	1.53	1.45
31	B	846	CLA	OBD-CAD	3.36	1.28	1.22
32	9	322	CHL	C3D-C4D	-3.36	1.36	1.44
36	8	302	LUT	C28-C29	3.36	1.53	1.45
31	9	316	CLA	C3D-C2D	3.36	1.48	1.39
32	6	309	CHL	OBD-CAD	3.36	1.28	1.22
31	b	313	CLA	C3D-C2D	3.36	1.48	1.39
32	4	317	CHL	CHB-C1B	3.36	1.46	1.39
31	B	843	CLA	C3D-C2D	3.36	1.48	1.39
31	3	309	CLA	C3D-C2D	3.35	1.48	1.39
32	6	320	CHL	CHD-C4C	3.35	1.46	1.39
31	7	314	CLA	C3D-C2D	3.35	1.48	1.39
31	A	815	CLA	OBD-CAD	3.35	1.28	1.22
31	a	322	CLA	OBD-CAD	3.35	1.28	1.22
31	7	314	CLA	OBD-CAD	3.35	1.28	1.22
31	A	817	CLA	MG-NB	3.35	2.12	2.05
32	8	319	CHL	OBD-CAD	3.35	1.28	1.22
32	7	317	CHL	MG-NA	3.35	2.14	2.06
31	A	828	CLA	OBD-CAD	3.35	1.28	1.22
31	B	817	CLA	OBD-CAD	3.35	1.28	1.22
32	a	320	CHL	C3D-C4D	-3.35	1.36	1.44
32	6	309	CHL	C3D-C4D	-3.35	1.36	1.44
31	A	843	CLA	C3D-C2D	3.35	1.48	1.39
31	8	321	CLA	C3D-C2D	3.35	1.48	1.39
31	2	308	CLA	OBD-CAD	3.35	1.28	1.22
32	5	317	CHL	OBD-CAD	3.35	1.28	1.22
31	F	305	CLA	C3D-C2D	3.35	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	317	CHL	C3D-C4D	-3.35	1.36	1.44
31	B	827	CLA	C1D-ND	-3.35	1.33	1.37
31	A	846	CLA	C1D-ND	-3.35	1.33	1.37
31	B	820	CLA	C1D-ND	-3.35	1.33	1.37
31	B	825	CLA	C1D-ND	-3.34	1.33	1.37
31	B	836	CLA	MG-NB	3.34	2.12	2.05
32	7	318	CHL	C3D-C4D	-3.34	1.36	1.44
36	7	305	LUT	C32-C33	3.34	1.53	1.45
32	8	319	CHL	CHD-C4C	3.34	1.46	1.39
32	4	317	CHL	C3D-C4D	-3.34	1.36	1.44
31	2	314	CLA	C3D-C2D	3.34	1.48	1.39
36	9	302	LUT	C11-C10	3.34	1.53	1.43
31	6	312	CLA	C3D-C2D	3.34	1.48	1.39
31	a	314	CLA	C3D-C2D	3.34	1.48	1.39
31	O	203	CLA	C3D-C2D	3.34	1.48	1.39
31	b	312	CLA	C3D-C2D	3.34	1.48	1.39
32	6	319	CHL	C3D-C4D	-3.34	1.36	1.44
31	3	319	CLA	C3D-C2D	3.34	1.48	1.39
31	4	314	CLA	C3D-C2D	3.34	1.48	1.39
31	A	816	CLA	C3D-C2D	3.34	1.48	1.39
31	5	310	CLA	OBD-CAD	3.34	1.28	1.22
32	8	319	CHL	C3D-C4D	-3.33	1.36	1.44
31	3	320	CLA	C3D-C2D	3.33	1.48	1.39
31	7	316	CLA	C3D-C2D	3.33	1.48	1.39
31	4	318	CLA	C3D-C2D	3.33	1.48	1.39
31	K	204	CLA	OBD-CAD	3.33	1.28	1.22
31	G	205	CLA	C3D-C2D	3.33	1.48	1.39
32	b	309	CHL	C3D-C4D	-3.33	1.36	1.44
31	B	841	CLA	C3D-C2D	3.33	1.48	1.39
31	2	309	CLA	C3D-C2D	3.33	1.48	1.39
31	B	812	CLA	C1B-NB	-3.33	1.33	1.37
32	5	319	CHL	C3D-C4D	-3.33	1.36	1.44
31	H	902	CLA	OBD-CAD	3.33	1.28	1.22
36	F	304	LUT	C11-C10	3.33	1.53	1.43
31	2	312	CLA	C3D-C2D	3.33	1.48	1.39
31	A	842	CLA	MG-ND	-3.33	1.99	2.05
31	3	320	CLA	MG-ND	-3.33	1.99	2.05
31	B	836	CLA	C1B-NB	-3.33	1.33	1.37
31	L	305	CLA	C3D-C2D	3.33	1.48	1.39
31	A	849	CLA	OBD-CAD	3.33	1.28	1.22
32	6	317	CHL	C3D-C4D	-3.33	1.36	1.44
31	2	306	CLA	MG-NC	3.32	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	824	CLA	OBD-CAD	3.32	1.28	1.22
31	8	312	CLA	C3D-C2D	3.32	1.48	1.39
31	7	315	CLA	C3D-C2D	3.32	1.48	1.39
31	a	311	CLA	OBD-CAD	3.32	1.28	1.22
31	6	310	CLA	C3D-C2D	3.32	1.48	1.39
32	6	318	CHL	CHD-C4C	3.32	1.46	1.39
31	3	314	CLA	C3D-C2D	3.32	1.48	1.39
36	8	303	LUT	C26-C27	3.32	1.55	1.50
31	A	845	CLA	C3D-C2D	3.32	1.48	1.39
31	8	308	CLA	C3D-C2D	3.32	1.48	1.39
31	2	304	CLA	C3D-C2D	3.32	1.48	1.39
31	A	817	CLA	OBD-CAD	3.32	1.28	1.22
36	8	303	LUT	C32-C33	3.32	1.53	1.45
32	9	320	CHL	C3D-C4D	-3.32	1.36	1.44
31	2	310	CLA	C3D-C2D	3.32	1.48	1.39
31	B	828	CLA	OBD-CAD	3.32	1.28	1.22
31	A	829	CLA	CHB-C1B	3.32	1.46	1.39
31	2	307	CLA	C3D-C2D	3.31	1.48	1.39
32	9	320	CHL	OBD-CAD	3.31	1.28	1.22
26	2	302	BCR	C1-C6	-3.31	1.49	1.53
31	O	204	CLA	C3D-C2D	3.31	1.48	1.39
31	5	323	CLA	C3D-C2D	3.31	1.48	1.39
31	3	319	CLA	OBD-CAD	3.31	1.28	1.22
31	8	311	CLA	OBD-CAD	3.31	1.28	1.22
31	A	816	CLA	OBD-CAD	3.31	1.28	1.22
31	b	306	CLA	C3D-C2D	3.31	1.48	1.39
31	a	316	CLA	C1D-ND	-3.31	1.33	1.37
31	A	855	CLA	OBD-CAD	3.31	1.28	1.22
31	8	310	CLA	OBD-CAD	3.31	1.28	1.22
31	9	319	CLA	C3D-C2D	3.31	1.48	1.39
31	B	839	CLA	C3D-C2D	3.31	1.48	1.39
31	B	817	CLA	C1D-ND	-3.31	1.33	1.37
31	b	304	CLA	C3D-C2D	3.31	1.48	1.39
31	5	309	CLA	C3D-C2D	3.31	1.48	1.39
31	b	305	CLA	C3D-C2D	3.31	1.48	1.39
31	7	313	CLA	OBD-CAD	3.31	1.28	1.22
36	6	304	LUT	C26-C27	3.31	1.55	1.50
31	B	850	CLA	C1D-ND	-3.31	1.33	1.37
36	9	303	LUT	C7-C6	3.30	1.56	1.45
32	A	839	CHL	C3D-C4D	-3.30	1.36	1.44
31	3	316	CLA	C3D-C2D	3.30	1.48	1.39
32	a	318	CHL	OBD-CAD	3.30	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	322	CHL	C3D-C4D	-3.30	1.36	1.44
31	A	853	CLA	OBD-CAD	3.30	1.28	1.22
31	B	834	CLA	CHD-C4C	3.30	1.46	1.39
31	b	310	CLA	C3D-C2D	3.30	1.48	1.39
31	5	314	CLA	C3D-C2D	3.30	1.48	1.39
31	A	824	CLA	C3D-C2D	3.30	1.48	1.39
36	7	305	LUT	C12-C13	3.30	1.53	1.45
31	A	848	CLA	C3D-C2D	3.30	1.48	1.39
31	8	315	CLA	C3D-C2D	3.30	1.48	1.39
32	7	319	CHL	C1D-ND	-3.30	1.33	1.37
31	A	815	CLA	C3D-C2D	3.30	1.48	1.39
31	B	826	CLA	OBD-CAD	3.30	1.28	1.22
31	3	314	CLA	C1D-ND	-3.30	1.33	1.37
31	A	837	CLA	C3D-C2D	3.29	1.48	1.39
31	a	311	CLA	C3D-C2D	3.29	1.48	1.39
31	6	315	CLA	C3D-C2D	3.29	1.48	1.39
31	A	823	CLA	C1D-ND	-3.29	1.33	1.37
31	B	833	CLA	C1D-ND	-3.29	1.33	1.37
31	6	306	CLA	C1D-ND	-3.29	1.33	1.37
31	B	831	CLA	OBD-CAD	3.29	1.28	1.22
31	6	308	CLA	C3D-C2D	3.29	1.48	1.39
31	A	816	CLA	C1D-ND	-3.29	1.33	1.37
31	7	312	CLA	C3D-C2D	3.29	1.48	1.39
31	a	319	CLA	C3D-C2D	3.29	1.48	1.39
31	2	305	CLA	C3D-C2D	3.29	1.48	1.39
31	3	317	CLA	C3D-C2D	3.29	1.48	1.39
31	7	322	CLA	C3D-C2D	3.29	1.48	1.39
31	5	311	CLA	C3D-C2D	3.29	1.48	1.39
31	A	849	CLA	C3D-C2D	3.29	1.48	1.39
32	8	316	CHL	C3D-C4D	-3.29	1.36	1.44
32	a	320	CHL	CHD-C4C	3.29	1.46	1.39
31	B	816	CLA	OBD-CAD	3.29	1.28	1.22
31	9	313	CLA	C3D-C2D	3.29	1.48	1.39
36	8	303	LUT	C11-C10	3.29	1.53	1.43
31	L	307	CLA	C3D-C2D	3.29	1.48	1.39
31	4	306	CLA	C3D-C2D	3.29	1.48	1.39
32	a	317	CHL	CHD-C4C	3.29	1.46	1.39
31	8	313	CLA	C3D-C2D	3.29	1.48	1.39
42	4	304	SQD	O47-C7	3.28	1.43	1.34
36	8	302	LUT	C11-C10	3.28	1.53	1.43
31	A	837	CLA	C1D-ND	-3.28	1.33	1.37
36	3	305	LUT	C11-C10	3.28	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	816	CLA	C1D-ND	-3.28	1.33	1.37
31	B	842	CLA	C1D-ND	-3.28	1.33	1.37
31	5	310	CLA	C3D-C2D	3.28	1.48	1.39
31	B	829	CLA	OBD-CAD	3.28	1.28	1.22
31	3	310	CLA	C3D-C2D	3.28	1.48	1.39
31	4	315	CLA	C3D-C2D	3.28	1.48	1.39
31	B	830	CLA	C1D-ND	-3.28	1.33	1.37
31	G	206	CLA	C1D-ND	-3.28	1.33	1.37
31	8	310	CLA	C3D-C2D	3.28	1.48	1.39
31	4	308	CLA	C3D-C2D	3.28	1.48	1.39
32	6	318	CHL	C3D-C4D	-3.28	1.36	1.44
31	B	835	CLA	MG-NC	3.27	2.14	2.06
31	A	835	CLA	OBD-CAD	3.27	1.28	1.22
31	8	318	CLA	C1D-ND	-3.27	1.33	1.37
39	7	301	3PH	P-O11	3.27	1.70	1.60
31	A	856	CLA	C3D-C2D	3.27	1.48	1.39
31	5	315	CLA	C3D-C2D	3.27	1.48	1.39
31	B	828	CLA	C3D-C2D	3.27	1.48	1.39
31	A	827	CLA	OBD-CAD	3.27	1.28	1.22
32	7	320	CHL	CHB-C1B	3.27	1.46	1.39
31	B	840	CLA	OBD-CAD	3.27	1.28	1.22
32	a	320	CHL	CHB-C1B	3.27	1.46	1.39
31	B	836	CLA	C1D-ND	-3.27	1.33	1.37
40	7	306	XAT	C34-C33	3.27	1.40	1.35
36	7	305	LUT	C11-C10	3.27	1.53	1.43
31	B	822	CLA	MG-NB	3.27	2.12	2.05
32	5	319	CHL	CHB-C1B	3.26	1.46	1.39
31	A	826	CLA	C1D-ND	-3.26	1.33	1.37
31	A	832	CLA	C1D-ND	-3.26	1.33	1.37
31	A	826	CLA	C3D-C2D	3.26	1.48	1.39
31	9	318	CLA	C3D-C2D	3.26	1.48	1.39
31	A	841	CLA	OBD-CAD	3.26	1.28	1.22
31	A	857	CLA	OBD-CAD	3.26	1.28	1.22
32	7	324	CHL	C3D-C4D	-3.26	1.36	1.44
32	8	319	CHL	CHB-C1B	3.26	1.46	1.39
32	9	322	CHL	OBD-CAD	3.26	1.28	1.22
31	A	817	CLA	C3D-C2D	3.26	1.48	1.39
31	6	316	CLA	C3D-C2D	3.26	1.48	1.39
26	3	302	BCR	C1-C6	-3.26	1.49	1.53
32	7	317	CHL	C3D-C4D	-3.26	1.36	1.44
31	B	847	CLA	OBD-CAD	3.26	1.28	1.22
31	B	826	CLA	C3D-C2D	3.26	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	318	CLA	OBD-CAD	3.25	1.28	1.22
31	A	851	CLA	C3D-C2D	3.25	1.48	1.39
32	6	320	CHL	C3D-C4D	-3.25	1.36	1.44
31	B	844	CLA	C1D-ND	-3.25	1.33	1.37
32	4	313	CHL	C3D-C4D	-3.25	1.36	1.44
32	7	317	CHL	CHD-C4C	3.25	1.46	1.39
31	A	847	CLA	C3D-C2D	3.25	1.48	1.39
31	5	313	CLA	C3D-C2D	3.25	1.48	1.39
31	B	813	CLA	OBD-CAD	3.25	1.28	1.22
32	5	319	CHL	OBD-CAD	3.25	1.28	1.22
32	7	324	CHL	CHD-C4C	3.25	1.46	1.39
31	K	205	CLA	C3D-C2D	3.25	1.48	1.39
32	7	319	CHL	C3D-C4D	-3.25	1.36	1.44
32	7	318	CHL	MG-NC	-3.25	1.98	2.06
31	A	845	CLA	C1D-ND	-3.25	1.33	1.37
31	F	301	CLA	OBD-CAD	3.25	1.28	1.22
31	4	321	CLA	C3D-C2D	3.25	1.48	1.39
31	6	307	CLA	C3D-C2D	3.25	1.48	1.39
31	6	322	CLA	C3D-C2D	3.25	1.48	1.39
31	G	206	CLA	C3D-C2D	3.25	1.48	1.39
31	A	823	CLA	C3D-C2D	3.25	1.48	1.39
31	A	822	CLA	C1B-NB	-3.25	1.33	1.37
31	8	318	CLA	OBD-CAD	3.25	1.28	1.22
31	B	825	CLA	C3D-C2D	3.25	1.48	1.39
31	A	836	CLA	OBD-CAD	3.25	1.28	1.22
31	B	845	CLA	C3D-C2D	3.25	1.48	1.39
31	4	312	CLA	C3D-C2D	3.24	1.48	1.39
31	8	314	CLA	OBD-CAD	3.24	1.28	1.22
31	B	836	CLA	C3D-C2D	3.24	1.48	1.39
31	B	822	CLA	OBD-CAD	3.24	1.28	1.22
32	A	839	CHL	MG-NA	3.24	2.14	2.06
31	B	820	CLA	C3D-C2D	3.24	1.48	1.39
31	A	821	CLA	C3D-C2D	3.24	1.48	1.39
31	a	322	CLA	C3D-C2D	3.24	1.48	1.39
32	7	317	CHL	OBD-CAD	3.24	1.28	1.22
36	2	301	LUT	C11-C10	3.24	1.53	1.43
32	6	321	CHL	C3D-C4D	-3.24	1.36	1.44
31	B	814	CLA	C1D-ND	-3.24	1.33	1.37
31	A	838	CLA	C3D-C2D	3.24	1.48	1.39
31	A	853	CLA	C3D-C2D	3.24	1.48	1.39
31	B	821	CLA	C3D-C2D	3.24	1.48	1.39
32	7	320	CHL	CHD-C4C	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	314	CLA	C3D-C2D	3.23	1.47	1.39
36	2	301	LUT	C12-C13	3.23	1.52	1.45
32	A	831	CHL	CHC-C4B	3.23	1.46	1.39
31	B	837	CLA	OBD-CAD	3.23	1.28	1.22
32	a	317	CHL	OBD-CAD	3.23	1.28	1.22
31	B	814	CLA	OBD-CAD	3.23	1.28	1.22
31	a	321	CLA	C3D-C2D	3.23	1.47	1.39
31	b	305	CLA	OBD-CAD	3.23	1.28	1.22
31	A	832	CLA	C3D-C2D	3.23	1.47	1.39
31	B	838	CLA	C3D-C2D	3.23	1.47	1.39
31	7	309	CLA	C3D-C2D	3.23	1.47	1.39
31	3	308	CLA	C3D-C2D	3.23	1.47	1.39
36	8	303	LUT	C28-C29	3.23	1.52	1.45
31	8	311	CLA	C3D-C2D	3.22	1.47	1.39
31	B	848	CLA	MG-NC	3.22	2.13	2.06
31	B	823	CLA	C1D-ND	-3.22	1.33	1.37
32	4	313	CHL	CHB-C1B	3.22	1.46	1.39
31	A	857	CLA	C3D-C2D	3.22	1.47	1.39
31	A	845	CLA	MG-NB	3.22	2.12	2.05
31	A	828	CLA	C3D-C2D	3.22	1.47	1.39
31	B	847	CLA	C3D-C2D	3.22	1.47	1.39
31	5	321	CLA	C3D-C2D	3.22	1.47	1.39
31	B	834	CLA	C1D-ND	-3.22	1.33	1.37
31	A	832	CLA	OBD-CAD	3.22	1.28	1.22
31	A	822	CLA	OBD-CAD	3.22	1.28	1.22
31	L	307	CLA	C4D-CHA	3.22	1.49	1.38
31	B	837	CLA	C1D-ND	-3.22	1.33	1.37
31	B	811	CLA	C3D-C2D	3.22	1.47	1.39
31	4	316	CLA	C3D-C2D	3.21	1.47	1.39
36	5	304	LUT	C7-C6	3.21	1.56	1.45
32	5	316	CHL	CHD-C4C	3.21	1.46	1.39
31	A	852	CLA	C3D-C2D	3.21	1.47	1.39
31	3	307	CLA	C3D-C2D	3.21	1.47	1.39
32	8	316	CHL	CHB-C1B	3.21	1.46	1.39
32	b	309	CHL	CHC-C4B	3.21	1.46	1.39
31	A	828	CLA	C1D-ND	-3.21	1.33	1.37
31	B	842	CLA	C3D-C2D	3.21	1.47	1.39
31	8	317	CLA	MG-NC	-3.21	1.98	2.06
31	9	312	CLA	C3D-C2D	3.21	1.47	1.39
32	7	317	CHL	CHB-C1B	3.21	1.46	1.39
31	2	315	CLA	C1D-ND	-3.21	1.33	1.37
31	B	843	CLA	C1D-ND	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	831	CHL	C3D-C4D	-3.21	1.36	1.44
31	B	836	CLA	OBD-CAD	3.21	1.28	1.22
31	9	317	CLA	C4D-CHA	3.21	1.49	1.38
36	9	302	LUT	C12-C13	3.21	1.52	1.45
32	5	317	CHL	CHC-C4B	3.21	1.46	1.39
32	7	318	CHL	CHB-C1B	3.21	1.46	1.39
36	F	304	LUT	C28-C29	3.21	1.52	1.45
31	A	830	CLA	OBD-CAD	3.21	1.28	1.22
32	6	318	CHL	OBD-CAD	3.21	1.28	1.22
32	6	321	CHL	CHC-C4B	3.21	1.46	1.39
32	5	322	CHL	CHB-C1B	3.20	1.46	1.39
31	A	825	CLA	C3D-C2D	3.20	1.47	1.39
31	A	843	CLA	OBD-CAD	3.20	1.28	1.22
31	B	839	CLA	OBD-CAD	3.20	1.28	1.22
31	4	309	CLA	C3D-C2D	3.20	1.47	1.39
31	B	816	CLA	C3D-C2D	3.20	1.47	1.39
31	6	313	CLA	C3D-C2D	3.20	1.47	1.39
31	A	830	CLA	C3D-C2D	3.20	1.47	1.39
36	a	305	LUT	C7-C6	3.20	1.56	1.45
31	5	312	CLA	C4D-CHA	3.20	1.49	1.38
31	B	827	CLA	C3D-C2D	3.20	1.47	1.39
31	7	321	CLA	C3D-C2D	3.20	1.47	1.39
32	A	840	CHL	C3D-C4D	-3.20	1.37	1.44
32	K	201	CHL	CHC-C4B	3.20	1.46	1.39
31	8	318	CLA	C3D-C2D	3.19	1.47	1.39
32	9	320	CHL	CHD-C4C	3.19	1.46	1.39
26	K	203	BCR	C30-C25	-3.19	1.49	1.53
31	A	822	CLA	C1D-ND	-3.19	1.33	1.37
31	A	843	CLA	C1D-ND	-3.19	1.33	1.37
31	B	813	CLA	C3D-C2D	3.19	1.47	1.39
32	8	316	CHL	CHD-C4C	3.19	1.46	1.39
31	B	818	CLA	C3D-C2D	3.19	1.47	1.39
32	A	840	CHL	CHD-C1D	3.19	1.44	1.38
31	6	310	CLA	C4D-CHA	3.19	1.49	1.38
31	8	308	CLA	OBD-CAD	3.19	1.28	1.22
32	6	309	CHL	CHB-C1B	3.19	1.46	1.39
31	9	321	CLA	C3B-C4B	3.19	1.50	1.42
31	A	825	CLA	C1D-ND	-3.19	1.33	1.37
31	A	827	CLA	C3D-C2D	3.19	1.47	1.39
31	9	321	CLA	C3D-C2D	3.19	1.47	1.39
31	b	302	CLA	C3D-C2D	3.19	1.47	1.39
31	A	818	CLA	C3D-C2D	3.19	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	309	CLA	OBD-CAD	3.19	1.28	1.22
31	B	822	CLA	C3D-C2D	3.19	1.47	1.39
31	B	848	CLA	C3D-C2D	3.19	1.47	1.39
32	8	316	CHL	OBD-CAD	3.18	1.28	1.22
31	8	309	CLA	C3D-C2D	3.18	1.47	1.39
31	A	838	CLA	OBD-CAD	3.18	1.28	1.22
31	a	312	CLA	C3D-C2D	3.18	1.47	1.39
31	B	821	CLA	C1D-ND	-3.18	1.33	1.37
31	B	845	CLA	C1D-ND	-3.18	1.33	1.37
31	4	318	CLA	C4D-CHA	3.18	1.49	1.38
31	A	854	CLA	C3D-C2D	3.18	1.47	1.39
31	5	310	CLA	C4D-CHA	3.18	1.49	1.38
31	A	833	CLA	C3D-C2D	3.18	1.47	1.39
31	B	833	CLA	OBD-CAD	3.18	1.28	1.22
31	B	832	CLA	OBD-CAD	3.18	1.28	1.22
31	B	829	CLA	C3D-C2D	3.18	1.47	1.39
31	B	814	CLA	C1B-NB	-3.18	1.33	1.37
31	A	837	CLA	OBD-CAD	3.17	1.27	1.22
31	a	310	CLA	OBD-CAD	3.17	1.27	1.22
32	a	320	CHL	CHC-C4B	3.17	1.46	1.39
31	B	814	CLA	C3D-C2D	3.17	1.47	1.39
31	A	819	CLA	OBD-CAD	3.17	1.27	1.22
31	7	316	CLA	C1D-ND	-3.17	1.33	1.37
32	a	317	CHL	CHB-C1B	3.17	1.46	1.39
36	F	304	LUT	C32-C33	3.17	1.52	1.45
31	8	317	CLA	C3D-C2D	3.17	1.47	1.39
36	J	103	LUT	C7-C6	3.17	1.56	1.45
31	5	313	CLA	C4D-CHA	3.17	1.49	1.38
31	7	310	CLA	C3D-C2D	3.17	1.47	1.39
31	B	848	CLA	C1D-ND	-3.17	1.33	1.37
31	B	849	CLA	C3D-C2D	3.17	1.47	1.39
31	b	302	CLA	C4D-CHA	3.17	1.49	1.38
31	L	306	CLA	C1D-ND	-3.17	1.33	1.37
32	A	840	CHL	CHD-C4C	3.17	1.46	1.39
31	A	821	CLA	C1D-ND	-3.16	1.33	1.37
31	a	313	CLA	C3D-C2D	3.16	1.47	1.39
36	6	304	LUT	C7-C6	3.16	1.56	1.45
31	B	818	CLA	C1D-ND	-3.16	1.33	1.37
31	b	313	CLA	C1D-ND	-3.16	1.33	1.37
31	B	840	CLA	C3D-C2D	3.16	1.47	1.39
32	6	321	CHL	CHB-C1B	3.16	1.46	1.39
31	B	823	CLA	C3D-C2D	3.16	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	850	CLA	C3D-C2D	3.16	1.47	1.39
31	8	314	CLA	C3D-C2D	3.15	1.47	1.39
32	b	309	CHL	CHB-C1B	3.15	1.46	1.39
31	A	853	CLA	MG-NB	-3.15	1.99	2.05
32	5	316	CHL	OBD-CAD	3.15	1.27	1.22
31	A	842	CLA	C3D-C2D	3.15	1.47	1.39
31	7	322	CLA	C1D-ND	-3.15	1.33	1.37
31	8	309	CLA	C4D-CHA	3.15	1.49	1.38
31	2	310	CLA	C4D-CHA	3.15	1.49	1.38
31	G	204	CLA	C3D-C2D	3.15	1.47	1.39
31	7	313	CLA	C3D-C2D	3.15	1.47	1.39
31	B	845	CLA	C1B-NB	-3.15	1.33	1.37
31	6	308	CLA	C4C-C3C	3.15	1.50	1.45
31	H	903	CLA	C1D-ND	-3.15	1.33	1.37
31	B	838	CLA	C1D-ND	-3.15	1.33	1.37
31	B	831	CLA	C3D-C2D	3.15	1.47	1.39
31	8	321	CLA	C1D-ND	-3.15	1.33	1.37
31	F	301	CLA	C3D-C2D	3.15	1.47	1.39
32	4	310	CHL	CHB-C1B	3.15	1.46	1.39
31	A	819	CLA	C3D-C2D	3.15	1.47	1.39
31	K	205	CLA	MG-ND	3.15	2.12	2.05
36	8	303	LUT	C7-C6	3.15	1.56	1.45
31	A	850	CLA	C1D-ND	-3.14	1.33	1.37
31	b	303	CLA	C4D-CHA	3.14	1.49	1.38
31	A	855	CLA	C1D-ND	-3.14	1.33	1.37
32	7	324	CHL	OBD-CAD	3.14	1.27	1.22
36	5	303	LUT	C28-C29	3.14	1.52	1.45
31	A	822	CLA	C3D-C2D	3.14	1.47	1.39
31	B	828	CLA	C1D-ND	-3.14	1.33	1.37
26	A	805	BCR	C1-C6	-3.14	1.49	1.53
36	4	302	LUT	C7-C6	3.14	1.56	1.45
32	7	320	CHL	OBD-CAD	3.14	1.27	1.22
31	F	306	CLA	C3D-C2D	3.14	1.47	1.39
31	a	310	CLA	C3D-C2D	3.13	1.47	1.39
31	B	844	CLA	C3D-C2D	3.13	1.47	1.39
36	L	304	LUT	C7-C6	3.13	1.56	1.45
31	A	848	CLA	C1D-ND	-3.13	1.33	1.37
31	b	304	CLA	C1D-ND	-3.13	1.33	1.37
31	A	845	CLA	OBD-CAD	3.13	1.27	1.22
31	A	829	CLA	C3D-C2D	3.13	1.47	1.39
31	a	309	CLA	C3D-C2D	3.13	1.47	1.39
31	5	320	CLA	C3D-C2D	3.13	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	835	CLA	C3D-C2D	3.13	1.47	1.39
31	8	313	CLA	C1D-ND	-3.13	1.33	1.37
31	F	301	CLA	C3B-C4B	3.13	1.50	1.42
31	A	826	CLA	C1B-NB	-3.13	1.33	1.37
31	4	316	CLA	MG-ND	3.13	2.12	2.05
31	J	105	CLA	C3D-C2D	3.13	1.47	1.39
31	b	313	CLA	C4C-C3C	3.13	1.50	1.45
31	A	838	CLA	C4D-CHA	3.13	1.49	1.38
31	8	315	CLA	C1D-ND	-3.13	1.33	1.37
31	B	819	CLA	C1D-ND	-3.13	1.33	1.37
31	A	823	CLA	OBD-CAD	3.13	1.27	1.22
31	F	301	CLA	C1D-ND	-3.13	1.33	1.37
31	F	305	CLA	C1D-ND	-3.13	1.33	1.37
31	A	855	CLA	C3B-C4B	3.12	1.50	1.42
31	B	829	CLA	C4D-CHA	3.12	1.49	1.38
31	A	855	CLA	C3D-C2D	3.12	1.47	1.39
32	a	320	CHL	OBD-CAD	3.12	1.27	1.22
31	8	320	CLA	C1D-ND	-3.12	1.33	1.37
31	8	321	CLA	C1B-NB	-3.12	1.33	1.37
31	A	830	CLA	C4D-CHA	3.12	1.49	1.38
31	a	311	CLA	C1D-ND	-3.12	1.33	1.37
36	8	303	LUT	C23-C24	3.12	1.54	1.50
32	6	320	CHL	CHB-C1B	3.12	1.46	1.39
31	A	818	CLA	OBD-CAD	3.12	1.27	1.22
31	B	845	CLA	OBD-CAD	3.12	1.27	1.22
31	8	308	CLA	C1D-ND	-3.12	1.33	1.37
31	F	306	CLA	C4D-CHA	3.12	1.49	1.38
26	K	202	BCR	C1-C6	-3.12	1.49	1.53
32	7	319	CHL	OBD-CAD	3.12	1.27	1.22
31	9	317	CLA	C3D-C2D	3.12	1.47	1.39
31	B	835	CLA	OBD-CAD	3.12	1.27	1.22
31	A	835	CLA	C4D-CHA	3.11	1.49	1.38
32	6	318	CHL	CHB-C1B	3.11	1.46	1.39
31	a	309	CLA	C4D-CHA	3.11	1.49	1.38
32	4	313	CHL	CHC-C4B	3.11	1.46	1.39
31	6	306	CLA	C3D-C2D	3.11	1.47	1.39
36	4	303	LUT	C26-C27	3.11	1.54	1.50
31	A	814	CLA	C3D-C2D	3.11	1.47	1.39
32	7	318	CHL	C1D-ND	-3.11	1.34	1.37
31	B	824	CLA	C3D-C2D	3.11	1.47	1.39
31	A	844	CLA	C1D-ND	-3.11	1.34	1.37
31	B	845	CLA	C3B-C4B	3.11	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	308	CLA	C3D-C2D	3.11	1.47	1.39
32	A	839	CHL	C1D-ND	-3.11	1.34	1.37
31	7	310	CLA	C4D-CHA	3.11	1.49	1.38
31	3	310	CLA	C1D-ND	-3.11	1.34	1.37
36	5	303	LUT	C7-C6	3.10	1.56	1.45
32	6	320	CHL	CHC-C4B	3.10	1.46	1.39
31	3	307	CLA	C1D-ND	-3.10	1.34	1.37
31	3	316	CLA	C1D-ND	-3.10	1.34	1.37
36	2	301	LUT	C26-C27	3.10	1.54	1.50
31	O	202	CLA	MG-ND	3.10	2.11	2.05
32	9	322	CHL	CHB-C1B	3.10	1.46	1.39
32	a	317	CHL	C1D-ND	-3.10	1.34	1.37
31	a	321	CLA	C1D-ND	-3.10	1.34	1.37
31	9	315	CLA	C4D-CHA	3.10	1.49	1.38
31	3	320	CLA	C4D-CHA	3.10	1.49	1.38
31	A	818	CLA	MG-NB	3.10	2.11	2.05
32	A	840	CHL	CHC-C4B	3.10	1.46	1.39
32	5	322	CHL	CHC-C4B	3.10	1.46	1.39
31	a	322	CLA	C1D-ND	-3.10	1.34	1.37
31	2	307	CLA	C4D-CHA	3.10	1.49	1.38
26	6	302	BCR	C1-C6	-3.10	1.49	1.53
31	G	204	CLA	C4D-CHA	3.10	1.49	1.38
31	3	313	CLA	C1D-ND	-3.10	1.34	1.37
31	H	902	CLA	C3D-C2D	3.10	1.47	1.39
31	b	307	CLA	C4D-CHA	3.10	1.49	1.38
31	3	308	CLA	C1D-ND	-3.10	1.34	1.37
31	B	822	CLA	C1D-ND	-3.09	1.34	1.37
36	b	301	LUT	C23-C24	3.09	1.54	1.50
31	9	321	CLA	C4D-CHA	3.09	1.49	1.38
31	A	829	CLA	CHC-C1C	3.09	1.44	1.38
31	A	836	CLA	C3D-C2D	3.09	1.47	1.39
31	B	824	CLA	C4D-CHA	3.09	1.49	1.38
31	a	319	CLA	C1D-ND	-3.09	1.34	1.37
31	O	203	CLA	C4D-CHA	3.09	1.49	1.38
31	B	815	CLA	C3D-C2D	3.09	1.47	1.39
31	3	307	CLA	OBD-CAD	3.09	1.27	1.22
32	3	315	CHL	OBD-CAD	3.09	1.27	1.22
31	B	843	CLA	C1B-NB	-3.09	1.34	1.37
31	4	309	CLA	C1D-ND	-3.09	1.34	1.37
31	F	301	CLA	C4D-CHA	3.09	1.49	1.38
31	8	311	CLA	C4D-CHA	3.09	1.49	1.38
31	b	312	CLA	C4D-CHA	3.09	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	309	CLA	C1D-ND	-3.09	1.34	1.37
31	9	311	CLA	C1D-ND	-3.08	1.34	1.37
32	6	319	CHL	CHB-C1B	3.08	1.46	1.39
31	B	849	CLA	C3B-C4B	3.08	1.50	1.42
31	H	901	CLA	C4D-CHA	3.08	1.49	1.38
31	A	817	CLA	C3B-C4B	3.08	1.50	1.42
31	O	204	CLA	C4D-CHA	3.08	1.49	1.38
32	A	831	CHL	C1D-ND	-3.08	1.34	1.37
32	A	840	CHL	CHB-C1B	3.08	1.46	1.39
31	3	317	CLA	C4D-CHA	3.08	1.49	1.38
30	A	813	CL0	CHD-C1D	3.08	1.44	1.38
32	7	320	CHL	CHC-C4B	3.08	1.46	1.39
31	2	306	CLA	C4D-CHA	3.08	1.49	1.38
31	A	815	CLA	C1B-NB	-3.08	1.34	1.37
31	A	816	CLA	C1B-NB	-3.08	1.34	1.37
31	4	315	CLA	C4D-CHA	3.08	1.49	1.38
31	A	821	CLA	OBD-CAD	3.08	1.27	1.22
31	4	308	CLA	C4D-CHA	3.08	1.49	1.38
32	7	319	CHL	CHC-C4B	3.08	1.46	1.39
31	4	308	CLA	C1D-ND	-3.08	1.34	1.37
31	B	848	CLA	OBD-CAD	3.08	1.27	1.22
31	A	849	CLA	C1D-ND	-3.07	1.34	1.37
31	8	317	CLA	C1B-NB	-3.07	1.34	1.37
36	a	303	LUT	C7-C6	3.07	1.56	1.45
31	B	833	CLA	C3D-C2D	3.07	1.47	1.39
32	6	317	CHL	C1D-ND	-3.07	1.34	1.37
32	5	319	CHL	MG-ND	3.07	2.11	2.05
26	G	203	BCR	C30-C25	-3.07	1.49	1.53
31	9	313	CLA	C4D-CHA	3.07	1.49	1.38
31	A	827	CLA	C1D-ND	-3.07	1.34	1.37
31	A	834	CLA	C1B-NB	-3.07	1.34	1.37
26	B	803	BCR	C1-C6	-3.07	1.49	1.53
31	A	844	CLA	C3D-C2D	3.07	1.47	1.39
31	A	836	CLA	MG-ND	3.07	2.11	2.05
31	O	202	CLA	C4D-CHA	3.07	1.49	1.38
32	7	317	CHL	CHC-C4B	3.07	1.46	1.39
31	9	319	CLA	C4D-CHA	3.07	1.49	1.38
32	A	831	CHL	OBD-CAD	3.07	1.27	1.22
31	A	854	CLA	C1D-ND	-3.07	1.34	1.37
31	7	315	CLA	C4D-CHA	3.07	1.49	1.38
31	A	833	CLA	C1D-ND	-3.07	1.34	1.37
31	H	901	CLA	C1D-ND	-3.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	815	CLA	C4D-CHA	3.06	1.49	1.38
31	A	851	CLA	C1D-ND	-3.06	1.34	1.37
31	5	308	CLA	C4D-CHA	3.06	1.49	1.38
36	9	302	LUT	C26-C27	3.06	1.54	1.50
31	B	811	CLA	C1B-NB	-3.06	1.34	1.37
31	7	313	CLA	C1D-ND	-3.06	1.34	1.37
31	6	314	CLA	C4D-CHA	3.06	1.49	1.38
31	A	820	CLA	C3D-C2D	3.06	1.47	1.39
31	5	311	CLA	C4D-CHA	3.06	1.49	1.38
36	F	304	LUT	C7-C6	3.06	1.56	1.45
31	2	315	CLA	MG-ND	3.06	2.11	2.05
32	8	316	CHL	C1D-ND	-3.06	1.34	1.37
36	5	304	LUT	C26-C27	3.06	1.54	1.50
31	B	846	CLA	C3D-C2D	3.06	1.47	1.39
31	6	312	CLA	C4D-CHA	3.06	1.49	1.38
32	3	315	CHL	CHB-C1B	3.06	1.46	1.39
31	B	817	CLA	C1B-NB	-3.06	1.34	1.37
31	B	817	CLA	C3D-C2D	3.06	1.47	1.39
31	5	318	CLA	C1D-ND	-3.06	1.34	1.37
31	B	850	CLA	C3B-C4B	3.05	1.49	1.42
32	3	315	CHL	CHC-C4B	3.05	1.46	1.39
31	A	847	CLA	C1D-ND	-3.05	1.34	1.37
31	4	312	CLA	C4D-CHA	3.05	1.49	1.38
31	b	310	CLA	C4D-CHA	3.05	1.49	1.38
32	4	310	CHL	C1D-ND	-3.05	1.34	1.37
26	A	804	BCR	C1-C6	-3.05	1.49	1.53
31	B	823	CLA	OBD-CAD	3.05	1.27	1.22
31	2	312	CLA	C4D-CHA	3.05	1.49	1.38
31	6	313	CLA	C4D-CHA	3.05	1.49	1.38
31	2	311	CLA	C1D-ND	-3.05	1.34	1.37
31	6	308	CLA	C1D-ND	-3.05	1.34	1.37
31	A	824	CLA	C4D-CHA	3.05	1.49	1.38
32	5	319	CHL	CHC-C4B	3.05	1.46	1.39
31	3	313	CLA	C4D-CHA	3.04	1.49	1.38
31	B	836	CLA	MG-ND	3.04	2.11	2.05
31	4	306	CLA	C4D-CHA	3.04	1.49	1.38
32	A	831	CHL	CHB-C1B	3.04	1.46	1.39
31	8	307	CLA	C1D-ND	-3.04	1.34	1.37
31	4	305	CLA	CHB-C4A	-3.04	1.30	1.37
32	4	317	CHL	CHC-C4B	3.04	1.46	1.39
31	a	310	CLA	C4D-CHA	3.04	1.49	1.38
31	5	307	CLA	C1D-ND	-3.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	311	CLA	C1D-ND	-3.04	1.34	1.37
31	F	305	CLA	MG-NB	-3.04	1.99	2.05
31	a	313	CLA	OBD-CAD	3.04	1.27	1.22
31	7	321	CLA	C1D-ND	-3.04	1.34	1.37
31	A	851	CLA	C4D-CHA	3.04	1.49	1.38
36	8	302	LUT	C23-C24	3.04	1.54	1.50
31	A	835	CLA	C1D-ND	-3.04	1.34	1.37
31	3	308	CLA	C4D-CHA	3.04	1.49	1.38
32	A	839	CHL	CHD-C4C	3.03	1.46	1.39
32	7	324	CHL	CHB-C1B	3.03	1.46	1.39
31	B	818	CLA	OBD-CAD	3.03	1.27	1.22
31	A	836	CLA	C1D-ND	-3.03	1.34	1.37
31	A	849	CLA	C4D-CHA	3.03	1.49	1.38
31	A	828	CLA	C4D-CHA	3.03	1.49	1.38
36	9	302	LUT	C7-C6	3.03	1.55	1.45
31	9	316	CLA	C4D-CHA	3.03	1.49	1.38
31	3	309	CLA	C1D-ND	-3.03	1.34	1.37
31	5	323	CLA	C1D-ND	-3.03	1.34	1.37
31	5	314	CLA	C4D-CHA	3.03	1.49	1.38
31	A	819	CLA	C4D-CHA	3.03	1.49	1.38
31	3	318	CLA	C1D-ND	-3.03	1.34	1.37
32	A	839	CHL	CHD-C1D	3.03	1.44	1.38
32	A	839	CHL	CHC-C4B	3.03	1.46	1.39
32	a	317	CHL	CHC-C4B	3.03	1.46	1.39
31	2	314	CLA	C1D-ND	-3.03	1.34	1.37
31	6	312	CLA	C1D-ND	-3.03	1.34	1.37
31	4	314	CLA	C4D-CHA	3.03	1.49	1.38
31	9	312	CLA	C4D-CHA	3.03	1.49	1.38
31	8	320	CLA	MG-NB	3.03	2.11	2.05
31	7	316	CLA	C4D-CHA	3.03	1.49	1.38
31	6	308	CLA	C4D-CHA	3.03	1.49	1.38
31	G	205	CLA	MG-NB	-3.02	1.99	2.05
36	a	305	LUT	C23-C24	3.02	1.54	1.50
31	2	309	CLA	C1D-ND	-3.02	1.34	1.37
32	3	315	CHL	C1D-ND	-3.02	1.34	1.37
31	8	315	CLA	C4D-CHA	3.02	1.49	1.38
32	9	322	CHL	CHC-C4B	3.02	1.46	1.39
31	B	815	CLA	C1D-ND	-3.02	1.34	1.37
31	7	312	CLA	C4D-CHA	3.02	1.49	1.38
31	H	902	CLA	C1D-ND	-3.02	1.34	1.37
32	a	318	CHL	CHB-C1B	3.02	1.46	1.39
31	B	838	CLA	C4D-CHA	3.02	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	321	CLA	C4D-CHA	3.02	1.49	1.38
31	4	311	CLA	C4D-CHA	3.02	1.49	1.38
31	A	820	CLA	C1D-ND	-3.02	1.34	1.37
31	2	309	CLA	C4D-CHA	3.02	1.49	1.38
31	8	312	CLA	C4D-CHA	3.02	1.49	1.38
31	B	816	CLA	MG-NA	3.01	2.13	2.06
31	a	312	CLA	C4D-CHA	3.01	1.49	1.38
31	A	821	CLA	C1B-NB	-3.01	1.34	1.37
31	B	824	CLA	C1D-ND	-3.01	1.34	1.37
31	B	849	CLA	C4D-CHA	3.01	1.49	1.38
36	9	305	LUT	C23-C24	3.01	1.54	1.50
31	K	206	CLA	C1D-ND	-3.01	1.34	1.37
31	9	312	CLA	C1D-ND	-3.01	1.34	1.37
31	A	846	CLA	C3D-C2D	3.01	1.47	1.39
31	B	849	CLA	C1D-ND	-3.01	1.34	1.37
31	B	819	CLA	MG-ND	3.01	2.11	2.05
31	A	822	CLA	C4D-CHA	3.01	1.49	1.38
31	B	832	CLA	C4D-CHA	3.01	1.49	1.38
31	a	312	CLA	C1D-ND	-3.01	1.34	1.37
31	6	322	CLA	C4D-CHA	3.01	1.49	1.38
31	7	311	CLA	C1D-ND	-3.00	1.34	1.37
31	A	852	CLA	OBD-CAD	3.00	1.27	1.22
31	B	845	CLA	C4D-CHA	3.00	1.49	1.38
31	a	319	CLA	C4D-CHA	3.00	1.49	1.38
31	F	306	CLA	OBD-CAD	3.00	1.27	1.22
31	B	830	CLA	C1B-NB	-3.00	1.34	1.37
31	5	323	CLA	C4D-CHA	3.00	1.49	1.38
26	6	302	BCR	C30-C25	-3.00	1.49	1.53
36	8	302	LUT	C7-C6	3.00	1.55	1.45
31	3	307	CLA	C4D-CHA	3.00	1.49	1.38
31	2	304	CLA	C1D-ND	-3.00	1.34	1.37
31	a	311	CLA	C4D-CHA	3.00	1.49	1.38
31	2	311	CLA	C4D-CHA	3.00	1.49	1.38
31	K	205	CLA	C1D-ND	-3.00	1.34	1.37
31	2	305	CLA	C1D-ND	-3.00	1.34	1.37
32	A	839	CHL	OBD-CAD	3.00	1.27	1.22
31	A	841	CLA	C3D-C2D	3.00	1.47	1.39
31	8	320	CLA	C4D-CHA	3.00	1.49	1.38
31	3	312	CLA	C4D-CHA	3.00	1.49	1.38
31	A	823	CLA	C1B-NB	-3.00	1.34	1.37
30	A	813	CL0	C3D-C2D	3.00	1.47	1.39
31	A	854	CLA	C4D-CHA	3.00	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	324	CHL	CHC-C4B	3.00	1.46	1.39
31	8	307	CLA	C4D-CHA	3.00	1.49	1.38
31	A	837	CLA	C4D-CHA	3.00	1.49	1.38
31	G	205	CLA	C4D-CHA	3.00	1.49	1.38
31	7	321	CLA	C4D-CHA	2.99	1.49	1.38
31	6	306	CLA	C1D-C2D	2.99	1.51	1.45
31	8	308	CLA	C4D-CHA	2.99	1.49	1.38
31	F	305	CLA	C4D-CHA	2.99	1.49	1.38
31	6	315	CLA	C1D-ND	-2.99	1.34	1.37
31	2	314	CLA	C4D-CHA	2.99	1.49	1.38
31	6	311	CLA	C4D-CHA	2.99	1.49	1.38
31	A	852	CLA	C4D-CHA	2.99	1.49	1.38
31	9	311	CLA	C4D-CHA	2.99	1.49	1.38
31	A	842	CLA	OBD-CAD	2.99	1.27	1.22
31	3	320	CLA	C1D-ND	-2.99	1.34	1.37
31	8	317	CLA	MG-NB	2.99	2.11	2.05
31	K	205	CLA	C4D-CHA	2.99	1.49	1.38
31	4	319	CLA	C4D-CHA	2.99	1.49	1.38
31	3	309	CLA	C4D-CHA	2.99	1.49	1.38
31	2	305	CLA	C4D-CHA	2.98	1.49	1.38
30	A	813	CL0	CHC-C1C	2.98	1.44	1.38
31	K	206	CLA	C4D-CHA	2.98	1.49	1.38
31	B	832	CLA	C1D-ND	-2.98	1.34	1.37
31	A	850	CLA	C1B-NB	-2.98	1.34	1.37
36	2	301	LUT	C7-C6	2.98	1.55	1.45
31	7	314	CLA	C4D-CHA	2.98	1.49	1.38
31	5	321	CLA	C4D-CHA	2.98	1.49	1.38
31	A	824	CLA	C1D-ND	-2.98	1.34	1.37
32	6	309	CHL	MG-NC	-2.98	1.99	2.06
31	9	315	CLA	C3D-C2D	2.98	1.47	1.39
31	2	308	CLA	C4D-CHA	2.98	1.49	1.38
31	7	314	CLA	C1D-ND	-2.98	1.34	1.37
26	8	301	BCR	C30-C25	-2.97	1.49	1.53
31	B	841	CLA	C1B-NB	-2.97	1.34	1.37
31	A	842	CLA	C4D-CHA	2.97	1.49	1.38
31	A	833	CLA	C4D-CHA	2.97	1.49	1.38
26	G	203	BCR	C1-C6	-2.97	1.49	1.53
31	3	312	CLA	C1D-ND	-2.97	1.34	1.37
32	9	320	CHL	C1D-ND	-2.97	1.34	1.37
31	A	819	CLA	C3B-C4B	2.97	1.49	1.42
31	7	313	CLA	C4D-CHA	2.97	1.48	1.38
31	2	304	CLA	C4D-CHA	2.97	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	310	CLA	C1B-NB	-2.97	1.34	1.37
32	5	317	CHL	C1D-ND	-2.97	1.34	1.37
31	A	847	CLA	C4D-CHA	2.97	1.48	1.38
32	7	317	CHL	C1D-ND	-2.97	1.34	1.37
31	B	822	CLA	C4D-CHA	2.97	1.48	1.38
31	A	845	CLA	C4D-CHA	2.97	1.48	1.38
31	5	320	CLA	C1D-ND	-2.97	1.34	1.37
31	b	306	CLA	C4D-CHA	2.97	1.48	1.38
31	5	315	CLA	C4D-CHA	2.97	1.48	1.38
31	5	309	CLA	C4D-CHA	2.96	1.48	1.38
31	a	321	CLA	C4D-CHA	2.96	1.48	1.38
32	5	317	CHL	CHB-C1B	2.96	1.46	1.39
31	9	318	CLA	C4D-CHA	2.96	1.48	1.38
32	6	317	CHL	CHC-C4B	2.96	1.46	1.39
31	L	306	CLA	C4D-CHA	2.96	1.48	1.38
31	H	902	CLA	C4D-CHA	2.96	1.48	1.38
32	7	318	CHL	CHC-C4B	2.96	1.46	1.39
31	B	833	CLA	C3B-C4B	2.96	1.49	1.42
31	B	832	CLA	C3D-C2D	2.96	1.47	1.39
31	9	319	CLA	C1D-ND	-2.96	1.34	1.37
31	2	313	CLA	C1D-ND	-2.96	1.34	1.37
31	B	836	CLA	C4D-CHA	2.96	1.48	1.38
31	A	843	CLA	C4D-CHA	2.96	1.48	1.38
31	A	852	CLA	C1D-ND	-2.96	1.34	1.37
31	6	315	CLA	C4D-CHA	2.96	1.48	1.38
31	a	310	CLA	C1D-ND	-2.96	1.34	1.37
31	B	818	CLA	C4D-CHA	2.96	1.48	1.38
31	b	311	CLA	C4D-CHA	2.96	1.48	1.38
31	B	839	CLA	C1B-NB	-2.96	1.34	1.37
31	b	304	CLA	C3B-C4B	2.96	1.49	1.42
31	B	847	CLA	C3B-C4B	2.96	1.49	1.42
31	8	311	CLA	C1D-ND	-2.96	1.34	1.37
31	B	819	CLA	C3D-C2D	2.95	1.47	1.39
31	8	314	CLA	C4D-CHA	2.95	1.48	1.38
31	2	315	CLA	MG-NA	-2.95	1.99	2.06
31	3	316	CLA	C4D-CHA	2.95	1.48	1.38
31	4	308	CLA	MG-NB	-2.95	1.99	2.05
31	3	314	CLA	C4D-CHA	2.95	1.48	1.38
32	8	319	CHL	CHC-C4B	2.95	1.46	1.39
31	B	819	CLA	OBD-CAD	2.95	1.27	1.22
36	9	305	LUT	C7-C6	2.95	1.55	1.45
31	b	308	CLA	C1D-ND	-2.95	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	814	CLA	C3B-C4B	2.95	1.49	1.42
26	L	303	BCR	C30-C25	-2.95	1.49	1.53
31	B	829	CLA	C1D-ND	-2.95	1.34	1.37
36	3	305	LUT	C26-C27	2.95	1.54	1.50
31	B	823	CLA	C4D-CHA	2.95	1.48	1.38
31	B	834	CLA	C4D-CHA	2.95	1.48	1.38
31	B	828	CLA	C3B-C4B	2.95	1.49	1.42
31	4	312	CLA	MG-ND	2.95	2.11	2.05
27	A	807	LMT	O3'-C3'	-2.95	1.36	1.43
32	4	310	CHL	CHC-C4B	2.94	1.46	1.39
33	B	808	DGD	C3G-C2G	2.94	1.59	1.50
31	A	850	CLA	C3D-C2D	2.94	1.47	1.39
26	3	303	BCR	C30-C25	-2.94	1.49	1.53
31	a	315	CLA	C4D-CHA	2.94	1.48	1.38
31	3	318	CLA	C4D-CHA	2.94	1.48	1.38
31	8	310	CLA	C4D-CHA	2.94	1.48	1.38
31	4	307	CLA	C4D-CHA	2.94	1.48	1.38
31	3	311	CLA	C4D-CHA	2.94	1.48	1.38
31	6	314	CLA	C1D-ND	-2.94	1.34	1.37
31	H	903	CLA	C4D-CHA	2.94	1.48	1.38
31	8	312	CLA	C1D-ND	-2.94	1.34	1.37
31	9	316	CLA	MG-NB	-2.94	2.00	2.05
32	5	322	CHL	MG-NC	2.94	2.13	2.06
31	A	828	CLA	C1B-NB	-2.94	1.34	1.37
31	A	834	CLA	OBD-CAD	2.94	1.27	1.22
31	5	314	CLA	C1D-ND	-2.94	1.34	1.37
31	7	311	CLA	C4D-CHA	2.94	1.48	1.38
31	7	312	CLA	C1D-ND	-2.94	1.34	1.37
31	A	823	CLA	C4D-CHA	2.94	1.48	1.38
31	B	849	CLA	C1B-NB	-2.94	1.34	1.37
32	6	318	CHL	CHC-C4B	2.94	1.46	1.39
32	7	318	CHL	OBD-CAD	2.94	1.27	1.22
31	B	818	CLA	C1B-NB	-2.94	1.34	1.37
31	5	318	CLA	C4D-CHA	2.93	1.48	1.38
31	B	826	CLA	C4D-CHA	2.93	1.48	1.38
26	I	801	BCR	C1-C6	-2.93	1.49	1.53
31	B	835	CLA	C4D-CHA	2.93	1.48	1.38
31	a	316	CLA	C4D-CHA	2.93	1.48	1.38
31	B	847	CLA	C1B-NB	-2.93	1.34	1.37
31	A	826	CLA	C4D-CHA	2.93	1.48	1.38
31	A	844	CLA	C4D-CHA	2.93	1.48	1.38
31	2	313	CLA	C4D-CHA	2.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	313	CHL	C1D-ND	-2.93	1.34	1.37
31	2	309	CLA	C3B-C4B	2.93	1.49	1.42
31	8	311	CLA	MG-ND	-2.93	2.00	2.05
31	B	819	CLA	C4D-CHA	2.93	1.48	1.38
31	B	833	CLA	C1B-NB	-2.93	1.34	1.37
31	G	205	CLA	C1D-ND	-2.93	1.34	1.37
31	6	312	CLA	MG-NC	-2.93	1.99	2.06
31	B	813	CLA	C4D-CHA	2.93	1.48	1.38
31	7	310	CLA	C1D-ND	-2.93	1.34	1.37
32	8	319	CHL	C1D-ND	-2.93	1.34	1.37
31	A	820	CLA	C4D-CHA	2.93	1.48	1.38
31	B	843	CLA	C4D-CHA	2.93	1.48	1.38
31	A	832	CLA	C1B-NB	-2.93	1.34	1.37
31	B	840	CLA	C1B-NB	-2.93	1.34	1.37
31	9	314	CLA	C1D-ND	-2.93	1.34	1.37
31	a	309	CLA	MG-NC	-2.93	1.99	2.06
31	A	821	CLA	C4D-CHA	2.93	1.48	1.38
31	b	308	CLA	C4C-C3C	2.93	1.50	1.45
31	A	830	CLA	C1D-ND	-2.93	1.34	1.37
31	4	307	CLA	C1D-ND	-2.93	1.34	1.37
32	5	316	CHL	CHB-C1B	2.93	1.46	1.39
31	a	315	CLA	C1D-ND	-2.93	1.34	1.37
31	3	314	CLA	C3B-C4B	2.93	1.49	1.42
31	4	305	CLA	CHD-C1D	2.93	1.44	1.38
31	A	844	CLA	MG-NA	2.93	2.13	2.06
31	b	313	CLA	C4D-CHA	2.92	1.48	1.38
31	4	320	CLA	C3B-C4B	2.92	1.49	1.42
31	4	309	CLA	C4D-CHA	2.92	1.48	1.38
31	a	313	CLA	C4D-CHA	2.92	1.48	1.38
31	B	832	CLA	C1C-NC	-2.92	1.33	1.37
42	4	304	SQD	C24-C23	2.92	1.59	1.50
31	A	855	CLA	C4D-CHA	2.92	1.48	1.38
31	B	846	CLA	C4D-CHA	2.92	1.48	1.38
31	3	319	CLA	C3B-C4B	2.92	1.49	1.42
31	B	820	CLA	C4D-CHA	2.92	1.48	1.38
31	5	307	CLA	C4D-CHA	2.92	1.48	1.38
30	A	813	CL0	C1B-C2B	2.92	1.50	1.43
31	8	314	CLA	C1D-ND	-2.92	1.34	1.37
31	A	838	CLA	C1D-ND	-2.92	1.34	1.37
32	6	321	CHL	C1D-ND	-2.92	1.34	1.37
31	A	818	CLA	C3B-C4B	2.92	1.49	1.42
31	A	838	CLA	C1B-NB	-2.92	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	204	CLA	C3A-C2A	-2.92	1.51	1.54
31	5	307	CLA	MG-NC	2.92	2.13	2.06
31	b	312	CLA	C4C-C3C	2.92	1.50	1.45
31	B	842	CLA	C1B-NB	-2.92	1.34	1.37
31	9	314	CLA	C4D-CHA	2.92	1.48	1.38
31	6	307	CLA	C4D-CHA	2.92	1.48	1.38
31	4	314	CLA	C1D-ND	-2.92	1.34	1.37
36	9	302	LUT	C23-C24	2.92	1.54	1.50
31	B	842	CLA	C4D-CHA	2.92	1.48	1.38
31	8	318	CLA	C4D-CHA	2.91	1.48	1.38
31	B	830	CLA	C3D-C2D	2.91	1.47	1.39
31	b	305	CLA	C4D-CHA	2.91	1.48	1.38
31	A	850	CLA	C4D-CHA	2.91	1.48	1.38
31	4	320	CLA	C4D-CHA	2.91	1.48	1.38
32	7	319	CHL	CHB-C1B	2.91	1.45	1.39
32	6	309	CHL	CHC-C4B	2.91	1.45	1.39
31	8	310	CLA	C3B-C4B	2.91	1.49	1.42
31	A	852	CLA	C1B-NB	-2.91	1.34	1.37
31	B	828	CLA	C4D-CHA	2.91	1.48	1.38
31	9	316	CLA	C1D-ND	-2.91	1.34	1.37
32	9	320	CHL	CHB-C1B	2.91	1.45	1.39
31	2	312	CLA	C1D-ND	-2.91	1.34	1.37
31	2	306	CLA	C1D-ND	-2.91	1.34	1.37
32	6	317	CHL	CHB-C1B	2.91	1.45	1.39
31	B	850	CLA	C4D-CHA	2.91	1.48	1.38
31	b	306	CLA	C1D-ND	-2.91	1.34	1.37
31	7	312	CLA	C3B-C4B	2.91	1.49	1.42
31	2	311	CLA	C3B-C4B	2.91	1.49	1.42
31	8	321	CLA	C4D-CHA	2.91	1.48	1.38
31	A	842	CLA	C1B-NB	-2.91	1.34	1.37
31	a	314	CLA	C1D-ND	-2.91	1.34	1.37
31	a	314	CLA	C4D-CHA	2.90	1.48	1.38
31	L	306	CLA	C1B-NB	-2.90	1.34	1.37
31	5	320	CLA	C4D-CHA	2.90	1.48	1.38
31	8	313	CLA	C4D-CHA	2.90	1.48	1.38
31	B	812	CLA	C3B-C4B	2.90	1.49	1.42
31	6	313	CLA	C1D-ND	-2.90	1.34	1.37
31	A	857	CLA	C4D-CHA	2.90	1.48	1.38
26	G	201	BCR	C1-C6	-2.90	1.49	1.53
32	6	319	CHL	CHC-C4B	2.90	1.45	1.39
31	B	821	CLA	C4D-CHA	2.90	1.48	1.38
36	9	303	LUT	C26-C27	2.90	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	314	CLA	C3B-C4B	2.90	1.49	1.42
32	K	201	CHL	CHB-C1B	2.90	1.45	1.39
31	A	854	CLA	C1B-NB	-2.89	1.34	1.37
31	O	203	CLA	MG-ND	2.89	2.11	2.05
32	6	320	CHL	C1D-ND	-2.89	1.34	1.37
31	7	309	CLA	C3B-C4B	2.89	1.49	1.42
31	F	301	CLA	C1B-NB	-2.89	1.34	1.37
31	7	315	CLA	C1D-ND	-2.89	1.34	1.37
31	A	853	CLA	C3B-C4B	2.89	1.49	1.42
31	B	847	CLA	C4D-CHA	2.89	1.48	1.38
31	9	315	CLA	OBD-CAD	2.89	1.27	1.22
31	A	824	CLA	C1B-NB	-2.89	1.34	1.37
31	2	315	CLA	C4D-CHA	2.89	1.48	1.38
31	B	825	CLA	C4D-CHA	2.89	1.48	1.38
36	b	301	LUT	C7-C6	2.89	1.55	1.45
31	b	308	CLA	C4D-CHA	2.89	1.48	1.38
32	8	316	CHL	CHC-C4B	2.89	1.45	1.39
31	A	844	CLA	C1B-NB	-2.89	1.34	1.37
31	6	311	CLA	C4C-C3C	2.89	1.50	1.45
31	7	311	CLA	C3B-C4B	2.89	1.49	1.42
30	A	813	CL0	OBD-CAD	2.89	1.27	1.22
31	B	840	CLA	C3B-C4B	2.89	1.49	1.42
31	B	845	CLA	C1C-NC	-2.89	1.33	1.37
31	A	847	CLA	C1B-NB	-2.89	1.34	1.37
31	9	318	CLA	C1D-ND	-2.89	1.34	1.37
31	A	817	CLA	C4D-CHA	2.89	1.48	1.38
31	G	206	CLA	C4D-CHA	2.89	1.48	1.38
31	b	313	CLA	C3B-C4B	2.89	1.49	1.42
31	3	311	CLA	OBD-CAD	2.88	1.27	1.22
31	A	846	CLA	C1B-NB	-2.88	1.34	1.37
31	A	829	CLA	MG-NB	2.88	2.11	2.05
32	a	320	CHL	C1D-ND	-2.88	1.34	1.37
31	A	856	CLA	C1B-NB	-2.88	1.34	1.37
31	3	311	CLA	C3D-C2D	2.88	1.47	1.39
31	A	848	CLA	C4D-CHA	2.88	1.48	1.38
31	6	307	CLA	C1D-ND	-2.88	1.34	1.37
36	F	304	LUT	C26-C27	2.88	1.54	1.50
31	A	836	CLA	C4D-CHA	2.88	1.48	1.38
31	L	307	CLA	C4C-C3C	2.88	1.50	1.45
31	L	306	CLA	C3B-C4B	2.87	1.49	1.42
31	A	814	CLA	OBD-CAD	2.87	1.27	1.22
31	A	843	CLA	C1B-NB	-2.87	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	311	CLA	C1D-ND	-2.87	1.34	1.37
31	5	315	CLA	C1D-ND	-2.87	1.34	1.37
31	A	815	CLA	C3B-C4B	2.87	1.49	1.42
31	8	309	CLA	C1C-NC	-2.87	1.33	1.37
31	B	848	CLA	C4D-CHA	2.87	1.48	1.38
31	a	322	CLA	C4D-CHA	2.87	1.48	1.38
31	A	819	CLA	C1D-ND	-2.87	1.34	1.37
31	3	317	CLA	C1D-ND	-2.87	1.34	1.37
31	2	308	CLA	C3B-C4B	2.87	1.49	1.42
31	B	834	CLA	C3D-C2D	2.87	1.47	1.39
31	3	320	CLA	C3B-C4B	2.87	1.49	1.42
36	5	303	LUT	C26-C27	2.87	1.54	1.50
31	B	821	CLA	C1B-NB	-2.87	1.34	1.37
26	M	101	BCR	C1-C6	-2.87	1.49	1.53
31	b	304	CLA	C4D-CHA	2.87	1.48	1.38
26	3	301	BCR	C30-C25	-2.87	1.49	1.53
31	B	846	CLA	C3B-C4B	2.87	1.49	1.42
31	4	320	CLA	C1D-ND	-2.87	1.34	1.37
32	a	318	CHL	CHC-C4B	2.86	1.45	1.39
31	4	305	CLA	CHC-C1C	2.86	1.44	1.38
31	F	306	CLA	C1D-ND	-2.86	1.34	1.37
31	2	308	CLA	C1D-ND	-2.86	1.34	1.37
36	6	303	LUT	C7-C6	2.86	1.55	1.45
31	a	309	CLA	C1D-ND	-2.86	1.34	1.37
31	7	309	CLA	C4D-CHA	2.86	1.48	1.38
31	A	832	CLA	C4D-CHA	2.86	1.48	1.38
31	J	105	CLA	C4D-CHA	2.86	1.48	1.38
31	B	822	CLA	C3B-C4B	2.86	1.49	1.42
30	A	813	CL0	CHD-C4C	2.86	1.45	1.39
31	A	853	CLA	C1B-NB	-2.86	1.34	1.37
31	B	838	CLA	C1B-NB	-2.86	1.34	1.37
31	B	837	CLA	C4C-C3C	2.86	1.50	1.45
31	G	205	CLA	C3B-C4B	2.86	1.49	1.42
31	4	321	CLA	C1D-ND	-2.86	1.34	1.37
31	8	308	CLA	C3B-C4B	2.86	1.49	1.42
31	b	310	CLA	C3B-C4B	2.86	1.49	1.42
31	b	305	CLA	C3B-C4B	2.86	1.49	1.42
31	A	836	CLA	C3B-C4B	2.86	1.49	1.42
36	7	305	LUT	C26-C27	2.86	1.54	1.50
31	B	811	CLA	C4D-CHA	2.86	1.48	1.38
31	B	831	CLA	C4D-CHA	2.86	1.48	1.38
32	5	316	CHL	CHC-C4B	2.85	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	103	LUT	C26-C27	2.85	1.54	1.50
36	5	303	LUT	C23-C24	2.85	1.54	1.50
31	8	307	CLA	MG-NB	-2.85	2.00	2.05
26	L	302	BCR	C1-C6	-2.85	1.49	1.53
31	3	319	CLA	C1B-NB	-2.85	1.34	1.37
31	5	321	CLA	C1D-ND	-2.85	1.34	1.37
31	A	825	CLA	C3B-C4B	2.85	1.49	1.42
31	A	823	CLA	C3B-C4B	2.85	1.49	1.42
31	G	204	CLA	C1D-ND	-2.85	1.34	1.37
31	4	319	CLA	C1D-ND	-2.85	1.34	1.37
31	8	317	CLA	C4D-CHA	2.85	1.48	1.38
36	8	303	LUT	C38-C25	2.85	1.55	1.50
31	b	310	CLA	C1D-ND	-2.85	1.34	1.37
31	9	317	CLA	C1D-ND	-2.85	1.34	1.37
31	A	827	CLA	C4D-CHA	2.85	1.48	1.38
32	A	840	CHL	C1D-ND	-2.85	1.34	1.37
32	4	317	CHL	C1D-ND	-2.85	1.34	1.37
31	7	322	CLA	C4D-CHA	2.85	1.48	1.38
26	G	201	BCR	C30-C25	-2.84	1.49	1.53
36	3	305	LUT	C7-C6	2.84	1.55	1.45
31	6	316	CLA	C4D-CHA	2.84	1.48	1.38
31	A	848	CLA	C1B-NB	-2.84	1.34	1.37
31	A	846	CLA	C4D-CHA	2.84	1.48	1.38
31	B	827	CLA	C4D-CHA	2.84	1.48	1.38
31	B	831	CLA	C1C-NC	-2.84	1.33	1.37
31	B	813	CLA	C3B-C4B	2.84	1.49	1.42
31	9	315	CLA	C1D-ND	-2.84	1.34	1.37
31	2	313	CLA	C3B-C4B	2.84	1.49	1.42
31	A	835	CLA	C3B-C4B	2.84	1.49	1.42
31	A	841	CLA	C4D-CHA	2.84	1.48	1.38
31	A	826	CLA	C3B-C4B	2.84	1.49	1.42
31	L	307	CLA	C3B-C4B	2.84	1.49	1.42
31	B	832	CLA	C1B-NB	-2.84	1.34	1.37
31	3	307	CLA	C3B-C4B	2.84	1.49	1.42
31	3	310	CLA	C4D-CHA	2.84	1.48	1.38
31	O	204	CLA	C3B-C4B	2.84	1.49	1.42
26	A	803	BCR	C30-C25	-2.84	1.49	1.53
31	b	303	CLA	C4C-C3C	2.84	1.49	1.45
31	A	853	CLA	C4D-CHA	2.84	1.48	1.38
31	6	312	CLA	C3B-C4B	2.84	1.49	1.42
31	B	814	CLA	C4D-CHA	2.83	1.48	1.38
31	O	204	CLA	C1D-ND	-2.83	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	203	CLA	C1D-ND	-2.83	1.34	1.37
31	3	310	CLA	MG-NA	2.83	2.13	2.06
31	L	305	CLA	C3B-C4B	2.83	1.49	1.42
31	2	313	CLA	C4C-C3C	2.83	1.49	1.45
31	4	311	CLA	C1D-ND	-2.83	1.34	1.37
32	6	309	CHL	C1D-ND	-2.83	1.34	1.37
31	B	844	CLA	C4D-CHA	2.83	1.48	1.38
31	B	834	CLA	C1B-NB	-2.83	1.34	1.37
31	A	818	CLA	C4B-NB	-2.83	1.34	1.37
26	A	804	BCR	C30-C25	-2.83	1.49	1.53
28	A	811	LHG	O7-C5	-2.83	1.39	1.46
31	A	849	CLA	C3B-C4B	2.83	1.49	1.42
31	6	308	CLA	C3B-C4B	2.83	1.49	1.42
31	B	833	CLA	C4D-CHA	2.83	1.48	1.38
31	L	306	CLA	MG-ND	2.82	2.11	2.05
31	B	839	CLA	C4D-CHA	2.82	1.48	1.38
31	A	856	CLA	C3B-C4B	2.82	1.49	1.42
31	5	320	CLA	C3B-C4B	2.82	1.49	1.42
31	A	856	CLA	C4D-CHA	2.82	1.48	1.38
31	5	309	CLA	MG-NC	2.82	2.13	2.06
31	A	819	CLA	C1B-NB	-2.82	1.34	1.37
31	A	834	CLA	C4D-CHA	2.82	1.48	1.38
31	9	321	CLA	C1D-ND	-2.82	1.34	1.37
31	5	311	CLA	C1D-ND	-2.82	1.34	1.37
31	A	843	CLA	C1C-NC	-2.82	1.33	1.37
31	A	855	CLA	C1C-NC	-2.82	1.33	1.37
31	A	856	CLA	OBD-CAD	2.82	1.27	1.22
31	9	321	CLA	C1B-NB	-2.82	1.34	1.37
36	2	301	LUT	C18-C5	2.82	1.55	1.50
31	B	830	CLA	C3B-C4B	2.82	1.49	1.42
31	b	303	CLA	C4D-ND	2.82	1.41	1.37
31	B	820	CLA	C3B-C4B	2.82	1.49	1.42
31	b	307	CLA	C1D-ND	-2.82	1.34	1.37
31	A	825	CLA	C1B-NB	-2.81	1.34	1.37
32	6	320	CHL	MG-NB	2.81	2.11	2.05
31	6	315	CLA	C3B-C4B	2.81	1.49	1.42
31	A	817	CLA	C1B-NB	-2.81	1.34	1.37
31	A	824	CLA	C3B-C4B	2.81	1.49	1.42
31	4	319	CLA	C3B-C4B	2.81	1.49	1.42
31	B	834	CLA	OBD-CAD	2.81	1.27	1.22
31	B	837	CLA	C4D-CHA	2.81	1.48	1.38
31	3	309	CLA	C3B-C4B	2.81	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	311	CLA	C1B-NB	-2.81	1.34	1.37
31	B	846	CLA	C1B-NB	-2.81	1.34	1.37
31	J	105	CLA	C1B-NB	-2.81	1.34	1.37
31	A	825	CLA	C4D-CHA	2.81	1.48	1.38
31	2	305	CLA	C3B-C4B	2.81	1.49	1.42
31	A	850	CLA	OBD-CAD	2.81	1.27	1.22
31	B	835	CLA	C3B-C4B	2.81	1.49	1.42
31	6	307	CLA	C3B-C4B	2.81	1.49	1.42
31	A	827	CLA	C1B-NB	-2.81	1.34	1.37
32	6	318	CHL	C1D-ND	-2.81	1.34	1.37
31	b	306	CLA	C3B-C4B	2.80	1.49	1.42
31	b	302	CLA	C3B-C4B	2.80	1.49	1.42
31	2	306	CLA	C3B-C4B	2.80	1.49	1.42
31	B	828	CLA	C1B-NB	-2.80	1.34	1.37
31	2	310	CLA	C1D-ND	-2.80	1.34	1.37
31	B	842	CLA	C3B-C4B	2.80	1.49	1.42
31	b	311	CLA	C3B-C4B	2.80	1.49	1.42
31	B	837	CLA	C3D-C2D	2.80	1.46	1.39
31	B	812	CLA	C4D-CHA	2.80	1.48	1.38
31	8	315	CLA	C3B-C4B	2.80	1.49	1.42
31	9	317	CLA	C1D-C2D	2.80	1.50	1.45
31	B	816	CLA	C4D-CHA	2.80	1.48	1.38
31	A	834	CLA	C3B-C4B	2.80	1.49	1.42
31	B	830	CLA	C4D-CHA	2.80	1.48	1.38
31	7	310	CLA	C1C-NC	-2.80	1.33	1.37
31	3	311	CLA	C1B-NB	-2.80	1.34	1.37
31	A	850	CLA	C3B-C4B	2.80	1.49	1.42
31	9	317	CLA	C4C-C3C	2.80	1.49	1.45
30	A	813	CL0	CHB-C1B	2.80	1.45	1.39
31	B	848	CLA	C3B-C4B	2.80	1.49	1.42
31	B	813	CLA	C1B-NB	-2.79	1.34	1.37
32	5	319	CHL	C1D-ND	-2.79	1.34	1.37
36	7	305	LUT	C18-C5	2.79	1.55	1.50
31	2	304	CLA	C3B-C4B	2.79	1.49	1.42
31	K	205	CLA	C3B-C4B	2.79	1.49	1.42
31	A	816	CLA	C4D-CHA	2.79	1.48	1.38
32	A	839	CHL	CHB-C1B	2.79	1.45	1.39
32	7	324	CHL	MG-NA	2.79	2.12	2.06
31	A	827	CLA	C3B-C4B	2.79	1.49	1.42
31	3	310	CLA	C3B-C4B	2.79	1.49	1.42
31	5	314	CLA	C3B-C4B	2.79	1.49	1.42
31	b	308	CLA	C3B-C4B	2.79	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	822	CLA	C1C-NC	-2.79	1.33	1.37
31	4	315	CLA	C3B-C4B	2.79	1.49	1.42
31	F	306	CLA	C3B-C4B	2.78	1.49	1.42
31	5	310	CLA	C1D-ND	-2.78	1.34	1.37
31	K	204	CLA	C4D-CHA	2.78	1.48	1.38
31	5	309	CLA	C1D-ND	-2.78	1.34	1.37
36	9	302	LUT	C18-C5	2.78	1.55	1.50
31	G	204	CLA	C3B-C4B	2.78	1.49	1.42
31	8	321	CLA	C3B-C4B	2.78	1.49	1.42
31	2	307	CLA	C1D-ND	-2.78	1.34	1.37
32	6	319	CHL	C1D-ND	-2.78	1.34	1.37
32	K	201	CHL	C1D-C2D	2.78	1.50	1.45
31	B	811	CLA	C4B-NB	-2.78	1.34	1.37
31	B	822	CLA	C1B-NB	-2.78	1.34	1.37
31	B	837	CLA	C3B-C4B	2.78	1.49	1.42
32	5	322	CHL	C1D-ND	-2.78	1.34	1.37
31	K	204	CLA	C3B-C4B	2.78	1.49	1.42
31	8	313	CLA	C3B-C4B	2.78	1.49	1.42
31	6	316	CLA	C3B-C4B	2.78	1.49	1.42
31	7	314	CLA	C1B-NB	-2.78	1.34	1.37
31	A	841	CLA	C1C-NC	-2.78	1.33	1.37
31	B	840	CLA	C4D-CHA	2.78	1.48	1.38
36	a	303	LUT	C18-C5	2.78	1.55	1.50
31	5	312	CLA	C3B-C4B	2.78	1.49	1.42
31	O	202	CLA	C3B-C4B	2.78	1.49	1.42
31	3	319	CLA	C4D-CHA	2.78	1.48	1.38
36	4	303	LUT	C23-C24	2.78	1.54	1.50
31	B	815	CLA	MG-NB	-2.78	2.00	2.05
31	b	307	CLA	C3B-C4B	2.77	1.49	1.42
31	B	817	CLA	C4D-CHA	2.77	1.48	1.38
31	A	828	CLA	MG-NB	2.77	2.11	2.05
31	9	318	CLA	C3B-C4B	2.77	1.49	1.42
31	5	309	CLA	C4C-C3C	2.77	1.49	1.45
36	J	103	LUT	C18-C5	2.77	1.55	1.50
31	9	313	CLA	C1D-ND	-2.77	1.34	1.37
31	A	814	CLA	C3B-C4B	2.77	1.49	1.42
31	B	835	CLA	C1C-NC	-2.77	1.33	1.37
32	7	320	CHL	C1D-ND	-2.77	1.34	1.37
32	b	309	CHL	C1D-ND	-2.77	1.34	1.37
31	4	312	CLA	C3B-C4B	2.77	1.49	1.42
31	6	322	CLA	C3B-C4B	2.76	1.49	1.42
31	B	839	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	318	CLA	C1B-NB	-2.76	1.34	1.37
31	H	903	CLA	C3B-C4B	2.76	1.49	1.42
31	2	312	CLA	C3B-C4B	2.76	1.49	1.42
31	A	851	CLA	OBD-CAD	2.76	1.27	1.22
31	3	312	CLA	C1B-NB	-2.76	1.34	1.37
31	B	819	CLA	C1B-NB	-2.76	1.34	1.37
31	B	824	CLA	C1C-NC	-2.76	1.33	1.37
31	A	838	CLA	C1C-NC	-2.76	1.33	1.37
31	H	903	CLA	C4C-C3C	2.76	1.49	1.45
31	G	204	CLA	C4C-C3C	2.76	1.49	1.45
31	H	901	CLA	C3B-C4B	2.76	1.49	1.42
31	7	312	CLA	C1B-NB	-2.76	1.34	1.37
31	L	305	CLA	C4D-CHA	2.76	1.48	1.38
32	5	319	CHL	MG-NB	-2.76	2.00	2.05
31	8	315	CLA	C1B-NB	-2.76	1.34	1.37
31	a	315	CLA	C3B-C4B	2.76	1.49	1.42
31	3	320	CLA	MG-NC	-2.75	1.99	2.06
31	5	312	CLA	C1D-ND	-2.75	1.34	1.37
31	6	311	CLA	C1D-ND	-2.75	1.34	1.37
31	2	310	CLA	C3B-C4B	2.75	1.49	1.42
27	A	808	LMT	O3'-C3'	-2.75	1.36	1.43
27	9	306	LMT	O3'-C3'	-2.75	1.36	1.43
31	B	823	CLA	C3B-C4B	2.75	1.49	1.42
31	8	307	CLA	C3B-C4B	2.75	1.49	1.42
36	3	305	LUT	C23-C24	2.75	1.54	1.50
31	8	311	CLA	C3B-C4B	2.75	1.49	1.42
31	B	824	CLA	C1B-NB	-2.75	1.34	1.37
31	4	306	CLA	C1D-ND	-2.75	1.34	1.37
31	9	312	CLA	C3B-C4B	2.75	1.49	1.42
31	a	313	CLA	MG-ND	-2.75	2.00	2.05
31	8	309	CLA	C1D-ND	-2.75	1.34	1.37
31	4	312	CLA	C1D-ND	-2.75	1.34	1.37
31	6	310	CLA	C1D-ND	-2.75	1.34	1.37
31	B	820	CLA	C1B-NB	-2.74	1.34	1.37
31	A	842	CLA	C3B-C4B	2.74	1.49	1.42
31	B	825	CLA	C3B-C4B	2.74	1.49	1.42
31	3	313	CLA	C3B-C4B	2.74	1.49	1.42
31	A	814	CLA	C4D-CHA	2.74	1.48	1.38
31	A	841	CLA	C3B-C4B	2.74	1.49	1.42
31	A	828	CLA	C3B-C4B	2.74	1.49	1.42
31	9	313	CLA	C3B-C4B	2.74	1.49	1.42
31	4	306	CLA	C3B-C4B	2.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	204	CLA	C4C-C3C	2.74	1.49	1.45
31	B	814	CLA	C1C-NC	-2.74	1.33	1.37
31	A	841	CLA	C1B-NB	-2.74	1.34	1.37
31	A	821	CLA	C3B-C4B	2.74	1.49	1.42
32	K	201	CHL	C3D-C2D	2.74	1.46	1.39
31	B	844	CLA	OBD-CAD	2.73	1.27	1.22
31	4	311	CLA	C4D-ND	2.73	1.41	1.37
31	K	205	CLA	C1B-NB	-2.73	1.34	1.37
31	3	313	CLA	C4C-C3C	2.73	1.49	1.45
31	8	314	CLA	C1C-NC	-2.73	1.33	1.37
31	A	852	CLA	C3B-C4B	2.73	1.49	1.42
31	4	305	CLA	C3D-C2D	2.73	1.46	1.39
26	L	301	BCR	C1-C6	-2.73	1.50	1.53
31	A	837	CLA	C1C-NC	-2.73	1.33	1.37
31	B	822	CLA	C4C-C3C	2.73	1.49	1.45
31	8	314	CLA	C4C-C3C	2.73	1.49	1.45
31	3	317	CLA	C3B-C4B	2.73	1.49	1.42
31	B	834	CLA	C1C-NC	-2.73	1.33	1.37
31	A	835	CLA	C4C-C3C	2.73	1.49	1.45
31	A	818	CLA	C4D-CHA	2.73	1.48	1.38
31	4	315	CLA	C1D-ND	-2.73	1.34	1.37
31	A	848	CLA	C1C-NC	-2.73	1.33	1.37
31	A	820	CLA	C1B-NB	-2.72	1.34	1.37
31	4	318	CLA	C4C-C3C	2.72	1.49	1.45
31	B	836	CLA	C3B-C4B	2.72	1.49	1.42
31	5	310	CLA	C1C-NC	-2.72	1.33	1.37
31	a	313	CLA	C3B-C4B	2.72	1.49	1.42
36	J	103	LUT	C23-C24	2.72	1.54	1.50
36	9	305	LUT	C38-C25	2.72	1.55	1.50
31	A	851	CLA	C1C-NC	-2.72	1.33	1.37
31	4	311	CLA	C3B-C4B	2.72	1.49	1.42
31	5	318	CLA	C1B-NB	-2.72	1.34	1.37
31	3	316	CLA	C3B-C4B	2.72	1.49	1.42
31	G	206	CLA	C1B-NB	-2.72	1.34	1.37
31	A	845	CLA	C3B-C4B	2.72	1.49	1.42
31	B	826	CLA	C3B-C4B	2.72	1.49	1.42
31	B	815	CLA	C1C-NC	-2.72	1.33	1.37
31	b	305	CLA	C1D-ND	-2.72	1.34	1.37
31	4	307	CLA	C4C-C3C	2.72	1.49	1.45
31	9	316	CLA	C1B-NB	-2.72	1.34	1.37
31	5	315	CLA	C3B-C4B	2.72	1.49	1.42
31	6	306	CLA	C1B-NB	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	312	CLA	C3B-C4B	2.71	1.49	1.42
31	4	318	CLA	C3B-C4B	2.71	1.49	1.42
31	A	822	CLA	C3B-C4B	2.71	1.49	1.42
31	a	313	CLA	C1B-NB	-2.71	1.34	1.37
31	3	312	CLA	C4C-C3C	2.71	1.49	1.45
31	A	843	CLA	C3B-C4B	2.71	1.49	1.42
31	5	308	CLA	C1D-ND	-2.71	1.34	1.37
31	7	316	CLA	C3B-C4B	2.71	1.49	1.42
31	O	202	CLA	C1D-ND	-2.71	1.34	1.37
31	6	314	CLA	C3B-C4B	2.71	1.49	1.42
31	a	322	CLA	C4C-C3C	2.71	1.49	1.45
31	9	318	CLA	C4C-C3C	2.71	1.49	1.45
31	a	309	CLA	C3B-C4B	2.71	1.49	1.42
31	2	307	CLA	C3B-C4B	2.71	1.49	1.42
31	G	206	CLA	C3B-C4B	2.71	1.49	1.42
32	9	322	CHL	C1D-ND	-2.70	1.34	1.37
31	A	830	CLA	C1C-NC	-2.70	1.33	1.37
31	a	322	CLA	C3B-C4B	2.70	1.49	1.42
31	9	316	CLA	C3B-C4B	2.70	1.49	1.42
31	4	308	CLA	C3B-C4B	2.70	1.49	1.42
31	9	311	CLA	C3B-C4B	2.70	1.49	1.42
31	H	901	CLA	MG-ND	-2.70	2.00	2.05
31	J	105	CLA	C3B-C4B	2.70	1.49	1.42
32	7	324	CHL	C1D-ND	-2.70	1.34	1.37
31	a	316	CLA	C3B-C4B	2.70	1.49	1.42
31	A	833	CLA	C3B-C4B	2.70	1.49	1.42
31	A	851	CLA	C3B-C4B	2.70	1.49	1.42
26	B	806	BCR	C1-C6	-2.70	1.50	1.53
31	B	849	CLA	OBD-CAD	2.69	1.27	1.22
31	9	315	CLA	C1C-NC	-2.69	1.33	1.37
31	A	857	CLA	C1C-NC	-2.69	1.33	1.37
31	5	321	CLA	C3B-C4B	2.69	1.49	1.42
31	4	307	CLA	C3B-C4B	2.69	1.49	1.42
31	A	833	CLA	C4C-C3C	2.69	1.49	1.45
31	B	847	CLA	MG-NB	2.69	2.11	2.05
31	4	314	CLA	C4C-C3C	2.69	1.49	1.45
31	B	824	CLA	C3B-C4B	2.69	1.49	1.42
36	F	304	LUT	C18-C5	2.69	1.55	1.50
31	B	811	CLA	C3B-C4B	2.69	1.49	1.42
36	3	304	LUT	C23-C24	2.69	1.54	1.50
31	B	844	CLA	C3B-C4B	2.69	1.49	1.42
31	6	311	CLA	C3B-C4B	2.69	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	843	CLA	C4C-C3C	2.68	1.49	1.45
31	O	203	CLA	C3B-C4B	2.68	1.49	1.42
31	4	305	CLA	MG-NB	2.68	2.11	2.05
31	B	848	CLA	C1B-NB	-2.68	1.34	1.37
31	A	830	CLA	C1B-NB	-2.68	1.34	1.37
31	B	841	CLA	C3B-C4B	2.68	1.49	1.42
36	a	305	LUT	C18-C5	2.68	1.55	1.50
31	5	318	CLA	C4C-C3C	2.68	1.49	1.45
31	A	853	CLA	C1C-NC	-2.68	1.33	1.37
31	B	821	CLA	C3B-C4B	2.68	1.49	1.42
31	7	321	CLA	C1B-NB	-2.68	1.34	1.37
31	4	321	CLA	C3B-C4B	2.68	1.49	1.42
31	a	313	CLA	C1D-ND	-2.68	1.34	1.37
31	A	814	CLA	C1C-NC	-2.68	1.33	1.37
31	B	816	CLA	C1C-NC	-2.68	1.33	1.37
31	6	322	CLA	C1D-ND	-2.68	1.34	1.37
31	B	841	CLA	C4D-CHA	2.67	1.47	1.38
31	B	844	CLA	C4B-NB	-2.67	1.34	1.37
31	3	308	CLA	C1B-NB	-2.67	1.34	1.37
31	K	205	CLA	C4C-C3C	2.67	1.49	1.45
31	B	837	CLA	C1B-NB	-2.67	1.34	1.37
31	B	834	CLA	C3B-C4B	2.67	1.49	1.42
31	A	855	CLA	C1B-NB	-2.67	1.34	1.37
31	b	307	CLA	C4C-C3C	2.67	1.49	1.45
31	a	311	CLA	C4C-C3C	2.67	1.49	1.45
31	8	320	CLA	C3B-C4B	2.67	1.49	1.42
31	9	319	CLA	C3B-C4B	2.67	1.49	1.42
31	4	312	CLA	C4C-C3C	2.67	1.49	1.45
31	9	314	CLA	C1B-NB	-2.67	1.34	1.37
31	9	319	CLA	C4C-C3C	2.67	1.49	1.45
31	6	313	CLA	MG-ND	-2.67	2.00	2.05
31	5	307	CLA	C3B-C4B	2.67	1.49	1.42
27	5	301	LMT	O2'-C2'	-2.67	1.36	1.43
31	7	314	CLA	C3B-C4B	2.67	1.49	1.42
31	2	315	CLA	C3B-C4B	2.66	1.49	1.42
31	5	323	CLA	C3B-C4B	2.66	1.49	1.42
31	A	816	CLA	C1C-NC	-2.66	1.33	1.37
31	B	835	CLA	MG-ND	2.66	2.11	2.05
31	O	202	CLA	C4C-C3C	2.66	1.49	1.44
31	3	312	CLA	C3B-C4B	2.66	1.49	1.42
31	A	815	CLA	C4D-CHA	2.66	1.47	1.38
31	B	815	CLA	C1B-NB	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	307	CLA	C1B-NB	-2.66	1.34	1.37
26	O	201	BCR	C1-C6	-2.66	1.50	1.53
31	3	314	CLA	C1B-NB	-2.66	1.34	1.37
31	b	302	CLA	C1D-ND	-2.66	1.34	1.37
31	H	901	CLA	C4C-C3C	2.66	1.49	1.45
31	a	312	CLA	C3B-C4B	2.66	1.49	1.42
31	8	308	CLA	C1B-NB	-2.66	1.34	1.37
31	9	315	CLA	C1B-NB	-2.66	1.34	1.37
26	B	802	BCR	C1-C6	-2.66	1.50	1.53
31	5	313	CLA	C1C-NC	-2.66	1.33	1.37
31	B	825	CLA	C1B-NB	-2.66	1.34	1.37
31	B	825	CLA	MG-ND	2.65	2.11	2.05
31	a	314	CLA	C3B-C4B	2.65	1.49	1.42
31	A	835	CLA	C1B-NB	-2.65	1.34	1.37
31	2	311	CLA	C4C-C3C	2.65	1.49	1.45
31	3	318	CLA	C3B-C4B	2.65	1.49	1.42
31	B	844	CLA	C1B-NB	-2.65	1.34	1.37
31	a	319	CLA	C3B-C4B	2.65	1.49	1.42
31	8	314	CLA	MG-NC	2.65	2.12	2.06
31	a	321	CLA	C3B-C4B	2.65	1.49	1.42
31	7	315	CLA	C1C-NC	-2.65	1.33	1.37
31	B	817	CLA	C1C-NC	-2.65	1.33	1.37
26	F	302	BCR	C1-C6	-2.65	1.50	1.53
31	2	314	CLA	C3B-C4B	2.65	1.49	1.42
31	a	310	CLA	C1C-NC	-2.64	1.33	1.37
31	8	315	CLA	C4C-C3C	2.64	1.49	1.45
27	5	301	LMT	O3'-C3'	-2.64	1.36	1.43
31	7	321	CLA	C3B-C4B	2.64	1.49	1.42
31	4	305	CLA	MG-NC	2.64	2.12	2.06
31	7	314	CLA	C4C-C3C	2.64	1.49	1.44
31	A	847	CLA	C3B-C4B	2.64	1.48	1.42
31	a	312	CLA	C1C-NC	-2.64	1.33	1.37
31	5	313	CLA	C1D-ND	-2.64	1.34	1.37
31	6	310	CLA	C3B-C4B	2.64	1.48	1.42
31	B	846	CLA	C1C-NC	-2.64	1.33	1.37
31	A	845	CLA	C1B-NB	-2.64	1.34	1.37
31	4	309	CLA	C1B-NB	-2.64	1.34	1.37
31	A	847	CLA	C1C-NC	-2.64	1.33	1.37
31	A	854	CLA	C3B-C4B	2.64	1.48	1.42
31	B	843	CLA	C4C-C3C	2.64	1.49	1.45
31	B	838	CLA	C1C-NC	-2.64	1.33	1.37
31	3	317	CLA	C4C-C3C	2.64	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	830	CLA	C1C-NC	-2.64	1.33	1.37
31	F	305	CLA	C4C-C3C	2.64	1.49	1.45
36	5	304	LUT	C23-C24	2.64	1.53	1.50
31	B	836	CLA	C1C-NC	-2.64	1.33	1.37
31	K	206	CLA	C3B-C4B	2.63	1.48	1.42
26	K	203	BCR	C1-C6	-2.63	1.50	1.53
31	a	322	CLA	C1B-NB	-2.63	1.34	1.37
31	b	312	CLA	C1D-ND	-2.63	1.34	1.37
31	B	823	CLA	C1C-NC	-2.63	1.33	1.37
31	B	838	CLA	C4C-C3C	2.63	1.49	1.45
31	5	321	CLA	C4C-C3C	2.63	1.49	1.45
31	B	826	CLA	C1B-NB	-2.63	1.34	1.37
31	8	312	CLA	C3B-C4B	2.63	1.48	1.42
31	3	320	CLA	C4D-ND	2.63	1.41	1.37
31	9	321	CLA	C4C-C3C	2.63	1.49	1.45
31	O	203	CLA	C4C-C3C	2.63	1.49	1.45
31	7	311	CLA	C1B-NB	-2.63	1.34	1.37
31	a	311	CLA	C3B-C4B	2.63	1.48	1.42
35	F	303	QTB	C09-C02	-2.63	1.40	1.45
31	2	309	CLA	C4C-C3C	2.63	1.49	1.45
31	a	321	CLA	C1B-NB	-2.63	1.34	1.37
31	F	305	CLA	C1B-NB	-2.63	1.34	1.37
31	G	204	CLA	C1B-NB	-2.63	1.34	1.37
32	5	316	CHL	C1D-ND	-2.63	1.34	1.37
31	b	307	CLA	C4D-ND	2.63	1.41	1.37
31	2	309	CLA	MG-NB	-2.63	2.00	2.05
31	6	312	CLA	C1B-NB	-2.63	1.34	1.37
31	b	306	CLA	C4C-C3C	2.63	1.49	1.45
26	M	101	BCR	C30-C25	-2.62	1.50	1.53
31	L	306	CLA	MG-NB	-2.62	2.00	2.05
31	5	313	CLA	MG-ND	2.62	2.11	2.05
38	a	304	AXT	C4-C5	-2.62	1.47	1.51
31	2	314	CLA	MG-NC	2.62	2.12	2.06
26	B	805	BCR	C1-C6	-2.62	1.50	1.53
31	A	837	CLA	C1B-NB	-2.62	1.34	1.37
31	A	815	CLA	C1C-NC	-2.62	1.33	1.37
31	A	827	CLA	MG-NB	2.62	2.11	2.05
31	7	310	CLA	C3B-C4B	2.62	1.48	1.42
26	B	803	BCR	C30-C25	-2.62	1.50	1.53
31	H	902	CLA	C3B-C4B	2.62	1.48	1.42
36	2	301	LUT	C23-C24	2.62	1.53	1.50
31	B	815	CLA	OBD-CAD	2.62	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	314	CLA	C3B-C4B	2.62	1.48	1.42
31	A	832	CLA	C3B-C4B	2.62	1.48	1.42
31	5	318	CLA	C3B-C4B	2.62	1.48	1.42
31	J	105	CLA	C1C-NC	-2.62	1.33	1.37
31	A	832	CLA	C1C-NC	-2.61	1.33	1.37
31	8	309	CLA	C3B-C4B	2.61	1.48	1.42
31	4	308	CLA	C1B-NB	-2.61	1.34	1.37
31	4	311	CLA	C4C-C3C	2.61	1.49	1.45
31	B	817	CLA	C3B-C4B	2.61	1.48	1.42
27	A	807	LMT	O2'-C2'	-2.61	1.36	1.43
32	9	320	CHL	CHC-C4B	2.61	1.45	1.39
31	L	305	CLA	C4C-C3C	2.61	1.49	1.45
31	B	815	CLA	C3B-C4B	2.61	1.48	1.42
31	3	316	CLA	C1C-NC	-2.61	1.33	1.37
31	A	830	CLA	C3B-C4B	2.61	1.48	1.42
31	a	312	CLA	C1B-NB	-2.61	1.34	1.37
31	8	310	CLA	C1B-NB	-2.61	1.34	1.37
31	2	306	CLA	C4C-C3C	2.61	1.49	1.45
36	a	305	LUT	C38-C25	2.61	1.55	1.50
31	8	317	CLA	C3B-C4B	2.61	1.48	1.42
31	B	823	CLA	C1B-NB	-2.60	1.34	1.37
31	B	831	CLA	C1B-NB	-2.60	1.34	1.37
31	L	307	CLA	C1D-ND	-2.60	1.34	1.37
31	4	309	CLA	C3B-C4B	2.60	1.48	1.42
31	B	812	CLA	C4B-NB	-2.60	1.34	1.37
31	B	837	CLA	C1C-NC	-2.60	1.33	1.37
31	5	308	CLA	C3B-C4B	2.60	1.48	1.42
31	6	313	CLA	C3B-C4B	2.60	1.48	1.42
31	B	850	CLA	C1B-NB	-2.60	1.34	1.37
31	a	311	CLA	C1B-NB	-2.60	1.34	1.37
31	9	314	CLA	C3B-C4B	2.60	1.48	1.42
31	B	821	CLA	C4C-C3C	2.60	1.49	1.45
31	3	308	CLA	C3B-C4B	2.60	1.48	1.42
36	5	303	LUT	C18-C5	2.60	1.55	1.50
36	8	302	LUT	C18-C5	2.60	1.55	1.50
31	4	319	CLA	MG-ND	2.60	2.10	2.05
31	2	315	CLA	C1B-NB	-2.60	1.34	1.37
31	a	319	CLA	C1C-NC	-2.60	1.33	1.37
31	A	838	CLA	C3B-C4B	2.60	1.48	1.42
32	b	309	CHL	MG-ND	-2.60	2.00	2.05
31	F	301	CLA	C4C-C3C	2.60	1.49	1.45
26	5	302	BCR	C1-C6	-2.59	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	307	CLA	C1B-NB	-2.59	1.34	1.37
31	A	844	CLA	C1C-NC	-2.59	1.33	1.37
31	8	308	CLA	C1C-NC	-2.59	1.33	1.37
31	5	321	CLA	C4D-ND	2.59	1.41	1.37
31	B	827	CLA	C1B-NB	-2.59	1.34	1.37
31	4	319	CLA	C4C-C3C	2.59	1.49	1.45
31	A	822	CLA	C1C-NC	-2.59	1.33	1.37
31	A	821	CLA	C4B-NB	-2.59	1.34	1.37
31	2	314	CLA	C4C-C3C	2.59	1.49	1.45
31	G	204	CLA	C1C-NC	-2.59	1.33	1.37
31	A	857	CLA	C1B-NB	-2.59	1.34	1.37
31	8	320	CLA	C1B-NB	-2.59	1.34	1.37
31	B	850	CLA	C1C-NC	-2.59	1.33	1.37
40	7	306	XAT	C8-C9	-2.59	1.40	1.45
31	B	829	CLA	C1C-NC	-2.59	1.33	1.37
31	8	320	CLA	C1C-NC	-2.59	1.33	1.37
31	6	314	CLA	MG-ND	2.59	2.10	2.05
31	b	303	CLA	C3B-C4B	2.59	1.48	1.42
31	5	309	CLA	C3B-C4B	2.59	1.48	1.42
31	b	305	CLA	C1B-NB	-2.59	1.34	1.37
32	4	310	CHL	C4C-C3C	2.59	1.49	1.45
31	L	307	CLA	C4D-ND	2.59	1.41	1.37
31	5	311	CLA	C3B-C4B	2.59	1.48	1.42
31	B	816	CLA	C1B-NB	-2.58	1.34	1.37
31	7	313	CLA	C1B-NB	-2.58	1.34	1.37
36	8	302	LUT	C26-C27	2.58	1.54	1.50
31	A	849	CLA	C4C-C3C	2.58	1.49	1.45
31	7	314	CLA	C1C-NC	-2.58	1.34	1.37
31	A	835	CLA	C1C-NC	-2.58	1.34	1.37
31	9	311	CLA	C1B-NB	-2.58	1.34	1.37
31	5	308	CLA	C4D-ND	2.58	1.41	1.37
31	A	819	CLA	C1C-NC	-2.57	1.34	1.37
31	5	312	CLA	C4C-C3C	2.57	1.49	1.45
31	b	302	CLA	C4D-ND	2.57	1.41	1.37
31	B	817	CLA	C4B-NB	-2.57	1.34	1.37
31	a	319	CLA	C4C-C3C	2.57	1.49	1.45
36	a	305	LUT	C1-C6	2.57	1.57	1.53
31	O	204	CLA	C4D-ND	2.57	1.41	1.37
36	7	305	LUT	C23-C24	2.57	1.53	1.50
36	9	303	LUT	C23-C24	2.57	1.53	1.50
31	A	829	CLA	MG-ND	2.57	2.10	2.05
31	A	820	CLA	C3B-C4B	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	849	CLA	C1B-NB	-2.57	1.34	1.37
31	7	322	CLA	MG-NA	2.57	2.12	2.06
31	F	301	CLA	C1C-NC	-2.57	1.34	1.37
26	B	804	BCR	C30-C25	-2.57	1.50	1.53
27	9	306	LMT	O2'-C2'	-2.57	1.36	1.43
31	B	831	CLA	C3B-C4B	2.57	1.48	1.42
32	A	840	CHL	OBD-CAD	2.57	1.26	1.22
31	F	306	CLA	C4C-C3C	2.57	1.49	1.45
31	b	312	CLA	C4D-ND	2.57	1.41	1.37
31	A	851	CLA	C1B-NB	-2.56	1.34	1.37
36	L	304	LUT	C18-C5	2.56	1.55	1.50
26	B	804	BCR	C1-C6	-2.56	1.50	1.53
31	5	313	CLA	C1D-C2D	2.56	1.50	1.45
26	B	806	BCR	C30-C25	-2.56	1.50	1.53
31	7	313	CLA	C1C-NC	-2.56	1.34	1.37
31	A	841	CLA	C4C-C3C	2.56	1.49	1.45
31	B	818	CLA	C4C-C3C	2.56	1.49	1.45
31	a	309	CLA	C1C-NC	-2.56	1.34	1.37
31	H	902	CLA	C4C-C3C	2.56	1.49	1.45
31	A	845	CLA	C1C-NC	-2.56	1.34	1.37
36	3	304	LUT	C26-C27	2.56	1.54	1.50
31	2	307	CLA	C4C-C3C	2.56	1.49	1.45
31	A	848	CLA	C3B-C4B	2.56	1.48	1.42
40	7	306	XAT	C32-C33	-2.56	1.40	1.45
31	A	838	CLA	C4C-C3C	2.56	1.49	1.45
31	b	311	CLA	C4C-C3C	2.56	1.49	1.45
31	7	313	CLA	C3B-C4B	2.56	1.48	1.42
31	2	307	CLA	C1C-NC	-2.56	1.34	1.37
31	5	313	CLA	MG-NB	2.56	2.10	2.05
26	A	806	BCR	C30-C25	-2.56	1.50	1.53
26	3	303	BCR	C1-C6	-2.56	1.50	1.53
36	4	302	LUT	C18-C5	2.56	1.55	1.50
31	a	316	CLA	C1B-NB	-2.56	1.34	1.37
31	A	814	CLA	C1B-NB	-2.55	1.34	1.37
31	3	317	CLA	C1B-NB	-2.55	1.34	1.37
26	3	301	BCR	C1-C6	-2.55	1.50	1.53
31	a	319	CLA	C1B-NB	-2.55	1.34	1.37
31	5	311	CLA	C1B-NB	-2.55	1.34	1.37
31	7	322	CLA	C3B-C4B	2.55	1.48	1.42
31	A	815	CLA	C4B-NB	-2.55	1.34	1.37
31	3	307	CLA	MG-NC	2.55	2.12	2.06
31	A	824	CLA	C4C-C3C	2.55	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	825	CLA	C1C-NC	-2.55	1.34	1.37
31	7	321	CLA	C1C-NC	-2.55	1.34	1.37
31	B	849	CLA	C4C-C3C	2.55	1.49	1.45
31	b	310	CLA	C1B-NB	-2.55	1.34	1.37
31	3	311	CLA	C1C-NC	-2.55	1.34	1.37
31	3	320	CLA	C1B-NB	-2.55	1.34	1.37
40	7	306	XAT	C28-C29	-2.55	1.40	1.45
31	B	811	CLA	C1B-C2B	2.54	1.49	1.43
32	a	320	CHL	MG-ND	2.54	2.10	2.05
31	K	206	CLA	C1B-NB	-2.54	1.34	1.37
31	5	311	CLA	C1C-NC	-2.54	1.34	1.37
31	A	857	CLA	C3B-C4B	2.54	1.48	1.42
31	8	307	CLA	C1B-NB	-2.54	1.34	1.37
31	A	837	CLA	C3B-C4B	2.54	1.48	1.42
31	5	312	CLA	C1B-NB	-2.54	1.34	1.37
40	7	306	XAT	C12-C13	-2.54	1.40	1.45
31	A	841	CLA	C4B-NB	-2.54	1.34	1.37
31	a	315	CLA	C1B-NB	-2.54	1.34	1.37
31	3	316	CLA	C1B-NB	-2.54	1.34	1.37
31	F	305	CLA	C1C-NC	-2.54	1.34	1.37
31	9	312	CLA	C1B-NB	-2.54	1.34	1.37
31	8	318	CLA	C3B-C4B	2.54	1.48	1.42
31	6	311	CLA	MG-NC	-2.53	2.00	2.06
31	B	812	CLA	C1C-NC	-2.53	1.34	1.37
31	B	838	CLA	C3B-C4B	2.53	1.48	1.42
31	a	310	CLA	C3B-C4B	2.53	1.48	1.42
32	6	309	CHL	MG-ND	-2.53	2.00	2.05
31	4	305	CLA	C4D-ND	2.53	1.41	1.37
31	8	320	CLA	C4C-C3C	2.53	1.49	1.45
31	6	314	CLA	C4C-C3C	2.53	1.49	1.45
31	A	836	CLA	C1C-NC	-2.53	1.34	1.37
31	9	314	CLA	C1C-NC	-2.53	1.34	1.37
36	5	304	LUT	C18-C5	2.53	1.55	1.50
31	2	310	CLA	C4D-ND	2.53	1.41	1.37
31	A	854	CLA	C1C-NC	-2.53	1.34	1.37
31	B	844	CLA	C1C-NC	-2.53	1.34	1.37
31	J	105	CLA	C1B-C2B	2.53	1.49	1.43
31	B	818	CLA	C1C-NC	-2.53	1.34	1.37
31	B	833	CLA	C1C-NC	-2.53	1.34	1.37
31	5	310	CLA	C1B-NB	-2.53	1.34	1.37
31	a	311	CLA	C1B-C2B	2.53	1.49	1.43
31	G	206	CLA	C4C-C3C	2.53	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	314	CLA	C4C-C3C	2.53	1.49	1.45
31	7	322	CLA	C1B-C2B	2.53	1.49	1.43
36	b	301	LUT	C38-C25	2.53	1.55	1.50
35	7	303	QTB	C09-C02	-2.52	1.40	1.45
31	A	843	CLA	MG-NB	-2.52	2.00	2.05
31	A	852	CLA	C1C-NC	-2.52	1.34	1.37
31	A	823	CLA	C4B-NB	-2.52	1.34	1.37
31	3	309	CLA	C1B-NB	-2.52	1.34	1.37
31	a	314	CLA	C1B-NB	-2.52	1.34	1.37
31	4	315	CLA	C4C-C3C	2.52	1.49	1.45
31	9	316	CLA	C1C-NC	-2.52	1.34	1.37
26	B	802	BCR	C30-C25	-2.52	1.50	1.53
31	F	306	CLA	C1B-NB	-2.52	1.34	1.37
31	b	310	CLA	C4C-C3C	2.52	1.49	1.45
31	F	305	CLA	C3B-C4B	2.52	1.48	1.42
31	B	832	CLA	C3B-C4B	2.51	1.48	1.42
31	3	318	CLA	C1B-NB	-2.51	1.34	1.37
31	A	823	CLA	C1C-NC	-2.51	1.34	1.37
31	7	322	CLA	C1B-NB	-2.51	1.34	1.37
31	b	302	CLA	C4C-C3C	2.51	1.49	1.45
36	7	305	LUT	C1-C6	2.51	1.57	1.53
31	5	312	CLA	C4D-ND	2.51	1.41	1.37
31	B	826	CLA	C1C-NC	-2.51	1.34	1.37
31	4	312	CLA	C1B-NB	-2.51	1.34	1.37
31	2	304	CLA	C4C-C3C	2.51	1.49	1.45
31	K	206	CLA	C4C-C3C	2.51	1.49	1.45
26	L	303	BCR	C1-C6	-2.51	1.50	1.53
31	7	310	CLA	C4D-ND	2.51	1.41	1.37
31	3	318	CLA	C4C-C3C	2.51	1.49	1.45
31	A	846	CLA	C3B-C4B	2.51	1.48	1.42
31	2	313	CLA	C1B-NB	-2.51	1.34	1.37
31	A	846	CLA	C1C-NC	-2.51	1.34	1.37
31	4	308	CLA	C1C-NC	-2.51	1.34	1.37
31	A	830	CLA	C4C-C3C	2.51	1.49	1.45
31	B	841	CLA	C1C-NC	-2.51	1.34	1.37
32	5	322	CHL	C3D-C2D	2.51	1.46	1.39
31	9	313	CLA	C4C-C3C	2.51	1.49	1.45
31	B	835	CLA	C4C-C3C	2.51	1.49	1.45
31	6	310	CLA	C4C-C3C	2.51	1.49	1.45
31	5	315	CLA	C4C-C3C	2.50	1.49	1.45
31	6	316	CLA	C1B-C2B	2.50	1.49	1.43
31	A	823	CLA	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	307	CLA	C4C-C3C	2.50	1.49	1.45
31	4	305	CLA	CHD-C4C	2.50	1.44	1.39
32	4	310	CHL	MG-NC	-2.50	2.00	2.06
31	7	315	CLA	C3B-C4B	2.50	1.48	1.42
31	B	844	CLA	C4C-C3C	2.50	1.49	1.45
30	A	813	CL0	CHB-C4A	-2.50	1.31	1.37
31	B	835	CLA	C1B-NB	-2.50	1.34	1.37
31	9	315	CLA	C3B-C4B	2.50	1.48	1.42
26	2	302	BCR	C30-C25	-2.50	1.50	1.53
31	A	833	CLA	C1B-NB	-2.50	1.34	1.37
31	B	842	CLA	C1C-NC	-2.50	1.34	1.37
27	5	301	LMT	O3B-C3B	-2.50	1.37	1.43
37	G	202	LMG	C4-C5	2.50	1.58	1.53
36	9	303	LUT	C38-C25	2.50	1.55	1.50
32	K	201	CHL	C1B-C2B	2.50	1.49	1.43
31	A	825	CLA	C1C-NC	-2.49	1.34	1.37
31	4	308	CLA	C4C-C3C	2.49	1.49	1.45
31	2	310	CLA	C1C-NC	-2.49	1.34	1.37
31	b	313	CLA	C1B-NB	-2.49	1.34	1.37
26	A	806	BCR	C1-C6	-2.49	1.50	1.53
31	3	309	CLA	C4C-C3C	2.49	1.49	1.45
31	6	313	CLA	C4C-C3C	2.49	1.49	1.45
26	8	301	BCR	C1-C6	-2.49	1.50	1.53
31	B	849	CLA	C1C-NC	-2.49	1.34	1.37
31	6	308	CLA	C1B-NB	-2.49	1.34	1.37
31	6	311	CLA	C1C-NC	-2.49	1.34	1.37
31	7	309	CLA	C1B-NB	-2.49	1.34	1.37
31	2	308	CLA	C1C-NC	-2.49	1.34	1.37
31	4	320	CLA	C4C-C3C	2.49	1.49	1.45
31	A	848	CLA	C4B-NB	-2.49	1.34	1.37
31	5	310	CLA	C4C-C3C	2.49	1.49	1.45
31	5	320	CLA	C4C-C3C	2.49	1.49	1.45
36	7	305	LUT	C38-C25	2.49	1.55	1.50
31	8	313	CLA	C1C-NC	-2.49	1.34	1.37
31	9	319	CLA	C1B-NB	-2.48	1.34	1.37
31	5	321	CLA	C1C-NC	-2.48	1.34	1.37
31	B	833	CLA	C4B-NB	-2.48	1.34	1.37
31	3	311	CLA	C3B-C4B	2.48	1.48	1.42
31	A	842	CLA	C1C-NC	-2.48	1.34	1.37
32	9	322	CHL	C3D-C2D	2.48	1.45	1.39
31	8	318	CLA	C1C-NC	-2.48	1.34	1.37
31	5	310	CLA	C3B-C4B	2.48	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	807	LMT	O2B-C2B	-2.48	1.37	1.43
31	5	315	CLA	C1C-NC	-2.48	1.34	1.37
31	6	307	CLA	C4D-ND	2.48	1.41	1.37
31	9	316	CLA	C4C-C3C	2.48	1.49	1.45
31	9	316	CLA	MG-ND	2.48	2.10	2.05
31	5	307	CLA	C1C-NC	-2.48	1.34	1.37
26	7	304	BCR	C30-C25	-2.48	1.50	1.53
27	9	306	LMT	O3B-C3B	-2.48	1.37	1.43
31	A	844	CLA	C3B-C4B	2.48	1.48	1.42
26	7	304	BCR	C1-C6	-2.48	1.50	1.53
31	A	854	CLA	MG-NB	-2.48	2.00	2.05
31	a	310	CLA	C1B-NB	-2.48	1.34	1.37
31	6	316	CLA	C1B-NB	-2.48	1.34	1.37
31	L	305	CLA	C1C-NC	-2.48	1.34	1.37
26	A	805	BCR	C30-C25	-2.48	1.50	1.53
31	2	310	CLA	C4C-C3C	2.47	1.49	1.45
31	A	822	CLA	C4B-NB	-2.47	1.34	1.37
31	A	834	CLA	C4C-C3C	2.47	1.49	1.45
31	B	827	CLA	C1C-NC	-2.47	1.34	1.37
26	A	803	BCR	C1-C6	-2.47	1.50	1.53
31	A	828	CLA	C1C-NC	-2.47	1.34	1.37
31	4	312	CLA	C4D-ND	2.47	1.41	1.37
32	a	318	CHL	C3D-C2D	2.47	1.45	1.39
31	B	821	CLA	C1C-NC	-2.47	1.34	1.37
31	F	306	CLA	C1C-NC	-2.47	1.34	1.37
31	B	843	CLA	C1C-NC	-2.47	1.34	1.37
31	6	322	CLA	C4D-ND	2.47	1.41	1.37
31	O	203	CLA	C1C-NC	-2.47	1.34	1.37
31	B	827	CLA	C3B-C4B	2.47	1.48	1.42
31	a	316	CLA	MG-NB	2.47	2.10	2.05
31	A	849	CLA	C1C-NC	-2.47	1.34	1.37
31	3	312	CLA	C1C-NC	-2.47	1.34	1.37
32	6	309	CHL	C3D-C2D	2.47	1.45	1.39
36	6	304	LUT	C23-C24	2.46	1.53	1.50
31	9	317	CLA	C1C-NC	-2.46	1.34	1.37
31	A	848	CLA	C4C-C3C	2.46	1.49	1.45
31	B	847	CLA	C4C-C3C	2.46	1.49	1.45
31	2	312	CLA	C4C-C3C	2.46	1.49	1.45
31	2	313	CLA	C1C-NC	-2.46	1.34	1.37
31	A	826	CLA	C4C-C3C	2.46	1.49	1.45
31	b	308	CLA	C4D-ND	2.46	1.41	1.37
31	4	319	CLA	C4D-ND	2.46	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	309	CLA	C1C-NC	-2.46	1.34	1.37
31	B	841	CLA	C4B-NB	-2.46	1.34	1.37
31	7	312	CLA	C4C-C3C	2.46	1.49	1.45
31	2	306	CLA	C1B-NB	-2.46	1.34	1.37
36	4	302	LUT	C38-C25	2.46	1.55	1.50
31	8	312	CLA	C1C-NC	-2.46	1.34	1.37
31	9	311	CLA	C1C-NC	-2.46	1.34	1.37
36	6	304	LUT	C38-C25	2.46	1.55	1.50
31	A	853	CLA	C4B-NB	-2.46	1.34	1.37
32	A	839	CHL	MG-NB	-2.46	2.00	2.05
31	5	323	CLA	C1B-NB	-2.46	1.34	1.37
31	B	847	CLA	C1C-NC	-2.45	1.34	1.37
31	2	308	CLA	C1B-NB	-2.45	1.34	1.37
31	3	307	CLA	C1C-NC	-2.45	1.34	1.37
31	B	850	CLA	C4C-C3C	2.45	1.49	1.45
31	B	819	CLA	C1C-NC	-2.45	1.34	1.37
31	2	305	CLA	C4C-C3C	2.45	1.49	1.45
31	B	814	CLA	C4C-C3C	2.45	1.49	1.45
31	A	836	CLA	C1B-NB	-2.45	1.34	1.37
31	4	315	CLA	C4D-ND	2.45	1.41	1.37
31	6	311	CLA	C4D-ND	2.45	1.41	1.37
31	9	318	CLA	C1C-NC	-2.45	1.34	1.37
31	4	311	CLA	C1C-NC	-2.45	1.34	1.37
31	A	832	CLA	C4C-C3C	2.45	1.49	1.45
31	B	836	CLA	C4C-C3C	2.45	1.49	1.45
31	7	322	CLA	C1C-NC	-2.45	1.34	1.37
31	L	307	CLA	C1C-NC	-2.45	1.34	1.37
31	b	303	CLA	C1D-ND	-2.45	1.34	1.37
31	4	306	CLA	C4C-C3C	2.45	1.49	1.45
31	8	311	CLA	C4C-C3C	2.44	1.49	1.45
31	3	318	CLA	C4D-ND	2.44	1.41	1.37
31	9	321	CLA	C1C-NC	-2.44	1.34	1.37
36	3	305	LUT	C38-C25	2.44	1.55	1.50
32	A	831	CHL	MG-NA	2.44	2.12	2.06
31	B	849	CLA	C4B-NB	-2.44	1.34	1.37
26	O	201	BCR	C30-C25	-2.44	1.50	1.53
36	5	304	LUT	C38-C25	2.44	1.55	1.50
31	3	320	CLA	C4C-C3C	2.44	1.49	1.45
31	4	315	CLA	C1C-NC	-2.44	1.34	1.37
31	A	833	CLA	C1C-NC	-2.44	1.34	1.37
31	8	307	CLA	C1C-NC	-2.44	1.34	1.37
31	6	310	CLA	C4D-ND	2.44	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	308	CLA	MG-NC	2.44	2.12	2.06
31	B	831	CLA	C4C-C3C	2.44	1.49	1.45
31	a	313	CLA	C4C-C3C	2.44	1.49	1.45
31	7	316	CLA	C1B-NB	-2.44	1.34	1.37
31	K	205	CLA	C1B-C2B	2.43	1.49	1.43
31	4	306	CLA	MG-NC	2.43	2.12	2.06
31	B	812	CLA	C4C-C3C	2.43	1.49	1.45
32	5	319	CHL	C3D-C2D	2.43	1.45	1.39
31	B	832	CLA	C1B-C2B	2.43	1.49	1.43
31	4	318	CLA	C4D-ND	2.43	1.41	1.37
31	B	829	CLA	C3B-C4B	2.43	1.48	1.42
31	9	312	CLA	C1C-NC	-2.43	1.34	1.37
36	9	305	LUT	C18-C5	2.43	1.54	1.50
31	3	308	CLA	C4D-ND	2.43	1.41	1.37
31	A	854	CLA	C4C-C3C	2.43	1.49	1.45
31	9	313	CLA	C1B-NB	-2.43	1.34	1.37
31	B	828	CLA	C4C-C3C	2.43	1.49	1.45
36	6	304	LUT	C18-C5	2.43	1.54	1.50
31	5	323	CLA	C4D-ND	2.43	1.41	1.37
31	B	823	CLA	C4C-C3C	2.43	1.49	1.45
31	A	850	CLA	C1C-NC	-2.43	1.34	1.37
27	9	306	LMT	O2B-C2B	-2.43	1.37	1.43
31	K	204	CLA	C1B-NB	-2.43	1.34	1.37
31	3	317	CLA	C1C-NC	-2.43	1.34	1.37
31	B	813	CLA	C4B-NB	-2.43	1.34	1.37
31	A	834	CLA	C1C-NC	-2.43	1.34	1.37
31	A	856	CLA	C1C-NC	-2.43	1.34	1.37
31	5	308	CLA	C1B-NB	-2.42	1.34	1.37
31	A	824	CLA	C1C-NC	-2.42	1.34	1.37
31	7	315	CLA	C4C-C3C	2.42	1.49	1.45
31	B	843	CLA	C3B-C4B	2.42	1.48	1.42
31	B	829	CLA	C1B-NB	-2.42	1.34	1.37
31	8	317	CLA	C4B-NB	-2.42	1.34	1.37
31	5	310	CLA	C4D-ND	2.42	1.41	1.37
32	9	320	CHL	C1B-NB	-2.42	1.34	1.37
36	b	301	LUT	C18-C5	2.42	1.54	1.50
31	A	836	CLA	C4C-C3C	2.42	1.49	1.45
31	a	316	CLA	C4C-C3C	2.42	1.49	1.45
31	4	321	CLA	C4C-C3C	2.42	1.49	1.45
31	A	821	CLA	C1C-NC	-2.42	1.34	1.37
31	3	309	CLA	C1C-NC	-2.42	1.34	1.37
31	H	901	CLA	C1B-NB	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	315	CLA	C1B-NB	-2.42	1.34	1.37
31	2	309	CLA	C1B-NB	-2.42	1.34	1.37
31	4	318	CLA	C1D-ND	-2.42	1.34	1.37
31	G	205	CLA	C4C-C3C	2.42	1.49	1.45
36	3	304	LUT	C18-C5	2.42	1.54	1.50
31	2	305	CLA	C4D-ND	2.42	1.41	1.37
31	A	817	CLA	C4B-NB	-2.42	1.34	1.37
32	4	317	CHL	C3D-C2D	2.42	1.45	1.39
31	B	829	CLA	C1B-C2B	2.42	1.49	1.43
31	7	322	CLA	C4C-C3C	2.42	1.49	1.45
27	A	808	LMT	O2B-C2B	-2.42	1.37	1.43
31	8	321	CLA	C1C-NC	-2.42	1.34	1.37
31	B	816	CLA	C4C-C3C	2.42	1.49	1.45
31	a	321	CLA	C4C-C3C	2.42	1.49	1.45
31	5	308	CLA	C4C-C3C	2.42	1.49	1.45
31	8	307	CLA	C1B-C2B	2.42	1.48	1.43
31	A	830	CLA	C4D-ND	2.42	1.41	1.37
31	6	315	CLA	C4C-C3C	2.42	1.49	1.45
32	a	317	CHL	C3D-C2D	2.42	1.45	1.39
31	A	852	CLA	C4C-C3C	2.41	1.49	1.45
31	6	306	CLA	C4C-C3C	2.41	1.49	1.45
31	B	816	CLA	C3B-C4B	2.41	1.48	1.42
31	4	307	CLA	C1C-NC	-2.41	1.34	1.37
31	8	309	CLA	C4D-ND	2.41	1.41	1.37
31	3	308	CLA	C1C-NC	-2.41	1.34	1.37
31	7	316	CLA	C4C-C3C	2.41	1.49	1.45
31	2	312	CLA	C1B-NB	-2.41	1.34	1.37
31	8	311	CLA	C1C-NC	-2.41	1.34	1.37
31	6	310	CLA	C1C-NC	-2.41	1.34	1.37
31	5	308	CLA	C1C-NC	-2.41	1.34	1.37
31	8	318	CLA	C4C-C3C	2.41	1.49	1.45
31	3	313	CLA	C1B-NB	-2.41	1.34	1.37
31	A	818	CLA	C4C-C3C	2.41	1.49	1.45
31	B	830	CLA	C4C-C3C	2.41	1.49	1.45
31	B	840	CLA	C4B-NB	-2.41	1.34	1.37
31	a	310	CLA	C4D-ND	2.41	1.41	1.37
31	K	206	CLA	C4D-ND	2.41	1.41	1.37
31	6	313	CLA	C1C-NC	-2.41	1.34	1.37
31	9	316	CLA	C1B-C2B	2.41	1.48	1.43
31	B	811	CLA	C4C-C3C	2.41	1.49	1.45
31	a	309	CLA	C4D-ND	2.41	1.41	1.37
32	9	322	CHL	C4C-C3C	2.41	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	314	CLA	C1C-NC	-2.41	1.34	1.37
31	O	202	CLA	C4D-ND	2.40	1.41	1.37
31	5	311	CLA	C4C-C3C	2.40	1.49	1.45
31	B	847	CLA	C4B-NB	-2.40	1.34	1.37
26	F	302	BCR	C30-C25	-2.40	1.50	1.53
31	b	303	CLA	C1C-NC	-2.40	1.34	1.37
31	7	309	CLA	C4C-C3C	2.40	1.49	1.45
31	B	819	CLA	C3B-C4B	2.40	1.48	1.42
31	B	846	CLA	C4C-C3C	2.40	1.49	1.45
31	a	315	CLA	C4C-C3C	2.40	1.49	1.45
31	B	839	CLA	C4B-NB	-2.40	1.34	1.37
31	3	311	CLA	C4C-C3C	2.40	1.49	1.45
31	B	840	CLA	C1B-C2B	2.40	1.48	1.43
31	H	903	CLA	C4D-ND	2.40	1.40	1.37
31	5	318	CLA	C1C-NC	-2.40	1.34	1.37
32	6	321	CHL	C3D-C2D	2.40	1.45	1.39
31	A	846	CLA	C4C-C3C	2.40	1.49	1.45
31	B	826	CLA	C1B-C2B	2.40	1.48	1.43
31	3	314	CLA	C4C-C3C	2.40	1.49	1.45
31	4	309	CLA	C1B-C2B	2.40	1.48	1.43
31	B	840	CLA	C1C-NC	-2.40	1.34	1.37
31	a	310	CLA	C4C-C3C	2.40	1.49	1.45
31	5	313	CLA	C4C-C3C	2.40	1.49	1.45
32	7	319	CHL	C3D-C2D	2.40	1.45	1.39
31	2	315	CLA	C1B-C2B	2.39	1.48	1.43
31	a	314	CLA	C1C-NC	-2.39	1.34	1.37
32	K	201	CHL	C1D-ND	-2.39	1.34	1.37
31	B	824	CLA	C4C-C3C	2.39	1.49	1.45
31	B	848	CLA	C4C-C3C	2.39	1.49	1.45
31	b	311	CLA	C1C-NC	-2.39	1.34	1.37
31	b	307	CLA	C1B-C2B	2.39	1.48	1.43
31	3	308	CLA	C4C-C3C	2.39	1.49	1.45
31	3	311	CLA	C4D-ND	2.39	1.40	1.37
31	A	818	CLA	C1C-NC	-2.39	1.34	1.37
31	2	304	CLA	C1B-NB	-2.39	1.34	1.37
31	b	305	CLA	C4C-C3C	2.39	1.49	1.45
31	5	313	CLA	C3B-C4B	2.39	1.48	1.42
31	2	315	CLA	C4C-C3C	2.39	1.49	1.45
31	B	814	CLA	C4B-NB	-2.39	1.34	1.37
32	b	309	CHL	C3D-C2D	2.39	1.45	1.39
32	5	316	CHL	C1B-NB	-2.39	1.34	1.37
31	8	312	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	322	CLA	C4C-C3C	2.39	1.49	1.45
31	B	813	CLA	C1C-NC	-2.39	1.34	1.37
27	5	301	LMT	O4'-C4B	-2.39	1.37	1.43
31	B	818	CLA	C3B-C4B	2.39	1.48	1.42
31	L	306	CLA	C4C-C3C	2.39	1.49	1.45
31	9	319	CLA	C1B-C2B	2.39	1.48	1.43
31	K	204	CLA	C1C-NC	-2.38	1.34	1.37
31	8	314	CLA	C1B-NB	-2.38	1.34	1.37
31	a	313	CLA	C1C-NC	-2.38	1.34	1.37
32	9	320	CHL	C3D-C2D	2.38	1.45	1.39
32	6	317	CHL	C3D-C2D	2.38	1.45	1.39
31	A	837	CLA	C4C-C3C	2.38	1.49	1.45
31	4	314	CLA	C4D-ND	2.38	1.40	1.37
31	5	321	CLA	C1B-NB	-2.38	1.34	1.37
31	G	206	CLA	C1C-NC	-2.38	1.34	1.37
31	a	319	CLA	C1B-C2B	2.38	1.48	1.43
31	2	311	CLA	C1B-NB	-2.38	1.34	1.37
31	5	307	CLA	C4C-C3C	2.38	1.49	1.45
31	6	316	CLA	C4C-C3C	2.38	1.49	1.45
26	B	805	BCR	C30-C25	-2.38	1.50	1.53
31	L	305	CLA	MG-NB	2.38	2.10	2.05
31	B	819	CLA	C1B-C2B	2.38	1.48	1.43
31	B	831	CLA	MG-ND	2.38	2.10	2.05
31	B	811	CLA	C1C-NC	-2.38	1.34	1.37
31	O	202	CLA	C1C-NC	-2.38	1.34	1.37
31	a	309	CLA	C1B-NB	-2.38	1.34	1.37
32	A	831	CHL	C4C-C3C	2.38	1.49	1.45
27	A	808	LMT	O4'-C4B	-2.37	1.37	1.43
31	5	309	CLA	C4D-ND	2.37	1.40	1.37
31	b	303	CLA	C1B-C2B	2.37	1.48	1.43
31	A	825	CLA	C1B-C2B	2.37	1.48	1.43
31	b	306	CLA	C4D-ND	2.37	1.40	1.37
31	6	310	CLA	C1B-C2B	2.37	1.48	1.43
31	7	311	CLA	C1C-NC	-2.37	1.34	1.37
31	A	851	CLA	C4B-NB	-2.37	1.34	1.37
31	5	323	CLA	C1C-NC	-2.37	1.34	1.37
31	b	304	CLA	C4C-C3C	2.37	1.49	1.45
36	8	303	LUT	C18-C5	2.37	1.54	1.50
31	2	314	CLA	C1B-NB	-2.37	1.34	1.37
31	5	313	CLA	C1B-C2B	2.37	1.48	1.43
31	A	842	CLA	C4B-NB	-2.37	1.34	1.37
31	K	205	CLA	C1C-NC	-2.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	314	CLA	C1C-NC	-2.37	1.34	1.37
31	L	305	CLA	C1B-NB	-2.37	1.34	1.37
31	K	206	CLA	C1C-NC	-2.37	1.34	1.37
31	7	321	CLA	MG-NC	-2.37	2.00	2.06
31	6	313	CLA	C4D-ND	2.37	1.40	1.37
31	A	820	CLA	C1C-NC	-2.37	1.34	1.37
31	9	311	CLA	C4C-C3C	2.37	1.49	1.45
31	6	314	CLA	C4D-ND	2.37	1.40	1.37
31	A	816	CLA	C4C-C3C	2.37	1.49	1.45
31	A	827	CLA	C4C-C3C	2.37	1.49	1.45
31	8	308	CLA	C4C-C3C	2.36	1.49	1.45
32	4	313	CHL	C3D-C2D	2.36	1.45	1.39
31	A	820	CLA	C1B-C2B	2.36	1.48	1.43
32	6	319	CHL	C3D-C2D	2.36	1.45	1.39
31	2	315	CLA	C1C-NC	-2.36	1.34	1.37
31	4	319	CLA	C1C-NC	-2.36	1.34	1.37
31	H	901	CLA	C4D-ND	2.36	1.40	1.37
32	7	318	CHL	C3D-C2D	2.36	1.45	1.39
31	5	320	CLA	C4D-ND	2.36	1.40	1.37
31	3	307	CLA	C4C-C3C	2.36	1.49	1.45
32	6	320	CHL	C3D-C2D	2.36	1.45	1.39
32	4	317	CHL	MG-NA	-2.36	2.00	2.06
32	7	319	CHL	C1B-NB	-2.36	1.34	1.37
36	L	304	LUT	C38-C25	2.36	1.55	1.50
31	A	827	CLA	C4B-NB	-2.36	1.34	1.37
31	H	903	CLA	C1C-NC	-2.36	1.34	1.37
31	2	314	CLA	C4D-ND	2.36	1.40	1.37
31	4	306	CLA	C4D-ND	2.36	1.40	1.37
31	B	840	CLA	C4C-C3C	2.35	1.49	1.45
31	G	205	CLA	C1C-NC	-2.35	1.34	1.37
31	2	307	CLA	C1B-NB	-2.35	1.34	1.37
31	B	850	CLA	MG-NB	2.35	2.10	2.05
31	A	820	CLA	C4C-C3C	2.35	1.49	1.45
31	B	839	CLA	C4C-C3C	2.35	1.49	1.45
28	7	307	LHG	O7-C5	-2.35	1.40	1.46
32	6	318	CHL	C3D-C2D	2.35	1.45	1.39
32	7	319	CHL	CHB-C4A	-2.35	1.32	1.37
31	H	901	CLA	C1C-NC	-2.35	1.34	1.37
31	5	320	CLA	C1B-C2B	2.35	1.48	1.43
31	B	842	CLA	C4B-NB	-2.35	1.34	1.37
31	B	823	CLA	C1B-C2B	2.35	1.48	1.43
31	B	831	CLA	C4B-NB	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	305	CLA	C1B-NB	-2.35	1.34	1.37
26	L	302	BCR	C30-C25	-2.35	1.50	1.53
31	5	315	CLA	C4D-ND	2.35	1.40	1.37
31	4	318	CLA	C1B-NB	-2.35	1.34	1.37
31	5	323	CLA	C4C-C3C	2.35	1.49	1.45
31	A	827	CLA	C1C-NC	-2.35	1.34	1.37
30	A	813	CL0	C1D-C2D	2.35	1.50	1.45
31	5	314	CLA	C4C-C3C	2.35	1.49	1.45
31	L	307	CLA	C1B-C2B	2.35	1.48	1.43
31	B	834	CLA	C4B-NB	-2.35	1.34	1.37
32	5	317	CHL	C3D-C2D	2.35	1.45	1.39
31	A	847	CLA	C4B-NB	-2.35	1.34	1.37
31	9	313	CLA	C1C-NC	-2.34	1.34	1.37
31	8	317	CLA	C1B-C2B	2.34	1.48	1.43
32	8	319	CHL	C1B-C2B	2.34	1.48	1.43
31	A	814	CLA	C4C-C3C	2.34	1.49	1.45
31	B	825	CLA	C4C-C3C	2.34	1.49	1.45
31	4	309	CLA	C4C-C3C	2.34	1.49	1.45
31	H	901	CLA	C1B-C2B	2.34	1.48	1.43
30	A	813	CL0	CHC-C4B	2.34	1.44	1.39
31	9	312	CLA	C4C-C3C	2.34	1.49	1.45
31	b	302	CLA	C1B-NB	-2.34	1.34	1.37
31	9	317	CLA	C1B-C2B	2.34	1.48	1.43
31	A	851	CLA	C4C-C3C	2.34	1.49	1.45
36	6	303	LUT	C18-C5	2.34	1.54	1.50
32	7	319	CHL	C3A-C2A	-2.34	1.47	1.54
31	B	817	CLA	C1B-C2B	2.34	1.48	1.43
31	2	307	CLA	C4D-ND	2.34	1.40	1.37
31	5	312	CLA	C1C-NC	-2.34	1.34	1.37
32	6	309	CHL	C4C-C3C	2.34	1.49	1.45
31	a	309	CLA	C4C-C3C	2.34	1.49	1.45
31	5	309	CLA	C1C-NC	-2.34	1.34	1.37
31	b	312	CLA	C1C-NC	-2.34	1.34	1.37
31	7	312	CLA	C1C-NC	-2.34	1.34	1.37
32	5	317	CHL	C3B-C4B	2.33	1.48	1.42
27	A	807	LMT	O3B-C3B	-2.33	1.37	1.43
31	2	312	CLA	C1B-C2B	2.33	1.48	1.43
31	A	817	CLA	C4C-C3C	2.33	1.49	1.45
31	B	833	CLA	C4C-C3C	2.33	1.49	1.45
31	7	310	CLA	C4C-C3C	2.33	1.49	1.44
31	2	311	CLA	C4D-ND	2.33	1.40	1.37
31	9	314	CLA	C4C-C3C	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	321	CLA	C4D-ND	2.33	1.40	1.37
31	4	307	CLA	C4D-ND	2.33	1.40	1.37
31	H	903	CLA	C1B-NB	-2.33	1.34	1.37
31	9	311	CLA	C4B-NB	-2.33	1.34	1.37
31	H	903	CLA	C1B-C2B	2.33	1.48	1.43
36	3	305	LUT	C18-C5	2.33	1.54	1.50
31	8	309	CLA	C4C-C3C	2.33	1.49	1.45
32	3	315	CHL	C3D-C2D	2.33	1.45	1.39
31	K	204	CLA	C1B-C2B	2.33	1.48	1.43
36	J	103	LUT	C4-C5	2.33	1.54	1.51
31	6	312	CLA	C4C-C3C	2.33	1.49	1.45
31	2	305	CLA	C1B-C2B	2.33	1.48	1.43
31	O	203	CLA	C4D-ND	2.33	1.40	1.37
31	A	849	CLA	MG-NC	2.33	2.11	2.06
31	A	850	CLA	C4B-NB	-2.33	1.34	1.37
31	3	310	CLA	C1C-NC	-2.33	1.34	1.37
35	9	304	QTB	C09-C02	-2.33	1.40	1.45
32	K	201	CHL	C3B-C4B	2.33	1.48	1.42
31	A	842	CLA	C4C-C3C	2.33	1.49	1.45
31	A	844	CLA	C4C-C3C	2.33	1.49	1.45
31	A	822	CLA	C4C-C3C	2.33	1.49	1.45
31	A	826	CLA	C1C-NC	-2.33	1.34	1.37
31	4	307	CLA	C1B-NB	-2.33	1.34	1.37
31	a	322	CLA	C4D-ND	2.33	1.40	1.37
35	a	302	QTB	C09-C02	-2.33	1.40	1.45
31	a	322	CLA	C1C-NC	-2.33	1.34	1.37
31	6	307	CLA	C1C-NC	-2.33	1.34	1.37
31	A	837	CLA	C4B-NB	-2.33	1.34	1.37
31	a	311	CLA	C1C-NC	-2.33	1.34	1.37
31	4	315	CLA	C1B-NB	-2.32	1.34	1.37
27	A	808	LMT	O3B-C3B	-2.32	1.37	1.43
31	8	307	CLA	C4C-C3C	2.32	1.49	1.45
31	7	310	CLA	C1B-NB	-2.32	1.34	1.37
28	A	810	LHG	P-O6	2.32	1.68	1.59
31	7	311	CLA	C4C-C3C	2.32	1.49	1.45
31	b	313	CLA	C1C-NC	-2.32	1.34	1.37
31	B	835	CLA	C1B-C2B	2.32	1.48	1.43
31	b	306	CLA	C1C-NC	-2.32	1.34	1.37
31	4	321	CLA	C1C-NC	-2.32	1.34	1.37
31	3	316	CLA	MG-NB	-2.32	2.01	2.05
31	B	847	CLA	C1B-C2B	2.32	1.48	1.43
31	7	316	CLA	C1C-NC	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	320	CHL	C3D-C2D	2.32	1.45	1.39
30	A	813	CL0	C4B-NB	-2.32	1.34	1.37
31	A	851	CLA	C1B-C2B	2.32	1.48	1.43
31	b	302	CLA	C1B-C2B	2.32	1.48	1.43
31	b	307	CLA	C1B-NB	-2.32	1.34	1.37
31	A	833	CLA	C1B-C2B	2.32	1.48	1.43
31	B	842	CLA	C4C-C3C	2.32	1.49	1.45
31	a	315	CLA	C1C-NC	-2.32	1.34	1.37
31	9	315	CLA	C4D-ND	2.32	1.40	1.37
31	B	816	CLA	C1B-C2B	2.32	1.48	1.43
31	A	857	CLA	C1B-C2B	2.32	1.48	1.43
31	A	824	CLA	C4B-NB	-2.32	1.34	1.37
31	B	829	CLA	C4C-C3C	2.32	1.49	1.45
31	3	317	CLA	C1B-C2B	2.32	1.48	1.43
36	F	304	LUT	C38-C25	2.32	1.54	1.50
31	B	841	CLA	MG-ND	2.32	2.10	2.05
31	b	310	CLA	C1B-C2B	2.32	1.48	1.43
31	A	853	CLA	C4C-C3C	2.32	1.49	1.45
31	J	105	CLA	C4C-C3C	2.32	1.49	1.45
31	3	320	CLA	C1B-C2B	2.32	1.48	1.43
31	2	305	CLA	C1C-NC	-2.31	1.34	1.37
31	A	815	CLA	C4C-C3C	2.31	1.49	1.45
31	6	314	CLA	C1C-NC	-2.31	1.34	1.37
31	a	316	CLA	C1B-C2B	2.31	1.48	1.43
31	7	311	CLA	C1B-C2B	2.31	1.48	1.43
31	8	321	CLA	C1B-C2B	2.31	1.48	1.43
31	B	833	CLA	MG-ND	2.31	2.10	2.05
31	6	315	CLA	C4D-ND	2.31	1.40	1.37
31	8	310	CLA	C1C-NC	-2.31	1.34	1.37
31	4	318	CLA	C1B-C2B	2.31	1.48	1.43
31	6	322	CLA	C1B-NB	-2.31	1.34	1.37
31	b	303	CLA	C1B-NB	-2.31	1.34	1.37
36	6	303	LUT	C38-C25	2.31	1.54	1.50
31	B	836	CLA	C4B-NB	-2.31	1.34	1.37
31	2	306	CLA	C4D-ND	2.31	1.40	1.37
31	3	308	CLA	C1B-C2B	2.31	1.48	1.43
31	A	817	CLA	C1C-NC	-2.31	1.34	1.37
31	b	302	CLA	C1C-NC	-2.31	1.34	1.37
31	4	320	CLA	MG-NB	2.31	2.10	2.05
31	4	320	CLA	C4D-ND	2.31	1.40	1.37
31	B	820	CLA	C1C-NC	-2.31	1.34	1.37
31	8	320	CLA	C1B-C2B	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	314	CLA	C1B-C2B	2.31	1.48	1.43
31	b	304	CLA	C1B-NB	-2.31	1.34	1.37
31	6	312	CLA	C4D-ND	2.30	1.40	1.37
31	A	856	CLA	C4B-NB	-2.30	1.35	1.37
31	A	820	CLA	MG-ND	2.30	2.10	2.05
31	G	205	CLA	C1B-NB	-2.30	1.35	1.37
31	9	317	CLA	C1B-NB	-2.30	1.35	1.37
31	J	105	CLA	C4D-ND	2.30	1.40	1.37
31	b	308	CLA	C1B-C2B	2.30	1.48	1.43
31	B	819	CLA	C4B-NB	-2.30	1.35	1.37
31	G	205	CLA	C4D-ND	2.30	1.40	1.37
27	A	808	LMT	O2'-C2'	-2.30	1.37	1.43
32	A	839	CHL	C1B-NB	-2.30	1.35	1.37
31	3	316	CLA	C4C-C3C	2.30	1.49	1.45
27	5	301	LMT	O2B-C2B	-2.30	1.37	1.43
31	7	309	CLA	C1C-NC	-2.30	1.34	1.37
31	B	845	CLA	C4C-C3C	2.30	1.49	1.45
31	A	815	CLA	MG-ND	2.30	2.10	2.05
31	G	206	CLA	C4B-NB	-2.30	1.35	1.37
32	7	317	CHL	C3D-C2D	2.30	1.45	1.39
31	8	309	CLA	C1B-C2B	2.30	1.48	1.43
36	3	304	LUT	C1-C6	2.30	1.56	1.53
31	7	316	CLA	C1B-C2B	2.30	1.48	1.43
31	4	321	CLA	C1B-C2B	2.30	1.48	1.43
31	A	838	CLA	C1B-C2B	2.30	1.48	1.43
31	A	846	CLA	C1B-C2B	2.30	1.48	1.43
31	5	310	CLA	C1B-C2B	2.30	1.48	1.43
31	B	822	CLA	C1B-C2B	2.30	1.48	1.43
37	J	104	LMG	C1-C2	2.30	1.59	1.52
31	B	819	CLA	C4C-C3C	2.29	1.49	1.45
31	b	313	CLA	C4D-ND	2.29	1.40	1.37
31	a	312	CLA	C4C-C3C	2.29	1.49	1.45
31	5	314	CLA	C1B-NB	-2.29	1.35	1.37
31	A	856	CLA	C4C-C3C	2.29	1.49	1.45
31	4	306	CLA	C1C-NC	-2.29	1.34	1.37
31	2	306	CLA	C1B-C2B	2.29	1.48	1.43
31	4	307	CLA	C1B-C2B	2.29	1.48	1.43
31	6	314	CLA	C1B-NB	-2.29	1.35	1.37
31	L	306	CLA	C1B-C2B	2.29	1.48	1.43
31	9	318	CLA	C4D-ND	2.29	1.40	1.37
31	8	312	CLA	C1B-NB	-2.29	1.35	1.37
32	8	319	CHL	C3D-C2D	2.29	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	319	CLA	C4B-NB	-2.29	1.35	1.37
31	7	315	CLA	C1B-C2B	2.29	1.48	1.43
31	4	319	CLA	C1B-C2B	2.29	1.48	1.43
31	B	823	CLA	C4B-NB	-2.29	1.35	1.37
31	8	312	CLA	C4D-ND	2.29	1.40	1.37
31	b	308	CLA	C1C-NC	-2.29	1.34	1.37
31	A	847	CLA	C4C-C3C	2.29	1.49	1.45
32	7	324	CHL	C1B-NB	-2.28	1.35	1.37
31	6	306	CLA	C1C-C2C	2.28	1.49	1.44
31	2	311	CLA	C1B-C2B	2.28	1.48	1.43
31	4	312	CLA	C1C-NC	-2.28	1.34	1.37
31	A	818	CLA	C1B-C2B	2.28	1.48	1.43
31	a	322	CLA	C1B-C2B	2.28	1.48	1.43
31	A	837	CLA	C1B-C2B	2.28	1.48	1.43
31	G	204	CLA	C4D-ND	2.28	1.40	1.37
32	5	316	CHL	C3A-C2A	-2.28	1.48	1.54
31	4	305	CLA	C4C-C3C	2.28	1.49	1.45
31	8	314	CLA	C1B-C2B	2.28	1.48	1.43
31	H	902	CLA	C4D-ND	2.28	1.40	1.37
31	3	307	CLA	C4D-ND	2.28	1.40	1.37
32	A	839	CHL	CHB-C4A	-2.28	1.32	1.37
31	B	832	CLA	C4C-C3C	2.28	1.49	1.45
31	a	315	CLA	C1B-C2B	2.28	1.48	1.43
31	5	309	CLA	C1B-C2B	2.28	1.48	1.43
31	4	321	CLA	C4D-ND	2.28	1.40	1.37
31	8	317	CLA	C1C-NC	-2.28	1.34	1.37
31	4	316	CLA	C4B-NB	-2.28	1.35	1.37
31	4	319	CLA	C1C-C2C	2.28	1.49	1.44
31	7	310	CLA	C1B-C2B	2.28	1.48	1.43
31	A	845	CLA	C4C-C3C	2.28	1.49	1.45
36	L	304	LUT	C4-C5	2.28	1.54	1.51
31	4	311	CLA	C1B-C2B	2.28	1.48	1.43
31	5	318	CLA	C4D-ND	2.28	1.40	1.37
31	A	835	CLA	C4D-ND	2.28	1.40	1.37
31	2	312	CLA	C4D-ND	2.28	1.40	1.37
32	7	319	CHL	C3B-C4B	2.28	1.48	1.42
31	8	313	CLA	C1B-NB	-2.28	1.35	1.37
31	5	312	CLA	C1B-C2B	2.28	1.48	1.43
31	5	314	CLA	C4D-ND	2.27	1.40	1.37
36	4	303	LUT	C38-C25	2.27	1.54	1.50
31	B	826	CLA	C4C-C3C	2.27	1.49	1.45
31	A	821	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	820	CLA	C1B-C2B	2.27	1.48	1.43
31	B	837	CLA	C1B-C2B	2.27	1.48	1.43
31	F	306	CLA	C1B-C2B	2.27	1.48	1.43
31	5	307	CLA	C4D-ND	2.27	1.40	1.37
36	8	302	LUT	C38-C25	2.27	1.54	1.50
31	9	318	CLA	C1B-NB	-2.27	1.35	1.37
31	3	318	CLA	C1B-C2B	2.27	1.48	1.43
32	A	839	CHL	C3B-C4B	2.27	1.48	1.42
32	a	320	CHL	MG-NA	2.27	2.11	2.06
31	4	306	CLA	C1B-NB	-2.27	1.35	1.37
31	4	320	CLA	C1B-NB	-2.27	1.35	1.37
32	4	313	CHL	C1B-C2B	2.27	1.48	1.43
32	4	317	CHL	C4C-C3C	2.27	1.49	1.45
31	G	205	CLA	C1B-C2B	2.27	1.48	1.43
31	6	322	CLA	C1C-NC	-2.27	1.34	1.37
31	A	850	CLA	C4C-C3C	2.27	1.48	1.45
31	9	313	CLA	C4D-ND	2.27	1.40	1.37
31	4	312	CLA	C1B-C2B	2.27	1.48	1.43
32	A	840	CHL	C1B-NB	-2.27	1.35	1.37
31	8	313	CLA	C1B-C2B	2.27	1.48	1.43
31	B	824	CLA	C4B-NB	-2.26	1.35	1.37
31	6	313	CLA	C1B-NB	-2.26	1.35	1.37
31	A	855	CLA	C1B-C2B	2.26	1.48	1.43
31	4	308	CLA	C4D-ND	2.26	1.40	1.37
31	6	306	CLA	C1B-C2B	2.26	1.48	1.43
32	7	324	CHL	C3D-C2D	2.26	1.45	1.39
36	8	303	LUT	C4-C5	2.26	1.54	1.51
31	4	316	CLA	C4D-ND	2.26	1.40	1.37
31	B	832	CLA	C4B-NB	-2.26	1.35	1.37
31	b	306	CLA	C1B-NB	-2.26	1.35	1.37
31	b	305	CLA	C4D-ND	2.26	1.40	1.37
26	J	102	BCR	C30-C25	-2.26	1.50	1.53
31	A	854	CLA	C1B-C2B	2.26	1.48	1.43
31	6	308	CLA	C1B-C2B	2.26	1.48	1.43
31	H	902	CLA	C1B-C2B	2.26	1.48	1.43
31	K	204	CLA	C4C-C3C	2.26	1.48	1.45
31	3	318	CLA	C1C-NC	-2.26	1.34	1.37
32	b	309	CHL	C4C-C3C	2.26	1.48	1.45
32	8	316	CHL	C3D-C2D	2.26	1.45	1.39
32	6	318	CHL	C3A-C2A	-2.26	1.48	1.54
31	F	305	CLA	C1B-C2B	2.25	1.48	1.43
31	B	826	CLA	C4B-NB	-2.25	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	319	CHL	C4C-C3C	2.25	1.48	1.45
31	3	312	CLA	C4D-ND	2.25	1.40	1.37
31	6	312	CLA	C1C-NC	-2.25	1.34	1.37
31	6	313	CLA	C1B-C2B	2.25	1.48	1.43
31	H	902	CLA	C1C-NC	-2.25	1.34	1.37
31	9	311	CLA	C4D-ND	2.25	1.40	1.37
31	6	314	CLA	C1B-C2B	2.25	1.48	1.43
32	5	316	CHL	C3D-C2D	2.25	1.45	1.39
31	4	318	CLA	C1C-NC	-2.25	1.34	1.37
31	b	312	CLA	C1B-C2B	2.25	1.48	1.43
36	3	304	LUT	C38-C25	2.25	1.54	1.50
31	a	316	CLA	C1C-NC	-2.25	1.34	1.37
31	O	204	CLA	C1C-NC	-2.25	1.34	1.37
31	B	844	CLA	C1B-C2B	2.25	1.48	1.43
31	6	315	CLA	C1C-NC	-2.25	1.34	1.37
31	8	308	CLA	C4D-ND	2.24	1.40	1.37
31	8	313	CLA	C4C-C3C	2.24	1.48	1.45
31	B	824	CLA	C1B-C2B	2.24	1.48	1.43
32	a	318	CHL	C1B-NB	-2.24	1.35	1.37
31	A	830	CLA	C4B-NB	-2.24	1.35	1.37
31	9	319	CLA	C1C-NC	-2.24	1.34	1.37
31	5	315	CLA	C1B-NB	-2.24	1.35	1.37
32	7	317	CHL	C1B-C2B	2.24	1.48	1.43
31	4	305	CLA	C4B-NB	-2.24	1.35	1.37
31	B	831	CLA	C1B-C2B	2.24	1.48	1.43
31	9	312	CLA	C1B-C2B	2.24	1.48	1.43
31	A	828	CLA	C4C-C3C	2.24	1.48	1.45
31	B	842	CLA	C1B-C2B	2.24	1.48	1.43
32	6	320	CHL	CHB-C4A	-2.24	1.32	1.37
32	b	309	CHL	C1B-C2B	2.24	1.48	1.43
32	8	319	CHL	C1B-NB	-2.24	1.35	1.37
31	9	313	CLA	C1B-C2B	2.24	1.48	1.43
31	b	304	CLA	C1C-NC	-2.24	1.34	1.37
32	3	315	CHL	CHB-C4A	-2.24	1.32	1.37
31	2	312	CLA	C1C-NC	-2.23	1.34	1.37
32	A	831	CHL	C3D-C2D	2.23	1.45	1.39
26	J	102	BCR	C1-C6	-2.23	1.50	1.53
31	3	319	CLA	C1B-C2B	2.23	1.48	1.43
31	6	313	CLA	MG-NB	2.23	2.10	2.05
31	3	310	CLA	C4B-NB	-2.23	1.35	1.37
31	5	313	CLA	C1B-NB	-2.23	1.35	1.37
31	3	319	CLA	C1C-NC	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	316	CLA	C1C-NC	-2.23	1.34	1.37
31	A	825	CLA	C4C-C3C	2.23	1.48	1.45
31	b	311	CLA	C1B-C2B	2.23	1.48	1.43
31	3	316	CLA	C4D-ND	2.23	1.40	1.37
31	9	319	CLA	C4D-ND	2.23	1.40	1.37
31	b	305	CLA	C1C-NC	-2.23	1.34	1.37
31	O	204	CLA	C1B-C2B	2.23	1.48	1.43
28	6	305	LHG	O7-C5	-2.23	1.41	1.46
31	4	320	CLA	C1C-NC	-2.23	1.34	1.37
31	5	314	CLA	C1C-NC	-2.23	1.34	1.37
31	3	313	CLA	C1B-C2B	2.23	1.48	1.43
31	4	308	CLA	C1B-C2B	2.23	1.48	1.43
31	7	312	CLA	C4B-NB	-2.23	1.35	1.37
31	8	315	CLA	C4D-ND	2.23	1.40	1.37
31	8	315	CLA	C1C-NC	-2.23	1.34	1.37
31	A	833	CLA	C4B-NB	-2.23	1.35	1.37
31	A	826	CLA	C1B-C2B	2.23	1.48	1.43
32	K	201	CHL	MG-NA	-2.23	2.01	2.06
31	F	301	CLA	C4B-NB	-2.23	1.35	1.37
32	8	316	CHL	C1B-NB	-2.23	1.35	1.37
31	B	839	CLA	C1B-C2B	2.23	1.48	1.43
31	2	306	CLA	C1C-NC	-2.23	1.34	1.37
32	5	322	CHL	C4C-C3C	2.23	1.48	1.45
31	b	306	CLA	C1B-C2B	2.23	1.48	1.43
31	A	830	CLA	C1B-C2B	2.22	1.48	1.43
31	A	853	CLA	C1B-C2B	2.22	1.48	1.43
31	4	320	CLA	C1B-C2B	2.22	1.48	1.43
32	4	317	CHL	C1B-C2B	2.22	1.48	1.43
31	A	821	CLA	C4C-C3C	2.22	1.48	1.45
31	B	813	CLA	C1C-C2C	2.22	1.48	1.44
31	b	307	CLA	C1C-NC	-2.22	1.34	1.37
31	B	825	CLA	C1B-C2B	2.22	1.48	1.43
31	8	315	CLA	C4B-NB	-2.22	1.35	1.37
31	A	857	CLA	C4C-C3C	2.22	1.48	1.45
32	6	317	CHL	MG-ND	2.22	2.10	2.05
31	B	833	CLA	C1B-C2B	2.22	1.48	1.43
32	5	322	CHL	C1B-C2B	2.22	1.48	1.43
31	3	310	CLA	C4C-C3C	2.22	1.48	1.45
31	2	308	CLA	C4C-C3C	2.22	1.48	1.45
31	A	814	CLA	C4B-NB	-2.22	1.35	1.37
31	b	302	CLA	MG-ND	-2.22	2.01	2.05
31	a	321	CLA	C1C-NC	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	313	CHL	C4C-C3C	2.22	1.48	1.45
31	7	314	CLA	C1B-C2B	2.22	1.48	1.43
31	B	848	CLA	C1C-NC	-2.22	1.34	1.37
31	6	308	CLA	C1C-NC	-2.22	1.34	1.37
31	A	855	CLA	C4C-C3C	2.22	1.48	1.45
31	A	838	CLA	C4B-NB	-2.22	1.35	1.37
31	3	310	CLA	C1B-C2B	2.22	1.48	1.43
31	9	315	CLA	C1B-C2B	2.22	1.48	1.43
31	B	839	CLA	C1C-NC	-2.22	1.34	1.37
31	b	310	CLA	C4D-ND	2.22	1.40	1.37
32	9	320	CHL	CHB-C4A	-2.22	1.32	1.37
32	5	317	CHL	CHB-C4A	-2.22	1.32	1.37
31	G	204	CLA	C4B-NB	-2.22	1.35	1.37
31	a	312	CLA	C4D-ND	2.22	1.40	1.37
31	A	819	CLA	C4C-C3C	2.22	1.48	1.45
31	A	852	CLA	C4B-NB	-2.21	1.35	1.37
33	7	308	DGD	O2G-C2G	-2.21	1.41	1.46
31	8	312	CLA	C1B-C2B	2.21	1.48	1.43
31	a	319	CLA	C4D-ND	2.21	1.40	1.37
31	3	308	CLA	C1C-C2C	2.21	1.48	1.44
31	9	314	CLA	C1B-C2B	2.21	1.48	1.43
31	2	310	CLA	C1B-C2B	2.21	1.48	1.43
31	6	306	CLA	C3B-C2B	2.21	1.48	1.41
31	B	848	CLA	C1B-C2B	2.21	1.48	1.43
31	3	312	CLA	C1B-C2B	2.21	1.48	1.43
32	7	320	CHL	C1B-C2B	2.21	1.48	1.43
31	3	320	CLA	C1C-NC	-2.21	1.34	1.37
31	6	311	CLA	C1B-C2B	2.21	1.48	1.43
32	9	320	CHL	C3A-C2A	-2.21	1.48	1.54
32	6	319	CHL	C3A-C2A	-2.21	1.48	1.54
31	3	313	CLA	C4D-ND	2.21	1.40	1.37
31	A	822	CLA	C1B-C2B	2.21	1.48	1.43
31	7	315	CLA	C4D-ND	2.21	1.40	1.37
31	B	841	CLA	C1B-C2B	2.21	1.48	1.43
31	L	306	CLA	C1C-NC	-2.21	1.34	1.37
36	9	302	LUT	C38-C25	2.21	1.54	1.50
31	5	308	CLA	C1B-C2B	2.21	1.48	1.43
31	5	315	CLA	C1B-C2B	2.21	1.48	1.43
31	5	321	CLA	C1B-C2B	2.21	1.48	1.43
32	5	317	CHL	C1B-NB	-2.21	1.35	1.37
31	A	814	CLA	C1B-C2B	2.21	1.48	1.43
31	2	314	CLA	C1B-C2B	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	318	CLA	C1B-C2B	2.21	1.48	1.43
31	a	314	CLA	C4D-ND	2.21	1.40	1.37
36	5	303	LUT	C38-C25	2.21	1.54	1.50
31	B	843	CLA	C4B-NB	-2.21	1.35	1.37
32	7	320	CHL	C3D-C2D	2.21	1.45	1.39
31	8	320	CLA	C4D-ND	2.20	1.40	1.37
26	3	302	BCR	C30-C25	-2.20	1.50	1.53
31	3	311	CLA	C1B-C2B	2.20	1.48	1.43
32	4	310	CHL	C3D-C2D	2.20	1.45	1.39
31	8	310	CLA	C1C-C2C	2.20	1.48	1.44
32	6	319	CHL	C4C-C3C	2.20	1.48	1.45
31	b	311	CLA	C1B-NB	-2.20	1.35	1.37
32	K	201	CHL	C1B-NB	-2.20	1.35	1.37
31	3	311	CLA	C3D-C4D	-2.20	1.39	1.44
36	J	103	LUT	C38-C25	2.20	1.54	1.50
31	6	307	CLA	C1B-NB	-2.20	1.35	1.37
31	B	830	CLA	C4D-ND	2.20	1.40	1.37
31	9	318	CLA	C1B-C2B	2.20	1.48	1.43
31	4	314	CLA	C1B-C2B	2.20	1.48	1.43
31	B	848	CLA	C4B-NB	-2.20	1.35	1.37
31	5	320	CLA	C1B-NB	-2.20	1.35	1.37
31	2	308	CLA	C1B-C2B	2.20	1.48	1.43
31	6	315	CLA	C1B-NB	-2.20	1.35	1.37
31	B	846	CLA	C4B-NB	-2.20	1.35	1.37
31	5	314	CLA	MG-NC	2.20	2.11	2.06
31	2	304	CLA	C1C-NC	-2.20	1.34	1.37
31	2	304	CLA	C1B-C2B	2.20	1.48	1.43
31	4	316	CLA	C1C-NC	-2.20	1.34	1.37
31	7	322	CLA	C4D-ND	2.20	1.40	1.37
31	7	321	CLA	C4B-NB	-2.20	1.35	1.37
31	B	850	CLA	MG-ND	2.19	2.10	2.05
31	B	820	CLA	C4C-C3C	2.19	1.48	1.45
31	B	829	CLA	C4D-ND	2.19	1.40	1.37
31	B	825	CLA	C4B-NB	-2.19	1.35	1.37
31	a	321	CLA	C1B-C2B	2.19	1.48	1.43
31	B	821	CLA	C4B-NB	-2.19	1.35	1.37
31	H	902	CLA	C1B-NB	-2.19	1.35	1.37
31	8	315	CLA	C1B-C2B	2.19	1.48	1.43
31	B	832	CLA	C4D-ND	2.19	1.40	1.37
31	B	840	CLA	MG-ND	2.19	2.10	2.05
36	9	302	LUT	C1-C6	2.19	1.56	1.53
31	A	834	CLA	C4B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	321	CLA	C4B-NB	-2.19	1.35	1.37
31	2	309	CLA	C1B-C2B	2.19	1.48	1.43
31	B	824	CLA	C4D-ND	2.19	1.40	1.37
31	O	203	CLA	C1C-C2C	2.19	1.48	1.44
31	9	318	CLA	C1C-C2C	2.19	1.48	1.44
31	a	315	CLA	C4D-ND	2.19	1.40	1.37
31	5	320	CLA	C1C-C2C	2.19	1.48	1.44
36	2	301	LUT	C38-C25	2.19	1.54	1.50
27	9	306	LMT	O1'-C1'	-2.18	1.36	1.40
31	5	318	CLA	C4B-NB	-2.18	1.35	1.37
31	b	304	CLA	C4D-ND	2.18	1.40	1.37
32	a	320	CHL	C3B-C4B	2.18	1.47	1.42
32	6	317	CHL	C3A-C2A	-2.18	1.48	1.54
31	7	313	CLA	C4C-C3C	2.18	1.48	1.45
31	b	308	CLA	C1B-NB	-2.18	1.35	1.37
26	K	202	BCR	C30-C25	-2.18	1.50	1.53
31	O	202	CLA	C1B-NB	-2.18	1.35	1.37
31	A	854	CLA	C4B-NB	-2.18	1.35	1.37
31	O	202	CLA	C1B-C2B	2.18	1.48	1.43
31	4	305	CLA	CHC-C4B	2.18	1.44	1.39
31	a	322	CLA	MG-ND	-2.18	2.01	2.05
31	K	205	CLA	C4B-NB	-2.18	1.35	1.37
32	K	201	CHL	C4B-NB	-2.18	1.35	1.37
31	4	306	CLA	C1B-C2B	2.18	1.48	1.43
31	7	321	CLA	C1B-C2B	2.18	1.48	1.43
28	B	807	LHG	O7-C5	-2.18	1.41	1.46
31	b	304	CLA	C1B-C2B	2.18	1.48	1.43
31	B	838	CLA	C1B-C2B	2.18	1.48	1.43
31	6	312	CLA	C1B-C2B	2.18	1.48	1.43
31	3	313	CLA	C1C-NC	-2.18	1.34	1.37
32	A	840	CHL	CHB-C4A	-2.18	1.32	1.37
31	8	309	CLA	C1B-NB	-2.18	1.35	1.37
31	6	310	CLA	C1B-NB	-2.18	1.35	1.37
31	B	838	CLA	C4B-NB	-2.17	1.35	1.37
31	4	305	CLA	C3B-C4B	2.17	1.47	1.42
31	B	813	CLA	C4C-C3C	2.17	1.48	1.45
31	b	311	CLA	C4D-ND	2.17	1.40	1.37
31	O	203	CLA	C1B-C2B	2.17	1.48	1.43
31	A	820	CLA	C1C-C2C	2.17	1.48	1.44
31	A	814	CLA	MG-NC	2.17	2.11	2.06
42	4	304	SQD	O9-S	2.17	1.51	1.45
31	A	824	CLA	C1B-C2B	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	312	CLA	C1B-C2B	2.17	1.48	1.43
31	8	307	CLA	C4D-ND	2.17	1.40	1.37
31	B	815	CLA	C4C-C3C	2.17	1.48	1.45
31	B	814	CLA	C1B-C2B	2.17	1.48	1.43
31	7	315	CLA	C4B-NB	-2.17	1.35	1.37
31	9	312	CLA	C4D-ND	2.17	1.40	1.37
31	2	309	CLA	C4D-ND	2.17	1.40	1.37
31	B	838	CLA	C4D-ND	2.17	1.40	1.37
31	A	828	CLA	C1B-C2B	2.17	1.48	1.43
31	F	306	CLA	C4B-NB	-2.17	1.35	1.37
36	9	303	LUT	C18-C5	2.16	1.54	1.50
31	4	305	CLA	C1D-C2D	2.16	1.49	1.45
32	5	319	CHL	C1B-C2B	2.16	1.48	1.43
31	9	315	CLA	C3D-C4D	-2.16	1.39	1.44
31	b	306	CLA	C1C-C2C	2.16	1.48	1.44
31	A	857	CLA	C4B-NB	-2.16	1.35	1.37
31	8	308	CLA	C4B-NB	-2.16	1.35	1.37
31	a	310	CLA	C1B-C2B	2.16	1.48	1.43
36	a	303	LUT	C38-C25	2.16	1.54	1.50
31	A	849	CLA	C4D-ND	2.16	1.40	1.37
31	4	305	CLA	CHB-C1B	2.16	1.44	1.39
32	A	840	CHL	C3D-C2D	2.16	1.45	1.39
31	G	206	CLA	C1B-C2B	2.16	1.48	1.43
31	6	315	CLA	C1B-C2B	2.16	1.48	1.43
32	4	310	CHL	C1B-C2B	2.16	1.48	1.43
32	6	309	CHL	C1B-C2B	2.16	1.48	1.43
31	B	822	CLA	C4B-NB	-2.16	1.35	1.37
31	L	307	CLA	C1B-NB	-2.16	1.35	1.37
31	B	830	CLA	C4B-NB	-2.16	1.35	1.37
31	4	314	CLA	C1B-NB	-2.16	1.35	1.37
31	5	323	CLA	C1B-C2B	2.15	1.48	1.43
31	5	309	CLA	C1B-NB	-2.15	1.35	1.37
31	2	308	CLA	C1C-C2C	2.15	1.48	1.44
31	a	314	CLA	C1B-C2B	2.15	1.48	1.43
33	7	308	DGD	O1G-C1G	-2.15	1.40	1.45
32	a	317	CHL	C1B-C2B	2.15	1.48	1.43
31	A	843	CLA	C1B-C2B	2.15	1.48	1.43
31	6	306	CLA	C1C-NC	-2.15	1.34	1.37
32	9	322	CHL	C1B-C2B	2.15	1.48	1.43
31	8	311	CLA	C4B-NB	-2.15	1.35	1.37
31	B	835	CLA	C4B-NB	-2.15	1.35	1.37
32	7	318	CHL	C1B-NB	-2.15	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	825	CLA	MG-ND	-2.14	2.01	2.05
31	5	312	CLA	C1C-C2C	2.14	1.48	1.44
31	A	830	CLA	MG-ND	-2.14	2.01	2.05
31	8	318	CLA	C4B-NB	-2.14	1.35	1.37
31	5	320	CLA	C1C-NC	-2.14	1.34	1.37
31	A	828	CLA	C4D-ND	2.14	1.40	1.37
31	4	319	CLA	C1B-NB	-2.14	1.35	1.37
32	A	840	CHL	C3B-C4B	2.14	1.47	1.42
32	6	321	CHL	C3B-C4B	2.14	1.47	1.42
31	9	314	CLA	C4D-ND	2.14	1.40	1.37
31	2	307	CLA	C1B-C2B	2.14	1.48	1.43
32	5	316	CHL	C1B-C2B	2.14	1.48	1.43
32	4	310	CHL	CHB-C4A	-2.14	1.32	1.37
28	8	304	LHG	O7-C5	-2.14	1.41	1.46
32	6	318	CHL	C4C-C3C	2.14	1.48	1.45
31	9	313	CLA	C3B-C2B	2.14	1.48	1.41
31	8	321	CLA	C3B-C2B	2.14	1.48	1.41
32	3	315	CHL	C3A-C2A	-2.14	1.48	1.54
31	F	305	CLA	C4B-NB	-2.14	1.35	1.37
31	L	305	CLA	C1B-C2B	2.13	1.48	1.43
32	6	317	CHL	CHB-C4A	-2.13	1.32	1.37
32	4	313	CHL	C3A-C2A	-2.13	1.48	1.54
31	F	306	CLA	C4D-ND	2.13	1.40	1.37
31	3	316	CLA	C1B-C2B	2.13	1.48	1.43
32	7	317	CHL	C1B-NB	-2.13	1.35	1.37
32	7	320	CHL	C1B-NB	-2.13	1.35	1.37
36	F	304	LUT	C4-C5	2.13	1.54	1.51
32	7	318	CHL	CHB-C4A	-2.13	1.32	1.37
31	A	826	CLA	C4B-NB	-2.13	1.35	1.37
31	A	816	CLA	C1B-C2B	2.13	1.48	1.43
31	7	309	CLA	C4B-NB	-2.13	1.35	1.37
27	A	807	LMT	O1'-C1'	-2.13	1.36	1.40
31	7	312	CLA	C1B-C2B	2.13	1.48	1.43
31	8	313	CLA	C4D-ND	2.13	1.40	1.37
31	B	812	CLA	C1B-C2B	2.13	1.48	1.43
32	6	321	CHL	C1B-C2B	2.13	1.48	1.43
31	7	313	CLA	C4D-ND	2.13	1.40	1.37
31	B	845	CLA	C4B-NB	-2.13	1.35	1.37
32	6	309	CHL	C3A-C2A	-2.13	1.48	1.54
32	A	839	CHL	C3A-C2A	-2.13	1.48	1.54
31	7	311	CLA	C4B-NB	-2.13	1.35	1.37
31	A	843	CLA	C4B-NB	-2.13	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	315	CLA	MG-ND	-2.13	2.01	2.05
31	3	312	CLA	C4B-NB	-2.13	1.35	1.37
32	a	318	CHL	CHB-C4A	-2.13	1.32	1.37
28	A	809	LHG	P-O6	2.13	1.67	1.59
32	6	319	CHL	CHB-C4A	-2.12	1.32	1.37
31	4	306	CLA	C1C-C2C	2.12	1.48	1.44
31	B	837	CLA	C3D-C4D	-2.12	1.39	1.44
31	A	835	CLA	C4B-NB	-2.12	1.35	1.37
32	A	831	CHL	C3B-C4B	2.12	1.47	1.42
31	A	819	CLA	C1B-C2B	2.12	1.48	1.43
32	8	319	CHL	C4C-C3C	2.12	1.48	1.45
31	A	834	CLA	MG-NC	2.12	2.11	2.06
31	9	313	CLA	C1C-C2C	2.12	1.48	1.44
31	A	827	CLA	C1B-C2B	2.12	1.48	1.43
32	8	316	CHL	C1B-C2B	2.12	1.48	1.43
32	b	309	CHL	C3A-C2A	-2.12	1.48	1.54
31	G	204	CLA	C1B-C2B	2.12	1.48	1.43
31	B	820	CLA	C1C-C2C	2.12	1.48	1.44
31	4	316	CLA	C1B-NB	-2.12	1.35	1.37
31	A	850	CLA	C1B-C2B	2.12	1.48	1.43
31	7	321	CLA	C4D-ND	2.12	1.40	1.37
31	A	825	CLA	C3B-C2B	2.12	1.48	1.41
31	3	317	CLA	C4D-ND	2.12	1.40	1.37
32	8	316	CHL	C3A-C2A	-2.12	1.48	1.54
31	B	813	CLA	MG-NB	-2.12	2.01	2.05
31	2	311	CLA	C1C-NC	-2.12	1.34	1.37
31	4	309	CLA	C4B-NB	-2.12	1.35	1.37
31	8	320	CLA	MG-ND	-2.12	2.01	2.05
31	B	820	CLA	C4B-NB	-2.11	1.35	1.37
31	4	311	CLA	C1B-NB	-2.11	1.35	1.37
31	K	205	CLA	C3B-C2B	2.11	1.48	1.41
31	A	845	CLA	MG-ND	-2.11	2.01	2.05
31	A	820	CLA	C3B-C2B	2.11	1.48	1.41
31	B	850	CLA	C4B-NB	-2.11	1.35	1.37
31	a	311	CLA	C4D-ND	2.11	1.40	1.37
31	4	312	CLA	C1C-C2C	2.11	1.48	1.44
31	A	838	CLA	C4D-ND	2.11	1.40	1.37
31	7	309	CLA	C4D-ND	2.11	1.40	1.37
31	a	322	CLA	C4B-NB	-2.11	1.35	1.37
31	B	825	CLA	C4D-ND	2.11	1.40	1.37
31	3	317	CLA	C3B-C2B	2.11	1.48	1.41
31	4	321	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	320	CHL	C3A-C2A	-2.11	1.48	1.54
32	A	840	CHL	C3A-C2A	-2.11	1.48	1.54
31	4	309	CLA	MG-ND	-2.11	2.01	2.05
31	5	314	CLA	C1C-C2C	2.11	1.48	1.44
31	6	311	CLA	C1B-NB	-2.11	1.35	1.37
36	4	303	LUT	C18-C5	2.11	1.54	1.50
31	A	821	CLA	MG-NB	2.11	2.10	2.05
31	9	321	CLA	C1B-C2B	2.11	1.48	1.43
31	b	312	CLA	C1B-NB	-2.11	1.35	1.37
31	L	306	CLA	C4D-ND	2.11	1.40	1.37
28	a	306	LHG	O7-C5	-2.11	1.41	1.46
32	a	317	CHL	C3A-C2A	-2.11	1.48	1.54
32	a	320	CHL	C3A-C2A	-2.11	1.48	1.54
31	7	316	CLA	C4D-ND	2.11	1.40	1.37
31	b	311	CLA	C1C-C2C	2.11	1.48	1.44
31	B	834	CLA	C1B-C2B	2.11	1.48	1.43
31	8	310	CLA	C1B-C2B	2.11	1.48	1.43
32	6	318	CHL	C1B-C2B	2.11	1.48	1.43
31	3	309	CLA	C4D-ND	2.10	1.40	1.37
31	J	105	CLA	C4B-NB	-2.10	1.35	1.37
31	5	311	CLA	C4B-NB	-2.10	1.35	1.37
31	A	836	CLA	C3D-C4D	-2.10	1.39	1.44
31	3	311	CLA	C4B-NB	-2.10	1.35	1.37
31	B	846	CLA	C1B-C2B	2.10	1.48	1.43
31	A	854	CLA	C4D-ND	2.10	1.40	1.37
31	B	815	CLA	C4B-NB	-2.10	1.35	1.37
31	B	829	CLA	C4B-NB	-2.10	1.35	1.37
31	3	314	CLA	C1B-C2B	2.10	1.48	1.43
31	2	308	CLA	C3B-C2B	2.10	1.48	1.41
30	A	813	CL0	C1C-C2C	2.10	1.48	1.44
32	b	309	CHL	C3B-C4B	2.10	1.47	1.42
31	8	307	CLA	MG-NC	2.10	2.11	2.06
31	B	845	CLA	C1B-C2B	2.10	1.48	1.43
32	6	319	CHL	C1B-C2B	2.10	1.48	1.43
31	2	308	CLA	C4D-ND	2.10	1.40	1.37
31	3	316	CLA	C4B-NB	-2.10	1.35	1.37
32	7	324	CHL	C1B-C2B	2.10	1.48	1.43
31	A	825	CLA	C1C-C2C	2.10	1.48	1.44
31	B	838	CLA	MG-ND	-2.10	2.01	2.05
31	2	312	CLA	C1C-C2C	2.10	1.48	1.44
31	B	830	CLA	C3D-C4D	-2.10	1.39	1.44
31	B	840	CLA	C3B-C2B	2.10	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	320	CLA	C3B-C2B	2.10	1.48	1.41
31	B	827	CLA	C4C-C3C	2.10	1.48	1.45
32	7	318	CHL	C1B-C2B	2.09	1.48	1.43
31	4	311	CLA	C1C-C2C	2.09	1.48	1.44
32	a	318	CHL	C3A-C2A	-2.09	1.48	1.54
31	A	836	CLA	C1B-C2B	2.09	1.48	1.43
37	J	101	LMG	C7-C8	2.09	1.57	1.50
32	9	322	CHL	C3A-C2A	-2.09	1.48	1.54
31	A	828	CLA	C4B-NB	-2.09	1.35	1.37
31	9	315	CLA	C4C-C3C	2.09	1.48	1.45
31	B	834	CLA	MG-NC	-2.09	2.01	2.06
31	a	313	CLA	C1B-C2B	2.09	1.48	1.43
31	A	825	CLA	C4B-NB	-2.09	1.35	1.37
31	5	311	CLA	C4D-ND	2.09	1.40	1.37
31	A	842	CLA	C1B-C2B	2.09	1.48	1.43
31	B	821	CLA	C1B-C2B	2.09	1.48	1.43
32	6	318	CHL	CHB-C4A	-2.09	1.32	1.37
31	6	315	CLA	C1C-C2C	2.09	1.48	1.44
31	A	852	CLA	C1B-C2B	2.09	1.48	1.43
31	b	305	CLA	C1B-C2B	2.09	1.48	1.43
31	G	205	CLA	C1C-C2C	2.09	1.48	1.44
31	a	313	CLA	C4D-ND	2.09	1.40	1.37
31	A	844	CLA	C4B-NB	-2.09	1.35	1.37
32	A	840	CHL	C4B-NB	-2.09	1.35	1.37
31	2	311	CLA	C1C-C2C	2.09	1.48	1.44
31	3	319	CLA	C3B-C2B	2.09	1.48	1.41
31	7	314	CLA	C4D-ND	2.09	1.40	1.37
31	7	321	CLA	C4C-C3C	2.09	1.48	1.45
31	3	309	CLA	C4B-NB	-2.09	1.35	1.37
31	8	307	CLA	C1C-C2C	2.09	1.48	1.44
31	A	819	CLA	C4B-NB	-2.09	1.35	1.37
31	a	315	CLA	C4B-NB	-2.08	1.35	1.37
31	2	304	CLA	C1C-C2C	2.08	1.48	1.44
32	8	316	CHL	C3B-C4B	2.08	1.47	1.42
31	B	826	CLA	C3B-C2B	2.08	1.48	1.41
31	O	204	CLA	C1B-NB	-2.08	1.35	1.37
31	2	315	CLA	C4B-NB	-2.08	1.35	1.37
31	a	316	CLA	C4D-ND	2.08	1.40	1.37
31	9	316	CLA	C4D-ND	2.08	1.40	1.37
31	2	304	CLA	C4D-ND	2.08	1.40	1.37
32	7	324	CHL	C3B-C4B	2.08	1.47	1.42
31	6	313	CLA	C3B-C2B	2.08	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	319	CHL	C3B-C4B	2.08	1.47	1.42
31	A	835	CLA	C1B-C2B	2.08	1.48	1.43
32	7	324	CHL	CHB-C4A	-2.08	1.32	1.37
31	B	843	CLA	C4D-ND	2.08	1.40	1.37
27	9	306	LMT	O4'-C4B	-2.08	1.38	1.43
42	4	304	SQD	O7-S	2.08	1.51	1.45
32	6	321	CHL	CHB-C4A	-2.08	1.32	1.37
31	L	305	CLA	C4B-NB	-2.08	1.35	1.37
31	7	313	CLA	C1B-C2B	2.08	1.48	1.43
31	9	316	CLA	C3B-C2B	2.08	1.48	1.41
31	2	313	CLA	C4D-ND	2.08	1.40	1.37
31	4	314	CLA	C1C-NC	-2.08	1.34	1.37
31	2	310	CLA	C1B-NB	-2.07	1.35	1.37
31	F	301	CLA	C1B-C2B	2.07	1.48	1.43
31	3	309	CLA	C1B-C2B	2.07	1.48	1.43
32	6	317	CHL	C1B-NB	-2.07	1.35	1.37
33	7	308	DGD	O3G-C3G	-2.07	1.40	1.43
31	7	309	CLA	C3D-C4D	-2.07	1.39	1.44
31	2	309	CLA	C1C-NC	-2.07	1.34	1.37
31	A	850	CLA	C3D-C4D	-2.07	1.39	1.44
31	6	308	CLA	C4D-ND	2.07	1.40	1.37
31	4	320	CLA	C1C-C2C	2.07	1.48	1.44
31	b	305	CLA	C1C-C2C	2.07	1.48	1.44
32	8	319	CHL	C3A-C2A	-2.07	1.48	1.54
31	A	836	CLA	C4D-ND	2.07	1.40	1.37
31	b	310	CLA	C3B-C2B	2.07	1.48	1.41
31	6	315	CLA	C3B-C2B	2.07	1.48	1.41
31	F	301	CLA	C4D-ND	2.07	1.40	1.37
32	6	321	CHL	C4C-C3C	2.07	1.48	1.45
32	a	318	CHL	C1B-C2B	2.07	1.48	1.43
31	6	316	CLA	C3B-C2B	2.07	1.48	1.41
31	7	311	CLA	C4D-ND	2.07	1.40	1.37
31	B	849	CLA	C3B-C2B	2.07	1.48	1.41
32	a	320	CHL	C1B-C2B	2.07	1.48	1.43
31	b	310	CLA	C1C-NC	-2.07	1.34	1.37
31	a	321	CLA	C4B-NB	-2.07	1.35	1.37
27	A	807	LMT	O4'-C4B	-2.07	1.38	1.43
32	6	317	CHL	C4C-C3C	2.06	1.48	1.45
31	4	320	CLA	C3B-C2B	2.06	1.48	1.41
32	5	319	CHL	C3A-C2A	-2.06	1.48	1.54
31	B	834	CLA	C4C-C3C	2.06	1.48	1.45
31	4	305	CLA	C1B-C2B	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	831	CHL	C1B-C2B	2.06	1.48	1.43
31	A	846	CLA	C4B-NB	-2.06	1.35	1.37
31	A	841	CLA	C1B-C2B	2.06	1.48	1.43
31	4	316	CLA	C1B-C2B	2.06	1.48	1.43
31	A	849	CLA	C1B-C2B	2.06	1.48	1.43
32	5	317	CHL	C3A-C2A	-2.06	1.48	1.54
31	7	312	CLA	C1C-C2C	2.06	1.48	1.44
31	O	202	CLA	C1C-C2C	2.06	1.48	1.44
31	8	313	CLA	C4B-NB	-2.06	1.35	1.37
32	9	322	CHL	C1B-NB	-2.06	1.35	1.37
31	5	311	CLA	C1B-C2B	2.06	1.48	1.43
31	G	205	CLA	C3B-C2B	2.06	1.48	1.41
31	b	305	CLA	C4B-NB	-2.06	1.35	1.37
31	B	828	CLA	C1C-NC	-2.06	1.34	1.37
31	b	307	CLA	C1C-C2C	2.06	1.48	1.44
32	7	317	CHL	C3B-C4B	2.06	1.47	1.42
31	4	316	CLA	C1C-C2C	2.06	1.48	1.44
31	8	308	CLA	C1B-C2B	2.06	1.48	1.43
31	3	317	CLA	C4B-NB	-2.06	1.35	1.37
32	7	320	CHL	C4B-NB	-2.06	1.35	1.37
32	7	317	CHL	C3A-C2A	-2.06	1.48	1.54
31	4	308	CLA	C3B-C2B	2.06	1.48	1.41
31	b	313	CLA	C1B-C2B	2.06	1.48	1.43
31	A	819	CLA	C1C-C2C	2.06	1.48	1.44
32	a	317	CHL	C4C-C3C	2.06	1.48	1.45
32	5	316	CHL	CHB-C4A	-2.06	1.32	1.37
31	3	309	CLA	C1C-C2C	2.05	1.48	1.44
31	B	846	CLA	C4D-ND	2.05	1.40	1.37
31	b	304	CLA	C3B-C2B	2.05	1.48	1.41
31	A	820	CLA	C4B-NB	-2.05	1.35	1.37
32	6	317	CHL	C1B-C2B	2.05	1.48	1.43
32	9	322	CHL	C3B-C4B	2.05	1.47	1.42
31	3	313	CLA	C1C-C2C	2.05	1.48	1.44
31	8	314	CLA	C4D-ND	2.05	1.40	1.37
32	9	322	CHL	MG-NC	-2.05	2.01	2.06
31	A	814	CLA	C3B-C2B	2.05	1.48	1.41
31	L	306	CLA	C3B-C2B	2.05	1.48	1.41
31	2	310	CLA	C1C-C2C	2.05	1.48	1.44
31	B	848	CLA	C3B-C2B	2.05	1.48	1.41
32	5	322	CHL	C3A-C2A	-2.05	1.48	1.54
32	6	321	CHL	C3A-C2A	-2.05	1.48	1.54
32	3	315	CHL	C1B-NB	-2.05	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	J	101	LMG	O2-C2	-2.05	1.38	1.43
31	4	305	CLA	C1C-C2C	2.05	1.48	1.44
31	A	817	CLA	C1B-C2B	2.05	1.48	1.43
31	b	310	CLA	C4B-NB	-2.05	1.35	1.37
26	2	302	BCR	C33-C5	-2.05	1.47	1.50
32	a	317	CHL	CHB-C4A	-2.05	1.32	1.37
31	A	832	CLA	C4B-NB	-2.05	1.35	1.37
31	H	902	CLA	C1C-C2C	2.05	1.48	1.44
31	6	310	CLA	C1C-C2C	2.05	1.48	1.44
31	A	844	CLA	C4D-ND	2.05	1.40	1.37
37	J	101	LMG	C4-C5	2.05	1.57	1.53
33	B	808	DGD	O1G-C1G	-2.05	1.40	1.45
28	A	809	LHG	O7-C5	-2.05	1.41	1.46
31	5	320	CLA	C3D-C4D	-2.05	1.39	1.44
32	b	309	CHL	CHB-C4A	-2.04	1.32	1.37
31	B	816	CLA	C4B-NB	-2.04	1.35	1.37
31	9	317	CLA	C1C-C2C	2.04	1.48	1.44
31	B	839	CLA	C3B-C2B	2.04	1.48	1.41
31	2	307	CLA	C3B-C2B	2.04	1.48	1.41
31	A	846	CLA	C1C-C2C	2.04	1.48	1.44
31	a	313	CLA	C4B-NB	-2.04	1.35	1.37
31	9	313	CLA	C4B-NB	-2.04	1.35	1.37
31	4	315	CLA	C1B-C2B	2.04	1.48	1.43
31	a	309	CLA	C1B-C2B	2.04	1.48	1.43
31	6	322	CLA	C1B-C2B	2.04	1.48	1.43
31	A	822	CLA	C3B-C2B	2.04	1.48	1.41
32	6	320	CHL	C3B-C4B	2.04	1.47	1.42
31	5	313	CLA	C1C-C2C	2.04	1.48	1.44
31	B	817	CLA	C4C-C3C	2.04	1.48	1.45
31	6	316	CLA	C1C-C2C	2.04	1.48	1.44
32	6	318	CHL	C1B-NB	-2.04	1.35	1.37
31	L	305	CLA	C3B-C2B	2.04	1.48	1.41
31	2	315	CLA	C4D-ND	2.04	1.40	1.37
32	6	318	CHL	C3B-C4B	2.04	1.47	1.42
31	O	204	CLA	C1C-C2C	2.04	1.48	1.44
31	8	307	CLA	C3B-C2B	2.04	1.48	1.41
31	K	204	CLA	C1C-C2C	2.04	1.48	1.44
31	2	306	CLA	C1C-C2C	2.03	1.48	1.44
33	7	308	DGD	O4D-C4D	-2.03	1.38	1.43
31	5	310	CLA	C1C-C2C	2.03	1.48	1.44
31	B	814	CLA	C3B-C2B	2.03	1.48	1.41
32	8	316	CHL	CHB-C4A	-2.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	309	CLA	C4D-ND	2.03	1.40	1.37
31	a	316	CLA	C4B-NB	-2.03	1.35	1.37
32	5	316	CHL	C4B-NB	-2.03	1.35	1.37
31	a	312	CLA	C1C-C2C	2.03	1.48	1.44
31	3	320	CLA	C1C-C2C	2.03	1.48	1.44
31	b	305	CLA	C3B-C2B	2.03	1.48	1.41
31	a	309	CLA	C1C-C2C	2.03	1.48	1.44
31	O	203	CLA	C1B-NB	-2.03	1.35	1.37
31	B	813	CLA	C1B-C2B	2.03	1.48	1.43
35	F	303	QTB	C17-C11	2.03	1.57	1.55
32	4	310	CHL	C3A-C2A	-2.03	1.48	1.54
31	4	316	CLA	C3B-C2B	2.03	1.48	1.41
32	7	319	CHL	C4C-C3C	2.03	1.48	1.45
31	7	321	CLA	C3B-C2B	2.03	1.48	1.41
31	2	304	CLA	C3B-C2B	2.03	1.48	1.41
31	B	830	CLA	C1B-C2B	2.03	1.48	1.43
31	b	308	CLA	C1C-C2C	2.03	1.48	1.44
32	A	831	CHL	CHB-C4A	-2.03	1.32	1.37
31	7	316	CLA	C1C-C2C	2.03	1.48	1.44
31	9	314	CLA	C3B-C2B	2.02	1.48	1.41
31	6	313	CLA	C1C-C2C	2.02	1.48	1.44
31	3	307	CLA	C3B-C2B	2.02	1.48	1.41
31	A	819	CLA	C4D-ND	2.02	1.40	1.37
31	B	828	CLA	C1B-C2B	2.02	1.48	1.43
31	9	311	CLA	C1B-C2B	2.02	1.48	1.43
31	3	307	CLA	C1C-C2C	2.02	1.48	1.44
31	3	319	CLA	C4C-C3C	2.02	1.48	1.45
31	7	312	CLA	C3B-C2B	2.02	1.48	1.41
31	2	306	CLA	C4B-NB	-2.02	1.35	1.37
32	K	201	CHL	C4C-C3C	2.02	1.48	1.45
31	8	308	CLA	C3B-C2B	2.02	1.48	1.41
31	6	312	CLA	C3B-C2B	2.02	1.48	1.41
31	a	315	CLA	C3B-C2B	2.02	1.48	1.41
31	B	819	CLA	C3D-C4D	-2.02	1.39	1.44
31	8	310	CLA	C3B-C2B	2.02	1.48	1.41
32	9	322	CHL	CHB-C4A	-2.02	1.32	1.37
31	B	840	CLA	C1C-C2C	2.02	1.48	1.44
31	B	841	CLA	C3B-C2B	2.02	1.48	1.41
32	7	320	CHL	C3B-C4B	2.02	1.47	1.42
31	8	313	CLA	C1C-C2C	2.02	1.48	1.44
31	5	307	CLA	C1B-C2B	2.02	1.48	1.43
31	B	820	CLA	C4D-ND	2.02	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	320	CHL	C4C-C3C	2.02	1.48	1.45
31	b	304	CLA	C1C-C2C	2.02	1.48	1.44
31	7	316	CLA	C4B-NB	-2.02	1.35	1.37
31	6	314	CLA	C4B-NB	-2.02	1.35	1.37
31	b	303	CLA	C3B-C2B	2.02	1.48	1.41
32	7	324	CHL	C3A-C2A	-2.02	1.48	1.54
31	8	308	CLA	C1C-C2C	2.02	1.48	1.44
31	9	314	CLA	C4B-NB	-2.02	1.35	1.37
32	6	309	CHL	C3B-C4B	2.02	1.47	1.42
32	6	309	CHL	CHB-C4A	-2.01	1.32	1.37
31	A	842	CLA	C3B-C2B	2.01	1.48	1.41
31	B	831	CLA	C3B-C2B	2.01	1.48	1.41
32	4	317	CHL	CHB-C4A	-2.01	1.32	1.37
31	8	311	CLA	C1B-C2B	2.01	1.48	1.43
31	B	815	CLA	C1B-C2B	2.01	1.48	1.43
31	B	831	CLA	C1C-C2C	2.01	1.48	1.44
31	A	833	CLA	C4D-ND	2.01	1.40	1.37
31	7	313	CLA	C1C-C2C	2.01	1.48	1.44
31	B	813	CLA	C3B-C2B	2.01	1.48	1.41
31	4	316	CLA	C3B-C4B	2.01	1.47	1.42
31	7	312	CLA	C4D-ND	2.01	1.40	1.37
31	H	901	CLA	C3B-C2B	2.01	1.48	1.41
31	a	309	CLA	C3B-C2B	2.01	1.48	1.41
31	A	845	CLA	C4B-NB	-2.01	1.35	1.37
31	B	837	CLA	C4B-NB	-2.01	1.35	1.37
32	7	324	CHL	C4B-NB	-2.01	1.35	1.37
31	5	321	CLA	C1C-C2C	2.01	1.48	1.44
31	3	314	CLA	C4D-ND	2.01	1.40	1.37
31	b	313	CLA	C3B-C2B	2.01	1.48	1.41
31	6	307	CLA	C1B-C2B	2.01	1.48	1.43
31	A	818	CLA	C3B-C2B	2.01	1.48	1.41
26	3	303	BCR	C33-C5	-2.00	1.47	1.50
31	5	315	CLA	C1C-C2C	2.00	1.48	1.44
31	a	312	CLA	C3B-C2B	2.00	1.48	1.41
32	5	316	CHL	C3B-C4B	2.00	1.47	1.42
31	8	320	CLA	C4B-NB	-2.00	1.35	1.37
32	9	320	CHL	C3B-C4B	2.00	1.47	1.42
31	B	838	CLA	C3D-C4D	-2.00	1.39	1.44
31	a	313	CLA	C3D-C4D	-2.00	1.39	1.44
31	5	310	CLA	C3B-C2B	2.00	1.48	1.41
31	F	305	CLA	C4D-ND	2.00	1.40	1.37
31	5	310	CLA	C4B-NB	-2.00	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	312	CLA	C4B-NB	-2.00	1.35	1.37
31	A	845	CLA	C1B-C2B	2.00	1.48	1.43
31	B	839	CLA	C3D-C4D	-2.00	1.39	1.44
31	3	314	CLA	C4B-NB	-2.00	1.35	1.37
31	A	828	CLA	C3B-C2B	2.00	1.48	1.41
31	K	205	CLA	C4D-ND	2.00	1.40	1.37
31	4	315	CLA	C1C-C2C	2.00	1.48	1.44
31	8	317	CLA	C3B-C2B	2.00	1.48	1.41

All (7142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	315	CLA	C4-C3-C5	-19.91	81.78	115.27
31	5	315	CLA	C5-C3-C2	19.18	159.93	121.12
31	5	315	CLA	C4-C3-C2	-17.67	78.34	123.68
36	7	305	LUT	C15-C14-C13	-17.12	102.87	127.31
36	2	301	LUT	C15-C14-C13	-16.15	104.26	127.31
36	9	305	LUT	C15-C35-C34	15.60	155.43	123.47
31	4	305	CLA	C1D-ND-C4D	-15.43	95.37	106.33
36	8	302	LUT	C15-C14-C13	-15.21	105.60	127.31
36	8	303	LUT	C15-C14-C13	-14.81	106.18	127.31
36	J	103	LUT	C15-C35-C34	14.38	152.93	123.47
36	3	305	LUT	C15-C14-C13	-14.36	106.82	127.31
36	9	302	LUT	C15-C35-C34	14.18	152.52	123.47
36	3	304	LUT	C15-C14-C13	-14.11	107.17	127.31
36	8	303	LUT	C18-C5-C6	-14.05	108.75	124.53
31	4	305	CLA	C4A-NA-C1A	-13.88	100.47	106.71
36	9	303	LUT	C15-C14-C13	-13.87	107.52	127.31
36	a	305	LUT	C15-C35-C34	13.74	151.62	123.47
36	b	301	LUT	C15-C35-C34	13.65	151.43	123.47
36	3	305	LUT	C18-C5-C6	-13.35	109.54	124.53
31	A	829	CLA	CHD-C1D-ND	-13.34	112.20	124.45
36	4	302	LUT	C15-C35-C34	13.26	150.64	123.47
31	4	305	CLA	C2B-C1B-NB	13.21	119.09	110.23
36	L	304	LUT	C15-C35-C34	13.07	150.25	123.47
36	a	305	LUT	C19-C9-C10	-12.96	104.77	122.92
36	F	304	LUT	C15-C35-C34	12.83	149.75	123.47
36	F	304	LUT	C18-C5-C6	-12.68	110.28	124.53
36	6	303	LUT	C18-C5-C6	-12.67	110.30	124.53
36	3	305	LUT	C11-C10-C9	-12.53	109.43	127.31
36	5	304	LUT	C15-C35-C34	12.46	148.99	123.47
36	6	303	LUT	C15-C35-C34	12.36	148.80	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	303	LUT	C15-C35-C34	12.36	148.79	123.47
36	9	303	LUT	C18-C5-C6	-12.35	110.66	124.53
36	6	304	LUT	C15-C35-C34	12.30	148.67	123.47
36	a	303	LUT	C15-C14-C13	-12.28	109.79	127.31
36	F	304	LUT	C11-C10-C9	-12.23	109.86	127.31
36	5	303	LUT	C15-C14-C13	-12.13	110.00	127.31
36	9	305	LUT	C35-C34-C33	-12.12	110.01	127.31
36	4	302	LUT	C31-C30-C29	-12.11	110.02	127.31
36	3	304	LUT	C31-C30-C29	-12.11	110.03	127.31
36	4	303	LUT	C18-C5-C6	-12.11	110.93	124.53
36	3	304	LUT	C11-C10-C9	-12.05	110.11	127.31
36	J	103	LUT	C31-C30-C29	-12.01	110.17	127.31
31	A	829	CLA	C4A-NA-C1A	11.99	112.10	106.71
36	8	303	LUT	C31-C30-C29	-11.86	110.39	127.31
36	9	305	LUT	C15-C14-C13	-11.85	110.41	127.31
31	4	316	CLA	CHD-C1D-ND	-11.84	113.57	124.45
36	9	302	LUT	C11-C10-C9	-11.81	110.45	127.31
36	F	304	LUT	C31-C30-C29	-11.73	110.57	127.31
36	4	303	LUT	C15-C35-C34	11.73	147.50	123.47
36	4	302	LUT	C15-C14-C13	-11.65	110.68	127.31
31	A	838	CLA	C4A-NA-C1A	11.54	111.89	106.71
36	2	301	LUT	C11-C10-C9	-11.51	110.89	127.31
36	a	303	LUT	C11-C10-C9	-11.47	110.94	127.31
36	a	303	LUT	C15-C35-C34	11.44	146.92	123.47
36	b	301	LUT	C11-C10-C9	-11.43	110.99	127.31
36	J	103	LUT	C11-C10-C9	-11.43	111.00	127.31
36	3	304	LUT	C15-C35-C34	11.40	146.84	123.47
36	a	305	LUT	C11-C12-C13	11.40	158.43	126.42
36	J	103	LUT	C15-C14-C13	-11.36	111.09	127.31
36	2	301	LUT	C31-C30-C29	-11.29	111.19	127.31
36	b	301	LUT	C18-C5-C6	-11.26	111.89	124.53
36	8	302	LUT	C15-C35-C34	11.18	146.38	123.47
30	A	813	CL0	C1D-ND-C4D	-11.16	98.40	106.33
36	8	302	LUT	C11-C10-C9	-11.15	111.39	127.31
36	L	304	LUT	C18-C5-C6	-11.09	112.08	124.53
36	5	303	LUT	C31-C30-C29	-11.09	111.49	127.31
36	8	302	LUT	C31-C30-C29	-11.06	111.53	127.31
36	4	303	LUT	C15-C14-C13	-11.06	111.53	127.31
36	9	305	LUT	C18-C5-C6	-11.05	112.12	124.53
36	L	304	LUT	C31-C30-C29	-11.05	111.54	127.31
36	6	303	LUT	C15-C14-C13	-11.05	111.54	127.31
36	9	303	LUT	C31-C30-C29	-11.05	111.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	7	305	LUT	C11-C10-C9	-11.01	111.59	127.31
36	7	305	LUT	C15-C35-C34	11.00	146.02	123.47
36	8	303	LUT	C15-C35-C34	10.99	145.99	123.47
36	5	304	LUT	C18-C5-C6	-10.97	112.21	124.53
36	3	305	LUT	C31-C30-C29	-10.97	111.66	127.31
36	4	302	LUT	C18-C5-C6	-10.91	112.28	124.53
36	9	302	LUT	C18-C5-C6	-10.85	112.35	124.53
36	5	304	LUT	C31-C30-C29	-10.84	111.84	127.31
31	B	832	CLA	C4A-NA-C1A	10.84	111.58	106.71
36	J	103	LUT	C18-C5-C6	-10.77	112.43	124.53
36	5	303	LUT	C18-C5-C6	-10.74	112.47	124.53
36	F	304	LUT	C11-C12-C13	10.73	156.55	126.42
36	L	304	LUT	C15-C14-C13	-10.72	112.01	127.31
36	a	303	LUT	C31-C32-C33	10.64	156.30	126.42
36	4	302	LUT	C11-C10-C9	-10.61	112.17	127.31
31	4	305	CLA	C2C-C1C-NC	10.58	119.89	109.97
36	5	303	LUT	C11-C10-C9	-10.58	112.22	127.31
36	8	302	LUT	C18-C5-C6	-10.58	112.65	124.53
36	3	305	LUT	C15-C35-C34	10.57	145.12	123.47
31	A	833	CLA	C4A-NA-C1A	10.53	111.44	106.71
31	A	841	CLA	C4A-NA-C1A	10.51	111.43	106.71
36	4	303	LUT	C11-C10-C9	-10.49	112.34	127.31
36	9	302	LUT	C15-C14-C13	-10.48	112.35	127.31
36	7	305	LUT	C31-C30-C29	-10.45	112.39	127.31
36	6	304	LUT	C18-C5-C6	-10.45	112.79	124.53
31	B	847	CLA	C4A-NA-C1A	10.38	111.37	106.71
31	A	852	CLA	C4A-NA-C1A	10.37	111.37	106.71
36	9	305	LUT	C31-C32-C33	10.37	155.56	126.42
36	5	303	LUT	C35-C34-C33	-10.35	112.53	127.31
32	K	201	CHL	C2B-C1B-NB	10.35	117.17	110.23
31	A	855	CLA	C4A-NA-C1A	10.34	111.35	106.71
36	4	303	LUT	C11-C12-C13	10.34	155.45	126.42
36	b	301	LUT	C31-C30-C29	-10.33	112.57	127.31
36	a	305	LUT	C18-C5-C6	-10.33	112.93	124.53
30	A	813	CL0	C2B-C1B-NB	10.29	117.13	110.23
36	6	304	LUT	C31-C30-C29	-10.29	112.63	127.31
36	9	302	LUT	C39-C29-C30	-10.27	108.54	122.92
36	6	303	LUT	C11-C12-C13	10.26	155.25	126.42
36	4	302	LUT	C35-C34-C33	-10.25	112.68	127.31
36	2	301	LUT	C15-C35-C34	10.24	144.46	123.47
36	L	304	LUT	C11-C12-C13	10.24	155.18	126.42
31	5	313	CLA	C4A-NA-C1A	10.22	111.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	304	LUT	C11-C10-C9	-10.18	112.78	127.31
31	A	822	CLA	C4A-NA-C1A	10.17	111.28	106.71
36	2	301	LUT	C18-C5-C6	-10.15	113.13	124.53
31	B	829	CLA	C4A-NA-C1A	10.14	111.27	106.71
36	L	304	LUT	C19-C9-C10	-10.14	108.72	122.92
36	a	305	LUT	C15-C14-C13	-10.11	112.88	127.31
36	J	103	LUT	C11-C12-C13	10.09	154.77	126.42
36	6	304	LUT	C15-C14-C13	-10.08	112.92	127.31
36	F	304	LUT	C19-C9-C10	-10.00	108.92	122.92
31	B	826	CLA	C4A-NA-C1A	9.97	111.19	106.71
36	9	303	LUT	C15-C35-C34	9.97	143.89	123.47
36	9	305	LUT	C20-C13-C14	-9.96	108.97	122.92
36	9	305	LUT	C31-C30-C29	-9.91	113.16	127.31
36	a	305	LUT	C31-C30-C29	-9.90	113.18	127.31
36	9	302	LUT	C31-C30-C29	-9.89	113.19	127.31
31	A	826	CLA	C4A-NA-C1A	9.87	111.14	106.71
36	4	303	LUT	C31-C30-C29	-9.86	113.23	127.31
31	8	309	CLA	C4A-NA-C1A	9.83	111.13	106.71
36	L	304	LUT	C40-C33-C34	-9.83	109.15	122.92
31	3	317	CLA	C4A-NA-C1A	9.83	111.13	106.71
31	A	851	CLA	C4A-NA-C1A	9.83	111.12	106.71
31	b	303	CLA	C4A-NA-C1A	9.80	111.11	106.71
36	a	303	LUT	C18-C5-C6	-9.80	113.53	124.53
36	6	303	LUT	C31-C30-C29	-9.79	113.34	127.31
36	9	303	LUT	C11-C10-C9	-9.78	113.35	127.31
31	B	845	CLA	C4A-NA-C1A	9.76	111.09	106.71
36	5	304	LUT	C11-C12-C13	9.72	153.72	126.42
31	A	856	CLA	C4A-NA-C1A	9.68	111.06	106.71
31	a	319	CLA	C4A-NA-C1A	9.66	111.05	106.71
31	B	840	CLA	C4A-NA-C1A	9.64	111.04	106.71
31	A	857	CLA	C4A-NA-C1A	9.64	111.04	106.71
36	L	304	LUT	C35-C34-C33	-9.63	113.57	127.31
31	6	306	CLA	C4A-NA-C1A	9.63	111.03	106.71
36	L	304	LUT	C20-C13-C14	-9.61	109.46	122.92
31	9	317	CLA	C4A-NA-C1A	9.61	111.03	106.71
31	F	306	CLA	C4A-NA-C1A	9.59	111.02	106.71
31	L	307	CLA	C4A-NA-C1A	9.58	111.02	106.71
36	3	304	LUT	C31-C32-C33	9.58	153.34	126.42
31	A	814	CLA	C4A-NA-C1A	9.58	111.01	106.71
31	B	823	CLA	C4A-NA-C1A	9.57	111.01	106.71
31	8	307	CLA	C4A-NA-C1A	9.52	110.99	106.71
36	J	103	LUT	C39-C29-C30	-9.51	109.60	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	301	LUT	C40-C33-C34	-9.51	109.61	122.92
36	a	305	LUT	C31-C32-C33	9.50	153.11	126.42
31	A	830	CLA	C4A-NA-C1A	9.50	110.97	106.71
31	3	308	CLA	C4A-NA-C1A	9.49	110.97	106.71
31	7	311	CLA	C4A-NA-C1A	9.46	110.96	106.71
31	A	820	CLA	C4A-NA-C1A	9.44	110.95	106.71
36	8	303	LUT	C11-C10-C9	-9.42	113.87	127.31
36	4	302	LUT	C39-C29-C30	-9.42	109.73	122.92
31	3	320	CLA	C4A-NA-C1A	9.41	110.94	106.71
31	9	313	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	A	827	CLA	C4A-NA-C1A	9.38	110.92	106.71
36	5	303	LUT	C40-C33-C34	-9.37	109.80	122.92
36	b	301	LUT	C19-C9-C10	-9.37	109.80	122.92
36	4	302	LUT	C31-C32-C33	9.37	152.73	126.42
36	L	304	LUT	C11-C10-C9	-9.36	113.95	127.31
30	A	813	CL0	C2C-C1C-NC	9.36	118.74	109.97
31	J	105	CLA	C4A-NA-C1A	9.36	110.91	106.71
31	b	302	CLA	C4A-NA-C1A	9.36	110.91	106.71
31	A	825	CLA	C4A-NA-C1A	9.35	110.91	106.71
31	F	301	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	B	824	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	b	307	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	4	314	CLA	C4A-NA-C1A	9.33	110.90	106.71
31	6	310	CLA	C4A-NA-C1A	9.33	110.90	106.71
36	a	305	LUT	C20-C13-C14	-9.31	109.88	122.92
31	7	321	CLA	C4A-NA-C1A	9.31	110.89	106.71
36	6	303	LUT	C40-C33-C34	-9.29	109.90	122.92
36	J	103	LUT	C19-C9-C10	-9.29	109.91	122.92
31	B	825	CLA	C4A-NA-C1A	9.28	110.88	106.71
36	9	305	LUT	C40-C33-C34	-9.28	109.92	122.92
36	a	305	LUT	C39-C29-C30	-9.25	109.96	122.92
31	B	811	CLA	C4A-NA-C1A	9.25	110.86	106.71
31	4	316	CLA	C4A-NA-C1A	9.25	110.86	106.71
31	6	313	CLA	C4A-NA-C1A	9.24	110.86	106.71
36	F	304	LUT	C35-C34-C33	-9.23	114.14	127.31
36	6	303	LUT	C31-C32-C33	9.20	152.27	126.42
36	9	305	LUT	C19-C9-C10	-9.19	110.05	122.92
36	L	304	LUT	C31-C32-C33	9.18	152.21	126.42
31	3	313	CLA	C4A-NA-C1A	9.18	110.83	106.71
36	3	305	LUT	C31-C32-C33	9.16	152.14	126.42
31	A	842	CLA	C4A-NA-C1A	9.16	110.82	106.71
31	5	321	CLA	C4A-NA-C1A	9.15	110.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	4	303	LUT	C19-C9-C10	-9.15	110.11	122.92
36	9	305	LUT	C39-C29-C30	-9.15	110.11	122.92
36	8	302	LUT	C40-C33-C34	-9.14	110.12	122.92
36	7	305	LUT	C31-C32-C33	9.13	152.06	126.42
36	5	303	LUT	C39-C29-C30	-9.12	110.14	122.92
31	B	816	CLA	C4A-NA-C1A	9.12	110.81	106.71
36	J	103	LUT	C20-C13-C14	-9.10	110.17	122.92
31	8	312	CLA	C4A-NA-C1A	9.10	110.80	106.71
36	9	305	LUT	C11-C12-C13	9.08	151.92	126.42
36	9	302	LUT	C35-C34-C33	-9.08	114.36	127.31
31	B	835	CLA	C4A-NA-C1A	9.05	110.77	106.71
31	5	312	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	5	323	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	6	315	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	9	316	CLA	C4A-NA-C1A	9.03	110.76	106.71
36	F	304	LUT	C15-C14-C13	-9.02	114.43	127.31
36	J	103	LUT	C40-C33-C34	-9.02	110.29	122.92
31	7	316	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	B	846	CLA	C4A-NA-C1A	9.01	110.75	106.71
31	2	310	CLA	C4A-NA-C1A	9.01	110.75	106.71
31	O	204	CLA	C4A-NA-C1A	9.00	110.75	106.71
36	2	301	LUT	C40-C33-C34	-9.00	110.31	122.92
31	A	854	CLA	C4A-NA-C1A	9.00	110.75	106.71
36	6	303	LUT	C11-C10-C9	-8.98	114.49	127.31
31	A	828	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	A	837	CLA	C4A-NA-C1A	8.97	110.74	106.71
31	A	821	CLA	C4A-NA-C1A	8.97	110.74	106.71
36	6	304	LUT	C11-C12-C13	8.96	151.60	126.42
31	B	818	CLA	C4A-NA-C1A	8.96	110.74	106.71
31	a	311	CLA	C4A-NA-C1A	8.96	110.73	106.71
36	9	302	LUT	C31-C32-C33	8.94	151.54	126.42
31	2	312	CLA	C4A-NA-C1A	8.94	110.73	106.71
31	9	312	CLA	C4A-NA-C1A	8.94	110.72	106.71
36	a	303	LUT	C39-C29-C30	-8.94	110.41	122.92
31	A	835	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	A	843	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	A	850	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	5	309	CLA	C4A-NA-C1A	8.93	110.72	106.71
36	8	303	LUT	C38-C25-C24	-8.93	104.46	123.56
31	L	305	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	2	315	CLA	C4A-NA-C1A	8.93	110.72	106.71
36	9	305	LUT	C11-C10-C9	-8.92	114.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	303	LUT	C31-C32-C33	8.92	151.48	126.42
31	A	853	CLA	C4A-NA-C1A	8.92	110.72	106.71
31	B	843	CLA	C4A-NA-C1A	8.92	110.72	106.71
36	2	301	LUT	C31-C32-C33	8.91	151.45	126.42
36	b	301	LUT	C31-C32-C33	8.91	151.45	126.42
36	6	303	LUT	C39-C29-C30	-8.91	110.44	122.92
31	B	822	CLA	C4A-NA-C1A	8.90	110.71	106.71
36	5	304	LUT	C40-C33-C34	-8.90	110.45	122.92
31	6	308	CLA	C4A-NA-C1A	8.89	110.70	106.71
36	4	302	LUT	C40-C33-C34	-8.89	110.47	122.92
36	6	303	LUT	C19-C9-C10	-8.89	110.47	122.92
36	9	303	LUT	C1-C6-C5	-8.89	110.09	122.61
31	4	318	CLA	C4A-NA-C1A	8.89	110.70	106.71
36	L	304	LUT	C39-C29-C30	-8.88	110.48	122.92
36	5	304	LUT	C15-C14-C13	-8.88	114.63	127.31
36	2	301	LUT	C20-C13-C14	-8.87	110.50	122.92
36	3	304	LUT	C40-C33-C34	-8.85	110.52	122.92
31	A	845	CLA	C4A-NA-C1A	8.84	110.68	106.71
31	A	846	CLA	C4A-NA-C1A	8.83	110.67	106.71
31	7	310	CLA	C4A-NA-C1A	8.82	110.67	106.71
36	F	304	LUT	C20-C13-C14	-8.80	110.59	122.92
31	8	310	CLA	C4A-NA-C1A	8.80	110.66	106.71
36	a	303	LUT	C31-C30-C29	-8.76	114.81	127.31
31	A	817	CLA	C4A-NA-C1A	8.75	110.64	106.71
36	F	304	LUT	C40-C33-C34	-8.75	110.66	122.92
36	8	302	LUT	C31-C32-C33	8.75	150.99	126.42
31	a	310	CLA	C4A-NA-C1A	8.75	110.64	106.71
36	9	302	LUT	C20-C13-C14	-8.74	110.67	122.92
36	b	301	LUT	C35-C34-C33	-8.74	114.83	127.31
36	3	304	LUT	C39-C29-C30	-8.74	110.68	122.92
31	2	305	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	B	842	CLA	C4A-NA-C1A	8.74	110.63	106.71
36	b	301	LUT	C15-C14-C13	-8.72	114.87	127.31
31	b	312	CLA	C4A-NA-C1A	8.71	110.62	106.71
36	2	301	LUT	C32-C33-C34	-8.71	105.57	118.94
31	F	305	CLA	C4A-NA-C1A	8.71	110.62	106.71
36	a	305	LUT	C40-C33-C34	-8.71	110.73	122.92
31	5	308	CLA	C4A-NA-C1A	8.70	110.62	106.71
31	H	901	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	5	320	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	2	311	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	6	311	CLA	C4A-NA-C1A	8.68	110.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	2	301	LUT	C39-C29-C30	-8.68	110.77	122.92
31	A	818	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	a	312	CLA	C4A-NA-C1A	8.65	110.60	106.71
36	9	302	LUT	C11-C12-C13	8.64	150.70	126.42
31	A	819	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	B	813	CLA	C4A-NA-C1A	8.63	110.59	106.71
31	A	824	CLA	C4A-NA-C1A	8.63	110.58	106.71
36	9	303	LUT	C19-C9-C10	-8.63	110.84	122.92
36	9	303	LUT	C11-C12-C13	8.61	150.59	126.42
32	A	839	CHL	O2D-CGD-O1D	-8.60	107.02	123.84
36	5	304	LUT	C19-C9-C10	-8.60	110.88	122.92
31	A	836	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	a	315	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	9	318	CLA	C4A-NA-C1A	8.58	110.56	106.71
36	F	304	LUT	C31-C32-C33	8.58	150.51	126.42
31	9	321	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	K	206	CLA	C4A-NA-C1A	8.55	110.55	106.71
36	b	301	LUT	C39-C29-C30	-8.55	110.95	122.92
36	5	304	LUT	C31-C32-C33	8.54	150.42	126.42
31	3	312	CLA	C4A-NA-C1A	8.54	110.55	106.71
31	6	314	CLA	C4A-NA-C1A	8.52	110.54	106.71
31	B	838	CLA	C4A-NA-C1A	8.52	110.54	106.71
36	4	302	LUT	C19-C9-C10	-8.51	111.00	122.92
36	4	302	LUT	C20-C13-C14	-8.51	111.00	122.92
31	B	812	CLA	C4A-NA-C1A	8.49	110.52	106.71
36	6	303	LUT	C20-C13-C14	-8.49	111.04	122.92
31	K	205	CLA	C4A-NA-C1A	8.47	110.51	106.71
31	7	314	CLA	C4A-NA-C1A	8.46	110.51	106.71
31	5	314	CLA	C4A-NA-C1A	8.46	110.51	106.71
31	B	850	CLA	C4A-NA-C1A	8.45	110.51	106.71
31	G	204	CLA	C4A-NA-C1A	8.43	110.49	106.71
36	F	304	LUT	C12-C13-C14	-8.42	106.01	118.94
31	B	819	CLA	C4A-NA-C1A	8.42	110.49	106.71
31	B	814	CLA	C4A-NA-C1A	8.41	110.49	106.71
36	8	302	LUT	C39-C29-C30	-8.40	111.16	122.92
31	G	205	CLA	C4A-NA-C1A	8.37	110.47	106.71
31	7	322	CLA	C4A-NA-C1A	8.37	110.47	106.71
31	B	815	CLA	C4A-NA-C1A	8.36	110.46	106.71
36	3	304	LUT	C35-C34-C33	-8.36	115.38	127.31
31	4	311	CLA	C4A-NA-C1A	8.35	110.46	106.71
36	3	304	LUT	C32-C33-C34	-8.35	106.12	118.94
31	4	319	CLA	C4A-NA-C1A	8.35	110.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	303	LUT	C20-C13-C14	-8.35	111.22	122.92
31	3	309	CLA	C4A-NA-C1A	8.34	110.45	106.71
31	2	314	CLA	C4A-NA-C1A	8.34	110.45	106.71
36	7	305	LUT	C35-C34-C33	-8.33	115.42	127.31
31	A	849	CLA	C4A-NA-C1A	8.32	110.45	106.71
36	b	301	LUT	C11-C12-C13	8.32	149.78	126.42
31	3	310	CLA	C4A-NA-C1A	8.31	110.44	106.71
31	B	820	CLA	C4A-NA-C1A	8.31	110.44	106.71
31	B	844	CLA	C4A-NA-C1A	8.30	110.44	106.71
31	H	902	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	B	848	CLA	C4A-NA-C1A	8.28	110.43	106.71
31	8	313	CLA	C4A-NA-C1A	8.28	110.43	106.71
31	8	317	CLA	C4A-NA-C1A	8.28	110.43	106.71
31	A	844	CLA	C4A-NA-C1A	8.27	110.43	106.71
31	8	311	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	9	319	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	4	312	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	B	828	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	H	903	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	7	312	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	7	315	CLA	C4A-NA-C1A	8.25	110.42	106.71
36	6	304	LUT	C19-C9-C10	-8.25	111.36	122.92
36	9	302	LUT	C40-C33-C34	-8.24	111.39	122.92
36	3	304	LUT	C20-C13-C14	-8.23	111.39	122.92
36	5	303	LUT	C11-C12-C13	8.23	149.53	126.42
36	7	305	LUT	C39-C29-C30	-8.22	111.40	122.92
31	4	308	CLA	C4A-NA-C1A	8.22	110.40	106.71
36	6	304	LUT	C38-C25-C24	-8.22	105.97	123.56
36	F	304	LUT	C32-C33-C34	-8.22	106.33	118.94
31	B	817	CLA	C4A-NA-C1A	8.22	110.40	106.71
36	4	302	LUT	C11-C12-C13	8.21	149.49	126.42
31	B	836	CLA	C4A-NA-C1A	8.21	110.40	106.71
31	B	849	CLA	C4A-NA-C1A	8.20	110.39	106.71
31	5	313	CLA	C2B-C1B-NB	8.20	115.73	110.23
36	4	303	LUT	C1-C6-C5	-8.20	111.07	122.61
32	K	201	CHL	CMD-C2D-C1D	8.19	139.14	124.71
36	a	305	LUT	C35-C34-C33	-8.18	115.63	127.31
36	4	303	LUT	C39-C29-C30	-8.18	111.46	122.92
36	7	305	LUT	C20-C13-C14	-8.18	111.46	122.92
31	a	314	CLA	C4A-NA-C1A	8.18	110.38	106.71
36	3	305	LUT	C39-C29-C30	-8.18	111.47	122.92
36	7	305	LUT	C40-C33-C34	-8.18	111.47	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	847	CLA	C4A-NA-C1A	8.16	110.37	106.71
36	6	304	LUT	C31-C32-C33	8.15	149.32	126.42
31	b	311	CLA	C4A-NA-C1A	8.15	110.37	106.71
36	a	303	LUT	C40-C33-C34	-8.14	111.51	122.92
31	2	308	CLA	C4A-NA-C1A	8.14	110.36	106.71
31	6	316	CLA	C4A-NA-C1A	8.13	110.36	106.71
36	9	303	LUT	C20-C13-C14	-8.10	111.58	122.92
36	5	304	LUT	C35-C34-C33	-8.10	115.75	127.31
36	3	305	LUT	C32-C33-C34	-8.09	106.53	118.94
31	O	203	CLA	C4A-NA-C1A	8.08	110.34	106.71
36	6	304	LUT	C20-C13-C14	-8.08	111.60	122.92
31	B	821	CLA	C4A-NA-C1A	8.08	110.34	106.71
36	5	304	LUT	C38-C25-C24	-8.07	106.29	123.56
36	4	303	LUT	C31-C32-C33	8.06	149.07	126.42
31	5	310	CLA	C4A-NA-C1A	8.06	110.33	106.71
31	A	815	CLA	C4A-NA-C1A	8.04	110.32	106.71
31	a	313	CLA	C4A-NA-C1A	8.02	110.31	106.71
36	8	303	LUT	C31-C32-C33	8.02	148.94	126.42
31	2	307	CLA	C4A-NA-C1A	8.01	110.31	106.71
36	J	103	LUT	C31-C32-C33	8.01	148.90	126.42
31	A	823	CLA	C4A-NA-C1A	8.00	110.30	106.71
31	8	321	CLA	C4A-NA-C1A	8.00	110.30	106.71
31	9	314	CLA	C4A-NA-C1A	7.99	110.30	106.71
31	4	305	CLA	CMD-C2D-C1D	7.99	138.80	124.71
36	2	301	LUT	C8-C9-C10	-7.99	106.68	118.94
36	5	303	LUT	C19-C9-C10	-7.99	111.73	122.92
31	B	834	CLA	C4A-NA-C1A	7.98	110.30	106.71
31	4	307	CLA	C4A-NA-C1A	7.98	110.29	106.71
31	A	816	CLA	C4A-NA-C1A	7.97	110.29	106.71
31	B	839	CLA	C4A-NA-C1A	7.97	110.29	106.71
31	5	315	CLA	C4A-NA-C1A	7.96	110.29	106.71
31	7	313	CLA	C4A-NA-C1A	7.95	110.28	106.71
32	A	839	CHL	O1D-CGD-CBD	-7.95	108.22	124.48
31	A	832	CLA	C4A-NA-C1A	7.94	110.27	106.71
31	B	830	CLA	C4A-NA-C1A	7.93	110.27	106.71
31	B	833	CLA	C4A-NA-C1A	7.92	110.27	106.71
36	3	305	LUT	C20-C13-C14	-7.91	111.85	122.92
36	b	301	LUT	C38-C25-C24	-7.89	106.68	123.56
36	9	302	LUT	C38-C25-C24	-7.89	106.68	123.56
36	6	304	LUT	C8-C9-C10	-7.89	106.83	118.94
31	b	310	CLA	C4A-NA-C1A	7.89	110.25	106.71
36	5	304	LUT	C39-C29-C30	-7.86	111.91	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	303	LUT	C20-C13-C14	-7.85	111.92	122.92
36	3	305	LUT	C40-C33-C34	-7.85	111.92	122.92
36	2	301	LUT	C19-C9-C10	-7.85	111.92	122.92
32	K	201	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
31	8	315	CLA	C4A-NA-C1A	7.83	110.23	106.71
31	8	314	CLA	C4A-NA-C1A	7.82	110.22	106.71
31	a	321	CLA	C4A-NA-C1A	7.82	110.22	106.71
36	8	302	LUT	C19-C9-C10	-7.81	111.98	122.92
36	4	303	LUT	C20-C13-C14	-7.80	111.99	122.92
31	8	318	CLA	C4A-NA-C1A	7.80	110.21	106.71
31	B	837	CLA	C4A-NA-C1A	7.79	110.21	106.71
36	3	304	LUT	C19-C9-C10	-7.76	112.05	122.92
36	F	304	LUT	C39-C29-C30	-7.76	112.05	122.92
31	2	309	CLA	C4A-NA-C1A	7.75	110.19	106.71
36	6	304	LUT	C11-C10-C9	-7.73	116.28	127.31
31	4	305	CLA	C3C-C4C-NC	7.70	119.21	110.57
36	2	301	LUT	C38-C25-C24	-7.70	107.09	123.56
36	4	303	LUT	C40-C33-C34	-7.70	112.14	122.92
31	K	204	CLA	C4A-NA-C1A	7.69	110.16	106.71
32	7	319	CHL	O2D-CGD-CBD	7.69	124.93	111.27
36	6	303	LUT	C1-C6-C5	-7.69	111.79	122.61
36	7	305	LUT	C11-C12-C13	7.68	147.99	126.42
31	3	311	CLA	C4A-NA-C1A	7.67	110.15	106.71
36	3	305	LUT	C38-C25-C24	-7.66	107.18	123.56
31	A	829	CLA	CMD-C2D-C1D	7.64	138.18	124.71
36	2	301	LUT	C20-C13-C12	-7.64	106.04	118.08
31	9	315	CLA	C4A-NA-C1A	7.63	110.14	106.71
31	a	309	CLA	C4A-NA-C1A	7.63	110.14	106.71
31	L	306	CLA	C4A-NA-C1A	7.62	110.13	106.71
36	3	305	LUT	C19-C9-C10	-7.62	112.25	122.92
31	4	320	CLA	C4A-NA-C1A	7.62	110.13	106.71
36	6	303	LUT	C32-C33-C34	-7.60	107.28	118.94
36	a	303	LUT	C19-C9-C10	-7.58	112.31	122.92
36	7	305	LUT	C38-C25-C24	-7.58	107.35	123.56
31	4	309	CLA	C4A-NA-C1A	7.58	110.11	106.71
31	3	316	CLA	C4A-NA-C1A	7.57	110.11	106.71
36	b	301	LUT	C40-C33-C32	-7.57	106.15	118.08
31	b	308	CLA	C4A-NA-C1A	7.57	110.11	106.71
36	8	303	LUT	C19-C9-C10	-7.55	112.35	122.92
36	a	303	LUT	C38-C25-C24	-7.55	107.41	123.56
32	A	831	CHL	O2D-CGD-O1D	-7.55	109.09	123.84
36	8	303	LUT	C20-C13-C14	-7.54	112.36	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	8	303	LUT	C40-C33-C34	-7.52	112.39	122.92
36	a	303	LUT	C32-C33-C34	-7.52	107.40	118.94
31	4	321	CLA	C4A-NA-C1A	7.51	110.08	106.71
31	6	306	CLA	CMD-C2D-C1D	7.51	137.94	124.71
36	a	305	LUT	C11-C10-C9	-7.50	116.60	127.31
31	O	202	CLA	C4A-NA-C1A	7.49	110.08	106.71
31	B	831	CLA	C4A-NA-C1A	7.48	110.07	106.71
36	9	303	LUT	C38-C25-C24	-7.47	107.58	123.56
36	a	303	LUT	C8-C9-C10	-7.47	107.48	118.94
31	8	309	CLA	CHC-C4B-NB	7.45	132.14	124.26
36	5	303	LUT	C38-C25-C24	-7.45	107.63	123.56
31	B	827	CLA	C4A-NA-C1A	7.44	110.05	106.71
31	5	311	CLA	C4A-NA-C1A	7.44	110.05	106.71
31	8	308	CLA	C4A-NA-C1A	7.43	110.05	106.71
36	8	302	LUT	C8-C9-C10	-7.43	107.54	118.94
36	b	301	LUT	C20-C13-C14	-7.43	112.52	122.92
31	b	306	CLA	C4A-NA-C1A	7.42	110.04	106.71
31	2	313	CLA	C4A-NA-C1A	7.42	110.04	106.71
36	8	302	LUT	C35-C34-C33	-7.42	116.71	127.31
36	4	303	LUT	C38-C25-C24	-7.42	107.69	123.56
36	9	302	LUT	C19-C9-C10	-7.40	112.56	122.92
36	5	304	LUT	C20-C13-C14	-7.39	112.56	122.92
31	6	322	CLA	C4A-NA-C1A	7.39	110.03	106.71
36	3	304	LUT	C11-C12-C13	7.39	147.17	126.42
36	7	305	LUT	C32-C33-C34	-7.37	107.62	118.94
31	G	206	CLA	C4A-NA-C1A	7.36	110.01	106.71
32	3	315	CHL	O2D-CGD-O1D	-7.34	109.49	123.84
36	6	304	LUT	C40-C33-C34	-7.34	112.64	122.92
32	6	319	CHL	O2D-CGD-CBD	7.32	124.28	111.27
31	b	304	CLA	C4A-NA-C1A	7.32	110.00	106.71
31	6	306	CLA	CHD-C1D-ND	-7.29	117.76	124.45
36	8	302	LUT	C20-C13-C14	-7.27	112.74	122.92
31	a	322	CLA	C4A-NA-C1A	7.26	109.97	106.71
31	3	318	CLA	C4A-NA-C1A	7.26	109.97	106.71
36	6	304	LUT	C39-C29-C30	-7.26	112.76	122.92
31	3	307	CLA	C4A-NA-C1A	7.24	109.96	106.71
36	6	303	LUT	C35-C34-C33	-7.24	116.98	127.31
31	6	312	CLA	C4A-NA-C1A	7.22	109.95	106.71
31	4	315	CLA	C4A-NA-C1A	7.21	109.95	106.71
31	B	812	CLA	C2B-C1B-NB	7.21	115.06	110.23
36	8	302	LUT	C11-C12-C13	7.17	146.56	126.42
36	a	303	LUT	C11-C12-C13	7.16	146.54	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	303	LUT	C20-C13-C12	-7.16	106.79	118.08
36	6	304	LUT	C35-C34-C33	-7.15	117.11	127.31
31	B	841	CLA	C4A-NA-C1A	7.15	109.92	106.71
36	F	304	LUT	C35-C15-C14	-7.15	108.84	123.47
36	b	301	LUT	C20-C13-C12	-7.14	106.83	118.08
32	A	831	CHL	O1D-CGD-CBD	-7.14	109.87	124.48
31	4	305	CLA	C3B-C4B-NB	7.13	117.13	110.52
31	4	306	CLA	C4A-NA-C1A	7.11	109.90	106.71
36	8	303	LUT	C40-C33-C32	-7.11	106.88	118.08
36	6	303	LUT	C20-C13-C12	-7.10	106.89	118.08
31	9	317	CLA	CMD-C2D-C1D	7.09	137.22	124.71
31	2	304	CLA	C4A-NA-C1A	7.09	109.89	106.71
36	8	302	LUT	C20-C13-C12	-7.09	106.91	118.08
32	A	839	CHL	C4A-NA-C1A	7.09	109.89	106.71
36	9	303	LUT	C40-C33-C34	-7.06	113.03	122.92
31	7	315	CLA	CHC-C4B-NB	7.06	131.74	124.26
36	9	303	LUT	C39-C29-C30	-7.06	113.03	122.92
36	8	303	LUT	C39-C29-C30	-7.06	113.03	122.92
31	8	320	CLA	C4A-NA-C1A	7.05	109.88	106.71
32	7	319	CHL	O2D-CGD-O1D	-7.03	110.09	123.84
31	7	310	CLA	CHC-C4B-NB	7.02	131.68	124.26
32	7	324	CHL	C4A-NA-C1A	7.00	109.85	106.71
36	8	303	LUT	C20-C13-C12	-6.99	107.07	118.08
31	A	848	CLA	C4A-NA-C1A	6.99	109.85	106.71
36	6	303	LUT	C38-C25-C24	-6.98	108.62	123.56
32	7	320	CHL	C4A-NA-C1A	6.97	109.84	106.71
31	A	847	CLA	C2B-C1B-NB	6.96	114.90	110.23
36	7	305	LUT	C39-C29-C28	-6.96	107.12	118.08
36	7	305	LUT	C19-C9-C10	-6.94	113.21	122.92
36	a	303	LUT	C35-C34-C33	-6.93	117.42	127.31
31	A	835	CLA	C2B-C1B-NB	6.93	114.88	110.23
32	7	319	CHL	O1D-CGD-CBD	-6.92	110.33	124.48
36	3	304	LUT	C38-C25-C24	-6.92	108.77	123.56
36	7	305	LUT	C20-C13-C12	-6.91	107.19	118.08
36	3	305	LUT	C8-C9-C10	-6.90	108.35	118.94
32	4	313	CHL	CHC-C4B-NB	6.90	131.56	124.26
36	9	302	LUT	C32-C33-C34	-6.89	108.37	118.94
31	3	314	CLA	C4A-NA-C1A	6.89	109.80	106.71
31	7	309	CLA	C4A-NA-C1A	6.84	109.78	106.71
36	6	304	LUT	C20-C13-C12	-6.83	107.31	118.08
32	a	320	CHL	O2D-CGD-CBD	6.83	123.40	111.27
31	6	310	CLA	CHC-C4B-NB	6.83	131.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	849	CLA	C2B-C1B-NB	6.82	114.80	110.23
31	A	817	CLA	C2B-C1B-NB	6.81	114.80	110.23
36	J	103	LUT	C40-C33-C32	-6.81	107.35	118.08
36	a	305	LUT	C32-C33-C34	-6.81	108.50	118.94
31	O	203	CLA	CHC-C4B-NB	6.79	131.45	124.26
36	9	303	LUT	C31-C32-C33	6.79	145.49	126.42
31	B	814	CLA	C2B-C1B-NB	6.79	114.78	110.23
36	L	304	LUT	C38-C25-C24	-6.78	109.05	123.56
31	5	310	CLA	O2D-CGD-CBD	6.78	123.31	111.27
31	B	829	CLA	CHC-C4B-NB	6.76	131.42	124.26
36	J	103	LUT	C38-C25-C24	-6.76	109.09	123.56
31	B	816	CLA	CHC-C4B-NB	6.76	131.41	124.26
36	4	302	LUT	C38-C25-C24	-6.74	109.14	123.56
31	9	311	CLA	C2B-C1B-NB	6.73	114.75	110.23
36	8	303	LUT	C11-C12-C13	6.72	145.30	126.42
36	9	303	LUT	C39-C29-C28	-6.71	107.50	118.08
36	3	304	LUT	C18-C5-C6	-6.71	116.99	124.53
36	3	305	LUT	C1-C6-C5	-6.71	113.16	122.61
31	4	315	CLA	C2B-C1B-NB	6.70	114.72	110.23
32	7	318	CHL	O2D-CGD-CBD	6.69	123.16	111.27
32	6	318	CHL	O2D-CGD-CBD	6.69	123.15	111.27
36	9	302	LUT	C8-C9-C10	-6.69	108.68	118.94
36	3	305	LUT	C11-C12-C13	6.68	145.18	126.42
36	8	302	LUT	C32-C33-C34	-6.68	108.69	118.94
36	9	305	LUT	C38-C25-C24	-6.68	109.28	123.56
31	5	307	CLA	C2B-C1B-NB	6.67	114.70	110.23
31	B	843	CLA	CHC-C4B-NB	6.67	131.31	124.26
31	b	313	CLA	C2B-C1B-NB	6.67	114.70	110.23
36	9	303	LUT	C40-C33-C32	-6.67	107.58	118.08
36	3	304	LUT	C7-C8-C9	-6.66	116.17	126.23
31	9	319	CLA	O2D-CGD-CBD	6.66	123.10	111.27
31	2	307	CLA	C2B-C1B-NB	6.65	114.69	110.23
36	J	103	LUT	C35-C34-C33	-6.65	117.82	127.31
36	8	303	LUT	C35-C34-C33	-6.64	117.83	127.31
31	6	307	CLA	C4A-NA-C1A	6.64	109.69	106.71
36	a	303	LUT	C20-C13-C12	-6.63	107.63	118.08
36	8	303	LUT	C8-C9-C10	-6.63	108.77	118.94
31	B	819	CLA	CHC-C4B-NB	6.61	131.26	124.26
31	G	204	CLA	C2B-C1B-NB	6.60	114.66	110.23
31	4	321	CLA	CHC-C4B-NB	6.60	131.24	124.26
31	B	844	CLA	C2B-C1B-NB	6.59	114.65	110.23
31	H	902	CLA	CHC-C4B-NB	6.59	131.23	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	818	CLA	C2B-C1B-NB	6.58	114.65	110.23
36	9	305	LUT	C8-C9-C10	-6.58	108.84	118.94
31	A	841	CLA	C2B-C1B-NB	6.57	114.64	110.23
32	8	319	CHL	O2D-CGD-CBD	6.57	122.94	111.27
32	9	322	CHL	C4A-NA-C1A	6.56	109.65	106.71
31	5	311	CLA	C2B-C1B-NB	6.55	114.62	110.23
36	2	301	LUT	C11-C12-C13	6.54	144.79	126.42
31	5	308	CLA	CHC-C4B-NB	6.53	131.17	124.26
31	9	315	CLA	CHC-C4B-NB	6.53	131.17	124.26
36	3	305	LUT	C20-C13-C12	-6.52	107.81	118.08
31	5	309	CLA	CHC-C4B-NB	6.52	131.16	124.26
36	4	303	LUT	C40-C33-C32	-6.51	107.81	118.08
36	3	305	LUT	C35-C34-C33	-6.51	118.02	127.31
36	8	302	LUT	C38-C25-C24	-6.51	109.64	123.56
36	9	302	LUT	C39-C29-C28	-6.51	107.83	118.08
31	6	313	CLA	CHC-C4B-NB	6.50	131.14	124.26
31	A	824	CLA	C2B-C1B-NB	6.50	114.59	110.23
30	A	813	CL0	C3C-C4C-NC	6.50	117.86	110.57
31	8	311	CLA	C2B-C1B-NB	6.50	114.59	110.23
31	A	819	CLA	C2B-C1B-NB	6.49	114.58	110.23
31	A	815	CLA	C2B-C1B-NB	6.48	114.58	110.23
31	8	308	CLA	C2B-C1B-NB	6.47	114.57	110.23
31	O	202	CLA	CHC-C4B-NB	6.47	131.11	124.26
31	5	313	CLA	CMD-C2D-C1D	6.47	136.12	124.71
31	a	310	CLA	CHC-C4B-NB	6.47	131.10	124.26
31	b	303	CLA	CHC-C4B-NB	6.46	131.10	124.26
36	8	302	LUT	C40-C33-C32	-6.46	107.90	118.08
31	B	836	CLA	C2B-C1B-NB	6.46	114.56	110.23
36	7	305	LUT	C8-C9-C10	-6.45	109.04	118.94
31	4	307	CLA	CHC-C4B-NB	6.45	131.09	124.26
32	5	319	CHL	CHC-C4B-NB	6.45	131.09	124.26
36	7	305	LUT	C18-C5-C6	-6.45	117.29	124.53
31	A	816	CLA	O2D-CGD-CBD	6.44	122.72	111.27
31	8	312	CLA	CHC-C4B-NB	6.44	131.07	124.26
31	7	313	CLA	CHC-C4B-NB	6.44	131.07	124.26
31	B	818	CLA	CHC-C4B-NB	6.44	131.07	124.26
31	2	307	CLA	CHC-C4B-NB	6.44	131.07	124.26
32	K	201	CHL	CHD-C1D-ND	-6.44	118.54	124.45
31	2	314	CLA	CHC-C4B-NB	6.43	131.07	124.26
31	K	205	CLA	C2B-C1B-NB	6.42	114.54	110.23
31	5	310	CLA	CHC-C4B-NB	6.42	131.05	124.26
36	5	303	LUT	C28-C29-C30	-6.41	109.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	315	CLA	C2B-C1B-NB	6.41	114.53	110.23
30	A	813	CL0	CMD-C2D-C1D	6.41	136.01	124.71
31	A	842	CLA	C2B-C1B-NB	6.40	114.52	110.23
32	5	322	CHL	CHC-C4B-NB	6.40	131.03	124.26
36	5	304	LUT	C40-C33-C32	-6.40	108.00	118.08
31	9	315	CLA	C2B-C1B-NB	6.40	114.52	110.23
31	2	315	CLA	CHC-C4B-NB	6.40	131.03	124.26
31	4	308	CLA	CHC-C4B-NB	6.39	131.03	124.26
31	3	309	CLA	C2B-C1B-NB	6.39	114.52	110.23
36	3	305	LUT	C39-C29-C28	-6.39	108.01	118.08
31	G	206	CLA	C2B-C1B-NB	6.39	114.51	110.23
31	b	305	CLA	C2B-C1B-NB	6.39	114.51	110.23
36	a	305	LUT	C28-C29-C30	-6.39	109.14	118.94
31	a	309	CLA	CHC-C4B-NB	6.39	131.02	124.26
31	7	316	CLA	CHC-C4B-NB	6.38	131.02	124.26
36	4	303	LUT	C35-C34-C33	-6.38	118.20	127.31
36	4	303	LUT	C39-C29-C28	-6.38	108.02	118.08
31	b	311	CLA	CHC-C4B-NB	6.38	131.01	124.26
31	A	834	CLA	C4A-NA-C1A	6.38	109.57	106.71
36	3	304	LUT	C20-C13-C12	-6.38	108.03	118.08
31	O	204	CLA	CHC-C4B-NB	6.36	130.99	124.26
31	b	302	CLA	CHC-C4B-NB	6.36	130.99	124.26
36	J	103	LUT	C20-C13-C12	-6.36	108.05	118.08
36	F	304	LUT	C39-C29-C28	-6.36	108.06	118.08
32	8	319	CHL	C4A-NA-C1A	6.36	109.56	106.71
36	6	303	LUT	C28-C29-C30	-6.36	109.19	118.94
31	F	301	CLA	C2B-C1B-NB	6.36	114.49	110.23
31	B	827	CLA	CHC-C4B-NB	6.36	130.99	124.26
31	5	318	CLA	C2B-C1B-NB	6.35	114.49	110.23
32	4	317	CHL	C4A-NA-C1A	6.35	109.56	106.71
31	B	813	CLA	C2B-C1B-NB	6.35	114.49	110.23
30	A	813	CL0	C3B-C4B-NB	6.34	116.40	110.52
36	8	302	LUT	C39-C29-C28	-6.34	108.08	118.08
31	4	306	CLA	C2B-C1B-NB	6.34	114.48	110.23
31	6	311	CLA	CHC-C4B-NB	6.32	130.94	124.26
31	F	305	CLA	CHC-C4B-NB	6.31	130.94	124.26
36	b	301	LUT	C8-C9-C10	-6.31	109.26	118.94
31	A	852	CLA	C2B-C1B-NB	6.31	114.46	110.23
31	4	315	CLA	CHC-C4B-NB	6.31	130.94	124.26
31	B	839	CLA	C2B-C1B-NB	6.31	114.46	110.23
31	4	308	CLA	C2B-C1B-NB	6.30	114.46	110.23
31	B	819	CLA	C2B-C1B-NB	6.29	114.45	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	321	CLA	C2B-C1B-NB	6.29	114.45	110.23
36	9	305	LUT	C19-C9-C8	-6.29	108.17	118.08
31	7	322	CLA	CHC-C4B-NB	6.29	130.91	124.26
36	J	103	LUT	C39-C29-C28	-6.28	108.18	118.08
31	a	313	CLA	C2B-C1B-NB	6.28	114.44	110.23
31	B	833	CLA	C2B-C1B-NB	6.27	114.44	110.23
36	5	303	LUT	C8-C9-C10	-6.27	109.32	118.94
31	3	311	CLA	CHC-C4B-NB	6.27	130.89	124.26
36	9	302	LUT	C12-C13-C14	-6.27	109.33	118.94
31	6	322	CLA	CHC-C4B-NB	6.25	130.88	124.26
31	3	311	CLA	C2B-C1B-NB	6.25	114.42	110.23
31	A	857	CLA	CHC-C4B-NB	6.24	130.87	124.26
31	A	849	CLA	C2B-C1B-NB	6.24	114.41	110.23
31	a	315	CLA	C2B-C1B-NB	6.24	114.41	110.23
31	L	306	CLA	O2D-CGD-CBD	6.24	122.35	111.27
31	a	310	CLA	C2B-C1B-NB	6.24	114.41	110.23
36	5	303	LUT	C39-C29-C28	-6.23	108.26	118.08
31	4	309	CLA	C2B-C1B-NB	6.23	114.41	110.23
36	7	305	LUT	C7-C8-C9	-6.23	116.82	126.23
31	A	830	CLA	CHC-C4B-NB	6.23	130.85	124.26
31	5	307	CLA	O2D-CGD-CBD	6.23	122.34	111.27
32	5	316	CHL	O2D-CGD-CBD	6.23	122.34	111.27
31	4	306	CLA	CHC-C4B-NB	6.23	130.85	124.26
32	A	831	CHL	C4A-NA-C1A	6.23	109.50	106.71
32	5	319	CHL	C4A-NA-C1A	6.23	109.50	106.71
31	B	841	CLA	C2B-C1B-NB	6.22	114.40	110.23
31	A	823	CLA	C2B-C1B-NB	6.22	114.40	110.23
31	6	322	CLA	C2B-C1B-NB	6.22	114.40	110.23
31	6	312	CLA	C2B-C1B-NB	6.21	114.39	110.23
31	5	311	CLA	CHC-C4B-NB	6.21	130.83	124.26
31	4	314	CLA	C4D-CHA-C1A	-6.20	113.70	121.25
31	B	848	CLA	C2B-C1B-NB	6.20	114.39	110.23
31	A	828	CLA	C2B-C1B-NB	6.20	114.39	110.23
36	a	305	LUT	C38-C25-C24	-6.20	110.30	123.56
31	A	847	CLA	O2D-CGD-CBD	6.19	122.28	111.27
31	a	316	CLA	C2B-C1B-NB	6.19	114.38	110.23
32	9	320	CHL	C2B-C1B-NB	6.19	114.38	110.23
31	5	323	CLA	CHC-C4B-NB	6.19	130.81	124.26
31	b	310	CLA	C2B-C1B-NB	6.19	114.38	110.23
31	3	319	CLA	C4A-NA-C1A	6.19	109.49	106.71
36	L	304	LUT	C12-C13-C14	-6.19	109.45	118.94
36	6	304	LUT	C39-C29-C28	-6.18	108.34	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	307	CLA	C2B-C1B-NB	6.18	114.38	110.23
31	3	319	CLA	C2B-C1B-NB	6.18	114.37	110.23
31	9	318	CLA	CHC-C4B-NB	6.17	130.79	124.26
31	A	821	CLA	C2B-C1B-NB	6.17	114.37	110.23
31	b	313	CLA	C4A-NA-C1A	6.17	109.48	106.71
36	a	303	LUT	C39-C29-C28	-6.16	108.36	118.08
36	9	303	LUT	C19-C9-C8	-6.16	108.37	118.08
31	4	321	CLA	C2B-C1B-NB	6.16	114.36	110.23
31	O	203	CLA	C2B-C1B-NB	6.16	114.36	110.23
31	A	820	CLA	CHC-C4B-NB	6.15	130.77	124.26
31	2	309	CLA	C2B-C1B-NB	6.15	114.36	110.23
31	a	321	CLA	C2B-C1B-NB	6.15	114.35	110.23
31	3	313	CLA	O2D-CGD-CBD	6.15	122.19	111.27
31	5	315	CLA	CHC-C4B-NB	6.15	130.76	124.26
36	b	301	LUT	C28-C29-C30	-6.15	109.51	118.94
31	7	313	CLA	C2B-C1B-NB	6.13	114.34	110.23
31	6	313	CLA	C2B-C1B-NB	6.13	114.34	110.23
36	F	304	LUT	C38-C25-C24	-6.13	110.44	123.56
31	B	817	CLA	C2B-C1B-NB	6.13	114.34	110.23
31	8	317	CLA	C2B-C1B-NB	6.13	114.34	110.23
36	J	103	LUT	C32-C33-C34	-6.13	109.53	118.94
32	7	318	CHL	CHC-C4B-NB	6.13	130.75	124.26
31	B	844	CLA	CHC-C4B-NB	6.13	130.74	124.26
31	B	829	CLA	C2B-C1B-NB	6.13	114.34	110.23
31	J	105	CLA	CHC-C4B-NB	6.12	130.74	124.26
31	3	316	CLA	C2B-C1B-NB	6.12	114.33	110.23
31	A	830	CLA	C2B-C1B-NB	6.11	114.33	110.23
36	F	304	LUT	C28-C29-C30	-6.11	109.57	118.94
31	6	314	CLA	CHC-C4B-NB	6.10	130.72	124.26
31	4	311	CLA	CHC-C4B-NB	6.10	130.72	124.26
32	a	317	CHL	CHC-C4B-NB	6.10	130.72	124.26
31	A	844	CLA	C2B-C1B-NB	6.10	114.32	110.23
31	F	305	CLA	C2B-C1B-NB	6.10	114.32	110.23
31	a	309	CLA	C2B-C1B-NB	6.10	114.32	110.23
32	6	318	CHL	CHC-C4B-NB	6.10	130.71	124.26
31	b	304	CLA	C2B-C1B-NB	6.09	114.32	110.23
31	9	313	CLA	CHC-C4B-NB	6.09	130.71	124.26
31	8	318	CLA	C2B-C1B-NB	6.09	114.31	110.23
31	B	815	CLA	CHC-C4B-NB	6.09	130.70	124.26
36	5	304	LUT	C20-C13-C12	-6.08	108.49	118.08
31	A	845	CLA	CHC-C4B-NB	6.08	130.70	124.26
36	9	305	LUT	C20-C13-C12	-6.08	108.49	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	9	302	LUT	C20-C13-C12	-6.08	108.50	118.08
31	L	307	CLA	CHC-C4B-NB	6.08	130.69	124.26
31	b	308	CLA	CHC-C4B-NB	6.08	130.69	124.26
36	5	304	LUT	C8-C9-C10	-6.07	109.62	118.94
31	9	319	CLA	CHC-C4B-NB	6.07	130.69	124.26
31	9	313	CLA	C2B-C1B-NB	6.07	114.30	110.23
31	B	838	CLA	CHC-C4B-NB	6.07	130.68	124.26
32	7	317	CHL	C4A-NA-C1A	6.07	109.43	106.71
31	b	312	CLA	CHC-C4B-NB	6.07	130.68	124.26
31	a	319	CLA	CHC-C4B-NB	6.07	130.68	124.26
31	3	316	CLA	CHC-C4B-NB	6.07	130.68	124.26
31	9	312	CLA	C2B-C1B-NB	6.07	114.30	110.23
31	8	321	CLA	C2B-C1B-NB	6.06	114.30	110.23
31	5	321	CLA	CHC-C4B-NB	6.06	130.68	124.26
31	A	854	CLA	C2B-C1B-NB	6.06	114.30	110.23
31	3	310	CLA	C2B-C1B-NB	6.06	114.29	110.23
36	5	304	LUT	C39-C29-C28	-6.06	108.54	118.08
36	2	301	LUT	C35-C34-C33	-6.06	118.67	127.31
31	B	850	CLA	C2B-C1B-NB	6.05	114.29	110.23
31	3	317	CLA	C2B-C1B-NB	6.05	114.29	110.23
31	2	308	CLA	O2D-CGD-CBD	6.05	122.02	111.27
31	L	306	CLA	C2B-C1B-NB	6.05	114.29	110.23
31	B	834	CLA	C2D-C1D-ND	6.05	114.56	110.10
36	6	304	LUT	C40-C33-C32	-6.04	108.56	118.08
31	B	823	CLA	CHC-C4B-NB	6.04	130.65	124.26
36	a	305	LUT	C40-C33-C32	-6.04	108.56	118.08
31	A	841	CLA	CHC-C4B-NB	6.04	130.65	124.26
31	4	319	CLA	CHC-C4B-NB	6.04	130.65	124.26
31	A	847	CLA	CHC-C4B-NB	6.03	130.64	124.26
31	8	314	CLA	CHC-C4B-NB	6.03	130.64	124.26
31	B	827	CLA	C2B-C1B-NB	6.02	114.27	110.23
31	a	322	CLA	C2B-C1B-NB	6.02	114.27	110.23
31	5	320	CLA	CHC-C4B-NB	6.02	130.63	124.26
31	b	302	CLA	C2B-C1B-NB	6.02	114.27	110.23
31	a	316	CLA	CHC-C4B-NB	6.02	130.63	124.26
32	a	320	CHL	CHC-C4B-NB	6.02	130.63	124.26
31	5	318	CLA	C4A-NA-C1A	6.02	109.41	106.71
31	8	307	CLA	CHC-C4B-NB	6.02	130.63	124.26
31	A	854	CLA	CHC-C4B-NB	6.01	130.62	124.26
31	5	314	CLA	CHC-C4B-NB	6.01	130.62	124.26
31	B	824	CLA	CHC-C4B-NB	6.01	130.62	124.26
31	A	837	CLA	CHC-C4B-NB	6.01	130.62	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	312	CLA	C2B-C1B-NB	6.00	114.26	110.23
31	8	307	CLA	C2B-C1B-NB	6.00	114.25	110.23
31	2	304	CLA	C2B-C1B-NB	6.00	114.25	110.23
31	6	315	CLA	CHC-C4B-NB	6.00	130.60	124.26
31	7	314	CLA	CHC-C4B-NB	6.00	130.60	124.26
31	2	306	CLA	CHC-C4B-NB	5.99	130.60	124.26
31	A	844	CLA	CHC-C4B-NB	5.99	130.60	124.26
31	6	307	CLA	C2B-C1B-NB	5.99	114.25	110.23
31	7	315	CLA	C2B-C1B-NB	5.99	114.25	110.23
31	A	834	CLA	C2B-C1B-NB	5.99	114.25	110.23
31	A	850	CLA	C2B-C1B-NB	5.99	114.25	110.23
31	A	827	CLA	C2B-C1B-NB	5.98	114.24	110.23
31	B	811	CLA	C2B-C1B-NB	5.98	114.24	110.23
31	9	311	CLA	O2D-CGD-CBD	5.98	121.90	111.27
32	7	319	CHL	C2B-C1B-NB	5.98	114.24	110.23
31	2	306	CLA	C4A-NA-C1A	5.98	109.39	106.71
31	5	312	CLA	C2B-C1B-NB	5.98	114.24	110.23
32	b	309	CHL	CHC-C4B-NB	5.98	130.59	124.26
36	L	304	LUT	C32-C33-C34	-5.98	109.77	118.94
31	B	838	CLA	C2B-C1B-NB	5.98	114.24	110.23
31	B	834	CLA	C2B-C1B-NB	5.97	114.24	110.23
31	a	314	CLA	CHC-C4B-NB	5.97	130.58	124.26
31	H	901	CLA	CHC-C4B-NB	5.97	130.57	124.26
31	B	824	CLA	C2B-C1B-NB	5.96	114.23	110.23
31	9	316	CLA	C2B-C1B-NB	5.96	114.23	110.23
36	a	305	LUT	C12-C13-C14	-5.96	109.80	118.94
32	A	831	CHL	O2D-CGD-CBD	5.96	121.85	111.27
31	A	851	CLA	CHC-C4B-NB	5.95	130.56	124.26
36	3	304	LUT	C39-C29-C28	-5.95	108.70	118.08
31	B	815	CLA	C2B-C1B-NB	5.95	114.22	110.23
31	b	305	CLA	C4A-NA-C1A	5.95	109.38	106.71
31	a	311	CLA	O2D-CGD-CBD	5.95	121.84	111.27
31	B	835	CLA	CHC-C4B-NB	5.95	130.55	124.26
32	3	315	CHL	C4A-NA-C1A	5.94	109.38	106.71
36	4	302	LUT	C20-C13-C12	-5.94	108.72	118.08
31	7	314	CLA	O2D-CGD-CBD	5.94	121.82	111.27
31	7	309	CLA	C2B-C1B-NB	5.94	114.21	110.23
31	9	311	CLA	CHC-C4B-NB	5.94	130.54	124.26
36	6	304	LUT	C32-C33-C34	-5.94	109.83	118.94
31	B	831	CLA	CHC-C4B-NB	5.93	130.54	124.26
31	a	311	CLA	CHC-C4B-NB	5.93	130.54	124.26
31	A	822	CLA	C2B-C1B-NB	5.93	114.20	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	8	303	LUT	C1-C6-C5	-5.92	114.28	122.61
31	2	310	CLA	CHC-C4B-NB	5.92	130.52	124.26
31	8	317	CLA	CHD-C1D-ND	-5.92	119.02	124.45
31	G	205	CLA	C2B-C1B-NB	5.91	114.20	110.23
32	8	316	CHL	C4A-NA-C1A	5.91	109.36	106.71
31	2	308	CLA	C2B-C1B-NB	5.91	114.19	110.23
31	A	828	CLA	O2D-CGD-CBD	5.91	121.77	111.27
31	3	320	CLA	O2D-CGD-CBD	5.91	121.77	111.27
31	2	304	CLA	CHC-C4B-NB	5.90	130.50	124.26
31	4	314	CLA	C2B-C1B-NB	5.89	114.18	110.23
31	2	314	CLA	C2B-C1B-NB	5.89	114.18	110.23
31	8	309	CLA	C2B-C1B-NB	5.89	114.18	110.23
31	A	846	CLA	CHC-C4B-NB	5.89	130.49	124.26
31	B	842	CLA	C2B-C1B-NB	5.88	114.18	110.23
31	b	306	CLA	C2B-C1B-NB	5.88	114.18	110.23
31	a	322	CLA	CHC-C4B-NB	5.88	130.48	124.26
31	3	312	CLA	CHC-C4B-NB	5.87	130.48	124.26
31	4	320	CLA	CHC-C4B-NB	5.87	130.48	124.26
31	3	318	CLA	CHC-C4B-NB	5.87	130.47	124.26
36	4	302	LUT	C8-C9-C10	-5.87	109.94	118.94
31	4	316	CLA	C2D-C1D-ND	-5.87	105.78	110.10
31	A	838	CLA	CHC-C4B-NB	5.86	130.46	124.26
32	5	316	CHL	C2B-C1B-NB	5.86	114.16	110.23
31	K	204	CLA	CHC-C4B-NB	5.86	130.46	124.26
31	6	312	CLA	CHC-C4B-NB	5.86	130.46	124.26
31	8	310	CLA	C2B-C1B-NB	5.86	114.16	110.23
32	5	316	CHL	O2D-CGD-O1D	-5.85	112.39	123.84
31	2	313	CLA	C2B-C1B-NB	5.85	114.16	110.23
31	H	902	CLA	C2B-C1B-NB	5.85	114.15	110.23
31	2	306	CLA	C2B-C1B-NB	5.85	114.15	110.23
31	5	315	CLA	C2B-C1B-NB	5.85	114.15	110.23
31	8	314	CLA	C2B-C1B-NB	5.84	114.15	110.23
31	L	305	CLA	C2D-C1D-ND	5.84	114.41	110.10
31	B	832	CLA	CHC-C4B-NB	5.84	130.44	124.26
32	5	319	CHL	O2D-CGD-CBD	5.84	121.64	111.27
31	2	310	CLA	C2B-C1B-NB	5.84	114.15	110.23
31	4	309	CLA	CHC-C4B-NB	5.83	130.43	124.26
31	B	825	CLA	C2B-C1B-NB	5.83	114.14	110.23
31	A	826	CLA	C2B-C1B-NB	5.83	114.14	110.23
31	3	309	CLA	CHC-C4B-NB	5.83	130.43	124.26
31	6	307	CLA	CHC-C4B-NB	5.83	130.43	124.26
31	9	314	CLA	CHC-C4B-NB	5.83	130.43	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	308	CLA	C2B-C1B-NB	5.83	114.14	110.23
36	J	103	LUT	C19-C9-C8	-5.83	108.90	118.08
31	6	313	CLA	O2D-CGD-CBD	5.82	121.62	111.27
36	8	303	LUT	C28-C29-C30	-5.82	110.00	118.94
31	A	845	CLA	C2B-C1B-NB	5.82	114.13	110.23
31	A	853	CLA	C2B-C1B-NB	5.82	114.13	110.23
31	b	310	CLA	CHC-C4B-NB	5.82	130.42	124.26
31	3	308	CLA	CHC-C4B-NB	5.82	130.41	124.26
31	K	206	CLA	CHC-C4B-NB	5.81	130.41	124.26
31	5	314	CLA	C2B-C1B-NB	5.81	114.13	110.23
31	O	202	CLA	C2B-C1B-NB	5.81	114.12	110.23
31	b	312	CLA	C2B-C1B-NB	5.81	114.12	110.23
32	5	317	CHL	C2B-C1B-NB	5.80	114.12	110.23
31	O	203	CLA	O2D-CGD-CBD	5.80	121.57	111.27
36	L	304	LUT	C39-C29-C28	-5.80	108.95	118.08
31	A	824	CLA	O2D-CGD-CBD	5.79	121.56	111.27
31	8	313	CLA	CHC-C4B-NB	5.79	130.39	124.26
31	b	311	CLA	C2B-C1B-NB	5.79	114.11	110.23
31	4	307	CLA	C2B-C1B-NB	5.79	114.11	110.23
32	5	322	CHL	C4A-NA-C1A	5.79	109.31	106.71
36	a	303	LUT	C28-C29-C30	-5.79	110.06	118.94
31	A	837	CLA	C2B-C1B-NB	5.79	114.11	110.23
31	A	820	CLA	C2B-C1B-NB	5.79	114.11	110.23
31	A	825	CLA	C2B-C1B-NB	5.79	114.11	110.23
36	6	303	LUT	C8-C9-C10	-5.78	110.06	118.94
31	A	815	CLA	C2D-C1D-ND	5.78	114.37	110.10
32	A	839	CHL	C2B-C1B-NB	5.78	114.11	110.23
31	A	842	CLA	CHC-C4B-NB	5.78	130.38	124.26
31	B	821	CLA	C2B-C1B-NB	5.78	114.11	110.23
32	4	310	CHL	CHC-C4B-NB	5.78	130.37	124.26
32	3	315	CHL	CHC-C4B-NB	5.78	130.37	124.26
31	B	846	CLA	CHC-C4B-NB	5.77	130.37	124.26
31	5	307	CLA	CHC-C4B-NB	5.77	130.37	124.26
31	4	318	CLA	C2B-C1B-NB	5.77	114.10	110.23
31	5	318	CLA	CHC-C4B-NB	5.77	130.37	124.26
32	b	309	CHL	C4A-NA-C1A	5.77	109.30	106.71
31	2	309	CLA	CHC-C4B-NB	5.77	130.36	124.26
31	9	314	CLA	C2B-C1B-NB	5.77	114.10	110.23
31	8	320	CLA	CHC-C4B-NB	5.77	130.36	124.26
31	4	312	CLA	CHC-C4B-NB	5.76	130.36	124.26
31	4	318	CLA	CHC-C4B-NB	5.76	130.36	124.26
31	6	307	CLA	O2D-CGD-CBD	5.76	121.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	305	CLA	C3D-C4D-ND	5.76	119.55	110.24
32	5	317	CHL	C4A-NA-C1A	5.76	109.30	106.71
31	B	840	CLA	C2B-C1B-NB	5.76	114.09	110.23
31	4	312	CLA	C2B-C1B-NB	5.76	114.09	110.23
31	b	311	CLA	O2D-CGD-CBD	5.76	121.50	111.27
31	3	309	CLA	O2D-CGD-CBD	5.75	121.49	111.27
31	A	814	CLA	C2B-C1B-NB	5.75	114.09	110.23
31	A	829	CLA	C1C-C2C-C3C	-5.74	100.92	106.96
31	3	317	CLA	CHC-C4B-NB	5.74	130.34	124.26
32	a	320	CHL	C4A-NA-C1A	5.74	109.29	106.71
32	4	313	CHL	C4A-NA-C1A	5.74	109.29	106.71
32	6	320	CHL	CHC-C4B-NB	5.74	130.33	124.26
31	B	832	CLA	C2B-C1B-NB	5.74	114.08	110.23
31	2	305	CLA	C2B-C1B-NB	5.74	114.08	110.23
31	4	311	CLA	C2B-C1B-NB	5.74	114.08	110.23
32	6	320	CHL	C2B-C1B-NB	5.74	114.08	110.23
31	9	316	CLA	CHC-C4B-NB	5.74	130.33	124.26
32	3	315	CHL	O2D-CGD-CBD	5.74	121.46	111.27
31	4	320	CLA	C2B-C1B-NB	5.73	114.08	110.23
31	7	321	CLA	CHC-C4B-NB	5.73	130.32	124.26
31	a	312	CLA	CHC-C4B-NB	5.73	130.32	124.26
31	a	321	CLA	CHC-C4B-NB	5.73	130.32	124.26
31	A	828	CLA	CHC-C4B-NB	5.73	130.32	124.26
32	6	318	CHL	C2B-C1B-NB	5.72	114.07	110.23
31	B	837	CLA	O2D-CGD-CBD	5.72	121.43	111.27
31	A	824	CLA	CHC-C4B-NB	5.72	130.31	124.26
31	H	901	CLA	C2B-C1B-NB	5.71	114.06	110.23
31	5	312	CLA	CHC-C4B-NB	5.71	130.30	124.26
31	A	825	CLA	CHC-C4B-NB	5.71	130.30	124.26
31	A	848	CLA	CHC-C4B-NB	5.71	130.30	124.26
31	5	308	CLA	C2B-C1B-NB	5.71	114.06	110.23
31	B	822	CLA	C2B-C1B-NB	5.71	114.06	110.23
31	3	313	CLA	CHC-C4B-NB	5.70	130.29	124.26
36	5	303	LUT	C32-C33-C34	-5.70	110.19	118.94
31	B	821	CLA	CHC-C4B-NB	5.70	130.29	124.26
36	5	304	LUT	C28-C29-C30	-5.70	110.19	118.94
31	4	305	CLA	C3B-C2B-C1B	-5.70	100.28	107.16
31	b	308	CLA	C2B-C1B-NB	5.70	114.05	110.23
32	7	320	CHL	CHC-C4B-NB	5.69	130.29	124.26
36	2	301	LUT	C40-C33-C32	-5.69	109.11	118.08
31	9	319	CLA	C2B-C1B-NB	5.69	114.05	110.23
31	4	305	CLA	CHD-C4C-C3C	-5.69	116.47	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	313	CLA	CHC-C4B-NB	5.69	130.28	124.26
32	4	317	CHL	CHC-C4B-NB	5.69	130.28	124.26
36	4	302	LUT	C32-C33-C34	-5.69	110.21	118.94
31	A	848	CLA	C2B-C1B-NB	5.69	114.05	110.23
31	3	318	CLA	O2D-CGD-CBD	5.69	121.37	111.27
31	b	303	CLA	C2B-C1B-NB	5.68	114.04	110.23
31	5	321	CLA	C2B-C1B-NB	5.68	114.04	110.23
31	6	311	CLA	C2B-C1B-NB	5.68	114.04	110.23
32	9	322	CHL	O2D-CGD-CBD	5.68	121.36	111.27
31	A	835	CLA	CHC-C4B-NB	5.67	130.26	124.26
31	H	903	CLA	CHC-C4B-NB	5.67	130.26	124.26
31	B	845	CLA	C2C-C1C-NC	5.67	115.28	109.97
32	A	839	CHL	O2D-CGD-CBD	5.67	121.34	111.27
31	3	318	CLA	C2B-C1B-NB	5.67	114.03	110.23
31	2	311	CLA	C2B-C1B-NB	5.67	114.03	110.23
31	A	833	CLA	CHC-C4B-NB	5.66	130.25	124.26
32	7	324	CHL	C2B-C1B-NB	5.66	114.03	110.23
31	B	826	CLA	C2B-C1B-NB	5.66	114.03	110.23
31	3	313	CLA	C2B-C1B-NB	5.66	114.03	110.23
31	K	204	CLA	C2B-C1B-NB	5.66	114.03	110.23
31	9	317	CLA	C2B-C1B-NB	5.66	114.02	110.23
31	9	321	CLA	C2B-C1B-NB	5.66	114.02	110.23
31	3	314	CLA	C2B-C1B-NB	5.65	114.02	110.23
31	4	305	CLA	C2D-C1D-ND	5.65	114.27	110.10
31	A	843	CLA	O2D-CGD-CBD	5.65	121.31	111.27
31	b	303	CLA	O2D-CGD-CBD	5.65	121.31	111.27
31	B	820	CLA	C2B-C1B-NB	5.65	114.02	110.23
31	4	305	CLA	O2D-CGD-CBD	5.65	121.30	111.27
31	L	305	CLA	C2B-C1B-NB	5.65	114.02	110.23
31	8	318	CLA	CHC-C4B-NB	5.65	130.23	124.26
31	B	831	CLA	C2B-C1B-NB	5.64	114.02	110.23
36	8	303	LUT	C32-C33-C34	-5.64	110.29	118.94
31	B	845	CLA	C2B-C1B-NB	5.64	114.01	110.23
31	b	306	CLA	CHC-C4B-NB	5.64	130.22	124.26
31	6	315	CLA	C2B-C1B-NB	5.63	114.01	110.23
31	2	312	CLA	C2B-C1B-NB	5.63	114.01	110.23
31	9	312	CLA	CHC-C4B-NB	5.63	130.22	124.26
31	3	308	CLA	C2B-C1B-NB	5.63	114.00	110.23
31	A	819	CLA	O2D-CGD-CBD	5.63	121.26	111.27
31	6	316	CLA	C2B-C1B-NB	5.63	114.00	110.23
32	K	201	CHL	O2D-CGD-CBD	5.62	121.26	111.27
31	A	838	CLA	O2D-CGD-CBD	5.62	121.26	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	814	CLA	CHC-C4B-NB	5.62	130.21	124.26
32	6	317	CHL	C2B-C1B-NB	5.62	114.00	110.23
31	2	312	CLA	CHC-C4B-NB	5.62	130.20	124.26
32	K	201	CHL	C3B-C2B-C1B	-5.62	100.38	107.16
31	b	305	CLA	CHC-C4B-NB	5.61	130.20	124.26
32	7	318	CHL	C4A-NA-C1A	5.61	109.23	106.71
32	A	831	CHL	CHC-C4B-NB	5.61	130.20	124.26
31	B	835	CLA	C2B-C1B-NB	5.61	113.99	110.23
31	A	836	CLA	C2B-C1B-NB	5.61	113.99	110.23
36	8	303	LUT	C39-C29-C28	-5.61	109.24	118.08
32	4	310	CHL	O2D-CGD-O1D	-5.60	112.88	123.84
31	2	311	CLA	CHC-C4B-NB	5.60	130.19	124.26
32	A	840	CHL	CHC-C4B-NB	5.60	130.18	124.26
31	G	204	CLA	CHC-C4B-NB	5.59	130.18	124.26
31	5	321	CLA	C4D-CHA-C1A	-5.59	114.45	121.25
31	5	310	CLA	C2B-C1B-NB	5.59	113.98	110.23
31	7	316	CLA	C2B-C1B-NB	5.59	113.98	110.23
32	6	309	CHL	C4A-NA-C1A	5.59	109.22	106.71
30	A	813	CL0	CHD-C4C-C3C	-5.58	116.63	124.84
31	a	315	CLA	O2D-CGD-O1D	-5.58	112.92	123.84
31	8	313	CLA	C2B-C1B-NB	5.58	113.97	110.23
32	6	321	CHL	CHC-C4B-NB	5.58	130.16	124.26
36	F	304	LUT	C7-C8-C9	-5.58	117.80	126.23
31	A	852	CLA	CHC-C4B-NB	5.57	130.16	124.26
31	A	838	CLA	C2B-C1B-NB	5.57	113.97	110.23
31	a	316	CLA	C4A-NA-C1A	5.57	109.21	106.71
31	B	837	CLA	CHC-C4B-NB	5.57	130.15	124.26
36	8	302	LUT	C28-C29-C30	-5.57	110.39	118.94
31	A	843	CLA	CHC-C4B-NB	5.57	130.15	124.26
31	B	811	CLA	CHC-C4B-NB	5.57	130.15	124.26
31	K	205	CLA	CHC-C4B-NB	5.57	130.15	124.26
36	6	303	LUT	C40-C33-C32	-5.57	109.31	118.08
36	2	301	LUT	C19-C9-C8	-5.57	109.31	118.08
31	A	832	CLA	C2B-C1B-NB	5.57	113.96	110.23
31	a	315	CLA	CHC-C4B-NB	5.56	130.15	124.26
31	B	818	CLA	C2C-C1C-NC	5.56	115.18	109.97
31	G	205	CLA	CHC-C4B-NB	5.56	130.14	124.26
31	F	306	CLA	CHC-C4B-NB	5.56	130.14	124.26
31	F	305	CLA	O2D-CGD-CBD	5.56	121.14	111.27
31	3	317	CLA	O2D-CGD-CBD	5.56	121.14	111.27
31	B	846	CLA	C2B-C1B-NB	5.55	113.96	110.23
32	6	321	CHL	C4A-NA-C1A	5.55	109.20	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	3	305	LUT	C4-C5-C6	-5.55	108.48	120.85
31	a	313	CLA	CHC-C4B-NB	5.55	130.13	124.26
31	3	319	CLA	CHD-C1D-ND	-5.55	119.36	124.45
32	a	317	CHL	C4A-NA-C1A	5.55	109.20	106.71
31	3	320	CLA	C2B-C1B-NB	5.54	113.95	110.23
31	7	310	CLA	C2B-C1B-NB	5.54	113.95	110.23
31	G	206	CLA	CHC-C4B-NB	5.54	130.12	124.26
32	6	321	CHL	O2D-CGD-CBD	5.54	121.11	111.27
32	7	319	CHL	C4A-NA-C1A	5.54	109.19	106.71
31	A	850	CLA	CHC-C4B-NB	5.53	130.11	124.26
31	B	842	CLA	CHC-C4B-NB	5.53	130.11	124.26
31	5	320	CLA	C2B-C1B-NB	5.53	113.94	110.23
30	A	813	CL0	C3D-C4D-ND	5.52	119.17	110.24
31	b	307	CLA	CHC-C4B-NB	5.52	130.10	124.26
31	2	306	CLA	O2D-CGD-CBD	5.52	121.08	111.27
31	F	306	CLA	C2B-C1B-NB	5.51	113.93	110.23
31	4	316	CLA	C2B-C1B-NB	5.51	113.93	110.23
31	B	826	CLA	CHC-C4B-NB	5.51	130.09	124.26
31	6	316	CLA	CHC-C4B-NB	5.51	130.09	124.26
32	6	319	CHL	C2B-C1B-NB	5.50	113.92	110.23
36	6	304	LUT	C28-C29-C30	-5.50	110.50	118.94
36	F	304	LUT	C40-C33-C32	-5.50	109.41	118.08
32	6	319	CHL	C4A-NA-C1A	5.50	109.18	106.71
31	B	830	CLA	C2B-C1B-NB	5.50	113.92	110.23
31	A	819	CLA	CHC-C4B-NB	5.49	130.07	124.26
31	8	315	CLA	CHC-C4B-NB	5.49	130.07	124.26
31	5	309	CLA	C2B-C1B-NB	5.49	113.91	110.23
31	8	312	CLA	C2B-C1B-NB	5.49	113.91	110.23
31	6	308	CLA	CHC-C4B-NB	5.49	130.06	124.26
36	4	303	LUT	C32-C33-C34	-5.48	110.53	118.94
31	a	319	CLA	O2D-CGD-CBD	5.48	121.01	111.27
30	A	813	CL0	C1C-C2C-C3C	-5.48	101.20	106.96
31	J	105	CLA	C2B-C1B-NB	5.48	113.91	110.23
31	O	204	CLA	C2B-C1B-NB	5.48	113.90	110.23
31	A	846	CLA	C2B-C1B-NB	5.47	113.90	110.23
31	2	308	CLA	CHC-C4B-NB	5.47	130.05	124.26
30	A	813	CL0	C3B-C2B-C1B	-5.47	100.56	107.16
32	9	322	CHL	CHC-C4B-NB	5.47	130.04	124.26
31	B	816	CLA	O2D-CGD-CBD	5.47	120.98	111.27
31	B	817	CLA	CHC-C4B-NB	5.46	130.04	124.26
32	6	319	CHL	CHC-C4B-NB	5.46	130.04	124.26
31	8	310	CLA	CHC-C4B-NB	5.46	130.04	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	2	301	LUT	C39-C29-C28	-5.46	109.47	118.08
31	A	849	CLA	CHC-C4B-NB	5.46	130.04	124.26
32	7	324	CHL	CHC-C4B-NB	5.46	130.04	124.26
31	4	316	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	6	314	CLA	C2B-C1B-NB	5.46	113.89	110.23
31	b	307	CLA	C2B-C1B-NB	5.46	113.89	110.23
31	7	310	CLA	C1C-C2C-C3C	-5.46	102.07	107.07
32	a	318	CHL	C2B-C1B-NB	5.46	113.89	110.23
32	4	310	CHL	O2D-CGD-CBD	5.45	120.96	111.27
31	B	822	CLA	CHC-C4B-NB	5.45	130.03	124.26
31	2	305	CLA	CHC-C4B-NB	5.45	130.03	124.26
31	A	833	CLA	C2B-C1B-NB	5.45	113.88	110.23
31	7	314	CLA	C2B-C1B-NB	5.45	113.88	110.23
32	7	317	CHL	CHC-C4B-NB	5.45	130.02	124.26
30	A	813	CL0	C2D-C1D-ND	5.44	114.12	110.10
36	9	303	LUT	C4-C5-C6	-5.44	108.72	120.85
31	B	827	CLA	CHD-C1D-ND	-5.44	119.45	124.45
36	9	305	LUT	C28-C29-C30	-5.44	110.59	118.94
31	6	316	CLA	O2D-CGD-CBD	5.44	120.93	111.27
36	9	303	LUT	C35-C34-C33	-5.44	119.55	127.31
31	3	312	CLA	C2B-C1B-NB	5.44	113.88	110.23
31	a	322	CLA	O2D-CGD-CBD	5.44	120.93	111.27
31	B	843	CLA	C2B-C1B-NB	5.43	113.88	110.23
31	8	311	CLA	CHC-C4B-NB	5.43	130.00	124.26
31	B	848	CLA	CHD-C1D-ND	-5.43	119.47	124.45
32	8	316	CHL	O2D-CGD-CBD	5.42	120.91	111.27
36	b	301	LUT	C19-C9-C8	-5.42	109.53	118.08
31	5	315	CLA	O2D-CGD-CBD	5.42	120.90	111.27
31	4	319	CLA	C2B-C1B-NB	5.42	113.86	110.23
31	a	321	CLA	CHD-C1D-ND	-5.42	119.47	124.45
32	6	317	CHL	CHC-C4B-NB	5.42	129.99	124.26
31	5	307	CLA	C4A-NA-C1A	5.42	109.14	106.71
31	a	312	CLA	C2B-C1B-NB	5.41	113.86	110.23
31	4	305	CLA	C4D-CHA-C1A	-5.41	114.66	121.25
31	9	311	CLA	C4A-NA-C1A	5.41	109.14	106.71
31	2	313	CLA	CHC-C4B-NB	5.41	129.99	124.26
31	5	323	CLA	C2B-C1B-NB	5.41	113.86	110.23
32	3	315	CHL	C2B-C1B-NB	5.41	113.86	110.23
32	8	319	CHL	CHC-C4B-NB	5.41	129.99	124.26
31	L	306	CLA	CHC-C4B-NB	5.41	129.98	124.26
31	A	856	CLA	CHD-C1D-ND	-5.41	119.48	124.45
31	A	836	CLA	CHC-C4B-NB	5.40	129.98	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	823	CLA	C2B-C1B-NB	5.40	113.85	110.23
31	8	312	CLA	O2D-CGD-CBD	5.40	120.86	111.27
36	9	303	LUT	C32-C33-C34	-5.40	110.66	118.94
31	B	843	CLA	C2C-C1C-NC	5.40	115.03	109.97
31	a	319	CLA	C2B-C1B-NB	5.40	113.85	110.23
31	B	819	CLA	C2C-C1C-NC	5.40	115.03	109.97
31	b	304	CLA	CHC-C4B-NB	5.39	129.97	124.26
32	6	309	CHL	CHC-C4B-NB	5.39	129.97	124.26
31	6	314	CLA	O2D-CGD-CBD	5.39	120.85	111.27
31	B	825	CLA	CHC-C4B-NB	5.39	129.96	124.26
31	7	315	CLA	O2D-CGD-CBD	5.39	120.84	111.27
31	4	314	CLA	CHC-C4B-NB	5.38	129.96	124.26
31	B	832	CLA	C2C-C1C-NC	5.38	115.01	109.97
31	3	307	CLA	CHC-C4B-NB	5.38	129.95	124.26
31	B	834	CLA	CHC-C4B-NB	5.37	129.94	124.26
36	4	302	LUT	C39-C29-C28	-5.37	109.62	118.08
31	B	841	CLA	CHC-C4B-NB	5.37	129.94	124.26
36	L	304	LUT	C28-C29-C30	-5.37	110.71	118.94
32	5	317	CHL	O2D-CGD-O1D	-5.36	113.35	123.84
36	5	303	LUT	C40-C33-C32	-5.36	109.63	118.08
31	7	322	CLA	C2B-C1B-NB	5.36	113.83	110.23
31	5	309	CLA	O2D-CGD-CBD	5.36	120.79	111.27
31	b	312	CLA	O2D-CGD-CBD	5.36	120.79	111.27
31	a	316	CLA	O2D-CGD-CBD	5.36	120.79	111.27
31	8	318	CLA	O2D-CGD-CBD	5.36	120.79	111.27
32	A	831	CHL	C2B-C1B-NB	5.36	113.82	110.23
32	K	201	CHL	C3C-C4C-NC	5.36	116.58	110.57
31	B	820	CLA	CHC-C4B-NB	5.36	129.93	124.26
32	8	316	CHL	CHC-C4B-NB	5.35	129.93	124.26
31	6	310	CLA	C2B-C1B-NB	5.35	113.82	110.23
31	A	822	CLA	CHC-C4B-NB	5.35	129.92	124.26
36	4	302	LUT	C40-C33-C32	-5.35	109.65	118.08
31	A	847	CLA	CHD-C1D-ND	-5.35	119.54	124.45
31	L	305	CLA	CHC-C4B-NB	5.34	129.91	124.26
31	3	310	CLA	CHD-C1D-ND	-5.34	119.55	124.45
36	7	305	LUT	C28-C29-C30	-5.34	110.75	118.94
31	6	311	CLA	O2D-CGD-CBD	5.34	120.75	111.27
31	G	206	CLA	CHD-C1D-ND	-5.34	119.55	124.45
31	7	311	CLA	C2B-C1B-NB	5.33	113.81	110.23
31	8	308	CLA	CHC-C4B-NB	5.33	129.90	124.26
31	A	823	CLA	CHC-C4B-NB	5.33	129.90	124.26
32	9	322	CHL	C2B-C1B-NB	5.33	113.80	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	832	CLA	CHC-C4B-NB	5.32	129.89	124.26
31	B	816	CLA	C2B-C1B-NB	5.32	113.80	110.23
31	A	833	CLA	C2C-C1C-NC	5.32	114.96	109.97
31	9	318	CLA	C2B-C1B-NB	5.32	113.80	110.23
31	4	319	CLA	O2D-CGD-CBD	5.32	120.72	111.27
32	6	309	CHL	C2B-C1B-NB	5.32	113.80	110.23
31	F	301	CLA	O2D-CGD-CBD	5.32	120.71	111.27
31	2	315	CLA	C2B-C1B-NB	5.31	113.79	110.23
30	A	813	CL0	O2D-CGD-CBD	5.31	120.71	111.27
31	B	813	CLA	CHC-C4B-NB	5.31	129.88	124.26
36	9	302	LUT	C40-C33-C32	-5.31	109.71	118.08
31	H	901	CLA	O2D-CGD-CBD	5.31	120.70	111.27
31	A	821	CLA	CHC-C4B-NB	5.30	129.87	124.26
31	5	321	CLA	O2D-CGD-CBD	5.30	120.69	111.27
32	7	320	CHL	O2D-CGD-CBD	5.29	120.67	111.27
36	6	303	LUT	C19-C9-C8	-5.29	109.74	118.08
31	B	832	CLA	O2D-CGD-CBD	5.29	120.67	111.27
31	8	310	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
32	4	313	CHL	O2D-CGD-CBD	5.29	120.66	111.27
31	7	314	CLA	C1C-C2C-C3C	-5.28	102.23	107.07
36	L	304	LUT	C40-C33-C32	-5.27	109.77	118.08
31	8	317	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
31	B	847	CLA	O2D-CGD-CBD	5.27	120.63	111.27
31	L	307	CLA	C2B-C1B-NB	5.27	113.76	110.23
31	B	845	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
32	a	318	CHL	O2D-CGD-CBD	5.26	120.61	111.27
31	3	314	CLA	CHC-C4B-NB	5.26	129.82	124.26
31	7	311	CLA	CHC-C4B-NB	5.26	129.82	124.26
31	A	851	CLA	C2B-C1B-NB	5.26	113.75	110.23
32	7	320	CHL	C2B-C1B-NB	5.26	113.75	110.23
32	5	316	CHL	C4A-NA-C1A	5.25	109.07	106.71
31	B	841	CLA	C2D-C1D-ND	5.25	113.97	110.10
31	5	313	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	B	819	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
36	F	304	LUT	C8-C9-C10	-5.24	110.90	118.94
32	A	840	CHL	C2B-C1B-NB	5.24	113.74	110.23
31	B	841	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
36	b	301	LUT	C39-C29-C28	-5.23	109.83	118.08
32	7	318	CHL	C2B-C1B-NB	5.23	113.74	110.23
31	8	320	CLA	C2B-C1B-NB	5.23	113.74	110.23
32	A	839	CHL	CHC-C4B-NB	5.23	129.79	124.26
31	a	316	CLA	CHD-C1D-ND	-5.23	119.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	9	304	QTB	C01-C02-C03	-5.22	115.61	122.92
32	6	321	CHL	C2B-C1B-NB	5.22	113.73	110.23
36	4	303	LUT	C20-C13-C12	-5.22	109.86	118.08
31	L	305	CLA	CHD-C1D-ND	-5.22	119.66	124.45
31	B	847	CLA	C2C-C1C-NC	5.22	114.86	109.97
32	9	320	CHL	CHC-C4B-NB	5.21	129.77	124.26
31	A	842	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	7	310	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	A	851	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	7	322	CLA	O2D-CGD-CBD	5.20	120.52	111.27
31	K	206	CLA	C2B-C1B-NB	5.20	113.72	110.23
31	B	827	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
36	9	305	LUT	C39-C29-C28	-5.20	109.89	118.08
31	b	307	CLA	O2D-CGD-O1D	-5.20	113.67	123.84
36	7	305	LUT	C17-C1-C6	5.20	118.73	110.30
31	8	321	CLA	O2D-CGD-CBD	5.19	120.50	111.27
31	K	205	CLA	CHD-C1D-ND	-5.19	119.68	124.45
31	9	317	CLA	CHD-C1D-ND	-5.19	119.68	124.45
31	B	812	CLA	C2D-C1D-ND	5.19	113.93	110.10
31	B	817	CLA	O2D-CGD-CBD	5.19	120.48	111.27
36	9	303	LUT	C7-C8-C9	-5.18	118.40	126.23
31	A	856	CLA	C2B-C1B-NB	5.18	113.70	110.23
32	a	317	CHL	C2B-C1B-NB	5.18	113.70	110.23
36	6	303	LUT	C39-C29-C28	-5.18	109.92	118.08
31	B	848	CLA	CHC-C4B-NB	5.17	129.73	124.26
31	B	819	CLA	CHD-C1D-ND	-5.17	119.70	124.45
31	6	322	CLA	O2D-CGD-CBD	5.17	120.45	111.27
32	4	317	CHL	O2D-CGD-CBD	5.17	120.45	111.27
31	a	321	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	2	304	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	B	811	CLA	O2D-CGD-CBD	5.16	120.44	111.27
32	b	309	CHL	O2D-CGD-CBD	5.16	120.43	111.27
31	A	835	CLA	O2D-CGD-CBD	5.15	120.43	111.27
31	4	316	CLA	C3B-C2B-C1B	-5.15	100.94	107.16
31	K	204	CLA	O2D-CGD-CBD	5.15	120.42	111.27
31	9	318	CLA	O2D-CGD-CBD	5.15	120.41	111.27
31	3	319	CLA	CHC-C4B-NB	5.15	129.70	124.26
31	A	826	CLA	CHC-C4B-NB	5.14	129.70	124.26
31	b	302	CLA	O2D-CGD-CBD	5.14	120.40	111.27
32	5	322	CHL	C2B-C1B-NB	5.13	113.67	110.23
31	O	202	CLA	C1C-C2C-C3C	-5.13	102.37	107.07
31	5	313	CLA	C3B-C2B-C1B	-5.13	100.97	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	814	CLA	CHC-C4B-NB	5.13	129.69	124.26
36	3	304	LUT	C19-C9-C8	-5.13	110.00	118.08
36	4	302	LUT	C28-C29-C30	-5.12	111.08	118.94
31	8	310	CLA	C2D-C1D-ND	5.12	113.88	110.10
31	4	320	CLA	O2D-CGD-CBD	5.12	120.37	111.27
36	b	301	LUT	C7-C6-C5	-5.11	109.08	121.46
31	B	811	CLA	C4D-CHA-C1A	-5.10	115.04	121.25
31	B	840	CLA	CHC-C4B-NB	5.10	129.66	124.26
31	6	310	CLA	O2D-CGD-CBD	5.09	120.32	111.27
31	b	310	CLA	CHD-C1D-ND	-5.09	119.77	124.45
31	4	307	CLA	O2D-CGD-CBD	5.09	120.31	111.27
30	A	813	CL0	CHD-C1D-ND	-5.09	119.78	124.45
31	A	855	CLA	C2D-C1D-ND	5.08	113.85	110.10
31	6	308	CLA	O2D-CGD-CBD	5.08	120.30	111.27
32	b	309	CHL	C2B-C1B-NB	5.08	113.64	110.23
31	B	841	CLA	CHD-C1D-ND	-5.07	119.79	124.45
31	A	847	CLA	C2C-C1C-NC	5.07	114.72	109.97
31	B	833	CLA	CHD-C1D-ND	-5.07	119.80	124.45
36	3	305	LUT	C40-C33-C32	-5.07	110.09	118.08
31	b	304	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	B	829	CLA	C2C-C1C-NC	5.07	114.72	109.97
31	7	311	CLA	O2D-CGD-CBD	5.07	120.27	111.27
31	b	306	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	3	320	CLA	CHC-C4B-NB	5.06	129.62	124.26
32	7	318	CHL	O2D-CGD-O1D	-5.06	113.94	123.84
31	a	312	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	A	845	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	8	317	CLA	C2D-C1D-ND	5.05	113.83	110.10
31	B	836	CLA	CHC-C4B-NB	5.05	129.61	124.26
31	J	105	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	a	314	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	7	309	CLA	CHC-C4B-NB	5.05	129.60	124.26
31	5	323	CLA	O2D-CGD-CBD	5.05	120.23	111.27
31	A	843	CLA	C2B-C1B-NB	5.04	113.61	110.23
31	B	848	CLA	O2D-CGD-CBD	5.04	120.23	111.27
31	B	850	CLA	C2D-C1D-ND	5.04	113.82	110.10
31	A	823	CLA	O2D-CGD-CBD	5.04	120.23	111.27
31	a	314	CLA	O2D-CGD-O1D	-5.04	113.98	123.84
31	A	827	CLA	CHC-C4B-NB	5.04	129.59	124.26
31	B	828	CLA	C2B-C1B-NB	5.04	113.61	110.23
31	6	316	CLA	CHD-C1D-ND	-5.04	119.83	124.45
31	L	307	CLA	O2D-CGD-CBD	5.04	120.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	827	CLA	C2C-C1C-NC	5.04	114.69	109.97
31	A	853	CLA	CHC-C4B-NB	5.03	129.59	124.26
31	A	817	CLA	C2D-C1D-ND	5.03	113.81	110.10
36	F	304	LUT	C1-C6-C5	-5.03	115.53	122.61
31	4	309	CLA	C2D-C1D-ND	5.03	113.81	110.10
36	9	302	LUT	C35-C15-C14	-5.03	113.17	123.47
31	9	315	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	B	829	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
32	7	319	CHL	CHD-C1D-ND	-5.02	119.84	124.45
31	B	831	CLA	O2D-CGD-CBD	5.02	120.18	111.27
36	3	304	LUT	C1-C6-C5	-5.02	115.55	122.61
31	A	841	CLA	C2D-C1D-ND	5.01	113.80	110.10
31	B	832	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
31	8	321	CLA	CHD-C1D-ND	-5.01	119.85	124.45
31	A	836	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	a	314	CLA	C2B-C1B-NB	5.01	113.59	110.23
31	A	844	CLA	C2C-C1C-NC	5.01	114.66	109.97
31	7	315	CLA	C2C-C1C-NC	5.00	114.66	109.97
32	8	316	CHL	C2B-C1B-NB	5.00	113.59	110.23
31	b	311	CLA	CHD-C1D-ND	-5.00	119.86	124.45
32	a	318	CHL	CHC-C4B-NB	5.00	129.55	124.26
31	3	319	CLA	C2D-C1D-ND	5.00	113.79	110.10
31	3	319	CLA	CHD-C4C-C3C	-5.00	117.50	124.84
31	2	313	CLA	O2D-CGD-CBD	4.99	120.14	111.27
36	9	303	LUT	C28-C29-C30	-4.99	111.28	118.94
31	A	841	CLA	CHD-C1D-ND	-4.99	119.87	124.45
31	A	825	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	B	817	CLA	C2C-C1C-NC	4.98	114.64	109.97
31	A	855	CLA	CHC-C4B-NB	4.98	129.53	124.26
31	A	856	CLA	CHC-C4B-NB	4.98	129.53	124.26
31	2	309	CLA	CHD-C1D-ND	-4.98	119.88	124.45
31	4	305	CLA	CAC-C3C-C4C	4.98	131.27	124.81
31	A	855	CLA	C2B-C1B-NB	4.97	113.57	110.23
31	B	821	CLA	CHD-C1D-ND	-4.97	119.88	124.45
31	A	846	CLA	C2D-C1D-ND	4.97	113.77	110.10
31	a	309	CLA	O1D-CGD-CBD	-4.97	114.31	124.48
31	A	854	CLA	O2D-CGD-CBD	4.97	120.10	111.27
32	a	320	CHL	C2B-C1B-NB	4.97	113.56	110.23
31	B	848	CLA	C2D-C1D-ND	4.97	113.76	110.10
36	5	304	LUT	C12-C13-C14	-4.97	111.32	118.94
31	3	308	CLA	O2D-CGD-CBD	4.97	120.09	111.27
32	6	309	CHL	O2D-CGD-CBD	4.97	120.09	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	814	CLA	C2D-C1D-ND	4.96	113.76	110.10
31	8	307	CLA	O2D-CGD-CBD	4.96	120.09	111.27
36	7	305	LUT	C40-C33-C32	-4.96	110.26	118.08
31	A	843	CLA	C2C-C1C-NC	4.96	114.62	109.97
31	B	839	CLA	CHD-C1D-ND	-4.96	119.90	124.45
31	3	310	CLA	CHC-C4B-NB	4.96	129.51	124.26
31	B	850	CLA	CHC-C4B-NB	4.96	129.50	124.26
31	B	816	CLA	C2D-C1D-ND	4.96	113.76	110.10
31	B	835	CLA	O2D-CGD-CBD	4.95	120.07	111.27
31	2	306	CLA	CHD-C1D-ND	-4.95	119.90	124.45
31	9	321	CLA	C2C-C1C-NC	4.95	114.61	109.97
31	3	319	CLA	O2D-CGD-CBD	4.95	120.06	111.27
31	B	843	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
31	L	306	CLA	CHD-C1D-ND	-4.94	119.91	124.45
31	G	204	CLA	O2D-CGD-CBD	4.94	120.05	111.27
32	5	322	CHL	C1C-C2C-C3C	-4.94	103.19	107.11
31	3	316	CLA	O2D-CGD-CBD	4.94	120.05	111.27
35	a	302	QTB	C01-C02-C03	-4.94	116.01	122.92
31	5	314	CLA	O2D-CGD-CBD	4.94	120.04	111.27
31	a	319	CLA	C2C-C1C-NC	4.94	114.60	109.97
31	b	304	CLA	CHD-C1D-ND	-4.94	119.92	124.45
31	A	822	CLA	C2D-C1D-ND	4.93	113.74	110.10
31	5	318	CLA	CHD-C1D-ND	-4.93	119.92	124.45
31	B	815	CLA	C2D-C1D-ND	4.93	113.73	110.10
31	A	817	CLA	CHD-C1D-ND	-4.93	119.93	124.45
36	L	304	LUT	C20-C13-C12	-4.92	110.32	118.08
31	A	834	CLA	CHC-C4B-NB	4.92	129.47	124.26
36	9	303	LUT	C20-C13-C12	-4.92	110.32	118.08
31	2	315	CLA	O2D-CGD-CBD	4.92	120.01	111.27
31	F	305	CLA	C2C-C1C-NC	4.92	114.58	109.97
31	2	314	CLA	O2D-CGD-CBD	4.92	120.00	111.27
31	A	814	CLA	C2D-C1D-ND	4.91	113.73	110.10
36	4	302	LUT	C19-C9-C8	-4.91	110.33	118.08
32	3	315	CHL	O1D-CGD-CBD	-4.91	114.43	124.48
31	9	315	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
31	2	305	CLA	O2D-CGD-CBD	4.91	120.00	111.27
31	7	316	CLA	O2D-CGD-O1D	-4.91	114.23	123.84
31	4	309	CLA	CHD-C1D-ND	-4.91	119.94	124.45
31	A	854	CLA	C2D-C1D-ND	4.91	113.72	110.10
31	B	828	CLA	CHD-C1D-ND	-4.90	119.95	124.45
31	a	311	CLA	C2B-C1B-NB	4.90	113.52	110.23
31	8	311	CLA	O2D-CGD-CBD	4.90	119.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	833	CLA	CHC-C4B-NB	4.90	129.44	124.26
31	a	321	CLA	C2C-C1C-NC	4.90	114.56	109.97
36	L	304	LUT	C19-C9-C8	-4.90	110.36	118.08
32	8	319	CHL	C2B-C1B-NB	4.90	113.52	110.23
32	6	320	CHL	O2D-CGD-CBD	4.90	119.97	111.27
32	7	317	CHL	C1-C2-C3	-4.90	117.57	126.04
36	9	302	LUT	C28-C29-C30	-4.90	111.43	118.94
31	A	847	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
31	8	310	CLA	O2D-CGD-CBD	4.89	119.97	111.27
31	7	310	CLA	C2C-C1C-NC	4.89	114.56	109.97
31	8	320	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	K	206	CLA	C2C-C1C-NC	4.89	114.55	109.97
31	9	316	CLA	C2C-C1C-NC	4.89	114.55	109.97
31	A	833	CLA	C1C-C2C-C3C	-4.88	101.82	106.96
31	A	829	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
32	5	317	CHL	O2D-CGD-CBD	4.88	119.94	111.27
31	B	840	CLA	CHD-C1D-ND	-4.88	119.97	124.45
32	6	318	CHL	C4A-NA-C1A	4.88	108.90	106.71
31	3	314	CLA	CHD-C1D-ND	-4.88	119.97	124.45
31	B	831	CLA	C2D-C1D-ND	4.88	113.70	110.10
31	H	902	CLA	O2D-CGD-CBD	4.88	119.94	111.27
31	3	310	CLA	CHD-C4C-C3C	-4.88	117.67	124.84
31	b	302	CLA	C2C-C1C-NC	4.88	114.54	109.97
31	6	313	CLA	C2C-C1C-NC	4.88	114.54	109.97
31	3	311	CLA	C2C-C1C-NC	4.87	114.54	109.97
31	2	312	CLA	CHD-C1D-ND	-4.87	119.97	124.45
31	B	844	CLA	CHD-C1D-ND	-4.87	119.98	124.45
31	B	823	CLA	C2C-C1C-NC	4.87	114.53	109.97
36	a	305	LUT	C19-C9-C8	-4.87	110.40	118.08
31	8	317	CLA	C2C-C1C-NC	4.87	114.53	109.97
31	B	848	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
32	4	317	CHL	C1C-C2C-C3C	-4.87	103.25	107.11
31	A	848	CLA	C2C-C1C-NC	4.86	114.53	109.97
32	3	315	CHL	C1-C2-C3	-4.86	117.63	126.04
31	B	818	CLA	C1C-C2C-C3C	-4.86	101.84	106.96
31	A	850	CLA	C2D-C1D-ND	4.86	113.69	110.10
31	2	308	CLA	C2D-C1D-ND	4.86	113.69	110.10
31	B	812	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
31	a	310	CLA	C2D-C1D-ND	4.86	113.69	110.10
31	A	856	CLA	C2D-C1D-ND	4.86	113.68	110.10
31	4	308	CLA	C2C-C1C-NC	4.86	114.52	109.97
31	B	846	CLA	O2D-CGD-CBD	4.86	119.90	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	817	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
31	5	323	CLA	C2D-C1D-ND	4.86	113.68	110.10
31	a	321	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
31	9	315	CLA	C2C-C1C-NC	4.85	114.52	109.97
31	2	309	CLA	O2D-CGD-CBD	4.85	119.88	111.27
31	A	821	CLA	CHD-C1D-ND	-4.85	120.00	124.45
31	4	311	CLA	O2D-CGD-CBD	4.84	119.87	111.27
31	B	836	CLA	C2C-C1C-NC	4.84	114.51	109.97
31	A	816	CLA	C2C-C1C-NC	4.84	114.50	109.97
31	3	310	CLA	C2C-C1C-NC	4.84	114.50	109.97
31	H	903	CLA	C2B-C1B-NB	4.84	113.47	110.23
31	2	315	CLA	C2D-C1D-ND	4.83	113.66	110.10
32	4	310	CHL	C2B-C1B-NB	4.83	113.47	110.23
31	6	315	CLA	C2D-C1D-ND	4.83	113.66	110.10
31	4	320	CLA	C4D-CHA-C1A	-4.83	115.38	121.25
32	a	318	CHL	C4A-NA-C1A	4.82	108.88	106.71
36	4	303	LUT	C19-C9-C8	-4.82	110.48	118.08
36	4	303	LUT	C8-C9-C10	-4.82	111.54	118.94
31	5	315	CLA	C1C-C2C-C3C	-4.82	101.89	106.96
31	8	308	CLA	O2D-CGD-CBD	4.82	119.83	111.27
31	2	307	CLA	O2D-CGD-CBD	4.81	119.82	111.27
31	3	318	CLA	C2C-C1C-NC	4.81	114.48	109.97
36	3	304	LUT	C8-C9-C10	-4.81	111.55	118.94
31	B	847	CLA	C2D-C1D-ND	4.81	113.65	110.10
31	8	317	CLA	CHC-C4B-NB	4.81	129.35	124.26
31	8	321	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
32	5	319	CHL	C2B-C1B-NB	4.81	113.46	110.23
31	5	311	CLA	C2C-C1C-NC	4.81	114.47	109.97
32	6	320	CHL	C1C-C2C-C3C	-4.80	103.30	107.11
31	a	310	CLA	C2C-C1C-NC	4.80	114.47	109.97
31	O	204	CLA	O2D-CGD-CBD	4.80	119.81	111.27
31	8	317	CLA	O2D-CGD-CBD	4.80	119.80	111.27
31	A	838	CLA	C2C-C1C-NC	4.80	114.47	109.97
31	3	307	CLA	O1D-CGD-CBD	-4.80	114.67	124.48
31	B	849	CLA	C2D-C1D-ND	4.80	113.64	110.10
31	3	310	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
31	b	312	CLA	C2C-C1C-NC	4.80	114.47	109.97
31	4	321	CLA	O2D-CGD-CBD	4.79	119.79	111.27
31	A	848	CLA	C1C-C2C-C3C	-4.79	101.92	106.96
31	B	838	CLA	O2D-CGD-CBD	4.79	119.78	111.27
32	5	319	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
31	B	837	CLA	C2B-C1B-NB	4.79	113.44	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	323	CLA	C2C-C1C-NC	4.79	114.46	109.97
31	4	309	CLA	C2C-C1C-NC	4.79	114.46	109.97
31	3	312	CLA	O2D-CGD-CBD	4.79	119.78	111.27
32	7	324	CHL	O2D-CGD-CBD	4.79	119.77	111.27
31	6	312	CLA	O2D-CGD-O1D	-4.78	114.48	123.84
32	A	840	CHL	C4A-NA-C1A	4.78	108.86	106.71
31	B	844	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
31	8	318	CLA	CHD-C1D-ND	-4.78	120.06	124.45
31	B	818	CLA	C2D-C1D-ND	4.78	113.63	110.10
36	9	305	LUT	C32-C33-C34	-4.78	111.61	118.94
36	3	304	LUT	C28-C29-C30	-4.78	111.61	118.94
31	B	823	CLA	C1C-C2C-C3C	-4.78	101.93	106.96
31	K	204	CLA	C1C-C2C-C3C	-4.78	101.93	106.96
31	a	319	CLA	C1C-C2C-C3C	-4.78	101.93	106.96
31	B	838	CLA	C2C-C1C-NC	4.77	114.44	109.97
31	a	309	CLA	C2D-C1D-ND	4.77	113.62	110.10
31	A	853	CLA	C2D-C1D-ND	4.77	113.62	110.10
36	7	305	LUT	C19-C9-C8	-4.77	110.57	118.08
31	A	814	CLA	O2D-CGD-CBD	4.76	119.73	111.27
31	A	832	CLA	CHD-C1D-ND	-4.76	120.08	124.45
33	7	308	DGD	O3G-C3G-C2G	-4.76	99.41	110.90
31	B	849	CLA	CHC-C4B-NB	4.76	129.30	124.26
31	b	310	CLA	O2D-CGD-CBD	4.76	119.73	111.27
31	8	321	CLA	CHC-C4B-NB	4.76	129.30	124.26
31	B	822	CLA	O2D-CGD-O1D	-4.76	114.53	123.84
31	A	834	CLA	CHD-C1D-ND	-4.76	120.08	124.45
31	B	845	CLA	C2D-C1D-ND	4.76	113.61	110.10
31	8	309	CLA	C2C-C1C-NC	4.76	114.43	109.97
31	4	320	CLA	C2C-C1C-NC	4.76	114.43	109.97
31	a	309	CLA	O2D-CGD-CBD	4.76	119.72	111.27
31	4	320	CLA	CHD-C1D-ND	-4.76	120.08	124.45
31	a	311	CLA	C1C-C2C-C3C	-4.75	101.96	106.96
31	9	314	CLA	O2D-CGD-CBD	4.75	119.72	111.27
36	a	305	LUT	C8-C9-C10	-4.75	111.65	118.94
31	6	306	CLA	C2B-C1B-NB	4.75	113.42	110.23
31	a	315	CLA	O1D-CGD-CBD	-4.75	114.76	124.48
36	4	303	LUT	C18-C5-C4	-4.75	105.55	114.36
31	5	313	CLA	CHD-C1D-ND	-4.75	120.09	124.45
31	b	303	CLA	C2C-C1C-NC	4.75	114.42	109.97
31	4	321	CLA	C2C-C1C-NC	4.75	114.42	109.97
36	9	305	LUT	C7-C6-C5	-4.74	109.97	121.46
31	F	301	CLA	CHC-C4B-NB	4.74	129.28	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	2	301	LUT	C28-C29-C30	-4.74	111.67	118.94
31	B	814	CLA	O2D-CGD-O1D	-4.74	114.57	123.84
31	A	842	CLA	CHD-C1D-ND	-4.74	120.10	124.45
31	6	313	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
31	2	315	CLA	C2C-C1C-NC	4.74	114.41	109.97
31	B	816	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
31	4	306	CLA	O2D-CGD-CBD	4.73	119.68	111.27
32	9	320	CHL	C4A-NA-C1A	4.73	108.83	106.71
31	B	826	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
31	8	314	CLA	C2C-C1C-NC	4.73	114.41	109.97
32	6	320	CHL	C4A-NA-C1A	4.73	108.83	106.71
31	4	312	CLA	O2D-CGD-CBD	4.73	119.67	111.27
31	B	829	CLA	C2D-C1D-ND	4.73	113.59	110.10
42	4	304	SQD	O9-S-C6	4.73	112.56	106.94
31	A	850	CLA	C1C-C2C-C3C	-4.73	101.99	106.96
31	8	320	CLA	C2C-C1C-NC	4.73	114.40	109.97
31	9	311	CLA	C1C-C2C-C3C	-4.73	101.99	106.96
31	H	903	CLA	C2C-C1C-NC	4.73	114.40	109.97
31	8	309	CLA	C2D-C1D-ND	4.73	113.59	110.10
31	B	842	CLA	CHD-C1D-ND	-4.73	120.11	124.45
31	b	305	CLA	CHD-C1D-ND	-4.72	120.11	124.45
31	3	320	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
31	b	313	CLA	CAC-C3C-C4C	4.72	130.94	124.81
31	3	314	CLA	C2C-C1C-NC	4.72	114.40	109.97
31	A	823	CLA	CHD-C1D-ND	-4.72	120.11	124.45
31	2	313	CLA	C2C-C1C-NC	4.72	114.39	109.97
31	B	816	CLA	C2C-C1C-NC	4.72	114.39	109.97
31	4	320	CLA	C1C-C2C-C3C	-4.72	102.00	106.96
31	3	311	CLA	O2D-CGD-CBD	4.72	119.65	111.27
31	A	820	CLA	C2D-C1D-ND	4.72	113.58	110.10
31	A	837	CLA	CHD-C1D-ND	-4.71	120.12	124.45
31	J	105	CLA	C2C-C1C-NC	4.71	114.39	109.97
31	B	834	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
32	7	319	CHL	CHC-C4B-NB	4.71	129.25	124.26
31	2	308	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
31	5	312	CLA	O2D-CGD-O1D	-4.71	114.63	123.84
31	A	837	CLA	O2D-CGD-CBD	4.71	119.64	111.27
31	A	836	CLA	CHD-C1D-ND	-4.71	120.13	124.45
31	3	312	CLA	C2C-C1C-NC	4.71	114.38	109.97
31	a	311	CLA	C2C-C1C-NC	4.71	114.38	109.97
31	9	312	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
31	A	841	CLA	C3B-C2B-C1B	-4.71	101.48	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	8	303	LUT	C18-C5-C4	-4.71	105.64	114.36
31	a	312	CLA	C2D-C1D-ND	4.71	113.57	110.10
31	3	310	CLA	C2D-C1D-ND	4.71	113.57	110.10
31	a	311	CLA	C4D-CHA-C1A	-4.70	115.53	121.25
31	B	849	CLA	CHD-C1D-ND	-4.70	120.13	124.45
31	A	857	CLA	C2D-C1D-ND	4.70	113.57	110.10
36	8	302	LUT	C8-C7-C6	-4.70	114.00	127.20
31	3	307	CLA	C2D-C1D-ND	4.70	113.57	110.10
31	5	315	CLA	C2C-C1C-NC	4.70	114.37	109.97
31	5	318	CLA	C2C-C1C-NC	4.70	114.37	109.97
31	A	821	CLA	C2D-C1D-ND	4.70	113.57	110.10
31	A	822	CLA	CHD-C4C-C3C	-4.70	117.94	124.84
32	6	317	CHL	C4A-NA-C1A	4.70	108.82	106.71
31	7	313	CLA	C2D-C1D-ND	4.70	113.56	110.10
31	3	310	CLA	C4D-CHA-C1A	-4.69	115.54	121.25
31	A	834	CLA	C2C-C1C-NC	4.69	114.37	109.97
31	7	309	CLA	CHD-C1D-ND	-4.69	120.14	124.45
31	A	815	CLA	O2D-CGD-CBD	4.69	119.61	111.27
31	6	314	CLA	C2C-C1C-NC	4.69	114.37	109.97
31	8	308	CLA	C2D-C1D-ND	4.69	113.56	110.10
31	3	314	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
31	3	309	CLA	CHD-C1D-ND	-4.69	120.15	124.45
31	b	308	CLA	O2D-CGD-CBD	4.68	119.59	111.27
31	B	817	CLA	C2D-C1D-ND	4.68	113.55	110.10
32	7	318	CHL	C1C-C2C-C3C	-4.68	103.40	107.11
31	4	316	CLA	O2D-CGD-CBD	4.68	119.58	111.27
31	A	815	CLA	CHC-C4B-NB	4.67	129.21	124.26
31	6	306	CLA	O2D-CGD-CBD	4.67	119.58	111.27
31	A	821	CLA	CHD-C4C-C3C	-4.67	117.97	124.84
31	7	315	CLA	C1C-C2C-C3C	-4.67	102.04	106.96
31	6	307	CLA	C1C-C2C-C3C	-4.67	102.04	106.96
31	2	307	CLA	C2C-C1C-NC	4.67	114.35	109.97
31	A	817	CLA	CHC-C4B-NB	4.67	129.20	124.26
31	9	314	CLA	C2D-C1D-ND	4.67	113.55	110.10
31	B	821	CLA	C2C-C1C-NC	4.67	114.34	109.97
31	B	833	CLA	C2D-C1D-ND	4.67	113.54	110.10
31	B	813	CLA	CHD-C1D-ND	-4.66	120.17	124.45
31	9	321	CLA	C1C-C2C-C3C	-4.66	102.05	106.96
31	8	313	CLA	C2D-C1D-ND	4.66	113.54	110.10
31	B	830	CLA	C4D-CHA-C1A	-4.66	115.57	121.25
31	A	832	CLA	C2C-C1C-NC	4.66	114.34	109.97
31	2	312	CLA	O2D-CGD-O1D	-4.66	114.72	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	311	CLA	O2D-CGD-CBD	4.66	119.55	111.27
31	B	825	CLA	O2D-CGD-CBD	4.66	119.55	111.27
31	B	826	CLA	CHD-C4C-C3C	-4.66	117.99	124.84
31	F	306	CLA	C2C-C1C-NC	4.66	114.34	109.97
31	4	305	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
31	b	307	CLA	C2C-C1C-NC	4.66	114.33	109.97
31	B	813	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
31	8	314	CLA	C2D-C1D-ND	4.66	113.53	110.10
31	8	311	CLA	CHD-C1D-ND	-4.66	120.18	124.45
31	B	830	CLA	CHC-C4B-NB	4.65	129.18	124.26
31	A	853	CLA	C2C-C1C-NC	4.65	114.33	109.97
31	B	826	CLA	C2C-C1C-NC	4.65	114.33	109.97
31	5	320	CLA	C4D-CHA-C1A	-4.65	115.59	121.25
31	b	313	CLA	O2D-CGD-CBD	4.65	119.53	111.27
31	B	847	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
31	B	817	CLA	C4D-CHA-C1A	-4.65	115.59	121.25
31	7	312	CLA	CHC-C4B-NB	4.65	129.18	124.26
31	K	206	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
31	7	312	CLA	O2D-CGD-CBD	4.64	119.52	111.27
32	A	839	CHL	CHD-C4C-C3C	-4.64	118.01	124.84
31	3	317	CLA	C2C-C1C-NC	4.64	114.32	109.97
31	B	840	CLA	C2D-C1D-ND	4.64	113.53	110.10
31	7	321	CLA	C2D-C1D-ND	4.64	113.53	110.10
31	B	811	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
31	B	813	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
31	5	308	CLA	O2D-CGD-CBD	4.64	119.51	111.27
31	4	315	CLA	O2D-CGD-CBD	4.64	119.51	111.27
31	9	311	CLA	C2C-C1C-NC	4.64	114.32	109.97
31	a	313	CLA	CHD-C1D-ND	-4.64	120.19	124.45
31	5	311	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
31	A	850	CLA	C2C-C1C-NC	4.63	114.31	109.97
31	J	105	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
31	7	314	CLA	C2C-C1C-NC	4.63	114.31	109.97
31	B	840	CLA	O2D-CGD-CBD	4.63	119.50	111.27
32	4	313	CHL	C2B-C1B-NB	4.63	113.34	110.23
31	A	825	CLA	CHD-C4C-C3C	-4.63	118.04	124.84
31	G	206	CLA	C2D-C1D-ND	4.63	113.52	110.10
31	A	845	CLA	C2C-C1C-NC	4.63	114.31	109.97
31	A	818	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
31	9	319	CLA	C2C-C1C-NC	4.63	114.31	109.97
31	4	307	CLA	C2C-C1C-NC	4.63	114.31	109.97
31	5	309	CLA	C2C-C1C-NC	4.63	114.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	819	CLA	C2D-C1D-ND	4.63	113.51	110.10
31	B	813	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
31	2	310	CLA	O2D-CGD-CBD	4.63	119.49	111.27
32	8	319	CHL	C1C-C2C-C3C	-4.63	103.44	107.11
31	B	812	CLA	CAC-C3C-C4C	4.62	130.81	124.81
31	A	844	CLA	C1C-C2C-C3C	-4.62	102.09	106.96
30	A	813	CL0	C3D-C2D-C1D	-4.62	99.52	105.83
31	2	314	CLA	C2C-C1C-NC	4.62	114.30	109.97
36	a	305	LUT	C35-C15-C14	-4.62	114.00	123.47
36	9	303	LUT	C7-C6-C5	-4.62	110.27	121.46
31	2	307	CLA	O2D-CGD-O1D	-4.62	114.80	123.84
31	K	204	CLA	C2C-C1C-NC	4.62	114.30	109.97
31	A	827	CLA	C2C-C1C-NC	4.62	114.30	109.97
31	9	312	CLA	C2D-C1D-ND	4.62	113.51	110.10
31	5	318	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
31	3	318	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
31	A	855	CLA	CHD-C4C-C3C	-4.62	118.06	124.84
36	a	305	LUT	C7-C6-C5	-4.62	110.28	121.46
31	6	307	CLA	CHD-C1D-ND	-4.61	120.21	124.45
31	8	313	CLA	O2D-CGD-O1D	-4.61	114.82	123.84
31	4	315	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
31	8	309	CLA	O2D-CGD-CBD	4.61	119.46	111.27
31	5	307	CLA	C2D-C1D-ND	4.61	113.50	110.10
31	A	818	CLA	C4D-CHA-C1A	-4.61	115.64	121.25
31	3	313	CLA	CHD-C1D-ND	-4.61	120.22	124.45
32	a	318	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
31	3	311	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
31	8	321	CLA	C2D-C1D-ND	4.61	113.50	110.10
31	B	821	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
31	5	311	CLA	O2D-CGD-CBD	4.61	119.46	111.27
32	3	315	CHL	C1C-C2C-C3C	-4.61	103.46	107.11
31	B	842	CLA	C2D-C1D-ND	4.61	113.50	110.10
31	6	311	CLA	C2C-C1C-NC	4.60	114.29	109.97
31	6	307	CLA	C2C-C1C-NC	4.60	114.28	109.97
31	A	857	CLA	CHD-C4C-C3C	-4.60	118.07	124.84
36	5	304	LUT	C18-C5-C4	-4.60	105.83	114.36
31	b	302	CLA	C2D-C1D-ND	4.60	113.50	110.10
32	a	320	CHL	C1C-C2C-C3C	-4.60	103.46	107.11
31	B	839	CLA	CHC-C4B-NB	4.60	129.13	124.26
31	9	317	CLA	O2D-CGD-CBD	4.60	119.44	111.27
31	a	312	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
31	A	845	CLA	C1C-C2C-C3C	-4.60	102.12	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	321	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
31	8	311	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
31	b	303	CLA	C4D-CHA-C1A	-4.60	115.65	121.25
31	7	310	CLA	C2D-C1D-ND	4.60	113.49	110.10
31	A	835	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
31	9	318	CLA	C2D-C1D-ND	4.59	113.49	110.10
31	8	313	CLA	CHD-C1D-ND	-4.59	120.23	124.45
31	6	310	CLA	C2C-C1C-NC	4.59	114.27	109.97
31	3	308	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
31	A	827	CLA	C2D-C1D-ND	4.59	113.49	110.10
31	8	318	CLA	C2C-C1C-NC	4.59	114.27	109.97
31	5	309	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
31	A	853	CLA	CHD-C1D-ND	-4.59	120.24	124.45
31	4	308	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
31	A	832	CLA	C1C-C2C-C3C	-4.59	102.14	106.96
31	B	828	CLA	CHC-C4B-NB	4.59	129.11	124.26
31	a	322	CLA	C2C-C1C-NC	4.59	114.27	109.97
31	4	306	CLA	CHD-C1D-ND	-4.59	120.24	124.45
31	A	825	CLA	C2D-C1D-ND	4.59	113.48	110.10
31	6	308	CLA	CAC-C3C-C4C	4.59	130.76	124.81
31	5	314	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
31	5	323	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
31	B	824	CLA	O2D-CGD-CBD	4.58	119.41	111.27
31	A	834	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
32	9	322	CHL	C1C-C2C-C3C	-4.58	103.48	107.11
31	O	203	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
32	6	317	CHL	O2D-CGD-CBD	4.58	119.41	111.27
31	B	813	CLA	C2D-C1D-ND	4.58	113.48	110.10
31	b	305	CLA	O2D-CGD-CBD	4.58	119.41	111.27
32	6	321	CHL	C1C-C2C-C3C	-4.58	103.48	107.11
31	F	305	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
31	8	311	CLA	C2C-C1C-NC	4.58	114.26	109.97
31	2	305	CLA	C2C-C1C-NC	4.58	114.26	109.97
36	8	303	LUT	C7-C8-C9	-4.58	119.32	126.23
31	A	830	CLA	O2D-CGD-O1D	-4.58	114.89	123.84
31	B	813	CLA	O2D-CGD-CBD	4.57	119.40	111.27
31	A	833	CLA	O2D-CGD-O1D	-4.57	114.89	123.84
31	b	306	CLA	C2C-C1C-NC	4.57	114.26	109.97
31	3	312	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
31	K	205	CLA	O2D-CGD-CBD	4.57	119.39	111.27
31	A	835	CLA	C2D-C1D-ND	4.57	113.47	110.10
36	L	304	LUT	C35-C15-C14	-4.57	114.11	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	320	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
31	3	320	CLA	C2C-C1C-NC	4.57	114.25	109.97
31	A	838	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
31	8	318	CLA	C2D-C1D-ND	4.56	113.47	110.10
31	B	841	CLA	C3B-C2B-C1B	-4.56	101.65	107.16
36	b	301	LUT	C12-C13-C14	-4.56	111.94	118.94
31	9	316	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
31	a	315	CLA	C2C-C1C-NC	4.56	114.25	109.97
31	4	307	CLA	CHD-C1D-ND	-4.56	120.26	124.45
32	4	317	CHL	C2B-C1B-NB	4.56	113.29	110.23
36	8	303	LUT	C19-C9-C8	-4.56	110.89	118.08
32	9	320	CHL	O2D-CGD-CBD	4.56	119.37	111.27
31	a	315	CLA	CHD-C1D-ND	-4.56	120.27	124.45
31	A	837	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
31	6	306	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
31	O	202	CLA	CHD-C1D-ND	-4.56	120.27	124.45
32	5	316	CHL	CHC-C4B-NB	4.55	129.08	124.26
31	K	205	CLA	C2C-C1C-NC	4.55	114.24	109.97
31	a	322	CLA	CHD-C1D-ND	-4.55	120.27	124.45
31	A	846	CLA	O2D-CGD-CBD	4.55	119.36	111.27
31	7	313	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
31	A	817	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
32	7	319	CHL	CGD-CBD-CAD	4.55	125.48	110.73
31	B	812	CLA	CHD-C1D-ND	-4.55	120.27	124.45
31	8	307	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
31	B	847	CLA	C2B-C1B-NB	4.55	113.28	110.23
31	3	314	CLA	O2D-CGD-O1D	-4.55	114.94	123.84
31	b	303	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
31	9	317	CLA	C2C-C1C-NC	4.55	114.23	109.97
31	5	308	CLA	C2C-C1C-NC	4.55	114.23	109.97
31	5	310	CLA	C2C-C1C-NC	4.55	114.23	109.97
31	A	816	CLA	C4D-CHA-C1A	-4.55	115.71	121.25
31	6	322	CLA	CHD-C1D-ND	-4.55	120.28	124.45
31	L	306	CLA	C2C-C1C-NC	4.55	114.23	109.97
31	4	319	CLA	C2C-C1C-NC	4.55	114.23	109.97
31	K	205	CLA	C3B-C2B-C1B	-4.54	101.67	107.16
31	4	306	CLA	C3B-C2B-C1B	-4.54	101.67	107.16
31	4	308	CLA	C2D-C1D-ND	4.54	113.45	110.10
31	A	855	CLA	O2D-CGD-CBD	4.54	119.34	111.27
31	H	903	CLA	O2D-CGD-O1D	-4.54	114.95	123.84
31	A	834	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
32	a	317	CHL	C1C-C2C-C3C	-4.54	103.51	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	311	CLA	C2D-C1D-ND	4.54	113.45	110.10
31	A	821	CLA	O2D-CGD-CBD	4.54	119.33	111.27
31	A	819	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
31	8	307	CLA	C2C-C1C-NC	4.54	114.22	109.97
31	A	845	CLA	C2D-C1D-ND	4.54	113.45	110.10
31	K	204	CLA	C4D-CHA-C1A	-4.54	115.73	121.25
32	7	317	CHL	C2B-C1B-NB	4.54	113.27	110.23
31	b	307	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
32	b	309	CHL	C1C-C2C-C3C	-4.54	103.51	107.11
31	9	312	CLA	C2C-C1C-NC	4.53	114.22	109.97
32	4	313	CHL	C1C-C2C-C3C	-4.53	103.52	107.11
31	A	828	CLA	C2D-C1D-ND	4.53	113.44	110.10
31	A	842	CLA	C2D-C1D-ND	4.53	113.44	110.10
31	A	836	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
31	B	825	CLA	C2D-C1D-ND	4.53	113.44	110.10
31	8	321	CLA	C2C-C1C-NC	4.53	114.22	109.97
31	L	307	CLA	C2C-C1C-NC	4.53	114.22	109.97
31	A	816	CLA	C2B-C1B-NB	4.53	113.27	110.23
31	A	833	CLA	C2D-C1D-ND	4.53	113.44	110.10
31	K	204	CLA	C2D-C1D-ND	4.53	113.44	110.10
31	b	302	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
32	4	310	CHL	C1C-C2C-C3C	-4.52	103.53	107.11
31	7	311	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
31	6	322	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
31	6	315	CLA	O2D-CGD-CBD	4.52	119.30	111.27
31	A	820	CLA	CHD-C4C-C3C	-4.52	118.20	124.84
31	B	826	CLA	C2D-C1D-ND	4.52	113.43	110.10
31	5	314	CLA	CHD-C4C-C3C	-4.52	118.20	124.84
31	B	836	CLA	C2D-C1D-ND	4.52	113.43	110.10
31	A	845	CLA	CHD-C1D-ND	-4.52	120.30	124.45
31	4	319	CLA	CHD-C1D-ND	-4.52	120.30	124.45
31	B	818	CLA	C2B-C1B-NB	4.52	113.26	110.23
31	b	306	CLA	C1C-C2C-C3C	-4.52	102.21	106.96
31	H	903	CLA	O2D-CGD-CBD	4.51	119.29	111.27
31	9	311	CLA	CHD-C1D-ND	-4.51	120.31	124.45
31	B	819	CLA	C3B-C2B-C1B	-4.51	101.71	107.16
31	4	312	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
31	9	312	CLA	CHD-C1D-ND	-4.51	120.31	124.45
31	b	312	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
31	5	320	CLA	CHD-C1D-ND	-4.51	120.31	124.45
31	A	852	CLA	C2D-C1D-ND	4.51	113.43	110.10
31	B	827	CLA	O2D-CGD-CBD	4.51	119.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	313	CLA	C4D-CHA-C1A	-4.51	115.76	121.25
36	6	304	LUT	C19-C9-C8	-4.51	110.97	118.08
31	8	315	CLA	CHD-C1D-ND	-4.51	120.31	124.45
31	2	312	CLA	O2D-CGD-CBD	4.51	119.28	111.27
31	B	829	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
31	H	903	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
32	8	316	CHL	O2D-CGD-O1D	-4.51	115.03	123.84
32	K	201	CHL	C3D-C2D-C1D	-4.50	99.68	105.83
32	a	318	CHL	O1D-CGD-CBD	-4.50	115.28	124.48
31	7	313	CLA	C2C-C1C-NC	4.50	114.19	109.97
31	4	309	CLA	C1C-C2C-C3C	-4.50	102.23	106.96
31	3	316	CLA	CHD-C1D-ND	-4.50	120.32	124.45
31	6	316	CLA	CHD-C4C-C3C	-4.50	118.23	124.84
31	A	821	CLA	C2C-C1C-NC	4.50	114.19	109.97
31	6	322	CLA	C2C-C1C-NC	4.50	114.19	109.97
31	8	307	CLA	C2D-C1D-ND	4.50	113.42	110.10
31	A	842	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
31	5	311	CLA	CHD-C1D-ND	-4.50	120.32	124.45
31	A	849	CLA	C2C-C1C-NC	4.49	114.18	109.97
31	L	306	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
31	J	105	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
31	B	839	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
31	5	318	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
31	A	826	CLA	C2D-C1D-ND	4.49	113.41	110.10
31	B	824	CLA	C2C-C1C-NC	4.49	114.18	109.97
31	A	827	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
32	7	320	CHL	C1C-C2C-C3C	-4.49	103.55	107.11
32	6	317	CHL	C1C-C2C-C3C	-4.49	103.55	107.11
31	7	321	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
31	2	307	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
31	A	824	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
31	B	811	CLA	C2D-C1D-ND	4.49	113.41	110.10
36	3	304	LUT	C17-C1-C6	4.49	117.58	110.30
31	8	314	CLA	O2D-CGD-O1D	-4.48	115.07	123.84
31	a	310	CLA	O2D-CGD-CBD	4.48	119.24	111.27
31	4	308	CLA	O2D-CGD-O1D	-4.48	115.07	123.84
31	8	312	CLA	C2C-C1C-NC	4.48	114.17	109.97
31	5	307	CLA	CHD-C1D-ND	-4.48	120.33	124.45
31	6	316	CLA	C2D-C1D-ND	4.48	113.41	110.10
36	3	305	LUT	C28-C29-C30	-4.48	112.07	118.94
31	F	301	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
32	A	831	CHL	C3B-C2B-C1B	-4.48	101.76	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	843	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
31	a	315	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
31	a	322	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
31	A	846	CLA	CHD-C4C-C3C	-4.48	118.26	124.84
31	G	206	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	5	321	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	B	815	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	B	837	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	B	842	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
31	5	314	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	4	314	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
31	A	820	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	A	854	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	K	206	CLA	O2D-CGD-CBD	4.47	119.21	111.27
31	b	307	CLA	O2D-CGD-CBD	4.47	119.21	111.27
31	B	835	CLA	C2D-C1D-ND	4.47	113.40	110.10
31	H	902	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	B	848	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
31	G	205	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
32	K	201	CHL	C3B-C4B-NB	4.47	114.66	110.52
31	3	319	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
31	a	314	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	7	322	CLA	C2C-C1C-NC	4.47	114.16	109.97
31	A	846	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
31	2	313	CLA	CHD-C1D-ND	-4.47	120.35	124.45
31	a	316	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
31	3	309	CLA	C2D-C1D-ND	4.46	113.39	110.10
31	9	313	CLA	C4D-CHA-C1A	-4.46	115.82	121.25
31	6	312	CLA	CHD-C1D-ND	-4.46	120.35	124.45
31	H	903	CLA	C4D-CHA-C1A	-4.46	115.82	121.25
31	b	310	CLA	C2C-C1C-NC	4.46	114.15	109.97
36	a	303	LUT	C40-C33-C32	-4.46	111.05	118.08
31	B	820	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
31	8	315	CLA	C2C-C1C-NC	4.46	114.15	109.97
31	B	831	CLA	C4D-CHA-C1A	-4.46	115.82	121.25
31	B	842	CLA	C2C-C1C-NC	4.46	114.15	109.97
31	4	312	CLA	C2C-C1C-NC	4.46	114.15	109.97
31	A	851	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
31	B	827	CLA	C2D-C1D-ND	4.46	113.39	110.10
31	2	312	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
31	b	306	CLA	C4D-CHA-C1A	-4.46	115.82	121.25
31	A	857	CLA	C2C-C1C-NC	4.46	114.15	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	820	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
31	2	310	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
31	3	309	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
31	4	305	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
31	8	315	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
31	B	816	CLA	CHD-C1D-ND	-4.45	120.36	124.45
31	B	820	CLA	C2D-C1D-ND	4.45	113.39	110.10
31	B	813	CLA	C1C-C2C-C3C	-4.45	102.27	106.96
31	G	205	CLA	CHD-C4C-C3C	-4.45	118.29	124.84
31	B	829	CLA	CHD-C1D-ND	-4.45	120.36	124.45
31	B	846	CLA	C2C-C1C-NC	4.45	114.14	109.97
31	A	830	CLA	C2D-C1D-ND	4.45	113.39	110.10
31	B	820	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
31	A	847	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
31	9	315	CLA	C2D-C1D-ND	4.45	113.38	110.10
31	A	841	CLA	C2C-C1C-NC	4.45	114.14	109.97
31	B	844	CLA	C2D-C1D-ND	4.45	113.38	110.10
31	B	847	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
31	b	305	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
31	B	824	CLA	O2D-CGD-O1D	-4.45	115.15	123.84
31	B	836	CLA	O2D-CGD-CBD	4.44	119.17	111.27
31	8	313	CLA	CHD-C4C-C3C	-4.44	118.31	124.84
31	4	314	CLA	C2C-C1C-NC	4.44	114.14	109.97
31	2	313	CLA	C1C-C2C-C3C	-4.44	102.28	106.96
31	b	310	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
31	9	321	CLA	CHD-C1D-ND	-4.44	120.37	124.45
31	A	823	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
36	4	303	LUT	C28-C29-C30	-4.44	112.13	118.94
31	B	817	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
31	5	321	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
31	B	812	CLA	O2D-CGD-CBD	4.44	119.16	111.27
31	J	105	CLA	C2D-C1D-ND	4.44	113.38	110.10
31	b	311	CLA	C2C-C1C-NC	4.44	114.13	109.97
31	a	313	CLA	O2D-CGD-CBD	4.44	119.15	111.27
31	8	315	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
31	7	321	CLA	C2C-C1C-NC	4.44	114.13	109.97
31	G	205	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
31	G	204	CLA	C2C-C1C-NC	4.44	114.13	109.97
31	B	831	CLA	C1C-C2C-C3C	-4.43	102.29	106.96
31	9	317	CLA	C1C-C2C-C3C	-4.43	102.29	106.96
32	8	316	CHL	CHD-C4C-C3C	-4.43	118.32	124.84
32	5	317	CHL	CHC-C4B-NB	4.43	128.95	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	321	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
31	6	312	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
31	B	832	CLA	O2D-CGD-O1D	-4.43	115.17	123.84
31	5	308	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
31	7	321	CLA	O2D-CGD-CBD	4.43	119.14	111.27
31	F	306	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
31	2	314	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
31	4	319	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
31	4	307	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
31	B	833	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
31	G	204	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
31	b	304	CLA	C2D-C1D-ND	4.43	113.37	110.10
31	9	311	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
31	a	313	CLA	C2C-C1C-NC	4.43	114.12	109.97
31	9	313	CLA	C2D-C1D-ND	4.43	113.37	110.10
31	F	301	CLA	C2C-C1C-NC	4.43	114.12	109.97
31	B	828	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
31	B	814	CLA	C3B-C2B-C1B	-4.43	101.82	107.16
36	L	304	LUT	C8-C9-C10	-4.43	112.15	118.94
31	A	818	CLA	CHD-C1D-ND	-4.43	120.39	124.45
31	9	314	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
32	7	320	CHL	O2D-CGD-O1D	-4.43	115.19	123.84
31	6	308	CLA	C2D-C1D-ND	4.43	113.36	110.10
31	b	304	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
31	7	315	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
31	2	307	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
31	A	853	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
31	B	820	CLA	CHD-C1D-ND	-4.42	120.39	124.45
31	F	305	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
31	3	313	CLA	C4D-CHA-C1A	-4.42	115.87	121.25
31	2	305	CLA	C4D-CHA-C1A	-4.42	115.87	121.25
31	5	318	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
31	A	847	CLA	C2D-C1D-ND	4.42	113.36	110.10
31	b	310	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
31	6	314	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
36	4	303	LUT	C4-C5-C6	-4.42	111.00	120.85
31	A	849	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
31	a	314	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
31	A	815	CLA	C4D-CHA-C1A	-4.42	115.87	121.25
31	3	311	CLA	C4D-CHA-C1A	-4.42	115.87	121.25
31	A	844	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
31	4	305	CLA	C1D-CHD-C4C	-4.42	116.53	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	811	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
31	F	306	CLA	C2D-C1D-ND	4.41	113.36	110.10
36	9	305	LUT	C40-C33-C32	-4.41	111.12	118.08
31	3	313	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
31	B	831	CLA	C2C-C1C-NC	4.41	114.11	109.97
31	7	309	CLA	C2D-C1D-ND	4.41	113.36	110.10
31	b	313	CLA	C2D-C1D-ND	4.41	113.36	110.10
31	4	306	CLA	C2C-C1C-NC	4.41	114.10	109.97
31	7	312	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
31	4	305	CLA	C6-C5-C3	-4.41	107.41	114.62
31	6	315	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
31	B	831	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
31	9	313	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
31	H	902	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
31	a	313	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
31	8	309	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
31	A	817	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
31	A	816	CLA	C1C-C2C-C3C	-4.41	102.33	106.96
31	A	837	CLA	C2D-C1D-ND	4.40	113.35	110.10
31	4	306	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
31	A	814	CLA	C3B-C2B-C1B	-4.40	101.84	107.16
31	B	814	CLA	O2D-CGD-CBD	4.40	119.09	111.27
31	5	312	CLA	C2C-C1C-NC	4.40	114.10	109.97
31	2	310	CLA	C2C-C1C-NC	4.40	114.10	109.97
31	7	309	CLA	O2D-CGD-CBD	4.40	119.09	111.27
31	b	313	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
31	H	901	CLA	C2C-C1C-NC	4.40	114.09	109.97
36	6	303	LUT	C4-C5-C6	-4.40	111.04	120.85
31	B	843	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
31	3	308	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
31	8	312	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
32	a	318	CHL	CHD-C1D-ND	-4.40	120.41	124.45
31	9	314	CLA	C2C-C1C-NC	4.40	114.09	109.97
31	b	308	CLA	CHD-C1D-ND	-4.40	120.41	124.45
31	B	835	CLA	C2C-C1C-NC	4.40	114.09	109.97
31	6	311	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
31	4	311	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
31	8	321	CLA	C4D-CHA-C1A	-4.40	115.90	121.25
31	3	309	CLA	C2C-C1C-NC	4.40	114.09	109.97
31	A	821	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
31	b	306	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
31	9	311	CLA	C2D-C1D-ND	4.40	113.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	828	CLA	O2D-CGD-CBD	4.39	119.08	111.27
31	B	828	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
31	A	830	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
31	2	308	CLA	CHD-C1D-ND	-4.39	120.42	124.45
31	8	313	CLA	C2C-C1C-NC	4.39	114.09	109.97
31	a	310	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
31	3	317	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
31	2	305	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
31	5	311	CLA	O2D-CGD-O1D	-4.39	115.25	123.84
31	A	816	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
31	B	831	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
31	7	321	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
31	B	845	CLA	CHD-C1D-ND	-4.39	120.42	124.45
31	B	817	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
31	a	319	CLA	C4D-CHA-C1A	-4.39	115.91	121.25
31	A	820	CLA	CHD-C1D-ND	-4.39	120.42	124.45
31	B	840	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
31	8	314	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
31	b	311	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
31	A	852	CLA	CHD-C1D-ND	-4.39	120.42	124.45
31	5	313	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
31	3	308	CLA	C2C-C1C-NC	4.39	114.08	109.97
31	2	309	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
31	2	304	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
36	9	303	LUT	C8-C9-C10	-4.39	112.21	118.94
31	5	312	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
31	A	829	CLA	O2D-CGD-CBD	4.38	119.06	111.27
31	4	316	CLA	CHC-C4B-NB	4.38	128.90	124.26
31	4	309	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
31	A	828	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
31	4	305	CLA	CHC-C4B-NB	-4.38	119.62	124.26
31	B	814	CLA	C2C-C1C-NC	4.38	114.08	109.97
32	7	317	CHL	C1C-C2C-C3C	-4.38	103.64	107.11
31	b	308	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
31	7	315	CLA	C2D-C1D-ND	4.38	113.33	110.10
31	8	318	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
31	5	311	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
31	a	315	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
31	7	313	CLA	CHD-C4C-C3C	-4.38	118.41	124.84
31	8	313	CLA	C1C-C2C-C3C	-4.38	102.36	106.96
31	b	305	CLA	C2C-C1C-NC	4.38	114.07	109.97
31	6	316	CLA	C3B-C2B-C1B	-4.38	101.88	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	841	CLA	O2D-CGD-CBD	4.37	119.04	111.27
31	b	306	CLA	CHD-C4C-C3C	-4.37	118.41	124.84
35	7	303	QTB	C01-C02-C03	-4.37	116.80	122.92
31	A	846	CLA	C2C-C1C-NC	4.37	114.07	109.97
31	5	312	CLA	O2D-CGD-CBD	4.37	119.04	111.27
31	9	319	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
32	3	315	CHL	CGD-CBD-CAD	4.37	124.89	110.73
31	A	816	CLA	C2D-C1D-ND	4.37	113.32	110.10
31	2	315	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
31	B	835	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
31	K	205	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
31	A	832	CLA	C2D-C1D-ND	4.37	113.32	110.10
31	A	822	CLA	CHD-C1D-ND	-4.37	120.44	124.45
31	B	815	CLA	C1C-C2C-C3C	-4.37	102.37	106.96
31	B	844	CLA	C2C-C1C-NC	4.36	114.06	109.97
31	A	834	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
31	4	321	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
31	9	316	CLA	CHD-C4C-C3C	-4.36	118.43	124.84
31	4	309	CLA	O2D-CGD-CBD	4.36	119.02	111.27
31	H	902	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
31	a	321	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
31	B	830	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
31	8	317	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
31	2	314	CLA	CHD-C1D-ND	-4.36	120.44	124.45
31	7	312	CLA	O2D-CGD-O1D	-4.36	115.31	123.84
31	B	849	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
31	4	318	CLA	C2C-C1C-NC	4.36	114.06	109.97
31	6	316	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
31	G	205	CLA	C2D-C1D-ND	4.36	113.32	110.10
36	5	304	LUT	C21-C26-C27	-4.36	107.19	112.70
31	A	828	CLA	C2C-C1C-NC	4.36	114.06	109.97
31	9	316	CLA	CHD-C1D-ND	-4.36	120.45	124.45
31	6	311	CLA	C4D-CHA-C1A	-4.36	115.94	121.25
31	5	307	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
31	F	305	CLA	C4D-CHA-C1A	-4.36	115.94	121.25
31	8	314	CLA	O2D-CGD-CBD	4.36	119.01	111.27
31	O	203	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
31	7	316	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
31	7	311	CLA	C2C-C1C-NC	4.36	114.05	109.97
31	8	307	CLA	CHD-C4C-C3C	-4.36	118.44	124.84
31	3	307	CLA	C4D-CHA-C1A	-4.36	115.95	121.25
31	9	314	CLA	O2D-CGD-O1D	-4.36	115.32	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	205	CLA	C2C-C1C-NC	4.35	114.05	109.97
31	5	307	CLA	C2C-C1C-NC	4.35	114.05	109.97
31	2	304	CLA	CHD-C1D-ND	-4.35	120.45	124.45
31	4	321	CLA	C2D-C1D-ND	4.35	113.31	110.10
31	B	836	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
31	b	305	CLA	C2D-C1D-ND	4.35	113.31	110.10
31	6	310	CLA	C2D-C1D-ND	4.35	113.31	110.10
31	A	826	CLA	C2C-C1C-NC	4.35	114.05	109.97
31	B	838	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
31	4	316	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
31	G	205	CLA	O1D-CGD-CBD	-4.35	115.58	124.48
31	9	319	CLA	CHD-C1D-ND	-4.35	120.46	124.45
31	b	307	CLA	CHD-C1D-ND	-4.35	120.46	124.45
31	3	316	CLA	C2D-C1D-ND	4.35	113.31	110.10
31	A	819	CLA	CHD-C4C-C3C	-4.35	118.45	124.84
31	A	823	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
31	A	842	CLA	C2C-C1C-NC	4.35	114.04	109.97
32	5	317	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
31	F	301	CLA	C2D-C1D-ND	4.35	113.31	110.10
31	A	842	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
32	5	322	CHL	O2D-CGD-CBD	4.35	118.99	111.27
31	5	323	CLA	CHD-C4C-C3C	-4.35	118.45	124.84
31	2	315	CLA	CHD-C4C-C3C	-4.35	118.45	124.84
31	A	819	CLA	C2C-C1C-NC	4.34	114.04	109.97
31	A	853	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
31	B	840	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
31	B	825	CLA	CHD-C1D-ND	-4.34	120.46	124.45
31	7	321	CLA	CHD-C1D-ND	-4.34	120.46	124.45
31	L	305	CLA	O2D-CGD-CBD	4.34	118.99	111.27
31	6	312	CLA	C2C-C1C-NC	4.34	114.04	109.97
31	B	831	CLA	CHD-C1D-ND	-4.34	120.46	124.45
31	7	316	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
31	8	321	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
31	A	827	CLA	CHD-C4C-C3C	-4.34	118.46	124.84
31	B	830	CLA	C2C-C1C-NC	4.34	114.04	109.97
31	4	306	CLA	C2D-C1D-ND	4.34	113.30	110.10
31	3	317	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
31	2	312	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
31	8	314	CLA	C4D-CHA-C1A	-4.34	115.97	121.25
31	8	310	CLA	CHD-C1D-ND	-4.34	120.47	124.45
31	2	307	CLA	O1D-CGD-CBD	-4.34	115.60	124.48
31	a	309	CLA	C3B-C2B-C1B	-4.34	101.92	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	849	CLA	O2D-CGD-CBD	4.34	118.98	111.27
31	B	833	CLA	O2D-CGD-CBD	4.34	118.97	111.27
31	5	314	CLA	C3B-C2B-C1B	-4.34	101.93	107.16
31	A	844	CLA	C2D-C1D-ND	4.34	113.30	110.10
31	F	305	CLA	C2D-C1D-ND	4.34	113.30	110.10
31	a	315	CLA	C2D-C1D-ND	4.34	113.30	110.10
31	a	322	CLA	C3B-C2B-C1B	-4.34	101.93	107.16
31	A	842	CLA	CHD-C4C-C3C	-4.34	118.47	124.84
31	L	307	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
31	A	836	CLA	C2C-C1C-NC	4.33	114.03	109.97
31	4	308	CLA	O2D-CGD-CBD	4.33	118.97	111.27
31	3	309	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
31	2	312	CLA	C2D-C1D-ND	4.33	113.30	110.10
31	a	316	CLA	C2C-C1C-NC	4.33	114.03	109.97
31	B	815	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
31	6	313	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
32	A	839	CHL	C3B-C2B-C1B	-4.33	101.93	107.16
31	A	836	CLA	C2D-C1D-ND	4.33	113.30	110.10
32	5	316	CHL	C4D-CHA-C1A	-4.33	115.98	121.25
31	4	318	CLA	C2D-C1D-ND	4.33	113.29	110.10
31	9	316	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
31	A	856	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
32	9	322	CHL	O2D-CGD-O1D	-4.33	115.38	123.84
31	b	307	CLA	C4D-CHA-C1A	-4.33	115.98	121.25
31	8	317	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
31	O	203	CLA	C2C-C1C-NC	4.32	114.02	109.97
31	B	850	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
32	6	319	CHL	C1C-C2C-C3C	-4.32	103.68	107.11
31	5	315	CLA	CHD-C1D-ND	-4.32	120.48	124.45
31	A	852	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
31	9	319	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
31	2	305	CLA	C2D-C1D-ND	4.32	113.29	110.10
31	9	315	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
31	L	306	CLA	C2D-C1D-ND	4.32	113.29	110.10
31	a	315	CLA	CHD-C4C-C3C	-4.32	118.49	124.84
31	L	305	CLA	C2C-C1C-NC	4.32	114.02	109.97
31	B	834	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
31	8	307	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
31	B	842	CLA	O2D-CGD-CBD	4.32	118.94	111.27
31	8	308	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
31	2	304	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
31	G	206	CLA	O2D-CGD-O1D	-4.32	115.40	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	309	CLA	C2C-C1C-NC	4.32	114.02	109.97
31	A	836	CLA	CHD-C4C-C3C	-4.32	118.50	124.84
31	9	319	CLA	C2D-C1D-ND	4.32	113.28	110.10
36	F	304	LUT	C19-C9-C8	-4.32	111.28	118.08
31	5	312	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
31	A	857	CLA	O2D-CGD-O1D	-4.31	115.40	123.84
31	6	313	CLA	C2D-C1D-ND	4.31	113.28	110.10
31	5	314	CLA	CHD-C1D-ND	-4.31	120.49	124.45
31	6	310	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
31	A	832	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
31	5	310	CLA	C2D-C1D-ND	4.31	113.28	110.10
31	B	825	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
31	K	206	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
31	b	308	CLA	C2C-C1C-NC	4.31	114.01	109.97
31	7	316	CLA	CHD-C1D-ND	-4.31	120.49	124.45
31	2	306	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
31	9	314	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
31	A	821	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
32	a	317	CHL	O2D-CGD-CBD	4.31	118.92	111.27
31	9	313	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
32	7	318	CHL	C1-C2-C3	-4.30	118.60	126.04
31	5	320	CLA	O2D-CGD-CBD	4.30	118.92	111.27
31	2	304	CLA	C2D-C1D-ND	4.30	113.28	110.10
31	9	313	CLA	C2C-C1C-NC	4.30	114.00	109.97
31	O	204	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
36	9	305	LUT	C35-C15-C14	-4.30	114.66	123.47
32	6	320	CHL	CHD-C4C-C3C	-4.30	118.52	124.84
31	9	316	CLA	C2D-C1D-ND	4.30	113.28	110.10
31	5	320	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
31	5	320	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
31	b	313	CLA	O2D-CGD-O1D	-4.30	115.43	123.84
31	A	822	CLA	C2C-C1C-NC	4.30	114.00	109.97
31	3	316	CLA	C2C-C1C-NC	4.30	114.00	109.97
31	6	308	CLA	CHD-C1D-ND	-4.30	120.50	124.45
31	4	319	CLA	C2D-C1D-ND	4.30	113.27	110.10
31	A	826	CLA	CHD-C4C-C3C	-4.30	118.52	124.84
31	a	310	CLA	CHD-C4C-C3C	-4.30	118.52	124.84
31	b	308	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
31	6	312	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
31	3	309	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
31	A	817	CLA	O2D-CGD-CBD	4.30	118.91	111.27
31	B	820	CLA	O2D-CGD-CBD	4.30	118.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	309	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
32	5	316	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
31	3	307	CLA	O2D-CGD-O1D	-4.29	115.44	123.84
31	B	828	CLA	C2C-C1C-NC	4.29	114.00	109.97
31	8	308	CLA	C4D-CHA-C1A	-4.29	116.02	121.25
31	3	313	CLA	C2C-C1C-NC	4.29	113.99	109.97
31	A	825	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
31	6	315	CLA	C2C-C1C-NC	4.29	113.99	109.97
31	B	823	CLA	CHD-C1D-ND	-4.29	120.51	124.45
31	5	314	CLA	C2D-C1D-ND	4.29	113.27	110.10
31	2	305	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
31	9	313	CLA	O2D-CGD-O1D	-4.29	115.45	123.84
36	5	304	LUT	C32-C33-C34	-4.29	112.36	118.94
31	K	206	CLA	C2D-C1D-ND	4.29	113.26	110.10
31	a	313	CLA	C2D-C1D-ND	4.29	113.26	110.10
31	4	305	CLA	CHD-C1D-ND	-4.29	120.51	124.45
32	5	317	CHL	C3B-C2B-C1B	-4.29	101.99	107.16
31	b	311	CLA	C2D-C1D-ND	4.29	113.26	110.10
31	A	851	CLA	C2C-C1C-NC	4.29	113.99	109.97
31	2	308	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
31	F	306	CLA	O2D-CGD-CBD	4.29	118.88	111.27
31	K	204	CLA	CHD-C4C-C3C	-4.29	118.54	124.84
31	4	318	CLA	C4D-CHA-C1A	-4.29	116.03	121.25
31	L	305	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
31	B	840	CLA	CHD-C4C-C3C	-4.28	118.54	124.84
31	5	310	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
31	3	307	CLA	CHD-C4C-C3C	-4.28	118.54	124.84
31	2	306	CLA	C3B-C2B-C1B	-4.28	101.99	107.16
32	5	316	CHL	C3B-C2B-C1B	-4.28	101.99	107.16
32	7	317	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
31	4	311	CLA	C2C-C1C-NC	4.28	113.98	109.97
32	a	318	CHL	O2D-CGD-O1D	-4.28	115.47	123.84
31	6	316	CLA	C2C-C1C-NC	4.28	113.98	109.97
31	5	318	CLA	O2D-CGD-CBD	4.28	118.87	111.27
31	2	309	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
31	3	319	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
31	a	309	CLA	C2C-C1C-NC	4.28	113.98	109.97
32	5	317	CHL	C1C-C2C-C3C	-4.28	103.72	107.11
31	a	309	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
31	A	819	CLA	C3B-C2B-C1B	-4.27	102.00	107.16
31	J	105	CLA	C4D-CHA-C1A	-4.27	116.05	121.25
31	3	311	CLA	C3B-C2B-C1B	-4.27	102.00	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	320	CLA	C4D-CHA-C1A	-4.27	116.05	121.25
31	6	306	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
31	3	320	CLA	C4D-CHA-C1A	-4.27	116.05	121.25
31	8	309	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
31	3	313	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
31	A	818	CLA	C2D-C1D-ND	4.27	113.25	110.10
31	4	320	CLA	C2D-C1D-ND	4.27	113.25	110.10
31	8	308	CLA	CHD-C4C-C3C	-4.27	118.57	124.84
31	A	820	CLA	O2D-CGD-CBD	4.27	118.85	111.27
31	B	812	CLA	C4D-CHA-C1A	-4.26	116.06	121.25
31	B	839	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
31	4	308	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
31	B	845	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
31	7	322	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
31	7	312	CLA	C2D-C1D-ND	4.26	113.24	110.10
31	B	826	CLA	O2D-CGD-CBD	4.26	118.84	111.27
31	b	303	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
31	A	824	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
31	O	202	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
31	2	314	CLA	C2D-C1D-ND	4.26	113.24	110.10
36	6	303	LUT	C10-C11-C12	-4.26	109.93	123.22
31	a	310	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
31	a	316	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
31	9	312	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
31	6	314	CLA	C4D-CHA-C1A	-4.26	116.07	121.25
31	4	311	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
31	F	305	CLA	O2D-CGD-O1D	-4.26	115.52	123.84
32	7	324	CHL	C3B-C2B-C1B	-4.26	102.02	107.16
31	B	823	CLA	O2D-CGD-CBD	4.25	118.83	111.27
31	O	204	CLA	C2C-C1C-NC	4.25	113.96	109.97
31	B	821	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
31	5	308	CLA	C2D-C1D-ND	4.25	113.24	110.10
31	7	314	CLA	C4D-CHA-C1A	-4.25	116.07	121.25
31	b	306	CLA	CHD-C1D-ND	-4.25	120.55	124.45
31	9	312	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
31	4	314	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
31	B	822	CLA	C2D-C1D-ND	4.25	113.24	110.10
31	9	314	CLA	O1D-CGD-CBD	-4.25	115.78	124.48
31	G	205	CLA	O2D-CGD-CBD	4.25	118.82	111.27
32	6	317	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
31	A	820	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
31	2	310	CLA	C2D-C1D-ND	4.25	113.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	835	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
31	7	310	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
32	6	309	CHL	C1C-C2C-C3C	-4.25	103.74	107.11
31	G	206	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
31	7	309	CLA	C4D-CHA-C1A	-4.25	116.08	121.25
31	5	308	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
31	B	826	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
31	7	313	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
31	2	306	CLA	C2C-C1C-NC	4.25	113.95	109.97
31	A	853	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
31	7	312	CLA	CHD-C1D-ND	-4.24	120.55	124.45
31	a	313	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
31	H	902	CLA	C2D-C1D-ND	4.24	113.23	110.10
31	A	856	CLA	O2D-CGD-CBD	4.24	118.81	111.27
31	5	321	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
32	7	318	CHL	C3B-C2B-C1B	-4.24	102.04	107.16
31	B	842	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
31	B	819	CLA	C2D-C1D-ND	4.24	113.23	110.10
31	B	833	CLA	CHD-C4C-C3C	-4.24	118.61	124.84
31	2	315	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
31	4	320	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
31	a	316	CLA	C2D-C1D-ND	4.24	113.23	110.10
31	2	310	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
31	H	901	CLA	CHD-C1D-ND	-4.24	120.56	124.45
31	B	821	CLA	C2D-C1D-ND	4.24	113.22	110.10
31	7	322	CLA	C2D-C1D-ND	4.24	113.22	110.10
31	6	308	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
31	5	307	CLA	C4D-CHA-C1A	-4.23	116.10	121.25
31	A	825	CLA	C1C-C2C-C3C	-4.23	102.50	106.96
31	3	312	CLA	CHD-C1D-ND	-4.23	120.56	124.45
31	3	318	CLA	CHD-C1D-ND	-4.23	120.56	124.45
31	b	307	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
31	A	844	CLA	O2D-CGD-CBD	4.23	118.79	111.27
31	A	852	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
31	B	815	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
31	3	308	CLA	C2D-C1D-ND	4.23	113.22	110.10
31	2	308	CLA	C2C-C1C-NC	4.23	113.93	109.97
31	B	813	CLA	C2C-C1C-NC	4.23	113.93	109.97
31	B	849	CLA	C2C-C1C-NC	4.23	113.93	109.97
31	b	307	CLA	O1D-CGD-CBD	-4.23	115.83	124.48
31	2	312	CLA	C2C-C1C-NC	4.23	113.93	109.97
31	4	315	CLA	C1C-C2C-C3C	-4.23	102.51	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	850	CLA	CHD-C4C-C3C	-4.23	118.63	124.84
31	a	319	CLA	C2D-C1D-ND	4.23	113.22	110.10
31	6	322	CLA	C2D-C1D-ND	4.23	113.22	110.10
31	6	314	CLA	CHD-C4C-C3C	-4.22	118.63	124.84
36	3	305	LUT	C7-C6-C5	-4.22	111.23	121.46
31	8	313	CLA	C3B-C2B-C1B	-4.22	102.06	107.16
32	9	320	CHL	C3B-C2B-C1B	-4.22	102.06	107.16
31	7	311	CLA	CHD-C4C-C3C	-4.22	118.63	124.84
31	B	840	CLA	C2C-C1C-NC	4.22	113.93	109.97
31	A	857	CLA	CHD-C1D-ND	-4.22	120.58	124.45
32	6	320	CHL	C3B-C2B-C1B	-4.22	102.07	107.16
31	A	816	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
31	H	901	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
31	O	202	CLA	C2C-C1C-NC	4.22	113.92	109.97
31	K	204	CLA	CHD-C1D-ND	-4.22	120.58	124.45
31	O	203	CLA	C2D-C1D-ND	4.22	113.21	110.10
28	6	305	LHG	O4-P-O5	4.22	133.09	112.24
32	K	201	CHL	CHD-C4C-C3C	-4.22	118.64	124.84
31	J	105	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
31	B	830	CLA	O2D-CGD-O1D	-4.22	115.60	123.84
32	5	317	CHL	CHD-C1D-ND	-4.22	120.58	124.45
31	A	855	CLA	C2C-C1C-NC	4.22	113.92	109.97
31	3	316	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
28	6	301	LHG	O4-P-O5	4.22	133.08	112.24
31	B	839	CLA	C1C-C2C-C3C	-4.22	102.53	106.96
31	b	306	CLA	C2D-C1D-ND	4.21	113.21	110.10
31	B	842	CLA	CHD-C4C-C3C	-4.21	118.64	124.84
31	B	820	CLA	C2C-C1C-NC	4.21	113.92	109.97
31	4	318	CLA	O2D-CGD-CBD	4.21	118.75	111.27
32	6	318	CHL	C1C-C2C-C3C	-4.21	103.77	107.11
31	2	310	CLA	C4D-CHA-C1A	-4.21	116.12	121.25
28	A	809	LHG	O4-P-O5	4.21	133.05	112.24
31	b	302	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
36	5	304	LUT	C7-C6-C5	-4.21	111.27	121.46
36	2	301	LUT	C7-C6-C5	-4.21	111.27	121.46
31	B	839	CLA	C2D-C1D-ND	4.21	113.20	110.10
31	4	318	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
31	b	302	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
31	b	305	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
31	b	304	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
31	A	852	CLA	C2C-C1C-NC	4.20	113.91	109.97
32	7	319	CHL	C3B-C2B-C1B	-4.20	102.09	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	849	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
31	a	310	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
31	G	205	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
32	A	840	CHL	C3B-C2B-C1B	-4.20	102.09	107.16
31	6	312	CLA	C2D-C1D-ND	4.20	113.20	110.10
31	4	312	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
32	a	320	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
31	4	314	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
31	5	308	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
36	7	305	LUT	C1-C6-C5	-4.20	116.70	122.61
31	A	834	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
31	4	309	CLA	CHD-C4C-C3C	-4.20	118.67	124.84
32	7	319	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
31	8	318	CLA	C3B-C2B-C1B	-4.20	102.10	107.16
28	7	307	LHG	O4-P-O5	4.19	132.98	112.24
31	3	310	CLA	O2D-CGD-CBD	4.19	118.72	111.27
31	6	307	CLA	C4D-CHA-C1A	-4.19	116.14	121.25
36	a	305	LUT	C1-C6-C5	-4.19	116.71	122.61
36	a	303	LUT	C7-C6-C5	-4.19	111.31	121.46
31	A	854	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
36	7	305	LUT	C16-C1-C6	-4.19	103.50	110.30
31	3	308	CLA	C4D-CHA-C1A	-4.19	116.15	121.25
31	G	204	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
31	4	306	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
31	B	821	CLA	O2D-CGD-CBD	4.19	118.72	111.27
31	A	817	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
32	6	318	CHL	C3B-C2B-C1B	-4.19	102.10	107.16
31	4	315	CLA	CHD-C1D-ND	-4.19	120.60	124.45
31	a	312	CLA	C2C-C1C-NC	4.19	113.90	109.97
31	b	311	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
32	4	310	CHL	C4D-CHA-C1A	-4.19	116.15	121.25
31	B	824	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
31	4	319	CLA	CHD-C4C-C3C	-4.19	118.69	124.84
31	L	306	CLA	CHD-C4C-C3C	-4.19	118.69	124.84
31	A	830	CLA	C2C-C1C-NC	4.19	113.89	109.97
31	3	317	CLA	C2D-C1D-ND	4.18	113.19	110.10
31	9	315	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
31	B	824	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
31	B	838	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
31	A	816	CLA	CHD-C1D-ND	-4.18	120.61	124.45
31	B	811	CLA	CHD-C1D-ND	-4.18	120.61	124.45
31	K	205	CLA	C2D-C1D-ND	4.18	113.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	825	CLA	CHD-C1D-ND	-4.18	120.61	124.45
32	7	318	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
31	8	310	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
31	4	308	CLA	O1D-CGD-CBD	-4.18	115.94	124.48
31	K	204	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
31	6	322	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
31	7	316	CLA	C2C-C1C-NC	4.17	113.88	109.97
31	A	844	CLA	CHD-C4C-C3C	-4.17	118.71	124.84
31	B	819	CLA	CHD-C4C-C3C	-4.17	118.71	124.84
31	A	828	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
31	6	315	CLA	CHD-C1D-ND	-4.17	120.62	124.45
31	B	837	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
31	4	315	CLA	C2D-C1D-ND	4.17	113.18	110.10
31	A	856	CLA	C2C-C1C-NC	4.17	113.88	109.97
31	B	844	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
31	A	846	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
32	7	320	CHL	C3B-C2B-C1B	-4.17	102.13	107.16
32	7	318	CHL	CGD-CBD-CAD	4.17	124.24	110.73
31	8	311	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
31	8	314	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
36	L	304	LUT	C7-C6-C5	-4.17	111.36	121.46
31	A	822	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
31	A	814	CLA	C2C-C1C-NC	4.17	113.88	109.97
31	B	832	CLA	C4D-CHA-C1A	-4.17	116.18	121.25
28	a	306	LHG	O4-P-O5	4.17	132.84	112.24
36	3	304	LUT	C40-C33-C32	-4.17	111.51	118.08
32	5	319	CHL	CGD-CBD-CAD	4.16	124.22	110.73
31	8	308	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
31	6	312	CLA	O1D-CGD-CBD	-4.16	115.97	124.48
31	B	820	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
31	B	829	CLA	O2D-CGD-CBD	4.16	118.67	111.27
31	9	318	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
31	3	318	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
36	4	302	LUT	C35-C15-C14	-4.16	114.95	123.47
31	7	309	CLA	O1D-CGD-CBD	-4.16	115.97	124.48
31	A	823	CLA	C2C-C1C-NC	4.16	113.87	109.97
31	3	320	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
36	F	304	LUT	C20-C13-C12	-4.16	111.53	118.08
31	8	311	CLA	C2D-C1D-ND	4.16	113.17	110.10
31	A	824	CLA	C2C-C1C-NC	4.16	113.87	109.97
31	5	309	CLA	C4D-CHA-C1A	-4.16	116.19	121.25
31	B	824	CLA	C2D-C1D-ND	4.16	113.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	321	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
31	8	308	CLA	O1D-CGD-CBD	-4.15	115.98	124.48
31	A	833	CLA	C4D-CHA-C1A	-4.15	116.19	121.25
31	2	311	CLA	C2C-C1C-NC	4.15	113.86	109.97
31	4	315	CLA	C2C-C1C-NC	4.15	113.86	109.97
31	a	314	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
31	5	320	CLA	C2C-C1C-NC	4.15	113.86	109.97
28	7	302	LHG	O4-P-O5	4.15	132.76	112.24
31	b	310	CLA	C2D-C1D-ND	4.15	113.16	110.10
31	A	854	CLA	CHD-C1D-ND	-4.15	120.64	124.45
31	6	308	CLA	C2C-C1C-NC	4.15	113.86	109.97
31	A	845	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
31	4	321	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
31	B	839	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
31	5	309	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
31	2	311	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
31	4	311	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
36	5	304	LUT	C19-C9-C8	-4.15	111.54	118.08
31	B	837	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
31	8	320	CLA	CAA-C2A-C3A	-4.15	101.42	112.78
31	6	322	CLA	CHD-C4C-C3C	-4.15	118.75	124.84
31	B	826	CLA	CHD-C1D-ND	-4.15	120.64	124.45
31	2	311	CLA	C2D-C1D-ND	4.14	113.16	110.10
31	6	314	CLA	C2D-C1D-ND	4.14	113.16	110.10
31	3	308	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
31	A	837	CLA	C2C-C1C-NC	4.14	113.85	109.97
31	B	849	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
31	B	814	CLA	CHD-C1D-ND	-4.14	120.65	124.45
31	A	833	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
31	a	313	CLA	O2D-CGD-O1D	-4.14	115.74	123.84
31	3	320	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
31	A	852	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
36	F	304	LUT	C18-C5-C4	-4.14	106.69	114.36
31	a	312	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
31	3	310	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
31	a	314	CLA	C4D-CHA-C1A	-4.14	116.21	121.25
32	6	319	CHL	CHD-C1D-ND	-4.14	120.65	124.45
31	6	311	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
31	B	826	CLA	O2D-CGD-O1D	-4.14	115.75	123.84
31	9	312	CLA	O2D-CGD-CBD	4.14	118.62	111.27
31	3	311	CLA	C2D-C1D-ND	4.14	113.15	110.10
31	4	307	CLA	C3B-C2B-C1B	-4.14	102.17	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	317	CHL	O2D-CGD-CBD	4.14	118.62	111.27
31	L	305	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
31	6	315	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
31	5	307	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
31	b	304	CLA	C2C-C1C-NC	4.13	113.84	109.97
31	A	818	CLA	CHC-C4B-NB	4.13	128.63	124.26
31	B	829	CLA	CHD-C4C-C3C	-4.13	118.77	124.84
32	7	324	CHL	C1C-C2C-C3C	-4.13	103.84	107.11
31	B	828	CLA	C2D-C1D-ND	4.13	113.15	110.10
31	A	854	CLA	CHD-C4C-C3C	-4.13	118.77	124.84
31	b	304	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
31	4	321	CLA	CHD-C1D-ND	-4.13	120.66	124.45
31	L	306	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
31	2	308	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
31	A	834	CLA	C2D-C1D-ND	4.13	113.14	110.10
31	B	846	CLA	C2D-C1D-ND	4.13	113.14	110.10
31	b	305	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
31	A	841	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
31	b	312	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
31	A	848	CLA	C2D-C1D-ND	4.12	113.14	110.10
31	A	826	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
31	A	851	CLA	C2D-C1D-ND	4.12	113.14	110.10
31	7	311	CLA	C2D-C1D-ND	4.12	113.14	110.10
31	2	304	CLA	C4D-CHA-C1A	-4.12	116.24	121.25
31	7	322	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
31	9	313	CLA	CHD-C4C-C3C	-4.12	118.79	124.84
36	4	302	LUT	C12-C13-C14	-4.12	112.62	118.94
31	2	311	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
31	8	312	CLA	C2D-C1D-ND	4.12	113.14	110.10
31	B	814	CLA	CHD-C4C-C3C	-4.12	118.79	124.84
31	B	820	CLA	C3B-C2B-C1B	-4.11	102.19	107.16
31	A	817	CLA	O2D-CGD-O1D	-4.11	115.80	123.84
31	L	307	CLA	CHA-C4D-ND	4.11	141.10	132.50
31	7	312	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	A	817	CLA	C2C-C1C-NC	4.11	113.82	109.97
28	8	304	LHG	O4-P-O5	4.11	132.56	112.24
31	3	307	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	2	314	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	a	313	CLA	CHD-C4C-C3C	-4.11	118.80	124.84
28	B	807	LHG	O4-P-O5	4.11	132.56	112.24
31	5	320	CLA	CHD-C4C-C3C	-4.11	118.80	124.84
31	6	312	CLA	CHD-C4C-C3C	-4.11	118.80	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	308	CLA	CHD-C4C-C3C	-4.11	118.80	124.84
31	9	313	CLA	O2D-CGD-CBD	4.11	118.57	111.27
31	b	310	CLA	CHD-C4C-C3C	-4.11	118.80	124.84
31	a	309	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
31	A	827	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	B	816	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	a	319	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
36	8	302	LUT	C19-C9-C8	-4.11	111.61	118.08
31	9	314	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	2	305	CLA	CHD-C1D-ND	-4.11	120.68	124.45
31	5	310	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
31	3	316	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
31	2	310	CLA	O2D-CGD-O1D	-4.10	115.82	123.84
32	8	316	CHL	C1C-C2C-C3C	-4.10	103.86	107.11
36	a	303	LUT	C19-C9-C8	-4.10	111.62	118.08
31	3	316	CLA	CHD-C4C-C3C	-4.10	118.81	124.84
31	7	322	CLA	CHD-C1D-ND	-4.10	120.69	124.45
31	A	818	CLA	O2D-CGD-O1D	-4.10	115.83	123.84
31	L	307	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
31	A	829	CLA	C2B-C1B-NB	4.10	112.98	110.23
31	B	844	CLA	CHD-C4C-C3C	-4.10	118.82	124.84
32	6	319	CHL	C3B-C2B-C1B	-4.10	102.22	107.16
31	3	318	CLA	CHD-C4C-C3C	-4.10	118.82	124.84
31	B	825	CLA	CHD-C4C-C3C	-4.09	118.82	124.84
31	6	315	CLA	CHD-C4C-C3C	-4.09	118.82	124.84
31	6	314	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
31	6	308	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
36	6	303	LUT	C7-C6-C5	-4.09	111.55	121.46
31	4	319	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
31	3	314	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
31	A	857	CLA	C2B-C1B-NB	4.09	112.97	110.23
31	O	204	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
31	B	823	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
31	7	322	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
36	4	302	LUT	C1-C6-C5	-4.09	116.86	122.61
31	8	315	CLA	O2D-CGD-CBD	4.09	118.53	111.27
36	J	103	LUT	C35-C15-C14	-4.09	115.10	123.47
32	6	321	CHL	C3B-C2B-C1B	-4.09	102.23	107.16
31	B	844	CLA	O2D-CGD-CBD	4.09	118.53	111.27
31	8	308	CLA	C2C-C1C-NC	4.09	113.80	109.97
31	A	857	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
31	B	841	CLA	O2D-CGD-O1D	-4.08	115.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	305	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
32	5	317	CHL	O1D-CGD-CBD	-4.08	116.13	124.48
31	8	310	CLA	CHD-C4C-NC	4.08	130.64	124.20
31	B	830	CLA	O2D-CGD-CBD	4.08	118.53	111.27
31	5	315	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
31	A	836	CLA	C4D-CHA-C1A	-4.08	116.28	121.25
31	7	311	CLA	CHD-C1D-ND	-4.08	120.70	124.45
31	B	846	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
31	A	835	CLA	C2C-C1C-NC	4.08	113.79	109.97
31	B	833	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
32	8	319	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
35	F	303	QTB	C01-C02-C03	-4.08	117.21	122.92
31	H	901	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
31	A	851	CLA	CHD-C1D-ND	-4.08	120.71	124.45
31	B	829	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
31	F	306	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
28	A	811	LHG	O4-P-O5	4.07	132.36	112.24
32	9	322	CHL	C3B-C2B-C1B	-4.07	102.25	107.16
31	a	316	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
36	5	303	LUT	C19-C9-C8	-4.07	111.67	118.08
31	8	310	CLA	CMC-C2C-C1C	4.07	131.23	125.04
31	A	843	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
32	a	318	CHL	C3B-C2B-C1B	-4.07	102.25	107.16
31	K	206	CLA	C4D-CHA-C1A	-4.07	116.30	121.25
31	A	850	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
31	B	825	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
31	B	846	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
32	6	317	CHL	C3B-C2B-C1B	-4.06	102.26	107.16
31	3	320	CLA	CHD-C1D-ND	-4.06	120.72	124.45
31	A	828	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
31	A	827	CLA	CHD-C1D-ND	-4.06	120.72	124.45
31	G	206	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
31	5	311	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
31	4	318	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
31	A	828	CLA	CHD-C1D-ND	-4.06	120.72	124.45
31	4	311	CLA	C2D-C1D-ND	4.06	113.09	110.10
31	B	839	CLA	O2D-CGD-CBD	4.06	118.48	111.27
32	A	840	CHL	CHD-C4C-C3C	-4.06	118.88	124.84
31	B	827	CLA	CHD-C4C-C3C	-4.06	118.88	124.84
36	9	305	LUT	C12-C13-C14	-4.06	112.72	118.94
31	A	829	CLA	C4D-CHA-C1A	-4.06	116.31	121.25
31	B	822	CLA	C3B-C2B-C1B	-4.05	102.27	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	826	CLA	C4D-CHA-C1A	-4.05	116.31	121.25
31	B	833	CLA	C2C-C1C-NC	4.05	113.77	109.97
31	A	846	CLA	CHD-C1D-ND	-4.05	120.73	124.45
31	A	835	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
31	A	846	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
31	A	851	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
32	b	309	CHL	C3B-C2B-C1B	-4.05	102.27	107.16
31	a	315	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
31	6	306	CLA	C2D-C1D-ND	4.05	113.09	110.10
31	3	312	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
31	A	837	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
31	A	825	CLA	C2C-C1C-NC	4.05	113.76	109.97
32	3	315	CHL	C3B-C2B-C1B	-4.05	102.28	107.16
31	4	320	CLA	CHD-C4C-C3C	-4.05	118.89	124.84
32	A	840	CHL	CHD-C1D-ND	-4.04	120.74	124.45
31	6	310	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
36	a	303	LUT	C8-C7-C6	-4.04	115.84	127.20
31	4	312	CLA	CHD-C1D-ND	-4.04	120.74	124.45
31	2	304	CLA	C2C-C1C-NC	4.04	113.76	109.97
32	a	318	CHL	C1C-C2C-C3C	-4.04	103.91	107.11
31	5	315	CLA	C4D-CHA-C1A	-4.04	116.33	121.25
31	b	304	CLA	C4D-CHA-C1A	-4.04	116.33	121.25
31	B	825	CLA	C2C-C1C-NC	4.04	113.76	109.97
31	A	854	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
31	5	318	CLA	C4D-CHA-C1A	-4.03	116.34	121.25
31	6	310	CLA	CHD-C4C-C3C	-4.03	118.91	124.84
31	A	849	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
32	A	831	CHL	CGD-CBD-CAD	4.03	123.80	110.73
31	6	308	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
31	B	849	CLA	CHD-C4C-C3C	-4.03	118.91	124.84
31	9	315	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
31	B	836	CLA	CHD-C4C-C3C	-4.03	118.91	124.84
31	K	206	CLA	CHD-C4C-C3C	-4.03	118.91	124.84
31	5	312	CLA	C2D-C1D-ND	4.03	113.08	110.10
31	b	305	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
31	A	857	CLA	C4D-CHA-C1A	-4.03	116.34	121.25
31	2	307	CLA	C2D-C1D-ND	4.03	113.07	110.10
31	6	307	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
31	A	824	CLA	C2D-C1D-ND	4.03	113.07	110.10
31	B	821	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
31	G	206	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
32	3	315	CHL	CHD-C4C-C3C	-4.02	118.92	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	850	CLA	CAC-C3C-C4C	4.02	130.03	124.81
31	A	814	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
31	A	855	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
31	8	313	CLA	C4D-CHA-C1A	-4.02	116.35	121.25
32	A	831	CHL	C1C-C2C-C3C	-4.02	103.92	107.11
31	B	842	CLA	C4D-CHA-C1A	-4.02	116.35	121.25
31	4	311	CLA	O2D-CGD-O1D	-4.02	115.97	123.84
31	a	314	CLA	O1D-CGD-CBD	-4.02	116.26	124.48
32	8	319	CHL	C3B-C2B-C1B	-4.02	102.31	107.16
31	G	204	CLA	CHD-C1D-ND	-4.02	120.76	124.45
31	8	318	CLA	CHD-C4C-C3C	-4.02	118.93	124.84
31	B	814	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
31	5	309	CLA	C2D-C1D-ND	4.02	113.06	110.10
31	6	314	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
32	a	317	CHL	CHD-C4C-C3C	-4.02	118.94	124.84
31	4	312	CLA	C4D-CHA-C1A	-4.02	116.36	121.25
31	B	812	CLA	CHC-C4B-NB	4.02	128.51	124.26
31	A	849	CLA	CHD-C1D-ND	-4.02	120.76	124.45
31	A	829	CLA	C1D-ND-C4D	-4.01	103.48	106.33
31	9	314	CLA	CHD-C1D-ND	-4.01	120.77	124.45
31	b	307	CLA	C2D-C1D-ND	4.01	113.06	110.10
31	B	835	CLA	CHD-C1D-ND	-4.01	120.77	124.45
31	5	320	CLA	C2D-C1D-ND	4.01	113.06	110.10
32	6	309	CHL	C3B-C2B-C1B	-4.01	102.32	107.16
31	2	305	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
31	3	320	CLA	C2D-C1D-ND	4.01	113.06	110.10
31	B	839	CLA	C2C-C1C-NC	4.01	113.73	109.97
31	b	313	CLA	C2C-C1C-NC	4.01	113.73	109.97
28	A	810	LHG	O4-P-O5	4.01	132.05	112.24
31	9	318	CLA	C3B-C2B-C1B	-4.01	102.33	107.16
31	3	318	CLA	C4D-CHA-C1A	-4.00	116.38	121.25
31	B	816	CLA	C4D-CHA-C1A	-4.00	116.38	121.25
32	5	322	CHL	C3B-C2B-C1B	-4.00	102.33	107.16
31	O	204	CLA	CHD-C1D-ND	-4.00	120.78	124.45
31	B	836	CLA	CHD-C1D-ND	-4.00	120.78	124.45
32	a	318	CHL	CGD-CBD-CAD	4.00	123.69	110.73
32	A	839	CHL	C4D-C3D-CAD	4.00	112.81	108.10
31	3	314	CLA	C2D-C1D-ND	4.00	113.05	110.10
31	8	312	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
31	A	825	CLA	C1-O2A-CGA	4.00	126.94	116.44
31	G	205	CLA	C4D-CHA-C1A	-4.00	116.38	121.25
31	6	308	CLA	C4D-CHA-C1A	-4.00	116.38	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	304	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
32	b	309	CHL	CGD-CBD-CAD	4.00	123.68	110.73
40	7	306	XAT	C39-C29-C30	-4.00	117.33	122.92
31	A	856	CLA	CHD-C4C-C3C	-4.00	118.97	124.84
32	7	324	CHL	CHD-C4C-C3C	-4.00	118.97	124.84
31	G	204	CLA	C2D-C1D-ND	3.99	113.05	110.10
31	B	814	CLA	O1D-CGD-CBD	-3.99	116.31	124.48
31	8	308	CLA	CHD-C1D-ND	-3.99	120.78	124.45
32	3	315	CHL	CHD-C1D-ND	-3.99	120.78	124.45
36	L	304	LUT	C1-C6-C5	-3.99	116.99	122.61
31	A	830	CLA	CAC-C3C-C4C	3.99	129.99	124.81
26	A	803	BCR	C2-C1-C6	3.99	116.62	110.48
31	A	848	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
31	9	315	CLA	CHA-C4D-ND	3.99	140.85	132.50
31	6	313	CLA	CHD-C4C-C3C	-3.99	118.97	124.84
40	7	306	XAT	C19-C9-C10	-3.99	117.33	122.92
36	6	304	LUT	C1-C6-C5	-3.99	116.99	122.61
31	B	847	CLA	CHD-C1D-ND	-3.99	120.79	124.45
31	A	815	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
36	3	305	LUT	C19-C9-C8	-3.99	111.79	118.08
31	B	837	CLA	CHD-C1D-ND	-3.99	120.79	124.45
32	9	320	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
31	A	827	CLA	O2D-CGD-CBD	3.99	118.35	111.27
31	B	845	CLA	C1-C2-C3	-3.99	120.30	126.75
31	B	843	CLA	C2D-C1D-ND	3.99	113.04	110.10
31	B	850	CLA	O2D-CGD-CBD	3.99	118.35	111.27
31	9	321	CLA	O2D-CGD-CBD	3.99	118.35	111.27
31	6	312	CLA	O2D-CGD-CBD	3.99	118.35	111.27
36	b	301	LUT	C32-C33-C34	-3.98	112.83	118.94
31	7	322	CLA	C4D-CHA-C1A	-3.98	116.40	121.25
31	5	315	CLA	C2D-C1D-ND	3.98	113.04	110.10
31	2	310	CLA	CHD-C4C-C3C	-3.98	118.99	124.84
31	9	315	CLA	C4D-CHA-C1A	-3.98	116.41	121.25
31	A	838	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
31	B	823	CLA	CHD-C4C-C3C	-3.98	118.99	124.84
36	6	303	LUT	C12-C13-C14	-3.98	112.84	118.94
32	7	319	CHL	C1C-C2C-C3C	-3.97	103.96	107.11
31	3	317	CLA	C4-C3-C5	3.97	120.53	115.98
31	A	820	CLA	C4D-CHA-C1A	-3.97	116.41	121.25
31	a	314	CLA	CHD-C1D-ND	-3.97	120.80	124.45
31	B	841	CLA	C2C-C1C-NC	3.97	113.69	109.97
31	8	310	CLA	O2D-CGD-O1D	-3.97	116.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	812	CLA	CHB-C1B-NB	-3.97	120.05	124.26
31	a	312	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
31	B	832	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
31	2	313	CLA	C4D-CHA-C1A	-3.97	116.42	121.25
31	5	307	CLA	O1D-CGD-CBD	-3.97	116.36	124.48
31	L	305	CLA	CHD-C4C-C3C	-3.97	119.01	124.84
31	3	318	CLA	C2D-C1D-ND	3.97	113.03	110.10
31	5	321	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
36	6	304	LUT	C12-C13-C14	-3.97	112.85	118.94
31	4	314	CLA	CHD-C1D-ND	-3.97	120.81	124.45
31	A	843	CLA	C4D-CHA-C1A	-3.96	116.42	121.25
31	A	826	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
31	B	845	CLA	O2D-CGD-CBD	3.96	118.31	111.27
31	8	317	CLA	CHD-C4C-NC	3.96	130.45	124.20
31	A	844	CLA	C4D-CHA-C1A	-3.96	116.43	121.25
31	2	313	CLA	C2D-C1D-ND	3.96	113.02	110.10
31	4	314	CLA	C2D-C1D-ND	3.96	113.02	110.10
31	B	836	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
31	a	319	CLA	CHD-C4C-C3C	-3.96	119.02	124.84
32	a	320	CHL	CGD-CBD-CAD	3.96	123.56	110.73
36	2	301	LUT	C7-C8-C9	-3.96	120.25	126.23
31	A	837	CLA	CHD-C4C-C3C	-3.96	119.02	124.84
31	A	814	CLA	CHD-C1D-ND	-3.96	120.82	124.45
31	A	844	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
31	A	823	CLA	C2D-C1D-ND	3.96	113.02	110.10
31	A	835	CLA	CHD-C1D-ND	-3.96	120.82	124.45
31	L	307	CLA	C2D-C1D-ND	3.95	113.02	110.10
31	B	822	CLA	C2C-C1C-NC	3.95	113.67	109.97
36	b	301	LUT	C7-C8-C9	-3.95	120.26	126.23
31	a	312	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
31	5	312	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
32	a	317	CHL	C3B-C2B-C1B	-3.95	102.39	107.16
31	B	850	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
31	6	315	CLA	C4D-CHA-C1A	-3.95	116.44	121.25
31	B	832	CLA	C2D-C1D-ND	3.95	113.01	110.10
31	B	846	CLA	CHD-C4C-C3C	-3.95	119.04	124.84
31	K	206	CLA	CHD-C1D-ND	-3.95	120.83	124.45
32	9	320	CHL	O2D-CGD-O1D	-3.95	116.12	123.84
31	2	311	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
32	6	317	CHL	CGD-CBD-CAD	3.95	123.52	110.73
31	4	312	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
31	A	815	CLA	C2C-C1C-NC	3.95	113.67	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	848	CLA	C2C-C1C-NC	3.95	113.67	109.97
31	a	312	CLA	CHD-C1D-ND	-3.95	120.83	124.45
31	B	834	CLA	C2C-C1C-NC	3.95	113.67	109.97
31	2	308	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
31	B	830	CLA	O1D-CGD-CBD	-3.94	116.41	124.48
31	O	202	CLA	CBD-CHA-C1A	3.94	133.15	128.50
31	5	312	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
31	7	316	CLA	CHD-C4C-C3C	-3.94	119.04	124.84
31	H	902	CLA	CHD-C1D-ND	-3.94	120.83	124.45
31	3	313	CLA	C2D-C1D-ND	3.94	113.01	110.10
31	6	311	CLA	C2D-C1D-ND	3.94	113.01	110.10
31	A	815	CLA	CHD-C4C-C3C	-3.94	119.04	124.84
31	7	309	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
31	L	307	CLA	CHD-C1D-ND	-3.94	120.83	124.45
31	8	318	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
31	A	818	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
31	A	845	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
31	4	314	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
31	a	319	CLA	CHD-C1D-ND	-3.94	120.84	124.45
31	B	823	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
31	F	301	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
31	3	307	CLA	O2D-CGD-CBD	3.93	118.26	111.27
36	6	304	LUT	C21-C26-C27	-3.93	107.73	112.70
31	B	848	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
31	5	323	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
31	2	309	CLA	C2D-C1D-ND	3.93	113.00	110.10
31	A	833	CLA	CHD-C4C-C3C	-3.93	119.06	124.84
31	H	903	CLA	CHD-C4C-C3C	-3.93	119.06	124.84
31	7	311	CLA	C3B-C2B-C1B	-3.93	102.42	107.16
32	6	321	CHL	CGD-CBD-CAD	3.93	123.47	110.73
31	2	309	CLA	CHD-C4C-C3C	-3.93	119.06	124.84
31	H	902	CLA	C4D-CHA-C1A	-3.93	116.47	121.25
32	A	839	CHL	CHD-C1D-ND	-3.93	120.84	124.45
31	A	847	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
31	B	834	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
31	B	824	CLA	CHD-C1D-ND	-3.93	120.84	124.45
31	5	312	CLA	CHD-C1D-ND	-3.93	120.84	124.45
31	8	312	CLA	CHD-C4C-C3C	-3.93	119.07	124.84
36	6	303	LUT	C7-C8-C9	-3.93	120.30	126.23
31	A	824	CLA	CHD-C1D-ND	-3.93	120.85	124.45
31	9	318	CLA	C2C-C1C-NC	3.93	113.65	109.97
31	A	818	CLA	O2D-CGD-CBD	3.93	118.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	842	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
31	7	314	CLA	C3B-C2B-C1B	-3.92	102.42	107.16
31	a	309	CLA	CHD-C4C-C3C	-3.92	119.07	124.84
31	A	850	CLA	CHD-C1D-ND	-3.92	120.85	124.45
31	A	850	CLA	C4-C3-C5	3.92	120.47	115.98
31	B	817	CLA	CHD-C1D-ND	-3.92	120.85	124.45
31	3	312	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
31	B	815	CLA	CHD-C1D-ND	-3.92	120.85	124.45
31	5	308	CLA	CHD-C1D-ND	-3.92	120.85	124.45
31	B	819	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
31	A	849	CLA	C2D-C1D-ND	3.92	112.99	110.10
31	a	311	CLA	C2D-C1D-ND	3.92	112.99	110.10
31	A	830	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
31	B	843	CLA	C4D-CHA-C1A	-3.92	116.48	121.25
31	A	834	CLA	O1D-CGD-CBD	-3.91	116.47	124.48
31	A	826	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
31	A	836	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
31	A	854	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
31	L	307	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
31	B	822	CLA	CHD-C1D-ND	-3.91	120.86	124.45
30	A	813	CL0	C2A-C1A-CHA	-3.91	117.02	123.86
31	B	834	CLA	CHD-C1D-ND	-3.91	120.86	124.45
31	A	841	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
31	3	307	CLA	C2C-C1C-NC	3.91	113.63	109.97
32	a	320	CHL	C3B-C2B-C1B	-3.91	102.44	107.16
31	3	317	CLA	CHD-C4C-C3C	-3.91	119.10	124.84
31	A	848	CLA	C4D-CHA-C1A	-3.91	116.50	121.25
31	5	310	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
31	B	818	CLA	CHD-C4C-C3C	-3.90	119.10	124.84
32	4	310	CHL	C4A-NA-C1A	3.90	108.46	106.71
31	B	843	CLA	CHD-C1D-ND	-3.90	120.87	124.45
32	K	201	CHL	C2D-C1D-ND	3.90	112.98	110.10
31	2	307	CLA	CHD-C1D-ND	-3.90	120.87	124.45
31	B	811	CLA	C2C-C1C-NC	3.90	113.62	109.97
32	7	320	CHL	CGD-CBD-CAD	3.90	123.36	110.73
31	7	315	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
31	3	307	CLA	CHD-C1D-ND	-3.90	120.87	124.45
31	9	321	CLA	C4D-CHA-C1A	-3.90	116.51	121.25
32	4	310	CHL	CHD-C1D-ND	-3.90	120.87	124.45
31	A	833	CLA	O2D-CGD-CBD	3.89	118.19	111.27
31	A	838	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
31	9	321	CLA	O2D-CGD-O1D	-3.89	116.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	7	305	LUT	C21-C26-C27	-3.89	107.78	112.70
31	b	308	CLA	C4D-CHA-C1A	-3.89	116.51	121.25
31	9	321	CLA	CHC-C4B-NB	3.89	128.38	124.26
36	3	305	LUT	C21-C26-C27	-3.89	107.78	112.70
36	5	303	LUT	C1-C6-C5	-3.89	117.14	122.61
31	2	312	CLA	C4D-CHA-C1A	-3.89	116.52	121.25
31	9	317	CLA	C2D-C1D-ND	3.88	112.97	110.10
31	K	205	CLA	O2D-CGD-O1D	-3.88	116.24	123.84
31	A	822	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
31	3	319	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
31	A	849	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
31	H	902	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
31	5	307	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
31	B	841	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
31	a	311	CLA	CHD-C1D-ND	-3.88	120.89	124.45
31	B	832	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
31	8	308	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
31	3	311	CLA	CHA-C4D-ND	3.88	140.61	132.50
31	6	316	CLA	C4D-CHA-C1A	-3.87	116.53	121.25
31	a	311	CLA	C3B-C2B-C1B	-3.87	102.48	107.16
32	4	313	CHL	C3B-C2B-C1B	-3.87	102.48	107.16
31	B	845	CLA	CHC-C4B-NB	3.87	128.36	124.26
32	4	317	CHL	C3B-C2B-C1B	-3.87	102.49	107.16
31	7	309	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
31	B	830	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
31	b	311	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
32	5	319	CHL	C3B-C2B-C1B	-3.87	102.49	107.16
31	9	318	CLA	CHD-C1D-ND	-3.87	120.90	124.45
31	7	316	CLA	O2D-CGD-CBD	3.87	118.14	111.27
31	3	317	CLA	CHD-C1D-ND	-3.87	120.90	124.45
31	B	811	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
31	3	308	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
31	3	319	CLA	CHD-C4C-NC	3.87	130.30	124.20
32	7	318	CHL	O1D-CGD-CBD	-3.87	116.57	124.48
31	A	821	CLA	C4D-CHA-C1A	-3.87	116.54	121.25
31	4	315	CLA	CHA-C4D-ND	3.87	140.59	132.50
31	8	320	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
31	5	308	CLA	O1D-CGD-CBD	-3.87	116.57	124.48
31	A	814	CLA	CHD-C4C-C3C	-3.87	119.16	124.84
31	B	825	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
31	3	314	CLA	O1D-CGD-CBD	-3.86	116.58	124.48
31	9	313	CLA	O1D-CGD-CBD	-3.86	116.58	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	321	CLA	C2D-C1D-ND	3.86	112.95	110.10
31	A	857	CLA	O2D-CGD-CBD	3.86	118.13	111.27
31	a	311	CLA	CHD-C4C-C3C	-3.86	119.17	124.84
31	6	311	CLA	CHD-C1D-ND	-3.86	120.91	124.45
31	2	304	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
31	F	305	CLA	CHD-C4C-C3C	-3.86	119.17	124.84
31	9	318	CLA	C4D-CHA-C1A	-3.86	116.55	121.25
32	a	318	CHL	CHD-C4C-NC	3.85	130.28	124.20
31	A	815	CLA	CHD-C1D-ND	-3.85	120.91	124.45
31	8	315	CLA	C2D-C1D-ND	3.85	112.94	110.10
31	4	321	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
31	3	307	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
32	7	317	CHL	C3B-C2B-C1B	-3.85	102.51	107.16
31	5	310	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
31	a	322	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
31	8	307	CLA	CHD-C1D-ND	-3.85	120.92	124.45
31	8	312	CLA	C4D-CHA-C1A	-3.85	116.57	121.25
31	6	307	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
32	9	320	CHL	C1C-C2C-C3C	-3.85	104.06	107.11
31	3	314	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
31	5	323	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
31	B	821	CLA	CHD-C4C-C3C	-3.85	119.19	124.84
31	8	311	CLA	CHD-C4C-C3C	-3.85	119.19	124.84
42	4	304	SQD	O47-C7-C8	3.84	119.79	111.50
31	4	305	CLA	C2A-C3A-C4A	-3.84	95.66	101.87
31	4	316	CLA	C2C-C1C-NC	3.84	113.57	109.97
31	5	318	CLA	O1D-CGD-CBD	-3.84	116.62	124.48
31	6	310	CLA	CHA-C4D-ND	3.84	140.54	132.50
31	9	314	CLA	C4D-CHA-C1A	-3.84	116.57	121.25
31	B	848	CLA	CHD-C4C-NC	3.84	130.25	124.20
31	A	815	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
31	B	843	CLA	O2D-CGD-CBD	3.84	118.09	111.27
31	8	321	CLA	CHD-C4C-NC	3.84	130.25	124.20
31	6	314	CLA	CHD-C1D-ND	-3.84	120.93	124.45
31	b	312	CLA	C2D-C1D-ND	3.83	112.93	110.10
31	B	822	CLA	CHD-C4C-C3C	-3.83	119.20	124.84
32	5	317	CHL	CGD-CBD-CAD	3.83	123.15	110.73
31	O	203	CLA	CHD-C1D-ND	-3.83	120.93	124.45
31	2	315	CLA	C4D-CHA-C1A	-3.83	116.58	121.25
31	5	308	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
31	A	848	CLA	C3B-C2B-C1B	-3.83	102.53	107.16
31	B	823	CLA	C4D-CHA-C1A	-3.83	116.58	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	313	CLA	C4D-CHA-C1A	-3.83	116.58	121.25
31	9	319	CLA	CHA-C4D-ND	3.83	140.52	132.50
31	F	301	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
31	B	849	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
31	5	312	CLA	O1D-CGD-CBD	-3.83	116.65	124.48
31	a	316	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
31	5	315	CLA	CHD-C4C-C3C	-3.83	119.22	124.84
31	7	316	CLA	C2D-C1D-ND	3.83	112.92	110.10
31	3	318	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
31	2	306	CLA	CHD-C4C-C3C	-3.82	119.22	124.84
31	A	848	CLA	CHD-C1D-ND	-3.82	120.94	124.45
31	9	313	CLA	CHD-C1D-ND	-3.82	120.94	124.45
31	8	309	CLA	CHA-C4D-ND	3.82	140.50	132.50
31	A	833	CLA	O1D-CGD-CBD	-3.82	116.66	124.48
36	6	304	LUT	C7-C6-C5	-3.82	112.21	121.46
40	7	306	XAT	C35-C15-C14	3.82	131.30	123.47
36	6	304	LUT	C10-C11-C12	-3.82	111.30	123.22
31	8	311	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
31	7	321	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
31	B	835	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
31	4	314	CLA	O2D-CGD-CBD	3.82	118.05	111.27
31	A	841	CLA	O2D-CGD-CBD	3.81	118.04	111.27
31	2	311	CLA	CHD-C1D-ND	-3.81	120.95	124.45
31	a	314	CLA	C2D-C1D-ND	3.81	112.91	110.10
36	4	303	LUT	C7-C8-C9	-3.81	120.48	126.23
31	9	321	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
31	B	815	CLA	CHA-C4D-ND	3.81	140.47	132.50
32	6	317	CHL	CHD-C1D-ND	-3.81	120.95	124.45
31	A	818	CLA	CHB-C4A-NA	3.81	129.78	124.51
31	8	314	CLA	CHD-C1D-ND	-3.81	120.95	124.45
31	A	850	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
31	2	315	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
32	8	316	CHL	C3B-C2B-C1B	-3.81	102.56	107.16
42	4	304	SQD	O9-S-O7	-3.81	100.77	113.95
31	B	828	CLA	C4D-CHA-C1A	-3.81	116.62	121.25
31	6	307	CLA	C2D-C1D-ND	3.81	112.91	110.10
31	4	306	CLA	C4D-CHA-C1A	-3.81	116.62	121.25
32	4	313	CHL	CGD-CBD-CAD	3.81	123.06	110.73
31	B	818	CLA	CHD-C1D-ND	-3.81	120.96	124.45
31	4	308	CLA	CHD-C1D-ND	-3.80	120.96	124.45
36	F	304	LUT	C21-C26-C27	-3.80	107.89	112.70
31	A	829	CLA	C1-C2-C3	-3.80	120.60	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	854	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
31	8	320	CLA	CHD-C1D-ND	-3.80	120.96	124.45
31	5	318	CLA	C2D-C1D-ND	3.80	112.91	110.10
31	8	313	CLA	O2D-CGD-CBD	3.80	118.02	111.27
31	a	311	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
31	3	312	CLA	C3B-C2B-C1B	-3.80	102.58	107.16
31	4	305	CLA	C1-C2-C3	-3.80	119.48	126.04
36	b	301	LUT	C1-C6-C5	-3.79	117.27	122.61
36	9	302	LUT	C19-C9-C8	-3.79	112.10	118.08
31	4	315	CLA	C4D-CHA-C1A	-3.79	116.63	121.25
31	7	309	CLA	C2C-C1C-NC	3.79	113.53	109.97
31	b	307	CLA	CHD-C4C-C3C	-3.79	119.26	124.84
31	a	321	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
31	O	204	CLA	C4D-CHA-C1A	-3.79	116.63	121.25
26	K	203	BCR	C2-C1-C6	3.79	116.32	110.48
31	b	308	CLA	C2D-C1D-ND	3.79	112.90	110.10
31	2	311	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	A	827	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
31	3	311	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	4	305	CLA	C4C-C3C-C2C	-3.79	101.37	106.90
31	2	313	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	8	309	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	2	314	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	4	312	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	2	312	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
31	6	306	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
31	6	311	CLA	O2D-CGD-O1D	-3.79	116.44	123.84
31	5	323	CLA	CHD-C1D-ND	-3.79	120.97	124.45
31	b	313	CLA	C4D-CHA-C1A	-3.79	116.64	121.25
32	7	320	CHL	CHD-C4C-C3C	-3.79	119.28	124.84
31	B	823	CLA	C2D-C1D-ND	3.78	112.89	110.10
31	F	306	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
31	a	321	CLA	CHD-C4C-C3C	-3.78	119.28	124.84
36	2	301	LUT	C1-C6-C5	-3.78	117.29	122.61
31	A	850	CLA	C4D-CHA-C1A	-3.78	116.65	121.25
31	a	310	CLA	O1D-CGD-CBD	-3.78	116.76	124.48
31	J	105	CLA	CHD-C1D-ND	-3.78	120.98	124.45
31	4	306	CLA	CHA-C4D-ND	3.77	140.39	132.50
31	A	825	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
31	B	813	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
31	O	202	CLA	C2D-C1D-ND	3.77	112.88	110.10
31	7	313	CLA	CHD-C1D-ND	-3.77	120.99	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	815	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
31	B	824	CLA	CHD-C4C-C3C	-3.77	119.30	124.84
31	2	312	CLA	CHA-C4D-ND	3.77	140.38	132.50
31	6	316	CLA	CHB-C1B-NB	-3.77	120.27	124.26
36	3	305	LUT	C8-C7-C6	-3.76	116.64	127.20
31	G	205	CLA	CHD-C1D-ND	-3.76	121.00	124.45
31	B	816	CLA	CHD-C4C-C3C	-3.76	119.31	124.84
31	2	313	CLA	C3B-C2B-C1B	-3.76	102.63	107.16
31	O	203	CLA	CHD-C4C-C3C	-3.76	119.32	124.84
26	5	302	BCR	C2-C1-C6	3.76	116.26	110.48
31	A	838	CLA	C2D-C1D-ND	3.75	112.87	110.10
31	A	822	CLA	O2D-CGD-CBD	3.75	117.93	111.27
32	9	322	CHL	CGD-CBD-CAD	3.75	122.88	110.73
31	B	812	CLA	C2C-C1C-NC	3.75	113.49	109.97
36	J	103	LUT	C3-C4-C5	3.75	119.33	111.85
36	a	305	LUT	C39-C29-C28	-3.75	112.17	118.08
31	4	312	CLA	C2D-C1D-ND	3.75	112.86	110.10
31	B	824	CLA	CHA-C4D-ND	3.75	140.34	132.50
31	3	319	CLA	O1D-CGD-CBD	-3.74	116.82	124.48
31	B	850	CLA	C4D-CHA-C1A	-3.74	116.69	121.25
31	9	312	CLA	C4D-CHA-C1A	-3.74	116.69	121.25
36	4	302	LUT	C7-C6-C5	-3.74	112.39	121.46
31	B	834	CLA	CHA-C4D-ND	3.74	140.33	132.50
31	B	825	CLA	C4D-CHA-C1A	-3.74	116.69	121.25
36	J	103	LUT	C8-C7-C6	-3.74	116.69	127.20
31	7	310	CLA	CHA-C4D-ND	3.74	140.33	132.50
31	B	843	CLA	O1D-CGD-CBD	-3.74	116.83	124.48
31	A	835	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
31	A	832	CLA	O2D-CGD-CBD	3.74	117.91	111.27
31	B	819	CLA	C4D-CHA-C1A	-3.74	116.70	121.25
31	8	314	CLA	O1D-CGD-CBD	-3.73	116.84	124.48
31	B	847	CLA	C4D-CHA-C1A	-3.73	116.70	121.25
31	5	311	CLA	C4D-CHA-C1A	-3.73	116.70	121.25
31	2	311	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
31	5	314	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
31	8	311	CLA	O1D-CGD-CBD	-3.73	116.85	124.48
31	A	838	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
36	9	302	LUT	C8-C7-C6	-3.73	116.72	127.20
31	7	314	CLA	CHD-C4C-C3C	-3.73	119.15	124.98
31	B	827	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
31	2	306	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
32	4	310	CHL	C3B-C2B-C1B	-3.73	102.66	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	312	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
32	6	318	CHL	CGD-CBD-CAD	3.73	122.80	110.73
31	5	312	CLA	CHA-C4D-ND	3.73	140.29	132.50
32	4	313	CHL	CHD-C1D-ND	-3.72	121.03	124.45
31	9	321	CLA	C2D-C1D-ND	3.72	112.85	110.10
36	a	303	LUT	C1-C6-C5	-3.72	117.37	122.61
31	B	837	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
31	2	312	CLA	CHB-C1B-NB	-3.72	120.32	124.26
30	A	813	CL0	C1-O2A-CGA	3.72	126.20	116.44
31	O	202	CLA	CHA-C4D-ND	3.72	140.28	132.50
31	B	834	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
31	b	302	CLA	CHA-C4D-ND	3.72	140.27	132.50
31	7	309	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
31	O	204	CLA	C2D-C1D-ND	3.72	112.84	110.10
31	5	311	CLA	O1D-CGD-CBD	-3.72	116.88	124.48
31	G	204	CLA	CHA-C4D-ND	3.71	140.27	132.50
31	2	310	CLA	CHA-C4D-ND	3.71	140.27	132.50
36	4	302	LUT	C7-C8-C9	-3.71	120.62	126.23
36	a	303	LUT	C30-C31-C32	-3.71	111.63	123.22
31	K	205	CLA	CHD-C4C-C3C	-3.71	119.38	124.84
31	8	313	CLA	O1D-CGD-CBD	-3.71	116.89	124.48
32	6	309	CHL	CGD-CBD-CAD	3.71	122.76	110.73
31	a	321	CLA	CHA-C4D-ND	3.71	140.26	132.50
31	F	306	CLA	CHD-C1D-ND	-3.71	121.05	124.45
31	6	313	CLA	CHD-C1D-ND	-3.71	121.05	124.45
31	b	305	CLA	C4D-CHA-C1A	-3.71	116.73	121.25
31	b	312	CLA	C4D-CHA-C1A	-3.71	116.74	121.25
31	2	306	CLA	C2D-C1D-ND	3.71	112.84	110.10
31	A	848	CLA	O1D-CGD-CBD	-3.71	116.90	124.48
31	A	830	CLA	CHD-C1D-ND	-3.71	121.05	124.45
31	F	306	CLA	CHA-C4D-ND	3.70	140.25	132.50
31	4	318	CLA	CHA-C4D-ND	3.70	140.25	132.50
36	a	305	LUT	C20-C13-C12	-3.70	112.24	118.08
31	a	314	CLA	C3B-C2B-C1B	-3.70	102.69	107.16
31	2	304	CLA	O1D-CGD-CBD	-3.70	116.91	124.48
32	7	318	CHL	CHD-C1D-ND	-3.70	121.05	124.45
32	b	309	CHL	CHD-C4C-C3C	-3.70	119.40	124.84
31	9	319	CLA	CHD-C4C-C3C	-3.70	119.40	124.84
31	B	818	CLA	C4D-CHA-C1A	-3.70	116.74	121.25
32	7	317	CHL	CHD-C1D-ND	-3.70	121.06	124.45
32	8	316	CHL	CGD-CBD-CAD	3.70	122.71	110.73
32	5	322	CHL	O2D-CGD-O1D	-3.70	116.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	4	317	CHL	CGD-CBD-CAD	3.70	122.71	110.73
32	4	317	CHL	C4D-CHA-C1A	-3.69	116.76	121.25
32	6	320	CHL	CGD-CBD-CAD	3.69	122.69	110.73
31	A	835	CLA	CHA-C4D-ND	3.69	140.22	132.50
31	B	835	CLA	CHD-C4C-C3C	-3.69	119.42	124.84
31	7	312	CLA	C2C-C1C-NC	3.69	113.43	109.97
31	8	320	CLA	C2D-C1D-ND	3.69	112.82	110.10
32	a	317	CHL	C1-C2-C3	-3.69	119.67	126.04
31	B	824	CLA	O1D-CGD-CBD	-3.69	116.94	124.48
31	3	310	CLA	CHD-C4C-NC	3.69	130.01	124.20
31	3	308	CLA	CHD-C1D-ND	-3.69	121.07	124.45
31	A	847	CLA	CHD-C4C-C3C	-3.69	119.42	124.84
36	9	303	LUT	C21-C26-C27	-3.69	108.04	112.70
31	B	845	CLA	C3B-C2B-C1B	-3.69	102.71	107.16
31	A	852	CLA	C4-C3-C5	3.69	120.20	115.98
31	H	903	CLA	C3B-C2B-C1B	-3.69	102.71	107.16
31	8	315	CLA	O2D-CGD-O1D	-3.68	116.63	123.84
32	K	201	CHL	C1D-ND-C4D	-3.68	103.72	106.33
31	L	305	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
31	2	314	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
31	H	901	CLA	C2D-C1D-ND	3.68	112.82	110.10
31	4	307	CLA	C2D-C1D-ND	3.68	112.82	110.10
31	4	319	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
31	5	310	CLA	CHA-C4D-ND	3.68	140.20	132.50
31	5	313	CLA	C2C-C1C-NC	3.68	113.42	109.97
31	a	309	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
31	A	830	CLA	C4-C3-C5	3.68	121.46	115.27
31	5	318	CLA	CHD-C4C-C3C	-3.68	119.43	124.84
36	a	305	LUT	C18-C5-C4	-3.68	107.54	114.36
31	A	855	CLA	C3B-C2B-C1B	-3.68	102.72	107.16
31	4	318	CLA	CHD-C1D-ND	-3.67	121.08	124.45
31	8	320	CLA	CHD-C4C-C3C	-3.67	119.44	124.84
31	7	314	CLA	C2D-C1D-ND	3.67	112.81	110.10
31	7	316	CLA	O1D-CGD-CBD	-3.67	116.97	124.48
31	2	307	CLA	CHA-C4D-ND	3.67	140.18	132.50
31	6	310	CLA	CHD-C1D-ND	-3.67	121.08	124.45
31	a	322	CLA	C2D-C1D-ND	3.67	112.81	110.10
31	5	321	CLA	C2D-C1D-ND	3.67	112.81	110.10
31	2	307	CLA	CHD-C4C-C3C	-3.67	119.45	124.84
36	5	303	LUT	C12-C13-C14	-3.67	113.31	118.94
31	b	305	CLA	O1D-CGD-CBD	-3.67	116.98	124.48
31	B	830	CLA	C2D-C1D-ND	3.67	112.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	840	CHL	C1C-C2C-C3C	-3.67	104.20	107.11
31	4	312	CLA	CHA-C4D-ND	3.67	140.17	132.50
31	5	320	CLA	O2D-CGD-O1D	-3.66	116.67	123.84
31	B	847	CLA	CHC-C4B-NB	3.66	128.14	124.26
31	3	313	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
32	5	322	CHL	CGD-CBD-CAD	3.66	122.60	110.73
31	b	302	CLA	CHD-C1D-ND	-3.66	121.09	124.45
31	8	320	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
31	3	320	CLA	CHA-C4D-ND	3.66	140.16	132.50
31	B	841	CLA	CHD-C4C-NC	3.66	129.97	124.20
32	8	319	CHL	CGD-CBD-CAD	3.66	122.59	110.73
31	A	855	CLA	C4-C3-C5	3.66	121.42	115.27
31	6	313	CLA	C4D-CHA-C1A	-3.66	116.80	121.25
31	A	819	CLA	CHA-C4D-ND	3.66	140.15	132.50
31	a	309	CLA	CHA-C4D-ND	3.66	140.15	132.50
31	b	303	CLA	CHA-C4D-ND	3.66	140.15	132.50
36	9	302	LUT	C10-C11-C12	-3.65	111.81	123.22
31	8	314	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
36	9	305	LUT	C4-C5-C6	-3.65	112.70	120.85
31	7	315	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
31	B	835	CLA	C1-O2A-CGA	3.65	126.02	116.44
31	B	811	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
31	8	310	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
31	A	843	CLA	C2D-C1D-ND	3.65	112.79	110.10
31	A	849	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
31	2	315	CLA	CHD-C1D-ND	-3.65	121.10	124.45
31	9	316	CLA	O2D-CGD-CBD	3.65	117.75	111.27
31	6	306	CLA	C2C-C1C-NC	3.65	113.39	109.97
31	B	828	CLA	CHD-C4C-NC	3.65	129.95	124.20
31	7	314	CLA	CHD-C1D-ND	-3.65	121.10	124.45
31	A	830	CLA	CHA-C4D-ND	3.65	140.12	132.50
31	a	310	CLA	CHA-C4D-ND	3.65	140.12	132.50
32	9	320	CHL	CGD-CBD-CAD	3.65	122.54	110.73
36	5	304	LUT	C1-C6-C5	-3.65	117.48	122.61
31	5	323	CLA	C4D-CHA-C1A	-3.65	116.81	121.25
32	a	317	CHL	O2D-CGD-O1D	-3.64	116.71	123.84
31	F	306	CLA	CHD-C4C-C3C	-3.64	119.48	124.84
31	9	317	CLA	C3B-C2B-C1B	-3.64	102.76	107.16
32	5	317	CHL	CHD-C4C-NC	3.64	129.94	124.20
31	5	310	CLA	C4D-CHA-C1A	-3.64	116.82	121.25
31	B	819	CLA	CHA-C4D-ND	3.64	140.12	132.50
31	b	312	CLA	CHA-C4D-ND	3.64	140.11	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	856	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
30	A	813	CL0	CMC-C2C-C1C	3.64	130.58	125.04
31	A	848	CLA	O2D-CGD-CBD	3.64	117.73	111.27
31	a	322	CLA	CHD-C4C-C3C	-3.64	119.49	124.84
32	8	316	CHL	O1D-CGD-CBD	-3.64	117.04	124.48
31	A	832	CLA	C4D-CHA-C1A	-3.64	116.82	121.25
31	F	301	CLA	CHA-C4D-ND	3.64	140.10	132.50
31	B	830	CLA	CHA-C4D-ND	3.63	140.10	132.50
32	A	839	CHL	C3D-C2D-C1D	-3.63	100.87	105.83
31	H	902	CLA	CHA-C4D-ND	3.63	140.10	132.50
31	a	312	CLA	O1D-CGD-CBD	-3.63	117.05	124.48
31	7	311	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
31	G	206	CLA	O2D-CGD-CBD	3.63	117.72	111.27
31	B	827	CLA	C3B-C2B-C1B	-3.63	102.78	107.16
31	5	314	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
32	A	839	CHL	C2D-C1D-ND	3.63	112.78	110.10
31	6	322	CLA	CHA-C4D-ND	3.63	140.09	132.50
31	9	321	CLA	CHA-C4D-ND	3.63	140.09	132.50
31	B	827	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
31	A	823	CLA	CHD-C4C-C3C	-3.63	119.51	124.84
31	8	315	CLA	CHD-C4C-C3C	-3.63	119.51	124.84
31	4	311	CLA	CHD-C4C-C3C	-3.63	119.51	124.84
31	B	839	CLA	C4D-CHA-C1A	-3.62	116.84	121.25
31	B	841	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
31	A	834	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
32	a	317	CHL	CGD-CBD-CAD	3.62	122.47	110.73
31	A	850	CLA	CHA-C4D-ND	3.62	140.07	132.50
31	6	313	CLA	CHA-C4D-ND	3.62	140.07	132.50
31	B	837	CLA	CHA-C4D-ND	3.62	140.07	132.50
31	A	819	CLA	CHD-C1D-ND	-3.62	121.13	124.45
31	B	826	CLA	C1-C2-C3	-3.62	120.90	126.75
31	A	851	CLA	CHA-C4D-ND	3.62	140.07	132.50
31	3	316	CLA	CHA-C4D-ND	3.62	140.07	132.50
36	J	103	LUT	C2-C3-C4	3.62	115.26	110.30
31	K	206	CLA	O1D-CGD-CBD	-3.62	117.08	124.48
31	b	302	CLA	C4D-CHA-C1A	-3.62	116.85	121.25
31	7	315	CLA	CHD-C1D-ND	-3.61	121.13	124.45
31	B	837	CLA	C3B-C2B-C1B	-3.61	102.80	107.16
31	b	313	CLA	O1D-CGD-CBD	-3.61	117.09	124.48
32	7	318	CHL	O2A-CGA-CBA	3.61	123.24	111.91
36	3	304	LUT	C16-C1-C6	-3.61	104.44	110.30
31	9	311	CLA	CHD-C4C-C3C	-3.61	119.53	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	309	CLA	CHD-C1D-ND	-3.61	121.14	124.45
31	6	316	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
31	O	204	CLA	CHD-C4C-C3C	-3.61	119.54	124.84
31	A	845	CLA	CHA-C4D-ND	3.61	140.05	132.50
31	O	203	CLA	CHA-C4D-ND	3.61	140.04	132.50
31	B	811	CLA	CHB-C1B-NB	-3.61	120.44	124.26
31	2	310	CLA	CHD-C1D-ND	-3.61	121.14	124.45
32	6	309	CHL	CHD-C1D-ND	-3.60	121.14	124.45
36	5	304	LUT	C10-C11-C12	-3.60	111.97	123.22
31	A	818	CLA	CAC-C3C-C4C	3.60	129.48	124.81
31	7	310	CLA	CHD-C4C-C3C	-3.60	119.35	124.98
31	5	321	CLA	CHA-C4D-ND	3.60	140.03	132.50
32	6	319	CHL	O2D-CGD-O1D	-3.60	116.80	123.84
31	8	307	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
30	A	813	CL0	C4D-CHA-C1A	-3.60	116.87	121.25
31	3	307	CLA	CHA-C4D-ND	3.60	140.03	132.50
31	A	836	CLA	CHA-C4D-ND	3.60	140.03	132.50
31	8	309	CLA	CHD-C1D-ND	-3.60	121.15	124.45
31	A	822	CLA	CHA-C4D-ND	3.60	140.02	132.50
31	F	301	CLA	CHD-C1D-ND	-3.60	121.15	124.45
31	A	852	CLA	CHA-C4D-ND	3.60	140.02	132.50
31	9	313	CLA	CHA-C4D-ND	3.60	140.02	132.50
31	a	312	CLA	C4D-CHA-C1A	-3.59	116.87	121.25
31	5	309	CLA	CHD-C1D-ND	-3.59	121.15	124.45
31	3	314	CLA	O2D-CGD-CBD	3.59	117.65	111.27
31	B	845	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
31	A	841	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
31	H	901	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
31	B	849	CLA	CHA-C4D-ND	3.59	140.01	132.50
31	B	830	CLA	C3B-C2B-C1B	-3.59	102.83	107.16
36	4	303	LUT	C12-C13-C14	-3.59	113.43	118.94
31	B	820	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
36	9	305	LUT	C8-C7-C6	-3.59	117.12	127.20
31	4	321	CLA	O1D-CGD-CBD	-3.59	117.14	124.48
31	b	307	CLA	CHA-C4D-ND	3.59	140.00	132.50
31	B	815	CLA	C4D-CHA-C1A	-3.58	116.89	121.25
31	B	829	CLA	CHA-C4D-ND	3.58	140.00	132.50
31	B	826	CLA	CHD-C4C-NC	3.58	129.85	124.20
31	8	311	CLA	O2A-CGA-CBA	3.58	123.15	111.91
32	A	840	CHL	C3D-C2D-C1D	-3.58	100.94	105.83
31	9	318	CLA	CHA-C4D-ND	3.58	139.99	132.50
31	b	311	CLA	C4D-CHA-C1A	-3.58	116.89	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	309	CHL	CHD-C1D-ND	-3.58	121.17	124.45
31	b	313	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
31	B	843	CLA	CHD-C4C-C3C	-3.58	119.58	124.84
31	B	812	CLA	CHD-C4C-C3C	-3.58	119.58	124.84
31	7	313	CLA	CHA-C4D-ND	3.58	139.98	132.50
31	7	316	CLA	CHA-C4D-ND	3.57	139.98	132.50
36	5	303	LUT	C30-C31-C32	-3.57	112.07	123.22
31	9	311	CLA	C4D-CHA-C1A	-3.57	116.90	121.25
31	6	313	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
32	6	318	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
31	8	315	CLA	CHA-C4D-ND	3.57	139.97	132.50
31	A	853	CLA	C4D-CHA-C1A	-3.57	116.91	121.25
31	3	308	CLA	CHA-C4D-ND	3.57	139.96	132.50
32	A	831	CHL	CHD-C1D-ND	-3.57	121.18	124.45
31	b	313	CLA	CHD-C1D-ND	-3.57	121.18	124.45
32	5	316	CHL	C1C-C2C-C3C	-3.57	104.28	107.11
31	2	306	CLA	CAA-C2A-C3A	-3.57	103.02	112.78
31	A	824	CLA	C4D-CHA-C1A	-3.56	116.91	121.25
31	9	316	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
31	A	852	CLA	O2D-CGD-CBD	3.56	117.60	111.27
32	4	317	CHL	CHC-C1C-NC	-3.56	118.80	124.20
31	b	310	CLA	CHA-C4D-ND	3.56	139.95	132.50
31	B	838	CLA	C2D-C1D-ND	3.56	112.73	110.10
31	A	819	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
31	7	321	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
31	B	827	CLA	CHD-C4C-NC	3.56	129.81	124.20
31	B	813	CLA	O1D-CGD-CBD	-3.55	117.21	124.48
32	A	831	CHL	C1-C2-C3	-3.55	119.90	126.04
31	5	311	CLA	CHA-C4D-ND	3.55	139.93	132.50
31	9	316	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
31	B	838	CLA	CHA-C4D-ND	3.55	139.93	132.50
31	B	840	CLA	O2A-CGA-CBA	3.55	123.04	111.91
31	4	309	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
31	A	827	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
31	K	205	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
31	4	320	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
31	A	826	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
31	B	818	CLA	O2D-CGD-CBD	3.54	117.56	111.27
32	7	317	CHL	CGD-CBD-CAD	3.54	122.21	110.73
36	J	103	LUT	C28-C29-C30	-3.54	113.51	118.94
31	O	204	CLA	CHA-C4D-ND	3.54	139.90	132.50
33	7	308	DGD	O6D-C1D-O3G	-3.54	101.59	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	309	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
31	5	309	CLA	CHA-C4D-ND	3.54	139.90	132.50
31	5	315	CLA	CHA-C4D-ND	3.54	139.90	132.50
31	A	824	CLA	CHA-C4D-ND	3.54	139.90	132.50
31	4	314	CLA	CHA-C4D-ND	3.54	139.90	132.50
31	A	817	CLA	C4D-CHA-C1A	-3.54	116.95	121.25
31	B	814	CLA	C4D-CHA-C1A	-3.54	116.95	121.25
31	4	318	CLA	CAC-C3C-C4C	3.54	129.40	124.81
31	9	318	CLA	CHD-C4C-C3C	-3.53	119.64	124.84
36	4	303	LUT	C21-C26-C27	-3.53	108.23	112.70
31	9	315	CLA	CHD-C1D-ND	-3.53	121.21	124.45
32	6	321	CHL	CHD-C4C-C3C	-3.53	119.65	124.84
32	4	310	CHL	CGD-CBD-CAD	3.53	122.17	110.73
31	6	315	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
36	7	305	LUT	C2-C3-C4	3.53	115.14	110.30
31	8	311	CLA	CHA-C4D-ND	3.53	139.88	132.50
32	7	324	CHL	CGD-CBD-CAD	3.53	122.17	110.73
31	2	313	CLA	CHA-C4D-ND	3.53	139.88	132.50
31	A	854	CLA	CAC-C3C-C4C	3.53	129.39	124.81
31	9	317	CLA	C3D-C2D-C1D	-3.53	101.02	105.83
32	5	319	CHL	CHD-C4C-C3C	-3.53	119.66	124.84
26	O	201	BCR	C2-C1-C6	3.53	115.91	110.48
31	F	301	CLA	CHD-C4C-C3C	-3.53	119.66	124.84
31	b	306	CLA	CHA-C4D-ND	3.53	139.87	132.50
31	B	832	CLA	CHA-C4D-ND	3.52	139.87	132.50
31	7	315	CLA	CHA-C4D-ND	3.52	139.87	132.50
32	8	319	CHL	CHD-C1D-ND	-3.52	121.22	124.45
31	6	307	CLA	CHA-C4D-ND	3.52	139.87	132.50
31	8	307	CLA	C4D-CHA-C1A	-3.52	116.96	121.25
31	A	851	CLA	CHD-C4C-C3C	-3.52	119.66	124.84
31	A	855	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	B	820	CLA	CHA-C4D-ND	3.52	139.87	132.50
32	7	319	CHL	CHD-C4C-NC	3.52	129.75	124.20
36	2	301	LUT	C21-C26-C27	-3.52	108.25	112.70
31	A	819	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
31	6	308	CLA	O1D-CGD-CBD	-3.52	117.29	124.48
31	a	313	CLA	CHA-C4D-ND	3.52	139.86	132.50
31	B	841	CLA	C1-C2-C3	-3.52	119.96	126.04
31	4	311	CLA	CHA-C4D-ND	3.52	139.85	132.50
31	B	815	CLA	O1D-CGD-CBD	-3.52	117.29	124.48
31	B	822	CLA	CHA-C4D-ND	3.52	139.85	132.50
32	K	201	CHL	C3D-C4D-ND	3.51	115.92	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	818	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
31	8	309	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
31	5	323	CLA	O1D-CGD-CBD	-3.51	117.30	124.48
36	9	305	LUT	C10-C11-C12	-3.51	112.26	123.22
31	A	836	CLA	CHD-C4C-NC	3.51	129.73	124.20
31	5	321	CLA	CHD-C4C-C3C	-3.51	119.69	124.84
32	8	316	CHL	CHD-C4C-NC	3.51	129.73	124.20
26	B	805	BCR	C15-C16-C17	-3.51	116.29	123.47
32	6	320	CHL	CHD-C4C-NC	3.51	129.73	124.20
31	9	317	CLA	CHC-C4B-NB	3.51	127.97	124.26
31	A	856	CLA	C3B-C2B-C1B	-3.51	102.93	107.16
31	6	312	CLA	CHA-C4D-ND	3.51	139.83	132.50
31	B	843	CLA	C3B-C2B-C1B	-3.50	102.93	107.16
31	6	314	CLA	CHA-C4D-ND	3.50	139.83	132.50
31	3	312	CLA	CHD-C4C-C3C	-3.50	119.69	124.84
31	4	307	CLA	CHD-C4C-C3C	-3.50	119.69	124.84
31	B	819	CLA	O2D-CGD-CBD	3.50	117.49	111.27
31	H	901	CLA	C4D-CHA-C1A	-3.50	116.99	121.25
31	3	316	CLA	C4D-CHA-C1A	-3.50	116.99	121.25
31	2	306	CLA	C4-C3-C5	3.50	121.15	115.27
31	6	315	CLA	CHA-C4D-ND	3.49	139.81	132.50
31	7	312	CLA	CHA-C4D-ND	3.49	139.81	132.50
31	8	312	CLA	CHA-C4D-ND	3.49	139.81	132.50
31	B	846	CLA	CHA-C4D-ND	3.49	139.81	132.50
31	a	316	CLA	CHA-C4D-ND	3.49	139.81	132.50
31	2	306	CLA	CHA-C4D-ND	3.49	139.80	132.50
31	5	308	CLA	CHA-C4D-ND	3.49	139.80	132.50
31	a	322	CLA	CHA-C4D-ND	3.49	139.80	132.50
31	b	311	CLA	CHA-C4D-ND	3.49	139.80	132.50
31	8	321	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
31	3	312	CLA	C2D-C1D-ND	3.49	112.68	110.10
31	H	901	CLA	CHA-C4D-ND	3.49	139.80	132.50
31	B	833	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
31	B	850	CLA	CHA-C4D-ND	3.49	139.79	132.50
31	4	307	CLA	CHA-C4D-ND	3.49	139.79	132.50
36	8	303	LUT	C16-C1-C6	-3.49	104.64	110.30
31	A	820	CLA	CHA-C4D-ND	3.49	139.79	132.50
32	6	318	CHL	CHD-C1D-ND	-3.49	121.25	124.45
31	3	318	CLA	CHA-C4D-ND	3.48	139.79	132.50
31	b	308	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
31	7	314	CLA	CHA-C4D-ND	3.48	139.79	132.50
31	7	321	CLA	CHA-C4D-ND	3.48	139.78	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	F	305	CLA	O1D-CGD-CBD	-3.48	117.36	124.48
31	5	309	CLA	CHD-C4C-C3C	-3.48	119.72	124.84
31	b	305	CLA	CHA-C4D-ND	3.48	139.78	132.50
31	7	312	CLA	C4D-CHA-C1A	-3.48	117.01	121.25
31	5	320	CLA	CHA-C4D-ND	3.48	139.78	132.50
31	A	847	CLA	CHA-C4D-ND	3.48	139.78	132.50
31	A	836	CLA	C4-C3-C5	3.48	121.12	115.27
31	A	848	CLA	C4-C3-C5	3.48	121.12	115.27
31	B	835	CLA	CHA-C4D-ND	3.48	139.78	132.50
31	B	844	CLA	CHA-C4D-ND	3.48	139.78	132.50
31	9	321	CLA	O1D-CGD-CBD	-3.48	117.37	124.48
31	F	305	CLA	CHA-C4D-ND	3.48	139.78	132.50
32	5	319	CHL	O2D-CGD-O1D	-3.48	117.04	123.84
31	A	855	CLA	C4D-CHA-C1A	-3.48	117.02	121.25
31	3	317	CLA	CHA-C4D-ND	3.47	139.77	132.50
31	4	319	CLA	CHA-C4D-ND	3.47	139.77	132.50
31	4	321	CLA	CHA-C4D-ND	3.47	139.77	132.50
31	A	825	CLA	CHD-C4C-NC	3.47	129.68	124.20
31	B	836	CLA	C4D-CHA-C1A	-3.47	117.02	121.25
31	O	204	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
31	4	318	CLA	CHD-C4C-C3C	-3.47	119.74	124.84
31	4	308	CLA	CHA-C4D-ND	3.47	139.76	132.50
31	B	834	CLA	O2D-CGD-CBD	3.47	117.43	111.27
31	a	319	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
31	B	846	CLA	CHD-C1D-ND	-3.47	121.27	124.45
31	6	316	CLA	CHD-C4C-NC	3.47	129.66	124.20
32	A	840	CHL	C4D-C3D-CAD	3.46	112.18	108.10
32	6	321	CHL	CHD-C1D-ND	-3.46	121.27	124.45
31	H	903	CLA	C2D-C1D-ND	3.46	112.65	110.10
31	A	825	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
31	B	815	CLA	O2D-CGD-CBD	3.46	117.42	111.27
31	5	314	CLA	CHD-C4C-NC	3.46	129.65	124.20
36	6	303	LUT	C18-C5-C4	-3.46	107.95	114.36
31	a	311	CLA	CHA-C4D-ND	3.46	139.73	132.50
31	4	315	CLA	CHD-C4C-C3C	-3.46	119.76	124.84
31	G	205	CLA	CHD-C4C-NC	3.46	129.65	124.20
31	4	305	CLA	O1D-CGD-CBD	-3.46	117.41	124.48
31	K	205	CLA	CHA-C4D-ND	3.46	139.73	132.50
31	9	311	CLA	CHA-C4D-ND	3.46	139.73	132.50
32	A	831	CHL	C4D-C3D-CAD	3.45	112.17	108.10
31	F	301	CLA	CAC-C3C-C4C	3.45	129.29	124.81
31	A	844	CLA	CHA-C4D-ND	3.45	139.72	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	9	305	LUT	C1-C6-C5	-3.45	117.75	122.61
31	8	313	CLA	CHA-C4D-ND	3.45	139.72	132.50
31	2	308	CLA	CHA-C4D-ND	3.45	139.72	132.50
31	A	845	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
36	L	304	LUT	C7-C8-C9	-3.45	121.02	126.23
31	A	823	CLA	CHA-C4D-ND	3.45	139.71	132.50
32	6	309	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
32	A	840	CHL	C1-C2-C3	-3.45	120.08	126.04
32	6	317	CHL	CHD-C4C-NC	3.45	129.63	124.20
31	A	828	CLA	O2D-CGD-O1D	-3.44	117.10	123.84
36	3	304	LUT	C2-C3-C4	3.44	115.02	110.30
31	9	312	CLA	CHA-C4D-ND	3.44	139.70	132.50
31	b	306	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
31	A	857	CLA	C3B-C2B-C1B	-3.44	103.01	107.16
31	A	814	CLA	C4D-CHA-C1A	-3.44	117.06	121.25
31	A	828	CLA	CHA-C4D-ND	3.44	139.70	132.50
31	A	834	CLA	CHD-C4C-NC	3.44	129.62	124.20
31	3	314	CLA	C4-C3-C5	3.44	121.06	115.27
31	B	815	CLA	C3D-C2D-C1D	-3.44	101.14	105.83
31	6	311	CLA	CHA-C4D-ND	3.44	139.70	132.50
36	9	302	LUT	C7-C6-C5	-3.44	113.13	121.46
31	5	323	CLA	CHA-C4D-ND	3.44	139.69	132.50
31	A	838	CLA	CHA-C4D-ND	3.44	139.69	132.50
31	8	315	CLA	C4D-CHA-C1A	-3.44	117.07	121.25
31	A	818	CLA	C2C-C1C-NC	3.44	113.19	109.97
31	B	832	CLA	O1D-CGD-CBD	-3.44	117.45	124.48
32	5	322	CHL	CHD-C1D-ND	-3.44	121.30	124.45
31	H	903	CLA	CHA-C4D-ND	3.43	139.69	132.50
31	4	309	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
31	B	817	CLA	CHB-C4A-NA	3.43	129.26	124.51
31	4	307	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
31	A	843	CLA	CHD-C1D-ND	-3.43	121.30	124.45
31	H	903	CLA	CHD-C1D-ND	-3.43	121.30	124.45
31	6	306	CLA	CHB-C1B-NB	-3.43	120.62	124.26
31	7	310	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
31	8	314	CLA	CHA-C4D-ND	3.43	139.67	132.50
31	6	308	CLA	CHA-C4D-ND	3.43	139.67	132.50
31	8	307	CLA	CHA-C4D-ND	3.43	139.67	132.50
31	B	817	CLA	CHD-C4C-NC	3.43	129.60	124.20
31	9	321	CLA	CHD-C4C-C3C	-3.43	119.80	124.84
32	A	839	CHL	CHD-C4C-NC	3.43	129.60	124.20
36	6	303	LUT	C30-C31-C32	-3.43	112.52	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	837	CLA	C2D-C1D-ND	3.43	112.63	110.10
31	3	312	CLA	CHA-C4D-ND	3.43	139.67	132.50
32	5	322	CHL	CHD-C4C-C3C	-3.43	119.81	124.84
36	6	304	LUT	C18-C5-C4	-3.43	108.01	114.36
31	8	310	CLA	C4D-CHA-C1A	-3.42	117.08	121.25
31	L	306	CLA	C4D-CHA-C1A	-3.42	117.08	121.25
31	2	311	CLA	CHA-C4D-ND	3.42	139.66	132.50
31	A	857	CLA	CHD-C4C-NC	3.42	129.60	124.20
31	2	309	CLA	CHA-C4D-ND	3.42	139.66	132.50
32	A	839	CHL	C1C-C2C-C3C	-3.42	104.40	107.11
31	A	821	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
31	A	837	CLA	CHA-C4D-ND	3.42	139.66	132.50
31	A	832	CLA	CHD-C4C-NC	3.42	129.59	124.20
36	8	302	LUT	C7-C6-C5	-3.42	113.18	121.46
31	A	842	CLA	C4D-CHA-C1A	-3.42	117.09	121.25
31	A	830	CLA	O2D-CGD-CBD	3.42	117.34	111.27
31	b	303	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
31	6	311	CLA	CHD-C4C-C3C	-3.42	119.82	124.84
31	A	833	CLA	CHD-C1D-ND	-3.42	121.31	124.45
32	A	840	CHL	OBD-CAD-C3D	3.42	136.75	128.52
31	5	318	CLA	CHA-C4D-ND	3.42	139.65	132.50
31	A	834	CLA	O2D-CGD-CBD	3.42	117.34	111.27
31	A	830	CLA	O1D-CGD-CBD	-3.42	117.49	124.48
31	b	303	CLA	C2D-C1D-ND	3.42	112.62	110.10
31	A	832	CLA	C3B-C2B-C1B	-3.42	103.04	107.16
31	5	314	CLA	CHA-C4D-ND	3.42	139.65	132.50
31	a	310	CLA	C4D-CHA-C1A	-3.41	117.09	121.25
31	G	204	CLA	C4D-CHA-C1A	-3.41	117.09	121.25
31	B	823	CLA	CHA-C4D-ND	3.41	139.64	132.50
31	2	314	CLA	CHA-C4D-ND	3.41	139.64	132.50
31	8	317	CLA	C1-C2-C3	-3.41	121.23	126.75
36	5	303	LUT	C7-C6-C5	-3.41	113.19	121.46
31	B	836	CLA	CHA-C4D-ND	3.41	139.64	132.50
31	B	825	CLA	CAC-C3C-C4C	3.41	129.24	124.81
31	a	312	CLA	CHA-C4D-ND	3.41	139.63	132.50
31	a	312	CLA	CHD-C4C-NC	3.41	129.58	124.20
31	A	849	CLA	CHA-C4D-ND	3.41	139.63	132.50
31	4	307	CLA	C4D-CHA-C1A	-3.41	117.10	121.25
31	J	105	CLA	CHD-C4C-NC	3.41	129.57	124.20
31	3	309	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
31	a	315	CLA	O2D-CGD-CBD	3.41	117.33	111.27
26	3	301	BCR	C2-C1-C6	3.41	115.73	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	4	317	CHL	CHD-C1D-ND	-3.41	121.32	124.45
31	A	852	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
31	9	314	CLA	CHA-C4D-ND	3.41	139.63	132.50
31	A	854	CLA	CHA-C4D-ND	3.41	139.62	132.50
31	B	845	CLA	CHA-C4D-ND	3.41	139.62	132.50
31	F	301	CLA	C4D-CHA-C1A	-3.41	117.10	121.25
36	b	301	LUT	C4-C5-C6	-3.41	113.26	120.85
31	B	850	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
31	9	316	CLA	CHA-C4D-ND	3.41	139.62	132.50
31	2	312	CLA	O1D-CGD-CBD	-3.40	117.52	124.48
31	B	828	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
31	7	309	CLA	CHA-C4D-ND	3.40	139.62	132.50
32	4	313	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
32	4	313	CHL	C4D-C3D-CAD	3.40	112.11	108.10
31	7	311	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
31	2	305	CLA	CHA-C4D-ND	3.40	139.62	132.50
31	B	813	CLA	CHD-C4C-NC	3.40	129.56	124.20
31	b	304	CLA	CHD-C4C-NC	3.40	129.56	124.20
36	2	301	LUT	C18-C5-C4	-3.40	108.06	114.36
31	a	316	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
36	a	305	LUT	C30-C31-C32	-3.40	112.62	123.22
31	2	304	CLA	CHA-C4D-ND	3.40	139.60	132.50
31	B	822	CLA	O2D-CGD-CBD	3.40	117.30	111.27
31	7	310	CLA	C4C-C3C-C2C	-3.39	103.96	107.07
31	B	838	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
31	B	820	CLA	CHD-C4C-NC	3.39	129.54	124.20
31	4	305	CLA	CMC-C2C-C1C	3.39	130.20	125.04
31	4	309	CLA	CHA-C4D-ND	3.39	139.59	132.50
31	B	816	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
31	8	317	CLA	C4D-CHA-C1A	-3.39	117.13	121.25
31	A	826	CLA	CHA-C4D-ND	3.39	139.59	132.50
31	8	308	CLA	CHA-C4D-ND	3.39	139.59	132.50
31	B	838	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	A	816	CLA	CHD-C4C-NC	3.39	129.54	124.20
31	A	821	CLA	CHD-C4C-NC	3.39	129.54	124.20
31	2	315	CLA	CHA-C4D-ND	3.38	139.58	132.50
31	A	830	CLA	C4D-CHA-C1A	-3.38	117.13	121.25
36	7	305	LUT	C10-C11-C12	-3.38	112.66	123.22
31	A	843	CLA	C3B-C2B-C1B	-3.38	103.08	107.16
31	A	821	CLA	CHA-C4D-ND	3.38	139.57	132.50
31	A	836	CLA	CMD-C2D-C1D	3.38	130.67	124.71
32	7	318	CHL	CHD-C4C-NC	3.38	129.53	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	317	CHL	CHD-C4C-NC	3.38	129.53	124.20
36	2	301	LUT	C8-C7-C6	-3.38	117.71	127.20
32	7	317	CHL	C4D-C3D-CAD	3.38	112.08	108.10
31	a	310	CLA	CHD-C1D-ND	-3.38	121.35	124.45
32	A	840	CHL	O2D-CGD-CBD	3.38	117.27	111.27
31	b	313	CLA	CHA-C4D-ND	3.38	139.56	132.50
32	a	317	CHL	O2A-CGA-CBA	3.38	122.50	111.91
31	b	312	CLA	CHD-C4C-C3C	-3.38	119.88	124.84
31	3	309	CLA	CHA-C4D-ND	3.37	139.56	132.50
31	3	319	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
31	G	205	CLA	CHA-C4D-ND	3.37	139.55	132.50
31	3	317	CLA	C4D-CHA-C1A	-3.37	117.15	121.25
36	a	305	LUT	C21-C26-C25	3.37	117.45	111.42
31	B	822	CLA	O1D-CGD-CBD	-3.37	117.59	124.48
31	B	817	CLA	CMB-C2B-C1B	3.37	130.50	125.37
31	L	307	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
32	a	320	CHL	CHD-C4C-NC	3.37	129.51	124.20
36	4	303	LUT	C10-C11-C12	-3.37	112.72	123.22
31	a	313	CLA	O1D-CGD-CBD	-3.36	117.60	124.48
31	3	308	CLA	CHD-C4C-NC	3.36	129.50	124.20
36	9	302	LUT	C21-C26-C27	-3.36	108.45	112.70
31	A	842	CLA	CHA-C4D-ND	3.36	139.54	132.50
31	B	839	CLA	CHD-C4C-NC	3.36	129.50	124.20
31	B	846	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
31	A	850	CLA	O1D-CGD-CBD	-3.36	117.60	124.48
31	9	319	CLA	O1D-CGD-CBD	-3.36	117.60	124.48
31	A	830	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
31	8	310	CLA	O1D-CGD-CBD	-3.36	117.61	124.48
31	A	826	CLA	CHD-C1D-ND	-3.36	121.36	124.45
32	8	319	CHL	CHD-C4C-NC	3.36	129.50	124.20
31	B	838	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
31	B	822	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
36	J	103	LUT	C7-C6-C5	-3.36	113.33	121.46
31	A	833	CLA	CHA-C4D-ND	3.36	139.52	132.50
31	7	312	CLA	O1D-CGD-CBD	-3.36	117.61	124.48
31	A	818	CLA	CHB-C1B-NB	-3.36	120.70	124.26
31	A	853	CLA	CHD-C4C-NC	3.36	129.49	124.20
26	6	302	BCR	C24-C23-C22	-3.35	121.17	126.23
31	K	205	CLA	CHB-C1B-NB	-3.35	120.71	124.26
32	8	319	CHL	C4D-C3D-CAD	3.35	112.05	108.10
31	b	313	CLA	O2A-CGA-CBA	3.35	122.43	111.91
31	a	314	CLA	CHA-C4D-ND	3.35	139.51	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	844	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
31	B	850	CLA	C2C-C1C-NC	3.35	113.11	109.97
31	A	825	CLA	CHA-C4D-ND	3.35	139.51	132.50
31	a	319	CLA	CHA-C4D-ND	3.35	139.51	132.50
31	2	305	CLA	O1D-CGD-CBD	-3.35	117.63	124.48
31	7	309	CLA	CHD-C4C-NC	3.35	129.48	124.20
31	B	828	CLA	CHA-C4D-ND	3.35	139.51	132.50
31	A	855	CLA	CHA-C4D-ND	3.35	139.51	132.50
31	b	303	CLA	CHD-C1D-ND	-3.35	121.38	124.45
36	F	304	LUT	C7-C6-C5	-3.35	113.35	121.46
32	8	316	CHL	C4D-C3D-CAD	3.35	112.04	108.10
31	3	313	CLA	CHA-C4D-ND	3.35	139.50	132.50
31	7	311	CLA	CHD-C4C-NC	3.35	129.47	124.20
31	B	849	CLA	O1D-CGD-CBD	-3.34	117.64	124.48
31	L	306	CLA	CHA-C4D-ND	3.34	139.50	132.50
32	A	839	CHL	C4-C3-C5	3.34	120.90	115.27
31	B	827	CLA	CHA-C4D-ND	3.34	139.49	132.50
31	3	311	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
31	B	825	CLA	CMC-C2C-C1C	3.34	130.13	125.04
32	K	201	CHL	CHB-C1B-NB	-3.34	120.72	124.26
32	a	317	CHL	C4D-C3D-CAD	3.34	112.04	108.10
31	A	827	CLA	CHD-C4C-NC	3.34	129.47	124.20
36	6	303	LUT	C35-C15-C14	-3.34	116.63	123.47
36	F	304	LUT	C30-C31-C32	-3.34	112.79	123.22
36	4	303	LUT	C7-C6-C5	-3.34	113.37	121.46
31	F	305	CLA	CHD-C1D-ND	-3.34	121.38	124.45
31	O	202	CLA	CHD-C4C-C3C	-3.34	119.76	124.98
31	4	320	CLA	CHA-C4D-ND	3.34	139.49	132.50
26	J	102	BCR	C2-C1-C6	3.34	115.62	110.48
31	B	821	CLA	CHA-C4D-ND	3.34	139.48	132.50
32	8	316	CHL	CHD-C1D-ND	-3.34	121.39	124.45
31	5	318	CLA	C4-C3-C5	3.34	120.89	115.27
31	2	306	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
31	A	846	CLA	CHD-C4C-NC	3.34	129.46	124.20
31	7	311	CLA	CHA-C4D-ND	3.34	139.48	132.50
31	3	319	CLA	CMC-C2C-C1C	3.34	130.12	125.04
36	6	304	LUT	C8-C7-C6	-3.34	117.83	127.20
31	B	813	CLA	CHA-C4D-ND	3.34	139.48	132.50
31	a	313	CLA	C4-C3-C5	3.34	120.88	115.27
32	A	839	CHL	C1-O2A-CGA	3.33	125.19	116.44
31	A	823	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
31	A	844	CLA	O1D-CGD-CBD	-3.33	117.66	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	317	CHL	CHD-C1D-ND	-3.33	121.39	124.45
31	A	843	CLA	CHA-C4D-ND	3.33	139.47	132.50
31	8	308	CLA	O2A-CGA-CBA	3.33	122.36	111.91
31	L	306	CLA	CHD-C4C-NC	3.33	129.45	124.20
32	6	320	CHL	C4D-C3D-CAD	3.33	112.02	108.10
31	B	826	CLA	CHA-C4D-ND	3.33	139.47	132.50
32	3	315	CHL	CHD-C4C-NC	3.33	129.45	124.20
31	B	849	CLA	C3D-C2D-C1D	-3.33	101.29	105.83
37	J	104	LMG	O6-C1-O1	-3.33	102.09	109.97
32	a	320	CHL	CHD-C1D-ND	-3.33	121.40	124.45
31	B	828	CLA	C3B-C2B-C1B	-3.33	103.14	107.16
43	5	306	PTY	C6-O7-C8	3.33	125.98	117.79
32	K	201	CHL	O2D-CGD-O1D	-3.33	117.34	123.84
31	A	857	CLA	CMB-C2B-C1B	3.32	130.43	125.37
36	6	304	LUT	C17-C1-C6	-3.32	104.91	110.30
31	a	315	CLA	CHA-C4D-ND	3.32	139.45	132.50
31	8	313	CLA	CHD-C4C-NC	3.32	129.44	124.20
31	K	204	CLA	C1-C2-C3	-3.32	121.38	126.75
31	A	817	CLA	CHD-C4C-NC	3.32	129.43	124.20
31	4	308	CLA	C4D-CHA-C1A	-3.32	117.21	121.25
31	A	814	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
31	K	204	CLA	CHD-C4C-NC	3.32	129.43	124.20
31	3	314	CLA	CHA-C4D-ND	3.32	139.43	132.50
32	5	322	CHL	O1D-CGD-CBD	-3.31	117.70	124.48
31	7	321	CLA	CHD-C4C-NC	3.31	129.43	124.20
31	A	856	CLA	C4D-CHA-C1A	-3.31	117.22	121.25
31	6	312	CLA	C4D-CHA-C1A	-3.31	117.22	121.25
31	B	842	CLA	O2A-CGA-CBA	3.31	122.30	111.91
31	7	312	CLA	CHD-C4C-NC	3.31	129.42	124.20
31	B	847	CLA	CHD-C4C-NC	3.31	129.42	124.20
31	4	321	CLA	C4D-CHA-C1A	-3.31	117.22	121.25
31	A	832	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
32	A	840	CHL	C2D-C1D-ND	3.31	112.54	110.10
31	K	206	CLA	CHA-C4D-ND	3.31	139.42	132.50
31	A	848	CLA	CHD-C4C-C3C	-3.31	119.98	124.84
31	A	841	CLA	C3D-C2D-C1D	-3.30	101.32	105.83
31	J	105	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
31	A	856	CLA	CHA-C4D-ND	3.30	139.41	132.50
31	5	307	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
31	A	850	CLA	CHD-C4C-NC	3.30	129.41	124.20
31	B	843	CLA	CHA-C4D-ND	3.30	139.41	132.50
32	6	318	CHL	O2D-CGD-O1D	-3.30	117.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	318	CLA	CHA-C4D-ND	3.30	139.41	132.50
31	8	321	CLA	CHA-C4D-ND	3.30	139.41	132.50
32	7	324	CHL	CHD-C1D-ND	-3.30	121.42	124.45
30	A	813	CL0	C4A-NA-C1A	-3.30	105.22	106.71
30	A	813	CL0	CHB-C1B-NB	-3.30	120.76	124.26
31	L	305	CLA	C3D-C2D-C1D	-3.30	101.33	105.83
31	B	833	CLA	CHD-C4C-NC	3.30	129.40	124.20
31	2	311	CLA	O1D-CGD-CBD	-3.30	117.73	124.48
36	4	302	LUT	C30-C31-C32	-3.30	112.92	123.22
32	a	320	CHL	C4D-C3D-CAD	3.30	111.98	108.10
31	F	306	CLA	O1D-CGD-CBD	-3.30	117.73	124.48
31	A	841	CLA	C4D-CHA-C1A	-3.30	117.23	121.25
31	2	304	CLA	CHD-C4C-NC	3.30	129.40	124.20
31	A	857	CLA	CHA-C4D-ND	3.30	139.40	132.50
40	7	306	XAT	C20-C13-C14	-3.30	118.30	122.92
31	2	308	CLA	CHD-C4C-NC	3.30	129.40	124.20
31	B	833	CLA	CHA-C4D-ND	3.30	139.40	132.50
31	A	829	CLA	CHB-C4A-NA	3.30	129.07	124.51
36	8	302	LUT	C17-C1-C6	-3.30	104.95	110.30
31	A	836	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
31	5	307	CLA	CHA-C4D-ND	3.29	139.39	132.50
31	B	821	CLA	C4D-CHA-C1A	-3.29	117.24	121.25
31	6	322	CLA	C4D-CHA-C1A	-3.29	117.24	121.25
32	7	319	CHL	C3D-C2D-C1D	-3.29	101.34	105.83
31	A	822	CLA	CHD-C4C-NC	3.29	129.39	124.20
31	A	835	CLA	C4D-CHA-C1A	-3.29	117.24	121.25
32	4	310	CHL	C4D-C3D-CAD	3.29	111.97	108.10
31	B	817	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
31	B	833	CLA	C1-O2A-CGA	3.29	125.07	116.44
36	8	302	LUT	C2-C3-C4	3.29	114.81	110.30
36	J	103	LUT	C8-C9-C10	-3.29	113.90	118.94
32	7	324	CHL	C3D-C2D-C1D	-3.29	101.35	105.83
31	A	848	CLA	CHA-C4D-ND	3.29	139.37	132.50
31	b	308	CLA	CHA-C4D-ND	3.29	139.37	132.50
31	3	311	CLA	CHD-C1D-ND	-3.29	121.43	124.45
32	A	839	CHL	CGD-CBD-CAD	3.29	121.38	110.73
31	9	316	CLA	O1D-CGD-CBD	-3.29	117.76	124.48
31	3	313	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
36	9	302	LUT	C30-C31-C32	-3.28	112.98	123.22
32	a	318	CHL	C4D-C3D-CAD	3.28	111.96	108.10
32	6	319	CHL	O1D-CGD-CBD	-3.28	117.77	124.48
36	J	103	LUT	C12-C13-C14	-3.28	113.91	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	813	CL0	CMB-C2B-C1B	3.28	130.37	125.37
32	7	320	CHL	C4D-C3D-CAD	3.28	111.96	108.10
32	5	322	CHL	C4D-C3D-CAD	3.28	111.96	108.10
31	b	304	CLA	CHA-C4D-ND	3.28	139.35	132.50
31	A	818	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
35	7	303	QTB	C09-C02-C03	3.28	123.97	118.94
31	b	310	CLA	CHD-C4C-NC	3.28	129.37	124.20
31	B	811	CLA	CMB-C2B-C1B	3.28	130.36	125.37
36	F	304	LUT	C1-C6-C7	-3.27	106.51	115.78
32	6	320	CHL	CHD-C1D-ND	-3.27	121.44	124.45
31	7	309	CLA	O2A-CGA-CBA	3.27	122.18	111.91
31	8	320	CLA	CHA-C4D-ND	3.27	139.35	132.50
31	4	312	CLA	O1D-CGD-CBD	-3.27	117.79	124.48
31	B	825	CLA	O1D-CGD-CBD	-3.27	117.79	124.48
31	A	835	CLA	CHD-C4C-C3C	-3.27	120.03	124.84
31	B	819	CLA	O1D-CGD-CBD	-3.27	117.79	124.48
31	2	308	CLA	O1D-CGD-CBD	-3.27	117.79	124.48
31	A	827	CLA	CHA-C4D-ND	3.27	139.34	132.50
31	B	818	CLA	CHA-C4D-ND	3.27	139.34	132.50
31	K	204	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
31	3	314	CLA	CHD-C4C-NC	3.27	129.35	124.20
31	B	814	CLA	CHA-C4D-ND	3.27	139.34	132.50
31	a	315	CLA	CHD-C4C-NC	3.27	129.35	124.20
31	A	841	CLA	CHA-C4D-ND	3.27	139.33	132.50
31	4	315	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
31	J	105	CLA	CHA-C4D-ND	3.26	139.33	132.50
31	A	853	CLA	O2D-CGD-CBD	3.26	117.07	111.27
31	4	315	CLA	CAC-C3C-C4C	3.26	129.04	124.81
36	5	303	LUT	C35-C15-C14	-3.26	116.79	123.47
32	6	321	CHL	C4D-C3D-CAD	3.26	111.94	108.10
31	9	312	CLA	CHD-C4C-NC	3.26	129.34	124.20
32	9	320	CHL	C4D-C3D-CAD	3.26	111.94	108.10
31	A	822	CLA	O2A-CGA-CBA	3.26	122.14	111.91
31	A	817	CLA	O1D-CGD-CBD	-3.26	117.81	124.48
31	B	840	CLA	CHD-C4C-NC	3.26	129.34	124.20
31	9	314	CLA	CHD-C4C-NC	3.25	129.33	124.20
32	6	319	CHL	CGD-CBD-CAD	3.25	121.27	110.73
31	B	842	CLA	CHA-C4D-ND	3.25	139.31	132.50
31	H	903	CLA	O1D-CGD-CBD	-3.25	117.83	124.48
31	6	316	CLA	CHA-C4D-ND	3.25	139.30	132.50
32	4	317	CHL	CHD-C4C-C3C	-3.25	120.06	124.84
31	G	204	CLA	CHD-C4C-C3C	-3.25	120.07	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	834	CLA	C4D-CHA-C1A	-3.25	117.30	121.25
31	8	310	CLA	CHA-C4D-ND	3.25	139.29	132.50
31	9	318	CLA	C1-C2-C3	-3.25	120.43	126.04
31	A	820	CLA	CHD-C4C-NC	3.25	129.32	124.20
32	6	317	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
31	B	847	CLA	C3B-C2B-C1B	-3.24	103.25	107.16
36	5	304	LUT	C30-C31-C32	-3.24	113.10	123.22
31	B	845	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
31	b	304	CLA	O1D-CGD-CBD	-3.24	117.85	124.48
32	6	319	CHL	C4D-C3D-CAD	3.24	111.92	108.10
31	A	816	CLA	CHA-C4D-ND	3.24	139.28	132.50
31	G	206	CLA	CHA-C4D-ND	3.24	139.28	132.50
31	F	301	CLA	C1-C2-C3	-3.24	120.44	126.04
32	3	315	CHL	C4D-C3D-CAD	3.24	111.91	108.10
31	8	317	CLA	CHA-C4D-ND	3.24	139.27	132.50
31	B	825	CLA	CHA-C4D-ND	3.24	139.27	132.50
32	4	310	CHL	O1D-CGD-CBD	-3.24	117.86	124.48
31	O	203	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
31	6	314	CLA	O1D-CGD-CBD	-3.24	117.86	124.48
31	2	309	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
32	a	317	CHL	CHD-C4C-NC	3.24	129.30	124.20
31	B	848	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
31	B	834	CLA	C1-C2-C3	-3.23	120.45	126.04
42	4	304	SQD	O8-S-C6	3.23	110.89	105.74
31	B	818	CLA	O1D-CGD-CBD	-3.23	117.87	124.48
31	b	311	CLA	O1D-CGD-CBD	-3.23	117.87	124.48
31	A	829	CLA	C2C-C1C-NC	3.23	113.00	109.97
32	6	309	CHL	C4D-C3D-CAD	3.23	111.90	108.10
31	B	835	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
31	b	306	CLA	CHD-C4C-NC	3.23	129.29	124.20
31	B	837	CLA	CHD-C4C-C3C	-3.23	120.10	124.84
31	2	313	CLA	O1D-CGD-CBD	-3.23	117.88	124.48
36	9	302	LUT	C1-C6-C5	-3.22	118.07	122.61
36	L	304	LUT	C30-C31-C32	-3.22	113.16	123.22
31	A	852	CLA	C3D-C2D-C1D	-3.22	101.43	105.83
32	9	322	CHL	C4D-C3D-CAD	3.22	111.89	108.10
31	B	831	CLA	CHA-C4D-ND	3.22	139.24	132.50
31	6	312	CLA	CHD-C4C-NC	3.22	129.28	124.20
31	3	318	CLA	CHD-C4C-NC	3.22	129.28	124.20
32	5	316	CHL	CHD-C4C-NC	3.22	129.28	124.20
31	9	317	CLA	C1D-ND-C4D	-3.22	104.05	106.33
31	B	831	CLA	CHD-C4C-NC	3.22	129.28	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	317	CLA	O2A-CGA-CBA	3.22	122.01	111.91
31	A	845	CLA	C4-C3-C5	3.22	120.69	115.27
36	7	305	LUT	C4-C5-C6	-3.22	113.68	120.85
31	3	319	CLA	C2C-C1C-NC	3.22	112.99	109.97
31	9	319	CLA	C4D-CHA-C1A	-3.22	117.33	121.25
31	6	310	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
32	K	201	CHL	CAC-C3C-C4C	3.22	128.98	124.81
32	7	324	CHL	C4D-C3D-CAD	3.21	111.89	108.10
31	A	843	CLA	CHD-C4C-C3C	-3.21	120.11	124.84
32	5	317	CHL	C4D-C3D-CAD	3.21	111.88	108.10
31	A	845	CLA	CHD-C4C-NC	3.21	129.27	124.20
31	B	811	CLA	CHD-C4C-NC	3.21	129.26	124.20
31	a	314	CLA	CHD-C4C-NC	3.21	129.26	124.20
31	b	308	CLA	CHD-C4C-C3C	-3.21	120.12	124.84
31	A	841	CLA	C1-C2-C3	-3.21	120.49	126.04
31	A	824	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
31	8	317	CLA	C3D-C2D-C1D	-3.21	101.45	105.83
31	4	311	CLA	CHD-C1D-ND	-3.21	121.51	124.45
31	A	842	CLA	CHD-C4C-NC	3.21	129.26	124.20
31	B	813	CLA	C1-C2-C3	-3.20	120.50	126.04
31	3	316	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
31	F	301	CLA	O1D-CGD-CBD	-3.20	117.93	124.48
31	A	855	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
31	a	313	CLA	CHD-C4C-NC	3.20	129.25	124.20
31	3	320	CLA	CHD-C4C-NC	3.20	129.25	124.20
31	8	311	CLA	C4-C3-C5	3.20	120.66	115.27
31	B	841	CLA	O1D-CGD-CBD	-3.20	117.93	124.48
31	A	819	CLA	CHD-C4C-NC	3.20	129.25	124.20
31	B	811	CLA	CHA-C4D-ND	3.20	139.19	132.50
36	8	303	LUT	C4-C5-C6	-3.20	113.72	120.85
31	B	828	CLA	C4-C3-C5	3.20	120.65	115.27
32	6	318	CHL	C4D-C3D-CAD	3.20	111.86	108.10
31	8	315	CLA	C6-C5-C3	-3.20	109.39	114.62
31	b	312	CLA	CHD-C1D-ND	-3.20	121.52	124.45
32	7	317	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
31	A	823	CLA	C1-C2-C3	-3.19	120.52	126.04
31	A	837	CLA	C4D-CHA-C1A	-3.19	117.36	121.25
31	7	322	CLA	CHA-C4D-ND	3.19	139.17	132.50
31	B	831	CLA	C1-C2-C3	-3.19	121.59	126.75
31	B	839	CLA	O1D-CGD-CBD	-3.19	117.96	124.48
26	8	301	BCR	C3-C4-C5	-3.19	108.38	114.08
31	B	819	CLA	CHD-C4C-NC	3.19	129.23	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	318	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
32	8	319	CHL	O2D-CGD-O1D	-3.19	117.61	123.84
26	B	804	BCR	C2-C1-C6	3.19	115.39	110.48
31	2	308	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
31	7	315	CLA	C4D-CHA-C1A	-3.18	117.38	121.25
31	A	842	CLA	C4-C3-C5	3.18	120.62	115.27
36	7	305	LUT	C30-C31-C32	-3.18	113.29	123.22
31	A	846	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
31	B	829	CLA	C3D-C2D-C1D	-3.18	101.49	105.83
31	b	305	CLA	CHD-C4C-NC	3.18	129.21	124.20
31	B	816	CLA	CHA-C4D-ND	3.18	139.15	132.50
31	B	845	CLA	CHD-C4C-NC	3.18	129.21	124.20
31	4	316	CLA	CMD-C2D-C3D	-3.17	120.31	127.61
31	A	819	CLA	O2A-CGA-CBA	3.17	121.87	111.91
31	4	318	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
31	B	836	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
31	A	836	CLA	C1-C2-C3	-3.17	120.56	126.04
31	F	306	CLA	C4D-CHA-C1A	-3.17	117.39	121.25
31	A	838	CLA	O1D-CGD-CBD	-3.17	118.00	124.48
32	A	839	CHL	C2C-C3C-C4C	-3.17	104.23	106.49
31	9	316	CLA	CHD-C4C-NC	3.17	129.20	124.20
32	A	840	CHL	C4-C3-C5	3.17	120.60	115.27
31	A	846	CLA	CHA-C4D-ND	3.17	139.13	132.50
32	3	315	CHL	C3D-C2D-C1D	-3.17	101.50	105.83
31	A	828	CLA	C1-C2-C3	-3.17	120.56	126.04
31	B	829	CLA	O1D-CGD-CBD	-3.17	118.00	124.48
31	6	322	CLA	CHD-C4C-NC	3.17	129.19	124.20
31	B	813	CLA	CMC-C2C-C1C	3.17	129.86	125.04
31	B	838	CLA	O1D-CGD-CBD	-3.17	118.01	124.48
31	6	313	CLA	O1D-CGD-CBD	-3.16	118.01	124.48
31	2	314	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
31	A	850	CLA	C3D-C2D-C1D	-3.16	101.51	105.83
31	A	851	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
32	7	317	CHL	C3D-C2D-C1D	-3.16	101.51	105.83
31	7	310	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	a	312	CLA	CMC-C2C-C1C	3.16	129.85	125.04
36	2	301	LUT	C4-C5-C6	-3.16	113.81	120.85
31	a	311	CLA	CHD-C4C-NC	3.16	129.18	124.20
31	K	206	CLA	C3B-C2B-C1B	-3.16	103.35	107.16
31	B	825	CLA	CHD-C4C-NC	3.15	129.17	124.20
31	3	314	CLA	C4D-CHA-C1A	-3.15	117.41	121.25
31	A	852	CLA	CHD-C4C-NC	3.15	129.17	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	844	CLA	C4D-CHA-C1A	-3.15	117.42	121.25
31	H	902	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
36	b	301	LUT	C30-C31-C32	-3.15	113.39	123.22
31	B	814	CLA	C3D-C2D-C1D	-3.15	101.53	105.83
31	A	819	CLA	C1-O2A-CGA	3.15	124.71	116.44
31	8	310	CLA	C2C-C1C-NC	3.15	112.92	109.97
31	b	313	CLA	C1-C2-C3	-3.15	120.60	126.04
36	5	303	LUT	C7-C8-C9	-3.15	121.48	126.23
32	A	839	CHL	CMD-C2D-C1D	3.15	130.26	124.71
32	4	317	CHL	C4D-C3D-CAD	3.15	111.81	108.10
31	3	307	CLA	O2A-CGA-CBA	3.15	121.78	111.91
31	9	315	CLA	CHD-C4C-NC	3.15	129.16	124.20
31	7	314	CLA	C4C-C3C-C2C	-3.15	104.19	107.07
31	A	855	CLA	CHD-C4C-NC	3.15	129.16	124.20
31	B	829	CLA	CHD-C4C-NC	3.14	129.16	124.20
31	3	308	CLA	O1D-CGD-CBD	-3.14	118.05	124.48
31	3	310	CLA	CHB-C4A-NA	3.14	128.86	124.51
31	a	321	CLA	CHD-C4C-NC	3.14	129.15	124.20
31	6	314	CLA	CHD-C4C-NC	3.14	129.15	124.20
31	A	844	CLA	CHD-C1D-ND	-3.14	121.57	124.45
26	8	301	BCR	C2-C1-C6	3.14	115.31	110.48
31	A	817	CLA	CHA-C4D-ND	3.14	139.07	132.50
36	5	304	LUT	C35-C15-C14	-3.14	117.04	123.47
31	A	834	CLA	CHA-C4D-ND	3.14	139.07	132.50
31	3	309	CLA	CHD-C4C-NC	3.14	129.15	124.20
31	A	857	CLA	O1D-CGD-CBD	-3.14	118.06	124.48
31	A	832	CLA	CHA-C4D-ND	3.14	139.06	132.50
31	7	314	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
31	9	319	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
31	O	203	CLA	C4-C3-C5	3.13	120.54	115.27
31	A	850	CLA	O2D-CGD-CBD	3.13	116.84	111.27
36	8	302	LUT	C1-C6-C5	-3.13	118.20	122.61
31	4	314	CLA	CHD-C4C-NC	3.13	129.14	124.20
32	7	320	CHL	C3D-C2D-C1D	-3.13	101.56	105.83
31	B	844	CLA	CHD-C4C-NC	3.13	129.14	124.20
31	6	307	CLA	CHD-C4C-NC	3.13	129.14	124.20
36	L	304	LUT	C18-C5-C4	-3.13	108.55	114.36
31	B	848	CLA	CHA-C4D-ND	3.13	139.05	132.50
26	3	301	BCR	C3-C4-C5	-3.13	108.49	114.08
31	B	848	CLA	C4D-CHA-C1A	-3.13	117.44	121.25
31	2	313	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
31	8	307	CLA	CHD-C4C-NC	3.13	129.13	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	821	CLA	O1D-CGD-CBD	-3.13	118.08	124.48
32	b	309	CHL	C4D-C3D-CAD	3.13	111.78	108.10
32	5	316	CHL	C1-C2-C3	-3.13	120.64	126.04
31	9	318	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
32	b	309	CHL	O2D-CGD-O1D	-3.13	117.73	123.84
32	7	319	CHL	C4D-C3D-CAD	3.12	111.78	108.10
31	B	812	CLA	C3D-C2D-C1D	-3.12	101.57	105.83
31	a	309	CLA	O2A-CGA-CBA	3.12	121.71	111.91
31	7	322	CLA	CHD-C4C-NC	3.12	129.12	124.20
32	3	315	CHL	C4-C3-C5	3.12	120.52	115.27
31	K	206	CLA	CHD-C4C-NC	3.12	129.12	124.20
32	6	319	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
36	5	303	LUT	C10-C11-C12	-3.12	113.48	123.22
31	A	826	CLA	O2D-CGD-CBD	3.12	116.81	111.27
31	B	822	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
31	5	308	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
32	8	319	CHL	C4D-CHA-C1A	-3.12	117.45	121.25
31	6	310	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
32	6	319	CHL	C3D-C2D-C1D	-3.12	101.58	105.83
36	J	103	LUT	C1-C6-C5	-3.12	118.22	122.61
31	3	307	CLA	CHD-C4C-NC	3.12	129.11	124.20
31	A	827	CLA	C1-C2-C3	-3.11	120.66	126.04
31	7	313	CLA	CHD-C4C-NC	3.11	129.11	124.20
31	B	812	CLA	O2A-CGA-CBA	3.11	121.68	111.91
31	B	833	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
31	8	315	CLA	O1D-CGD-CBD	-3.11	118.12	124.48
32	5	317	CHL	C3D-C2D-C1D	-3.11	101.58	105.83
32	5	319	CHL	CHD-C1D-ND	-3.11	121.59	124.45
32	a	320	CHL	O2D-CGD-O1D	-3.11	117.76	123.84
31	B	840	CLA	CHA-C4D-ND	3.11	139.01	132.50
31	2	315	CLA	CHD-C4C-NC	3.11	129.10	124.20
31	A	856	CLA	CHD-C4C-NC	3.11	129.10	124.20
31	A	854	CLA	O1D-CGD-CBD	-3.11	118.13	124.48
31	A	822	CLA	C3D-C2D-C1D	-3.11	101.59	105.83
26	2	302	BCR	C11-C10-C9	-3.11	122.88	127.31
31	5	311	CLA	CHD-C4C-NC	3.11	129.10	124.20
31	B	850	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
31	G	204	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
31	3	312	CLA	O1D-CGD-CBD	-3.10	118.13	124.48
36	9	305	LUT	C21-C26-C25	3.10	116.98	111.42
32	5	316	CHL	C3D-C2D-C1D	-3.10	101.59	105.83
31	5	323	CLA	CHD-C4C-NC	3.10	129.09	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	303	CLA	CHD-C4C-C3C	-3.10	120.28	124.84
31	2	305	CLA	CHD-C4C-NC	3.10	129.09	124.20
31	A	856	CLA	C3D-C2D-C1D	-3.10	101.60	105.83
31	8	312	CLA	CHD-C1D-ND	-3.10	121.61	124.45
31	A	845	CLA	C3D-C2D-C1D	-3.10	101.61	105.83
31	B	813	CLA	C3D-C2D-C1D	-3.10	101.61	105.83
31	B	847	CLA	CHA-C4D-ND	3.10	138.98	132.50
31	3	319	CLA	C1-C2-C3	-3.10	120.69	126.04
32	4	317	CHL	O2D-CGD-O1D	-3.09	117.79	123.84
31	5	310	CLA	O1D-CGD-CBD	-3.09	118.15	124.48
31	A	853	CLA	CHA-C4D-ND	3.09	138.97	132.50
31	B	815	CLA	CHD-C4C-NC	3.09	129.08	124.20
36	J	103	LUT	C17-C1-C6	-3.09	105.28	110.30
36	a	303	LUT	C17-C1-C6	-3.09	105.28	110.30
31	8	315	CLA	C4-C3-C5	3.09	120.47	115.27
32	5	316	CHL	C4D-C3D-CAD	3.09	111.74	108.10
31	8	310	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
31	B	848	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
31	3	310	CLA	CHA-C4D-ND	3.09	138.96	132.50
31	A	817	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
31	B	813	CLA	O2A-CGA-CBA	3.09	121.60	111.91
36	5	303	LUT	C18-C5-C4	-3.09	108.63	114.36
31	B	820	CLA	O1D-CGD-CBD	-3.09	118.17	124.48
32	7	324	CHL	C1-C2-C3	-3.09	120.70	126.04
40	7	306	XAT	C40-C33-C34	-3.09	118.60	122.92
31	B	845	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
31	4	306	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
32	7	324	CHL	CHD-C4C-NC	3.09	129.07	124.20
31	5	315	CLA	CHD-C4C-NC	3.09	129.06	124.20
31	B	846	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
31	2	309	CLA	C4D-CHA-C1A	-3.08	117.50	121.25
30	A	813	CL0	CBC-CAC-C3C	-3.08	103.93	112.43
31	4	309	CLA	CHD-C4C-NC	3.08	129.06	124.20
31	A	822	CLA	C4D-CHA-C1A	-3.08	117.50	121.25
31	5	313	CLA	CHC-C4B-NB	3.08	127.52	124.26
31	A	841	CLA	CHB-C1B-NB	-3.08	121.00	124.26
31	6	315	CLA	CHD-C4C-NC	3.08	129.06	124.20
31	6	311	CLA	CAC-C3C-C4C	3.08	128.80	124.81
32	K	201	CHL	CHB-C4A-NA	3.08	128.77	124.51
32	K	201	CHL	C2A-C1A-CHA	-3.08	118.48	123.86
31	A	818	CLA	O2A-CGA-CBA	3.08	121.56	111.91
31	3	318	CLA	C4-C3-C5	3.08	119.50	115.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	O	203	CLA	O2A-CGA-CBA	3.07	121.56	111.91
31	A	828	CLA	CHD-C4C-NC	3.07	129.05	124.20
26	L	303	BCR	C2-C1-C6	3.07	115.21	110.48
31	A	853	CLA	O2A-CGA-CBA	3.07	121.55	111.91
31	a	316	CLA	CHD-C4C-NC	3.07	129.04	124.20
31	G	206	CLA	CHD-C4C-NC	3.07	129.04	124.20
31	7	316	CLA	CHD-C4C-NC	3.07	129.04	124.20
31	5	320	CLA	CHD-C4C-NC	3.07	129.04	124.20
31	B	826	CLA	O1D-CGD-CBD	-3.07	118.20	124.48
31	3	310	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
31	A	826	CLA	C4-C3-C5	3.07	120.43	115.27
31	4	321	CLA	CHD-C4C-NC	3.07	129.03	124.20
31	9	311	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
31	A	818	CLA	CHD-C4C-NC	3.06	129.03	124.20
31	b	308	CLA	CAC-C3C-C4C	3.06	128.79	124.81
31	3	316	CLA	CHD-C4C-NC	3.06	129.03	124.20
31	7	311	CLA	O1D-CGD-CBD	-3.06	118.22	124.48
31	B	849	CLA	C4D-CHA-C1A	-3.06	117.52	121.25
36	9	303	LUT	C18-C5-C4	-3.06	108.68	114.36
31	A	815	CLA	C3D-C2D-C1D	-3.06	101.65	105.83
31	B	817	CLA	CHA-C4D-ND	3.06	138.91	132.50
31	B	819	CLA	CMD-C2D-C1D	3.06	130.11	124.71
31	A	847	CLA	C3D-C2D-C1D	-3.06	101.65	105.83
31	A	820	CLA	C3D-C2D-C1D	-3.06	101.65	105.83
36	3	304	LUT	C18-C5-C4	-3.06	108.69	114.36
31	A	835	CLA	CAC-C3C-C4C	3.06	128.78	124.81
31	8	318	CLA	CHD-C4C-NC	3.06	129.02	124.20
31	H	901	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
32	4	310	CHL	CHD-C4C-C3C	-3.06	120.35	124.84
31	B	824	CLA	C4D-CHA-C1A	-3.06	117.53	121.25
31	4	306	CLA	CHD-C4C-NC	3.05	129.02	124.20
31	B	840	CLA	C3D-C2D-C1D	-3.05	101.66	105.83
32	6	317	CHL	C4D-CHA-C1A	-3.05	117.53	121.25
32	A	831	CHL	CAC-C3C-C4C	3.05	128.77	124.81
31	B	822	CLA	C4-C3-C5	3.05	120.41	115.27
32	9	322	CHL	CHD-C4C-C3C	-3.05	120.35	124.84
31	9	313	CLA	CHD-C4C-NC	3.05	129.01	124.20
31	b	304	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
31	7	316	CLA	C4D-CHA-C1A	-3.05	117.54	121.25
31	B	850	CLA	C3D-C2D-C1D	-3.05	101.67	105.83
26	7	304	BCR	C28-C27-C26	-3.05	108.63	114.08
31	B	837	CLA	CAC-C3C-C4C	3.05	128.76	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	839	CLA	CHA-C4D-ND	3.05	138.88	132.50
36	3	304	LUT	C30-C31-C32	-3.05	113.71	123.22
31	A	841	CLA	C6-C5-C3	-3.05	105.47	113.45
31	A	815	CLA	C1-C2-C3	-3.05	120.77	126.04
31	7	309	CLA	C1-C2-C3	-3.05	120.77	126.04
31	A	828	CLA	O1D-CGD-CBD	-3.05	118.25	124.48
31	F	306	CLA	C3D-C2D-C1D	-3.05	101.67	105.83
31	2	309	CLA	CHD-C4C-NC	3.05	129.00	124.20
31	5	309	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
31	A	818	CLA	C4-C3-C5	3.04	120.39	115.27
36	5	303	LUT	C21-C26-C27	-3.04	108.85	112.70
31	5	310	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	A	837	CLA	CHD-C4C-NC	3.04	129.00	124.20
31	A	851	CLA	C4D-CHA-C1A	-3.04	117.55	121.25
32	8	316	CHL	C3D-C2D-C1D	-3.04	101.68	105.83
31	A	823	CLA	O1D-CGD-CBD	-3.04	118.26	124.48
31	B	849	CLA	C1-C2-C3	-3.04	121.83	126.75
31	4	316	CLA	CHA-C4D-ND	3.04	138.86	132.50
32	7	318	CHL	C4D-C3D-CAD	3.04	111.68	108.10
31	5	320	CLA	CHB-C1B-NB	-3.04	121.04	124.26
32	b	309	CHL	CHD-C4C-NC	3.04	128.99	124.20
31	B	834	CLA	O1D-CGD-CBD	-3.04	118.27	124.48
31	8	317	CLA	CHB-C1B-NB	-3.04	121.04	124.26
31	A	849	CLA	CHD-C4C-NC	3.04	128.99	124.20
31	B	817	CLA	CHB-C1B-NB	-3.04	121.04	124.26
36	a	303	LUT	C12-C13-C14	-3.03	114.28	118.94
31	A	838	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
36	b	301	LUT	C18-C5-C4	-3.03	108.74	114.36
31	A	821	CLA	C3D-C2D-C1D	-3.03	101.69	105.83
31	2	306	CLA	CHD-C4C-NC	3.03	128.98	124.20
31	L	307	CLA	CHD-C4C-C3C	-3.03	120.38	124.84
31	B	818	CLA	C3D-C2D-C1D	-3.03	101.69	105.83
31	B	850	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	B	816	CLA	CMC-C2C-C1C	3.03	129.65	125.04
31	3	319	CLA	CHA-C4D-ND	3.03	138.84	132.50
31	9	318	CLA	CHC-C1C-NC	-3.03	119.61	124.20
31	B	845	CLA	O2A-CGA-CBA	3.03	121.41	111.91
31	3	320	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
31	4	309	CLA	O1D-CGD-CBD	-3.03	118.29	124.48
31	B	823	CLA	O1D-CGD-CBD	-3.03	118.29	124.48
31	9	311	CLA	O2A-CGA-CBA	3.03	121.40	111.91
31	6	311	CLA	O1D-CGD-CBD	-3.02	118.30	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	309	CHL	C4D-CHA-C1A	-3.02	117.57	121.25
31	O	202	CLA	C4C-C3C-C2C	-3.02	104.30	107.07
32	6	317	CHL	C4D-C3D-CAD	3.02	111.66	108.10
31	J	105	CLA	CMB-C2B-C1B	3.02	129.97	125.37
36	3	305	LUT	C2-C3-C4	3.02	114.44	110.30
36	4	303	LUT	C2-C3-C4	3.02	114.44	110.30
31	A	853	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
31	3	318	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
31	6	310	CLA	CHC-C1C-NC	-3.02	119.62	124.20
31	A	819	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
26	3	303	BCR	C11-C10-C9	-3.02	123.00	127.31
31	B	812	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	a	311	CLA	CMB-C2B-C1B	3.02	129.96	125.37
31	B	849	CLA	CHD-C4C-NC	3.01	128.95	124.20
31	9	315	CLA	C3D-C2D-C1D	-3.01	101.72	105.83
32	A	831	CHL	C3D-C2D-C1D	-3.01	101.72	105.83
31	4	316	CLA	CHC-C1C-NC	-3.01	119.63	124.20
32	9	320	CHL	CHD-C4C-NC	3.01	128.95	124.20
32	6	309	CHL	CHD-C4C-NC	3.01	128.95	124.20
31	F	305	CLA	CED-O2D-CGD	3.01	122.75	115.94
36	5	304	LUT	C17-C1-C6	-3.01	105.42	110.30
31	A	815	CLA	CAC-C3C-C4C	3.01	128.71	124.81
31	B	841	CLA	C3D-C2D-C1D	-3.01	101.72	105.83
31	B	841	CLA	CHA-C4D-ND	3.01	138.79	132.50
31	B	816	CLA	C3D-C2D-C1D	-3.01	101.73	105.83
31	6	307	CLA	C1-C2-C3	-3.01	121.89	126.75
31	A	824	CLA	CHD-C4C-C3C	-3.01	120.42	124.84
32	9	320	CHL	C3D-C2D-C1D	-3.01	101.73	105.83
31	3	319	CLA	O2A-CGA-CBA	3.01	121.34	111.91
31	B	820	CLA	C4-C3-C5	3.01	120.33	115.27
31	A	842	CLA	C1-C2-C3	-3.01	120.84	126.04
31	9	312	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
32	6	318	CHL	C3D-C2D-C1D	-3.00	101.73	105.83
31	5	315	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	3	319	CLA	C3D-C2D-C1D	-3.00	101.73	105.83
32	4	310	CHL	CMD-C2D-C1D	3.00	130.00	124.71
31	a	319	CLA	CHD-C4C-NC	3.00	128.93	124.20
36	a	303	LUT	C18-C5-C4	-3.00	108.80	114.36
32	6	320	CHL	CHC-C1C-NC	-3.00	119.65	124.20
26	L	301	BCR	C2-C1-C6	3.00	115.10	110.48
31	6	306	CLA	CHC-C4B-NB	3.00	127.43	124.26
31	7	312	CLA	C4-C3-C5	3.00	120.31	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	831	CLA	C3D-C2D-C1D	-3.00	101.74	105.83
31	8	311	CLA	C3D-C2D-C1D	-3.00	101.74	105.83
31	B	830	CLA	CHD-C1D-ND	-2.99	121.70	124.45
31	A	835	CLA	C3D-C2D-C1D	-2.99	101.75	105.83
31	3	313	CLA	C4-C3-C5	2.99	120.31	115.27
31	B	842	CLA	CHD-C4C-NC	2.99	128.92	124.20
31	2	308	CLA	C3D-C2D-C1D	-2.99	101.75	105.83
31	B	834	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
31	a	311	CLA	CHB-C4A-NA	2.99	128.65	124.51
31	a	322	CLA	CHD-C4C-NC	2.99	128.91	124.20
31	5	307	CLA	O2A-CGA-CBA	2.99	121.29	111.91
31	4	316	CLA	CHD-C4C-C3C	-2.99	120.45	124.84
31	a	319	CLA	C4-C3-C5	2.99	120.30	115.27
31	A	854	CLA	C3D-C2D-C1D	-2.99	101.75	105.83
32	5	319	CHL	C3D-C2D-C1D	-2.99	101.75	105.83
32	a	320	CHL	C3D-C2D-C1D	-2.99	101.76	105.83
32	b	309	CHL	C3D-C2D-C1D	-2.99	101.76	105.83
31	3	307	CLA	CMC-C2C-C1C	2.99	129.59	125.04
31	A	818	CLA	CHA-C4D-ND	2.98	138.74	132.50
31	A	842	CLA	C3D-C2D-C1D	-2.98	101.76	105.83
31	A	826	CLA	CHD-C4C-NC	2.98	128.90	124.20
31	B	827	CLA	C4-C3-C5	2.98	120.29	115.27
32	4	313	CHL	CMB-C2B-C1B	2.98	129.91	125.37
32	5	319	CHL	C4D-C3D-CAD	2.98	111.61	108.10
31	B	823	CLA	CHD-C4C-NC	2.98	128.90	124.20
26	L	303	BCR	C24-C23-C22	-2.98	121.74	126.23
32	A	840	CHL	CHD-C4C-NC	2.98	128.89	124.20
31	8	313	CLA	C3D-C2D-C1D	-2.98	101.77	105.83
31	H	903	CLA	CHD-C4C-NC	2.98	128.89	124.20
31	L	305	CLA	CHA-C4D-ND	2.98	138.72	132.50
31	5	321	CLA	CHC-C1C-NC	-2.97	119.69	124.20
26	O	201	BCR	C3-C4-C5	-2.97	108.77	114.08
31	8	311	CLA	CHD-C4C-NC	2.97	128.89	124.20
31	A	835	CLA	O1D-CGD-CBD	-2.97	118.40	124.48
31	B	811	CLA	C4-C3-C5	2.97	120.27	115.27
32	6	320	CHL	C3D-C2D-C1D	-2.97	101.78	105.83
31	4	320	CLA	CHD-C4C-NC	2.97	128.89	124.20
31	B	848	CLA	C1-C2-C3	-2.97	120.91	126.04
32	7	318	CHL	C3D-C2D-C1D	-2.97	101.78	105.83
31	K	204	CLA	O2A-CGA-CBA	2.97	121.23	111.91
31	B	829	CLA	C4-C3-C5	2.97	120.27	115.27
31	B	830	CLA	CHD-C4C-NC	2.97	128.88	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	311	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
31	4	305	CLA	CHB-C1B-C2B	-2.97	118.86	127.24
31	A	837	CLA	CMB-C2B-C1B	2.97	129.88	125.37
31	8	309	CLA	C3D-C2D-C1D	-2.96	101.78	105.83
32	A	840	CHL	CGD-CBD-CAD	2.96	120.34	110.73
31	b	312	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
31	B	815	CLA	C1-C2-C3	-2.96	120.92	126.04
31	2	310	CLA	CHD-C4C-NC	2.96	128.87	124.20
31	7	321	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
31	2	306	CLA	O2A-CGA-CBA	2.96	121.21	111.91
32	5	316	CHL	C2C-C3C-C4C	-2.96	104.38	106.49
31	6	308	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
31	9	315	CLA	O1D-CGD-CBD	-2.96	118.43	124.48
32	5	317	CHL	C4D-CHA-C1A	-2.96	117.65	121.25
31	B	812	CLA	C1-C2-C3	-2.96	120.92	126.04
36	3	304	LUT	C12-C13-C14	-2.96	114.40	118.94
32	9	322	CHL	C4D-CHA-C1A	-2.96	117.65	121.25
31	A	837	CLA	CAC-C3C-C4C	2.96	128.65	124.81
31	B	823	CLA	C4-C3-C5	2.96	120.25	115.27
31	A	844	CLA	CHD-C4C-NC	2.96	128.86	124.20
36	8	302	LUT	C10-C11-C12	-2.96	113.99	123.22
31	a	309	CLA	C1-C2-C3	-2.96	120.93	126.04
31	a	321	CLA	C4D-CHA-C1A	-2.95	117.65	121.25
31	B	827	CLA	C3D-C2D-C1D	-2.95	101.80	105.83
32	6	317	CHL	C3D-C2D-C1D	-2.95	101.80	105.83
36	9	305	LUT	C17-C1-C6	-2.95	105.51	110.30
31	A	837	CLA	C3D-C2D-C1D	-2.95	101.81	105.83
31	A	855	CLA	C3D-C2D-C1D	-2.95	101.81	105.83
32	8	319	CHL	C3D-C2D-C1D	-2.95	101.81	105.83
32	5	322	CHL	CHD-C4C-NC	2.95	128.85	124.20
36	J	103	LUT	C21-C26-C27	-2.94	108.98	112.70
31	B	844	CLA	C3D-C2D-C1D	-2.94	101.81	105.83
31	3	319	CLA	CAA-C2A-C1A	-2.94	102.33	111.97
31	8	308	CLA	CHD-C4C-NC	2.94	128.84	124.20
31	A	836	CLA	C3D-C2D-C1D	-2.94	101.81	105.83
31	5	311	CLA	C3D-C2D-C1D	-2.94	101.81	105.83
36	6	304	LUT	C35-C15-C14	-2.94	117.45	123.47
36	5	303	LUT	C8-C7-C6	-2.94	118.94	127.20
31	B	817	CLA	O2A-CGA-CBA	2.94	121.14	111.91
31	a	316	CLA	O1D-CGD-CBD	-2.94	118.47	124.48
36	3	305	LUT	C12-C13-C14	-2.94	114.43	118.94
31	B	829	CLA	C4D-CHA-C1A	-2.94	117.67	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	833	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
31	8	321	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
26	2	302	BCR	C15-C16-C17	-2.94	117.45	123.47
31	3	313	CLA	CHD-C4C-NC	2.94	128.83	124.20
32	7	320	CHL	O2A-CGA-CBA	2.94	121.13	111.91
31	B	842	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	B	835	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
31	A	833	CLA	CHD-C4C-NC	2.94	128.83	124.20
31	B	839	CLA	C1-C2-C3	-2.94	120.97	126.04
32	7	320	CHL	CHD-C4C-NC	2.94	128.83	124.20
31	A	845	CLA	C4D-CHA-C1A	-2.94	117.68	121.25
36	3	305	LUT	C30-C31-C32	-2.93	114.06	123.22
31	6	306	CLA	CHD-C4C-C3C	-2.93	120.53	124.84
36	5	304	LUT	C8-C7-C6	-2.93	118.96	127.20
31	B	812	CLA	CHA-C4D-ND	2.93	138.63	132.50
31	6	307	CLA	O1D-CGD-CBD	-2.93	118.48	124.48
31	5	323	CLA	C3D-C2D-C1D	-2.93	101.83	105.83
31	A	841	CLA	O2A-CGA-CBA	2.93	121.11	111.91
31	6	315	CLA	CHC-C1C-NC	-2.93	119.76	124.20
32	a	318	CHL	C3D-C2D-C1D	-2.93	101.83	105.83
31	O	203	CLA	C4D-CHA-C1A	-2.93	117.68	121.25
31	5	321	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	5	312	CLA	CHD-C4C-NC	2.93	128.82	124.20
31	B	821	CLA	CHD-C4C-NC	2.93	128.82	124.20
31	A	854	CLA	CHD-C4C-NC	2.93	128.81	124.20
31	G	204	CLA	CAC-C3C-C4C	2.93	128.61	124.81
31	L	305	CLA	C1-C2-C3	-2.93	120.98	126.04
31	G	206	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
32	6	309	CHL	O2A-CGA-CBA	2.92	121.08	111.91
31	B	820	CLA	C1-C2-C3	-2.92	120.99	126.04
31	A	828	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
31	8	318	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
31	9	319	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
36	8	303	LUT	C30-C31-C32	-2.92	114.09	123.22
31	A	827	CLA	O1D-CGD-CBD	-2.92	118.50	124.48
31	4	319	CLA	CHD-C4C-NC	2.92	128.81	124.20
36	6	304	LUT	C4-C5-C6	-2.92	114.33	120.85
31	A	820	CLA	CMC-C2C-C1C	2.92	129.49	125.04
31	7	313	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
31	8	314	CLA	O2A-CGA-CBA	2.92	121.08	111.91
31	2	310	CLA	O1D-CGD-CBD	-2.92	118.50	124.48
32	9	320	CHL	CHD-C1D-ND	-2.92	121.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	837	CLA	CMD-C2D-C1D	2.92	129.86	124.71
31	A	846	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
31	8	314	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
31	4	318	CLA	C3D-C2D-C1D	-2.92	101.84	105.83
31	A	853	CLA	O1D-CGD-CBD	-2.92	118.51	124.48
31	9	312	CLA	C3D-C2D-C1D	-2.92	101.85	105.83
31	O	204	CLA	CHD-C4C-NC	2.92	128.80	124.20
31	7	314	CLA	CHD-C4C-NC	2.92	128.80	124.20
31	O	203	CLA	O1D-CGD-CBD	-2.92	118.51	124.48
31	2	311	CLA	CAC-C3C-C4C	2.92	128.60	124.81
31	a	315	CLA	CHB-C1B-NB	-2.92	121.17	124.26
26	6	302	BCR	C11-C10-C9	-2.92	123.15	127.31
31	B	834	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
32	a	320	CHL	CHC-C1C-NC	-2.92	119.78	124.20
31	6	316	CLA	C1-C2-C3	-2.92	122.03	126.75
37	G	202	LMG	O6-C1-O1	-2.92	103.07	109.97
31	B	816	CLA	CHD-C4C-NC	2.92	128.80	124.20
31	B	835	CLA	CAC-C3C-C4C	2.92	128.59	124.81
31	J	105	CLA	CHB-C1B-NB	-2.92	121.17	124.26
31	A	857	CLA	C4-C3-C5	2.91	120.17	115.27
31	6	315	CLA	CMC-C2C-C1C	2.91	129.47	125.04
36	L	304	LUT	C10-C11-C12	-2.91	114.13	123.22
26	G	201	BCR	C27-C26-C25	2.91	126.96	122.73
31	4	309	CLA	C3D-C2D-C1D	-2.91	101.86	105.83
31	A	832	CLA	C3D-C2D-C1D	-2.91	101.86	105.83
31	b	307	CLA	CHB-C1B-NB	-2.91	121.18	124.26
31	6	313	CLA	CHD-C4C-NC	2.91	128.79	124.20
30	A	813	CL0	C4-C3-C5	2.91	120.17	115.27
31	5	318	CLA	CHD-C4C-NC	2.91	128.79	124.20
31	4	307	CLA	CMB-C2B-C1B	2.91	129.80	125.37
31	a	312	CLA	C4-C3-C5	2.91	120.16	115.27
31	4	309	CLA	CHB-C1B-NB	-2.91	121.18	124.26
31	B	838	CLA	C4D-CHA-C1A	-2.91	117.71	121.25
31	L	306	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	A	818	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
31	A	828	CLA	C4D-CHA-C1A	-2.91	117.71	121.25
31	K	204	CLA	CMC-C2C-C1C	2.91	129.47	125.04
31	A	843	CLA	C1-C2-C3	-2.91	121.02	126.04
31	3	312	CLA	C1-C2-C3	-2.91	121.02	126.04
31	A	826	CLA	O1D-CGD-CBD	-2.90	118.54	124.48
31	7	310	CLA	CHC-C1C-NC	-2.90	119.80	124.20
31	B	847	CLA	C3D-C2D-C1D	-2.90	101.87	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	309	CLA	C1-C2-C3	-2.90	122.05	126.75
31	3	310	CLA	C3D-C2D-C1D	-2.90	101.87	105.83
32	6	319	CHL	C1D-CHD-C4C	-2.90	119.80	126.06
31	4	312	CLA	CHD-C4C-NC	2.90	128.78	124.20
31	b	302	CLA	CHD-C4C-NC	2.90	128.78	124.20
31	B	846	CLA	C1-O2A-CGA	2.90	124.05	116.44
31	B	835	CLA	O2A-C1-C2	-2.90	101.01	108.64
31	4	311	CLA	O1D-CGD-CBD	-2.90	118.55	124.48
31	A	820	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	L	305	CLA	CHD-C4C-NC	2.90	128.77	124.20
32	7	324	CHL	C4-C3-C5	2.90	120.15	115.27
30	A	813	CL0	CHC-C1C-C2C	-2.90	118.68	126.73
31	a	309	CLA	C3D-C2D-C1D	-2.90	101.88	105.83
31	B	832	CLA	CHD-C4C-NC	2.90	128.77	124.20
32	4	313	CHL	C3D-C2D-C1D	-2.90	101.88	105.83
31	a	309	CLA	CHC-C1C-NC	-2.90	119.81	124.20
31	B	820	CLA	C3D-C2D-C1D	-2.90	101.88	105.83
31	A	814	CLA	CHA-C4D-ND	2.90	138.56	132.50
31	A	857	CLA	CMC-C2C-C1C	2.90	129.45	125.04
32	A	840	CHL	CMD-C2D-C1D	2.90	129.82	124.71
31	3	317	CLA	CHD-C4C-NC	2.89	128.76	124.20
32	A	831	CHL	CMB-C2B-C1B	2.89	129.78	125.37
36	b	301	LUT	C8-C7-C6	-2.89	119.08	127.20
31	A	847	CLA	CHD-C4C-NC	2.89	128.76	124.20
31	B	832	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	4	315	CLA	CMC-C2C-C1C	2.89	129.44	125.04
31	B	812	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
31	3	307	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	4	314	CLA	O1D-CGD-CBD	-2.89	118.57	124.48
31	K	204	CLA	CHC-C1C-NC	-2.89	119.82	124.20
31	A	852	CLA	O1D-CGD-CBD	-2.89	118.57	124.48
31	a	312	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	2	315	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	a	310	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	6	307	CLA	CMC-C2C-C1C	2.89	129.44	125.04
31	A	816	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	A	830	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	9	314	CLA	C3D-C2D-C1D	-2.89	101.89	105.83
31	B	844	CLA	C1-C2-C3	-2.88	121.06	126.04
31	b	302	CLA	C3D-C2D-C1D	-2.88	101.90	105.83
31	4	308	CLA	CHD-C4C-NC	2.88	128.75	124.20
31	B	836	CLA	C3D-C2D-C1D	-2.88	101.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	K	205	CLA	CHD-C4C-NC	2.88	128.75	124.20
32	6	321	CHL	C1D-CHD-C4C	-2.88	119.84	126.06
31	B	840	CLA	C4D-CHA-C1A	-2.88	117.74	121.25
31	8	317	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	a	313	CLA	C3D-C2D-C1D	-2.88	101.90	105.83
31	A	838	CLA	CHD-C1D-ND	-2.88	121.81	124.45
32	5	317	CHL	CHC-C1C-NC	-2.88	119.83	124.20
31	B	836	CLA	CHD-C4C-NC	2.88	128.74	124.20
31	B	817	CLA	C1-C2-C3	-2.88	121.07	126.04
31	B	829	CLA	CMD-C2D-C1D	2.88	129.78	124.71
31	B	815	CLA	C4-C3-C5	2.88	120.11	115.27
31	2	307	CLA	C4D-CHA-C1A	-2.88	117.75	121.25
31	A	816	CLA	C3B-C2B-C1B	-2.88	103.69	107.16
32	8	316	CHL	C4-C3-C5	2.88	120.11	115.27
31	A	820	CLA	CMD-C2D-C1D	2.88	129.78	124.71
31	A	824	CLA	CAC-C3C-C4C	2.88	128.54	124.81
31	4	305	CLA	CHC-C1C-NC	-2.88	119.84	124.20
31	5	323	CLA	C1-C2-C3	-2.87	121.07	126.04
31	b	312	CLA	CAC-C3C-C4C	2.87	128.54	124.81
31	3	307	CLA	CAC-C3C-C4C	2.87	128.54	124.81
31	8	315	CLA	CHD-C4C-NC	2.87	128.73	124.20
31	F	305	CLA	CMB-C2B-C1B	2.87	129.74	125.37
31	3	320	CLA	CHC-C1C-NC	-2.87	119.84	124.20
31	A	843	CLA	CAC-C3C-C4C	2.87	128.54	124.81
31	A	851	CLA	C3D-C2D-C1D	-2.87	101.91	105.83
31	A	821	CLA	C4-C3-C5	2.87	120.10	115.27
27	5	301	LMT	C3'-C4'-C5'	-2.87	104.34	110.93
42	4	304	SQD	O7-S-C6	2.87	110.35	106.94
31	9	318	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
31	A	815	CLA	C4-C3-C5	2.87	120.10	115.27
31	F	301	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
31	b	303	CLA	CAC-C3C-C4C	2.87	128.53	124.81
31	4	312	CLA	CHC-C1C-NC	-2.87	119.85	124.20
31	3	317	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	9	302	LUT	C18-C5-C4	-2.87	109.04	114.36
31	8	321	CLA	O1D-CGD-CBD	-2.87	118.62	124.48
32	6	321	CHL	CHD-C4C-NC	2.87	128.72	124.20
31	5	313	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
31	A	838	CLA	CAC-C3C-C4C	2.86	128.53	124.81
31	7	313	CLA	CHC-C1C-NC	-2.86	119.86	124.20
31	B	822	CLA	C3D-C2D-C1D	-2.86	101.92	105.83
31	8	312	CLA	O2D-CGD-O1D	-2.86	118.24	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	310	CLA	C4-C3-C5	2.86	120.09	115.27
31	B	818	CLA	C4-C3-C5	2.86	120.08	115.27
31	9	316	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
31	A	833	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
31	F	305	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
31	9	313	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
31	3	312	CLA	CHD-C4C-NC	2.86	128.71	124.20
31	5	312	CLA	C1-C2-C3	-2.86	122.12	126.75
32	5	316	CHL	CGD-CBD-CAD	2.86	120.00	110.73
31	A	846	CLA	C4-C3-C5	2.86	120.08	115.27
31	A	847	CLA	CMD-C2D-C1D	2.86	129.75	124.71
38	a	304	AXT	C3-C4-C5	2.86	117.55	111.85
31	B	828	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
32	6	321	CHL	CHC-C1C-NC	-2.85	119.87	124.20
31	8	320	CLA	O1D-CGD-CBD	-2.85	118.64	124.48
31	5	321	CLA	O1D-CGD-CBD	-2.85	118.64	124.48
31	8	312	CLA	CHD-C4C-NC	2.85	128.70	124.20
31	7	321	CLA	O2A-CGA-CBA	2.85	120.86	111.91
31	B	831	CLA	CHB-C1B-NB	-2.85	121.24	124.26
31	7	310	CLA	CMB-C2B-C1B	2.85	129.71	125.37
31	A	815	CLA	CHD-C4C-NC	2.85	128.69	124.20
31	8	320	CLA	CHD-C4C-NC	2.85	128.69	124.20
31	A	842	CLA	O1D-CGD-CBD	-2.85	118.66	124.48
32	A	831	CHL	CHB-C1B-NB	-2.85	121.24	124.26
31	4	308	CLA	C3D-C2D-C1D	-2.85	101.94	105.83
31	B	842	CLA	C3D-C2D-C1D	-2.85	101.95	105.83
31	a	321	CLA	CMD-C2D-C1D	2.85	129.73	124.71
31	6	312	CLA	C1-C2-C3	-2.85	121.12	126.04
31	A	819	CLA	O1D-CGD-CBD	-2.85	118.66	124.48
31	A	814	CLA	C3D-C2D-C1D	-2.84	101.95	105.83
31	4	305	CLA	CMD-C2D-C3D	-2.84	121.08	127.61
31	A	844	CLA	C1-C2-C3	-2.84	122.16	126.75
31	4	308	CLA	C4-C3-C5	2.84	120.05	115.27
31	G	206	CLA	C4D-CHA-C1A	-2.84	117.79	121.25
31	4	311	CLA	CHC-C1C-NC	-2.84	119.89	124.20
31	B	828	CLA	O1D-CGD-CBD	-2.84	118.67	124.48
31	7	312	CLA	C3D-C2D-C1D	-2.84	101.96	105.83
31	2	312	CLA	CMB-C2B-C1B	2.84	129.69	125.37
32	A	840	CHL	C2C-C3C-C4C	-2.84	104.47	106.49
31	K	204	CLA	CHA-C4D-ND	2.84	138.43	132.50
31	5	320	CLA	CMD-C2D-C1D	2.84	129.71	124.71
31	6	315	CLA	C3D-C2D-C1D	-2.83	101.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	317	CLA	CHD-C4C-C3C	-2.83	120.67	124.84
31	B	844	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
32	5	319	CHL	CHD-C4C-NC	2.83	128.67	124.20
31	A	852	CLA	O2A-CGA-CBA	2.83	120.80	111.91
31	A	832	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
31	b	311	CLA	CHD-C4C-NC	2.83	128.66	124.20
31	3	313	CLA	O2A-CGA-CBA	2.83	120.79	111.91
31	5	313	CLA	CHB-C1B-NB	-2.83	121.26	124.26
31	8	309	CLA	CMB-C2B-C1B	2.83	129.68	125.37
31	A	841	CLA	CMD-C2D-C1D	2.83	129.70	124.71
31	7	316	CLA	CMB-C2B-C1B	2.83	129.68	125.37
31	B	826	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
31	A	815	CLA	CHA-C4D-ND	2.83	138.41	132.50
31	A	825	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
31	A	841	CLA	CAC-C3C-C4C	2.83	128.48	124.81
31	A	857	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
32	4	310	CHL	C3D-C2D-C1D	-2.83	101.97	105.83
31	A	816	CLA	CMB-C2B-C1B	2.83	129.67	125.37
31	9	316	CLA	C1-C2-C3	-2.83	122.18	126.75
32	4	317	CHL	C3D-C2D-C1D	-2.82	101.98	105.83
31	a	314	CLA	CED-O2D-CGD	2.82	122.33	115.94
31	A	826	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
31	B	824	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
31	3	318	CLA	O2A-CGA-CBA	2.82	120.77	111.91
31	B	847	CLA	C4-C3-C5	2.82	120.02	115.27
31	A	825	CLA	CMC-C2C-C1C	2.82	129.34	125.04
35	a	302	QTB	C09-C02-C03	2.82	123.27	118.94
31	7	309	CLA	CMD-C2D-C1D	2.82	129.69	124.71
31	B	850	CLA	CMC-C2C-C1C	2.82	129.34	125.04
31	3	318	CLA	O1D-CGD-CBD	-2.82	118.71	124.48
31	8	309	CLA	C1D-CHD-C4C	-2.82	119.97	126.06
36	4	302	LUT	C18-C5-C4	-2.82	109.13	114.36
32	6	319	CHL	CHB-C1B-NB	-2.82	121.27	124.26
31	3	308	CLA	CHC-C1C-NC	-2.82	119.93	124.20
31	9	318	CLA	CAC-C3C-C4C	2.82	128.47	124.81
31	B	819	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
31	4	319	CLA	CHC-C1C-NC	-2.82	119.93	124.20
31	B	833	CLA	CHB-C1B-NB	-2.82	121.28	124.26
26	3	303	BCR	C2-C1-C6	2.82	114.82	110.48
28	7	307	LHG	O8-C23-C24	2.81	120.74	111.91
32	5	316	CHL	O2A-CGA-CBA	2.81	120.74	111.91
31	b	308	CLA	O1D-CGD-CBD	-2.81	118.73	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	827	CLA	CMC-C2C-C1C	2.81	129.32	125.04
36	b	301	LUT	C35-C15-C14	-2.81	117.71	123.47
31	A	824	CLA	C3D-C2D-C1D	-2.81	101.99	105.83
32	a	320	CHL	O2A-CGA-CBA	2.81	120.73	111.91
31	A	829	CLA	C2A-C3A-C4A	2.81	106.41	101.87
31	2	312	CLA	CHD-C4C-NC	2.81	128.63	124.20
31	B	847	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
31	7	314	CLA	O2A-CGA-CBA	2.81	120.73	111.91
31	a	321	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
32	5	322	CHL	CHC-C1C-NC	-2.81	119.94	124.20
31	6	322	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	A	831	CHL	C4-C3-C5	2.81	120.00	115.27
36	b	301	LUT	C10-C11-C12	-2.81	114.45	123.22
31	a	316	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
31	L	306	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
32	6	318	CHL	CHD-C4C-NC	2.81	128.63	124.20
31	b	310	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
31	9	315	CLA	CMD-C2D-C1D	2.81	129.66	124.71
26	G	203	BCR	C27-C26-C25	2.81	126.81	122.73
31	3	309	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
31	A	857	CLA	CAC-C3C-C4C	2.81	128.45	124.81
31	H	902	CLA	CHD-C4C-NC	2.81	128.63	124.20
31	a	319	CLA	CHC-C1C-NC	-2.81	119.94	124.20
31	8	311	CLA	CMD-C2D-C1D	2.81	129.66	124.71
31	a	322	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
31	A	838	CLA	CHD-C4C-NC	2.81	128.62	124.20
31	6	307	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
31	3	309	CLA	C4-C3-C5	2.80	119.99	115.27
31	A	823	CLA	C3D-C2D-C1D	-2.80	102.00	105.83
31	K	205	CLA	O1D-CGD-CBD	-2.80	118.75	124.48
31	a	309	CLA	CMC-C2C-C1C	2.80	129.31	125.04
31	3	319	CLA	CAC-C3C-C4C	2.80	128.44	124.81
31	B	850	CLA	C1-C2-C3	-2.80	121.20	126.04
31	A	837	CLA	C1-C2-C3	-2.80	121.20	126.04
32	6	321	CHL	C3D-C2D-C1D	-2.80	102.01	105.83
31	A	830	CLA	CMC-C2C-C1C	2.80	129.30	125.04
31	6	306	CLA	CMD-C2D-C3D	-2.80	121.17	127.61
32	7	320	CHL	O1D-CGD-CBD	-2.80	118.75	124.48
32	5	322	CHL	C4D-CHA-C1A	-2.80	117.84	121.25
32	5	316	CHL	O1D-CGD-CBD	-2.80	118.76	124.48
31	2	304	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
36	F	304	LUT	C10-C11-C12	-2.80	114.48	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	K	201	CHL	CMD-C2D-C3D	-2.80	121.18	127.61
31	4	312	CLA	CMD-C2D-C1D	2.80	129.64	124.71
31	7	309	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
36	9	303	LUT	C12-C13-C14	-2.80	114.65	118.94
31	4	315	CLA	C3D-C2D-C1D	-2.80	102.02	105.83
31	B	844	CLA	CAC-C3C-C4C	2.80	128.44	124.81
32	A	831	CHL	CHD-C4C-C3C	-2.80	120.73	124.84
31	O	203	CLA	CHC-C1C-NC	-2.80	119.96	124.20
31	L	305	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
31	A	827	CLA	C3D-C2D-C1D	-2.80	102.02	105.83
31	A	817	CLA	C1-O2A-CGA	2.79	123.78	116.44
31	2	312	CLA	C3D-C2D-C1D	-2.79	102.02	105.83
31	A	817	CLA	CAC-C3C-C4C	2.79	128.44	124.81
31	2	311	CLA	CHD-C4C-NC	2.79	128.61	124.20
31	A	816	CLA	CAC-C3C-C4C	2.79	128.44	124.81
36	8	302	LUT	C30-C31-C32	-2.79	114.50	123.22
31	6	313	CLA	C3D-C2D-C1D	-2.79	102.02	105.83
36	9	302	LUT	C4-C5-C6	-2.79	114.62	120.85
31	b	307	CLA	CHD-C4C-NC	2.79	128.60	124.20
31	7	316	CLA	CMC-C2C-C1C	2.79	129.29	125.04
31	8	307	CLA	C3D-C2D-C1D	-2.79	102.02	105.83
31	2	307	CLA	C1-C2-C3	-2.79	121.22	126.04
36	3	304	LUT	C4-C5-C6	-2.79	114.63	120.85
31	K	205	CLA	C3D-C2D-C1D	-2.79	102.03	105.83
31	F	305	CLA	CHD-C4C-NC	2.79	128.60	124.20
31	8	317	CLA	CMD-C2D-C1D	2.79	129.63	124.71
31	3	316	CLA	C3D-C2D-C1D	-2.79	102.03	105.83
31	8	308	CLA	C3D-C2D-C1D	-2.79	102.03	105.83
31	8	309	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
31	6	313	CLA	CHC-C1C-NC	-2.79	119.97	124.20
31	9	319	CLA	CHD-C4C-NC	2.79	128.60	124.20
31	B	841	CLA	CHB-C1B-NB	-2.79	121.31	124.26
31	H	903	CLA	CHC-C1C-NC	-2.79	119.98	124.20
31	7	321	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
31	B	834	CLA	CHD-C4C-NC	2.78	128.59	124.20
36	4	302	LUT	C10-C11-C12	-2.78	114.53	123.22
32	6	320	CHL	C4D-CHA-C1A	-2.78	117.86	121.25
31	A	851	CLA	C4-C3-C5	2.78	119.95	115.27
31	9	321	CLA	CMD-C2D-C1D	2.78	129.62	124.71
31	O	204	CLA	O1D-CGD-CBD	-2.78	118.79	124.48
31	B	830	CLA	C4-C3-C5	2.78	119.95	115.27
31	9	312	CLA	O1D-CGD-CBD	-2.78	118.79	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	308	CLA	CHC-C1C-NC	-2.78	119.98	124.20
32	a	317	CHL	C3D-C2D-C1D	-2.78	102.04	105.83
31	2	313	CLA	CHD-C4C-NC	2.78	128.58	124.20
31	4	307	CLA	CHD-C4C-NC	2.78	128.58	124.20
31	8	318	CLA	C1-C2-C3	-2.78	122.25	126.75
26	6	302	BCR	C27-C26-C25	2.78	126.77	122.73
31	A	823	CLA	C4D-CHA-C1A	-2.78	117.87	121.25
36	3	304	LUT	C21-C26-C27	-2.78	109.19	112.70
26	G	201	BCR	C7-C8-C9	-2.78	122.04	126.23
31	B	818	CLA	CAC-C3C-C4C	2.78	128.41	124.81
31	B	821	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
31	9	311	CLA	CHD-C4C-NC	2.78	128.58	124.20
31	A	818	CLA	C1-C2-C3	-2.78	121.24	126.04
31	5	308	CLA	CHD-C4C-NC	2.78	128.58	124.20
32	7	318	CHL	C4-C3-C5	2.78	119.94	115.27
32	a	320	CHL	O1D-CGD-CBD	-2.78	118.80	124.48
31	B	811	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
28	a	306	LHG	O8-C23-C24	2.77	120.61	111.91
31	6	316	CLA	C3D-C2D-C1D	-2.77	102.05	105.83
36	8	303	LUT	C21-C26-C25	2.77	116.38	111.42
31	B	850	CLA	C4-C3-C5	2.77	119.93	115.27
31	F	306	CLA	C1-C2-C3	-2.77	122.27	126.75
31	7	315	CLA	C3D-C2D-C1D	-2.77	102.05	105.83
31	3	316	CLA	C1-C2-C3	-2.77	122.27	126.75
31	2	314	CLA	CHD-C4C-NC	2.77	128.57	124.20
31	B	846	CLA	O2A-CGA-CBA	2.77	120.60	111.91
40	7	306	XAT	C12-C13-C14	2.77	123.19	118.94
31	A	817	CLA	C4-C3-C5	2.77	119.92	115.27
31	B	825	CLA	C3D-C2D-C1D	-2.77	102.06	105.83
31	A	823	CLA	CHD-C4C-NC	2.77	128.56	124.20
31	B	814	CLA	CHB-C4A-NA	2.77	128.34	124.51
31	4	314	CLA	CHB-C1B-NB	-2.76	121.33	124.26
31	9	311	CLA	C4-C3-C5	2.76	119.92	115.27
32	5	322	CHL	C3D-C2D-C1D	-2.76	102.06	105.83
31	5	310	CLA	CHC-C1C-NC	-2.76	120.01	124.20
31	5	307	CLA	CHD-C4C-NC	2.76	128.56	124.20
31	4	316	CLA	O2A-CGA-CBA	2.76	120.58	111.91
31	B	836	CLA	C1-O2A-CGA	2.76	123.70	116.44
31	A	837	CLA	CHB-C1B-NB	-2.76	121.33	124.26
31	5	323	CLA	CHC-C1C-NC	-2.76	120.01	124.20
31	B	816	CLA	CAC-C3C-C4C	2.76	128.40	124.81
31	4	320	CLA	CHB-C1B-NB	-2.76	121.33	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	H	902	CLA	CHC-C1C-NC	-2.76	120.01	124.20
31	5	308	CLA	CMB-C2B-C1B	2.76	129.57	125.37
32	7	317	CHL	CMD-C2D-C1D	2.76	129.58	124.71
31	3	308	CLA	C3D-C2D-C1D	-2.76	102.06	105.83
31	7	322	CLA	CMB-C2B-C1B	2.76	129.57	125.37
31	B	849	CLA	O2D-CGD-CBD	2.76	116.17	111.27
31	6	310	CLA	CHD-C4C-NC	2.76	128.55	124.20
31	a	315	CLA	C3D-C2D-C1D	-2.76	102.06	105.83
31	7	310	CLA	C1D-CHD-C4C	-2.76	120.11	126.06
32	7	319	CHL	C2D-C1D-ND	2.76	112.14	110.10
31	B	814	CLA	CHD-C4C-NC	2.76	128.55	124.20
31	6	307	CLA	CMD-C2D-C1D	2.76	129.57	124.71
31	4	320	CLA	C3D-C2D-C1D	-2.76	102.07	105.83
31	7	310	CLA	C3D-C2D-C1D	-2.76	102.07	105.83
36	2	301	LUT	C30-C31-C32	-2.76	114.61	123.22
31	b	313	CLA	CHD-C4C-C3C	-2.76	120.79	124.84
31	5	309	CLA	CHD-C4C-NC	2.76	128.55	124.20
31	8	320	CLA	O2A-CGA-CBA	2.76	120.56	111.91
31	B	827	CLA	O1D-CGD-CBD	-2.76	118.85	124.48
31	2	310	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
31	G	204	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
31	8	315	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
31	6	312	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
31	6	308	CLA	O2A-CGA-CBA	2.75	120.55	111.91
31	6	310	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
31	B	838	CLA	CAC-C3C-C4C	2.75	128.38	124.81
31	8	314	CLA	C1-C2-C3	-2.75	121.28	126.04
31	B	839	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
31	5	312	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
31	B	824	CLA	C4-C3-C5	2.75	119.90	115.27
31	9	315	CLA	CHC-C1C-NC	-2.75	120.03	124.20
31	B	818	CLA	CHD-C4C-NC	2.75	128.54	124.20
31	a	319	CLA	CMB-C2B-C1B	2.75	129.56	125.37
26	L	301	BCR	C29-C30-C25	2.75	114.71	110.48
36	8	303	LUT	C7-C6-C5	-2.75	114.80	121.46
31	2	310	CLA	CHC-C1C-NC	-2.75	120.03	124.20
31	4	318	CLA	CHD-C4C-NC	2.75	128.53	124.20
31	b	305	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
31	4	306	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
31	B	816	CLA	CHC-C1C-NC	-2.75	120.03	124.20
31	A	829	CLA	O2A-CGA-CBA	2.75	120.53	111.91
32	9	320	CHL	O2A-CGA-CBA	2.75	120.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	308	CLA	CHC-C1C-NC	-2.75	120.04	124.20
31	4	319	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
31	A	853	CLA	CED-O2D-CGD	2.75	122.15	115.94
31	B	821	CLA	C1-O2A-CGA	2.74	123.64	116.44
31	b	311	CLA	C3D-C2D-C1D	-2.74	102.09	105.83
31	O	202	CLA	C4D-CHA-C1A	-2.74	117.91	121.25
31	A	842	CLA	CMC-C2C-C1C	2.74	129.21	125.04
31	4	305	CLA	C4B-CHC-C1C	-2.74	119.84	126.34
31	a	312	CLA	CHC-C1C-NC	-2.74	120.04	124.20
31	8	307	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
31	A	850	CLA	CMD-C2D-C1D	2.74	129.54	124.71
31	6	322	CLA	CMD-C2D-C1D	2.74	129.54	124.71
33	7	308	DGD	C1E-O6E-C5E	2.74	119.07	113.69
36	4	302	LUT	C17-C1-C6	-2.74	105.86	110.30
31	5	313	CLA	CMB-C2B-C1B	2.74	129.54	125.37
26	5	302	BCR	C27-C26-C25	2.74	126.71	122.73
31	L	307	CLA	C3D-C2D-C1D	-2.74	102.09	105.83
31	A	853	CLA	C4-C3-C5	2.74	119.88	115.27
31	6	315	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
31	3	313	CLA	CAC-C3C-C4C	2.74	128.36	124.81
36	J	103	LUT	C10-C11-C12	-2.74	114.68	123.22
31	7	322	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
31	5	320	CLA	CMC-C2C-C1C	2.74	129.21	125.04
32	7	320	CHL	CHC-C1C-NC	-2.74	120.05	124.20
31	B	818	CLA	C3B-C2B-C1B	-2.74	103.86	107.16
31	L	307	CLA	CMD-C2D-C1D	2.73	129.53	124.71
31	O	203	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
36	3	304	LUT	C35-C15-C14	-2.73	117.88	123.47
28	A	811	LHG	O8-C23-C24	2.73	120.48	111.91
31	4	305	CLA	O2A-CGA-CBA	2.73	120.48	111.91
31	A	847	CLA	O1D-CGD-CBD	-2.73	118.89	124.48
31	8	307	CLA	CMC-C2C-C1C	2.73	129.20	125.04
36	F	304	LUT	C2-C3-C4	2.73	114.04	110.30
32	b	309	CHL	CHC-C1C-NC	-2.73	120.06	124.20
32	9	320	CHL	C2C-C3C-C4C	-2.73	104.54	106.49
31	3	317	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
31	B	822	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
31	a	313	CLA	CMD-C2D-C1D	2.73	129.52	124.71
26	B	805	BCR	C31-C1-C6	2.73	114.72	110.30
32	7	324	CHL	C2D-C1D-ND	2.73	112.11	110.10
31	b	307	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
31	A	821	CLA	O1D-CGD-CBD	-2.73	118.91	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	310	CLA	CMD-C2D-C1D	2.73	129.52	124.71
31	b	310	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
26	A	805	BCR	C28-C27-C26	-2.72	109.21	114.08
32	3	315	CHL	CHC-C1C-NC	-2.72	120.07	124.20
31	A	852	CLA	C4D-CHA-C1A	-2.72	117.93	121.25
28	7	302	LHG	O8-C23-C24	2.72	120.45	111.91
32	6	309	CHL	C4-C3-C5	2.72	119.85	115.27
31	7	309	CLA	CMC-C2C-C1C	2.72	129.18	125.04
31	b	306	CLA	CHC-C1C-NC	-2.72	120.08	124.20
31	8	311	CLA	C4D-CHA-C1A	-2.72	117.94	121.25
31	a	315	CLA	C1-C2-C3	-2.72	121.34	126.04
31	4	309	CLA	C1-C2-C3	-2.72	121.34	126.04
32	7	320	CHL	C4D-CHA-C1A	-2.72	117.94	121.25
31	5	314	CLA	O1D-CGD-CBD	-2.72	118.92	124.48
36	9	305	LUT	C30-C31-C32	-2.72	114.73	123.22
31	A	849	CLA	C3D-C2D-C1D	-2.72	102.12	105.83
31	5	313	CLA	CHD-C4C-C3C	-2.72	120.84	124.84
32	a	318	CHL	O2A-CGA-CBA	2.72	120.44	111.91
31	2	305	CLA	C3D-C2D-C1D	-2.72	102.12	105.83
31	5	310	CLA	CMC-C2C-C1C	2.72	129.18	125.04
31	5	310	CLA	C3D-C2D-C1D	-2.72	102.12	105.83
31	5	313	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
31	F	305	CLA	CAC-C3C-C4C	2.72	128.33	124.81
31	B	843	CLA	CHC-C1C-NC	-2.71	120.08	124.20
31	B	835	CLA	O1D-CGD-CBD	-2.71	118.93	124.48
31	b	304	CLA	C3D-C2D-C1D	-2.71	102.13	105.83
31	A	832	CLA	C1-C2-C3	-2.71	121.35	126.04
33	7	308	DGD	CDB-CCB-CBB	-2.71	100.65	114.42
31	b	311	CLA	CHC-C1C-NC	-2.71	120.09	124.20
31	5	309	CLA	CMD-C2D-C1D	2.71	129.49	124.71
31	B	811	CLA	CHB-C4A-NA	2.71	128.26	124.51
31	3	313	CLA	C3D-C2D-C1D	-2.71	102.13	105.83
26	K	202	BCR	C27-C26-C25	2.71	126.67	122.73
31	5	309	CLA	CAC-C3C-C4C	2.71	128.33	124.81
31	6	312	CLA	CED-O2D-CGD	2.71	122.07	115.94
31	A	822	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
36	8	302	LUT	C18-C5-C4	-2.71	109.33	114.36
31	7	314	CLA	C4-C3-C5	2.71	119.83	115.27
31	7	311	CLA	C1-C2-C3	-2.71	121.36	126.04
31	a	311	CLA	C3D-C2D-C1D	-2.71	102.14	105.83
31	a	316	CLA	CHB-C1B-NB	-2.71	121.39	124.26
31	2	308	CLA	O2A-CGA-CBA	2.71	122.92	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	307	CLA	CHD-C4C-NC	2.71	128.47	124.20
31	G	205	CLA	CHC-C1C-NC	-2.70	120.10	124.20
31	9	321	CLA	C3D-C2D-C1D	-2.70	102.14	105.83
31	J	105	CLA	CHB-C4A-NA	2.70	128.25	124.51
31	A	820	CLA	C4-C3-C5	2.70	119.82	115.27
31	A	829	CLA	CHB-C1B-NB	2.70	127.12	124.26
31	a	309	CLA	CHD-C4C-NC	2.70	128.46	124.20
31	O	203	CLA	CHD-C4C-NC	2.70	128.46	124.20
31	4	315	CLA	CHD-C4C-NC	2.70	128.46	124.20
31	a	310	CLA	CHD-C4C-NC	2.70	128.46	124.20
31	5	307	CLA	C3D-C2D-C1D	-2.70	102.14	105.83
31	5	313	CLA	C4D-CHA-C1A	-2.70	117.96	121.25
31	9	321	CLA	O2A-CGA-CBA	2.70	120.38	111.91
31	b	308	CLA	CMC-C2C-C1C	2.70	129.15	125.04
31	9	319	CLA	CED-O2D-CGD	2.70	122.04	115.94
31	5	314	CLA	C3D-C2D-C1D	-2.70	102.15	105.83
31	A	821	CLA	C1-C2-C3	-2.70	121.38	126.04
31	B	835	CLA	CHD-C4C-NC	2.70	128.46	124.20
36	L	304	LUT	C4-C5-C6	-2.70	114.83	120.85
31	B	820	CLA	CMC-C2C-C1C	2.70	129.15	125.04
32	6	318	CHL	O1D-CGD-CBD	-2.70	118.96	124.48
31	O	202	CLA	CHD-C4C-NC	2.70	128.45	124.20
32	3	315	CHL	O2A-CGA-CBA	2.70	120.37	111.91
31	B	825	CLA	C1-C2-C3	-2.69	121.38	126.04
31	3	307	CLA	C1-C2-C3	-2.69	121.38	126.04
31	3	313	CLA	CMC-C2C-C1C	2.69	129.14	125.04
32	7	317	CHL	CHC-C1C-NC	-2.69	120.12	124.20
31	B	813	CLA	CMD-C2D-C1D	2.69	129.46	124.71
31	6	307	CLA	O2A-CGA-CBA	2.69	120.36	111.91
32	4	313	CHL	CHD-C4C-NC	2.69	128.45	124.20
31	6	311	CLA	CHC-C1C-NC	-2.69	120.12	124.20
31	B	824	CLA	CHD-C4C-NC	2.69	128.44	124.20
32	5	316	CHL	C4-C3-C5	2.69	119.80	115.27
36	8	303	LUT	C10-C11-C12	-2.69	114.82	123.22
31	B	823	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
32	9	322	CHL	O1D-CGD-CBD	-2.69	118.98	124.48
31	3	319	CLA	CHB-C1B-NB	-2.69	121.41	124.26
31	B	819	CLA	C4-C3-C5	2.69	119.79	115.27
31	2	307	CLA	C4-C3-C5	2.69	119.79	115.27
32	6	321	CHL	C4D-CHA-C1A	-2.69	117.98	121.25
31	B	834	CLA	C1D-CHD-C4C	-2.69	120.26	126.06
31	6	322	CLA	C3D-C2D-C1D	-2.69	102.17	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	205	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
31	7	311	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
36	6	304	LUT	C30-C31-C32	-2.68	114.84	123.22
31	B	811	CLA	CAC-C3C-C4C	2.68	128.29	124.81
31	O	202	CLA	O2D-CGD-O1D	-2.68	118.00	124.09
36	a	303	LUT	C35-C15-C14	-2.68	117.98	123.47
31	A	843	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
26	5	302	BCR	C3-C4-C5	-2.68	109.29	114.08
31	F	301	CLA	O2A-CGA-CBA	2.68	120.33	111.91
36	a	303	LUT	C36-C21-C26	2.68	113.61	109.55
31	O	204	CLA	CAC-C3C-C4C	2.68	128.29	124.81
31	2	313	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
31	6	314	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
31	3	314	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
31	B	835	CLA	CMC-C2C-C1C	2.68	129.12	125.04
31	A	829	CLA	CHB-C1B-C2B	-2.68	119.67	127.24
31	9	321	CLA	CHB-C1B-NB	-2.68	121.42	124.26
31	5	312	CLA	CHB-C1B-NB	-2.68	121.42	124.26
26	B	806	BCR	C27-C26-C25	2.68	126.62	122.73
31	B	825	CLA	C4-C3-C5	2.68	119.78	115.27
32	8	316	CHL	C2D-C1D-ND	2.68	112.08	110.10
36	8	303	LUT	C22-C23-C24	2.67	114.78	111.74
31	b	306	CLA	C3D-C2D-C1D	-2.67	102.18	105.83
31	2	306	CLA	C3D-C2D-C1D	-2.67	102.18	105.83
31	O	202	CLA	CMD-C2D-C1D	2.67	129.43	124.71
31	3	312	CLA	CAC-C3C-C4C	2.67	128.28	124.81
31	8	310	CLA	CAC-C3C-C4C	2.67	128.28	124.81
31	4	312	CLA	O2A-CGA-CBA	2.67	120.29	111.91
31	B	849	CLA	CMD-C2D-C1D	2.67	129.42	124.71
32	6	320	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
31	A	837	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
31	4	320	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
31	2	306	CLA	CMB-C2B-C1B	2.67	129.44	125.37
31	b	310	CLA	C4D-CHA-C1A	-2.67	118.00	121.25
31	6	313	CLA	CMC-C2C-C1C	2.67	129.10	125.04
36	9	303	LUT	C16-C1-C6	2.67	114.63	110.30
31	A	822	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
28	8	304	LHG	O8-C23-C24	2.67	120.28	111.91
32	7	324	CHL	O2A-CGA-CBA	2.67	120.28	111.91
31	H	902	CLA	C3D-C2D-C1D	-2.67	102.19	105.83
32	A	840	CHL	O2A-CGA-CBA	2.67	120.28	111.91
32	3	315	CHL	C2D-C1D-ND	2.67	112.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	305	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
31	6	316	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
33	B	808	DGD	CDB-CCB-CBB	-2.67	100.89	114.42
32	5	317	CHL	C2D-C1D-ND	2.67	112.07	110.10
31	A	841	CLA	C4-C3-C5	2.67	119.76	115.27
32	6	309	CHL	C1-C2-C3	-2.67	121.43	126.04
31	A	817	CLA	CMC-C2C-C1C	2.67	129.10	125.04
31	7	312	CLA	CMC-C2C-C1C	2.67	129.10	125.04
31	3	311	CLA	C4-C3-C5	2.67	119.75	115.27
31	B	844	CLA	CMD-C2D-C1D	2.67	129.41	124.71
31	3	311	CLA	C3D-C2D-C1D	-2.67	102.19	105.83
31	b	312	CLA	CHC-C1C-NC	-2.66	120.16	124.20
31	a	321	CLA	O2A-CGA-CBA	2.66	120.27	111.91
31	2	309	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
31	L	307	CLA	CAC-C3C-C4C	2.66	128.26	124.81
31	6	307	CLA	CHC-C1C-NC	-2.66	120.16	124.20
31	5	309	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
31	9	317	CLA	CHB-C1B-NB	-2.66	121.44	124.26
31	L	306	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
36	9	303	LUT	C2-C3-C4	2.66	113.95	110.30
31	B	827	CLA	CMD-C2D-C1D	2.66	129.40	124.71
36	9	305	LUT	C18-C5-C4	-2.66	109.43	114.36
31	2	307	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
26	6	302	BCR	C7-C8-C9	-2.66	122.22	126.23
31	a	319	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
31	9	311	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
31	4	306	CLA	CHC-C1C-NC	-2.66	120.17	124.20
31	6	306	CLA	C1D-ND-C4D	-2.66	104.45	106.33
31	G	206	CLA	CAC-C3C-C4C	2.66	128.26	124.81
31	K	206	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
31	5	321	CLA	CAC-C3C-C4C	2.66	128.26	124.81
30	A	813	CL0	C1D-CHD-C4C	-2.66	120.33	126.06
31	5	323	CLA	O2A-CGA-CBA	2.66	120.24	111.91
31	5	308	CLA	C3D-C2D-C1D	-2.66	102.21	105.83
32	4	317	CHL	CHD-C4C-NC	2.66	128.39	124.20
31	8	312	CLA	C1-C2-C3	-2.66	122.46	126.75
31	A	838	CLA	C3D-C2D-C1D	-2.65	102.21	105.83
31	7	316	CLA	C3D-C2D-C1D	-2.65	102.21	105.83
36	9	303	LUT	C10-C11-C12	-2.65	114.93	123.22
35	a	302	QTB	C11-C10-C09	2.65	131.23	125.47
31	A	853	CLA	C1-C2-C3	-2.65	121.45	126.04
31	A	816	CLA	C4-C3-C5	2.65	119.73	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	203	BCR	C24-C23-C22	-2.65	122.23	126.23
31	5	310	CLA	CAC-C3C-C4C	2.65	128.25	124.81
31	9	318	CLA	CHD-C4C-NC	2.65	128.38	124.20
31	B	834	CLA	CMD-C2D-C1D	2.65	129.39	124.71
31	9	317	CLA	O2A-CGA-CBA	2.65	120.23	111.91
31	4	308	CLA	CHC-C1C-NC	-2.65	120.18	124.20
32	7	318	CHL	CHC-C1C-NC	-2.65	120.18	124.20
31	B	847	CLA	C1-C2-C3	-2.65	121.46	126.04
31	A	848	CLA	C4-C3-C2	-2.65	116.88	123.68
32	4	317	CHL	C1D-CHD-C4C	-2.65	120.34	126.06
31	B	842	CLA	CAC-C3C-C4C	2.65	128.25	124.81
31	G	204	CLA	CMD-C2D-C1D	2.65	129.38	124.71
31	6	310	CLA	CMB-C2B-C1B	2.65	129.40	125.37
31	A	852	CLA	CAC-C3C-C4C	2.65	128.24	124.81
31	H	901	CLA	CHD-C4C-NC	2.65	128.37	124.20
37	a	301	LMG	O6-C1-O1	-2.65	103.71	109.97
31	8	320	CLA	C4-C3-C5	2.64	119.72	115.27
32	A	839	CHL	CHB-C1B-NB	-2.64	121.46	124.26
32	5	317	CHL	CMD-C2D-C1D	2.64	129.37	124.71
31	A	830	CLA	O2A-CGA-CBA	2.64	120.20	111.91
31	A	856	CLA	CMC-C2C-C1C	2.64	129.06	125.04
31	B	818	CLA	CMC-C2C-C1C	2.64	129.06	125.04
31	B	830	CLA	C1-C2-C3	-2.64	121.47	126.04
31	6	308	CLA	CHD-C4C-C3C	-2.64	120.96	124.84
31	5	315	CLA	C1-C2-C3	-2.64	121.48	126.04
31	B	817	CLA	C3D-C2D-C1D	-2.64	102.23	105.83
31	7	314	CLA	C1-C2-C3	-2.64	121.48	126.04
31	F	306	CLA	CAC-C3C-C4C	2.64	128.24	124.81
31	b	308	CLA	CHD-C4C-NC	2.64	128.36	124.20
31	6	311	CLA	O2A-CGA-CBA	2.64	120.19	111.91
31	B	819	CLA	CMB-C2B-C1B	2.64	129.39	125.37
31	B	814	CLA	O2A-CGA-CBA	2.64	120.19	111.91
31	5	308	CLA	CHC-C1C-NC	-2.64	120.20	124.20
31	B	833	CLA	CMD-C2D-C1D	2.64	129.36	124.71
31	4	306	CLA	CMD-C2D-C1D	2.64	129.36	124.71
31	A	815	CLA	O2A-CGA-CBA	2.64	120.19	111.91
32	6	309	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
31	G	204	CLA	C1-C2-C3	-2.64	122.48	126.75
31	B	833	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
31	4	312	CLA	CMC-C2C-C1C	2.64	129.05	125.04
31	A	847	CLA	C4-C3-C5	2.64	119.70	115.27
32	A	831	CHL	CHC-C1C-NC	-2.64	120.20	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	316	CLA	CAC-C3C-C4C	2.64	128.23	124.81
32	4	313	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
31	2	311	CLA	CMC-C2C-C1C	2.63	129.05	125.04
31	2	314	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
32	5	316	CHL	CHD-C1D-ND	-2.63	122.03	124.45
36	9	302	LUT	C17-C1-C6	-2.63	106.03	110.30
31	B	828	CLA	CMD-C2D-C1D	2.63	129.35	124.71
32	7	320	CHL	CMD-C2D-C1D	2.63	129.35	124.71
31	9	317	CLA	CMD-C2D-C3D	-2.63	121.56	127.61
31	4	307	CLA	CMD-C2D-C1D	2.63	129.35	124.71
31	A	834	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
31	A	814	CLA	C4-C3-C5	2.63	119.69	115.27
31	8	308	CLA	CMC-C2C-C1C	2.63	129.04	125.04
31	4	309	CLA	O2A-CGA-CBA	2.63	120.16	111.91
26	3	302	BCR	C7-C8-C9	-2.63	122.26	126.23
32	9	320	CHL	O1D-CGD-CBD	-2.63	119.11	124.48
31	3	309	CLA	O2A-CGA-CBA	2.63	120.15	111.91
31	5	318	CLA	CMD-C2D-C1D	2.63	129.34	124.71
31	5	310	CLA	CHD-C4C-NC	2.63	128.34	124.20
31	5	307	CLA	C1-C2-C3	-2.63	121.50	126.04
31	b	307	CLA	CHC-C1C-NC	-2.63	120.22	124.20
31	b	307	CLA	CED-O2D-CGD	2.63	121.88	115.94
31	6	311	CLA	CHD-C4C-NC	2.63	128.34	124.20
31	A	829	CLA	CMD-C2D-C3D	-2.63	121.57	127.61
31	8	320	CLA	CMB-C2B-C1B	2.63	129.37	125.37
31	B	821	CLA	C1-C2-C3	-2.63	121.50	126.04
31	B	836	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
30	A	813	CL0	CHB-C4A-NA	2.62	128.14	124.51
31	B	815	CLA	CHC-C1C-NC	-2.62	120.22	124.20
36	b	301	LUT	C22-C23-C24	2.62	114.72	111.74
32	7	317	CHL	C2D-C1D-ND	2.62	112.04	110.10
31	B	836	CLA	C4-C3-C5	2.62	119.68	115.27
26	3	303	BCR	C27-C26-C25	2.62	126.54	122.73
31	a	321	CLA	C5-C3-C4	2.62	120.39	114.60
31	B	845	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
31	4	315	CLA	CMD-C2D-C1D	2.62	129.33	124.71
31	5	308	CLA	CED-O2D-CGD	2.62	121.86	115.94
31	4	314	CLA	CHC-C1C-NC	-2.62	120.23	124.20
32	7	324	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
31	G	205	CLA	CMC-C2C-C1C	2.62	129.03	125.04
31	a	316	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
31	7	312	CLA	CAC-C3C-C4C	2.62	128.21	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	315	CLA	CHC-C1C-NC	-2.62	120.23	124.20
31	G	204	CLA	O2A-CGA-CBA	2.62	120.12	111.91
31	8	312	CLA	CHC-C1C-NC	-2.62	120.23	124.20
31	8	320	CLA	CAC-C3C-C4C	2.62	128.21	124.81
31	4	308	CLA	CED-O2D-CGD	2.62	121.86	115.94
31	8	309	CLA	C1-O2A-CGA	2.62	123.31	116.44
31	A	823	CLA	C1D-CHD-C4C	-2.62	120.41	126.06
31	4	308	CLA	C1-C2-C3	-2.62	121.52	126.04
31	A	852	CLA	CMD-C2D-C1D	2.62	129.32	124.71
31	2	308	CLA	CMD-C2D-C1D	2.62	129.32	124.71
31	5	320	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
31	A	853	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
37	J	101	LMG	O6-C1-O1	-2.62	103.78	109.97
32	a	317	CHL	CAA-CBA-CGA	-2.62	105.61	113.25
31	B	828	CLA	C11-C10-C8	-2.62	107.47	115.92
31	O	202	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
31	B	850	CLA	CHD-C4C-NC	2.61	128.32	124.20
32	6	319	CHL	CMD-C2D-C1D	2.61	129.32	124.71
31	B	834	CLA	C4-C3-C5	2.61	119.67	115.27
31	4	321	CLA	CED-O2D-CGD	2.61	121.85	115.94
31	b	313	CLA	C3D-C2D-C1D	-2.61	102.26	105.83
31	B	840	CLA	CHB-C1B-NB	-2.61	121.49	124.26
32	7	317	CHL	O2A-CGA-CBA	2.61	120.11	111.91
31	A	834	CLA	CED-O2D-CGD	2.61	121.85	115.94
31	B	832	CLA	CMD-C2D-C1D	2.61	129.32	124.71
31	8	313	CLA	CMD-C2D-C1D	2.61	129.32	124.71
32	9	322	CHL	CHD-C1D-ND	-2.61	122.05	124.45
26	K	202	BCR	C39-C30-C25	2.61	114.54	110.30
36	6	303	LUT	C8-C7-C6	-2.61	119.87	127.20
31	H	902	CLA	CMC-C2C-C1C	2.61	129.02	125.04
31	9	316	CLA	CHB-C1B-NB	-2.61	121.49	124.26
36	a	305	LUT	C4-C5-C6	-2.61	115.03	120.85
31	A	851	CLA	CHD-C4C-NC	2.61	128.32	124.20
31	B	834	CLA	C3C-C4C-NC	2.61	113.50	110.57
36	2	301	LUT	C10-C11-C12	-2.61	115.07	123.22
31	B	832	CLA	C4-C3-C5	2.61	119.66	115.27
31	9	314	CLA	C1-C2-C3	-2.61	121.53	126.04
31	G	204	CLA	C5-C3-C4	2.61	120.36	114.60
32	5	316	CHL	OMC-CMC-C2C	-2.61	119.79	125.69
35	7	303	QTB	C03-C04-C05	2.61	131.36	123.22
32	4	310	CHL	CHD-C4C-NC	2.61	128.31	124.20
37	G	202	LMG	O1-C7-C8	-2.61	104.61	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	840	CHL	C1D-CHD-C4C	-2.61	120.43	126.06
31	5	315	CLA	O2A-CGA-CBA	2.61	120.09	111.91
31	a	319	CLA	C1-O2A-CGA	2.61	123.28	116.44
31	A	818	CLA	C3D-C2D-C1D	-2.61	102.28	105.83
31	a	311	CLA	CMD-C2D-C1D	2.61	129.31	124.71
31	9	321	CLA	CHD-C4C-NC	2.61	128.31	124.20
31	5	321	CLA	CHD-C4C-NC	2.61	128.31	124.20
31	A	829	CLA	C5-C3-C4	2.61	120.36	114.60
31	4	314	CLA	C3D-C2D-C1D	-2.61	102.28	105.83
31	3	316	CLA	O2A-CGA-CBA	2.60	120.08	111.91
31	b	306	CLA	CED-O2D-CGD	2.60	121.83	115.94
36	5	303	LUT	C1-C6-C7	-2.60	108.41	115.78
31	2	315	CLA	CMC-C2C-C1C	2.60	129.00	125.04
32	7	318	CHL	O2A-CGA-O1A	-2.60	117.02	123.59
31	8	308	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
31	6	314	CLA	O2A-CGA-CBA	2.60	120.07	111.91
31	B	816	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
31	F	306	CLA	CHD-C4C-NC	2.60	128.30	124.20
31	B	813	CLA	C4-C3-C5	2.60	119.64	115.27
31	B	816	CLA	C1-C2-C3	-2.60	121.55	126.04
31	B	818	CLA	CHC-C4B-C3B	-2.60	116.16	127.71
31	B	819	CLA	CHB-C1B-NB	-2.60	121.51	124.26
31	3	313	CLA	CHC-C1C-NC	-2.60	120.26	124.20
36	J	103	LUT	C18-C5-C4	-2.60	109.55	114.36
32	A	840	CHL	O2D-CGD-O1D	-2.60	118.76	123.84
31	4	315	CLA	O1D-CGD-CBD	-2.60	119.17	124.48
31	3	310	CLA	CMD-C2D-C1D	2.60	129.29	124.71
31	8	312	CLA	C3D-C2D-C1D	-2.59	102.29	105.83
28	6	305	LHG	O8-C23-C24	2.59	120.05	111.91
31	3	320	CLA	C3D-C2D-C1D	-2.59	102.29	105.83
31	4	321	CLA	C3D-C2D-C1D	-2.59	102.29	105.83
31	B	827	CLA	O2A-CGA-CBA	2.59	120.05	111.91
31	B	819	CLA	C1-C2-C3	-2.59	121.56	126.04
31	A	838	CLA	O2A-CGA-CBA	2.59	120.05	111.91
31	F	306	CLA	O2A-CGA-CBA	2.59	120.05	111.91
31	6	316	CLA	CMB-C2B-C1B	2.59	129.32	125.37
31	A	814	CLA	CHD-C4C-NC	2.59	128.29	124.20
31	8	307	CLA	CHB-C1B-NB	-2.59	121.51	124.26
32	8	319	CHL	CMD-C2D-C1D	2.59	129.28	124.71
31	B	814	CLA	CHB-C1B-NB	-2.59	121.51	124.26
31	2	306	CLA	CMD-C2D-C1D	2.59	129.28	124.71
32	6	317	CHL	C2D-C1D-ND	2.59	112.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	314	CLA	CHD-C4C-NC	2.59	128.28	124.20
32	K	201	CHL	C4D-CHA-C1A	-2.59	118.10	121.25
31	5	315	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
31	A	821	CLA	C6-C5-C3	-2.59	106.67	113.45
31	b	303	CLA	CHC-C1C-NC	-2.59	120.28	124.20
31	2	311	CLA	C3D-C2D-C1D	-2.59	102.30	105.83
31	7	309	CLA	CAC-C3C-C4C	2.59	128.17	124.81
31	a	310	CLA	CHC-C1C-NC	-2.59	120.28	124.20
31	B	823	CLA	CHC-C1C-NC	-2.59	120.28	124.20
32	9	320	CHL	C2D-C1D-ND	2.59	112.01	110.10
32	9	320	CHL	CHB-C1B-NB	-2.59	121.52	124.26
26	J	102	BCR	C24-C23-C22	-2.58	122.33	126.23
31	B	843	CLA	CHC-C4B-C3B	-2.58	116.21	127.71
31	B	842	CLA	C1-C2-C3	-2.58	121.57	126.04
31	3	311	CLA	CHD-C4C-NC	2.58	128.28	124.20
31	4	311	CLA	CHD-C4C-NC	2.58	128.28	124.20
31	B	843	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
31	6	313	CLA	CMD-C2D-C1D	2.58	129.27	124.71
36	4	302	LUT	C22-C23-C24	2.58	114.68	111.74
31	4	308	CLA	CMC-C2C-C1C	2.58	128.97	125.04
31	b	305	CLA	CMD-C2D-C1D	2.58	129.26	124.71
31	9	313	CLA	CHC-C1C-NC	-2.58	120.29	124.20
32	7	320	CHL	CHD-C1D-ND	-2.58	122.08	124.45
31	8	313	CLA	CMB-C2B-C1B	2.58	129.30	125.37
32	6	320	CHL	C2D-C1D-ND	2.58	112.01	110.10
31	4	307	CLA	O2A-CGA-CBA	2.58	120.00	111.91
31	5	315	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
31	5	310	CLA	C1-C2-C3	-2.58	121.58	126.04
26	K	203	BCR	C15-C16-C17	-2.58	118.19	123.47
31	9	315	CLA	C4-C3-C5	2.58	119.61	115.27
31	K	204	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
36	b	301	LUT	C36-C21-C26	2.58	113.45	109.55
31	A	856	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
31	9	319	CLA	CAC-C3C-C4C	2.58	128.15	124.81
32	5	319	CHL	CHC-C1C-NC	-2.58	120.29	124.20
31	5	309	CLA	CHC-C1C-NC	-2.58	120.30	124.20
31	6	311	CLA	C3D-C2D-C1D	-2.57	102.32	105.83
31	A	845	CLA	CMC-C2C-C1C	2.57	128.96	125.04
32	7	319	CHL	CMD-C2D-C1D	2.57	129.25	124.71
26	K	202	BCR	C24-C23-C22	-2.57	122.35	126.23
31	B	846	CLA	CHD-C4C-NC	2.57	128.26	124.20
31	A	848	CLA	C3D-C2D-C1D	-2.57	102.32	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	844	CLA	CMC-C2C-C1C	2.57	128.96	125.04
32	7	324	CHL	CED-O2D-CGD	2.57	121.76	115.94
31	5	320	CLA	O1D-CGD-CBD	-2.57	119.22	124.48
30	A	813	CL0	C4C-C3C-C2C	-2.57	103.15	106.90
31	8	308	CLA	CHC-C1C-NC	-2.57	120.30	124.20
31	B	843	CLA	CHD-C4C-NC	2.57	128.25	124.20
31	9	314	CLA	O2A-CGA-CBA	2.57	119.97	111.91
31	B	818	CLA	C1-C2-C3	-2.57	121.60	126.04
36	F	304	LUT	C4-C5-C6	-2.57	115.12	120.85
31	2	307	CLA	O2A-CGA-CBA	2.57	119.97	111.91
31	2	305	CLA	CHC-C1C-NC	-2.57	120.31	124.20
31	4	305	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
31	a	314	CLA	C1-O2A-CGA	2.57	123.18	116.44
31	F	301	CLA	C4-C3-C5	2.57	119.59	115.27
32	9	322	CHL	C3D-C2D-C1D	-2.57	102.33	105.83
31	A	820	CLA	CHC-C1C-NC	-2.57	120.31	124.20
31	9	321	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
31	7	314	CLA	CHC-C1C-NC	-2.57	120.31	124.20
31	9	318	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
31	5	310	CLA	C4-C3-C5	2.57	119.59	115.27
32	6	309	CHL	CMD-C2D-C1D	2.56	129.23	124.71
31	A	814	CLA	O2A-CGA-CBA	2.56	119.95	111.91
26	2	302	BCR	C33-C5-C6	-2.56	121.65	124.53
31	4	306	CLA	CMC-C2C-C1C	2.56	128.94	125.04
31	7	316	CLA	CAC-C3C-C4C	2.56	128.14	124.81
31	7	315	CLA	CHC-C4B-C3B	-2.56	116.31	127.71
31	7	315	CLA	CHD-C4C-NC	2.56	128.24	124.20
31	b	312	CLA	CHD-C4C-NC	2.56	128.24	124.20
31	A	819	CLA	CMC-C2C-C1C	2.56	128.94	125.04
31	B	847	CLA	CHB-C4A-NA	2.56	128.05	124.51
31	2	308	CLA	CED-O2D-CGD	2.56	121.73	115.94
36	5	303	LUT	C4-C5-C6	-2.56	115.14	120.85
31	L	305	CLA	CHC-C1C-NC	-2.56	120.32	124.20
31	8	320	CLA	C3D-C2D-C1D	-2.56	102.34	105.83
32	8	319	CHL	CMB-C2B-C1B	2.56	129.27	125.37
31	A	834	CLA	C4-C3-C5	2.56	119.58	115.27
31	A	856	CLA	C4-C3-C5	2.56	119.58	115.27
31	9	314	CLA	CED-O2D-CGD	2.56	121.72	115.94
31	8	309	CLA	CHC-C4B-C3B	-2.56	116.33	127.71
26	G	201	BCR	C11-C10-C9	-2.56	123.66	127.31
36	9	305	LUT	C7-C8-C9	-2.56	122.37	126.23
31	8	309	CLA	CHC-C1C-NC	-2.56	120.32	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	302	CLA	CHC-C1C-NC	-2.56	120.32	124.20
31	B	835	CLA	C4-C3-C5	2.56	119.57	115.27
31	7	310	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
31	a	321	CLA	C1-C2-C3	-2.55	122.62	126.75
31	K	205	CLA	CMD-C2D-C1D	2.55	129.22	124.71
31	B	824	CLA	C4-C3-C2	-2.55	117.13	123.68
31	B	824	CLA	C1D-CHD-C4C	-2.55	120.55	126.06
31	A	844	CLA	C3D-C2D-C1D	-2.55	102.35	105.83
31	B	812	CLA	C1D-CHD-C4C	-2.55	120.55	126.06
31	5	312	CLA	O2A-CGA-CBA	2.55	119.92	111.91
36	4	302	LUT	C36-C21-C26	2.55	113.41	109.55
31	5	315	CLA	CMD-C2D-C1D	2.55	129.21	124.71
32	6	309	CHL	C4D-CHA-C1A	-2.55	118.14	121.25
36	4	302	LUT	C4-C5-C6	-2.55	115.16	120.85
37	G	202	LMG	C38-C37-C36	-2.55	101.47	114.42
31	H	902	CLA	CMD-C2D-C1D	2.55	129.21	124.71
31	7	311	CLA	CMC-C2C-C1C	2.55	128.92	125.04
31	5	313	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
31	7	311	CLA	CMB-C2B-C1B	2.55	129.25	125.37
31	A	836	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
31	A	835	CLA	C1-O2A-CGA	2.55	123.13	116.44
31	B	829	CLA	CHC-C4B-C3B	-2.55	116.38	127.71
31	7	314	CLA	C3D-C2D-C1D	-2.55	102.36	105.83
31	8	320	CLA	CHC-C1C-NC	-2.55	120.34	124.20
31	9	312	CLA	CHC-C1C-NC	-2.55	120.34	124.20
31	4	319	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
32	6	309	CHL	O2D-CGD-O1D	-2.55	118.86	123.84
31	B	828	CLA	C1-C2-C3	-2.55	121.64	126.04
32	a	317	CHL	CHC-C1C-NC	-2.55	120.34	124.20
31	F	305	CLA	CMC-C2C-C1C	2.55	128.91	125.04
31	2	309	CLA	CMD-C2D-C1D	2.54	129.20	124.71
33	7	308	DGD	O6D-C5D-C6D	-2.54	101.53	106.67
31	a	312	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	A	849	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
31	2	315	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
31	b	307	CLA	CMD-C2D-C1D	2.54	129.20	124.71
31	A	846	CLA	CHB-C4A-NA	2.54	128.03	124.51
31	B	821	CLA	CMD-C2D-C1D	2.54	129.19	124.71
31	B	821	CLA	C4-C3-C5	2.54	119.55	115.27
31	4	307	CLA	CAC-C3C-C4C	2.54	128.11	124.81
32	9	322	CHL	CHD-C4C-NC	2.54	128.21	124.20
31	4	318	CLA	O1D-CGD-CBD	-2.54	119.28	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	303	CLA	CMB-C2B-C1B	2.54	129.24	125.37
31	7	321	CLA	CHC-C1C-NC	-2.54	120.35	124.20
32	4	313	CHL	CHB-C1B-NB	-2.54	121.57	124.26
31	4	309	CLA	C1-O2A-CGA	2.54	123.11	116.44
26	3	301	BCR	C27-C26-C25	2.54	126.42	122.73
32	4	317	CHL	O1D-CGD-CBD	-2.54	119.28	124.48
36	b	301	LUT	C17-C1-C6	-2.54	106.18	110.30
31	a	321	CLA	CMB-C2B-C1B	2.54	129.24	125.37
31	A	849	CLA	CMD-C2D-C1D	2.54	129.19	124.71
31	B	819	CLA	CHC-C4B-C3B	-2.54	116.42	127.71
32	4	313	CHL	CHC-C1C-NC	-2.54	120.35	124.20
31	O	202	CLA	CHC-C1C-NC	-2.54	120.35	124.20
32	6	319	CHL	CMB-C2B-C1B	2.54	129.23	125.37
31	8	310	CLA	CHC-C1C-NC	-2.54	120.35	124.20
31	a	313	CLA	C4-C3-C2	-2.54	117.17	123.68
31	B	816	CLA	C4-C3-C5	2.54	119.54	115.27
31	2	314	CLA	CHC-C1C-NC	-2.54	120.36	124.20
26	2	302	BCR	C27-C26-C25	2.54	126.41	122.73
31	4	319	CLA	O1D-CGD-CBD	-2.54	119.30	124.48
26	O	201	BCR	C24-C23-C22	-2.54	122.40	126.23
32	b	309	CHL	O1D-CGD-CBD	-2.53	119.30	124.48
28	7	302	LHG	C11-C10-C9	-2.53	101.56	114.42
31	B	814	CLA	C4-C3-C5	2.53	119.53	115.27
31	2	307	CLA	CED-O2D-CGD	2.53	121.67	115.94
31	A	814	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
32	a	320	CHL	CMD-C2D-C1D	2.53	129.18	124.71
31	b	306	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
31	9	315	CLA	O2A-CGA-CBA	2.53	119.85	111.91
31	A	843	CLA	C4-C3-C5	2.53	119.53	115.27
31	8	314	CLA	CMD-C2D-C1D	2.53	129.18	124.71
31	6	316	CLA	CHC-C1C-NC	-2.53	120.36	124.20
31	4	314	CLA	CMC-C2C-C1C	2.53	128.89	125.04
31	B	812	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	7	313	CLA	CMC-C2C-C1C	2.53	128.89	125.04
31	5	315	CLA	CBC-CAC-C3C	-2.53	105.46	112.43
31	A	829	CLA	CMC-C2C-C1C	2.53	128.89	125.04
31	2	309	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
31	2	311	CLA	CHC-C1C-NC	-2.53	120.37	124.20
31	B	840	CLA	CMD-C2D-C1D	2.53	129.17	124.71
31	G	206	CLA	CMD-C2D-C1D	2.53	129.17	124.71
32	5	316	CHL	CMD-C2D-C1D	2.53	129.17	124.71
31	A	814	CLA	CAC-C3C-C4C	2.53	128.09	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	303	CLA	CHB-C1B-NB	-2.53	121.58	124.26
31	B	850	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
31	b	312	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
32	8	319	CHL	O1D-CGD-CBD	-2.53	119.31	124.48
31	B	842	CLA	CHB-C1B-NB	-2.53	121.58	124.26
31	B	812	CLA	C4C-C3C-C2C	-2.53	103.22	106.90
32	3	315	CHL	CMD-C2D-C1D	2.52	129.16	124.71
31	3	309	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
31	4	307	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
31	9	315	CLA	CHC-C4B-C3B	-2.52	116.48	127.71
31	7	315	CLA	CAC-C3C-C4C	2.52	128.08	124.81
31	3	313	CLA	CMD-C2D-C1D	2.52	129.16	124.71
31	3	318	CLA	C1-C2-C3	-2.52	121.68	126.04
31	A	833	CLA	CMB-C2B-C1B	2.52	129.21	125.37
31	B	835	CLA	CHC-C1C-NC	-2.52	120.38	124.20
32	7	324	CHL	CMD-C2D-C1D	2.52	129.16	124.71
31	b	303	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
31	4	309	CLA	CMB-C2B-C1B	2.52	129.21	125.37
31	B	832	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
31	L	307	CLA	CMB-C2B-C1B	2.52	129.21	125.37
31	4	315	CLA	CHC-C1C-NC	-2.52	120.38	124.20
32	4	313	CHL	O2A-CGA-CBA	2.52	119.81	111.91
31	b	302	CLA	CHB-C1B-NB	-2.52	121.59	124.26
26	8	301	BCR	C27-C26-C25	2.52	126.39	122.73
31	5	314	CLA	CHC-C1C-NC	-2.52	120.38	124.20
31	4	312	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
31	6	308	CLA	CMC-C2C-C1C	2.52	128.87	125.04
31	B	847	CLA	CMB-C2B-C1B	2.52	129.20	125.37
31	B	824	CLA	O2A-CGA-CBA	2.52	119.80	111.91
31	4	321	CLA	C5-C3-C4	2.52	120.16	114.60
31	6	312	CLA	O2A-CGA-CBA	2.52	119.80	111.91
31	9	314	CLA	CHC-C1C-NC	-2.52	120.39	124.20
31	A	835	CLA	C4-C3-C5	2.52	119.50	115.27
31	H	901	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
31	4	311	CLA	CHB-C1B-NB	-2.51	121.59	124.26
31	A	825	CLA	CHB-C4A-NA	2.51	127.99	124.51
31	5	314	CLA	CMB-C2B-C1B	2.51	129.20	125.37
32	9	322	CHL	CHC-C1C-NC	-2.51	120.39	124.20
31	b	302	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
36	9	302	LUT	C7-C8-C9	-2.51	122.44	126.23
31	A	855	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
31	4	311	CLA	CMB-C2B-C1B	2.51	129.19	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	318	CLA	CMD-C2D-C1D	2.51	129.14	124.71
32	A	831	CHL	C2D-C1D-ND	2.51	111.95	110.10
31	4	318	CLA	CMB-C2B-C1B	2.51	129.19	125.37
26	B	805	BCR	C15-C14-C13	-2.51	123.73	127.31
26	K	203	BCR	C27-C26-C25	2.51	126.38	122.73
31	B	818	CLA	O2A-CGA-CBA	2.51	119.78	111.91
31	4	309	CLA	CMC-C2C-C1C	2.51	128.86	125.04
31	A	814	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
31	A	837	CLA	C4-C3-C5	2.51	119.49	115.27
31	B	839	CLA	CAC-C3C-C4C	2.51	128.06	124.81
31	5	318	CLA	C3D-C2D-C1D	-2.51	102.41	105.83
31	A	852	CLA	CMC-C2C-C1C	2.51	128.85	125.04
31	5	307	CLA	C1D-CHD-C4C	-2.51	120.65	126.06
31	6	306	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
31	B	844	CLA	C4-C3-C5	2.51	119.49	115.27
31	H	901	CLA	CMB-C2B-C1B	2.51	129.19	125.37
31	b	306	CLA	CMD-C2D-C1D	2.51	129.13	124.71
31	6	322	CLA	CMC-C2C-C1C	2.51	128.85	125.04
31	A	833	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	4	309	CLA	C1D-CHD-C4C	-2.50	120.66	126.06
31	4	314	CLA	CMD-C2D-C1D	2.50	129.13	124.71
31	A	847	CLA	C1D-CHD-C4C	-2.50	120.66	126.06
40	7	306	XAT	C15-C35-C34	2.50	128.60	123.47
31	A	846	CLA	O2A-CGA-CBA	2.50	119.76	111.91
32	b	309	CHL	CMD-C2D-C1D	2.50	129.12	124.71
32	4	313	CHL	CMD-C2D-C1D	2.50	129.12	124.71
31	4	321	CLA	CHC-C1C-NC	-2.50	120.41	124.20
31	A	845	CLA	C1-C2-C3	-2.50	121.71	126.04
31	4	320	CLA	CHC-C1C-NC	-2.50	120.41	124.20
31	5	323	CLA	CMC-C2C-C1C	2.50	128.85	125.04
31	4	319	CLA	CMB-C2B-C1B	2.50	129.18	125.37
31	4	309	CLA	C4-C3-C5	2.50	119.48	115.27
32	6	321	CHL	C2D-C1D-ND	2.50	111.95	110.10
26	L	303	BCR	C27-C26-C25	2.50	126.36	122.73
31	B	848	CLA	O2A-CGA-CBA	2.50	119.75	111.91
31	8	309	CLA	C5-C3-C4	2.50	120.12	114.60
32	6	321	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
31	A	852	CLA	C1-C2-C3	-2.50	121.72	126.04
31	A	848	CLA	CHD-C4C-NC	2.50	128.14	124.20
31	B	848	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
31	6	312	CLA	CMC-C2C-C1C	2.50	128.84	125.04
32	5	319	CHL	C4D-CHA-C1A	-2.50	118.21	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	319	CHL	CMB-C2B-C1B	2.50	129.17	125.37
31	B	829	CLA	C1-C2-C3	-2.50	121.72	126.04
31	B	841	CLA	C4-C3-C5	2.50	119.47	115.27
31	3	311	CLA	CMD-C2D-C1D	2.50	129.11	124.71
31	b	302	CLA	CMD-C2D-C1D	2.50	129.11	124.71
31	A	854	CLA	CMC-C2C-C1C	2.50	128.84	125.04
31	9	315	CLA	CMC-C2C-C1C	2.50	128.84	125.04
31	9	318	CLA	CMC-C2C-C1C	2.50	128.84	125.04
31	4	314	CLA	CED-O2D-CGD	2.49	121.58	115.94
32	4	310	CHL	CAC-C3C-C4C	2.49	128.05	124.81
31	A	821	CLA	CHB-C1B-NB	-2.49	121.62	124.26
31	3	312	CLA	CMC-C2C-C1C	2.49	128.84	125.04
31	6	310	CLA	O2A-CGA-CBA	2.49	119.73	111.91
31	b	304	CLA	CHC-C1C-NC	-2.49	120.42	124.20
31	8	313	CLA	CMC-C2C-C1C	2.49	128.84	125.04
31	5	312	CLA	CHC-C1C-NC	-2.49	120.42	124.20
31	b	304	CLA	CMC-C2C-C1C	2.49	128.84	125.04
31	4	311	CLA	CAC-C3C-C4C	2.49	128.04	124.81
28	8	304	LHG	C11-C10-C9	-2.49	101.77	114.42
31	A	846	CLA	CHB-C1B-NB	-2.49	121.62	124.26
31	9	318	CLA	CMD-C2D-C1D	2.49	129.10	124.71
31	3	316	CLA	CMD-C2D-C1D	2.49	129.10	124.71
31	B	841	CLA	C1D-CHD-C4C	-2.49	120.69	126.06
31	A	822	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
31	a	311	CLA	CHC-C1C-NC	-2.49	120.43	124.20
31	a	312	CLA	CAC-C3C-C4C	2.49	128.04	124.81
31	B	848	CLA	CMC-C2C-C1C	2.49	128.83	125.04
31	9	311	CLA	CMC-C2C-C1C	2.49	128.83	125.04
31	2	304	CLA	CMC-C2C-C1C	2.49	128.83	125.04
31	B	828	CLA	C6-C7-C8	-2.49	107.88	115.92
31	A	844	CLA	C1-O2A-CGA	2.49	122.97	116.44
31	B	839	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	A	836	CLA	O2A-CGA-CBA	2.48	119.71	111.91
31	6	316	CLA	CMD-C2D-C1D	2.48	129.09	124.71
31	B	816	CLA	CHC-C4B-C3B	-2.48	116.66	127.71
31	5	315	CLA	CHC-C1C-NC	-2.48	120.44	124.20
31	3	319	CLA	CHB-C4A-NA	2.48	127.95	124.51
31	B	834	CLA	CAC-C3C-C4C	2.48	128.03	124.81
26	M	101	BCR	C27-C26-C25	2.48	126.34	122.73
31	A	851	CLA	O2A-CGA-CBA	2.48	119.70	111.91
31	B	848	CLA	CMD-C2D-C1D	2.48	129.09	124.71
32	a	318	CHL	C4D-CHA-C1A	-2.48	118.23	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	831	CHL	C1D-CHD-C4C	-2.48	120.70	126.06
31	3	313	CLA	C1-C2-C3	-2.48	121.75	126.04
31	A	829	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	4	314	CLA	CMB-C2B-C1B	2.48	129.15	125.37
26	A	803	BCR	C27-C26-C25	2.48	126.33	122.73
31	B	831	CLA	CHC-C1C-NC	-2.48	120.44	124.20
31	a	311	CLA	CMC-C2C-C1C	2.48	128.81	125.04
31	5	312	CLA	CMC-C2C-C1C	2.48	128.81	125.04
31	B	846	CLA	CAC-C3C-C4C	2.48	128.03	124.81
32	A	839	CHL	CMB-C2B-C1B	2.48	129.15	125.37
30	A	813	CL0	O2D-CGD-O1D	-2.48	118.99	123.84
31	9	318	CLA	C4-C3-C5	2.48	119.44	115.27
31	K	206	CLA	CHC-C1C-NC	-2.48	120.44	124.20
31	B	815	CLA	O2A-CGA-CBA	2.48	119.68	111.91
31	B	827	CLA	CHC-C4B-C3B	-2.48	116.69	127.71
26	B	803	BCR	C27-C26-C25	2.48	126.33	122.73
31	A	847	CLA	C4D-CHA-C1A	-2.48	118.23	121.25
28	A	811	LHG	C11-C10-C9	-2.48	101.85	114.42
32	8	316	CHL	O2A-CGA-CBA	2.48	119.68	111.91
31	B	813	CLA	CHC-C1C-NC	-2.48	120.45	124.20
31	3	311	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
37	a	301	LMG	C38-C37-C36	-2.47	101.86	114.42
31	a	313	CLA	O2A-CGA-CBA	2.47	119.67	111.91
31	8	315	CLA	CMD-C2D-C1D	2.47	129.07	124.71
31	B	826	CLA	O2A-CGA-CBA	2.47	119.67	111.91
36	7	305	LUT	C18-C5-C4	-2.47	109.77	114.36
32	5	319	CHL	O1D-CGD-CBD	-2.47	119.42	124.48
31	6	312	CLA	C4-C3-C5	2.47	119.43	115.27
31	A	835	CLA	CHD-C4C-NC	2.47	128.10	124.20
31	B	832	CLA	C3B-C4B-NB	2.47	112.81	110.52
31	A	838	CLA	CHC-C1C-NC	-2.47	120.45	124.20
31	4	311	CLA	CMC-C2C-C1C	2.47	128.80	125.04
31	B	845	CLA	CMD-C2D-C1D	2.47	129.07	124.71
31	A	850	CLA	CMC-C2C-C1C	2.47	128.80	125.04
31	5	314	CLA	CMC-C2C-C1C	2.47	128.80	125.04
31	O	204	CLA	C3D-C2D-C1D	-2.47	102.46	105.83
32	8	319	CHL	CHB-C1B-NB	-2.47	121.64	124.26
32	7	324	CHL	CHC-C1C-NC	-2.47	120.46	124.20
36	L	304	LUT	C36-C21-C26	2.47	113.28	109.55
32	5	317	CHL	CHB-C1B-NB	-2.47	121.64	124.26
31	O	204	CLA	CMD-C2D-C1D	2.47	129.06	124.71
36	8	303	LUT	C21-C26-C27	-2.47	109.58	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	206	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
26	K	202	BCR	C7-C8-C9	-2.47	122.51	126.23
31	B	837	CLA	C1-O2A-CGA	2.47	122.92	116.44
32	5	316	CHL	CHB-C1B-NB	-2.47	121.65	124.26
31	A	819	CLA	CHC-C1C-NC	-2.47	120.46	124.20
31	A	822	CLA	C4-C3-C5	2.47	119.42	115.27
31	6	313	CLA	CHC-C4B-C3B	-2.47	116.74	127.71
31	A	816	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
31	A	856	CLA	C1D-CHD-C4C	-2.46	120.74	126.06
32	a	320	CHL	C4D-CHA-C1A	-2.46	118.25	121.25
31	9	314	CLA	C4-C3-C5	2.46	119.42	115.27
31	9	321	CLA	CAC-C3C-C4C	2.46	128.01	124.81
31	B	832	CLA	CHC-C4B-C3B	-2.46	116.75	127.71
31	B	834	CLA	O2A-CGA-CBA	2.46	119.64	111.91
31	2	313	CLA	CHC-C1C-NC	-2.46	120.47	124.20
31	6	311	CLA	C4-C3-C5	2.46	119.41	115.27
31	3	319	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
31	B	815	CLA	CMC-C2C-C1C	2.46	128.79	125.04
32	6	318	CHL	C1D-CHD-C4C	-2.46	120.75	126.06
31	A	857	CLA	C1-C2-C3	-2.46	121.79	126.04
31	B	817	CLA	C4-C3-C5	2.46	119.41	115.27
32	6	319	CHL	CHD-C4C-NC	2.46	128.08	124.20
31	b	311	CLA	CED-O2D-CGD	2.46	121.50	115.94
31	4	311	CLA	C3D-C2D-C1D	-2.46	102.47	105.83
31	3	312	CLA	CMD-C2D-C1D	2.46	129.05	124.71
31	7	311	CLA	CHC-C1C-NC	-2.46	120.47	124.20
31	3	311	CLA	CHC-C4B-C3B	-2.46	116.78	127.71
31	B	824	CLA	CAC-C3C-C4C	2.46	128.00	124.81
28	B	807	LHG	C11-C10-C9	-2.46	101.95	114.42
31	B	822	CLA	CHD-C4C-NC	2.46	128.08	124.20
31	b	305	CLA	CED-O2D-CGD	2.46	121.50	115.94
28	A	809	LHG	C11-C10-C9	-2.46	101.95	114.42
31	B	815	CLA	CMD-C2D-C1D	2.46	129.04	124.71
36	4	303	LUT	C35-C15-C14	-2.46	118.44	123.47
31	a	314	CLA	C1-C2-C3	-2.45	122.78	126.75
31	6	311	CLA	CMD-C2D-C1D	2.45	129.04	124.71
31	9	312	CLA	CMD-C2D-C1D	2.45	129.04	124.71
31	6	307	CLA	CAC-C3C-C4C	2.45	127.99	124.81
32	6	317	CHL	CHC-C1C-NC	-2.45	120.48	124.20
31	5	310	CLA	CHC-C4B-C3B	-2.45	116.79	127.71
31	4	316	CLA	CMC-C2C-C1C	2.45	128.78	125.04
32	5	316	CHL	CMB-C2B-C1B	2.45	129.11	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	309	CLA	O2A-CGA-CBA	2.45	119.61	111.91
28	a	306	LHG	C11-C10-C9	-2.45	101.97	114.42
31	B	845	CLA	CHC-C1C-NC	-2.45	120.48	124.20
31	F	305	CLA	CHC-C1C-NC	-2.45	120.48	124.20
31	9	321	CLA	CMB-C2B-C1B	2.45	129.10	125.37
31	b	307	CLA	CMB-C2B-C1B	2.45	129.10	125.37
31	5	318	CLA	C1-O2A-CGA	2.45	122.88	116.44
31	3	320	CLA	CMB-C2B-C1B	2.45	129.10	125.37
31	O	203	CLA	CMC-C2C-C1C	2.45	128.77	125.04
31	B	816	CLA	CMB-C2B-C1B	2.45	129.10	125.37
31	A	825	CLA	CHC-C1C-NC	-2.45	120.49	124.20
31	4	321	CLA	CMB-C2B-C1B	2.45	129.10	125.37
28	A	809	LHG	C18-C17-C16	-2.45	101.99	114.42
31	H	901	CLA	C3D-C2D-C1D	-2.45	102.49	105.83
31	9	318	CLA	O2A-CGA-CBA	2.45	119.59	111.91
31	A	833	CLA	CAC-C3C-C4C	2.45	127.99	124.81
31	6	314	CLA	CED-O2D-CGD	2.45	121.47	115.94
31	6	316	CLA	O2A-CGA-CBA	2.45	119.59	111.91
31	3	307	CLA	C4-C3-C5	2.45	119.39	115.27
31	3	313	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
31	6	310	CLA	CMC-C2C-C1C	2.45	128.76	125.04
31	9	313	CLA	CMD-C2D-C1D	2.45	129.03	124.71
31	2	312	CLA	C1D-CHD-C4C	-2.45	120.78	126.06
31	3	312	CLA	C3D-C2D-C1D	-2.45	102.49	105.83
31	B	832	CLA	C1-C2-C3	-2.45	121.81	126.04
31	3	320	CLA	CMD-C2D-C1D	2.44	129.02	124.71
36	3	305	LUT	C18-C5-C4	-2.44	109.83	114.36
31	5	311	CLA	CMD-C2D-C1D	2.44	129.02	124.71
31	a	322	CLA	C3D-C2D-C1D	-2.44	102.50	105.83
28	A	810	LHG	C11-C10-C9	-2.44	102.02	114.42
28	7	307	LHG	C11-C10-C9	-2.44	102.02	114.42
31	5	309	CLA	CMC-C2C-C1C	2.44	128.76	125.04
31	6	311	CLA	CMC-C2C-C1C	2.44	128.76	125.04
31	L	307	CLA	CHC-C1C-NC	-2.44	120.50	124.20
31	A	814	CLA	C1-C2-C3	-2.44	121.82	126.04
31	3	318	CLA	C3D-C2D-C1D	-2.44	102.50	105.83
31	B	815	CLA	CED-O2D-CGD	2.44	121.46	115.94
32	K	201	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
31	6	314	CLA	CHC-C1C-NC	-2.44	120.50	124.20
32	4	317	CHL	C4B-CHC-C1C	-2.44	120.55	126.34
31	6	310	CLA	CHC-C4B-C3B	-2.44	116.85	127.71
31	2	305	CLA	CED-O2D-CGD	2.44	121.46	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	313	CLA	CMD-C2D-C1D	2.44	129.01	124.71
24	B	801	PQN	C11-C3-C4	-2.44	115.89	118.50
31	4	308	CLA	CHC-C4B-C3B	-2.44	116.86	127.71
31	a	316	CLA	CMB-C2B-C1B	2.44	129.08	125.37
31	A	822	CLA	CHB-C4A-NA	2.44	127.89	124.51
31	5	323	CLA	CED-O2D-CGD	2.44	121.45	115.94
31	3	311	CLA	O2A-CGA-CBA	2.44	119.56	111.91
31	5	320	CLA	CHC-C1C-NC	-2.44	120.50	124.20
31	B	840	CLA	C1-C2-C3	-2.44	121.83	126.04
31	A	846	CLA	CMB-C2B-C1B	2.44	129.08	125.37
31	A	841	CLA	CHD-C4C-NC	2.44	128.04	124.20
31	3	318	CLA	CED-O2D-CGD	2.44	121.45	115.94
31	3	317	CLA	C1-C2-C3	-2.44	121.83	126.04
31	a	314	CLA	C3D-C2D-C1D	-2.44	102.51	105.83
31	A	843	CLA	CHC-C1C-NC	-2.43	120.51	124.20
31	A	836	CLA	CMB-C2B-C1B	2.43	129.08	125.37
31	B	828	CLA	CMC-C2C-C1C	2.43	128.75	125.04
31	B	814	CLA	C1-O2A-CGA	2.43	122.83	116.44
36	a	303	LUT	C4-C5-C6	-2.43	115.42	120.85
31	9	317	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
31	B	818	CLA	C3B-C4B-NB	2.43	112.77	110.52
32	7	320	CHL	C4-C3-C5	2.43	119.36	115.27
31	A	836	CLA	CHC-C1C-NC	-2.43	120.51	124.20
31	A	846	CLA	CHC-C1C-NC	-2.43	120.51	124.20
32	a	317	CHL	CED-O2D-CGD	2.43	121.44	115.94
31	4	316	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
31	3	313	CLA	CMB-C2B-C1B	2.43	129.07	125.37
32	a	318	CHL	CMD-C2D-C1D	2.43	129.00	124.71
32	a	318	CHL	C2D-C1D-ND	2.43	111.90	110.10
31	2	306	CLA	CHB-C1B-NB	-2.43	121.68	124.26
32	6	309	CHL	CMB-C2B-C1B	2.43	129.07	125.37
32	5	317	CHL	C1D-CHD-C4C	-2.43	120.81	126.06
31	6	312	CLA	CMD-C2D-C1D	2.43	129.00	124.71
32	4	313	CHL	CHC-C4B-C3B	-2.43	116.90	127.71
31	b	304	CLA	CMD-C2D-C1D	2.43	129.00	124.71
31	B	812	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
31	7	310	CLA	CHC-C4B-C3B	-2.43	116.91	127.71
32	a	318	CHL	CHB-C1B-NB	-2.43	121.69	124.26
31	A	847	CLA	O2A-CGA-CBA	2.43	119.53	111.91
31	A	850	CLA	O2A-CGA-CBA	2.43	119.53	111.91
31	4	308	CLA	CAC-C3C-C4C	2.43	127.96	124.81
31	B	829	CLA	CHC-C1C-NC	-2.43	120.52	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	320	CHL	C2D-C1D-ND	2.43	111.89	110.10
31	8	317	CLA	C1D-CHD-C4C	-2.43	120.82	126.06
31	4	321	CLA	CHC-C4B-C3B	-2.43	116.92	127.71
31	4	308	CLA	O2A-CGA-CBA	2.43	119.52	111.91
32	7	317	CHL	CED-O2D-CGD	2.43	121.42	115.94
39	7	301	3PH	O13-P-O11	-2.42	100.28	106.73
31	A	824	CLA	CED-O2D-CGD	2.42	121.42	115.94
31	8	314	CLA	C6-C5-C3	-2.42	110.66	114.62
31	B	846	CLA	C3D-C2D-C1D	-2.42	102.52	105.83
36	4	302	LUT	C8-C7-C6	-2.42	120.40	127.20
31	H	901	CLA	CAC-C3C-C4C	2.42	127.95	124.81
32	9	322	CHL	CAC-C3C-C4C	2.42	127.95	124.81
31	4	316	CLA	CHB-C1B-NB	-2.42	121.69	124.26
31	A	848	CLA	O2A-CGA-CBA	2.42	119.51	111.91
28	8	304	LHG	C20-C19-C18	-2.42	102.13	114.42
31	A	815	CLA	CHB-C4A-NA	2.42	127.86	124.51
31	4	316	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
31	F	301	CLA	CMB-C2B-C1B	2.42	129.06	125.37
31	a	321	CLA	CHB-C1B-NB	-2.42	121.69	124.26
31	6	316	CLA	CMC-C2C-C1C	2.42	128.73	125.04
31	9	319	CLA	CMB-C2B-C1B	2.42	129.06	125.37
31	B	846	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
31	J	105	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
31	A	816	CLA	CMC-C2C-C1C	2.42	128.72	125.04
26	2	302	BCR	C15-C14-C13	-2.42	123.86	127.31
31	3	311	CLA	CHC-C1C-NC	-2.42	120.53	124.20
42	4	304	SQD	O48-C23-C24	2.42	119.50	111.91
31	B	831	CLA	CMB-C2B-C1B	2.42	129.05	125.37
31	A	830	CLA	CHD-C4C-NC	2.42	128.01	124.20
31	a	314	CLA	C5-C3-C4	2.42	119.94	114.60
31	8	320	CLA	C4-C3-C2	-2.42	117.47	123.68
31	6	311	CLA	CMB-C2B-C1B	2.42	129.05	125.37
31	L	307	CLA	CED-O2D-CGD	2.42	121.40	115.94
31	2	305	CLA	CMB-C2B-C1B	2.42	129.05	125.37
31	B	834	CLA	C16-C15-C13	-2.42	108.11	115.92
31	B	836	CLA	CAC-C3C-C4C	2.42	127.94	124.81
31	B	838	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
31	a	319	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
32	4	310	CHL	CHB-C1B-NB	-2.42	121.70	124.26
31	A	824	CLA	C1-O2A-CGA	2.42	122.78	116.44
31	6	307	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
26	3	301	BCR	C15-C16-C17	-2.41	118.53	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	845	CLA	CAC-C3C-C4C	2.41	127.94	124.81
31	3	314	CLA	CMC-C2C-C1C	2.41	128.72	125.04
26	L	302	BCR	C15-C16-C17	-2.41	118.53	123.47
31	2	315	CLA	CHB-C1B-NB	-2.41	121.70	124.26
31	b	303	CLA	CHC-C4B-C3B	-2.41	116.97	127.71
31	5	314	CLA	CMD-C2D-C1D	2.41	128.97	124.71
31	b	308	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
31	5	312	CLA	CMB-C2B-C1B	2.41	129.04	125.37
31	a	312	CLA	CMD-C2D-C1D	2.41	128.97	124.71
31	B	831	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
31	K	205	CLA	C1D-CHD-C4C	-2.41	120.85	126.06
31	B	850	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
31	K	205	CLA	CAC-C3C-C4C	2.41	127.94	124.81
31	8	314	CLA	CAC-C3C-C4C	2.41	127.94	124.81
31	B	842	CLA	CMB-C2B-C1B	2.41	129.04	125.37
31	3	320	CLA	CHB-C1B-NB	-2.41	121.70	124.26
31	B	842	CLA	CMD-C2D-C1D	2.41	128.96	124.71
32	8	319	CHL	C2D-C1D-ND	2.41	111.88	110.10
31	7	310	CLA	CHD-C4C-NC	2.41	128.00	124.20
31	7	321	CLA	CMD-C2D-C1D	2.41	128.96	124.71
31	A	841	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
31	4	314	CLA	CAC-C3C-C4C	2.41	127.94	124.81
32	6	318	CHL	C2D-C1D-ND	2.41	111.88	110.10
31	a	321	CLA	CED-O2D-CGD	2.41	121.39	115.94
31	8	307	CLA	CHC-C1C-NC	-2.41	120.55	124.20
32	6	319	CHL	CAC-C3C-C4C	2.41	127.93	124.81
31	B	817	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
31	4	312	CLA	CAC-C3C-C4C	2.41	127.93	124.81
32	A	839	CHL	CMA-C3A-C4A	-2.41	105.31	111.77
31	2	312	CLA	CMD-C2D-C1D	2.41	128.95	124.71
36	F	304	LUT	C22-C23-C24	2.40	114.48	111.74
31	7	313	CLA	CMD-C2D-C1D	2.40	128.95	124.71
31	F	301	CLA	C6-C5-C3	-2.40	107.15	113.45
36	5	304	LUT	C7-C8-C9	-2.40	122.60	126.23
31	A	834	CLA	O2A-CGA-CBA	2.40	119.45	111.91
31	A	832	CLA	CMD-C2D-C1D	2.40	128.95	124.71
31	7	312	CLA	CMD-C2D-C1D	2.40	128.95	124.71
31	B	831	CLA	O2A-CGA-CBA	2.40	119.45	111.91
32	6	319	CHL	C2D-C1D-ND	2.40	111.88	110.10
31	L	307	CLA	CHB-C1B-NB	-2.40	121.71	124.26
31	5	318	CLA	C6-C5-C3	-2.40	107.15	113.45
36	3	305	LUT	C10-C11-C12	-2.40	115.72	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	316	CLA	CHC-C1C-NC	-2.40	120.56	124.20
31	A	857	CLA	O2A-CGA-CBA	2.40	119.44	111.91
31	5	321	CLA	CMC-C2C-C1C	2.40	128.69	125.04
32	a	320	CHL	C2D-C1D-ND	2.40	111.87	110.10
31	B	819	CLA	C1-O2A-CGA	2.40	122.74	116.44
31	9	316	CLA	C5-C3-C4	2.40	119.91	114.60
31	A	851	CLA	CMD-C2D-C1D	2.40	128.94	124.71
31	3	307	CLA	CHC-C1C-NC	-2.40	120.56	124.20
32	4	317	CHL	CMB-C2B-C1B	2.40	129.02	125.37
32	7	324	CHL	C2C-C3C-C4C	-2.40	104.78	106.49
31	B	831	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	A	818	CLA	CMC-C2C-C1C	2.40	128.69	125.04
31	A	825	CLA	CMD-C2D-C1D	2.40	128.94	124.71
31	7	313	CLA	O2D-CGD-O1D	-2.40	118.65	124.09
32	8	316	CHL	CHC-C1C-NC	-2.40	120.57	124.20
31	B	822	CLA	CMD-C2D-C1D	2.40	128.94	124.71
31	A	842	CLA	CHC-C1C-NC	-2.40	120.57	124.20
31	9	321	CLA	C1D-CHD-C4C	-2.39	120.89	126.06
26	6	302	BCR	C16-C15-C14	-2.39	118.57	123.47
31	2	307	CLA	CHC-C4B-C3B	-2.39	117.06	127.71
31	a	310	CLA	CHC-C4B-C3B	-2.39	117.07	127.71
26	B	804	BCR	C27-C26-C25	2.39	126.20	122.73
31	3	319	CLA	C4-C3-C5	2.39	119.30	115.27
31	5	310	CLA	CHB-C1B-NB	-2.39	121.72	124.26
32	4	313	CHL	CAC-C3C-C4C	2.39	127.91	124.81
31	B	823	CLA	CMD-C2D-C1D	2.39	128.93	124.71
31	5	311	CLA	CHC-C4B-C3B	-2.39	117.07	127.71
36	4	302	LUT	C1-C6-C7	-2.39	109.01	115.78
31	4	321	CLA	CMC-C2C-C1C	2.39	128.68	125.04
31	B	824	CLA	CMD-C2D-C1D	2.39	128.93	124.71
31	6	322	CLA	CHC-C1C-NC	-2.39	120.58	124.20
31	3	319	CLA	CED-O2D-CGD	2.39	121.34	115.94
31	B	832	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
31	7	322	CLA	CHC-C4B-C3B	-2.39	117.08	127.71
31	2	314	CLA	CHC-C4B-C3B	-2.39	117.08	127.71
31	O	204	CLA	CHC-C1C-NC	-2.39	120.58	124.20
31	4	312	CLA	CMB-C2B-C1B	2.39	129.01	125.37
31	A	821	CLA	CHB-C4A-NA	2.39	127.81	124.51
32	5	322	CHL	CMB-C2B-C1B	2.39	129.01	125.37
31	B	843	CLA	CAC-C3C-C4C	2.39	127.91	124.81
31	2	309	CLA	CAC-C3C-C4C	2.39	127.91	124.81
31	b	312	CLA	CMC-C2C-C1C	2.39	128.67	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	F	301	CLA	CED-O2D-CGD	2.39	121.33	115.94
31	5	309	CLA	CMB-C2B-C1B	2.39	129.00	125.37
32	8	316	CHL	CMD-C2D-C1D	2.39	128.92	124.71
31	A	838	CLA	CMC-C2C-C1C	2.38	128.67	125.04
32	4	310	CHL	CHC-C1C-NC	-2.38	120.58	124.20
31	6	311	CLA	C1-C2-C3	-2.38	121.92	126.04
31	b	305	CLA	CMC-C2C-C1C	2.38	128.67	125.04
31	3	307	CLA	CMD-C2D-C1D	2.38	128.91	124.71
31	A	816	CLA	CHC-C4B-NB	2.38	126.78	124.26
26	A	804	BCR	C24-C23-C22	-2.38	122.63	126.23
28	A	809	LHG	C20-C19-C18	-2.38	102.33	114.42
31	B	848	CLA	CHB-C1B-NB	-2.38	121.73	124.26
31	b	313	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
31	L	307	CLA	C3D-C4D-CHA	-2.38	107.27	112.72
31	L	306	CLA	CMC-C2C-C1C	2.38	128.67	125.04
32	5	319	CHL	CMD-C2D-C1D	2.38	128.91	124.71
31	B	825	CLA	CHC-C1C-NC	-2.38	120.59	124.20
31	A	856	CLA	CMD-C2D-C1D	2.38	128.91	124.71
31	4	307	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
31	b	308	CLA	CMB-C2B-C1B	2.38	128.99	125.37
31	B	826	CLA	CHC-C1C-NC	-2.38	120.59	124.20
26	5	302	BCR	C34-C9-C10	-2.38	119.59	122.92
31	A	820	CLA	CHC-C4B-C3B	-2.38	117.13	127.71
31	7	313	CLA	CHC-C4B-C3B	-2.38	117.13	127.71
31	A	846	CLA	CMC-C2C-C1C	2.38	128.66	125.04
31	6	307	CLA	CED-O2D-CGD	2.38	121.32	115.94
32	8	316	CHL	C2C-C3C-C4C	-2.38	104.79	106.49
31	8	312	CLA	CMC-C2C-C1C	2.38	128.66	125.04
31	A	844	CLA	CHC-C4B-C3B	-2.38	117.14	127.71
31	7	322	CLA	C3D-C2D-C1D	-2.38	102.59	105.83
31	8	311	CLA	CMC-C2C-C1C	2.38	128.66	125.04
31	2	306	CLA	CAC-C3C-C4C	2.38	127.89	124.81
36	5	303	LUT	C17-C1-C6	-2.38	106.44	110.30
31	B	819	CLA	O2A-CGA-CBA	2.38	119.36	111.91
31	B	840	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
31	2	312	CLA	CHC-C1C-NC	-2.37	120.60	124.20
31	5	320	CLA	CAC-C3C-C4C	2.37	127.89	124.81
31	A	816	CLA	C1-C2-C3	-2.37	121.94	126.04
31	B	834	CLA	CHB-C1B-NB	-2.37	121.75	124.26
31	A	833	CLA	O2A-CGA-CBA	2.37	119.35	111.91
31	7	309	CLA	C4-C3-C5	2.37	119.26	115.27
31	a	322	CLA	CMD-C2D-C1D	2.37	128.89	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	317	CHL	CMB-C2B-C1B	2.37	128.98	125.37
31	5	307	CLA	CAC-C3C-C4C	2.37	127.89	124.81
31	F	305	CLA	CHB-C1B-NB	-2.37	121.75	124.26
31	a	309	CLA	CMD-C2D-C1D	2.37	128.89	124.71
31	A	855	CLA	CMB-C2B-C1B	2.37	128.98	125.37
32	6	319	CHL	O2A-CGA-CBA	2.37	121.60	112.23
31	A	847	CLA	CHC-C4B-C3B	-2.37	117.17	127.71
37	G	202	LMG	O2-C2-C1	-2.37	104.29	110.05
32	5	322	CHL	CHC-C4B-C3B	-2.37	117.17	127.71
31	B	837	CLA	CHC-C1C-NC	-2.37	120.61	124.20
28	A	811	LHG	C18-C17-C16	-2.37	102.40	114.42
26	3	302	BCR	C27-C26-C25	2.37	126.17	122.73
31	b	302	CLA	CHC-C4B-C3B	-2.37	117.18	127.71
31	b	310	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
31	A	854	CLA	CHC-C4B-C3B	-2.37	117.18	127.71
31	7	315	CLA	CHC-C1C-NC	-2.37	120.61	124.20
31	4	307	CLA	CHC-C4B-C3B	-2.37	117.18	127.71
31	B	816	CLA	O2A-CGA-CBA	2.37	119.33	111.91
31	a	314	CLA	CMD-C2D-C1D	2.37	128.88	124.71
31	4	315	CLA	C3D-C4D-CHA	-2.37	107.31	112.72
31	B	840	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
31	B	812	CLA	CHD-C4C-NC	2.37	127.93	124.20
31	5	309	CLA	CHC-C4B-C3B	-2.37	117.19	127.71
31	8	308	CLA	C4-C3-C5	2.37	119.25	115.27
31	a	311	CLA	C4-C3-C5	2.36	119.25	115.27
26	3	303	BCR	C24-C23-C22	-2.36	122.66	126.23
31	a	315	CLA	O2A-CGA-CBA	2.36	119.33	111.91
36	8	302	LUT	C1-C2-C3	2.36	118.98	113.64
31	7	322	CLA	CHB-C1B-NB	-2.36	121.75	124.26
31	4	306	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
32	A	839	CHL	C1D-CHD-C4C	-2.36	120.96	126.06
31	a	311	CLA	CAC-C3C-C4C	2.36	127.88	124.81
31	8	318	CLA	C5-C3-C4	2.36	119.82	114.60
31	3	309	CLA	CHC-C1C-NC	-2.36	120.62	124.20
31	8	312	CLA	CHC-C4B-C3B	-2.36	117.20	127.71
31	9	311	CLA	C1-C2-C3	-2.36	121.96	126.04
31	A	828	CLA	C4-C3-C5	2.36	119.24	115.27
31	F	305	CLA	CHB-C4A-NA	2.36	127.78	124.51
31	a	321	CLA	C1D-CHD-C4C	-2.36	120.97	126.06
31	9	319	CLA	CMC-C2C-C1C	2.36	128.63	125.04
31	8	315	CLA	CAC-C3C-C4C	2.36	127.87	124.81
31	a	315	CLA	CHC-C1C-NC	-2.36	120.62	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	306	CLA	CMC-C2C-C1C	2.36	128.63	125.04
31	H	902	CLA	CHC-C4B-C3B	-2.36	117.22	127.71
28	A	811	LHG	C20-C19-C18	-2.36	102.45	114.42
32	a	317	CHL	C2D-C1D-ND	2.36	111.84	110.10
32	5	316	CHL	CHB-C4A-NA	2.36	127.77	124.51
31	5	321	CLA	CMB-C2B-C1B	2.36	128.96	125.37
31	A	822	CLA	CHB-C1B-NB	-2.36	121.76	124.26
31	6	308	CLA	CMD-C2D-C1D	2.36	128.87	124.71
31	A	827	CLA	O2A-CGA-CBA	2.36	119.31	111.91
31	5	315	CLA	CMB-C2B-C1B	2.36	128.96	125.37
36	3	304	LUT	C8-C7-C6	2.36	133.82	127.20
28	A	810	LHG	O8-C23-C24	2.36	119.30	111.91
31	3	314	CLA	O2A-CGA-CBA	2.36	119.30	111.91
31	B	820	CLA	C1-O2A-CGA	2.36	122.62	116.44
31	a	322	CLA	CAC-C3C-C4C	2.36	127.87	124.81
31	B	830	CLA	CMD-C2D-C1D	2.36	128.86	124.71
31	5	308	CLA	CMC-C2C-C1C	2.35	128.62	125.04
31	B	837	CLA	C4-C3-C5	2.35	119.23	115.27
31	8	311	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
31	F	305	CLA	CHC-C4B-C3B	-2.35	117.24	127.71
31	9	314	CLA	CMD-C2D-C1D	2.35	128.86	124.71
31	7	309	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
32	A	831	CHL	CMD-C2D-C1D	2.35	128.86	124.71
31	A	814	CLA	CHB-C1B-NB	-2.35	121.77	124.26
31	4	306	CLA	C3D-C4D-CHA	-2.35	107.34	112.72
31	2	306	CLA	CMC-C2C-C1C	2.35	128.62	125.04
31	F	306	CLA	CMB-C2B-C1B	2.35	128.95	125.37
33	B	808	DGD	O6D-C1D-O3G	-2.35	104.41	109.97
31	4	318	CLA	CMD-C2D-C1D	2.35	128.85	124.71
37	J	104	LMG	O3-C3-C2	-2.35	104.92	110.35
28	a	306	LHG	C20-C19-C18	-2.35	102.50	114.42
26	7	304	BCR	C15-C16-C17	-2.35	118.66	123.47
32	6	317	CHL	CED-O2D-CGD	2.35	121.25	115.94
31	A	838	CLA	CHC-C4B-C3B	-2.35	117.27	127.71
31	8	312	CLA	O2A-CGA-CBA	2.35	119.28	111.91
31	9	311	CLA	C1D-CHD-C4C	-2.35	120.99	126.06
31	3	310	CLA	C1-C2-C3	-2.35	121.98	126.04
31	9	314	CLA	CMC-C2C-C1C	2.35	128.61	125.04
31	3	318	CLA	CHC-C1C-NC	-2.35	120.64	124.20
32	3	315	CHL	CMB-C2B-C1B	2.35	128.94	125.37
32	6	309	CHL	CHB-C1B-NB	-2.35	121.77	124.26
31	7	316	CLA	CMD-C2D-C1D	2.35	128.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	311	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
31	O	202	CLA	CMC-C2C-C1C	2.34	128.61	125.04
33	7	308	DGD	C3G-C2G-C1G	-2.34	106.24	111.79
32	A	840	CHL	CHC-C1C-NC	-2.34	120.65	124.20
31	B	840	CLA	C6-C7-C8	-2.34	108.34	115.92
31	A	830	CLA	CHC-C4B-C3B	-2.34	117.28	127.71
31	F	306	CLA	CMC-C2C-C1C	2.34	128.61	125.04
31	a	310	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
32	9	320	CHL	C1D-CHD-C4C	-2.34	121.00	126.06
31	b	303	CLA	CHD-C4C-NC	2.34	127.89	124.20
31	A	844	CLA	CHC-C1C-NC	-2.34	120.65	124.20
31	8	314	CLA	CHC-C4B-C3B	-2.34	117.29	127.71
32	4	313	CHL	O1D-CGD-CBD	-2.34	119.69	124.48
31	8	309	CLA	O2A-CGA-CBA	2.34	119.26	111.91
31	O	204	CLA	CMC-C2C-C1C	2.34	128.60	125.04
31	B	826	CLA	CHB-C4A-NA	2.34	127.75	124.51
31	B	830	CLA	C3D-C4D-CHA	-2.34	107.37	112.72
31	A	823	CLA	CMD-C2D-C1D	2.34	128.84	124.71
31	A	837	CLA	CMD-C2D-C1D	2.34	128.84	124.71
31	4	309	CLA	CMD-C2D-C1D	2.34	128.84	124.71
31	B	838	CLA	CHC-C4B-C3B	-2.34	117.30	127.71
31	5	321	CLA	CED-O2D-CGD	2.34	121.23	115.94
31	B	825	CLA	CMD-C2D-C1D	2.34	128.84	124.71
31	B	824	CLA	CHC-C4B-C3B	-2.34	117.30	127.71
31	3	312	CLA	CHC-C4B-C3B	-2.34	117.30	127.71
31	5	313	CLA	CHC-C1C-NC	-2.34	120.65	124.20
31	B	849	CLA	CAC-C3C-C4C	2.34	127.85	124.81
32	5	319	CHL	CHC-C4B-C3B	-2.34	117.30	127.71
31	4	305	CLA	CHC-C1C-C2C	-2.34	120.23	126.73
31	8	308	CLA	CAC-C3C-C4C	2.34	127.84	124.81
31	7	310	CLA	CMC-C2C-C1C	2.34	128.60	125.04
36	a	303	LUT	C10-C11-C12	-2.34	115.92	123.22
32	A	831	CHL	CHD-C4C-NC	2.34	127.89	124.20
31	4	319	CLA	CMD-C2D-C1D	2.34	128.83	124.71
31	A	857	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
31	K	206	CLA	CHC-C4B-C3B	-2.34	117.31	127.71
31	5	323	CLA	C4-C3-C5	2.34	119.20	115.27
32	5	316	CHL	CHA-C4D-ND	2.34	137.38	132.50
31	A	852	CLA	CAA-CBA-CGA	-2.34	106.43	113.25
31	A	842	CLA	CED-O2D-CGD	2.33	121.22	115.94
31	4	309	CLA	CHC-C4B-C3B	-2.33	117.33	127.71
31	3	311	CLA	C1-C2-C3	-2.33	122.01	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	311	CLA	C1-O2A-CGA	2.33	122.57	116.44
36	F	304	LUT	C16-C1-C6	-2.33	106.51	110.30
31	H	901	CLA	CHB-C1B-NB	-2.33	121.79	124.26
31	A	827	CLA	CMD-C2D-C1D	2.33	128.82	124.71
36	3	304	LUT	C10-C11-C12	-2.33	115.94	123.22
26	M	101	BCR	C2-C1-C6	2.33	114.07	110.48
26	L	301	BCR	C11-C10-C9	-2.33	123.98	127.31
31	K	204	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
31	A	841	CLA	CHB-C4A-NA	2.33	127.74	124.51
31	B	825	CLA	O2A-CGA-CBA	2.33	119.22	111.91
31	4	309	CLA	CHC-C1C-NC	-2.33	120.67	124.20
31	B	841	CLA	CAC-C3C-C4C	2.33	127.83	124.81
26	5	302	BCR	C11-C10-C9	-2.33	123.98	127.31
28	6	301	LHG	O8-C23-C24	2.33	119.22	111.91
31	A	814	CLA	CHC-C1C-NC	-2.33	120.67	124.20
31	B	814	CLA	CMD-C2D-C1D	2.33	128.82	124.71
31	H	902	CLA	CAC-C3C-C4C	2.33	127.83	124.81
32	a	317	CHL	OBD-CAD-C3D	2.33	134.12	128.52
31	G	204	CLA	CHD-C4C-NC	2.33	127.87	124.20
31	a	309	CLA	C4-C3-C5	2.33	119.19	115.27
36	8	302	LUT	C21-C26-C27	-2.33	109.76	112.70
31	8	321	CLA	CMD-C2D-C1D	2.33	128.82	124.71
40	7	306	XAT	C32-C33-C34	2.33	122.51	118.94
31	A	844	CLA	C5-C3-C4	2.33	119.74	114.60
32	A	831	CHL	C2C-C3C-C4C	-2.33	104.83	106.49
31	3	312	CLA	O2A-CGA-CBA	2.33	119.21	111.91
31	J	105	CLA	CHC-C1C-NC	-2.33	120.67	124.20
31	A	847	CLA	CHB-C1B-NB	-2.33	121.80	124.26
31	a	321	CLA	O1D-CGD-CBD	-2.33	119.73	124.48
31	B	815	CLA	CMB-C2B-C1B	2.33	128.91	125.37
31	B	835	CLA	CMD-C2D-C1D	2.32	128.81	124.71
31	L	306	CLA	CMD-C2D-C1D	2.32	128.81	124.71
31	A	832	CLA	O2A-CGA-CBA	2.32	119.20	111.91
31	9	311	CLA	CHC-C4B-C3B	-2.32	117.37	127.71
31	O	203	CLA	CHC-C4B-C3B	-2.32	117.37	127.71
31	B	840	CLA	CHB-C4A-NA	2.32	127.72	124.51
31	A	834	CLA	C7-C6-C5	-2.32	107.05	113.36
31	a	311	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	3	312	CLA	C4-C3-C5	2.32	119.18	115.27
31	F	301	CLA	CMC-C2C-C1C	2.32	128.57	125.04
31	5	308	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
31	3	311	CLA	CAC-C3C-C4C	2.32	127.82	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	323	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
31	8	310	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	3	311	CLA	CMC-C2C-C1C	2.32	128.57	125.04
31	9	321	CLA	C4-C3-C5	2.32	119.17	115.27
31	4	307	CLA	C4-C3-C5	2.32	119.17	115.27
26	8	301	BCR	C15-C16-C17	-2.32	118.72	123.47
31	3	320	CLA	CED-O2D-CGD	2.32	121.18	115.94
31	6	315	CLA	CMD-C2D-C1D	2.32	128.80	124.71
32	9	322	CHL	O2A-CGA-CBA	2.32	121.39	112.23
31	B	820	CLA	CMD-C2D-C1D	2.32	128.80	124.71
26	F	302	BCR	C27-C26-C25	2.32	126.10	122.73
31	A	843	CLA	CHC-C4B-C3B	-2.32	117.40	127.71
31	2	314	CLA	CAC-C3C-C4C	2.32	127.82	124.81
36	8	302	LUT	C4-C5-C6	-2.32	115.69	120.85
31	B	819	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
31	4	306	CLA	CMB-C2B-C1B	2.32	128.90	125.37
31	8	307	CLA	CHC-C4B-C3B	-2.32	117.41	127.71
31	b	313	CLA	CED-O2D-CGD	2.32	121.17	115.94
31	B	832	CLA	O2A-CGA-CBA	2.32	119.17	111.91
31	9	319	CLA	CMD-C2D-C1D	2.32	128.79	124.71
31	4	305	CLA	C4-C3-C5	2.31	119.17	115.27
31	A	857	CLA	CHC-C4B-C3B	-2.31	117.41	127.71
31	A	829	CLA	CHD-C1D-C2D	2.31	130.34	125.48
31	6	311	CLA	CHC-C4B-C3B	-2.31	117.42	127.71
31	B	842	CLA	CMC-C2C-C1C	2.31	128.56	125.04
31	7	315	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
31	9	319	CLA	CHC-C1C-NC	-2.31	120.69	124.20
31	B	838	CLA	CHD-C4C-NC	2.31	127.85	124.20
31	4	321	CLA	C1-C2-C3	-2.31	123.01	126.75
31	B	832	CLA	CHB-C4A-NA	2.31	127.71	124.51
31	5	312	CLA	C5-C3-C4	2.31	119.71	114.60
31	A	845	CLA	CMD-C2D-C1D	2.31	128.79	124.71
32	7	320	CHL	CHA-C4D-ND	2.31	137.34	132.50
32	7	320	CHL	CHB-C1B-NB	-2.31	121.81	124.26
31	6	322	CLA	CHC-C4B-C3B	-2.31	117.43	127.71
31	9	311	CLA	CAC-C3C-C4C	2.31	127.81	124.81
31	5	311	CLA	CED-O2D-CGD	2.31	121.16	115.94
31	A	836	CLA	CMC-C2C-C1C	2.31	128.56	125.04
31	4	306	CLA	C1D-CHD-C4C	-2.31	121.07	126.06
31	a	310	CLA	CMB-C2B-C1B	2.31	128.89	125.37
31	2	310	CLA	CMC-C2C-C1C	2.31	128.56	125.04
32	7	317	CHL	O1D-CGD-CBD	-2.31	119.76	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	303	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
26	L	302	BCR	C28-C27-C26	-2.31	109.95	114.08
31	3	314	CLA	CMD-C2D-C1D	2.31	128.78	124.71
32	A	831	CHL	C1-O2A-CGA	2.31	122.50	116.44
32	7	318	CHL	C2D-C1D-ND	2.31	111.81	110.10
31	8	309	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
31	A	845	CLA	CHC-C4B-C3B	-2.31	117.45	127.71
31	A	854	CLA	CMD-C2D-C1D	2.31	128.78	124.71
32	a	317	CHL	CHC-C4B-C3B	-2.31	117.45	127.71
31	A	822	CLA	CAC-C3C-C4C	2.31	127.80	124.81
31	3	317	CLA	CAC-C3C-C4C	2.31	127.80	124.81
31	2	311	CLA	CMB-C2B-C1B	2.31	128.88	125.37
36	L	304	LUT	C1-C6-C7	-2.31	109.25	115.78
31	3	316	CLA	CHC-C4B-C3B	-2.31	117.45	127.71
31	3	308	CLA	CMC-C2C-C1C	2.31	128.55	125.04
31	A	846	CLA	CMD-C2D-C1D	2.31	128.78	124.71
31	4	320	CLA	CMD-C2D-C1D	2.31	128.78	124.71
31	3	317	CLA	CMD-C2D-C1D	2.30	128.78	124.71
32	A	839	CHL	CHB-C4A-NA	2.30	127.70	124.51
31	3	308	CLA	CMD-C2D-C1D	2.30	128.77	124.71
31	3	314	CLA	C1-O2A-CGA	2.30	122.49	116.44
31	A	824	CLA	C1D-CHD-C4C	-2.30	121.09	126.06
31	B	823	CLA	CHC-C4B-C3B	-2.30	117.46	127.71
31	B	837	CLA	CHD-C4C-NC	2.30	127.83	124.20
31	8	312	CLA	C5-C3-C4	2.30	119.69	114.60
31	A	847	CLA	C1-O2A-CGA	2.30	122.48	116.44
28	A	809	LHG	O8-C23-C24	2.30	119.13	111.91
31	2	315	CLA	CHC-C4B-C3B	-2.30	117.47	127.71
32	6	318	CHL	CMD-C2D-C1D	2.30	128.77	124.71
31	B	814	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
31	6	312	CLA	CAC-C3C-C4C	2.30	127.80	124.81
26	K	202	BCR	C15-C14-C13	-2.30	124.03	127.31
31	7	312	CLA	O2A-CGA-CBA	2.30	119.12	111.91
31	J	105	CLA	CHC-C4B-C3B	-2.30	117.48	127.71
32	4	317	CHL	C2D-C1D-ND	2.30	111.80	110.10
31	2	307	CLA	CAC-C3C-C4C	2.30	127.79	124.81
31	5	315	CLA	CHC-C4B-C3B	-2.30	117.49	127.71
31	8	312	CLA	CAC-C3C-C4C	2.30	127.79	124.81
32	9	322	CHL	CHB-C1B-NB	-2.30	121.83	124.26
31	8	313	CLA	CHC-C1C-NC	-2.30	120.72	124.20
31	8	321	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	I	801	BCR	C28-C27-C26	-2.30	109.98	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	309	CLA	CHC-C4B-C3B	-2.30	117.50	127.71
31	B	844	CLA	CHC-C4B-C3B	-2.30	117.50	127.71
31	b	307	CLA	CMC-C2C-C1C	2.29	128.53	125.04
31	b	306	CLA	CMB-C2B-C1B	2.29	128.86	125.37
31	2	315	CLA	CAC-C3C-C4C	2.29	127.79	124.81
31	B	829	CLA	C1-O2A-CGA	2.29	122.46	116.44
26	A	804	BCR	C11-C10-C9	-2.29	124.04	127.31
31	F	306	CLA	CMD-C2D-C1D	2.29	128.75	124.71
31	A	830	CLA	C6-C7-C8	-2.29	108.51	115.92
31	6	307	CLA	C3D-C4D-CHA	-2.29	107.48	112.72
31	A	855	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
31	B	823	CLA	CMB-C2B-C1B	2.29	128.86	125.37
31	6	313	CLA	CAC-C3C-C4C	2.29	127.78	124.81
32	7	324	CHL	CAC-C3C-C4C	2.29	127.78	124.81
26	B	803	BCR	C24-C23-C22	-2.29	122.77	126.23
31	A	838	CLA	C4-C3-C5	2.29	119.12	115.27
31	A	824	CLA	CHD-C4C-NC	2.29	127.81	124.20
31	a	310	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
31	B	843	CLA	CED-O2D-CGD	2.29	121.12	115.94
36	8	303	LUT	C36-C21-C26	2.29	113.01	109.55
31	B	813	CLA	CAC-C3C-C4C	2.29	127.78	124.81
32	3	315	CHL	C1D-CHD-C4C	-2.29	121.12	126.06
31	2	306	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
26	G	203	BCR	C24-C23-C22	-2.29	122.78	126.23
31	3	318	CLA	CMB-C2B-C1B	2.29	128.85	125.37
31	5	313	CLA	C2D-C1D-ND	2.29	111.79	110.10
31	A	821	CLA	CMD-C2D-C1D	2.29	128.75	124.71
31	5	308	CLA	C1D-CHD-C4C	-2.29	121.12	126.06
31	5	318	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
31	G	204	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
35	9	304	QTB	C03-C04-C05	2.29	130.35	123.22
32	6	318	CHL	CHB-C1B-NB	-2.29	121.84	124.26
31	8	318	CLA	CMB-C2B-C1B	2.29	128.85	125.37
32	8	316	CHL	C4-C3-C2	-2.28	117.82	123.68
31	2	313	CLA	C3D-C4D-CHA	-2.28	107.50	112.72
31	A	821	CLA	CMC-C2C-C1C	2.28	128.52	125.04
31	O	202	CLA	CHC-C4B-C3B	-2.28	117.55	127.71
32	6	309	CHL	CAC-C3C-C4C	2.28	127.77	124.81
36	2	301	LUT	C17-C1-C6	-2.28	106.59	110.30
31	8	310	CLA	C1-C2-C3	-2.28	122.09	126.04
32	6	318	CHL	CMB-C2B-C1B	2.28	128.85	125.37
36	6	303	LUT	C22-C23-C24	2.28	114.34	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	312	CLA	CMD-C2D-C1D	2.28	128.74	124.71
32	8	319	CHL	CHC-C1C-NC	-2.28	120.74	124.20
35	7	303	QTB	C11-C10-C09	2.28	130.43	125.47
31	B	842	CLA	C4-C3-C5	2.28	119.11	115.27
31	3	310	CLA	C4-C3-C5	2.28	119.11	115.27
31	B	844	CLA	O2A-CGA-CBA	2.28	119.07	111.91
31	2	310	CLA	CMB-C2B-C1B	2.28	128.84	125.37
31	6	314	CLA	CMB-C2B-C1B	2.28	128.84	125.37
31	a	312	CLA	C1-C2-C3	-2.28	122.10	126.04
31	A	833	CLA	CHC-C1C-NC	-2.28	120.74	124.20
31	A	829	CLA	CHD-C4C-C3C	-2.28	121.49	124.84
31	9	314	CLA	CHC-C4B-C3B	-2.28	117.56	127.71
31	B	849	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
31	5	308	CLA	CAC-C3C-C4C	2.28	127.77	124.81
31	B	843	CLA	CMC-C2C-C1C	2.28	128.51	125.04
26	3	301	BCR	C15-C14-C13	-2.28	124.06	127.31
31	a	309	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
32	7	320	CHL	CMB-C2B-C1B	2.28	128.84	125.37
32	6	318	CHL	C2C-C3C-C4C	-2.28	104.86	106.49
31	B	831	CLA	CMD-C2D-C1D	2.28	128.73	124.71
32	8	316	CHL	C4D-CHA-C1A	-2.28	118.48	121.25
31	b	311	CLA	CMB-C2B-C1B	2.28	128.84	125.37
32	7	317	CHL	CMB-C2B-C1B	2.28	128.84	125.37
31	B	826	CLA	CMC-C2C-C1C	2.28	128.51	125.04
31	A	820	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	8	309	CLA	CHD-C4C-NC	2.28	127.79	124.20
31	B	849	CLA	C5-C3-C4	2.28	119.63	114.60
31	B	838	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
31	A	849	CLA	CHC-C1C-NC	-2.28	120.75	124.20
31	B	848	CLA	C4-C3-C5	2.28	119.10	115.27
31	A	824	CLA	CMC-C2C-C1C	2.28	128.50	125.04
28	B	807	LHG	C27-C26-C25	-2.28	102.87	114.42
32	4	313	CHL	C2D-C1D-ND	2.28	111.78	110.10
26	K	202	BCR	C11-C10-C9	-2.28	124.06	127.31
32	a	317	CHL	C4-C3-C5	2.27	119.10	115.27
28	B	807	LHG	O8-C23-C24	2.27	119.05	111.91
31	9	313	CLA	CHC-C4B-C3B	-2.27	117.59	127.71
31	7	314	CLA	CED-O2D-CGD	2.27	121.08	115.94
31	a	315	CLA	CED-O2D-CGD	2.27	121.08	115.94
31	a	311	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
31	A	851	CLA	CHC-C4B-C3B	-2.27	117.60	127.71
31	3	317	CLA	O2A-CGA-CBA	2.27	119.04	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	314	CLA	CMC-C2C-C1C	2.27	128.50	125.04
26	3	303	BCR	C3-C4-C5	-2.27	110.02	114.08
31	B	837	CLA	C3D-C4D-CHA	-2.27	107.52	112.72
31	H	901	CLA	CED-O2D-CGD	2.27	121.08	115.94
31	8	315	CLA	CHB-C4A-NA	2.27	127.65	124.51
31	5	312	CLA	CAC-C3C-C4C	2.27	127.76	124.81
31	B	833	CLA	C1D-CHD-C4C	-2.27	121.16	126.06
31	6	314	CLA	CHC-C4B-C3B	-2.27	117.61	127.71
31	7	314	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
31	b	312	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
31	5	307	CLA	CHC-C1C-NC	-2.27	120.76	124.20
31	3	320	CLA	CMC-C2C-C1C	2.27	128.49	125.04
31	8	314	CLA	C4-C3-C5	2.27	119.09	115.27
31	a	311	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
31	A	848	CLA	CAC-C3C-C4C	2.27	127.75	124.81
28	6	305	LHG	C11-C10-C9	-2.27	102.91	114.42
31	O	204	CLA	CAA-C2A-C3A	-2.27	110.81	116.10
31	6	310	CLA	C3D-C4D-CHA	-2.27	107.54	112.72
32	4	317	CHL	CMD-C2D-C1D	2.27	128.71	124.71
31	4	312	CLA	C3D-C4D-CHA	-2.27	107.54	112.72
31	G	206	CLA	CHC-C4B-C3B	-2.27	117.63	127.71
31	5	313	CLA	CMC-C2C-C1C	2.27	128.49	125.04
31	6	308	CLA	CMB-C2B-C1B	2.27	128.82	125.37
31	A	850	CLA	CAC-C3C-C4C	2.27	127.75	124.81
31	a	316	CLA	CMC-C2C-C1C	2.26	128.49	125.04
31	7	321	CLA	CMC-C2C-C1C	2.26	128.49	125.04
31	b	311	CLA	CHC-C4B-C3B	-2.26	117.64	127.71
31	2	307	CLA	CHC-C1C-NC	-2.26	120.77	124.20
32	3	315	CHL	C4D-CHA-C1A	-2.26	118.49	121.25
31	A	829	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
31	A	820	CLA	CAC-C3C-C4C	2.26	127.75	124.81
32	6	318	CHL	CHC-C4B-C3B	-2.26	117.64	127.71
31	A	819	CLA	CMD-C2D-C1D	2.26	128.70	124.71
31	2	314	CLA	CMC-C2C-C1C	2.26	128.49	125.04
32	7	320	CHL	C2C-C3C-C4C	-2.26	104.88	106.49
36	2	301	LUT	C12-C13-C14	-2.26	115.47	118.94
31	2	312	CLA	C3D-C4D-CHA	-2.26	107.55	112.72
26	8	301	BCR	C15-C14-C13	-2.26	124.08	127.31
36	a	303	LUT	C1-C2-C3	2.26	118.75	113.64
31	a	319	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
27	A	808	LMT	O1'-C1'-C2'	2.26	111.83	108.30
31	a	316	CLA	CHC-C4B-C3B	-2.26	117.66	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	311	CLA	C1-C2-C3	-2.26	122.13	126.04
31	7	321	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
31	6	316	CLA	C5-C3-C4	2.26	119.59	114.60
31	A	828	CLA	CHC-C4B-C3B	-2.26	117.66	127.71
31	b	305	CLA	CHC-C1C-NC	-2.26	120.78	124.20
31	5	318	CLA	CHC-C4B-C3B	-2.26	117.66	127.71
31	5	307	CLA	CHC-C4B-C3B	-2.26	117.67	127.71
31	A	822	CLA	CMD-C2D-C1D	2.26	128.69	124.71
31	B	825	CLA	CHB-C4A-NA	2.26	127.63	124.51
31	B	837	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
31	B	844	CLA	CHB-C1B-NB	-2.26	121.87	124.26
31	A	830	CLA	C4-C3-C2	-2.26	117.89	123.68
31	b	308	CLA	CMD-C2D-C1D	2.26	128.69	124.71
32	6	321	CHL	O1D-CGD-CBD	-2.26	119.87	124.48
31	b	305	CLA	CHC-C4B-C3B	-2.26	117.68	127.71
31	8	309	CLA	C4D-CHA-C1A	-2.26	118.50	121.25
31	B	817	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
31	8	320	CLA	CMD-C2D-C1D	2.25	128.69	124.71
31	b	303	CLA	CMD-C2D-C1D	2.25	128.69	124.71
32	8	316	CHL	C1-O2A-CGA	2.25	122.36	116.44
31	B	828	CLA	CED-O2D-CGD	2.25	121.04	115.94
37	G	202	LMG	O3-C3-C2	-2.25	105.14	110.35
31	a	315	CLA	CMD-C2D-C1D	2.25	128.68	124.71
32	a	320	CHL	CHA-C4D-ND	2.25	137.21	132.50
31	3	309	CLA	CMD-C2D-C1D	2.25	128.68	124.71
31	8	310	CLA	CED-O2D-CGD	2.25	121.03	115.94
33	B	808	DGD	CFB-CEB-CDB	-2.25	102.99	114.42
31	B	845	CLA	C5-C3-C4	2.25	119.58	114.60
32	4	310	CHL	CHC-C4B-C3B	-2.25	117.69	127.71
31	5	321	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
31	3	317	CLA	CED-O2D-CGD	2.25	121.03	115.94
31	A	855	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
31	A	856	CLA	CHC-C1C-NC	-2.25	120.79	124.20
31	2	304	CLA	CHC-C1C-NC	-2.25	120.79	124.20
31	a	316	CLA	CMD-C2D-C1D	2.25	128.68	124.71
31	6	315	CLA	CAC-C3C-C4C	2.25	127.73	124.81
31	A	823	CLA	C4-C3-C5	2.25	119.06	115.27
31	B	841	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
31	5	311	CLA	CHC-C1C-NC	-2.25	120.79	124.20
31	4	308	CLA	C6-C7-C8	-2.25	108.64	115.92
31	L	306	CLA	CAC-C3C-C4C	2.25	127.73	124.81
31	B	845	CLA	O2A-CGA-O1A	-2.25	117.92	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	822	CLA	C1-C2-C3	-2.25	122.15	126.04
31	A	820	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
31	9	311	CLA	CHB-C1B-NB	-2.25	121.88	124.26
31	B	836	CLA	CHB-C4A-NA	2.25	127.62	124.51
27	A	807	LMT	O1'-C1'-C2'	2.25	111.81	108.30
31	A	848	CLA	CHC-C1C-NC	-2.25	120.79	124.20
31	8	311	CLA	CAC-C3C-C4C	2.25	127.73	124.81
31	b	302	CLA	CMB-C2B-C1B	2.25	128.79	125.37
31	3	311	CLA	C3D-C4D-CHA	-2.25	107.58	112.72
31	3	317	CLA	CHB-C1B-NB	-2.25	121.88	124.26
31	B	841	CLA	O2A-CGA-CBA	2.25	118.96	111.91
31	9	319	CLA	CHC-C4B-C3B	-2.25	117.72	127.71
31	a	309	CLA	CAC-C3C-C4C	2.25	127.72	124.81
31	H	901	CLA	CHC-C4B-C3B	-2.25	117.72	127.71
31	A	853	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
31	5	320	CLA	O2A-CGA-CBA	2.25	121.11	112.23
31	G	205	CLA	CMD-C2D-C1D	2.25	128.67	124.71
31	B	831	CLA	CMC-C2C-C1C	2.25	128.46	125.04
31	b	310	CLA	CMC-C2C-C1C	2.25	128.46	125.04
32	6	317	CHL	CMD-C2D-C1D	2.25	128.67	124.71
31	4	318	CLA	CMC-C2C-C1C	2.24	128.46	125.04
31	9	316	CLA	CHC-C4B-C3B	-2.24	117.73	127.71
31	3	317	CLA	CHC-C4B-C3B	-2.24	117.73	127.71
31	a	322	CLA	CHC-C4B-C3B	-2.24	117.73	127.71
31	8	309	CLA	CMD-C2D-C1D	2.24	128.67	124.71
31	a	314	CLA	CHC-C1C-NC	-2.24	120.80	124.20
31	2	310	CLA	CMD-C2D-C1D	2.24	128.67	124.71
31	O	202	CLA	CMB-C2B-C1B	2.24	128.78	125.37
31	3	314	CLA	C1-C2-C3	-2.24	122.16	126.04
31	a	316	CLA	C1D-CHD-C4C	-2.24	121.22	126.06
31	3	312	CLA	CED-O2D-CGD	2.24	121.01	115.94
31	A	842	CLA	CMD-C2D-C1D	2.24	128.66	124.71
31	A	853	CLA	CMD-C2D-C1D	2.24	128.66	124.71
31	O	204	CLA	CMB-C2B-C1B	2.24	128.78	125.37
31	3	310	CLA	O2A-CGA-CBA	2.24	118.94	111.91
31	b	312	CLA	CED-O2D-CGD	2.24	121.01	115.94
31	4	309	CLA	CED-O2D-CGD	2.24	121.01	115.94
31	A	856	CLA	C1-C2-C3	-2.24	122.17	126.04
31	F	301	CLA	C1D-CHD-C4C	-2.24	121.22	126.06
31	b	312	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
31	8	314	CLA	CHC-C1C-NC	-2.24	120.81	124.20
31	7	315	CLA	CMC-C2C-C1C	2.24	128.45	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L	302	BCR	C29-C30-C25	2.24	113.93	110.48
31	B	846	CLA	CHC-C1C-NC	-2.24	120.81	124.20
31	G	204	CLA	CHB-C1B-NB	-2.24	121.89	124.26
31	B	822	CLA	O2A-CGA-CBA	2.24	118.93	111.91
31	7	316	CLA	CHC-C4B-C3B	-2.24	117.75	127.71
31	B	846	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
31	a	314	CLA	CHC-C4B-C3B	-2.24	117.75	127.71
32	6	320	CHL	CMD-C2D-C1D	2.24	128.66	124.71
31	2	305	CLA	CMD-C2D-C1D	2.24	128.66	124.71
31	A	833	CLA	CMD-C2D-C1D	2.24	128.66	124.71
31	9	316	CLA	CMD-C2D-C1D	2.24	128.66	124.71
32	4	313	CHL	CED-O2D-CGD	2.24	121.00	115.94
31	J	105	CLA	CMC-C2C-C1C	2.24	128.44	125.04
31	F	301	CLA	CHD-C4C-NC	2.24	127.73	124.20
36	a	303	LUT	C22-C23-C24	2.24	114.28	111.74
31	B	812	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
31	O	203	CLA	CMD-C2D-C1D	2.24	128.65	124.71
31	7	315	CLA	CHB-C1B-NB	-2.23	121.89	124.26
26	A	806	BCR	C15-C16-C17	-2.23	118.90	123.47
31	A	823	CLA	O2A-CGA-CBA	2.23	118.92	111.91
31	b	302	CLA	CMC-C2C-C1C	2.23	128.44	125.04
31	5	307	CLA	CMC-C2C-C1C	2.23	128.44	125.04
31	4	306	CLA	CHC-C4B-C3B	-2.23	117.77	127.71
31	A	855	CLA	CAA-C2A-C1A	2.23	119.29	111.97
31	3	318	CLA	CHC-C4B-C3B	-2.23	117.78	127.71
35	a	302	QTB	C03-C04-C05	2.23	130.18	123.22
32	6	319	CHL	CHA-C4D-ND	2.23	137.17	132.50
31	3	308	CLA	CHC-C4B-C3B	-2.23	117.78	127.71
31	O	204	CLA	CHC-C4B-C3B	-2.23	117.78	127.71
32	7	318	CHL	CMB-C2B-C1B	2.23	128.77	125.37
31	B	836	CLA	C1D-CHD-C4C	-2.23	121.25	126.06
31	b	303	CLA	CMC-C2C-C1C	2.23	128.44	125.04
31	A	818	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
32	b	309	CHL	CMB-C2B-C1B	2.23	128.76	125.37
31	9	315	CLA	C1-O2A-CGA	2.23	122.29	116.44
31	A	825	CLA	O2A-CGA-CBA	2.23	118.90	111.91
31	L	307	CLA	CHD-C4C-NC	2.23	127.72	124.20
31	7	321	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
31	B	839	CLA	CMC-C2C-C1C	2.23	128.43	125.04
31	A	819	CLA	C4-C3-C5	2.23	119.02	115.27
31	8	320	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
31	H	903	CLA	CMB-C2B-C1B	2.23	128.76	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	312	CLA	CMB-C2B-C1B	2.23	128.76	125.37
31	K	205	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
31	7	315	CLA	C7-C6-C5	-2.23	109.65	114.49
31	5	320	CLA	C1D-CHD-C4C	-2.23	121.25	126.06
31	B	821	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
31	A	848	CLA	CHC-C4B-C3B	-2.23	117.81	127.71
31	4	314	CLA	C3D-C4D-CHA	-2.23	107.63	112.72
31	2	309	CLA	CMC-C2C-C1C	2.23	128.43	125.04
31	9	313	CLA	CAC-C3C-C4C	2.23	127.70	124.81
31	3	309	CLA	CED-O2D-CGD	2.22	120.97	115.94
31	A	846	CLA	CHC-C4B-C3B	-2.22	117.81	127.71
31	B	815	CLA	CHC-C4B-C3B	-2.22	117.81	127.71
31	4	307	CLA	CHB-C1B-NB	-2.22	121.90	124.26
31	A	838	CLA	C1-C2-C3	-2.22	122.20	126.04
37	a	301	LMG	O2-C2-C1	-2.22	104.64	110.05
31	4	316	CLA	CAA-CBA-CGA	-2.22	106.75	113.25
31	5	321	CLA	C3D-C4D-CHA	-2.22	107.64	112.72
31	7	315	CLA	CMB-C2B-C1B	2.22	128.76	125.37
32	7	324	CHL	CHB-C1B-NB	-2.22	121.90	124.26
31	3	309	CLA	CMC-C2C-C1C	2.22	128.42	125.04
31	b	306	CLA	C3D-C4D-CHA	-2.22	107.64	112.72
31	B	829	CLA	CMB-C2B-C1B	2.22	128.75	125.37
36	6	303	LUT	C1-C6-C7	-2.22	109.49	115.78
31	A	857	CLA	CHC-C1C-NC	-2.22	120.83	124.20
26	I	801	BCR	C29-C30-C25	2.22	113.90	110.48
31	8	315	CLA	CMC-C2C-C1C	2.22	128.42	125.04
31	2	308	CLA	CMC-C2C-C1C	2.22	128.42	125.04
31	a	314	CLA	CMB-C2B-C1B	2.22	128.75	125.37
26	A	804	BCR	C27-C26-C25	2.22	125.96	122.73
31	4	315	CLA	CHC-C4B-C3B	-2.22	117.83	127.71
31	A	824	CLA	O2A-CGA-CBA	2.22	118.88	111.91
32	7	318	CHL	CHC-C4B-C3B	-2.22	117.83	127.71
33	7	308	DGD	CFB-CEB-CDB	-2.22	103.16	114.42
32	9	320	CHL	CED-O2D-CGD	2.22	120.96	115.94
31	a	313	CLA	C1-O2A-CGA	2.22	122.27	116.44
32	K	201	CHL	CMB-C2B-C1B	2.22	128.75	125.37
31	4	318	CLA	CHC-C4B-C3B	-2.22	117.84	127.71
31	a	313	CLA	C1-C2-C3	-2.22	122.21	126.04
31	8	311	CLA	CHC-C4B-C3B	-2.22	117.84	127.71
31	A	815	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	A	822	CLA	C4C-C3C-C2C	-2.22	103.67	106.90
31	L	305	CLA	C4-C3-C5	2.22	119.00	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	322	CHL	CMD-C2D-C1D	2.22	128.62	124.71
31	A	819	CLA	CMB-C2B-C1B	2.22	128.75	125.37
31	A	857	CLA	CHB-C1B-NB	-2.22	121.91	124.26
31	B	832	CLA	CHC-C1C-NC	-2.22	120.84	124.20
31	A	849	CLA	CED-O2D-CGD	2.22	120.95	115.94
31	4	321	CLA	CAA-CBA-CGA	-2.22	106.78	113.25
31	3	309	CLA	CMB-C2B-C1B	2.21	128.74	125.37
28	8	304	LHG	C27-C26-C25	-2.21	103.19	114.42
31	B	832	CLA	CAC-C3C-C4C	2.21	127.68	124.81
31	6	312	CLA	CHC-C4B-C3B	-2.21	117.86	127.71
31	6	310	CLA	CED-O2D-CGD	2.21	120.94	115.94
31	A	814	CLA	C4C-C3C-C2C	-2.21	103.67	106.90
31	A	841	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
31	A	850	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
31	2	306	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
31	5	315	CLA	CMC-C2C-C1C	2.21	128.41	125.04
36	9	302	LUT	C1-C6-C7	-2.21	109.53	115.78
31	B	831	CLA	CHC-C4B-C3B	-2.21	117.88	127.71
31	3	310	CLA	CHC-C1C-NC	-2.21	120.85	124.20
31	B	831	CLA	C5-C3-C4	2.21	119.48	114.60
26	A	805	BCR	C15-C14-C13	-2.21	124.16	127.31
31	B	813	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
31	2	307	CLA	CMC-C2C-C1C	2.21	128.40	125.04
31	A	832	CLA	CHC-C4B-C3B	-2.21	117.89	127.71
31	A	828	CLA	CAC-C3C-C4C	2.21	127.67	124.81
31	A	824	CLA	CMD-C2D-C1D	2.21	128.60	124.71
31	5	315	CLA	C3D-C4D-CHA	-2.21	107.68	112.72
31	2	307	CLA	C1D-CHD-C4C	-2.21	121.30	126.06
31	B	817	CLA	CHC-C4B-C3B	-2.21	117.90	127.71
32	5	316	CHL	C2D-C1D-ND	2.21	111.73	110.10
31	9	312	CLA	C1D-CHD-C4C	-2.20	121.30	126.06
33	7	308	DGD	O2D-C2D-C1D	-2.20	104.69	110.05
31	5	310	CLA	O2A-CGA-CBA	2.20	118.83	111.91
31	B	850	CLA	CHC-C1C-NC	-2.20	120.86	124.20
31	8	315	CLA	C1-C2-C3	-2.20	122.23	126.04
31	G	206	CLA	C1D-CHD-C4C	-2.20	121.30	126.06
31	B	827	CLA	CAC-C3C-C4C	2.20	127.67	124.81
26	J	102	BCR	C27-C26-C25	2.20	125.93	122.73
31	6	316	CLA	CED-O2D-CGD	2.20	120.92	115.94
31	5	321	CLA	CHB-C1B-NB	-2.20	121.92	124.26
31	B	845	CLA	CMC-C2C-C1C	2.20	128.39	125.04
31	9	318	CLA	CHC-C4B-C3B	-2.20	117.91	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	314	CLA	CHC-C4B-C3B	-2.20	117.91	127.71
32	7	320	CHL	CHC-C4B-C3B	-2.20	117.91	127.71
31	b	310	CLA	CHB-C1B-NB	-2.20	121.93	124.26
31	B	835	CLA	CHC-C4B-C3B	-2.20	117.92	127.71
26	K	202	BCR	C15-C16-C17	-2.20	118.97	123.47
31	7	315	CLA	O2A-CGA-CBA	2.20	118.81	111.91
31	6	312	CLA	CHC-C1C-NC	-2.20	120.86	124.20
31	8	320	CLA	CMC-C2C-C1C	2.20	128.39	125.04
31	a	315	CLA	CHC-C4B-C3B	-2.20	117.92	127.71
32	b	309	CHL	CHC-C4B-C3B	-2.20	117.92	127.71
31	F	306	CLA	C5-C3-C4	2.20	119.46	114.60
26	L	303	BCR	C15-C16-C17	-2.20	118.97	123.47
31	6	315	CLA	CHC-C4B-C3B	-2.20	117.93	127.71
31	5	311	CLA	CMC-C2C-C1C	2.20	128.39	125.04
31	B	826	CLA	CHC-C4B-C3B	-2.20	117.93	127.71
31	5	321	CLA	CHC-C4B-C3B	-2.20	117.93	127.71
31	B	846	CLA	C4-C3-C5	2.20	118.97	115.27
32	7	317	CHL	C2C-C3C-C4C	-2.20	104.92	106.49
26	B	802	BCR	C15-C16-C17	-2.20	118.97	123.47
31	F	306	CLA	CHC-C1C-NC	-2.20	120.87	124.20
31	5	318	CLA	CHB-C1B-NB	-2.20	121.93	124.26
31	A	846	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
31	2	308	CLA	C1D-CHD-C4C	-2.20	121.32	126.06
31	L	305	CLA	CAC-C3C-C4C	2.20	127.66	124.81
31	a	312	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
31	B	842	CLA	CHB-C4A-NA	2.20	127.55	124.51
31	b	310	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
31	5	307	CLA	C4-C3-C5	2.20	118.97	115.27
31	6	310	CLA	CMD-C2D-C1D	2.20	128.58	124.71
31	8	318	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
31	8	307	CLA	C1D-CHD-C4C	-2.20	121.32	126.06
31	4	311	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
31	4	320	CLA	C1D-CHD-C4C	-2.20	121.32	126.06
28	8	304	LHG	C18-C17-C16	-2.20	103.28	114.42
31	B	812	CLA	CMB-C2B-C1B	2.19	128.71	125.37
33	B	808	DGD	O5D-C6D-C5D	-2.19	104.99	109.05
31	B	824	CLA	CHB-C1B-NB	-2.19	121.93	124.26
31	A	819	CLA	C1D-CHD-C4C	-2.19	121.32	126.06
31	F	301	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
31	a	315	CLA	C4-C3-C5	2.19	118.96	115.27
31	G	204	CLA	CHC-C4B-C3B	-2.19	117.95	127.71
32	5	322	CHL	CED-O2D-CGD	2.19	120.90	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	310	CLA	C1-O2A-CGA	2.19	122.20	116.44
32	4	317	CHL	CHC-C4B-C3B	-2.19	117.95	127.71
31	H	902	CLA	C3D-C4D-CHA	-2.19	107.70	112.72
31	9	315	CLA	C1D-CHD-C4C	-2.19	121.33	126.06
31	B	848	CLA	CAC-C3C-C4C	2.19	127.66	124.81
31	B	849	CLA	CMC-C2C-C1C	2.19	128.38	125.04
31	9	315	CLA	C3D-C4D-CHA	-2.19	107.71	112.72
31	B	839	CLA	C4-C3-C5	2.19	118.96	115.27
31	A	849	CLA	CMB-C2B-C1B	2.19	128.71	125.37
31	9	321	CLA	CHB-C4A-NA	2.19	127.54	124.51
31	J	105	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
31	3	317	CLA	CHB-C4A-NA	2.19	127.54	124.51
32	A	839	CHL	CAC-C3C-C4C	2.19	127.65	124.81
31	2	310	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
31	A	837	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
31	A	850	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
32	6	319	CHL	CHC-C1C-NC	-2.19	120.88	124.20
31	a	321	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
31	A	824	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
31	8	318	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
36	L	304	LUT	C17-C1-C6	-2.19	106.75	110.30
26	O	201	BCR	C28-C27-C26	-2.19	110.17	114.08
31	K	204	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
26	A	806	BCR	C38-C26-C27	-2.19	109.41	113.62
31	2	314	CLA	C1D-CHD-C4C	-2.19	121.34	126.06
31	B	831	CLA	C1-O2A-CGA	2.19	122.18	116.44
31	A	824	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
31	B	835	CLA	CHB-C1B-NB	-2.19	121.94	124.26
31	3	310	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
36	L	304	LUT	C22-C23-C24	2.19	114.23	111.74
26	3	302	BCR	C15-C16-C17	-2.19	119.00	123.47
31	B	811	CLA	CHC-C4B-C3B	-2.19	117.98	127.71
31	b	308	CLA	CHC-C4B-C3B	-2.19	117.99	127.71
31	8	308	CLA	C4C-C3C-C2C	-2.19	103.71	106.90
31	H	902	CLA	CMB-C2B-C1B	2.19	128.70	125.37
32	a	317	CHL	CHB-C1B-NB	-2.19	121.94	124.26
31	H	903	CLA	CHC-C4B-C3B	-2.19	117.99	127.71
31	6	322	CLA	C3D-C4D-CHA	-2.19	107.72	112.72
31	5	313	CLA	CAC-C3C-C4C	2.18	127.64	124.81
31	A	842	CLA	CHC-C4B-C3B	-2.18	117.99	127.71
27	5	301	LMT	O5B-C5B-C6B	2.18	111.87	106.44
26	L	302	BCR	C15-C14-C13	-2.18	124.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	316	CLA	O2A-CGA-CBA	2.18	120.86	112.23
31	B	820	CLA	CHC-C1C-NC	-2.18	120.89	124.20
31	O	202	CLA	C3D-C4D-CHA	-2.18	107.73	112.72
31	9	316	CLA	CHC-C1C-NC	-2.18	120.89	124.20
31	4	319	CLA	CHC-C4B-C3B	-2.18	118.00	127.71
31	9	311	CLA	CHC-C1C-NC	-2.18	120.89	124.20
31	B	839	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
31	B	847	CLA	CHB-C1B-NB	-2.18	121.95	124.26
31	4	309	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
31	B	842	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
31	A	833	CLA	CHC-C4B-C3B	-2.18	118.01	127.71
31	A	822	CLA	CHC-C4B-C3B	-2.18	118.01	127.71
31	H	902	CLA	O2A-CGA-CBA	2.18	120.85	112.23
32	9	320	CHL	C4D-CHA-C1A	-2.18	118.60	121.25
33	7	308	DGD	C5B-C4B-C3B	-2.18	103.36	114.42
31	9	319	CLA	C3D-C4D-CHA	-2.18	107.74	112.72
31	b	311	CLA	CMD-C2D-C1D	2.18	128.55	124.71
31	4	318	CLA	CED-O2D-CGD	2.18	120.86	115.94
31	8	308	CLA	C1-C2-C3	-2.18	122.28	126.04
31	L	307	CLA	CHC-C4B-C3B	-2.18	118.02	127.71
31	A	855	CLA	CHC-C1C-NC	-2.18	120.90	124.20
31	5	311	CLA	O2A-CGA-CBA	2.18	120.84	112.23
31	B	841	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
35	F	303	QTB	C03-C04-C05	2.18	130.01	123.22
26	B	802	BCR	C28-C27-C26	-2.18	110.19	114.08
26	B	805	BCR	C11-C10-C9	-2.18	124.20	127.31
31	A	835	CLA	CHC-C4B-C3B	-2.18	118.02	127.71
31	B	836	CLA	CHC-C4B-C3B	-2.18	118.02	127.71
31	A	844	CLA	CMC-C2C-C1C	2.18	128.35	125.04
31	9	312	CLA	CHC-C4B-C3B	-2.18	118.03	127.71
36	4	303	LUT	C30-C31-C32	-2.18	116.42	123.22
31	B	826	CLA	CHB-C1B-NB	-2.18	121.95	124.26
31	A	830	CLA	CMD-C2D-C1D	2.18	128.55	124.71
31	a	310	CLA	C3C-C4C-NC	2.18	113.01	110.57
31	A	815	CLA	CHB-C1B-NB	-2.18	121.95	124.26
31	2	309	CLA	CHB-C1B-NB	-2.18	121.95	124.26
37	J	104	LMG	O7-C10-O9	-2.17	118.45	123.70
31	9	313	CLA	CMC-C2C-C1C	2.17	128.35	125.04
31	3	319	CLA	C1D-CHD-C4C	-2.17	121.37	126.06
31	A	828	CLA	CMD-C2D-C1D	2.17	128.54	124.71
31	2	304	CLA	CMD-C2D-C1D	2.17	128.54	124.71
31	B	811	CLA	C1D-CHD-C4C	-2.17	121.37	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	311	CLA	O2A-CGA-CBA	2.17	120.82	112.23
31	B	827	CLA	CHC-C1C-NC	-2.17	120.91	124.20
31	3	314	CLA	CHC-C1C-NC	-2.17	120.91	124.20
31	3	316	CLA	C3D-C4D-CHA	-2.17	107.75	112.72
31	a	319	CLA	CED-O2D-CGD	2.17	120.85	115.94
27	A	807	LMT	O5B-C5B-C4B	2.17	113.64	109.69
32	6	318	CHL	C2A-C1A-CHA	-2.17	120.06	123.86
31	a	313	CLA	CHC-C4B-C3B	-2.17	118.04	127.71
32	7	318	CHL	CMD-C2D-C1D	2.17	128.54	124.71
31	A	838	CLA	CHB-C4A-NA	2.17	127.52	124.51
31	8	318	CLA	CAC-C3C-C4C	2.17	127.63	124.81
31	3	318	CLA	CHB-C1B-NB	-2.17	121.96	124.26
31	B	837	CLA	CHC-C4B-C3B	-2.17	118.05	127.71
32	5	317	CHL	O2A-CGA-CBA	2.17	120.81	112.23
31	F	301	CLA	CMD-C2D-C1D	2.17	128.54	124.71
31	A	815	CLA	CMC-C2C-C1C	2.17	128.35	125.04
31	A	836	CLA	C3D-C4D-CHA	-2.17	107.76	112.72
31	b	313	CLA	CHC-C4B-C3B	-2.17	118.06	127.71
31	6	307	CLA	CMB-C2B-C1B	2.17	128.67	125.37
31	6	307	CLA	CHC-C4B-C3B	-2.17	118.06	127.71
31	7	309	CLA	CHC-C1C-NC	-2.17	120.91	124.20
31	5	311	CLA	CAC-C3C-C4C	2.17	127.62	124.81
31	2	310	CLA	O2A-CGA-CBA	2.17	121.00	114.03
28	a	306	LHG	C18-C17-C16	-2.17	103.41	114.42
31	4	307	CLA	C1-C2-C3	-2.17	122.29	126.04
31	A	852	CLA	CHC-C4B-C3B	-2.17	118.06	127.71
31	a	309	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
31	9	317	CLA	CMB-C2B-C1B	2.17	128.67	125.37
31	7	311	CLA	C4-C3-C5	2.17	118.92	115.27
31	L	306	CLA	CHC-C4B-C3B	-2.17	118.07	127.71
31	2	304	CLA	CHC-C4B-C3B	-2.17	118.07	127.71
26	5	302	BCR	C24-C23-C22	-2.17	122.96	126.23
31	A	825	CLA	CHC-C4B-C3B	-2.17	118.07	127.71
31	3	317	CLA	CHC-C1C-NC	-2.17	120.92	124.20
31	9	317	CLA	CHC-C1C-NC	-2.17	120.92	124.20
31	2	314	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
31	b	305	CLA	C3D-C4D-CHA	-2.17	107.77	112.72
31	B	829	CLA	CMC-C2C-C1C	2.17	128.34	125.04
31	A	849	CLA	CHC-C4B-C3B	-2.17	118.08	127.71
31	H	901	CLA	CMD-C2D-C1D	2.17	128.53	124.71
32	9	322	CHL	CMD-C2D-C1D	2.16	128.53	124.71
32	9	322	CHL	CHA-C4D-ND	2.16	137.03	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	309	CHL	C2D-C1D-ND	2.16	111.70	110.10
26	O	201	BCR	C15-C16-C17	-2.16	119.04	123.47
26	B	802	BCR	C31-C1-C6	2.16	113.81	110.30
31	b	313	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
31	4	314	CLA	O2A-CGA-CBA	2.16	120.98	114.03
31	A	853	CLA	CMB-C2B-C1B	2.16	128.66	125.37
31	4	311	CLA	O2A-CGA-CBA	2.16	120.77	112.23
31	B	842	CLA	C1D-CHD-C4C	-2.16	121.39	126.06
31	A	843	CLA	C1-O2A-CGA	2.16	122.11	116.44
26	L	303	BCR	C11-C10-C9	-2.16	124.23	127.31
31	6	308	CLA	CHD-C4C-NC	2.16	127.61	124.20
31	A	828	CLA	CMC-C2C-C1C	2.16	128.33	125.04
31	B	824	CLA	CED-O2D-CGD	2.16	120.82	115.94
26	G	203	BCR	C16-C15-C14	-2.16	119.05	123.47
37	J	101	LMG	O3-C3-C2	-2.16	105.36	110.35
28	7	302	LHG	C20-C19-C18	-2.16	103.46	114.42
31	A	826	CLA	CMC-C2C-C1C	2.16	128.33	125.04
26	8	301	BCR	C7-C8-C9	-2.16	122.97	126.23
31	A	816	CLA	O2A-CGA-CBA	2.16	118.68	111.91
31	4	321	CLA	O2A-CGA-CBA	2.16	118.68	111.91
31	2	314	CLA	CHB-C1B-NB	-2.16	121.97	124.26
32	A	831	CHL	O2A-CGA-CBA	2.16	118.68	111.91
31	A	826	CLA	O2A-CGA-CBA	2.16	118.68	111.91
31	A	845	CLA	CHC-C1C-NC	-2.16	120.93	124.20
32	6	318	CHL	CHA-C4D-ND	2.16	137.01	132.50
31	8	317	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
31	4	321	CLA	C1D-CHD-C4C	-2.16	121.40	126.06
26	A	806	BCR	C27-C26-C25	2.16	125.86	122.73
28	A	809	LHG	C27-C26-C25	-2.16	103.48	114.42
31	A	843	CLA	CHD-C4C-NC	2.16	127.60	124.20
31	7	310	CLA	CHB-C1B-NB	-2.16	121.97	124.26
31	4	305	CLA	CHB-C1B-NB	-2.16	121.97	124.26
31	A	817	CLA	CHB-C4A-NA	2.16	127.49	124.51
31	5	320	CLA	CHC-C4B-C3B	-2.16	118.12	127.71
31	a	321	CLA	C3D-C4D-CHA	-2.16	107.79	112.72
31	9	311	CLA	C3D-C4D-CHA	-2.16	107.79	112.72
31	A	851	CLA	CHC-C1C-NC	-2.16	120.93	124.20
32	5	319	CHL	CHA-C4D-ND	2.16	137.01	132.50
26	I	801	BCR	C33-C5-C6	-2.16	122.11	124.53
32	9	322	CHL	CHC-C4B-C3B	-2.16	118.12	127.71
32	9	322	CHL	CMB-C2B-C1B	2.15	128.65	125.37
32	7	320	CHL	CAC-C3C-C4C	2.15	127.61	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	311	CLA	O2A-CGA-CBA	2.15	118.67	111.91
31	A	821	CLA	CHC-C4B-C3B	-2.15	118.13	127.71
31	4	312	CLA	CHC-C4B-C3B	-2.15	118.13	127.71
31	9	321	CLA	CED-O2D-CGD	2.15	120.81	115.94
31	3	310	CLA	CHB-C1B-NB	-2.15	121.98	124.26
32	9	320	CHL	CHC-C4B-C3B	-2.15	118.13	127.71
32	6	317	CHL	CHC-C4B-C3B	-2.15	118.13	127.71
28	7	302	LHG	C27-C26-C25	-2.15	103.50	114.42
31	4	309	CLA	CAC-C3C-C4C	2.15	127.60	124.81
31	G	205	CLA	CHC-C4B-C3B	-2.15	118.14	127.71
31	B	812	CLA	C4-C3-C5	2.15	118.89	115.27
31	L	305	CLA	CMD-C2D-C1D	2.15	128.50	124.71
32	3	315	CHL	CHC-C4B-C3B	-2.15	118.14	127.71
32	6	319	CHL	CHC-C4B-C3B	-2.15	118.14	127.71
35	F	303	QTB	C11-C10-C09	2.15	130.14	125.47
32	5	322	CHL	C2D-C1D-ND	2.15	111.69	110.10
31	8	321	CLA	CED-O2D-CGD	2.15	120.80	115.94
31	B	846	CLA	CMC-C2C-C1C	2.15	128.31	125.04
32	a	320	CHL	CHC-C4B-C3B	-2.15	118.15	127.71
31	A	828	CLA	C1D-CHD-C4C	-2.15	121.42	126.06
31	B	823	CLA	CMC-C2C-C1C	2.15	128.31	125.04
31	O	203	CLA	CMB-C2B-C1B	2.15	128.64	125.37
31	8	313	CLA	CHB-C1B-NB	-2.15	121.98	124.26
31	5	312	CLA	CHC-C4B-C3B	-2.15	118.15	127.71
31	6	306	CLA	CHD-C4C-NC	2.15	127.59	124.20
32	6	309	CHL	CHC-C1C-NC	-2.15	120.94	124.20
32	6	309	CHL	CHC-C4B-C3B	-2.15	118.16	127.71
31	9	311	CLA	CED-O2D-CGD	2.15	120.80	115.94
31	3	319	CLA	CMD-C2D-C1D	2.15	128.50	124.71
31	9	318	CLA	C3D-C4D-CHA	-2.15	107.81	112.72
31	H	903	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
26	7	304	BCR	C2-C1-C6	2.15	113.78	110.48
31	5	314	CLA	CED-O2D-CGD	2.15	120.79	115.94
31	L	306	CLA	CED-O2D-CGD	2.15	120.79	115.94
32	4	310	CHL	CMB-C2B-C1B	2.15	128.64	125.37
31	A	832	CLA	CHC-C1C-NC	-2.14	120.95	124.20
31	A	841	CLA	C4C-C3C-C2C	-2.14	103.77	106.90
31	3	317	CLA	C1-O2A-CGA	2.14	122.07	116.44
31	A	837	CLA	O2A-CGA-CBA	2.14	118.64	111.91
31	8	317	CLA	CHB-C4A-NA	2.14	127.48	124.51
31	8	307	CLA	CAC-C3C-C4C	2.14	127.59	124.81
31	3	309	CLA	CHC-C4B-C3B	-2.14	118.17	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	324	CHL	CHA-C4D-ND	2.14	136.98	132.50
31	6	314	CLA	CMC-C2C-C1C	2.14	128.30	125.04
31	b	302	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
31	F	306	CLA	CHC-C4B-C3B	-2.14	118.18	127.71
31	2	305	CLA	CHC-C4B-C3B	-2.14	118.18	127.71
31	B	822	CLA	CHC-C4B-C3B	-2.14	118.18	127.71
31	b	305	CLA	CAC-C3C-C4C	2.14	127.59	124.81
31	B	811	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
31	b	310	CLA	C1D-CHD-C4C	-2.14	121.44	126.06
31	6	322	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
32	b	309	CHL	CED-O2D-CGD	2.14	120.78	115.94
31	B	850	CLA	O2A-CGA-CBA	2.14	118.62	111.91
31	B	817	CLA	C1D-CHD-C4C	-2.14	121.44	126.06
31	A	846	CLA	C7-C6-C5	-2.14	107.55	113.36
31	B	847	CLA	CAC-C3C-C4C	2.14	127.58	124.81
32	6	320	CHL	CED-O2D-CGD	2.14	120.77	115.94
31	A	829	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
26	A	805	BCR	C33-C5-C6	-2.14	122.13	124.53
31	K	205	CLA	CMB-C2B-C1B	2.14	128.62	125.37
31	6	310	CLA	C1D-CHD-C4C	-2.14	121.45	126.06
31	8	313	CLA	CHC-C4B-C3B	-2.14	118.20	127.71
26	A	804	BCR	C15-C14-C13	-2.14	124.26	127.31
31	B	839	CLA	CMD-C2D-C1D	2.14	128.48	124.71
31	A	853	CLA	CHB-C4A-NA	2.14	127.47	124.51
31	H	903	CLA	C3D-C4D-CHA	-2.14	107.84	112.72
31	5	318	CLA	C3D-C4D-CHA	-2.14	107.84	112.72
31	A	849	CLA	CAC-C3C-C4C	2.14	127.58	124.81
31	A	827	CLA	CHC-C1C-NC	-2.14	120.96	124.20
32	6	319	CHL	C2C-C3C-C4C	-2.14	104.97	106.49
31	O	204	CLA	CED-O2D-CGD	2.13	120.77	115.94
31	3	307	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
32	a	320	CHL	CMB-C2B-C1B	2.13	128.62	125.37
31	A	854	CLA	C4C-C3C-C2C	-2.13	103.79	106.90
31	4	307	CLA	CMC-C2C-C1C	2.13	128.29	125.04
31	A	826	CLA	C1-O2A-CGA	2.13	122.04	116.44
32	6	309	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
31	B	818	CLA	CMD-C2D-C1D	2.13	128.47	124.71
31	K	206	CLA	CAC-C3C-C4C	2.13	127.58	124.81
31	O	204	CLA	C3D-C4D-CHA	-2.13	107.84	112.72
31	4	321	CLA	CMD-C2D-C1D	2.13	128.47	124.71
31	B	849	CLA	C1-O2A-CGA	2.13	122.04	116.44
31	B	826	CLA	C5-C3-C4	2.13	119.31	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	314	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
31	B	839	CLA	CED-O2D-CGD	2.13	120.75	115.94
31	B	832	CLA	CMC-C2C-C1C	2.13	128.28	125.04
31	A	855	CLA	C4-C3-C2	-2.13	118.22	123.68
31	B	842	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
31	A	825	CLA	O2A-C1-C2	-2.13	103.04	108.64
32	5	319	CHL	CAC-C3C-C4C	2.13	127.57	124.81
32	6	317	CHL	O2A-CGA-CBA	2.13	120.64	112.23
31	3	320	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
31	8	315	CLA	CHC-C4B-C3B	-2.13	118.24	127.71
31	G	206	CLA	CHB-C1B-NB	-2.13	122.00	124.26
31	A	826	CLA	CHC-C4B-C3B	-2.13	118.24	127.71
32	7	324	CHL	CHC-C4B-C3B	-2.13	118.25	127.71
31	5	321	CLA	O2A-CGA-CBA	2.13	120.64	112.23
31	4	321	CLA	C3D-C4D-CHA	-2.13	107.86	112.72
31	7	321	CLA	CED-O2D-CGD	2.13	120.75	115.94
31	8	315	CLA	C1-O2A-CGA	2.13	122.02	116.44
31	B	830	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
32	A	840	CHL	CHA-C4D-ND	2.13	136.95	132.50
31	O	203	CLA	CED-O2D-CGD	2.13	120.75	115.94
31	2	307	CLA	CMD-C2D-C1D	2.13	128.46	124.71
31	4	320	CLA	CHC-C4B-C3B	-2.13	118.26	127.71
31	5	309	CLA	C3D-C4D-CHA	-2.13	107.86	112.72
31	5	320	CLA	C3D-C4D-CHA	-2.13	107.86	112.72
31	9	312	CLA	C4C-C3C-C2C	-2.12	103.80	106.90
31	2	308	CLA	CHC-C4B-C3B	-2.12	118.26	127.71
31	4	311	CLA	C3D-C4D-CHA	-2.12	107.86	112.72
26	K	203	BCR	C15-C14-C13	-2.12	124.28	127.31
31	8	309	CLA	CHB-C1B-NB	-2.12	122.01	124.26
31	b	307	CLA	CAC-C3C-C4C	2.12	127.56	124.81
32	7	317	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
31	8	312	CLA	C1-O2A-CGA	2.12	122.01	116.44
31	A	815	CLA	C4C-C3C-C2C	-2.12	103.80	106.90
31	6	311	CLA	C3D-C4D-CHA	-2.12	107.87	112.72
32	4	313	CHL	CHA-C4D-ND	2.12	136.94	132.50
31	A	826	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
32	8	319	CHL	CHC-C4B-C3B	-2.12	118.27	127.71
32	4	317	CHL	CED-O2D-CGD	2.12	120.73	115.94
31	B	818	CLA	C1D-CHD-C4C	-2.12	121.48	126.06
31	B	832	CLA	CMB-C2B-C1B	2.12	128.60	125.37
32	6	320	CHL	CHC-C4B-C3B	-2.12	118.28	127.71
31	b	305	CLA	C1D-CHD-C4C	-2.12	121.48	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	318	CLA	CMB-C2B-C1B	2.12	128.60	125.37
31	A	816	CLA	C1-O2A-CGA	2.12	122.00	116.44
31	b	310	CLA	CAC-C3C-C4C	2.12	127.56	124.81
31	9	316	CLA	O2A-CGA-CBA	2.12	118.56	111.91
26	3	302	BCR	C33-C5-C6	-2.12	122.15	124.53
32	7	318	CHL	CHA-C4D-ND	2.12	136.93	132.50
31	8	308	CLA	CHC-C4B-C3B	-2.12	118.29	127.71
31	H	901	CLA	CHC-C1C-NC	-2.12	120.99	124.20
31	3	316	CLA	CHC-C1C-NC	-2.12	120.99	124.20
31	3	307	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
31	b	313	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
31	2	309	CLA	CHC-C4B-C3B	-2.12	118.29	127.71
31	B	836	CLA	CMD-C2D-C1D	2.12	128.44	124.71
31	7	309	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
31	6	314	CLA	CMD-C2D-C1D	2.12	128.44	124.71
26	K	203	BCR	C3-C4-C5	-2.12	110.30	114.08
31	a	322	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
32	8	316	CHL	CHC-C4B-C3B	-2.12	118.30	127.71
31	6	314	CLA	CAC-C3C-C4C	2.12	127.56	124.81
28	6	305	LHG	C27-C26-C25	-2.12	103.68	114.42
31	K	204	CLA	C5-C3-C4	2.12	119.28	114.60
31	b	311	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
32	a	317	CHL	C2C-C3C-C4C	-2.12	104.98	106.49
31	A	835	CLA	O2A-CGA-CBA	2.12	118.55	111.91
31	A	843	CLA	CMD-C2D-C1D	2.12	128.44	124.71
31	B	823	CLA	CHB-C4A-NA	2.12	127.44	124.51
32	4	313	CHL	C1D-CHD-C4C	-2.11	121.50	126.06
26	B	805	BCR	C29-C30-C25	2.11	113.74	110.48
31	6	307	CLA	C5-C3-C4	2.11	119.27	114.60
28	A	810	LHG	C27-C26-C25	-2.11	103.69	114.42
31	B	839	CLA	O2A-CGA-CBA	2.11	118.54	111.91
31	2	313	CLA	CHC-C4B-C3B	-2.11	118.31	127.71
26	M	101	BCR	C16-C15-C14	-2.11	119.14	123.47
31	3	312	CLA	CHC-C1C-NC	-2.11	121.00	124.20
31	6	308	CLA	CHC-C1C-NC	-2.11	121.00	124.20
31	L	305	CLA	CMC-C2C-C1C	2.11	128.26	125.04
31	5	311	CLA	CHB-C1B-NB	-2.11	122.02	124.26
31	A	834	CLA	C16-C15-C13	-2.11	109.09	115.92
31	B	828	CLA	O2A-CGA-CBA	2.11	118.54	111.91
31	b	312	CLA	C3D-C4D-CHA	-2.11	107.89	112.72
31	A	837	CLA	CMC-C2C-C1C	2.11	128.25	125.04
31	A	819	CLA	CHC-C4B-C3B	-2.11	118.32	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	320	CHL	C1-O2A-CGA	2.11	121.98	116.44
31	A	853	CLA	C11-C10-C8	-2.11	109.10	115.92
31	9	311	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
31	A	834	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
31	B	843	CLA	C3B-C4B-NB	2.11	112.47	110.52
36	8	303	LUT	C12-C13-C14	-2.11	115.70	118.94
31	8	314	CLA	CED-O2D-CGD	2.11	120.71	115.94
31	B	846	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
26	B	806	BCR	C16-C15-C14	-2.11	119.15	123.47
31	4	307	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
31	K	206	CLA	CMC-C2C-C1C	2.11	128.25	125.04
31	a	322	CLA	CMB-C2B-C1B	2.11	128.58	125.37
31	4	307	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
36	6	303	LUT	C36-C21-C26	2.11	112.74	109.55
26	A	805	BCR	C15-C16-C17	-2.11	119.16	123.47
31	A	855	CLA	C1-O2A-CGA	2.11	121.97	116.44
31	B	814	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
31	8	317	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
32	6	318	CHL	CHC-C1C-NC	-2.11	121.01	124.20
31	2	311	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
31	7	322	CLA	O2A-CGA-CBA	2.11	120.56	112.23
27	A	808	LMT	O5B-C5B-C6B	2.11	111.67	106.44
31	A	817	CLA	CMD-C2D-C1D	2.11	128.43	124.71
31	8	311	CLA	CED-O2D-CGD	2.11	120.70	115.94
31	B	819	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
31	8	318	CLA	CHC-C1C-NC	-2.11	121.01	124.20
26	2	302	BCR	C24-C23-C22	-2.11	123.05	126.23
31	A	834	CLA	CMD-C2D-C1D	2.11	128.42	124.71
31	B	826	CLA	CMD-C2D-C1D	2.11	128.42	124.71
31	A	821	CLA	C11-C10-C8	-2.11	109.11	115.92
26	5	302	BCR	C1-C6-C5	-2.11	119.65	122.61
31	A	841	CLA	CMC-C2C-C1C	2.10	128.24	125.04
31	B	819	CLA	CMC-C2C-C1C	2.10	128.24	125.04
31	3	318	CLA	CMC-C2C-C1C	2.10	128.24	125.04
31	2	315	CLA	CMB-C2B-C1B	2.10	128.57	125.37
31	B	843	CLA	CMB-C2B-C3B	2.10	131.68	126.59
31	7	321	CLA	CHB-C1B-NB	-2.10	122.03	124.26
32	a	317	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
31	8	309	CLA	CMC-C2C-C1C	2.10	128.24	125.04
32	4	313	CHL	C2C-C3C-C4C	-2.10	104.99	106.49
31	a	321	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
31	A	851	CLA	O1D-CGD-CBD	-2.10	120.18	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	837	CLA	C4D-C3D-CAD	2.10	110.57	108.10
31	3	307	CLA	CHC-C4B-C3B	-2.10	118.36	127.71
26	G	203	BCR	C38-C26-C25	-2.10	122.17	124.53
31	A	829	CLA	C4B-CHC-C1C	-2.10	121.36	126.34
31	9	311	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
31	A	816	CLA	CMD-C2D-C1D	2.10	128.41	124.71
31	8	307	CLA	O2A-CGA-CBA	2.10	120.53	112.23
31	A	850	CLA	C1-O2A-CGA	2.10	121.95	116.44
32	7	319	CHL	C2C-C3C-C4C	-2.10	104.99	106.49
31	3	310	CLA	CMB-C2B-C1B	2.10	128.57	125.37
31	a	322	CLA	O2A-CGA-CBA	2.10	120.53	112.23
31	a	321	CLA	CMC-C2C-C1C	2.10	128.24	125.04
32	5	319	CHL	C2D-C1D-ND	2.10	111.65	110.10
31	8	309	CLA	C3C-C4C-NC	2.10	112.92	110.57
31	2	306	CLA	CHC-C1C-NC	-2.10	121.02	124.20
31	A	816	CLA	CHB-C4A-NA	2.10	127.41	124.51
31	B	822	CLA	C6-C7-C8	-2.10	109.14	115.92
31	B	849	CLA	CMB-C2B-C3B	2.10	131.67	126.59
31	B	830	CLA	CMC-C2C-C1C	2.10	128.23	125.04
31	5	323	CLA	CAC-C3C-C4C	2.10	127.53	124.81
31	3	316	CLA	C5-C3-C4	2.10	119.23	114.60
31	B	823	CLA	C1-C2-C3	-2.10	122.42	126.04
32	6	320	CHL	O2A-CGA-CBA	2.10	120.51	112.23
31	A	819	CLA	CHB-C4A-NA	2.09	127.41	124.51
36	a	305	LUT	C16-C1-C6	-2.09	106.90	110.30
31	7	311	CLA	CMD-C2D-C1D	2.09	128.41	124.71
31	O	203	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
31	A	853	CLA	CHB-C1B-NB	-2.09	122.04	124.26
31	b	308	CLA	C3D-C4D-CHA	-2.09	107.93	112.72
31	9	315	CLA	CED-O2D-CGD	2.09	120.67	115.94
31	8	317	CLA	C5-C3-C4	2.09	119.23	114.60
31	B	825	CLA	CMB-C2B-C1B	2.09	128.56	125.37
31	6	316	CLA	CHC-C4B-C3B	-2.09	118.40	127.71
31	8	314	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
31	A	842	CLA	CAC-C3C-C4C	2.09	127.53	124.81
31	B	819	CLA	C1D-CHD-C4C	-2.09	121.54	126.06
31	A	853	CLA	CMC-C2C-C1C	2.09	128.22	125.04
31	A	832	CLA	C7-C6-C5	-2.09	107.68	113.36
31	4	308	CLA	CMD-C2D-C1D	2.09	128.40	124.71
31	5	323	CLA	CMD-C2D-C1D	2.09	128.40	124.71
31	3	311	CLA	C1D-CHD-C4C	-2.09	121.55	126.06
31	7	312	CLA	C1-O2A-CGA	2.09	121.93	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	312	CLA	CMC-C2C-C1C	2.09	128.22	125.04
31	B	830	CLA	O2A-CGA-CBA	2.09	118.47	111.91
31	B	820	CLA	CHC-C4B-C3B	-2.09	118.41	127.71
31	A	823	CLA	CAC-C3C-C4C	2.09	127.52	124.81
31	9	318	CLA	CMB-C2B-C1B	2.09	128.55	125.37
31	8	309	CLA	CAC-C3C-C4C	2.09	127.52	124.81
31	2	304	CLA	CAC-C3C-C4C	2.09	127.52	124.81
31	6	308	CLA	CHC-C4B-C3B	-2.09	118.42	127.71
32	b	309	CHL	CHA-C4D-ND	2.09	136.87	132.50
31	L	307	CLA	CMC-C2C-C1C	2.09	128.22	125.04
31	A	851	CLA	CAC-C3C-C4C	2.09	127.52	124.81
31	G	204	CLA	CBA-CAA-C2A	-2.09	107.70	113.86
26	K	202	BCR	C30-C25-C26	-2.09	119.67	122.61
31	b	313	CLA	CHC-C1C-NC	-2.09	121.04	124.20
31	7	316	CLA	CED-O2D-CGD	2.09	120.66	115.94
31	a	316	CLA	CHB-C4A-NA	2.09	127.40	124.51
31	B	834	CLA	CHC-C4B-C3B	-2.09	118.43	127.71
31	B	811	CLA	C1-C2-C3	-2.09	122.43	126.04
32	3	315	CHL	CHA-C4D-ND	2.09	136.86	132.50
31	5	310	CLA	CMB-C2B-C1B	2.09	128.55	125.37
26	3	301	BCR	C11-C10-C9	-2.09	124.33	127.31
32	6	319	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
31	B	841	CLA	CHC-C4B-C3B	-2.09	118.43	127.71
31	B	829	CLA	CHB-C1B-NB	-2.09	122.05	124.26
31	2	308	CLA	O2A-CGA-O1A	-2.09	116.61	123.14
31	b	303	CLA	C3D-C4D-CHA	-2.08	107.95	112.72
31	A	814	CLA	CMC-C2C-C1C	2.08	128.21	125.04
31	3	316	CLA	CAC-C3C-C4C	2.08	127.52	124.81
31	B	823	CLA	O2A-CGA-CBA	2.08	118.45	111.91
31	6	310	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
31	9	311	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
31	b	307	CLA	CHC-C4B-C3B	-2.08	118.44	127.71
31	A	826	CLA	CHC-C1C-NC	-2.08	121.04	124.20
31	3	313	CLA	CHC-C4B-C3B	-2.08	118.44	127.71
31	b	304	CLA	O2A-CGA-CBA	2.08	120.46	112.23
31	b	304	CLA	CHC-C4B-C3B	-2.08	118.44	127.71
31	6	322	CLA	C1D-CHD-C4C	-2.08	121.56	126.06
31	B	843	CLA	CMD-C2D-C1D	2.08	128.38	124.71
31	B	840	CLA	CMC-C2C-C1C	2.08	128.21	125.04
31	7	310	CLA	C3D-C4D-CHA	-2.08	107.96	112.72
31	2	305	CLA	CMC-C2C-C1C	2.08	128.21	125.04
26	I	801	BCR	C38-C26-C27	-2.08	109.62	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	312	CLA	CMD-C2D-C1D	2.08	128.38	124.71
31	A	855	CLA	CBA-CAA-C2A	2.08	120.00	113.86
31	A	850	CLA	CHC-C1C-NC	-2.08	121.05	124.20
31	2	314	CLA	CMD-C2D-C1D	2.08	128.38	124.71
31	B	824	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
31	3	308	CLA	CMB-C2B-C1B	2.08	128.54	125.37
31	A	825	CLA	C4-C3-C5	2.08	118.77	115.27
31	A	827	CLA	C4-C3-C5	2.08	118.77	115.27
31	O	203	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
31	A	819	CLA	C11-C10-C8	-2.08	109.20	115.92
31	6	313	CLA	O2A-CGA-CBA	2.08	120.44	112.23
32	A	831	CHL	CHA-C4D-ND	2.08	136.84	132.50
31	A	819	CLA	CHB-C1B-NB	-2.08	122.06	124.26
31	4	312	CLA	CHB-C1B-NB	-2.08	122.06	124.26
31	A	843	CLA	C3B-C4B-NB	2.08	112.44	110.52
31	B	841	CLA	CMC-C2C-C1C	2.08	128.20	125.04
31	6	313	CLA	CED-O2D-CGD	2.08	120.63	115.94
31	7	314	CLA	CMB-C2B-C1B	2.08	128.53	125.37
31	3	312	CLA	CHB-C4A-NA	2.08	127.38	124.51
31	3	320	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
36	3	305	LUT	C35-C15-C14	-2.08	119.22	123.47
31	5	308	CLA	CMD-C2D-C1D	2.08	128.37	124.71
31	7	315	CLA	C1D-CHD-C4C	-2.07	121.58	126.06
31	A	814	CLA	CHC-C4B-C3B	-2.07	118.48	127.71
31	8	321	CLA	CHC-C4B-C3B	-2.07	118.48	127.71
32	7	317	CHL	CHC-C4B-C3B	-2.07	118.49	127.71
31	A	824	CLA	C1-C2-C3	-2.07	122.46	126.04
31	5	311	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
31	2	310	CLA	CAC-C3C-C4C	2.07	127.50	124.81
31	B	820	CLA	C16-C15-C13	-2.07	109.22	115.92
31	B	846	CLA	C1D-CHD-C4C	-2.07	121.59	126.06
32	8	319	CHL	C2C-C3C-C4C	-2.07	105.01	106.49
31	b	313	CLA	CMC-C2C-C1C	2.07	128.19	125.04
31	A	853	CLA	CAC-C3C-C4C	2.07	127.50	124.81
31	A	842	CLA	CHB-C1B-NB	-2.07	122.06	124.26
32	6	320	CHL	CMB-C2B-C1B	2.07	128.52	125.37
31	4	319	CLA	CHB-C1B-NB	-2.07	122.06	124.26
31	a	316	CLA	C3D-C4D-CHA	-2.07	107.99	112.72
31	B	825	CLA	CHC-C4B-C3B	-2.07	118.50	127.71
31	3	313	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
31	B	823	CLA	CHB-C1B-NB	-2.07	122.07	124.26
31	b	306	CLA	CHC-C4B-C3B	-2.07	118.50	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	314	CLA	CHC-C4B-C3B	-2.07	118.50	127.71
31	8	312	CLA	CMB-C2B-C1B	2.07	128.52	125.37
31	7	322	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
32	4	310	CHL	CHA-C4D-ND	2.07	136.83	132.50
31	H	902	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
26	L	302	BCR	C2-C1-C6	2.07	113.67	110.48
31	5	313	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	6	322	CLA	CAC-C3C-C4C	2.07	127.49	124.81
31	7	310	CLA	CED-O2D-CGD	2.07	120.61	115.94
31	2	315	CLA	CED-O2D-CGD	2.07	120.61	115.94
31	A	827	CLA	CHC-C4B-C3B	-2.07	118.51	127.71
31	4	308	CLA	C6-C5-C3	-2.07	108.03	113.45
31	A	826	CLA	CHB-C4A-NA	2.07	127.37	124.51
40	7	306	XAT	C28-C29-C30	2.07	122.11	118.94
31	4	307	CLA	CHC-C1C-NC	-2.07	121.07	124.20
26	A	806	BCR	C2-C1-C6	2.07	113.66	110.48
31	2	309	CLA	CMB-C2B-C1B	2.07	128.52	125.37
31	3	310	CLA	CHC-C4B-C3B	-2.07	118.52	127.71
31	a	309	CLA	C6-C7-C8	-2.07	109.24	115.92
31	A	842	CLA	O2A-CGA-CBA	2.07	118.39	111.91
32	6	321	CHL	CHC-C4B-C3B	-2.07	118.52	127.71
32	a	318	CHL	CHC-C4B-C3B	-2.07	118.52	127.71
31	2	314	CLA	CMB-C2B-C1B	2.06	128.51	125.37
31	4	305	CLA	CMB-C2B-C3B	2.06	131.59	126.59
31	a	319	CLA	CHB-C4A-NA	2.06	127.37	124.51
31	3	316	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
31	5	307	CLA	CMD-C2D-C1D	2.06	128.35	124.71
31	A	836	CLA	CHC-C4B-C3B	-2.06	118.53	127.71
26	5	302	BCR	C15-C16-C17	-2.06	119.25	123.47
31	A	857	CLA	CED-O2D-CGD	2.06	120.61	115.94
32	9	320	CHL	CHA-C4D-ND	2.06	136.81	132.50
31	B	819	CLA	CHC-C1C-NC	-2.06	121.07	124.20
31	7	312	CLA	CHC-C1C-NC	-2.06	121.07	124.20
26	B	804	BCR	C3-C4-C5	-2.06	110.39	114.08
31	7	313	CLA	C3D-C4D-CHA	-2.06	108.00	112.72
31	B	827	CLA	C1-C2-C3	-2.06	122.48	126.04
31	B	818	CLA	CHC-C1C-NC	-2.06	121.08	124.20
26	L	301	BCR	C40-C30-C25	2.06	113.64	110.30
31	A	850	CLA	CHB-C4A-NA	2.06	127.36	124.51
31	3	312	CLA	C3D-C4D-CHA	-2.06	108.01	112.72
31	B	838	CLA	CHB-C1B-NB	-2.06	122.08	124.26
31	B	830	CLA	CAC-C3C-C4C	2.06	127.48	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	309	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
31	B	838	CLA	CMB-C2B-C1B	2.06	128.51	125.37
31	B	841	CLA	CMD-C2D-C1D	2.06	128.34	124.71
26	L	301	BCR	C27-C26-C25	2.06	125.72	122.73
32	a	317	CHL	C1D-CHD-C4C	-2.06	121.61	126.06
31	F	306	CLA	CHB-C4A-NA	2.06	127.36	124.51
31	5	312	CLA	C1D-CHD-C4C	-2.06	121.62	126.06
31	B	841	CLA	C3C-C4C-NC	2.06	112.88	110.57
31	7	311	CLA	CHC-C4B-C3B	-2.06	118.56	127.71
31	2	308	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
31	2	313	CLA	O2A-CGA-CBA	2.06	120.36	112.23
32	7	317	CHL	C6-C5-C3	-2.06	108.06	113.45
31	8	312	CLA	C3D-C4D-CHA	-2.06	108.02	112.72
31	b	308	CLA	CHB-C1B-NB	-2.06	122.08	124.26
31	A	825	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
31	a	313	CLA	C3D-C4D-CHA	-2.06	108.02	112.72
33	7	308	DGD	CAB-C9B-C8B	-2.06	103.99	114.42
31	7	314	CLA	C3D-C4D-CHA	-2.06	108.02	112.72
31	b	304	CLA	CED-O2D-CGD	2.06	120.59	115.94
35	F	303	QTB	C09-C02-C03	2.06	122.09	118.94
26	B	806	BCR	C2-C1-C6	2.06	113.64	110.48
31	O	203	CLA	C1D-CHD-C4C	-2.06	121.62	126.06
31	A	847	CLA	CAC-C3C-C4C	2.05	127.47	124.81
31	9	315	CLA	CHB-C4A-NA	2.05	127.35	124.51
37	a	301	LMG	O3-C3-C2	-2.05	105.60	110.35
31	a	309	CLA	C3D-C4D-CHA	-2.05	108.03	112.72
31	O	203	CLA	CAC-C3C-C4C	2.05	127.47	124.81
31	4	306	CLA	CAC-C3C-C4C	2.05	127.47	124.81
31	4	320	CLA	CMB-C2B-C1B	2.05	128.50	125.37
31	4	314	CLA	CHC-C4B-C3B	-2.05	118.58	127.71
31	A	822	CLA	C1D-CHD-C4C	-2.05	121.63	126.06
31	7	313	CLA	CMB-C2B-C1B	2.05	128.50	125.37
31	L	305	CLA	CHC-C4B-C3B	-2.05	118.58	127.71
31	B	832	CLA	C4D-C3D-CAD	2.05	110.51	108.10
26	7	304	BCR	C29-C30-C25	2.05	113.64	110.48
36	2	301	LUT	C1-C2-C3	2.05	118.28	113.64
31	A	847	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
31	4	306	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
31	7	321	CLA	C1D-CHD-C4C	-2.05	121.63	126.06
32	7	319	CHL	C1D-CHD-C4C	-2.05	121.63	126.06
31	K	205	CLA	C3D-C4D-CHA	-2.05	108.03	112.72
31	b	304	CLA	C3D-C4D-CHA	-2.05	108.03	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	856	CLA	CAC-C3C-C4C	2.05	127.47	124.81
31	A	818	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
27	A	807	LMT	O5B-C5B-C6B	2.05	111.53	106.44
31	9	317	CLA	C3B-C4B-NB	2.05	112.42	110.52
31	B	838	CLA	CMD-C2D-C1D	2.05	128.32	124.71
33	7	308	DGD	C7B-C6B-C5B	-2.05	104.03	114.42
31	3	318	CLA	CAC-C3C-C4C	2.05	127.47	124.81
31	A	819	CLA	C1-C2-C3	-2.05	122.50	126.04
31	8	317	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
31	B	827	CLA	C3D-C4D-CHA	-2.05	108.04	112.72
31	9	312	CLA	CMB-C2B-C1B	2.05	128.49	125.37
32	a	318	CHL	CMB-C2B-C1B	2.05	128.49	125.37
26	A	803	BCR	C16-C15-C14	-2.05	119.28	123.47
31	5	311	CLA	C1D-CHD-C4C	-2.05	121.64	126.06
32	7	318	CHL	C2C-C3C-C4C	-2.05	105.03	106.49
32	6	321	CHL	CMB-C2B-C1B	2.05	128.48	125.37
31	B	839	CLA	CHC-C4B-C3B	-2.05	118.61	127.71
30	A	813	CL0	O1D-CGD-CBD	-2.04	120.30	124.48
32	A	840	CHL	CHC-C4B-C3B	-2.04	118.61	127.71
31	A	833	CLA	CED-O2D-CGD	2.04	120.56	115.94
31	a	319	CLA	CMC-C2C-C1C	2.04	128.15	125.04
32	7	317	CHL	CHA-C4D-ND	2.04	136.78	132.50
31	B	845	CLA	CMB-C2B-C1B	2.04	128.48	125.37
31	K	206	CLA	CMD-C2D-C1D	2.04	128.32	124.71
31	B	830	CLA	CHB-C4A-NA	2.04	127.34	124.51
36	7	305	LUT	C8-C7-C6	2.04	132.94	127.20
32	a	318	CHL	C2C-C3C-C4C	-2.04	105.03	106.49
31	A	825	CLA	CAC-C3C-C4C	2.04	127.46	124.81
31	H	901	CLA	C3D-C4D-CHA	-2.04	108.05	112.72
31	2	310	CLA	C3D-C4D-CHA	-2.04	108.05	112.72
32	8	316	CHL	CMB-C2B-C1B	2.04	128.48	125.37
31	3	318	CLA	C3D-C4D-CHA	-2.04	108.05	112.72
26	F	302	BCR	C38-C26-C27	-2.04	109.69	113.62
31	a	310	CLA	CMD-C2D-C1D	2.04	128.31	124.71
31	A	823	CLA	CHB-C1B-NB	-2.04	122.10	124.26
31	6	322	CLA	CED-O2D-CGD	2.04	120.55	115.94
31	8	320	CLA	C1-O2A-CGA	2.04	121.80	116.44
31	A	856	CLA	CHC-C4B-C3B	-2.04	118.63	127.71
31	B	816	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
31	b	307	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
31	8	315	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
26	G	201	BCR	C38-C26-C27	-2.04	109.70	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	7	307	LHG	C27-C26-C25	-2.04	104.08	114.42
31	3	307	CLA	C4C-C3C-C2C	-2.04	103.93	106.90
32	4	310	CHL	C2C-C3C-C4C	-2.04	105.04	106.49
31	L	306	CLA	CHC-C1C-NC	-2.04	121.11	124.20
31	3	313	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
31	6	313	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
31	B	830	CLA	CMB-C2B-C1B	2.04	128.47	125.37
32	6	317	CHL	CMB-C2B-C1B	2.04	128.47	125.37
26	A	805	BCR	C29-C30-C25	2.04	113.61	110.48
31	7	313	CLA	C1D-CHD-C4C	-2.04	121.67	126.06
31	B	837	CLA	C4C-C3C-C2C	-2.03	103.93	106.90
33	B	808	DGD	CBB-CAB-C9B	-2.03	104.10	114.42
31	F	305	CLA	O2A-CGA-CBA	2.03	120.27	112.23
32	a	317	CHL	CMD-C2D-C1D	2.03	128.30	124.71
31	G	204	CLA	CHB-C4A-NA	2.03	127.32	124.51
31	8	313	CLA	CAC-C3C-C4C	2.03	127.45	124.81
31	A	835	CLA	CMC-C2C-C1C	2.03	128.13	125.04
32	A	839	CHL	CHA-C4D-ND	2.03	136.75	132.50
31	A	849	CLA	O2A-CGA-CBA	2.03	120.26	112.23
31	A	830	CLA	CHC-C1C-NC	-2.03	121.12	124.20
31	A	822	CLA	CMC-C2C-C1C	2.03	128.13	125.04
31	4	320	CLA	CMC-C2C-C1C	2.03	128.13	125.04
31	B	831	CLA	CAC-C3C-C4C	2.03	127.45	124.81
31	5	318	CLA	CHB-C4A-NA	2.03	127.32	124.51
32	6	317	CHL	C2C-C3C-C4C	-2.03	105.04	106.49
31	7	310	CLA	CMD-C2D-C1D	2.03	128.29	124.71
26	6	302	BCR	C33-C5-C6	-2.03	122.25	124.53
31	A	845	CLA	C3D-C4D-CHA	-2.03	108.08	112.72
32	7	324	CHL	O2A-CGA-O1A	-2.03	118.47	123.59
31	b	302	CLA	C1D-CHD-C4C	-2.03	121.68	126.06
36	a	303	LUT	C2-C3-C4	2.03	113.08	110.30
31	4	309	CLA	C3D-C4D-CHA	-2.03	108.08	112.72
31	7	312	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
31	A	815	CLA	CHC-C4B-C3B	-2.03	118.68	127.71
31	B	816	CLA	CHB-C1B-NB	-2.03	122.11	124.26
31	F	301	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
36	6	303	LUT	C2-C3-C4	2.03	113.08	110.30
36	8	303	LUT	C3-C4-C5	2.03	115.89	111.85
31	A	821	CLA	CAC-C3C-C4C	2.03	127.44	124.81
31	b	310	CLA	C3D-C4D-CHA	-2.03	108.08	112.72
26	2	302	BCR	C40-C30-C25	2.03	113.59	110.30
31	7	322	CLA	CHC-C1C-NC	-2.03	121.13	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	307	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	B	802	BCR	C27-C26-C25	2.03	125.67	122.73
31	6	316	CLA	C3D-C4D-CHA	-2.03	108.09	112.72
31	5	310	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
31	B	848	CLA	CHC-C4B-C3B	-2.03	118.70	127.71
31	9	319	CLA	C1D-CHD-C4C	-2.03	121.69	126.06
32	7	324	CHL	C1D-CHD-C4C	-2.03	121.69	126.06
31	5	312	CLA	C3D-C4D-CHA	-2.03	108.09	112.72
31	5	314	CLA	CHB-C1B-NB	-2.03	122.11	124.26
32	b	309	CHL	O2A-CGA-CBA	2.03	120.24	112.23
31	A	857	CLA	C6-C5-C3	-2.03	108.14	113.45
31	6	311	CLA	CED-O2D-CGD	2.03	120.52	115.94
31	2	312	CLA	CHC-C4B-C3B	-2.03	118.70	127.71
31	A	848	CLA	CED-O2D-CGD	2.02	120.52	115.94
32	A	831	CHL	CBB-CAB-C3B	-2.02	117.55	127.62
31	B	821	CLA	CAC-C3C-C4C	2.02	127.44	124.81
36	3	305	LUT	C1-C6-C7	-2.02	110.05	115.78
31	B	838	CLA	C3D-C4D-CHA	-2.02	108.09	112.72
31	B	850	CLA	CMB-C2B-C1B	2.02	128.45	125.37
26	B	806	BCR	C30-C25-C26	-2.02	119.76	122.61
31	B	842	CLA	CHC-C4B-C3B	-2.02	118.71	127.71
31	8	315	CLA	CED-O2D-CGD	2.02	120.51	115.94
31	A	857	CLA	CMD-C2D-C1D	2.02	128.28	124.71
31	B	828	CLA	CHC-C1C-NC	-2.02	121.14	124.20
27	9	306	LMT	C1'-O5'-C5'	-2.02	109.72	113.69
31	B	831	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
31	5	307	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
26	B	806	BCR	C10-C11-C12	-2.02	116.91	123.22
32	5	322	CHL	O2A-CGA-CBA	2.02	120.22	112.23
31	A	844	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
31	G	204	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
31	3	310	CLA	C1-O2A-CGA	2.02	121.74	116.44
31	B	844	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
31	A	826	CLA	C1-C2-C3	-2.02	122.55	126.04
31	8	318	CLA	C1D-CHD-C4C	-2.02	121.70	126.06
31	a	314	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
31	8	314	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
31	2	314	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
31	5	310	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
31	9	321	CLA	CMC-C2C-C1C	2.02	128.11	125.04
31	7	314	CLA	CMD-C2D-C1D	2.02	128.27	124.71
31	B	840	CLA	C4-C3-C5	2.02	118.67	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	319	CLA	C6-C5-C3	-2.02	108.16	113.45
32	A	839	CHL	O2A-C1-C2	-2.02	103.33	108.64
31	a	314	CLA	CMC-C2C-C1C	2.02	128.11	125.04
31	B	845	CLA	CHB-C4A-NA	2.02	127.30	124.51
32	9	322	CHL	CHB-C4A-NA	2.02	127.30	124.51
31	4	307	CLA	CED-O2D-CGD	2.02	120.50	115.94
32	7	324	CHL	CMB-C2B-C1B	2.02	128.44	125.37
31	6	315	CLA	C3D-C4D-CHA	-2.02	108.11	112.72
31	a	311	CLA	CHB-C1B-NB	-2.02	122.12	124.26
31	5	323	CLA	CMB-C2B-C1B	2.02	128.44	125.37
31	G	205	CLA	CAC-C3C-C4C	2.02	127.43	124.81
31	B	830	CLA	C6-C5-C3	-2.02	108.17	113.45
31	A	830	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
31	A	843	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
31	b	302	CLA	CED-O2D-CGD	2.02	120.50	115.94
31	8	315	CLA	CHC-C1C-NC	-2.02	121.14	124.20
31	A	846	CLA	C16-C15-C13	-2.02	109.40	115.92
31	3	314	CLA	CMB-C2B-C1B	2.02	128.44	125.37
31	b	305	CLA	O2A-CGA-CBA	2.02	120.19	112.23
31	a	322	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
31	4	320	CLA	C3D-C4D-CHA	-2.01	108.11	112.72
31	A	825	CLA	CHB-C1B-NB	-2.01	122.12	124.26
31	5	307	CLA	C3D-C4D-CHA	-2.01	108.11	112.72
31	A	841	CLA	C1D-CHD-C4C	-2.01	121.71	126.06
31	3	316	CLA	C4C-C3C-C2C	-2.01	103.96	106.90
31	H	903	CLA	CED-O2D-CGD	2.01	120.49	115.94
31	8	310	CLA	CHC-C4B-C3B	-2.01	118.75	127.71
31	B	820	CLA	C3D-C4D-CHA	-2.01	108.12	112.72
31	A	829	CLA	C3D-C4D-CHA	-2.01	108.12	112.72
31	9	313	CLA	C3D-C4D-CHA	-2.01	108.12	112.72
26	L	303	BCR	C3-C4-C5	-2.01	110.48	114.08
26	A	806	BCR	C10-C11-C12	-2.01	116.94	123.22
31	A	832	CLA	CAC-C3C-C4C	2.01	127.42	124.81
31	9	317	CLA	CAC-C3C-C4C	2.01	127.42	124.81
26	L	302	BCR	C33-C5-C6	-2.01	122.27	124.53
31	5	318	CLA	CHC-C1C-NC	-2.01	121.15	124.20
27	9	306	LMT	O5B-C5B-C6B	2.01	111.44	106.44
31	9	311	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
31	A	830	CLA	CHB-C1B-NB	-2.01	122.13	124.26
31	B	837	CLA	C1-C2-C3	-2.01	122.57	126.04
31	5	310	CLA	C1D-CHD-C4C	-2.01	121.72	126.06
31	B	840	CLA	CHC-C4B-C3B	-2.01	118.77	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	302	CLA	C3D-C4D-CHA	-2.01	108.13	112.72
30	A	813	CL0	CAC-C3C-C4C	2.01	127.42	124.81
32	6	321	CHL	CMD-C2D-C1D	2.01	128.25	124.71
31	B	842	CLA	CHC-C1C-NC	-2.01	121.16	124.20
31	2	309	CLA	O2A-CGA-CBA	2.01	120.17	112.23
31	3	308	CLA	CHB-C4A-NA	2.01	127.29	124.51
31	A	855	CLA	CMD-C2D-C1D	2.01	128.25	124.71
31	6	310	CLA	CAC-C3C-C4C	2.01	127.42	124.81
31	A	844	CLA	CAC-C3C-C4C	2.01	127.42	124.81
32	6	318	CHL	CAC-C3C-C4C	2.01	127.42	124.81
31	B	833	CLA	O2A-CGA-CBA	2.01	118.21	111.91
31	B	836	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
31	A	828	CLA	C7-C6-C5	-2.01	107.91	113.36
31	4	316	CLA	C3C-C4C-NC	2.01	112.82	110.57
31	a	319	CLA	C6-C7-C8	-2.01	109.43	115.92
31	A	832	CLA	C1-O2A-CGA	2.01	121.71	116.44
31	B	838	CLA	CMC-C2C-C1C	2.01	128.09	125.04
31	B	813	CLA	CHB-C4A-NA	2.01	127.29	124.51
31	K	204	CLA	CMB-C2B-C1B	2.01	128.42	125.37
31	8	311	CLA	C1-C2-C3	-2.01	122.57	126.04
31	a	321	CLA	CAC-C3C-C4C	2.01	127.41	124.81
31	A	815	CLA	CMB-C2B-C3B	2.01	131.44	126.59
31	3	309	CLA	C3D-C4D-CHA	-2.01	108.14	112.72
32	a	317	CHL	C2A-C1A-CHA	-2.01	120.35	123.86
31	7	322	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
31	B	824	CLA	CHC-C1C-NC	-2.00	121.16	124.20
31	B	830	CLA	CHC-C4B-C3B	-2.00	118.80	127.71
31	4	319	CLA	C1D-CHD-C4C	-2.00	121.73	126.06
31	F	305	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
31	4	319	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
32	5	322	CHL	CHA-C4D-ND	2.00	136.69	132.50
32	6	321	CHL	CHA-C4D-ND	2.00	136.69	132.50
31	A	824	CLA	CHB-C1B-NB	-2.00	122.14	124.26
31	H	901	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
31	3	309	CLA	C1-O2A-CGA	2.00	121.70	116.44
31	5	314	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
32	6	309	CHL	CHA-C4D-ND	2.00	136.69	132.50
31	L	305	CLA	O2A-CGA-CBA	2.00	118.19	111.91
31	A	817	CLA	C1-C2-C3	-2.00	122.58	126.04
33	7	308	DGD	CBB-CAB-C9B	-2.00	104.26	114.42
31	5	320	CLA	CMB-C2B-C1B	2.00	128.42	125.37
36	F	304	LUT	C3-C4-C5	2.00	115.84	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	321	CLA	CHC-C1C-NC	-2.00	121.17	124.20
31	8	318	CLA	CHB-C4A-NA	2.00	127.28	124.51
31	2	311	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
31	8	314	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
31	3	309	CLA	CHB-C4A-NA	2.00	127.28	124.51
31	7	309	CLA	CHC-C4B-C3B	-2.00	118.81	127.71
31	4	318	CLA	CHC-C1C-NC	-2.00	121.17	124.20
31	4	315	CLA	CED-O2D-CGD	2.00	120.46	115.94
31	4	319	CLA	CED-O2D-CGD	2.00	120.46	115.94
31	J	105	CLA	CAC-C3C-C4C	2.00	127.41	124.81
31	3	314	CLA	CAC-C3C-C4C	2.00	127.41	124.81
31	9	314	CLA	CAC-C3C-C4C	2.00	127.41	124.81
31	a	309	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
31	a	322	CLA	CHC-C1C-NC	-2.00	121.17	124.20

There are no chirality outliers.

All (2970) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	804	BCR	C7-C8-C9-C10
26	A	804	BCR	C7-C8-C9-C34
26	A	804	BCR	C20-C21-C22-C23
26	A	805	BCR	C7-C8-C9-C34
26	A	805	BCR	C20-C21-C22-C37
26	A	806	BCR	C21-C22-C23-C24
26	A	806	BCR	C37-C22-C23-C24
26	B	802	BCR	C7-C8-C9-C34
26	B	802	BCR	C21-C22-C23-C24
26	B	802	BCR	C37-C22-C23-C24
26	B	803	BCR	C7-C8-C9-C10
26	B	803	BCR	C11-C10-C9-C8
26	B	805	BCR	C7-C8-C9-C34
26	B	805	BCR	C23-C24-C25-C30
26	F	302	BCR	C7-C8-C9-C10
26	F	302	BCR	C7-C8-C9-C34
26	F	302	BCR	C37-C22-C23-C24
26	G	201	BCR	C7-C8-C9-C10
26	G	201	BCR	C7-C8-C9-C34
26	G	201	BCR	C21-C22-C23-C24
26	G	201	BCR	C37-C22-C23-C24
26	G	203	BCR	C1-C6-C7-C8
26	G	203	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	G	203	BCR	C20-C21-C22-C37
26	G	203	BCR	C21-C22-C23-C24
26	G	203	BCR	C37-C22-C23-C24
26	G	203	BCR	C22-C23-C24-C25
26	I	801	BCR	C1-C6-C7-C8
26	I	801	BCR	C7-C8-C9-C34
26	J	102	BCR	C7-C8-C9-C10
26	J	102	BCR	C7-C8-C9-C34
26	K	202	BCR	C7-C8-C9-C10
26	K	202	BCR	C23-C24-C25-C26
26	K	202	BCR	C23-C24-C25-C30
26	K	203	BCR	C23-C24-C25-C30
26	M	101	BCR	C7-C8-C9-C34
26	M	101	BCR	C23-C24-C25-C30
26	3	301	BCR	C1-C6-C7-C8
26	3	301	BCR	C7-C8-C9-C10
26	3	301	BCR	C23-C24-C25-C30
26	3	302	BCR	C1-C6-C7-C8
26	3	303	BCR	C7-C8-C9-C10
26	7	304	BCR	C20-C21-C22-C23
26	7	304	BCR	C20-C21-C22-C37
26	8	301	BCR	C20-C21-C22-C37
26	8	301	BCR	C23-C24-C25-C30
26	L	301	BCR	C7-C8-C9-C10
26	L	301	BCR	C7-C8-C9-C34
26	L	301	BCR	C21-C22-C23-C24
26	L	301	BCR	C37-C22-C23-C24
26	L	301	BCR	C23-C24-C25-C26
26	L	301	BCR	C23-C24-C25-C30
26	L	302	BCR	C1-C6-C7-C8
26	L	302	BCR	C11-C10-C9-C34
26	L	303	BCR	C17-C18-C19-C20
26	L	303	BCR	C23-C24-C25-C30
26	2	302	BCR	C6-C7-C8-C9
26	5	302	BCR	C6-C7-C8-C9
26	5	302	BCR	C7-C8-C9-C34
26	5	302	BCR	C11-C10-C9-C8
26	5	302	BCR	C17-C18-C19-C20
26	5	302	BCR	C18-C19-C20-C21
26	5	302	BCR	C20-C21-C22-C23
26	5	302	BCR	C20-C21-C22-C37
26	5	302	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	5	302	BCR	C23-C24-C25-C30
26	6	302	BCR	C1-C6-C7-C8
26	6	302	BCR	C11-C12-C13-C14
27	9	306	LMT	C2'-C1'-O1'-C1
27	9	306	LMT	O5'-C1'-O1'-C1
27	5	301	LMT	C2-C1-O1'-C1'
28	A	809	LHG	O1-C1-C2-C3
28	A	809	LHG	C3-O3-P-O4
28	A	810	LHG	O9-C7-O7-C5
28	A	811	LHG	C3-O3-P-O5
28	a	306	LHG	C4-O6-P-O4
28	7	302	LHG	C4-O6-P-O3
28	7	302	LHG	O9-C7-O7-C5
28	7	307	LHG	C4-O6-P-O5
28	5	305	LHG	O1-C1-C2-C3
28	5	305	LHG	C1-C2-C3-O3
28	5	305	LHG	O2-C2-C3-O3
28	5	305	LHG	C3-O3-P-O4
28	5	305	LHG	C3-O3-P-O5
28	5	305	LHG	C3-O3-P-O6
28	5	305	LHG	C4-O6-P-O4
28	6	301	LHG	C3-O3-P-O4
28	6	301	LHG	C3-O3-P-O6
28	6	305	LHG	C8-C7-O7-C5
31	A	818	CLA	CHA-CBD-CGD-O1D
31	A	818	CLA	CAD-CBD-CGD-O1D
31	A	819	CLA	C1A-C2A-CAA-CBA
31	A	819	CLA	C2B-C3B-CAB-CBB
31	A	819	CLA	C4B-C3B-CAB-CBB
31	A	821	CLA	CHA-CBD-CGD-O1D
31	A	822	CLA	C1A-C2A-CAA-CBA
31	A	824	CLA	C1A-C2A-CAA-CBA
31	A	824	CLA	CBD-CGD-O2D-CED
31	A	824	CLA	O1D-CGD-O2D-CED
31	A	830	CLA	C4-C3-C5-C6
31	A	832	CLA	CHA-CBD-CGD-O2D
31	A	833	CLA	C3A-C2A-CAA-CBA
31	A	833	CLA	C2B-C3B-CAB-CBB
31	A	833	CLA	C4B-C3B-CAB-CBB
31	A	833	CLA	CBD-CGD-O2D-CED
31	A	834	CLA	CHA-CBD-CGD-O2D
31	A	834	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	A	835	CLA	CBD-CGD-O2D-CED
31	A	836	CLA	C2B-C3B-CAB-CBB
31	A	836	CLA	C4B-C3B-CAB-CBB
31	A	836	CLA	CBD-CGD-O2D-CED
31	A	836	CLA	C4-C3-C5-C6
31	A	837	CLA	C2B-C3B-CAB-CBB
31	A	837	CLA	C4B-C3B-CAB-CBB
31	A	837	CLA	CHA-CBD-CGD-O2D
31	A	842	CLA	C2A-CAA-CBA-CGA
31	A	842	CLA	CBD-CGD-O2D-CED
31	A	843	CLA	CHA-CBD-CGD-O2D
31	A	845	CLA	CBD-CGD-O2D-CED
31	A	845	CLA	C2-C3-C5-C6
31	A	845	CLA	C4-C3-C5-C6
31	A	846	CLA	C1A-C2A-CAA-CBA
31	A	847	CLA	CHA-CBD-CGD-O1D
31	A	848	CLA	C2B-C3B-CAB-CBB
31	A	848	CLA	C4B-C3B-CAB-CBB
31	A	849	CLA	C2B-C3B-CAB-CBB
31	A	849	CLA	C4B-C3B-CAB-CBB
31	A	850	CLA	C2-C3-C5-C6
31	A	850	CLA	C4-C3-C5-C6
31	A	852	CLA	CHA-CBD-CGD-O2D
31	A	853	CLA	CHA-CBD-CGD-O2D
31	A	854	CLA	CHA-CBD-CGD-O1D
31	A	855	CLA	C1A-C2A-CAA-CBA
31	A	857	CLA	C2-C1-O2A-CGA
31	A	857	CLA	C2B-C3B-CAB-CBB
31	A	857	CLA	C4B-C3B-CAB-CBB
31	A	857	CLA	CHA-CBD-CGD-O2D
31	B	811	CLA	CHA-CBD-CGD-O2D
31	B	811	CLA	CBD-CGD-O2D-CED
31	B	813	CLA	CBD-CGD-O2D-CED
31	B	814	CLA	C1A-C2A-CAA-CBA
31	B	815	CLA	C2B-C3B-CAB-CBB
31	B	815	CLA	C4B-C3B-CAB-CBB
31	B	817	CLA	C2B-C3B-CAB-CBB
31	B	817	CLA	C4B-C3B-CAB-CBB
31	B	817	CLA	CHA-CBD-CGD-O1D
31	B	817	CLA	C6-C7-C8-C9
31	B	818	CLA	CHA-CBD-CGD-O2D
31	B	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	B	822	CLA	CBD-CGD-O2D-CED
31	B	826	CLA	C1A-C2A-CAA-CBA
31	B	828	CLA	C2B-C3B-CAB-CBB
31	B	828	CLA	C4B-C3B-CAB-CBB
31	B	830	CLA	CBD-CGD-O2D-CED
31	B	830	CLA	O1D-CGD-O2D-CED
31	B	831	CLA	CHA-CBD-CGD-O1D
31	B	831	CLA	CHA-CBD-CGD-O2D
31	B	832	CLA	CHA-CBD-CGD-O1D
31	B	833	CLA	CHA-CBD-CGD-O1D
31	B	836	CLA	CHA-CBD-CGD-O2D
31	B	841	CLA	CHA-CBD-CGD-O1D
31	B	842	CLA	C2B-C3B-CAB-CBB
31	B	842	CLA	C4B-C3B-CAB-CBB
31	B	846	CLA	C2B-C3B-CAB-CBB
31	B	846	CLA	C4B-C3B-CAB-CBB
31	B	847	CLA	CBD-CGD-O2D-CED
31	B	850	CLA	C2B-C3B-CAB-CBB
31	B	850	CLA	C4B-C3B-CAB-CBB
31	F	301	CLA	C4B-C3B-CAB-CBB
31	F	301	CLA	CBD-CGD-O2D-CED
31	F	305	CLA	CHA-CBD-CGD-O1D
31	F	305	CLA	CBD-CGD-O2D-CED
31	F	305	CLA	O1D-CGD-O2D-CED
31	F	306	CLA	C2B-C3B-CAB-CBB
31	F	306	CLA	C4B-C3B-CAB-CBB
31	G	204	CLA	CBD-CGD-O2D-CED
31	G	205	CLA	CBD-CGD-O2D-CED
31	G	206	CLA	CBD-CGD-O2D-CED
31	H	901	CLA	CBD-CGD-O2D-CED
31	H	901	CLA	O1D-CGD-O2D-CED
31	H	902	CLA	CHA-CBD-CGD-O2D
31	H	902	CLA	CBD-CGD-O2D-CED
31	H	902	CLA	O1D-CGD-O2D-CED
31	H	903	CLA	C1A-C2A-CAA-CBA
31	H	903	CLA	C3A-C2A-CAA-CBA
31	H	903	CLA	CHA-CBD-CGD-O2D
31	H	903	CLA	CBD-CGD-O2D-CED
31	J	105	CLA	C1A-C2A-CAA-CBA
31	J	105	CLA	C2B-C3B-CAB-CBB
31	J	105	CLA	C4B-C3B-CAB-CBB
31	J	105	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	J	105	CLA	CBD-CGD-O2D-CED
31	K	204	CLA	C2B-C3B-CAB-CBB
31	K	204	CLA	C4B-C3B-CAB-CBB
31	K	205	CLA	CBD-CGD-O2D-CED
31	a	309	CLA	CHA-CBD-CGD-O2D
31	a	311	CLA	C2B-C3B-CAB-CBB
31	a	311	CLA	C4B-C3B-CAB-CBB
31	a	311	CLA	CHA-CBD-CGD-O1D
31	a	311	CLA	CBD-CGD-O2D-CED
31	a	311	CLA	O1D-CGD-O2D-CED
31	a	314	CLA	CBD-CGD-O2D-CED
31	a	315	CLA	CHA-CBD-CGD-O2D
31	a	316	CLA	C1A-C2A-CAA-CBA
31	a	316	CLA	C3A-C2A-CAA-CBA
31	a	316	CLA	CBD-CGD-O2D-CED
31	a	319	CLA	C2B-C3B-CAB-CBB
31	a	319	CLA	C4B-C3B-CAB-CBB
31	a	319	CLA	CBD-CGD-O2D-CED
31	a	321	CLA	C2B-C3B-CAB-CBB
31	a	321	CLA	C4B-C3B-CAB-CBB
31	a	321	CLA	CHA-CBD-CGD-O2D
31	a	321	CLA	CBD-CGD-O2D-CED
31	a	321	CLA	O1D-CGD-O2D-CED
31	a	322	CLA	CBD-CGD-O2D-CED
31	3	307	CLA	CHA-CBD-CGD-O2D
31	3	307	CLA	CBD-CGD-O2D-CED
31	3	308	CLA	CBD-CGD-O2D-CED
31	3	309	CLA	C1A-C2A-CAA-CBA
31	3	309	CLA	C2B-C3B-CAB-CBB
31	3	309	CLA	C4B-C3B-CAB-CBB
31	3	309	CLA	CBD-CGD-O2D-CED
31	3	309	CLA	C6-C7-C8-C9
31	3	312	CLA	CHA-CBD-CGD-O2D
31	3	312	CLA	CBD-CGD-O2D-CED
31	3	313	CLA	CBA-CGA-O2A-C1
31	3	313	CLA	O1A-CGA-O2A-C1
31	3	313	CLA	C2B-C3B-CAB-CBB
31	3	313	CLA	C4B-C3B-CAB-CBB
31	3	313	CLA	CBD-CGD-O2D-CED
31	3	313	CLA	O1D-CGD-O2D-CED
31	3	314	CLA	C2B-C3B-CAB-CBB
31	3	314	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	3	316	CLA	CBD-CGD-O2D-CED
31	3	316	CLA	O1D-CGD-O2D-CED
31	3	317	CLA	CBD-CGD-O2D-CED
31	3	317	CLA	O1D-CGD-O2D-CED
31	3	317	CLA	C2-C3-C5-C6
31	3	317	CLA	C4-C3-C5-C6
31	3	318	CLA	C2B-C3B-CAB-CBB
31	3	318	CLA	C4B-C3B-CAB-CBB
31	3	318	CLA	CBD-CGD-O2D-CED
31	3	318	CLA	C2-C3-C5-C6
31	3	318	CLA	C4-C3-C5-C6
31	3	320	CLA	C2B-C3B-CAB-CBB
31	3	320	CLA	C4B-C3B-CAB-CBB
31	3	320	CLA	CBD-CGD-O2D-CED
31	3	320	CLA	O1D-CGD-O2D-CED
31	7	310	CLA	CBD-CGD-O2D-CED
31	7	311	CLA	C2B-C3B-CAB-CBB
31	7	311	CLA	C4B-C3B-CAB-CBB
31	7	311	CLA	CBD-CGD-O2D-CED
31	7	312	CLA	CBD-CGD-O2D-CED
31	7	314	CLA	CBD-CGD-O2D-CED
31	7	314	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	CBD-CGD-O2D-CED
31	7	316	CLA	CBD-CGD-O2D-CED
31	7	321	CLA	CBD-CGD-O2D-CED
31	7	321	CLA	O1D-CGD-O2D-CED
31	7	322	CLA	C3A-C2A-CAA-CBA
31	7	322	CLA	C2B-C3B-CAB-CBB
31	7	322	CLA	C4B-C3B-CAB-CBB
31	7	322	CLA	CBD-CGD-O2D-CED
31	8	307	CLA	CBD-CGD-O2D-CED
31	8	309	CLA	CBD-CGD-O2D-CED
31	8	311	CLA	C1A-C2A-CAA-CBA
31	8	311	CLA	CBD-CGD-O2D-CED
31	8	311	CLA	O1D-CGD-O2D-CED
31	8	312	CLA	CBD-CGD-O2D-CED
31	8	312	CLA	O1D-CGD-O2D-CED
31	8	313	CLA	C2B-C3B-CAB-CBB
31	8	313	CLA	C4B-C3B-CAB-CBB
31	8	313	CLA	CHA-CBD-CGD-O2D
31	8	314	CLA	CBD-CGD-O2D-CED
31	8	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	8	315	CLA	C2B-C3B-CAB-CBB
31	8	315	CLA	C4B-C3B-CAB-CBB
31	8	315	CLA	CHA-CBD-CGD-O2D
31	8	317	CLA	CBD-CGD-O2D-CED
31	8	320	CLA	C2B-C3B-CAB-CBB
31	8	320	CLA	C4B-C3B-CAB-CBB
31	8	320	CLA	CHA-CBD-CGD-O2D
31	8	320	CLA	CBD-CGD-O2D-CED
31	8	321	CLA	CHA-CBD-CGD-O2D
31	8	321	CLA	CBD-CGD-O2D-CED
31	9	311	CLA	CBD-CGD-O2D-CED
31	9	311	CLA	O1D-CGD-O2D-CED
31	9	312	CLA	CBD-CGD-O2D-CED
31	9	315	CLA	CBD-CGD-O2D-CED
31	9	316	CLA	CHA-CBD-CGD-O1D
31	9	317	CLA	C2B-C3B-CAB-CBB
31	9	317	CLA	C4B-C3B-CAB-CBB
31	9	318	CLA	CBD-CGD-O2D-CED
31	9	319	CLA	C1A-C2A-CAA-CBA
31	9	319	CLA	C2B-C3B-CAB-CBB
31	9	319	CLA	C4B-C3B-CAB-CBB
31	9	319	CLA	CBD-CGD-O2D-CED
31	9	319	CLA	O1D-CGD-O2D-CED
31	L	306	CLA	CBD-CGD-O2D-CED
31	L	307	CLA	C2B-C3B-CAB-CBB
31	L	307	CLA	C4B-C3B-CAB-CBB
31	L	307	CLA	CBD-CGD-O2D-CED
31	O	202	CLA	C2B-C3B-CAB-CBB
31	O	202	CLA	C4B-C3B-CAB-CBB
31	O	203	CLA	CHA-CBD-CGD-O2D
31	O	203	CLA	CBD-CGD-O2D-CED
31	O	203	CLA	C2-C3-C5-C6
31	O	203	CLA	C4-C3-C5-C6
31	O	204	CLA	C2B-C3B-CAB-CBB
31	O	204	CLA	C4B-C3B-CAB-CBB
31	O	204	CLA	CBD-CGD-O2D-CED
31	O	204	CLA	O1D-CGD-O2D-CED
31	b	302	CLA	CBD-CGD-O2D-CED
31	b	303	CLA	CHA-CBD-CGD-O1D
31	b	303	CLA	CBD-CGD-O2D-CED
31	b	304	CLA	C1A-C2A-CAA-CBA
31	b	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	305	CLA	CBD-CGD-O2D-CED
31	b	305	CLA	O1D-CGD-O2D-CED
31	b	306	CLA	C1A-C2A-CAA-CBA
31	b	306	CLA	C3A-C2A-CAA-CBA
31	b	306	CLA	C2B-C3B-CAB-CBB
31	b	306	CLA	C4B-C3B-CAB-CBB
31	b	306	CLA	CBD-CGD-O2D-CED
31	b	306	CLA	O1D-CGD-O2D-CED
31	b	307	CLA	C2B-C3B-CAB-CBB
31	b	307	CLA	C4B-C3B-CAB-CBB
31	b	307	CLA	CHA-CBD-CGD-O1D
31	b	307	CLA	CBD-CGD-O2D-CED
31	b	308	CLA	CHA-CBD-CGD-O2D
31	b	308	CLA	CBD-CGD-O2D-CED
31	b	310	CLA	CBD-CGD-O2D-CED
31	b	310	CLA	O1D-CGD-O2D-CED
31	b	311	CLA	C1A-C2A-CAA-CBA
31	b	311	CLA	C3A-C2A-CAA-CBA
31	b	311	CLA	CBD-CGD-O2D-CED
31	b	311	CLA	O1D-CGD-O2D-CED
31	b	312	CLA	C2B-C3B-CAB-CBB
31	b	312	CLA	C4B-C3B-CAB-CBB
31	b	312	CLA	CBD-CGD-O2D-CED
31	b	312	CLA	O1D-CGD-O2D-CED
31	2	304	CLA	C3A-C2A-CAA-CBA
31	2	304	CLA	CAD-CBD-CGD-O2D
31	2	304	CLA	CBD-CGD-O2D-CED
31	2	304	CLA	O1D-CGD-O2D-CED
31	2	305	CLA	C2B-C3B-CAB-CBB
31	2	305	CLA	C4B-C3B-CAB-CBB
31	2	305	CLA	CBD-CGD-O2D-CED
31	2	306	CLA	C2B-C3B-CAB-CBB
31	2	306	CLA	C4B-C3B-CAB-CBB
31	2	306	CLA	CBD-CGD-O2D-CED
31	2	306	CLA	C2-C3-C5-C6
31	2	306	CLA	C4-C3-C5-C6
31	2	307	CLA	O1D-CGD-O2D-CED
31	2	308	CLA	CBD-CGD-O2D-CED
31	2	309	CLA	CBD-CGD-O2D-CED
31	2	309	CLA	O1D-CGD-O2D-CED
31	2	310	CLA	CBD-CGD-O2D-CED
31	2	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	2	311	CLA	CHA-CBD-CGD-O1D
31	2	311	CLA	CBD-CGD-O2D-CED
31	2	311	CLA	O1D-CGD-O2D-CED
31	2	312	CLA	C2B-C3B-CAB-CBB
31	2	312	CLA	C4B-C3B-CAB-CBB
31	2	313	CLA	CHA-CBD-CGD-O1D
31	2	314	CLA	CBD-CGD-O2D-CED
31	2	314	CLA	O1D-CGD-O2D-CED
31	2	315	CLA	C1A-C2A-CAA-CBA
31	2	315	CLA	C3A-C2A-CAA-CBA
31	2	315	CLA	C2B-C3B-CAB-CBB
31	2	315	CLA	C4B-C3B-CAB-CBB
31	2	315	CLA	CHA-CBD-CGD-O1D
31	2	315	CLA	CBD-CGD-O2D-CED
31	4	305	CLA	C1A-C2A-CAA-CBA
31	4	305	CLA	CBD-CGD-O2D-CED
31	4	306	CLA	CBD-CGD-O2D-CED
31	4	307	CLA	C2B-C3B-CAB-CBB
31	4	307	CLA	C4B-C3B-CAB-CBB
31	4	307	CLA	CBD-CGD-O2D-CED
31	4	307	CLA	O1D-CGD-O2D-CED
31	4	308	CLA	O1D-CGD-O2D-CED
31	4	309	CLA	C2B-C3B-CAB-CBB
31	4	309	CLA	C4B-C3B-CAB-CBB
31	4	309	CLA	CBD-CGD-O2D-CED
31	4	309	CLA	O1D-CGD-O2D-CED
31	4	311	CLA	C1A-C2A-CAA-CBA
31	4	311	CLA	C2B-C3B-CAB-CBB
31	4	311	CLA	C4B-C3B-CAB-CBB
31	4	311	CLA	CHA-CBD-CGD-O1D
31	4	311	CLA	CBD-CGD-O2D-CED
31	4	312	CLA	C1A-C2A-CAA-CBA
31	4	312	CLA	C3A-C2A-CAA-CBA
31	4	312	CLA	C2B-C3B-CAB-CBB
31	4	312	CLA	C4B-C3B-CAB-CBB
31	4	312	CLA	CBD-CGD-O2D-CED
31	4	314	CLA	C2B-C3B-CAB-CBB
31	4	314	CLA	C4B-C3B-CAB-CBB
31	4	315	CLA	CHA-CBD-CGD-O2D
31	4	315	CLA	CBD-CGD-O2D-CED
31	4	315	CLA	O1D-CGD-O2D-CED
31	4	316	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	4	318	CLA	C2B-C3B-CAB-CBB
31	4	318	CLA	C4B-C3B-CAB-CBB
31	4	318	CLA	CBD-CGD-O2D-CED
31	4	318	CLA	O1D-CGD-O2D-CED
31	4	319	CLA	C2B-C3B-CAB-CBB
31	4	319	CLA	C4B-C3B-CAB-CBB
31	4	319	CLA	CBD-CGD-O2D-CED
31	4	319	CLA	O1D-CGD-O2D-CED
31	4	320	CLA	C2B-C3B-CAB-CBB
31	4	320	CLA	C4B-C3B-CAB-CBB
31	4	321	CLA	C2B-C3B-CAB-CBB
31	4	321	CLA	C4B-C3B-CAB-CBB
31	4	321	CLA	CBD-CGD-O2D-CED
31	5	307	CLA	CBD-CGD-O2D-CED
31	5	308	CLA	CBD-CGD-O2D-CED
31	5	309	CLA	CBD-CGD-O2D-CED
31	5	309	CLA	O1D-CGD-O2D-CED
31	5	310	CLA	CHA-CBD-CGD-O2D
31	5	311	CLA	CBD-CGD-O2D-CED
31	5	311	CLA	O1D-CGD-O2D-CED
31	5	312	CLA	C1A-C2A-CAA-CBA
31	5	312	CLA	C2A-CAA-CBA-CGA
31	5	312	CLA	C2B-C3B-CAB-CBB
31	5	312	CLA	C4B-C3B-CAB-CBB
31	5	314	CLA	CBD-CGD-O2D-CED
31	5	315	CLA	CBD-CGD-O2D-CED
31	5	315	CLA	O1D-CGD-O2D-CED
31	5	318	CLA	CHA-CBD-CGD-O2D
31	5	320	CLA	C2A-CAA-CBA-CGA
31	5	321	CLA	C2B-C3B-CAB-CBB
31	5	321	CLA	C4B-C3B-CAB-CBB
31	5	321	CLA	CBD-CGD-O2D-CED
31	5	323	CLA	C1A-C2A-CAA-CBA
31	5	323	CLA	C3A-C2A-CAA-CBA
31	5	323	CLA	CBD-CGD-O2D-CED
31	6	306	CLA	C3A-C2A-CAA-CBA
31	6	307	CLA	CBD-CGD-O2D-CED
31	6	307	CLA	O1D-CGD-O2D-CED
31	6	308	CLA	C2B-C3B-CAB-CBB
31	6	308	CLA	C4B-C3B-CAB-CBB
31	6	308	CLA	CBD-CGD-O2D-CED
31	6	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	6	310	CLA	CBD-CGD-O2D-CED
31	6	310	CLA	O1D-CGD-O2D-CED
31	6	311	CLA	C2B-C3B-CAB-CBB
31	6	311	CLA	C4B-C3B-CAB-CBB
31	6	311	CLA	CHA-CBD-CGD-O1D
31	6	311	CLA	CBD-CGD-O2D-CED
31	6	312	CLA	CHA-CBD-CGD-O2D
31	6	313	CLA	CBD-CGD-O2D-CED
31	6	314	CLA	CBD-CGD-O2D-CED
31	6	315	CLA	CBD-CGD-O2D-CED
31	6	316	CLA	CBD-CGD-O2D-CED
31	6	316	CLA	O1D-CGD-O2D-CED
31	6	322	CLA	C2B-C3B-CAB-CBB
31	6	322	CLA	C4B-C3B-CAB-CBB
31	6	322	CLA	CBD-CGD-O2D-CED
31	6	322	CLA	O1D-CGD-O2D-CED
32	A	831	CHL	C3A-C2A-CAA-CBA
32	A	831	CHL	C2B-C3B-CAB-CBB
32	A	831	CHL	C4B-C3B-CAB-CBB
32	A	831	CHL	C1C-C2C-CMC-OMC
32	A	831	CHL	C3C-C2C-CMC-OMC
32	A	839	CHL	C1C-C2C-CMC-OMC
32	A	839	CHL	C3C-C2C-CMC-OMC
32	A	839	CHL	CAD-CBD-CGD-O2D
32	A	839	CHL	CBD-CGD-O2D-CED
32	A	840	CHL	CHA-CBD-CGD-O1D
32	A	840	CHL	CBD-CGD-O2D-CED
32	A	840	CHL	O1D-CGD-O2D-CED
32	a	317	CHL	C3C-C2C-CMC-OMC
32	a	317	CHL	CHA-CBD-CGD-O1D
32	a	317	CHL	CBD-CGD-O2D-CED
32	a	317	CHL	O1D-CGD-O2D-CED
32	a	318	CHL	C3C-C2C-CMC-OMC
32	a	320	CHL	C1C-C2C-CMC-OMC
32	a	320	CHL	CBD-CGD-O2D-CED
32	3	315	CHL	CAD-CBD-CGD-O2D
32	3	315	CHL	C2-C3-C5-C6
32	3	315	CHL	C4-C3-C5-C6
32	7	317	CHL	C2B-C3B-CAB-CBB
32	7	317	CHL	C4B-C3B-CAB-CBB
32	7	317	CHL	C3C-C2C-CMC-OMC
32	7	317	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	7	317	CHL	CBD-CGD-O2D-CED
32	7	317	CHL	O1D-CGD-O2D-CED
32	7	317	CHL	C2-C3-C5-C6
32	7	317	CHL	C4-C3-C5-C6
32	7	318	CHL	C1A-C2A-CAA-CBA
32	7	318	CHL	C3A-C2A-CAA-CBA
32	7	318	CHL	C3C-C2C-CMC-OMC
32	7	320	CHL	CBD-CGD-O2D-CED
32	7	324	CHL	CHA-CBD-CGD-O1D
32	7	324	CHL	CBD-CGD-O2D-CED
32	7	324	CHL	O1D-CGD-O2D-CED
32	8	316	CHL	C3A-C2A-CAA-CBA
32	8	316	CHL	CBD-CGD-O2D-CED
32	8	319	CHL	CBD-CGD-O2D-CED
32	9	320	CHL	C2B-C3B-CAB-CBB
32	9	320	CHL	C4B-C3B-CAB-CBB
32	9	320	CHL	C1C-C2C-CMC-OMC
32	9	320	CHL	C3C-C2C-CMC-OMC
32	9	320	CHL	CHA-CBD-CGD-O1D
32	9	320	CHL	CBD-CGD-O2D-CED
32	9	322	CHL	C1C-C2C-CMC-OMC
32	9	322	CHL	C3C-C2C-CMC-OMC
32	9	322	CHL	CBD-CGD-O2D-CED
32	b	309	CHL	C2B-C3B-CAB-CBB
32	b	309	CHL	C4B-C3B-CAB-CBB
32	b	309	CHL	C1C-C2C-CMC-OMC
32	b	309	CHL	C3C-C2C-CMC-OMC
32	b	309	CHL	CHA-CBD-CGD-O1D
32	b	309	CHL	CBD-CGD-O2D-CED
32	b	309	CHL	O1D-CGD-O2D-CED
32	4	310	CHL	C1A-C2A-CAA-CBA
32	4	313	CHL	C2B-C3B-CAB-CBB
32	4	313	CHL	C4B-C3B-CAB-CBB
32	4	313	CHL	C1C-C2C-CMC-OMC
32	4	313	CHL	C3C-C2C-CMC-OMC
32	4	313	CHL	CHA-CBD-CGD-O1D
32	4	313	CHL	CHA-CBD-CGD-O2D
32	4	313	CHL	CBD-CGD-O2D-CED
32	4	317	CHL	C1A-C2A-CAA-CBA
32	4	317	CHL	C3A-C2A-CAA-CBA
32	4	317	CHL	C1C-C2C-CMC-OMC
32	4	317	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
32	4	317	CHL	CBD-CGD-O2D-CED
32	4	317	CHL	O1D-CGD-O2D-CED
32	5	316	CHL	C2B-C3B-CAB-CBB
32	5	316	CHL	C4B-C3B-CAB-CBB
32	5	316	CHL	C1C-C2C-CMC-OMC
32	5	316	CHL	C3C-C2C-CMC-OMC
32	5	316	CHL	CHA-CBD-CGD-O2D
32	5	317	CHL	C3C-C2C-CMC-OMC
32	5	319	CHL	CBD-CGD-O2D-CED
32	5	322	CHL	C3A-C2A-CAA-CBA
32	5	322	CHL	CBD-CGD-O2D-CED
32	5	322	CHL	O1D-CGD-O2D-CED
32	6	309	CHL	C1A-C2A-CAA-CBA
32	6	309	CHL	C3A-C2A-CAA-CBA
32	6	309	CHL	C1C-C2C-CMC-OMC
32	6	309	CHL	C3C-C2C-CMC-OMC
32	6	309	CHL	CBD-CGD-O2D-CED
32	6	309	CHL	O1D-CGD-O2D-CED
32	6	309	CHL	C2-C3-C5-C6
32	6	309	CHL	C4-C3-C5-C6
32	6	317	CHL	C2B-C3B-CAB-CBB
32	6	317	CHL	C4B-C3B-CAB-CBB
32	6	317	CHL	C1C-C2C-CMC-OMC
32	6	317	CHL	C3C-C2C-CMC-OMC
32	6	317	CHL	CHA-CBD-CGD-O1D
32	6	317	CHL	CBD-CGD-O2D-CED
32	6	317	CHL	O1D-CGD-O2D-CED
32	6	318	CHL	C1A-C2A-CAA-CBA
32	6	318	CHL	C3A-C2A-CAA-CBA
32	6	318	CHL	C2B-C3B-CAB-CBB
32	6	318	CHL	C4B-C3B-CAB-CBB
32	6	318	CHL	C1C-C2C-CMC-OMC
32	6	318	CHL	C3C-C2C-CMC-OMC
32	6	319	CHL	C1A-C2A-CAA-CBA
32	6	319	CHL	C3A-C2A-CAA-CBA
32	6	319	CHL	C2B-C3B-CAB-CBB
32	6	319	CHL	C4B-C3B-CAB-CBB
32	6	319	CHL	CHA-CBD-CGD-O1D
32	6	319	CHL	CHA-CBD-CGD-O2D
32	6	320	CHL	C1C-C2C-CMC-OMC
32	6	320	CHL	C3C-C2C-CMC-OMC
32	6	320	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	6	320	CHL	CHA-CBD-CGD-O2D
32	6	320	CHL	CBD-CGD-O2D-CED
32	6	320	CHL	O1D-CGD-O2D-CED
32	6	321	CHL	C2B-C3B-CAB-CBB
32	6	321	CHL	C4B-C3B-CAB-CBB
32	6	321	CHL	C3C-C2C-CMC-OMC
32	6	321	CHL	CBD-CGD-O2D-CED
32	6	321	CHL	O1D-CGD-O2D-CED
34	B	851	LAP	O2-C1-O1-C13
34	B	851	LAP	C15-O4-P9-O5
34	B	851	LAP	C15-O4-P9-O6
35	F	303	QTB	C01-C02-C03-C04
35	F	303	QTB	C09-C02-C03-C04
35	F	303	QTB	C01-C02-C09-C10
35	F	303	QTB	C03-C02-C09-C10
35	F	303	QTB	C02-C09-C10-C11
35	a	302	QTB	C09-C10-C11-C12
35	a	302	QTB	C09-C10-C11-C17
35	7	303	QTB	C01-C02-C09-C10
35	7	303	QTB	C04-C05-C06-C08
35	7	303	QTB	C02-C09-C10-C11
35	7	303	QTB	C09-C10-C11-C12
35	9	304	QTB	C03-C02-C09-C10
35	9	304	QTB	C03-C04-C05-C06
35	9	304	QTB	C04-C05-C06-C08
35	9	304	QTB	C04-C05-C06-O07
36	F	304	LUT	C5-C6-C7-C8
36	F	304	LUT	C7-C8-C9-C10
36	F	304	LUT	C7-C8-C9-C19
36	F	304	LUT	C11-C10-C9-C8
36	F	304	LUT	C20-C13-C14-C15
36	F	304	LUT	C39-C29-C30-C31
36	F	304	LUT	C31-C32-C33-C34
36	F	304	LUT	C31-C32-C33-C40
36	F	304	LUT	C40-C33-C34-C35
36	J	103	LUT	C5-C6-C7-C8
36	J	103	LUT	C11-C10-C9-C19
36	J	103	LUT	C11-C12-C13-C20
36	J	103	LUT	C20-C13-C14-C15
36	J	103	LUT	C27-C28-C29-C30
36	J	103	LUT	C39-C29-C30-C31
36	J	103	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	J	103	LUT	C33-C34-C35-C15
36	a	303	LUT	C5-C6-C7-C8
36	a	303	LUT	C7-C8-C9-C19
36	a	303	LUT	C11-C10-C9-C19
36	a	303	LUT	C11-C12-C13-C20
36	a	303	LUT	C20-C13-C14-C15
36	a	303	LUT	C27-C28-C29-C30
36	a	303	LUT	C28-C29-C30-C31
36	a	303	LUT	C39-C29-C30-C31
36	a	303	LUT	C31-C32-C33-C34
36	a	303	LUT	C31-C32-C33-C40
36	a	303	LUT	C40-C33-C34-C35
36	a	305	LUT	C5-C6-C7-C8
36	a	305	LUT	C7-C8-C9-C19
36	a	305	LUT	C11-C10-C9-C19
36	a	305	LUT	C20-C13-C14-C15
36	a	305	LUT	C21-C26-C27-C28
36	a	305	LUT	C25-C26-C27-C28
36	a	305	LUT	C27-C28-C29-C30
36	a	305	LUT	C27-C28-C29-C39
36	a	305	LUT	C28-C29-C30-C31
36	a	305	LUT	C40-C33-C34-C35
36	3	304	LUT	C11-C10-C9-C19
36	3	304	LUT	C11-C12-C13-C14
36	3	304	LUT	C20-C13-C14-C15
36	3	304	LUT	C39-C29-C30-C31
36	3	304	LUT	C40-C33-C34-C35
36	3	305	LUT	C5-C6-C7-C8
36	3	305	LUT	C7-C8-C9-C19
36	3	305	LUT	C11-C10-C9-C19
36	3	305	LUT	C11-C12-C13-C20
36	3	305	LUT	C20-C13-C14-C15
36	3	305	LUT	C27-C28-C29-C30
36	3	305	LUT	C39-C29-C30-C31
36	3	305	LUT	C40-C33-C34-C35
36	7	305	LUT	C11-C10-C9-C19
36	7	305	LUT	C20-C13-C14-C15
36	7	305	LUT	C39-C29-C30-C31
36	7	305	LUT	C40-C33-C34-C35
36	8	302	LUT	C5-C6-C7-C8
36	8	302	LUT	C7-C8-C9-C19
36	8	302	LUT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
36	8	302	LUT	C11-C12-C13-C14
36	8	302	LUT	C20-C13-C14-C15
36	8	302	LUT	C27-C28-C29-C39
36	8	302	LUT	C39-C29-C30-C31
36	8	302	LUT	C31-C32-C33-C34
36	8	302	LUT	C31-C32-C33-C40
36	8	302	LUT	C40-C33-C34-C35
36	8	303	LUT	C20-C13-C14-C15
36	8	303	LUT	C39-C29-C30-C31
36	8	303	LUT	C40-C33-C34-C35
36	9	302	LUT	C5-C6-C7-C8
36	9	302	LUT	C7-C8-C9-C10
36	9	302	LUT	C11-C10-C9-C19
36	9	302	LUT	C20-C13-C14-C15
36	9	302	LUT	C28-C29-C30-C31
36	9	302	LUT	C39-C29-C30-C31
36	9	302	LUT	C40-C33-C34-C35
36	9	303	LUT	C7-C8-C9-C10
36	9	303	LUT	C11-C10-C9-C19
36	9	303	LUT	C9-C10-C11-C12
36	9	303	LUT	C11-C12-C13-C14
36	9	303	LUT	C20-C13-C14-C15
36	9	303	LUT	C27-C28-C29-C39
36	9	303	LUT	C28-C29-C30-C31
36	9	303	LUT	C40-C33-C34-C35
36	9	305	LUT	C5-C6-C7-C8
36	9	305	LUT	C11-C10-C9-C19
36	9	305	LUT	C12-C13-C14-C15
36	9	305	LUT	C20-C13-C14-C15
36	9	305	LUT	C28-C29-C30-C31
36	9	305	LUT	C39-C29-C30-C31
36	9	305	LUT	C31-C32-C33-C34
36	9	305	LUT	C31-C32-C33-C40
36	9	305	LUT	C40-C33-C34-C35
36	L	304	LUT	C7-C8-C9-C10
36	L	304	LUT	C11-C10-C9-C8
36	L	304	LUT	C9-C10-C11-C12
36	L	304	LUT	C20-C13-C14-C15
36	L	304	LUT	C27-C28-C29-C30
36	L	304	LUT	C39-C29-C30-C31
36	L	304	LUT	C31-C32-C33-C40
36	L	304	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	b	301	LUT	C11-C10-C9-C8
36	b	301	LUT	C11-C10-C9-C19
36	b	301	LUT	C12-C13-C14-C15
36	b	301	LUT	C39-C29-C30-C31
36	b	301	LUT	C31-C32-C33-C34
36	b	301	LUT	C40-C33-C34-C35
36	2	301	LUT	C5-C6-C7-C8
36	2	301	LUT	C11-C10-C9-C19
36	2	301	LUT	C11-C12-C13-C20
36	2	301	LUT	C20-C13-C14-C15
36	2	301	LUT	C27-C28-C29-C30
36	2	301	LUT	C39-C29-C30-C31
36	2	301	LUT	C40-C33-C34-C35
36	4	302	LUT	C5-C6-C7-C8
36	4	302	LUT	C7-C8-C9-C10
36	4	302	LUT	C7-C8-C9-C19
36	4	302	LUT	C11-C10-C9-C19
36	4	302	LUT	C11-C12-C13-C20
36	4	302	LUT	C20-C13-C14-C15
36	4	302	LUT	C27-C28-C29-C30
36	4	302	LUT	C27-C28-C29-C39
36	4	302	LUT	C39-C29-C30-C31
36	4	302	LUT	C40-C33-C34-C35
36	4	303	LUT	C11-C10-C9-C8
36	4	303	LUT	C11-C10-C9-C19
36	4	303	LUT	C11-C12-C13-C20
36	4	303	LUT	C20-C13-C14-C15
36	4	303	LUT	C27-C28-C29-C39
36	4	303	LUT	C28-C29-C30-C31
36	4	303	LUT	C40-C33-C34-C35
36	5	303	LUT	C5-C6-C7-C8
36	5	303	LUT	C7-C8-C9-C19
36	5	303	LUT	C11-C10-C9-C19
36	5	303	LUT	C11-C12-C13-C14
36	5	303	LUT	C20-C13-C14-C15
36	5	303	LUT	C27-C28-C29-C30
36	5	303	LUT	C39-C29-C30-C31
36	5	303	LUT	C40-C33-C34-C35
36	5	304	LUT	C5-C6-C7-C8
36	5	304	LUT	C7-C8-C9-C19
36	5	304	LUT	C11-C10-C9-C8
36	5	304	LUT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
36	5	304	LUT	C9-C10-C11-C12
36	5	304	LUT	C11-C12-C13-C20
36	5	304	LUT	C12-C13-C14-C15
36	5	304	LUT	C27-C28-C29-C30
36	5	304	LUT	C39-C29-C30-C31
36	5	304	LUT	C40-C33-C34-C35
36	6	303	LUT	C5-C6-C7-C8
36	6	303	LUT	C7-C8-C9-C19
36	6	303	LUT	C11-C10-C9-C8
36	6	303	LUT	C11-C10-C9-C19
36	6	303	LUT	C20-C13-C14-C15
36	6	303	LUT	C39-C29-C30-C31
36	6	303	LUT	C31-C32-C33-C40
36	6	303	LUT	C40-C33-C34-C35
36	6	303	LUT	C33-C34-C35-C15
36	6	304	LUT	C5-C6-C7-C8
36	6	304	LUT	C7-C8-C9-C19
36	6	304	LUT	C11-C10-C9-C19
36	6	304	LUT	C11-C12-C13-C14
36	6	304	LUT	C27-C28-C29-C39
36	6	304	LUT	C28-C29-C30-C31
36	6	304	LUT	C40-C33-C34-C35
37	J	104	LMG	C2-C1-O1-C7
37	J	104	LMG	O6-C1-O1-C7
37	a	301	LMG	C2-C1-O1-C7
37	a	301	LMG	O6-C1-O1-C7
39	7	301	3PH	C1-O11-P-O13
39	7	301	3PH	C1-O11-P-O14
40	7	306	XAT	C10-C11-C12-C13
40	7	306	XAT	C11-C12-C13-C14
40	7	306	XAT	C11-C12-C13-C20
41	8	305	DGA	CG1-CG2-CG3-OXT
41	8	305	DGA	OG2-CG2-CG3-OXT
42	4	304	SQD	O5-C5-C6-S
43	5	306	PTY	C11-C8-O7-C6
43	5	306	PTY	C3-O11-P1-O12
43	5	306	PTY	C3-O11-P1-O13
43	5	306	PTY	C3-O11-P1-O14
31	A	819	CLA	O1D-CGD-O2D-CED
31	A	830	CLA	O1D-CGD-O2D-CED
31	A	835	CLA	O1D-CGD-O2D-CED
31	A	836	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	A	842	CLA	O1D-CGD-O2D-CED
31	A	848	CLA	O1D-CGD-O2D-CED
31	B	811	CLA	O1D-CGD-O2D-CED
31	B	813	CLA	O1D-CGD-O2D-CED
31	B	818	CLA	O1D-CGD-O2D-CED
31	B	819	CLA	O1D-CGD-O2D-CED
31	B	843	CLA	O1D-CGD-O2D-CED
31	J	105	CLA	O1D-CGD-O2D-CED
31	K	206	CLA	O1D-CGD-O2D-CED
31	a	309	CLA	O1D-CGD-O2D-CED
31	a	310	CLA	O1D-CGD-O2D-CED
31	a	316	CLA	O1D-CGD-O2D-CED
31	3	308	CLA	O1D-CGD-O2D-CED
31	3	312	CLA	O1D-CGD-O2D-CED
31	3	319	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	O1D-CGD-O2D-CED
31	8	313	CLA	O1D-CGD-O2D-CED
31	8	317	CLA	O1D-CGD-O2D-CED
31	8	321	CLA	O1D-CGD-O2D-CED
31	9	313	CLA	O1D-CGD-O2D-CED
31	9	314	CLA	O1D-CGD-O2D-CED
31	9	315	CLA	O1D-CGD-O2D-CED
31	9	321	CLA	O1D-CGD-O2D-CED
31	L	306	CLA	O1D-CGD-O2D-CED
31	O	203	CLA	O1D-CGD-O2D-CED
31	b	313	CLA	O1D-CGD-O2D-CED
31	2	310	CLA	O1D-CGD-O2D-CED
31	4	314	CLA	O1D-CGD-O2D-CED
31	5	312	CLA	O1D-CGD-O2D-CED
31	5	321	CLA	O1D-CGD-O2D-CED
31	5	323	CLA	O1D-CGD-O2D-CED
31	6	312	CLA	O1D-CGD-O2D-CED
31	6	313	CLA	O1D-CGD-O2D-CED
32	9	320	CHL	O1D-CGD-O2D-CED
32	4	313	CHL	O1D-CGD-O2D-CED
32	5	319	CHL	O1D-CGD-O2D-CED
31	A	823	CLA	O1D-CGD-O2D-CED
31	A	828	CLA	O1D-CGD-O2D-CED
31	A	833	CLA	O1D-CGD-O2D-CED
31	A	844	CLA	O1D-CGD-O2D-CED
31	A	854	CLA	O1D-CGD-O2D-CED
31	A	855	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	A	857	CLA	O1D-CGD-O2D-CED
31	B	822	CLA	O1D-CGD-O2D-CED
31	B	824	CLA	O1D-CGD-O2D-CED
31	B	825	CLA	O1D-CGD-O2D-CED
31	B	827	CLA	O1D-CGD-O2D-CED
31	B	828	CLA	O1D-CGD-O2D-CED
31	B	838	CLA	O1D-CGD-O2D-CED
31	B	839	CLA	O1D-CGD-O2D-CED
31	G	206	CLA	O1D-CGD-O2D-CED
31	H	903	CLA	O1D-CGD-O2D-CED
31	a	312	CLA	O1D-CGD-O2D-CED
31	a	314	CLA	O1D-CGD-O2D-CED
31	a	315	CLA	O1D-CGD-O2D-CED
31	3	307	CLA	O1D-CGD-O2D-CED
31	3	311	CLA	O1D-CGD-O2D-CED
31	3	314	CLA	O1D-CGD-O2D-CED
31	7	309	CLA	O1D-CGD-O2D-CED
31	7	311	CLA	O1D-CGD-O2D-CED
31	8	310	CLA	O1D-CGD-O2D-CED
31	b	303	CLA	O1D-CGD-O2D-CED
31	b	307	CLA	O1D-CGD-O2D-CED
31	2	305	CLA	O1D-CGD-O2D-CED
31	2	306	CLA	O1D-CGD-O2D-CED
31	2	308	CLA	O1D-CGD-O2D-CED
31	2	312	CLA	O1D-CGD-O2D-CED
31	2	313	CLA	O1D-CGD-O2D-CED
31	4	321	CLA	O1D-CGD-O2D-CED
31	5	307	CLA	O1D-CGD-O2D-CED
31	5	308	CLA	O1D-CGD-O2D-CED
31	5	314	CLA	O1D-CGD-O2D-CED
31	5	318	CLA	O1D-CGD-O2D-CED
31	5	320	CLA	O1D-CGD-O2D-CED
31	6	311	CLA	O1D-CGD-O2D-CED
31	6	314	CLA	O1D-CGD-O2D-CED
32	a	318	CHL	O1D-CGD-O2D-CED
32	a	320	CHL	O1D-CGD-O2D-CED
31	A	819	CLA	CBD-CGD-O2D-CED
31	A	823	CLA	CBD-CGD-O2D-CED
31	A	828	CLA	CBD-CGD-O2D-CED
31	A	830	CLA	CBD-CGD-O2D-CED
31	A	841	CLA	CBD-CGD-O2D-CED
31	A	846	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	A	847	CLA	CBD-CGD-O2D-CED
31	A	848	CLA	CBD-CGD-O2D-CED
31	A	854	CLA	CBD-CGD-O2D-CED
31	A	855	CLA	CBD-CGD-O2D-CED
31	A	857	CLA	CBD-CGD-O2D-CED
31	B	818	CLA	CBD-CGD-O2D-CED
31	B	820	CLA	CBD-CGD-O2D-CED
31	B	824	CLA	CBD-CGD-O2D-CED
31	B	825	CLA	CBD-CGD-O2D-CED
31	B	827	CLA	CBD-CGD-O2D-CED
31	B	828	CLA	CBD-CGD-O2D-CED
31	B	835	CLA	CBD-CGD-O2D-CED
31	B	838	CLA	CBD-CGD-O2D-CED
31	B	839	CLA	CBD-CGD-O2D-CED
31	B	843	CLA	CBD-CGD-O2D-CED
31	K	206	CLA	CBD-CGD-O2D-CED
31	a	309	CLA	CBD-CGD-O2D-CED
31	a	310	CLA	CBD-CGD-O2D-CED
31	a	312	CLA	CBD-CGD-O2D-CED
31	a	313	CLA	CBD-CGD-O2D-CED
31	a	315	CLA	CBD-CGD-O2D-CED
31	3	311	CLA	CBD-CGD-O2D-CED
31	3	319	CLA	CBD-CGD-O2D-CED
31	8	308	CLA	CBD-CGD-O2D-CED
31	8	310	CLA	CBD-CGD-O2D-CED
31	8	313	CLA	CBD-CGD-O2D-CED
31	9	313	CLA	CBD-CGD-O2D-CED
31	9	314	CLA	CBD-CGD-O2D-CED
31	9	321	CLA	CBD-CGD-O2D-CED
31	b	313	CLA	CBD-CGD-O2D-CED
31	2	307	CLA	CBD-CGD-O2D-CED
31	2	312	CLA	CBD-CGD-O2D-CED
31	2	313	CLA	CBD-CGD-O2D-CED
31	4	308	CLA	CBD-CGD-O2D-CED
31	4	314	CLA	CBD-CGD-O2D-CED
31	4	320	CLA	CBD-CGD-O2D-CED
31	5	310	CLA	CBD-CGD-O2D-CED
31	5	312	CLA	CBD-CGD-O2D-CED
31	5	318	CLA	CBD-CGD-O2D-CED
31	5	320	CLA	CBD-CGD-O2D-CED
31	6	312	CLA	CBD-CGD-O2D-CED
32	a	318	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	7	318	CHL	CBD-CGD-O2D-CED
32	5	316	CHL	CBD-CGD-O2D-CED
31	A	818	CLA	O1D-CGD-O2D-CED
31	A	827	CLA	O1D-CGD-O2D-CED
31	A	834	CLA	O1D-CGD-O2D-CED
31	A	841	CLA	O1D-CGD-O2D-CED
31	A	845	CLA	O1D-CGD-O2D-CED
31	A	846	CLA	O1D-CGD-O2D-CED
31	B	815	CLA	O1D-CGD-O2D-CED
31	B	820	CLA	O1D-CGD-O2D-CED
31	B	821	CLA	O1D-CGD-O2D-CED
31	B	826	CLA	O1D-CGD-O2D-CED
31	B	834	CLA	O1D-CGD-O2D-CED
31	B	835	CLA	O1D-CGD-O2D-CED
31	F	306	CLA	O1D-CGD-O2D-CED
31	G	204	CLA	O1D-CGD-O2D-CED
31	G	205	CLA	O1D-CGD-O2D-CED
31	a	313	CLA	O1D-CGD-O2D-CED
31	a	322	CLA	O1D-CGD-O2D-CED
31	3	309	CLA	O1D-CGD-O2D-CED
31	7	312	CLA	O1D-CGD-O2D-CED
31	7	316	CLA	O1D-CGD-O2D-CED
31	7	322	CLA	O1D-CGD-O2D-CED
31	8	307	CLA	O1D-CGD-O2D-CED
31	8	308	CLA	O1D-CGD-O2D-CED
31	8	309	CLA	O1D-CGD-O2D-CED
31	9	318	CLA	O1D-CGD-O2D-CED
31	b	304	CLA	O1D-CGD-O2D-CED
31	b	308	CLA	O1D-CGD-O2D-CED
31	2	315	CLA	O1D-CGD-O2D-CED
31	4	306	CLA	O1D-CGD-O2D-CED
31	4	320	CLA	O1D-CGD-O2D-CED
31	5	310	CLA	O1D-CGD-O2D-CED
32	8	319	CHL	O1D-CGD-O2D-CED
32	7	318	CHL	C4C-C3C-CAC-CBC
31	A	817	CLA	O1D-CGD-O2D-CED
31	A	838	CLA	O1D-CGD-O2D-CED
31	A	856	CLA	O1D-CGD-O2D-CED
31	B	829	CLA	O1D-CGD-O2D-CED
31	B	841	CLA	O1D-CGD-O2D-CED
31	F	301	CLA	O1D-CGD-O2D-CED
31	K	205	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	a	319	CLA	O1D-CGD-O2D-CED
31	3	318	CLA	O1D-CGD-O2D-CED
31	7	310	CLA	O1D-CGD-O2D-CED
31	8	320	CLA	O1D-CGD-O2D-CED
31	9	312	CLA	O1D-CGD-O2D-CED
31	L	307	CLA	O1D-CGD-O2D-CED
31	b	302	CLA	O1D-CGD-O2D-CED
31	4	305	CLA	O1D-CGD-O2D-CED
31	4	311	CLA	O1D-CGD-O2D-CED
31	4	312	CLA	O1D-CGD-O2D-CED
31	6	315	CLA	O1D-CGD-O2D-CED
32	7	320	CHL	O1D-CGD-O2D-CED
32	9	322	CHL	O1D-CGD-O2D-CED
34	B	851	LAP	C2-C1-O1-C13
31	A	818	CLA	CBD-CGD-O2D-CED
31	A	821	CLA	CBD-CGD-O2D-CED
31	A	827	CLA	CBD-CGD-O2D-CED
31	A	838	CLA	CBD-CGD-O2D-CED
31	A	844	CLA	CBD-CGD-O2D-CED
31	B	812	CLA	CBD-CGD-O2D-CED
31	B	815	CLA	CBD-CGD-O2D-CED
31	B	821	CLA	CBD-CGD-O2D-CED
31	B	826	CLA	CBD-CGD-O2D-CED
31	B	834	CLA	CBD-CGD-O2D-CED
31	B	840	CLA	CBD-CGD-O2D-CED
31	F	306	CLA	CBD-CGD-O2D-CED
31	3	314	CLA	CBD-CGD-O2D-CED
31	7	309	CLA	CBD-CGD-O2D-CED
32	A	831	CHL	CBD-CGD-O2D-CED
32	3	315	CHL	CBD-CGD-O2D-CED
32	7	319	CHL	CBD-CGD-O2D-CED
32	6	318	CHL	CBD-CGD-O2D-CED
32	7	318	CHL	C2C-C3C-CAC-CBC
28	A	809	LHG	O10-C23-O8-C6
31	A	857	CLA	O1A-CGA-O2A-C1
37	J	101	LMG	O10-C28-O8-C9
43	5	306	PTY	O30-C30-O4-C1
31	A	821	CLA	O1D-CGD-O2D-CED
31	A	847	CLA	O1D-CGD-O2D-CED
31	B	812	CLA	O1D-CGD-O2D-CED
31	B	847	CLA	O1D-CGD-O2D-CED
31	A	826	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	A	832	CLA	O1D-CGD-O2D-CED
31	B	842	CLA	O1D-CGD-O2D-CED
31	B	846	CLA	O1D-CGD-O2D-CED
31	B	842	CLA	CBD-CGD-O2D-CED
31	K	204	CLA	CBD-CGD-O2D-CED
31	B	823	CLA	O1D-CGD-O2D-CED
31	K	204	CLA	O1D-CGD-O2D-CED
28	6	305	LHG	O9-C7-O7-C5
37	J	104	LMG	O9-C10-O7-C8
43	5	306	PTY	O10-C8-O7-C6
31	B	844	CLA	O1D-CGD-O2D-CED
31	A	822	CLA	C3-C5-C6-C7
31	A	830	CLA	C3-C5-C6-C7
31	A	851	CLA	C3-C5-C6-C7
31	A	857	CLA	C3-C5-C6-C7
31	B	820	CLA	C3-C5-C6-C7
31	B	827	CLA	C3-C5-C6-C7
31	B	830	CLA	C3-C5-C6-C7
31	B	832	CLA	C3-C5-C6-C7
31	B	833	CLA	C3-C5-C6-C7
31	a	315	CLA	C3-C5-C6-C7
31	7	314	CLA	C3-C5-C6-C7
31	9	318	CLA	C3-C5-C6-C7
31	6	311	CLA	C3-C5-C6-C7
28	A	809	LHG	C24-C23-O8-C6
31	7	315	CLA	CBA-CGA-O2A-C1
37	J	101	LMG	C29-C28-O8-C9
43	5	306	PTY	C31-C30-O4-C1
28	A	810	LHG	C8-C7-O7-C5
28	7	302	LHG	C8-C7-O7-C5
32	6	318	CHL	O1D-CGD-O2D-CED
31	B	846	CLA	CBD-CGD-O2D-CED
31	B	841	CLA	C4-C3-C5-C6
31	8	311	CLA	C4-C3-C5-C6
31	A	836	CLA	C2-C3-C5-C6
31	B	837	CLA	CBD-CGD-O2D-CED
31	A	857	CLA	C2A-CAA-CBA-CGA
31	B	850	CLA	C2A-CAA-CBA-CGA
31	a	310	CLA	C2A-CAA-CBA-CGA
31	a	316	CLA	C2A-CAA-CBA-CGA
31	b	310	CLA	C2A-CAA-CBA-CGA
32	a	317	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	4	313	CHL	C2A-CAA-CBA-CGA
32	6	320	CHL	C2A-CAA-CBA-CGA
34	B	851	LAP	C5-C6-C7-C8
31	a	313	CLA	C3-C5-C6-C7
31	8	308	CLA	C3-C5-C6-C7
31	9	321	CLA	C3-C5-C6-C7
31	A	841	CLA	CBA-CGA-O2A-C1
31	A	848	CLA	CBA-CGA-O2A-C1
31	a	313	CLA	CBA-CGA-O2A-C1
31	3	309	CLA	CBA-CGA-O2A-C1
31	8	308	CLA	CBA-CGA-O2A-C1
31	A	825	CLA	O1D-CGD-O2D-CED
31	9	316	CLA	O1D-CGD-O2D-CED
31	B	831	CLA	CBD-CGD-O2D-CED
31	B	836	CLA	O1D-CGD-O2D-CED
31	B	840	CLA	O1D-CGD-O2D-CED
31	A	841	CLA	O1A-CGA-O2A-C1
31	A	850	CLA	O1A-CGA-O2A-C1
31	3	309	CLA	O1A-CGA-O2A-C1
31	7	315	CLA	O1A-CGA-O2A-C1
31	8	308	CLA	O1A-CGA-O2A-C1
36	J	103	LUT	C9-C10-C11-C12
36	a	303	LUT	C29-C30-C31-C32
36	3	304	LUT	C29-C30-C31-C32
36	8	302	LUT	C29-C30-C31-C32
36	8	303	LUT	C33-C34-C35-C15
36	9	303	LUT	C29-C30-C31-C32
36	9	305	LUT	C13-C14-C15-C35
36	9	305	LUT	C29-C30-C31-C32
36	L	304	LUT	C29-C30-C31-C32
36	b	301	LUT	C33-C34-C35-C15
36	4	303	LUT	C13-C14-C15-C35
36	4	303	LUT	C29-C30-C31-C32
36	5	303	LUT	C33-C34-C35-C15
36	5	304	LUT	C13-C14-C15-C35
36	6	304	LUT	C29-C30-C31-C32
28	6	305	LHG	C23-C24-C25-C26
31	A	817	CLA	CBD-CGD-O2D-CED
31	A	825	CLA	CBD-CGD-O2D-CED
31	A	837	CLA	CBD-CGD-O2D-CED
31	A	856	CLA	CBD-CGD-O2D-CED
31	B	841	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	5	317	CHL	CBD-CGD-O2D-CED
32	6	319	CHL	CBD-CGD-O2D-CED
28	7	307	LHG	O2-C2-C3-O3
31	A	821	CLA	C3-C5-C6-C7
31	A	836	CLA	C3-C5-C6-C7
31	B	823	CLA	C3-C5-C6-C7
31	A	834	CLA	CBA-CGA-O2A-C1
31	A	845	CLA	CBA-CGA-O2A-C1
31	A	857	CLA	CBA-CGA-O2A-C1
31	B	850	CLA	CBA-CGA-O2A-C1
31	8	311	CLA	CBA-CGA-O2A-C1
41	8	305	DGA	CA2-CA1-OG1-CG1
31	a	313	CLA	O1A-CGA-O2A-C1
33	B	808	DGD	O6E-C5E-C6E-O5E
28	5	305	LHG	C25-C26-C27-C28
31	A	845	CLA	O1A-CGA-O2A-C1
28	8	304	LHG	C23-C24-C25-C26
31	B	841	CLA	C3-C5-C6-C7
31	B	842	CLA	C3-C5-C6-C7
31	A	850	CLA	CBA-CGA-O2A-C1
27	A	807	LMT	O5B-C5B-C6B-O6B
37	G	202	LMG	O6-C5-C6-O5
33	B	808	DGD	C4E-C5E-C6E-O5E
31	A	834	CLA	O1A-CGA-O2A-C1
31	A	848	CLA	O1A-CGA-O2A-C1
31	B	850	CLA	O1A-CGA-O2A-C1
27	5	301	LMT	O5B-C5B-C6B-O6B
31	A	848	CLA	C4-C3-C5-C6
31	A	855	CLA	C4-C3-C5-C6
31	3	314	CLA	C4-C3-C5-C6
31	A	830	CLA	C2-C3-C5-C6
31	A	848	CLA	C2-C3-C5-C6
31	A	855	CLA	C2-C3-C5-C6
31	3	314	CLA	C2-C3-C5-C6
31	8	311	CLA	C2-C3-C5-C6
31	a	322	CLA	C2A-CAA-CBA-CGA
32	8	316	CHL	C2A-CAA-CBA-CGA
41	8	305	DGA	OA1-CA1-OG1-CG1
31	O	203	CLA	CBA-CGA-O2A-C1
31	5	323	CLA	CBA-CGA-O2A-C1
32	4	317	CHL	C2C-C3C-CAC-CBC
31	A	814	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	B	814	CLA	O1D-CGD-O2D-CED
31	8	311	CLA	O1A-CGA-O2A-C1
31	A	843	CLA	O1D-CGD-O2D-CED
31	A	820	CLA	O1D-CGD-O2D-CED
31	A	850	CLA	O1D-CGD-O2D-CED
28	A	809	LHG	C1-C2-C3-O3
27	A	807	LMT	C4B-C5B-C6B-O6B
31	O	203	CLA	O1A-CGA-O2A-C1
31	5	323	CLA	O1A-CGA-O2A-C1
34	B	851	LAP	C16-C17-N8-C19
31	B	849	CLA	O1D-CGD-O2D-CED
28	5	305	LHG	C24-C23-O8-C6
31	A	829	CLA	CBA-CGA-O2A-C1
31	5	315	CLA	CBA-CGA-O2A-C1
32	8	316	CHL	CBA-CGA-O2A-C1
27	5	301	LMT	O5'-C5'-C6'-O6'
31	A	832	CLA	CBD-CGD-O2D-CED
31	4	316	CLA	CBD-CGD-O2D-CED
37	G	202	LMG	C4-C5-C6-O5
36	F	304	LUT	C29-C30-C31-C32
36	a	305	LUT	C13-C14-C15-C35
36	3	304	LUT	C33-C34-C35-C15
36	7	305	LUT	C29-C30-C31-C32
36	8	302	LUT	C33-C34-C35-C15
36	8	303	LUT	C29-C30-C31-C32
36	9	302	LUT	C13-C14-C15-C35
36	4	303	LUT	C9-C10-C11-C12
36	6	304	LUT	C13-C14-C15-C35
27	9	306	LMT	O5'-C5'-C6'-O6'
31	A	826	CLA	C13-C15-C16-C17
31	7	315	CLA	C5-C6-C7-C8
31	5	315	CLA	C10-C11-C12-C13
28	A	809	LHG	O2-C2-C3-O3
28	7	302	LHG	O2-C2-C3-O3
31	B	822	CLA	C2C-C3C-CAC-CBC
32	8	316	CHL	O1A-CGA-O2A-C1
31	B	841	CLA	C2-C3-C5-C6
31	B	815	CLA	C6-C7-C8-C9
31	B	819	CLA	C14-C13-C15-C16
31	B	842	CLA	C11-C12-C13-C14
31	L	305	CLA	C6-C7-C8-C9
32	7	318	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	7	318	CHL	C11-C10-C8-C9
32	7	320	CHL	C11-C10-C8-C9
32	6	309	CHL	C14-C13-C15-C16
31	A	816	CLA	O1D-CGD-O2D-CED
32	7	318	CHL	O1D-CGD-O2D-CED
31	B	815	CLA	C5-C6-C7-C8
31	4	312	CLA	C2A-CAA-CBA-CGA
31	6	306	CLA	C2A-CAA-CBA-CGA
26	B	803	BCR	C7-C8-C9-C34
26	B	803	BCR	C37-C22-C23-C24
26	K	202	BCR	C37-C22-C23-C24
26	3	301	BCR	C7-C8-C9-C34
26	5	302	BCR	C37-C22-C23-C24
36	F	304	LUT	C11-C12-C13-C20
36	a	305	LUT	C31-C32-C33-C40
36	3	304	LUT	C7-C8-C9-C19
36	3	304	LUT	C27-C28-C29-C39
36	7	305	LUT	C7-C8-C9-C19
36	8	303	LUT	C7-C8-C9-C19
36	8	303	LUT	C11-C12-C13-C20
36	8	303	LUT	C27-C28-C29-C39
36	9	302	LUT	C7-C8-C9-C19
36	9	303	LUT	C31-C32-C33-C40
36	9	305	LUT	C7-C8-C9-C19
36	9	305	LUT	C27-C28-C29-C39
36	L	304	LUT	C27-C28-C29-C39
36	b	301	LUT	C7-C8-C9-C19
36	b	301	LUT	C27-C28-C29-C39
36	4	303	LUT	C7-C8-C9-C19
36	4	303	LUT	C31-C32-C33-C40
36	6	303	LUT	C11-C12-C13-C20
26	K	202	BCR	C21-C22-C23-C24
26	5	302	BCR	C7-C8-C9-C10
35	7	303	QTB	C03-C02-C09-C10
36	F	304	LUT	C27-C28-C29-C30
36	J	103	LUT	C31-C32-C33-C34
36	a	305	LUT	C11-C12-C13-C14
36	3	304	LUT	C31-C32-C33-C34
36	3	305	LUT	C31-C32-C33-C34
36	7	305	LUT	C11-C12-C13-C14
36	8	303	LUT	C31-C32-C33-C34
36	9	302	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	9	302	LUT	C27-C28-C29-C30
36	9	302	LUT	C31-C32-C33-C34
36	9	305	LUT	C11-C12-C13-C14
36	b	301	LUT	C11-C12-C13-C14
36	5	303	LUT	C31-C32-C33-C34
36	5	304	LUT	C31-C32-C33-C34
36	6	303	LUT	C31-C32-C33-C34
28	5	305	LHG	C8-C7-O7-C5
37	J	104	LMG	C11-C10-O7-C8
28	a	306	LHG	C32-C33-C34-C35
28	5	305	LHG	O10-C23-O8-C6
31	A	824	CLA	C8-C10-C11-C12
31	A	828	CLA	C15-C16-C17-C18
28	5	305	LHG	C10-C11-C12-C13
31	B	833	CLA	O1D-CGD-O2D-CED
31	B	815	CLA	C3-C5-C6-C7
31	B	839	CLA	C3-C5-C6-C7
31	a	312	CLA	C3-C5-C6-C7
31	A	827	CLA	C5-C6-C7-C8
31	B	814	CLA	C15-C16-C17-C18
31	B	820	CLA	C5-C6-C7-C8
31	B	840	CLA	C15-C16-C17-C18
31	a	319	CLA	C10-C11-C12-C13
31	3	307	CLA	C8-C10-C11-C12
31	8	310	CLA	C13-C15-C16-C17
32	a	317	CHL	C10-C11-C12-C13
32	7	320	CHL	C10-C11-C12-C13
28	A	809	LHG	C23-C24-C25-C26
31	A	829	CLA	C2C-C3C-CAC-CBC
32	5	317	CHL	C2C-C3C-CAC-CBC
24	A	801	PQN	C25-C26-C27-C28
31	A	836	CLA	C10-C11-C12-C13
31	B	832	CLA	C10-C11-C12-C13
31	B	833	CLA	C5-C6-C7-C8
31	B	840	CLA	C8-C10-C11-C12
31	3	307	CLA	C10-C11-C12-C13
31	3	311	CLA	C5-C6-C7-C8
31	7	314	CLA	C5-C6-C7-C8
31	9	318	CLA	C15-C16-C17-C18
31	L	305	CLA	C5-C6-C7-C8
27	5	301	LMT	C4B-C5B-C6B-O6B
28	5	305	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	a	306	LHG	C7-C8-C9-C10
37	J	101	LMG	C10-C11-C12-C13
37	a	301	LMG	C10-C11-C12-C13
37	a	301	LMG	C28-C29-C30-C31
42	4	304	SQD	C7-C8-C9-C10
32	a	318	CHL	C2C-C3C-CAC-CBC
31	A	835	CLA	C5-C6-C7-C8
31	a	312	CLA	C13-C15-C16-C17
32	a	317	CHL	C8-C10-C11-C12
31	8	312	CLA	CBA-CGA-O2A-C1
31	B	842	CLA	C10-C11-C12-C13
31	B	847	CLA	C5-C6-C7-C8
31	3	307	CLA	C13-C15-C16-C17
34	B	851	LAP	C16-C17-N8-C20
28	7	307	LHG	C23-C24-C25-C26
37	J	101	LMG	C28-C29-C30-C31
31	A	853	CLA	C11-C10-C8-C7
31	A	857	CLA	C6-C7-C8-C10
31	B	815	CLA	C11-C10-C8-C7
31	a	312	CLA	C6-C7-C8-C10
31	5	315	CLA	O1A-CGA-O2A-C1
26	6	302	BCR	C9-C10-C11-C12
36	a	305	LUT	C9-C10-C11-C12
36	a	305	LUT	C29-C30-C31-C32
36	a	305	LUT	C33-C34-C35-C15
36	b	301	LUT	C29-C30-C31-C32
36	2	301	LUT	C29-C30-C31-C32
36	5	303	LUT	C29-C30-C31-C32
36	5	304	LUT	C29-C30-C31-C32
36	6	304	LUT	C33-C34-C35-C15
31	A	821	CLA	C2A-CAA-CBA-CGA
31	9	319	CLA	C2A-CAA-CBA-CGA
31	4	321	CLA	C2A-CAA-CBA-CGA
32	b	309	CHL	C2A-CAA-CBA-CGA
31	B	837	CLA	O1D-CGD-O2D-CED
32	8	316	CHL	O1D-CGD-O2D-CED
31	a	315	CLA	C5-C6-C7-C8
31	8	313	CLA	CBA-CGA-O2A-C1
31	A	829	CLA	O1A-CGA-O2A-C1
28	B	807	LHG	C23-C24-C25-C26
26	6	302	BCR	C10-C11-C12-C13
32	7	320	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	B	824	CLA	CBA-CGA-O2A-C1
31	A	849	CLA	O1D-CGD-O2D-CED
31	B	819	CLA	C10-C11-C12-C13
31	B	824	CLA	C5-C6-C7-C8
31	B	830	CLA	C8-C10-C11-C12
31	B	832	CLA	C15-C16-C17-C18
31	3	309	CLA	C5-C6-C7-C8
31	B	829	CLA	CBD-CGD-O2D-CED
31	8	312	CLA	O1A-CGA-O2A-C1
31	A	837	CLA	C5-C6-C7-C8
31	A	837	CLA	C15-C16-C17-C18
31	A	842	CLA	C5-C6-C7-C8
31	B	825	CLA	C8-C10-C11-C12
31	a	319	CLA	C8-C10-C11-C12
31	9	314	CLA	C10-C11-C12-C13
31	5	315	CLA	C8-C10-C11-C12
28	7	302	LHG	C3-O3-P-O6
28	5	305	LHG	C4-O6-P-O3
34	B	851	LAP	C16-O6-P9-O4
28	B	807	LHG	C24-C23-O8-C6
39	7	301	3PH	C31-C32-C33-C34
28	5	305	LHG	O9-C7-O7-C5
32	6	320	CHL	C2C-C3C-CAC-CBC
31	A	814	CLA	C2A-CAA-CBA-CGA
31	A	824	CLA	C2A-CAA-CBA-CGA
31	B	826	CLA	C2A-CAA-CBA-CGA
31	9	321	CLA	C2A-CAA-CBA-CGA
31	b	313	CLA	C2A-CAA-CBA-CGA
31	2	312	CLA	C2A-CAA-CBA-CGA
37	J	104	LMG	C4-C5-C6-O5
31	A	830	CLA	CBA-CGA-O2A-C1
31	A	851	CLA	CBA-CGA-O2A-C1
32	6	321	CHL	C2C-C3C-CAC-CBC
31	A	823	CLA	C5-C6-C7-C8
31	B	827	CLA	C8-C10-C11-C12
35	F	303	QTB	C02-C03-C04-C05
35	a	302	QTB	C02-C03-C04-C05
35	9	304	QTB	C02-C03-C04-C05
36	3	305	LUT	C29-C30-C31-C32
36	7	305	LUT	C9-C10-C11-C12
36	9	302	LUT	C29-C30-C31-C32
36	b	301	LUT	C13-C14-C15-C35

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Mol	Chain	Res	Type	Atoms
36	6	303	LUT	C29-C30-C31-C32
37	G	202	LMG	C11-C10-O7-C8
26	A	804	BCR	C20-C21-C22-C37
26	B	803	BCR	C20-C21-C22-C37
26	B	805	BCR	C20-C21-C22-C37
26	3	301	BCR	C16-C17-C18-C36
36	a	305	LUT	C39-C29-C30-C31
36	8	303	LUT	C11-C10-C9-C19
36	9	303	LUT	C39-C29-C30-C31
36	4	303	LUT	C39-C29-C30-C31
36	6	304	LUT	C20-C13-C14-C15
36	6	304	LUT	C39-C29-C30-C31
27	A	808	LMT	C2-C3-C4-C5
28	A	810	LHG	C24-C25-C26-C27
33	7	308	DGD	CAB-CBB-CCB-CDB
33	7	308	DGD	CCB-CDB-CEB-CFB
31	B	839	CLA	C11-C12-C13-C14
28	8	304	LHG	C28-C29-C30-C31
28	5	305	LHG	C26-C27-C28-C29
32	4	317	CHL	C4C-C3C-CAC-CBC
37	J	101	LMG	C22-C23-C24-C25
31	B	836	CLA	CBD-CGD-O2D-CED
28	7	302	LHG	C11-C10-C9-C8
28	7	302	LHG	C27-C28-C29-C30
28	5	305	LHG	C12-C13-C14-C15
37	G	202	LMG	C16-C17-C18-C19
33	B	808	DGD	C7B-C8B-C9B-CAB
37	G	202	LMG	C17-C18-C19-C20
31	A	845	CLA	C5-C6-C7-C8
31	8	308	CLA	C13-C15-C16-C17
26	A	805	BCR	C20-C21-C22-C23
26	3	302	BCR	C12-C13-C14-C15
26	3	303	BCR	C11-C10-C9-C8
26	8	301	BCR	C20-C21-C22-C23
26	L	302	BCR	C11-C10-C9-C8
26	6	302	BCR	C12-C13-C14-C15
36	F	304	LUT	C28-C29-C30-C31
36	J	103	LUT	C11-C10-C9-C8
36	a	305	LUT	C11-C10-C9-C8
36	a	305	LUT	C32-C33-C34-C35
36	3	304	LUT	C28-C29-C30-C31
36	3	305	LUT	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	7	305	LUT	C28-C29-C30-C31
36	8	302	LUT	C28-C29-C30-C31
36	8	303	LUT	C11-C10-C9-C8
36	9	302	LUT	C12-C13-C14-C15
36	9	303	LUT	C11-C10-C9-C8
36	9	305	LUT	C11-C10-C9-C8
36	9	305	LUT	C32-C33-C34-C35
36	2	301	LUT	C11-C10-C9-C8
36	5	303	LUT	C12-C13-C14-C15
36	6	303	LUT	C12-C13-C14-C15
36	6	304	LUT	C12-C13-C14-C15
31	G	204	CLA	CBA-CGA-O2A-C1
31	4	321	CLA	CBA-CGA-O2A-C1
27	A	808	LMT	C3-C4-C5-C6
28	A	809	LHG	C27-C28-C29-C30
28	A	811	LHG	C34-C35-C36-C37
32	7	318	CHL	C8-C10-C11-C12
30	A	813	CL0	C16-C17-C18-C19
31	A	851	CLA	O1D-CGD-O2D-CED
31	3	310	CLA	C4-C3-C5-C6
28	7	307	LHG	C26-C27-C28-C29
31	A	814	CLA	C11-C10-C8-C9
31	A	814	CLA	C14-C13-C15-C16
31	B	815	CLA	C11-C12-C13-C14
31	a	312	CLA	C6-C7-C8-C9
31	5	318	CLA	C11-C10-C8-C9
28	6	301	LHG	C23-C24-C25-C26
28	7	307	LHG	C27-C28-C29-C30
37	J	101	LMG	C29-C30-C31-C32
41	8	305	DGA	CA6-CA7-CA8-CA9
31	9	313	CLA	C2A-CAA-CBA-CGA
31	A	830	CLA	O1A-CGA-O2A-C1
31	A	851	CLA	O1A-CGA-O2A-C1
31	B	824	CLA	O1A-CGA-O2A-C1
26	3	301	BCR	C37-C22-C23-C24
26	6	302	BCR	C11-C12-C13-C35
36	J	103	LUT	C7-C8-C9-C19
36	9	303	LUT	C7-C8-C9-C19
36	L	304	LUT	C11-C12-C13-C20
36	2	301	LUT	C7-C8-C9-C19
36	6	303	LUT	C27-C28-C29-C39
36	6	304	LUT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
28	A	810	LHG	C28-C29-C30-C31
28	8	304	LHG	C32-C33-C34-C35
33	B	808	DGD	C7A-C8A-C9A-CAA
37	J	101	LMG	C19-C20-C21-C22
28	A	810	LHG	O1-C1-C2-C3
28	6	301	LHG	O1-C1-C2-C3
28	6	305	LHG	O1-C1-C2-C3
26	3	302	BCR	C7-C8-C9-C10
36	J	103	LUT	C7-C8-C9-C10
36	7	305	LUT	C27-C28-C29-C30
36	7	305	LUT	C31-C32-C33-C34
36	8	302	LUT	C7-C8-C9-C10
36	2	301	LUT	C31-C32-C33-C34
36	4	302	LUT	C31-C32-C33-C34
36	4	303	LUT	C11-C12-C13-C14
36	6	303	LUT	C27-C28-C29-C30
31	B	817	CLA	C3-C5-C6-C7
32	7	317	CHL	C3-C5-C6-C7
31	B	813	CLA	C5-C6-C7-C8
31	B	822	CLA	C8-C10-C11-C12
28	B	807	LHG	C24-C25-C26-C27
37	a	301	LMG	C31-C32-C33-C34
28	5	305	LHG	C7-C8-C9-C10
28	5	305	LHG	C23-C24-C25-C26
27	5	301	LMT	C2-C3-C4-C5
28	A	809	LHG	C11-C10-C9-C8
28	A	810	LHG	C32-C33-C34-C35
28	a	306	LHG	C24-C25-C26-C27
37	a	301	LMG	C36-C37-C38-C39
31	A	855	CLA	C4B-C3B-CAB-CBB
31	B	847	CLA	C4B-C3B-CAB-CBB
31	6	307	CLA	C4B-C3B-CAB-CBB
31	B	823	CLA	C6-C7-C8-C9
31	B	823	CLA	C6-C7-C8-C10
31	A	837	CLA	C8-C10-C11-C12
28	a	306	LHG	C26-C27-C28-C29
28	7	307	LHG	C28-C29-C30-C31
28	8	304	LHG	C27-C28-C29-C30
28	5	305	LHG	C9-C10-C11-C12
37	J	101	LMG	C11-C12-C13-C14
37	a	301	LMG	C33-C34-C35-C36
28	a	306	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
28	8	304	LHG	C11-C12-C13-C14
42	4	304	SQD	C9-C10-C11-C12
34	B	851	LAP	C4-C5-C6-C7
31	3	314	CLA	CBA-CGA-O2A-C1
31	7	314	CLA	CBA-CGA-O2A-C1
28	a	306	LHG	C27-C28-C29-C30
31	B	817	CLA	O1D-CGD-O2D-CED
31	L	305	CLA	O1D-CGD-O2D-CED
31	A	819	CLA	C3A-C2A-CAA-CBA
31	A	822	CLA	C3A-C2A-CAA-CBA
31	A	824	CLA	C3A-C2A-CAA-CBA
31	A	846	CLA	C3A-C2A-CAA-CBA
31	A	855	CLA	C3A-C2A-CAA-CBA
31	B	826	CLA	C3A-C2A-CAA-CBA
31	a	310	CLA	C3A-C2A-CAA-CBA
31	3	309	CLA	C3A-C2A-CAA-CBA
31	9	319	CLA	C3A-C2A-CAA-CBA
31	9	321	CLA	C3A-C2A-CAA-CBA
31	L	307	CLA	C3A-C2A-CAA-CBA
31	b	302	CLA	C3A-C2A-CAA-CBA
31	4	305	CLA	C3A-C2A-CAA-CBA
31	4	311	CLA	C3A-C2A-CAA-CBA
37	a	301	LMG	O6-C5-C6-O5
36	8	302	LUT	C13-C14-C15-C35
27	9	306	LMT	C2-C3-C4-C5
27	9	306	LMT	C7-C8-C9-C10
28	A	811	LHG	C16-C17-C18-C19
28	7	302	LHG	C17-C18-C19-C20
32	9	320	CHL	C2C-C3C-CAC-CBC
28	a	306	LHG	C31-C32-C33-C34
28	8	304	LHG	C15-C16-C17-C18
28	8	304	LHG	C34-C35-C36-C37
31	B	844	CLA	CBD-CGD-O2D-CED
43	5	306	PTY	C31-C32-C33-C34
26	6	302	BCR	C14-C15-C16-C17
31	A	855	CLA	C3-C5-C6-C7
37	G	202	LMG	C11-C12-C13-C14
31	B	825	CLA	C4-C3-C5-C6
31	4	307	CLA	C4-C3-C5-C6
31	B	825	CLA	C2-C3-C5-C6
31	B	836	CLA	C2-C3-C5-C6
31	B	840	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	3	310	CLA	C2-C3-C5-C6
31	4	307	CLA	C2-C3-C5-C6
28	a	306	LHG	C29-C30-C31-C32
31	A	856	CLA	C2A-CAA-CBA-CGA
28	A	810	LHG	O1-C1-C2-O2
28	7	302	LHG	C26-C27-C28-C29
30	A	813	CL0	C16-C17-C18-C20
31	B	822	CLA	C4C-C3C-CAC-CBC
33	B	808	DGD	C2B-C3B-C4B-C5B
31	A	855	CLA	C2B-C3B-CAB-CBB
31	B	847	CLA	C2B-C3B-CAB-CBB
31	F	301	CLA	C2B-C3B-CAB-CBB
31	6	307	CLA	C2B-C3B-CAB-CBB
31	6	314	CLA	C2B-C3B-CAB-CBB
31	3	313	CLA	C8-C10-C11-C12
31	3	314	CLA	O1A-CGA-O2A-C1
33	B	808	DGD	C4A-C5A-C6A-C7A
31	3	309	CLA	C2-C1-O2A-CGA
31	A	853	CLA	C15-C16-C17-C18
31	B	830	CLA	C5-C6-C7-C8
35	F	303	QTB	C03-C04-C05-C06
35	a	302	QTB	C03-C04-C05-C06
35	7	303	QTB	C03-C04-C05-C06
31	4	321	CLA	O1A-CGA-O2A-C1
34	B	851	LAP	C16-C17-N8-C18
26	A	805	BCR	C23-C24-C25-C26
26	A	805	BCR	C23-C24-C25-C30
26	B	805	BCR	C23-C24-C25-C26
26	G	203	BCR	C5-C6-C7-C8
26	G	203	BCR	C23-C24-C25-C26
26	G	203	BCR	C23-C24-C25-C30
26	I	801	BCR	C5-C6-C7-C8
26	J	102	BCR	C23-C24-C25-C26
26	J	102	BCR	C23-C24-C25-C30
26	K	203	BCR	C23-C24-C25-C26
26	M	101	BCR	C23-C24-C25-C26
26	3	301	BCR	C5-C6-C7-C8
26	3	301	BCR	C23-C24-C25-C26
26	3	302	BCR	C5-C6-C7-C8
26	7	304	BCR	C23-C24-C25-C26
26	7	304	BCR	C23-C24-C25-C30
26	8	301	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	8	301	BCR	C23-C24-C25-C26
26	L	302	BCR	C5-C6-C7-C8
26	L	303	BCR	C23-C24-C25-C26
26	2	302	BCR	C1-C6-C7-C8
26	2	302	BCR	C5-C6-C7-C8
26	2	302	BCR	C23-C24-C25-C26
26	5	302	BCR	C23-C24-C25-C26
26	6	302	BCR	C5-C6-C7-C8
26	6	302	BCR	C23-C24-C25-C26
26	6	302	BCR	C23-C24-C25-C30
32	5	316	CHL	C3-C5-C6-C7
36	3	304	LUT	C1-C6-C7-C8
36	7	305	LUT	C1-C6-C7-C8
36	8	303	LUT	C5-C6-C7-C8
36	9	303	LUT	C1-C6-C7-C8
36	9	303	LUT	C5-C6-C7-C8
36	b	301	LUT	C5-C6-C7-C8
36	4	303	LUT	C1-C6-C7-C8
38	a	304	AXT	C25-C26-C27-C28
28	a	306	LHG	C34-C35-C36-C37
28	7	302	LHG	C32-C33-C34-C35
31	B	829	CLA	CBA-CGA-O2A-C1
31	b	313	CLA	CBA-CGA-O2A-C1
31	2	306	CLA	CBA-CGA-O2A-C1
31	A	821	CLA	C5-C6-C7-C8
31	B	848	CLA	C15-C16-C17-C18
31	4	309	CLA	C5-C6-C7-C8
32	7	318	CHL	C15-C16-C17-C18
28	A	811	LHG	C8-C7-O7-C5
37	J	101	LMG	C11-C10-O7-C8
31	G	204	CLA	O1A-CGA-O2A-C1
33	7	308	DGD	O1A-C1A-O1G-C1G
31	4	307	CLA	C11-C10-C8-C9
28	A	810	LHG	C23-C24-C25-C26
28	A	811	LHG	C11-C10-C9-C8
28	7	302	LHG	C25-C26-C27-C28
28	7	307	LHG	C29-C30-C31-C32
31	A	842	CLA	C13-C15-C16-C17
32	7	318	CHL	C13-C15-C16-C17
27	9	306	LMT	C3-C4-C5-C6
28	7	302	LHG	C28-C29-C30-C31
28	7	302	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	A	827	CLA	C4-C3-C5-C6
31	B	833	CLA	C4-C3-C5-C6
31	B	840	CLA	C4-C3-C5-C6
31	7	311	CLA	C4-C3-C5-C6
31	A	814	CLA	C11-C10-C8-C7
31	A	814	CLA	C12-C13-C15-C16
31	B	815	CLA	C11-C12-C13-C15
31	B	833	CLA	C2-C3-C5-C6
31	7	311	CLA	C2-C3-C5-C6
31	5	318	CLA	C11-C10-C8-C7
32	7	318	CHL	C12-C13-C15-C16
32	7	324	CHL	C11-C12-C13-C15
31	7	315	CLA	C2-C3-C5-C6
31	B	829	CLA	O1A-CGA-O2A-C1
31	7	314	CLA	O1A-CGA-O2A-C1
33	B	808	DGD	O1A-C1A-O1G-C1G
31	8	310	CLA	C8-C10-C11-C12
36	5	304	LUT	C33-C34-C35-C15
28	7	307	LHG	O9-C7-O7-C5
33	B	808	DGD	O1B-C1B-O2G-C2G
28	A	809	LHG	C7-C8-C9-C10
28	A	811	LHG	C12-C13-C14-C15
31	L	307	CLA	C2A-CAA-CBA-CGA
31	2	315	CLA	C2A-CAA-CBA-CGA
31	B	850	CLA	O1D-CGD-O2D-CED
31	9	311	CLA	C5-C6-C7-C8
33	7	308	DGD	C9B-CAB-CBB-CCB
41	8	305	DGA	CB1-CB2-CB3-CB4
37	G	202	LMG	C15-C16-C17-C18
37	a	301	LMG	C32-C33-C34-C35
27	A	807	LMT	C5-C6-C7-C8
26	A	805	BCR	C22-C23-C24-C25
37	G	202	LMG	O10-C28-O8-C9
31	B	837	CLA	C6-C7-C8-C10
28	B	807	LHG	C8-C7-O7-C5
39	7	301	3PH	C22-C21-O21-C2
41	8	305	DGA	CB2-CB1-OG2-CG2
37	J	104	LMG	O6-C5-C6-O5
26	L	303	BCR	C18-C19-C20-C21
28	7	307	LHG	C24-C25-C26-C27
31	A	818	CLA	C5-C6-C7-C8
33	7	308	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
39	7	301	3PH	O22-C21-O21-C2
41	8	305	DGA	OB1-CB1-OG2-CG2
28	A	811	LHG	C29-C30-C31-C32
31	B	815	CLA	C10-C11-C12-C13
28	7	302	LHG	O7-C5-C6-O8
33	B	808	DGD	O2G-C2G-C3G-O3G
43	5	306	PTY	C32-C33-C34-C35
28	A	810	LHG	C27-C28-C29-C30
31	B	836	CLA	C4-C3-C5-C6
31	A	827	CLA	C2-C3-C5-C6
28	7	307	LHG	C11-C10-C9-C8
31	A	837	CLA	C11-C10-C8-C9
31	A	853	CLA	C11-C10-C8-C9
31	A	857	CLA	C6-C7-C8-C9
31	B	819	CLA	C11-C12-C13-C14
31	B	824	CLA	C11-C10-C8-C9
31	7	312	CLA	C11-C10-C8-C9
32	7	324	CHL	C11-C12-C13-C14
31	A	853	CLA	O1D-CGD-O2D-CED
31	4	316	CLA	O1D-CGD-O2D-CED
31	A	822	CLA	C2A-CAA-CBA-CGA
32	6	319	CHL	C2A-CAA-CBA-CGA
31	4	309	CLA	CBA-CGA-O2A-C1
26	K	202	BCR	C7-C8-C9-C34
26	L	302	BCR	C37-C22-C23-C24
36	9	302	LUT	C31-C32-C33-C40
36	9	303	LUT	C11-C12-C13-C20
31	3	310	CLA	C2C-C3C-CAC-CBC
37	a	301	LMG	C11-C12-C13-C14
36	4	303	LUT	C7-C8-C9-C10
36	5	304	LUT	C11-C12-C13-C14
36	6	304	LUT	C27-C28-C29-C30
31	b	313	CLA	O1A-CGA-O2A-C1
31	2	306	CLA	O1A-CGA-O2A-C1
31	A	833	CLA	C1A-C2A-CAA-CBA
31	A	837	CLA	C1A-C2A-CAA-CBA
31	A	843	CLA	C1A-C2A-CAA-CBA
31	A	848	CLA	C1A-C2A-CAA-CBA
31	B	835	CLA	C1A-C2A-CAA-CBA
31	a	309	CLA	C1A-C2A-CAA-CBA
31	a	310	CLA	C1A-C2A-CAA-CBA
31	3	307	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	3	314	CLA	C1A-C2A-CAA-CBA
31	7	315	CLA	C1A-C2A-CAA-CBA
31	7	322	CLA	C1A-C2A-CAA-CBA
31	8	314	CLA	C1A-C2A-CAA-CBA
31	9	321	CLA	C1A-C2A-CAA-CBA
31	L	307	CLA	C1A-C2A-CAA-CBA
31	O	203	CLA	C1A-C2A-CAA-CBA
31	b	302	CLA	C1A-C2A-CAA-CBA
31	2	304	CLA	C1A-C2A-CAA-CBA
31	2	307	CLA	C1A-C2A-CAA-CBA
31	4	308	CLA	C1A-C2A-CAA-CBA
31	4	321	CLA	C1A-C2A-CAA-CBA
31	5	307	CLA	C1A-C2A-CAA-CBA
31	6	306	CLA	C1A-C2A-CAA-CBA
31	6	307	CLA	C1A-C2A-CAA-CBA
32	A	831	CHL	C1A-C2A-CAA-CBA
32	8	316	CHL	C1A-C2A-CAA-CBA
32	5	316	CHL	C1A-C2A-CAA-CBA
32	5	322	CHL	C1A-C2A-CAA-CBA
31	A	841	CLA	C16-C17-C18-C20
31	B	827	CLA	C11-C12-C13-C15
31	B	837	CLA	C6-C7-C8-C9
31	B	839	CLA	C11-C12-C13-C15
31	a	311	CLA	C11-C12-C13-C14
37	G	202	LMG	O9-C10-O7-C8
32	5	317	CHL	C4C-C3C-CAC-CBC
37	G	202	LMG	C31-C32-C33-C34
37	a	301	LMG	C14-C15-C16-C17
31	A	837	CLA	C10-C11-C12-C13
32	8	316	CHL	C10-C11-C12-C13
28	A	809	LHG	C3-O3-P-O6
28	a	306	LHG	C4-O6-P-O3
28	7	307	LHG	C4-O6-P-O3
28	6	301	LHG	C4-O6-P-O3
27	9	306	LMT	C4'-C5'-C6'-O6'
32	a	318	CHL	C4C-C3C-CAC-CBC
31	A	816	CLA	C13-C15-C16-C17
31	A	853	CLA	C8-C10-C11-C12
31	A	855	CLA	C5-C6-C7-C8
31	A	855	CLA	C8-C10-C11-C12
43	5	306	PTY	O14-C5-C6-C1
32	K	201	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	a	306	LHG	C23-C24-C25-C26
31	6	312	CLA	C16-C17-C18-C20
28	8	304	LHG	C16-C17-C18-C19
31	b	313	CLA	C2C-C3C-CAC-CBC
32	A	840	CHL	C3-C5-C6-C7
33	B	808	DGD	C3A-C4A-C5A-C6A
32	a	317	CHL	CBA-CGA-O2A-C1
32	7	320	CHL	CBA-CGA-O2A-C1
28	7	307	LHG	C1-C2-C3-O3
31	A	823	CLA	C4-C3-C5-C6
31	3	309	CLA	C4-C3-C5-C6
31	3	309	CLA	C2-C3-C5-C6
31	a	319	CLA	C13-C15-C16-C17
31	9	317	CLA	C2-C1-O2A-CGA
37	J	101	LMG	C18-C19-C20-C21
31	B	831	CLA	O1D-CGD-O2D-CED
31	B	832	CLA	O1D-CGD-O2D-CED
28	A	809	LHG	C18-C19-C20-C21
28	8	304	LHG	C4-C5-C6-O8
39	7	301	3PH	C1-C2-C3-O31
31	B	816	CLA	O1D-CGD-O2D-CED
31	A	857	CLA	C5-C6-C7-C8
31	A	852	CLA	O1D-CGD-O2D-CED
34	B	851	LAP	C6-C7-C8-C9
31	A	849	CLA	CBA-CGA-O2A-C1
28	A	809	LHG	O1-C1-C2-O2
27	A	807	LMT	C9-C10-C11-C12
37	G	202	LMG	C37-C38-C39-C40
37	J	101	LMG	C16-C17-C18-C19
33	7	308	DGD	C1A-C2A-C3A-C4A
28	7	307	LHG	C8-C7-O7-C5
26	B	804	BCR	C20-C21-C22-C37
26	F	302	BCR	C35-C13-C14-C15
26	I	801	BCR	C20-C21-C22-C37
31	8	313	CLA	O1A-CGA-O2A-C1
31	A	834	CLA	C4-C3-C5-C6
31	A	853	CLA	C4-C3-C5-C6
31	8	315	CLA	C4-C3-C5-C6
31	L	305	CLA	C4-C3-C5-C6
28	5	305	LHG	C27-C28-C29-C30
31	A	823	CLA	C2-C3-C5-C6
31	A	834	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	6	305	LHG	C7-C8-C9-C10
39	7	301	3PH	C21-C22-C23-C24
31	A	855	CLA	C16-C17-C18-C20
31	O	203	CLA	C6-C7-C8-C9
31	B	823	CLA	CBA-CGA-O2A-C1
31	3	316	CLA	CBA-CGA-O2A-C1
31	A	833	CLA	C2A-CAA-CBA-CGA
31	4	305	CLA	C2A-CAA-CBA-CGA
28	a	306	LHG	C9-C10-C11-C12
32	6	320	CHL	C4C-C3C-CAC-CBC
28	A	811	LHG	C23-C24-C25-C26
37	G	202	LMG	C28-C29-C30-C31
31	A	819	CLA	C3-C5-C6-C7
27	A	807	LMT	C4-C5-C6-C7
28	A	809	LHG	C10-C11-C12-C13
31	8	318	CLA	CBA-CGA-O2A-C1
39	7	301	3PH	C32-C31-O31-C3
28	6	301	LHG	O6-C4-C5-O7
31	B	847	CLA	C16-C17-C18-C20
31	a	311	CLA	C11-C12-C13-C15
31	4	309	CLA	O1A-CGA-O2A-C1
26	I	801	BCR	C20-C21-C22-C23
26	K	202	BCR	C20-C21-C22-C23
26	7	304	BCR	C16-C17-C18-C19
26	6	302	BCR	C11-C10-C9-C8
36	7	305	LUT	C11-C10-C9-C8
36	5	304	LUT	C28-C29-C30-C31
36	6	303	LUT	C28-C29-C30-C31
28	6	301	LHG	O7-C5-C6-O8
37	a	301	LMG	O1-C7-C8-O7
31	B	814	CLA	C8-C10-C11-C12
32	a	317	CHL	O1A-CGA-O2A-C1
31	A	818	CLA	C4-C3-C5-C6
31	a	315	CLA	C4-C3-C5-C6
31	a	319	CLA	C4-C3-C5-C6
31	3	313	CLA	C4-C3-C5-C6
32	a	317	CHL	C4-C3-C5-C6
31	F	301	CLA	C8-C10-C11-C12
31	3	311	CLA	C8-C10-C11-C12
31	A	818	CLA	C2-C3-C5-C6
31	A	826	CLA	C11-C10-C8-C7
31	A	837	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	A	841	CLA	C11-C12-C13-C15
31	A	853	CLA	C2-C3-C5-C6
31	B	815	CLA	C6-C7-C8-C10
31	B	820	CLA	C11-C10-C8-C7
31	B	824	CLA	C6-C7-C8-C10
31	B	825	CLA	C11-C10-C8-C7
31	B	842	CLA	C11-C12-C13-C15
31	B	844	CLA	C12-C13-C15-C16
31	a	312	CLA	C11-C10-C8-C7
31	3	307	CLA	C12-C13-C15-C16
31	3	309	CLA	C6-C7-C8-C10
31	3	311	CLA	C11-C10-C8-C7
31	3	313	CLA	C2-C3-C5-C6
31	7	312	CLA	C11-C10-C8-C7
31	8	308	CLA	C11-C10-C8-C7
31	8	310	CLA	C6-C7-C8-C10
31	L	305	CLA	C2-C3-C5-C6
32	A	831	CHL	C11-C10-C8-C7
32	7	318	CHL	C6-C7-C8-C10
28	6	305	LHG	C27-C28-C29-C30
32	6	321	CHL	C4C-C3C-CAC-CBC
37	J	101	LMG	C24-C25-C26-C27
31	A	815	CLA	C11-C12-C13-C14
31	A	826	CLA	C11-C10-C8-C9
31	A	838	CLA	C14-C13-C15-C16
31	A	841	CLA	C11-C12-C13-C14
31	B	820	CLA	C11-C10-C8-C9
31	B	824	CLA	C6-C7-C8-C9
31	B	825	CLA	C11-C10-C8-C9
31	B	840	CLA	C11-C12-C13-C14
31	B	844	CLA	C11-C12-C13-C14
31	B	844	CLA	C14-C13-C15-C16
31	B	848	CLA	C14-C13-C15-C16
31	7	311	CLA	C11-C10-C8-C9
31	7	311	CLA	C14-C13-C15-C16
31	8	308	CLA	C11-C10-C8-C9
31	8	310	CLA	C6-C7-C8-C9
31	9	314	CLA	C6-C7-C8-C9
31	9	321	CLA	C6-C7-C8-C9
31	A	855	CLA	CBA-CGA-O2A-C1
31	3	312	CLA	CBA-CGA-O2A-C1
31	9	318	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
42	4	304	SQD	C24-C23-O48-C46
28	a	306	LHG	C25-C26-C27-C28
31	B	823	CLA	O1A-CGA-O2A-C1
26	3	303	BCR	C7-C8-C9-C34
36	b	301	LUT	C31-C32-C33-C40
36	J	103	LUT	C11-C12-C13-C14
36	6	303	LUT	C11-C12-C13-C14
31	L	305	CLA	C3-C5-C6-C7
28	7	302	LHG	C1-C2-C3-O3
31	A	826	CLA	C15-C16-C17-C18
33	7	308	DGD	C2B-C1B-O2G-C2G
37	G	202	LMG	C13-C14-C15-C16
32	7	320	CHL	O1A-CGA-O2A-C1
37	a	301	LMG	C30-C31-C32-C33
31	B	847	CLA	C15-C16-C17-C18
31	a	313	CLA	C5-C6-C7-C8
31	9	315	CLA	C6-C7-C8-C9
28	A	809	LHG	C28-C29-C30-C31
30	A	813	CL0	C4B-C3B-CAB-CBB
31	A	846	CLA	C4B-C3B-CAB-CBB
31	H	901	CLA	C4B-C3B-CAB-CBB
31	a	316	CLA	C4B-C3B-CAB-CBB
31	7	316	CLA	C4B-C3B-CAB-CBB
31	9	318	CLA	C4B-C3B-CAB-CBB
31	5	308	CLA	C4B-C3B-CAB-CBB
31	6	314	CLA	C4B-C3B-CAB-CBB
28	A	810	LHG	O6-C4-C5-C6
28	6	301	LHG	O6-C4-C5-C6
31	A	823	CLA	CBA-CGA-O2A-C1
31	9	317	CLA	CBA-CGA-O2A-C1
32	9	320	CHL	C4C-C3C-CAC-CBC
31	A	837	CLA	C4-C3-C5-C6
31	B	816	CLA	C4-C3-C5-C6
31	B	846	CLA	C4-C3-C5-C6
32	7	318	CHL	C4-C3-C5-C6
31	a	315	CLA	C2-C3-C5-C6
31	a	319	CLA	C2-C3-C5-C6
31	8	315	CLA	C2-C3-C5-C6
32	a	317	CHL	C2-C3-C5-C6
31	B	822	CLA	C10-C11-C12-C13
28	A	811	LHG	O9-C7-O7-C5
31	3	316	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	B	818	CLA	C3-C5-C6-C7
32	8	316	CHL	C16-C17-C18-C20
28	A	811	LHG	C10-C11-C12-C13
31	A	841	CLA	C15-C16-C17-C18
31	7	321	CLA	CBA-CGA-O2A-C1
41	8	305	DGA	OG2-CB1-CB2-CB3
28	8	304	LHG	C7-C8-C9-C10
28	A	809	LHG	C13-C14-C15-C16
31	B	814	CLA	C3A-C2A-CAA-CBA
31	4	316	CLA	C3A-C2A-CAA-CBA
31	5	312	CLA	C3A-C2A-CAA-CBA
28	a	306	LHG	C33-C34-C35-C36
37	a	301	LMG	C15-C16-C17-C18
31	3	312	CLA	C15-C16-C17-C18
28	7	302	LHG	C4-C5-C6-O8
33	B	808	DGD	C1G-C2G-C3G-O3G
33	7	308	DGD	O1G-C1G-C2G-C3G
37	J	101	LMG	C7-C8-C9-O8
37	a	301	LMG	O1-C7-C8-C9
27	5	301	LMT	C6-C7-C8-C9
28	A	810	LHG	C7-C8-C9-C10
37	G	202	LMG	C8-C9-O8-C28
43	5	306	PTY	C14-C15-C16-C17
28	A	810	LHG	C29-C30-C31-C32
31	O	203	CLA	C6-C7-C8-C10
31	6	312	CLA	C16-C17-C18-C19
31	B	816	CLA	C2-C3-C5-C6
31	3	310	CLA	O1D-CGD-O2D-CED
27	9	306	LMT	C5-C6-C7-C8
28	7	307	LHG	C10-C11-C12-C13
31	3	310	CLA	C4C-C3C-CAC-CBC
32	7	320	CHL	C2C-C3C-CAC-CBC
31	8	315	CLA	O1D-CGD-O2D-CED
32	a	320	CHL	C3C-C2C-CMC-OMC
31	8	318	CLA	O1A-CGA-O2A-C1
28	6	305	LHG	O1-C1-C2-O2
31	5	310	CLA	C13-C15-C16-C17
37	G	202	LMG	C36-C37-C38-C39
42	4	304	SQD	C24-C25-C26-C27
28	A	810	LHG	O6-C4-C5-O7
31	7	315	CLA	C3-C5-C6-C7
39	7	301	3PH	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
42	4	304	SQD	O10-C23-O48-C46
31	A	855	CLA	C16-C17-C18-C19
32	A	840	CHL	C16-C17-C18-C19
42	4	304	SQD	C25-C26-C27-C28
31	H	901	CLA	CBA-CGA-O2A-C1
28	8	304	LHG	O2-C2-C3-O3
30	A	813	CL0	C2B-C3B-CAB-CBB
31	7	316	CLA	C2B-C3B-CAB-CBB
31	9	318	CLA	C2B-C3B-CAB-CBB
31	3	312	CLA	O1A-CGA-O2A-C1
31	9	318	CLA	O1A-CGA-O2A-C1
35	7	303	QTB	C04-C05-C06-O07
28	A	811	LHG	O7-C5-C6-O8
33	7	308	DGD	O1G-C1G-C2G-O2G
37	J	101	LMG	O1-C7-C8-O7
31	A	827	CLA	CBA-CGA-O2A-C1
31	B	827	CLA	C11-C12-C13-C14
32	A	840	CHL	C16-C17-C18-C20
28	A	811	LHG	C31-C32-C33-C34
42	4	304	SQD	O5-C1-O6-C44
31	B	827	CLA	C10-C11-C12-C13
34	B	851	LAP	C13-C14-C15-O4
31	B	814	CLA	C4-C3-C5-C6
31	A	816	CLA	C2-C1-O2A-CGA
31	A	820	CLA	C2-C1-O2A-CGA
32	6	309	CHL	C2-C1-O2A-CGA
31	A	837	CLA	C2-C3-C5-C6
31	B	814	CLA	C2-C3-C5-C6
31	2	313	CLA	C2C-C3C-CAC-CBC
31	B	812	CLA	C11-C10-C8-C9
31	B	812	CLA	C14-C13-C15-C16
31	B	814	CLA	C11-C12-C13-C14
31	B	815	CLA	C11-C10-C8-C9
31	a	312	CLA	C11-C10-C8-C9
31	3	311	CLA	C14-C13-C15-C16
31	L	305	CLA	C11-C10-C8-C9
31	b	313	CLA	C11-C10-C8-C9
32	a	317	CHL	C11-C10-C8-C9
28	6	301	LHG	C5-C4-O6-P
37	G	202	LMG	C12-C13-C14-C15
31	8	308	CLA	C2A-CAA-CBA-CGA
31	B	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	803	BCR	C5-C6-C7-C8
26	A	804	BCR	C23-C24-C25-C26
26	A	805	BCR	C1-C6-C7-C8
26	A	805	BCR	C5-C6-C7-C8
26	B	803	BCR	C1-C6-C7-C8
26	B	803	BCR	C5-C6-C7-C8
26	B	804	BCR	C23-C24-C25-C26
26	B	804	BCR	C23-C24-C25-C30
26	B	805	BCR	C5-C6-C7-C8
26	B	806	BCR	C1-C6-C7-C8
26	B	806	BCR	C5-C6-C7-C8
26	G	201	BCR	C5-C6-C7-C8
26	G	201	BCR	C23-C24-C25-C26
26	G	201	BCR	C23-C24-C25-C30
26	K	202	BCR	C1-C6-C7-C8
26	K	202	BCR	C5-C6-C7-C8
26	K	203	BCR	C1-C6-C7-C8
26	K	203	BCR	C5-C6-C7-C8
26	M	101	BCR	C1-C6-C7-C8
26	M	101	BCR	C5-C6-C7-C8
26	3	302	BCR	C23-C24-C25-C26
26	3	302	BCR	C23-C24-C25-C30
26	3	303	BCR	C5-C6-C7-C8
26	3	303	BCR	C23-C24-C25-C26
26	3	303	BCR	C23-C24-C25-C30
26	8	301	BCR	C1-C6-C7-C8
26	L	303	BCR	C5-C6-C7-C8
26	O	201	BCR	C1-C6-C7-C8
26	O	201	BCR	C5-C6-C7-C8
26	2	302	BCR	C23-C24-C25-C30
32	7	324	CHL	C3-C5-C6-C7
36	9	302	LUT	C1-C6-C7-C8
36	L	304	LUT	C5-C6-C7-C8
26	7	304	BCR	C7-C8-C9-C34
26	L	303	BCR	C36-C18-C19-C20
33	B	808	DGD	C8A-C9A-CAA-CBA
26	A	806	BCR	C7-C8-C9-C10
26	F	302	BCR	C21-C22-C23-C24
26	G	203	BCR	C17-C18-C19-C20
36	4	302	LUT	C11-C12-C13-C14
31	A	846	CLA	C10-C11-C12-C13
33	7	308	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
31	B	840	CLA	CAA-CBA-CGA-O2A
31	9	314	CLA	C11-C12-C13-C14
35	7	303	QTB	C09-C10-C11-C17
31	A	838	CLA	C8-C10-C11-C12
31	8	320	CLA	C13-C15-C16-C17
31	B	825	CLA	C10-C11-C12-C13
24	B	801	PQN	C16-C17-C18-C20
31	A	830	CLA	C6-C7-C8-C10
31	A	838	CLA	C12-C13-C15-C16
31	B	812	CLA	C11-C10-C8-C7
31	B	812	CLA	C12-C13-C15-C16
31	B	814	CLA	C11-C12-C13-C15
31	B	817	CLA	C6-C7-C8-C10
31	B	840	CLA	C11-C12-C13-C15
31	B	844	CLA	C11-C12-C13-C15
31	B	846	CLA	C2-C3-C5-C6
31	B	848	CLA	C12-C13-C15-C16
31	7	311	CLA	C12-C13-C15-C16
31	9	314	CLA	C6-C7-C8-C10
31	9	321	CLA	C6-C7-C8-C10
31	b	313	CLA	C11-C10-C8-C7
26	5	302	BCR	C19-C20-C21-C22
35	7	303	QTB	C02-C03-C04-C05
36	8	302	LUT	C9-C10-C11-C12
36	9	302	LUT	C33-C34-C35-C15
36	9	305	LUT	C9-C10-C11-C12
36	4	302	LUT	C33-C34-C35-C15
31	A	841	CLA	C16-C17-C18-C19
31	B	847	CLA	C16-C17-C18-C19
27	A	808	LMT	C1-C2-C3-C4
31	8	320	CLA	CBA-CGA-O2A-C1
31	B	839	CLA	C5-C6-C7-C8
31	7	312	CLA	C8-C10-C11-C12
26	3	301	BCR	C20-C21-C22-C37
27	A	807	LMT	C11-C10-C9-C8
27	A	808	LMT	O5'-C5'-C6'-O6'
35	7	303	QTB	C01-C02-C03-C04
35	9	304	QTB	C01-C02-C03-C04
32	8	316	CHL	C16-C17-C18-C19
28	A	810	LHG	C24-C23-O8-C6
31	A	837	CLA	CBA-CGA-O2A-C1
32	5	316	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	G	202	LMG	C29-C28-O8-C9
37	J	104	LMG	C29-C28-O8-C9
31	8	320	CLA	C8-C10-C11-C12
31	A	826	CLA	CAD-CBD-CGD-O2D
31	A	829	CLA	CAD-CBD-CGD-O2D
31	A	850	CLA	CAD-CBD-CGD-O2D
31	B	815	CLA	CAD-CBD-CGD-O2D
31	B	822	CLA	CAD-CBD-CGD-O2D
31	B	824	CLA	CAD-CBD-CGD-O2D
31	B	826	CLA	CAD-CBD-CGD-O2D
31	B	843	CLA	CAD-CBD-CGD-O2D
31	3	313	CLA	CAD-CBD-CGD-O2D
31	7	312	CLA	CAD-CBD-CGD-O2D
31	8	310	CLA	CAD-CBD-CGD-O2D
31	9	314	CLA	CAD-CBD-CGD-O2D
31	2	307	CLA	CAD-CBD-CGD-O2D
31	2	310	CLA	CAD-CBD-CGD-O2D
31	2	312	CLA	CAD-CBD-CGD-O2D
31	4	308	CLA	CAD-CBD-CGD-O2D
31	4	309	CLA	CAD-CBD-CGD-O2D
31	5	307	CLA	CAD-CBD-CGD-O2D
31	5	312	CLA	CAD-CBD-CGD-O2D
32	A	831	CHL	CAD-CBD-CGD-O2D
32	A	840	CHL	CAD-CBD-CGD-O2D
32	a	317	CHL	CAD-CBD-CGD-O2D
32	8	319	CHL	CAD-CBD-CGD-O2D
32	4	313	CHL	CAD-CBD-CGD-O2D
32	6	318	CHL	CAD-CBD-CGD-O2D
32	6	320	CHL	CAD-CBD-CGD-O2D
32	6	321	CHL	CAD-CBD-CGD-O2D
43	5	306	PTY	C5-C6-O7-C8
28	7	302	LHG	C13-C14-C15-C16
28	7	307	LHG	C7-C8-C9-C10
31	6	308	CLA	C2C-C3C-CAC-CBC
31	B	813	CLA	C4-C3-C5-C6
33	7	308	DGD	CBB-CCB-CDB-CEB
37	G	202	LMG	C7-C8-C9-O8
42	4	304	SQD	O6-C44-C45-C46
31	B	845	CLA	CBD-CGD-O2D-CED
28	5	305	LHG	O6-C4-C5-O7
43	5	306	PTY	O14-C5-C6-O7
31	B	840	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	B	814	CLA	CBA-CGA-O2A-C1
26	M	101	BCR	C14-C15-C16-C17
31	9	319	CLA	CBA-CGA-O2A-C1
28	8	304	LHG	C1-C2-C3-O3
31	A	817	CLA	CHA-CBD-CGD-O1D
31	A	826	CLA	CHA-CBD-CGD-O1D
31	A	828	CLA	CHA-CBD-CGD-O2D
31	A	830	CLA	CHA-CBD-CGD-O1D
31	A	835	CLA	CHA-CBD-CGD-O2D
31	A	838	CLA	CHA-CBD-CGD-O2D
31	A	843	CLA	CHA-CBD-CGD-O1D
31	A	847	CLA	CHA-CBD-CGD-O2D
31	A	848	CLA	CHA-CBD-CGD-O2D
31	A	849	CLA	CHA-CBD-CGD-O2D
31	A	850	CLA	CHA-CBD-CGD-O1D
31	B	813	CLA	CHA-CBD-CGD-O1D
31	B	822	CLA	CHA-CBD-CGD-O1D
31	B	824	CLA	CHA-CBD-CGD-O1D
31	B	834	CLA	CHA-CBD-CGD-O1D
31	B	838	CLA	CHA-CBD-CGD-O2D
31	B	848	CLA	CHA-CBD-CGD-O1D
31	B	849	CLA	CHA-CBD-CGD-O1D
31	G	205	CLA	CHA-CBD-CGD-O1D
31	K	206	CLA	CHA-CBD-CGD-O1D
31	a	312	CLA	CHA-CBD-CGD-O1D
31	a	316	CLA	CHA-CBD-CGD-O2D
31	3	313	CLA	CHA-CBD-CGD-O1D
31	9	313	CLA	CHA-CBD-CGD-O1D
31	9	314	CLA	CHA-CBD-CGD-O1D
31	9	315	CLA	CHA-CBD-CGD-O2D
31	L	306	CLA	CHA-CBD-CGD-O2D
31	b	303	CLA	CHA-CBD-CGD-O2D
31	b	313	CLA	CHA-CBD-CGD-O1D
31	2	304	CLA	CHA-CBD-CGD-O1D
31	2	304	CLA	CHA-CBD-CGD-O2D
31	2	307	CLA	CHA-CBD-CGD-O1D
31	4	308	CLA	CHA-CBD-CGD-O1D
31	4	319	CLA	CHA-CBD-CGD-O2D
31	4	320	CLA	CHA-CBD-CGD-O1D
31	4	320	CLA	CHA-CBD-CGD-O2D
31	5	310	CLA	CHA-CBD-CGD-O1D
31	5	312	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	5	323	CLA	CHA-CBD-CGD-O2D
31	6	313	CLA	CHA-CBD-CGD-O2D
31	6	322	CLA	CHA-CBD-CGD-O1D
32	K	201	CHL	CHA-CBD-CGD-O1D
32	K	201	CHL	CHA-CBD-CGD-O2D
32	7	324	CHL	CHA-CBD-CGD-O2D
32	b	309	CHL	CHA-CBD-CGD-O2D
32	4	310	CHL	CHA-CBD-CGD-O2D
32	6	317	CHL	CHA-CBD-CGD-O2D
31	9	317	CLA	O1A-CGA-O2A-C1
26	I	801	BCR	C16-C17-C18-C19
26	L	301	BCR	C20-C21-C22-C23
36	8	303	LUT	C28-C29-C30-C31
36	4	302	LUT	C12-C13-C14-C15
28	7	302	LHG	C11-C12-C13-C14
28	A	809	LHG	O7-C5-C6-O8
37	G	202	LMG	O7-C8-C9-O8
37	J	101	LMG	O7-C8-C9-O8
28	A	810	LHG	C33-C34-C35-C36
27	5	301	LMT	C4'-C5'-C6'-O6'
31	9	318	CLA	C13-C15-C16-C17
31	A	823	CLA	O1A-CGA-O2A-C1
31	A	855	CLA	O1A-CGA-O2A-C1
31	7	321	CLA	O1A-CGA-O2A-C1
31	a	312	CLA	C16-C17-C18-C20
37	J	101	LMG	C20-C21-C22-C23
31	B	832	CLA	C4-C3-C5-C6
31	B	835	CLA	C4-C3-C5-C6
31	5	318	CLA	C4-C3-C5-C6
31	B	835	CLA	C2-C3-C5-C6
31	7	312	CLA	C14-C13-C15-C16
31	8	310	CLA	C11-C10-C8-C9
31	8	320	CLA	O1A-CGA-O2A-C1
32	5	316	CHL	O1A-CGA-O2A-C1
31	B	812	CLA	C13-C15-C16-C17
31	A	834	CLA	C2A-CAA-CBA-CGA
31	A	843	CLA	CBD-CGD-O2D-CED
28	A	809	LHG	C16-C17-C18-C19
31	A	827	CLA	O1A-CGA-O2A-C1
26	2	302	BCR	C7-C8-C9-C34
26	2	302	BCR	C7-C8-C9-C10
31	A	835	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	A	847	CLA	C1A-C2A-CAA-CBA
31	B	822	CLA	C1A-C2A-CAA-CBA
31	B	847	CLA	C1A-C2A-CAA-CBA
31	F	305	CLA	C1A-C2A-CAA-CBA
31	a	312	CLA	C1A-C2A-CAA-CBA
31	a	321	CLA	C1A-C2A-CAA-CBA
31	8	315	CLA	C1A-C2A-CAA-CBA
31	9	311	CLA	C1A-C2A-CAA-CBA
31	6	322	CLA	C1A-C2A-CAA-CBA
24	B	801	PQN	C26-C27-C28-C29
31	B	846	CLA	C16-C17-C18-C20
31	A	843	CLA	C13-C15-C16-C17
33	B	808	DGD	C9B-CAB-CBB-CCB
31	A	841	CLA	C2-C1-O2A-CGA
31	B	846	CLA	C2-C1-O2A-CGA
31	5	323	CLA	C2-C1-O2A-CGA
41	8	305	DGA	CB3-CB4-CB5-CB6
36	F	304	LUT	C9-C10-C11-C12
36	3	305	LUT	C33-C34-C35-C15
41	8	305	DGA	CA5-CA6-CA7-CA8
28	A	809	LHG	C3-O3-P-O5
28	7	302	LHG	C3-O3-P-O5
28	7	302	LHG	C4-O6-P-O4
28	6	301	LHG	C3-O3-P-O5
28	6	301	LHG	C4-O6-P-O4
31	B	845	CLA	C4B-C3B-CAB-CBB
31	9	321	CLA	C4B-C3B-CAB-CBB
31	5	313	CLA	C4B-C3B-CAB-CBB
34	B	851	LAP	C16-O6-P9-O5
34	B	851	LAP	C16-O6-P9-O7
28	7	302	LHG	C23-C24-C25-C26
27	9	306	LMT	C11-C10-C9-C8
37	J	101	LMG	C23-C24-C25-C26
31	A	826	CLA	CAD-CBD-CGD-O1D
31	A	850	CLA	CAD-CBD-CGD-O1D
31	A	854	CLA	CAD-CBD-CGD-O1D
31	B	822	CLA	CAD-CBD-CGD-O1D
31	B	834	CLA	CAD-CBD-CGD-O1D
31	B	848	CLA	CAD-CBD-CGD-O1D
31	B	849	CLA	CAD-CBD-CGD-O1D
31	K	206	CLA	CAD-CBD-CGD-O1D
31	9	313	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	2	304	CLA	CAD-CBD-CGD-O1D
32	K	201	CHL	CAD-CBD-CGD-O1D
31	A	837	CLA	O1A-CGA-O2A-C1
27	5	301	LMT	C3-C4-C5-C6
43	5	306	PTY	C33-C34-C35-C36
24	A	801	PQN	C26-C27-C28-C30
28	A	811	LHG	O6-C4-C5-O7
28	7	302	LHG	O6-C4-C5-O7
31	A	821	CLA	C11-C10-C8-C7
31	A	821	CLA	C12-C13-C15-C16
31	B	813	CLA	C2-C3-C5-C6
31	B	822	CLA	C11-C10-C8-C7
31	B	822	CLA	C12-C13-C15-C16
31	B	827	CLA	C6-C7-C8-C10
31	3	319	CLA	C11-C12-C13-C15
31	7	311	CLA	C11-C10-C8-C7
31	8	311	CLA	C3A-C2A-CAA-CBA
31	6	312	CLA	C11-C12-C13-C15
32	7	318	CHL	C11-C10-C8-C7
32	6	309	CHL	C11-C12-C13-C15
41	8	305	DGA	CB2-CB3-CB4-CB5
31	3	311	CLA	C3-C5-C6-C7
33	7	308	DGD	C6B-C7B-C8B-C9B
31	B	841	CLA	C6-C7-C8-C10
31	9	317	CLA	C2C-C3C-CAC-CBC
32	a	317	CHL	C1C-C2C-CMC-OMC
32	a	318	CHL	C1C-C2C-CMC-OMC
32	7	317	CHL	C1C-C2C-CMC-OMC
32	7	318	CHL	C1C-C2C-CMC-OMC
32	5	317	CHL	C1C-C2C-CMC-OMC
32	6	321	CHL	C1C-C2C-CMC-OMC
34	B	851	LAP	O6-C16-C17-N8
37	J	101	LMG	O1-C7-C8-C9
28	8	304	LHG	O7-C5-C6-O8
39	7	301	3PH	O21-C2-C3-O31
42	4	304	SQD	O6-C44-C45-O47
31	2	313	CLA	C4C-C3C-CAC-CBC
32	A	831	CHL	CAA-CBA-CGA-O2A
31	9	314	CLA	C11-C12-C13-C15
31	A	848	CLA	C3-C5-C6-C7
31	2	304	CLA	CBA-CGA-O2A-C1
30	A	813	CL0	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	B	820	CLA	C15-C16-C17-C18
31	A	817	CLA	C4-C3-C5-C6
31	A	819	CLA	CBA-CGA-O2A-C1
31	B	832	CLA	C2-C3-C5-C6
24	B	801	PQN	C16-C17-C18-C19
31	A	830	CLA	C6-C7-C8-C9
31	A	851	CLA	C11-C10-C8-C9
31	B	827	CLA	C6-C7-C8-C9
31	B	835	CLA	C6-C7-C8-C9
31	3	309	CLA	C14-C13-C15-C16
31	3	311	CLA	C11-C10-C8-C9
28	7	302	LHG	C14-C15-C16-C17
31	A	837	CLA	O1D-CGD-O2D-CED
31	8	309	CLA	O1A-CGA-O2A-C1
36	F	304	LUT	C10-C11-C12-C13
36	a	305	LUT	C10-C11-C12-C13
36	a	305	LUT	C30-C31-C32-C33
36	9	305	LUT	C30-C31-C32-C33
36	L	304	LUT	C10-C11-C12-C13
32	A	840	CHL	C8-C10-C11-C12
31	B	814	CLA	O1A-CGA-O2A-C1
36	L	304	LUT	C31-C32-C33-C34
31	A	846	CLA	C2B-C3B-CAB-CBB
31	A	853	CLA	C2B-C3B-CAB-CBB
31	F	305	CLA	C2B-C3B-CAB-CBB
31	H	901	CLA	C2B-C3B-CAB-CBB
31	a	316	CLA	C2B-C3B-CAB-CBB
31	b	308	CLA	C2B-C3B-CAB-CBB
31	b	311	CLA	C2B-C3B-CAB-CBB
31	2	310	CLA	C2B-C3B-CAB-CBB
31	2	311	CLA	C2B-C3B-CAB-CBB
31	4	305	CLA	C2B-C3B-CAB-CBB
31	5	308	CLA	C2B-C3B-CAB-CBB
31	5	314	CLA	C2B-C3B-CAB-CBB
43	5	306	PTY	C34-C35-C36-C37
31	2	309	CLA	CBA-CGA-O2A-C1
32	7	318	CHL	C2-C3-C5-C6
31	B	820	CLA	C8-C10-C11-C12
39	7	301	3PH	C25-C26-C27-C28
31	A	849	CLA	O1A-CGA-O2A-C1
32	K	201	CHL	O1A-CGA-O2A-C1
28	7	302	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
31	B	832	CLA	C2A-CAA-CBA-CGA
31	b	305	CLA	C2A-CAA-CBA-CGA
31	9	317	CLA	C4C-C3C-CAC-CBC
31	A	819	CLA	C2-C1-O2A-CGA
31	A	829	CLA	C2-C1-O2A-CGA
31	3	310	CLA	C2-C1-O2A-CGA
31	8	311	CLA	C2-C1-O2A-CGA
31	O	203	CLA	C2-C1-O2A-CGA
32	7	318	CHL	C2-C1-O2A-CGA
32	7	320	CHL	C4C-C3C-CAC-CBC
42	4	304	SQD	C11-C10-C9-C8
28	B	807	LHG	O10-C23-O8-C6
28	B	807	LHG	C11-C10-C9-C8
31	8	309	CLA	CBA-CGA-O2A-C1
33	7	308	DGD	C2A-C1A-O1G-C1G
26	A	803	BCR	C1-C6-C7-C8
26	A	803	BCR	C23-C24-C25-C26
26	A	803	BCR	C23-C24-C25-C30
26	A	804	BCR	C23-C24-C25-C30
26	B	805	BCR	C1-C6-C7-C8
26	B	806	BCR	C23-C24-C25-C26
26	B	806	BCR	C23-C24-C25-C30
26	G	201	BCR	C1-C6-C7-C8
26	L	303	BCR	C1-C6-C7-C8
26	O	201	BCR	C23-C24-C25-C26
31	5	318	CLA	C2-C3-C5-C6
31	A	841	CLA	C13-C15-C16-C17
31	B	848	CLA	C13-C15-C16-C17
32	8	316	CHL	C5-C6-C7-C8
31	3	318	CLA	CAA-CBA-CGA-O2A
32	4	310	CHL	C2C-C3C-CAC-CBC
37	G	202	LMG	C32-C33-C34-C35
28	7	302	LHG	C34-C35-C36-C37
30	A	813	CL0	C13-C15-C16-C17
32	5	317	CHL	C2A-CAA-CBA-CGA
32	6	309	CHL	C2A-CAA-CBA-CGA
31	2	313	CLA	CBA-CGA-O2A-C1
26	A	804	BCR	C11-C10-C9-C8
36	3	304	LUT	C11-C10-C9-C8
36	4	302	LUT	C11-C10-C9-C8
37	a	301	LMG	O7-C8-C9-O8
28	A	810	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	A	811	LHG	C3-O3-P-O6
33	B	808	DGD	O1G-C1G-C2G-C3G
37	J	104	LMG	O1-C7-C8-C9
31	4	309	CLA	C4-C3-C5-C6
31	8	308	CLA	C8-C10-C11-C12
27	A	808	LMT	C4'-C5'-C6'-O6'
31	B	835	CLA	C6-C7-C8-C10
31	B	822	CLA	C11-C10-C8-C9
31	3	307	CLA	C14-C13-C15-C16
32	6	309	CHL	C11-C12-C13-C14
31	3	312	CLA	C13-C15-C16-C17
31	a	312	CLA	C16-C17-C18-C19
31	9	321	CLA	C5-C6-C7-C8
41	8	305	DGA	CA4-CA5-CA6-CA7
37	G	202	LMG	C34-C35-C36-C37
28	7	302	LHG	C2-C3-O3-P
28	7	302	LHG	C5-C4-O6-P
31	A	821	CLA	C13-C15-C16-C17
28	A	811	LHG	C18-C19-C20-C21
31	4	307	CLA	C11-C10-C8-C7
32	A	840	CHL	C4-C3-C5-C6
28	6	301	LHG	O1-C1-C2-O2
31	B	841	CLA	C6-C7-C8-C9
31	A	838	CLA	CBA-CGA-O2A-C1
31	7	311	CLA	CBA-CGA-O2A-C1
31	6	311	CLA	CBA-CGA-O2A-C1
32	3	315	CHL	O1A-CGA-O2A-C1
31	5	313	CLA	CBD-CGD-O2D-CED
28	5	305	LHG	C13-C14-C15-C16
26	3	302	BCR	C22-C23-C24-C25
31	A	819	CLA	O1A-CGA-O2A-C1
31	A	853	CLA	C4B-C3B-CAB-CBB
31	F	305	CLA	C4B-C3B-CAB-CBB
31	K	206	CLA	C4B-C3B-CAB-CBB
31	b	308	CLA	C4B-C3B-CAB-CBB
31	b	311	CLA	C4B-C3B-CAB-CBB
31	2	310	CLA	C4B-C3B-CAB-CBB
31	2	311	CLA	C4B-C3B-CAB-CBB
31	4	305	CLA	C4B-C3B-CAB-CBB
31	5	314	CLA	C4B-C3B-CAB-CBB
31	b	306	CLA	C2A-CAA-CBA-CGA
32	6	318	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
33	B	808	DGD	C2G-C1G-O1G-C1A
26	B	805	BCR	C19-C20-C21-C22
36	6	304	LUT	C9-C10-C11-C12
40	7	306	XAT	C29-C30-C31-C32
28	5	305	LHG	O6-C4-C5-C6
31	A	820	CLA	O1A-CGA-O2A-C1
39	7	301	3PH	C24-C25-C26-C27
41	8	305	DGA	CA7-CA8-CA9-CAA
31	a	316	CLA	CAA-CBA-CGA-O2A
31	4	306	CLA	CAA-CBA-CGA-O2A
31	O	203	CLA	C3-C5-C6-C7
31	9	311	CLA	C4-C3-C5-C6
32	7	320	CHL	C4-C3-C5-C6
31	4	314	CLA	CAA-CBA-CGA-O2A
31	A	832	CLA	C2-C3-C5-C6
31	5	323	CLA	C5-C6-C7-C8
31	7	310	CLA	CAA-CBA-CGA-O1A
31	2	311	CLA	CAA-CBA-CGA-O2A
31	A	853	CLA	C2-C1-O2A-CGA
31	B	818	CLA	C2-C1-O2A-CGA
31	B	841	CLA	C2-C1-O2A-CGA
31	B	850	CLA	C2-C1-O2A-CGA
31	G	204	CLA	C2-C1-O2A-CGA
31	B	811	CLA	C15-C16-C17-C18
31	L	305	CLA	C10-C11-C12-C13
31	2	305	CLA	CAA-CBA-CGA-O1A
31	B	816	CLA	C2A-CAA-CBA-CGA
31	3	318	CLA	C2A-CAA-CBA-CGA
31	2	308	CLA	C2A-CAA-CBA-CGA
31	4	311	CLA	C2A-CAA-CBA-CGA
32	A	831	CHL	C2A-CAA-CBA-CGA
37	a	301	LMG	C35-C36-C37-C38
31	B	813	CLA	C8-C10-C11-C12
37	a	301	LMG	C12-C13-C14-C15
31	A	818	CLA	C3A-C2A-CAA-CBA
32	b	309	CHL	C3A-C2A-CAA-CBA
31	7	313	CLA	CAA-CBA-CGA-O1A
31	L	307	CLA	CAA-CBA-CGA-O1A
31	4	315	CLA	CAA-CBA-CGA-O2A
31	5	318	CLA	CAA-CBA-CGA-O2A
36	a	303	LUT	C33-C34-C35-C15
31	A	832	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	6	311	CLA	C4-C3-C5-C6
31	A	817	CLA	C2-C3-C5-C6
31	A	821	CLA	C11-C10-C8-C9
31	B	822	CLA	C14-C13-C15-C16
31	a	319	CLA	C11-C10-C8-C9
31	6	312	CLA	C11-C12-C13-C14
31	7	310	CLA	CAA-CBA-CGA-O2A
26	A	806	BCR	C16-C17-C18-C36
26	B	803	BCR	C11-C10-C9-C34
26	B	806	BCR	C20-C21-C22-C37
26	6	302	BCR	C20-C21-C22-C37
36	L	304	LUT	C11-C10-C9-C19
37	a	301	LMG	C7-C8-C9-O8
31	4	314	CLA	CAA-CBA-CGA-O1A
32	6	318	CHL	CAA-CBA-CGA-O2A
31	5	309	CLA	C2A-CAA-CBA-CGA
31	5	314	CLA	C2A-CAA-CBA-CGA
33	B	808	DGD	C2A-C1A-O1G-C1G
33	B	808	DGD	O6E-C1E-O5D-C6D
26	G	203	BCR	C36-C18-C19-C20
26	K	203	BCR	C11-C12-C13-C35
31	2	305	CLA	CAA-CBA-CGA-O2A
31	4	315	CLA	CAA-CBA-CGA-O1A
36	5	303	LUT	C27-C28-C29-C39
26	M	101	BCR	C7-C8-C9-C10
28	7	302	LHG	C9-C10-C11-C12
31	3	312	CLA	C4-C3-C5-C6
31	9	315	CLA	C4-C3-C5-C6
32	A	839	CHL	C4-C3-C5-C6
31	A	818	CLA	C1A-C2A-CAA-CBA
31	A	844	CLA	C1A-C2A-CAA-CBA
31	A	849	CLA	C1A-C2A-CAA-CBA
31	B	836	CLA	C1A-C2A-CAA-CBA
31	B	837	CLA	C1A-C2A-CAA-CBA
31	3	318	CLA	C1A-C2A-CAA-CBA
31	7	309	CLA	C1A-C2A-CAA-CBA
31	7	312	CLA	C1A-C2A-CAA-CBA
31	8	308	CLA	C1A-C2A-CAA-CBA
31	8	310	CLA	C1A-C2A-CAA-CBA
31	9	317	CLA	C1A-C2A-CAA-CBA
31	2	310	CLA	C1A-C2A-CAA-CBA
31	6	314	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	b	309	CHL	C1A-C2A-CAA-CBA
31	A	815	CLA	C12-C13-C15-C16
31	B	814	CLA	C11-C10-C8-C7
31	B	817	CLA	C11-C10-C8-C7
31	6	312	CLA	C6-C7-C8-C10
32	7	324	CHL	C11-C10-C8-C7
28	a	306	LHG	C18-C19-C20-C21
24	B	801	PQN	C25-C26-C27-C28
31	7	313	CLA	CAA-CBA-CGA-O2A
31	L	307	CLA	CAA-CBA-CGA-O2A
31	5	313	CLA	O1D-CGD-O2D-CED
28	7	307	LHG	C30-C31-C32-C33
32	A	840	CHL	C3C-C2C-CMC-OMC
32	7	320	CHL	C3C-C2C-CMC-OMC
32	3	315	CHL	CBA-CGA-O2A-C1
31	7	311	CLA	O1A-CGA-O2A-C1
33	B	808	DGD	C8B-C9B-CAB-CBB
31	9	318	CLA	C2A-CAA-CBA-CGA
31	2	307	CLA	C2A-CAA-CBA-CGA
31	4	307	CLA	C2A-CAA-CBA-CGA
31	4	308	CLA	C2A-CAA-CBA-CGA
31	4	318	CLA	C2A-CAA-CBA-CGA
31	6	307	CLA	C2A-CAA-CBA-CGA
32	4	317	CHL	C2A-CAA-CBA-CGA
31	A	822	CLA	C5-C6-C7-C8
31	B	842	CLA	C5-C6-C7-C8
31	3	307	CLA	C15-C16-C17-C18
27	A	808	LMT	C9-C10-C11-C12
31	b	304	CLA	CBA-CGA-O2A-C1
31	3	309	CLA	C8-C10-C11-C12
31	B	847	CLA	C4-C3-C5-C6
31	B	845	CLA	C2B-C3B-CAB-CBB
31	3	310	CLA	C2B-C3B-CAB-CBB
31	9	321	CLA	C2B-C3B-CAB-CBB
31	5	313	CLA	C2B-C3B-CAB-CBB
32	K	201	CHL	C2B-C3B-CAB-CBB
32	5	319	CHL	C2B-C3B-CAB-CBB
31	A	826	CLA	C10-C11-C12-C13
32	8	316	CHL	C15-C16-C17-C18
31	B	831	CLA	O1A-CGA-O2A-C1
30	A	813	CL0	C3-C5-C6-C7
31	A	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	B	807	LHG	O9-C7-O7-C5
26	A	806	BCR	C11-C10-C9-C8
26	6	302	BCR	C20-C21-C22-C23
36	a	303	LUT	C12-C13-C14-C15
36	3	305	LUT	C9-C10-C11-C12
36	6	303	LUT	C13-C14-C15-C35
31	4	306	CLA	CAA-CBA-CGA-O1A
31	H	901	CLA	O1A-CGA-O2A-C1
31	a	316	CLA	CAA-CBA-CGA-O1A
31	2	311	CLA	CAA-CBA-CGA-O1A
31	8	314	CLA	C4-C3-C5-C6
31	A	824	CLA	C2-C1-O2A-CGA
31	B	811	CLA	C2-C1-O2A-CGA
31	B	826	CLA	C2-C1-O2A-CGA
31	9	315	CLA	C2-C3-C5-C6
31	4	309	CLA	C2-C3-C5-C6
31	6	311	CLA	C2-C3-C5-C6
32	A	839	CHL	C2-C3-C5-C6
32	A	840	CHL	C2-C3-C5-C6
32	7	320	CHL	C2-C3-C5-C6
31	a	314	CLA	O1A-CGA-O2A-C1
31	6	311	CLA	O1A-CGA-O2A-C1
31	A	841	CLA	C6-C7-C8-C9
32	6	309	CHL	C11-C10-C8-C9
31	4	319	CLA	C2C-C3C-CAC-CBC
31	3	311	CLA	C13-C15-C16-C17
31	B	812	CLA	C2A-CAA-CBA-CGA
28	6	305	LHG	C11-C10-C9-C8
31	A	838	CLA	O1A-CGA-O2A-C1
26	A	804	BCR	C1-C6-C7-C8
26	B	802	BCR	C1-C6-C7-C8
26	F	302	BCR	C1-C6-C7-C8
26	J	102	BCR	C1-C6-C7-C8
26	3	303	BCR	C1-C6-C7-C8
26	L	301	BCR	C1-C6-C7-C8
26	L	301	BCR	C5-C6-C7-C8
26	L	302	BCR	C23-C24-C25-C30
26	O	201	BCR	C23-C24-C25-C30
36	a	305	LUT	C1-C6-C7-C8
31	B	848	CLA	CAA-CBA-CGA-O2A
28	7	302	LHG	O1-C1-C2-C3
31	9	319	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	J	103	LUT	C13-C14-C15-C35
36	7	305	LUT	C33-C34-C35-C15
36	8	303	LUT	C9-C10-C11-C12
31	4	316	CLA	C2-C1-O2A-CGA
31	B	817	CLA	C4-C3-C5-C6
31	9	321	CLA	C4-C3-C5-C6
31	2	307	CLA	C4-C3-C5-C6
32	7	318	CHL	C16-C17-C18-C19
27	5	301	LMT	C1-C2-C3-C4
31	A	851	CLA	C13-C15-C16-C17
33	B	808	DGD	C5D-C6D-O5D-C1E
31	A	843	CLA	C16-C17-C18-C19
31	B	814	CLA	C16-C17-C18-C20
31	B	850	CLA	C10-C11-C12-C13
31	F	301	CLA	C15-C16-C17-C18
31	a	311	CLA	C10-C11-C12-C13
31	B	831	CLA	CBA-CGA-O2A-C1
31	A	827	CLA	C3-C5-C6-C7
31	5	314	CLA	CAA-CBA-CGA-O1A
31	a	310	CLA	C4B-C3B-CAB-CBB
31	3	310	CLA	C4B-C3B-CAB-CBB
31	5	309	CLA	C4B-C3B-CAB-CBB
32	K	201	CHL	C4B-C3B-CAB-CBB
32	5	319	CHL	C4B-C3B-CAB-CBB
32	6	320	CHL	C4B-C3B-CAB-CBB
31	A	818	CLA	C16-C17-C18-C20
33	B	808	DGD	C3B-C4B-C5B-C6B
31	B	821	CLA	C4-C3-C5-C6
31	B	844	CLA	C4-C3-C5-C6
31	5	318	CLA	C2C-C3C-CAC-CBC
31	A	851	CLA	C11-C10-C8-C7
31	B	817	CLA	C11-C12-C13-C15
31	B	830	CLA	C11-C10-C8-C7
31	7	312	CLA	C12-C13-C15-C16
31	a	314	CLA	CBA-CGA-O2A-C1
43	5	306	PTY	N1-C2-C3-O11
28	8	304	LHG	C9-C10-C11-C12
28	7	302	LHG	O1-C1-C2-O2
36	4	302	LUT	C29-C30-C31-C32
38	a	304	AXT	C29-C30-C31-C32
28	6	301	LHG	C7-C8-C9-C10
28	7	307	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
41	8	305	DGA	OB1-CB1-CB2-CB3
31	A	847	CLA	C13-C15-C16-C17
31	3	313	CLA	C3-C5-C6-C7
31	A	837	CLA	C2A-CAA-CBA-CGA
31	a	314	CLA	C2A-CAA-CBA-CGA
31	A	820	CLA	CBA-CGA-O2A-C1
26	A	806	BCR	C11-C10-C9-C34
26	B	806	BCR	C11-C10-C9-C34
26	3	302	BCR	C11-C10-C9-C34
36	F	304	LUT	C11-C10-C9-C19
31	B	846	CLA	CAA-CBA-CGA-O2A
37	J	101	LMG	O8-C28-C29-C30
31	A	822	CLA	C4-C3-C5-C6
31	A	856	CLA	C4-C3-C5-C6
31	B	829	CLA	C4-C3-C5-C6
31	B	837	CLA	C4-C3-C5-C6
31	B	842	CLA	C4-C3-C5-C6
31	6	312	CLA	C4-C3-C5-C6
32	7	324	CHL	C4-C3-C5-C6
37	J	104	LMG	C10-C11-C12-C13
31	A	854	CLA	CAA-CBA-CGA-O2A
31	A	815	CLA	C14-C13-C15-C16
31	A	821	CLA	C14-C13-C15-C16
31	B	830	CLA	C11-C10-C8-C9
32	A	831	CHL	C11-C10-C8-C9
32	7	318	CHL	C14-C13-C15-C16
31	4	319	CLA	C4C-C3C-CAC-CBC
39	7	301	3PH	C33-C34-C35-C36
31	B	822	CLA	C3A-C2A-CAA-CBA
31	H	901	CLA	C3A-C2A-CAA-CBA
31	b	304	CLA	C3A-C2A-CAA-CBA
31	b	310	CLA	C3A-C2A-CAA-CBA
31	4	318	CLA	C3A-C2A-CAA-CBA
28	7	307	LHG	O8-C23-C24-C25
31	H	901	CLA	CAA-CBA-CGA-O2A
31	3	308	CLA	CAA-CBA-CGA-O2A
31	8	309	CLA	CAA-CBA-CGA-O2A
31	A	817	CLA	CAD-CBD-CGD-O2D
31	A	827	CLA	CAD-CBD-CGD-O2D
31	A	830	CLA	CAD-CBD-CGD-O2D
31	B	813	CLA	CAD-CBD-CGD-O2D
31	B	814	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	B	834	CLA	CAD-CBD-CGD-O2D
31	B	839	CLA	CAD-CBD-CGD-O2D
31	B	848	CLA	CAD-CBD-CGD-O2D
31	B	849	CLA	CAD-CBD-CGD-O2D
31	G	205	CLA	CAD-CBD-CGD-O2D
31	K	206	CLA	CAD-CBD-CGD-O2D
31	a	312	CLA	CAD-CBD-CGD-O2D
31	3	319	CLA	CAD-CBD-CGD-O2D
31	9	313	CLA	CAD-CBD-CGD-O2D
31	9	316	CLA	CAD-CBD-CGD-O2D
31	b	313	CLA	CAD-CBD-CGD-O2D
31	2	309	CLA	CAD-CBD-CGD-O2D
31	4	316	CLA	CAD-CBD-CGD-O2D
31	5	311	CLA	CAD-CBD-CGD-O2D
31	6	308	CLA	CAD-CBD-CGD-O2D
31	6	311	CLA	CAD-CBD-CGD-O2D
32	a	320	CHL	CAD-CBD-CGD-O2D
32	7	317	CHL	CAD-CBD-CGD-O2D
32	7	324	CHL	CAD-CBD-CGD-O2D
32	b	309	CHL	CAD-CBD-CGD-O2D
32	4	317	CHL	CAD-CBD-CGD-O2D
32	6	317	CHL	CAD-CBD-CGD-O2D
31	B	815	CLA	C8-C10-C11-C12
31	5	315	CLA	C15-C16-C17-C18
31	b	311	CLA	C2A-CAA-CBA-CGA
31	6	311	CLA	C2A-CAA-CBA-CGA
31	3	310	CLA	C5-C6-C7-C8
31	A	822	CLA	CAA-CBA-CGA-O2A
31	B	820	CLA	CAA-CBA-CGA-O2A
31	b	307	CLA	CAA-CBA-CGA-O2A
32	a	320	CHL	CAA-CBA-CGA-O2A
31	A	821	CLA	C4-C3-C5-C6
31	B	839	CLA	C4-C3-C5-C6
31	F	301	CLA	C4-C3-C5-C6
31	a	311	CLA	C4-C3-C5-C6
31	7	314	CLA	C4-C3-C5-C6
31	A	814	CLA	C16-C17-C18-C19
31	8	311	CLA	C3-C5-C6-C7
31	A	822	CLA	C2-C3-C5-C6
31	A	838	CLA	C2-C3-C5-C6
31	B	847	CLA	C2-C3-C5-C6
31	3	312	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	9	321	CLA	C2-C3-C5-C6
31	A	826	CLA	CAA-CBA-CGA-O2A
31	A	833	CLA	CAA-CBA-CGA-O2A
31	A	838	CLA	CAA-CBA-CGA-O2A
31	B	815	CLA	CAA-CBA-CGA-O2A
31	8	308	CLA	CAA-CBA-CGA-O2A
31	6	306	CLA	CAA-CBA-CGA-O2A
32	A	831	CHL	C2C-C3C-CAC-CBC
26	3	303	BCR	C17-C18-C19-C20
28	A	809	LHG	C4-C5-C6-O8
28	6	301	LHG	C4-C5-C6-O8
39	7	301	3PH	C1-O11-P-O12
31	3	317	CLA	O1A-CGA-O2A-C1
30	A	813	CL0	CAA-CBA-CGA-O2A
31	G	205	CLA	CAA-CBA-CGA-O2A
31	9	315	CLA	CAA-CBA-CGA-O2A
31	b	313	CLA	CAA-CBA-CGA-O2A
31	4	312	CLA	CAA-CBA-CGA-O2A
31	A	857	CLA	C8-C10-C11-C12
31	3	319	CLA	C2A-CAA-CBA-CGA
31	B	823	CLA	C5-C6-C7-C8
31	6	310	CLA	CAA-CBA-CGA-O2A
31	6	313	CLA	CAA-CBA-CGA-O2A
32	K	201	CHL	CAA-CBA-CGA-O2A
37	J	104	LMG	O8-C28-C29-C30
31	9	315	CLA	C3-C5-C6-C7
31	2	306	CLA	C3-C5-C6-C7
31	5	315	CLA	C3-C5-C6-C7
34	B	851	LAP	O3-C14-C15-O4
31	A	814	CLA	CHA-CBD-CGD-O1D
31	A	816	CLA	CHA-CBD-CGD-O2D
31	A	826	CLA	CHA-CBD-CGD-O2D
31	A	828	CLA	CHA-CBD-CGD-O1D
31	A	837	CLA	CHA-CBD-CGD-O1D
31	A	841	CLA	CHA-CBD-CGD-O2D
31	A	849	CLA	CHA-CBD-CGD-O1D
31	A	851	CLA	CHA-CBD-CGD-O2D
31	B	814	CLA	CHA-CBD-CGD-O1D
31	B	816	CLA	CHA-CBD-CGD-O2D
31	B	817	CLA	CHA-CBD-CGD-O2D
31	B	823	CLA	CHA-CBD-CGD-O2D
31	B	826	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	B	833	CLA	CHA-CBD-CGD-O2D
31	B	835	CLA	CHA-CBD-CGD-O2D
31	B	841	CLA	CHA-CBD-CGD-O2D
31	B	844	CLA	CHA-CBD-CGD-O2D
31	K	204	CLA	CHA-CBD-CGD-O1D
31	K	205	CLA	CHA-CBD-CGD-O2D
31	a	310	CLA	CHA-CBD-CGD-O1D
31	a	311	CLA	CHA-CBD-CGD-O2D
31	a	314	CLA	CHA-CBD-CGD-O2D
31	a	316	CLA	CHA-CBD-CGD-O1D
31	a	319	CLA	CHA-CBD-CGD-O2D
31	a	322	CLA	CHA-CBD-CGD-O2D
31	3	308	CLA	CHA-CBD-CGD-O2D
31	3	317	CLA	CHA-CBD-CGD-O2D
31	3	319	CLA	CHA-CBD-CGD-O1D
31	7	309	CLA	CHA-CBD-CGD-O2D
31	7	312	CLA	CHA-CBD-CGD-O1D
31	7	316	CLA	CHA-CBD-CGD-O2D
31	7	321	CLA	CHA-CBD-CGD-O2D
31	8	307	CLA	CHA-CBD-CGD-O2D
31	9	321	CLA	CHA-CBD-CGD-O2D
31	L	305	CLA	CHA-CBD-CGD-O1D
31	O	203	CLA	CHA-CBD-CGD-O1D
31	b	305	CLA	CHA-CBD-CGD-O1D
31	b	310	CLA	CHA-CBD-CGD-O2D
31	2	305	CLA	CHA-CBD-CGD-O2D
31	4	307	CLA	CHA-CBD-CGD-O1D
31	4	308	CLA	CHA-CBD-CGD-O2D
31	5	312	CLA	CHA-CBD-CGD-O2D
31	5	315	CLA	CHA-CBD-CGD-O1D
31	5	321	CLA	CHA-CBD-CGD-O2D
31	6	307	CLA	CHA-CBD-CGD-O2D
31	6	314	CLA	CHA-CBD-CGD-O2D
31	6	315	CLA	CHA-CBD-CGD-O1D
32	A	840	CHL	CHA-CBD-CGD-O2D
32	a	317	CHL	CHA-CBD-CGD-O2D
32	7	317	CHL	CHA-CBD-CGD-O2D
32	4	310	CHL	CHA-CBD-CGD-O1D
32	5	316	CHL	CHA-CBD-CGD-O1D
32	6	309	CHL	CHA-CBD-CGD-O1D
32	6	309	CHL	CHA-CBD-CGD-O2D
31	B	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	B	839	CLA	C2-C3-C5-C6
28	A	811	LHG	C13-C14-C15-C16
37	G	202	LMG	C30-C31-C32-C33
26	A	806	BCR	C16-C17-C18-C19
26	B	803	BCR	C20-C21-C22-C23
28	7	307	LHG	C25-C26-C27-C28
31	2	309	CLA	O1A-CGA-O2A-C1
28	7	302	LHG	O7-C7-C8-C9
31	A	816	CLA	CAA-CBA-CGA-O2A
31	7	321	CLA	CAA-CBA-CGA-O2A
31	5	318	CLA	C4C-C3C-CAC-CBC
32	6	309	CHL	O1A-CGA-O2A-C1
31	7	312	CLA	C2A-CAA-CBA-CGA
31	b	303	CLA	C2A-CAA-CBA-CGA
31	b	302	CLA	CAA-CBA-CGA-O2A
31	b	305	CLA	CAA-CBA-CGA-O2A
31	B	848	CLA	C4-C3-C5-C6
31	5	321	CLA	CBA-CGA-O2A-C1
32	7	324	CHL	C2-C3-C5-C6
31	2	313	CLA	O1A-CGA-O2A-C1
31	4	320	CLA	C2C-C3C-CAC-CBC
31	B	814	CLA	C11-C10-C8-C9
31	B	817	CLA	C11-C10-C8-C9
31	F	301	CLA	C11-C12-C13-C14
31	a	309	CLA	C11-C10-C8-C9
31	6	312	CLA	C6-C7-C8-C9
26	B	804	BCR	C19-C20-C21-C22
36	F	304	LUT	C33-C34-C35-C15
31	4	320	CLA	C4C-C3C-CAC-CBC
32	6	309	CHL	C10-C11-C12-C13
31	A	856	CLA	C2B-C3B-CAB-CBB
31	K	206	CLA	C2B-C3B-CAB-CBB
31	8	311	CLA	C2B-C3B-CAB-CBB
31	5	309	CLA	C2B-C3B-CAB-CBB
28	8	304	LHG	C25-C26-C27-C28
31	3	317	CLA	CBA-CGA-O2A-C1
31	a	322	CLA	CAA-CBA-CGA-O2A
37	a	301	LMG	O7-C10-C11-C12
28	7	307	LHG	O10-C23-C24-C25
31	B	840	CLA	CAA-CBA-CGA-O1A
31	B	822	CLA	C3-C5-C6-C7
31	B	822	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	B	839	CLA	C2A-CAA-CBA-CGA
32	a	320	CHL	CAA-CBA-CGA-O1A
28	A	811	LHG	O8-C23-C24-C25
31	A	848	CLA	CAA-CBA-CGA-O2A
31	4	309	CLA	CAA-CBA-CGA-O2A
31	5	311	CLA	CAA-CBA-CGA-O2A
31	6	322	CLA	CAA-CBA-CGA-O2A
31	a	319	CLA	CBA-CGA-O2A-C1
36	2	301	LUT	C27-C28-C29-C39
32	7	318	CHL	C16-C17-C18-C20
31	B	844	CLA	C2-C3-C5-C6
31	5	314	CLA	CAA-CBA-CGA-O2A
31	A	826	CLA	CAA-CBA-CGA-O1A
31	A	833	CLA	CAA-CBA-CGA-O1A
31	B	815	CLA	CAA-CBA-CGA-O1A
31	G	205	CLA	CAA-CBA-CGA-O1A
26	A	803	BCR	C21-C22-C23-C24
26	6	302	BCR	C21-C22-C23-C24
35	a	302	QTB	C03-C02-C09-C10
31	A	826	CLA	C1A-C2A-CAA-CBA
31	A	856	CLA	C1A-C2A-CAA-CBA
31	H	901	CLA	C1A-C2A-CAA-CBA
31	8	313	CLA	C1A-C2A-CAA-CBA
31	8	320	CLA	C1A-C2A-CAA-CBA
31	b	308	CLA	C1A-C2A-CAA-CBA
31	b	310	CLA	C1A-C2A-CAA-CBA
31	2	306	CLA	C1A-C2A-CAA-CBA
31	4	318	CLA	C1A-C2A-CAA-CBA
31	6	316	CLA	C1A-C2A-CAA-CBA
32	6	317	CHL	C1A-C2A-CAA-CBA
31	B	812	CLA	C16-C17-C18-C20
31	A	854	CLA	CAA-CBA-CGA-O1A
31	9	315	CLA	CAA-CBA-CGA-O1A
31	4	312	CLA	CAA-CBA-CGA-O1A
31	6	310	CLA	CAA-CBA-CGA-O1A
28	6	301	LHG	O9-C7-C8-C9
31	A	822	CLA	CAA-CBA-CGA-O1A
31	A	848	CLA	CAA-CBA-CGA-O1A
31	3	308	CLA	CAA-CBA-CGA-O1A
31	3	319	CLA	C8-C10-C11-C12
31	3	317	CLA	C2A-CAA-CBA-CGA
31	9	314	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	O	203	CLA	C2A-CAA-CBA-CGA
31	5	310	CLA	C2A-CAA-CBA-CGA
32	K	201	CHL	CAA-CBA-CGA-O1A
31	B	840	CLA	C13-C15-C16-C17
32	3	315	CHL	C5-C6-C7-C8
32	7	318	CHL	C5-C6-C7-C8
31	9	316	CLA	C2C-C3C-CAC-CBC
41	8	305	DGA	CA9-CAA-CBA-CCA
31	A	847	CLA	C5-C6-C7-C8
28	a	306	LHG	C10-C11-C12-C13
31	B	846	CLA	CAA-CBA-CGA-O1A
31	b	307	CLA	CAA-CBA-CGA-O1A
31	2	304	CLA	O1A-CGA-O2A-C1
33	B	808	DGD	C2E-C1E-O5D-C6D
30	A	813	CL0	C10-C11-C12-C13
31	a	311	CLA	C8-C10-C11-C12
32	7	324	CHL	C5-C6-C7-C8
32	5	316	CHL	C2C-C3C-CAC-CBC
28	A	810	LHG	C3-O3-P-O5
28	a	306	LHG	C4-O6-P-O5
28	7	307	LHG	C4-O6-P-O4
31	a	322	CLA	C4B-C3B-CAB-CBB
43	5	306	PTY	C5-O14-P1-O13
31	6	313	CLA	CAA-CBA-CGA-O1A
26	3	303	BCR	C20-C21-C22-C37
26	A	804	BCR	C5-C6-C7-C8
26	B	802	BCR	C5-C6-C7-C8
26	B	804	BCR	C5-C6-C7-C8
26	F	302	BCR	C5-C6-C7-C8
26	J	102	BCR	C5-C6-C7-C8
26	7	304	BCR	C1-C6-C7-C8
32	5	316	CHL	C4C-C3C-CAC-CBC
31	A	816	CLA	CAA-CBA-CGA-O1A
31	B	820	CLA	CAA-CBA-CGA-O1A
31	7	321	CLA	CAA-CBA-CGA-O1A
31	b	302	CLA	CAA-CBA-CGA-O1A
31	5	311	CLA	CAA-CBA-CGA-O1A
31	A	828	CLA	O1A-CGA-O2A-C1
31	3	311	CLA	CAA-CBA-CGA-O2A
31	9	316	CLA	C4C-C3C-CAC-CBC
31	A	814	CLA	C16-C17-C18-C20
31	2	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	a	319	CLA	O1A-CGA-O2A-C1
31	5	318	CLA	C15-C16-C17-C18
28	6	301	LHG	O7-C7-C8-C9
31	8	309	CLA	CAA-CBA-CGA-O1A
31	2	307	CLA	C2-C3-C5-C6
31	A	828	CLA	C16-C17-C18-C19
37	J	101	LMG	C33-C34-C35-C36
31	B	843	CLA	CAA-CBA-CGA-O2A
31	A	814	CLA	CAD-CBD-CGD-O1D
31	A	832	CLA	CAD-CBD-CGD-O1D
31	A	843	CLA	CAD-CBD-CGD-O1D
31	A	849	CLA	CAD-CBD-CGD-O1D
31	B	819	CLA	CAD-CBD-CGD-O1D
31	B	826	CLA	CAD-CBD-CGD-O1D
31	B	832	CLA	CAD-CBD-CGD-O1D
31	L	305	CLA	CAD-CBD-CGD-O1D
31	L	306	CLA	CAD-CBD-CGD-O1D
31	b	312	CLA	CAD-CBD-CGD-O1D
31	4	320	CLA	CAD-CBD-CGD-O1D
31	5	315	CLA	CAD-CBD-CGD-O1D
31	6	308	CLA	CAD-CBD-CGD-O1D
32	4	310	CHL	CAD-CBD-CGD-O1D
31	A	838	CLA	CAA-CBA-CGA-O1A
31	8	308	CLA	CAA-CBA-CGA-O1A
31	b	305	CLA	CAA-CBA-CGA-O1A
31	6	306	CLA	CAA-CBA-CGA-O1A
28	7	302	LHG	C30-C31-C32-C33
31	5	313	CLA	CAA-CBA-CGA-O2A
31	A	851	CLA	C14-C13-C15-C16
31	A	857	CLA	C11-C12-C13-C14
31	B	817	CLA	C11-C12-C13-C14
31	b	313	CLA	C4C-C3C-CAC-CBC
31	5	309	CLA	CAA-CBA-CGA-O2A
33	7	308	DGD	O2G-C1B-C2B-C3B
31	B	843	CLA	CAA-CBA-CGA-O1A
31	5	307	CLA	C2A-CAA-CBA-CGA
31	4	308	CLA	CAA-CBA-CGA-O2A
42	4	304	SQD	O47-C7-C8-C9
31	B	811	CLA	C8-C10-C11-C12
31	3	310	CLA	C10-C11-C12-C13
39	7	301	3PH	C32-C33-C34-C35
31	5	309	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	A	843	CLA	C4-C3-C5-C6
31	B	820	CLA	O1A-CGA-O2A-C1
31	A	826	CLA	C3A-C2A-CAA-CBA
31	A	856	CLA	C3A-C2A-CAA-CBA
31	A	857	CLA	C11-C12-C13-C15
31	F	301	CLA	C11-C12-C13-C15
31	a	309	CLA	C11-C10-C8-C7
31	7	313	CLA	CHA-CBD-CGD-O1D
31	7	313	CLA	CAD-CBD-CGD-O2D
31	8	320	CLA	C3A-C2A-CAA-CBA
31	O	202	CLA	CHA-CBD-CGD-O1D
31	2	306	CLA	C3A-C2A-CAA-CBA
31	5	315	CLA	C12-C13-C15-C16
32	4	310	CHL	C3A-C2A-CAA-CBA
28	A	810	LHG	O8-C23-C24-C25
28	A	811	LHG	O7-C7-C8-C9
31	A	834	CLA	CAA-CBA-CGA-O2A
32	A	840	CHL	CAA-CBA-CGA-O2A
32	5	322	CHL	CAA-CBA-CGA-O2A
41	8	305	DGA	OG1-CA1-CA2-CA3
31	B	844	CLA	C5-C6-C7-C8
28	a	306	LHG	O10-C23-C24-C25
31	a	322	CLA	CAA-CBA-CGA-O1A
31	4	309	CLA	CAA-CBA-CGA-O1A
31	5	313	CLA	CAA-CBA-CGA-O1A
26	6	302	BCR	C13-C14-C15-C16
36	J	103	LUT	C29-C30-C31-C32
36	2	301	LUT	C9-C10-C11-C12
27	9	306	LMT	C6-C7-C8-C9
31	A	853	CLA	C13-C15-C16-C17
31	A	834	CLA	CAA-CBA-CGA-O1A
37	J	104	LMG	O9-C10-C11-C12
33	B	808	DGD	C2B-C1B-O2G-C2G
37	G	202	LMG	C14-C15-C16-C17
31	A	815	CLA	CAA-CBA-CGA-O2A
31	a	313	CLA	CAA-CBA-CGA-O2A
31	8	320	CLA	CAA-CBA-CGA-O2A
31	2	307	CLA	CAA-CBA-CGA-O2A
32	7	324	CHL	CAA-CBA-CGA-O2A
37	a	301	LMG	O8-C28-C29-C30
41	8	305	DGA	OA1-CA1-CA2-CA3
31	b	308	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	A	824	CLA	C10-C11-C12-C13
31	3	311	CLA	C10-C11-C12-C13
31	8	310	CLA	C10-C11-C12-C13
32	7	324	CHL	C10-C11-C12-C13
32	5	316	CHL	C5-C6-C7-C8
28	A	811	LHG	O9-C7-C8-C9
31	2	313	CLA	CAA-CBA-CGA-O2A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	F	303	QTB	C11-C12-C14-C15-C16-C17
35	7	303	QTB	C11-C12-C14-C15-C16-C17

268 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	5	305	LHG	1	0
31	6	308	CLA	1	0
31	7	321	CLA	1	0
31	a	314	CLA	2	0
32	5	316	CHL	6	0
41	8	305	DGA	2	0
31	A	838	CLA	1	0
31	B	843	CLA	2	0
26	O	201	BCR	2	0
32	6	318	CHL	5	0
31	A	820	CLA	2	0
31	5	311	CLA	2	0
32	a	318	CHL	4	0
31	G	204	CLA	1	0
31	A	823	CLA	4	0
36	2	301	LUT	4	0
31	a	310	CLA	1	0
31	5	308	CLA	1	0
31	A	825	CLA	4	0
31	A	845	CLA	4	0
26	2	302	BCR	3	0
31	B	834	CLA	3	0
31	5	323	CLA	3	0
31	A	835	CLA	3	0
31	A	856	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	823	CLA	1	0
31	2	313	CLA	2	0
31	4	318	CLA	5	0
26	K	203	BCR	3	0
31	3	318	CLA	1	0
31	B	814	CLA	3	0
38	a	304	AXT	1	0
26	A	803	BCR	3	0
31	4	308	CLA	1	0
31	G	205	CLA	1	0
31	a	321	CLA	1	0
36	4	302	LUT	7	0
31	a	312	CLA	2	0
31	3	313	CLA	2	0
28	B	807	LHG	1	0
32	3	315	CHL	1	0
36	a	305	LUT	6	0
26	B	802	BCR	4	0
31	b	305	CLA	1	0
31	7	313	CLA	1	0
32	A	831	CHL	2	0
36	3	305	LUT	7	0
31	5	307	CLA	2	0
31	3	311	CLA	2	0
32	8	316	CHL	8	0
31	8	317	CLA	1	0
32	5	319	CHL	4	0
31	3	308	CLA	2	0
31	J	105	CLA	1	0
31	3	314	CLA	1	0
31	A	816	CLA	2	0
36	4	303	LUT	4	0
32	b	309	CHL	1	0
31	A	814	CLA	5	0
31	A	821	CLA	3	0
31	K	206	CLA	1	0
27	A	807	LMT	4	0
31	A	830	CLA	2	0
31	7	311	CLA	3	0
31	B	838	CLA	1	0
31	4	305	CLA	5	0
26	3	303	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	L	304	LUT	1	0
31	A	834	CLA	6	0
31	B	847	CLA	2	0
31	H	902	CLA	6	0
31	4	314	CLA	5	0
31	8	307	CLA	1	0
31	A	848	CLA	1	0
31	B	833	CLA	1	0
31	3	320	CLA	2	0
31	A	849	CLA	1	0
31	B	832	CLA	2	0
31	7	309	CLA	1	0
31	A	850	CLA	2	0
32	4	317	CHL	7	0
31	8	314	CLA	1	0
31	6	322	CLA	3	0
31	4	319	CLA	1	0
32	8	319	CHL	1	0
26	M	101	BCR	3	0
32	4	313	CHL	3	0
32	4	310	CHL	7	0
36	6	304	LUT	3	0
33	B	808	DGD	4	0
31	a	311	CLA	1	0
31	B	819	CLA	2	0
26	B	805	BCR	5	0
26	G	201	BCR	1	0
31	A	837	CLA	4	0
32	9	320	CHL	3	0
31	A	826	CLA	3	0
28	a	306	LHG	9	0
31	5	309	CLA	1	0
31	B	811	CLA	1	0
31	B	837	CLA	4	0
37	G	202	LMG	4	0
31	2	314	CLA	3	0
32	7	319	CHL	3	0
32	a	317	CHL	6	0
32	7	324	CHL	3	0
31	B	826	CLA	1	0
31	2	311	CLA	1	0
31	A	853	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	F	302	BCR	1	0
31	2	304	CLA	4	0
31	A	822	CLA	2	0
36	9	305	LUT	1	0
32	A	840	CHL	5	0
31	B	818	CLA	2	0
26	B	804	BCR	4	0
31	A	815	CLA	3	0
31	A	819	CLA	3	0
31	A	846	CLA	3	0
26	B	806	BCR	2	0
31	A	832	CLA	2	0
26	8	301	BCR	4	0
31	4	315	CLA	2	0
31	G	206	CLA	6	0
31	B	848	CLA	2	0
26	K	202	BCR	4	0
31	b	313	CLA	3	0
36	J	103	LUT	3	0
31	A	836	CLA	3	0
32	6	319	CHL	2	0
31	4	321	CLA	1	0
31	2	310	CLA	1	0
36	7	305	LUT	3	0
31	4	316	CLA	4	0
28	7	307	LHG	4	0
31	F	301	CLA	3	0
36	9	302	LUT	1	0
36	3	304	LUT	3	0
31	b	308	CLA	1	0
31	5	313	CLA	1	0
28	A	810	LHG	2	0
31	7	315	CLA	4	0
31	H	903	CLA	2	0
36	F	304	LUT	2	0
36	5	304	LUT	6	0
31	8	321	CLA	2	0
31	A	857	CLA	3	0
36	8	303	LUT	2	0
31	2	312	CLA	1	0
39	7	301	3PH	1	0
26	L	301	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	315	CLA	1	0
26	3	302	BCR	4	0
26	A	806	BCR	4	0
36	5	303	LUT	3	0
32	5	317	CHL	4	0
31	B	850	CLA	4	0
32	5	322	CHL	4	0
31	a	309	CLA	3	0
31	L	305	CLA	6	0
32	6	320	CHL	1	0
30	A	813	CL0	3	0
31	4	312	CLA	1	0
31	A	828	CLA	2	0
31	B	817	CLA	2	0
31	A	854	CLA	1	0
31	B	831	CLA	2	0
31	H	901	CLA	2	0
31	B	845	CLA	4	0
31	B	815	CLA	1	0
31	8	320	CLA	1	0
32	6	309	CHL	7	0
24	A	801	PQN	1	0
32	6	317	CHL	3	0
37	a	301	LMG	2	0
32	6	321	CHL	2	0
31	6	314	CLA	2	0
31	6	315	CLA	1	0
31	B	813	CLA	4	0
26	J	102	BCR	1	0
31	a	315	CLA	3	0
43	5	306	PTY	1	0
31	B	844	CLA	2	0
32	a	320	CHL	3	0
31	8	313	CLA	1	0
31	2	306	CLA	3	0
31	A	855	CLA	3	0
26	3	301	BCR	1	0
31	3	309	CLA	6	0
31	B	840	CLA	2	0
28	A	809	LHG	2	0
36	9	303	LUT	6	0
26	6	302	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	841	CLA	3	0
31	6	316	CLA	1	0
31	4	311	CLA	1	0
26	B	803	BCR	1	0
31	B	816	CLA	2	0
36	6	303	LUT	2	0
31	7	322	CLA	1	0
31	A	833	CLA	3	0
26	A	804	BCR	2	0
31	5	320	CLA	1	0
31	6	312	CLA	1	0
31	8	308	CLA	3	0
31	5	315	CLA	1	0
31	8	310	CLA	3	0
31	b	302	CLA	1	0
31	3	310	CLA	1	0
31	A	843	CLA	2	0
31	6	306	CLA	5	0
31	5	310	CLA	4	0
31	B	839	CLA	2	0
31	B	812	CLA	2	0
36	a	303	LUT	4	0
31	B	836	CLA	1	0
26	L	302	BCR	2	0
37	J	101	LMG	4	0
32	7	317	CHL	6	0
31	A	852	CLA	1	0
31	9	314	CLA	2	0
28	6	301	LHG	2	0
31	A	851	CLA	3	0
31	A	827	CLA	2	0
31	8	315	CLA	1	0
31	b	311	CLA	1	0
42	4	304	SQD	1	0
31	9	313	CLA	1	0
31	B	822	CLA	3	0
31	8	311	CLA	4	0
26	5	302	BCR	2	0
31	a	313	CLA	1	0
24	B	801	PQN	2	0
31	6	313	CLA	1	0
31	a	319	CLA	3	0

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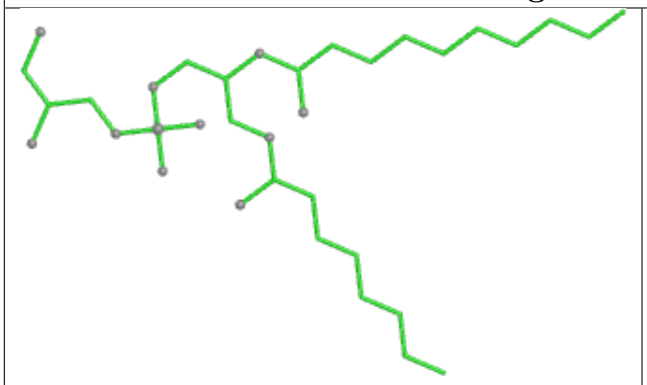
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	F	306	CLA	1	0
26	A	805	BCR	2	0
31	A	829	CLA	10	0
31	8	309	CLA	1	0
26	I	801	BCR	1	0
32	K	201	CHL	1	0
28	A	811	LHG	3	0
34	B	851	LAP	4	0
31	2	308	CLA	1	0
32	7	318	CHL	9	0
31	A	824	CLA	1	0
32	7	320	CHL	6	0
31	a	316	CLA	1	0
31	B	820	CLA	3	0
32	9	322	CHL	3	0
31	B	842	CLA	4	0
36	b	301	LUT	5	0
31	A	818	CLA	3	0
31	6	307	CLA	2	0
31	B	825	CLA	4	0
28	6	305	LHG	1	0
26	L	303	BCR	3	0
28	7	302	LHG	4	0
31	9	315	CLA	1	0
31	3	319	CLA	4	0
26	7	304	BCR	6	0
31	6	311	CLA	1	0
31	B	846	CLA	3	0
36	8	302	LUT	5	0
31	5	318	CLA	5	0
31	A	841	CLA	5	0
31	B	835	CLA	2	0
32	A	839	CHL	4	0

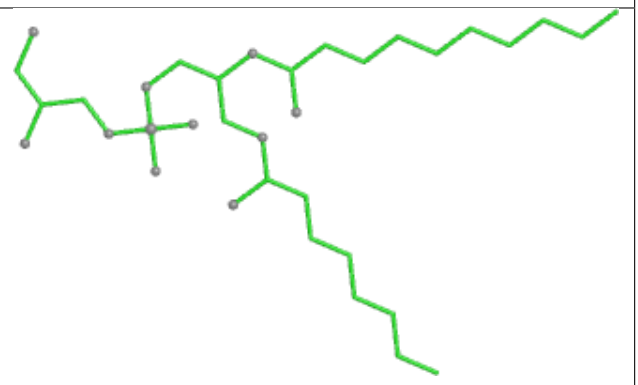
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

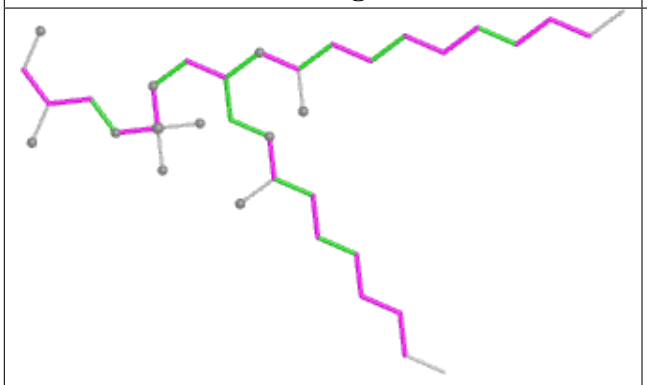
Ligand LHG 5 305



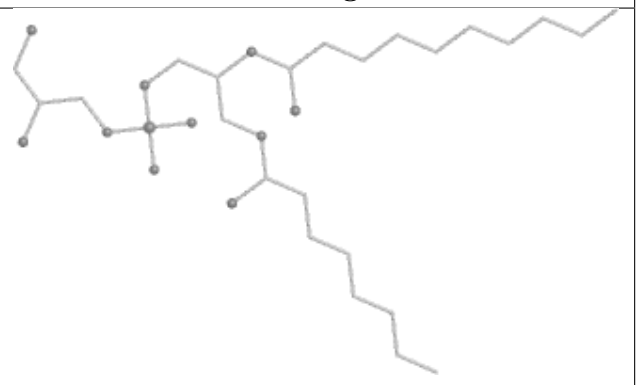
Bond lengths



Bond angles

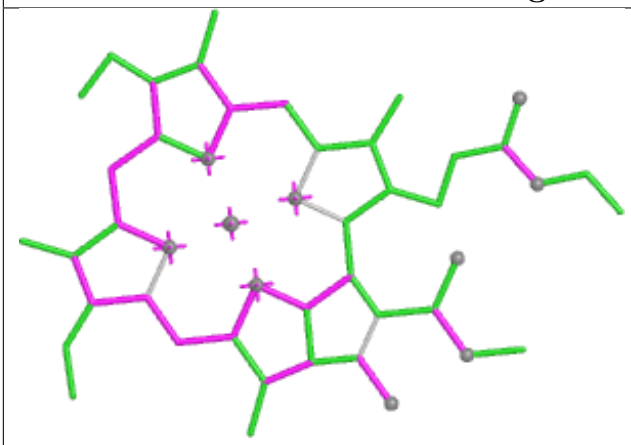


Torsions

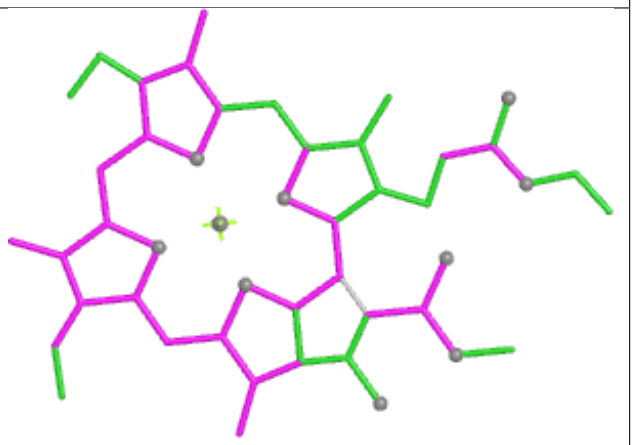


Rings

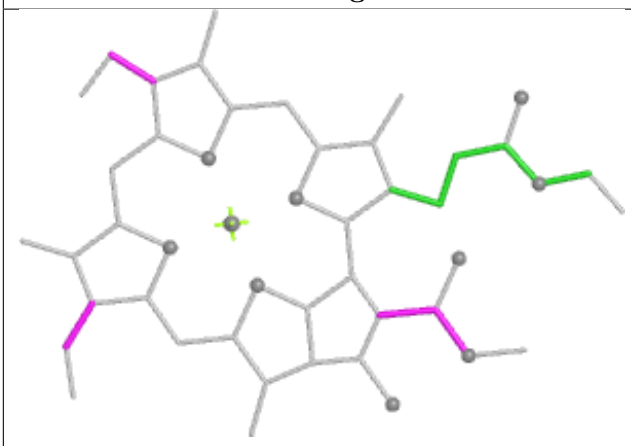
Ligand CLA 6 308



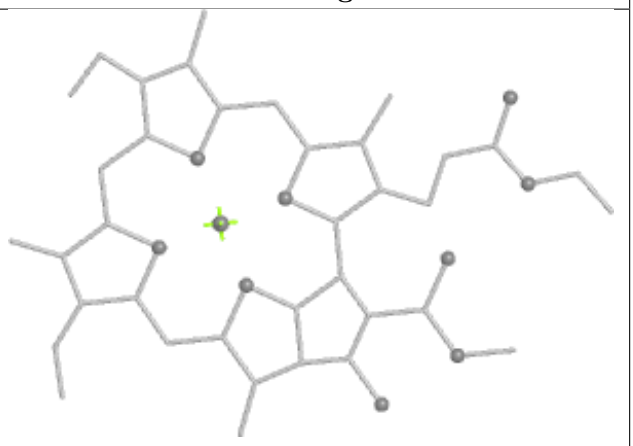
Bond lengths



Bond angles

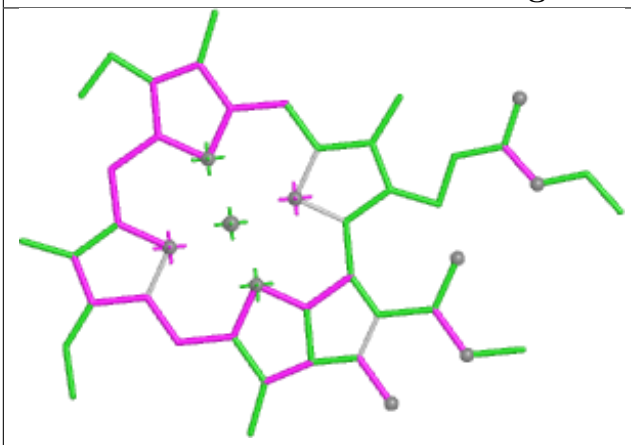


Torsions

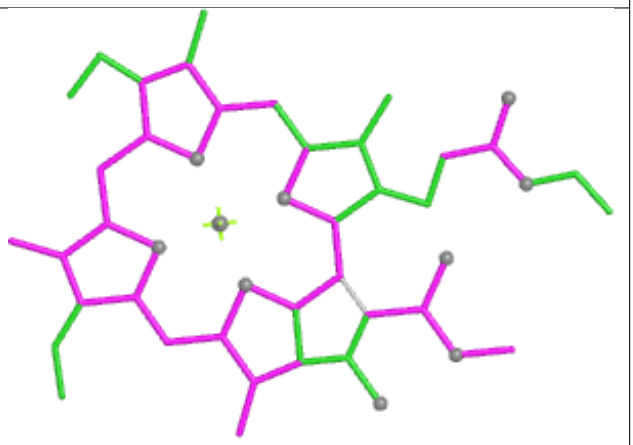


Rings

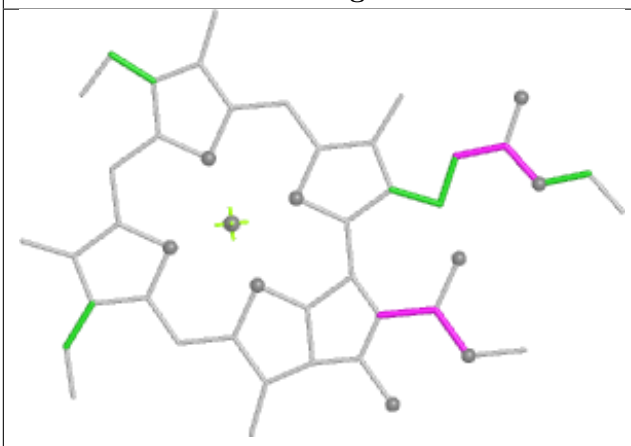
Ligand CLA 7 321



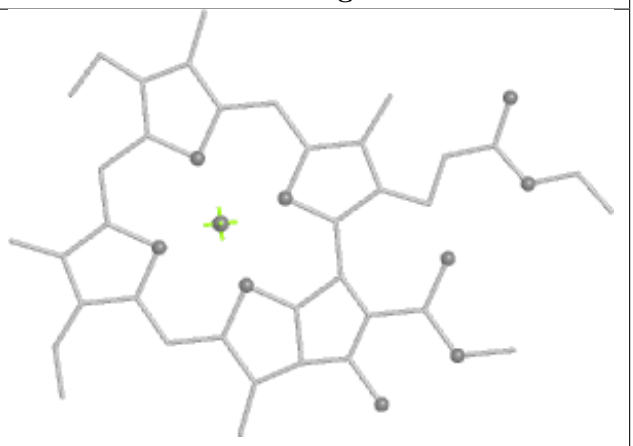
Bond lengths



Bond angles

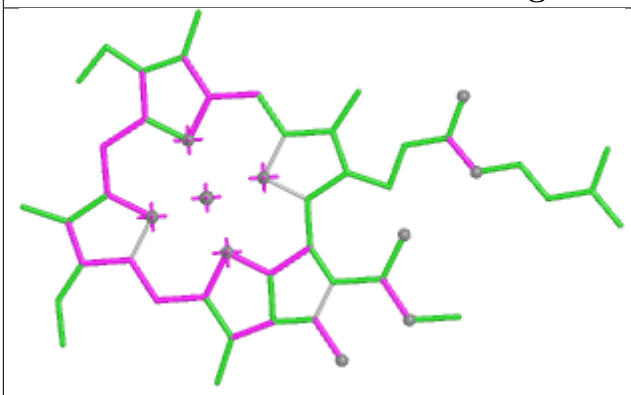


Torsions

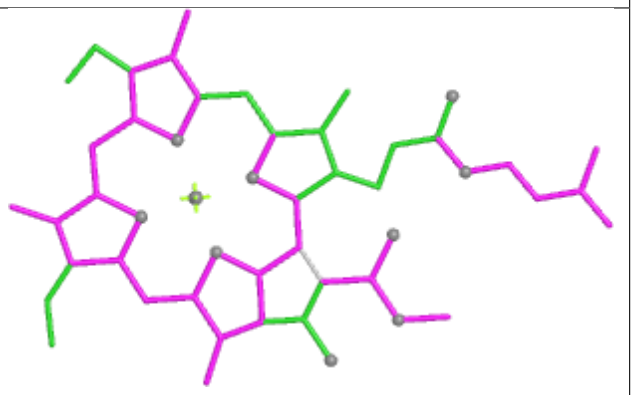


Rings

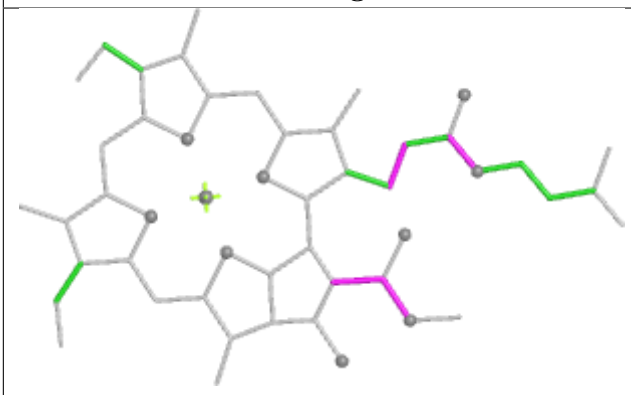
Ligand CLA a 314



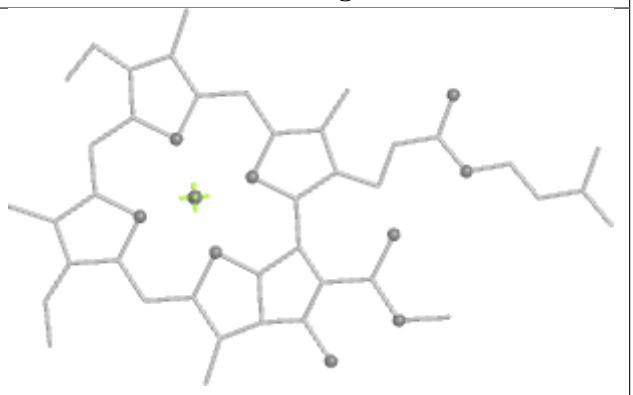
Bond lengths



Bond angles

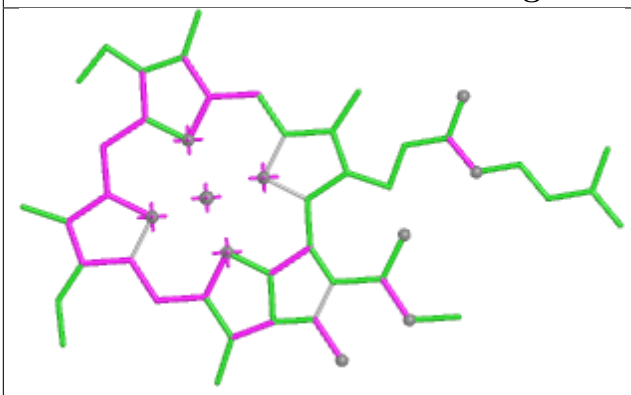


Torsions

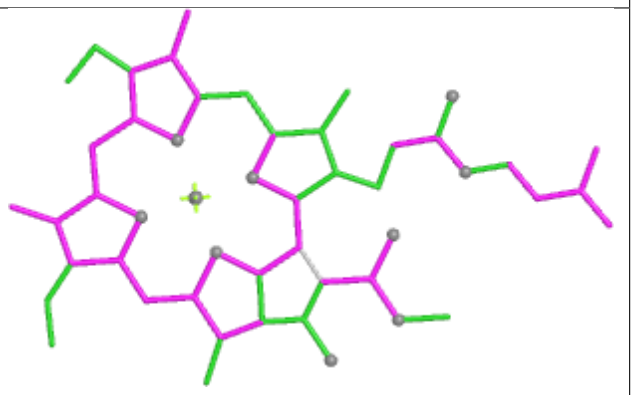


Rings

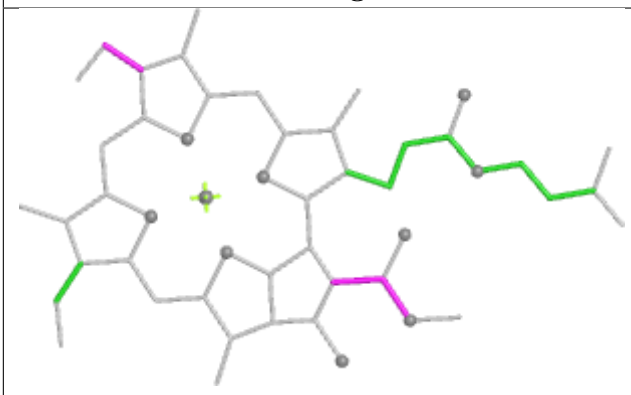
Ligand CLA K 204



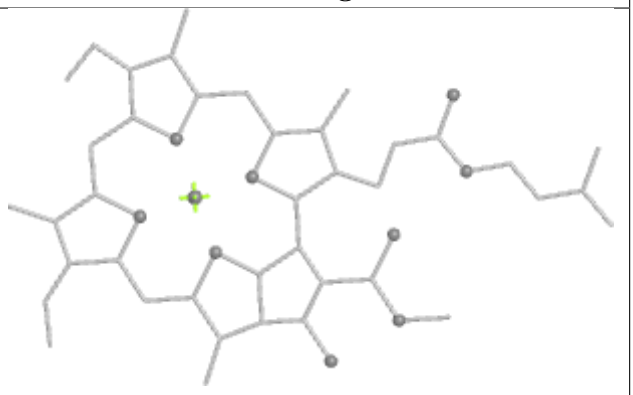
Bond lengths



Bond angles

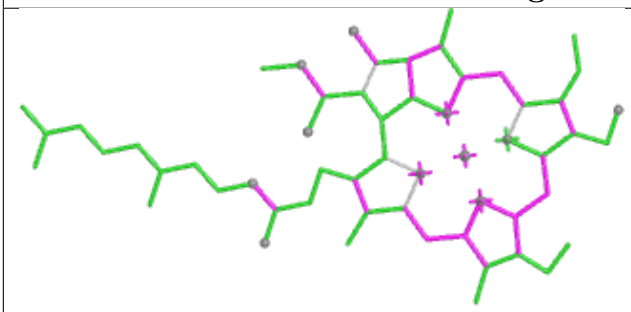


Torsions

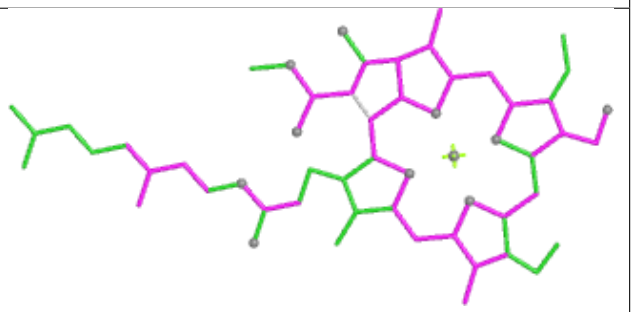


Rings

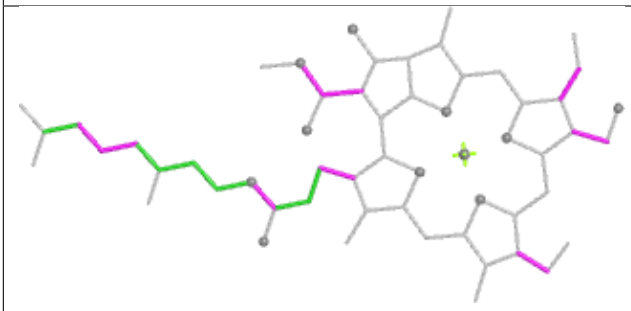
Ligand CHL 5 316



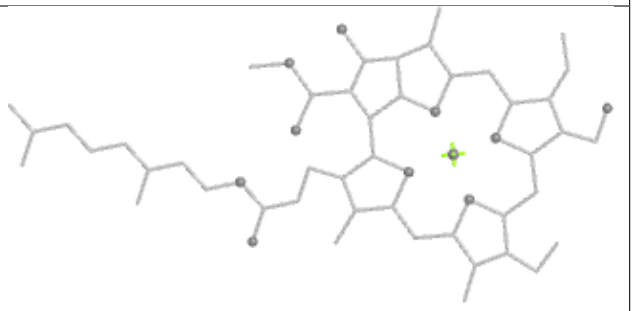
Bond lengths



Bond angles

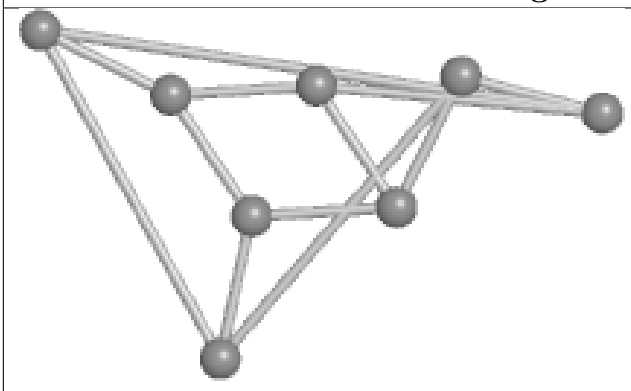


Torsions



Rings

Ligand SF4 A 802



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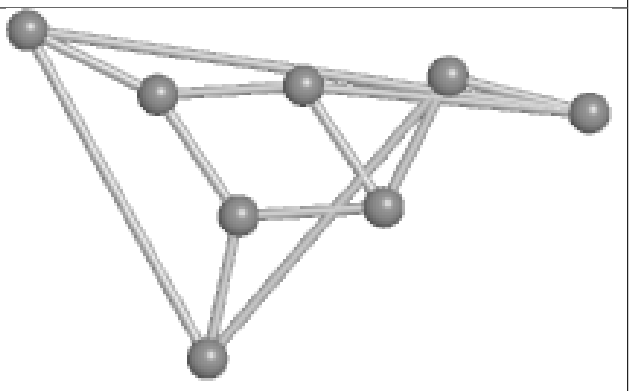
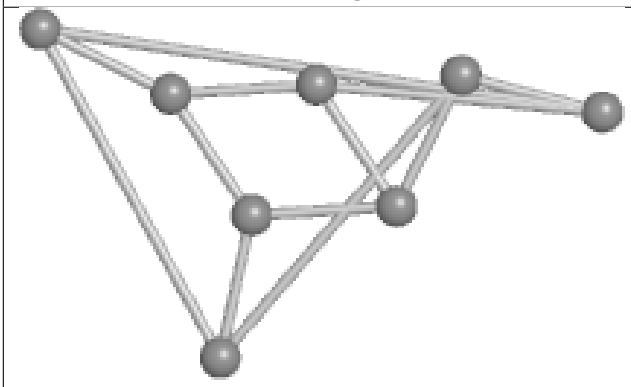


Bond angles



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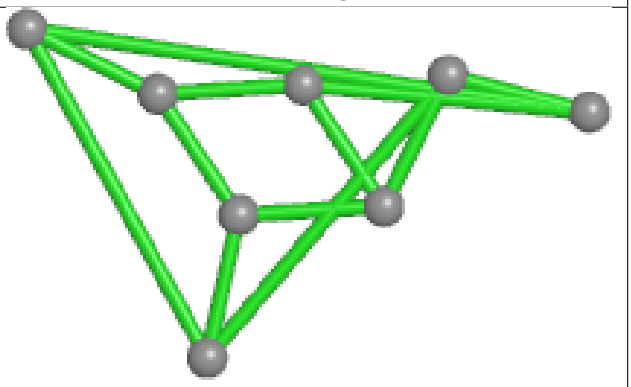
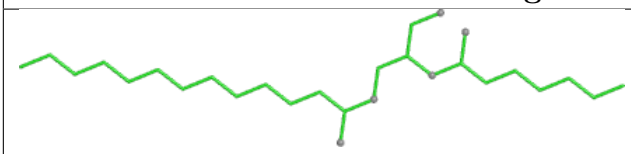


Rings

Ligand DGA 8 305



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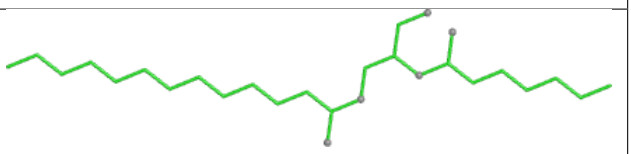
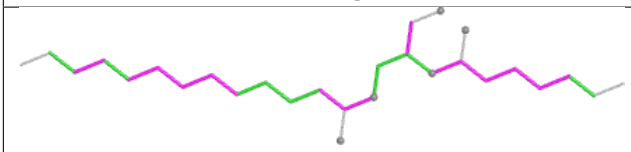
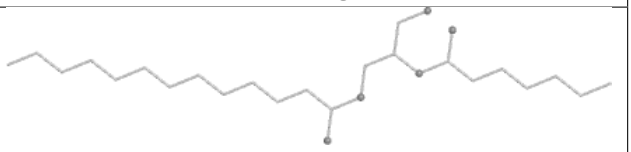


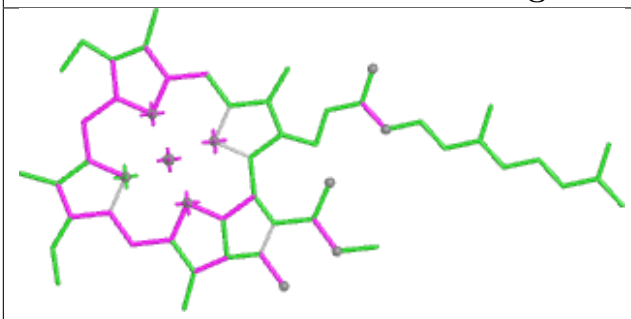
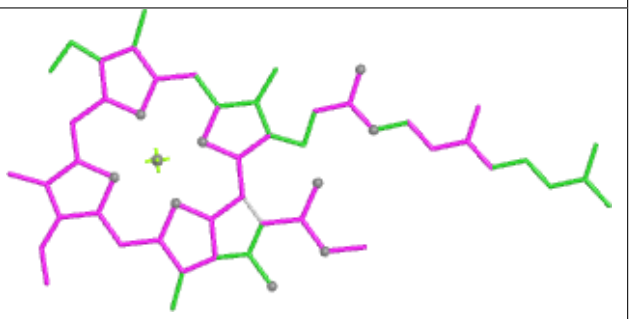
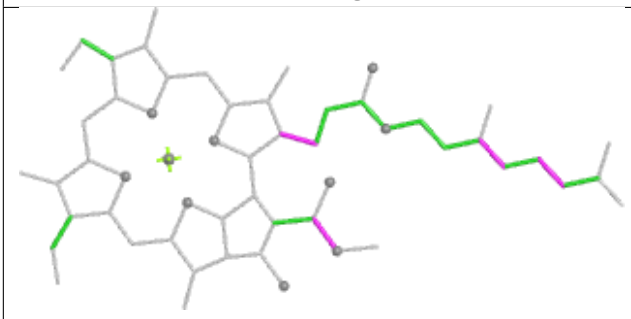
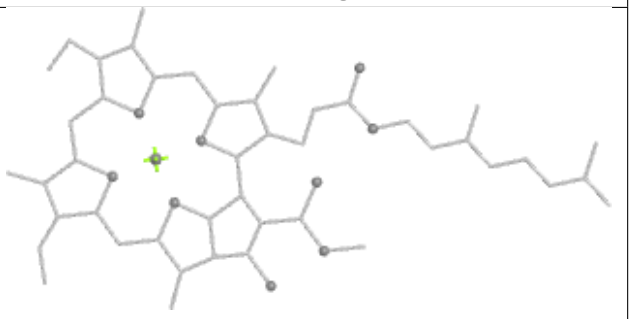
Bond angles

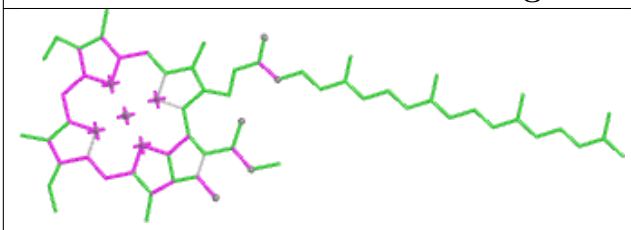
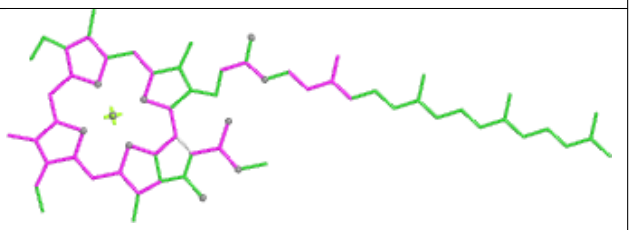
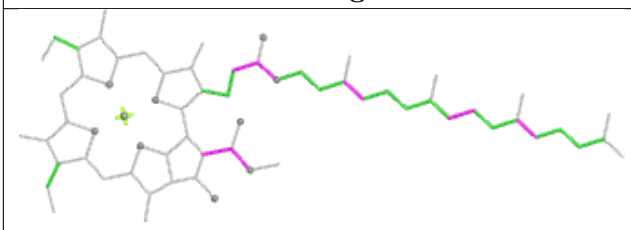
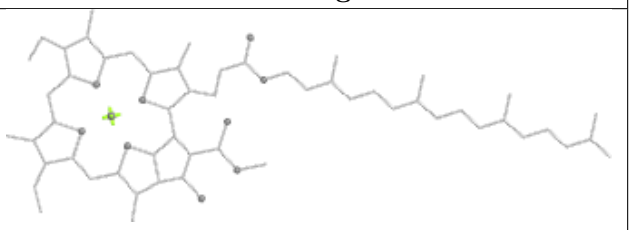


Torsions

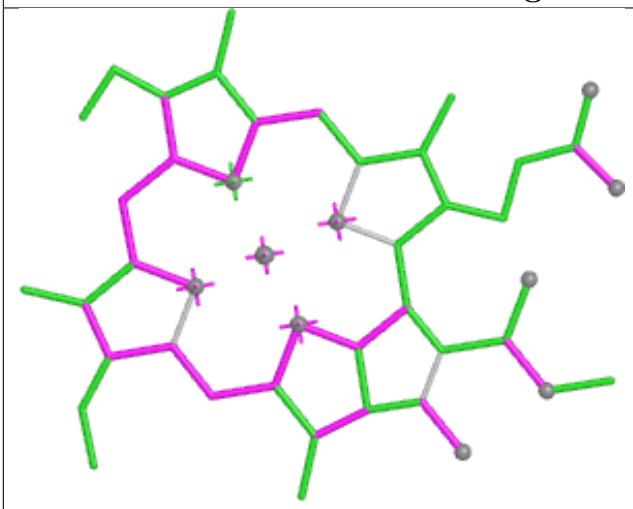


Rings

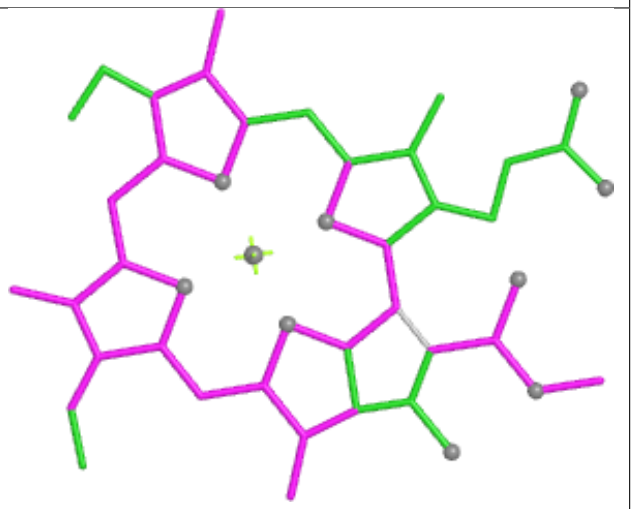
Ligand CLA 9 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

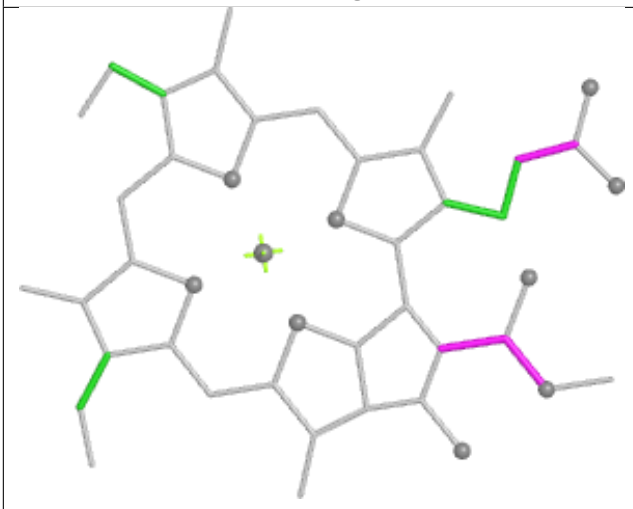
Ligand CLA B 843



Bond lengths



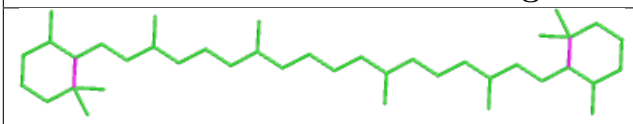
Bond angles



Torsions

Rings

Ligand BCR O 201



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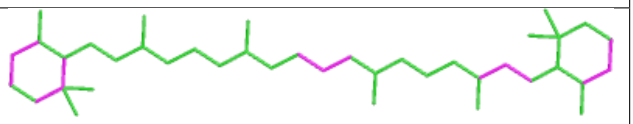

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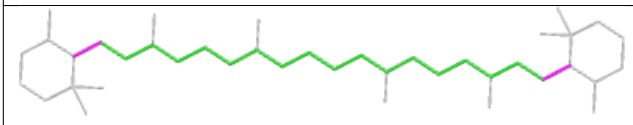

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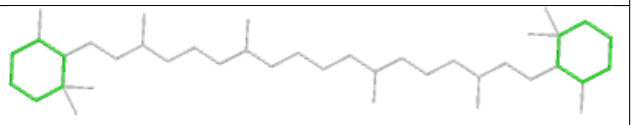
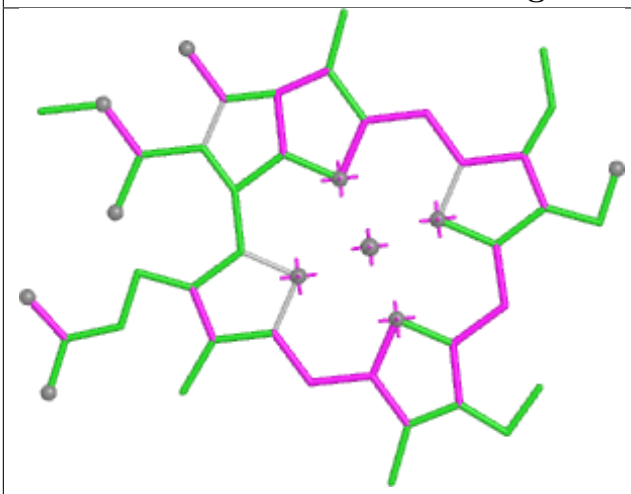


Rings

Ligand CHL 6 318



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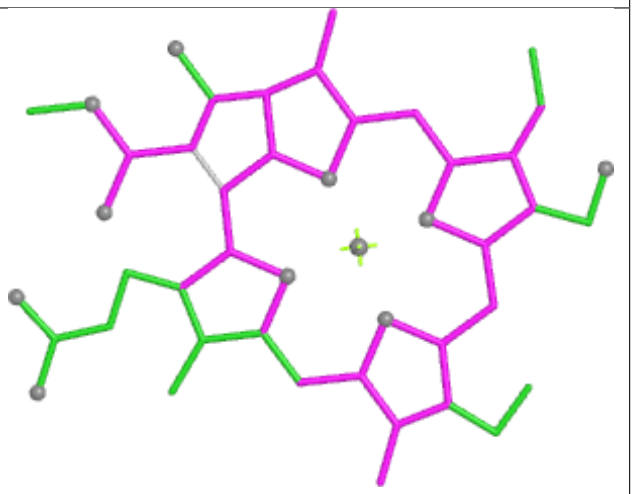
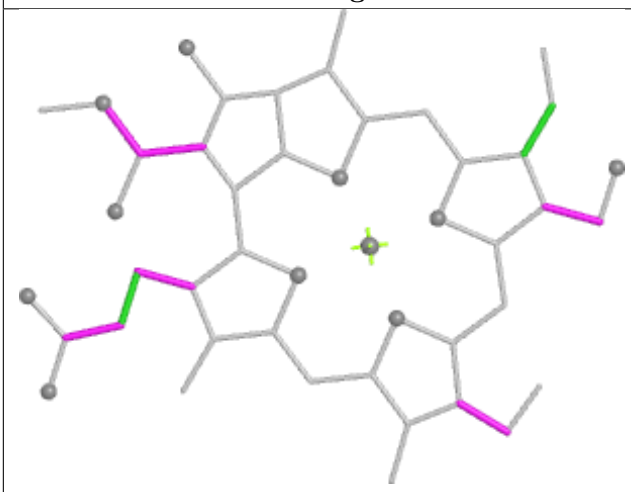


Bond angles



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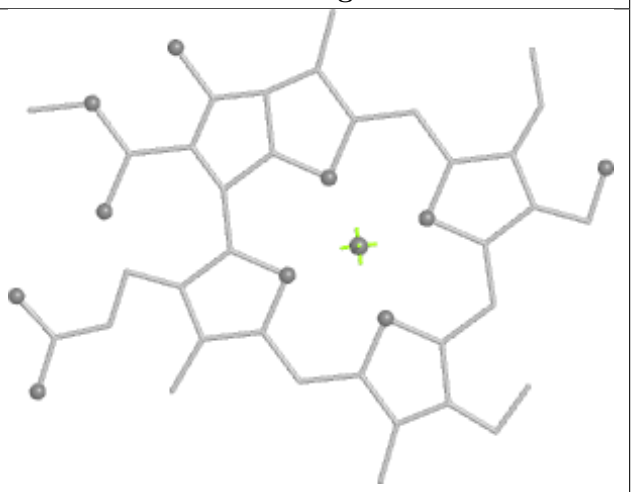
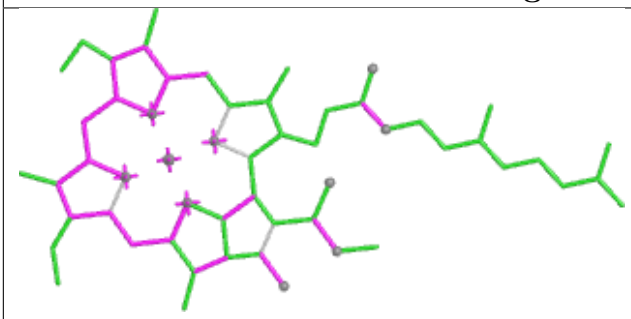
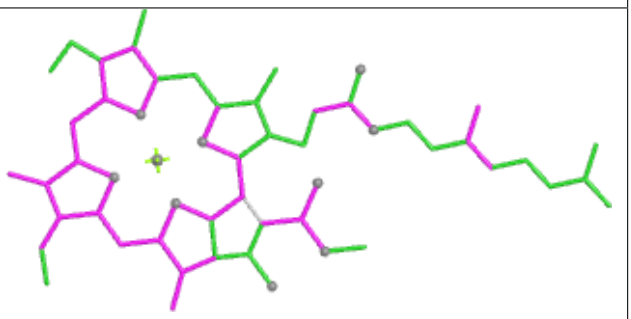


Rings

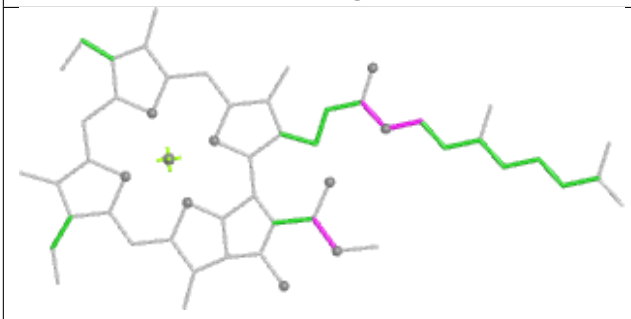
Ligand CLA A 820



Bond lengths



Bond angles



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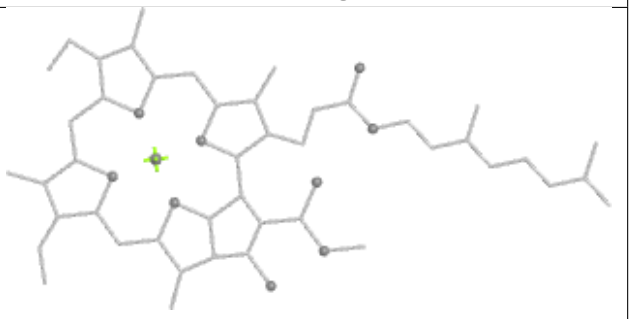
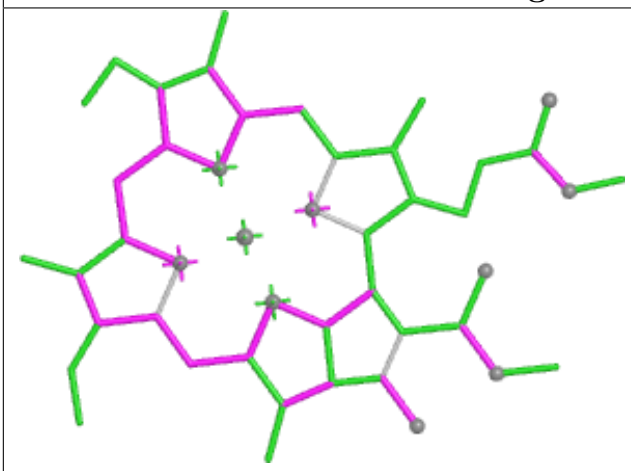


Rings

Ligand CLA 5 311



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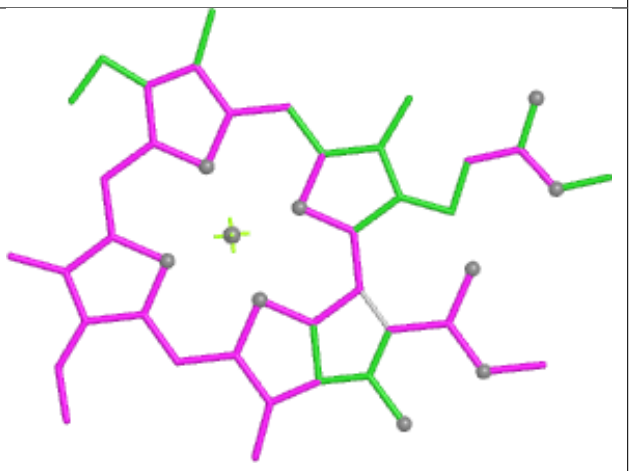
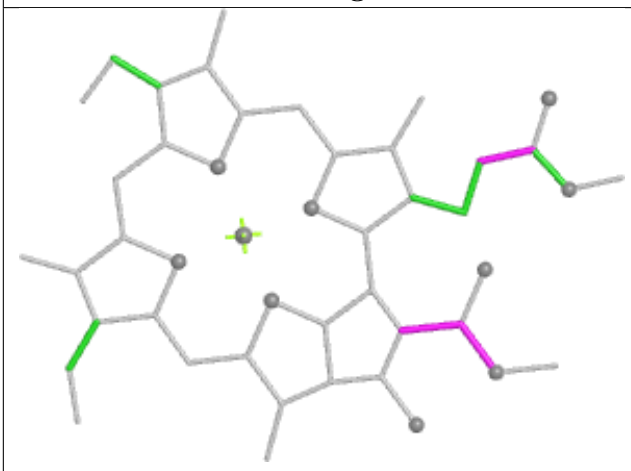
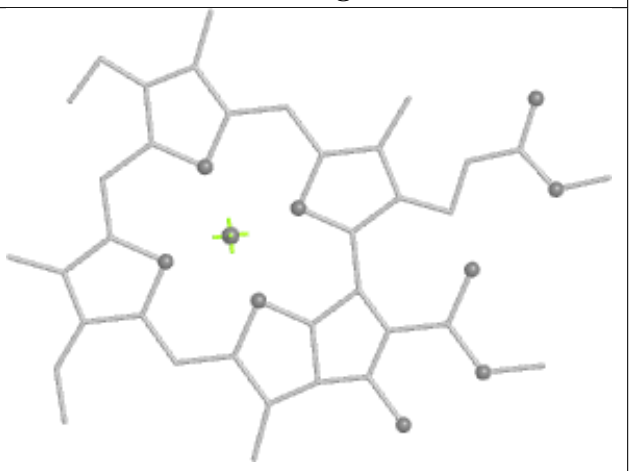


Bond angles

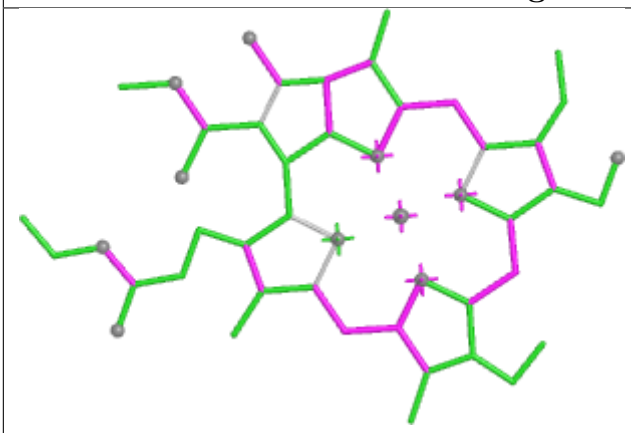


Torsions



Rings

Ligand CHL a 318



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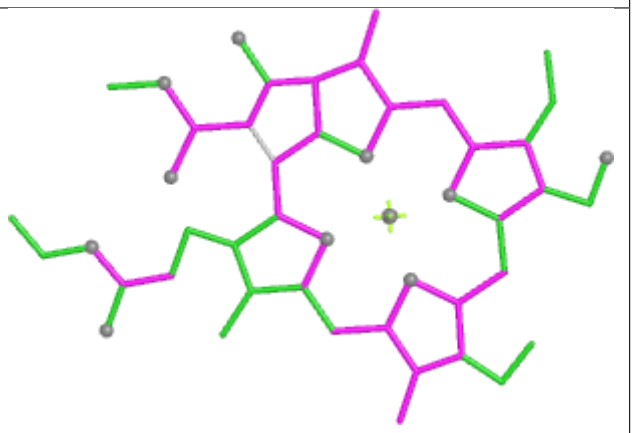
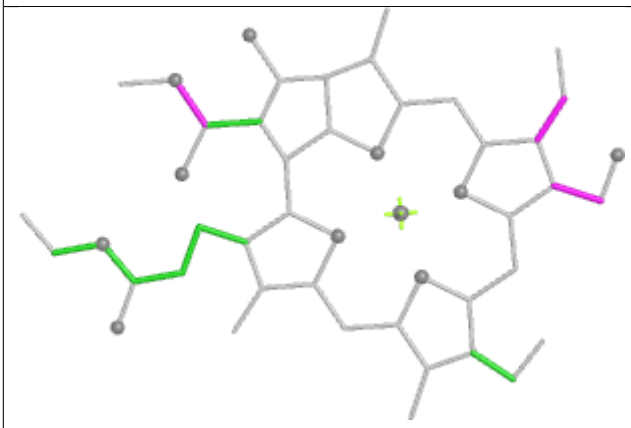


Bond angles



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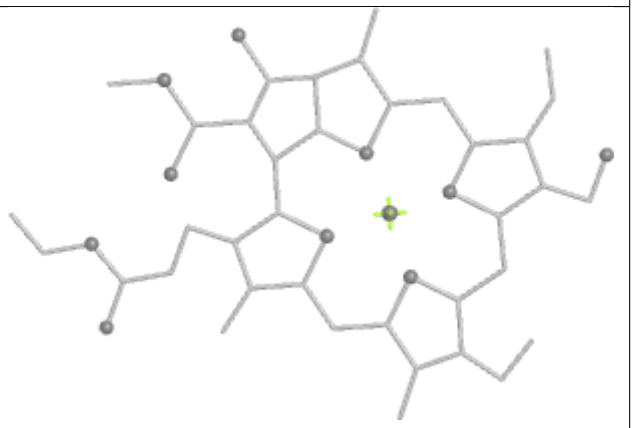
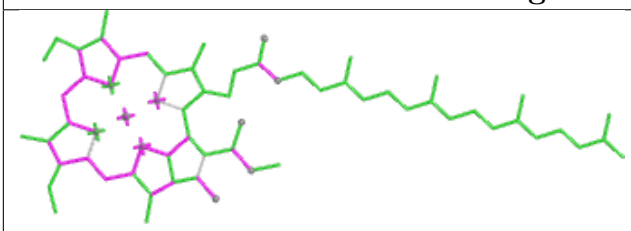


Rings

Ligand CLA 3 312



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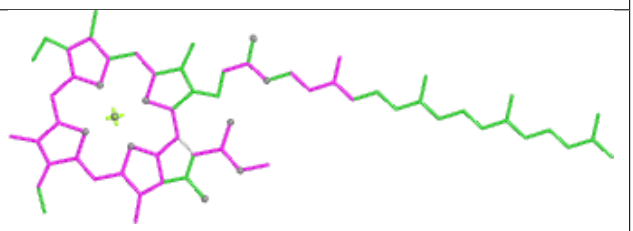
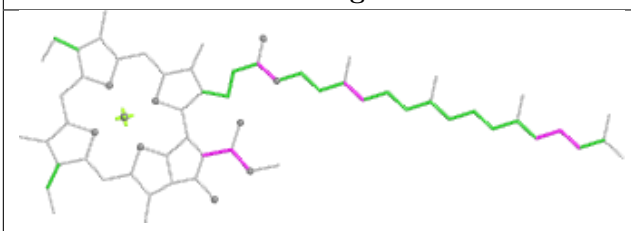
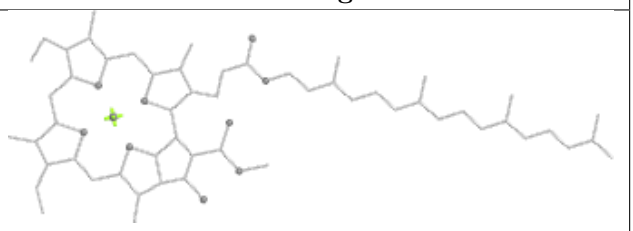


Bond angles

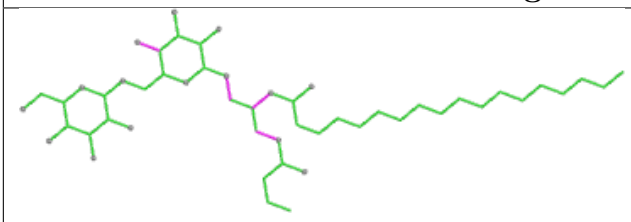


Torsions

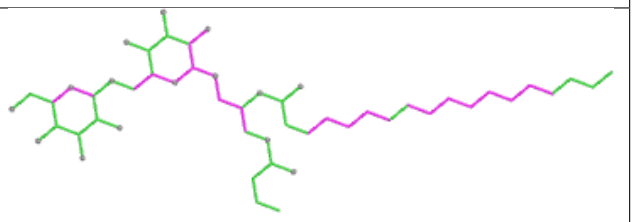


Rings

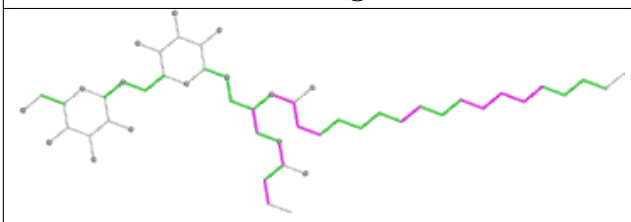
Ligand DGD 7 308



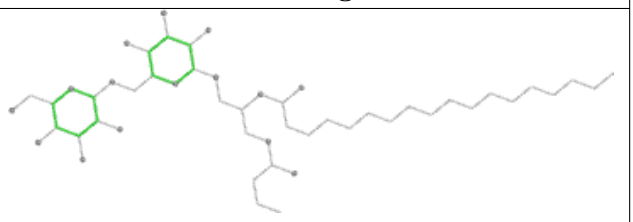
Bond lengths



Bond angles

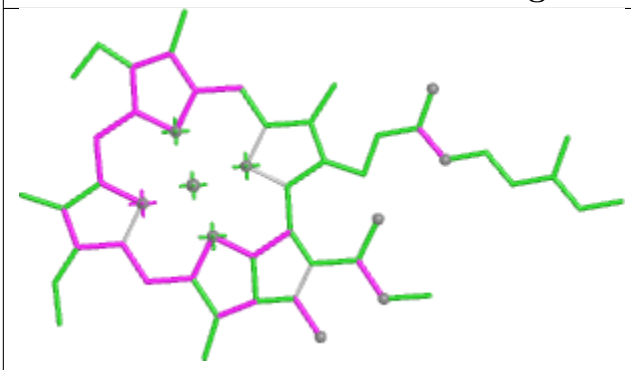


Torsions



Rings

Ligand CLA 3 317



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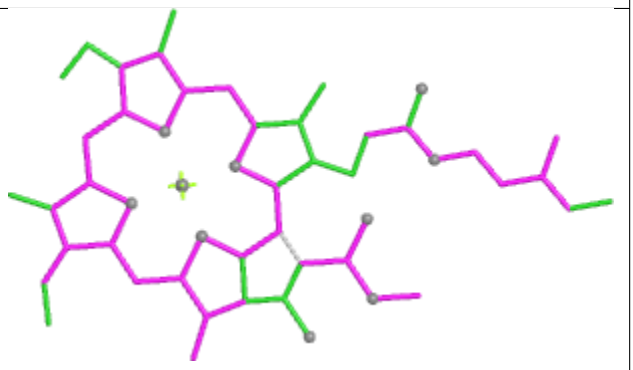
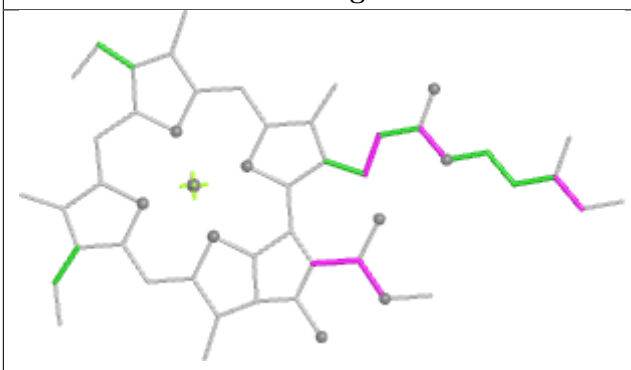
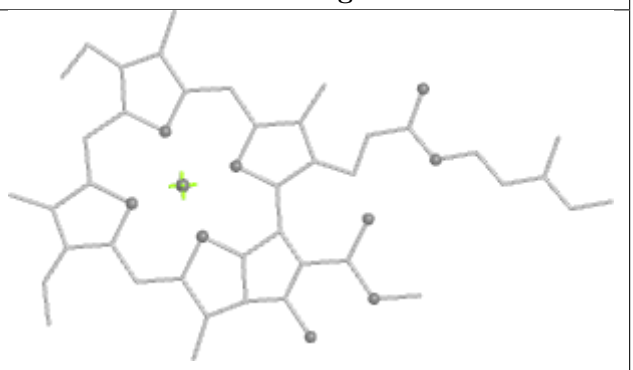


Bond angles

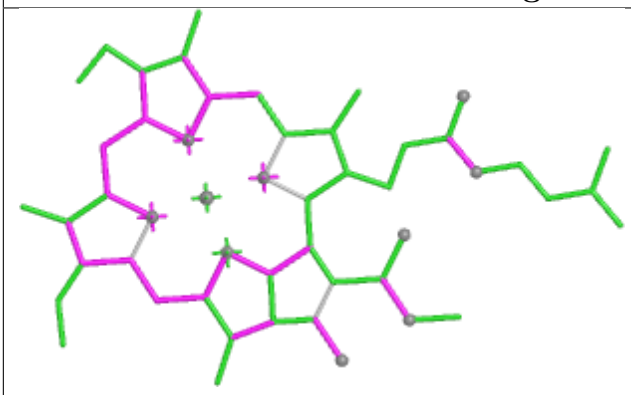


Torsions

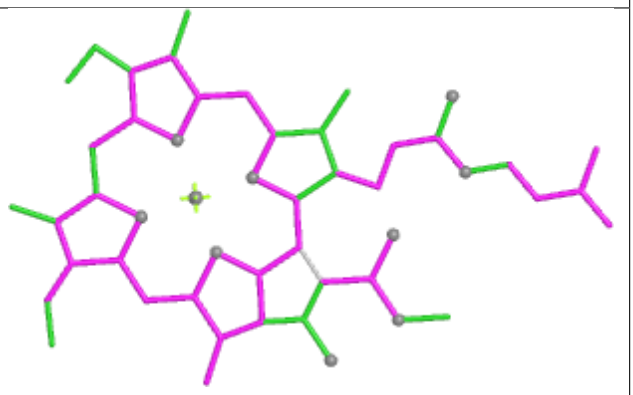


Rings

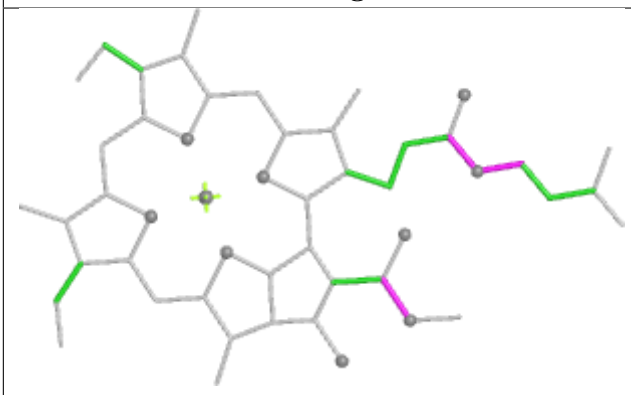
Ligand CLA G 204



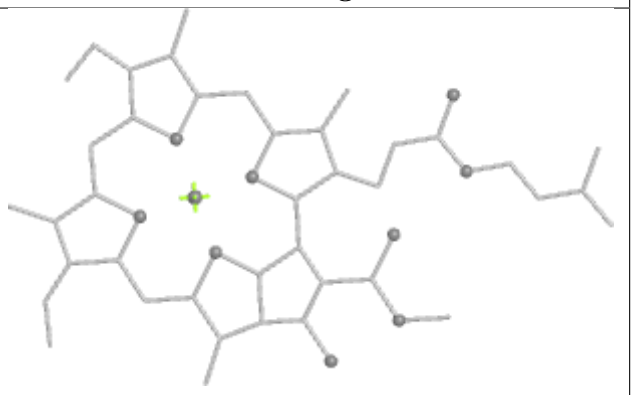
Bond lengths



Bond angles

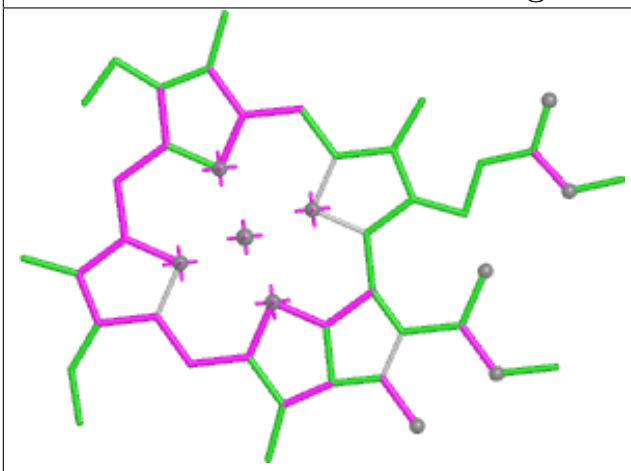


Torsions

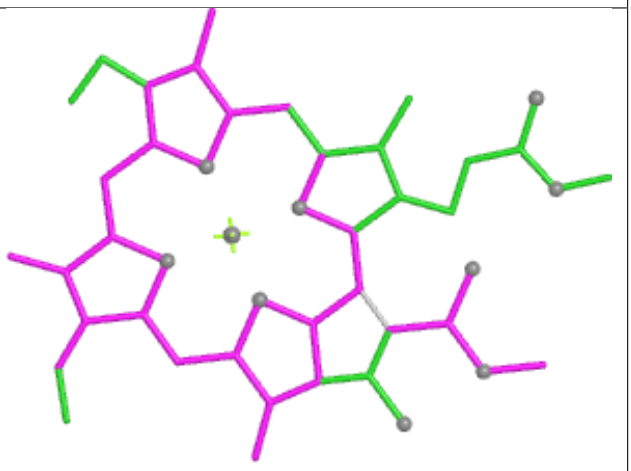


Rings

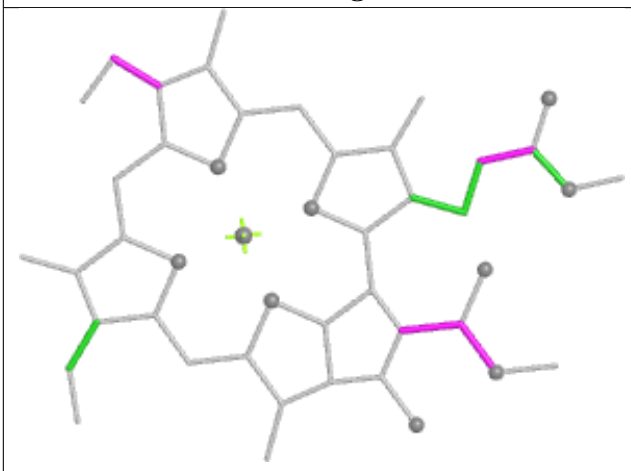
Ligand CLA b 307



Bond lengths



Bond angles



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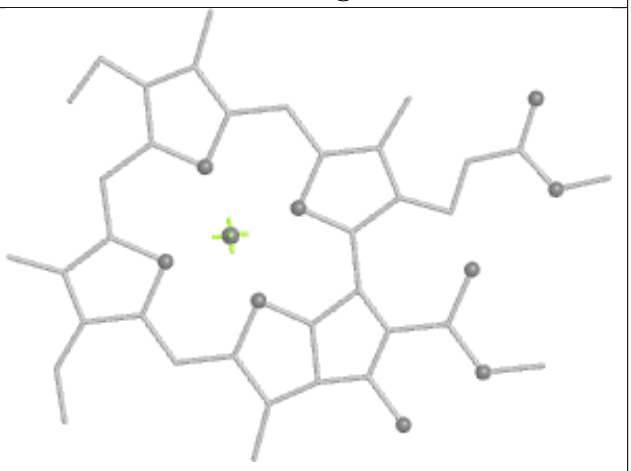
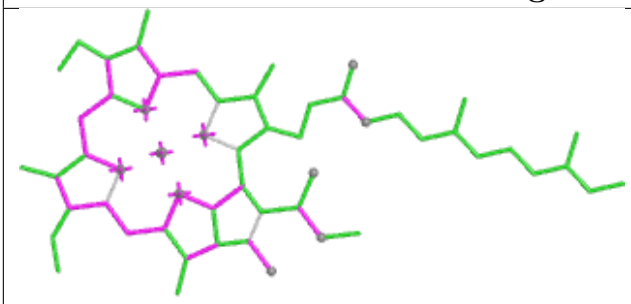
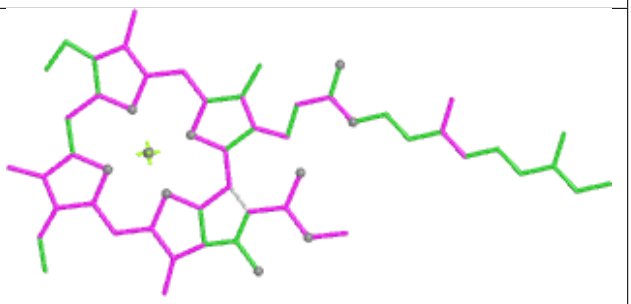


Rings

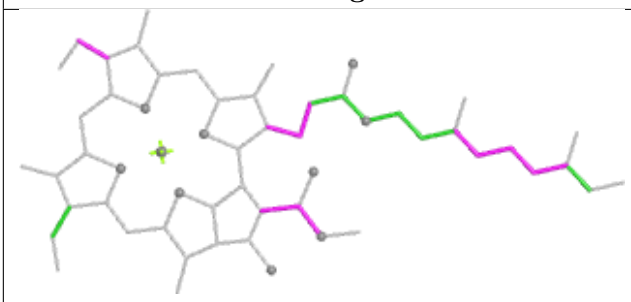
Ligand CLA 9 321



Bond lengths



Bond angles



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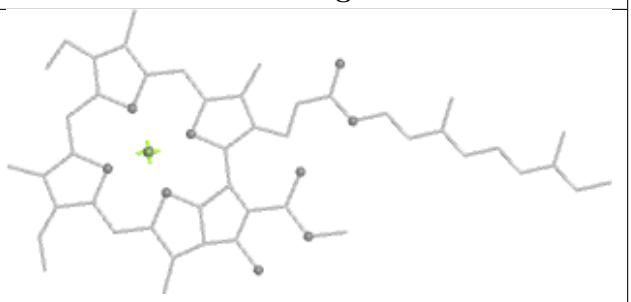
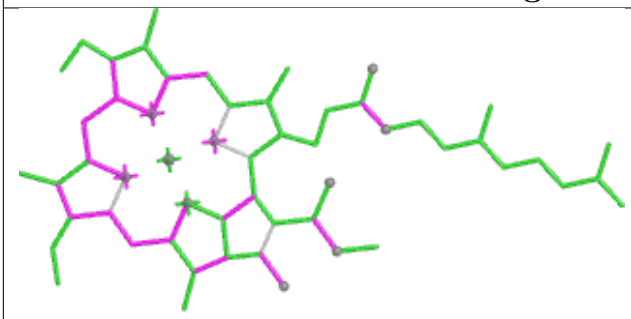
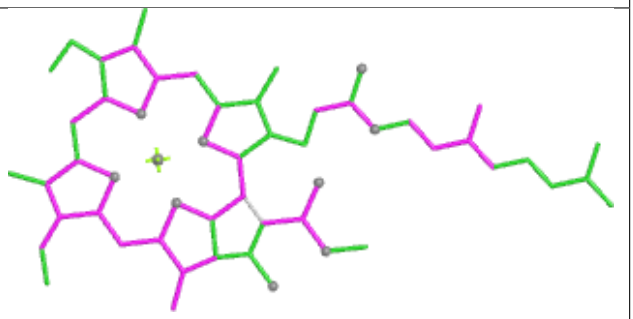


Rings

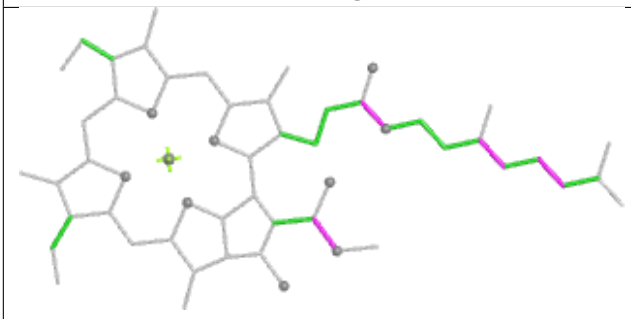
Ligand CLA A 823



Bond lengths



Bond angles



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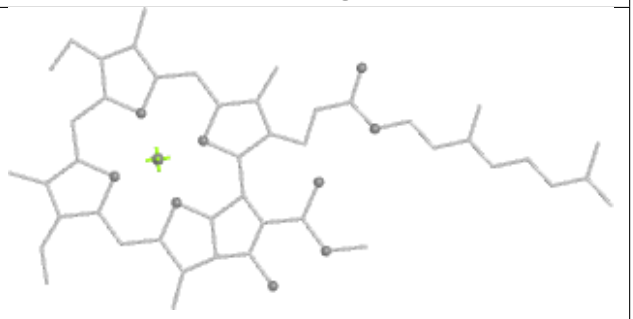
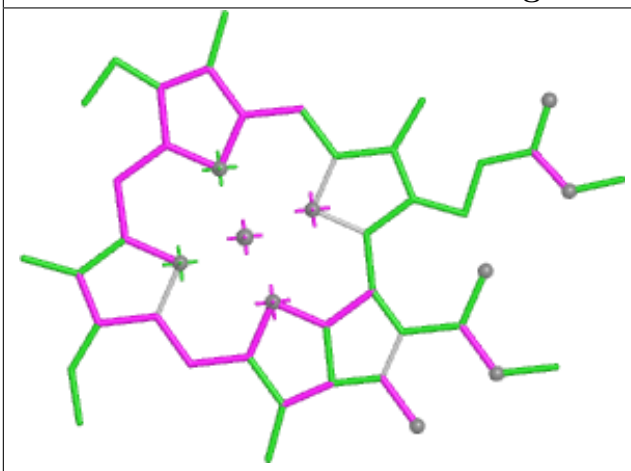


Rings

Ligand CLA K 205



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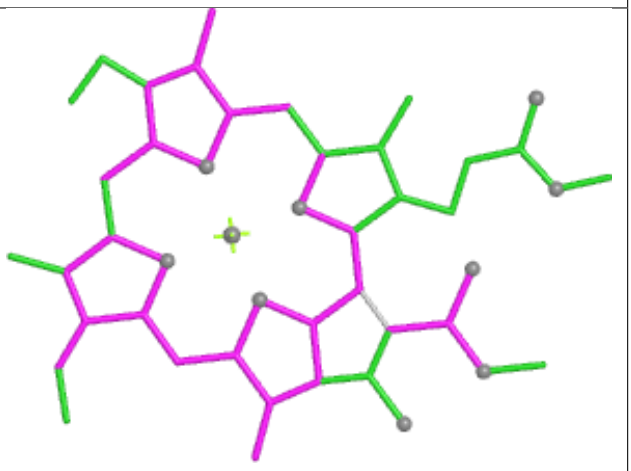
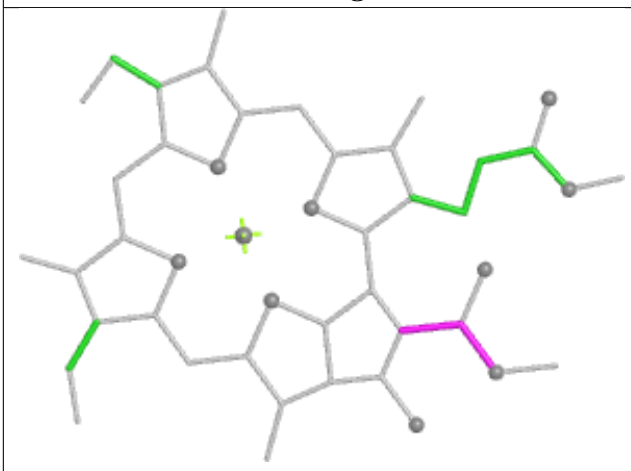


Bond angles



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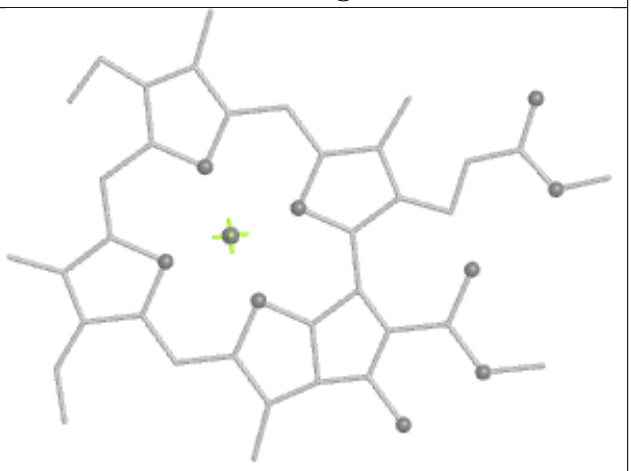
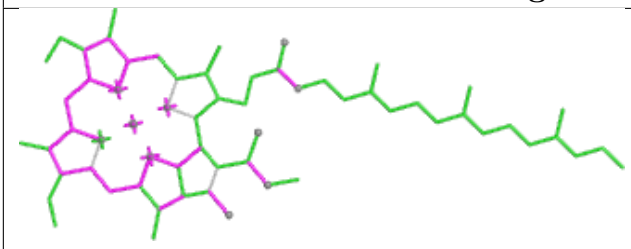


Rings

Ligand CLA 7 312



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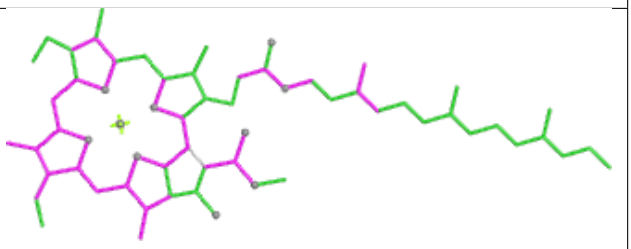
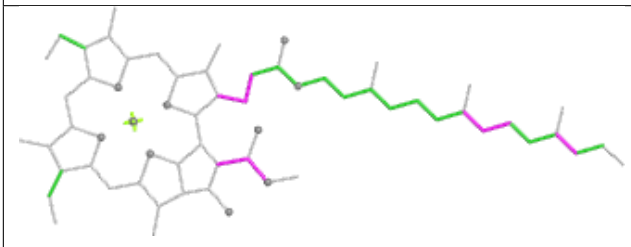


Bond angles



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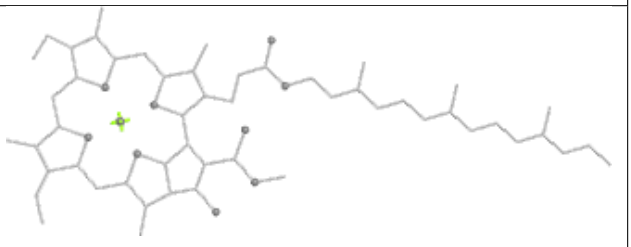
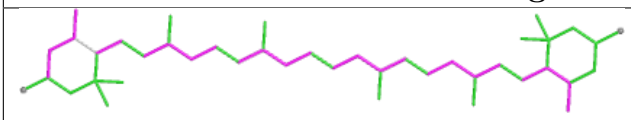


Rings

Ligand LUT 2 301



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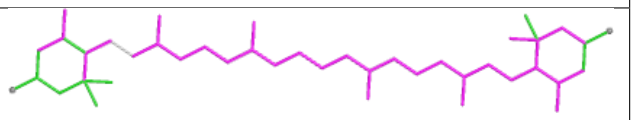
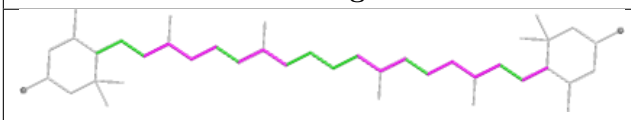


Bond angles



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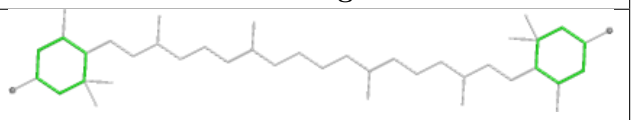
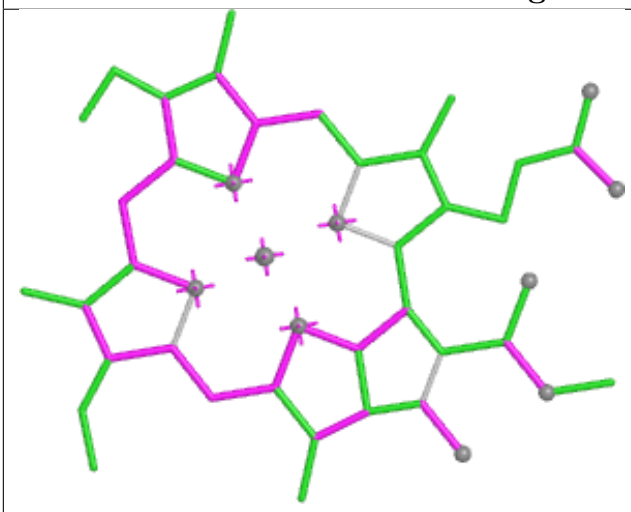


Rings

Ligand CLA a 310



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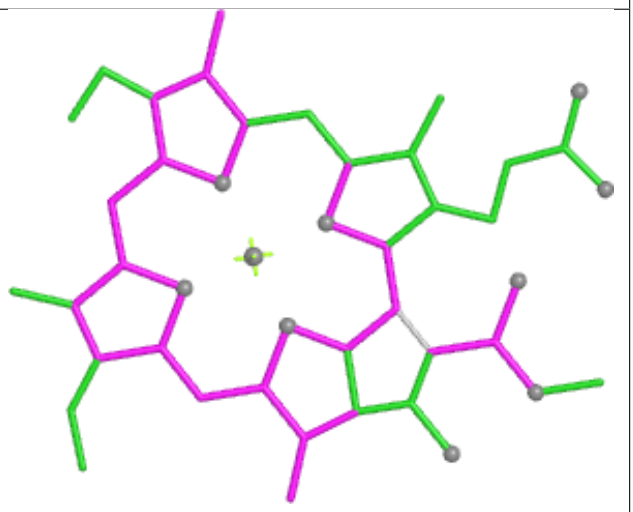
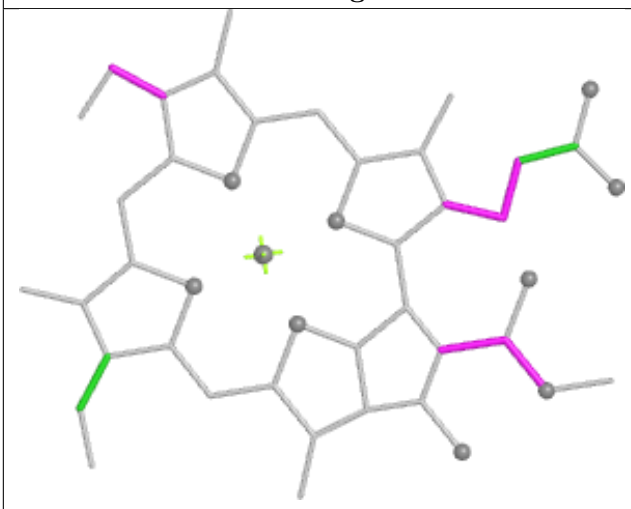


Bond angles



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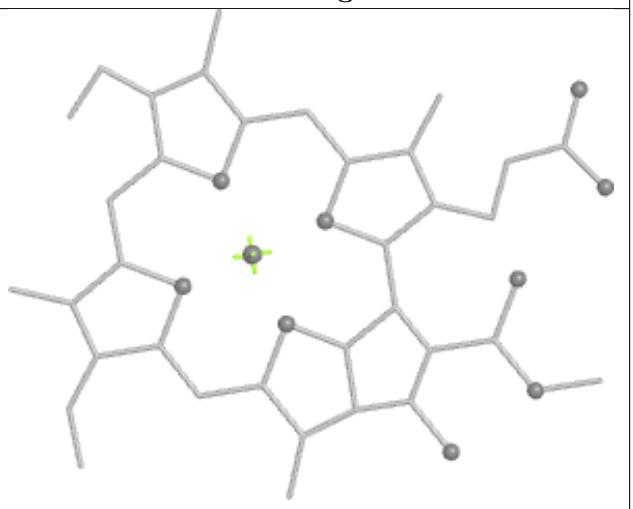
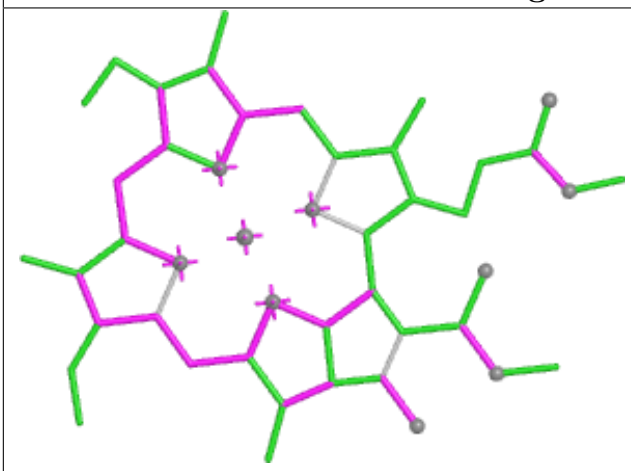


Rings

Ligand CLA 5 308



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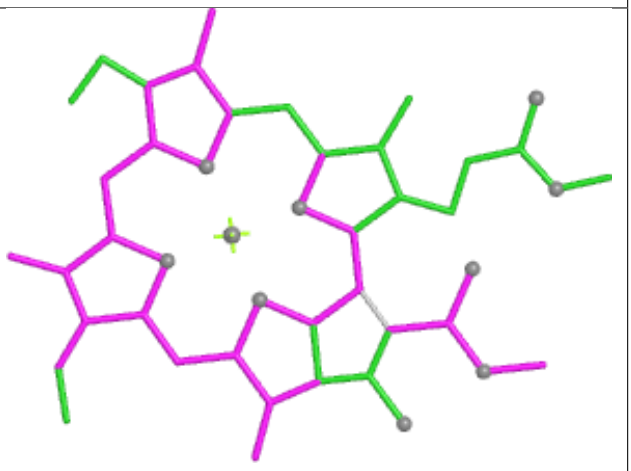

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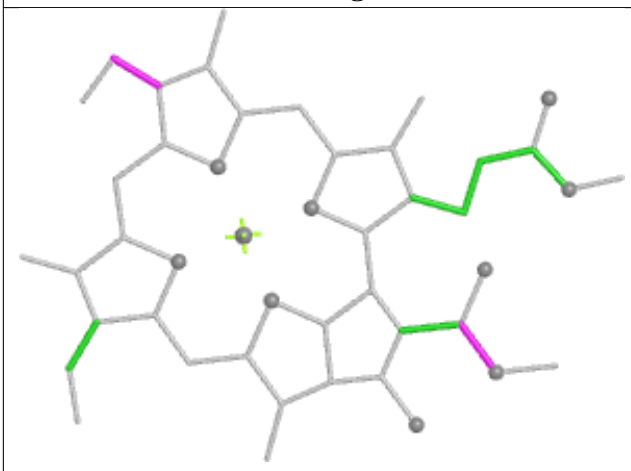

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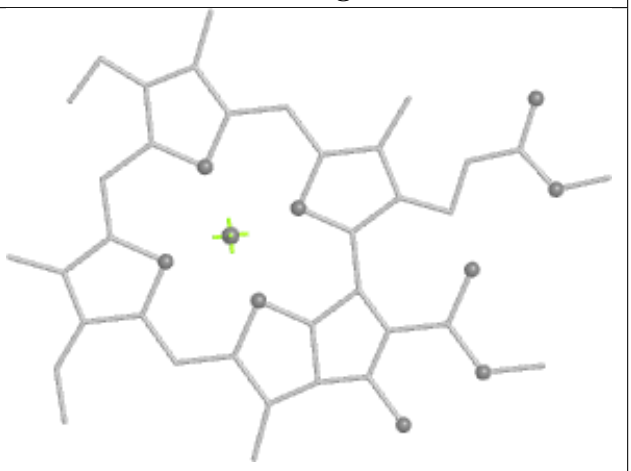
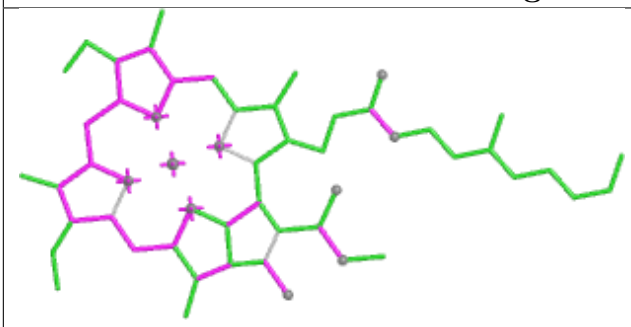


Rings

Ligand CLA A 825



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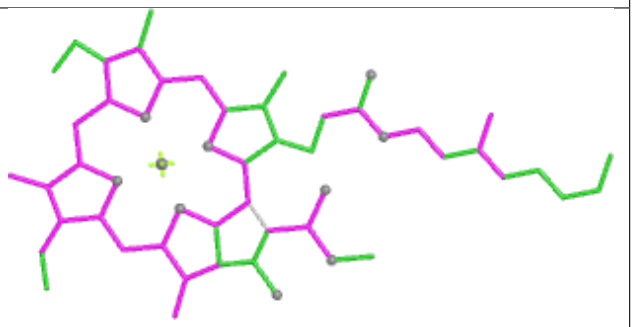
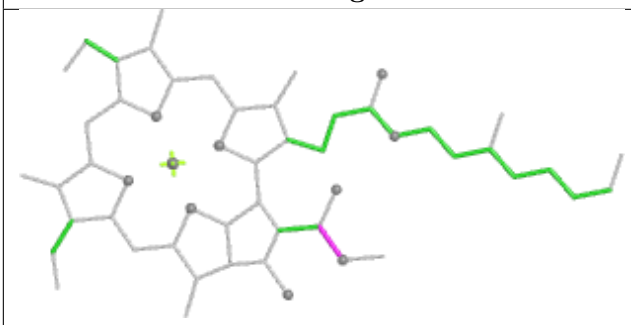


Bond angles



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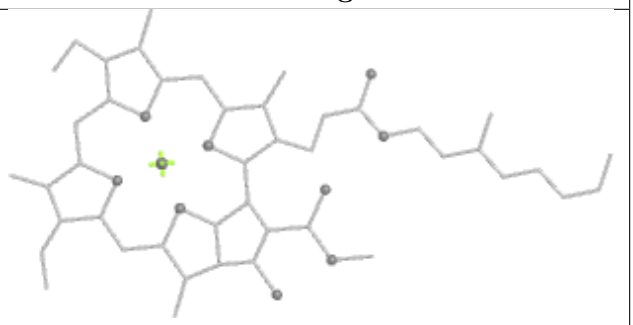
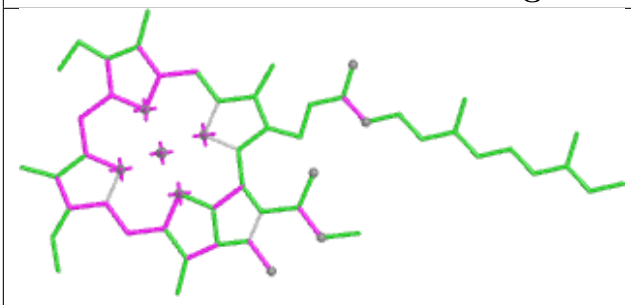


Rings

Ligand CLA A 845



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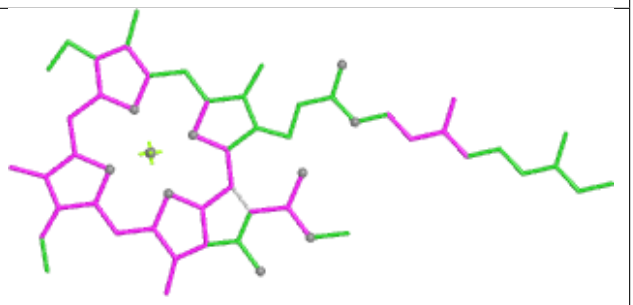
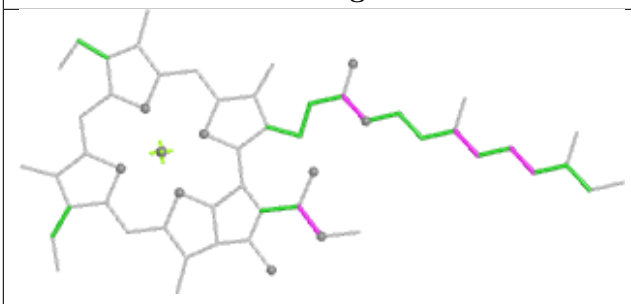


Bond angles



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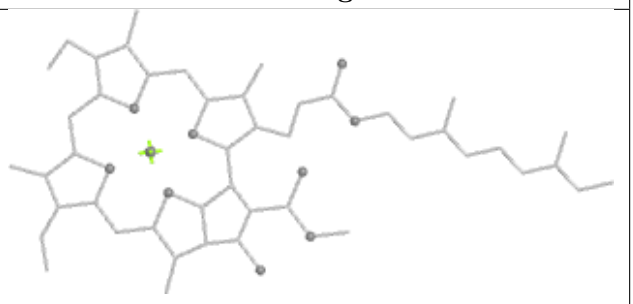
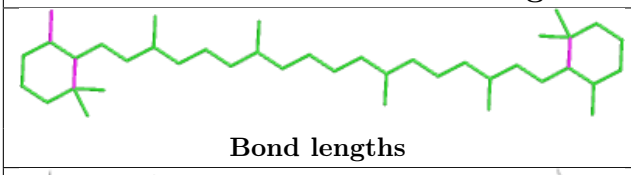


Rings

Ligand BCR 2 302



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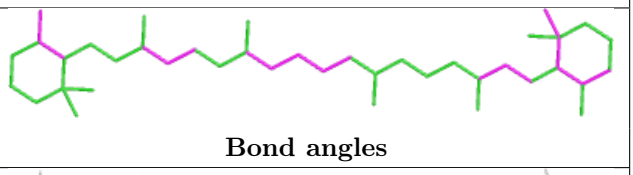
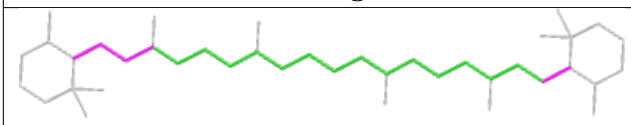
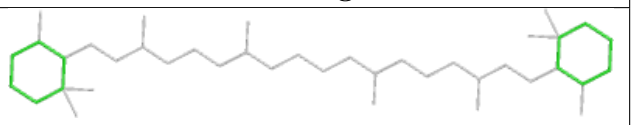


Bond angles

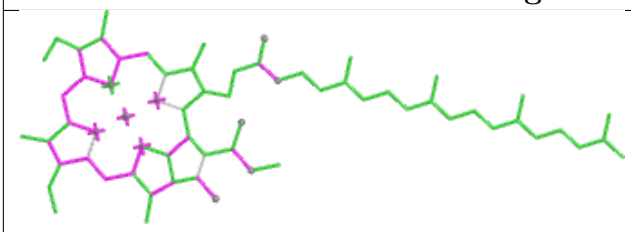


Torsions

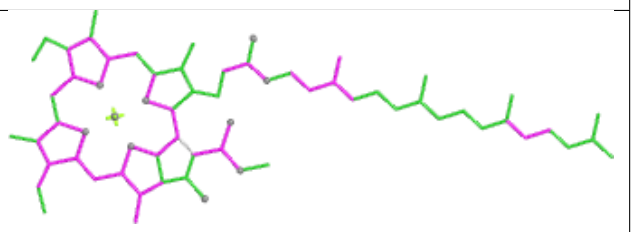


Rings

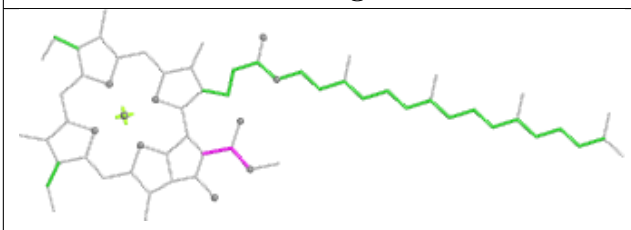
Ligand CLA B 834



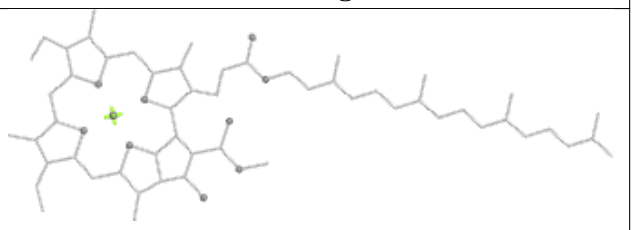
Bond lengths



Bond angles

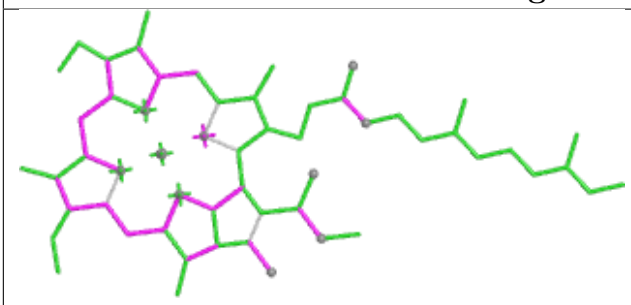


Torsions

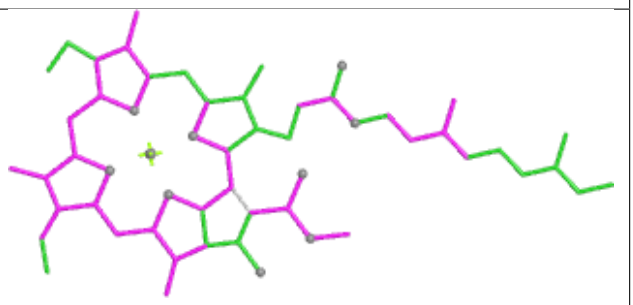


Rings

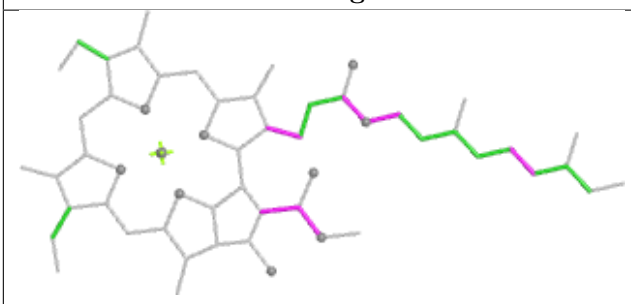
Ligand CLA 5 323



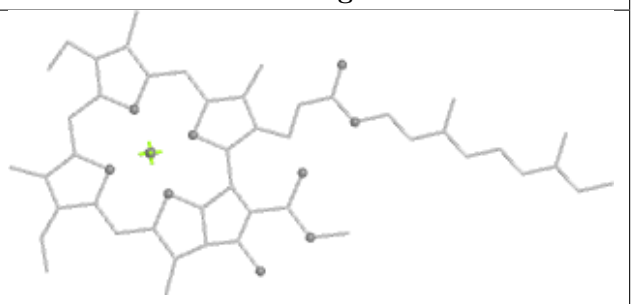
Bond lengths



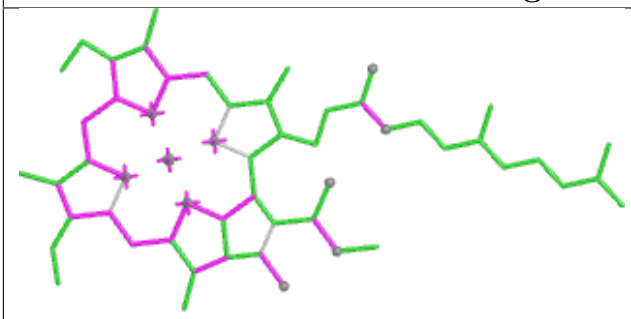
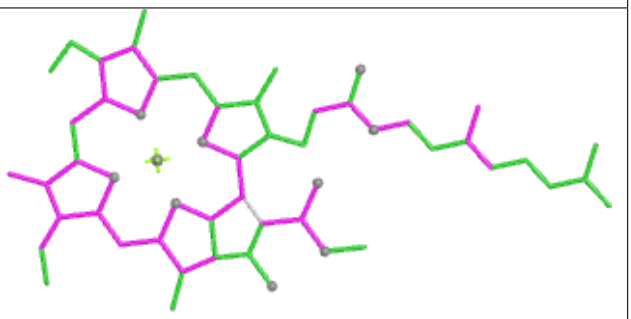
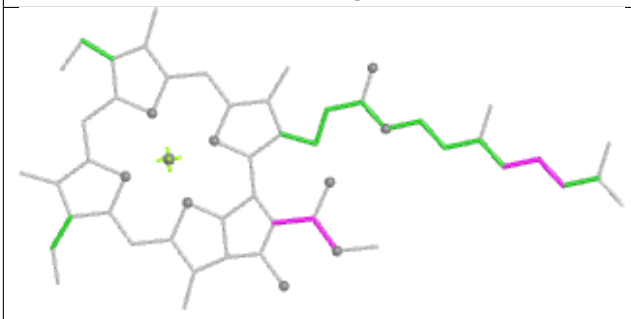
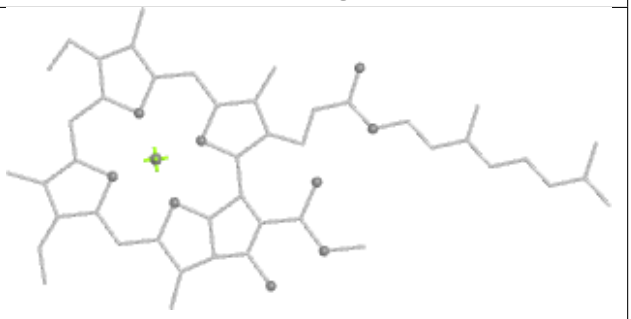
Bond angles

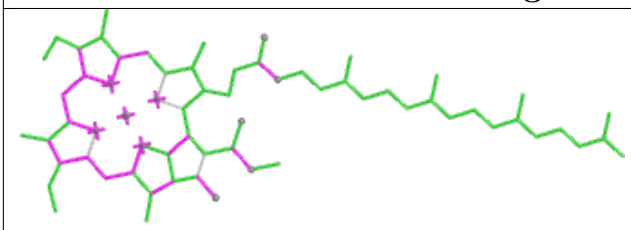
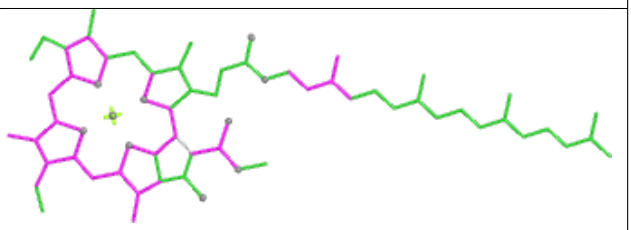
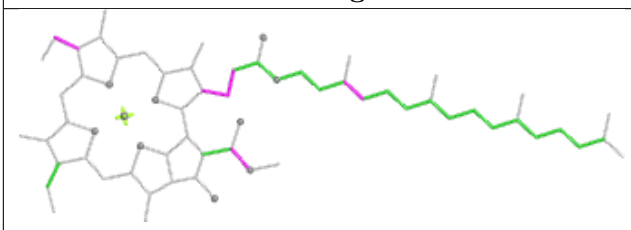
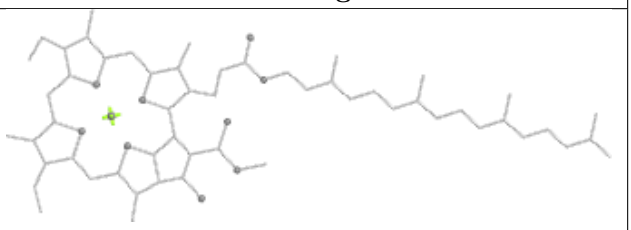


Torsions

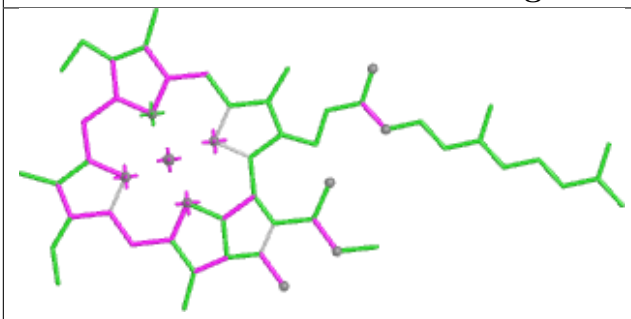


Rings

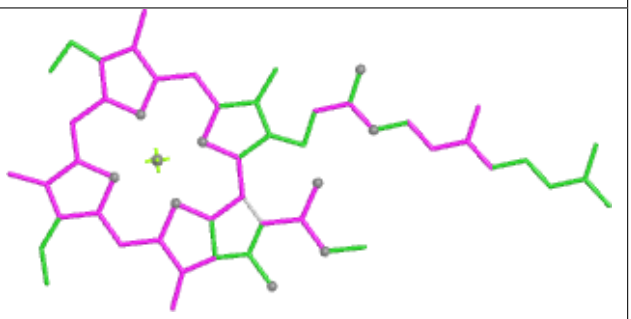
Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 856	
 Bond lengths	 Bond angles
 Torsions	 Rings

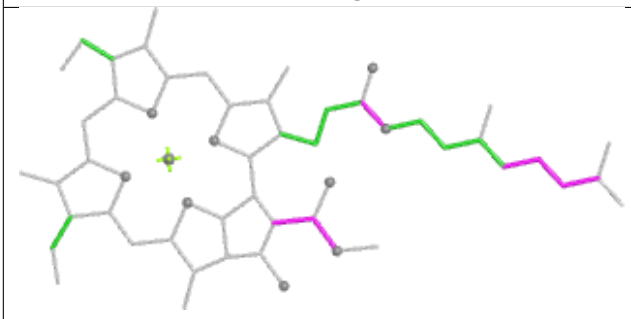
Ligand CLA B 823



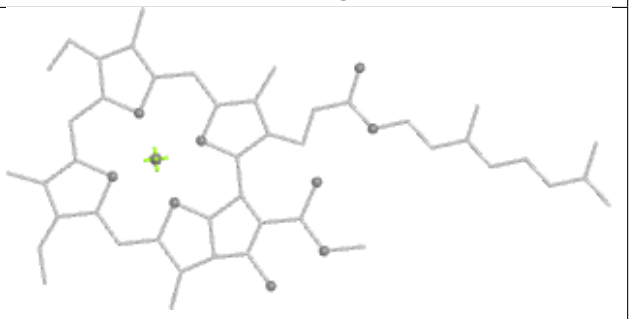
Bond lengths



Bond angles

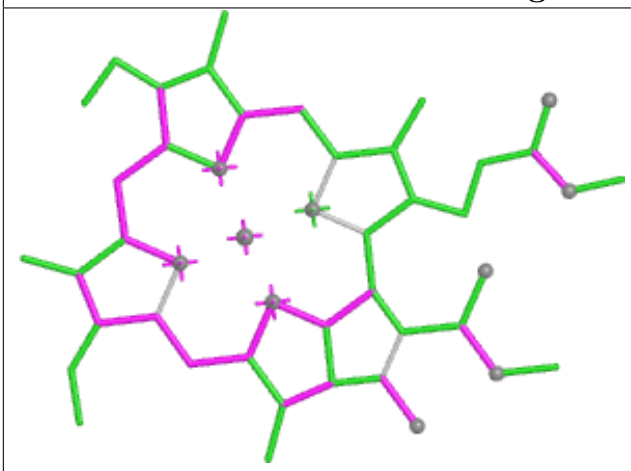


Torsions

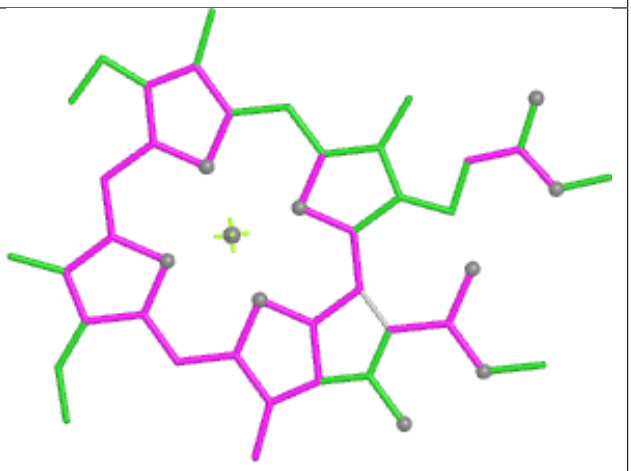


Rings

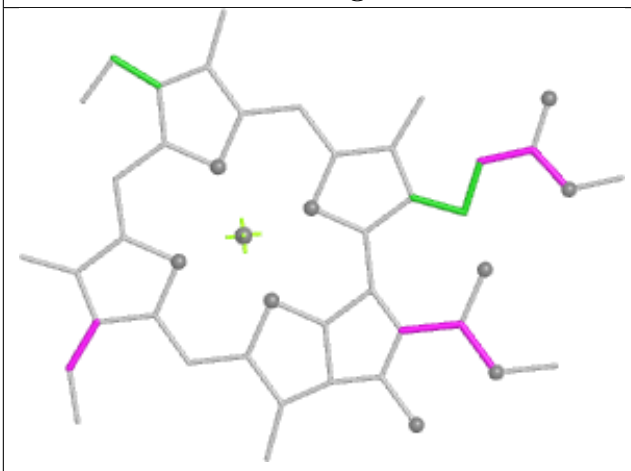
Ligand CLA 2 313



Bond lengths



Bond angles



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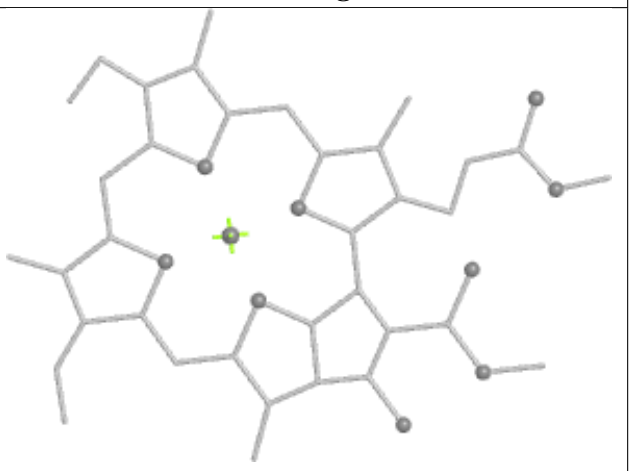
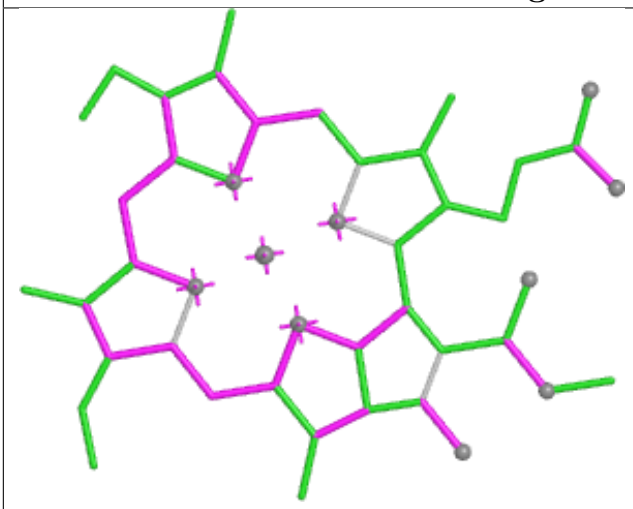


Rings

Ligand CLA 4 318



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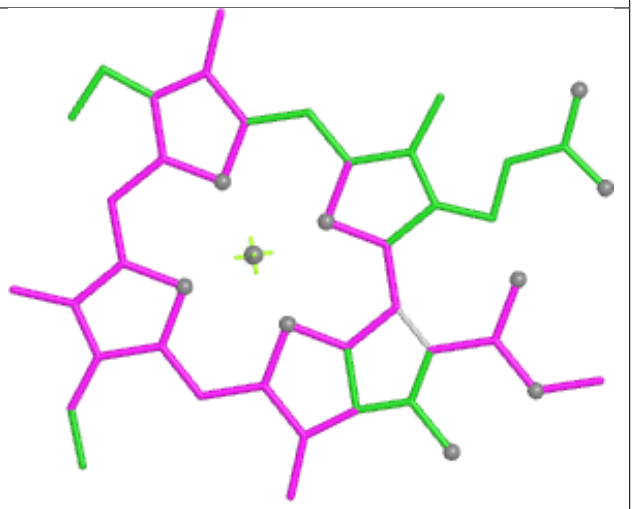
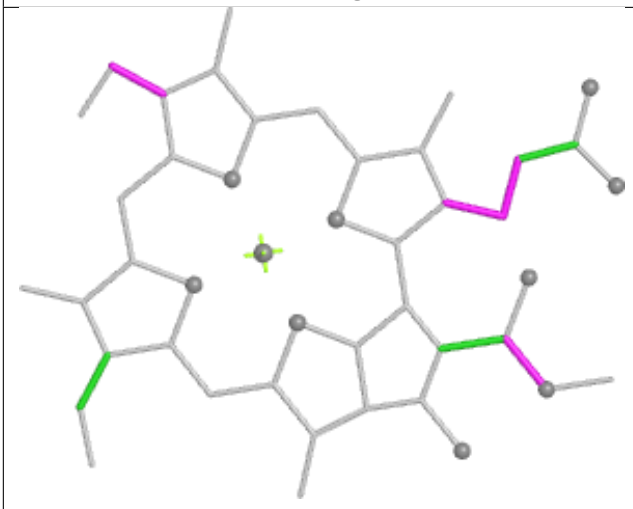


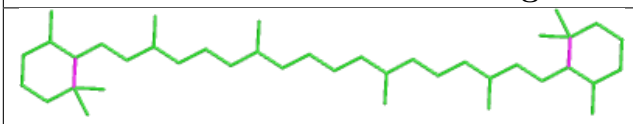
Bond angles



Torsions

Rings

Ligand BCR K 203



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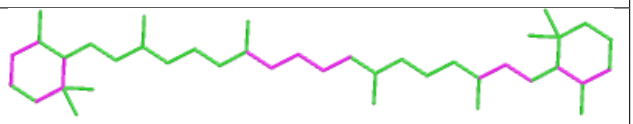

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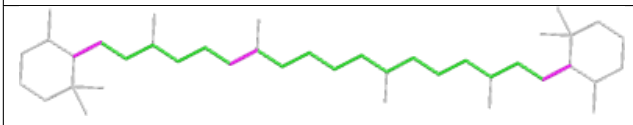

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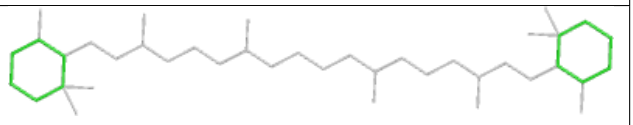
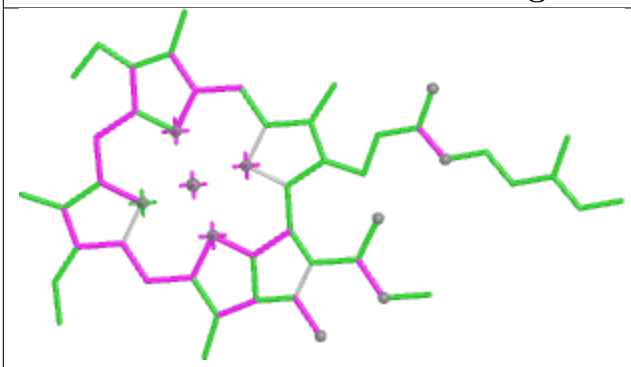


Rings

Ligand CLA 3 318



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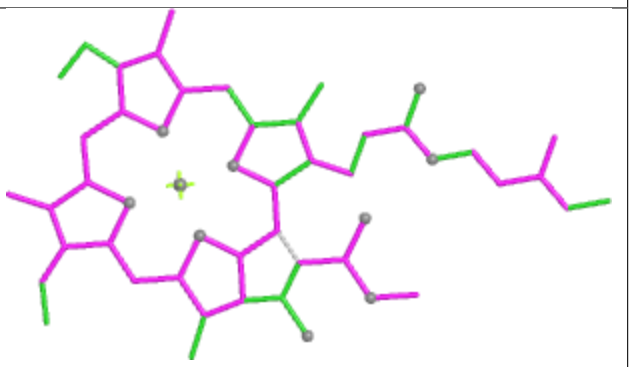
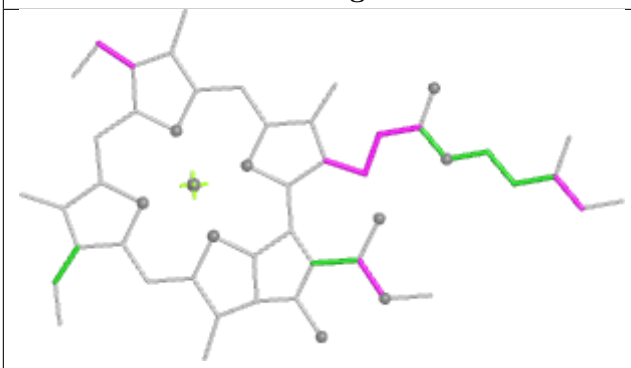


Bond angles



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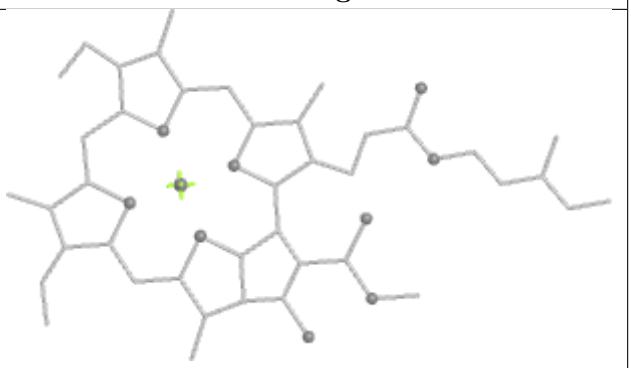
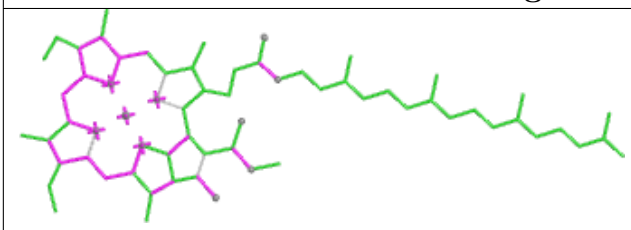


Rings

Ligand CLA B 814



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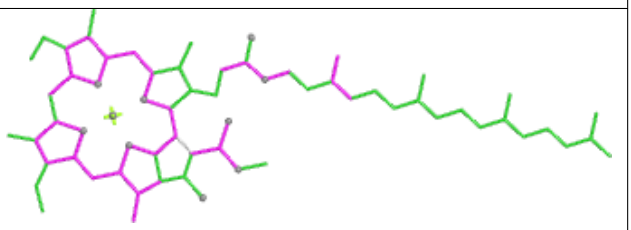
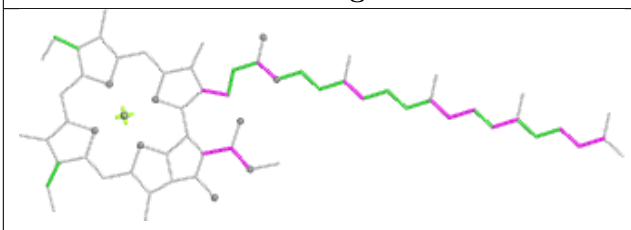


Bond angles



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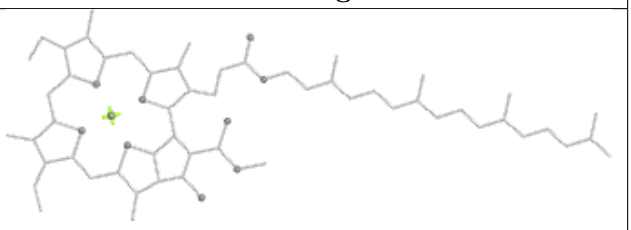
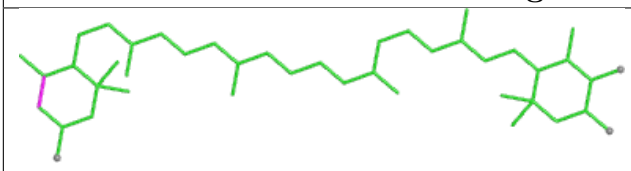


Rings

Ligand AXT a 304



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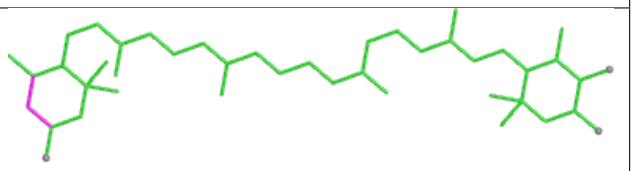
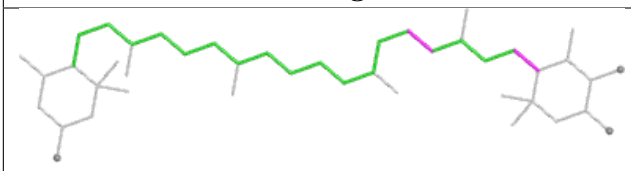
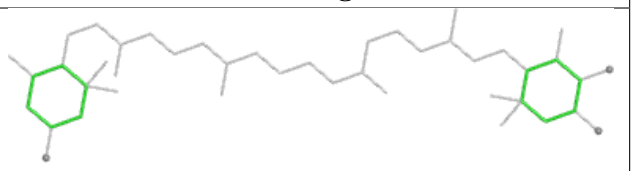


Bond angles

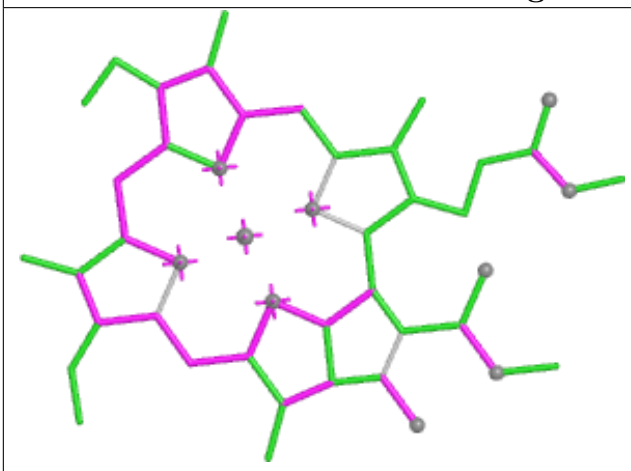


Torsions



Rings

Ligand CLA b 303



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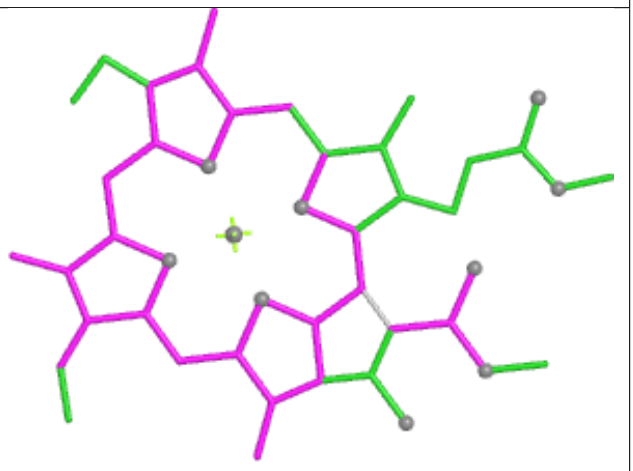
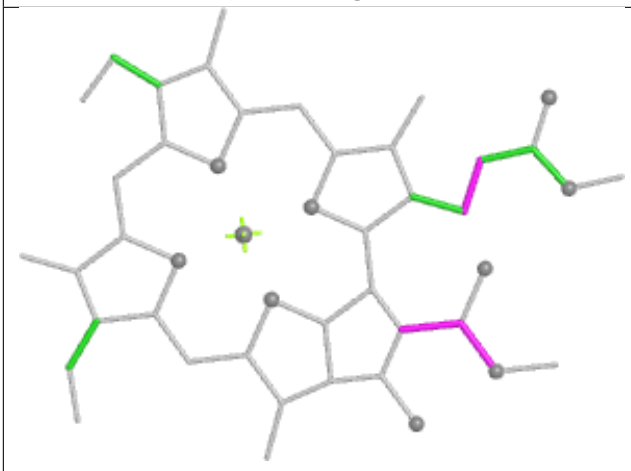
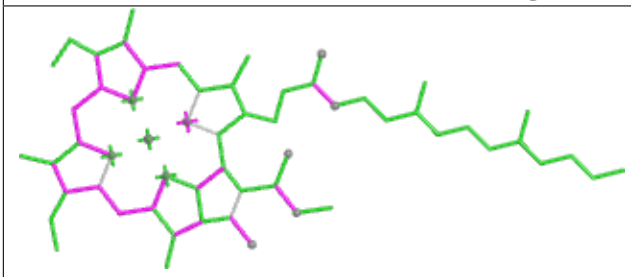
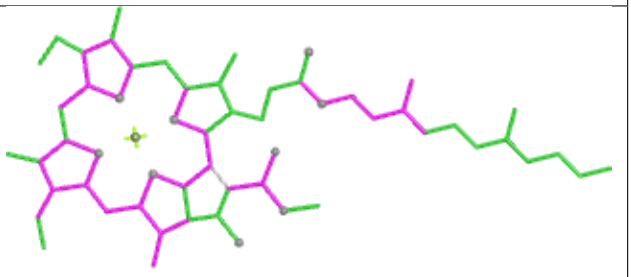
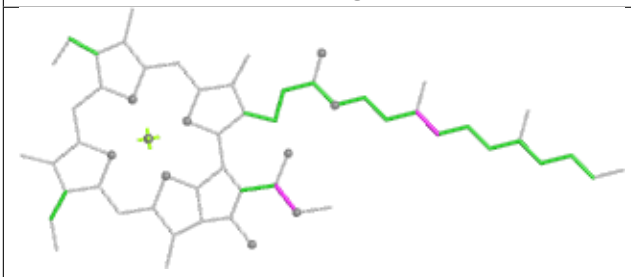
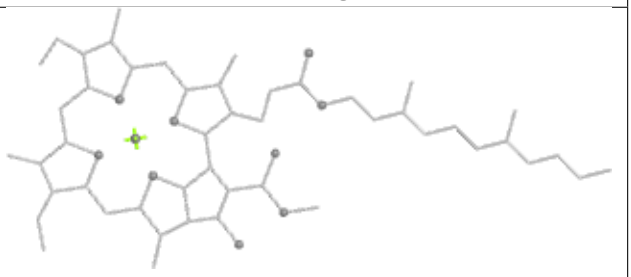


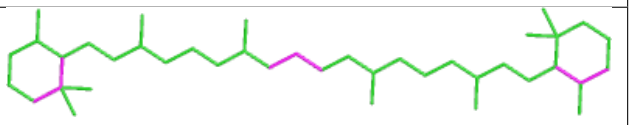
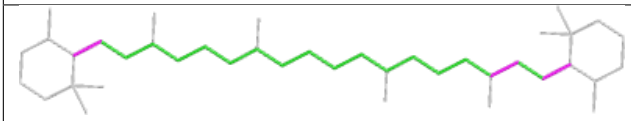
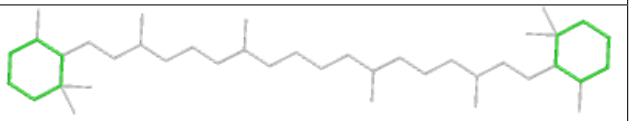
Bond angles



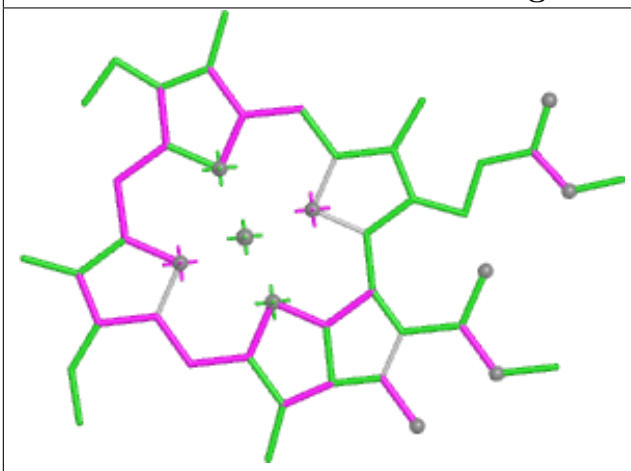
Torsions

Rings

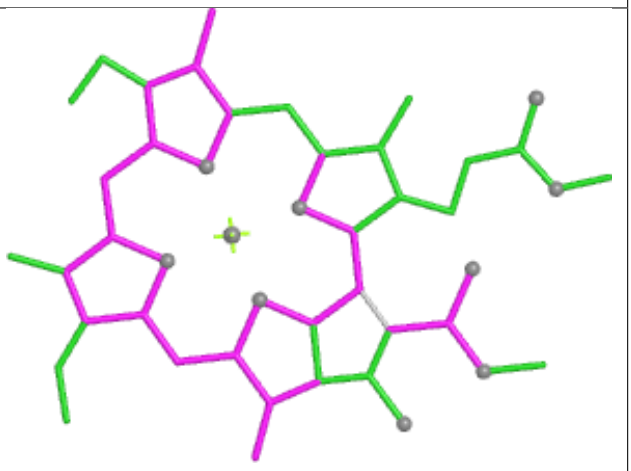
Ligand CLA B 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

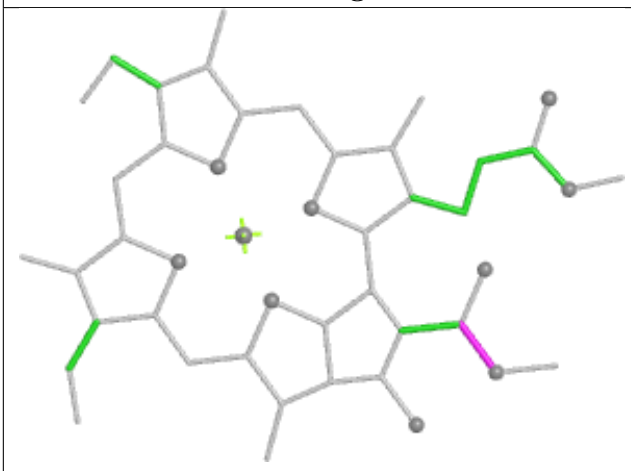
Ligand CLA 9 312



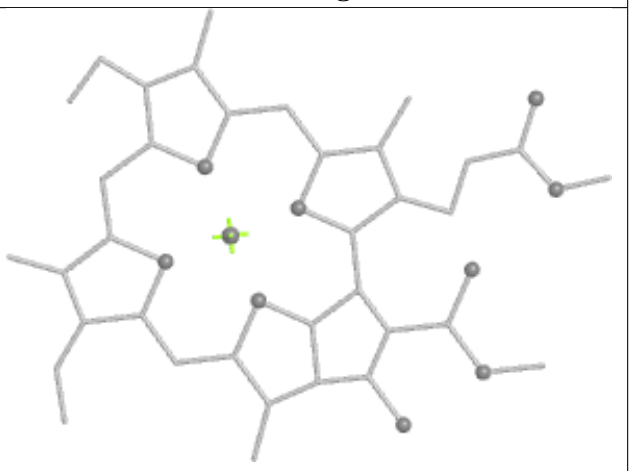
Bond lengths



Bond angles

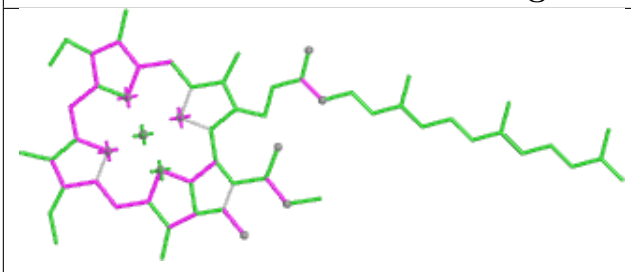


Torsions

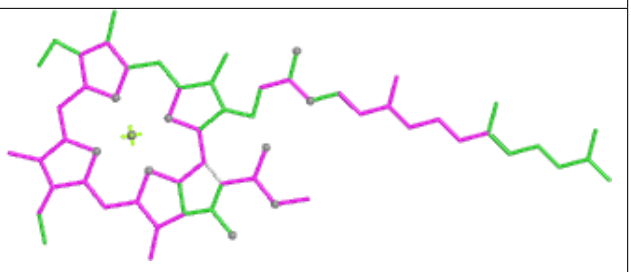


Rings

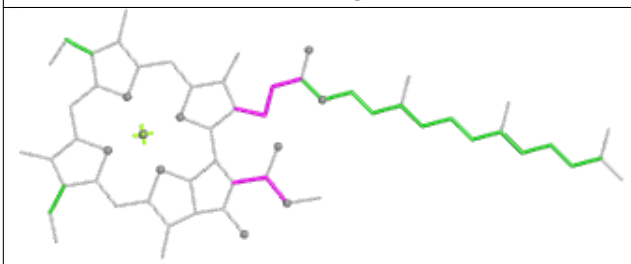
Ligand CLA 4 308



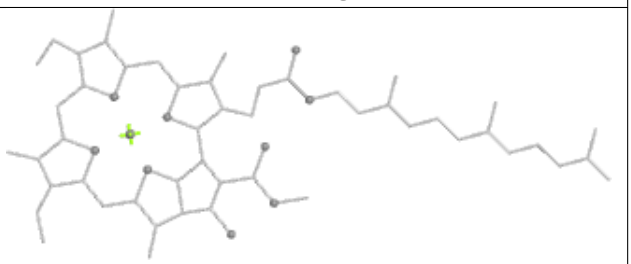
Bond lengths



Bond angles

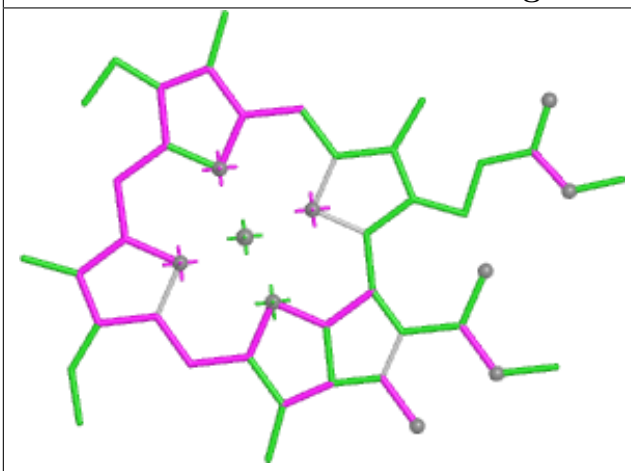


Torsions

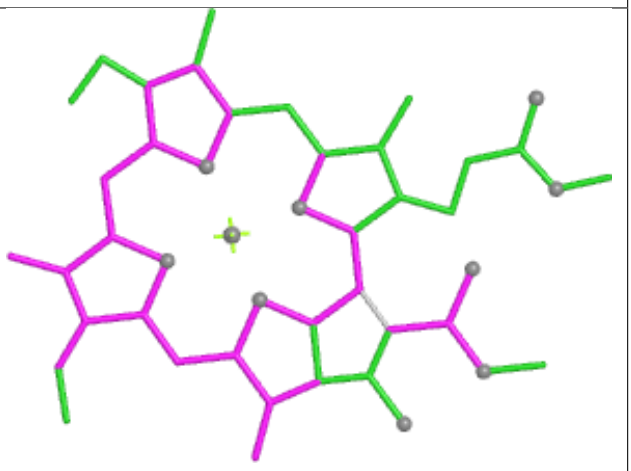


Rings

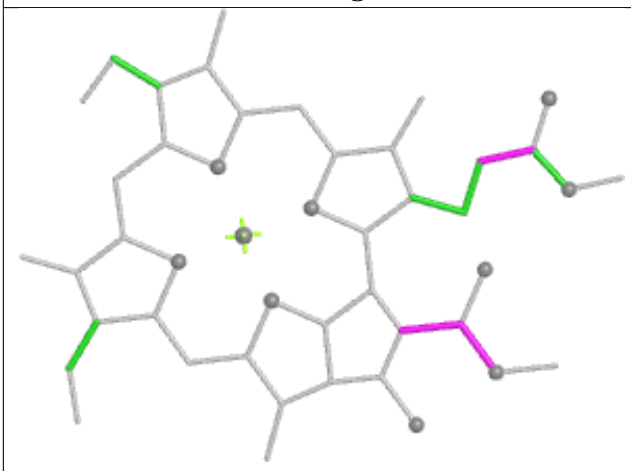
Ligand CLA G 205



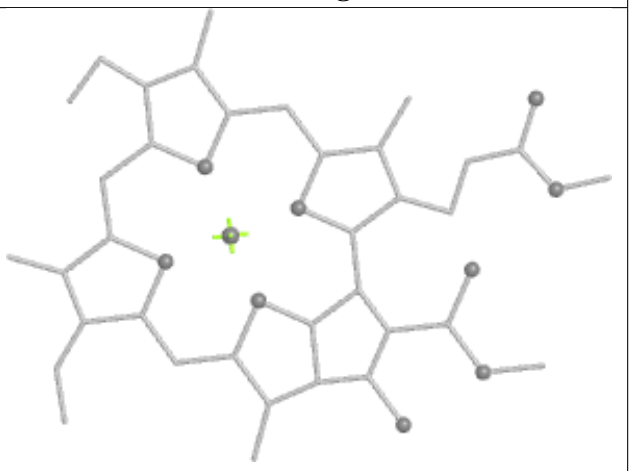
Bond lengths



Bond angles

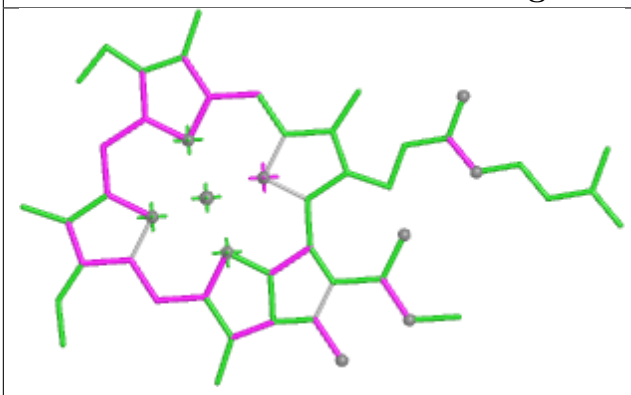


Torsions

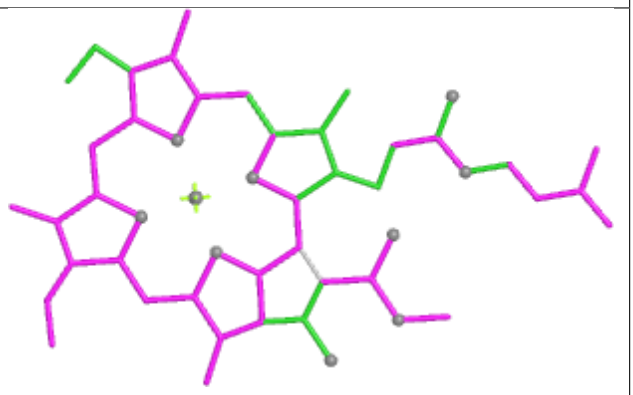


Rings

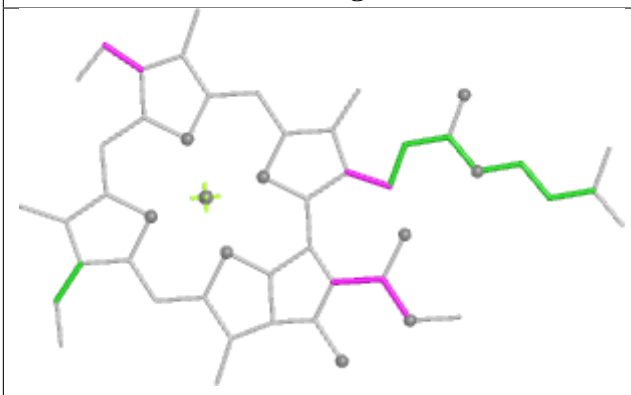
Ligand CLA a 321



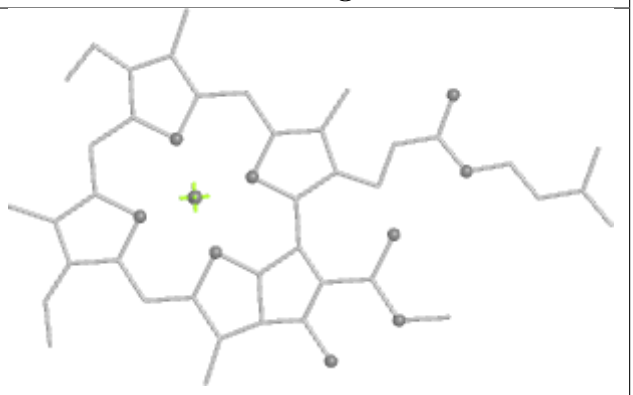
Bond lengths



Bond angles

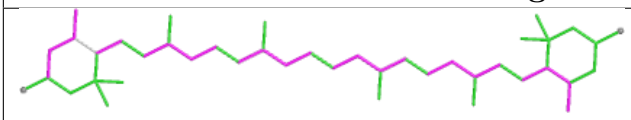


Torsions

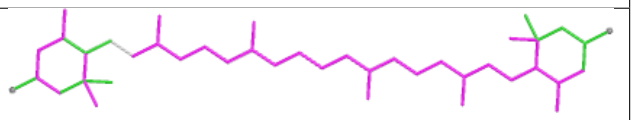


Rings

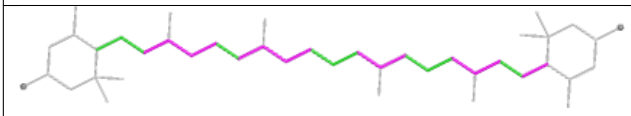
Ligand LUT 4 302



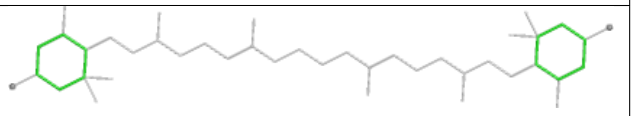
Bond lengths



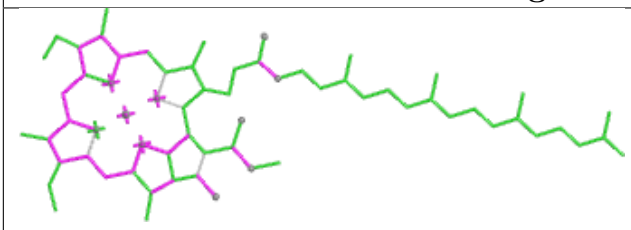
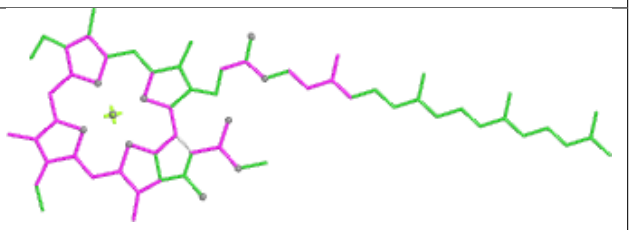
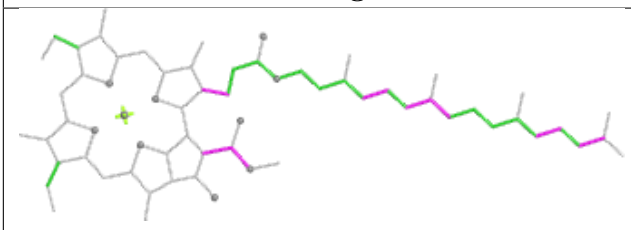
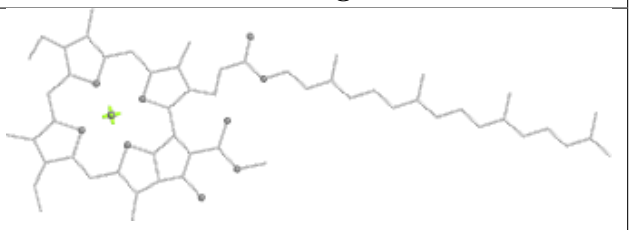
Bond angles

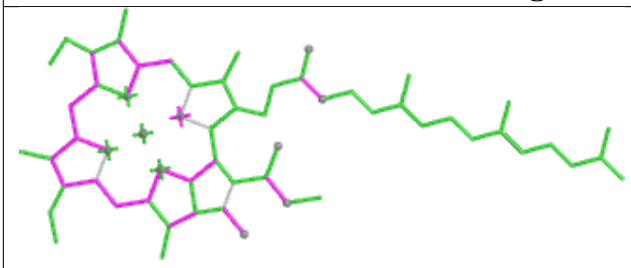
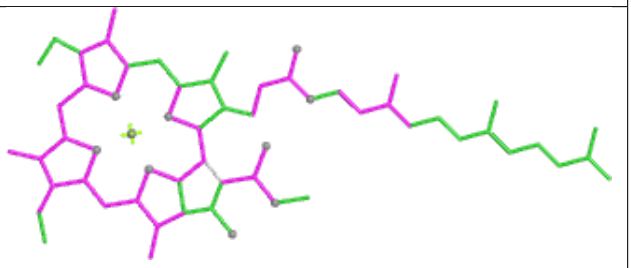
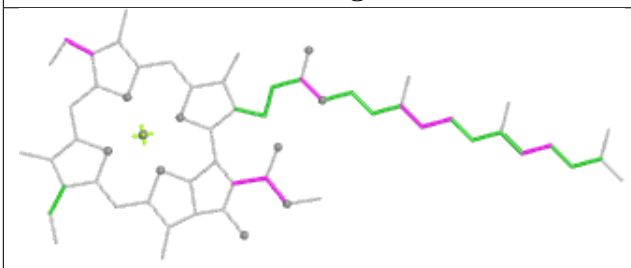
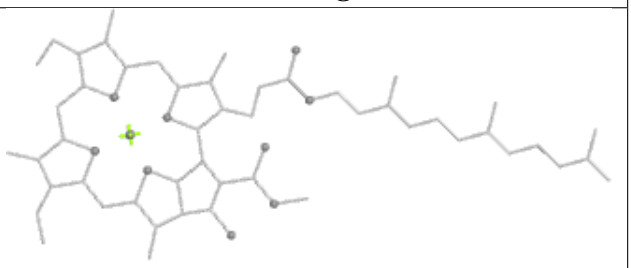


Torsions

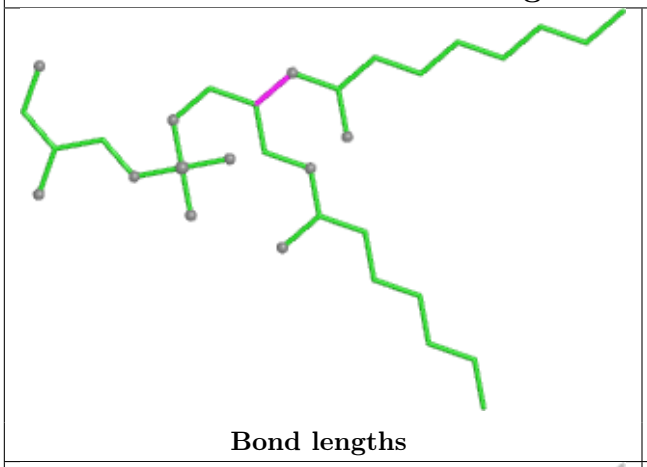


Rings

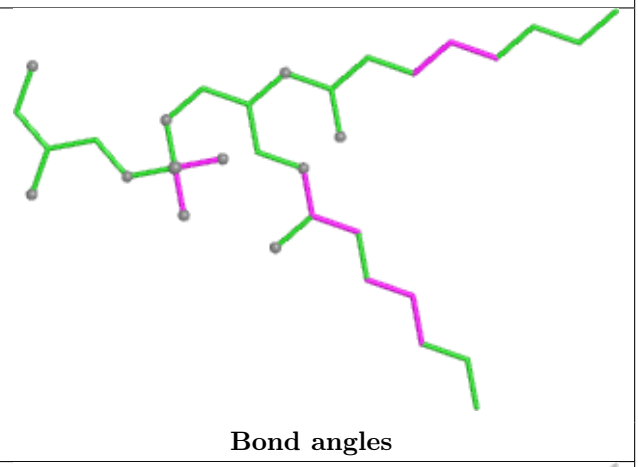
Ligand CLA a 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

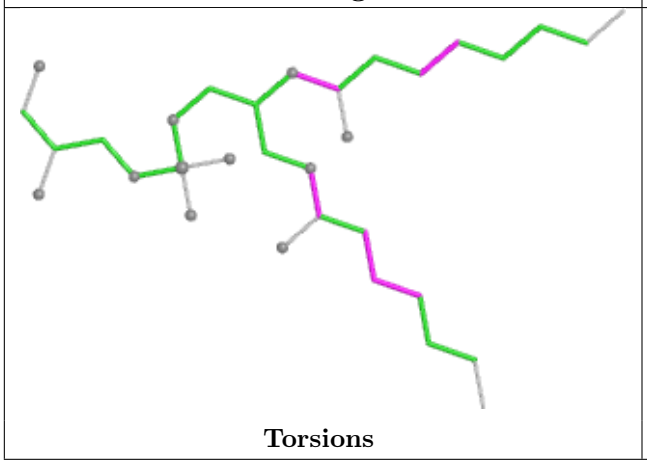
Ligand LHG B 807



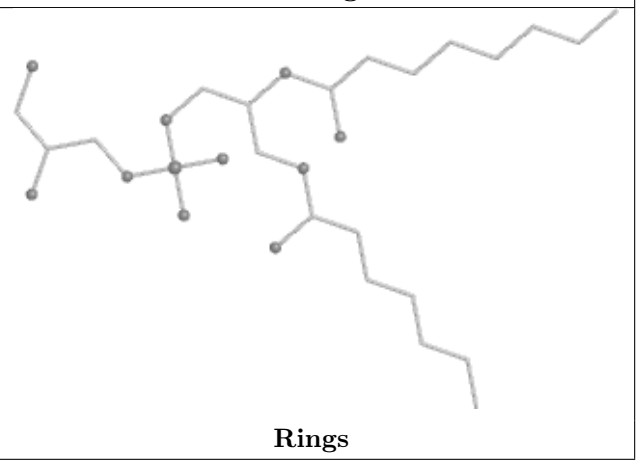
Bond lengths



Bond angles

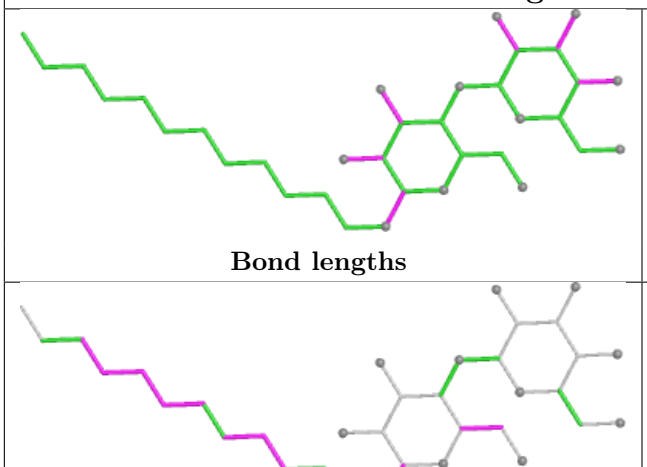


Torsions



Rings

Ligand LMT 9 306



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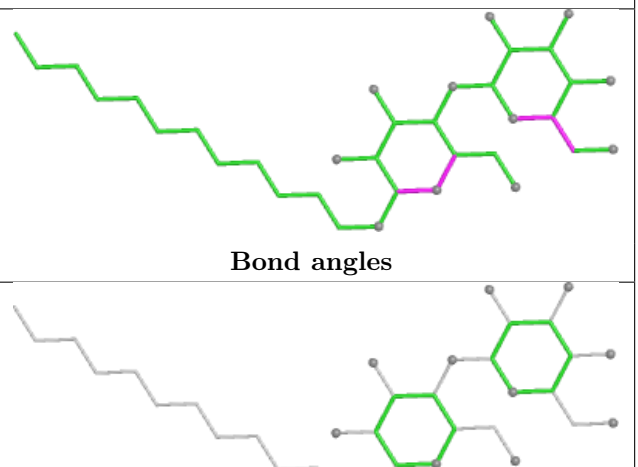
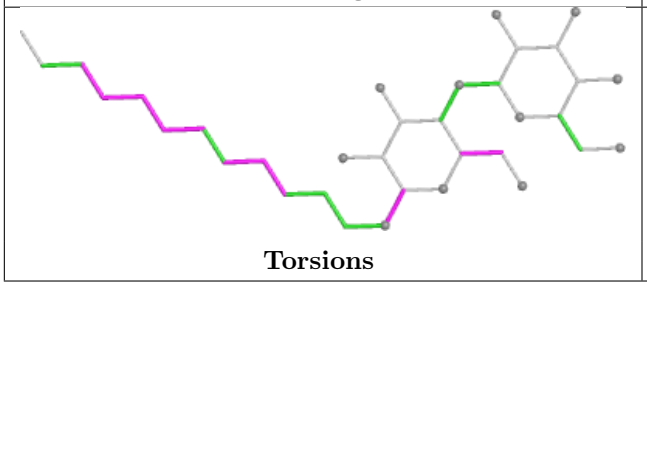


Bond angles



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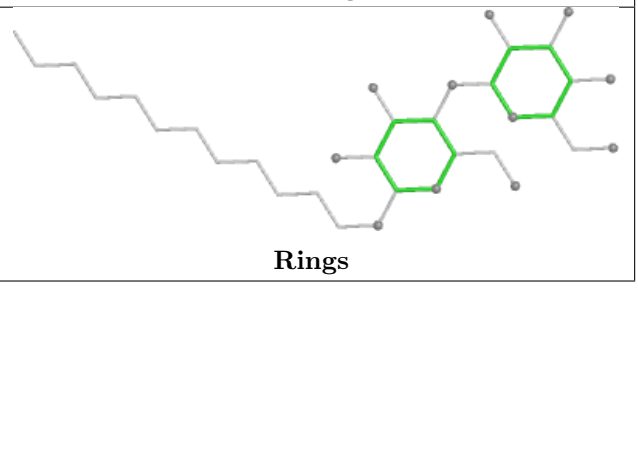
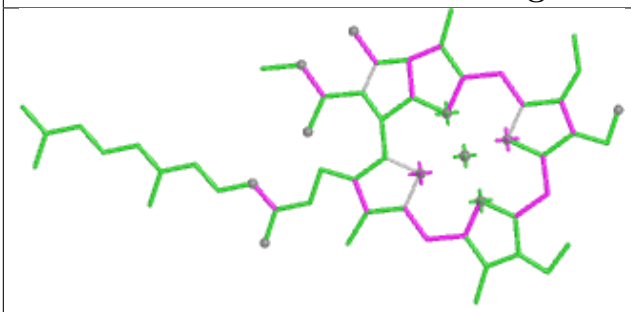
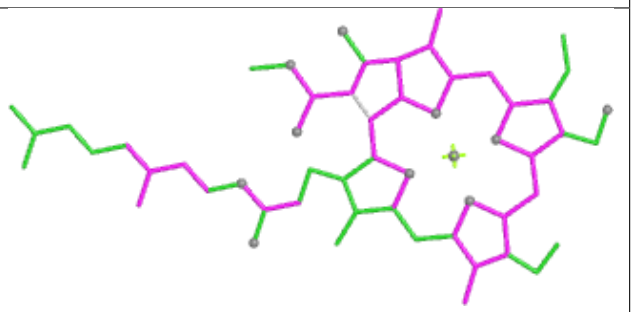


Rings

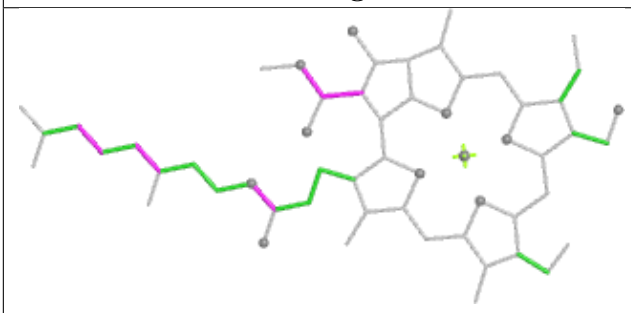
Ligand CHL 3 315



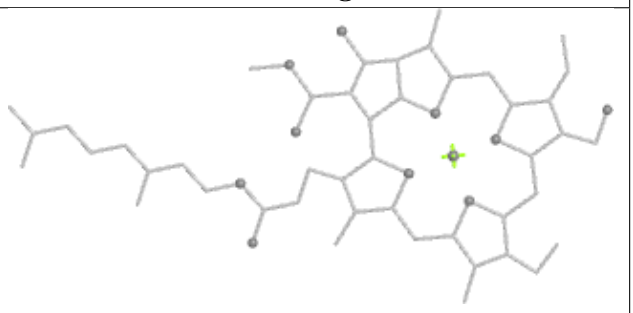
Bond lengths



Bond angles

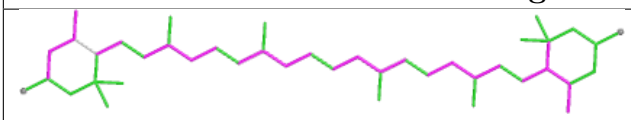


Torsions



Rings

Ligand LUT a 305



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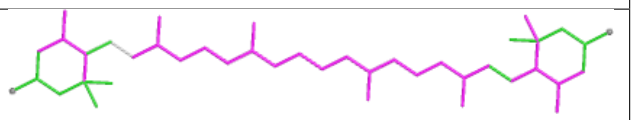
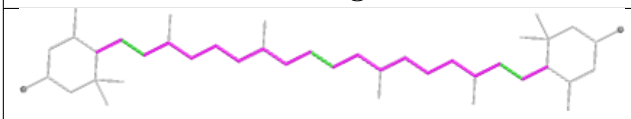


Bond angles



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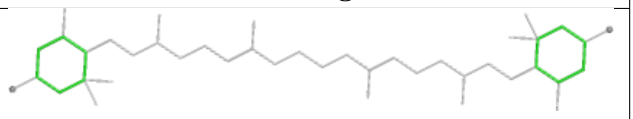
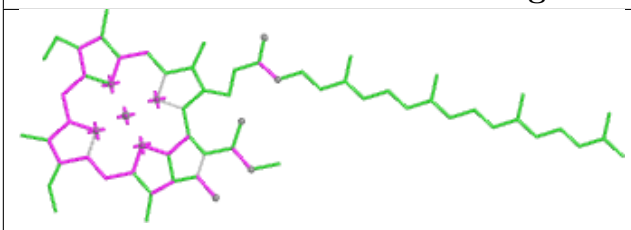
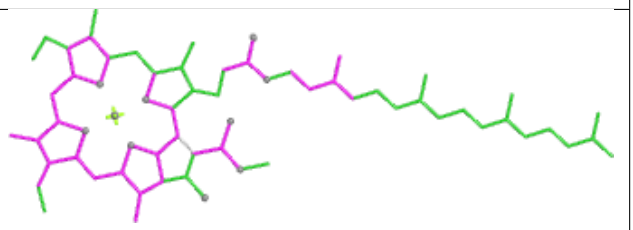


Rings

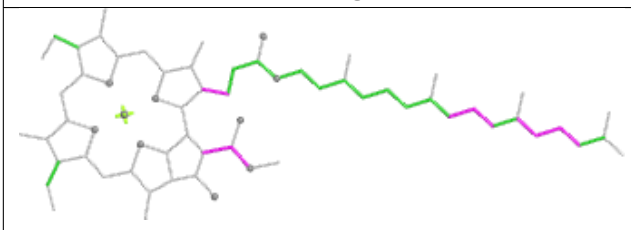
Ligand CLA 3 307



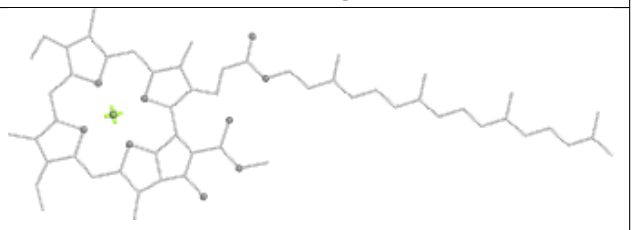
Bond lengths



Bond angles

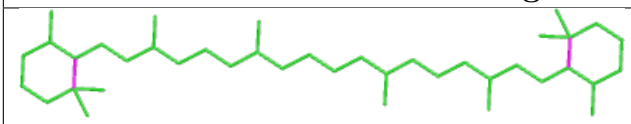


Torsions

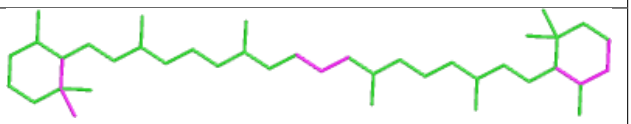


Rings

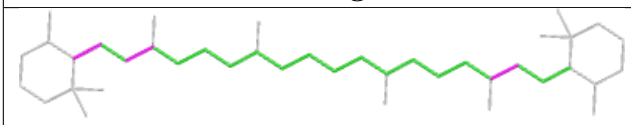
Ligand BCR B 802



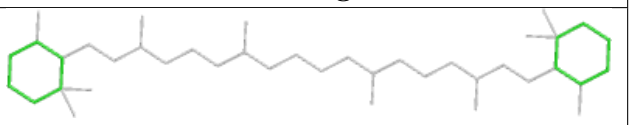
Bond lengths



Bond angles

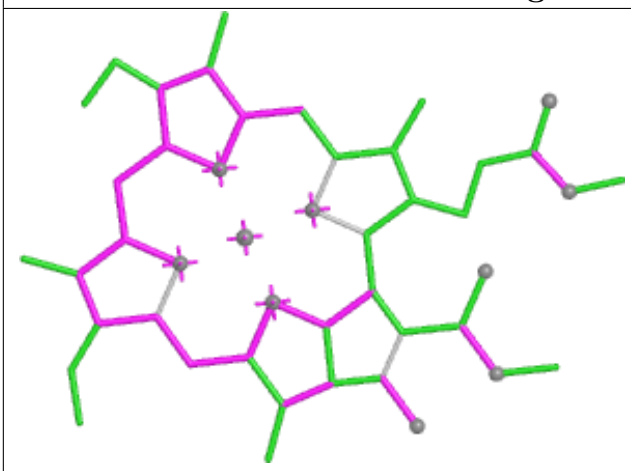


Torsions



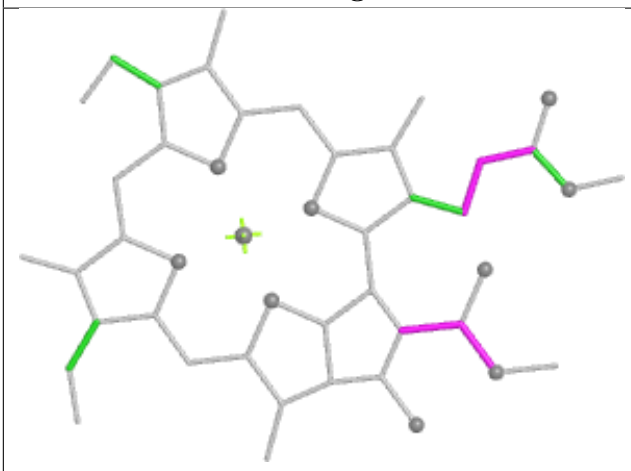
Rings

Ligand CLA b 305



Bond lengths

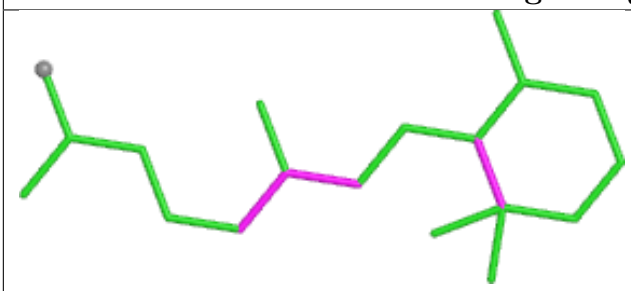
Bond angles



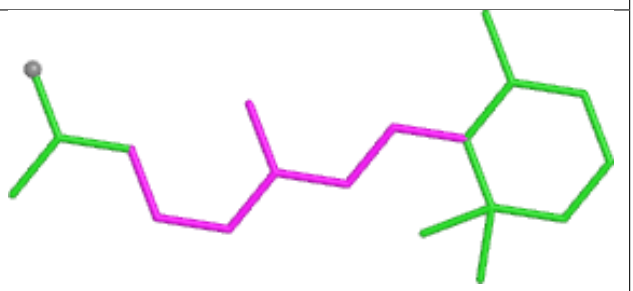
Torsions

Rings

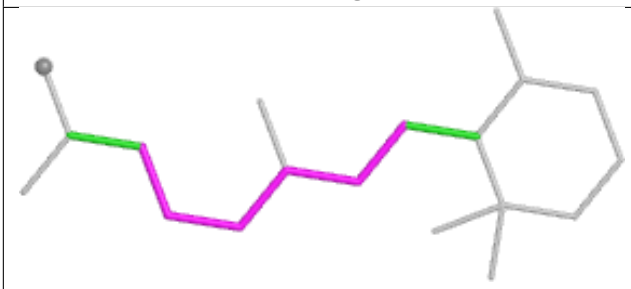
Ligand QTB F 303



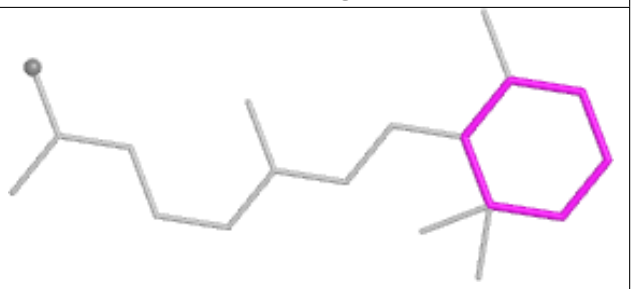
Bond lengths



Bond angles

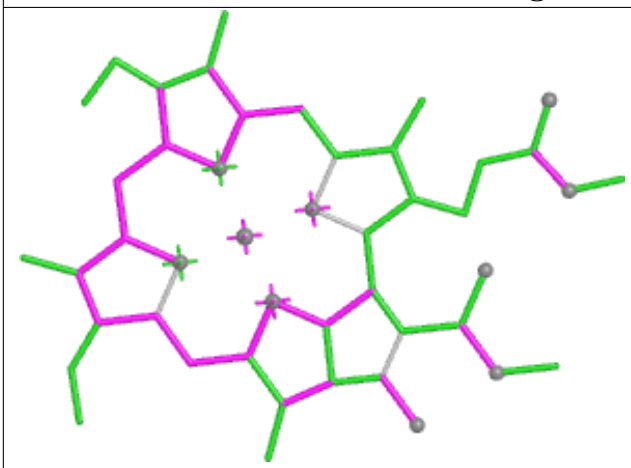


Torsions



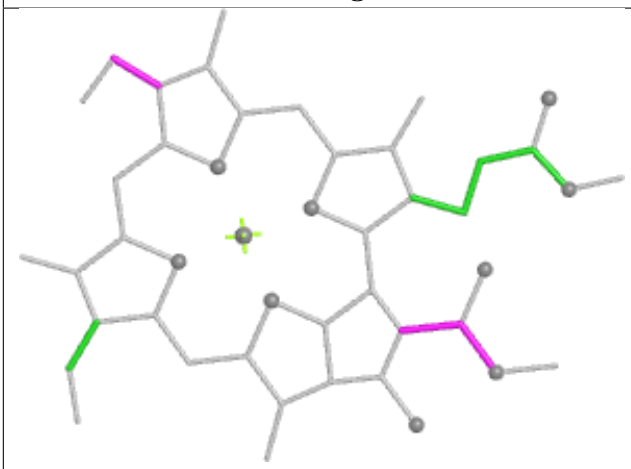
Rings

Ligand CLA 7 316



Bond lengths

Bond angles

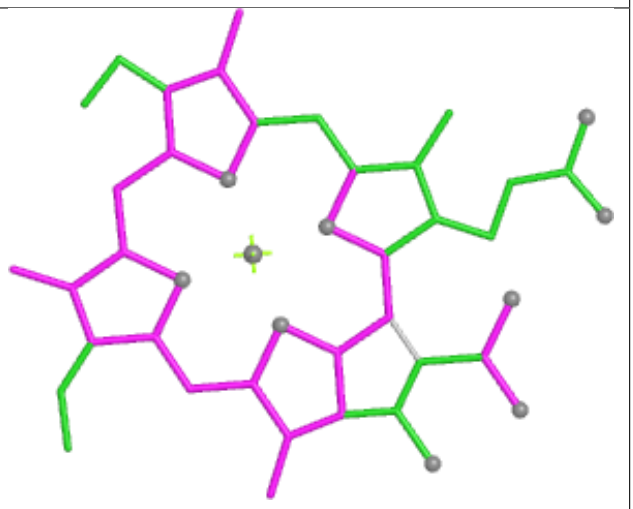


Torsions

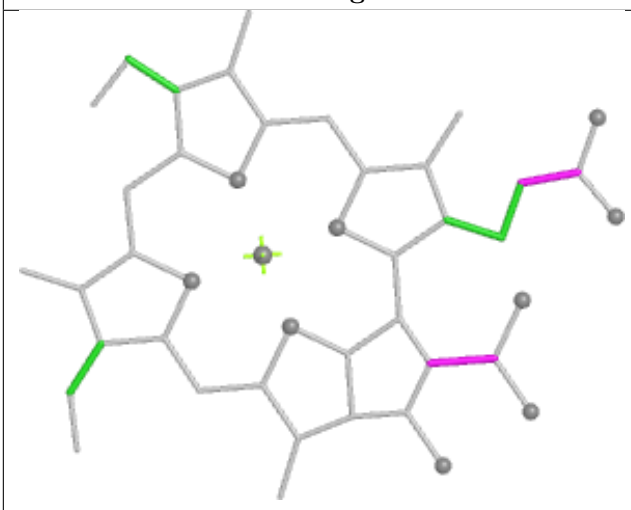
Rings

Ligand CLA 7 313

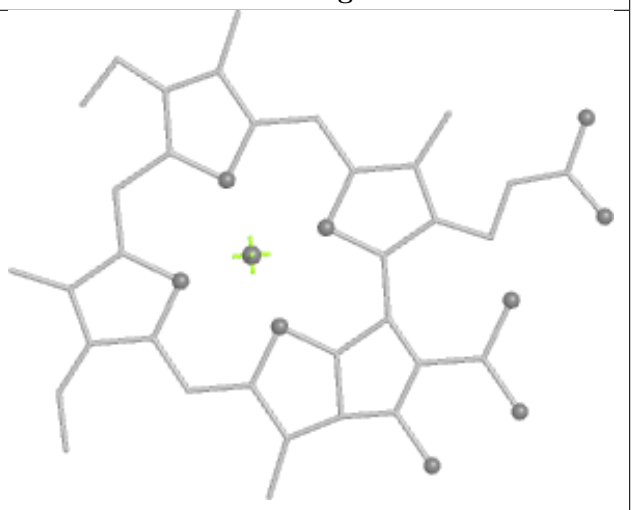
Bond lengths



Bond angles

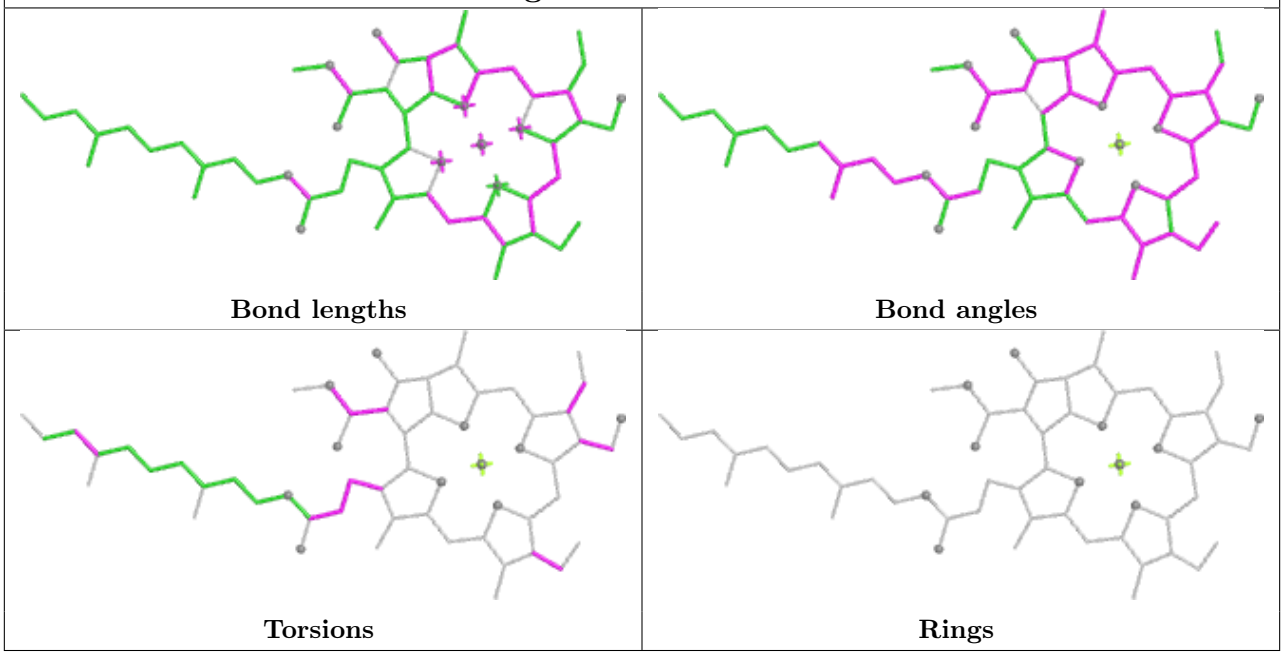


Torsions

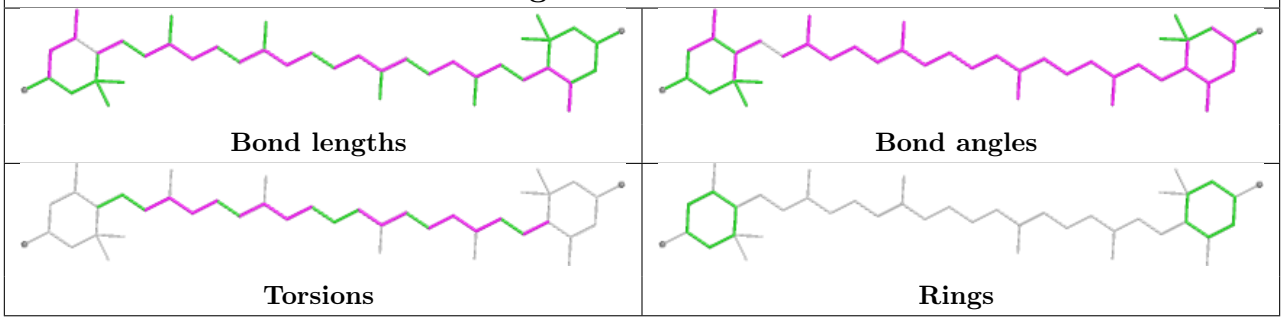


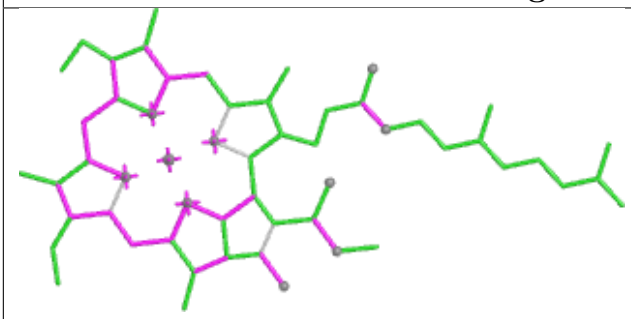
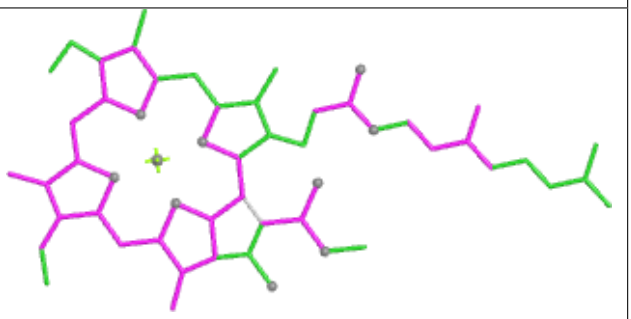
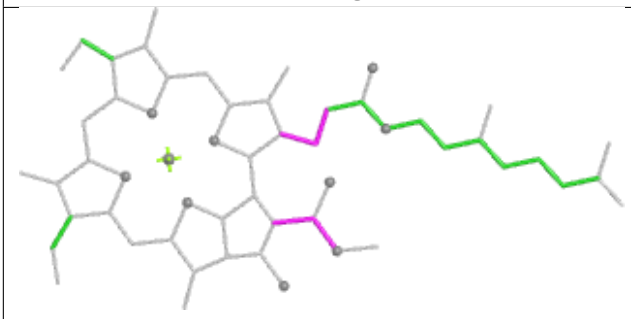
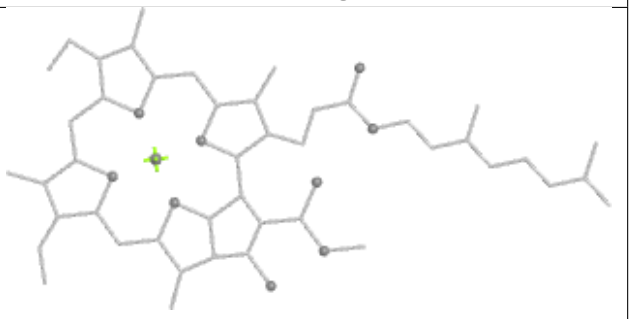
Rings

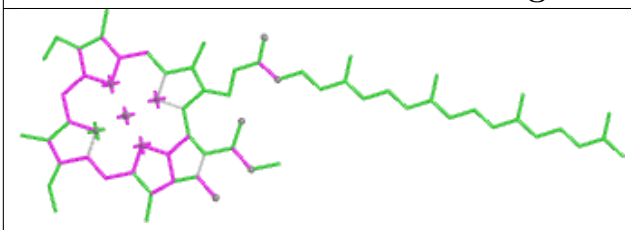
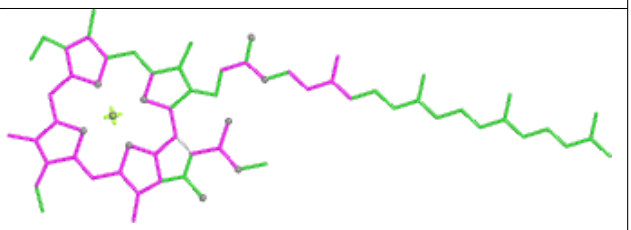
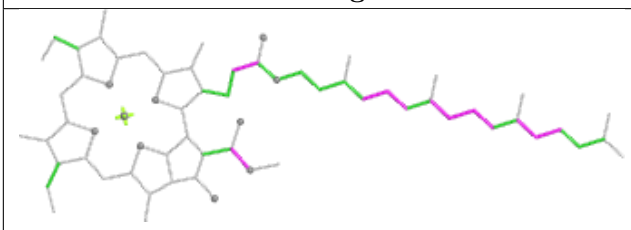
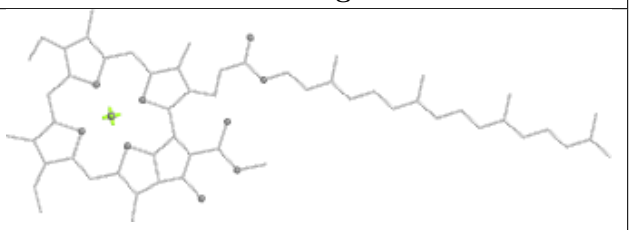
Ligand CHL A 831



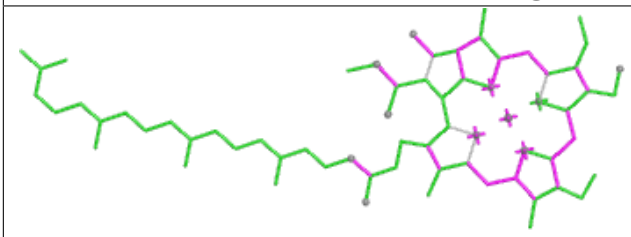
Ligand LUT 3 305



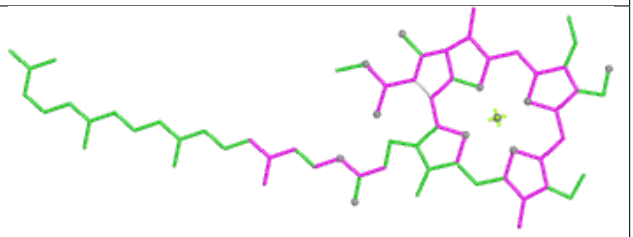
Ligand CLA 5 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

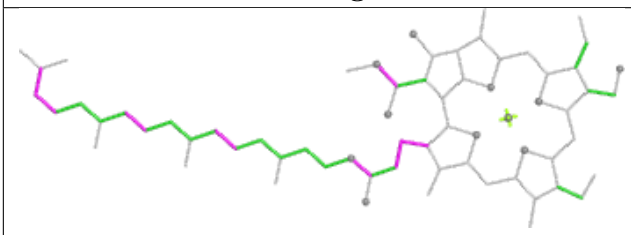
Ligand CHL 8 316



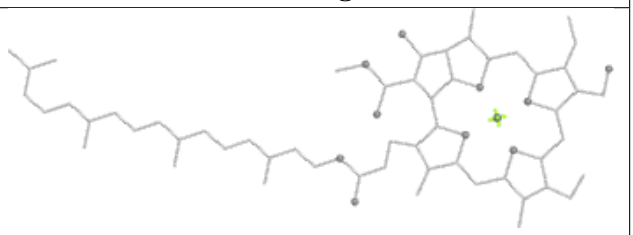
Bond lengths



Bond angles

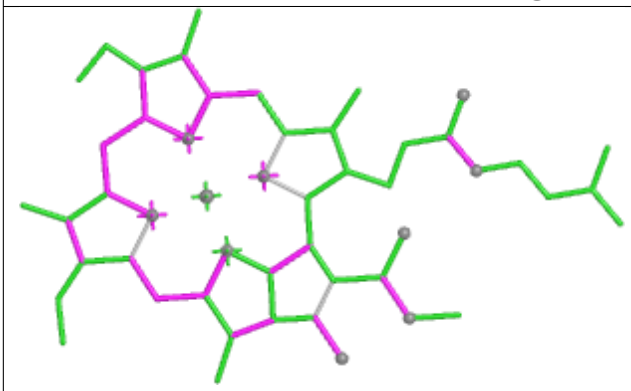


Torsions



Rings

Ligand CLA 8 317



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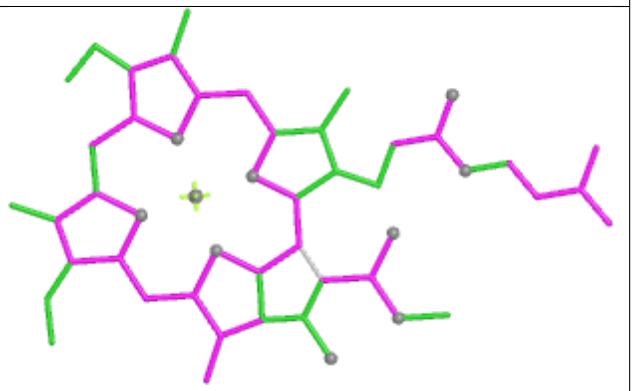

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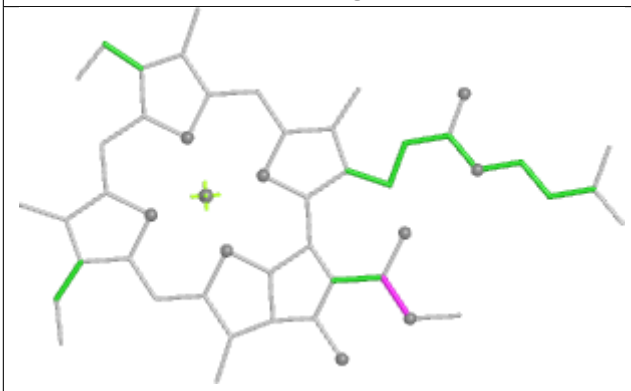

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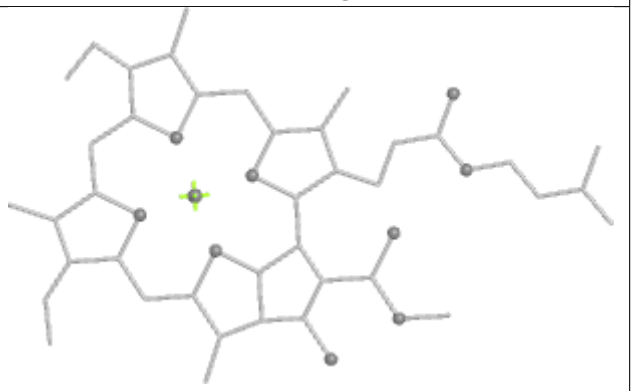
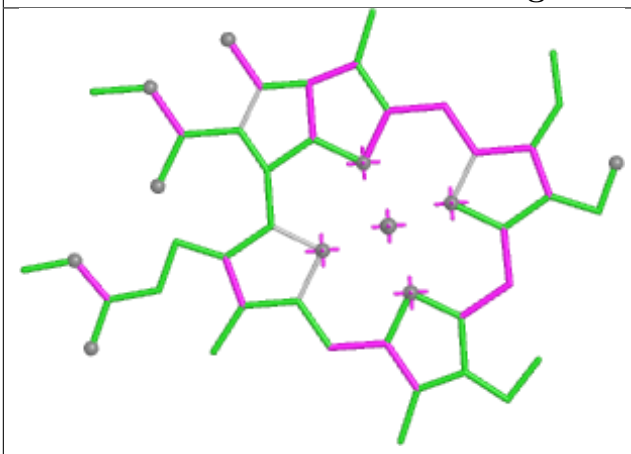


Rings

Ligand CHL 5 319



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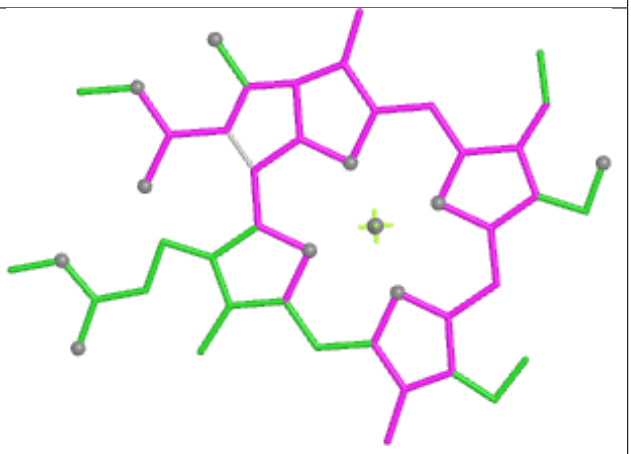
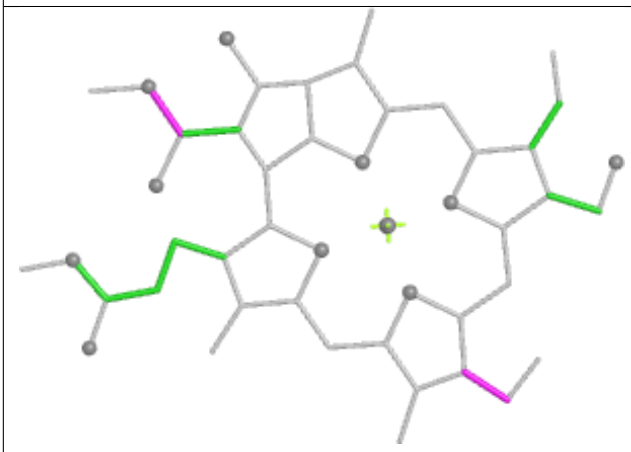


Bond angles



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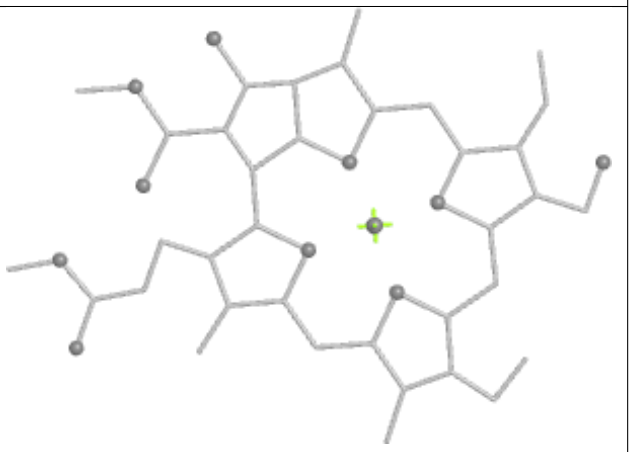
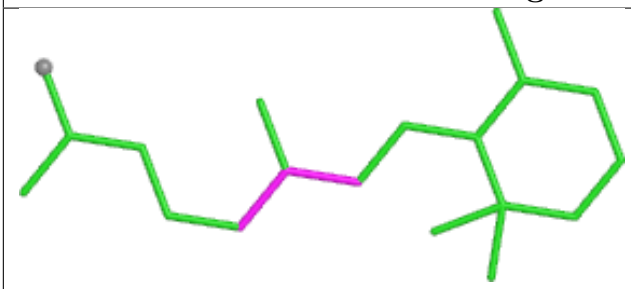


Rings

Ligand QTB 9 304



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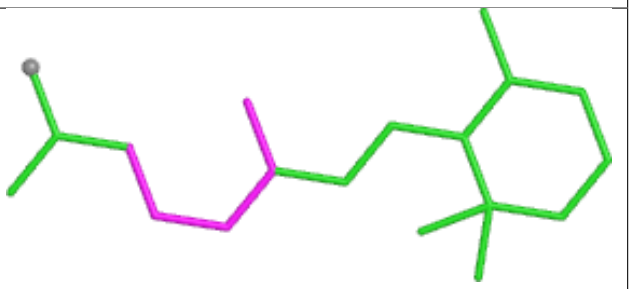
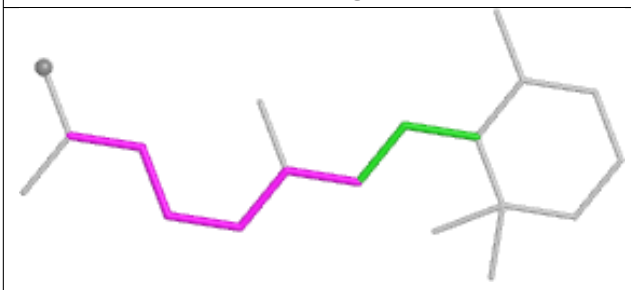


Bond angles



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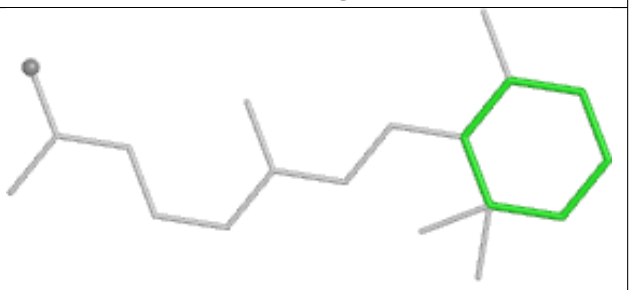
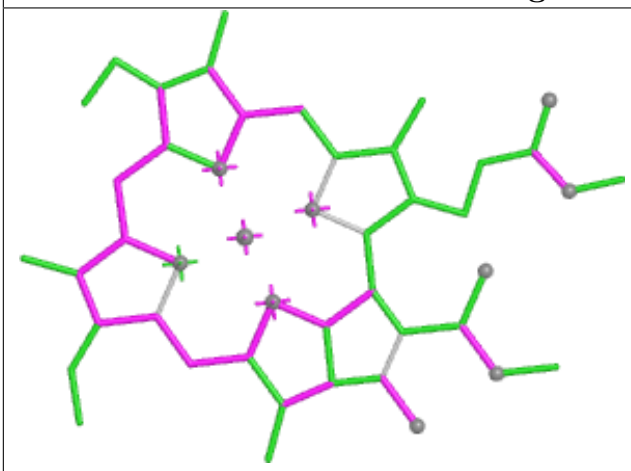
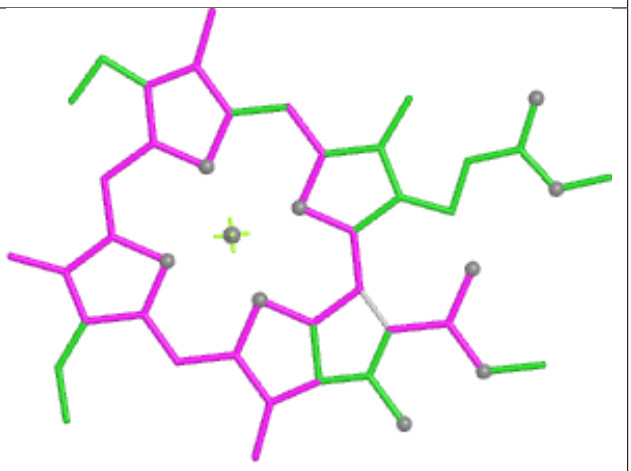


Rings

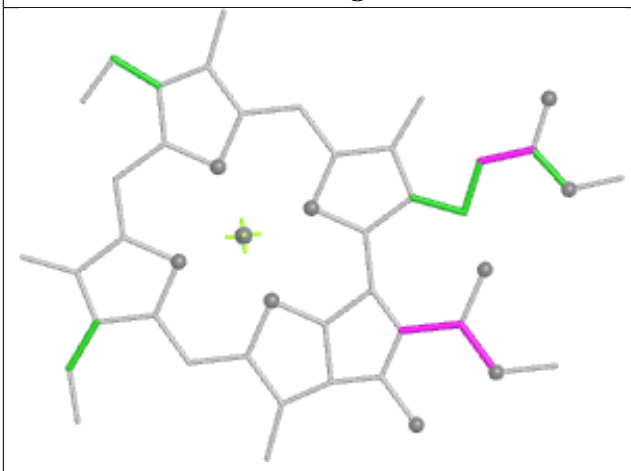
Ligand CLA 3 308



Bond lengths



Bond angles



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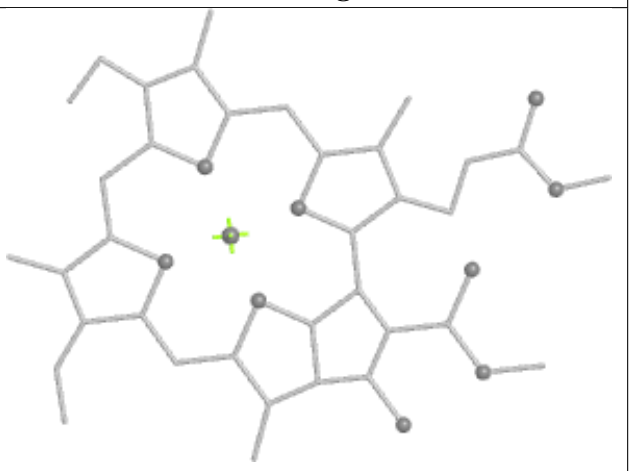
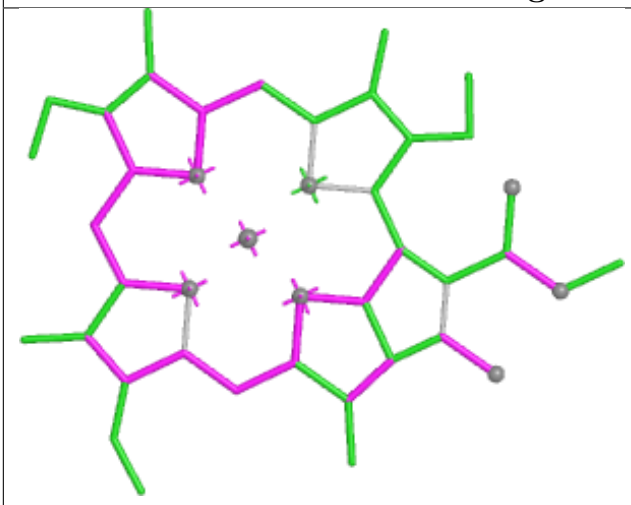


Rings

Ligand CLA J 105



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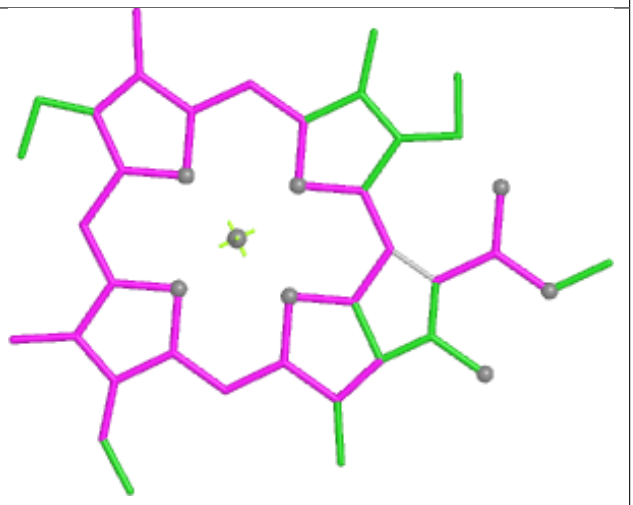
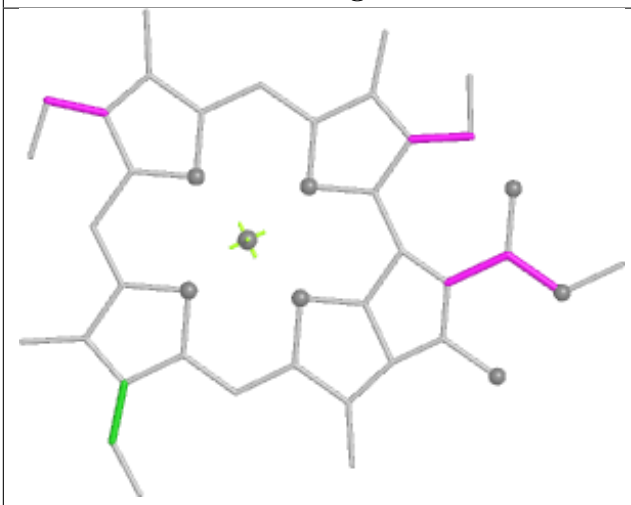


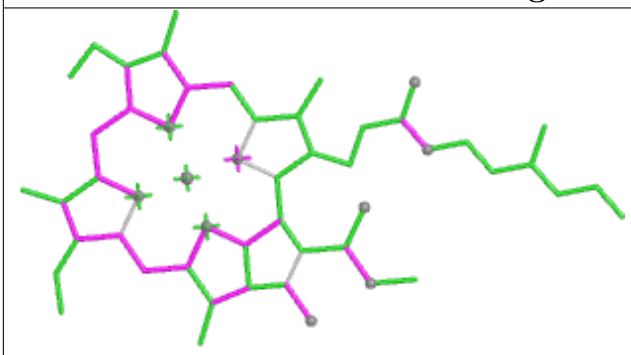
Bond angles



Torsions

Rings

Ligand CLA 3 314



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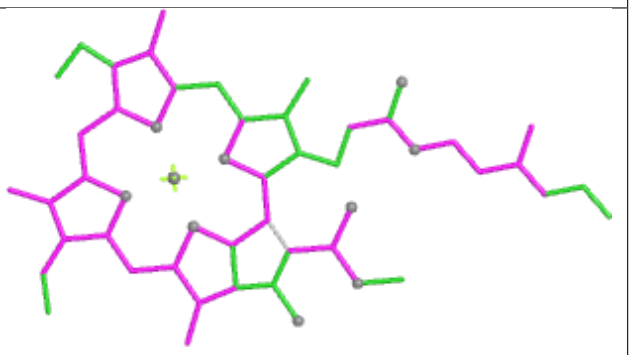
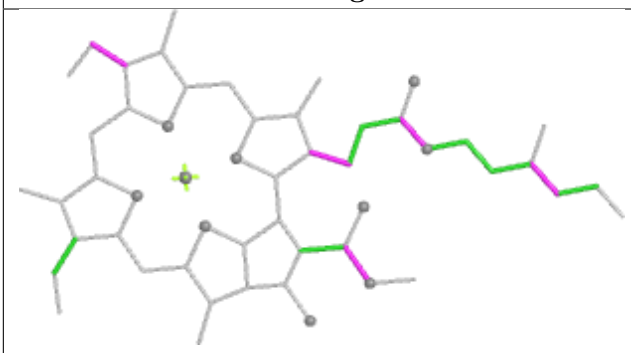


Bond angles



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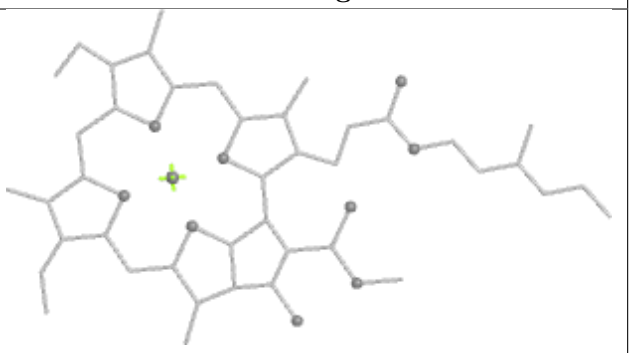
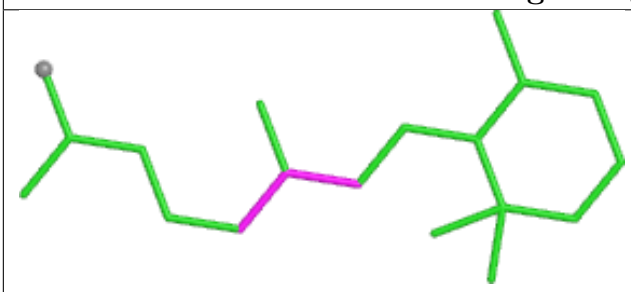


Rings

Ligand QTB a 302



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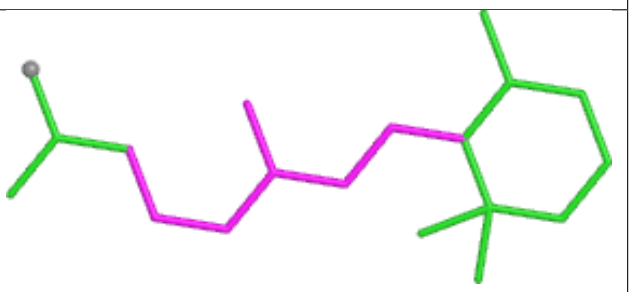
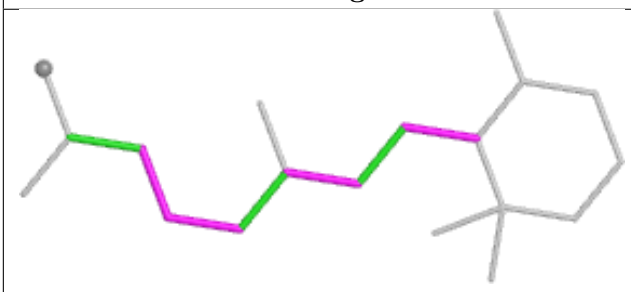


Bond angles



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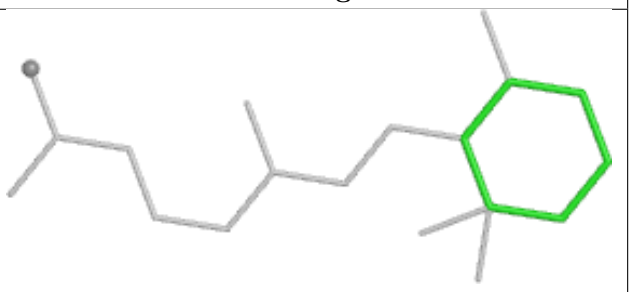
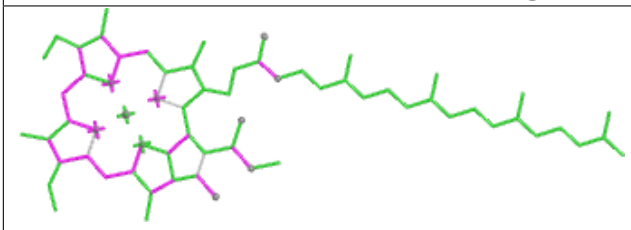


Rings

Ligand CLA A 816



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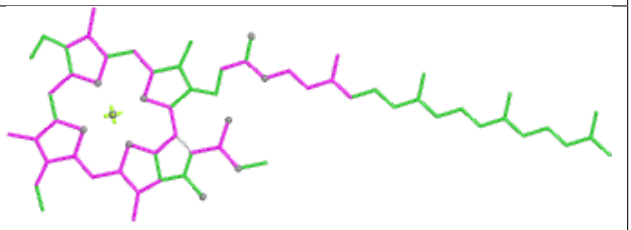
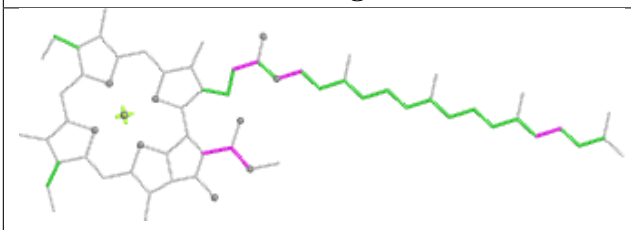


Bond angles



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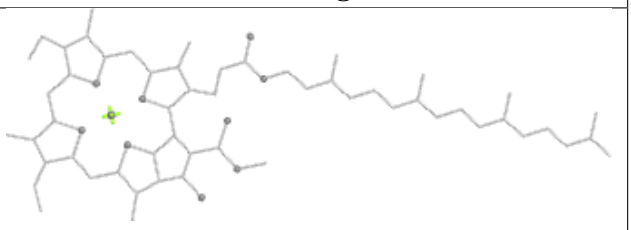
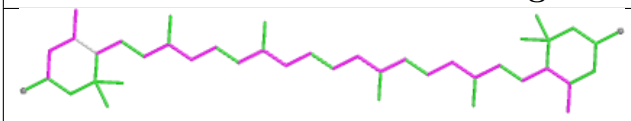


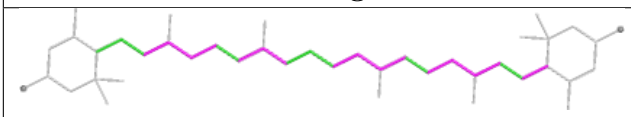
Rings

Ligand LUT 4 303



Bond lengths

Bond angles



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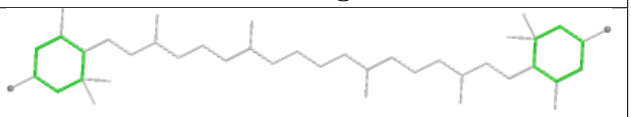
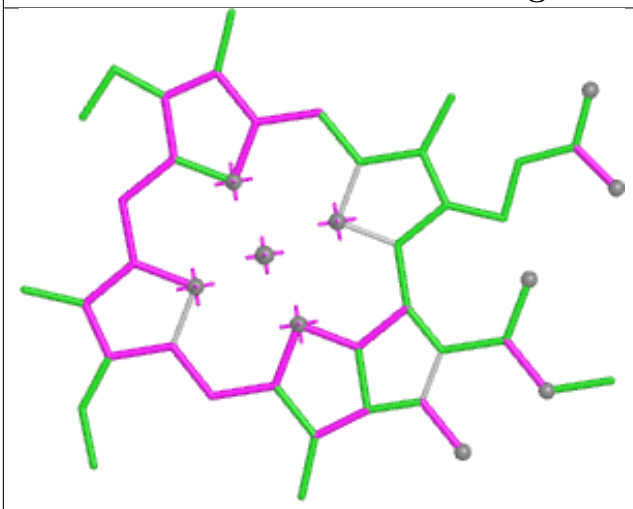
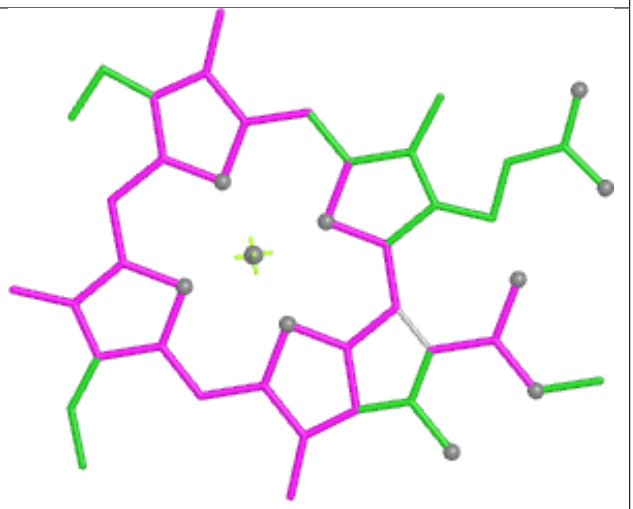


Rings

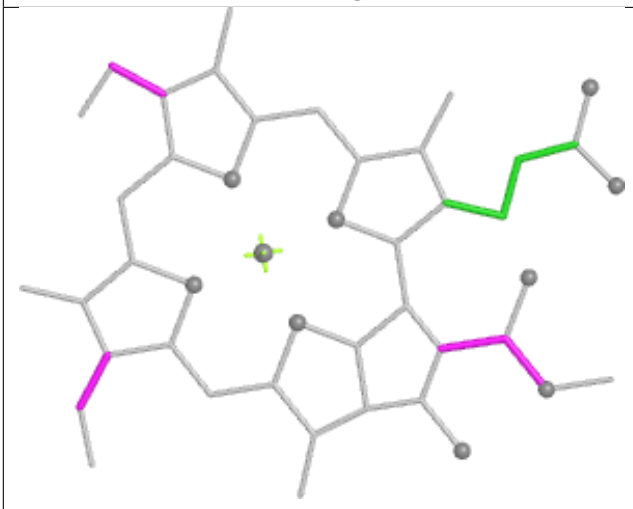
Ligand CLA 4 320



Bond lengths



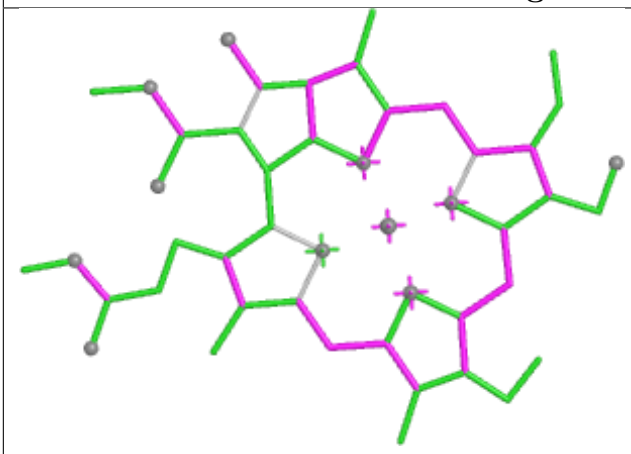
Bond angles



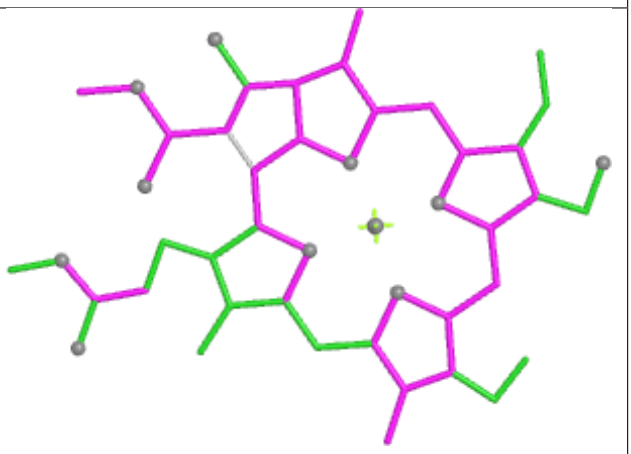
Torsions

Rings

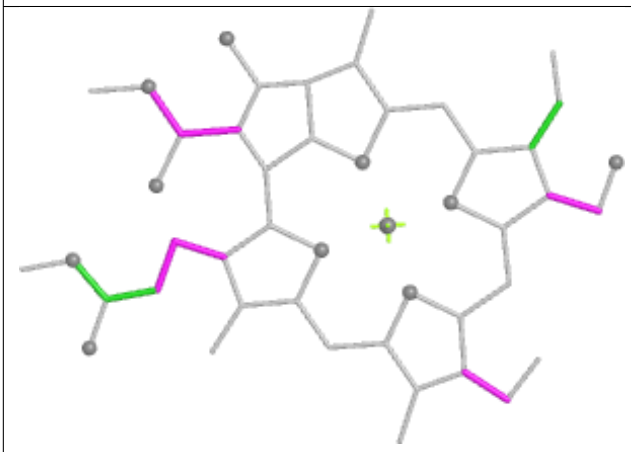
Ligand CHL b 309



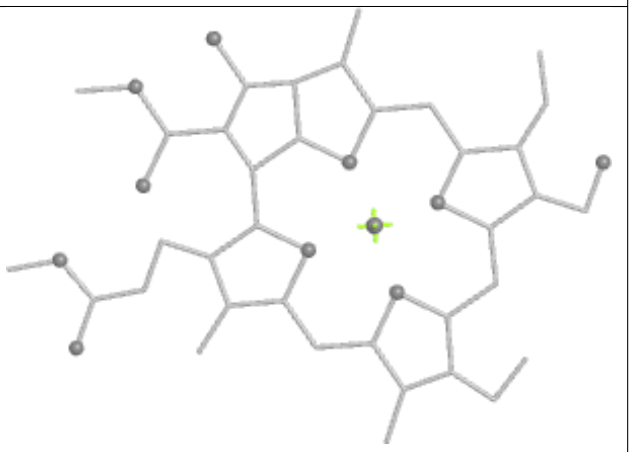
Bond lengths



Bond angles

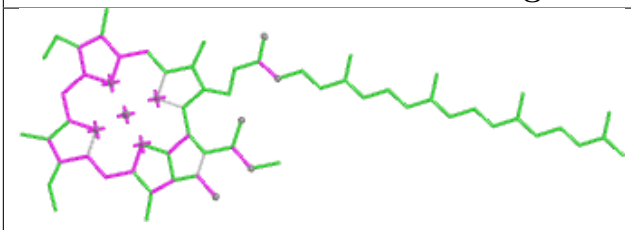


Torsions

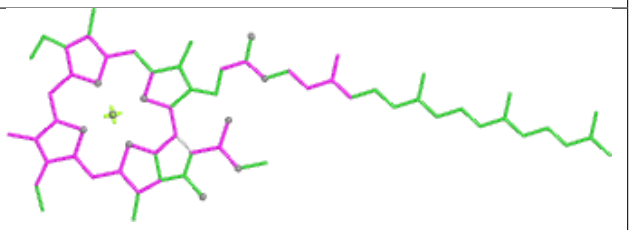


Rings

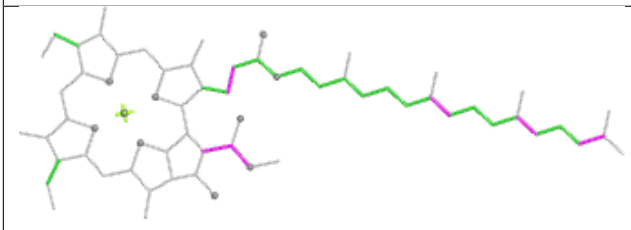
Ligand CLA A 814



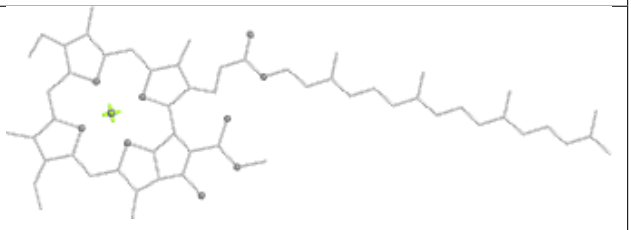
Bond lengths



Bond angles

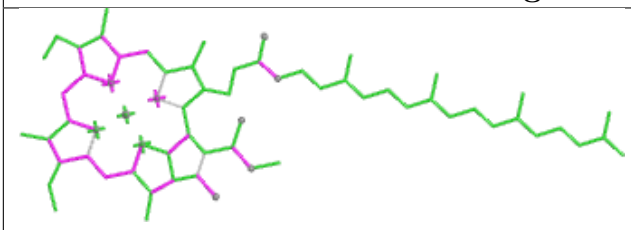


Torsions

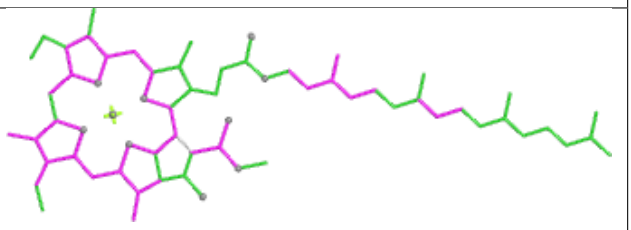


Rings

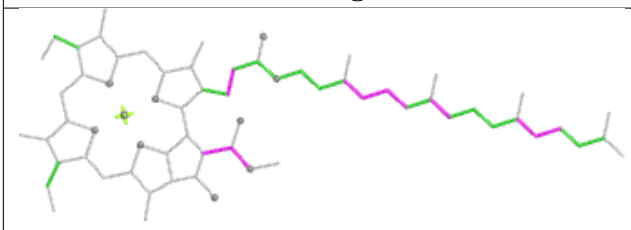
Ligand CLA A 821



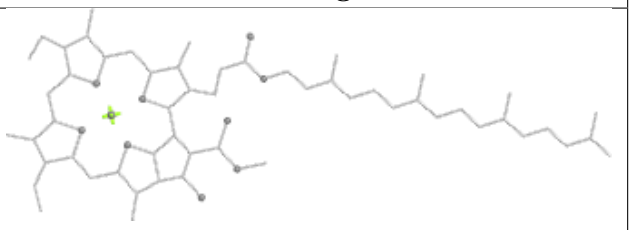
Bond lengths



Bond angles

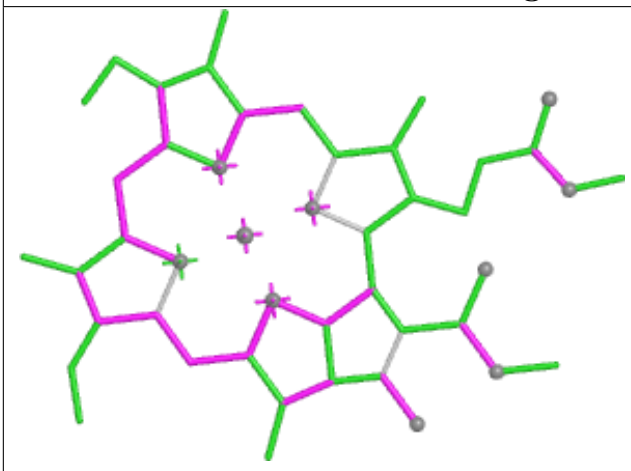


Torsions

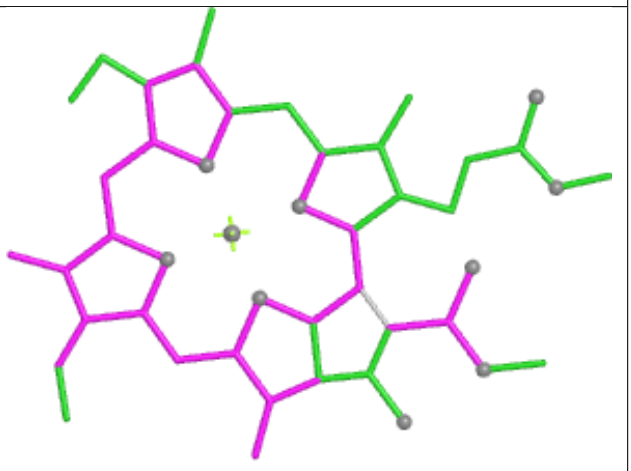


Rings

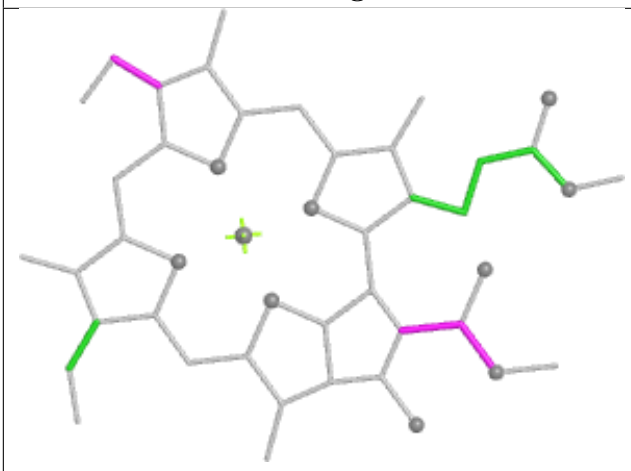
Ligand CLA K 206



Bond lengths



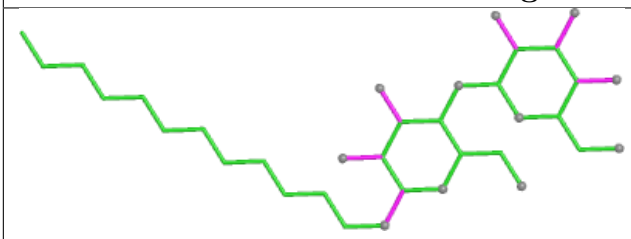
Bond angles



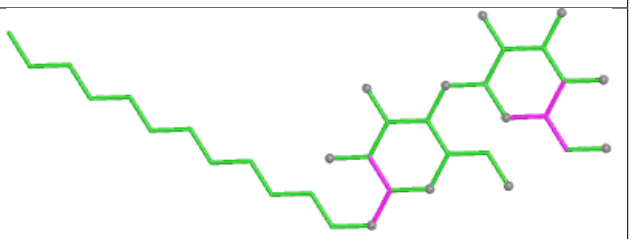
Torsions

Rings

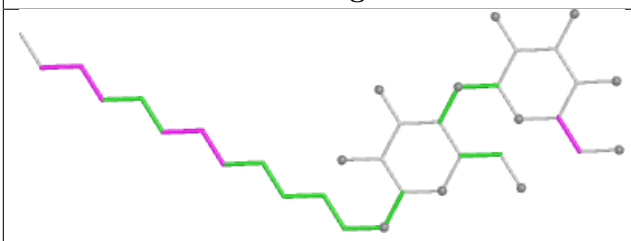
Ligand LMT A 807



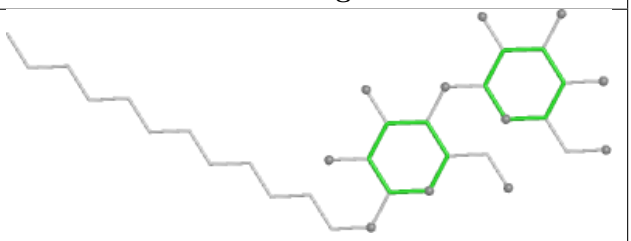
Bond lengths



Bond angles

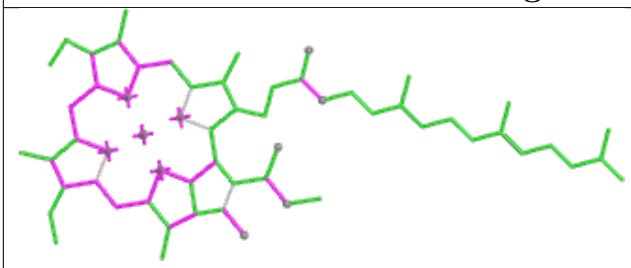


Torsions

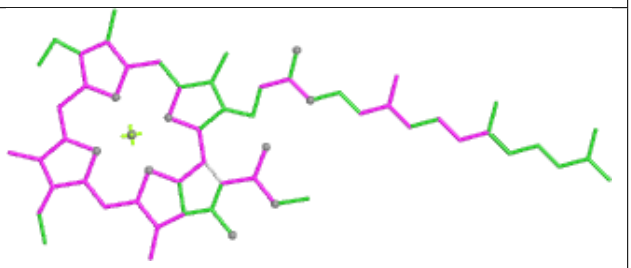


Rings

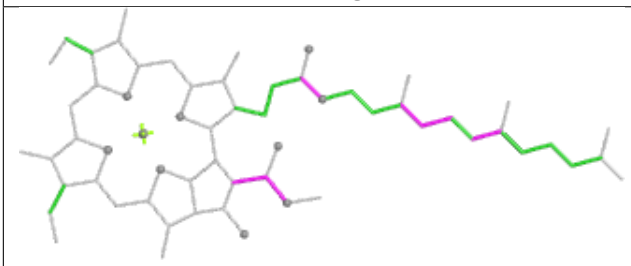
Ligand CLA A 830



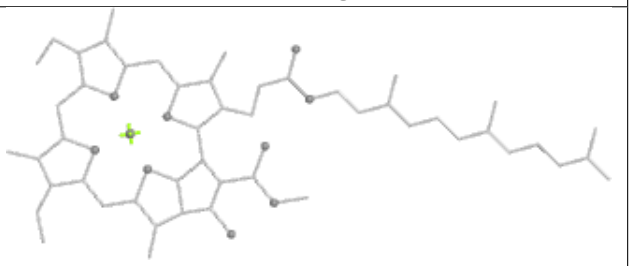
Bond lengths



Bond angles

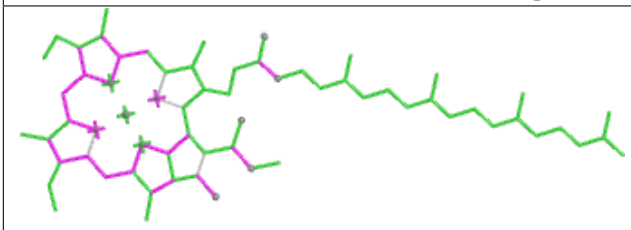


Torsions

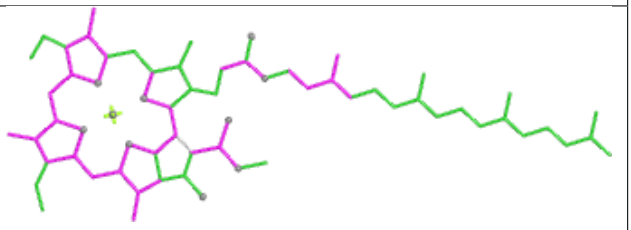


Rings

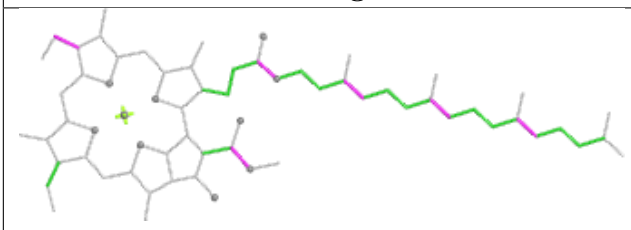
Ligand CLA 7 311



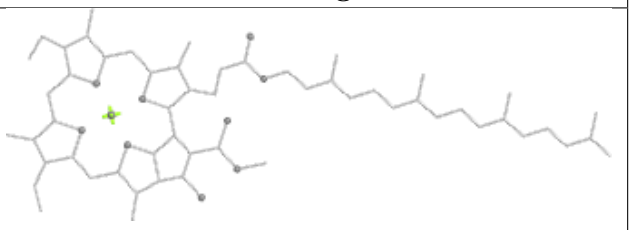
Bond lengths



Bond angles

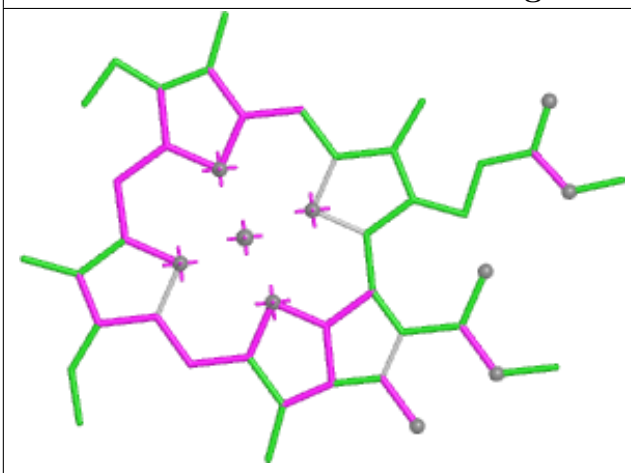


Torsions

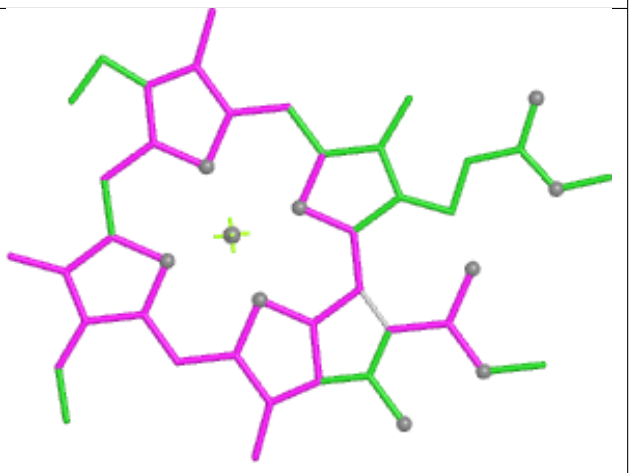


Rings

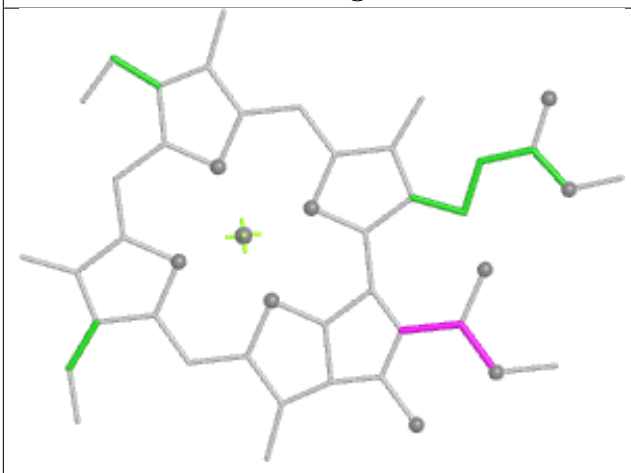
Ligand CLA B 838



Bond lengths



Bond angles



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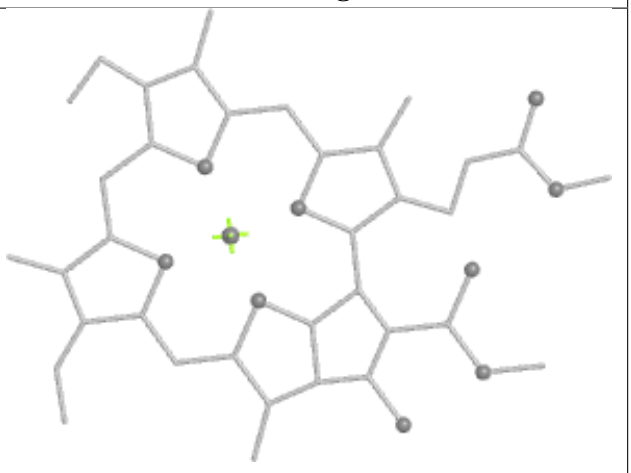
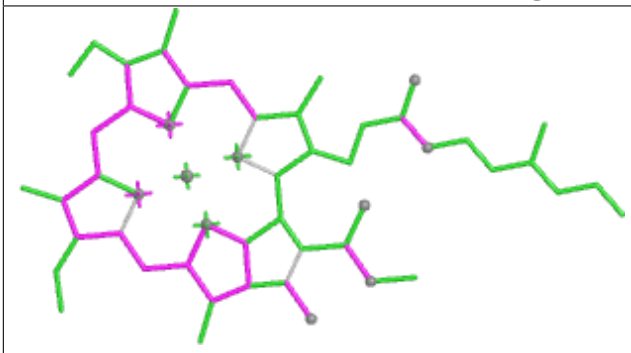
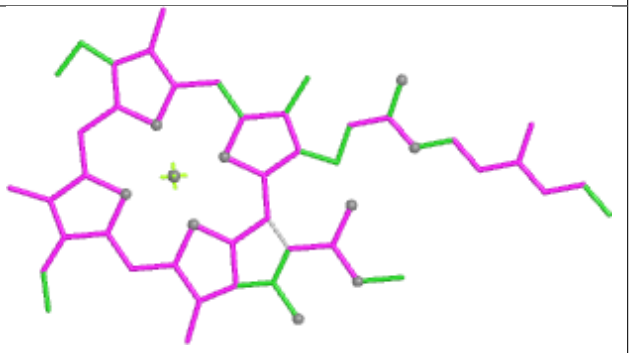
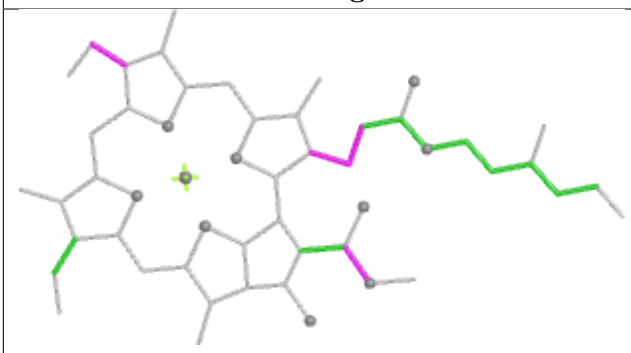
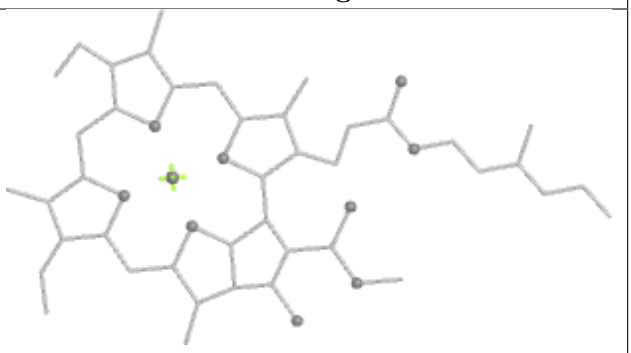
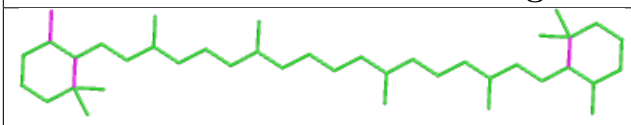
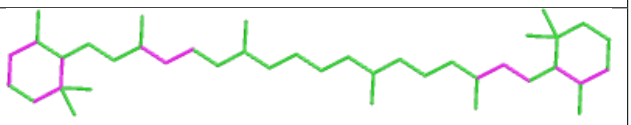
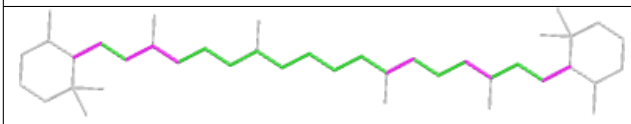
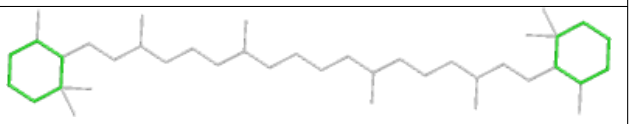
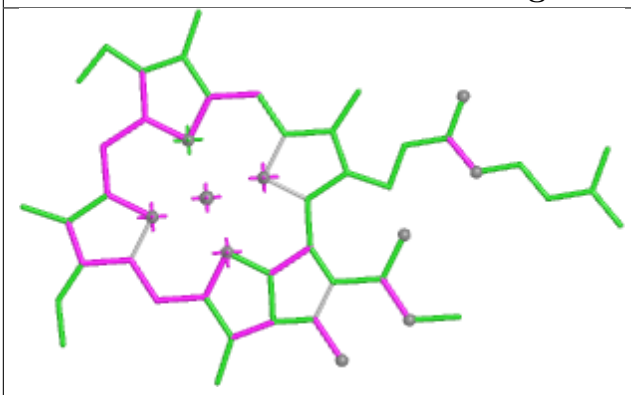


Rings

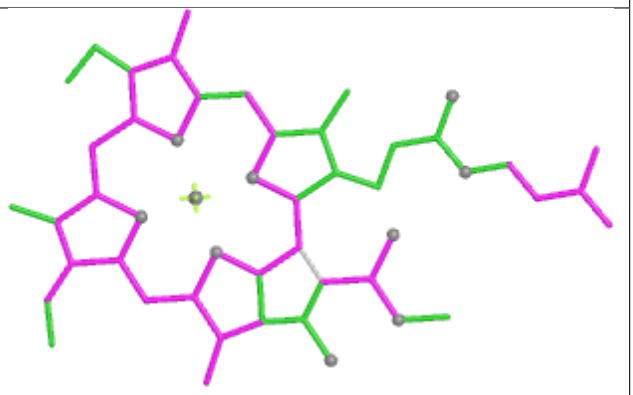
Ligand CLA 4 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 3 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

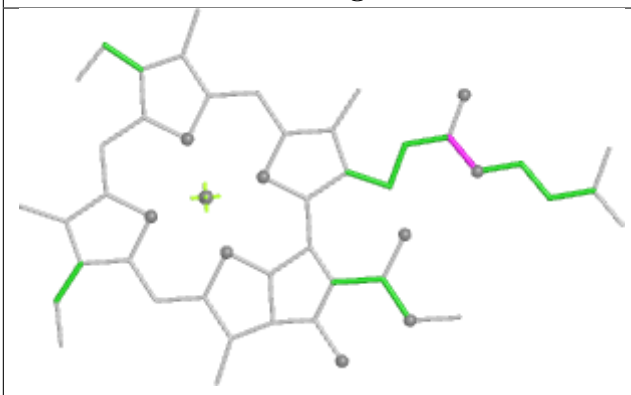
Ligand CLA 8 318



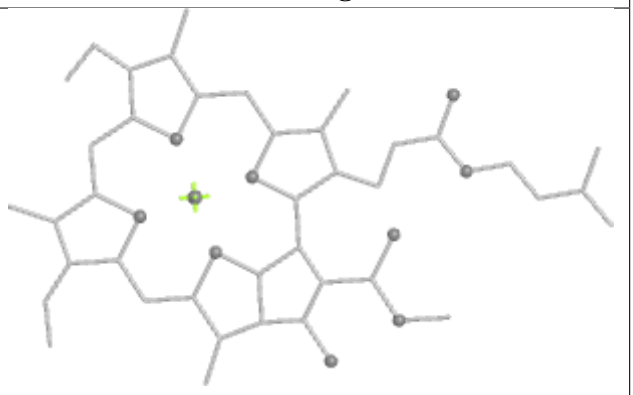
Bond lengths



Bond angles

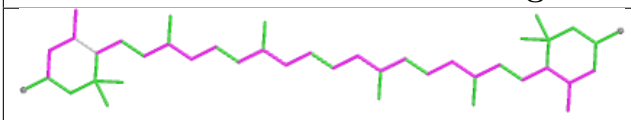


Torsions

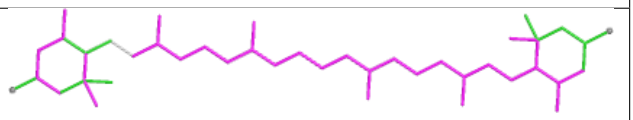


Rings

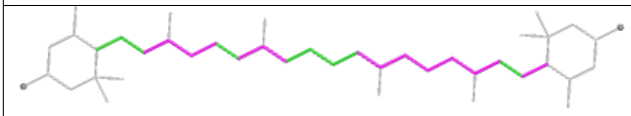
Ligand LUT L 304



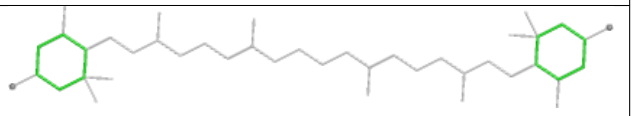
Bond lengths



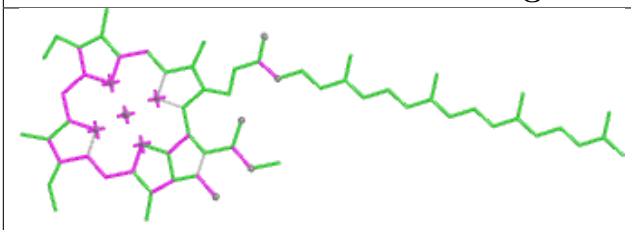
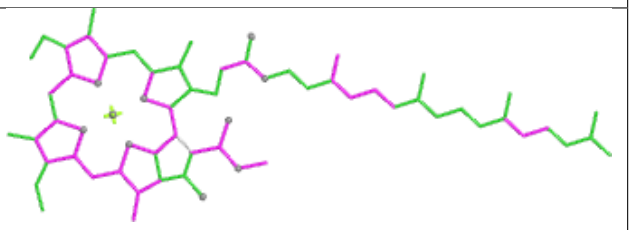
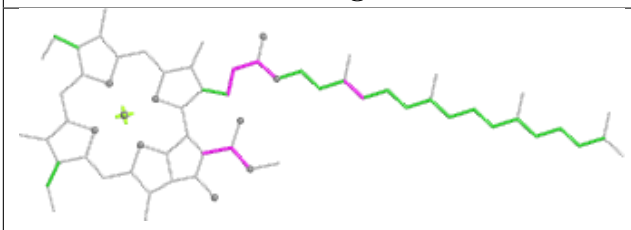
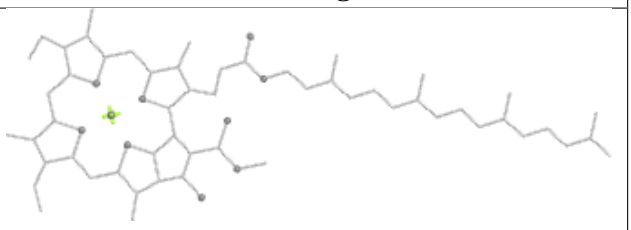
Bond angles

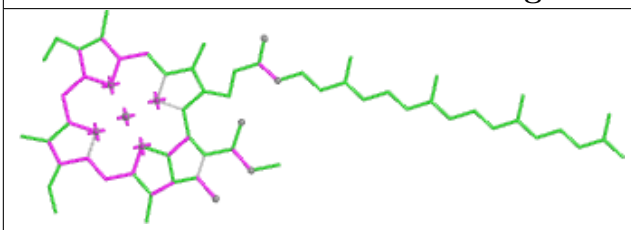
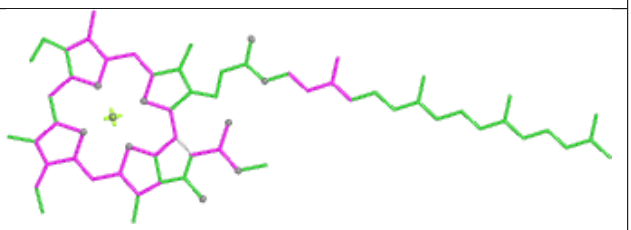
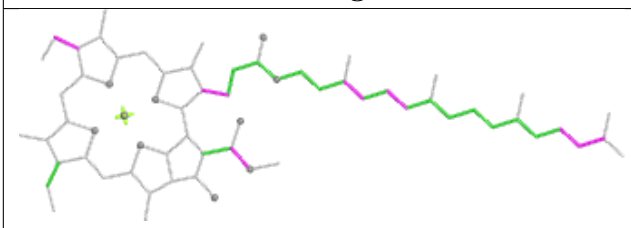
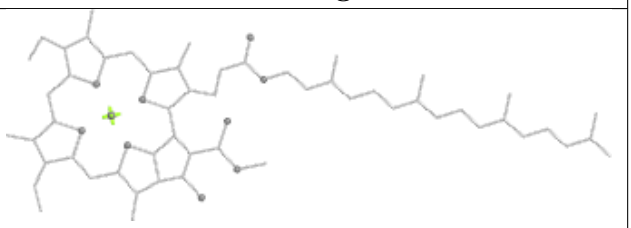


Torsions

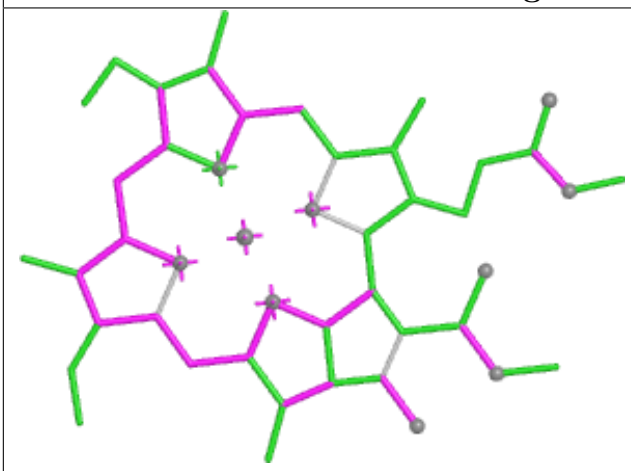


Rings

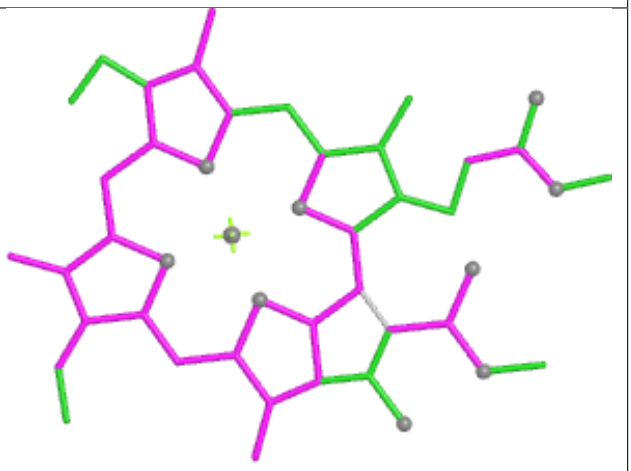
Ligand CLA A 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

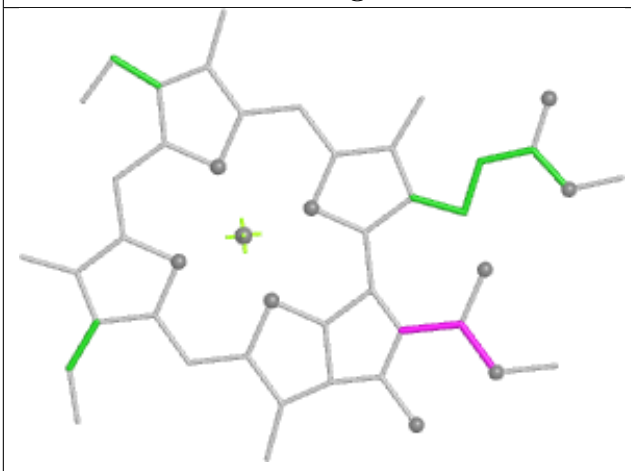
Ligand CLA H 902



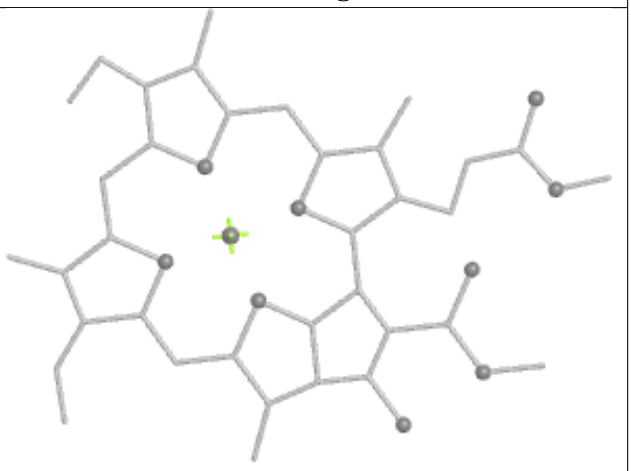
Bond lengths



Bond angles

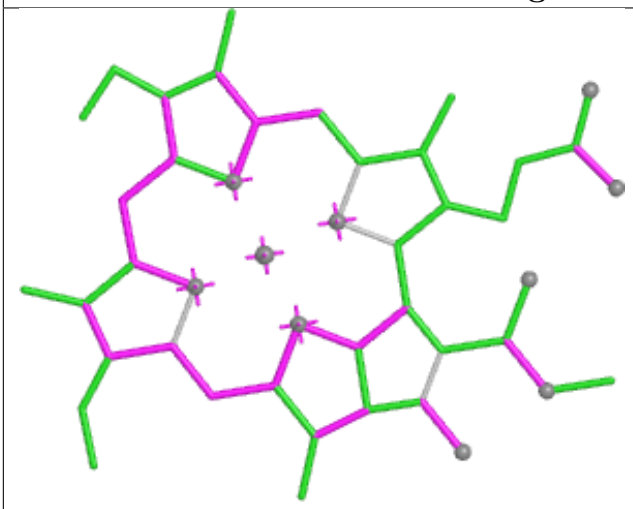


Torsions



Rings

Ligand CLA 4 314



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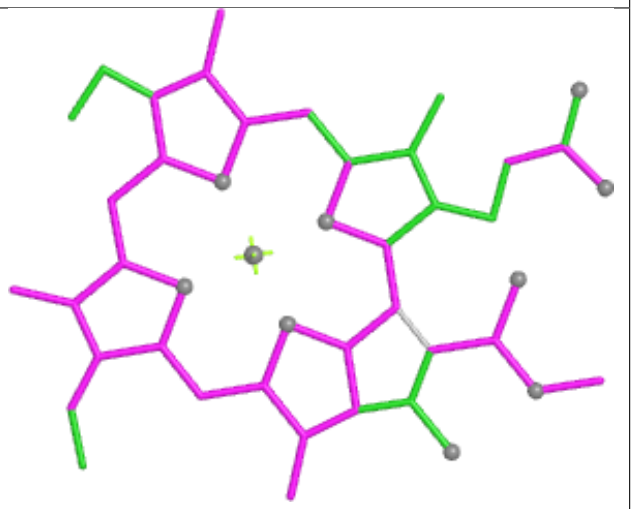
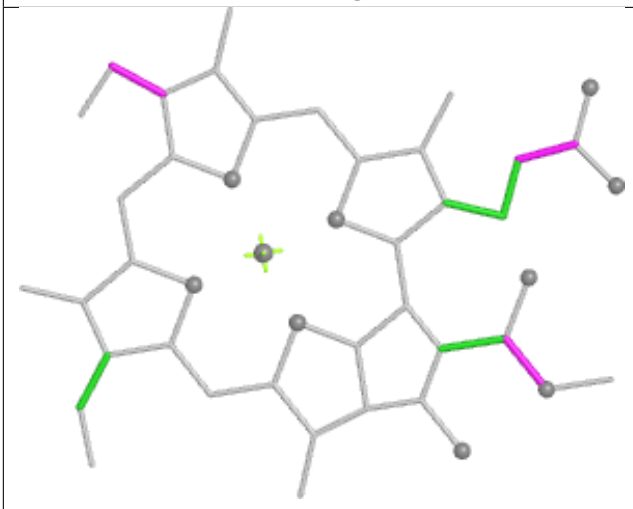


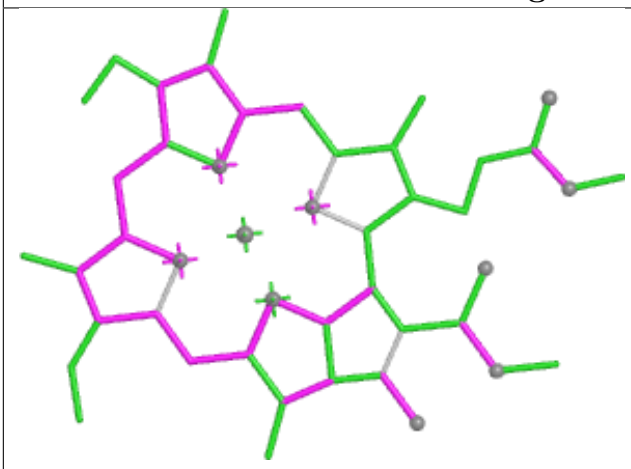
Bond angles



Torsions

Rings

Ligand CLA 8 307



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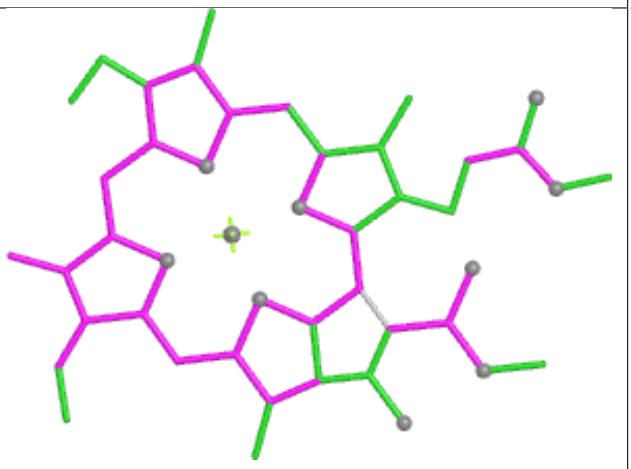
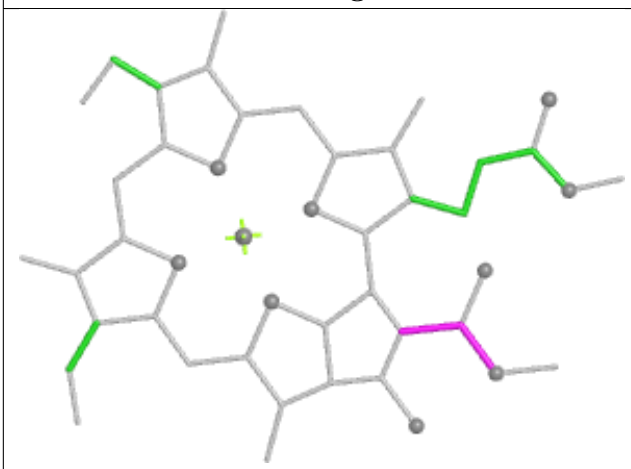


Bond angles



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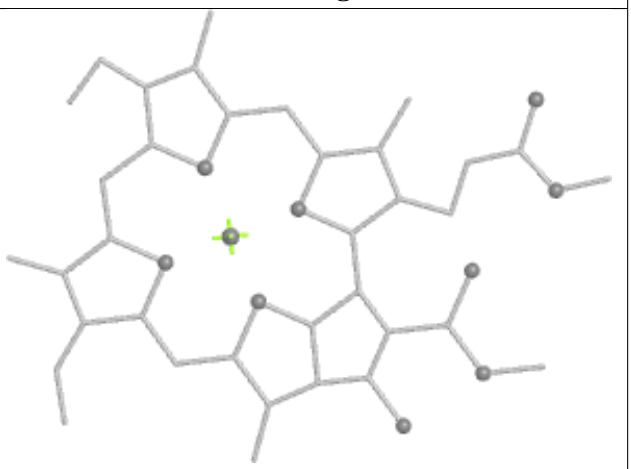
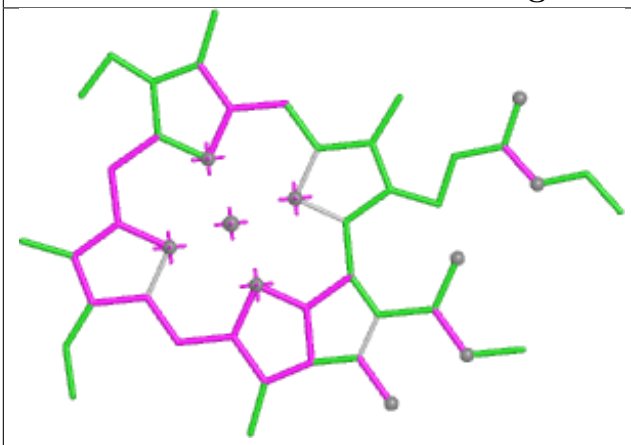


Rings

Ligand CLA 9 317



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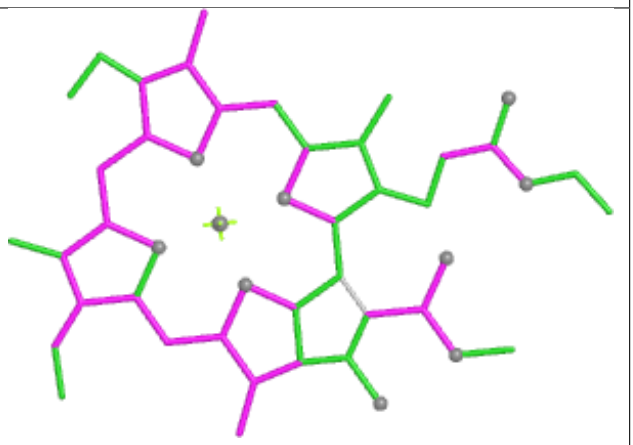

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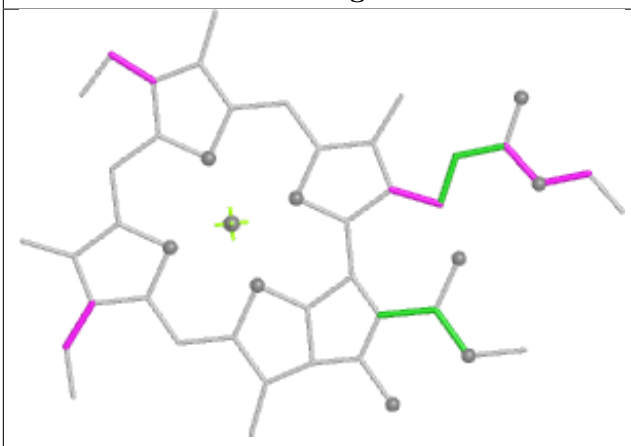
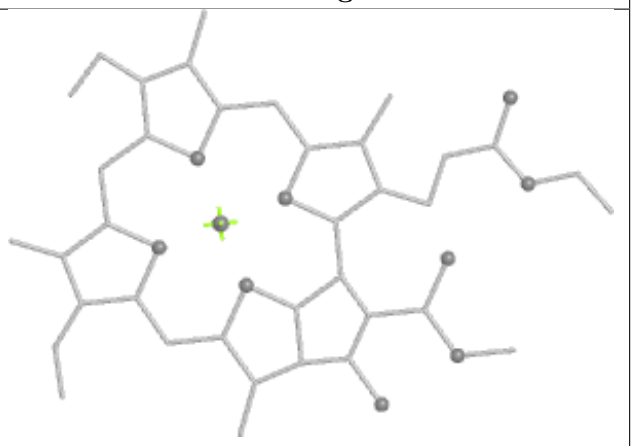
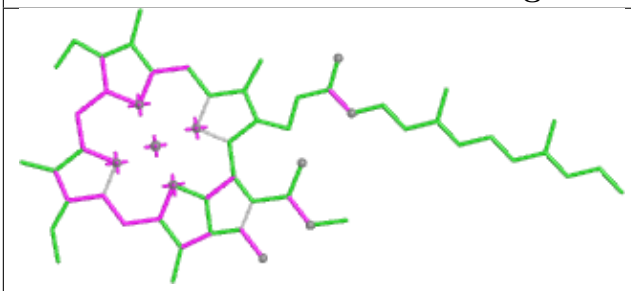


Torsions



Rings

Ligand CLA A 848



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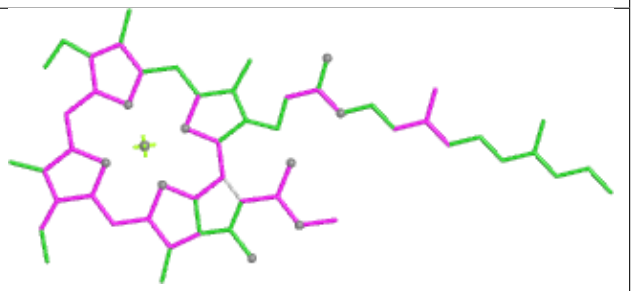
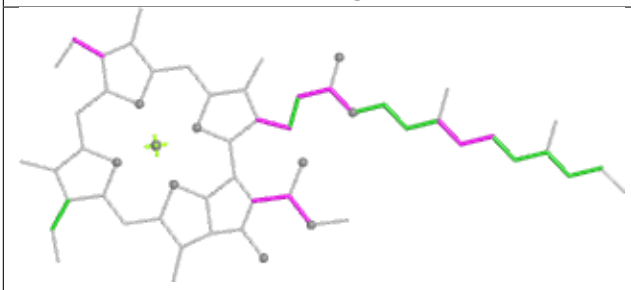


Bond angles



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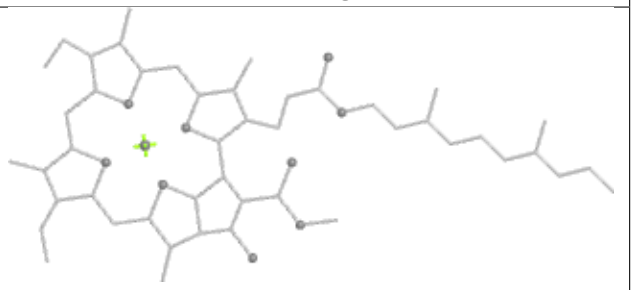
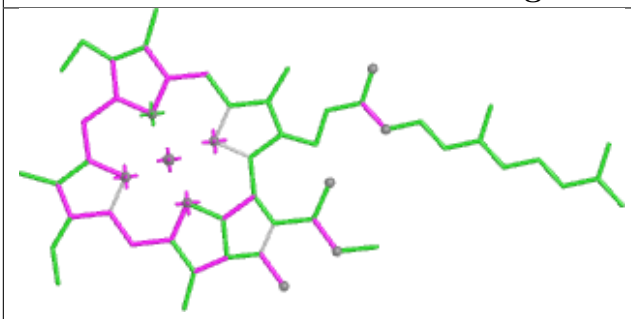


Rings

Ligand CLA B 833



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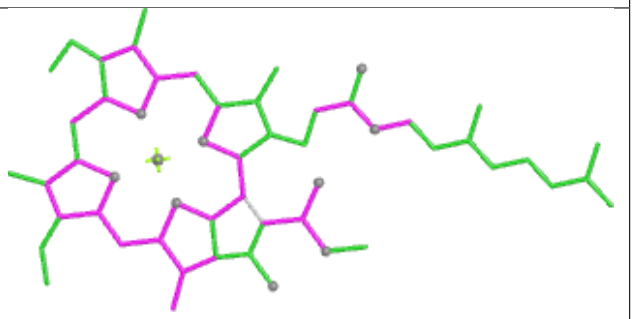

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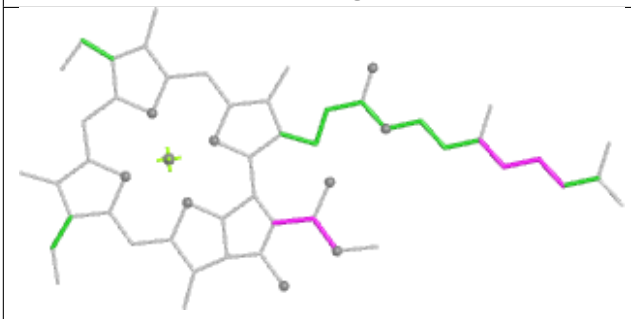

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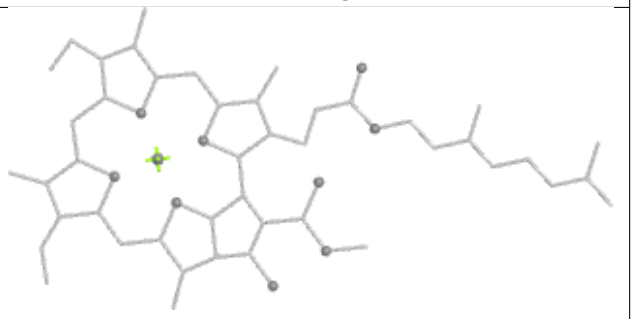
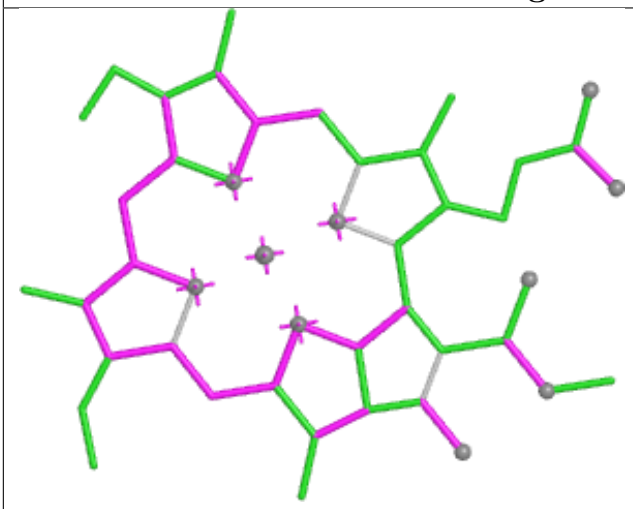


Rings

Ligand CLA 3 320



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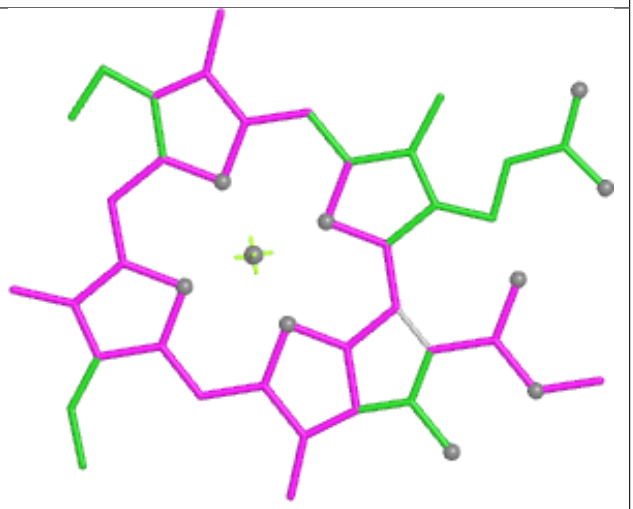

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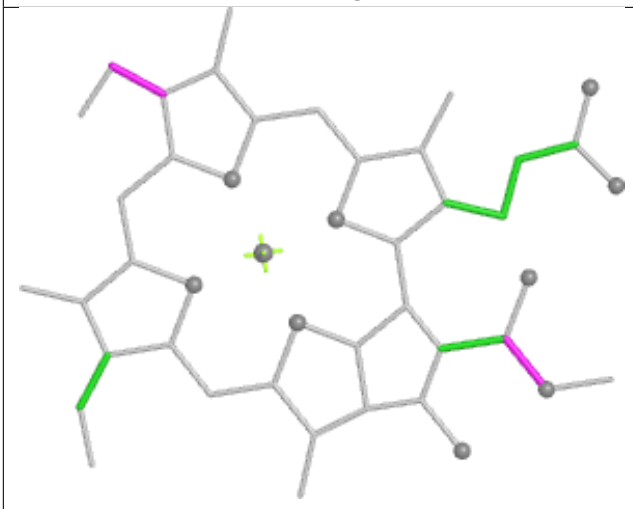
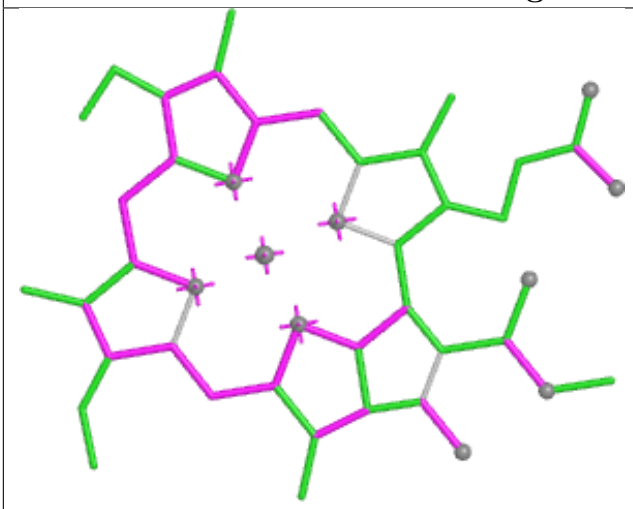


Torsions

Rings

Ligand CLA L 306



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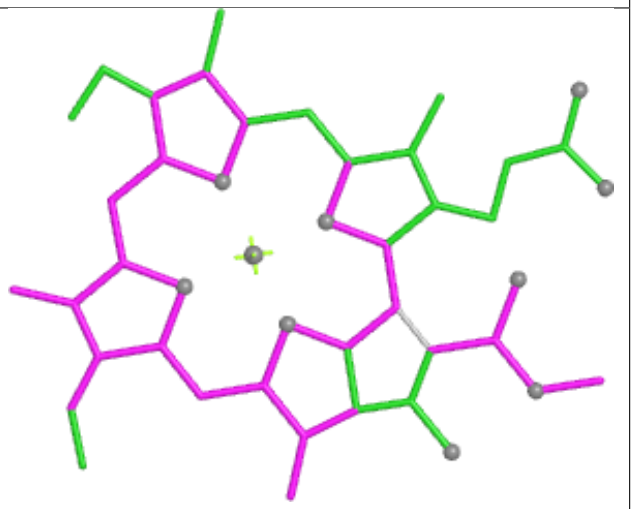

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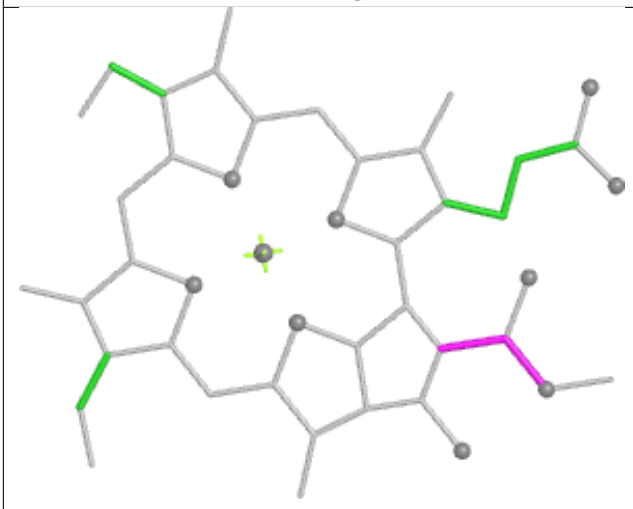
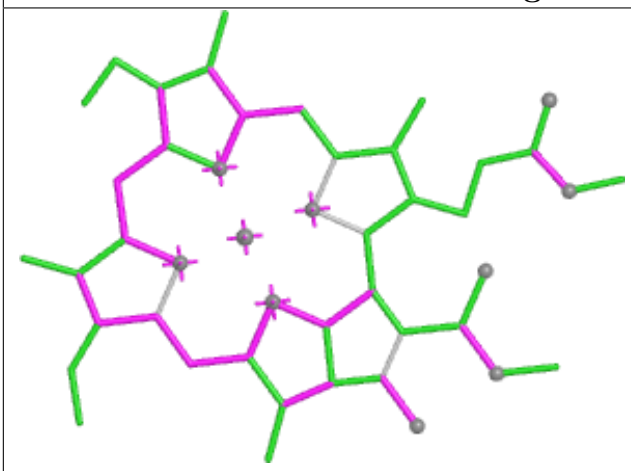


Torsions

Rings

Ligand CLA A 849



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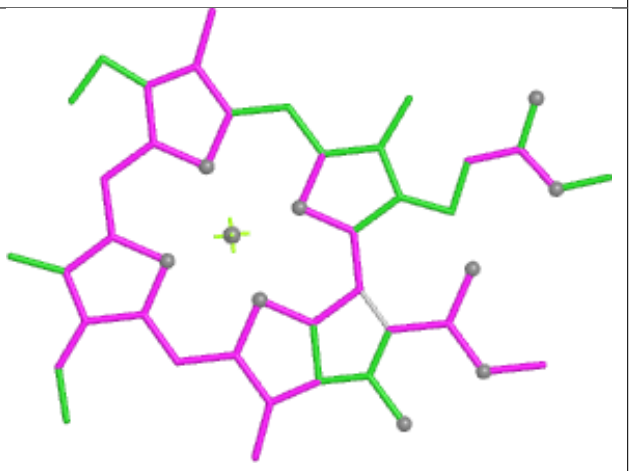

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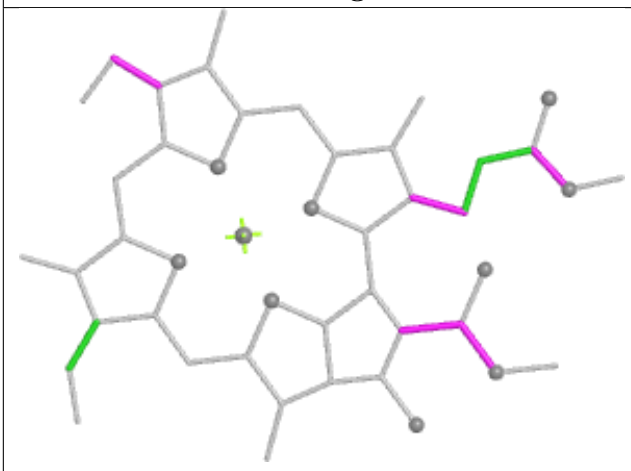
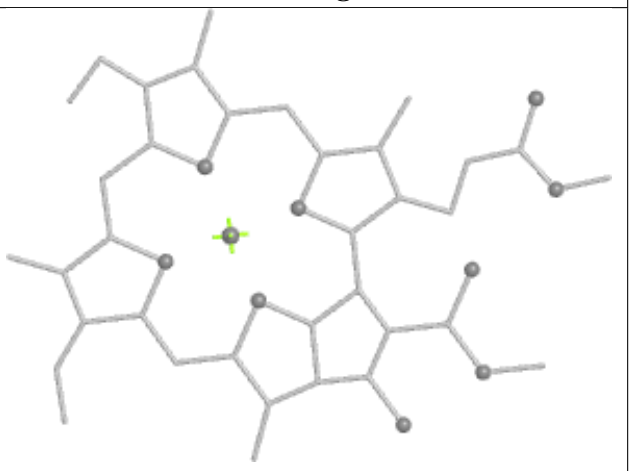
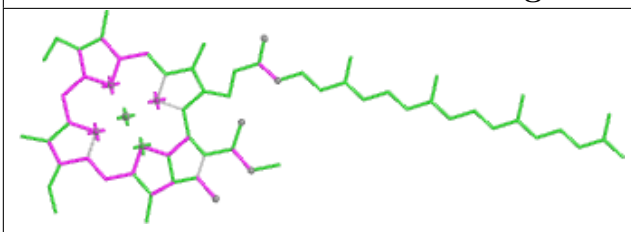


Torsions

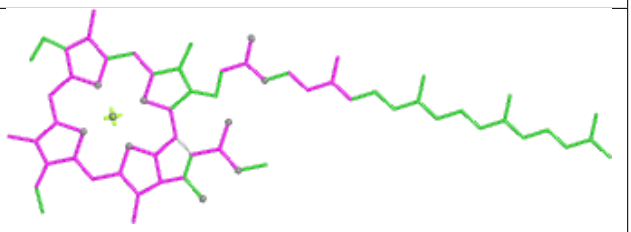


Rings

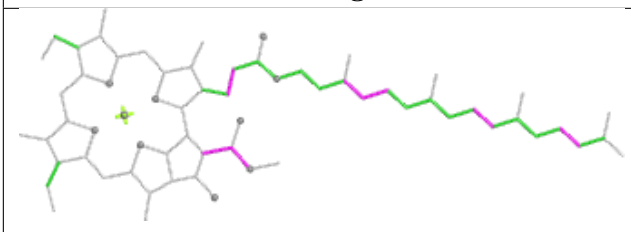
Ligand CLA B 832



Bond lengths



Bond angles



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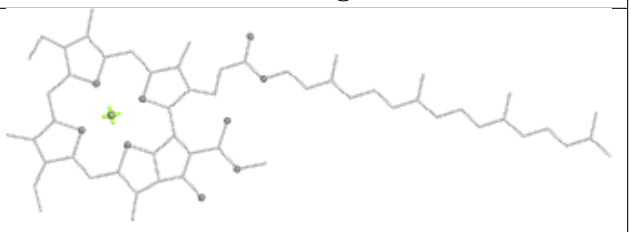
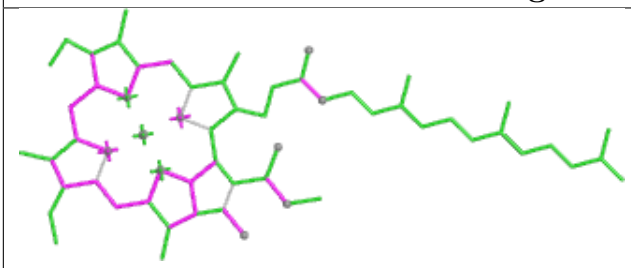
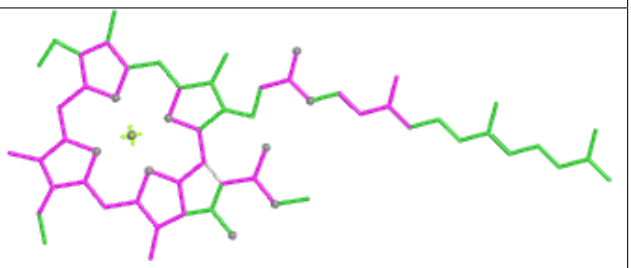
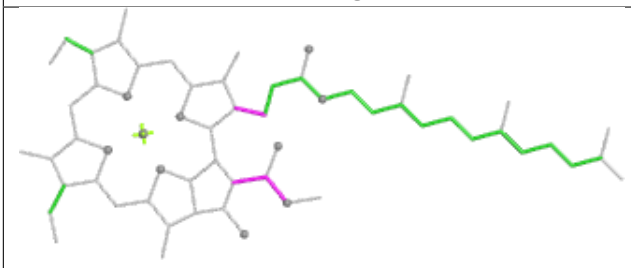
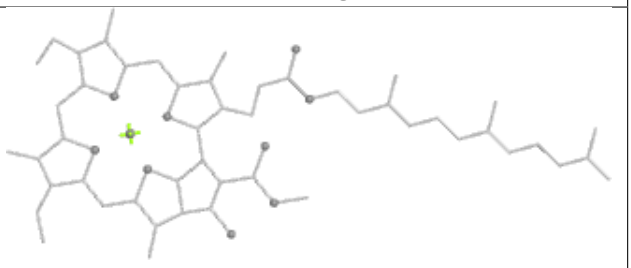
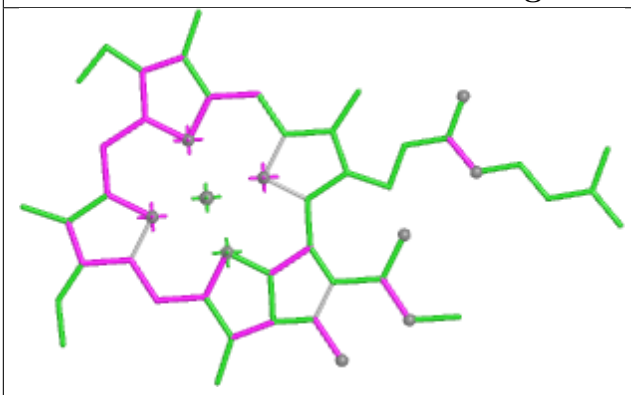
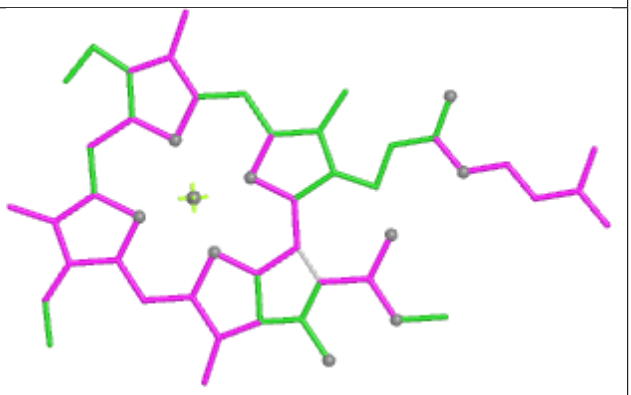
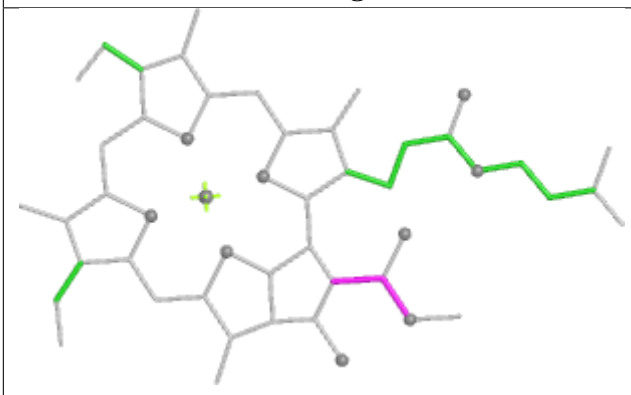
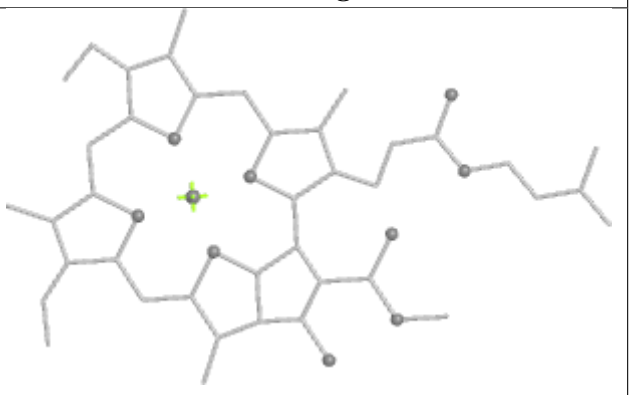
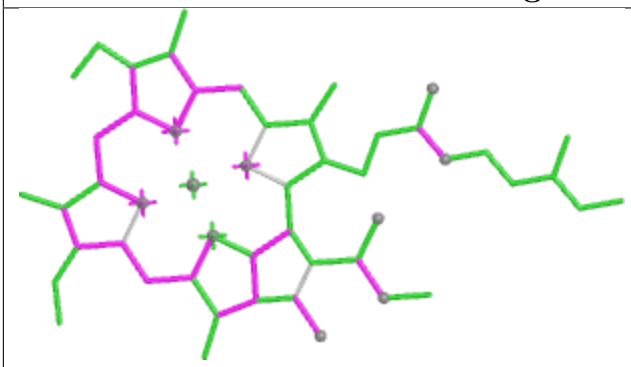


Rings

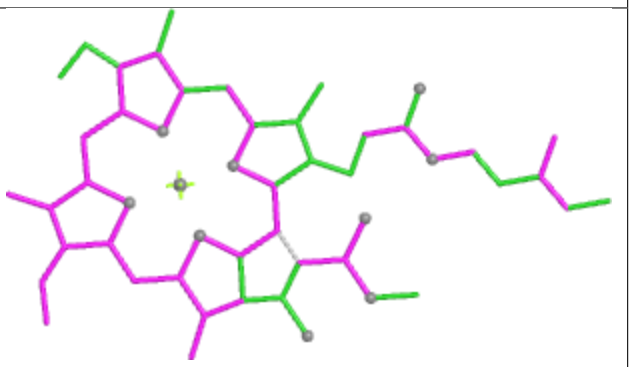
Ligand CLA 7 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

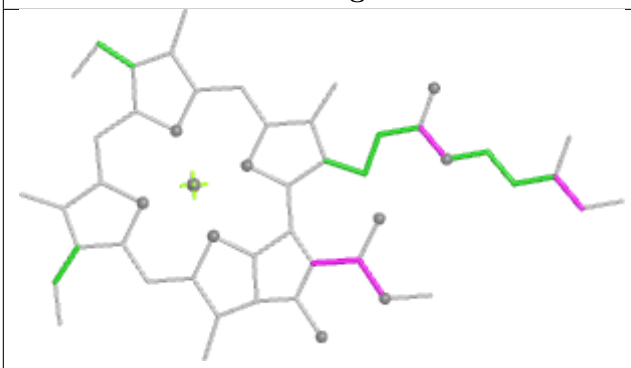
Ligand CLA A 850



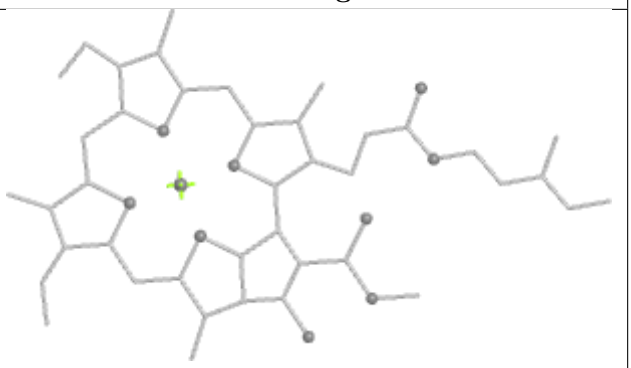
Bond lengths



Bond angles

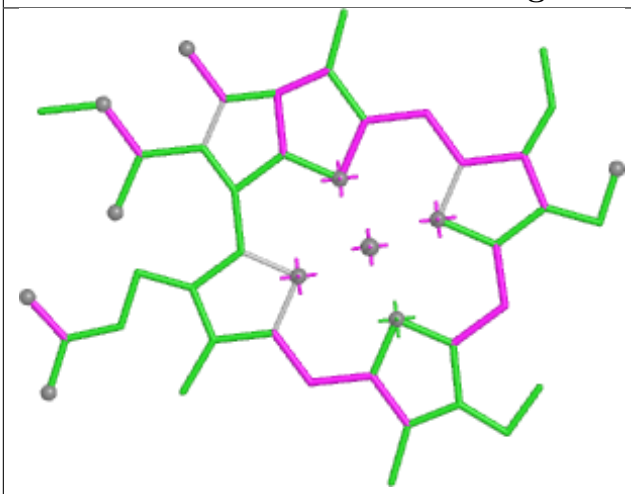


Torsions



Rings

Ligand CHL 4 317



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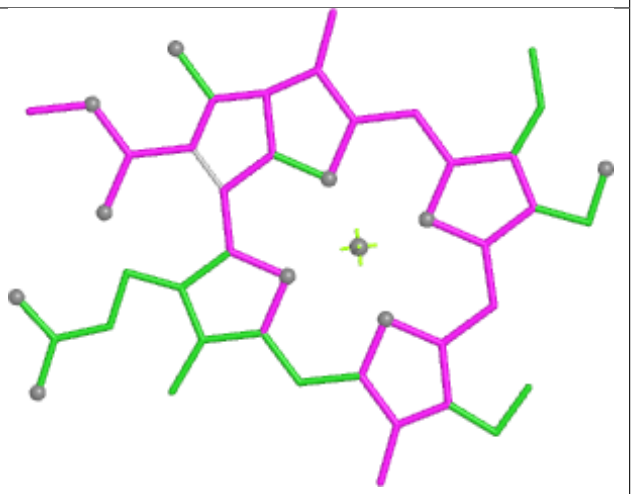
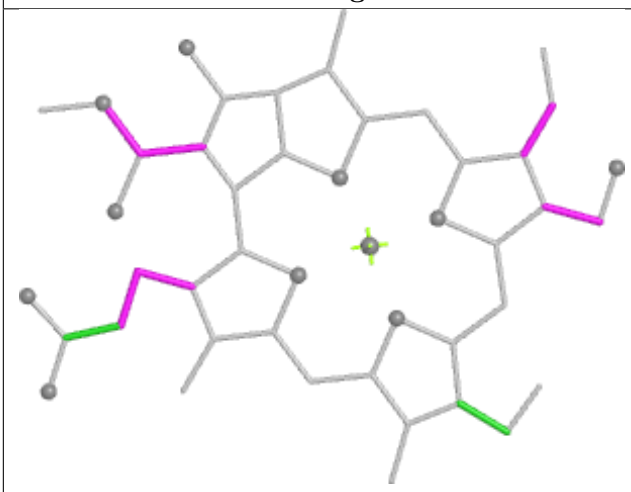


Bond angles



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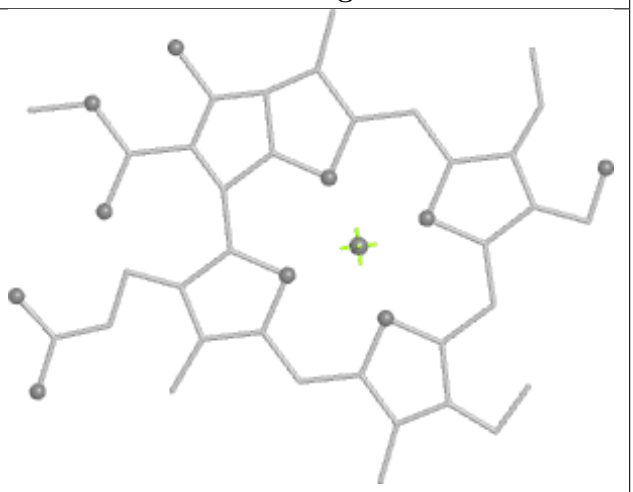
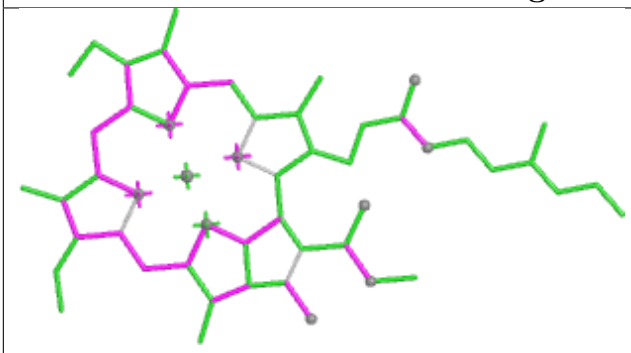


Rings

Ligand CLA 8 314



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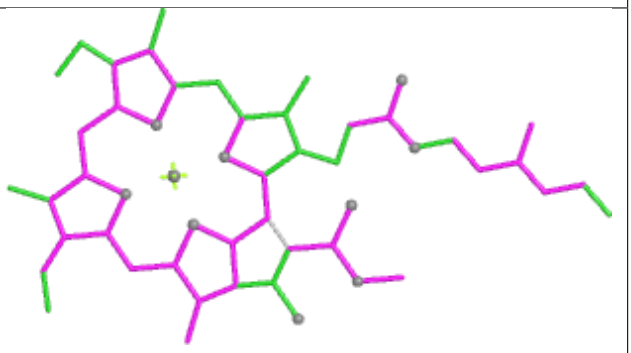
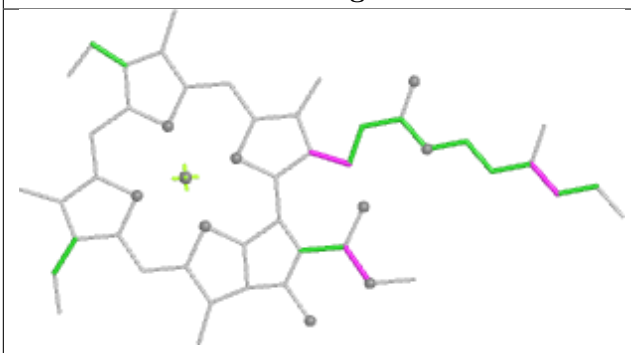
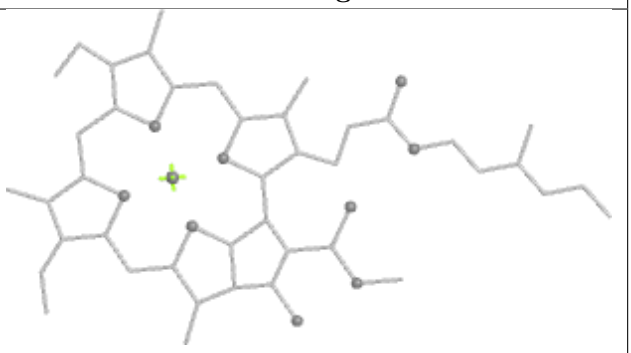


Bond angles

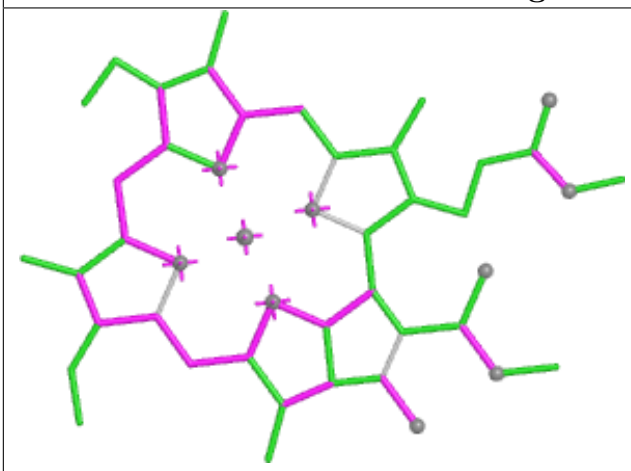


Torsions

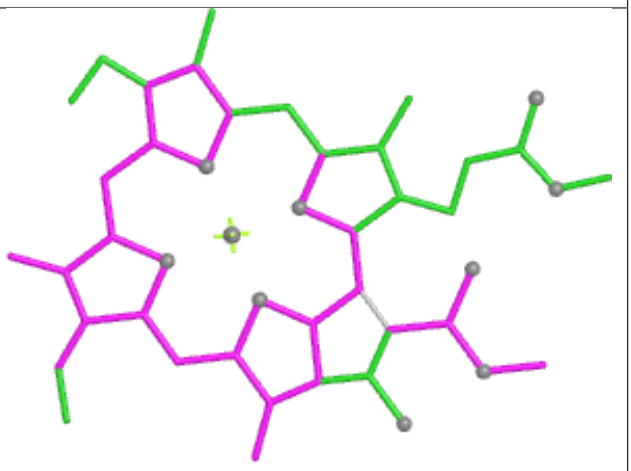


Rings

Ligand CLA 6 322



Bond lengths



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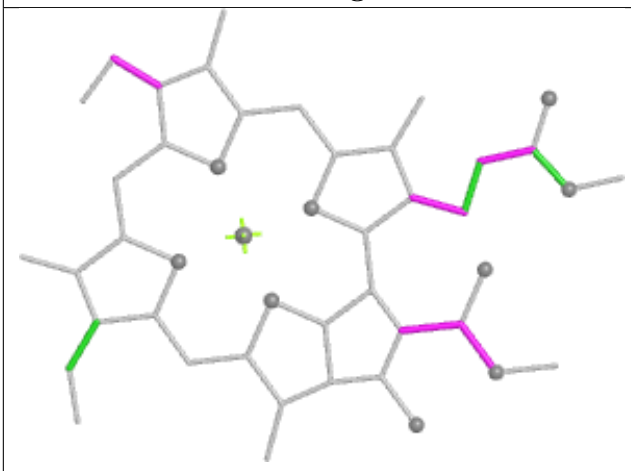

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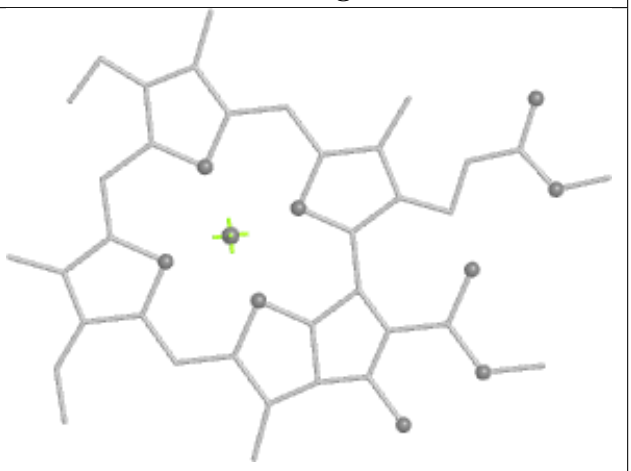
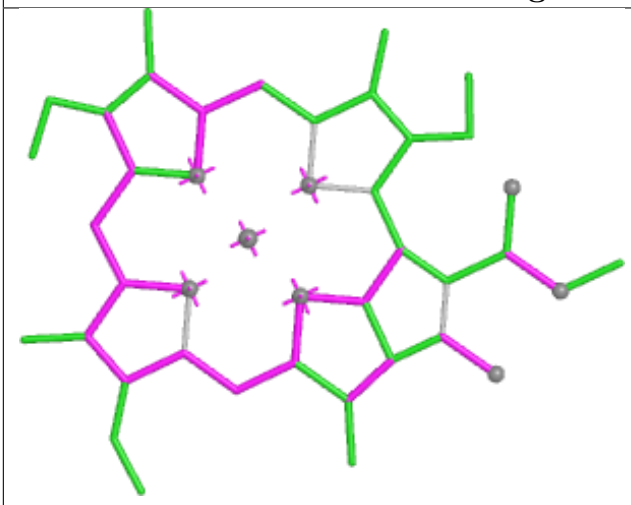


Rings

Ligand CLA 4 319



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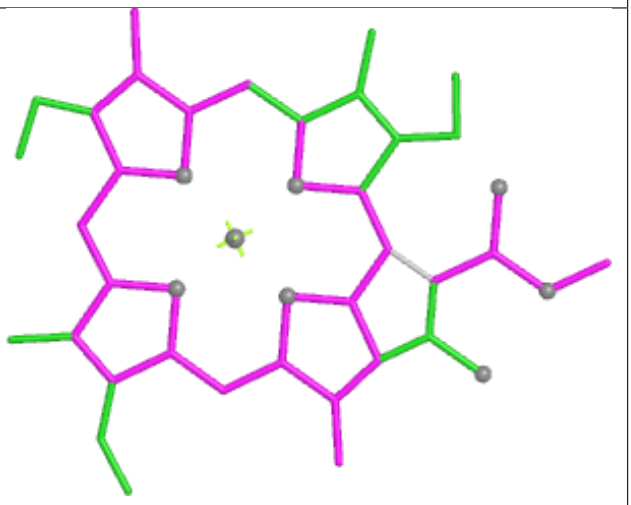
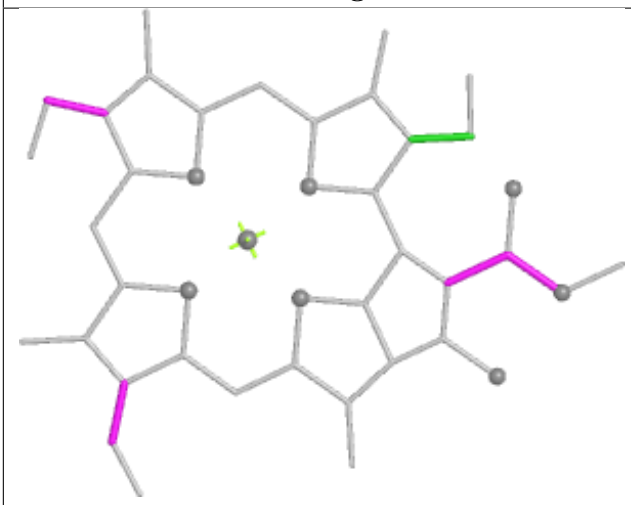


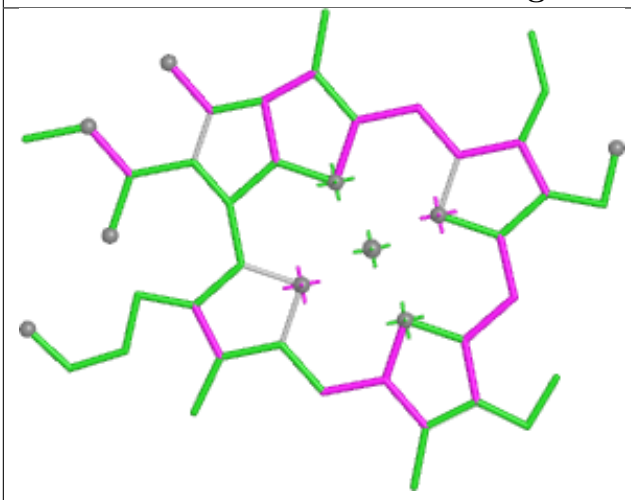
Bond angles



Torsions

Rings

Ligand CHL 8 319



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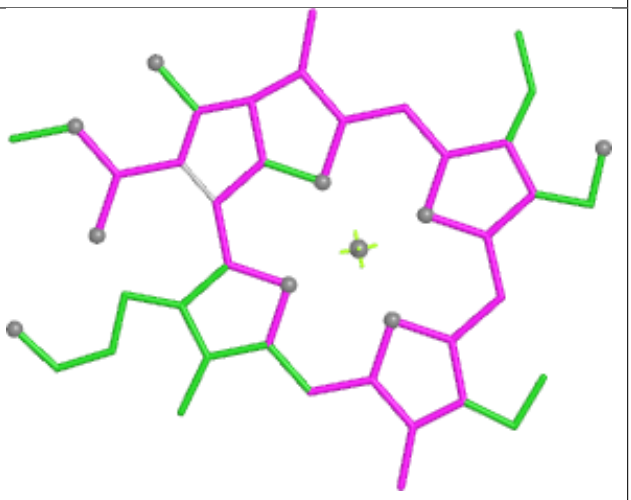
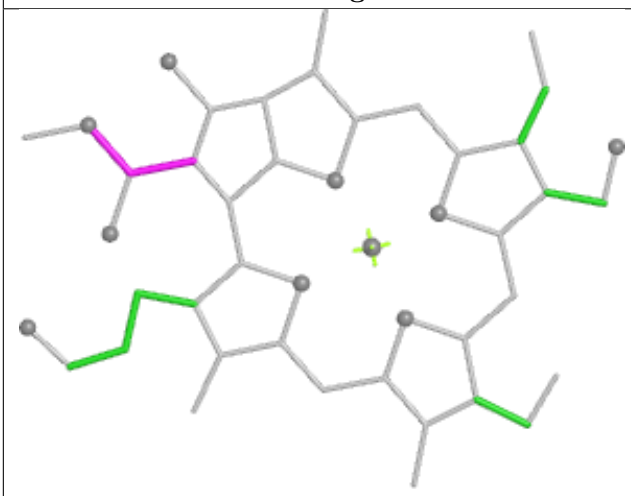
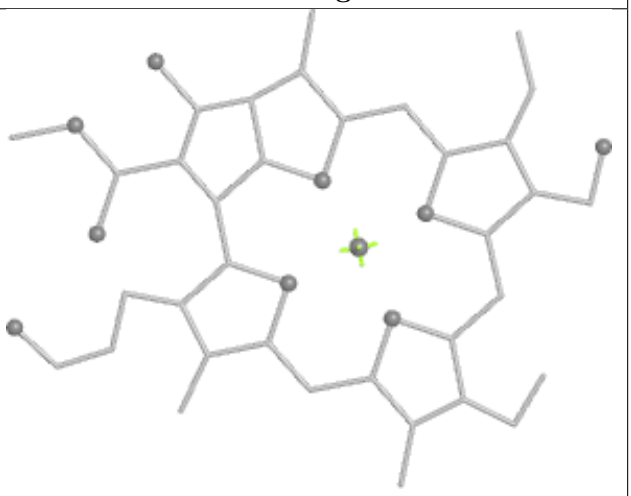


Bond angles



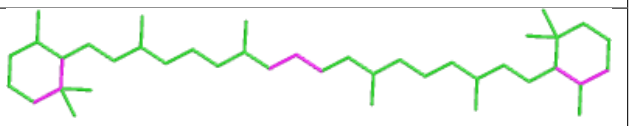
Torsions



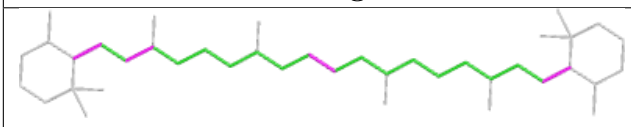
Rings

Ligand BCR M 101

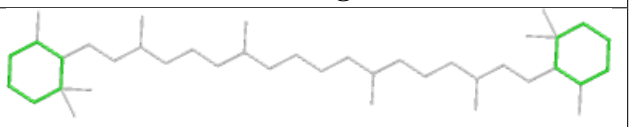
Bond lengths



Bond angles

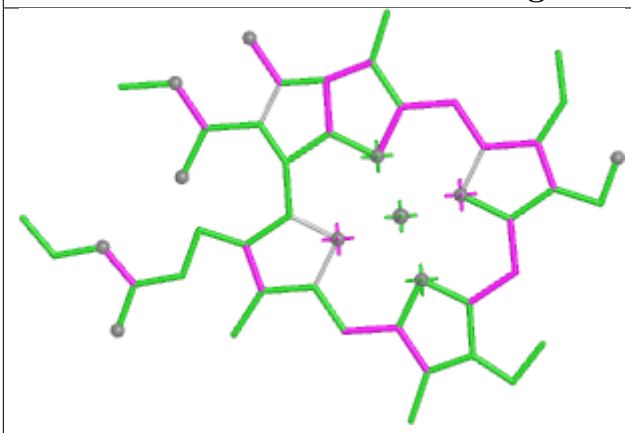


Torsions

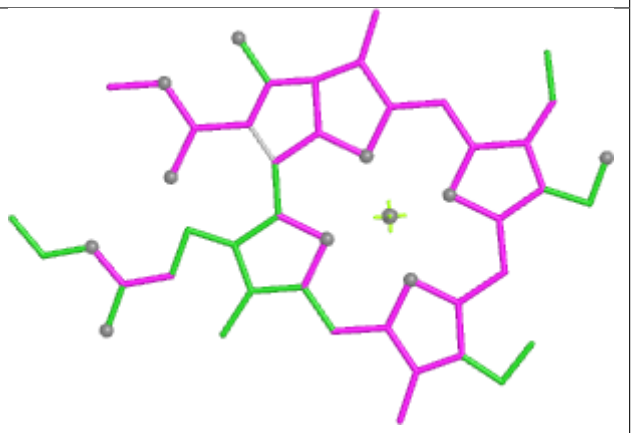


Rings

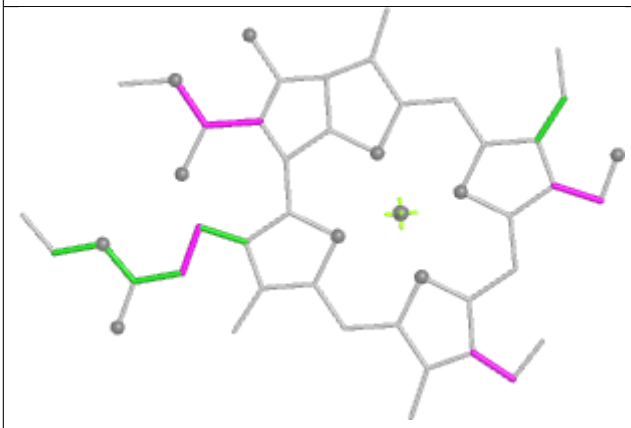
Ligand CHL 4 313



Bond lengths



Bond angles



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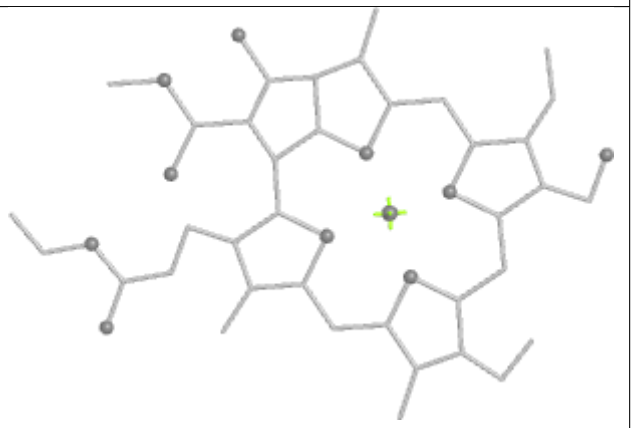
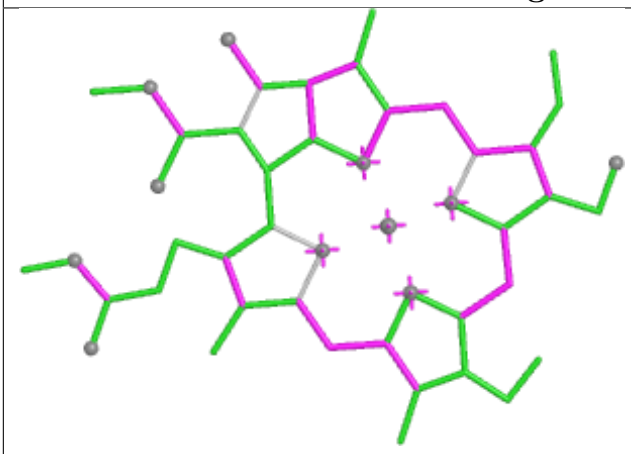
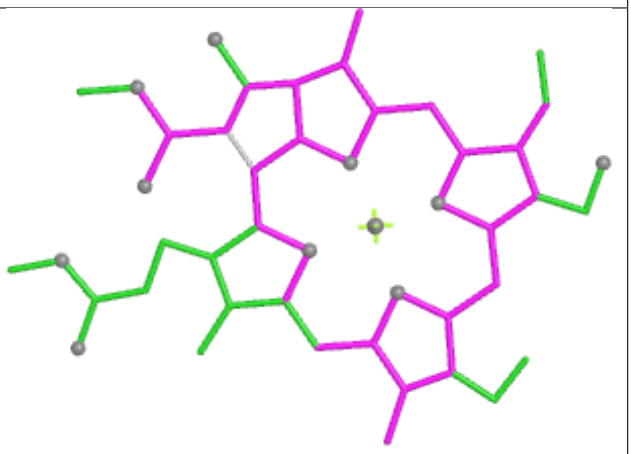


Rings

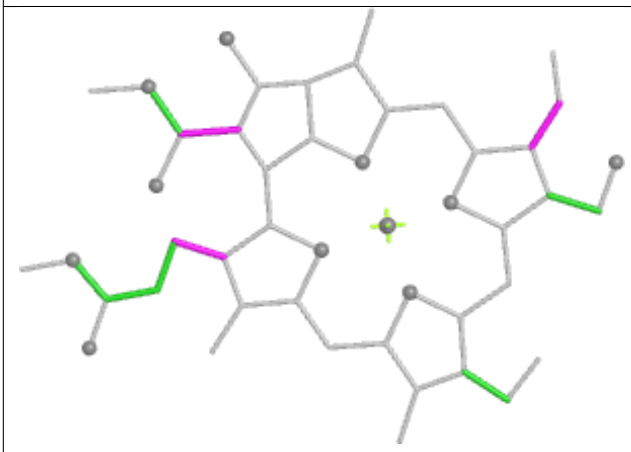
Ligand CHL 4 310



Bond lengths



Bond angles



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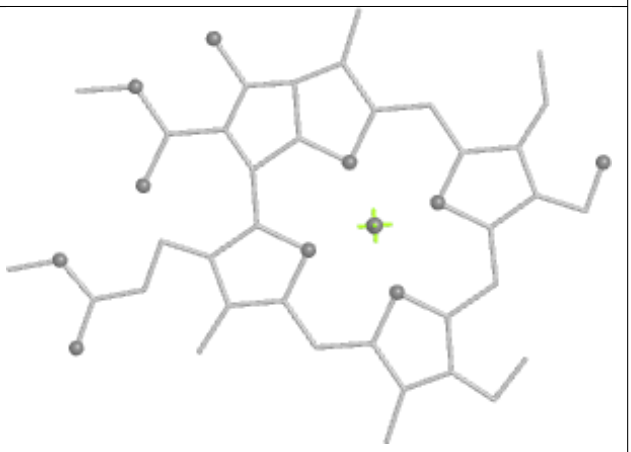
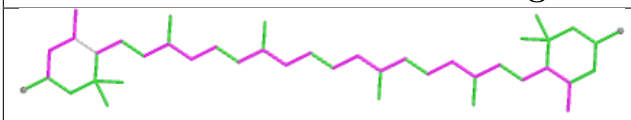


Rings

Ligand LUT 6 304



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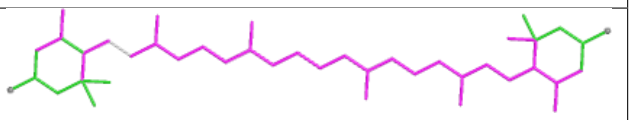
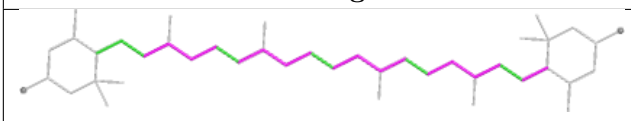


Bond angles



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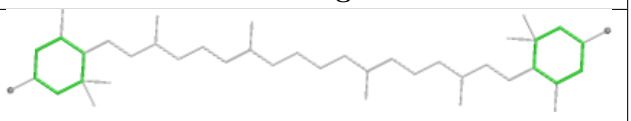
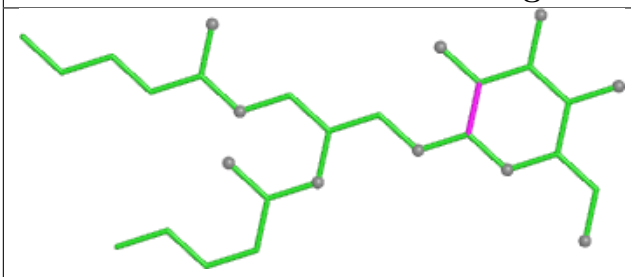


Rings

Ligand LMG J 104



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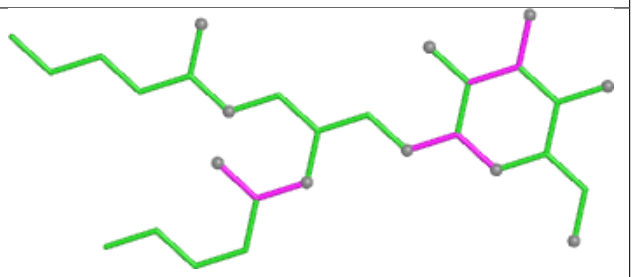
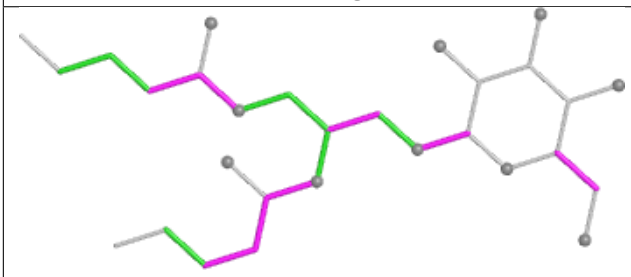


Bond angles



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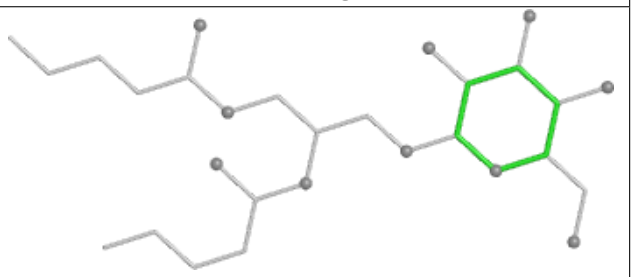
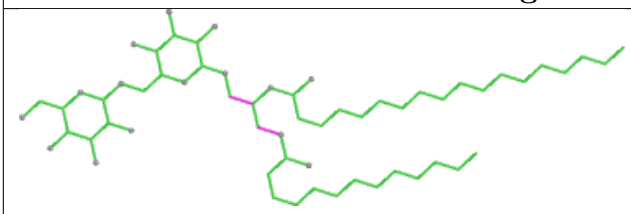


Rings

Ligand DGD B 808



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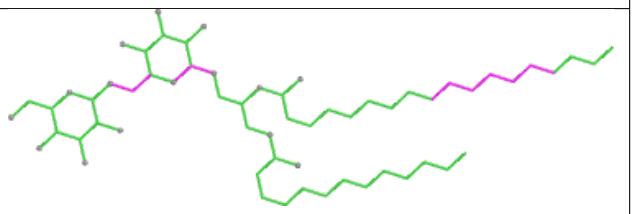
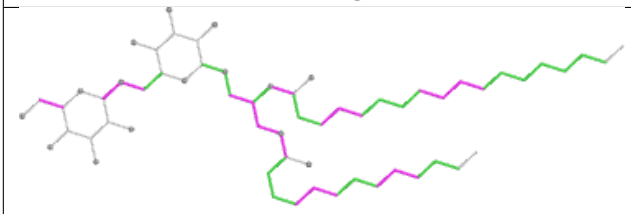


Bond angles



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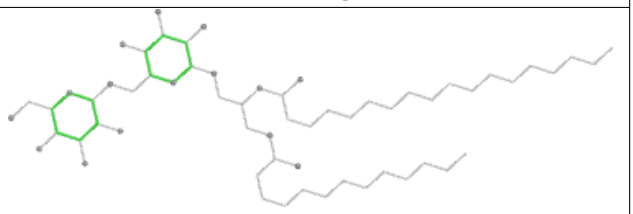
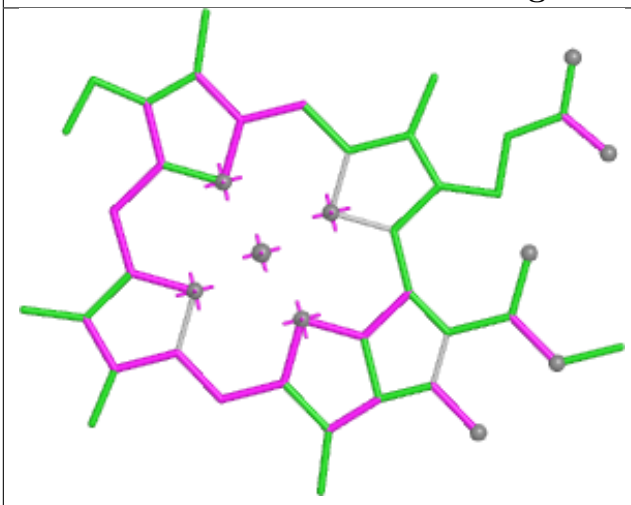


Rings

Ligand CLA 7 310



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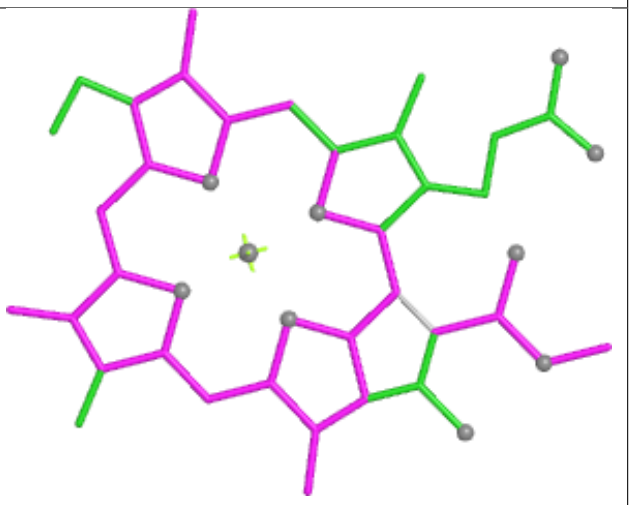
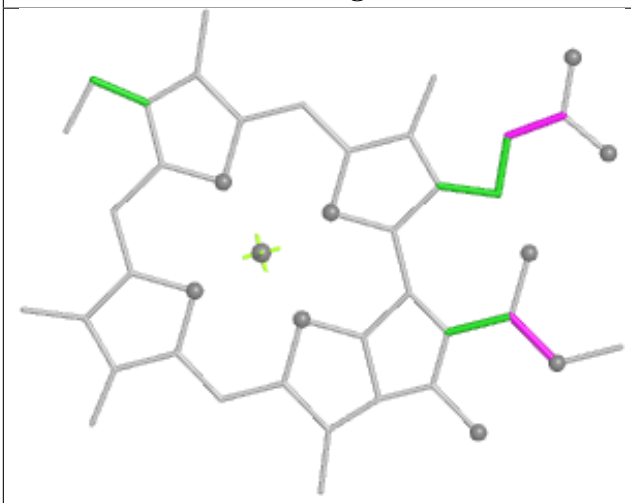


Bond angles



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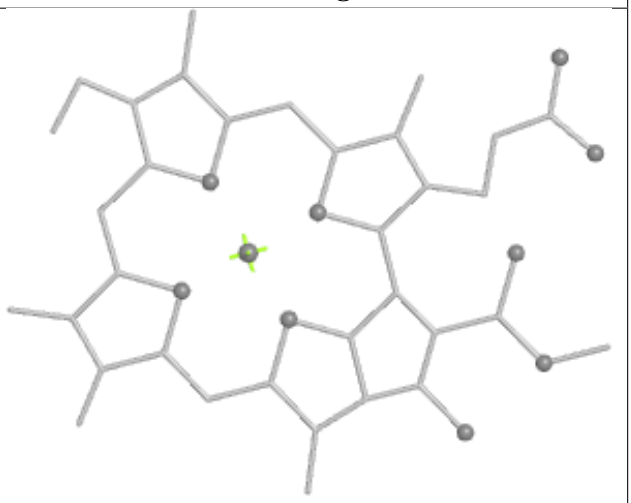
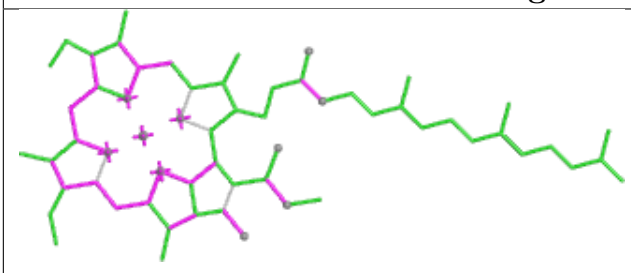


Rings

Ligand CLA a 311



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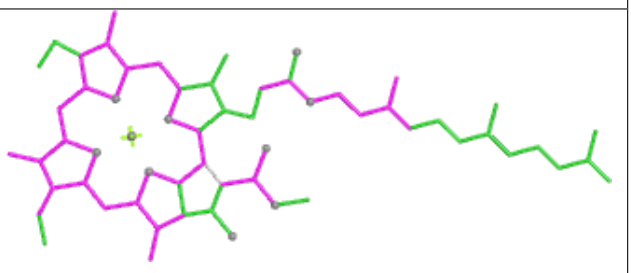
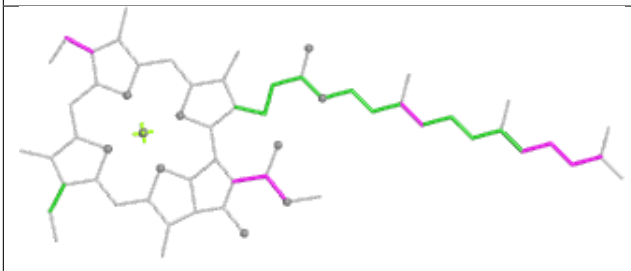
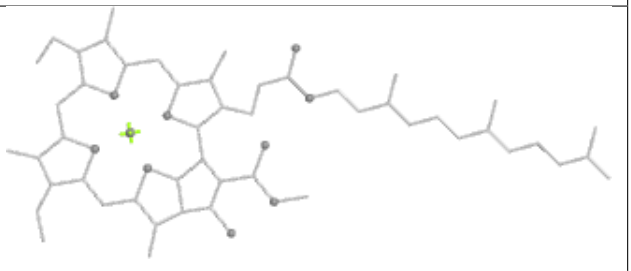


Bond angles

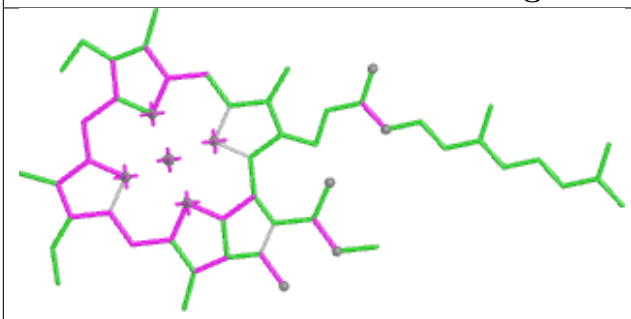


Torsions

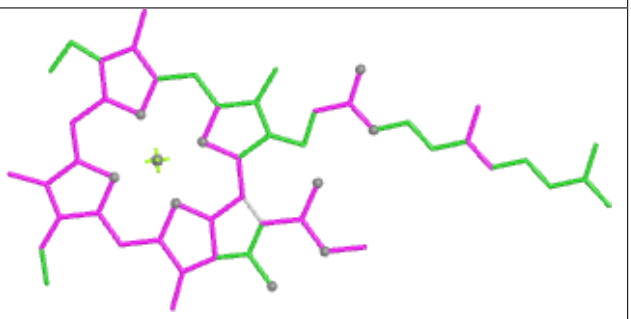


Rings

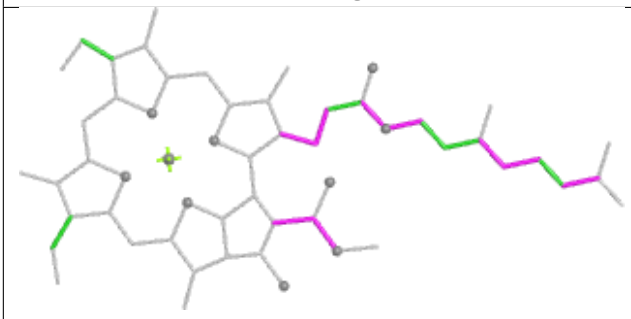
Ligand CLA O 203



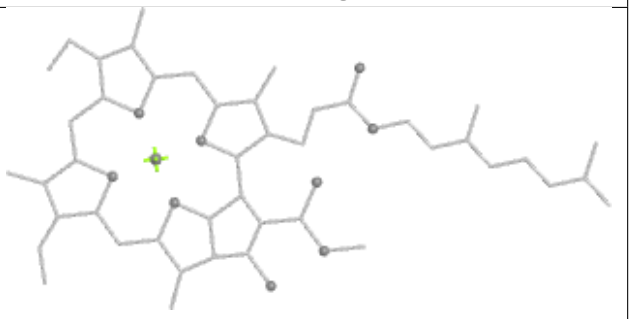
Bond lengths



Bond angles

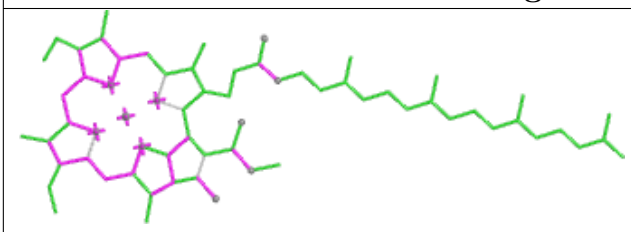


Torsions

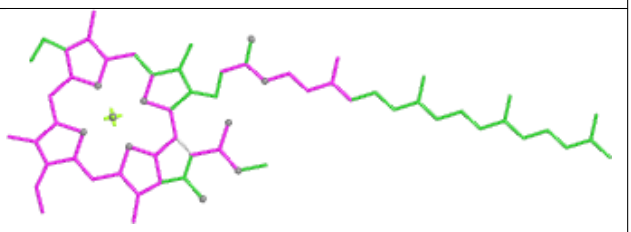


Rings

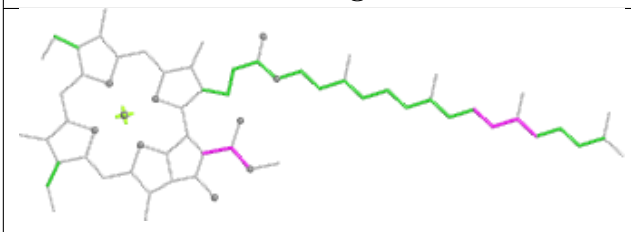
Ligand CLA B 819



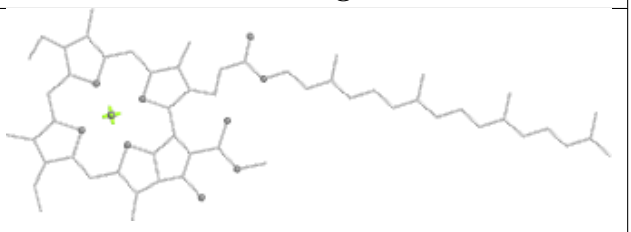
Bond lengths



Bond angles

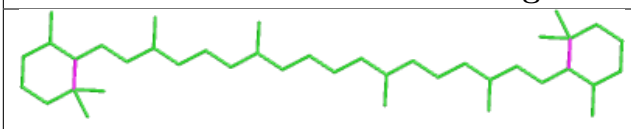


Torsions

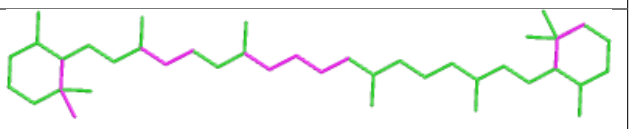


Rings

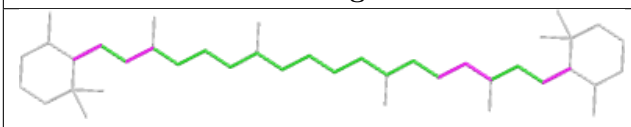
Ligand BCR B 805



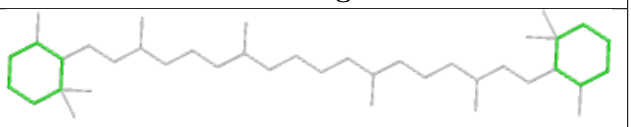
Bond lengths



Bond angles

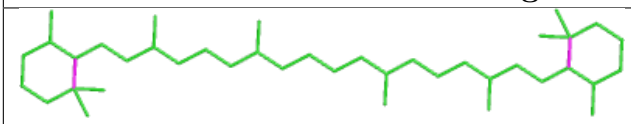


Torsions

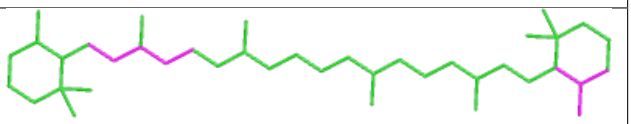


Rings

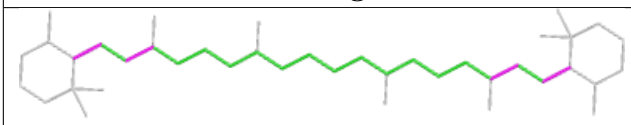
Ligand BCR G 201



Bond lengths



Bond angles



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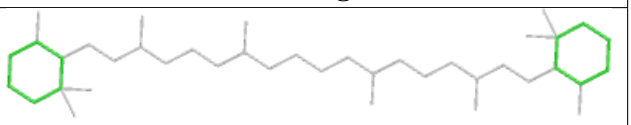
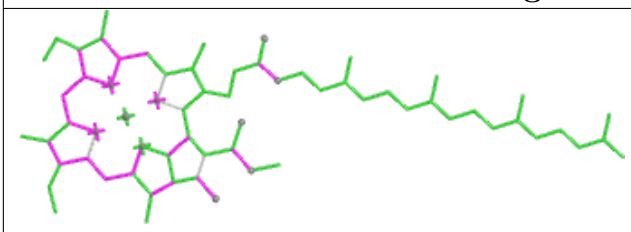


Rings

Ligand CLA A 837



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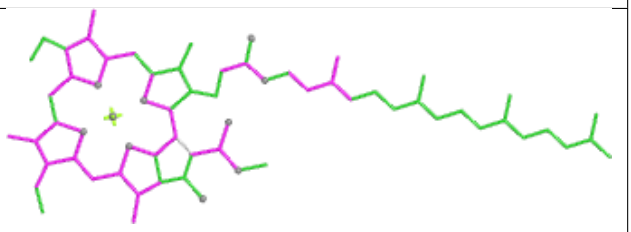
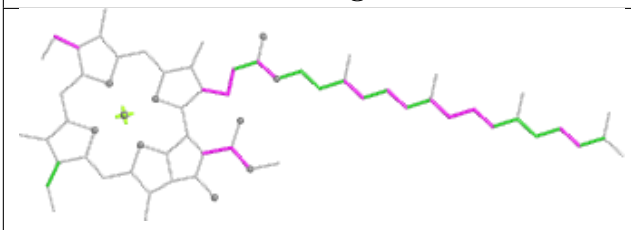


Bond angles



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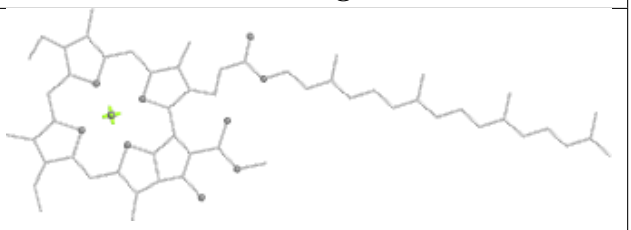
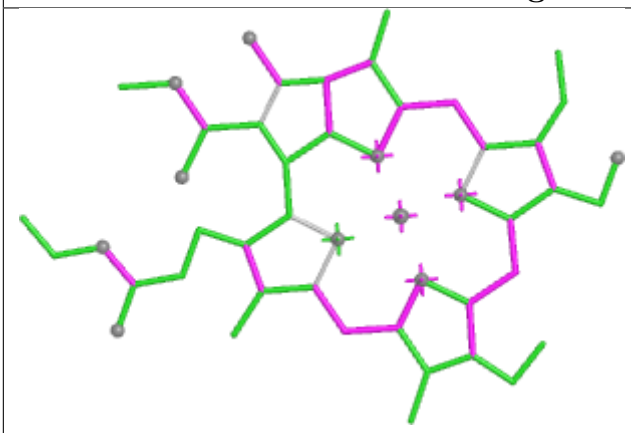


Rings

Ligand CHL 9 320



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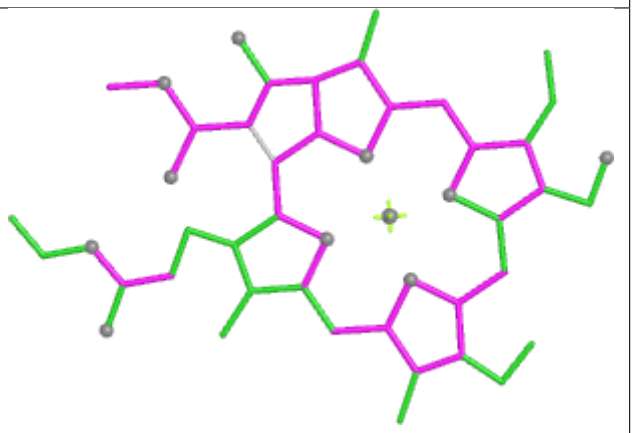
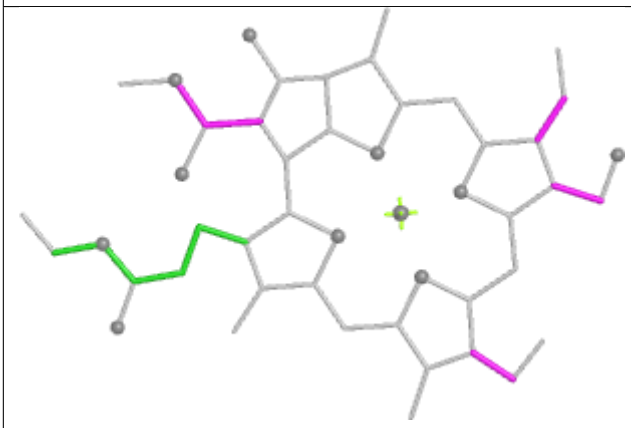


Bond angles



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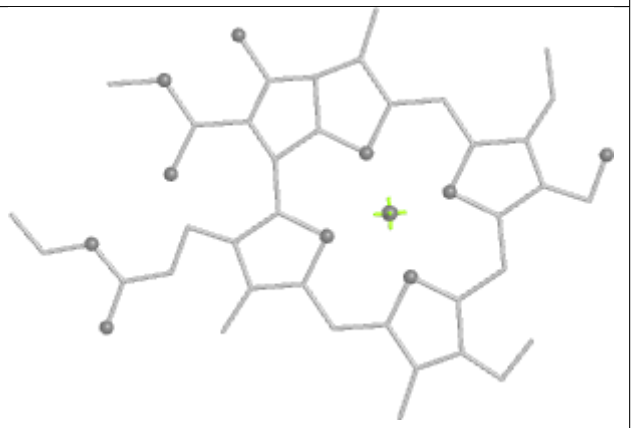
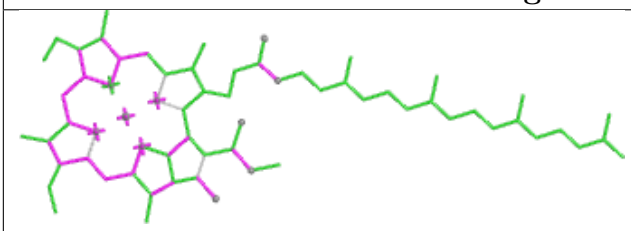


Rings

Ligand CLA A 826



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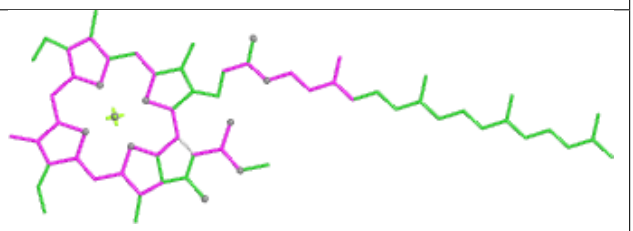
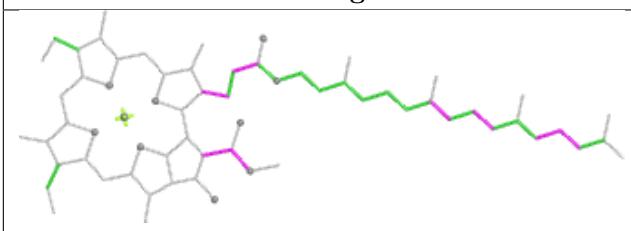


Bond angles



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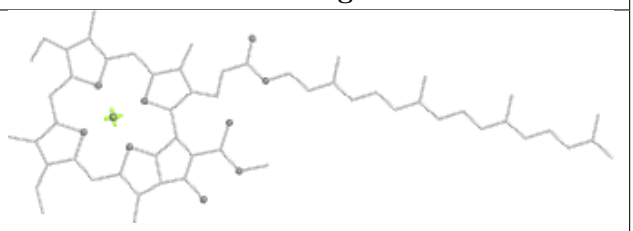
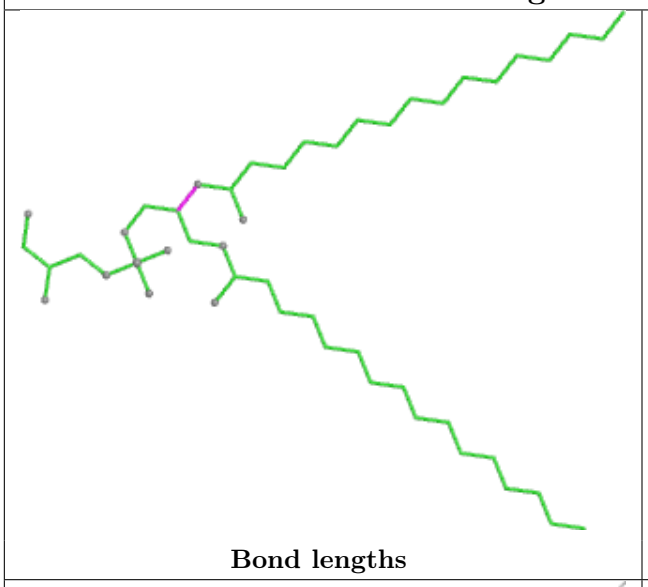


Rings

Ligand LHG a 306



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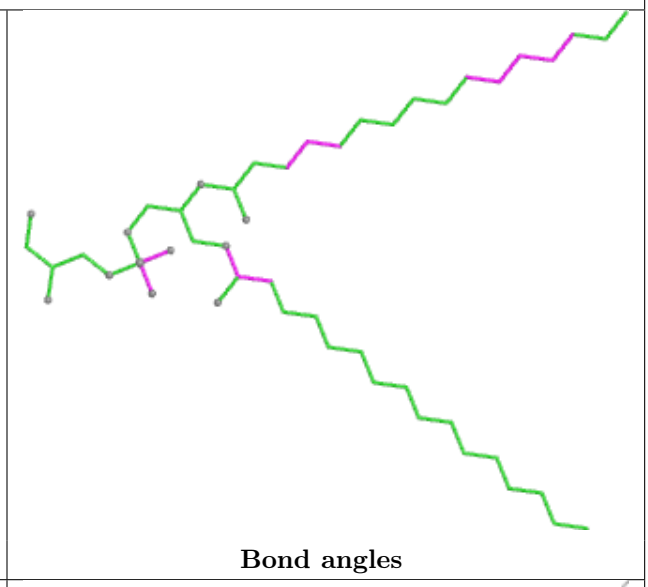
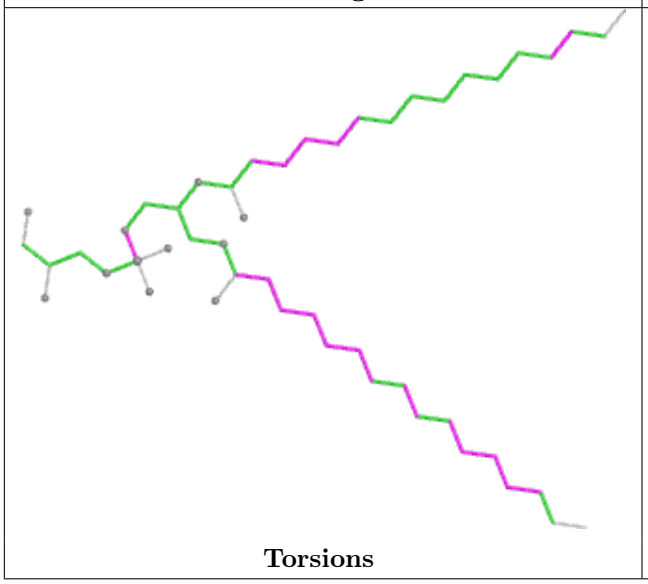


Bond angles



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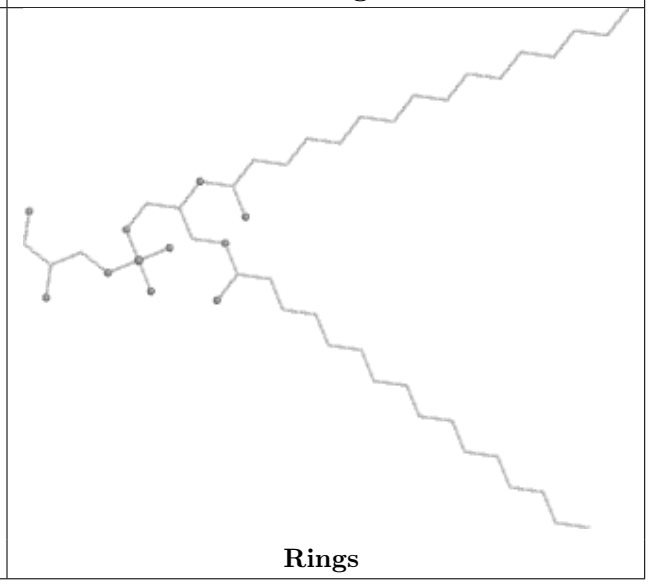
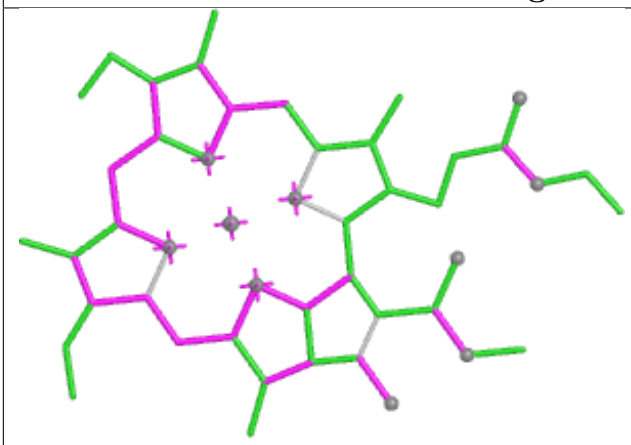


Rings

Ligand CLA 5 309



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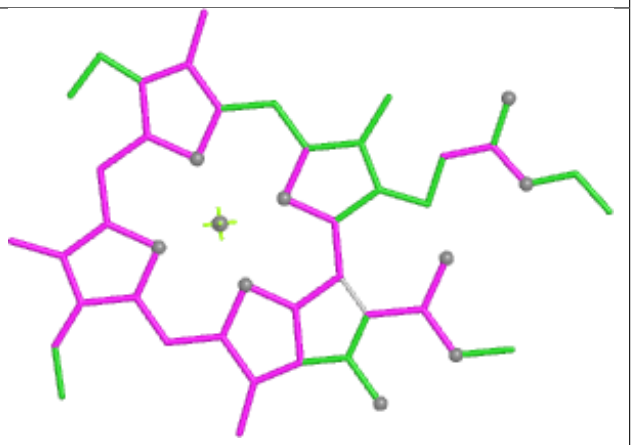

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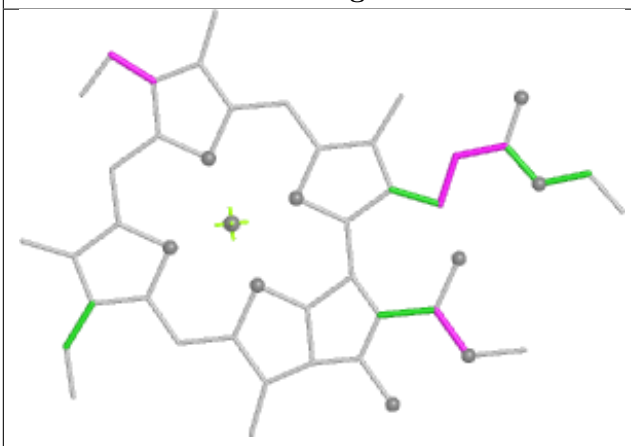

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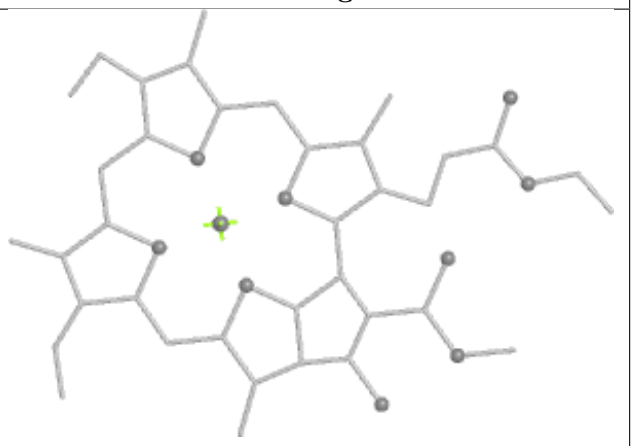
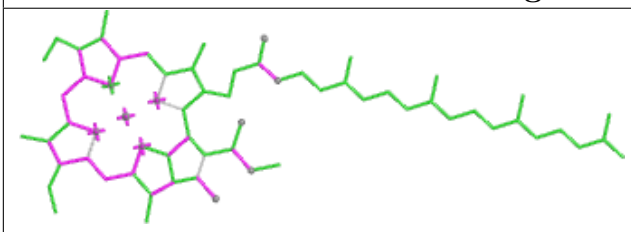


Rings

Ligand CLA B 811



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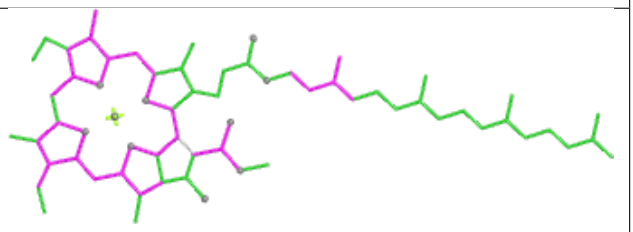
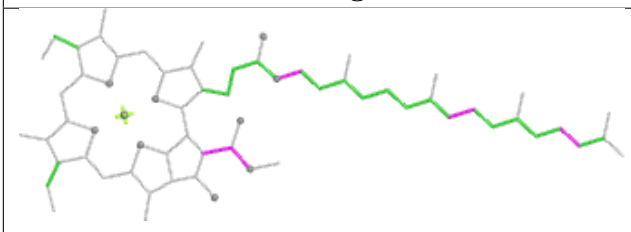


Bond angles



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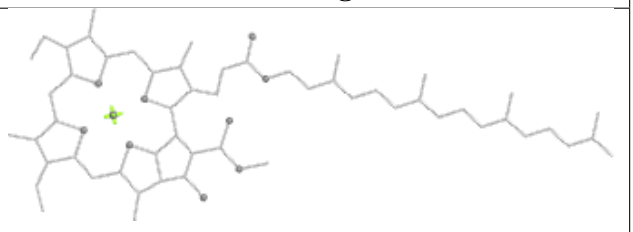
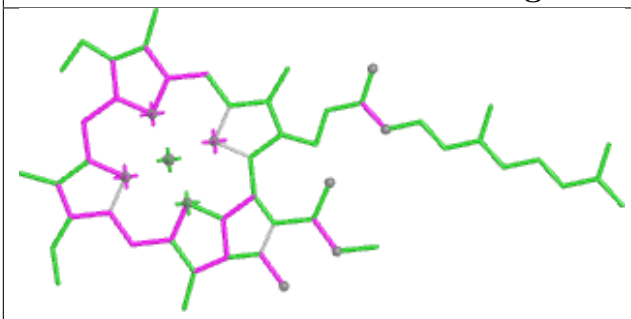


Rings

Ligand CLA B 837



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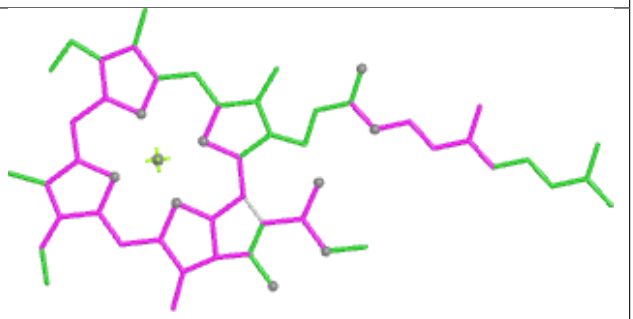
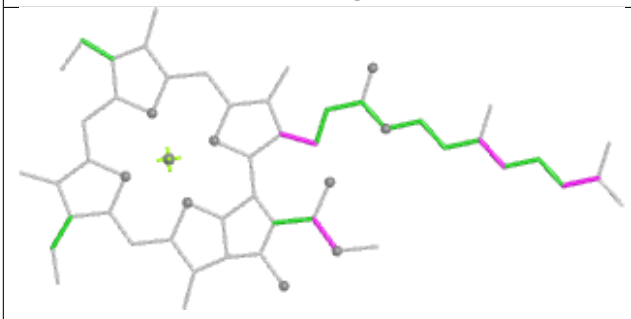
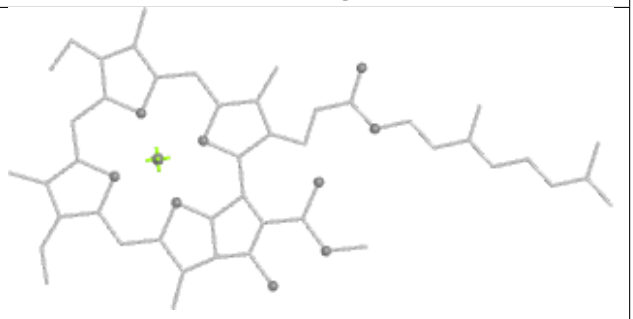


Bond angles

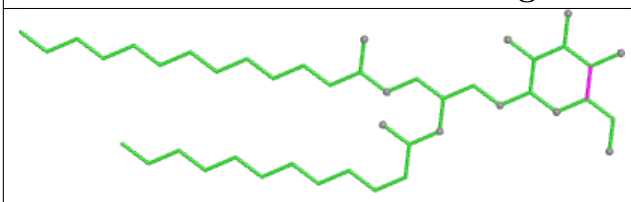


Torsions



Rings

Ligand LMG G 202



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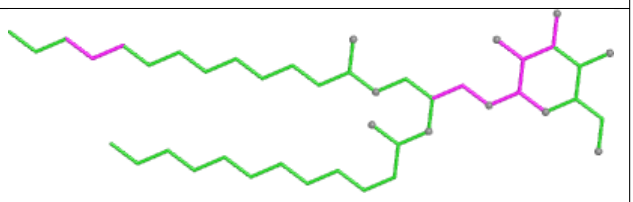

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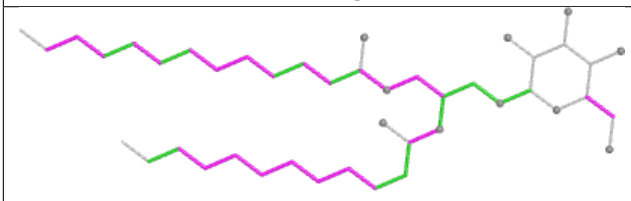

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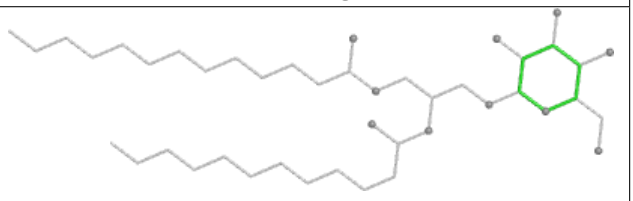
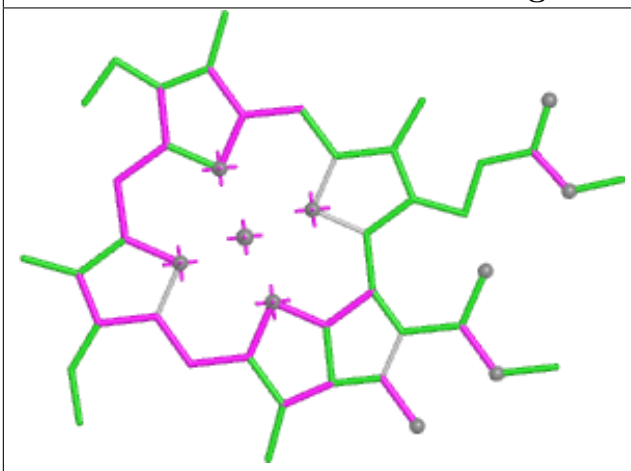


Rings

Ligand CLA 2 314



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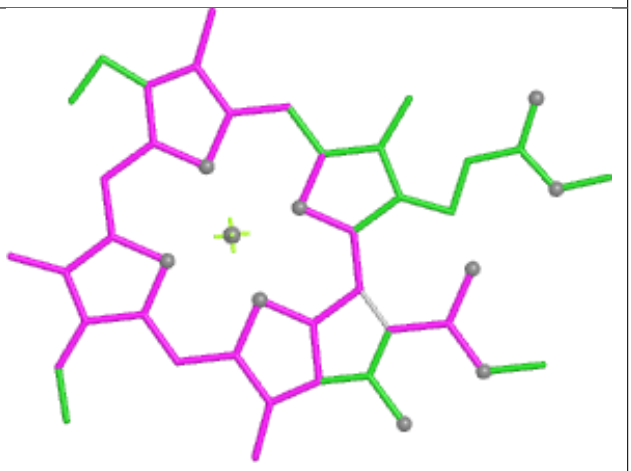
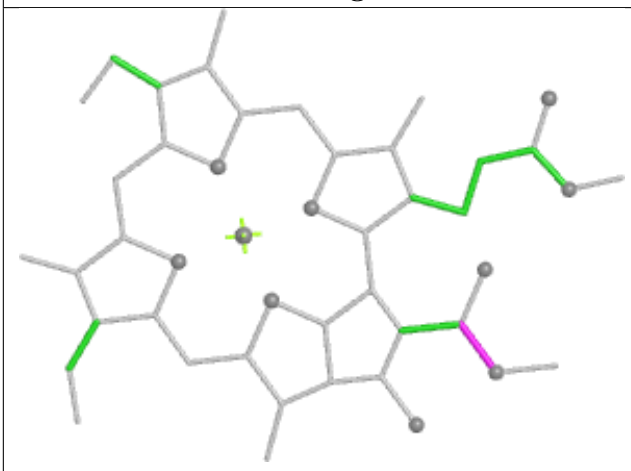


Bond angles



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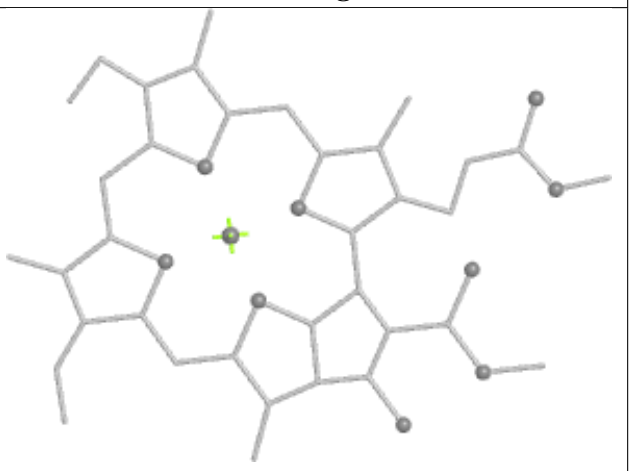
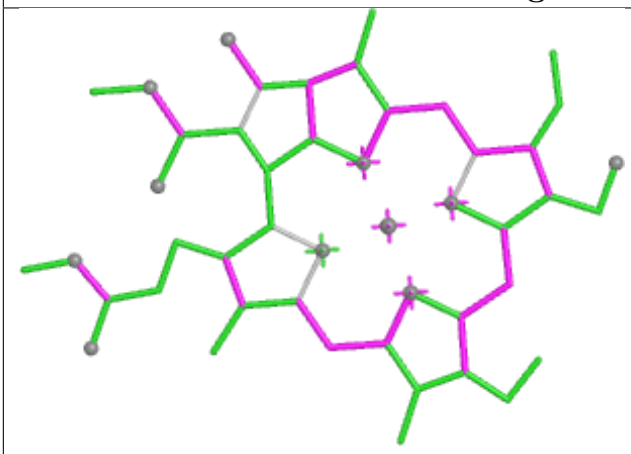


Rings

Ligand CHL 7 319



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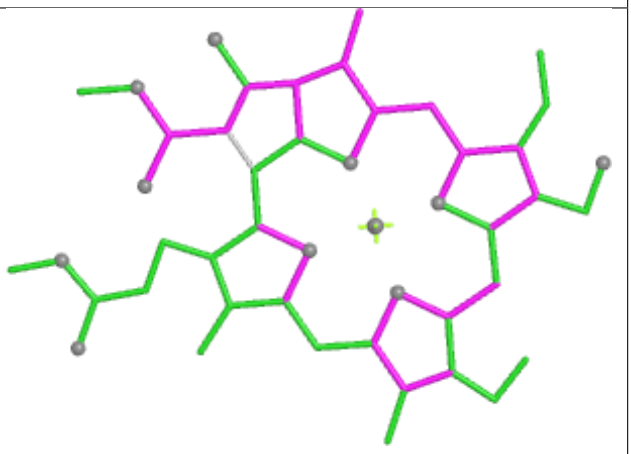
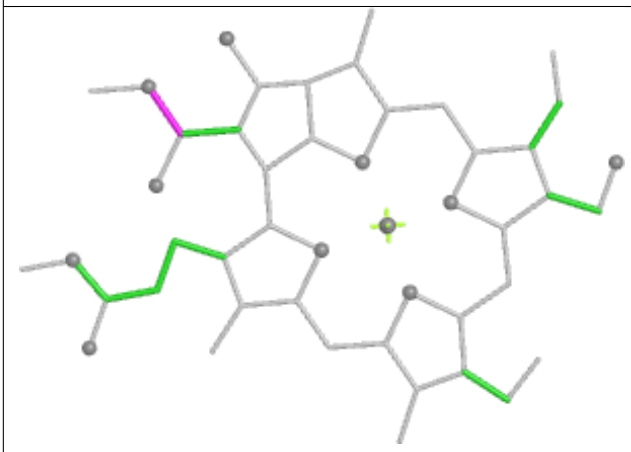


Bond angles



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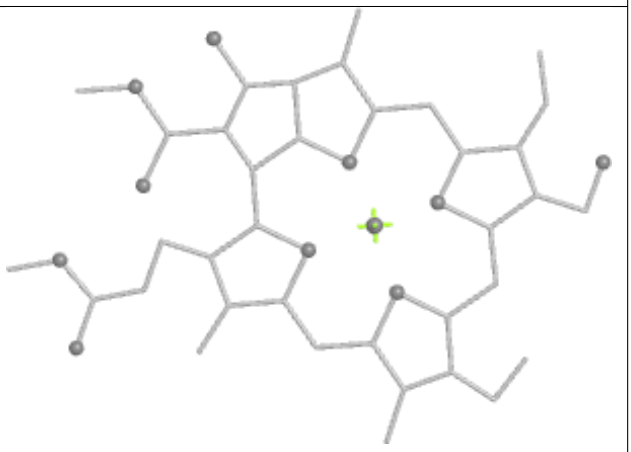
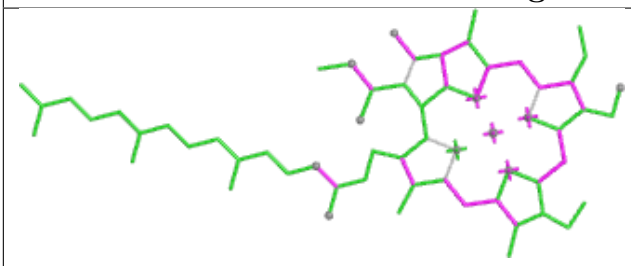


Rings

Ligand CHL a 317



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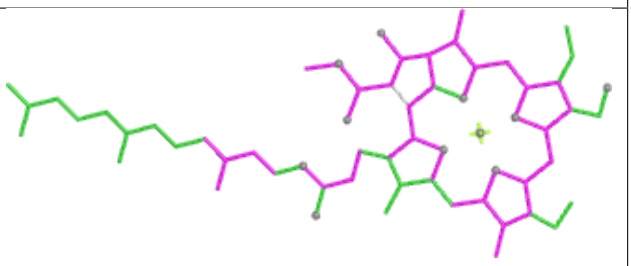
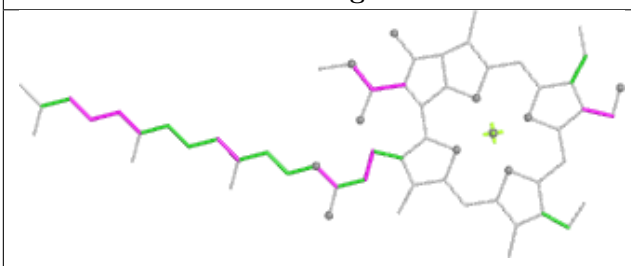
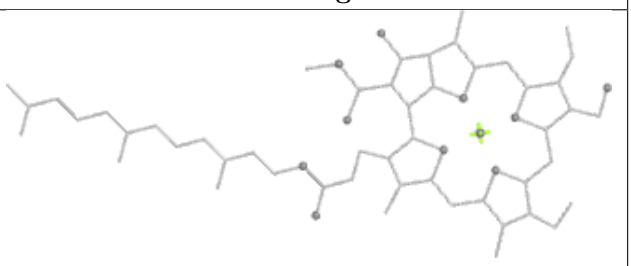


Bond angles

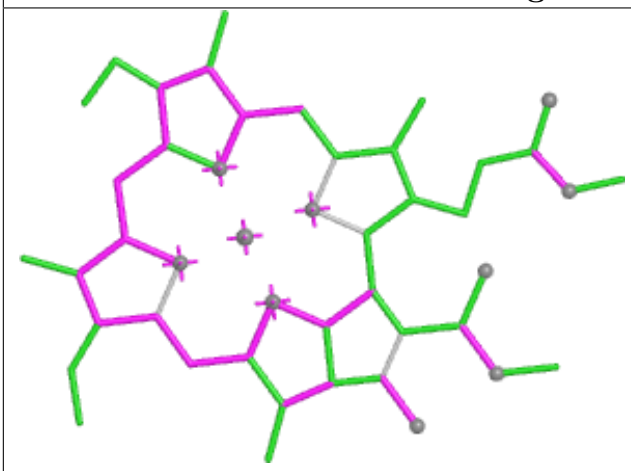


Torsions

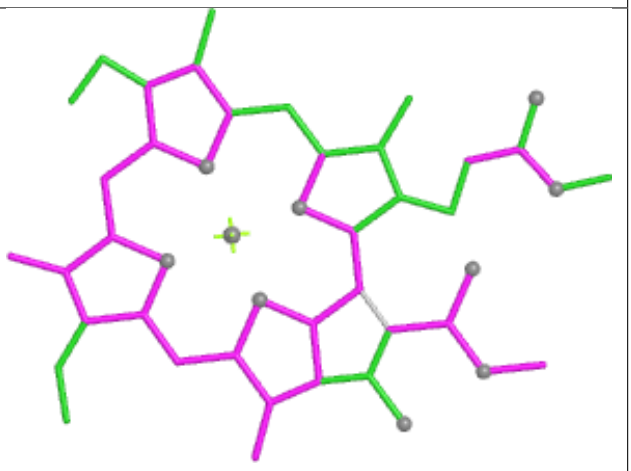


Rings

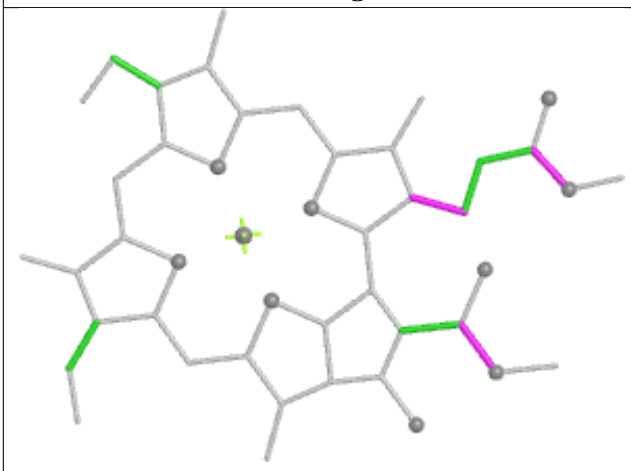
Ligand CLA b 304



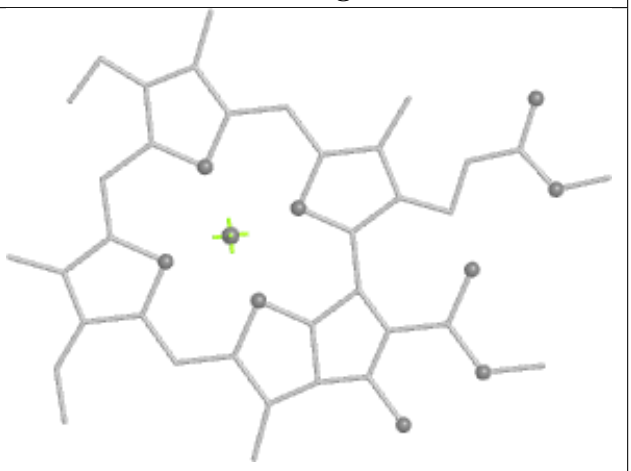
Bond lengths



Bond angles

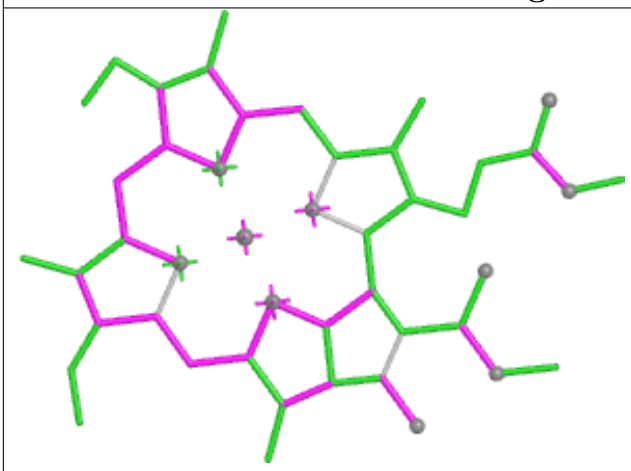


Torsions

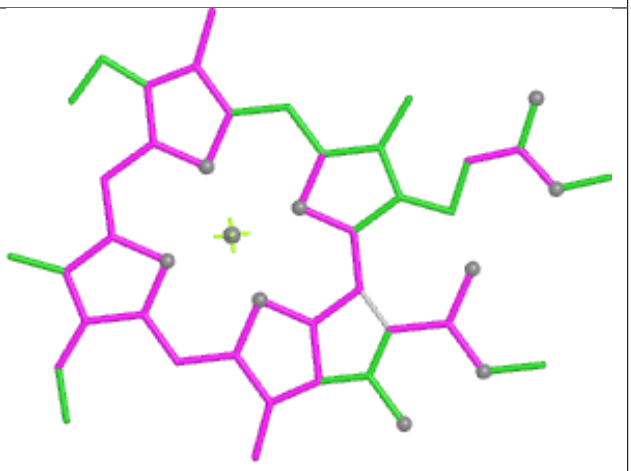


Rings

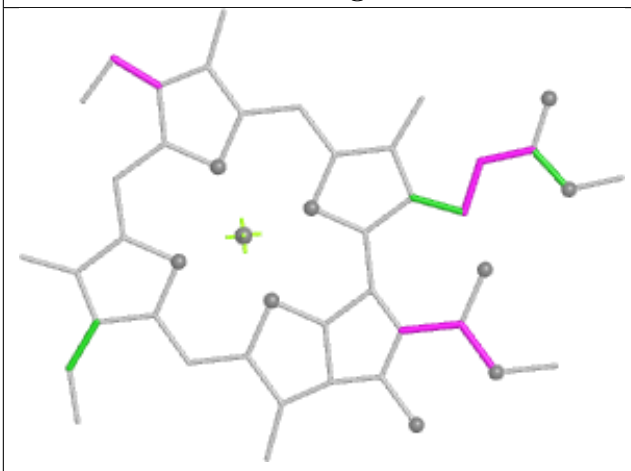
Ligand CLA a 322



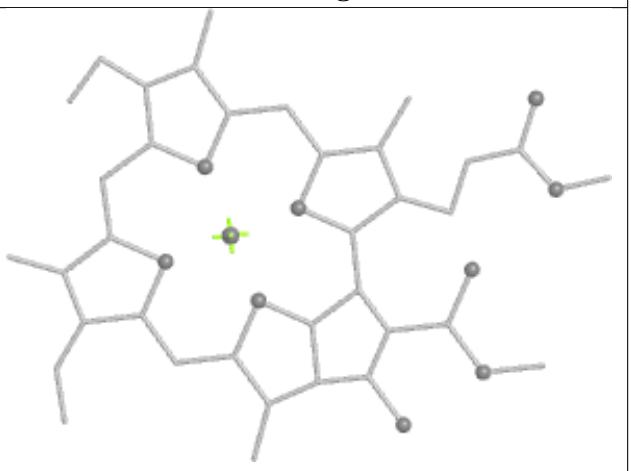
Bond lengths



Bond angles

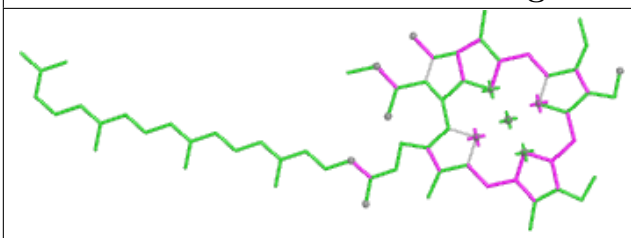


Torsions

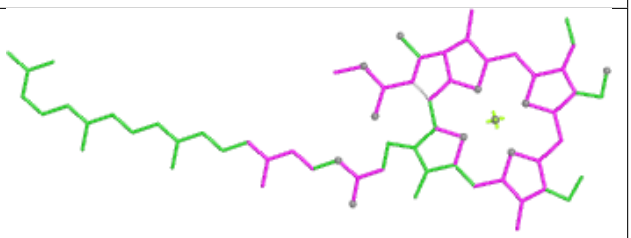


Rings

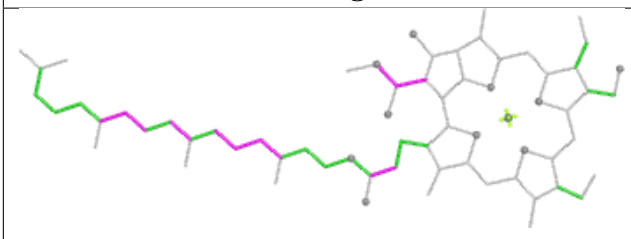
Ligand CHL 7 324



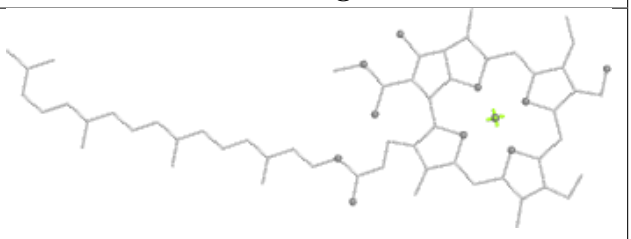
Bond lengths



Bond angles

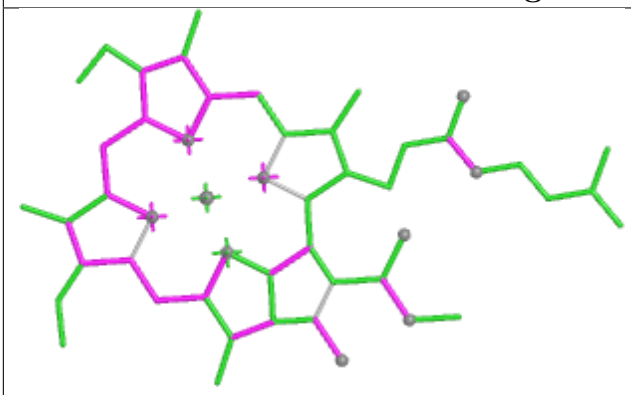


Torsions

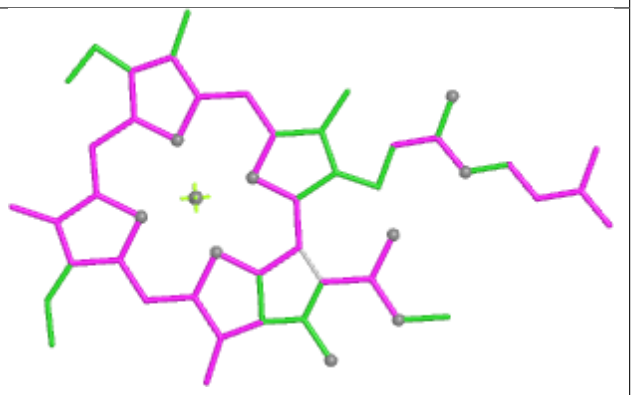


Rings

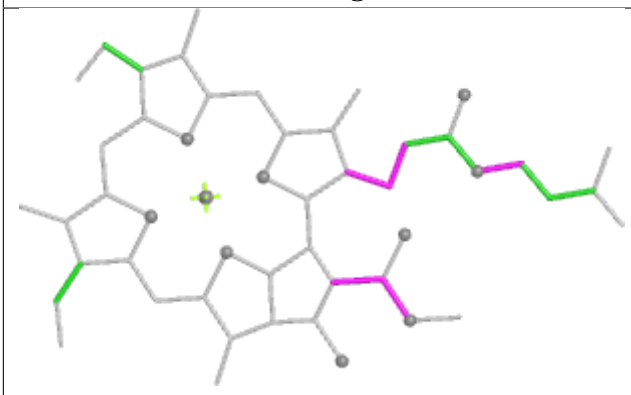
Ligand CLA B 826



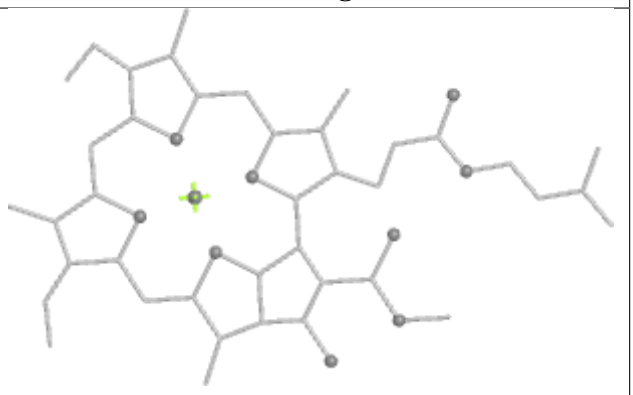
Bond lengths



Bond angles

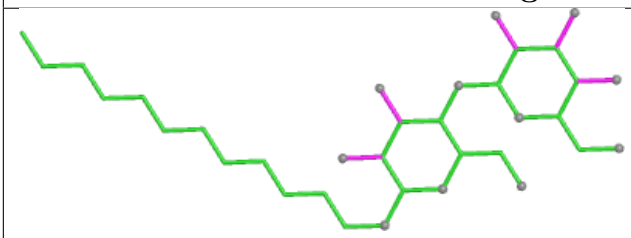


Torsions

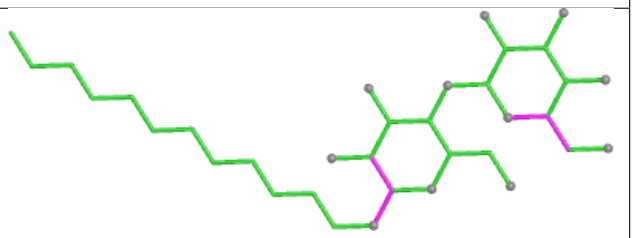


Rings

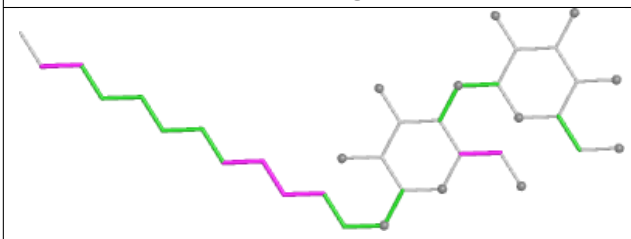
Ligand LMT A 808



Bond lengths



Bond angles



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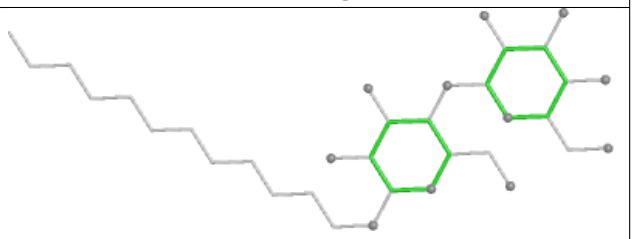
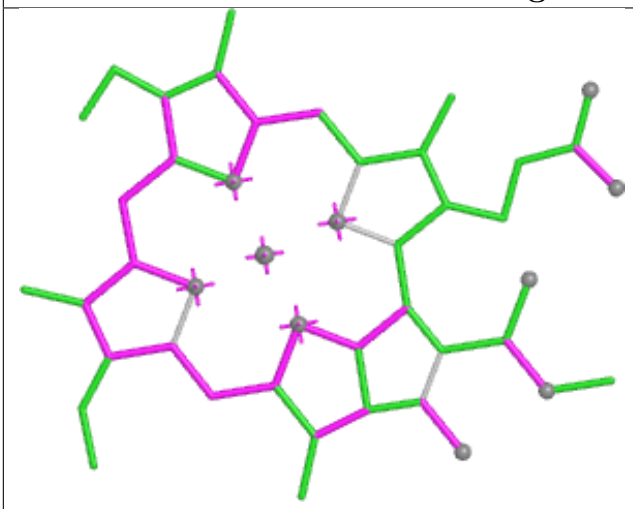


Rings

Ligand CLA 2 311



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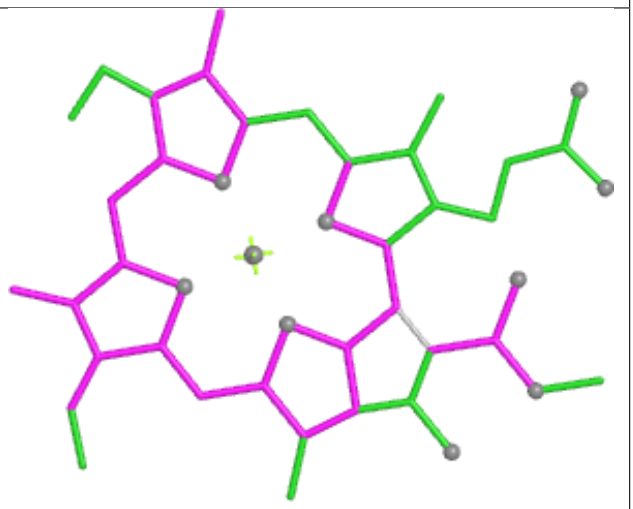
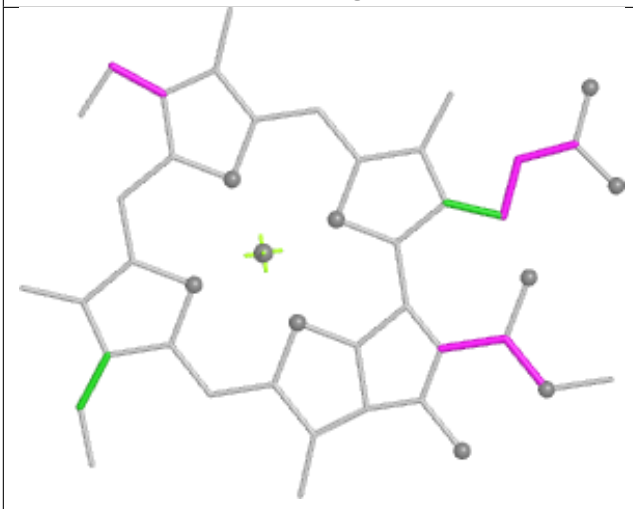


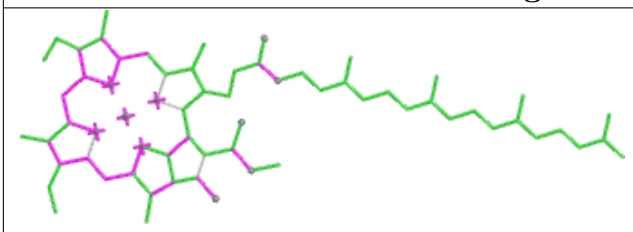
Bond angles



Torsions

Rings

Ligand CLA A 853



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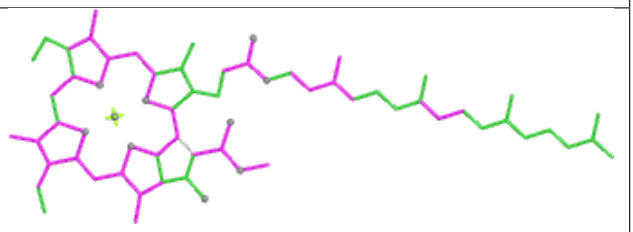
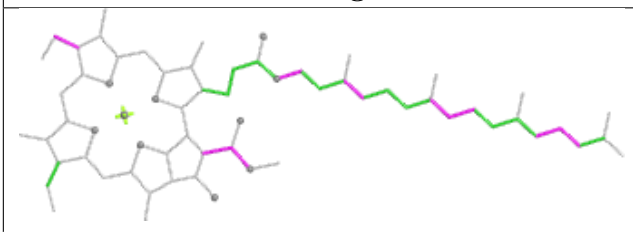
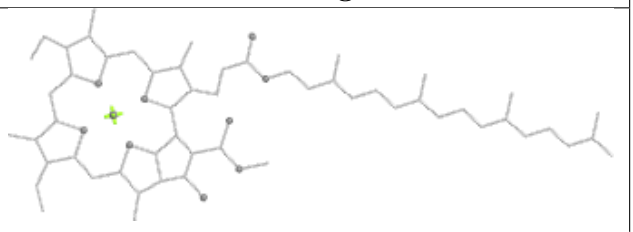


Bond angles

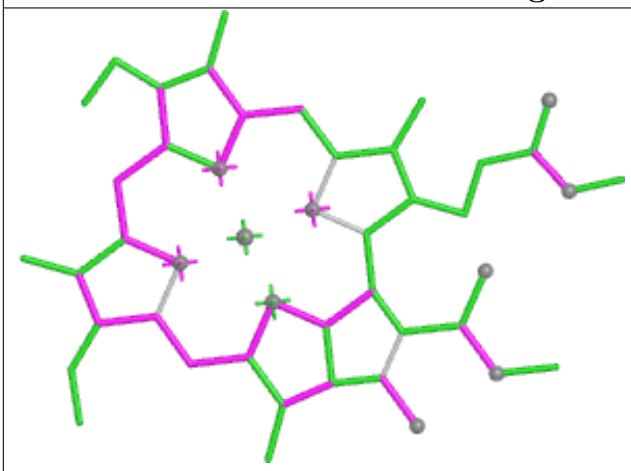


Torsions



Rings

Ligand CLA 2 309



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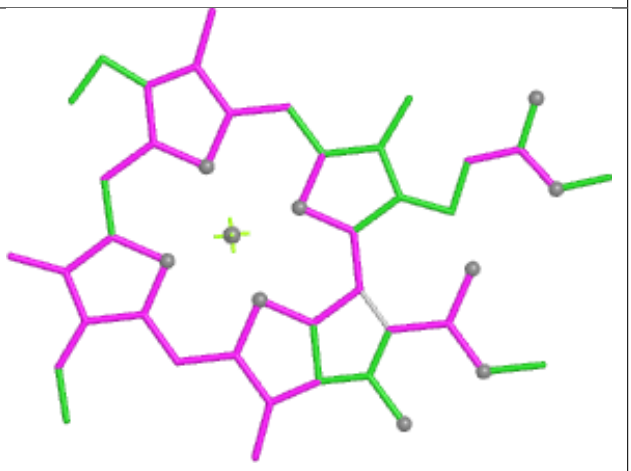
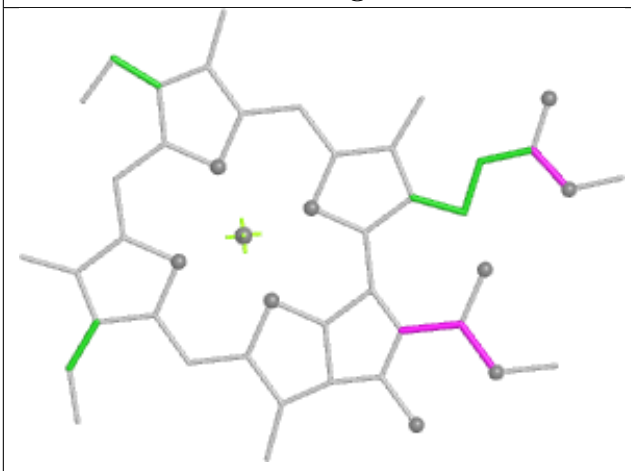


Bond angles



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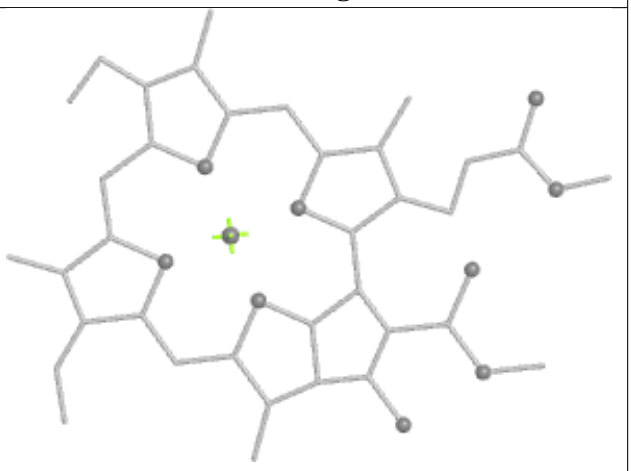
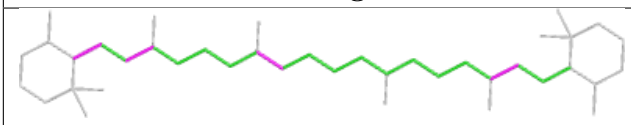


Rings

Ligand BCR F 302

Bond lengths

Bond angles



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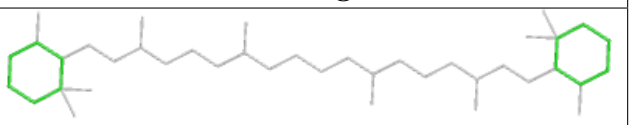
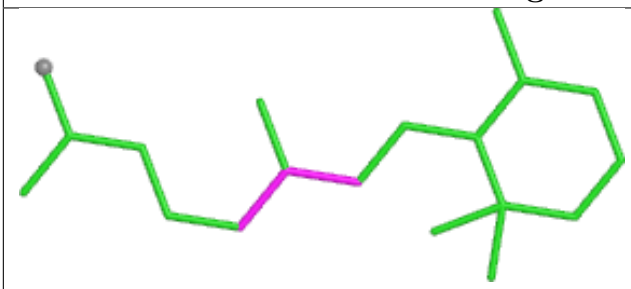


Rings

Ligand QTB 7 303



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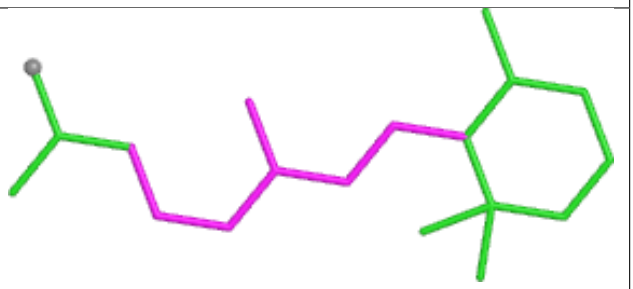
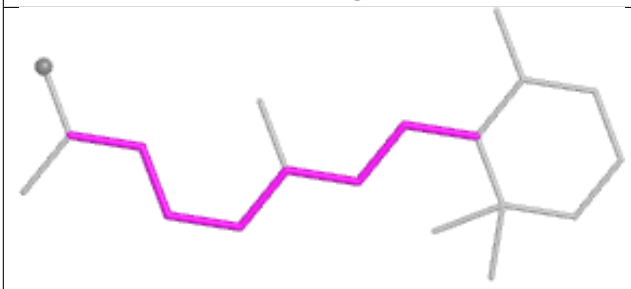
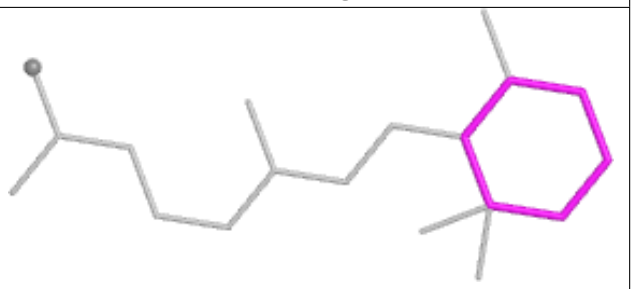


Bond angles

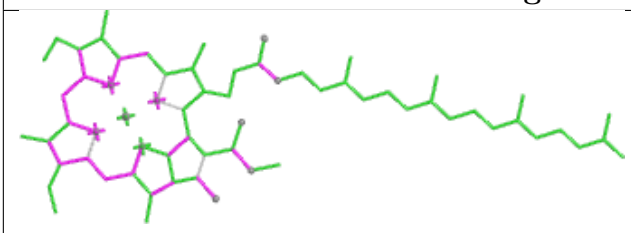


Torsions

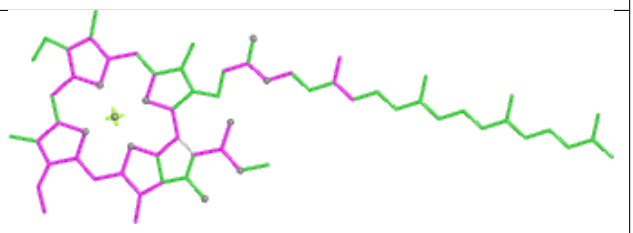


Rings

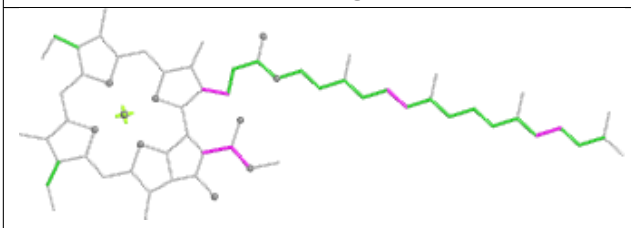
Ligand CLA A 847



Bond lengths



Bond angles



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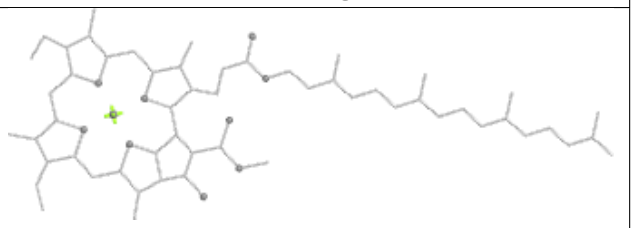
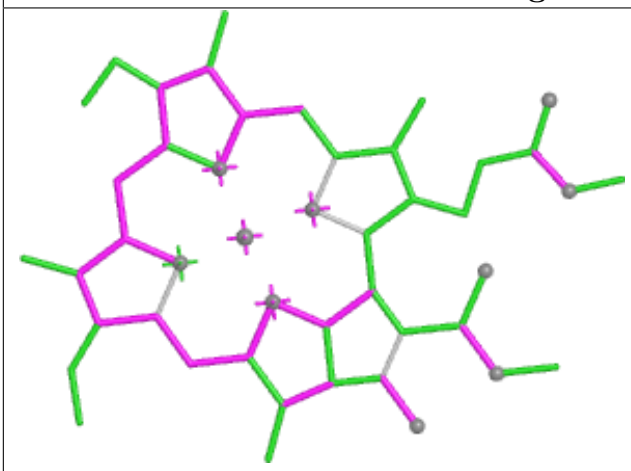
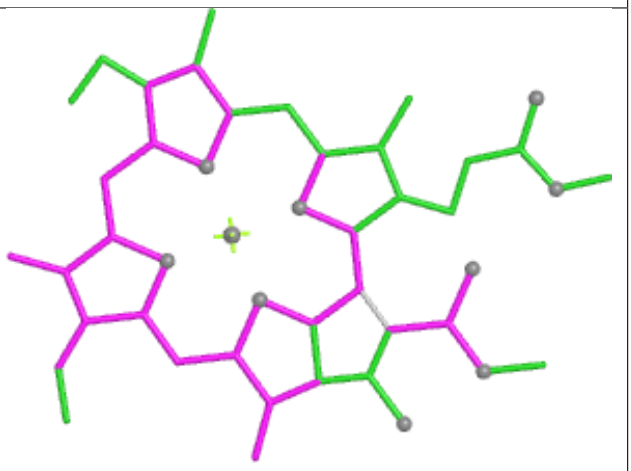


Rings

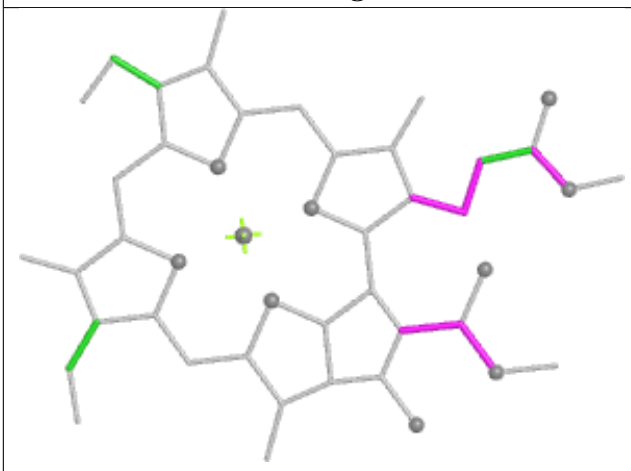
Ligand CLA 2 304



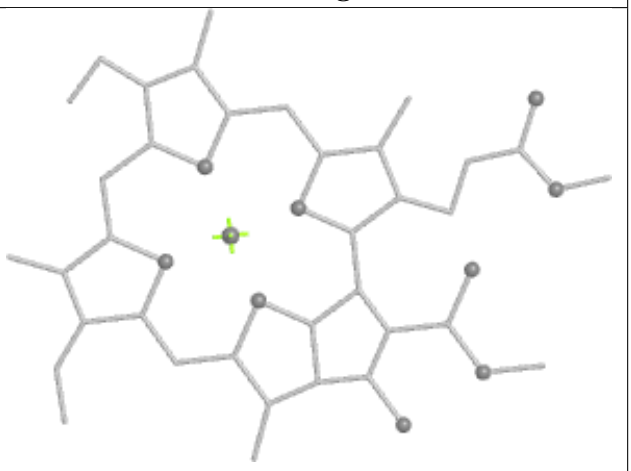
Bond lengths



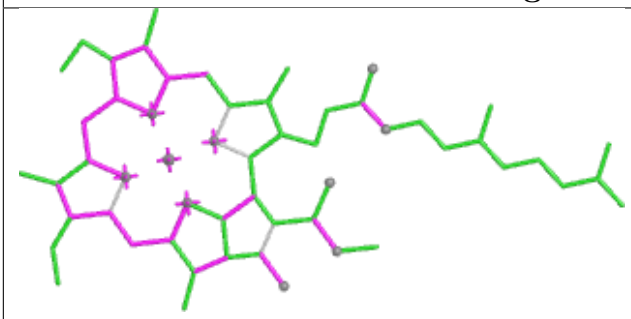
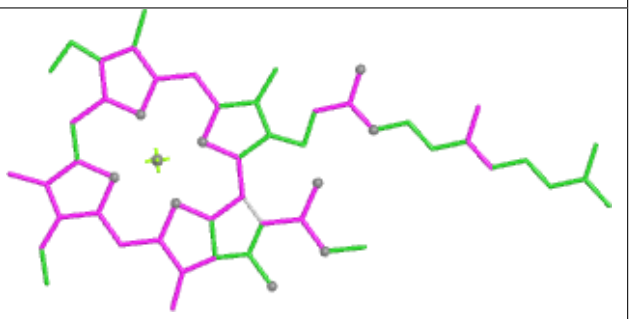
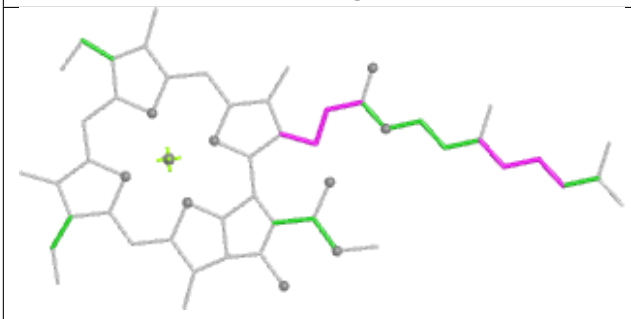
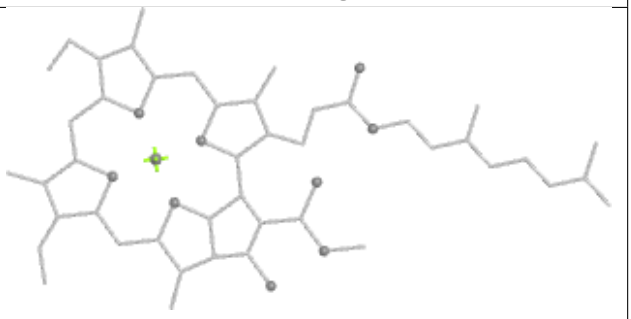
Bond angles

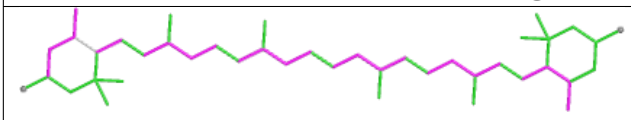
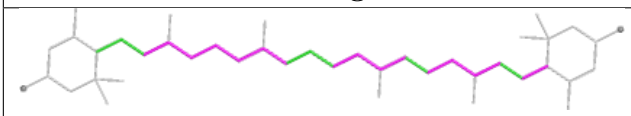
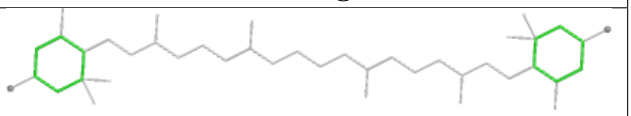


Torsions

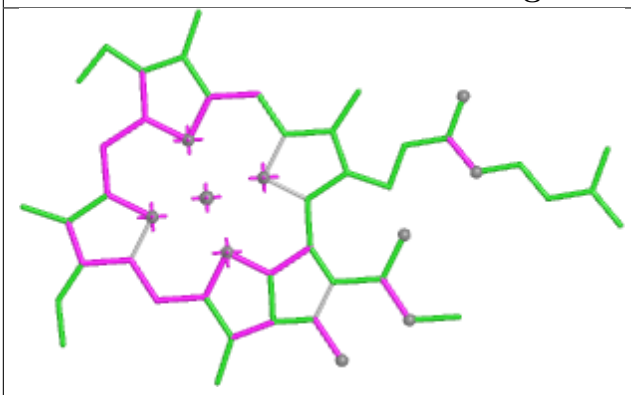


Rings

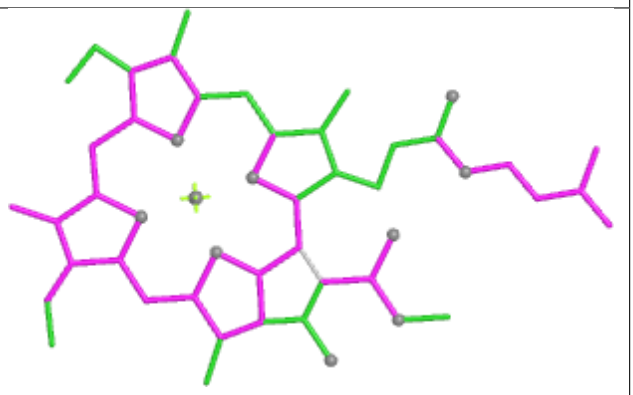
Ligand CLA A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 9 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

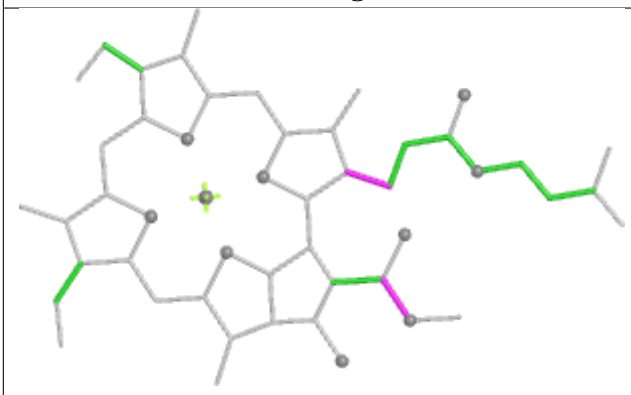
Ligand CLA A 844



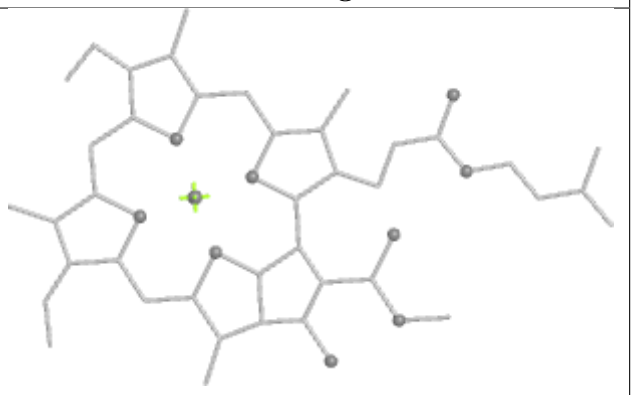
Bond lengths



Bond angles

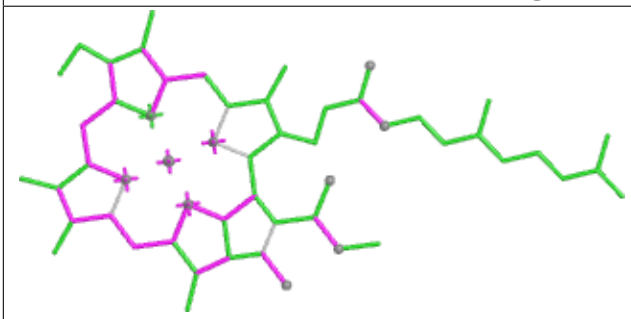


Torsions

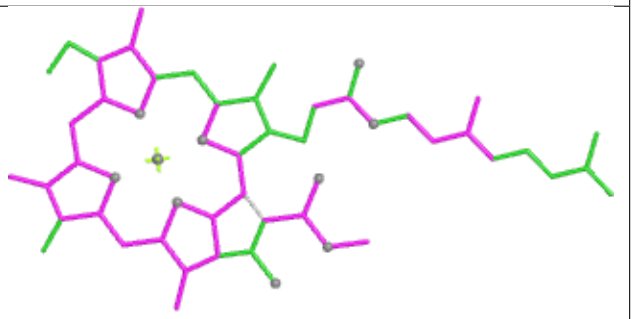


Rings

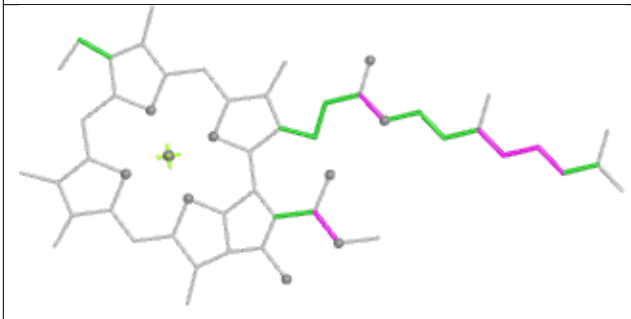
Ligand CLA 7 314



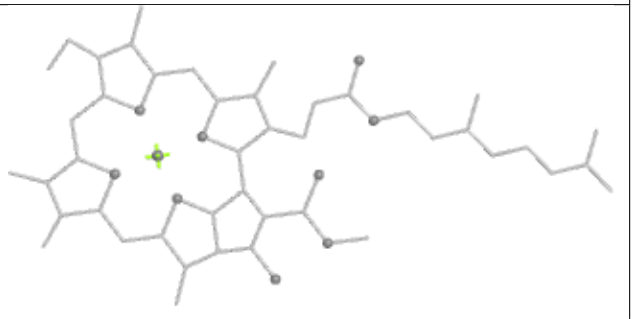
Bond lengths



Bond angles

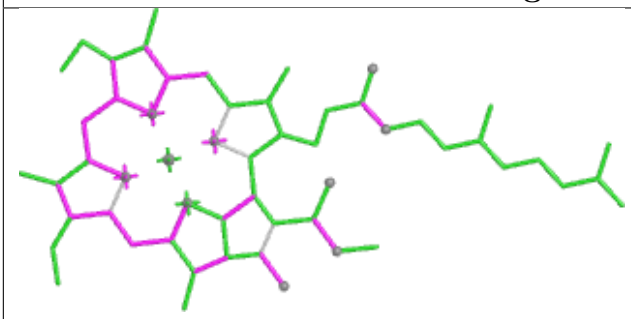


Torsions

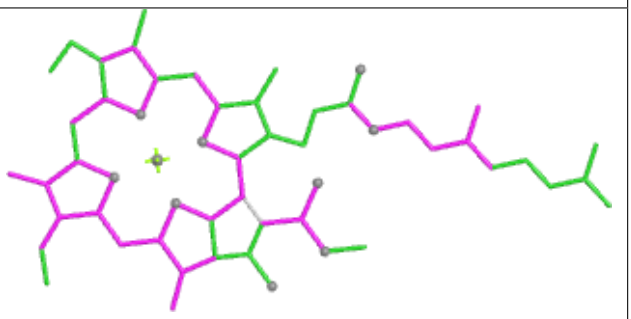


Rings

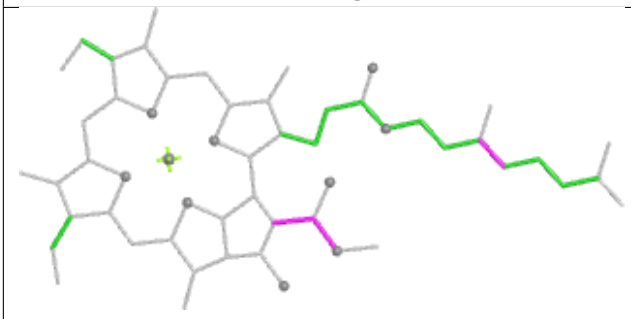
Ligand CLA A 817



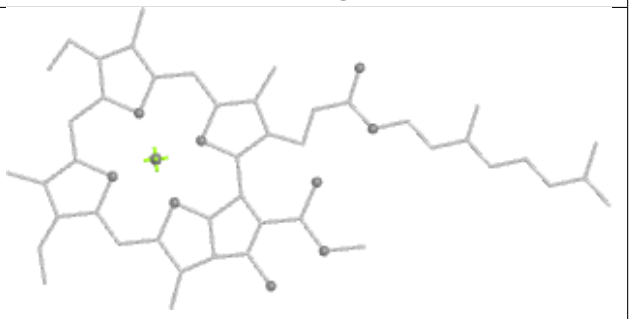
Bond lengths



Bond angles

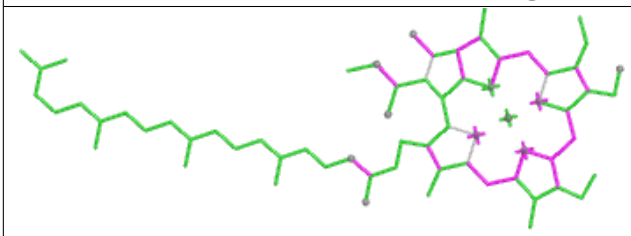


Torsions

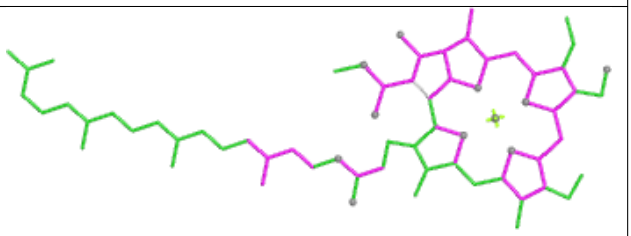


Rings

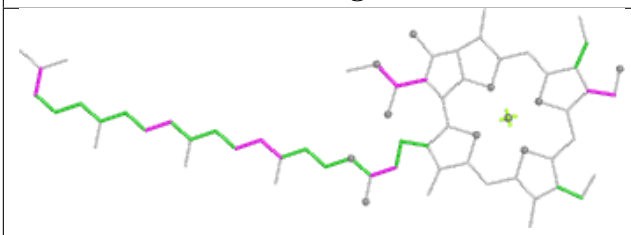
Ligand CHL A 840



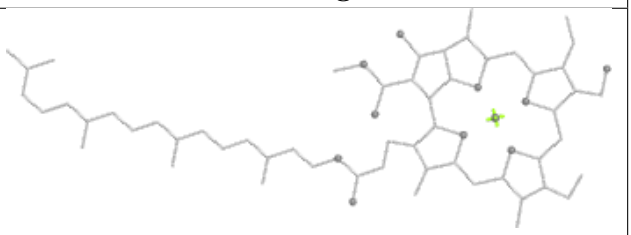
Bond lengths



Bond angles

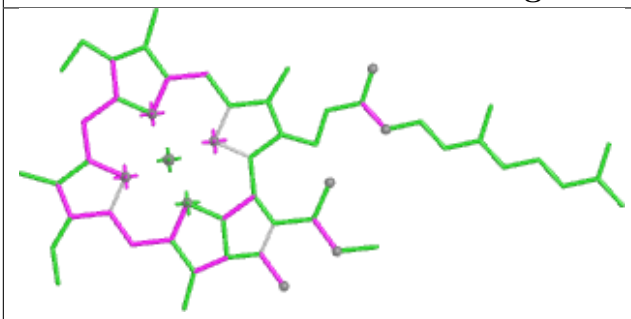


Torsions



Rings

Ligand CLA B 818



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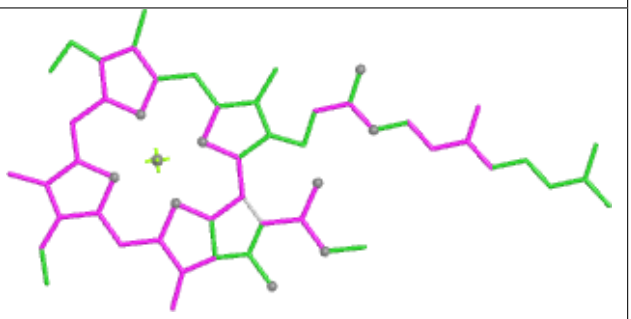
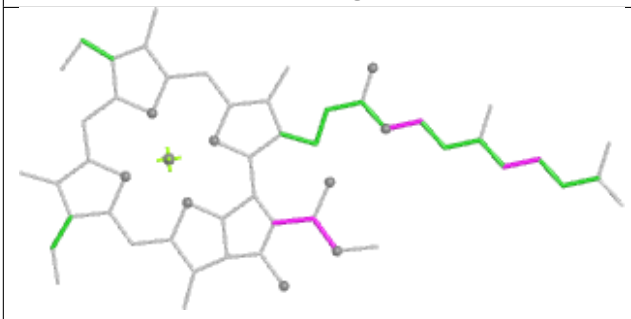
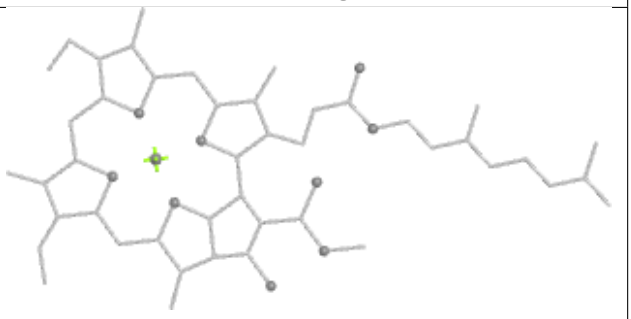


Bond angles

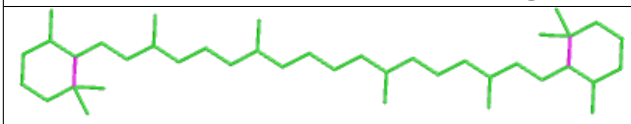


Torsions

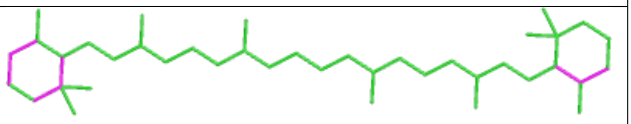


Rings

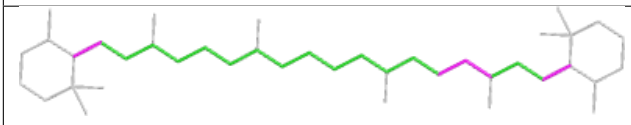
Ligand BCR B 804



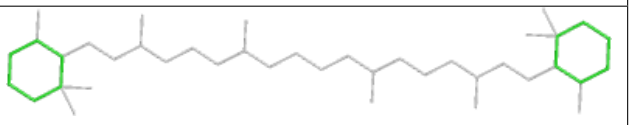
Bond lengths



Bond angles

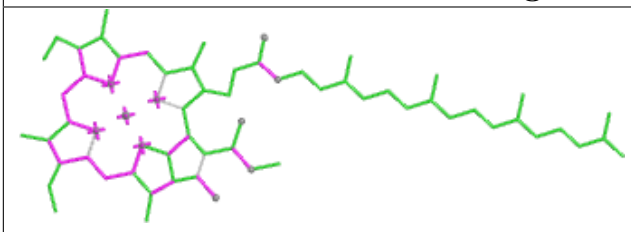


Torsions

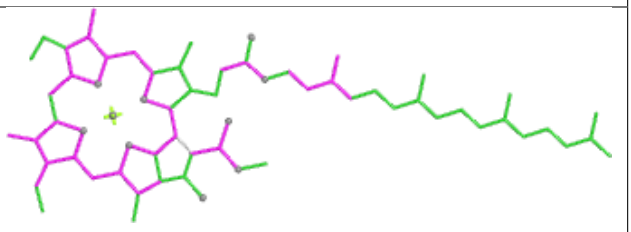


Rings

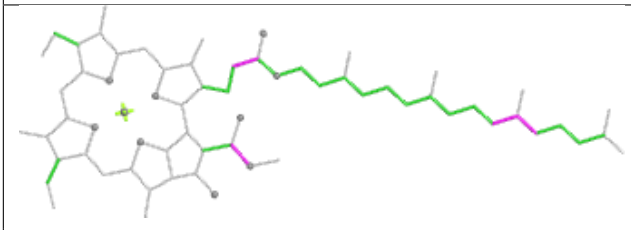
Ligand CLA A 815



Bond lengths



Bond angles



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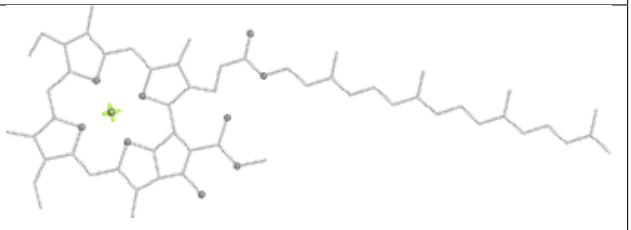
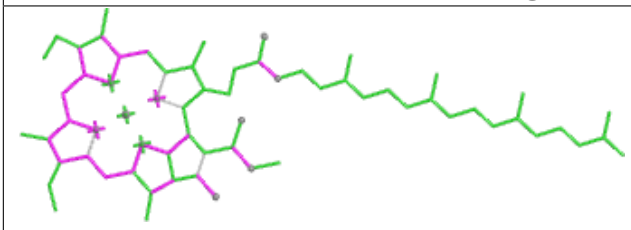
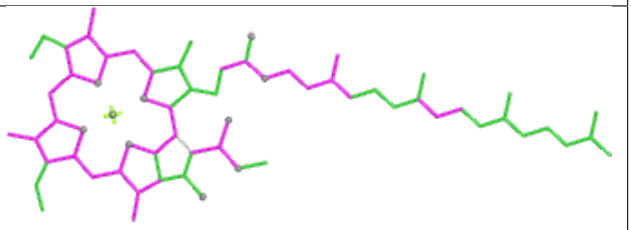


Rings

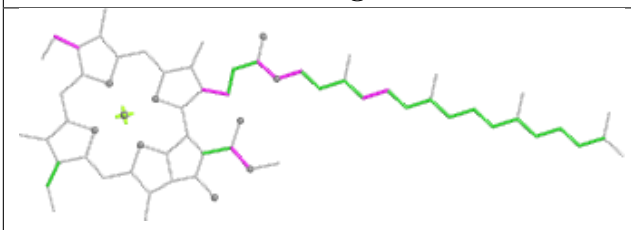
Ligand CLA A 819



Bond lengths



Bond angles



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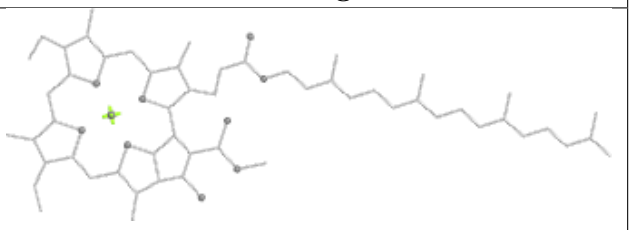
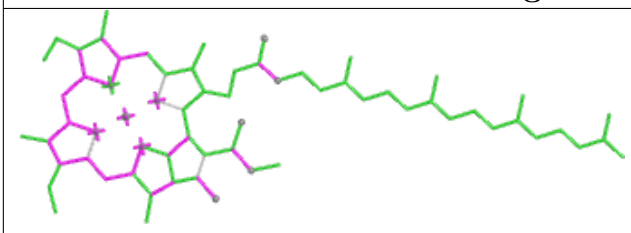
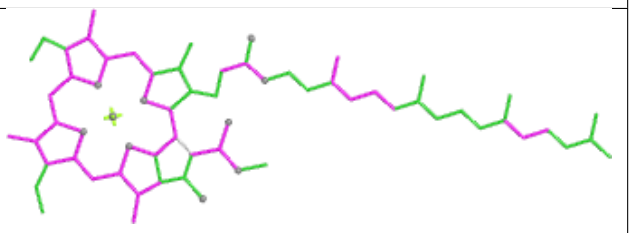


Rings

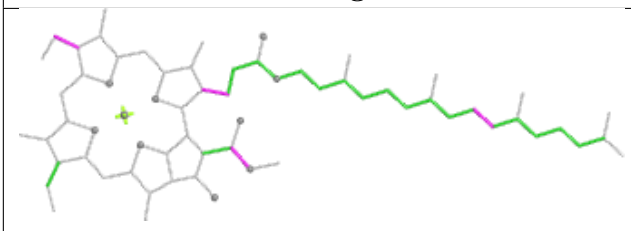
Ligand CLA A 846



Bond lengths



Bond angles



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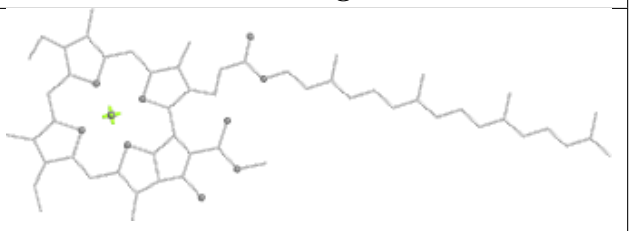
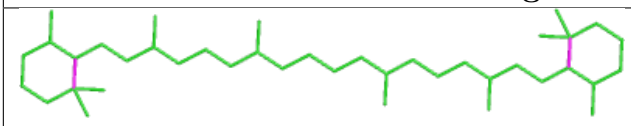
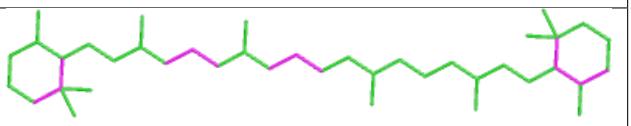


Rings

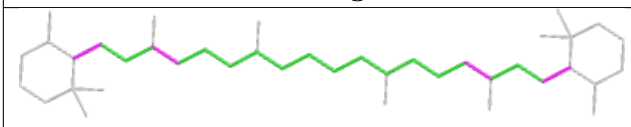
Ligand BCR B 806



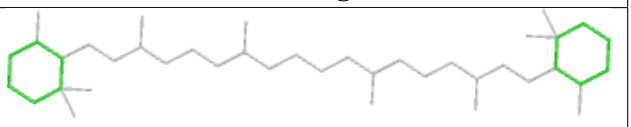
Bond lengths



Bond angles

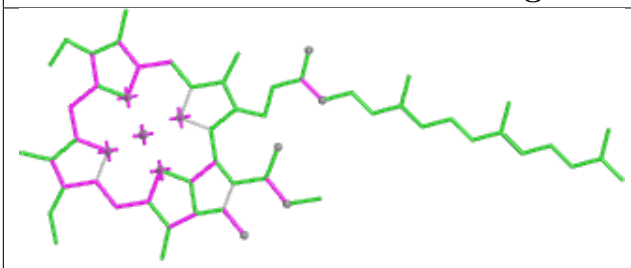


Torsions



Rings

Ligand CLA B 828



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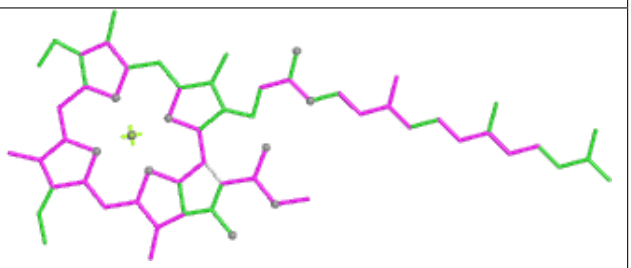
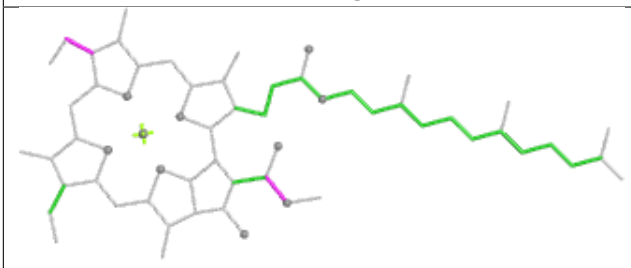


Bond angles



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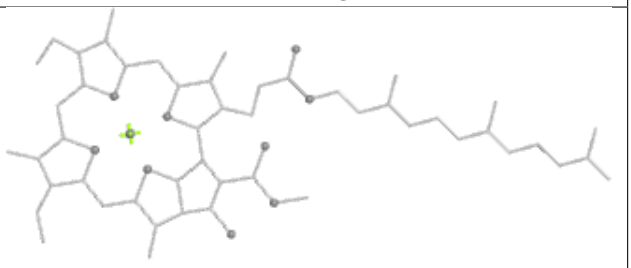
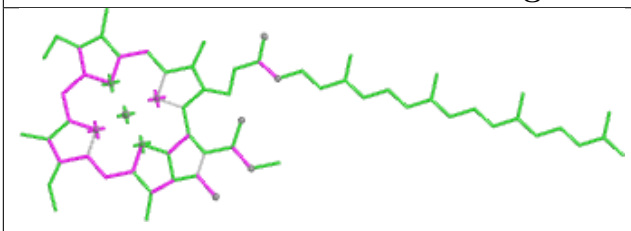


Rings

Ligand CLA A 832



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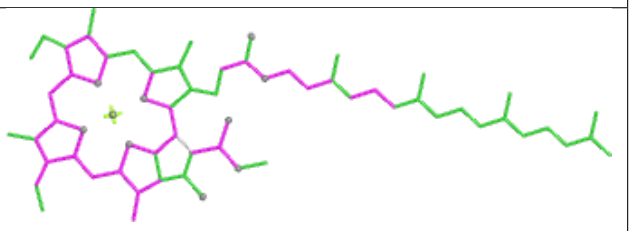
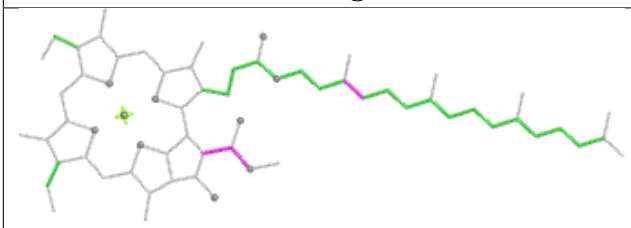


Bond angles



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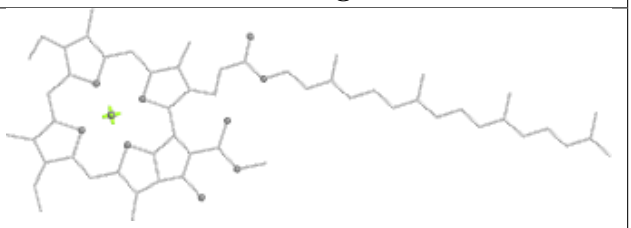
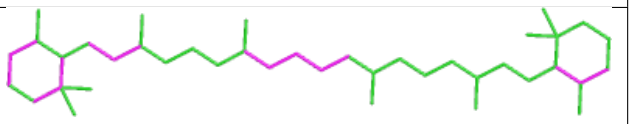


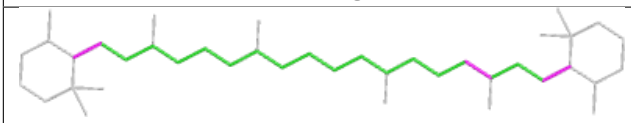
Rings

Ligand BCR 8 301

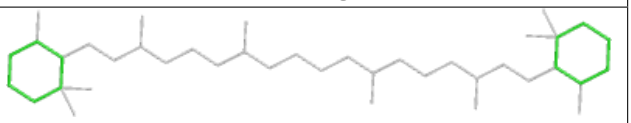
Bond lengths



Bond angles

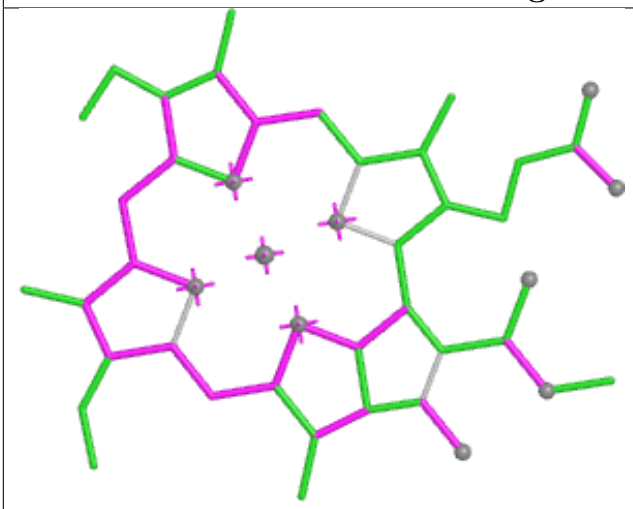


Torsions



Rings

Ligand CLA 4 315



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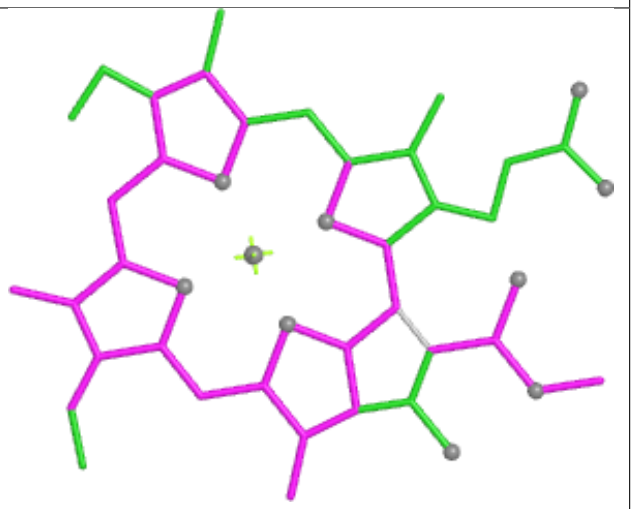
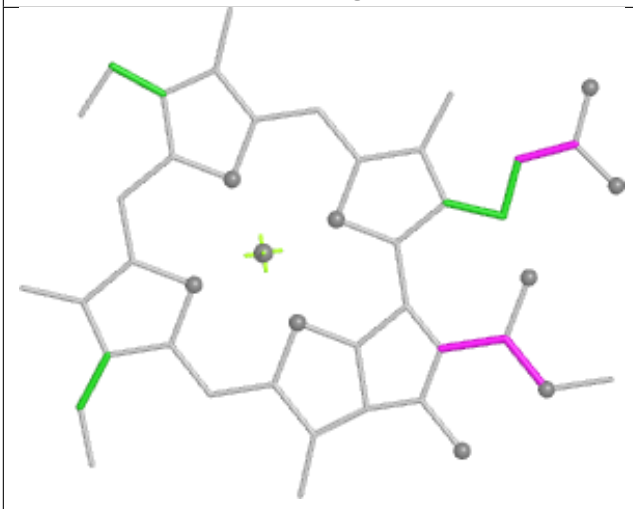


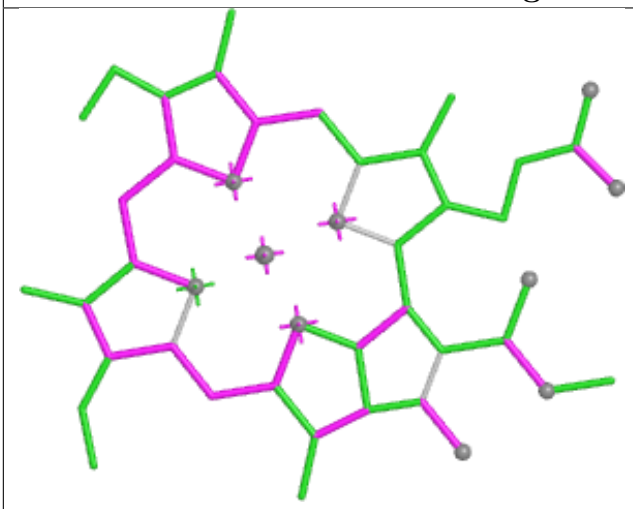
Bond angles



Torsions

Rings

Ligand CLA G 206



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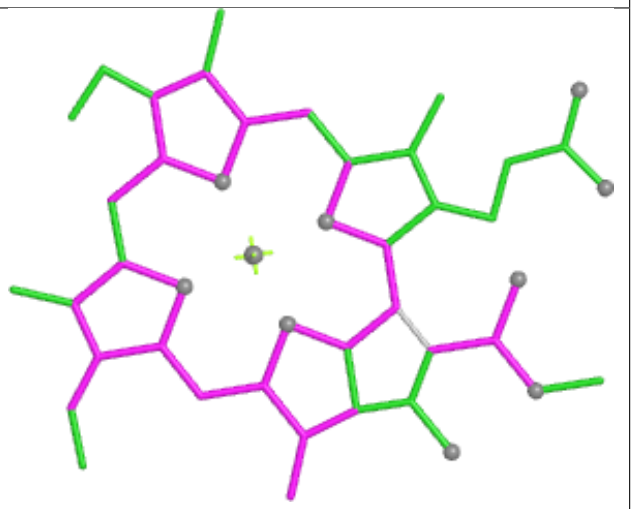
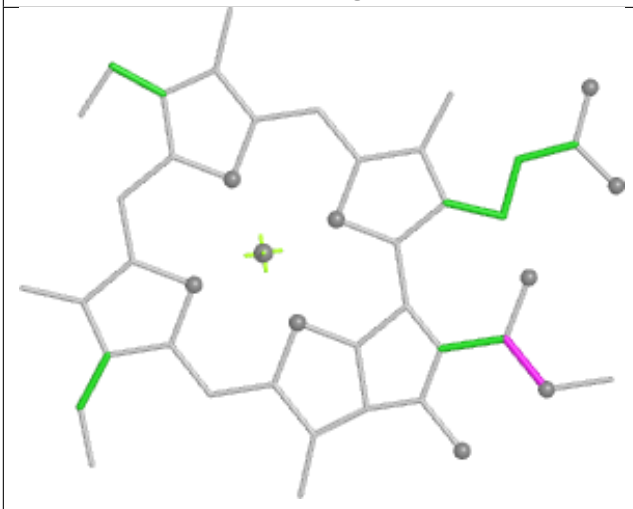


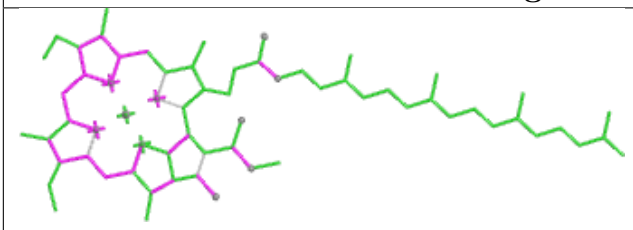
Bond angles



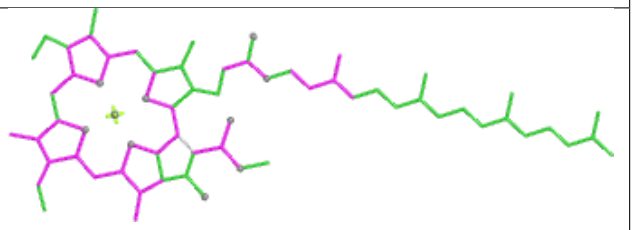
Torsions

Rings

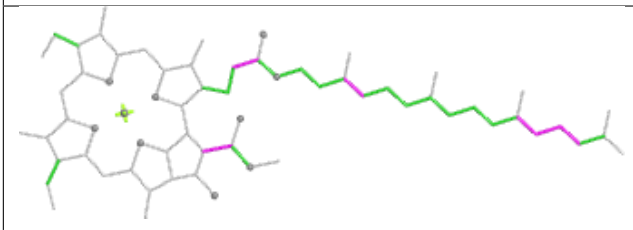
Ligand CLA B 848



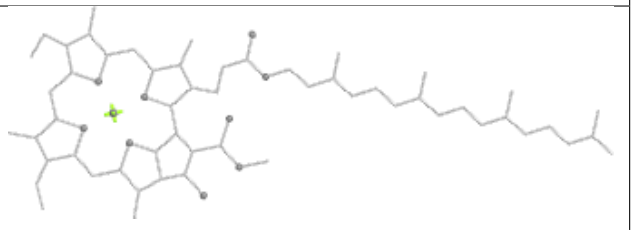
Bond lengths



Bond angles

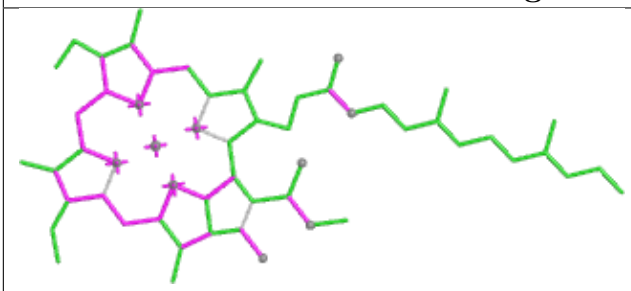


Torsions

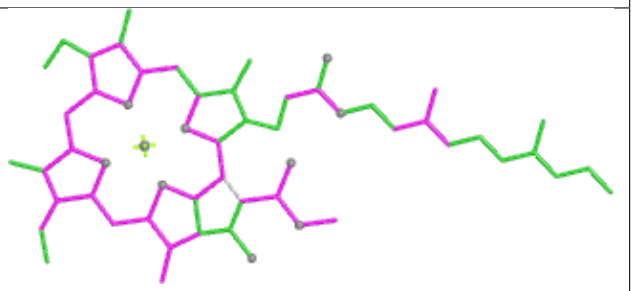


Rings

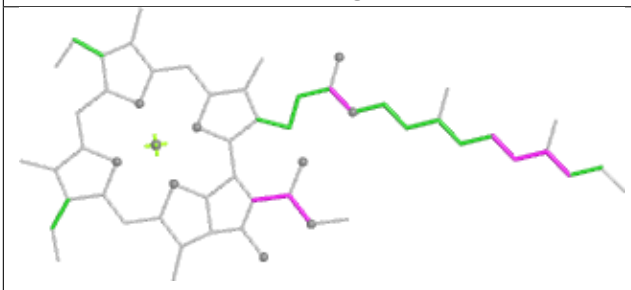
Ligand CLA B 824



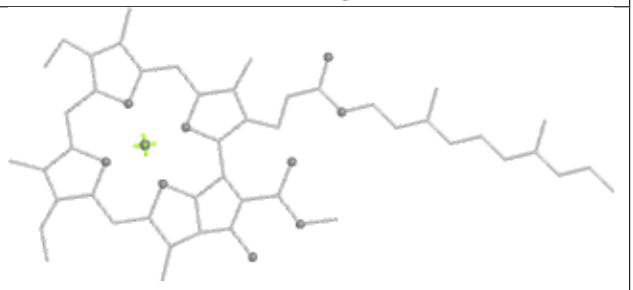
Bond lengths



Bond angles



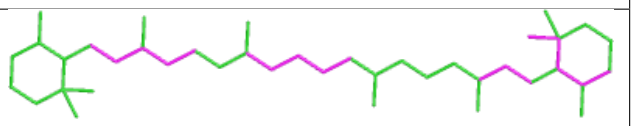
Torsions



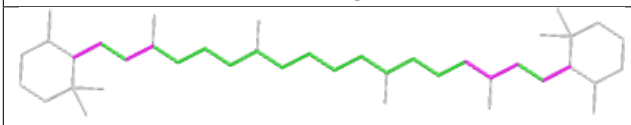
Rings

Ligand BCR K 202

Bond lengths



Bond angles



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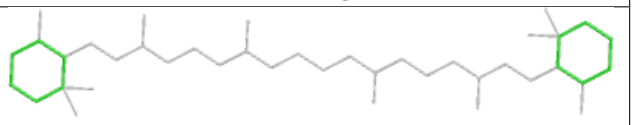
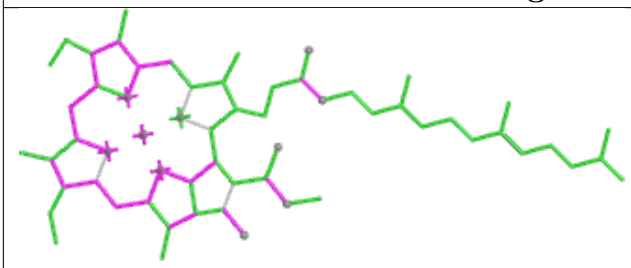


Rings

Ligand CLA b 313



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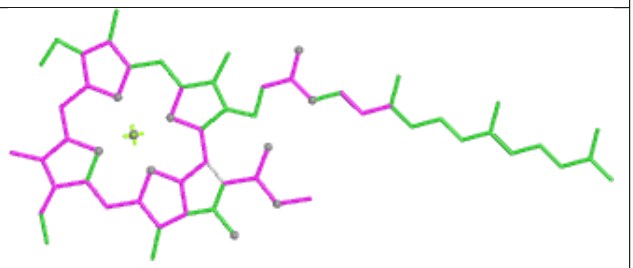
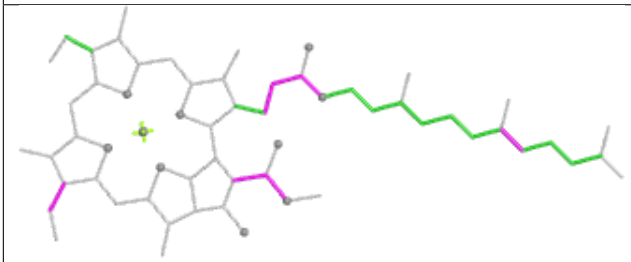


Bond angles



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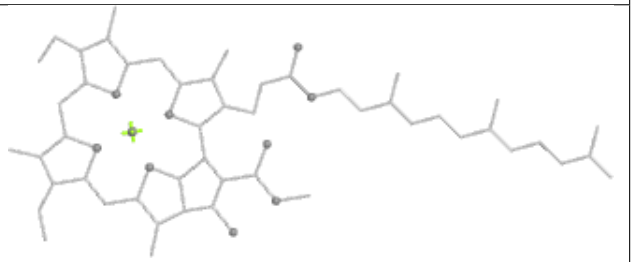
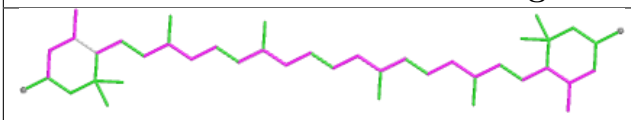


Rings

Ligand LUT J 103



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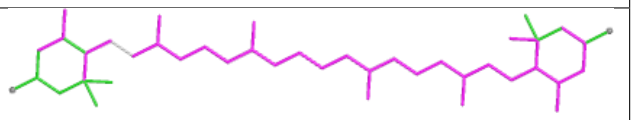
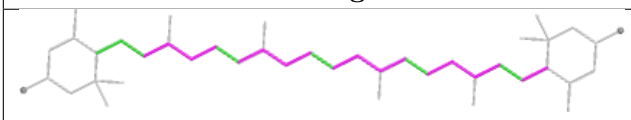


Bond angles



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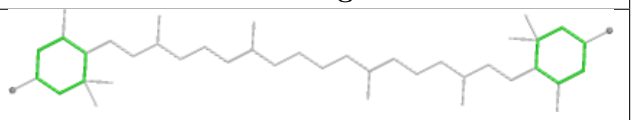
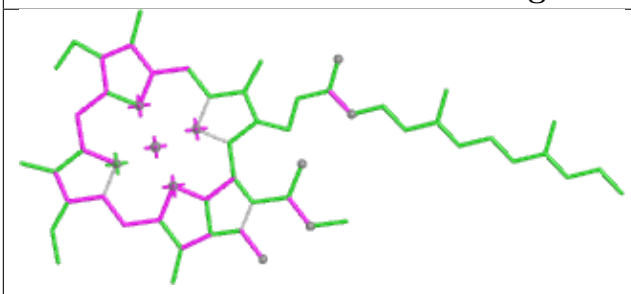


Rings

Ligand CLA 2 307



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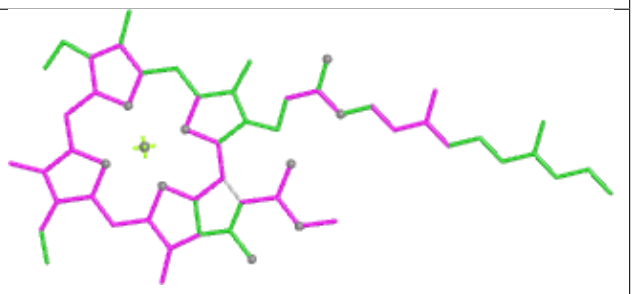
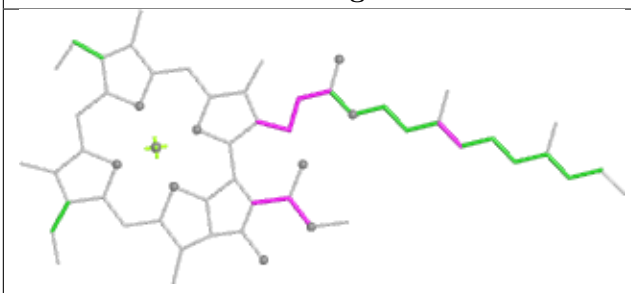


Bond angles



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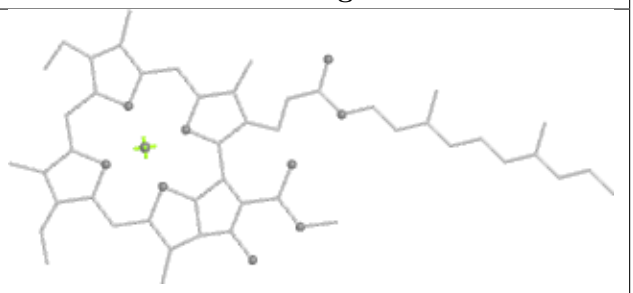
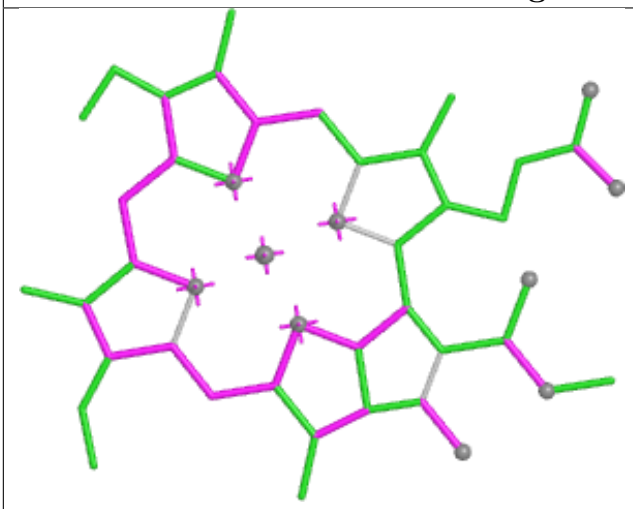


Rings

Ligand CLA 2 305



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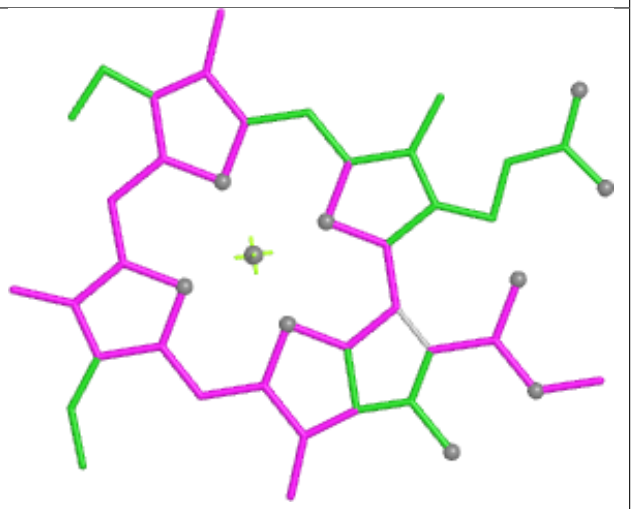

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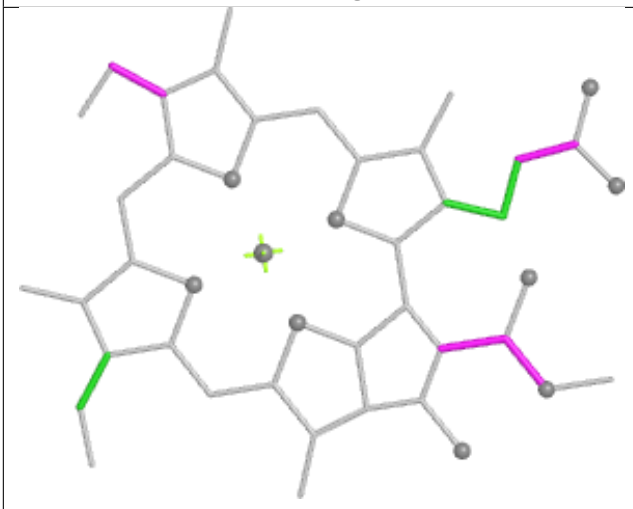
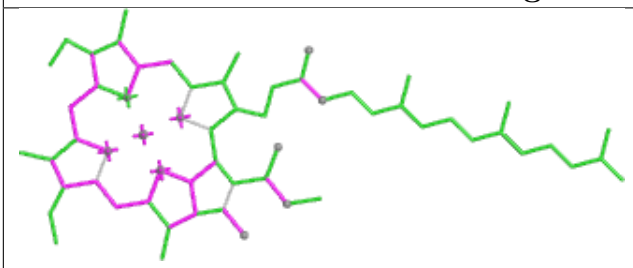


Torsions

Rings

Ligand CLA A 836



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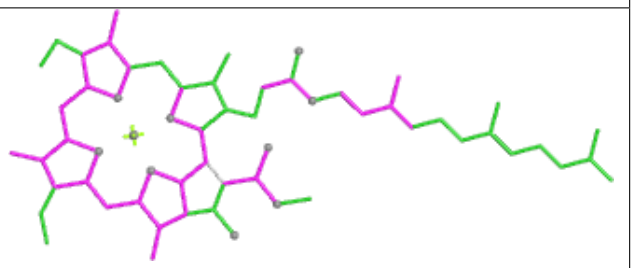
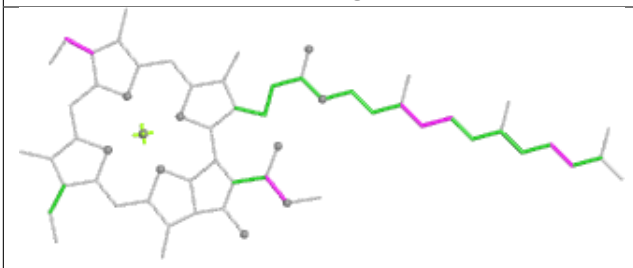


Bond angles



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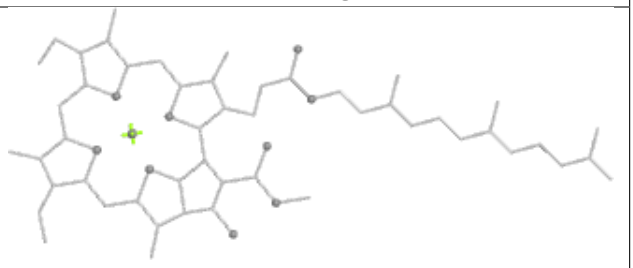
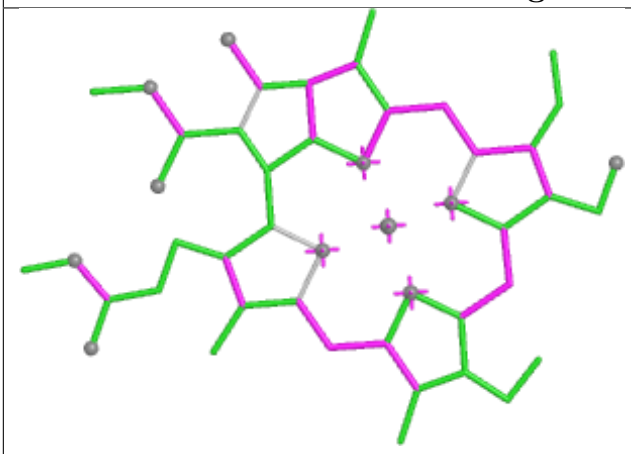


Rings

Ligand CHL 6 319



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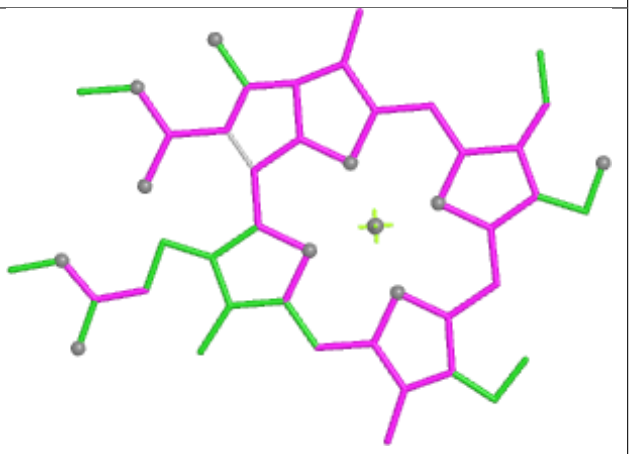
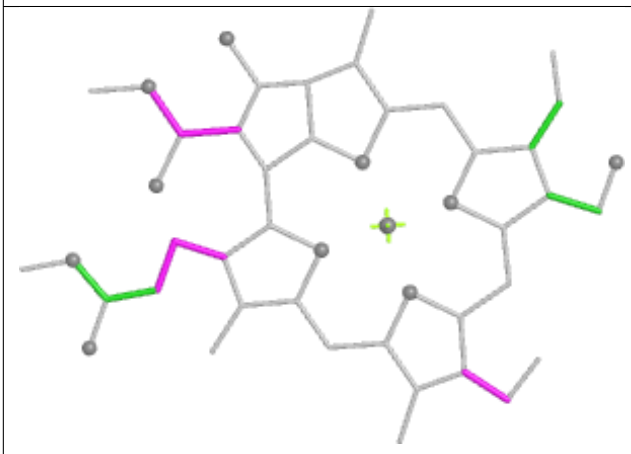


Bond angles



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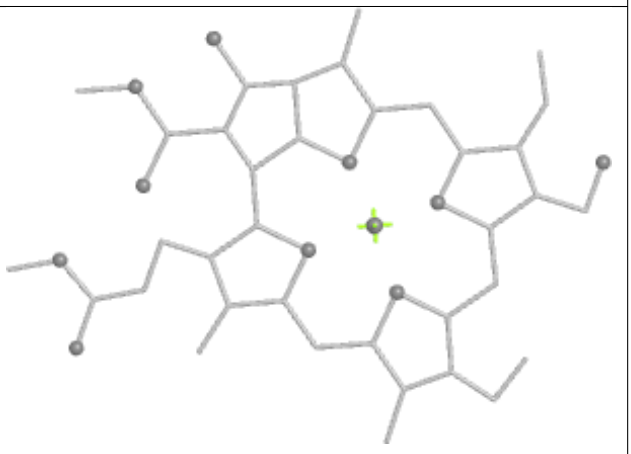
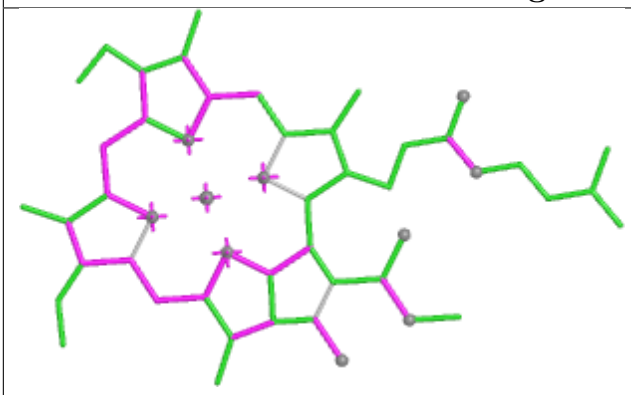


Rings

Ligand CLA 4 321



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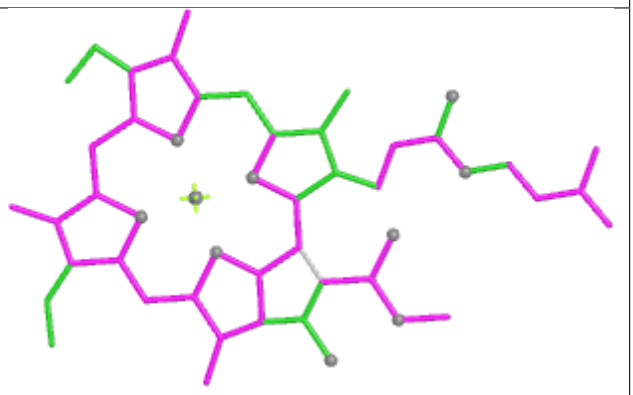
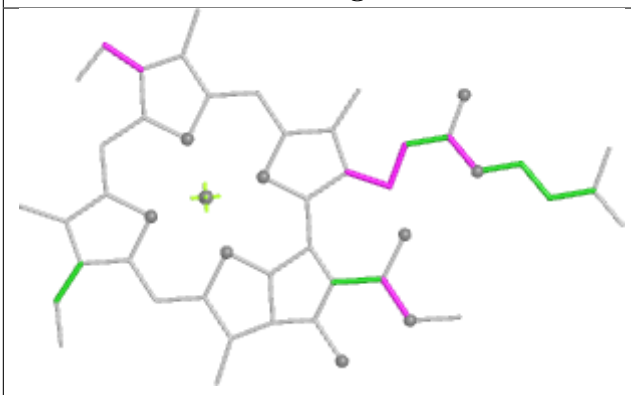


Bond angles



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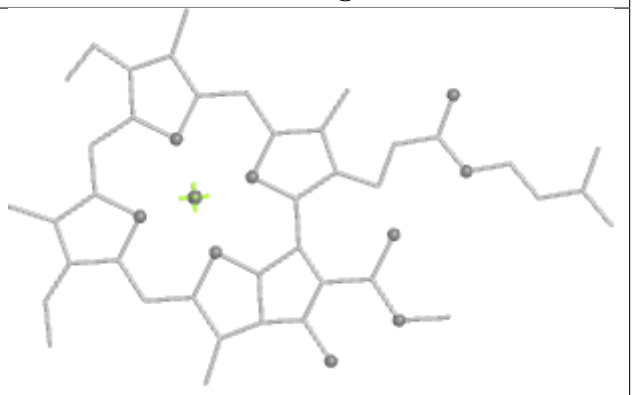
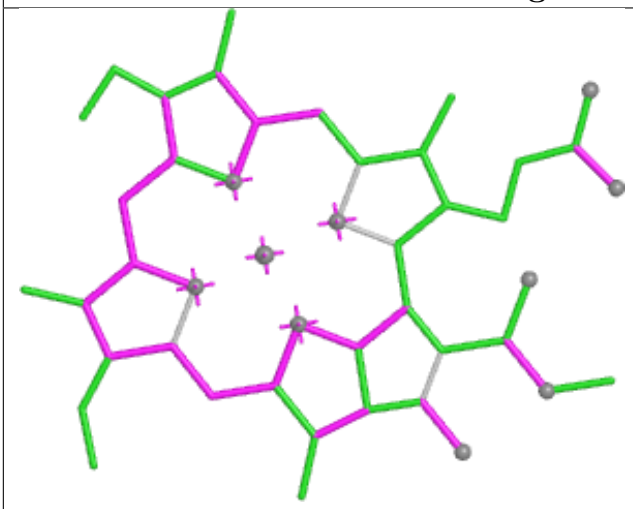


Rings

Ligand CLA 2 310



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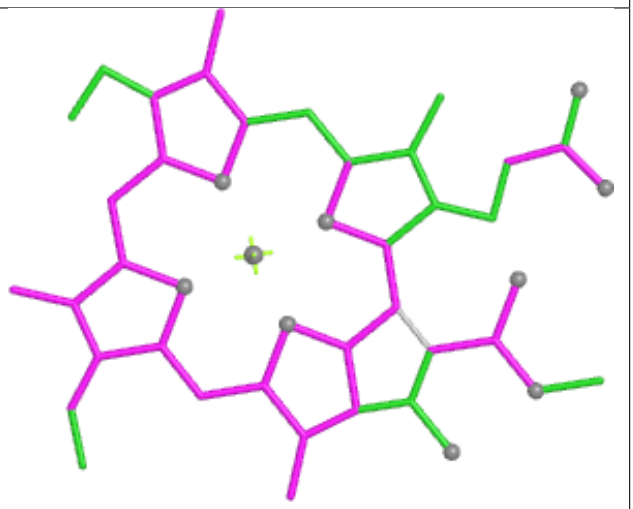
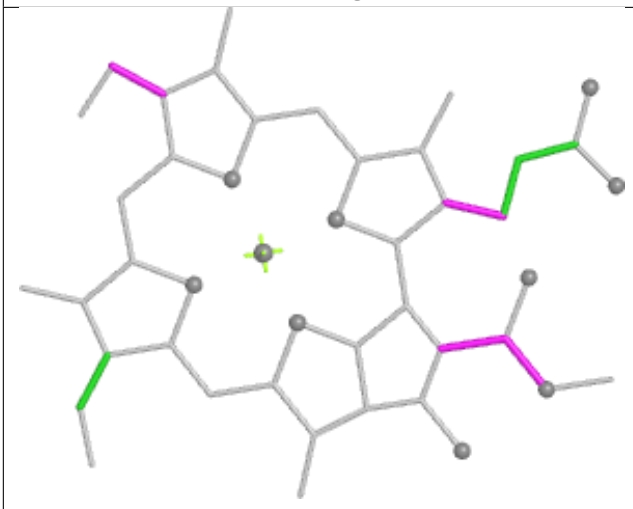


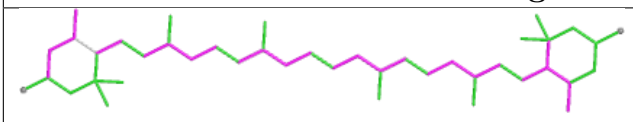
Bond angles



Torsions

Rings

Ligand LUT 7 305



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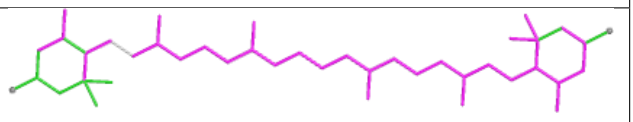

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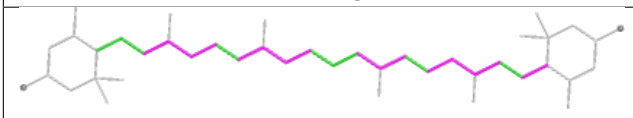
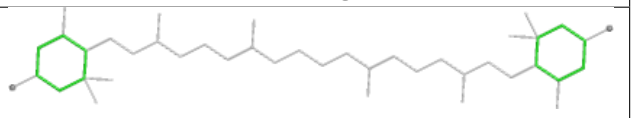
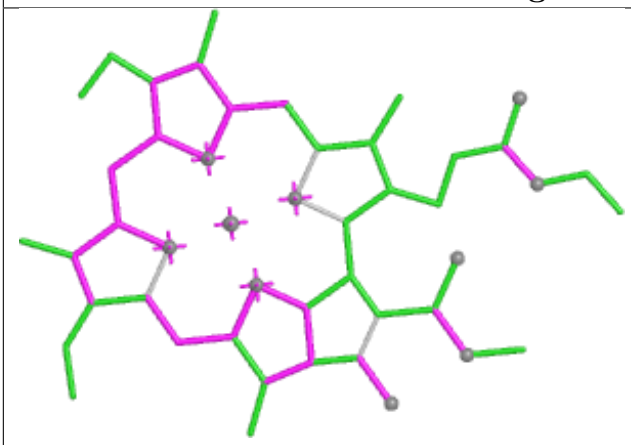


Torsions



Rings

Ligand CLA 4 316



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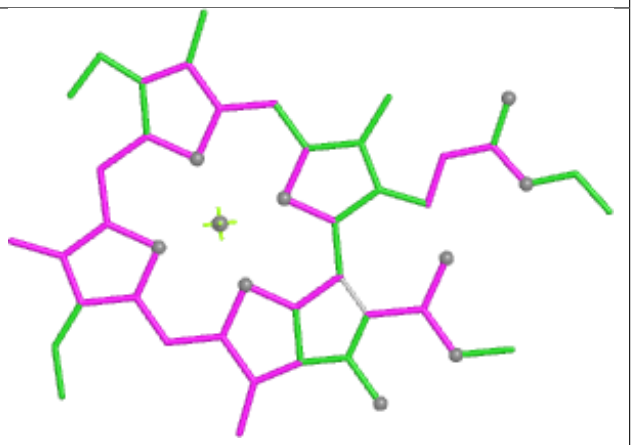
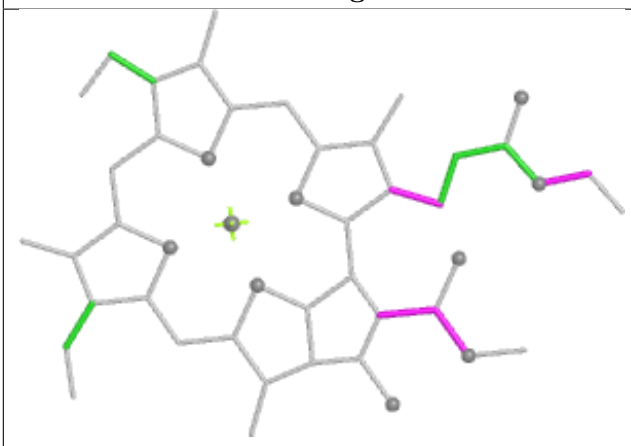


Bond angles



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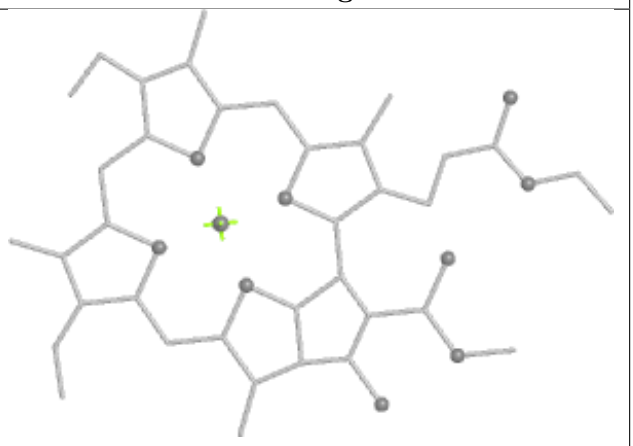
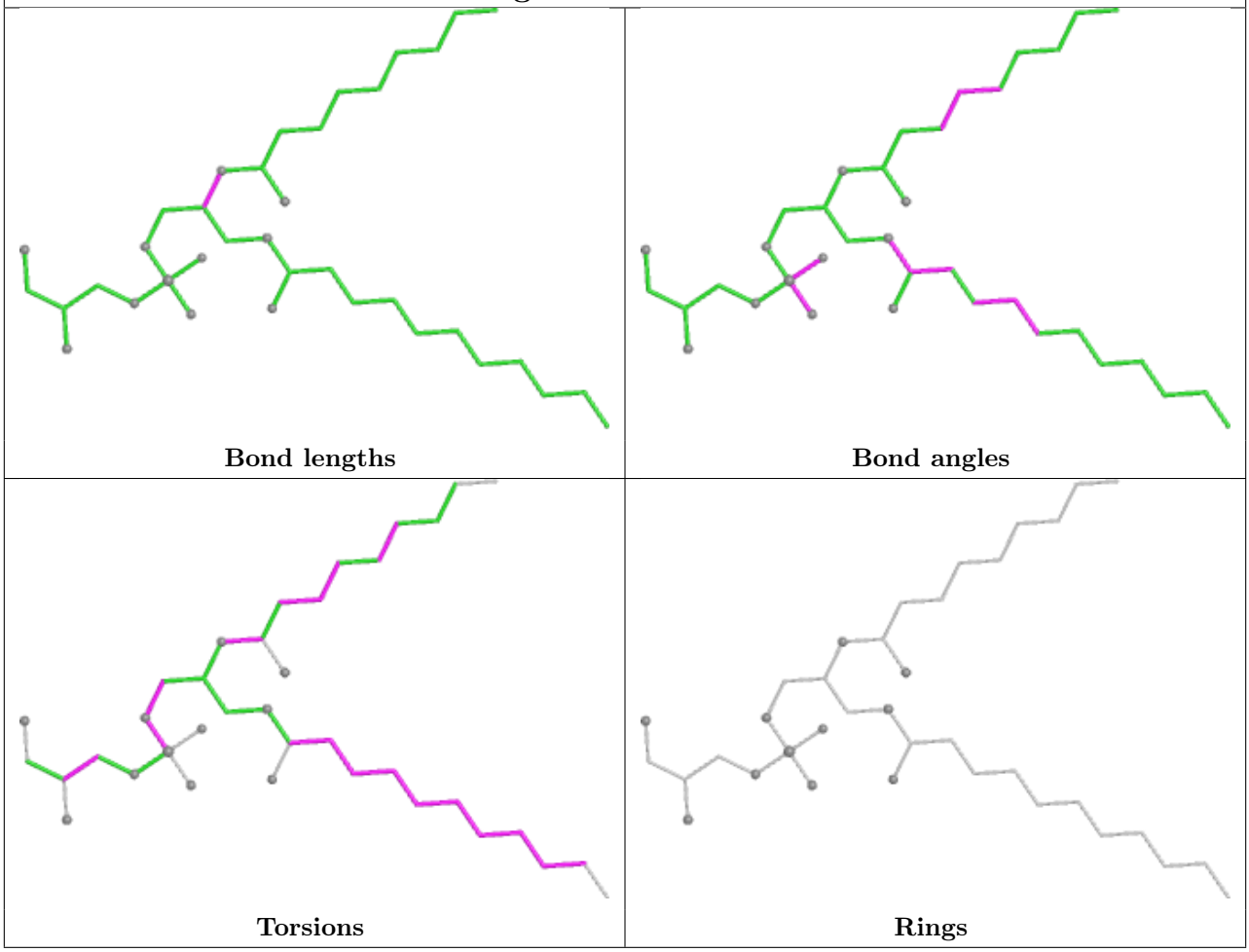
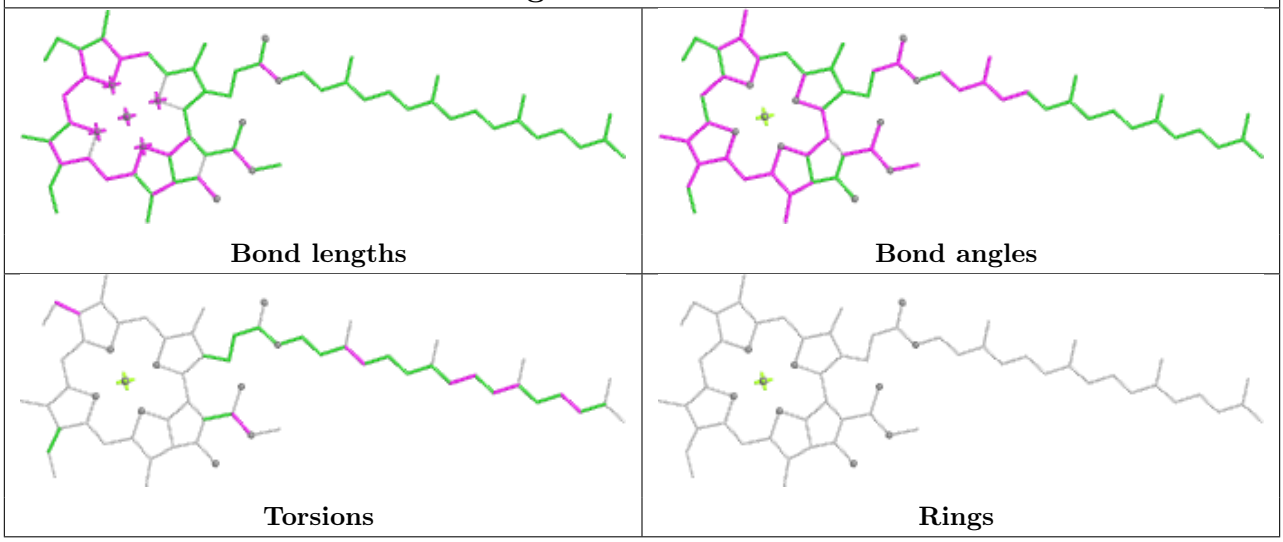


Rings

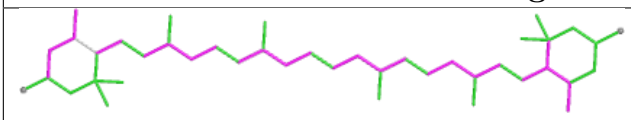
Ligand LHG 7 307



Ligand CLA F 301



Ligand LUT 9 302



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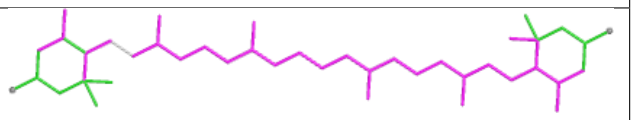
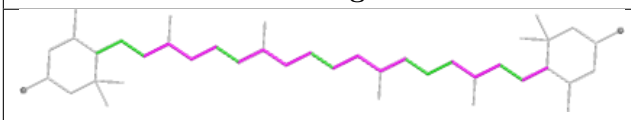


Bond angles



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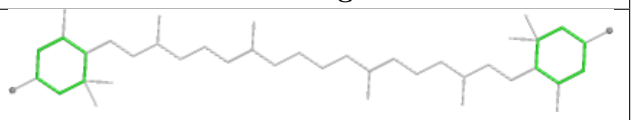
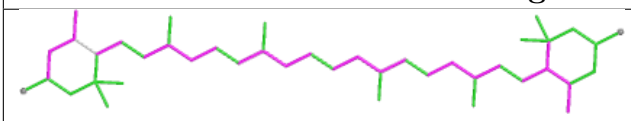


Rings

Ligand LUT 3 304



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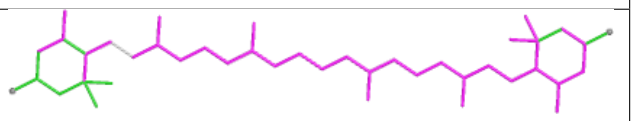
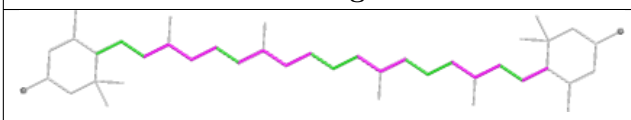
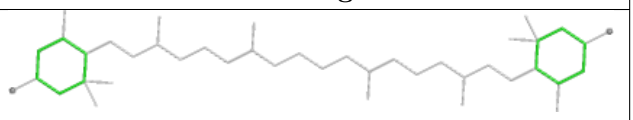


Bond angles

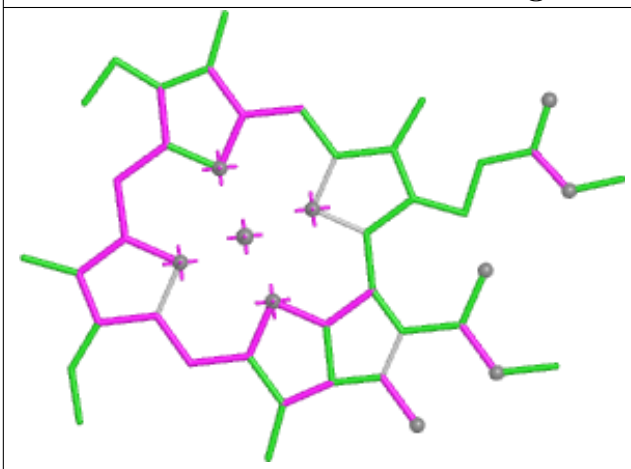


Torsions

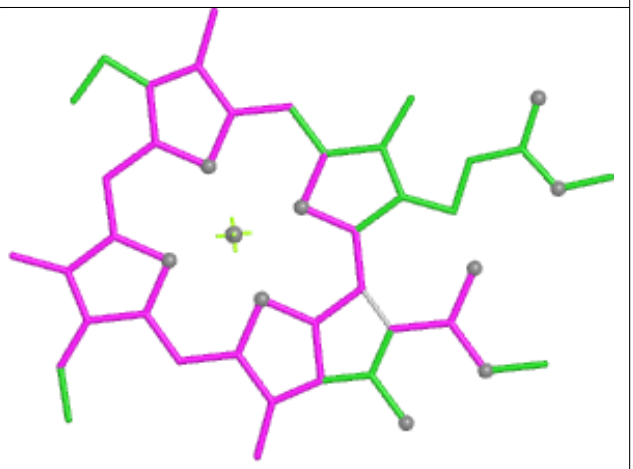


Rings

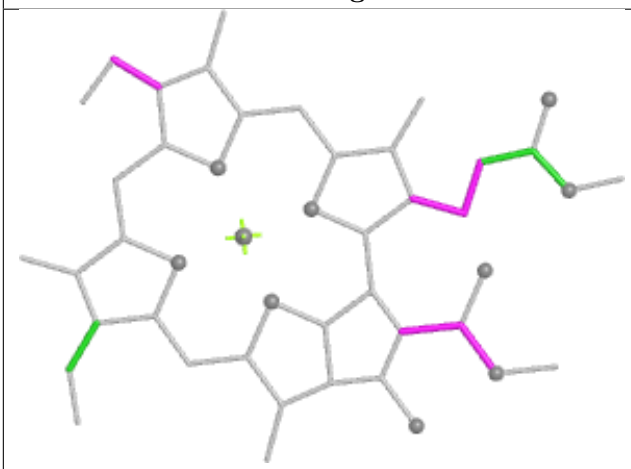
Ligand CLA b 308



Bond lengths



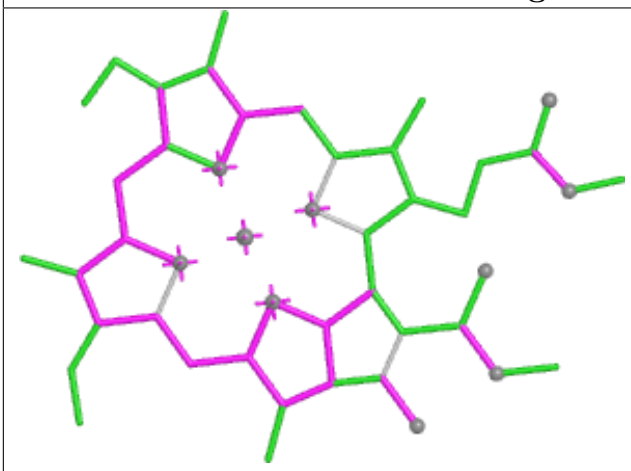
Bond angles



Torsions

Rings

Ligand CLA 5 313



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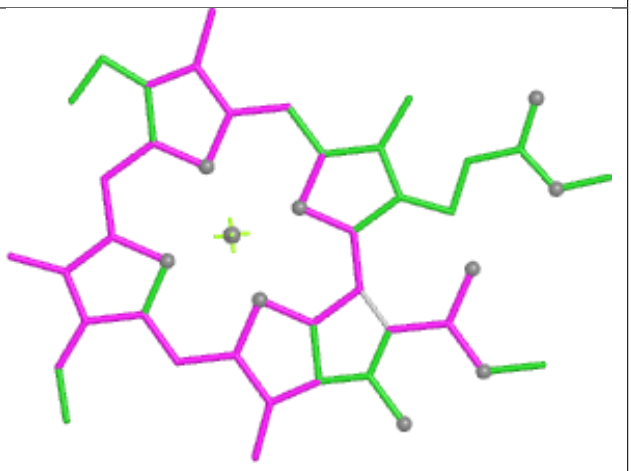

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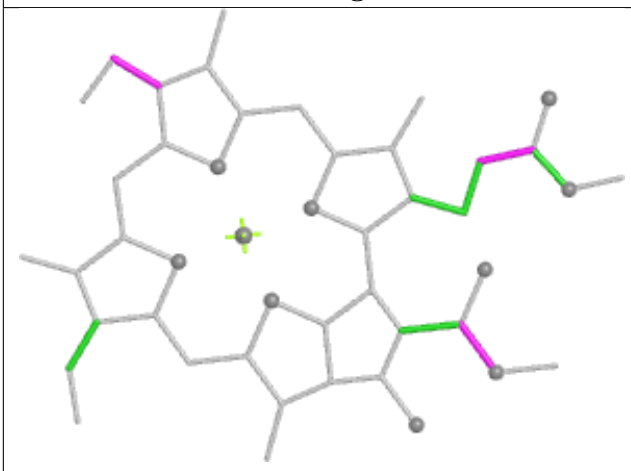
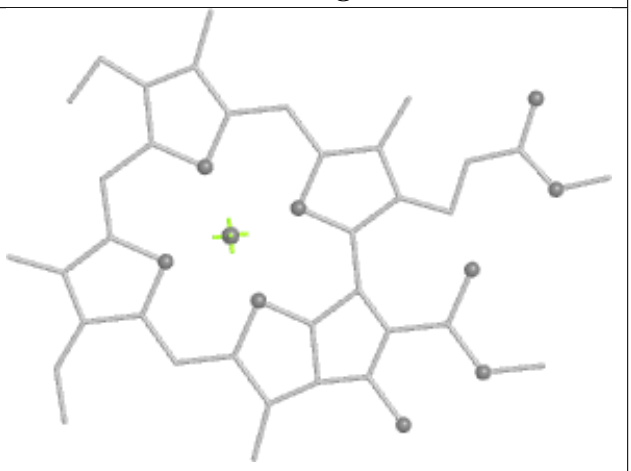
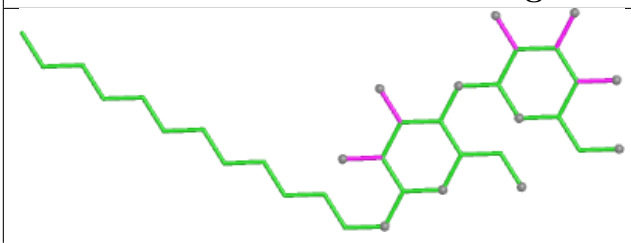


Torsions



Rings

Ligand LMT 5 301



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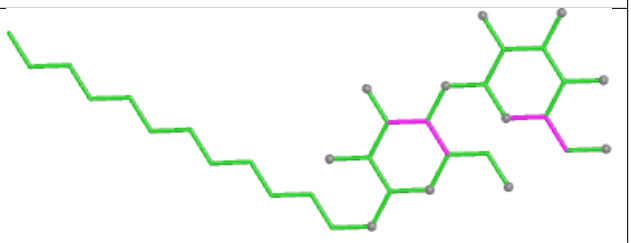
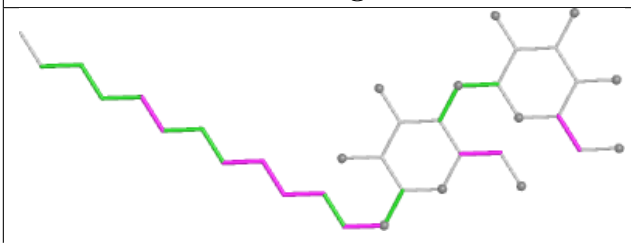
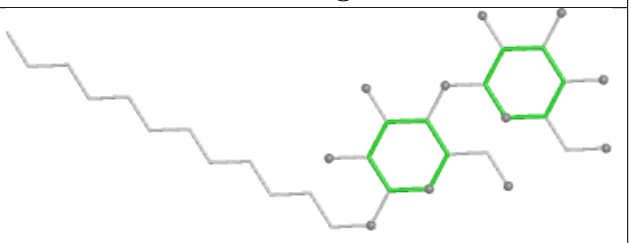


Bond angles

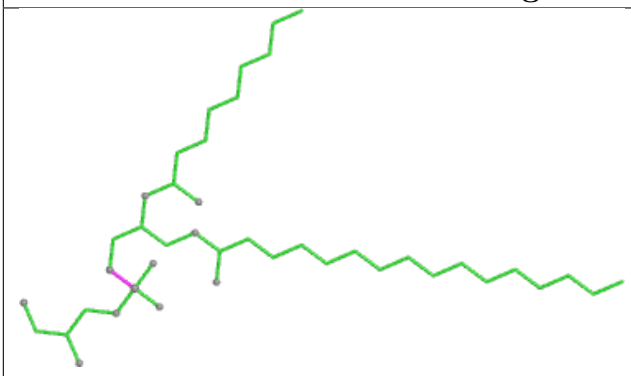


Torsions



Rings

Ligand LHG A 810



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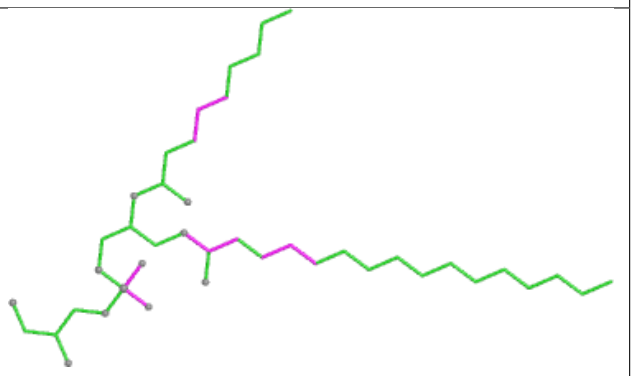

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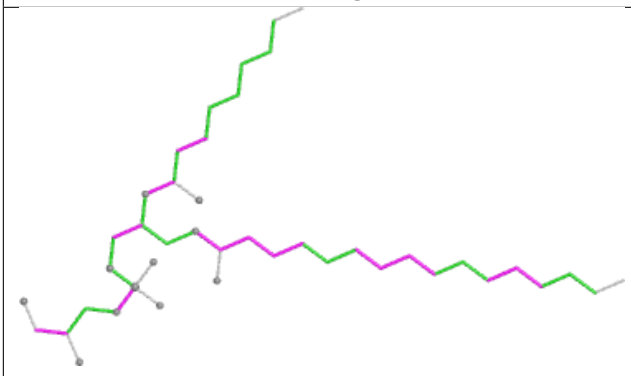

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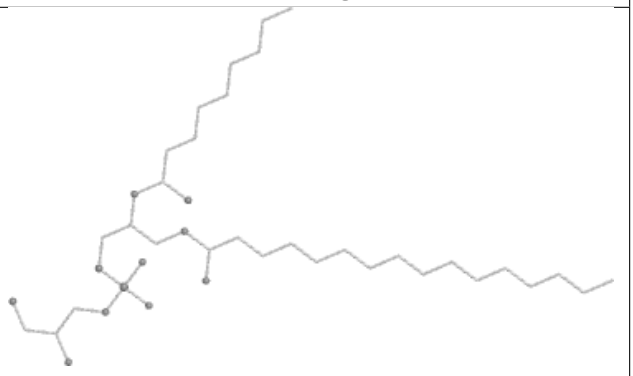
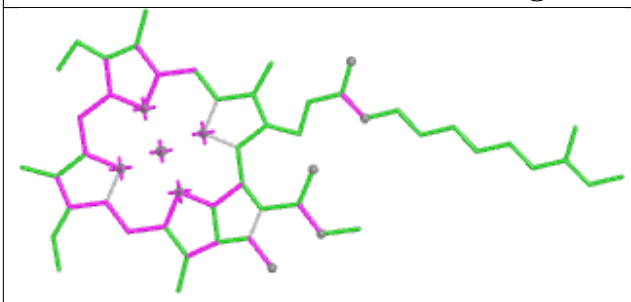


Rings

Ligand CLA 7 315



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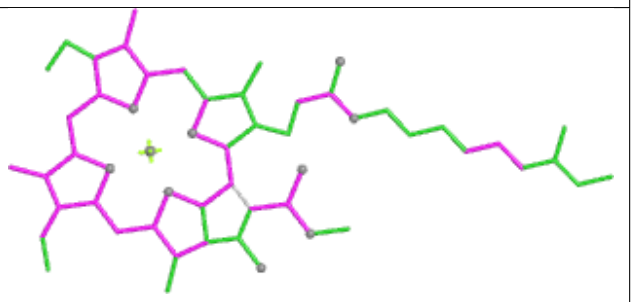
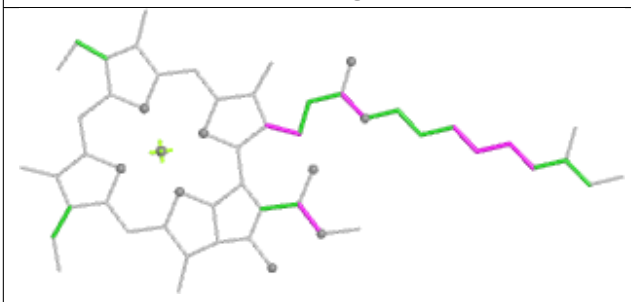


Bond angles



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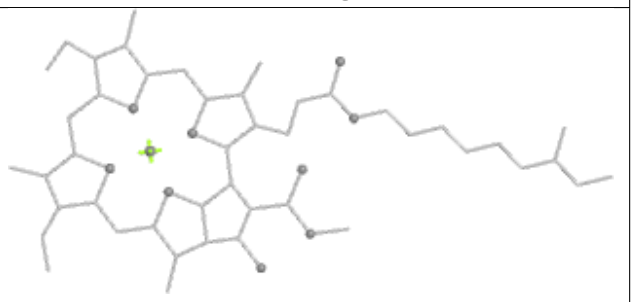
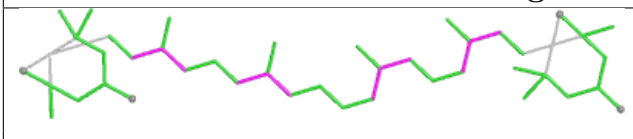


Rings

Ligand XAT 7 306



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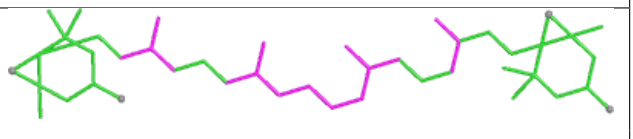
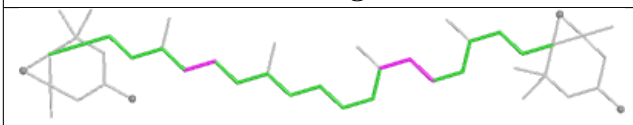


Bond angles



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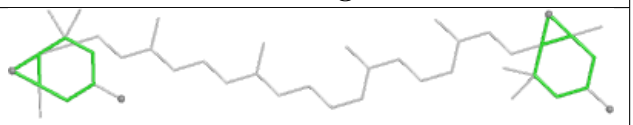
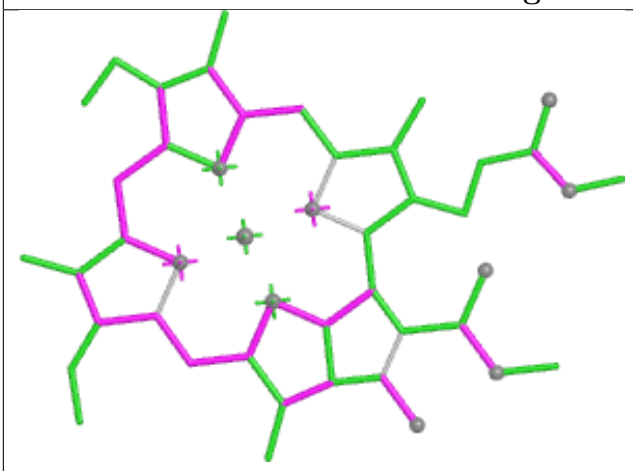


Rings

Ligand CLA H 903



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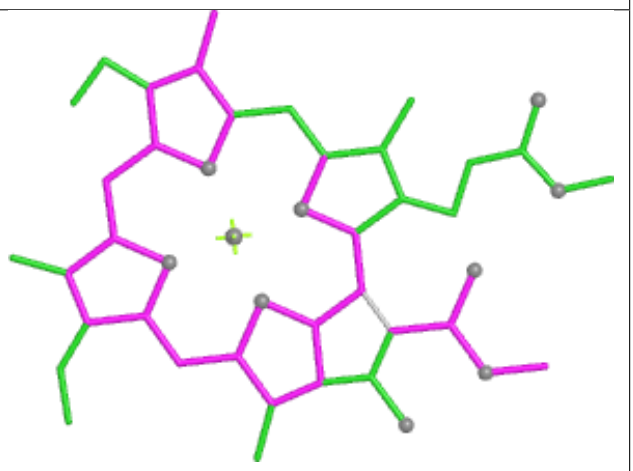

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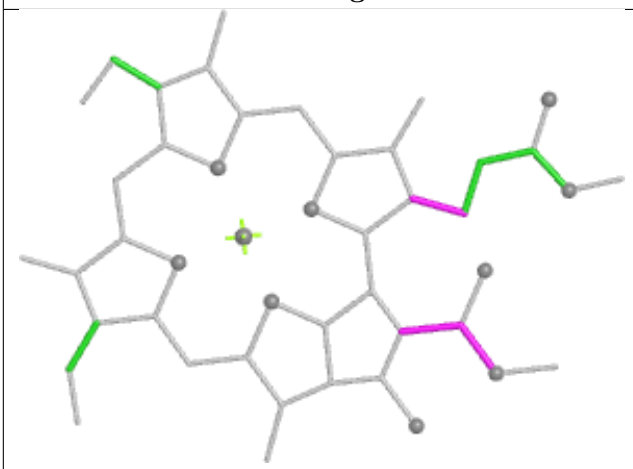
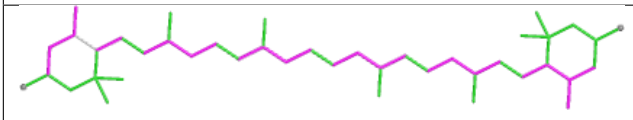


Torsions

Rings

Ligand LUT F 304



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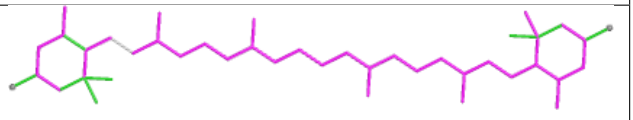
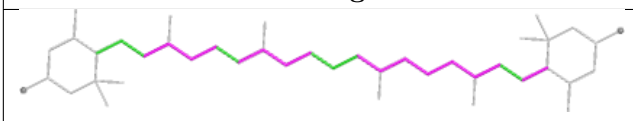


Bond angles



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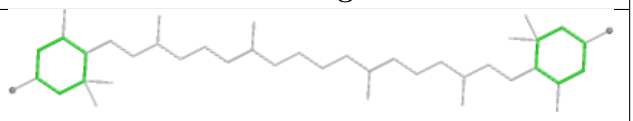
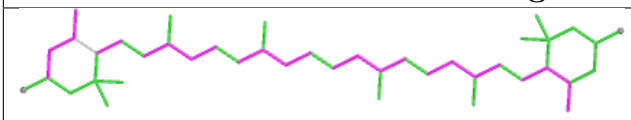


Rings

Ligand LUT 5 304



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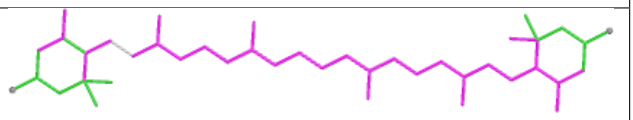
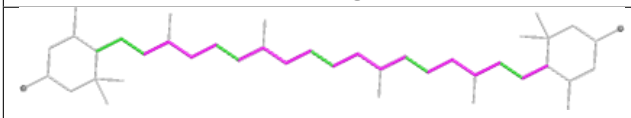


Bond angles



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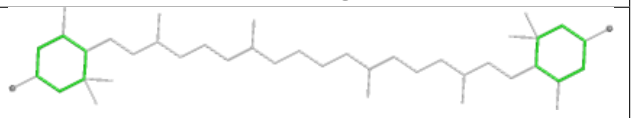
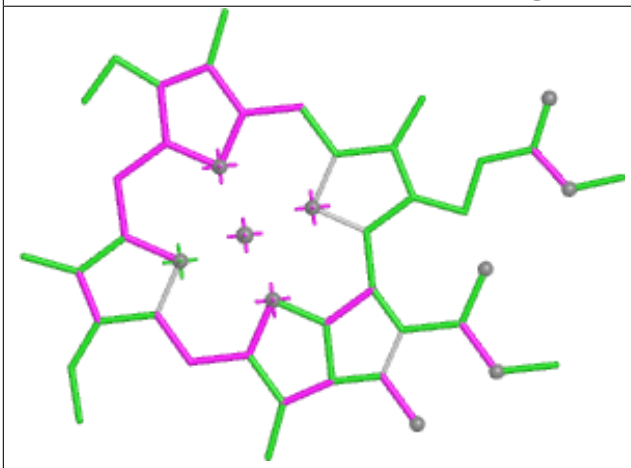


Rings

Ligand CLA 8 321



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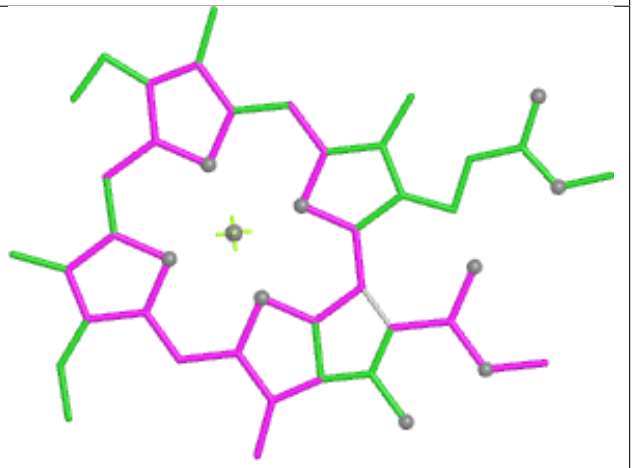
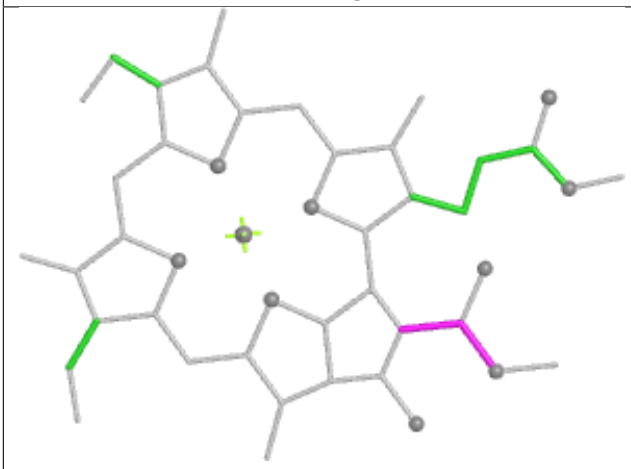


Bond angles



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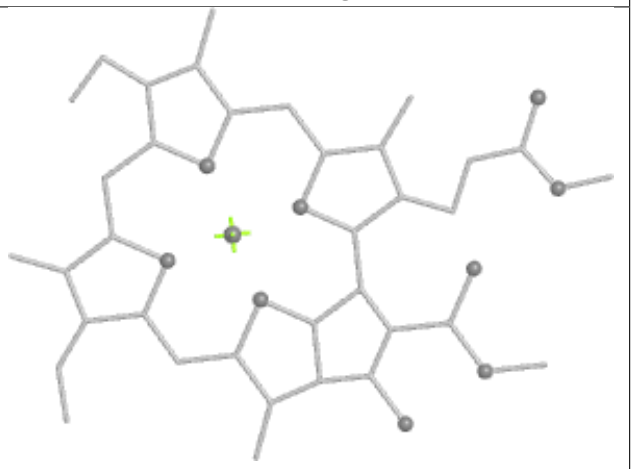
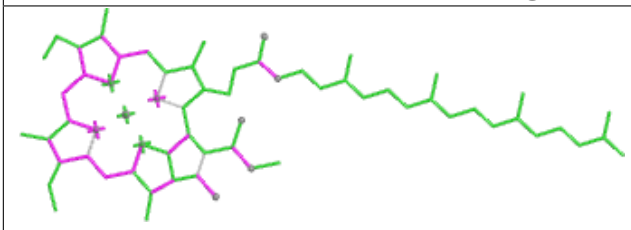


Rings

Ligand CLA A 857



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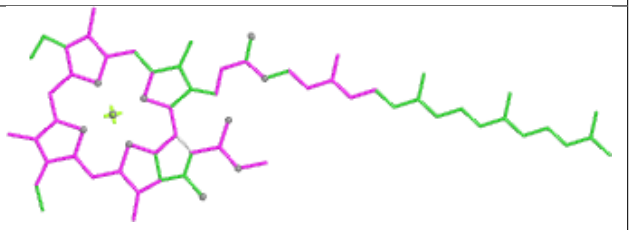
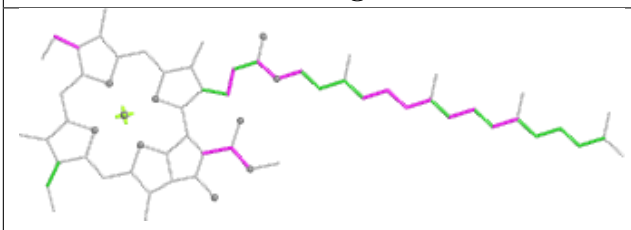


Bond angles



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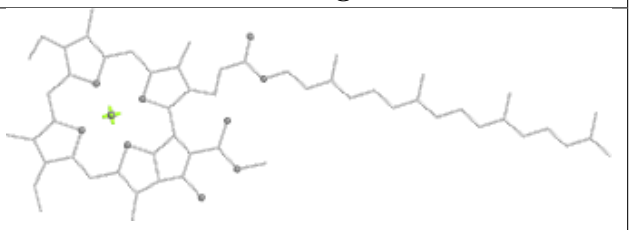
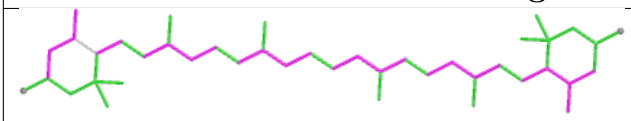


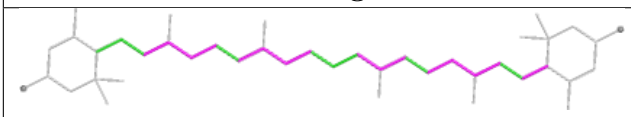
Rings

Ligand LUT 8 303



Bond lengths

Bond angles



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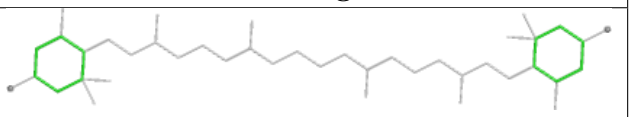
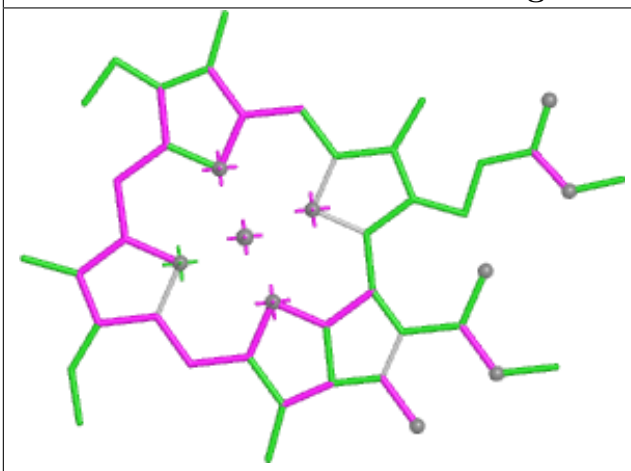


Rings

Ligand CLA b 306



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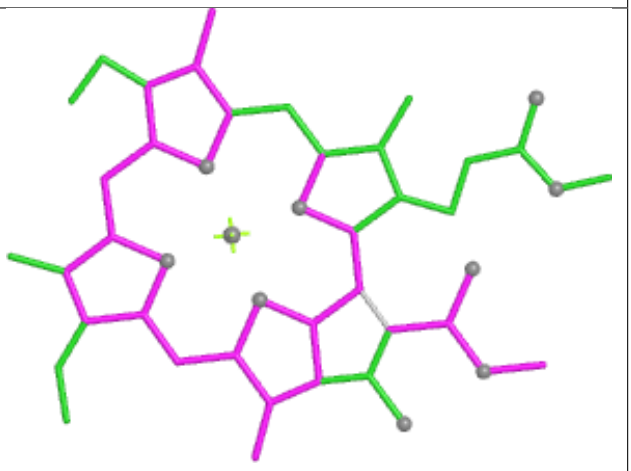
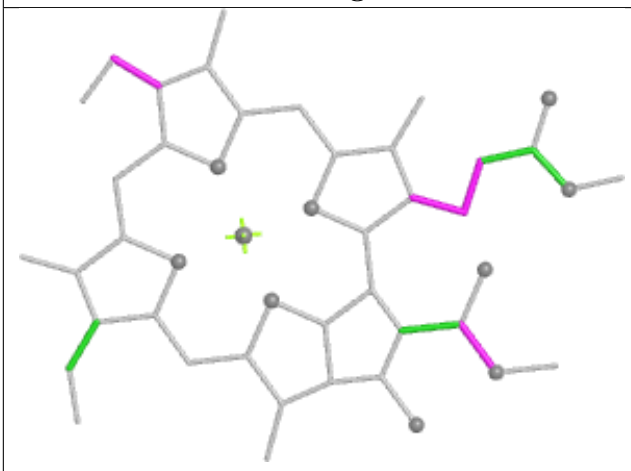


Bond angles



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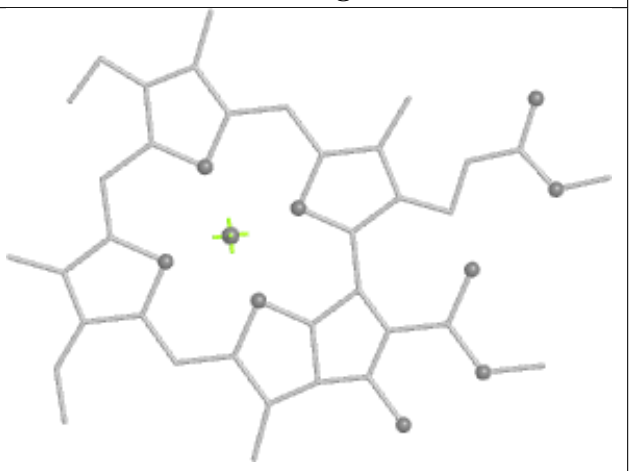
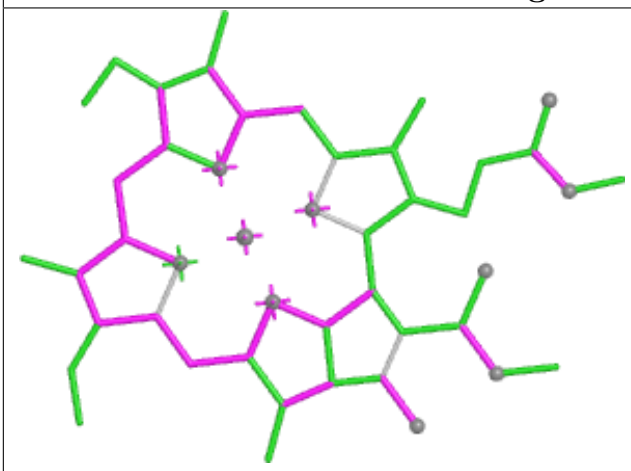


Rings

Ligand CLA 2 312



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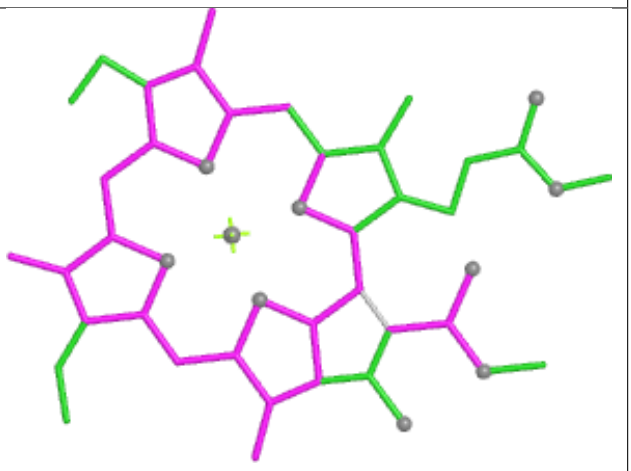
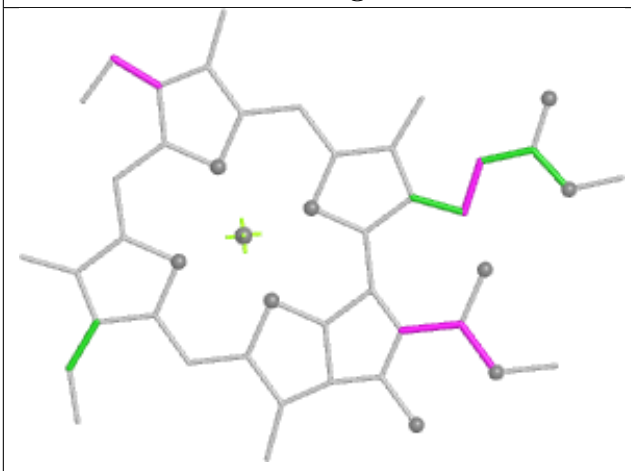


Bond angles



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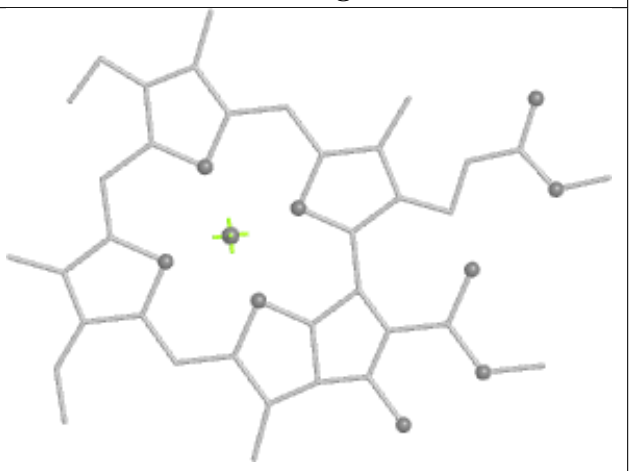
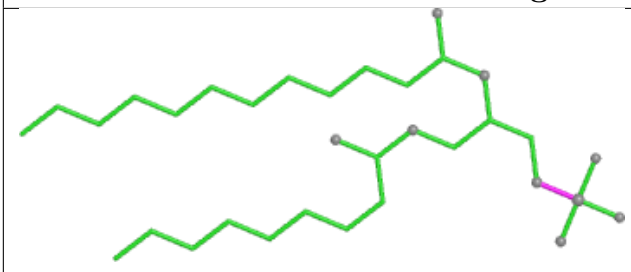


Rings

Ligand 3PH 7 301



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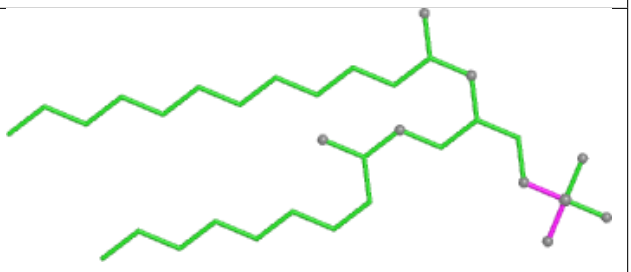
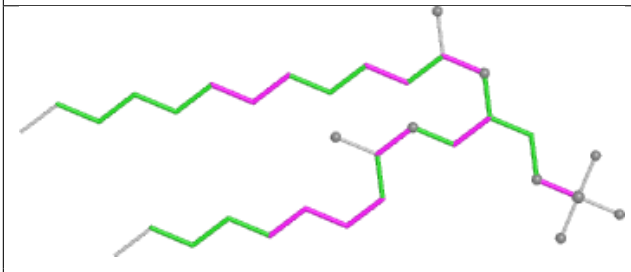
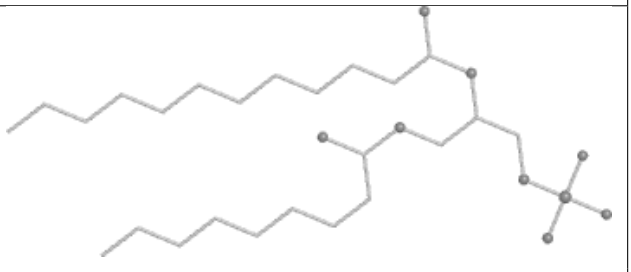


Bond angles

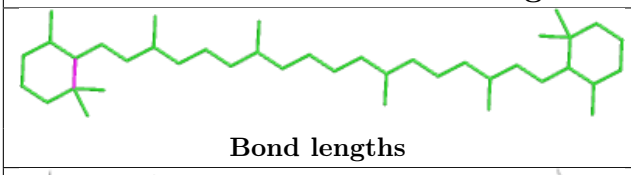


Torsions

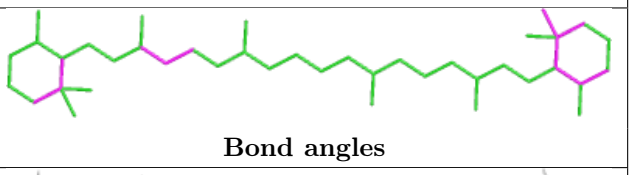


Rings

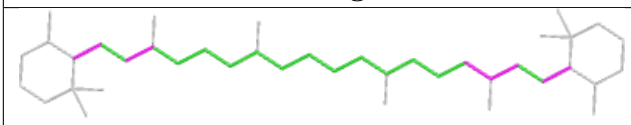
Ligand BCR L 301



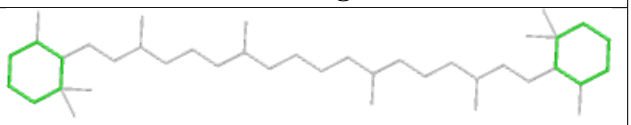
Bond lengths



Bond angles

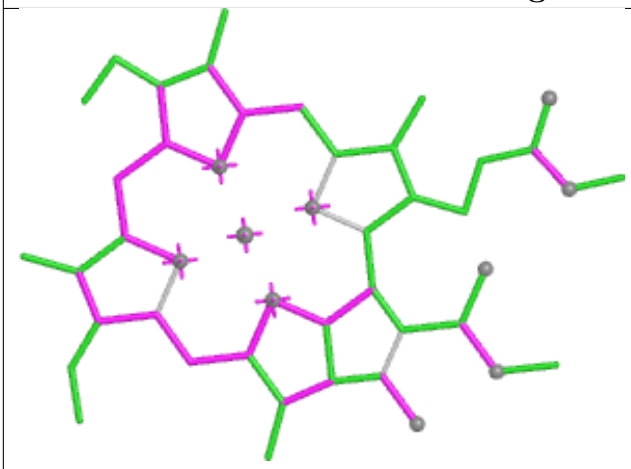


Torsions



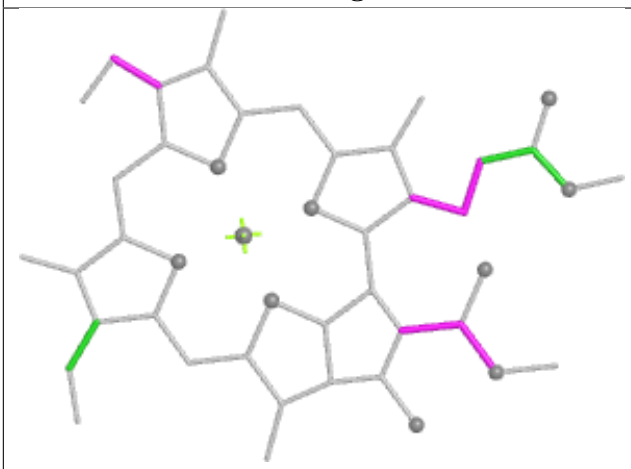
Rings

Ligand CLA 2 315



Bond lengths

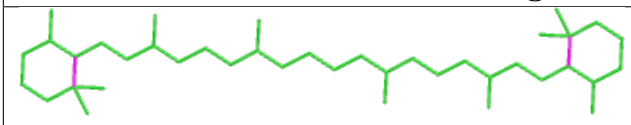
Bond angles



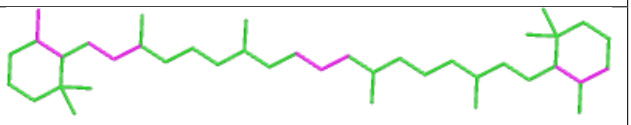
Torsions

Rings

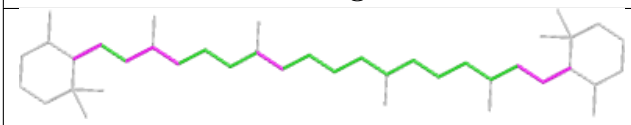
Ligand BCR 3 302



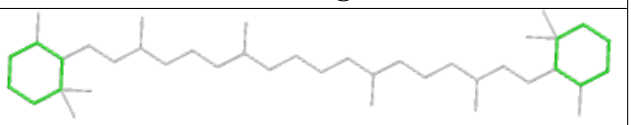
Bond lengths



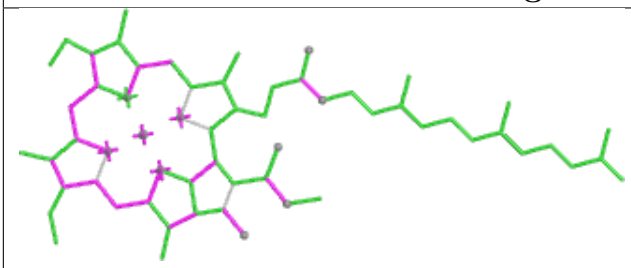
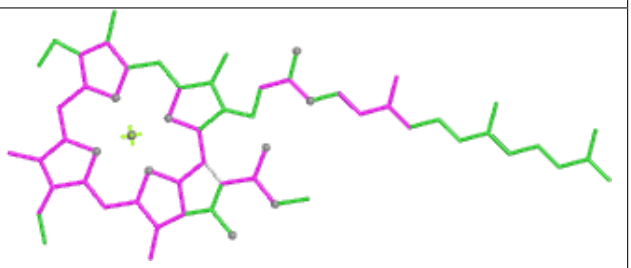
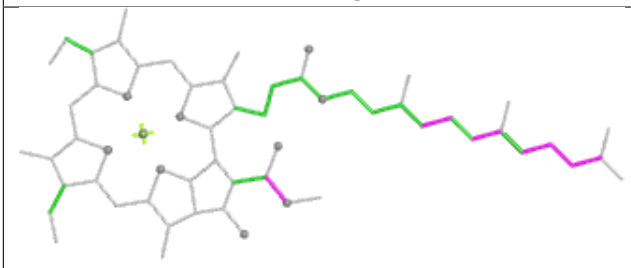
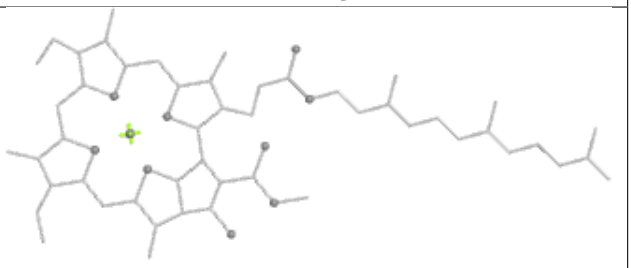
Bond angles

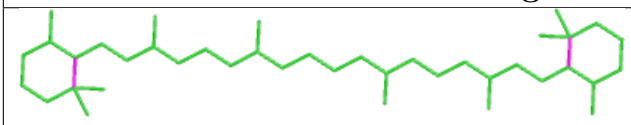
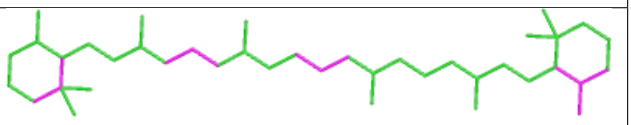
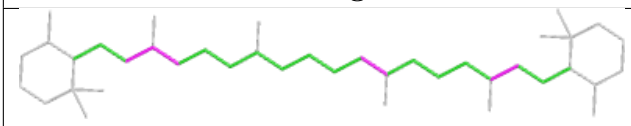
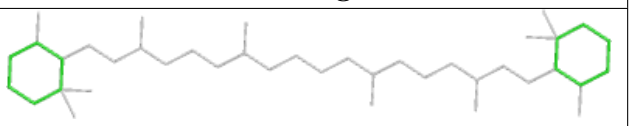


Torsions

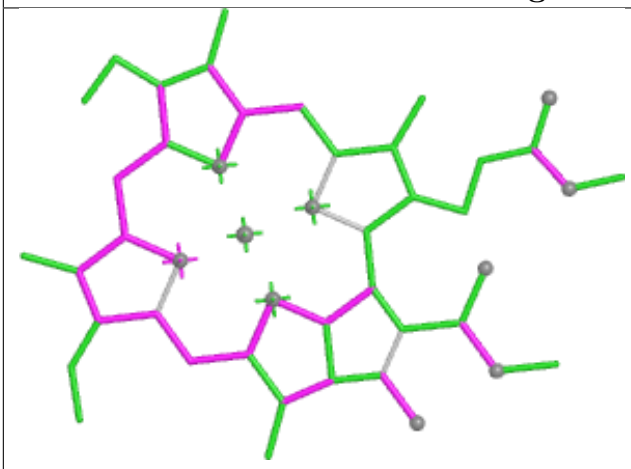


Rings

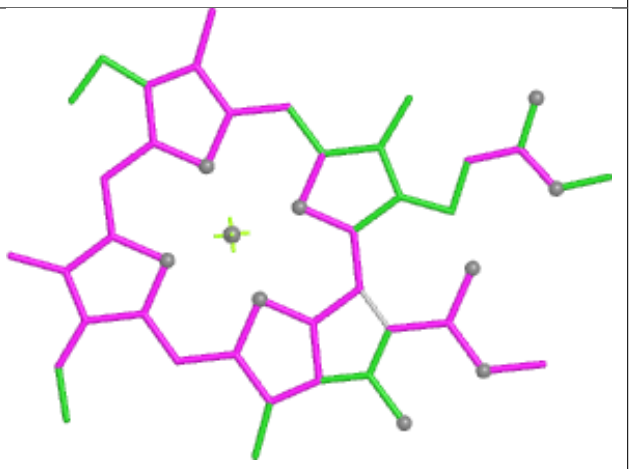
Ligand CLA B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

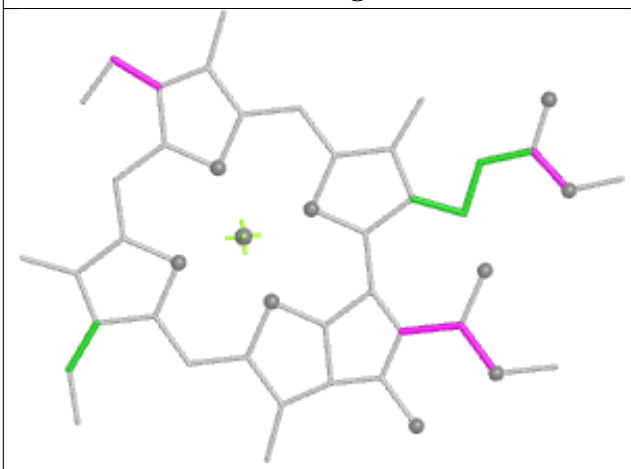
Ligand CLA 5 321



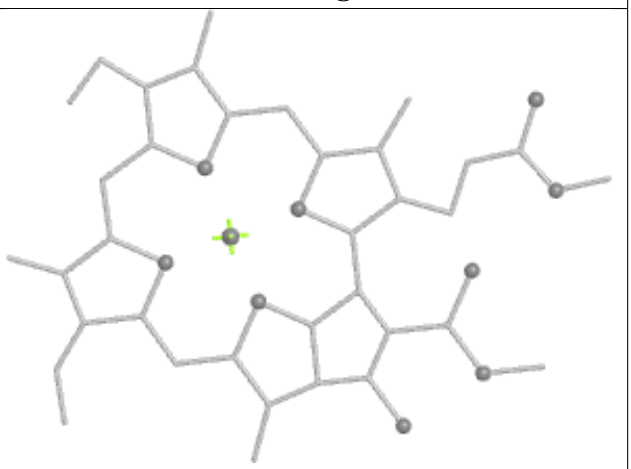
Bond lengths



Bond angles

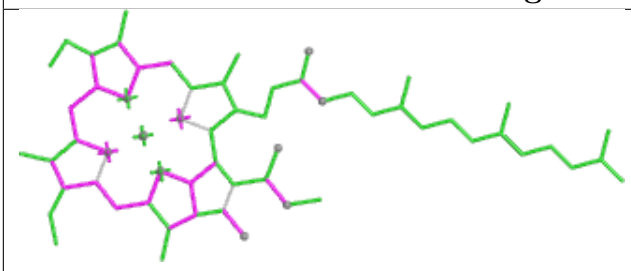


Torsions

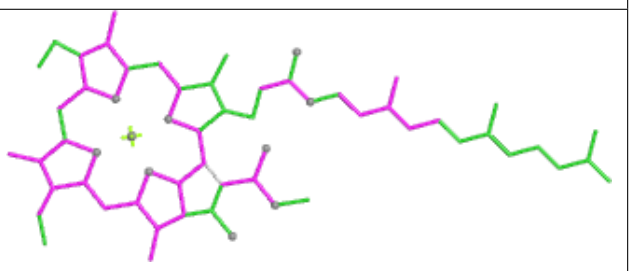


Rings

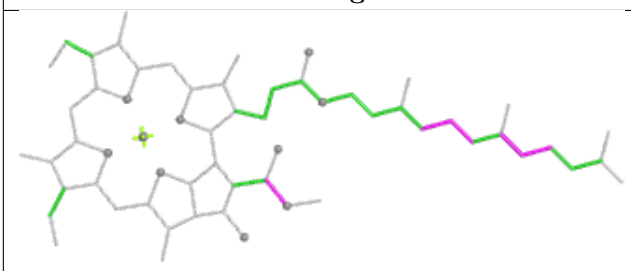
Ligand CLA B 830



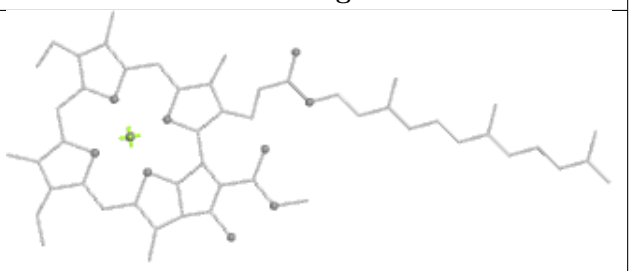
Bond lengths



Bond angles

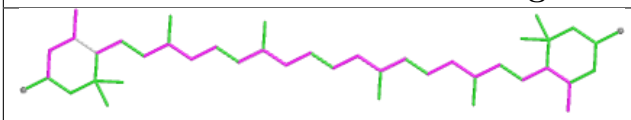


Torsions



Rings

Ligand LUT 5 303



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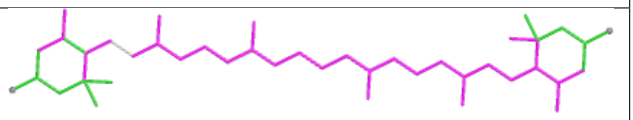
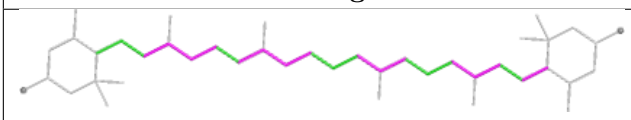


Bond angles



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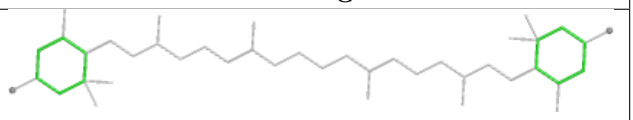
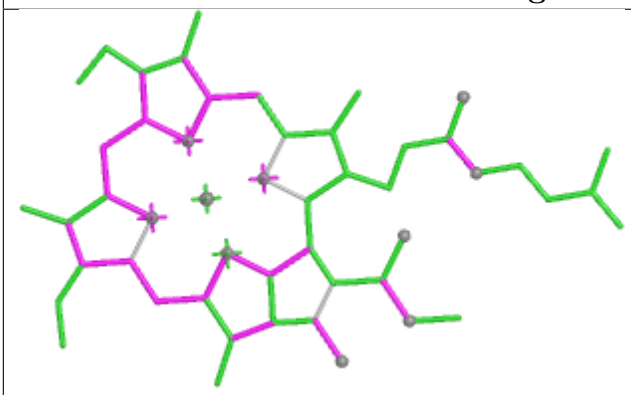
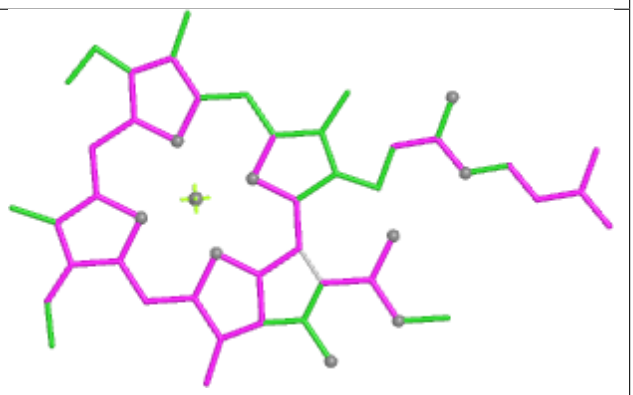


Rings

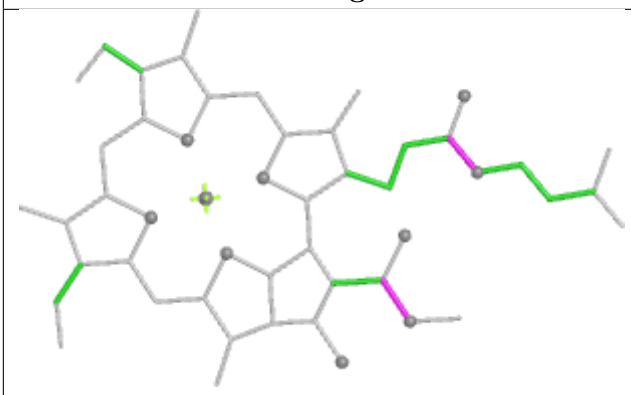
Ligand CLA 3 316



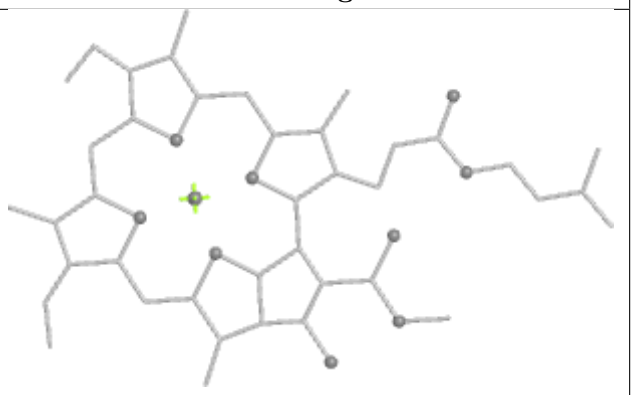
Bond lengths



Bond angles

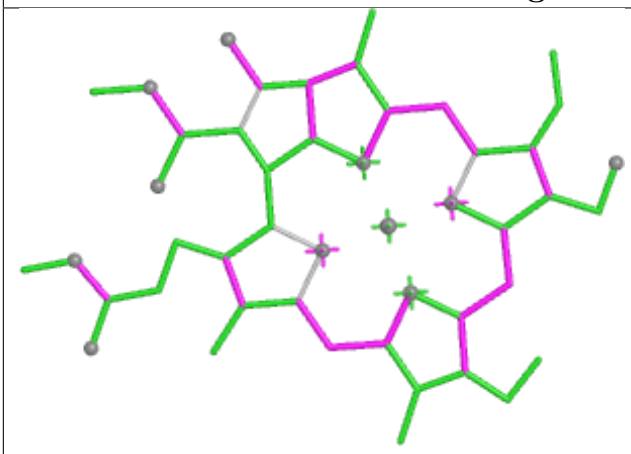


Torsions



Rings

Ligand CHL 5 317



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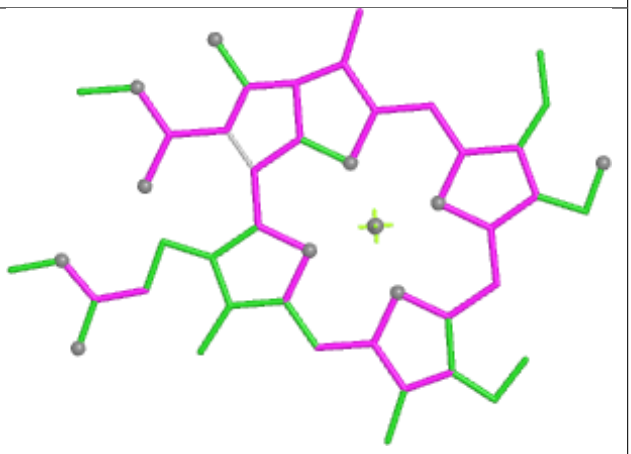
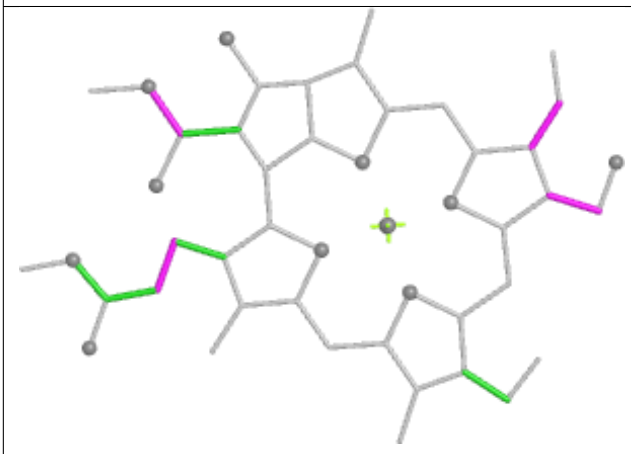


Bond angles



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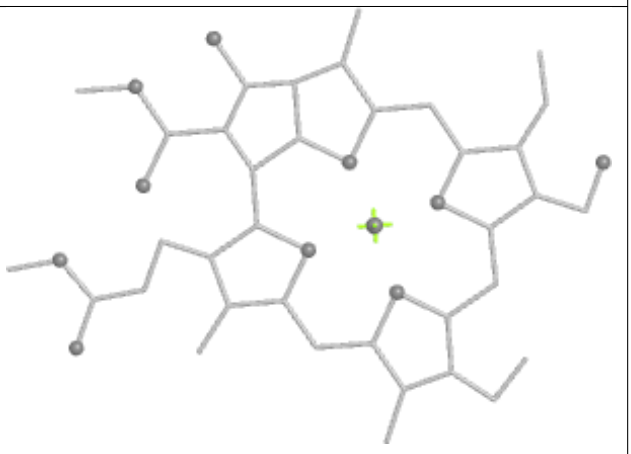
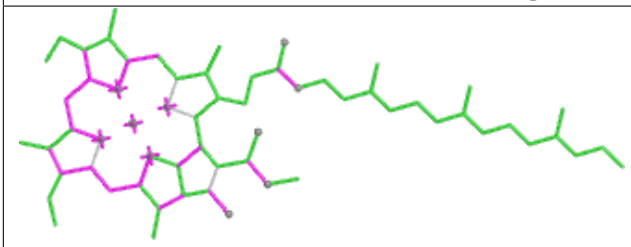
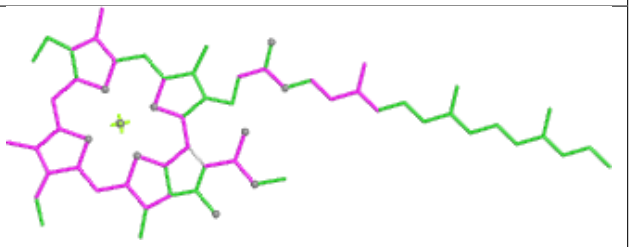


Rings

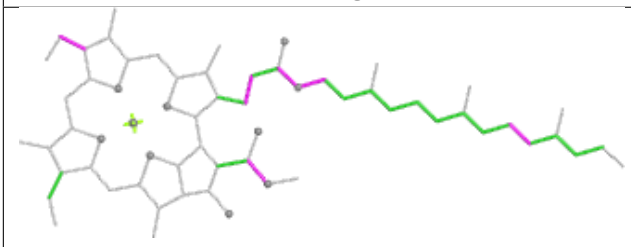
Ligand CLA B 850



Bond lengths



Bond angles



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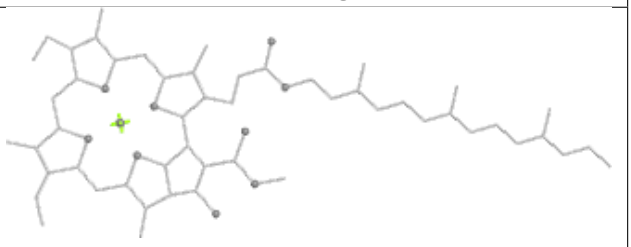
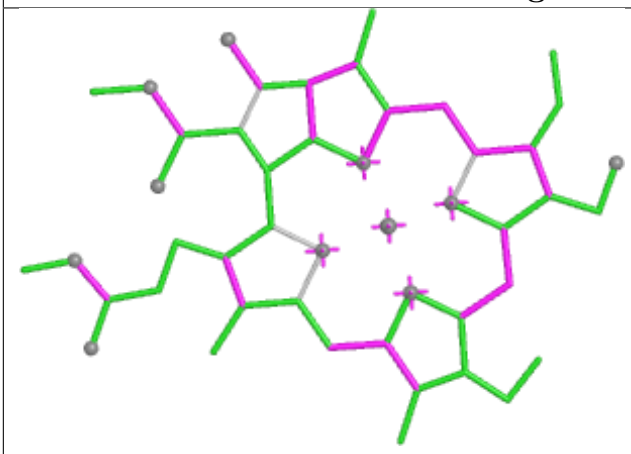
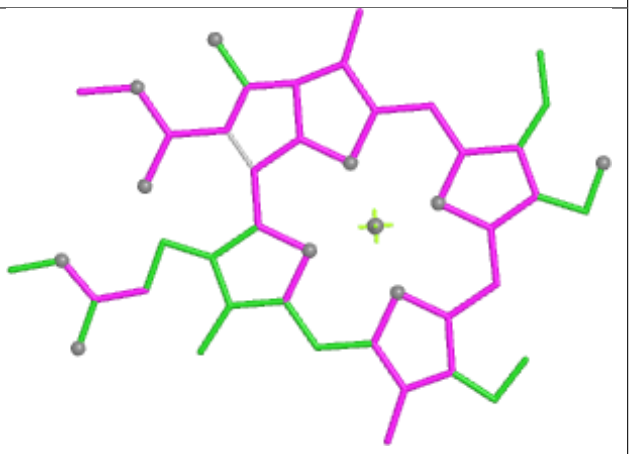


Rings

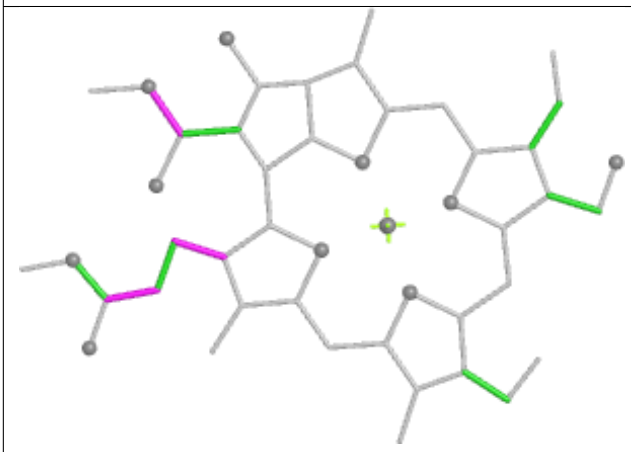
Ligand CHL 5 322



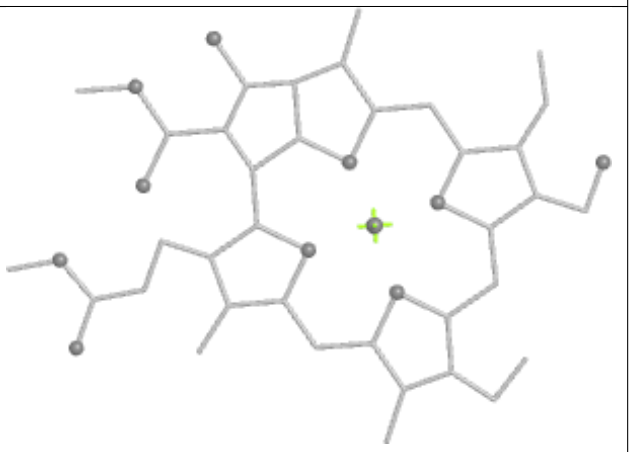
Bond lengths



Bond angles

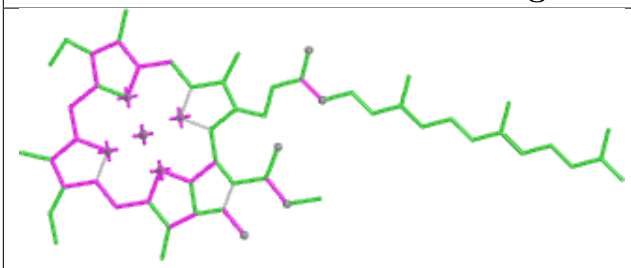


Torsions

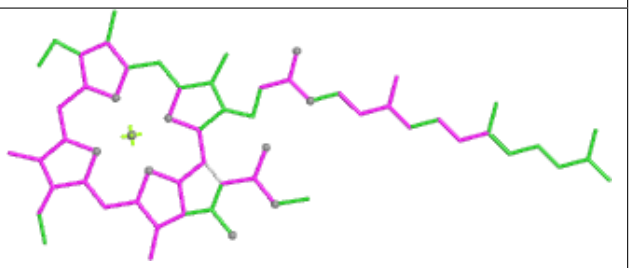


Rings

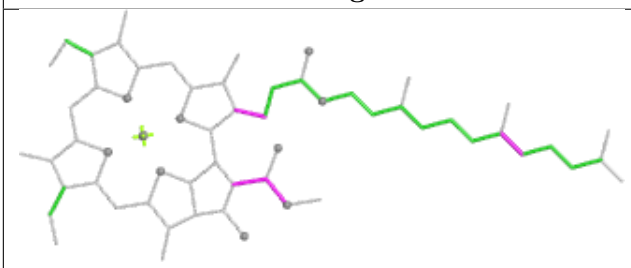
Ligand CLA a 309



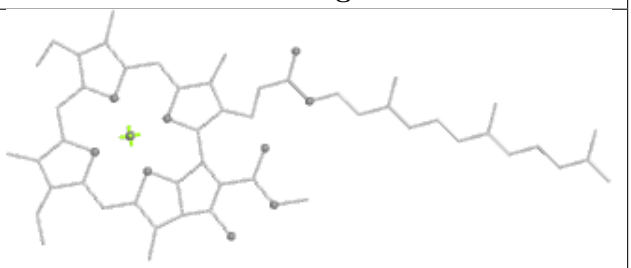
Bond lengths



Bond angles

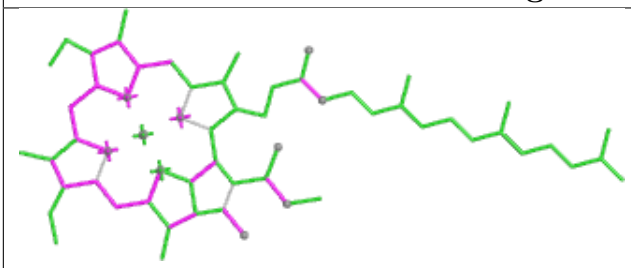


Torsions

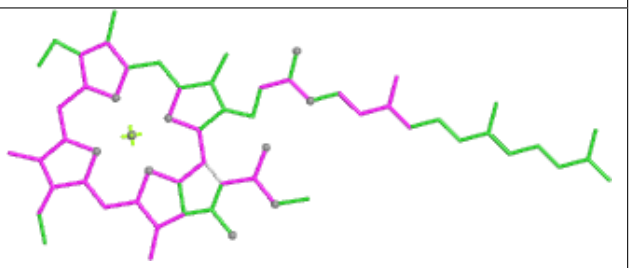


Rings

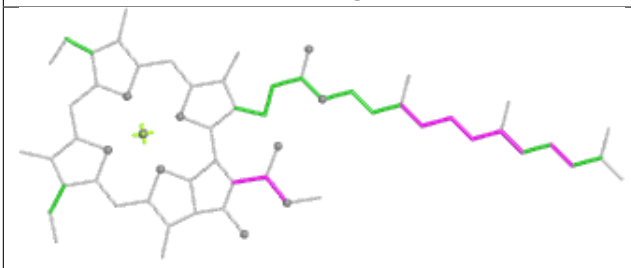
Ligand CLA L 305



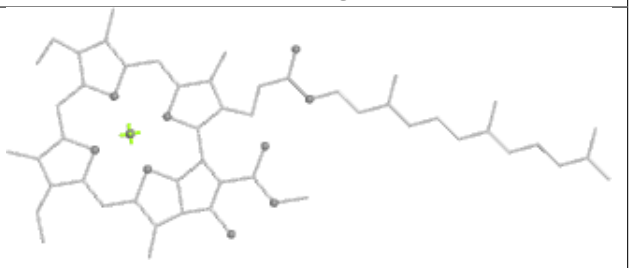
Bond lengths



Bond angles

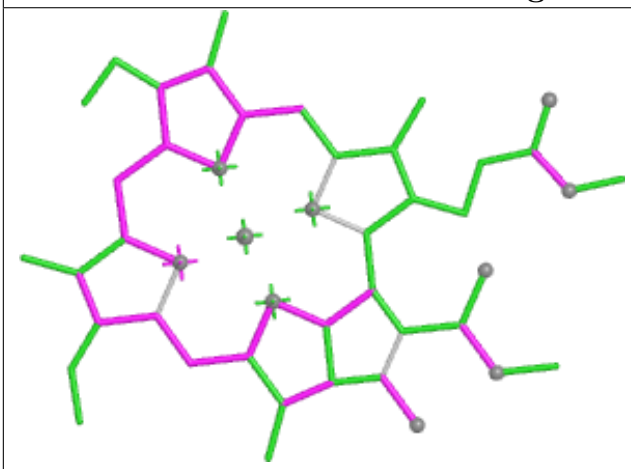


Torsions

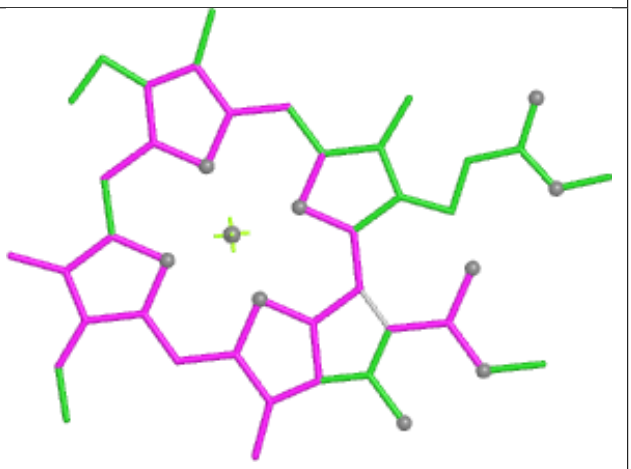


Rings

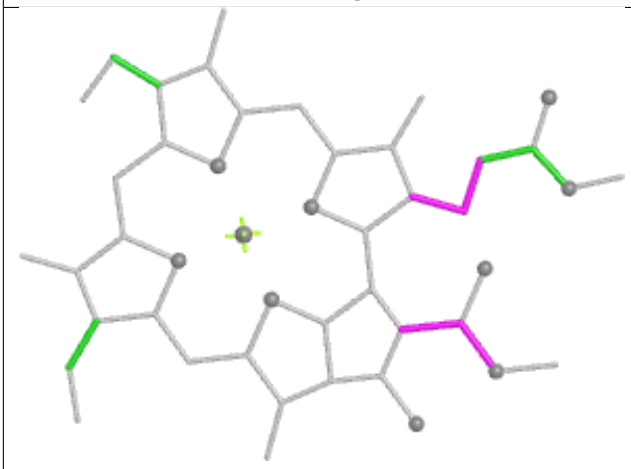
Ligand CLA b 310



Bond lengths



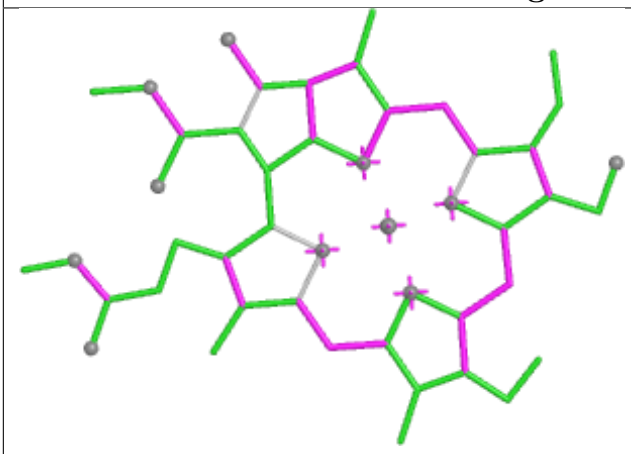
Bond angles



Torsions

Rings

Ligand CHL 6 320



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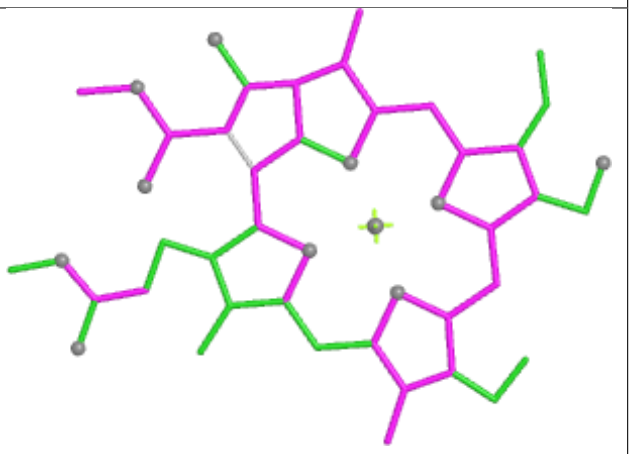
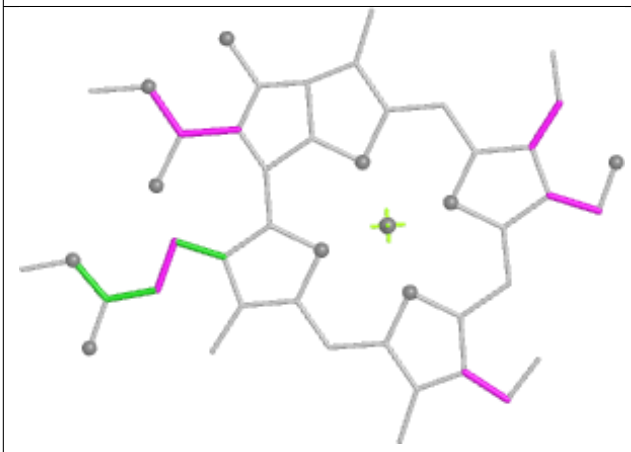
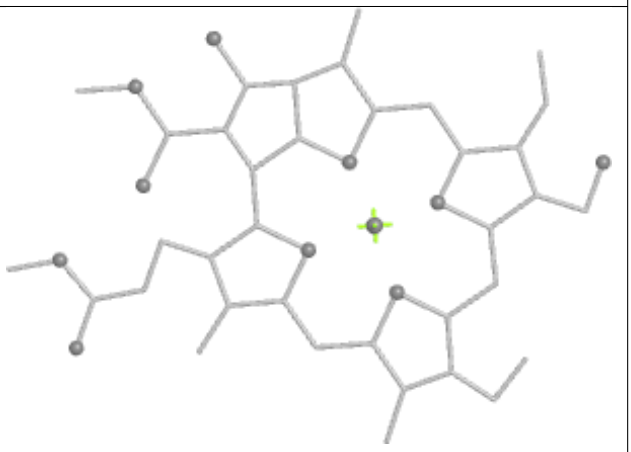


Bond angles

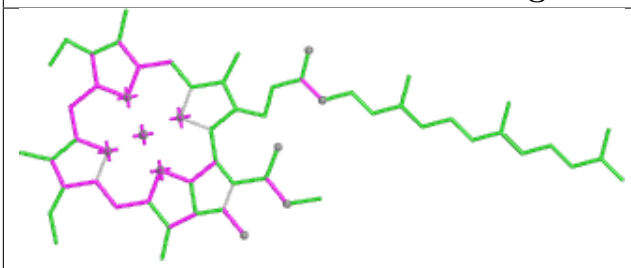


Torsions



Rings

Ligand CLA 4 309



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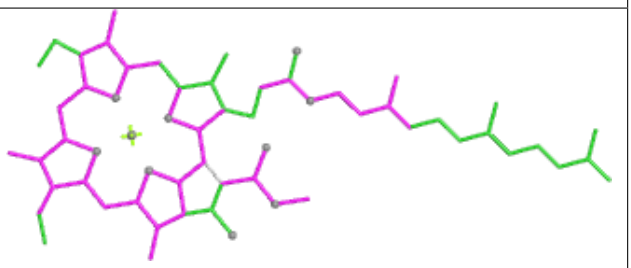
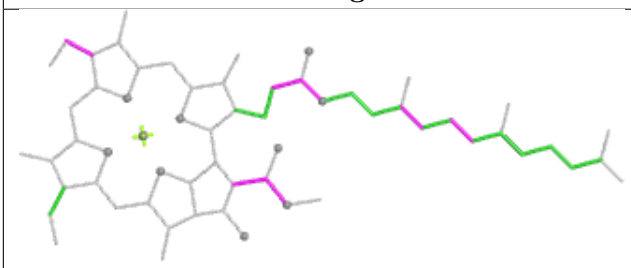
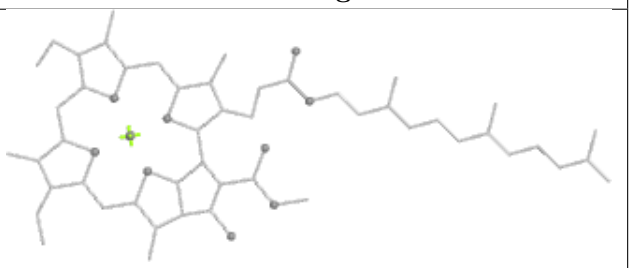


Bond angles

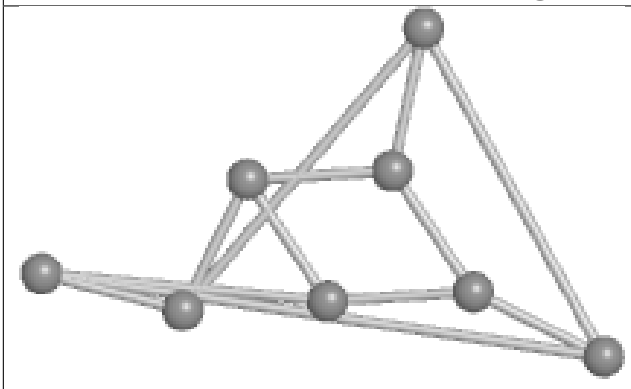


Torsions

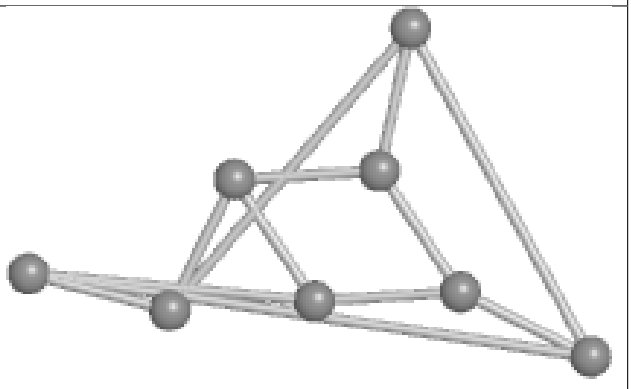


Rings

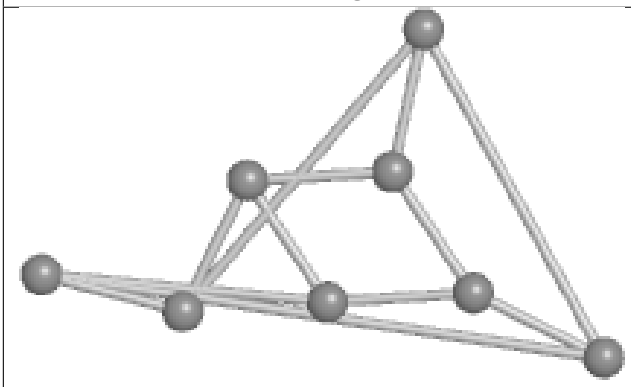
Ligand SF4 C 101



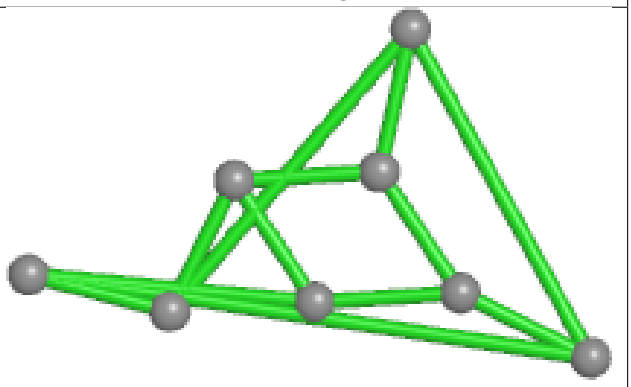
Bond lengths



Bond angles

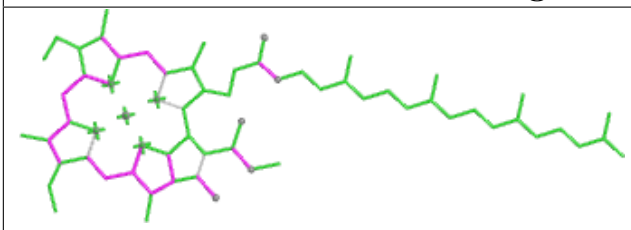


Torsions

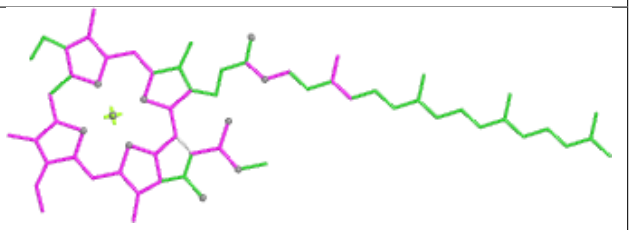


Rings

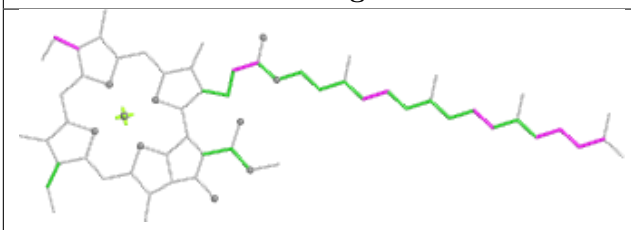
Ligand CL0 A 813



Bond lengths



Bond angles



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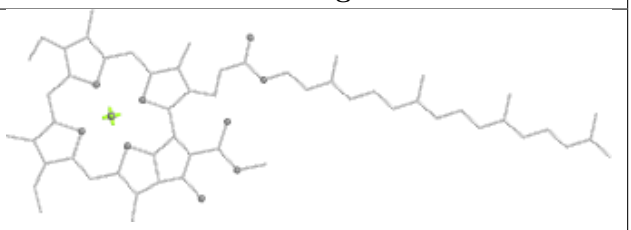
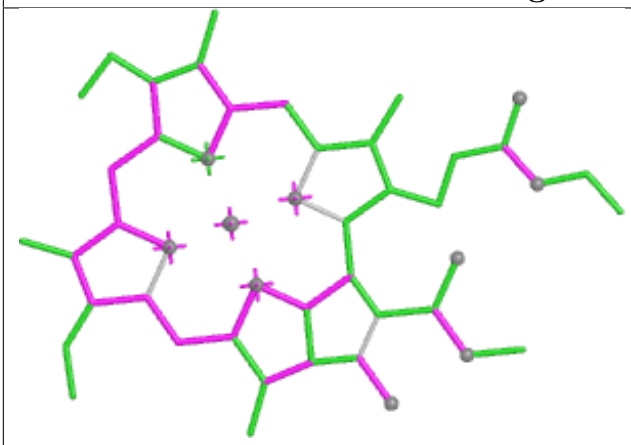


Rings

Ligand CLA 4 312



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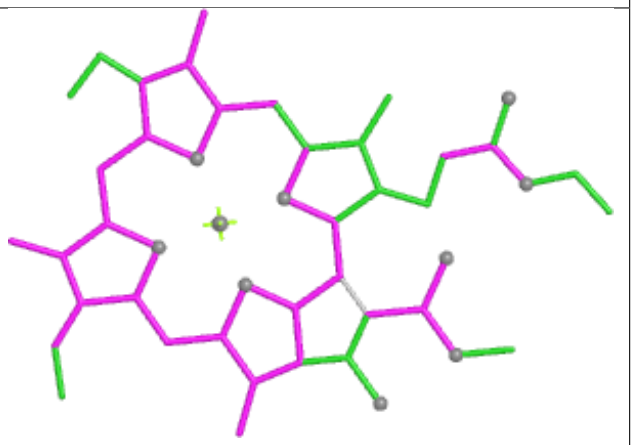
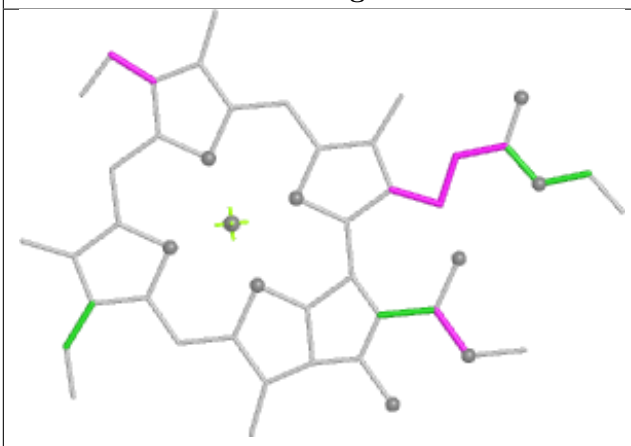


Bond angles



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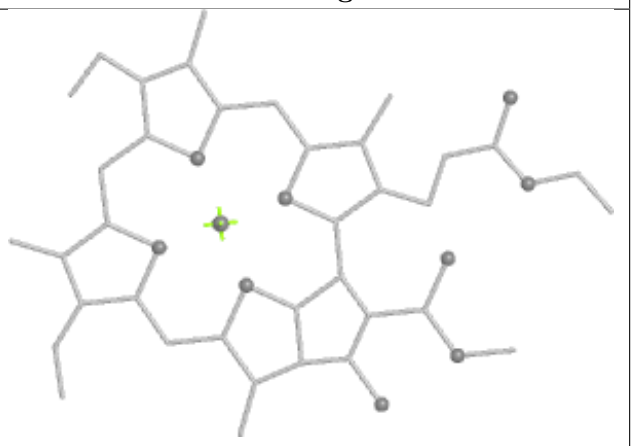
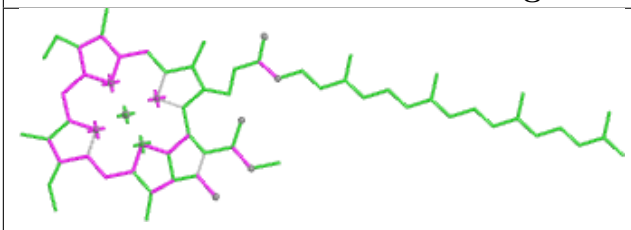


Rings

Ligand CLA A 828



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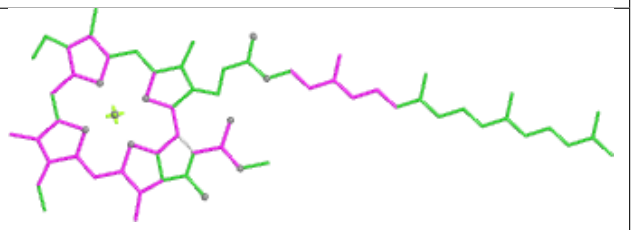
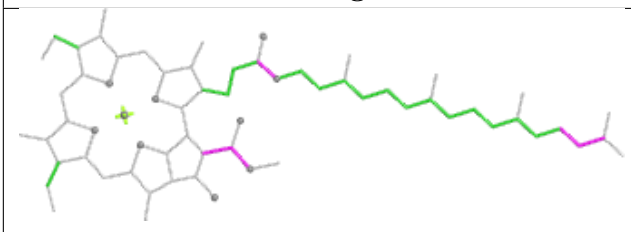


Bond angles



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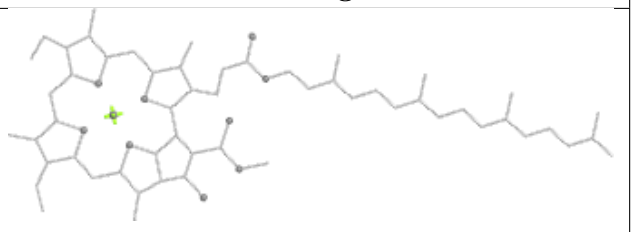
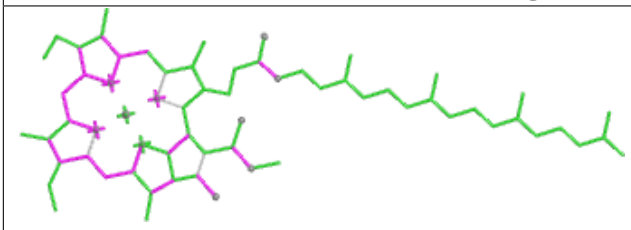


Rings

Ligand CLA B 817



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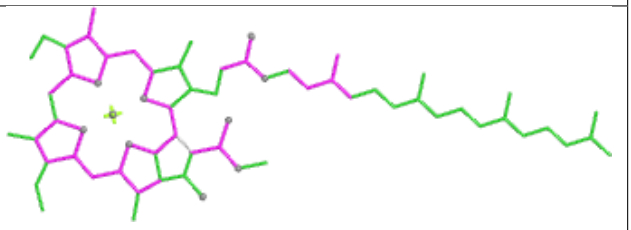
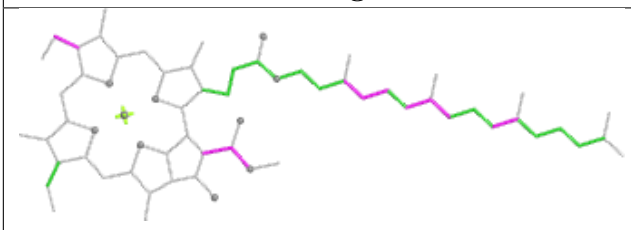
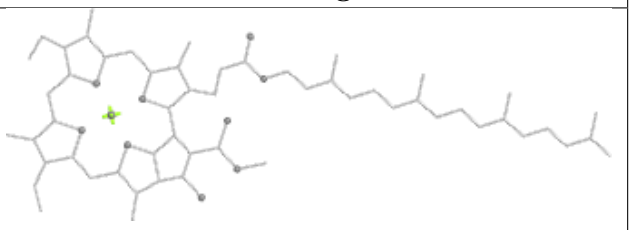


Bond angles

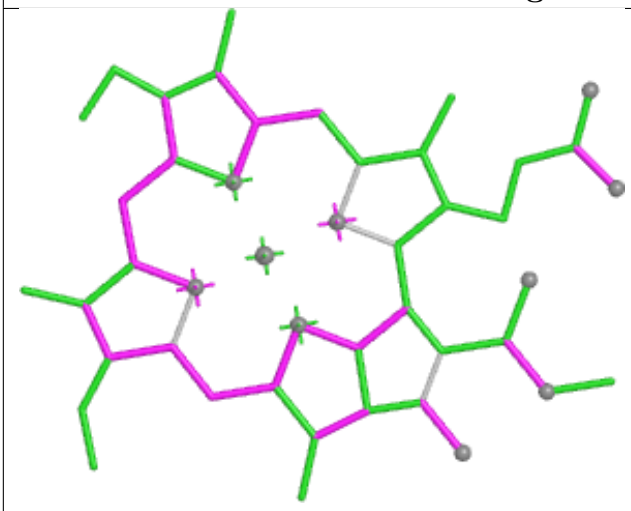


Torsions



Rings

Ligand CLA L 307



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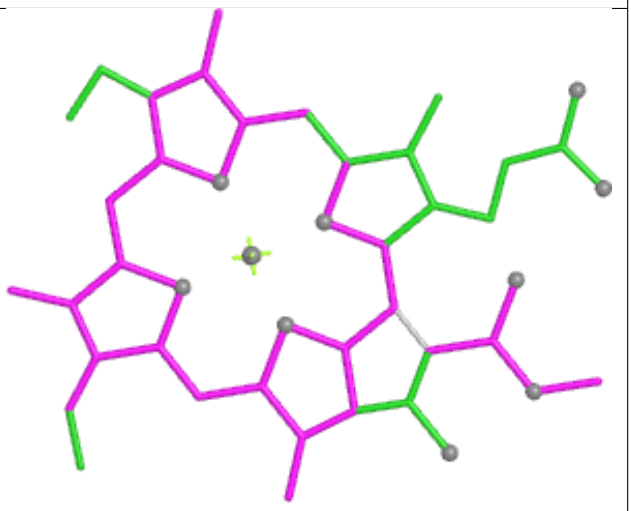
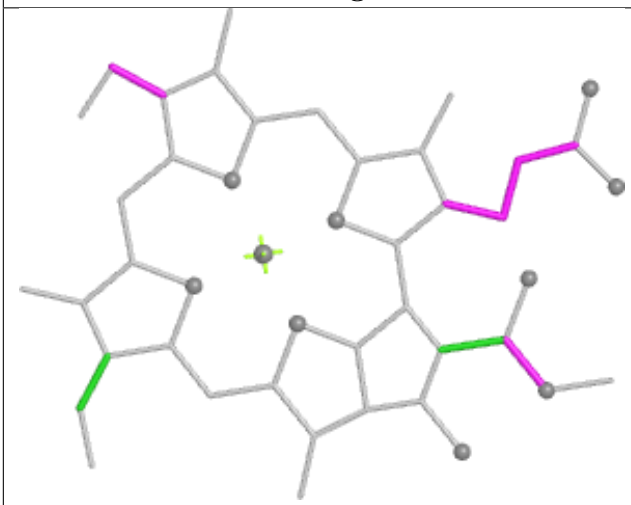


Bond angles



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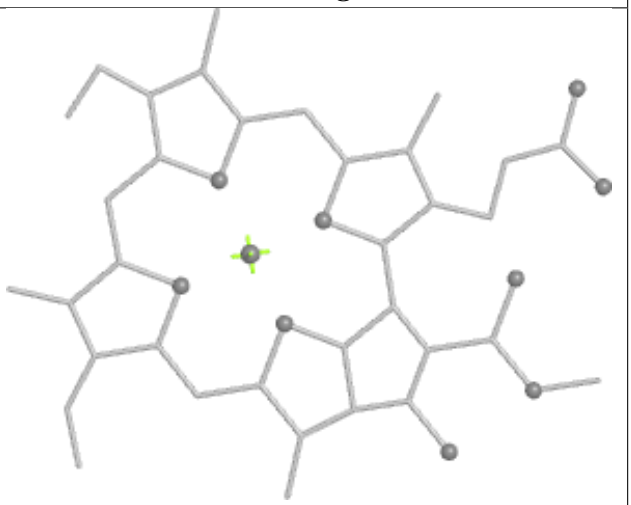
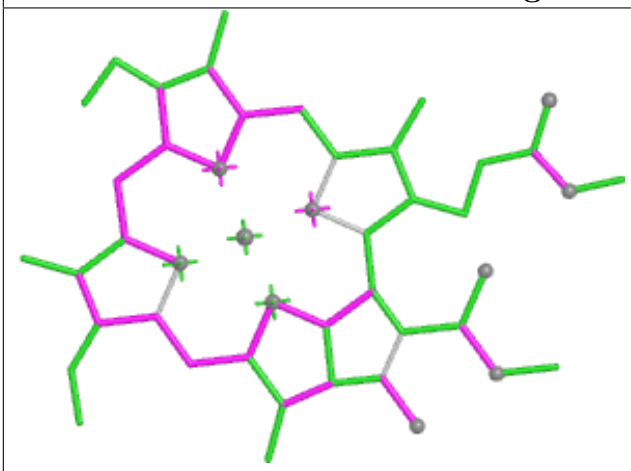


Rings

Ligand CLA A 854



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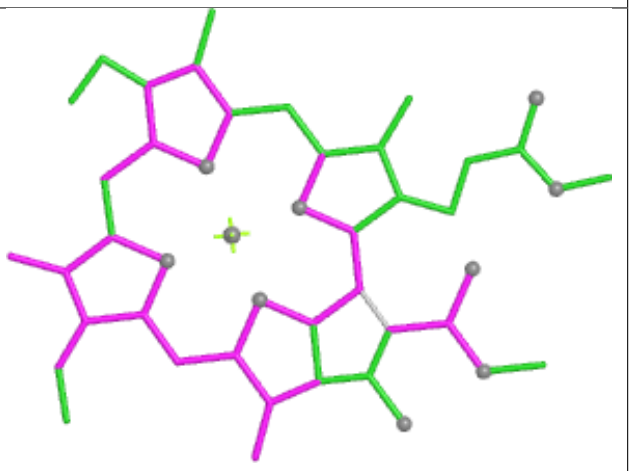
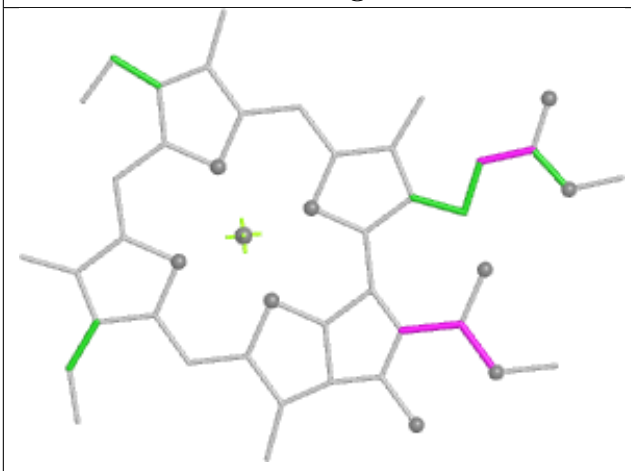


Bond angles



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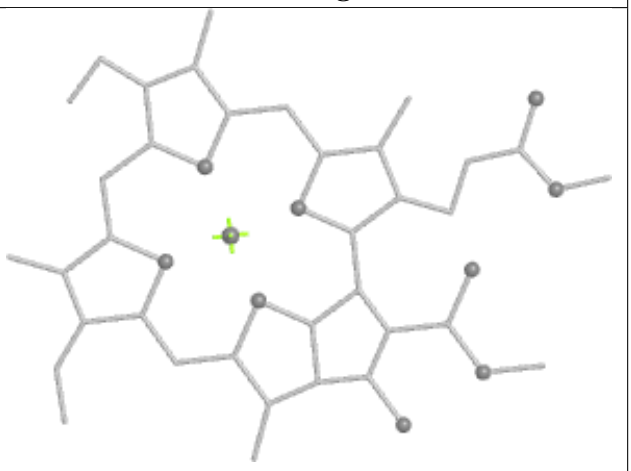
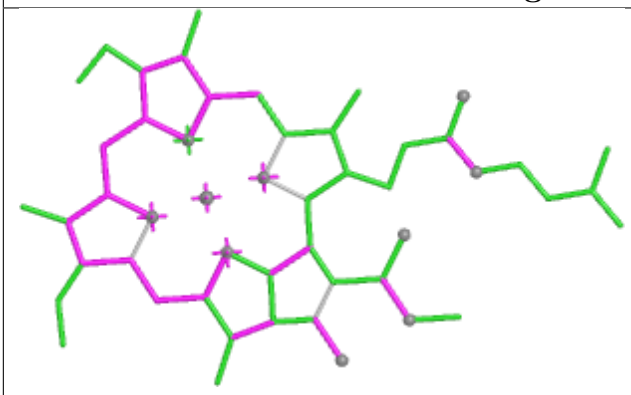


Rings

Ligand CLA B 831



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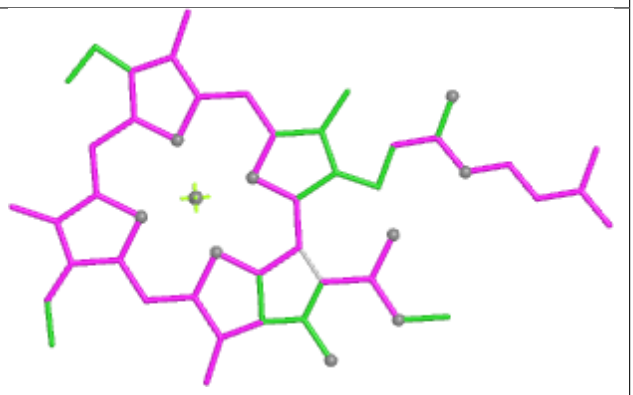
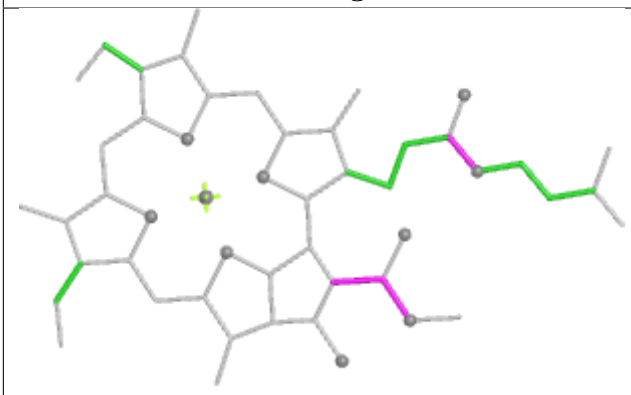


Bond angles



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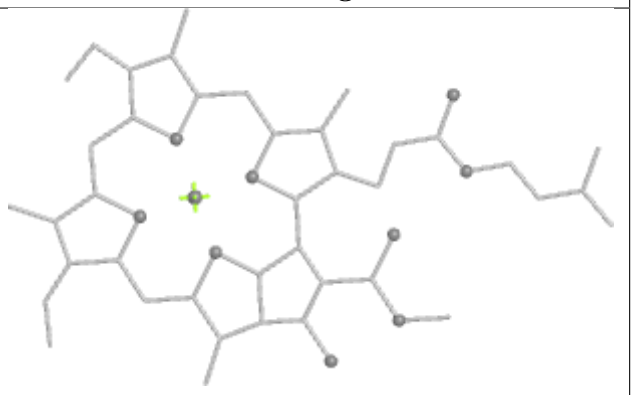
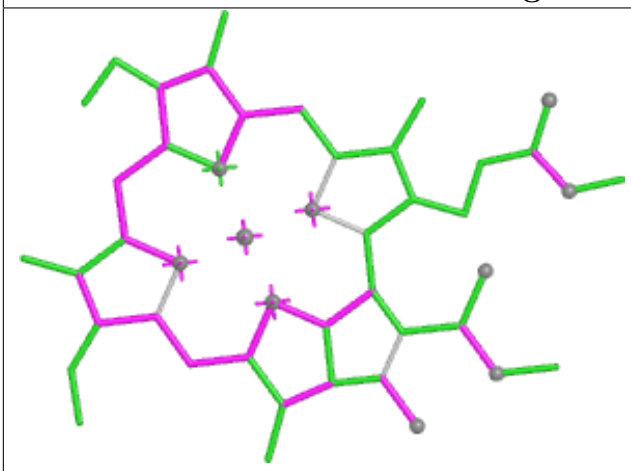
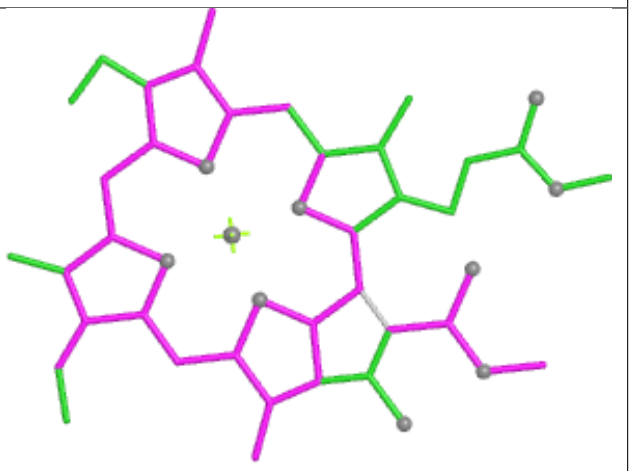


Rings

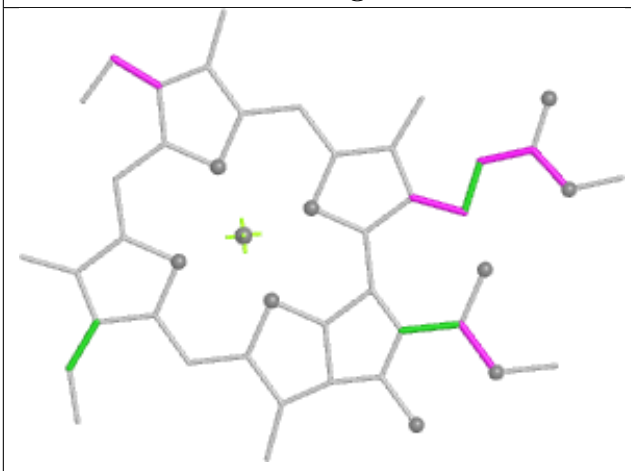
Ligand CLA H 901



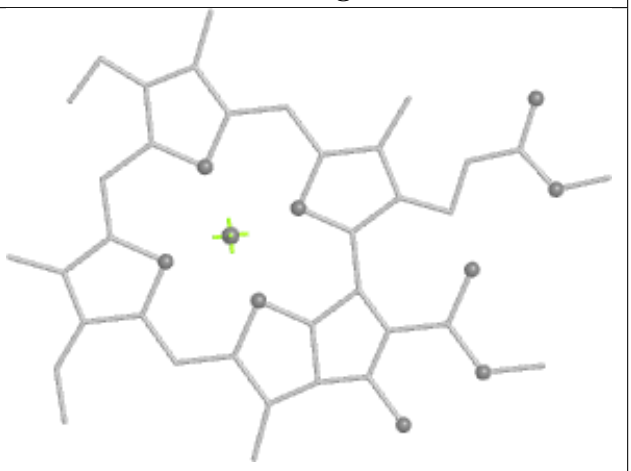
Bond lengths



Bond angles

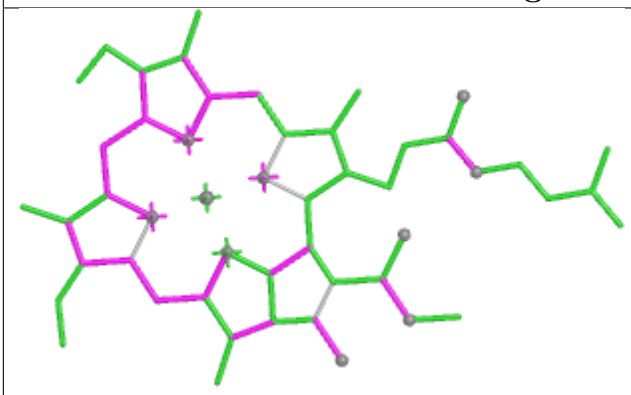


Torsions

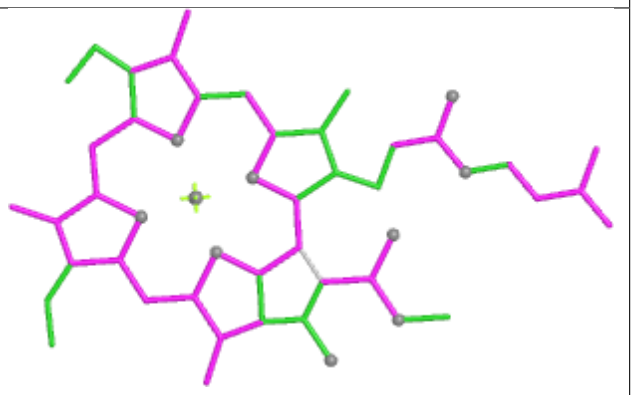


Rings

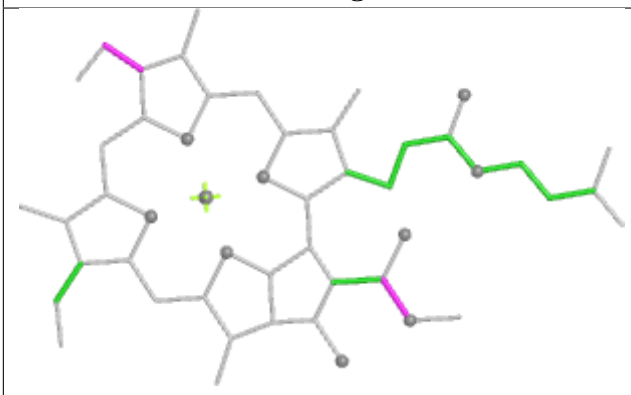
Ligand CLA B 845



Bond lengths



Bond angles



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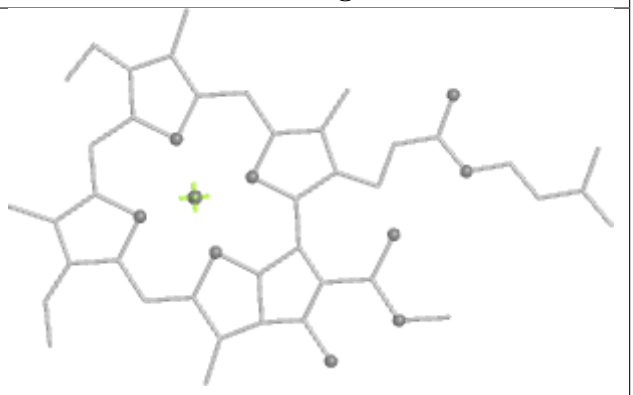
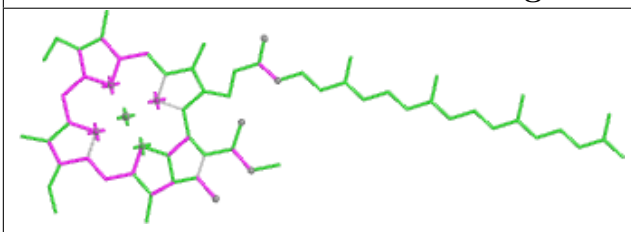
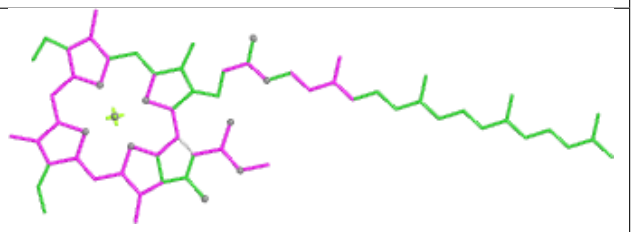


Rings

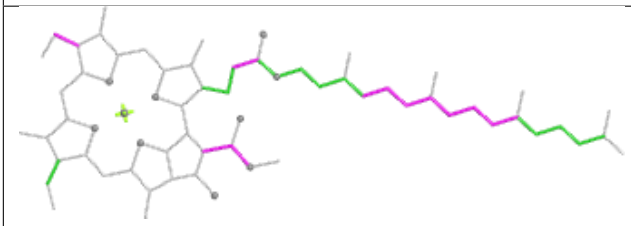
Ligand CLA B 815



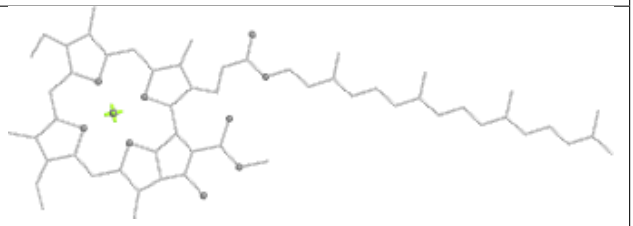
Bond lengths



Bond angles

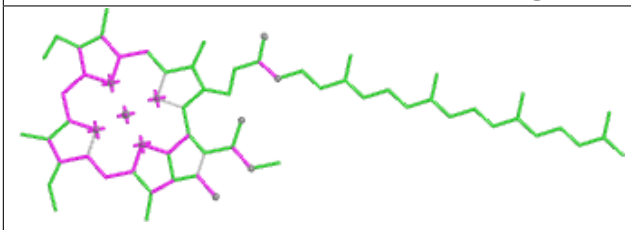


Torsions



Rings

Ligand CLA 8 320



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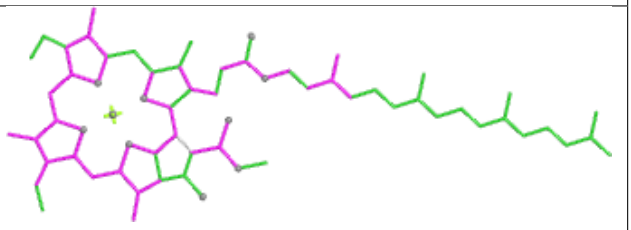

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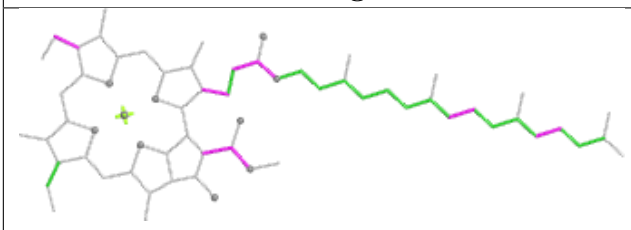

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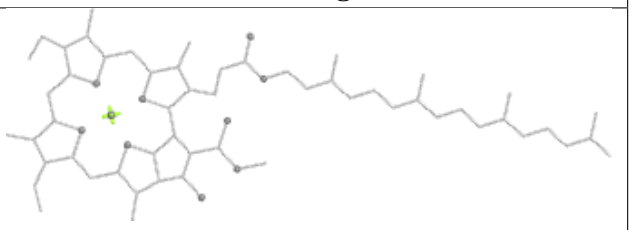
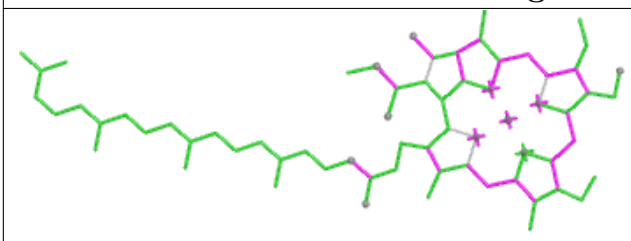


Rings

Ligand CHL 6 309



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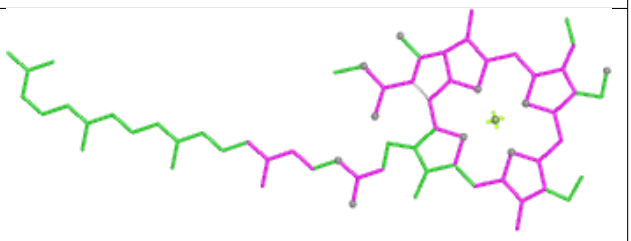

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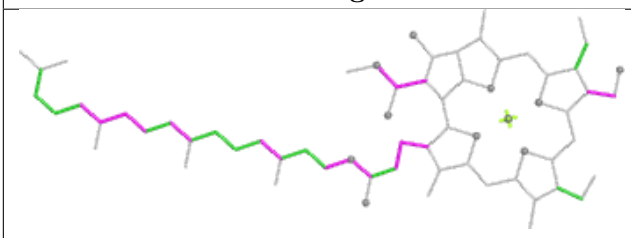

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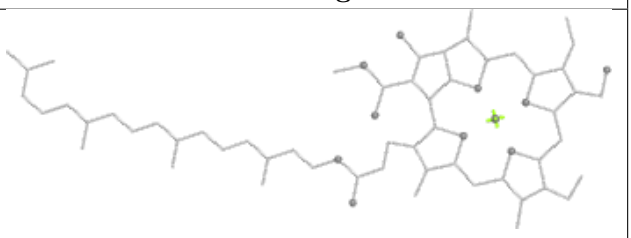
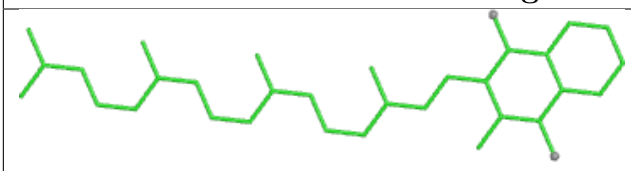


Rings

Ligand PQN A 801



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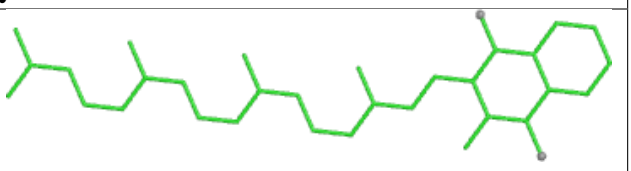

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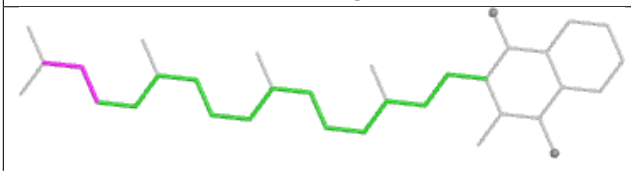

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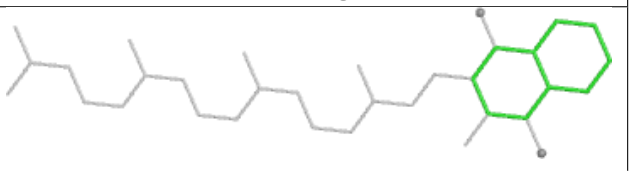
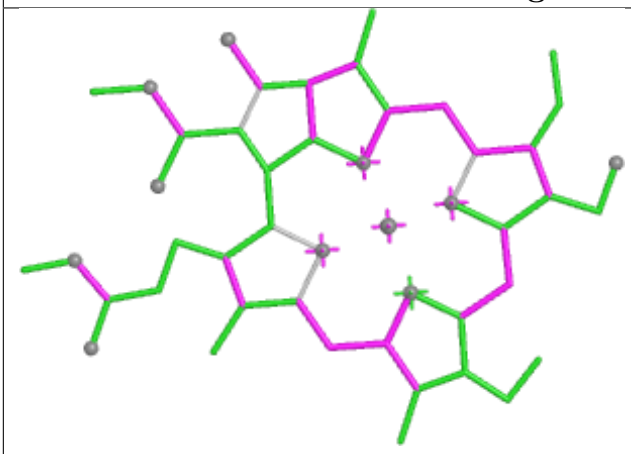


Rings

Ligand CHL 6 317



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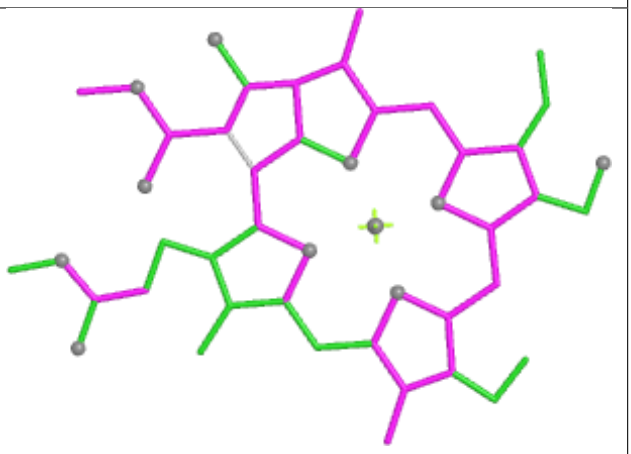
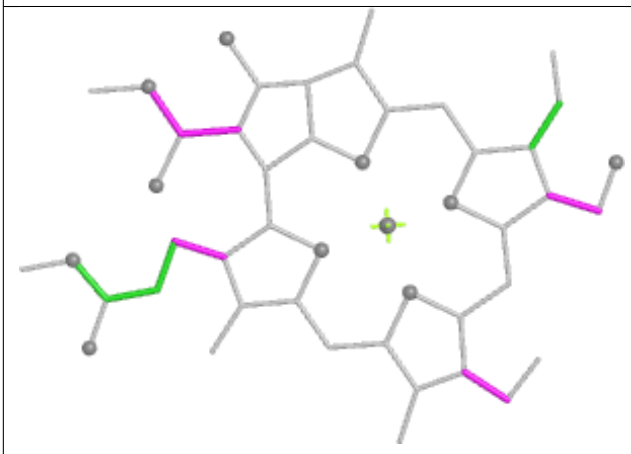


Bond angles



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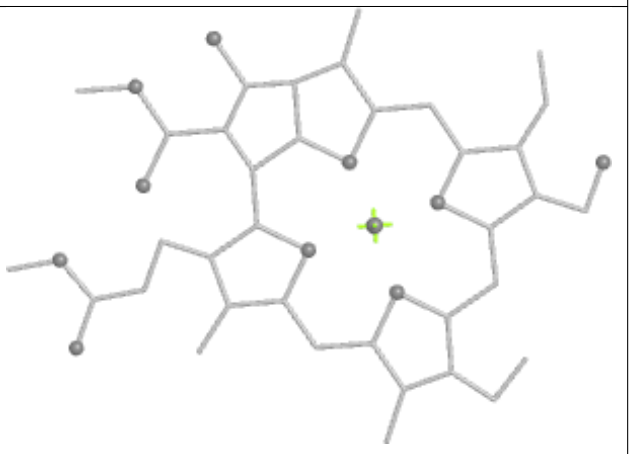
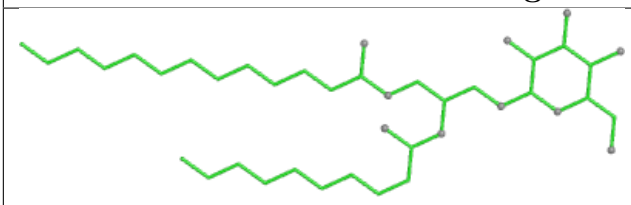


Rings

Ligand LMG a 301



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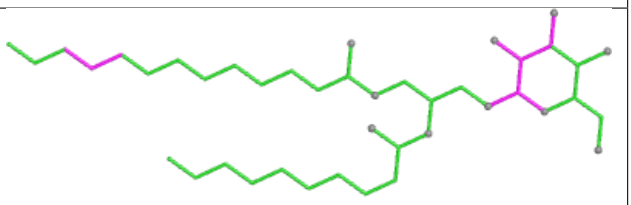
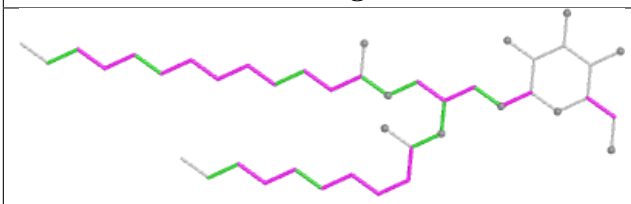


Bond angles



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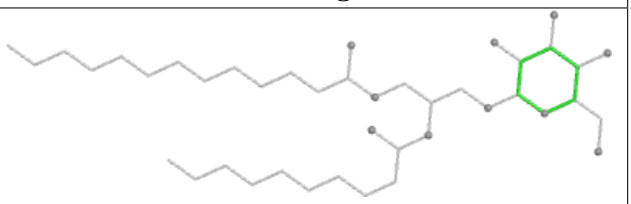
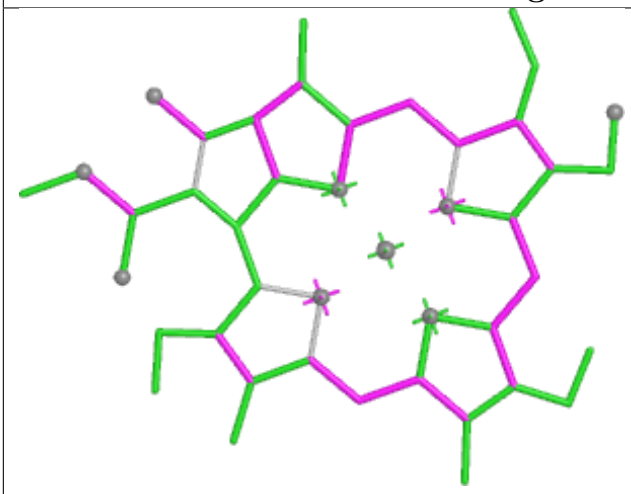


Rings

Ligand CHL 6 321



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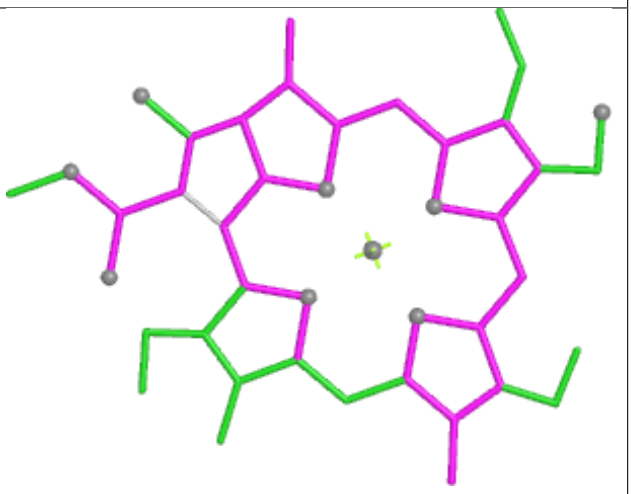
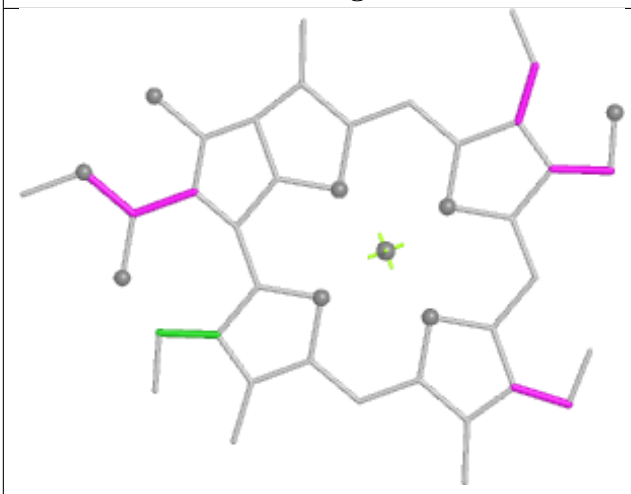


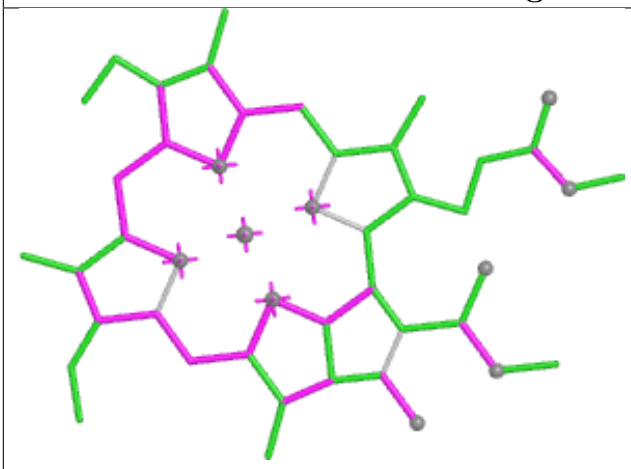
Bond angles



Torsions

Rings

Ligand CLA F 305



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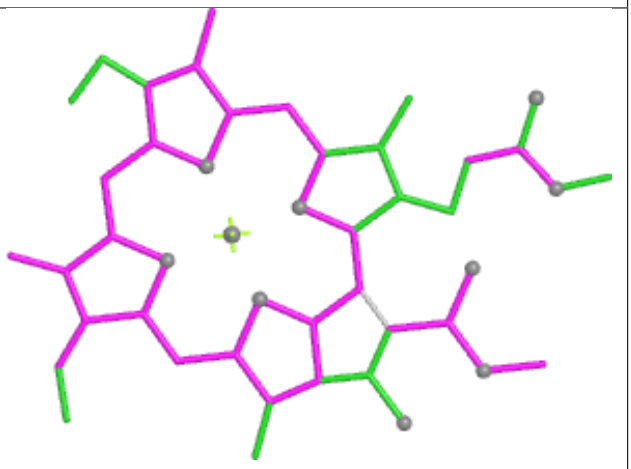

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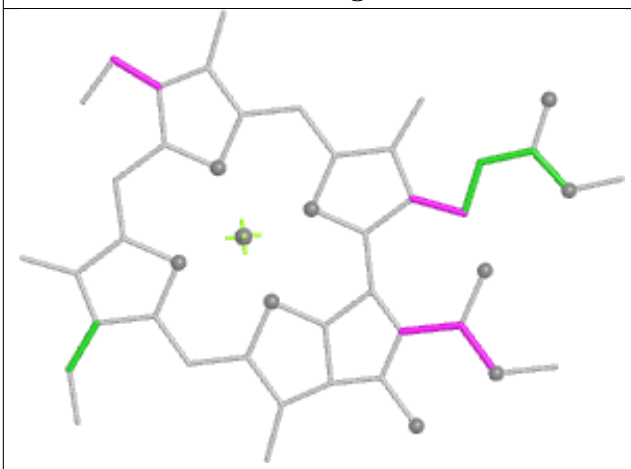

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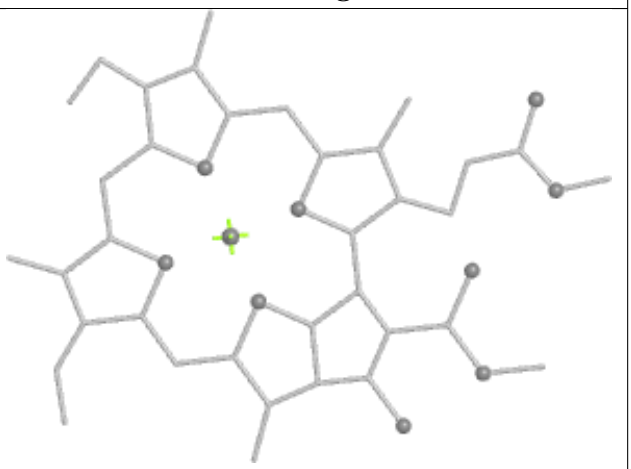
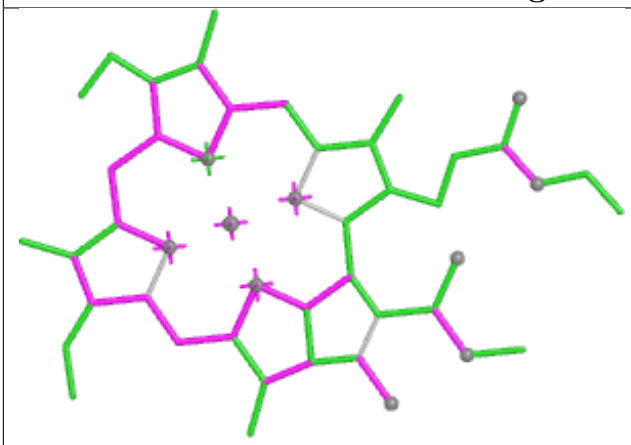


Rings

Ligand CLA 6 314



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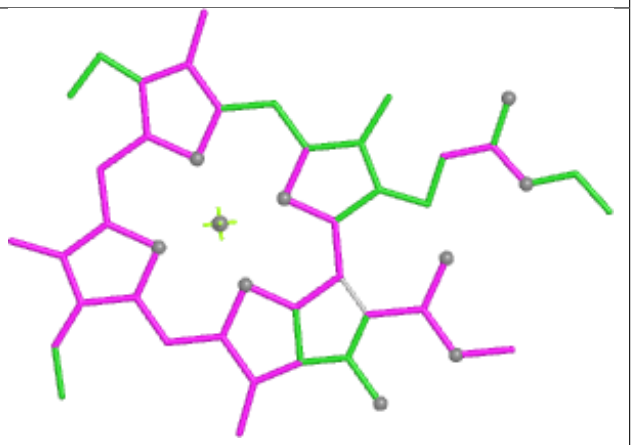
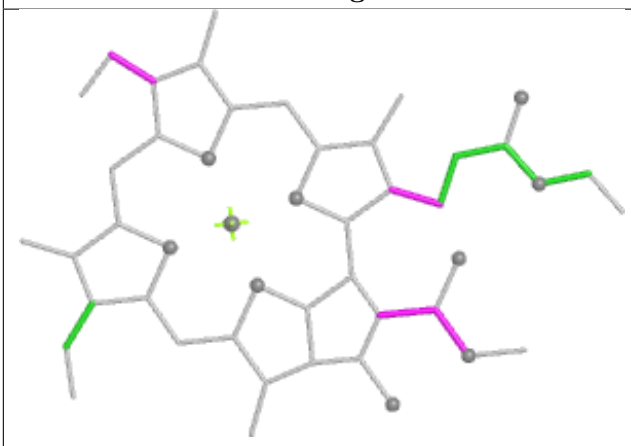


Bond angles



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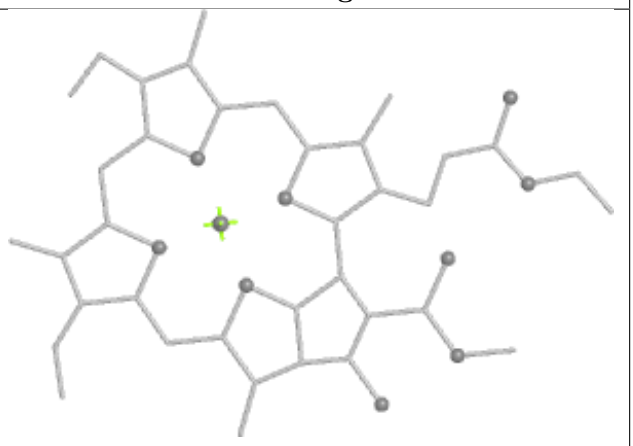
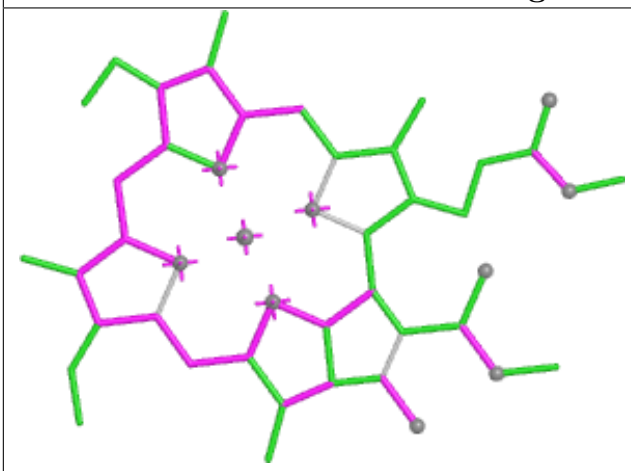


Rings

Ligand CLA 6 315



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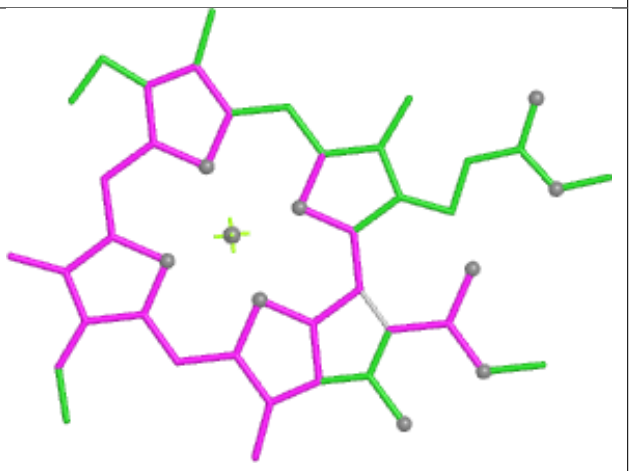

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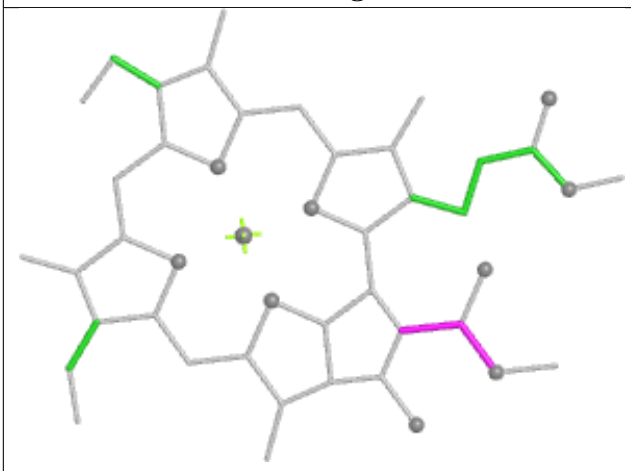

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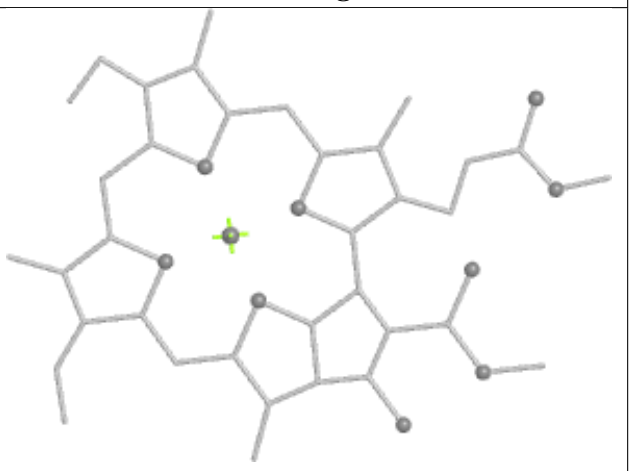
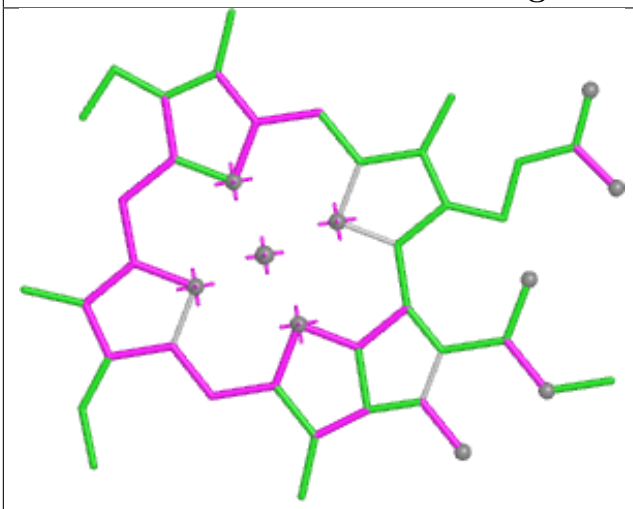


Rings

Ligand CLA 5 314



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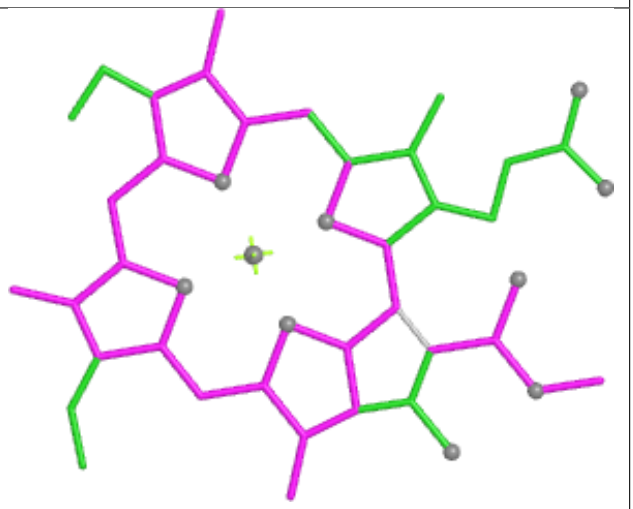

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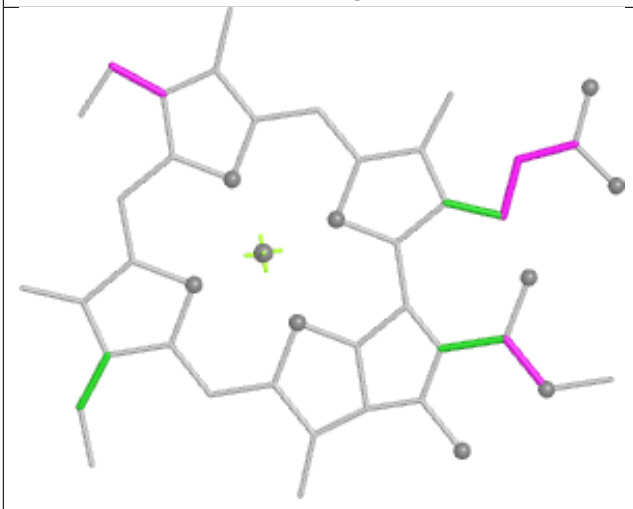
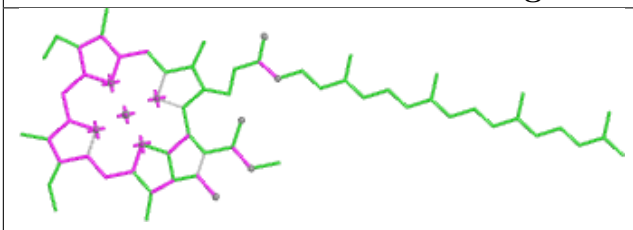


Torsions

Rings

Ligand CLA B 813



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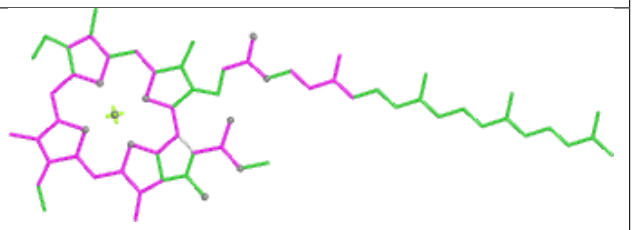
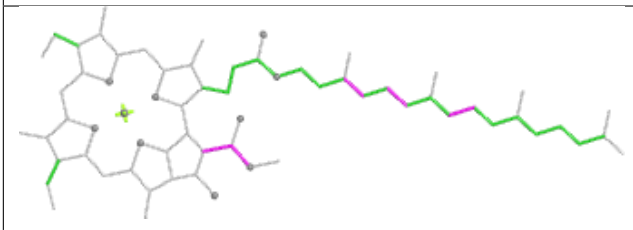


Bond angles



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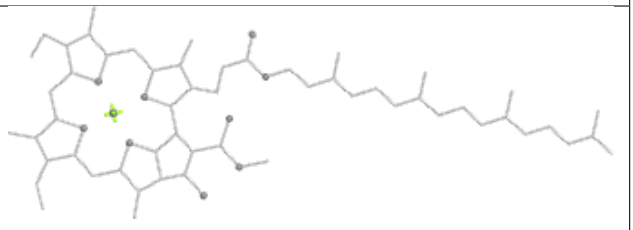
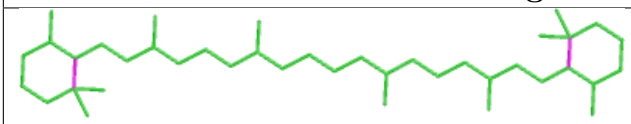


Rings

Ligand BCR J 102



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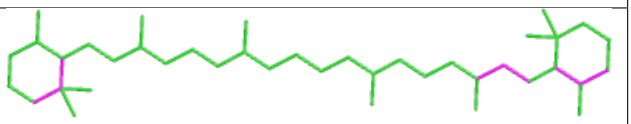
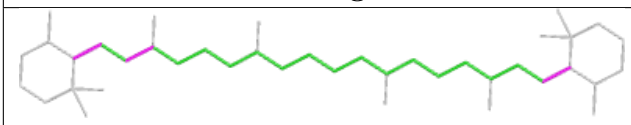


Bond angles



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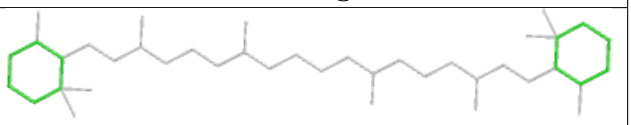
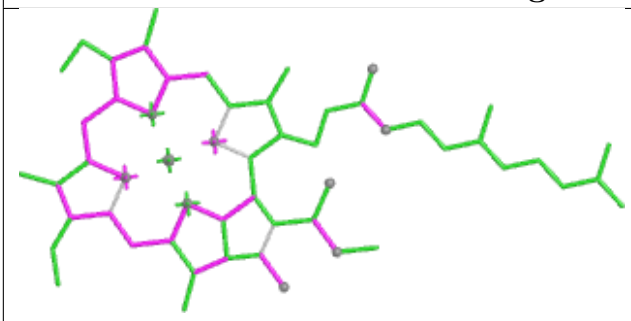


Rings

Ligand CLA a 315



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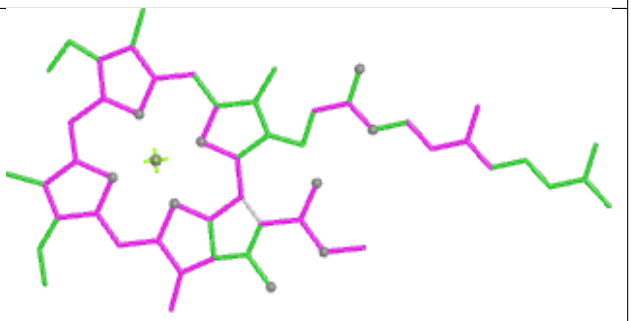
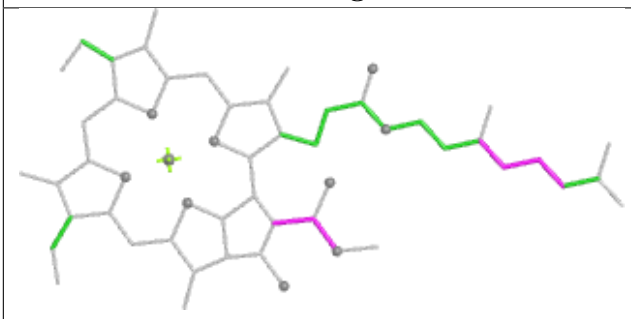


Bond angles



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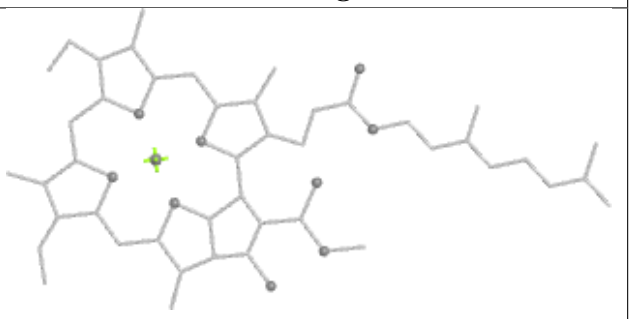
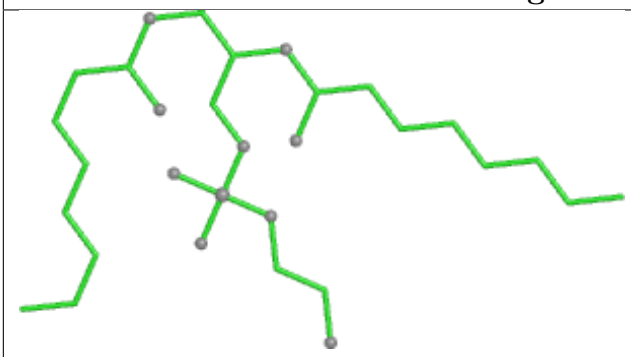
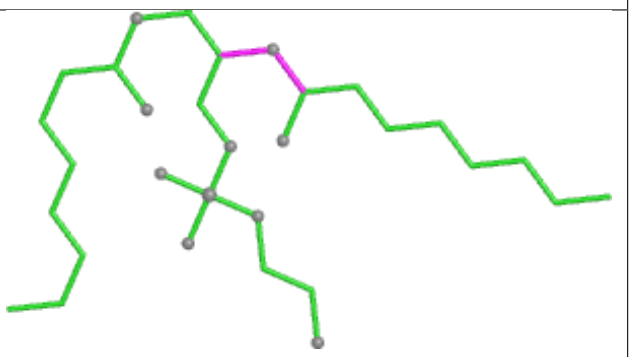


Rings

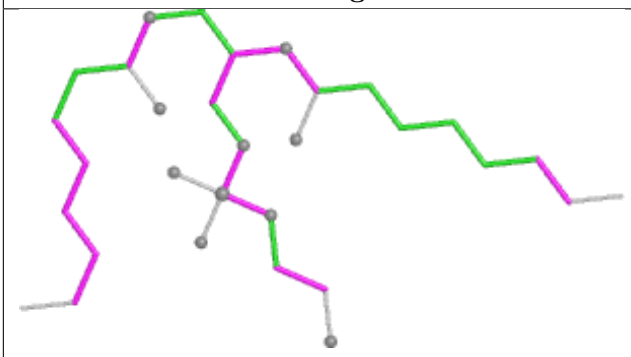
Ligand PTY 5 306



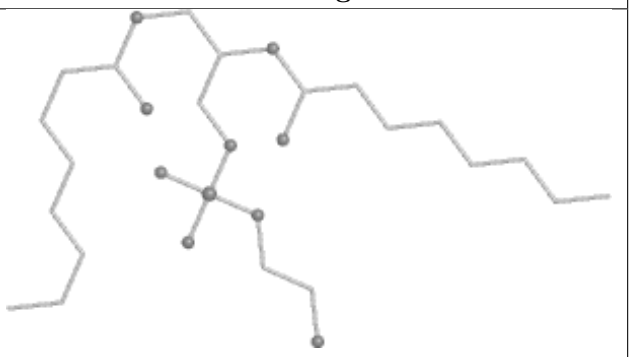
Bond lengths



Bond angles

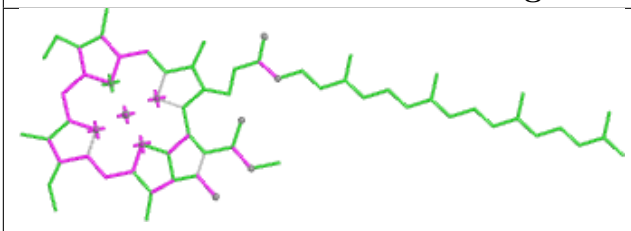


Torsions

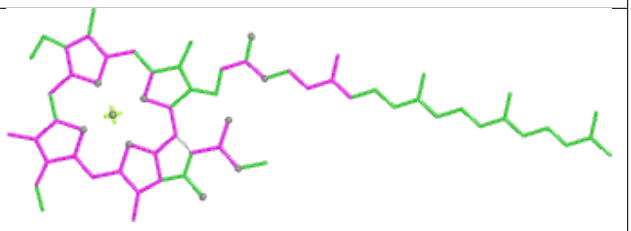


Rings

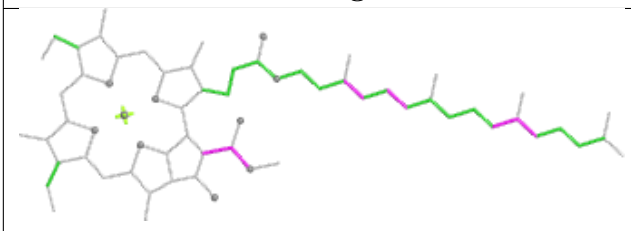
Ligand CLA B 844



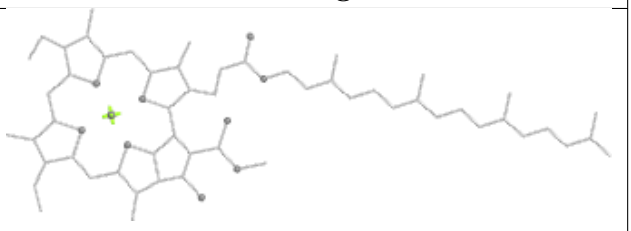
Bond lengths



Bond angles

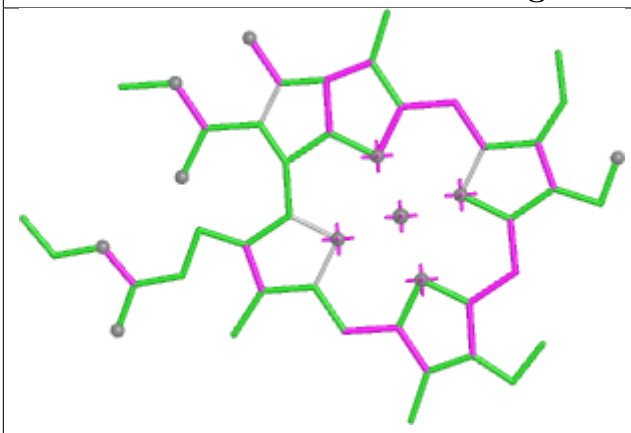


Torsions



Rings

Ligand CHL a 320



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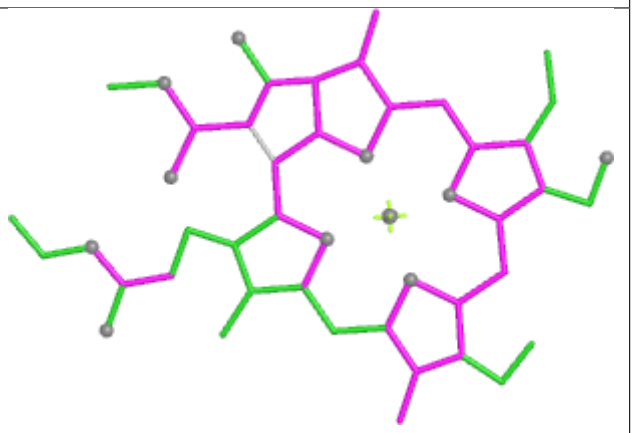
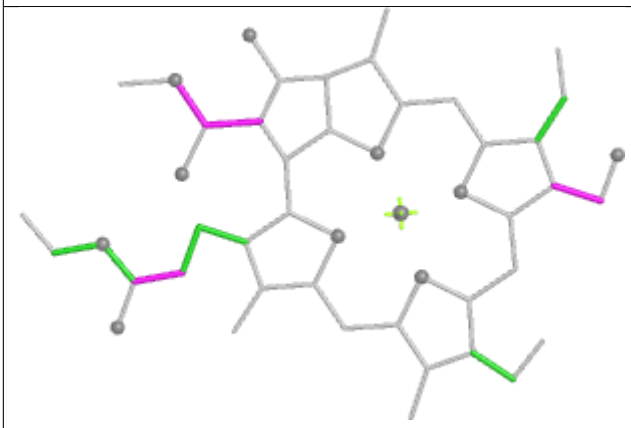
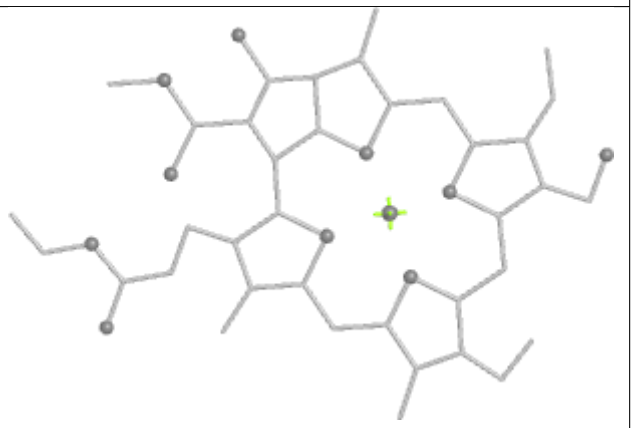


Bond angles

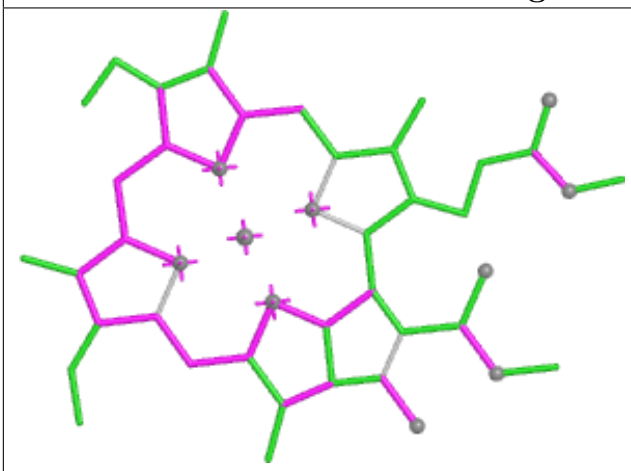


Torsions

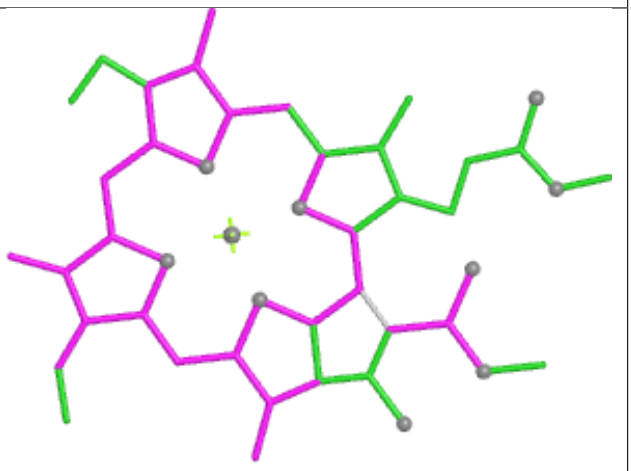


Rings

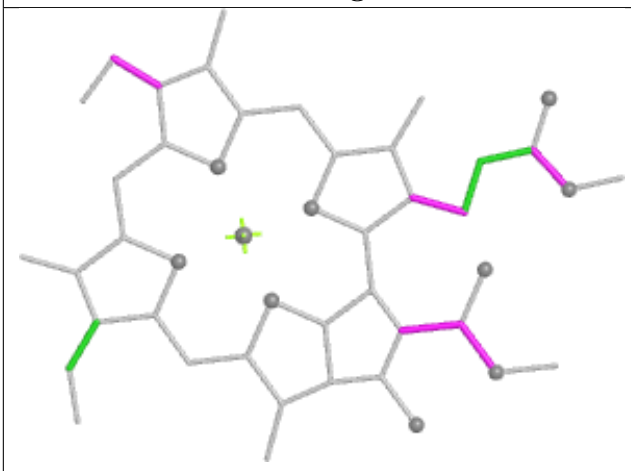
Ligand CLA 8 313



Bond lengths



Bond angles



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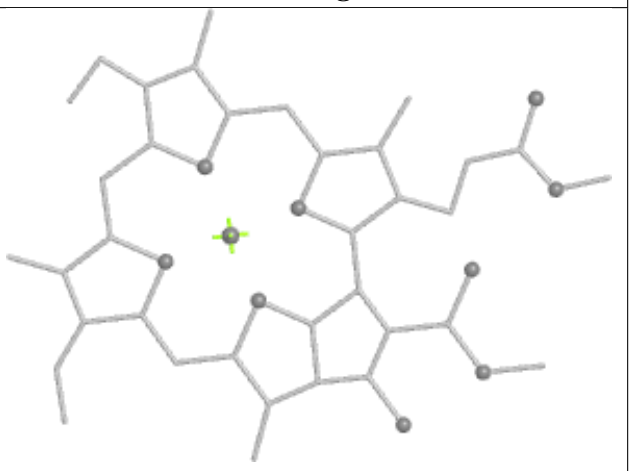
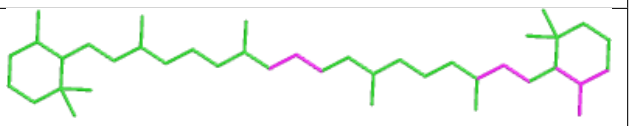


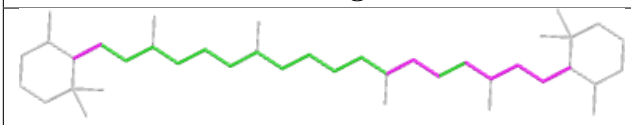
Rings

Ligand BCR G 203

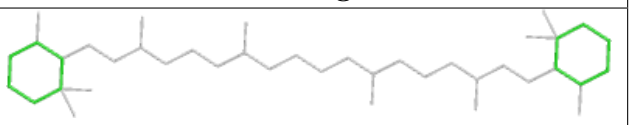
Bond lengths



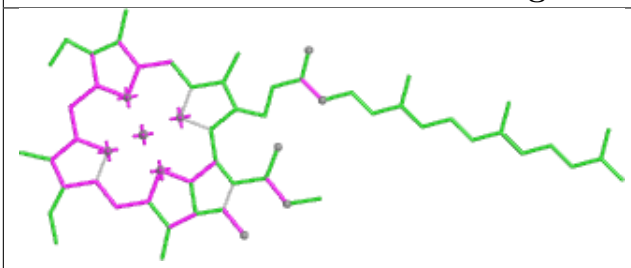
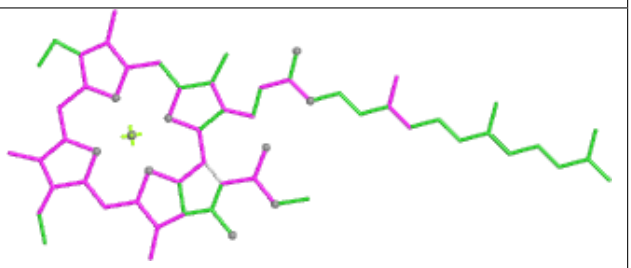
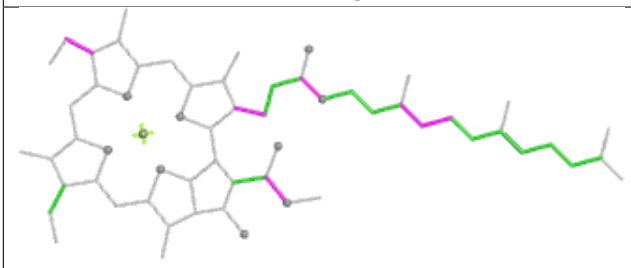
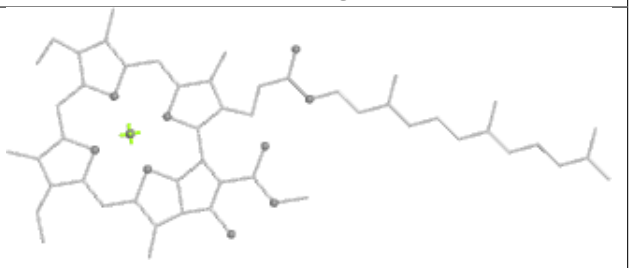
Bond angles

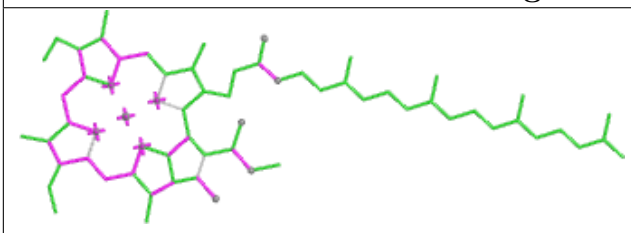
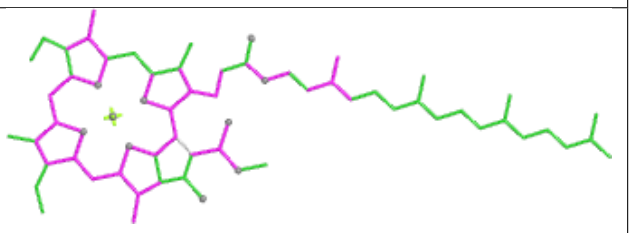
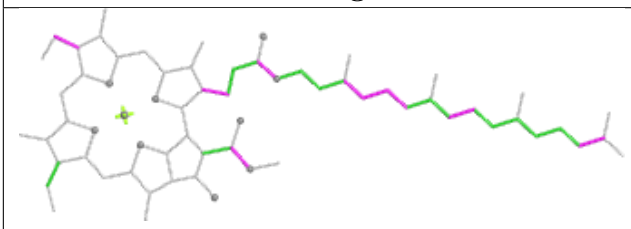
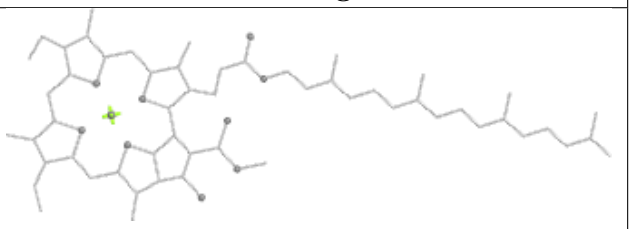


Torsions

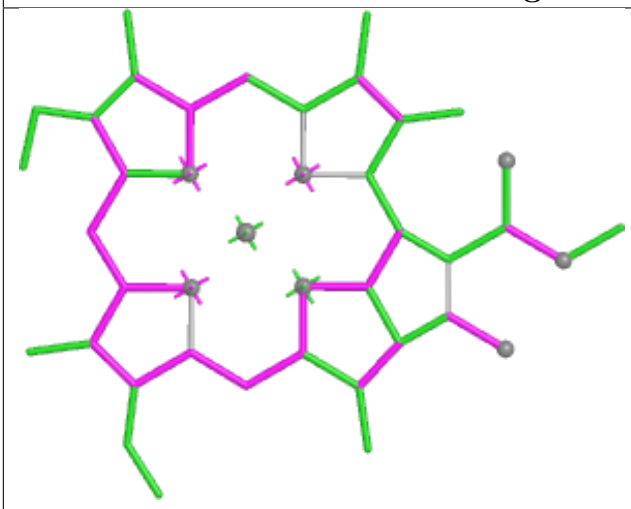


Rings

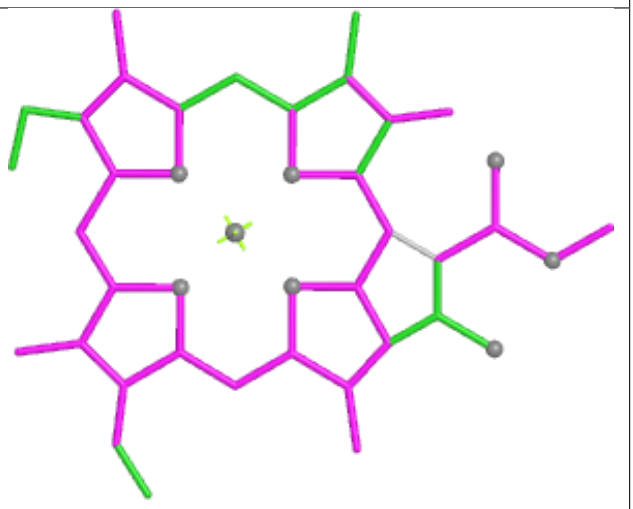
Ligand CLA 2 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 855	
	
Bond lengths	Bond angles
	
Torsions	Rings

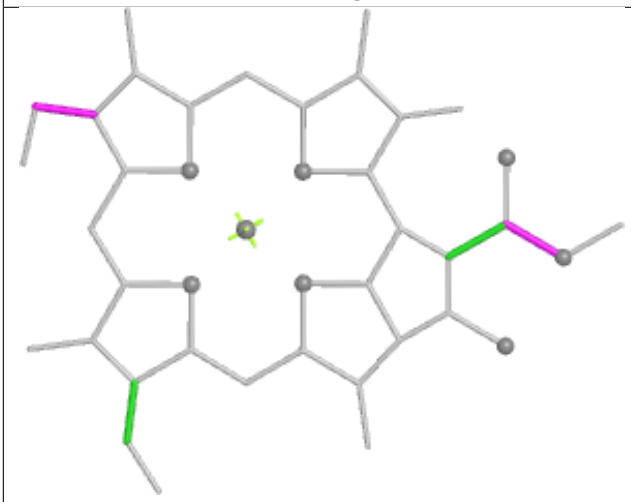
Ligand CLA O 204



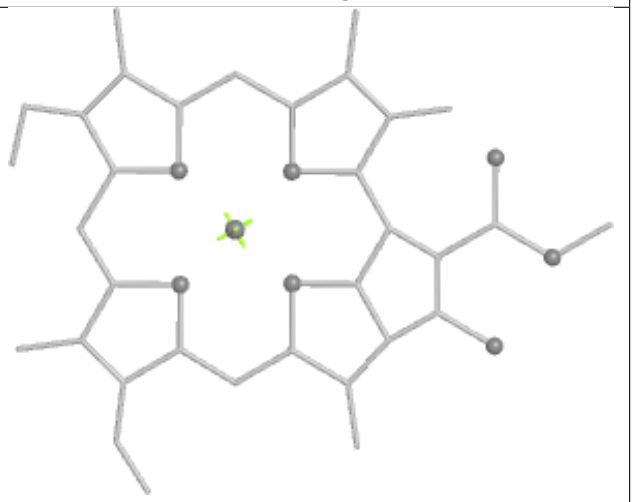
Bond lengths



Bond angles



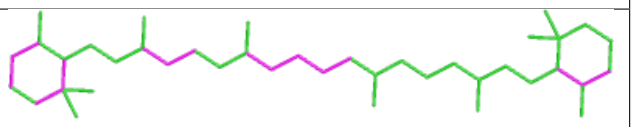
Torsions



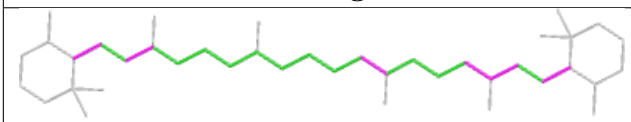
Rings

Ligand BCR 3 301

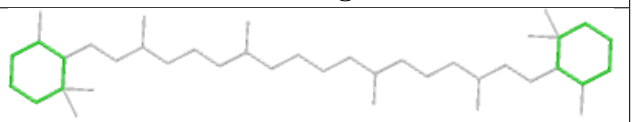
Bond lengths



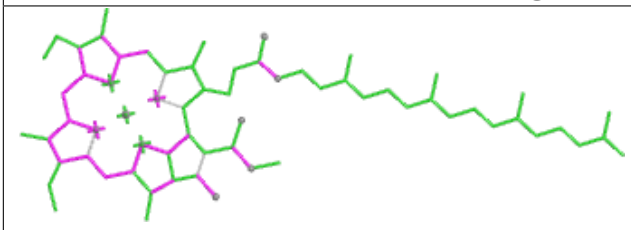
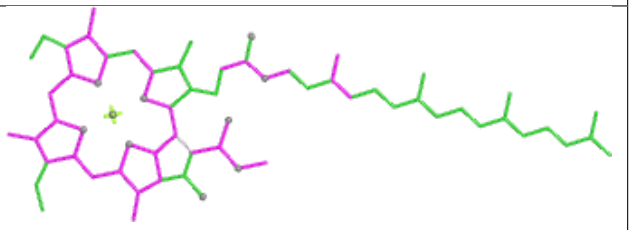
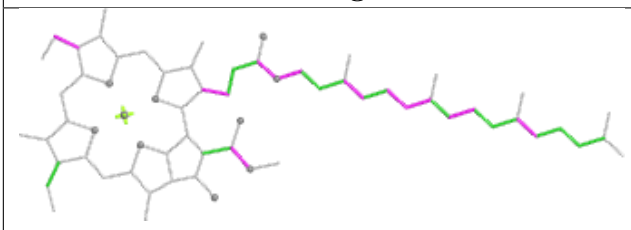
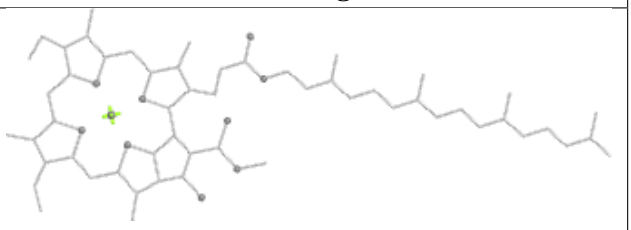
Bond angles

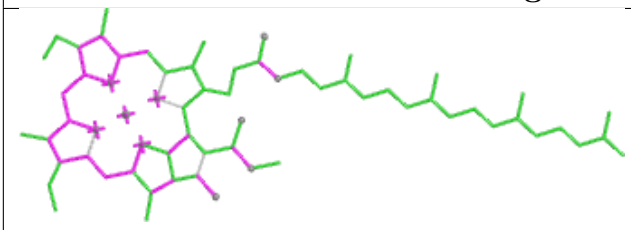
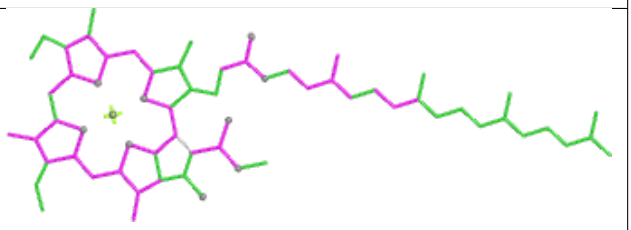
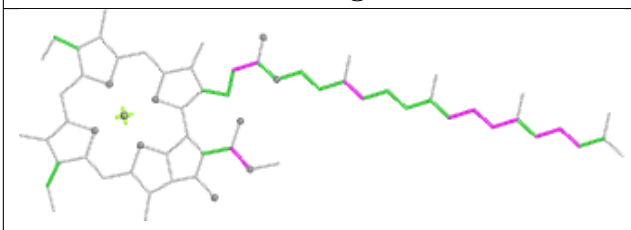
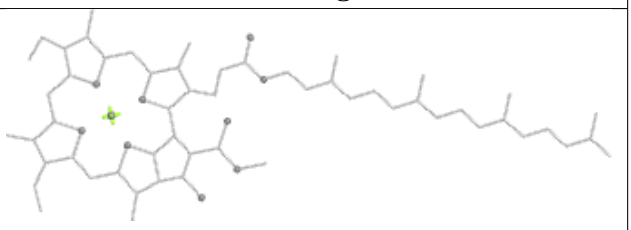


Torsions

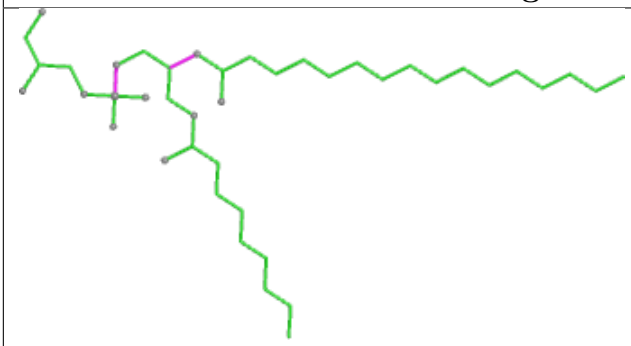


Rings

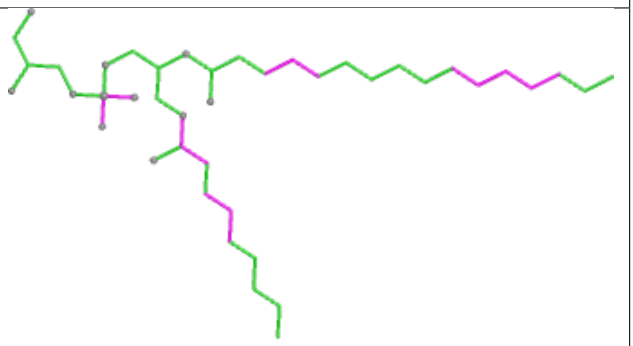
Ligand CLA 3 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

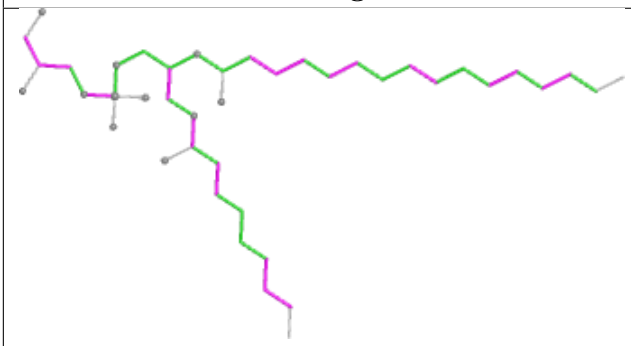
Ligand LHG A 809



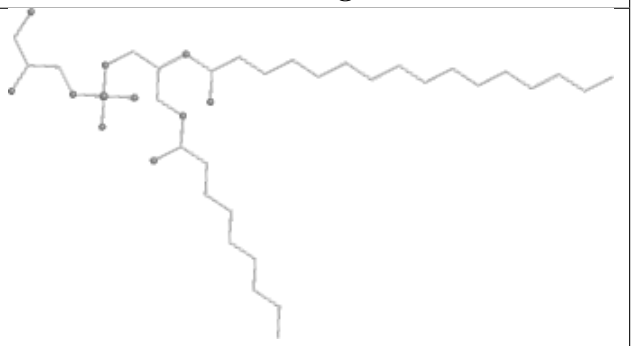
Bond lengths



Bond angles

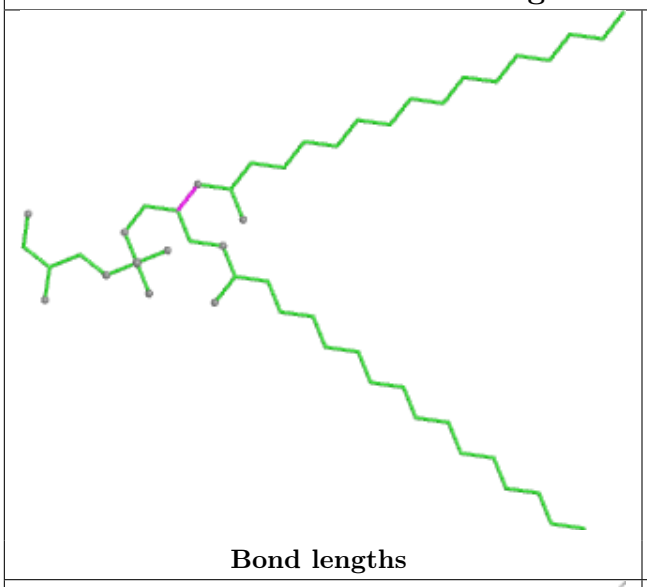


Torsions

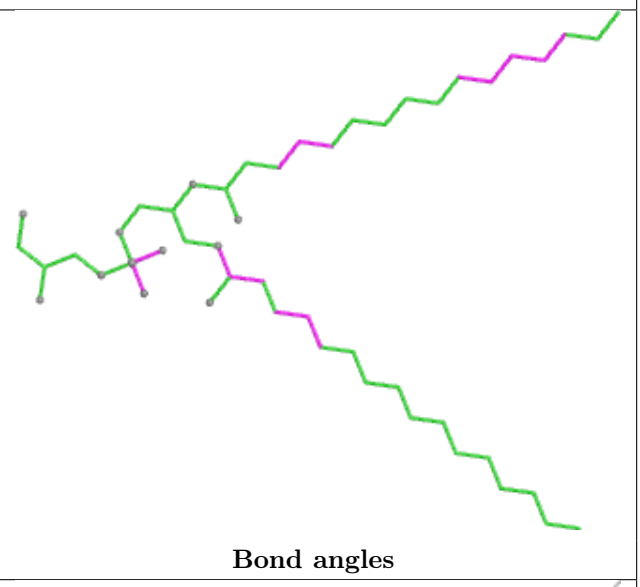


Rings

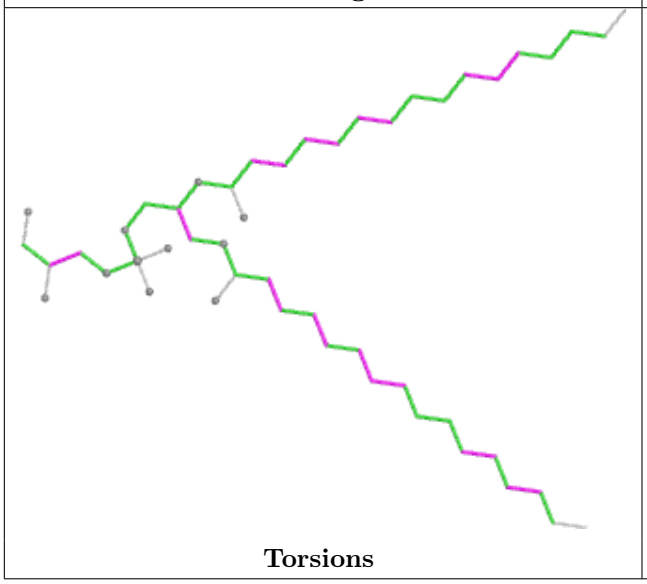
Ligand LHG 8 304



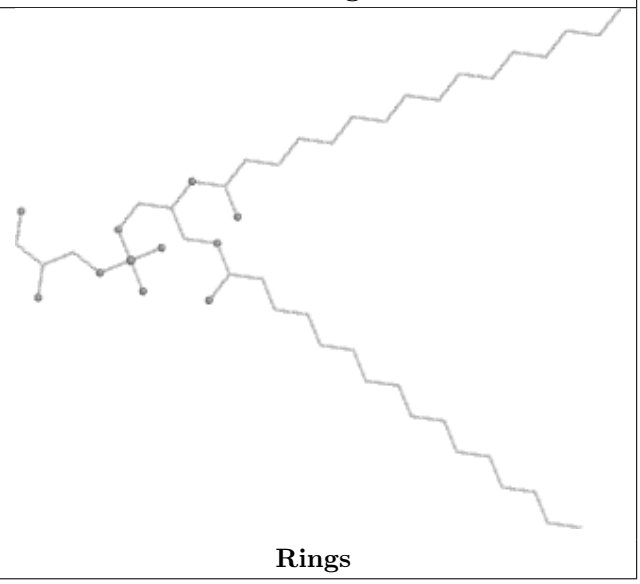
Bond lengths



Bond angles



Torsions

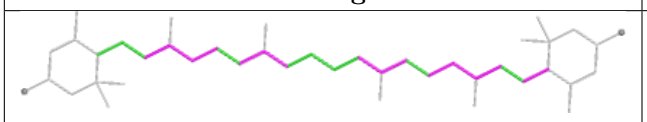


Rings

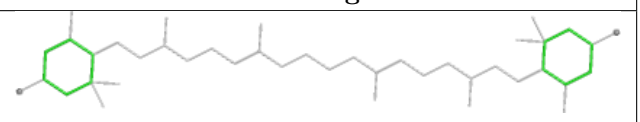
Ligand LUT 9 303

Bond lengths

Bond angles

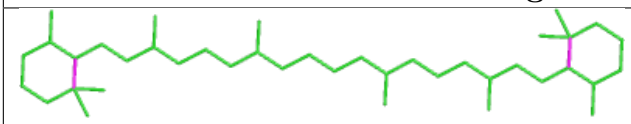


Torsions

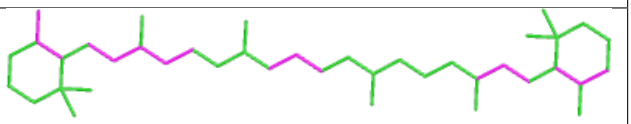


Rings

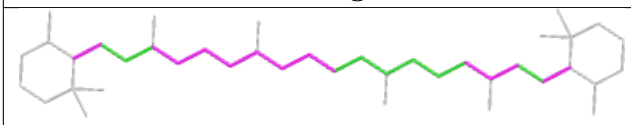
Ligand BCR 6 302



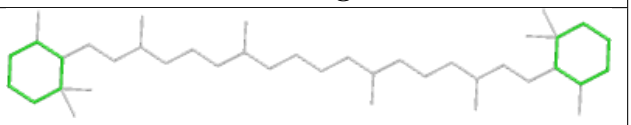
Bond lengths



Bond angles

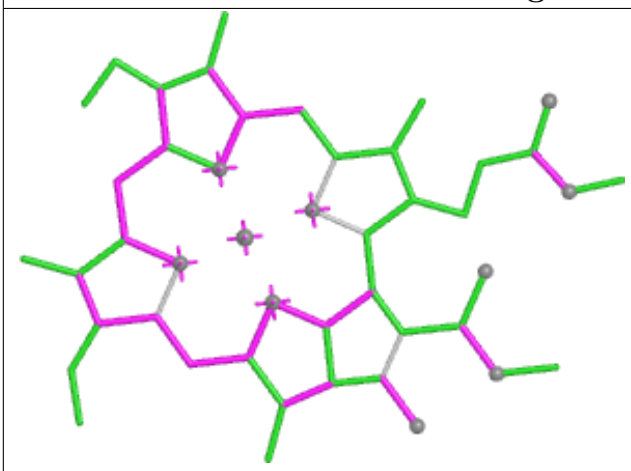


Torsions



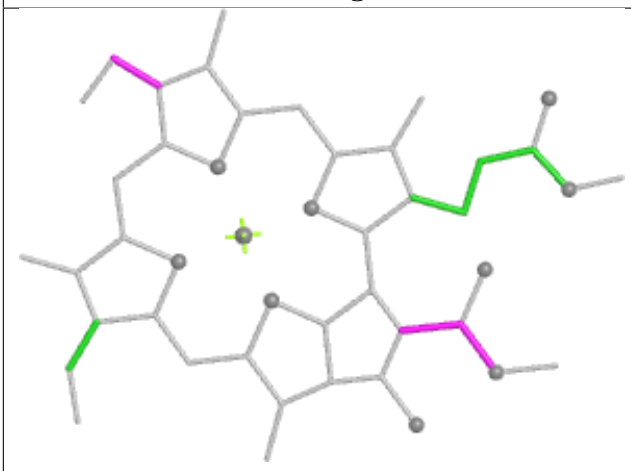
Rings

Ligand CLA b 312



Bond lengths

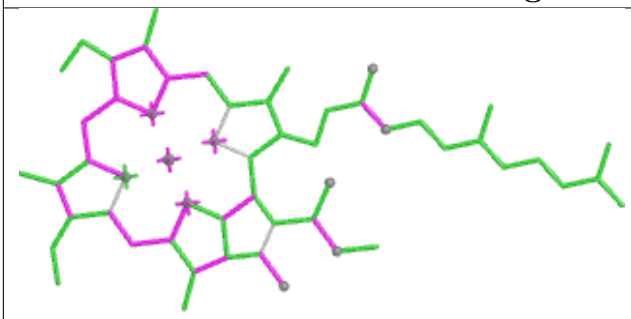
Bond angles



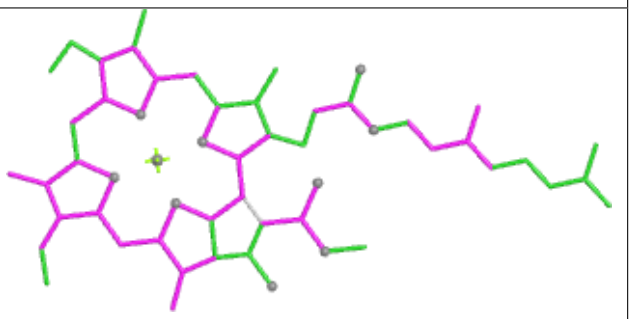
Torsions

Rings

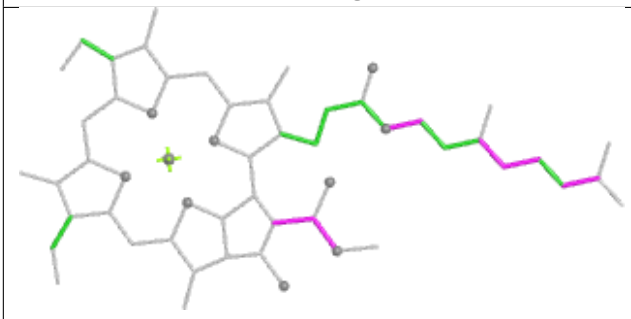
Ligand CLA B 841



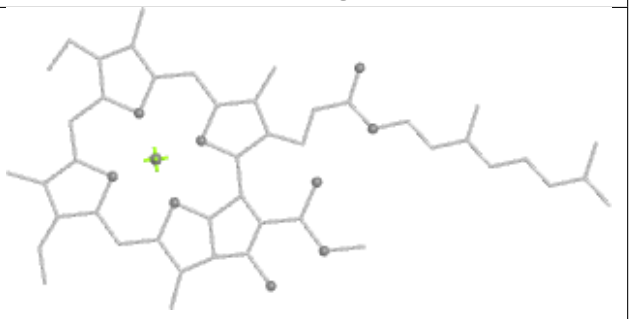
Bond lengths



Bond angles

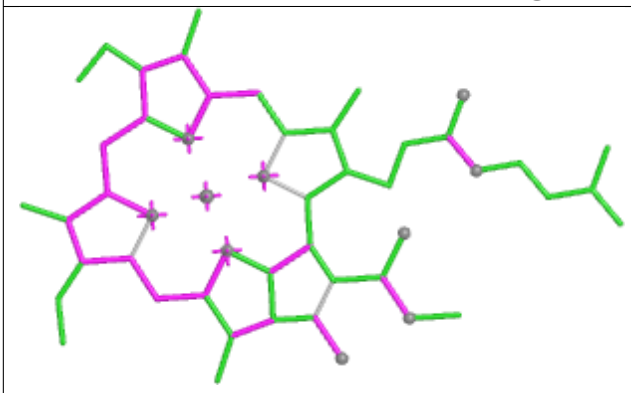


Torsions

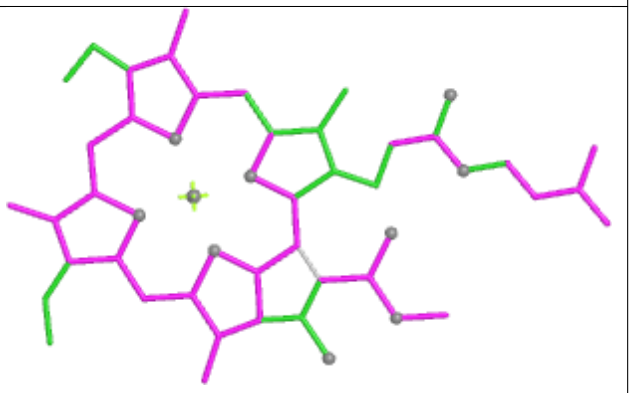


Rings

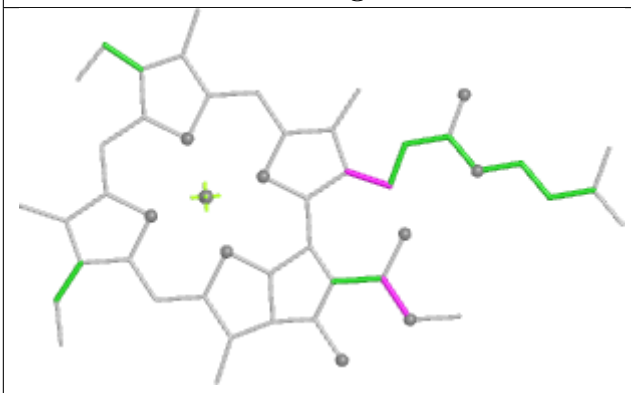
Ligand CLA 6 316



Bond lengths



Bond angles



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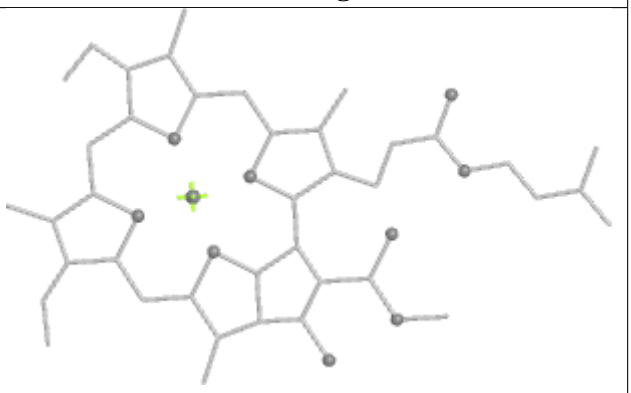
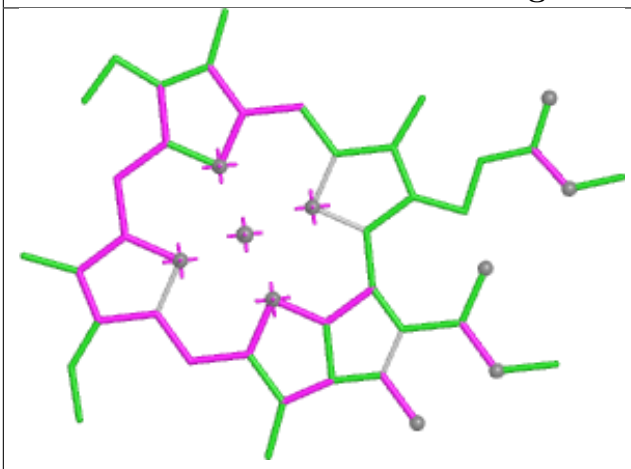
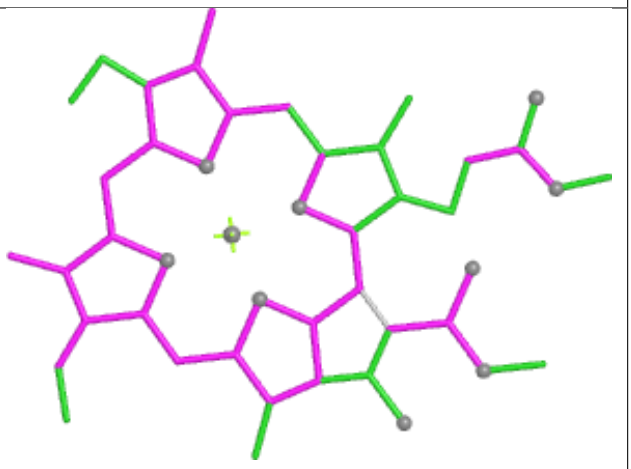


Rings

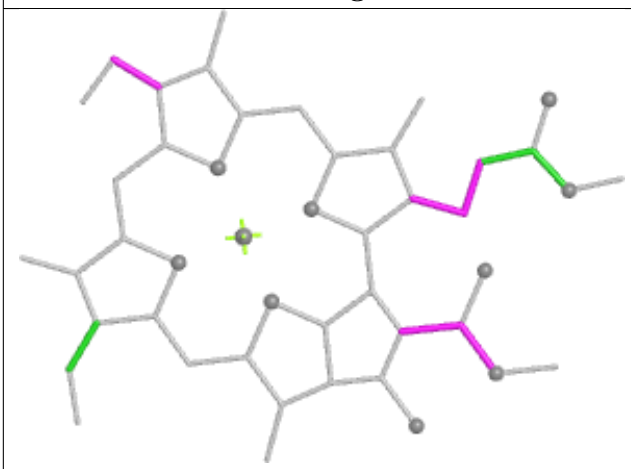
Ligand CLA 4 311



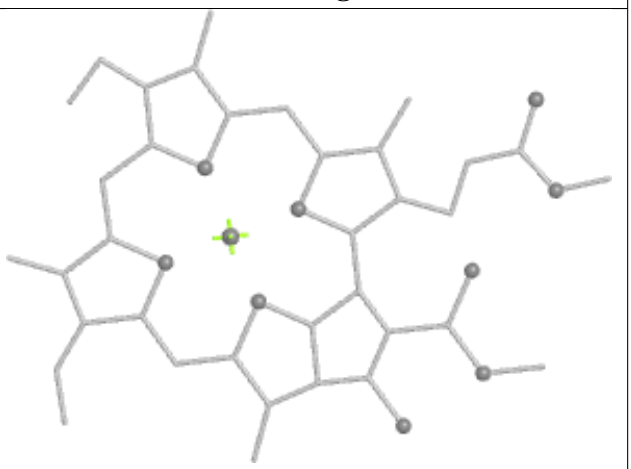
Bond lengths



Bond angles



Torsions

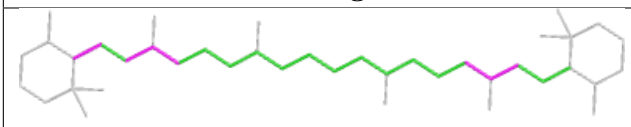


Rings

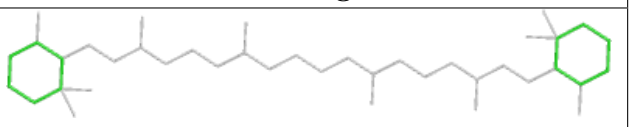
Ligand BCR B 803

Bond lengths

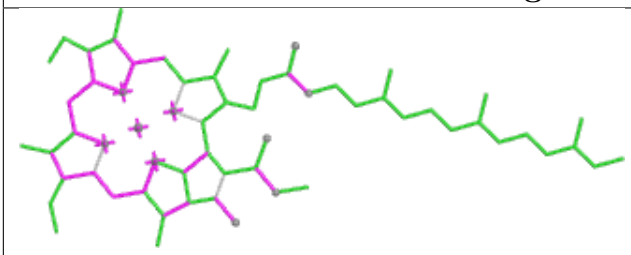
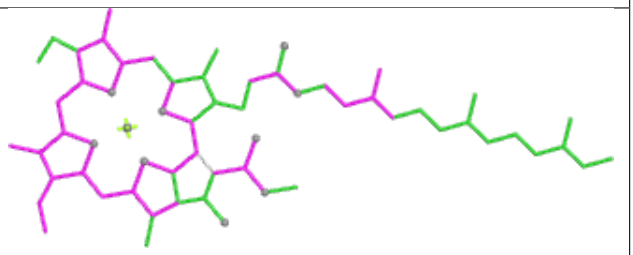
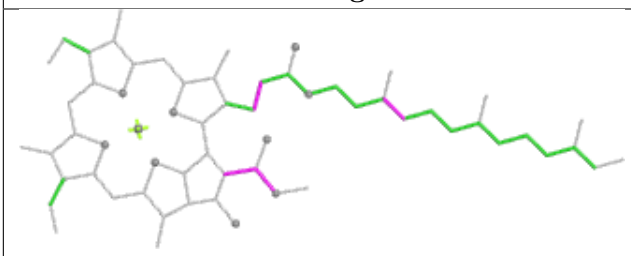
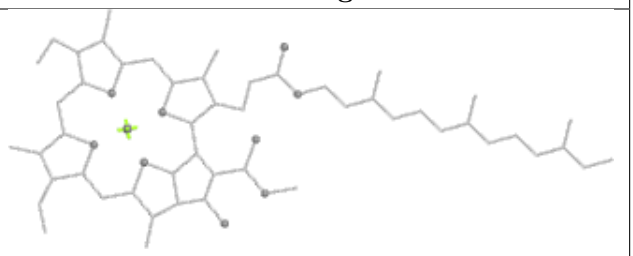
Bond angles

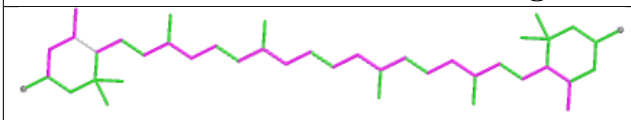
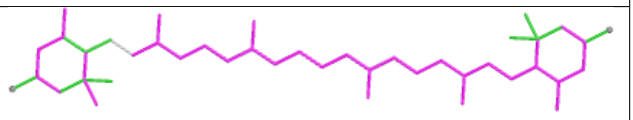
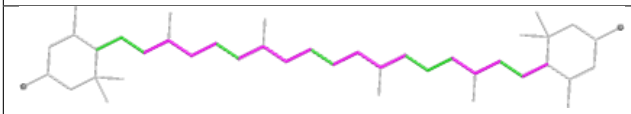
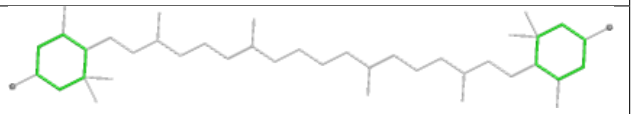


Torsions

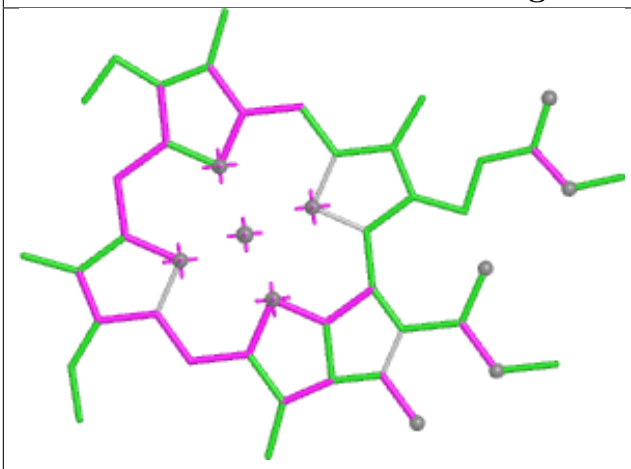


Rings

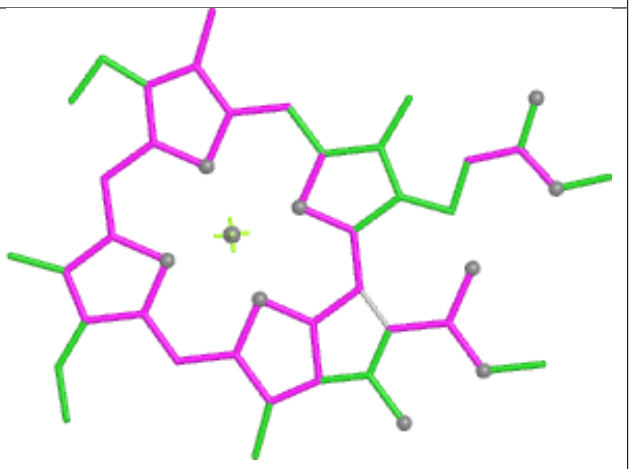
Ligand CLA B 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 6 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

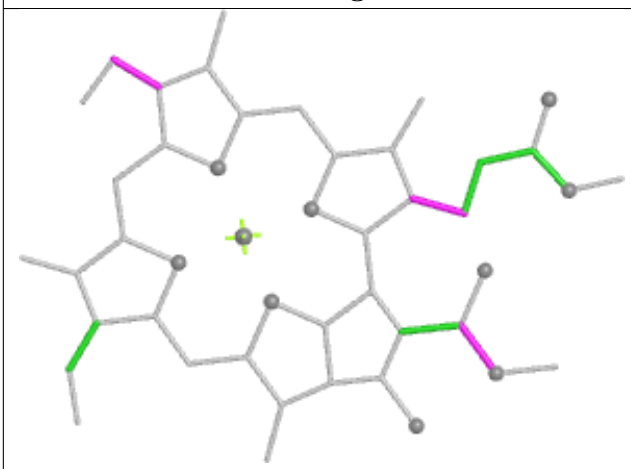
Ligand CLA 7 322



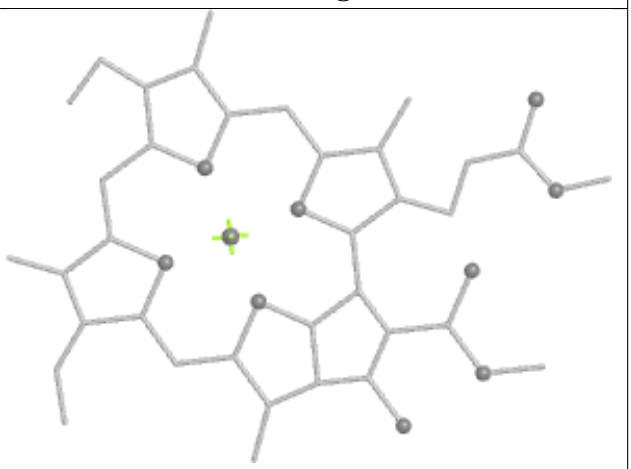
Bond lengths



Bond angles

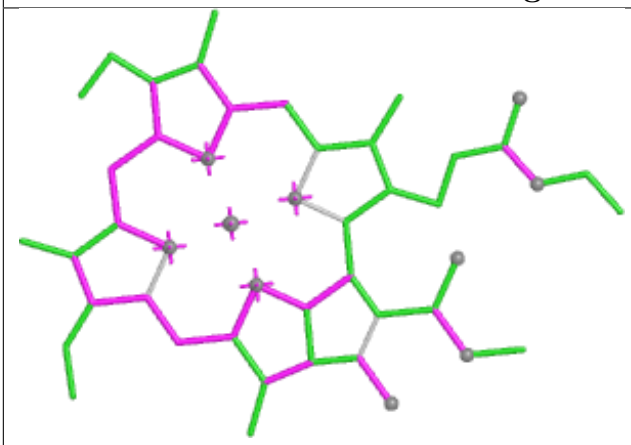


Torsions

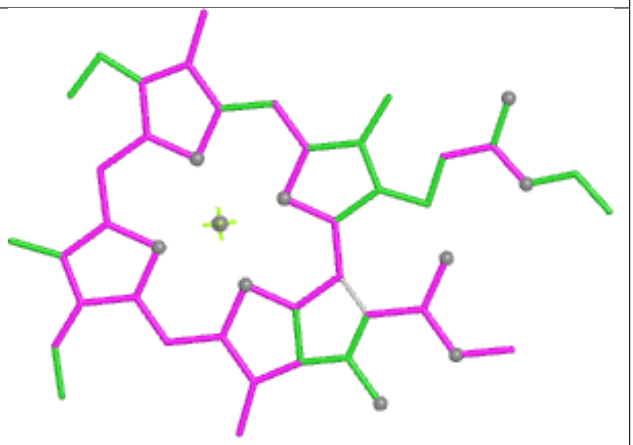


Rings

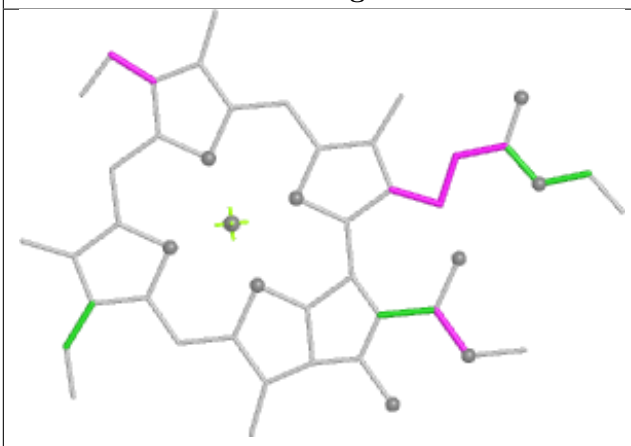
Ligand CLA A 833



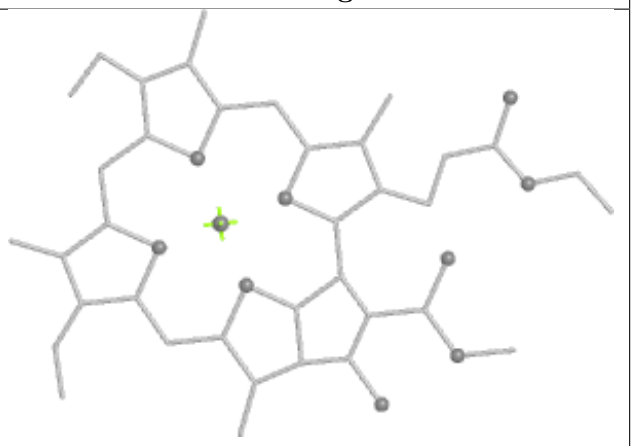
Bond lengths



Bond angles



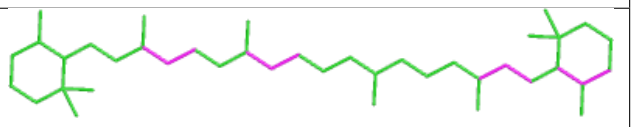
Torsions



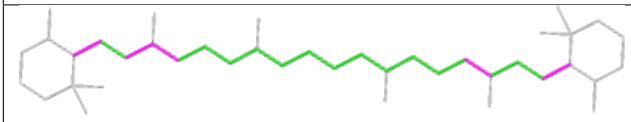
Rings

Ligand BCR A 804

Bond lengths



Bond angles



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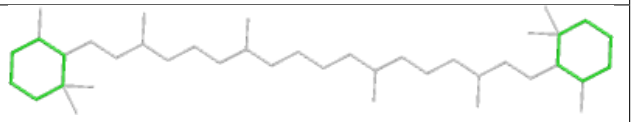
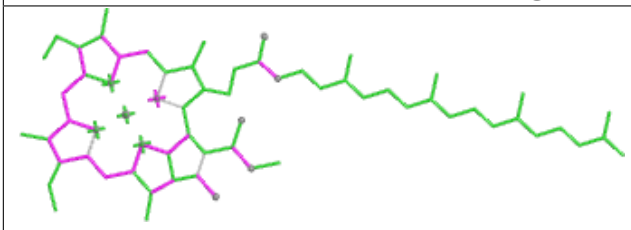
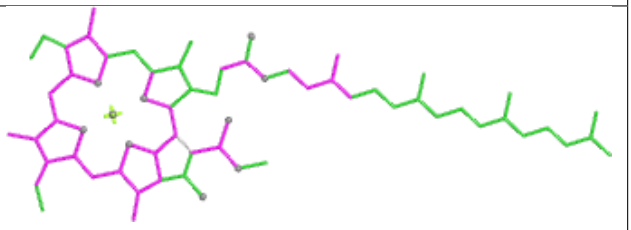


Rings

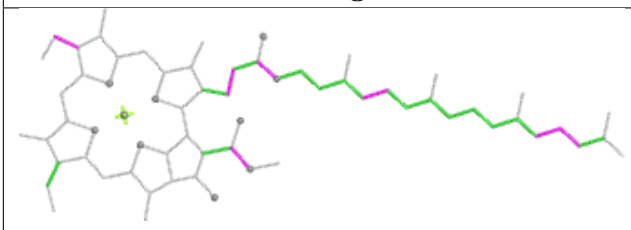
Ligand CLA 9 318



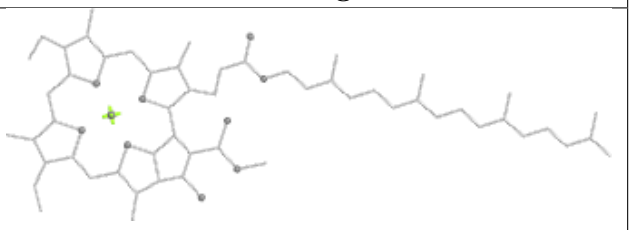
Bond lengths



Bond angles

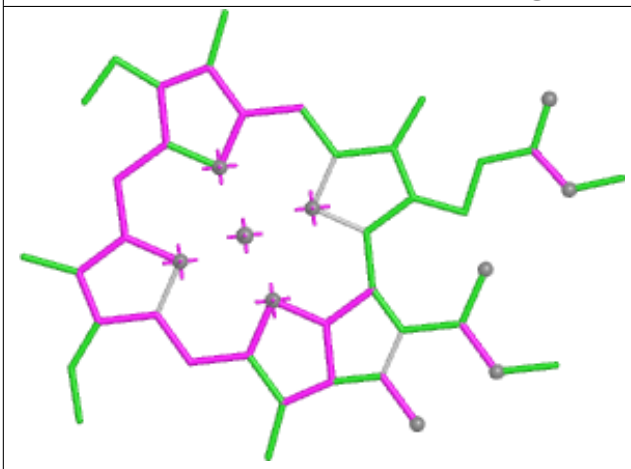


Torsions

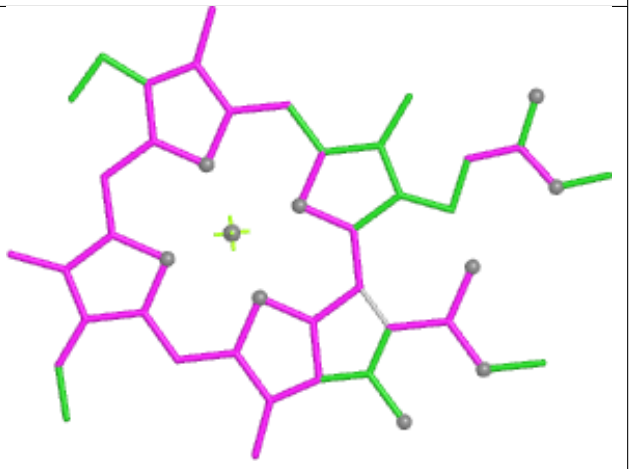


Rings

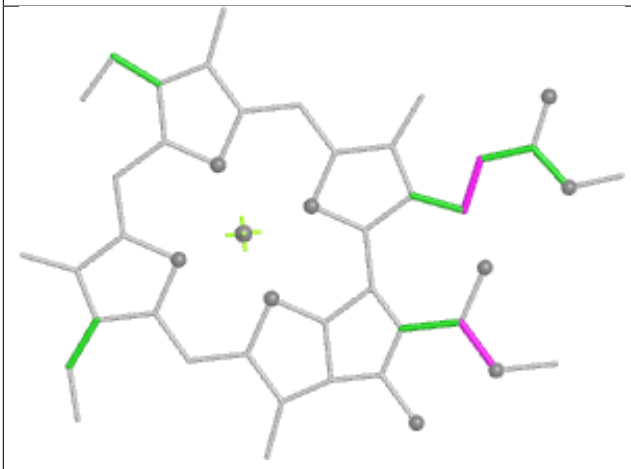
Ligand CLA 5 320



Bond lengths



Bond angles



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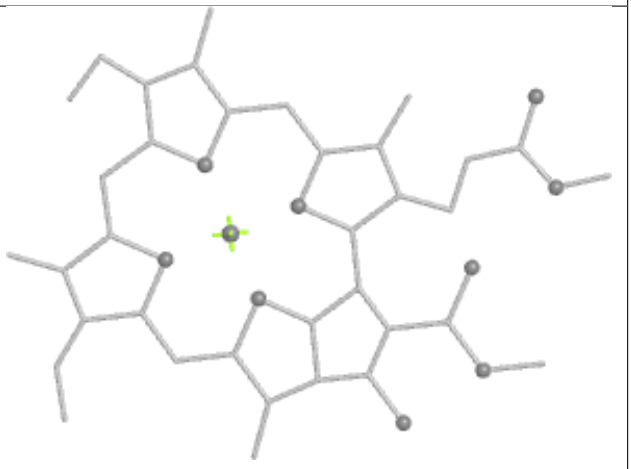
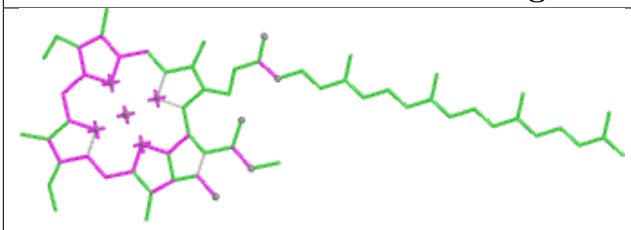
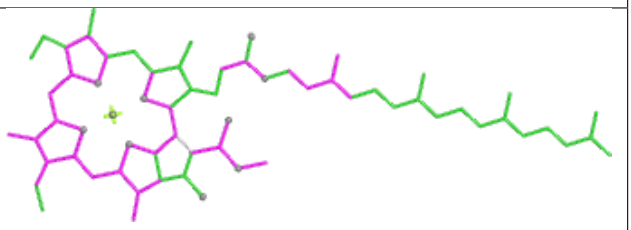


Rings

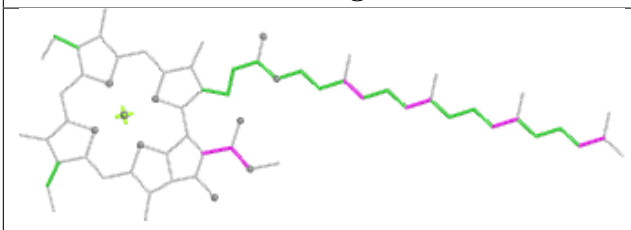
Ligand CLA 6 312



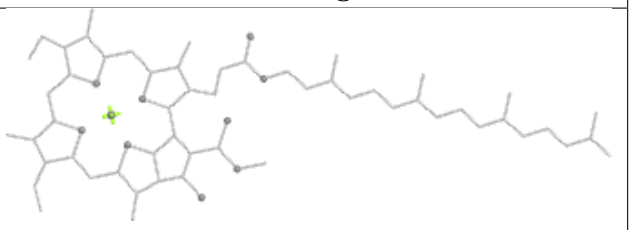
Bond lengths



Bond angles

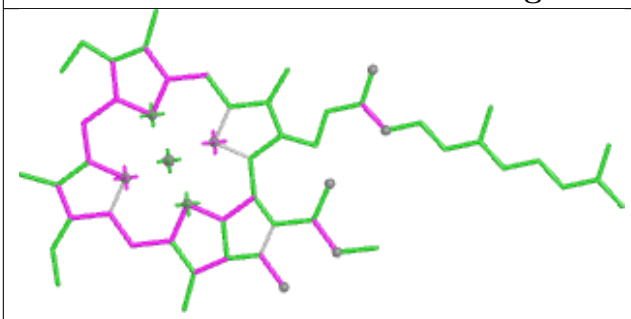


Torsions

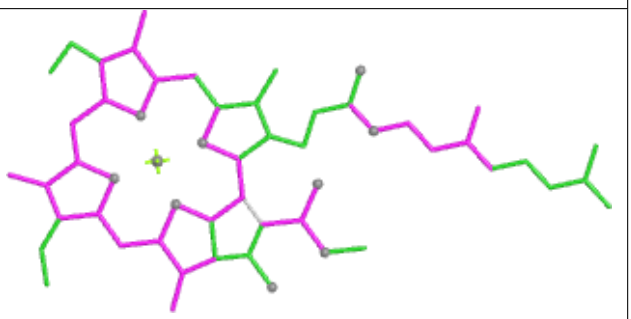


Rings

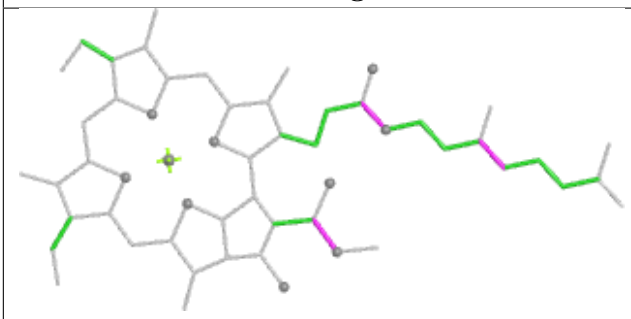
Ligand CLA B 829



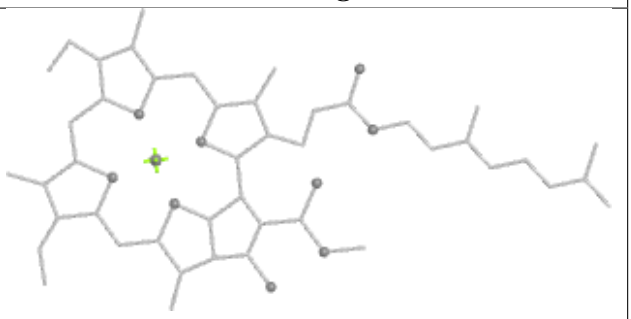
Bond lengths



Bond angles

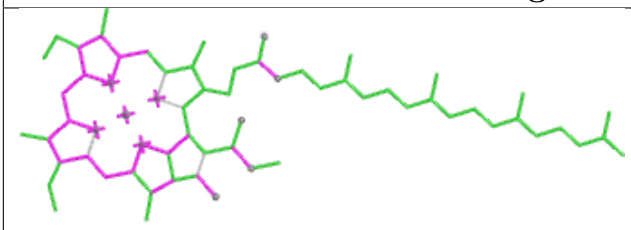


Torsions

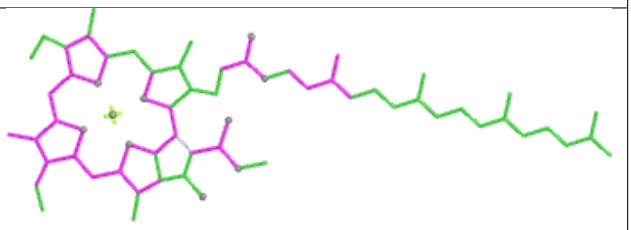


Rings

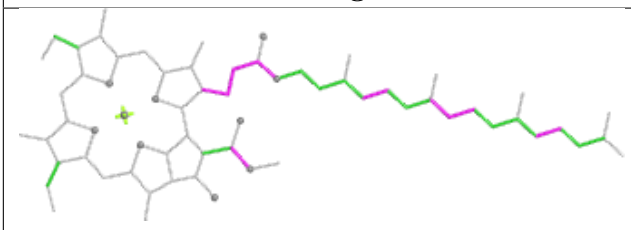
Ligand CLA 8 308



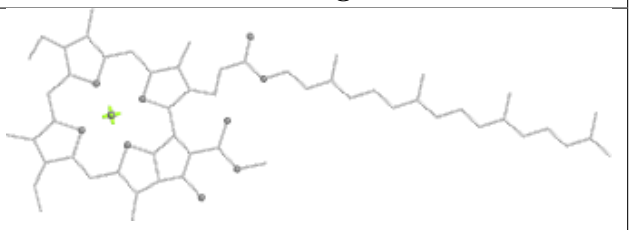
Bond lengths



Bond angles

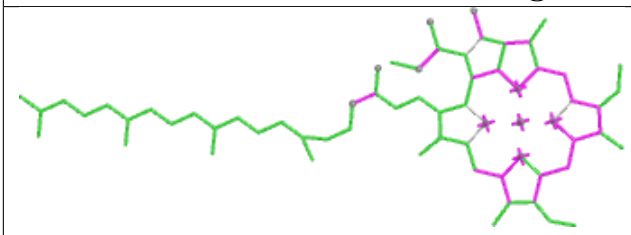


Torsions

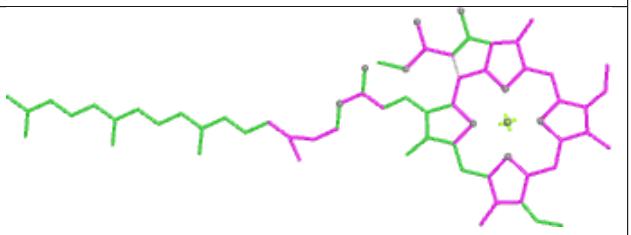


Rings

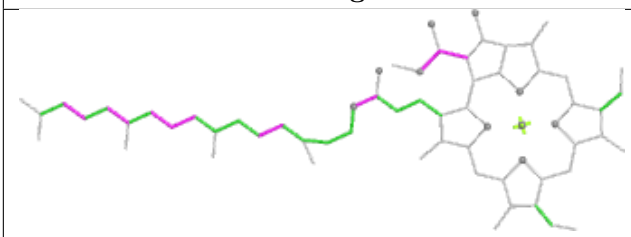
Ligand CLA 5 315



Bond lengths



Bond angles



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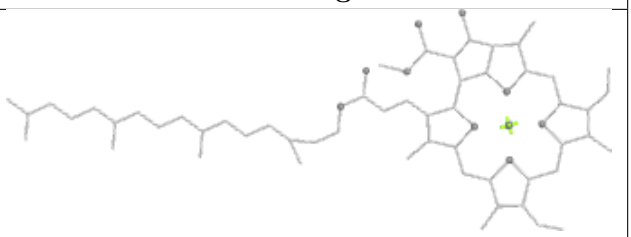
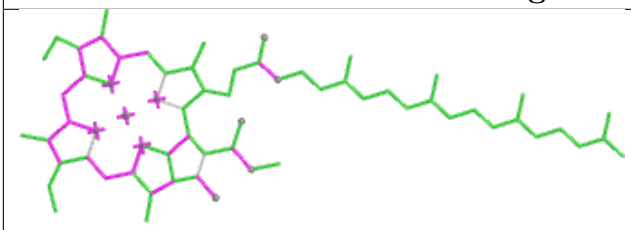
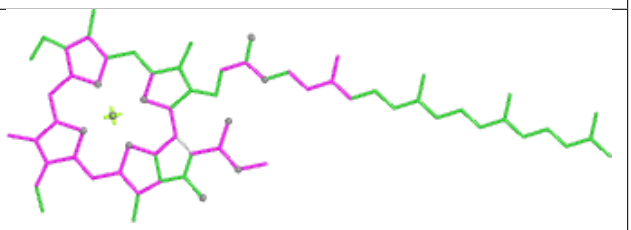


Rings

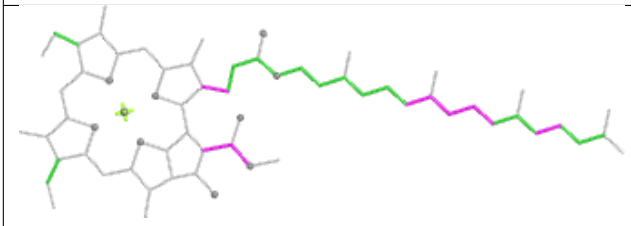
Ligand CLA 8 310



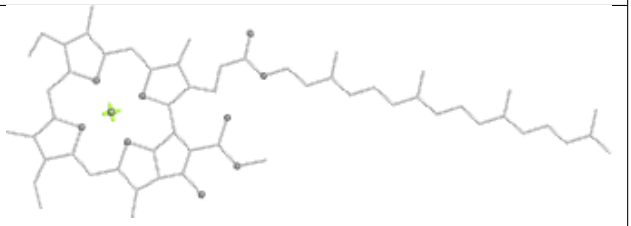
Bond lengths



Bond angles

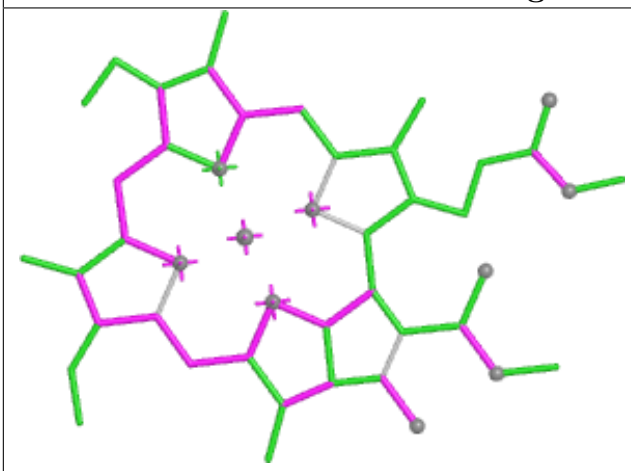


Torsions



Rings

Ligand CLA b 302



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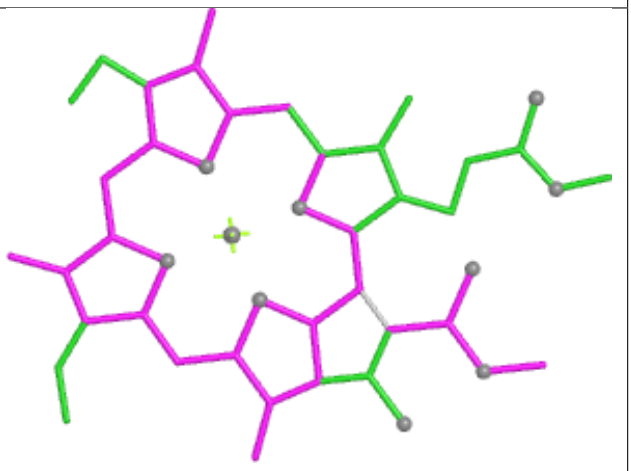
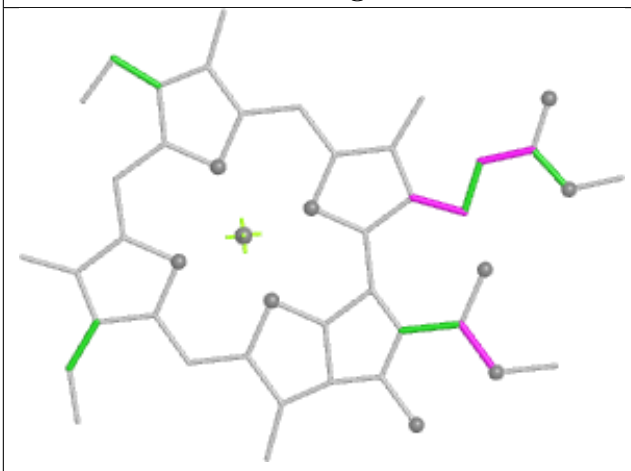


Bond angles



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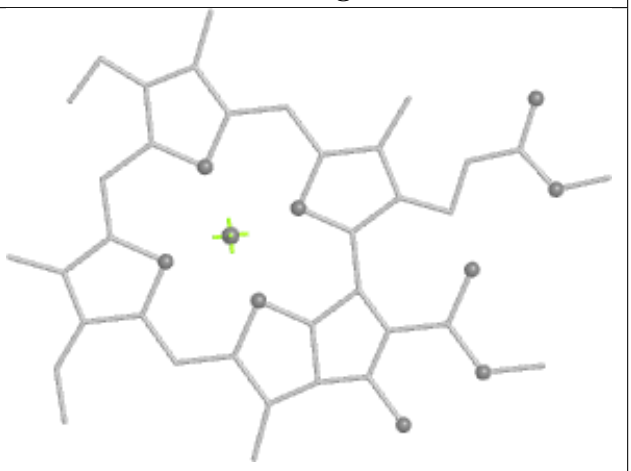
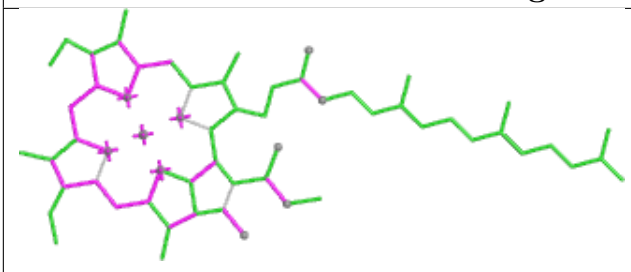
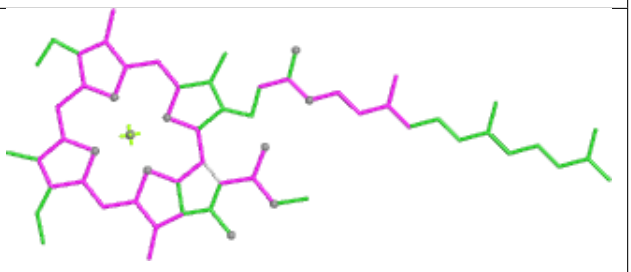


Rings

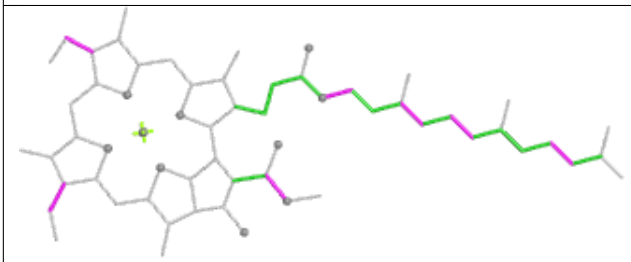
Ligand CLA 3 310



Bond lengths



Bond angles



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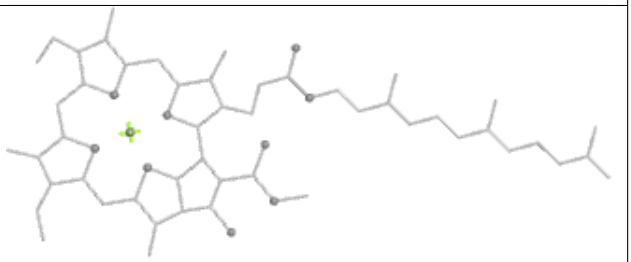
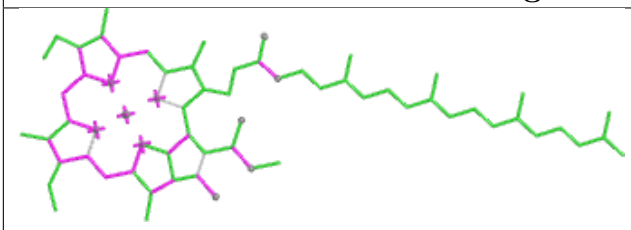


Rings

Ligand CLA A 843



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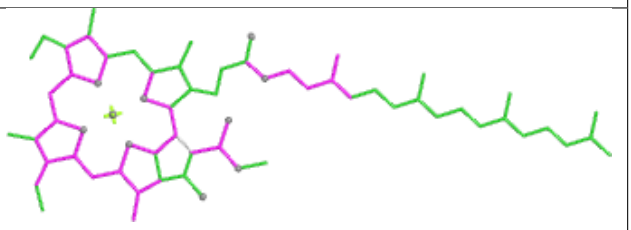
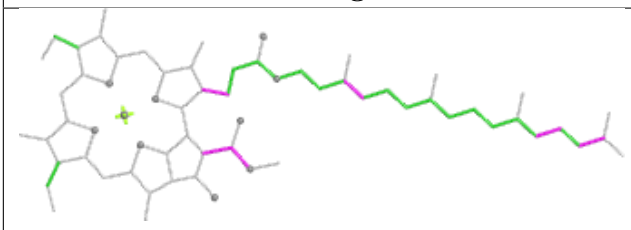


Bond angles



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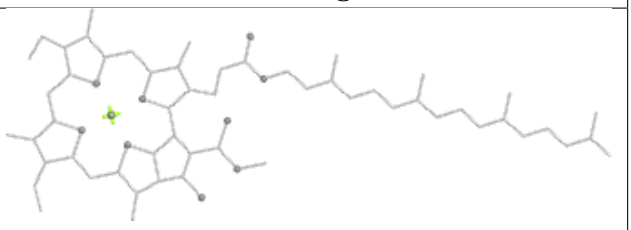
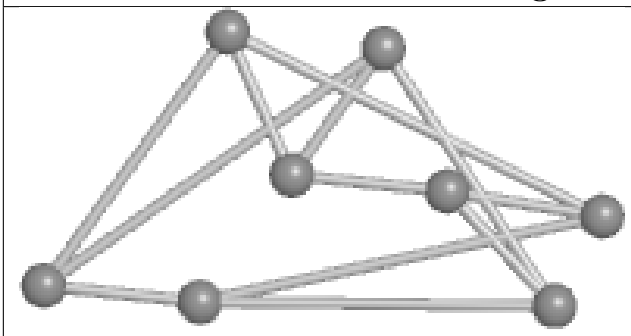


Rings

Ligand SF4 C 102



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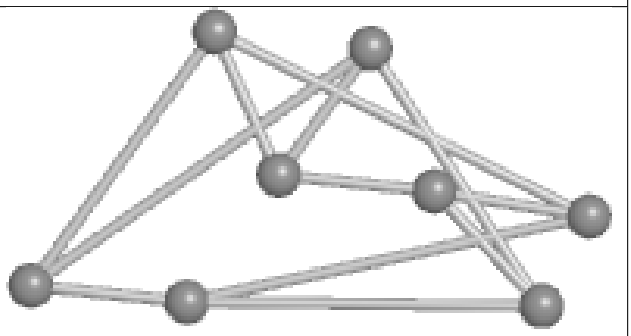
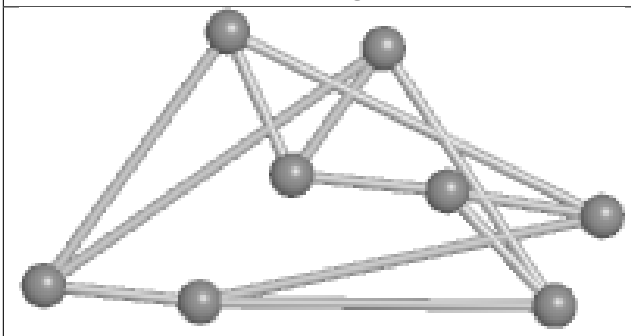


Bond angles



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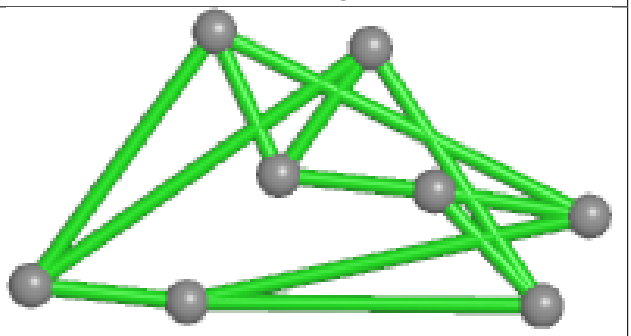
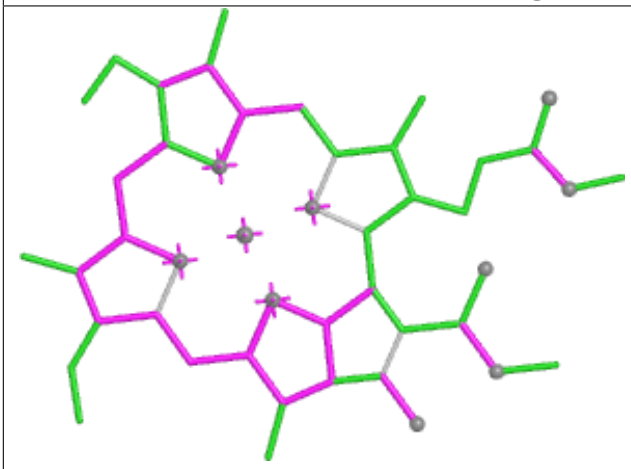


Rings

Ligand CLA 6 306



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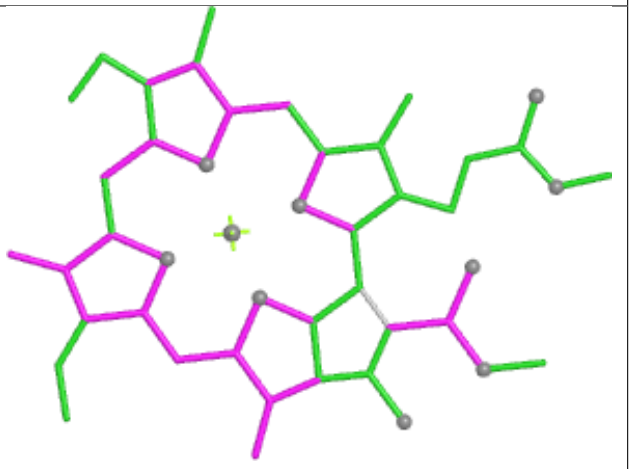
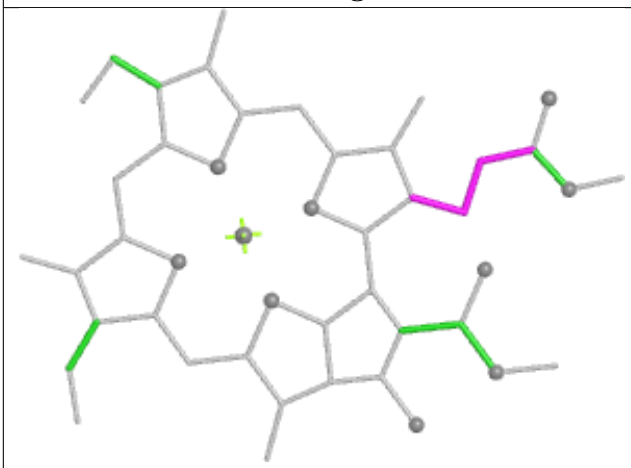


Bond angles



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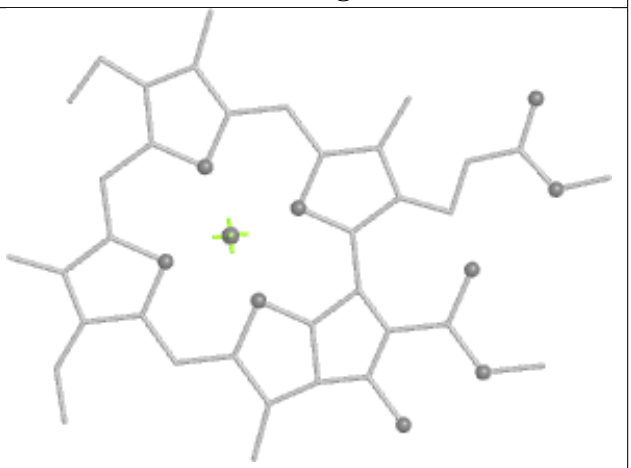
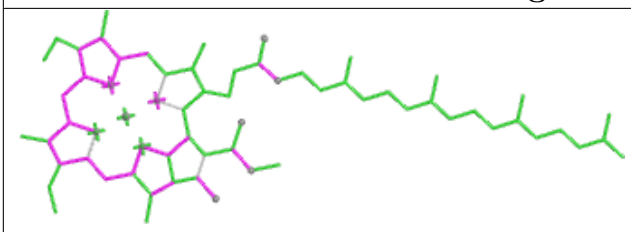


Rings

Ligand CLA 5 310



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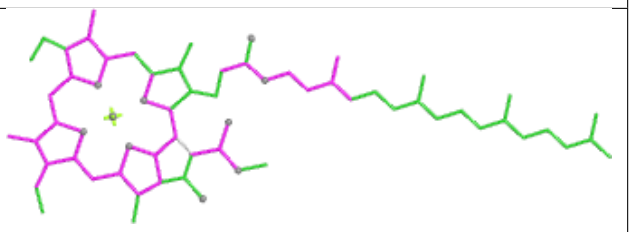
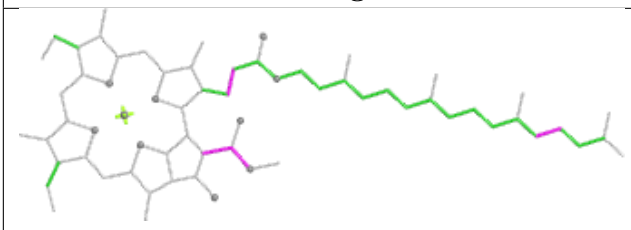
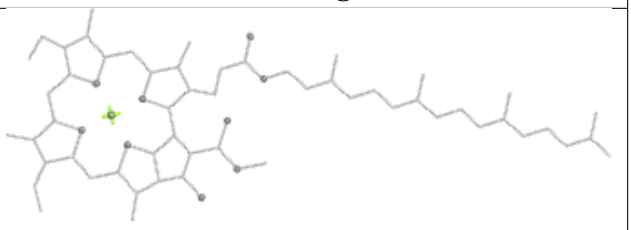


Bond angles

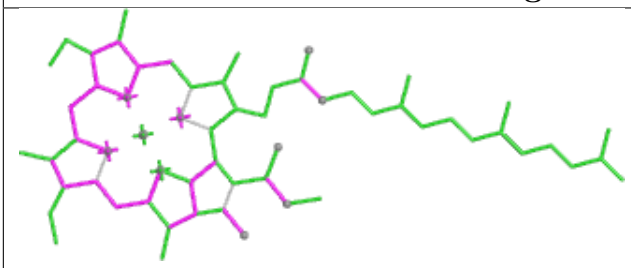


Torsions

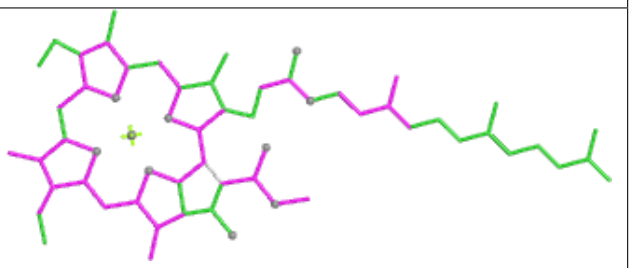


Rings

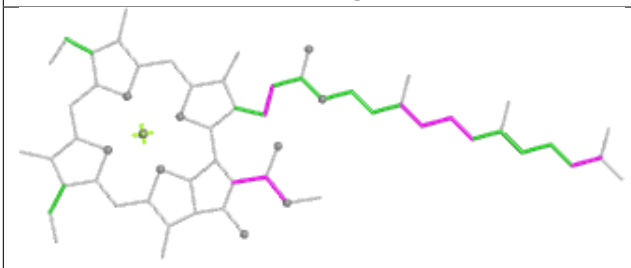
Ligand CLA B 839



Bond lengths



Bond angles



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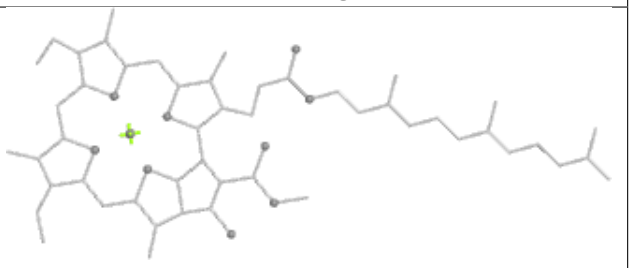
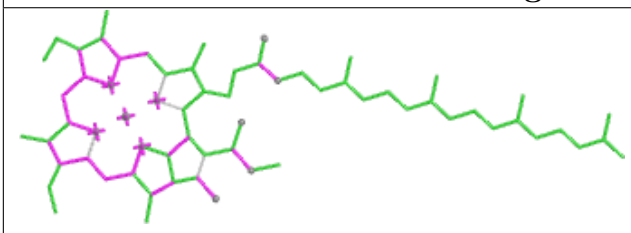


Rings

Ligand CLA B 812



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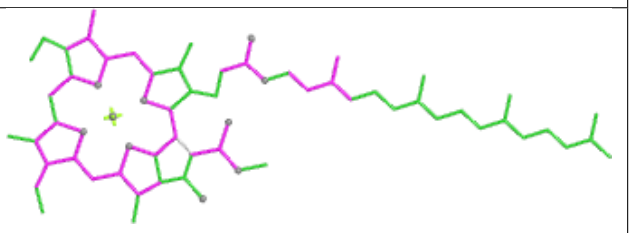
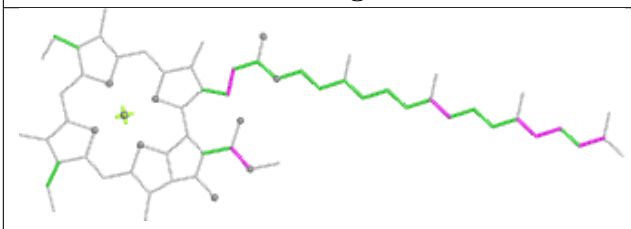
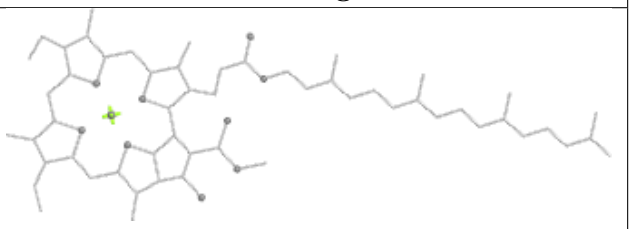


Bond angles

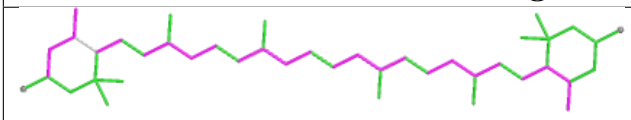


Torsions



Rings

Ligand LUT a 303



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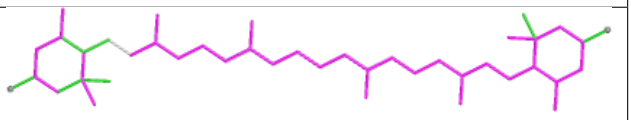
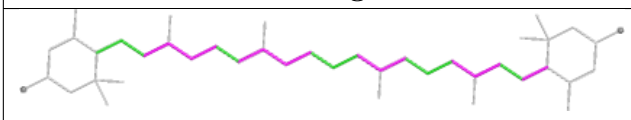


Bond angles



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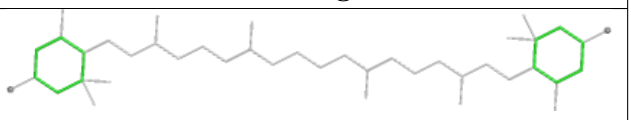
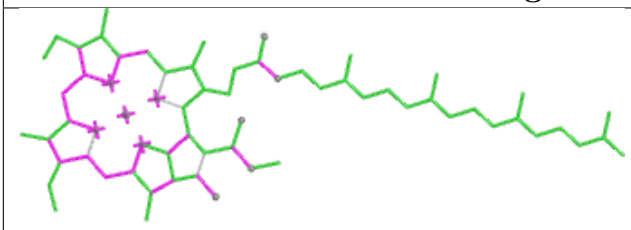
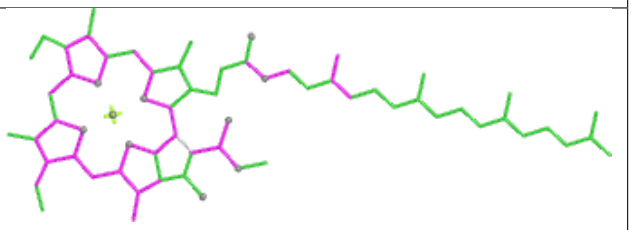


Rings

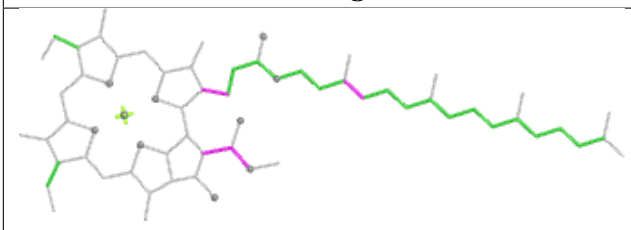
Ligand CLA B 836



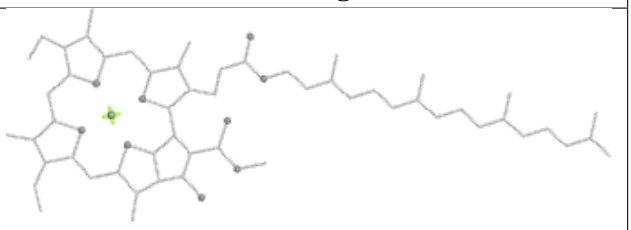
Bond lengths



Bond angles

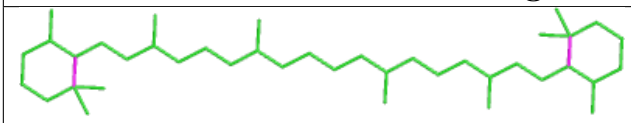


Torsions

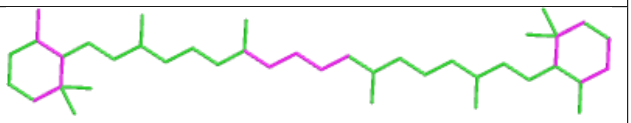


Rings

Ligand BCR L 302

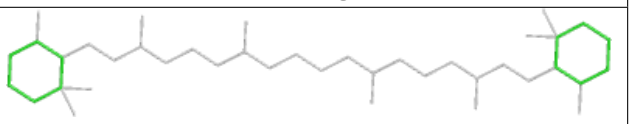


Bond lengths



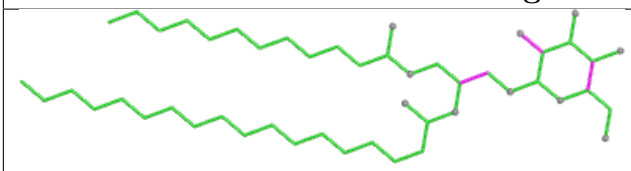
Bond angles

Torsions

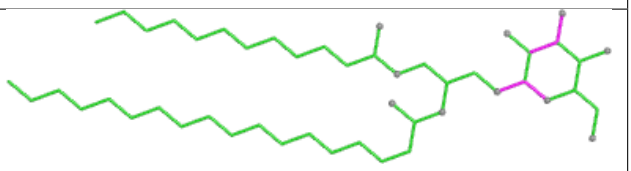


Rings

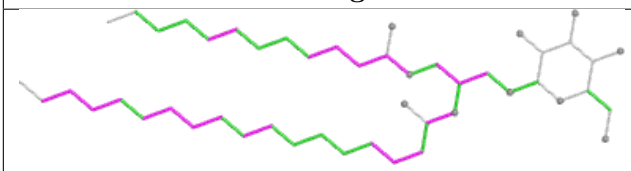
Ligand LMG J 101



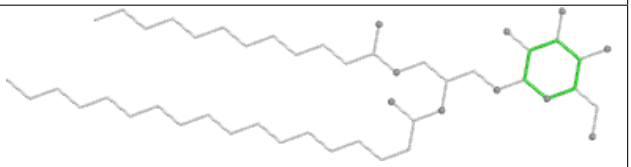
Bond lengths



Bond angles

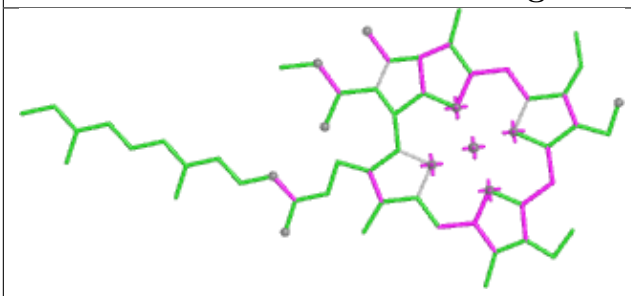


Torsions



Rings

Ligand CHL 7 317



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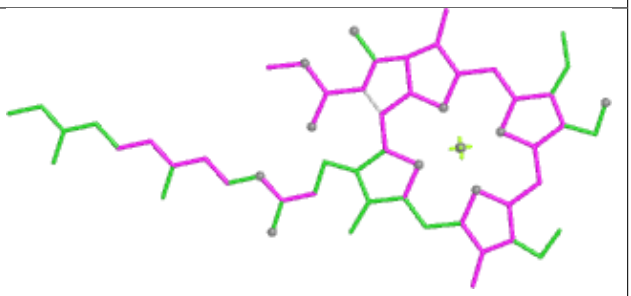

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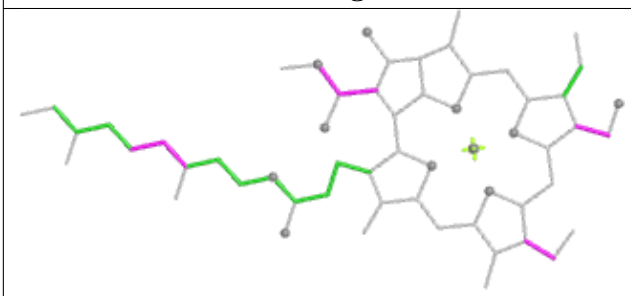
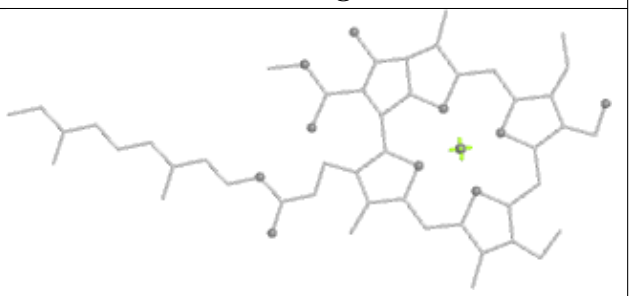
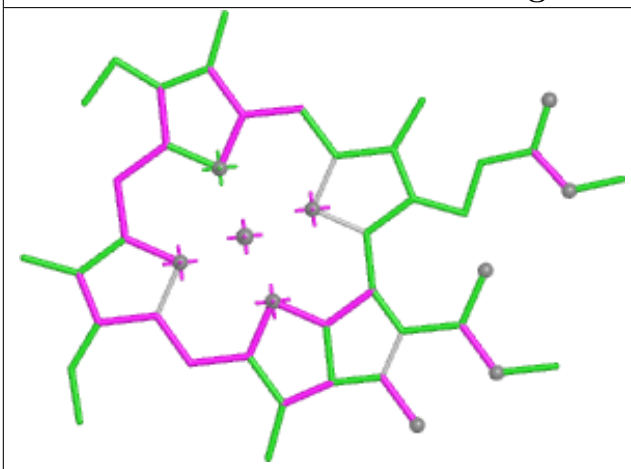


Torsions

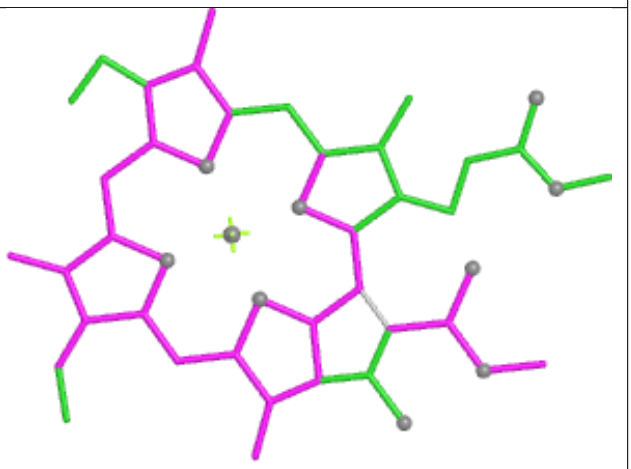


Rings

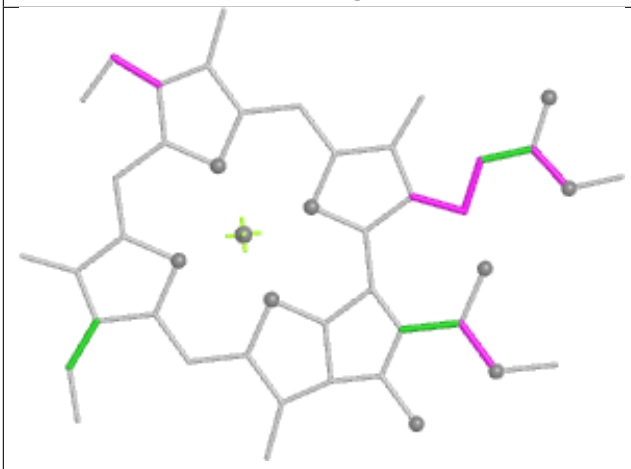
Ligand CLA 9 319



Bond lengths



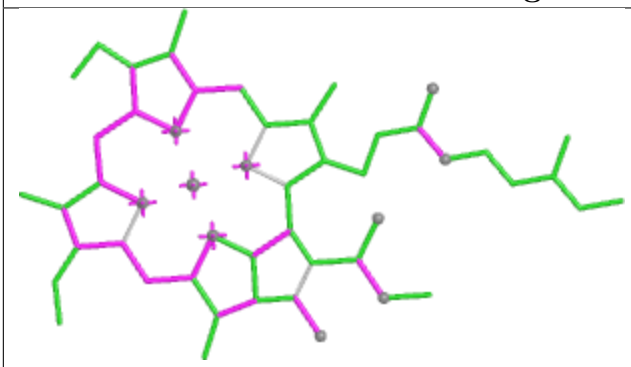
Bond angles



Torsions

Rings

Ligand CLA A 852



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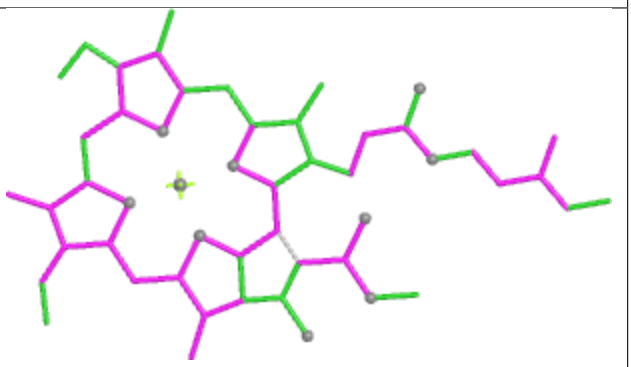
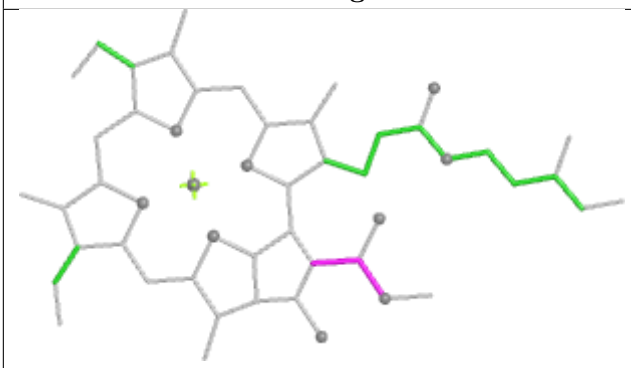
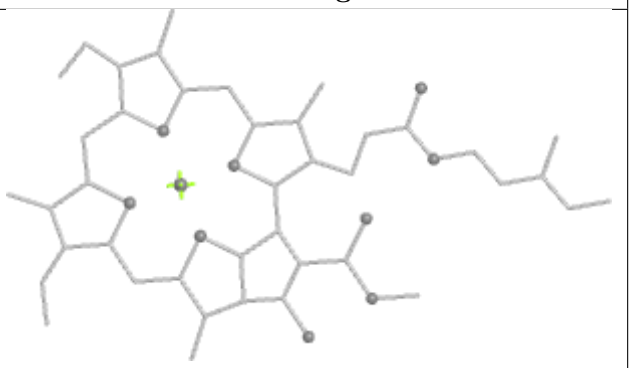


Bond angles



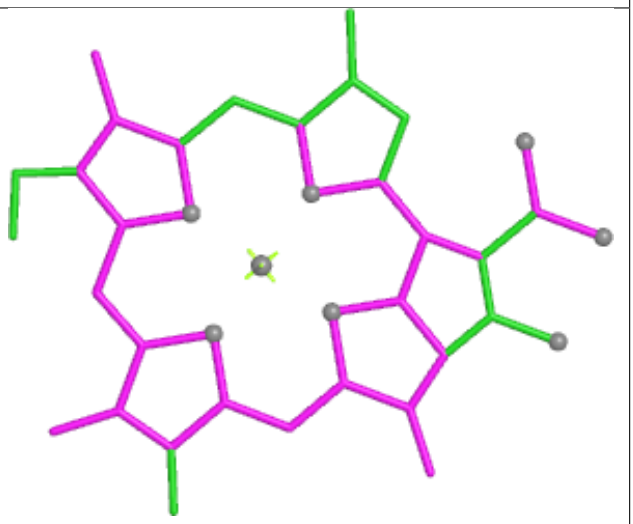
Torsions



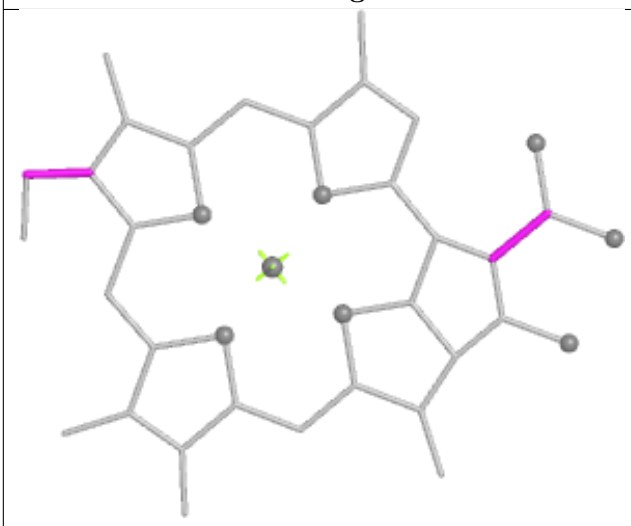
Rings

Ligand CLA O 202

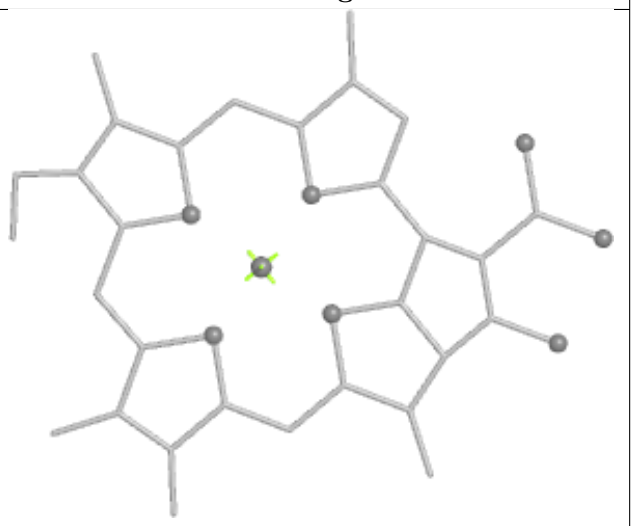
Bond lengths



Bond angles

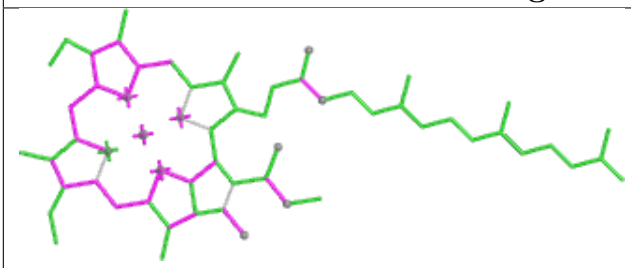


Torsions

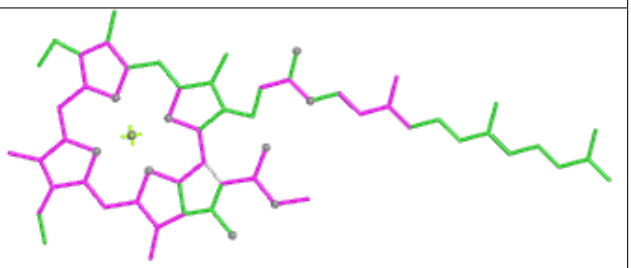


Rings

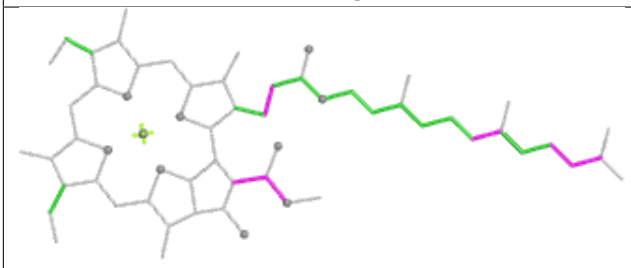
Ligand CLA 9 314



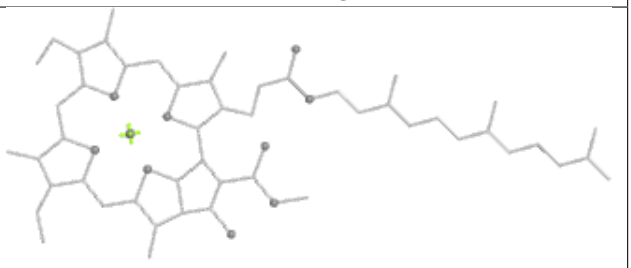
Bond lengths



Bond angles

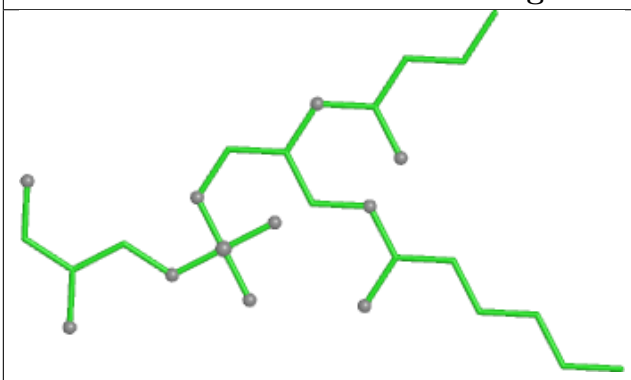


Torsions



Rings

Ligand LHG 6 301



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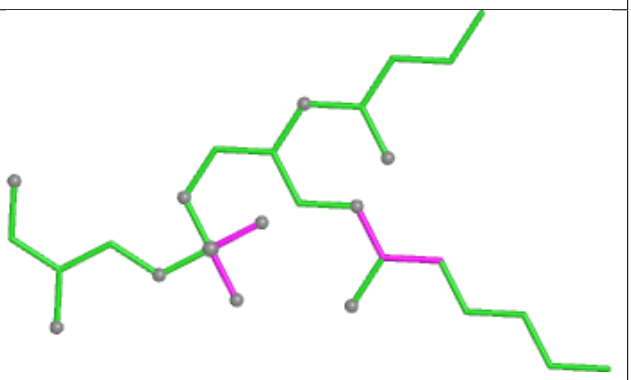
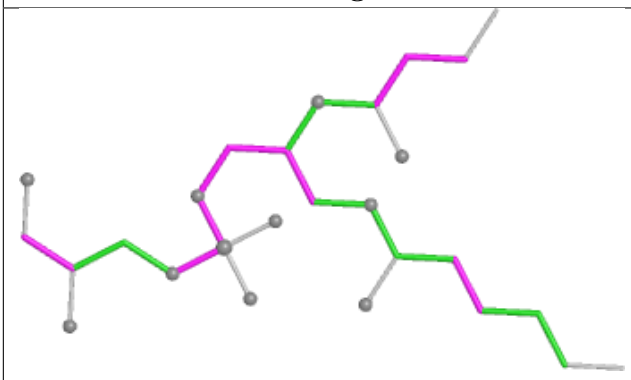
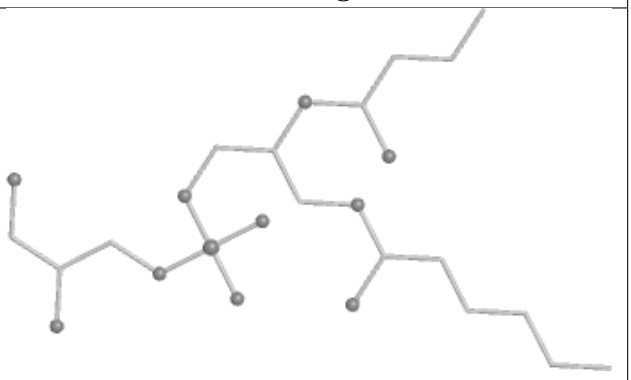


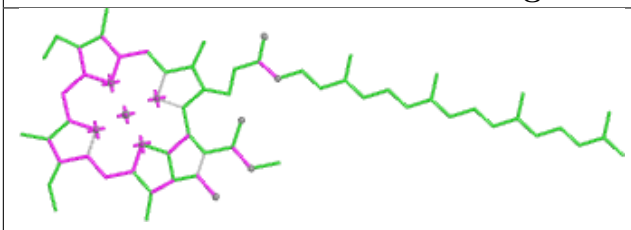
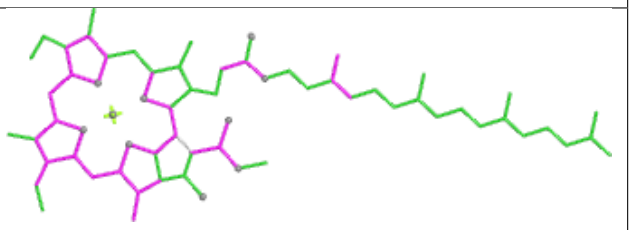
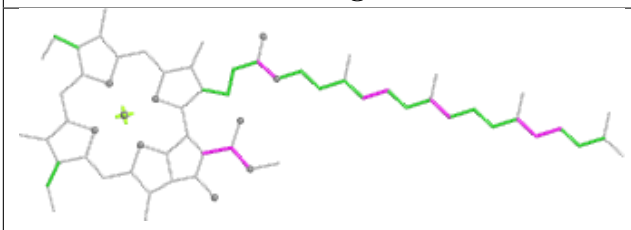
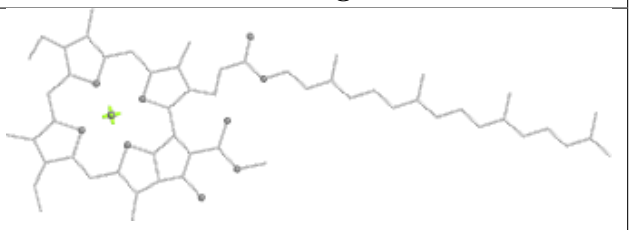
Bond angles

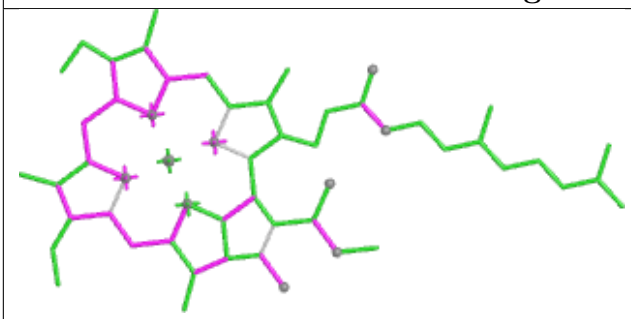
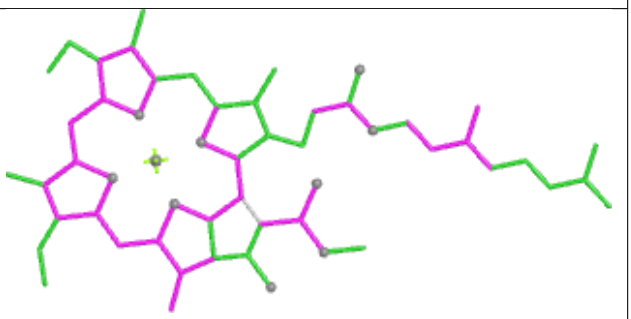
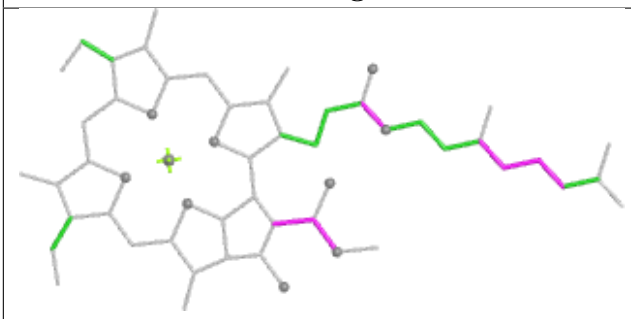
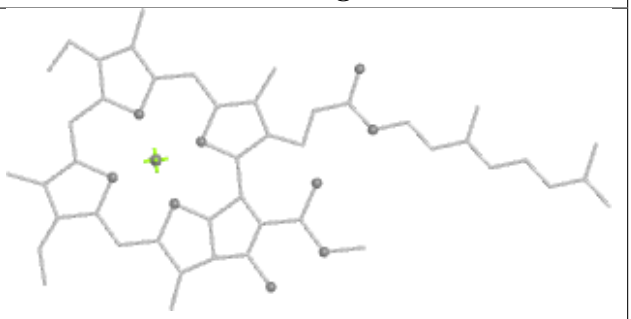


Torsions

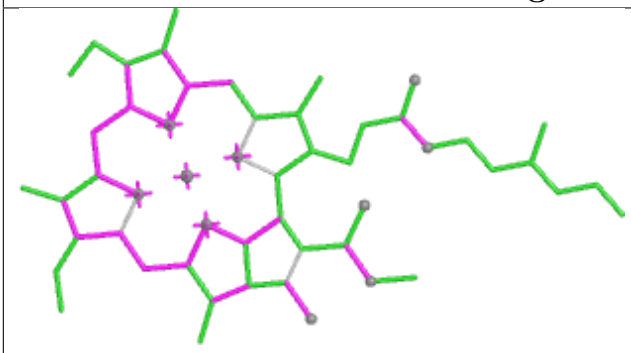


Rings

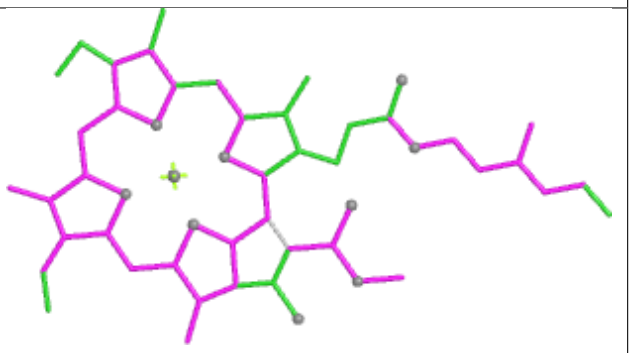
Ligand CLA A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

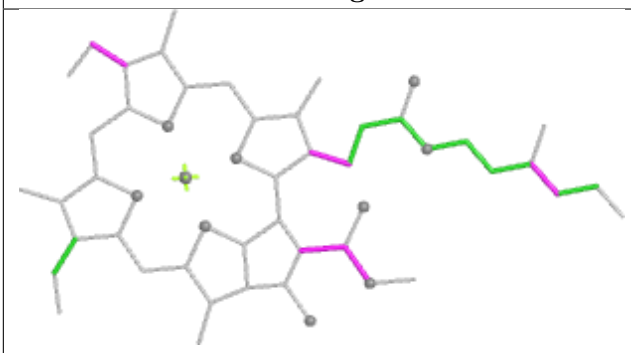
Ligand CLA 8 315



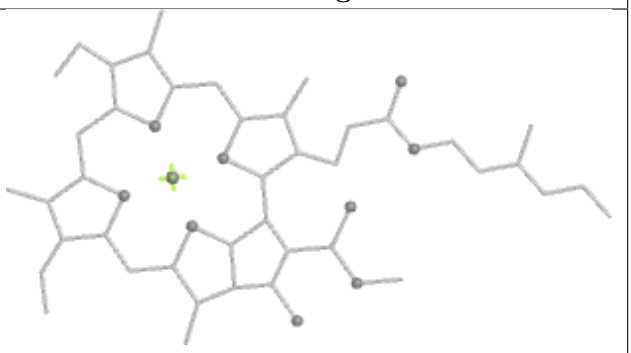
Bond lengths



Bond angles

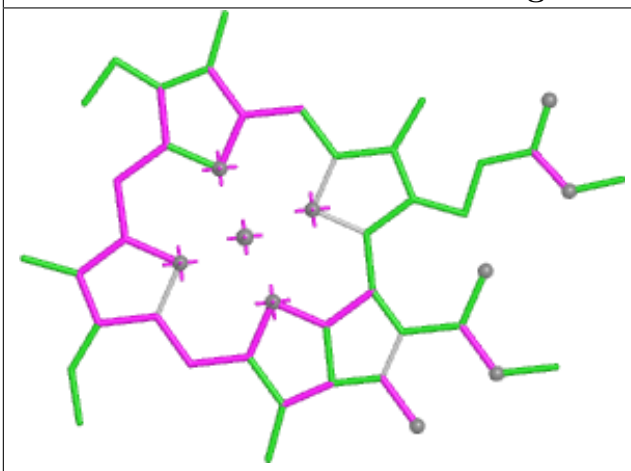


Torsions



Rings

Ligand CLA b 311



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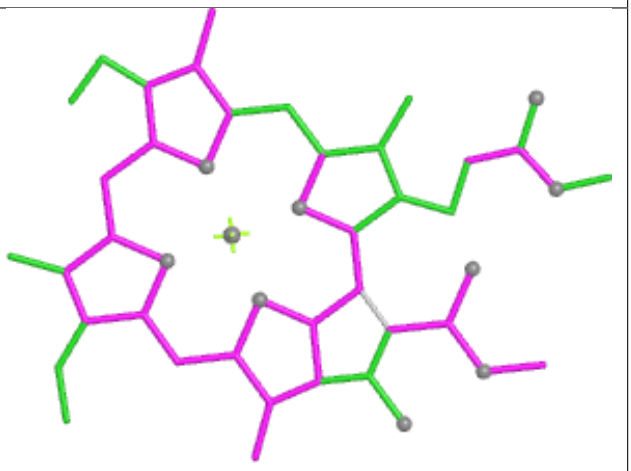
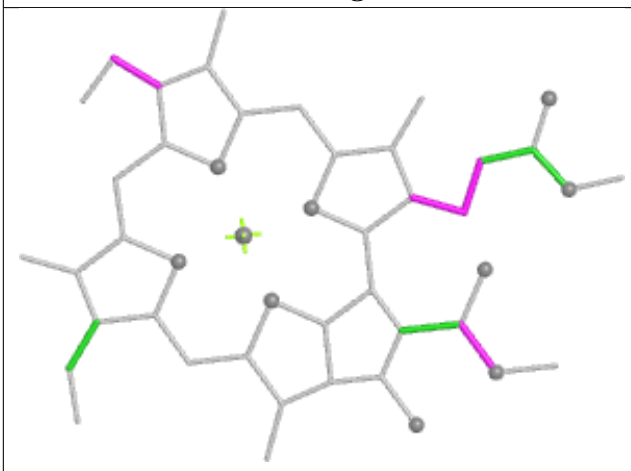
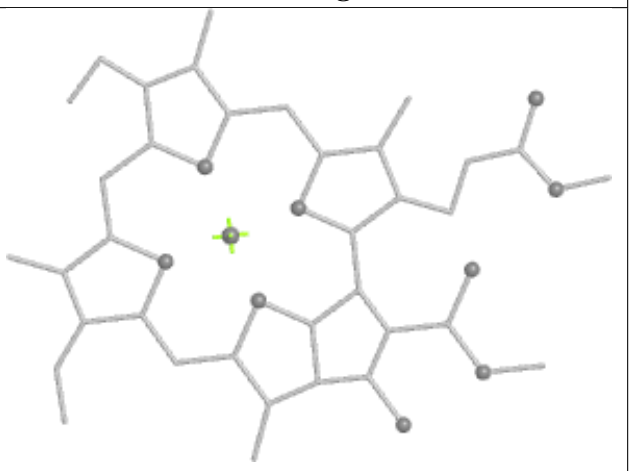


Bond angles

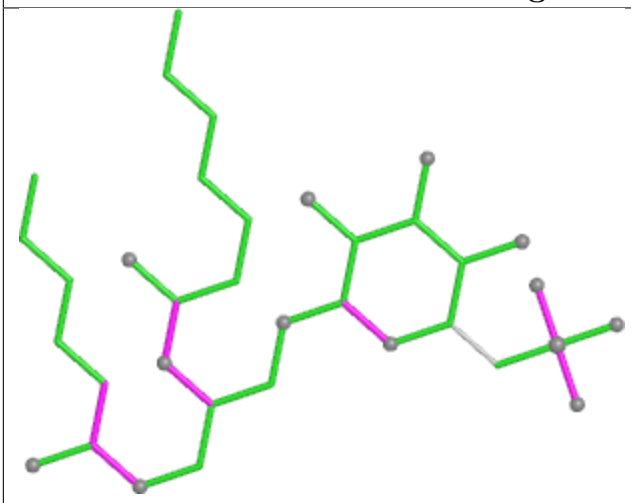


Torsions

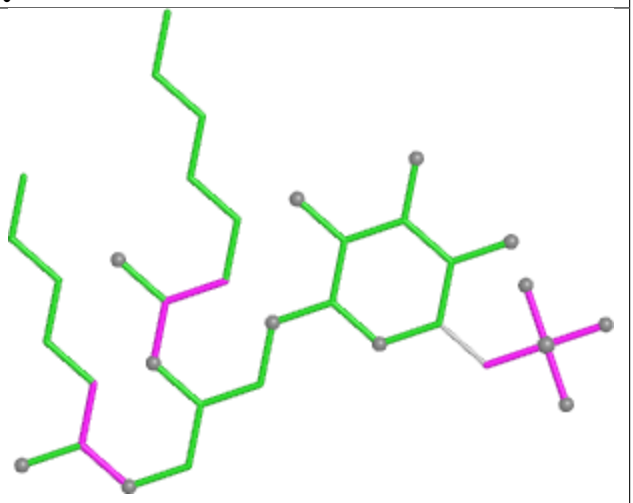


Rings

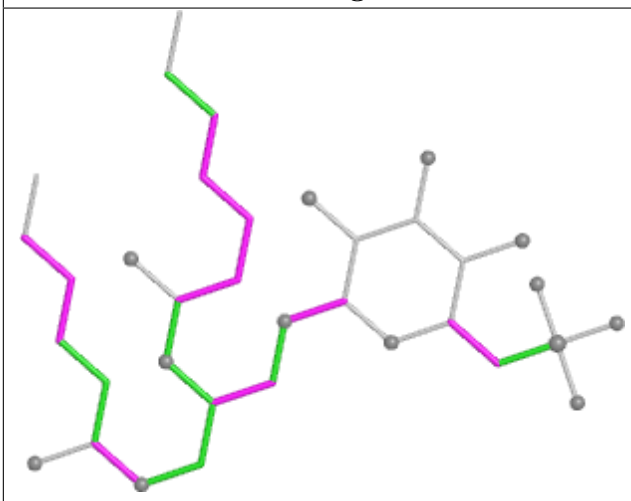
Ligand SQD 4 304



Bond lengths



Bond angles



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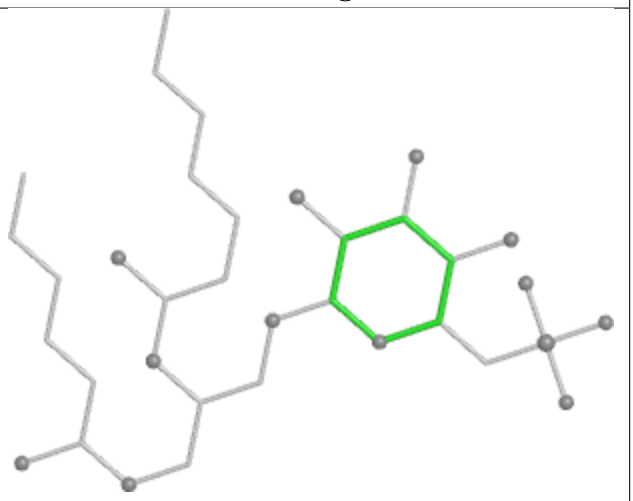
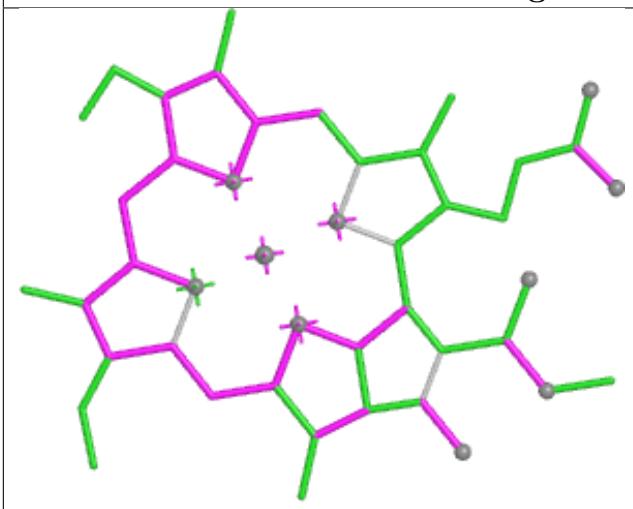
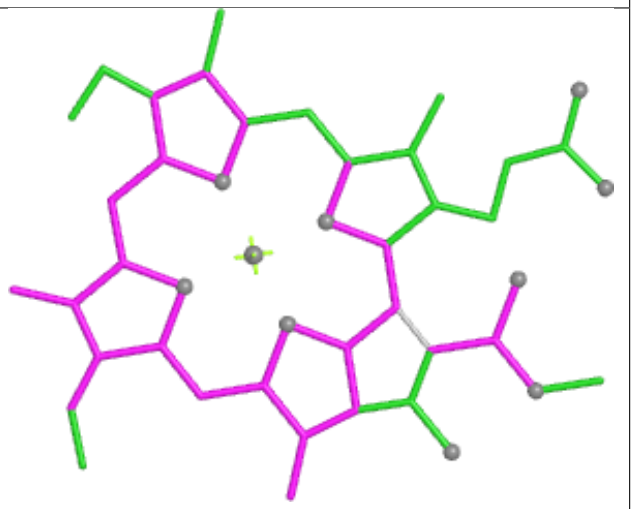


Rings

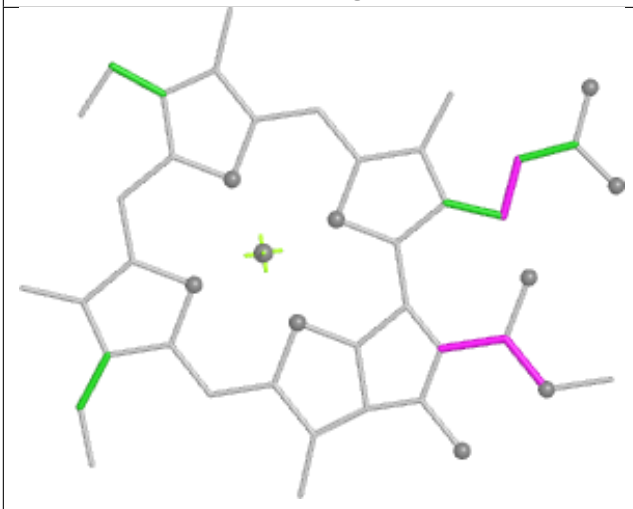
Ligand CLA 9 313



Bond lengths



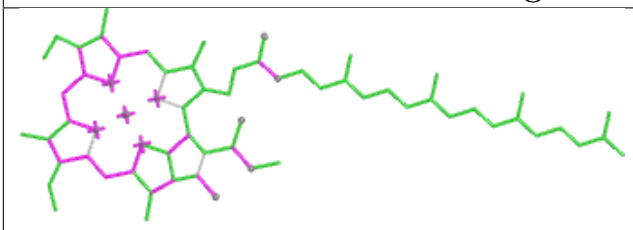
Bond angles



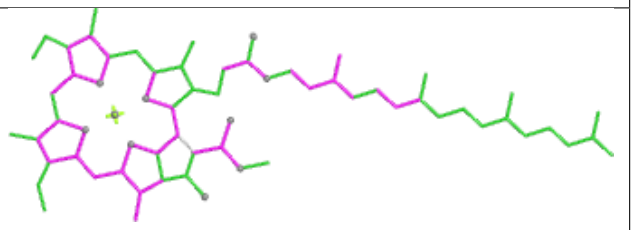
Torsions

Rings

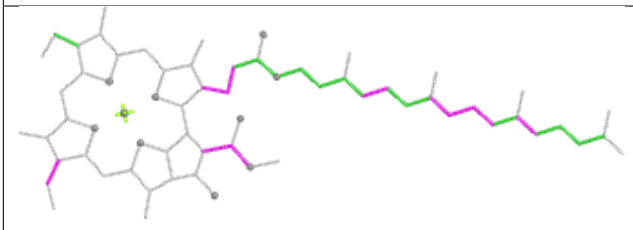
Ligand CLA B 822



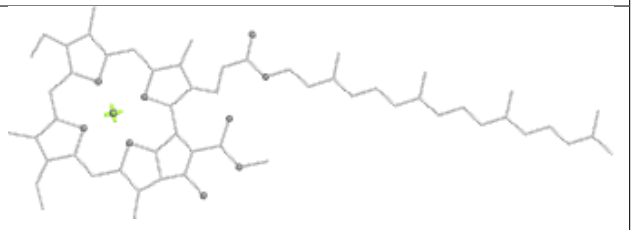
Bond lengths



Bond angles

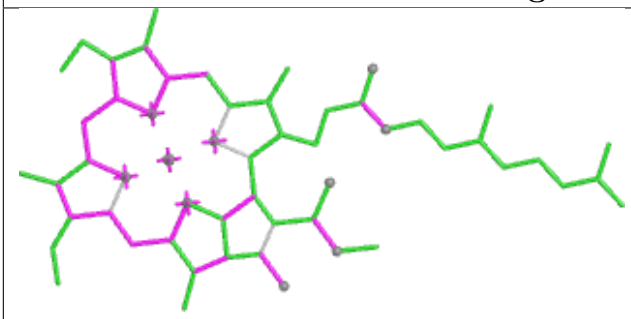


Torsions

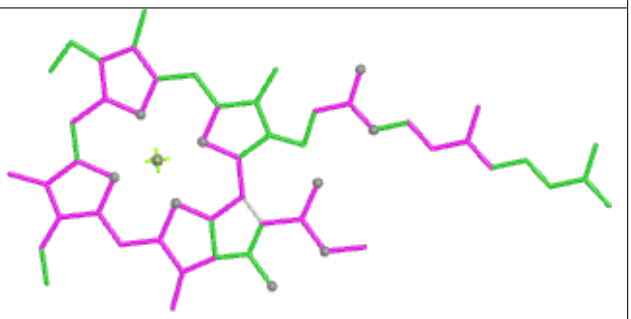


Rings

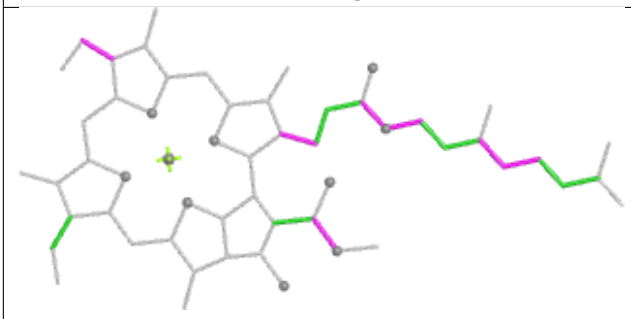
Ligand CLA 8 311



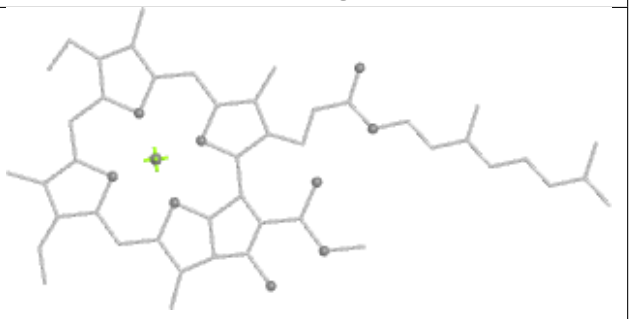
Bond lengths



Bond angles

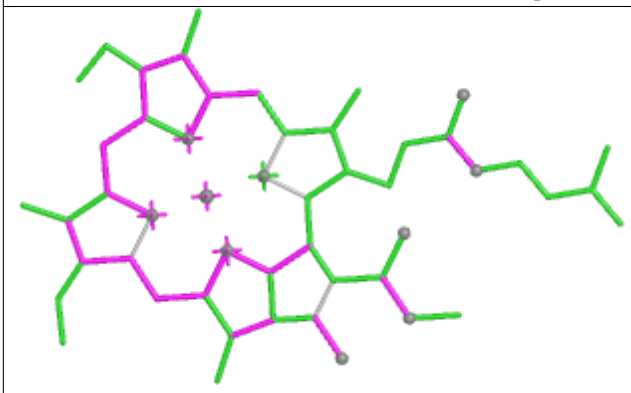


Torsions



Rings

Ligand CLA 9 316



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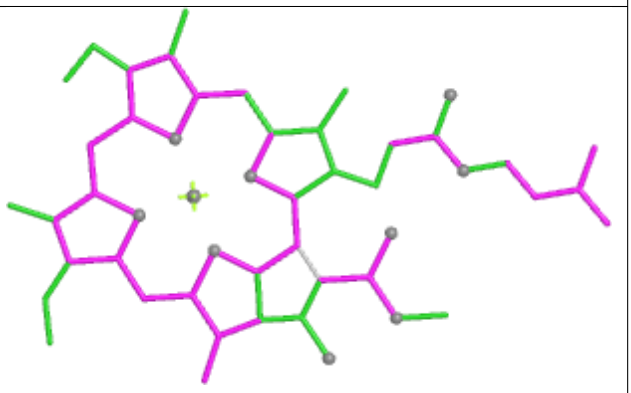

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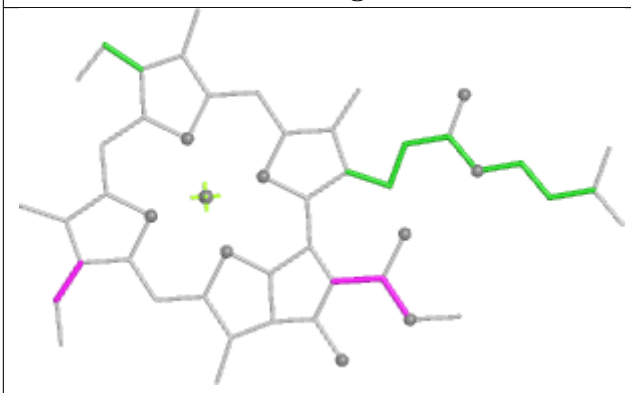

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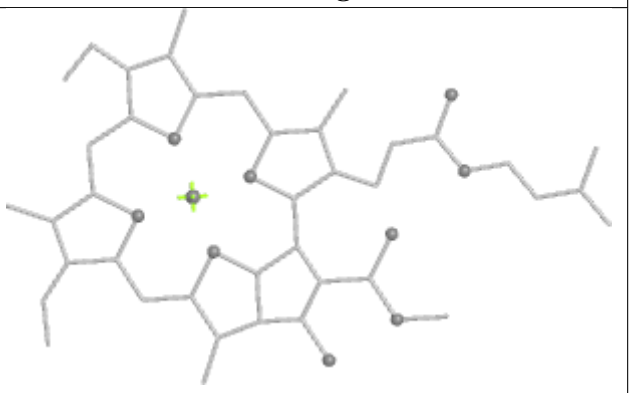
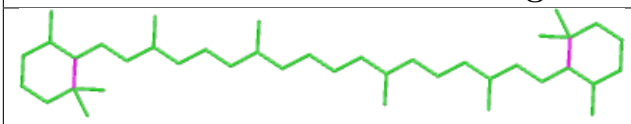


Rings

Ligand BCR 5 302



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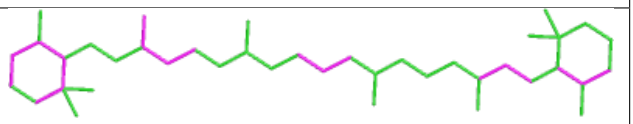
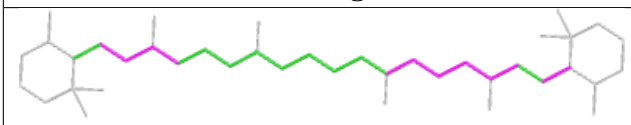


Bond angles



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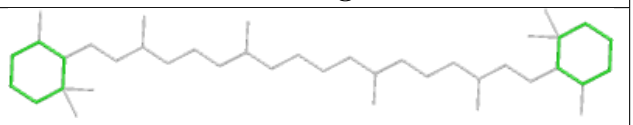
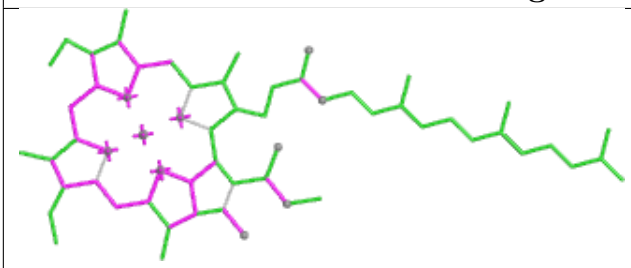


Rings

Ligand CLA a 313



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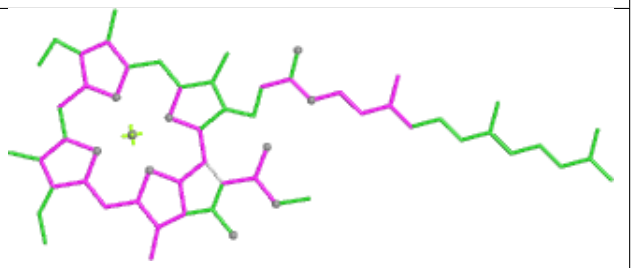
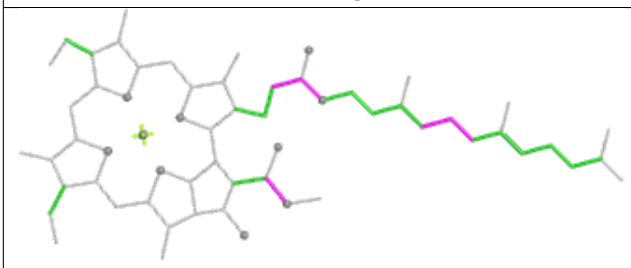


Bond angles



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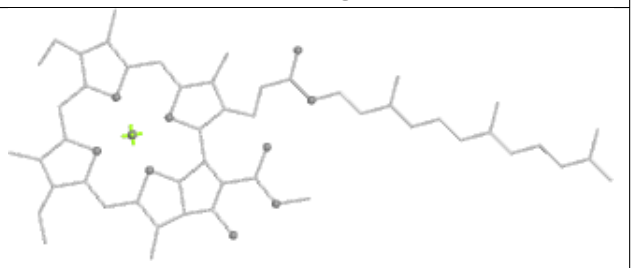
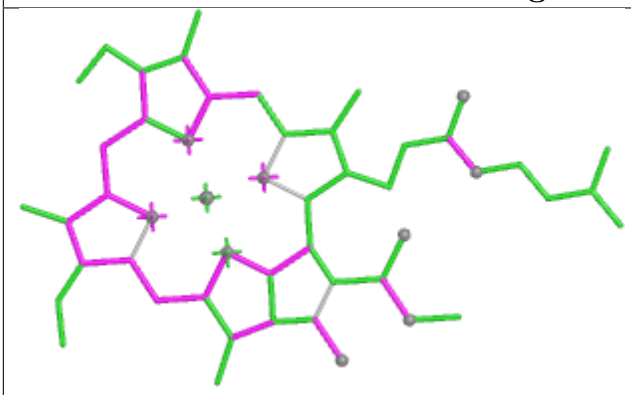


Rings

Ligand CLA 5 312



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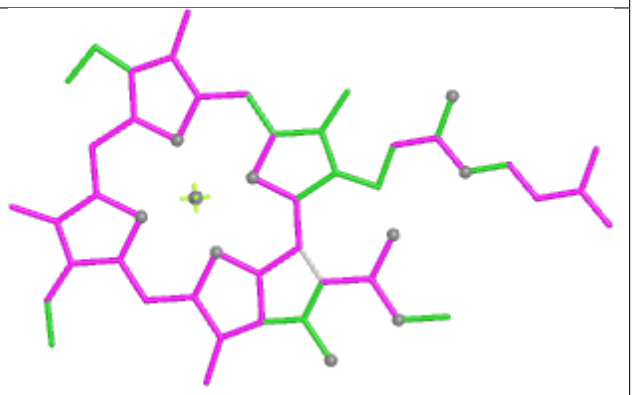
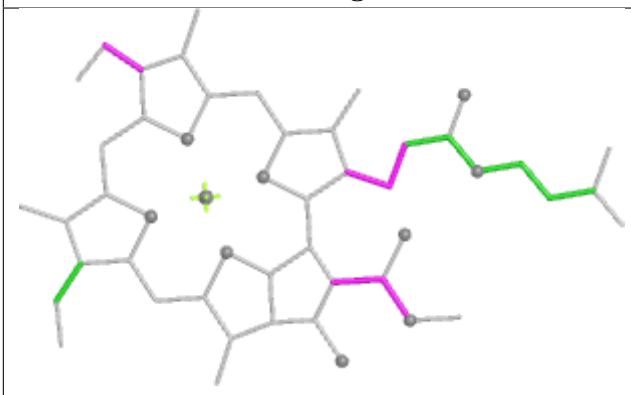
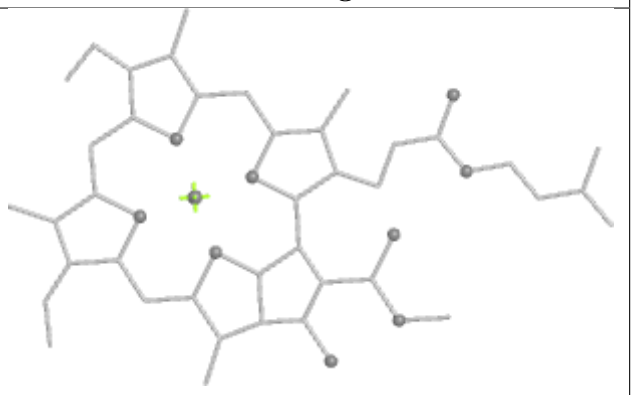


Bond angles

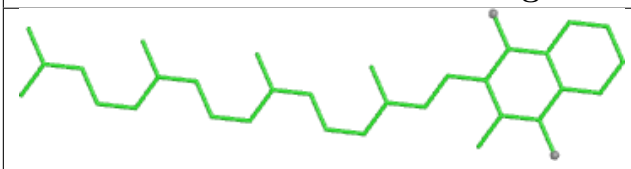


Torsions



Rings

Ligand PQN B 801



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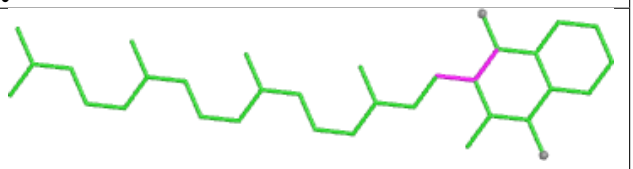
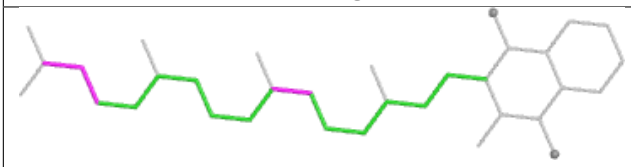


Bond angles



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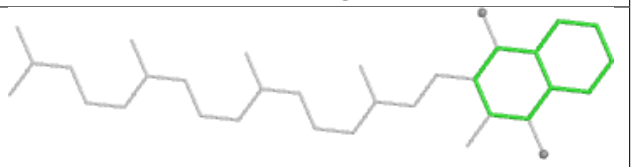
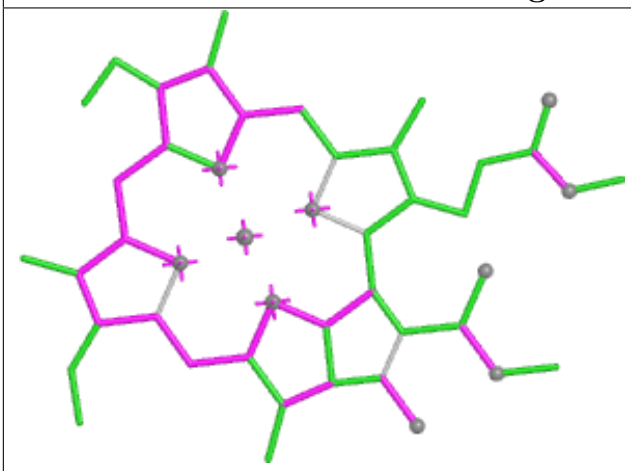
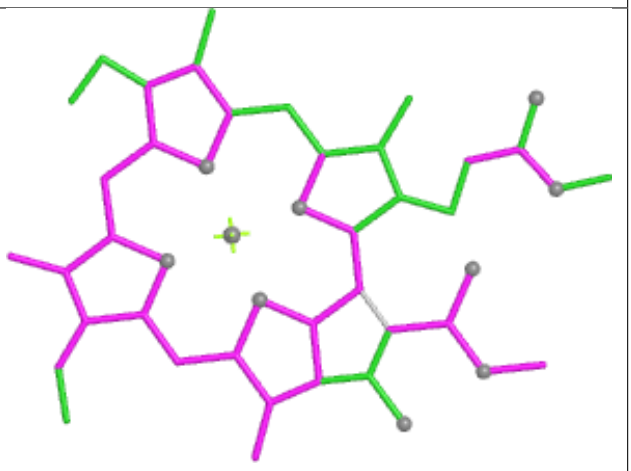


Rings

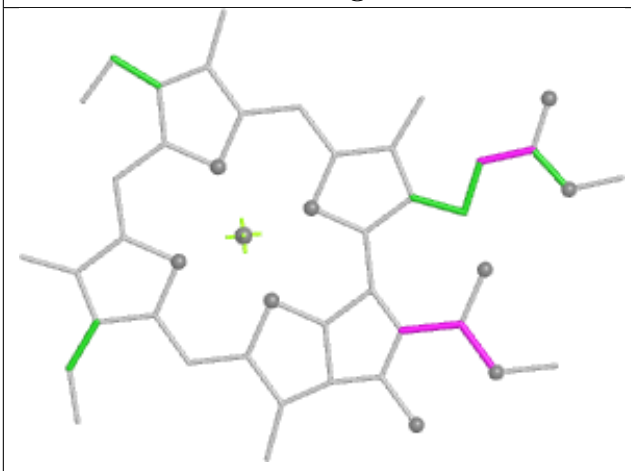
Ligand CLA 6 313



Bond lengths



Bond angles



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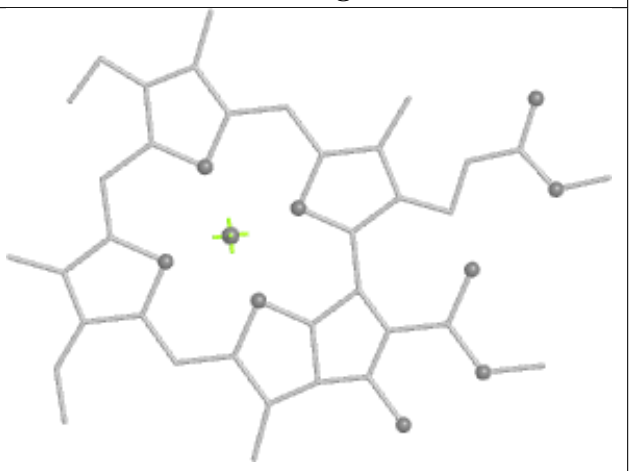
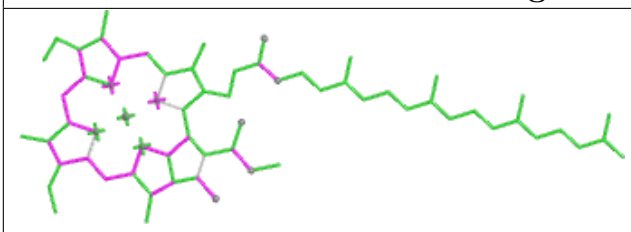


Rings

Ligand CLA a 319



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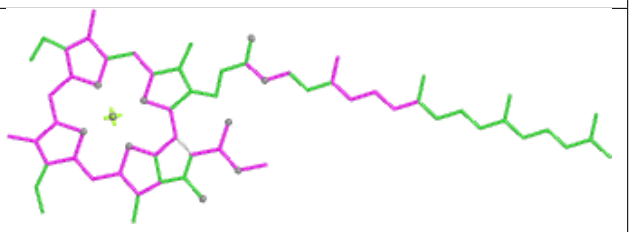
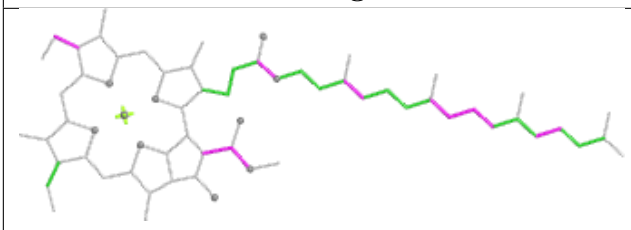


Bond angles



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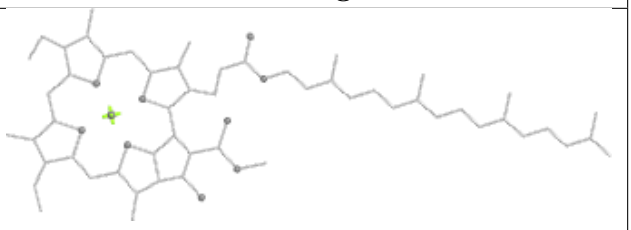
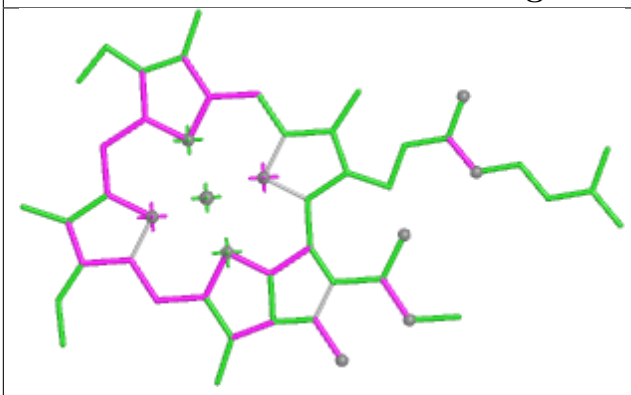


Rings

Ligand CLA F 306



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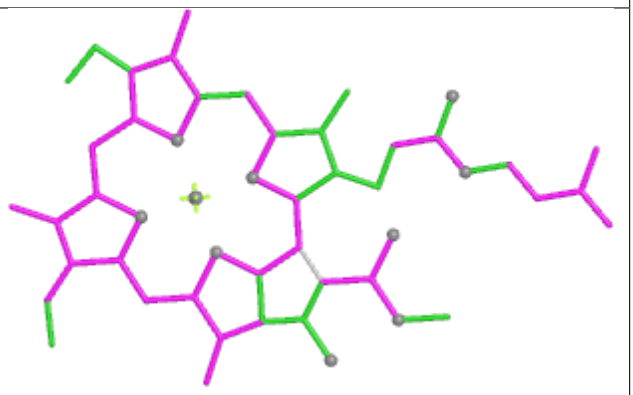
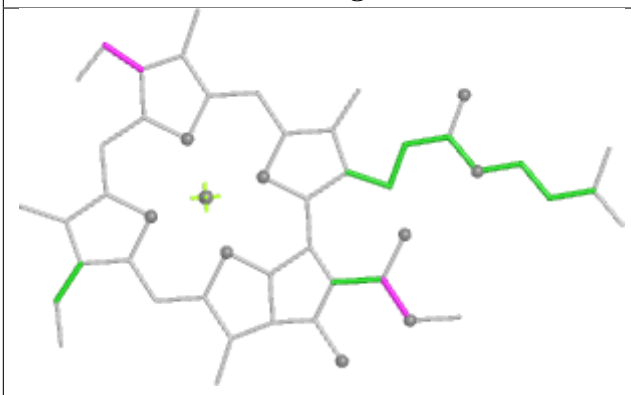
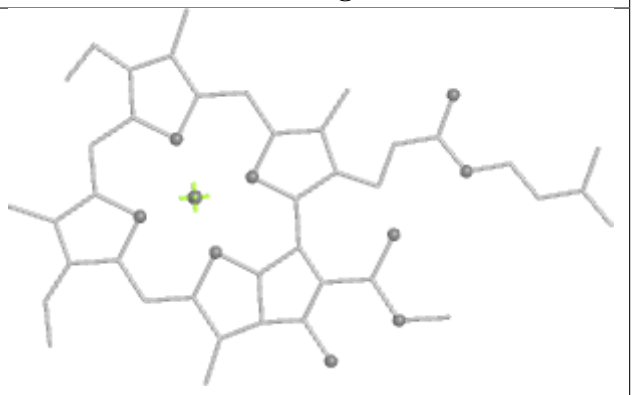


Bond angles



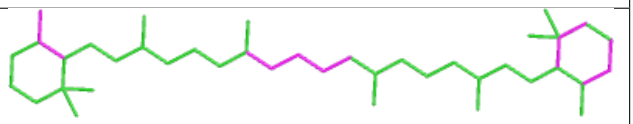
Torsions



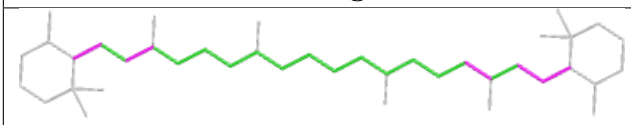
Rings

Ligand BCR A 805

Bond lengths



Bond angles



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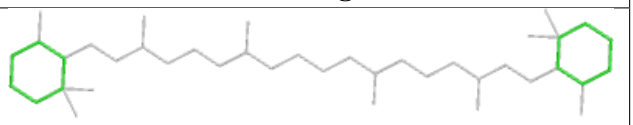
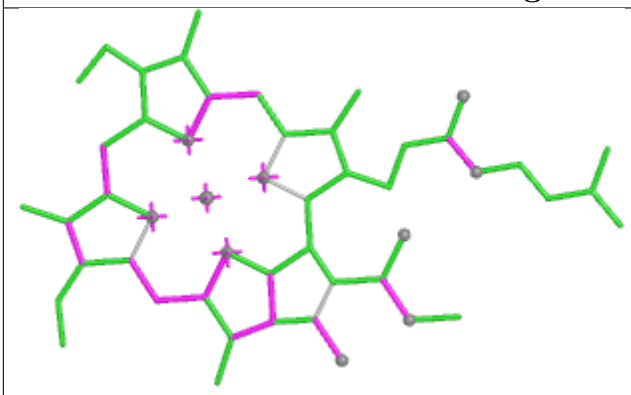


Rings

Ligand CLA A 829



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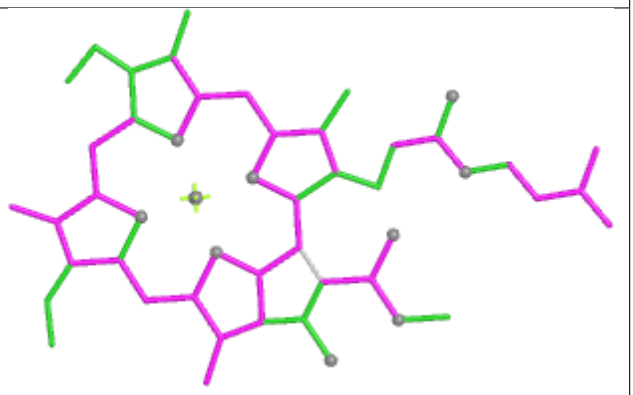
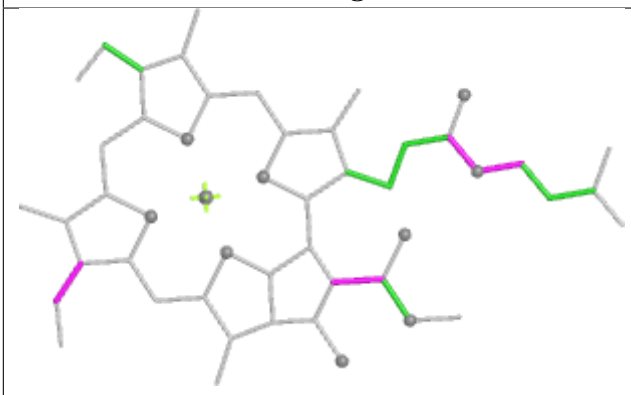
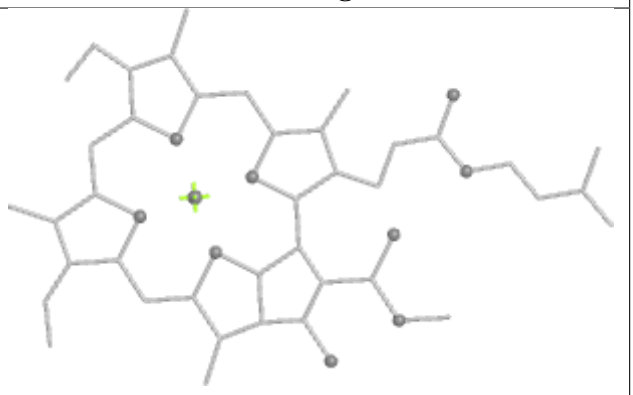


Bond angles

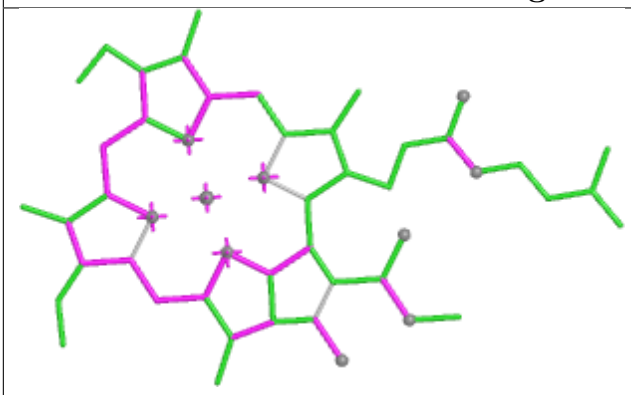


Torsions



Rings

Ligand CLA 8 309



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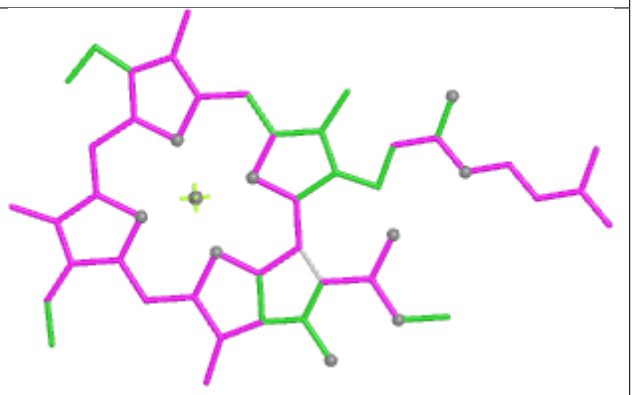
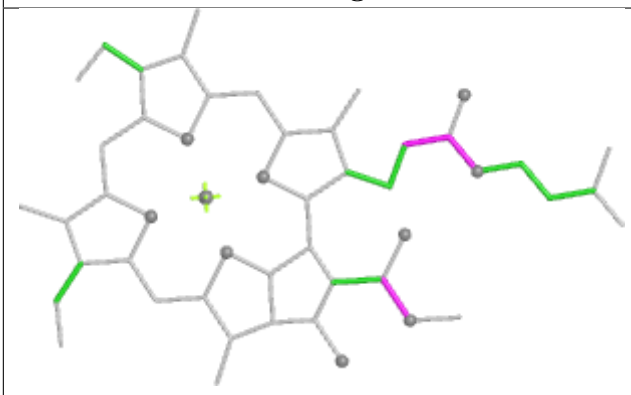
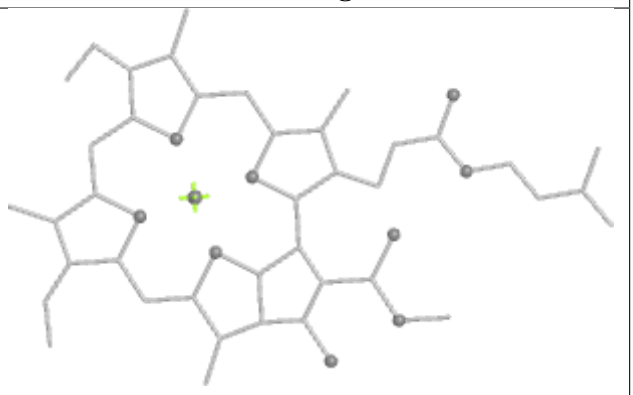


Bond angles



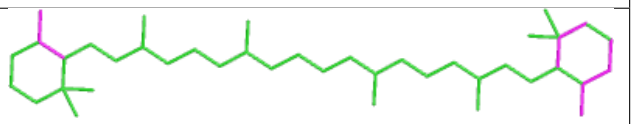
Torsions



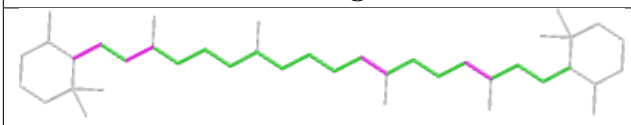
Rings

Ligand BCR I 801

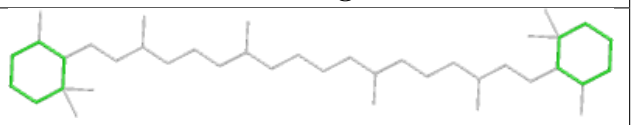
Bond lengths



Bond angles

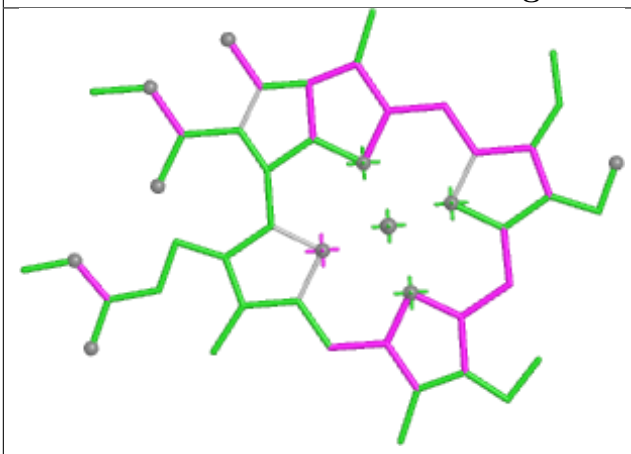


Torsions

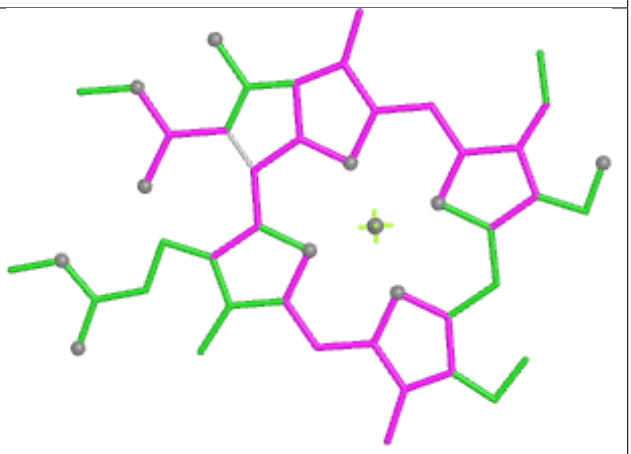


Rings

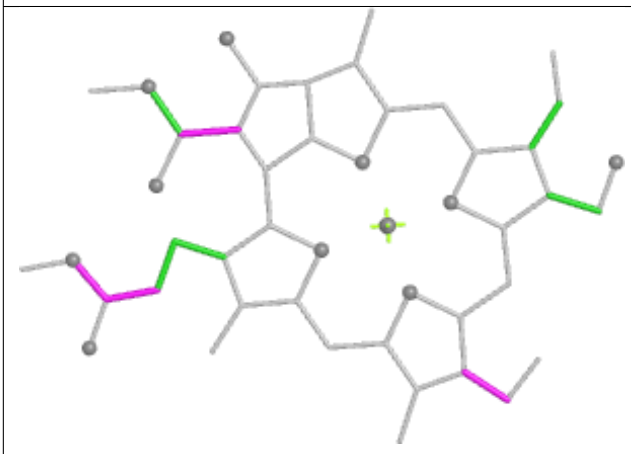
Ligand CHL K 201



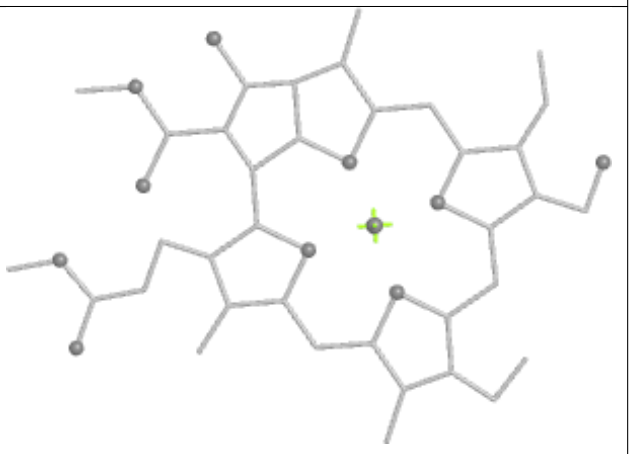
Bond lengths



Bond angles

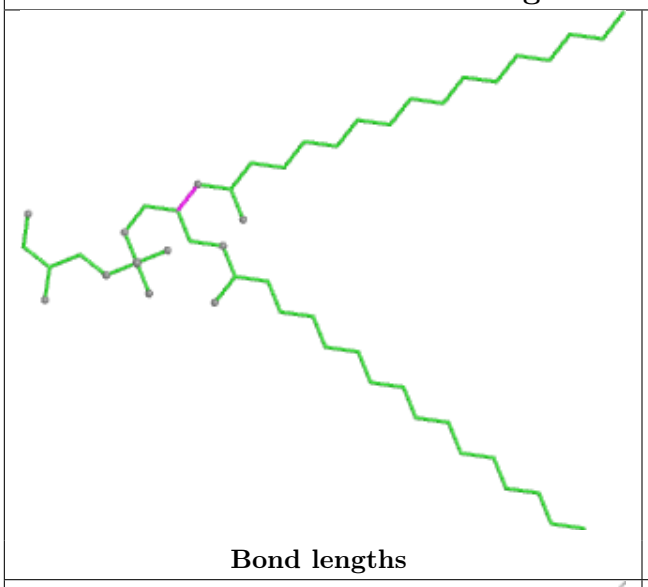


Torsions

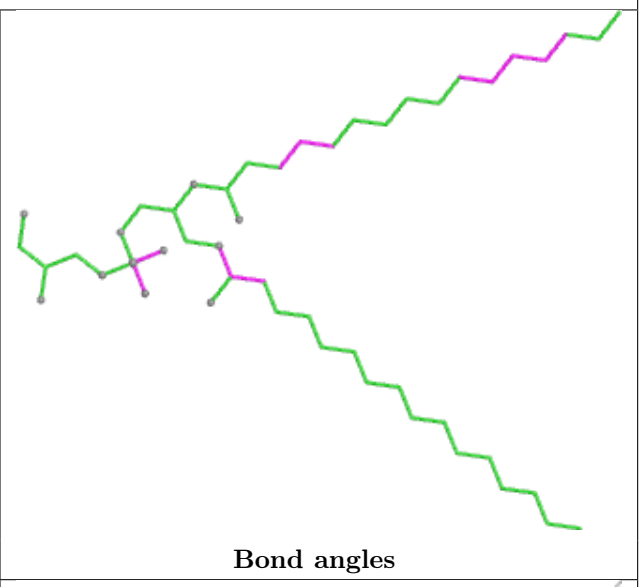


Rings

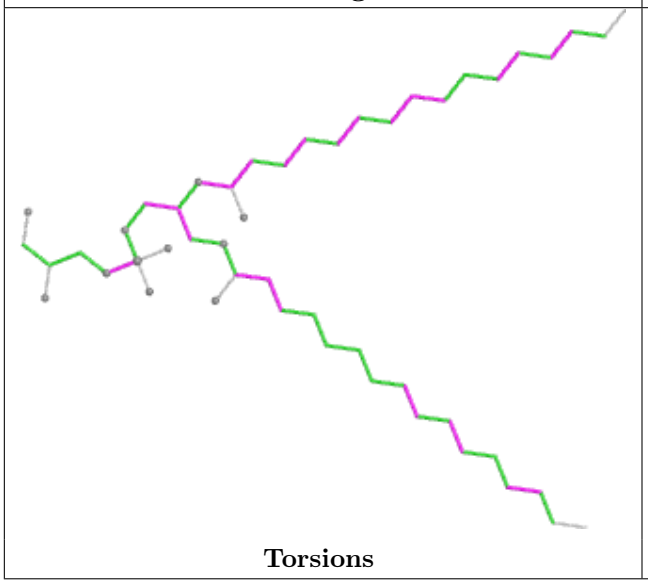
Ligand LHG A 811



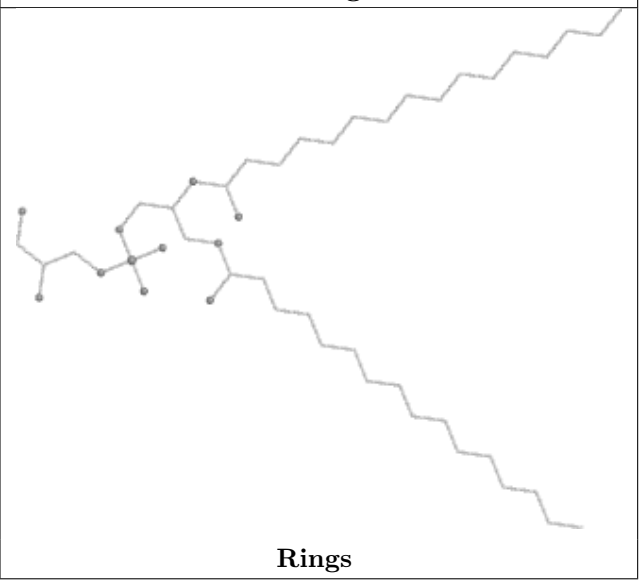
Bond lengths



Bond angles

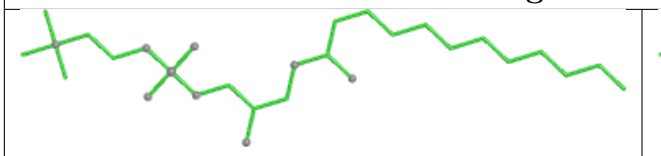


Torsions

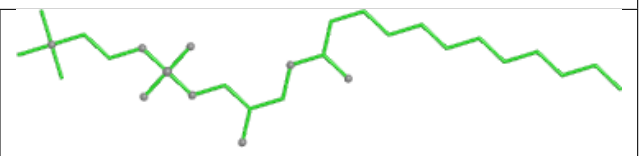


Rings

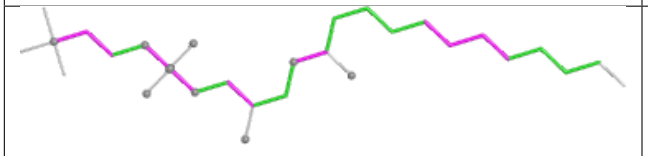
Ligand LAP B 851



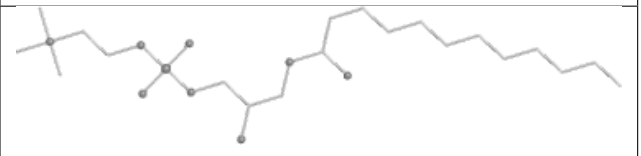
Bond lengths



Bond angles

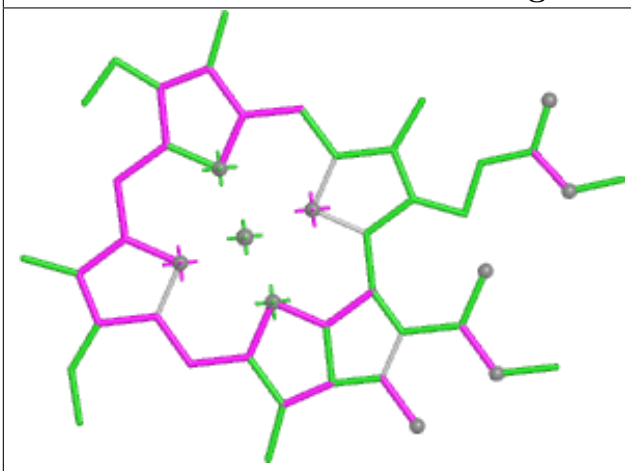


Torsions



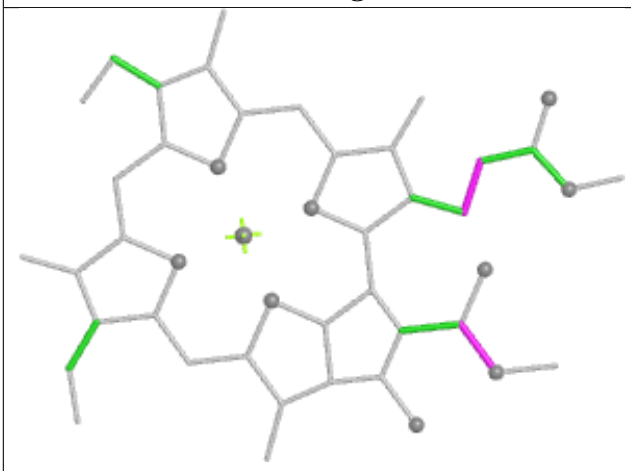
Rings

Ligand CLA 2 308

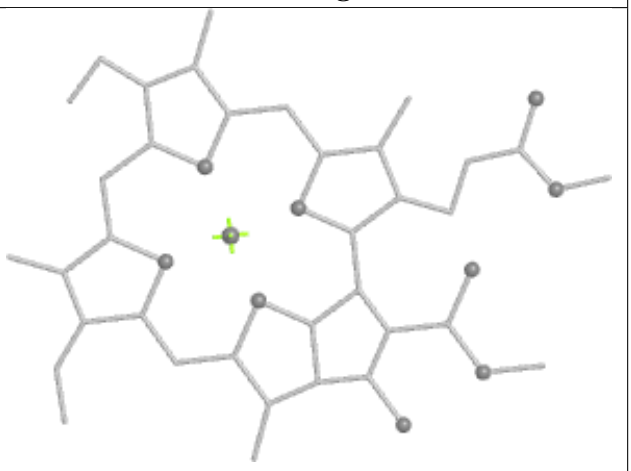


Bond lengths

Bond angles

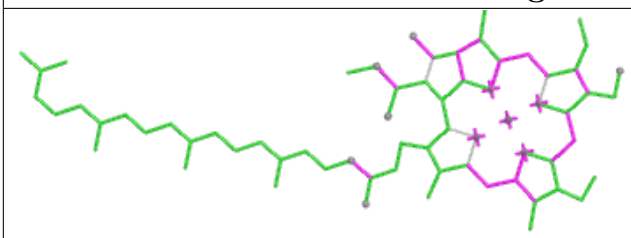


Torsions



Rings

Ligand CHL 7 318



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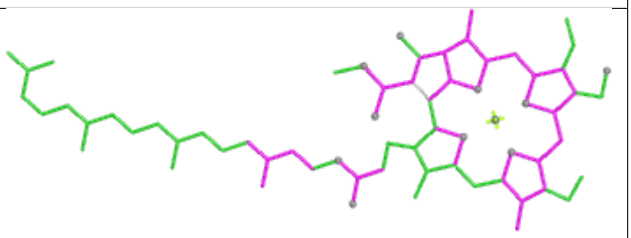
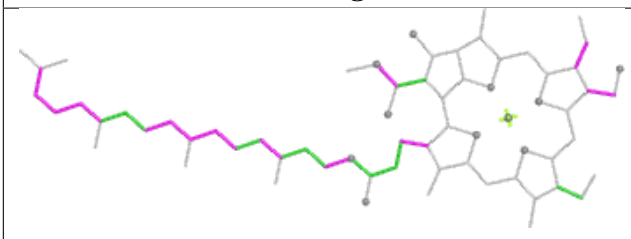
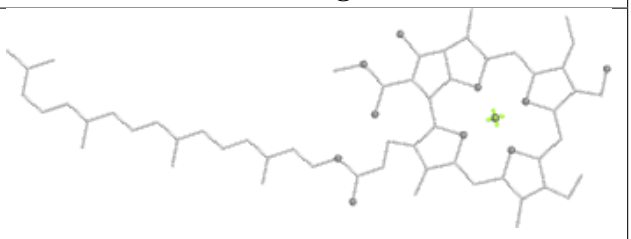


Bond angles

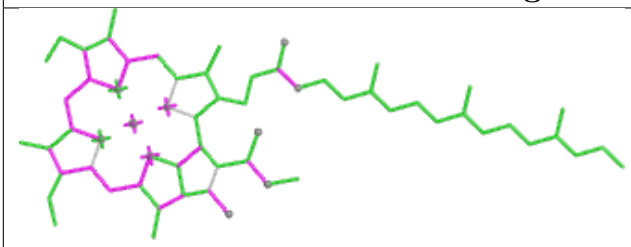


Torsions



Rings

Ligand CLA A 824



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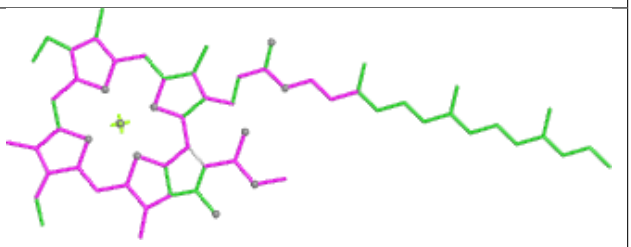
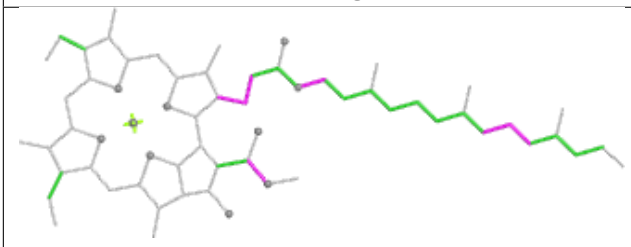
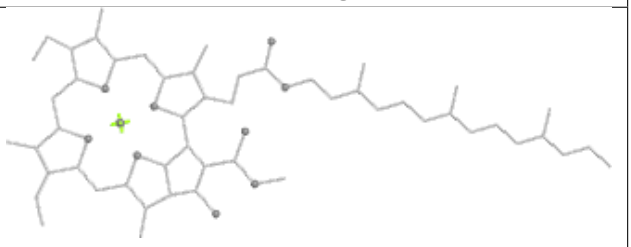


Bond angles

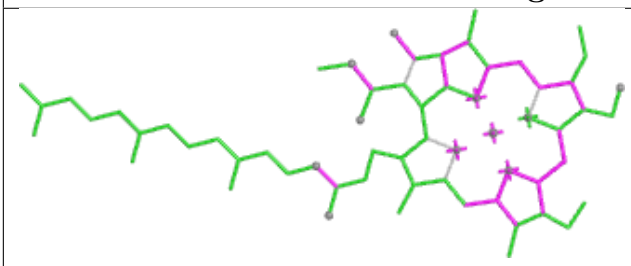


Torsions



Rings

Ligand CHL 7 320



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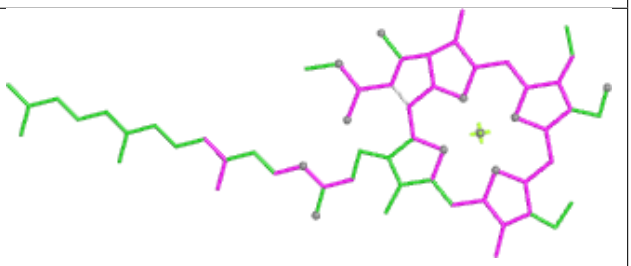
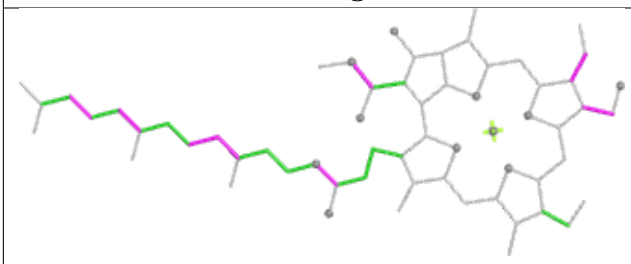


Bond angles



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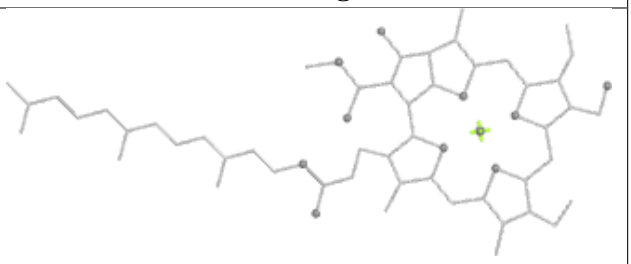
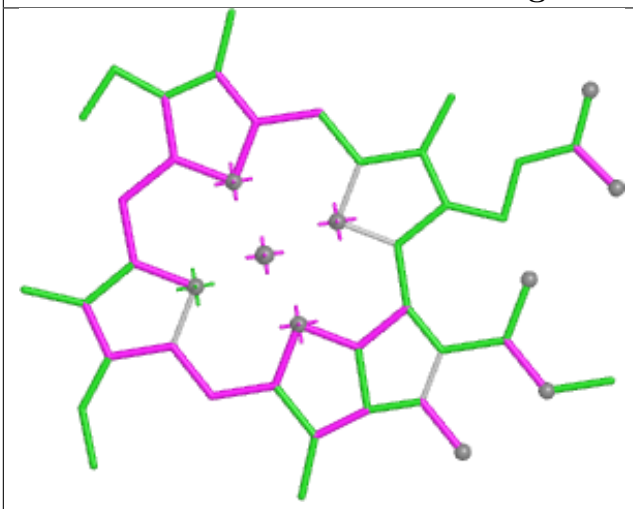
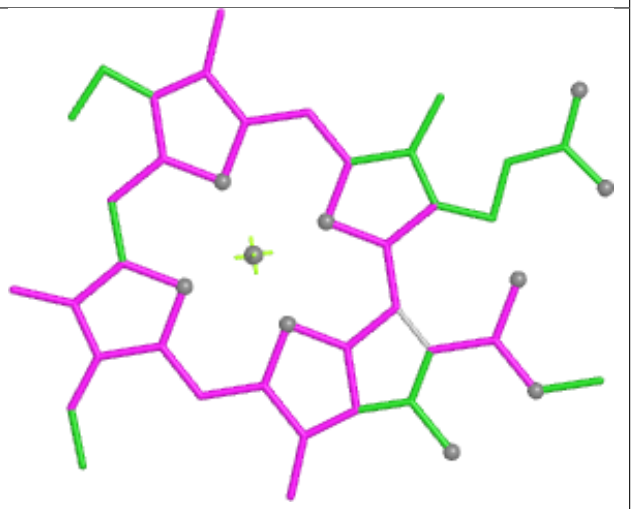


Rings

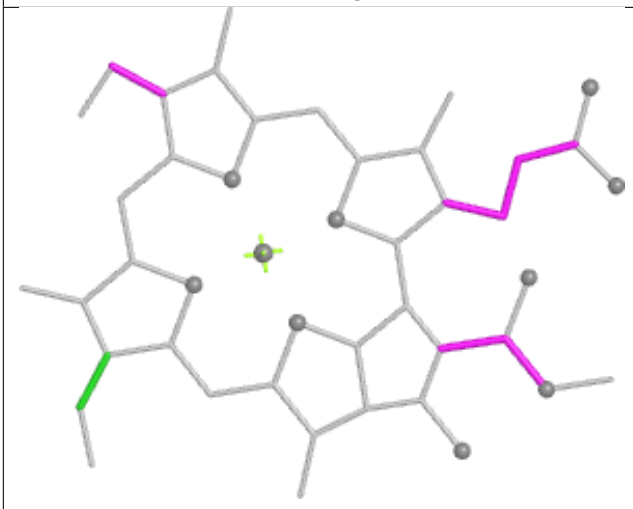
Ligand CLA a 316



Bond lengths



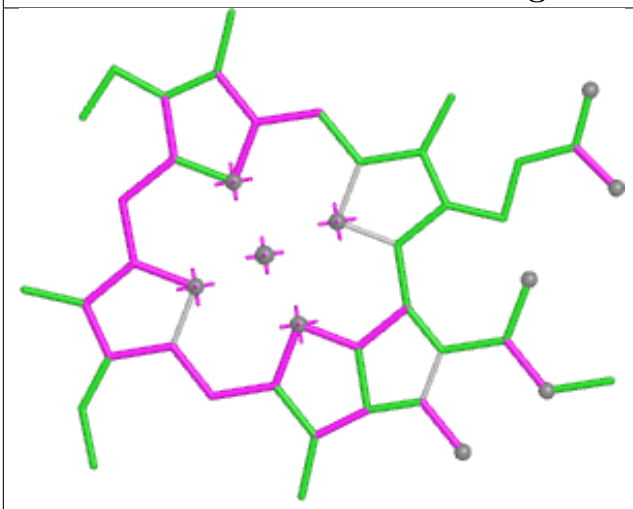
Bond angles



Torsions

Rings

Ligand CLA 4 306



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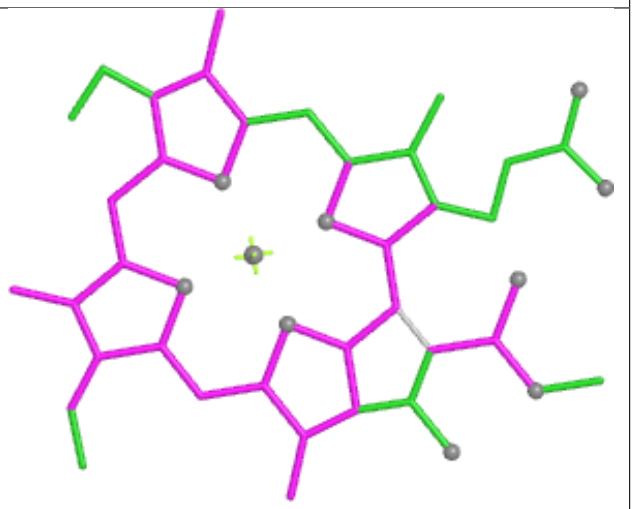
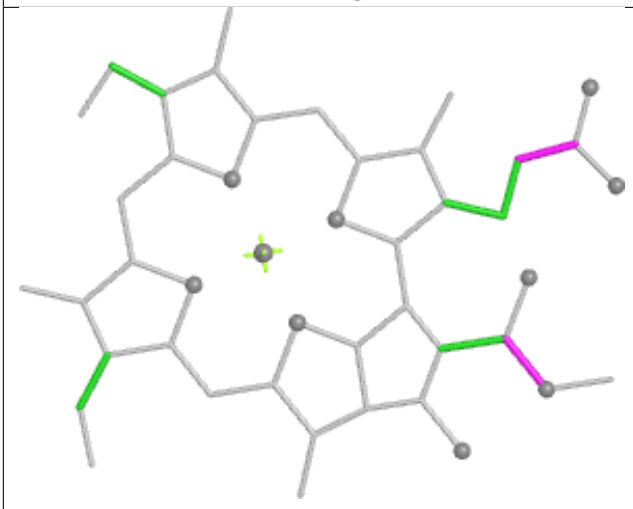


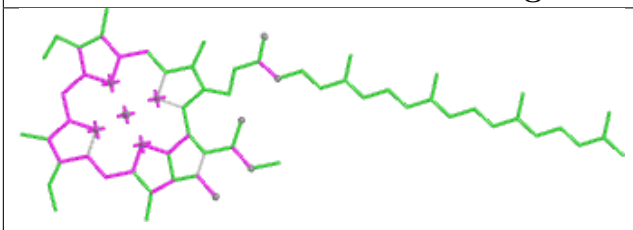
Bond angles



Torsions

Rings

Ligand CLA B 820



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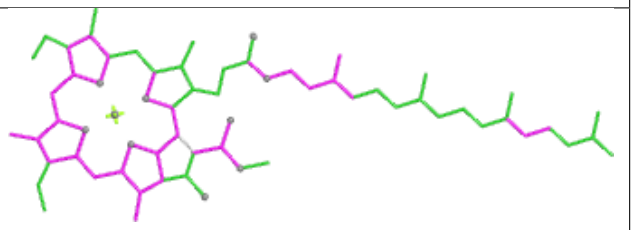
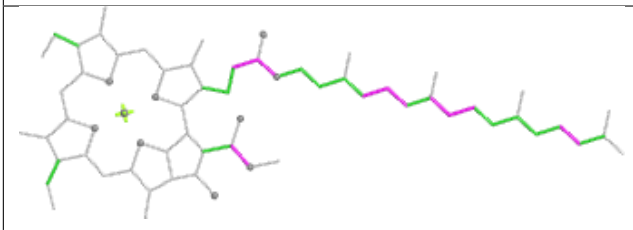
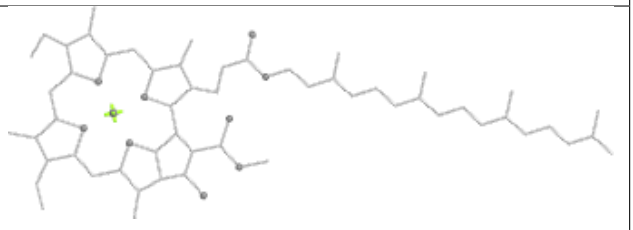


Bond angles

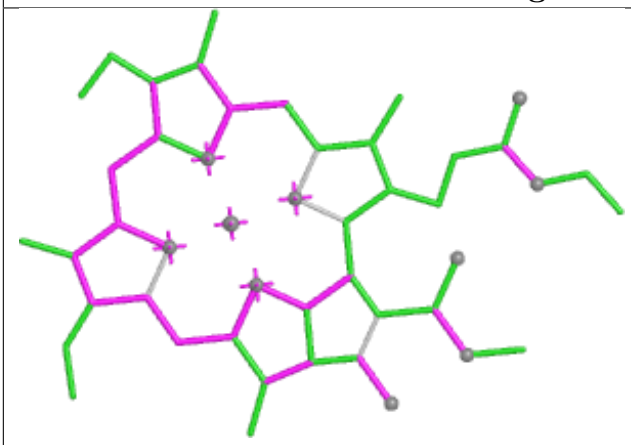


Torsions



Rings

Ligand CLA 6 310



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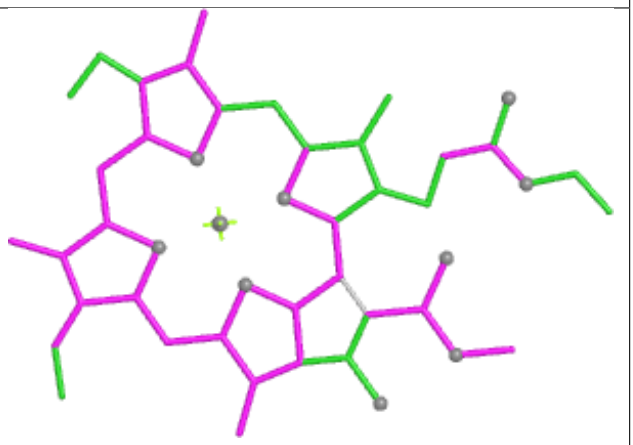
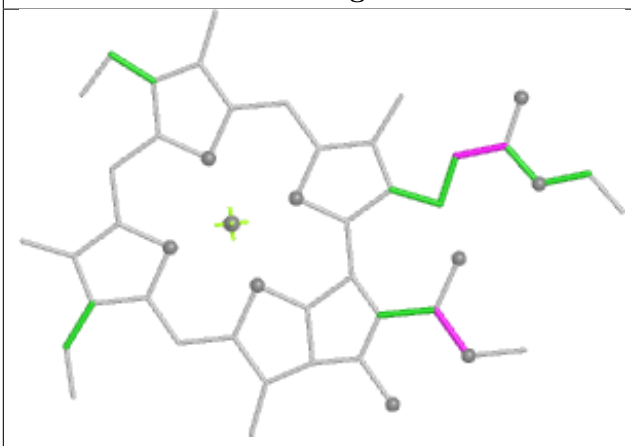
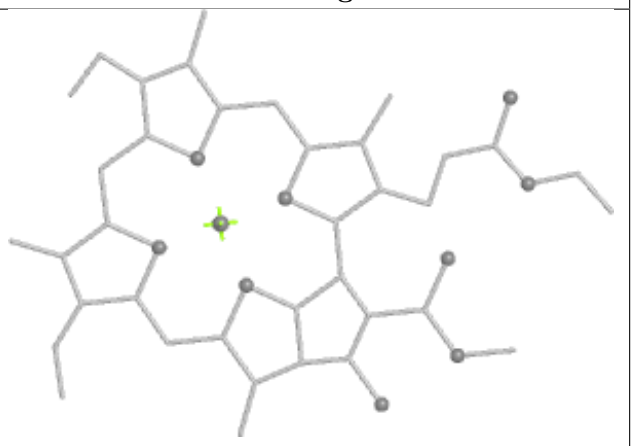


Bond angles

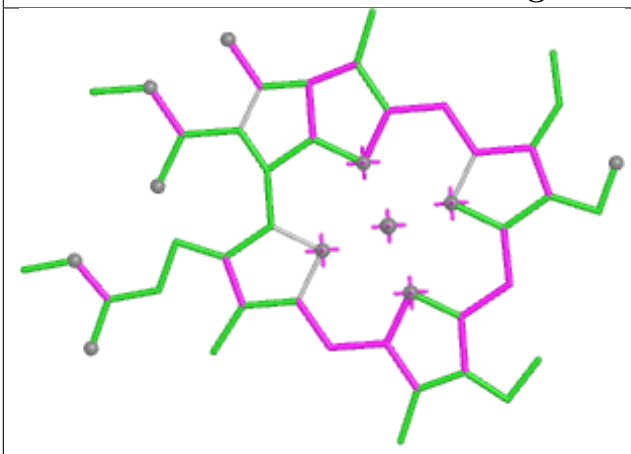


Torsions



Rings

Ligand CHL 9 322



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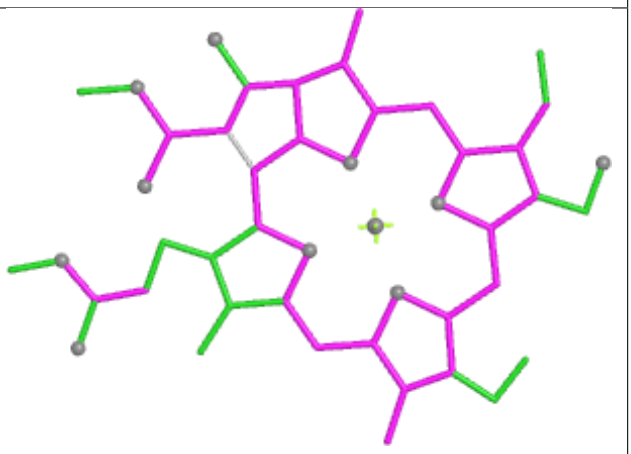
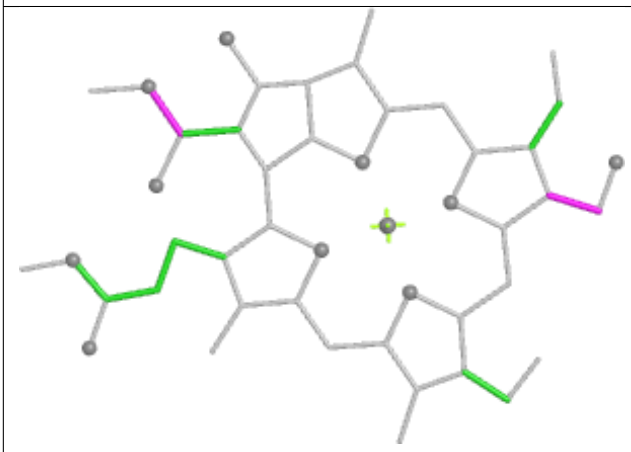


Bond angles



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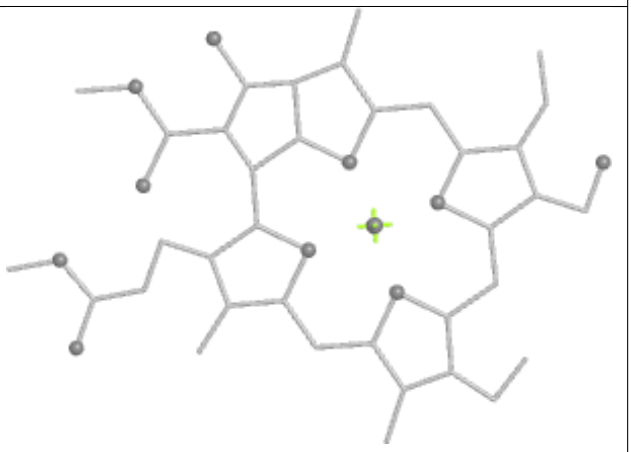
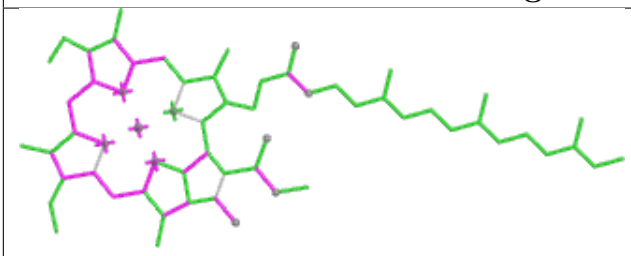
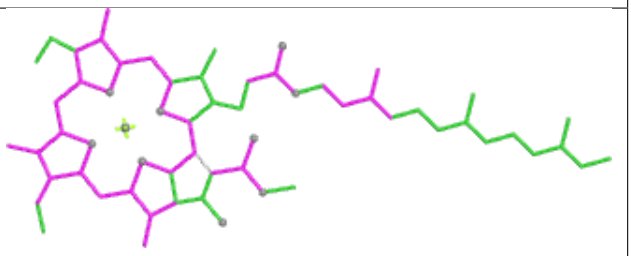


Rings

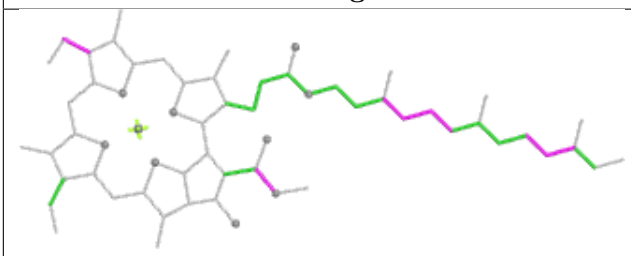
Ligand CLA B 842



Bond lengths



Bond angles



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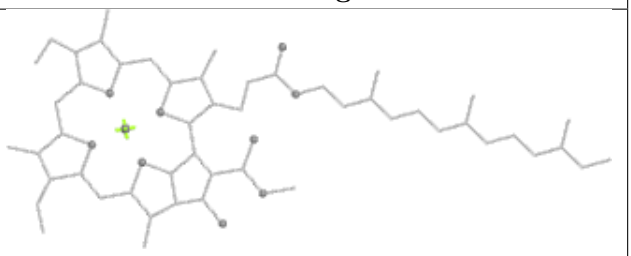
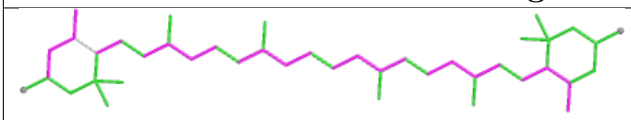


Rings

Ligand LUT b 301



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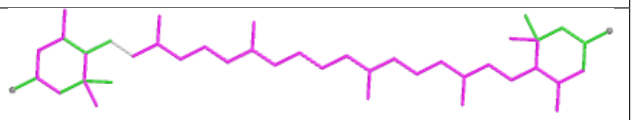
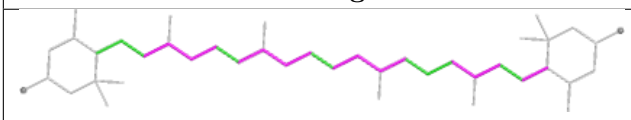
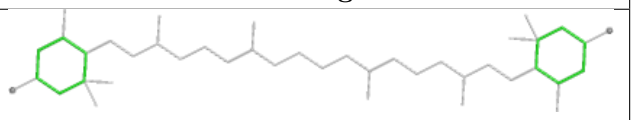


Bond angles

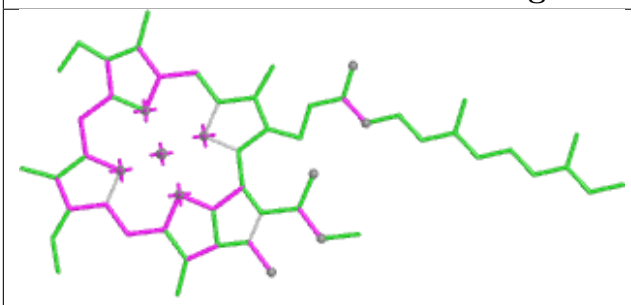


Torsions

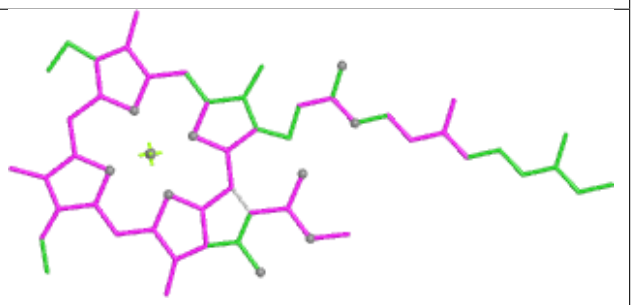


Rings

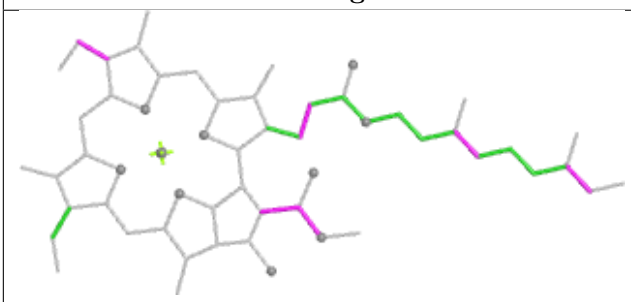
Ligand CLA 4 307



Bond lengths



Bond angles



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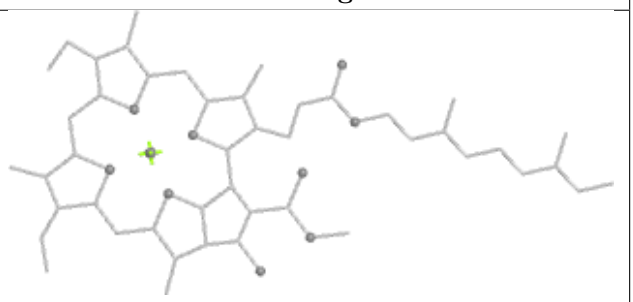
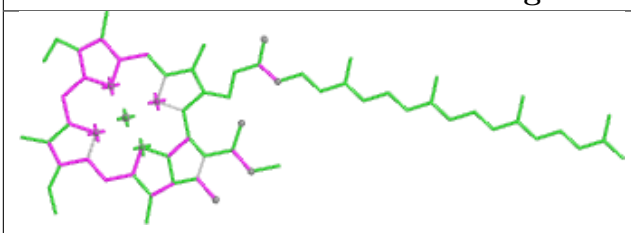
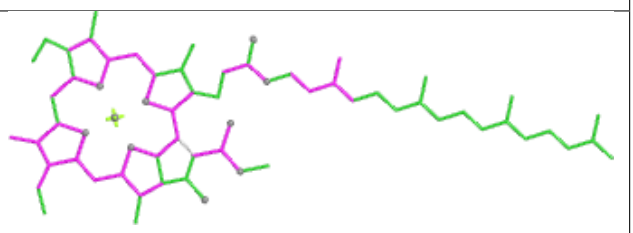


Rings

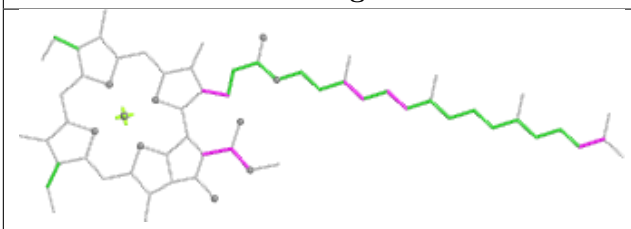
Ligand CLA A 818



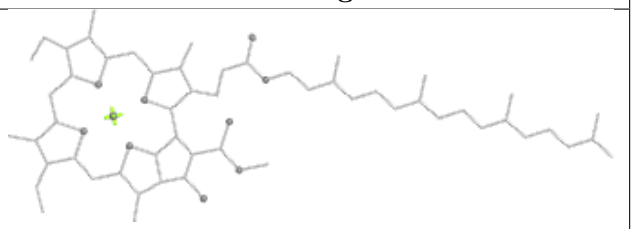
Bond lengths



Bond angles

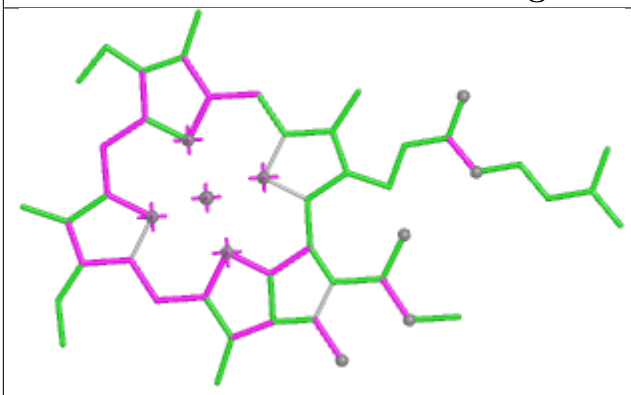


Torsions

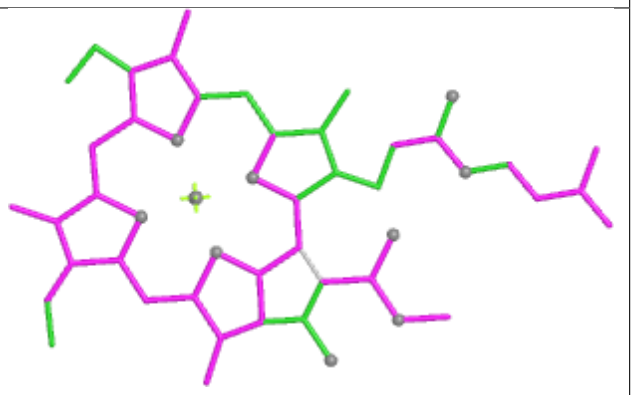


Rings

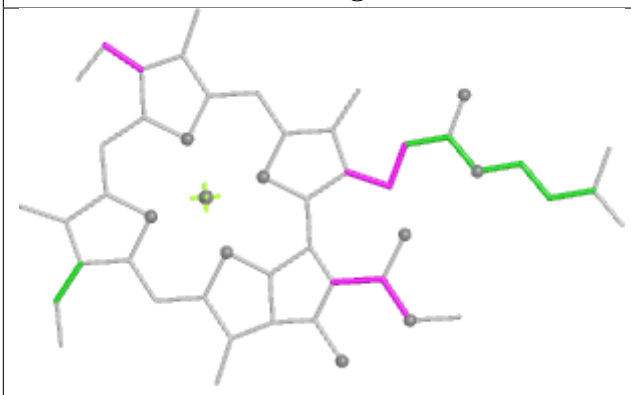
Ligand CLA 6 307



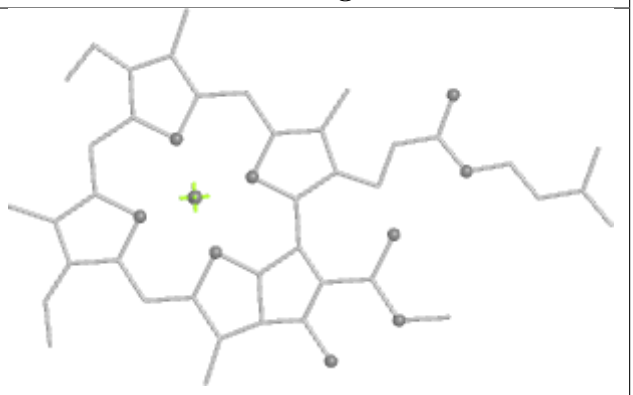
Bond lengths



Bond angles

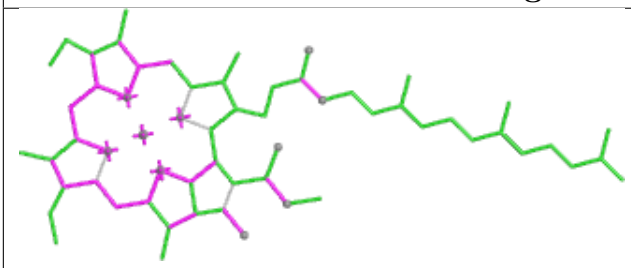


Torsions



Rings

Ligand CLA B 825



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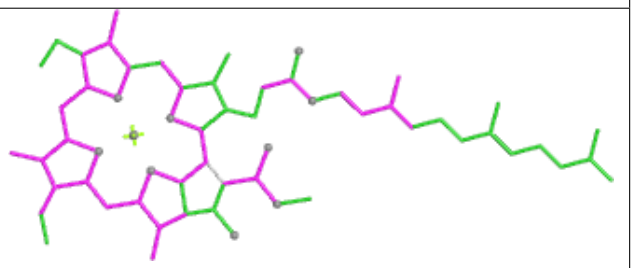
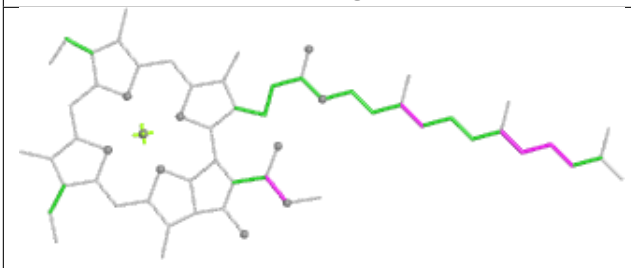
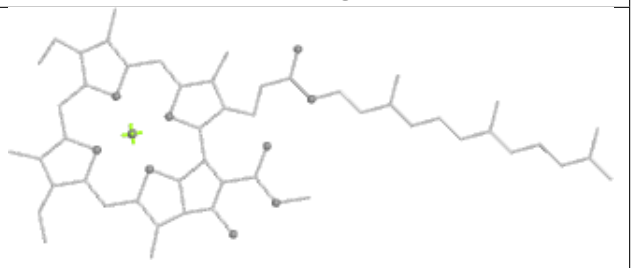


Bond angles

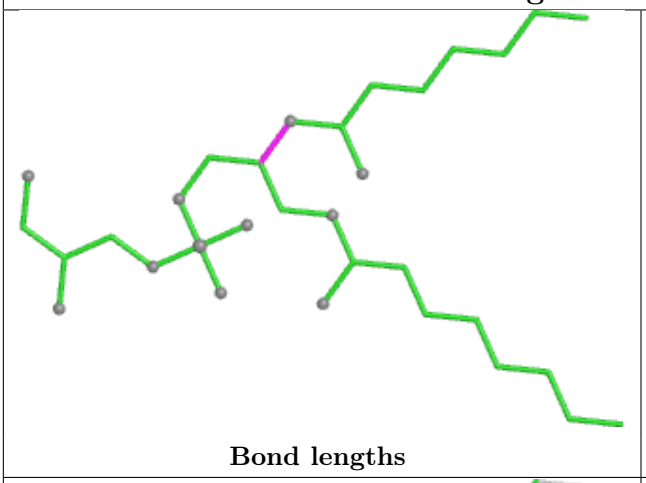


Torsions



Rings

Ligand LHG 6 305



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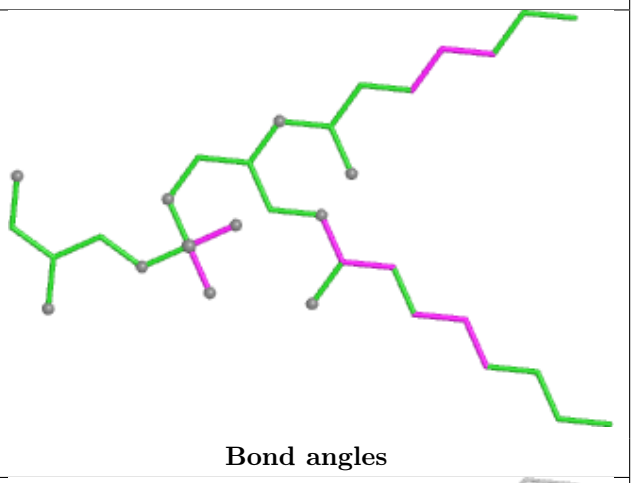
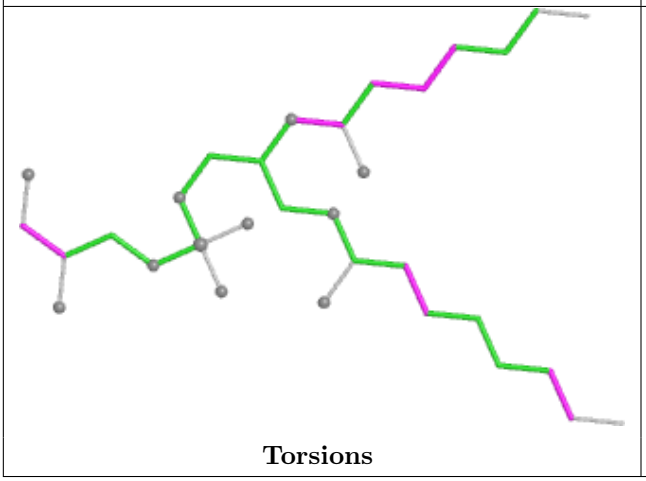


Bond angles



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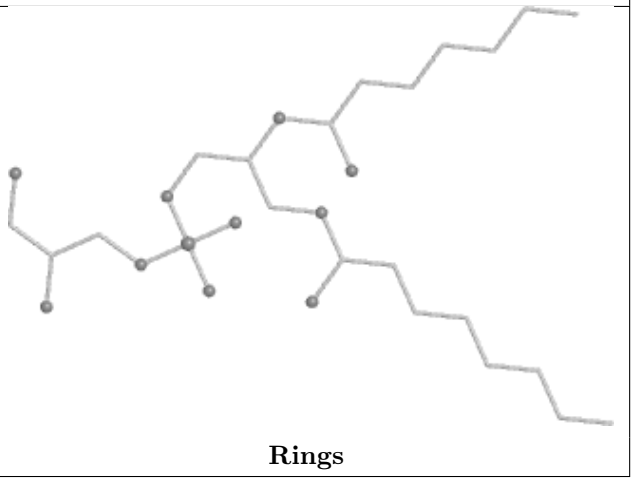
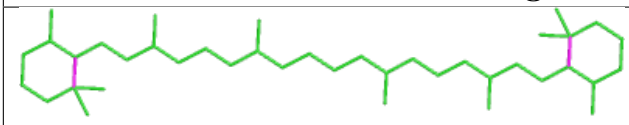


Rings

Ligand BCR L 303



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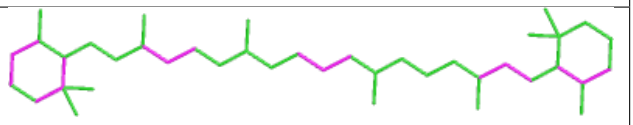
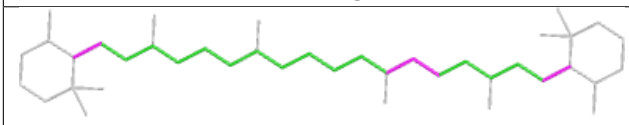


Bond angles



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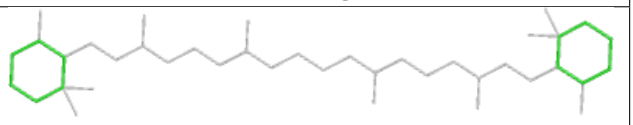
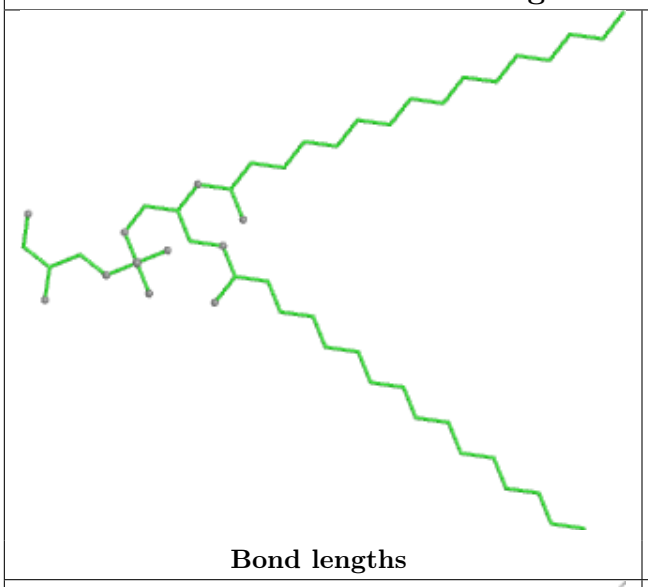


Rings

Ligand LHG 7 302



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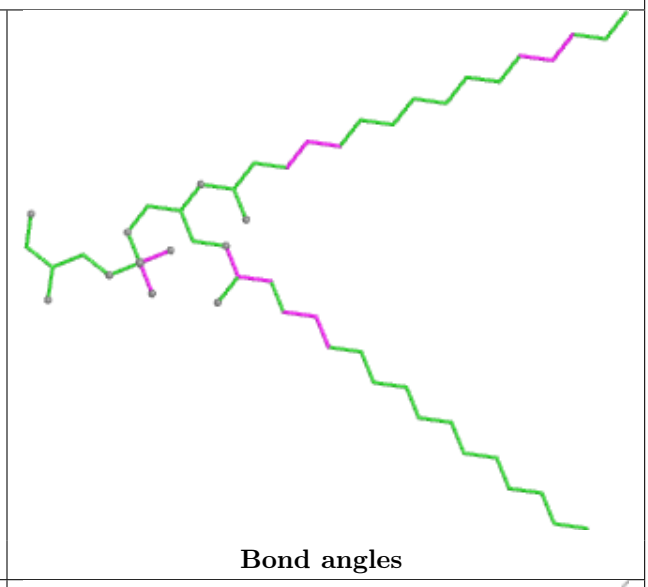
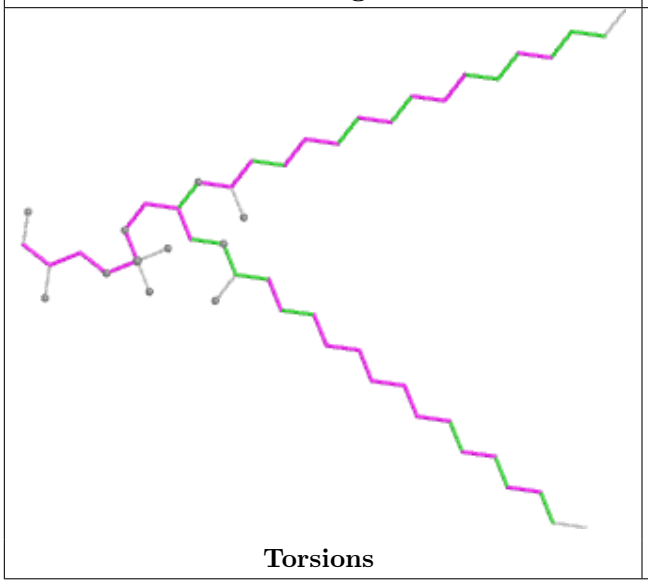


Bond angles



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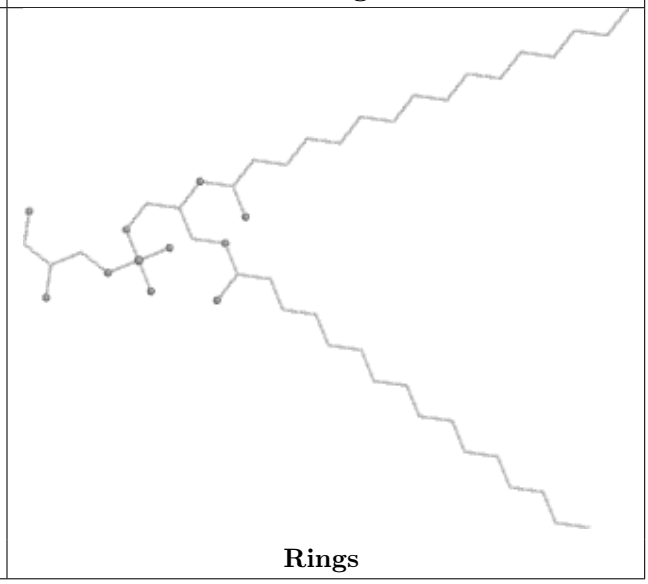
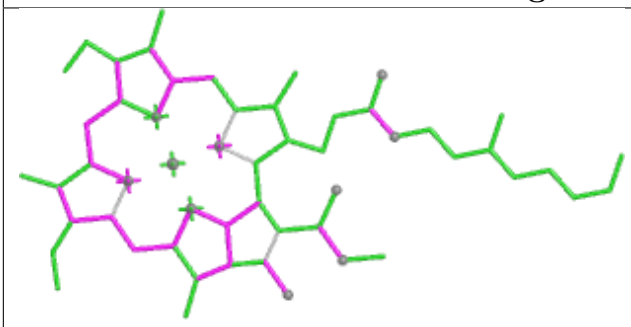


Rings

Ligand CLA 9 315



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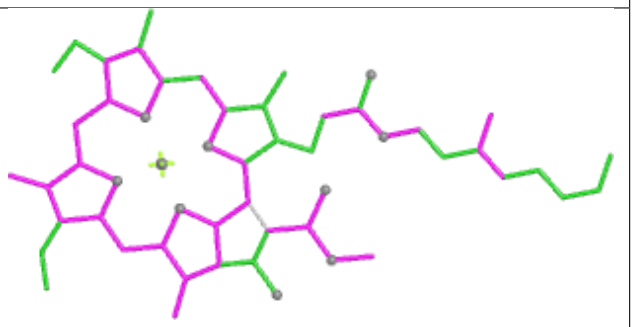
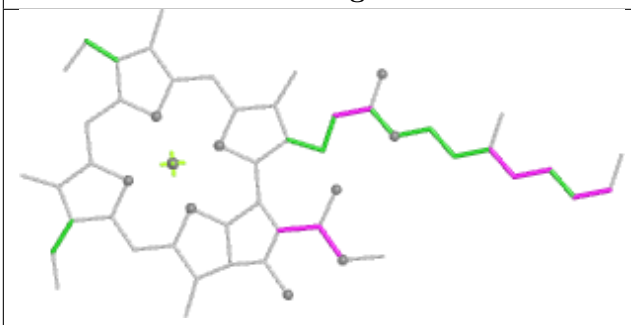


Bond angles



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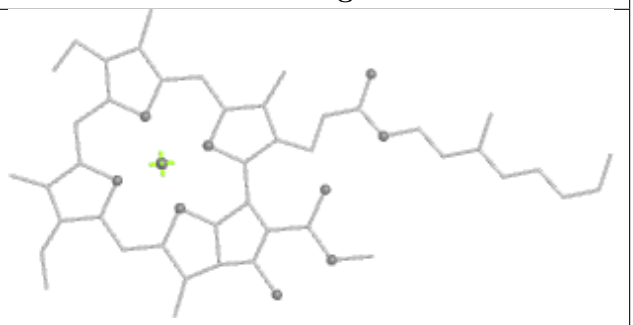
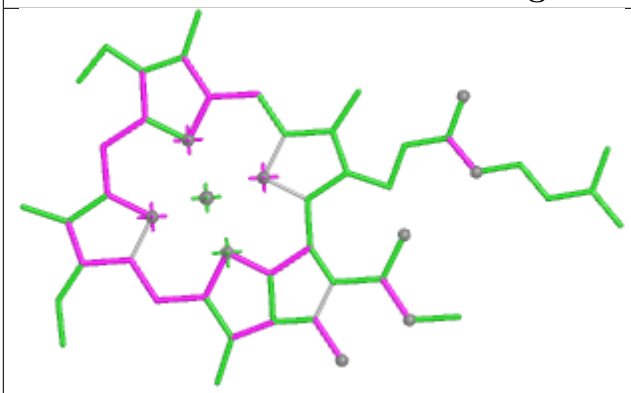


Rings

Ligand CLA 8 312



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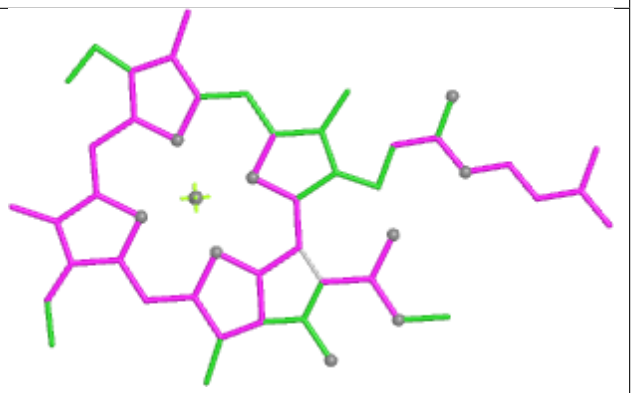
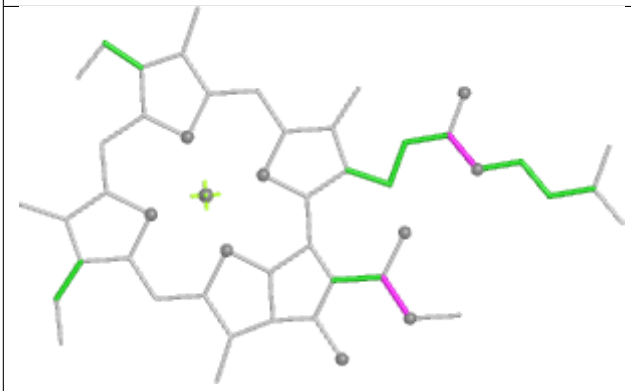


Bond angles



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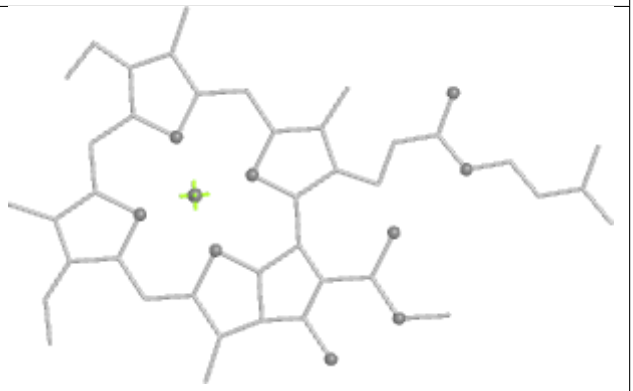
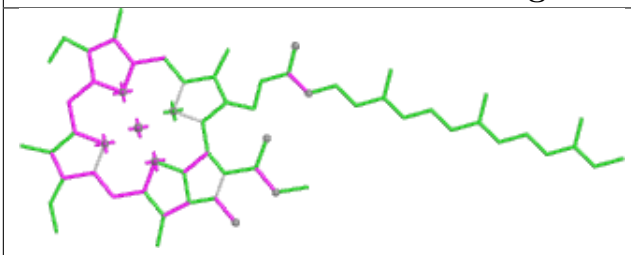
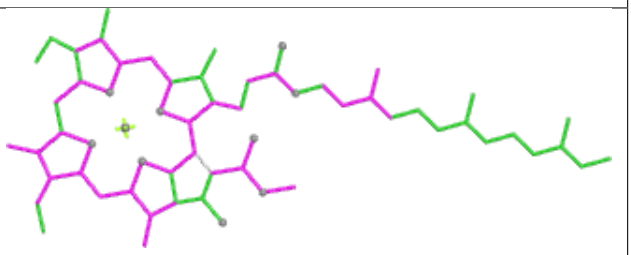


Rings

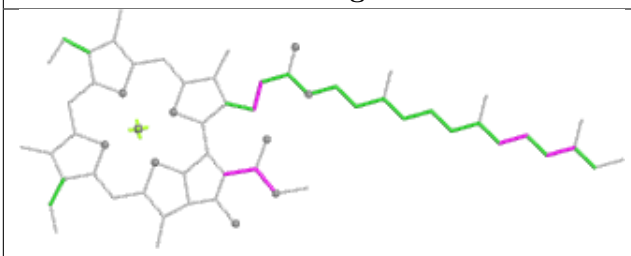
Ligand CLA 3 319



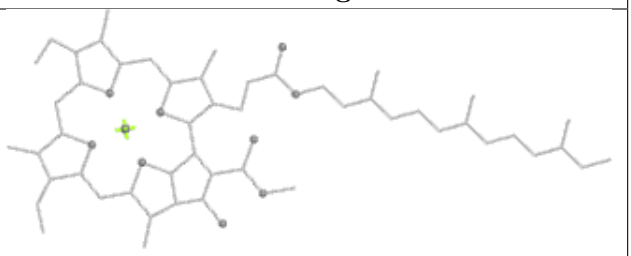
Bond lengths



Bond angles

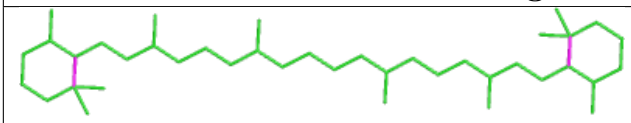


Torsions



Rings

Ligand BCR 7 304



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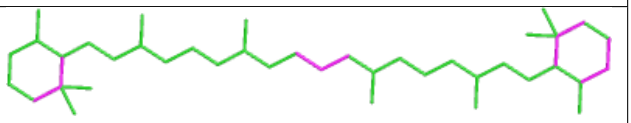

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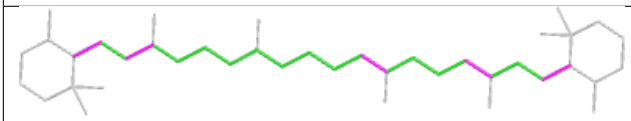

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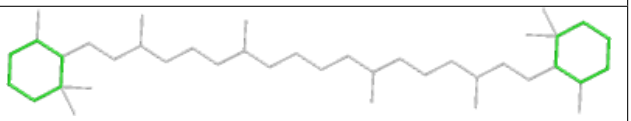
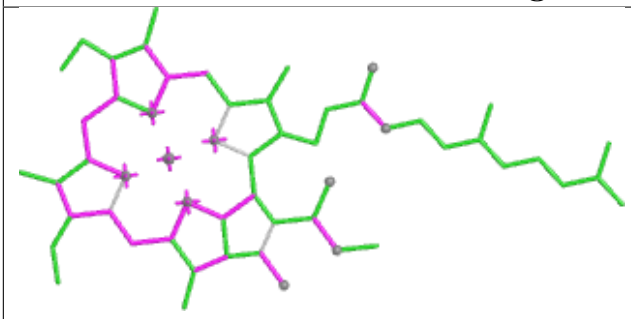


Rings

Ligand CLA 6 311



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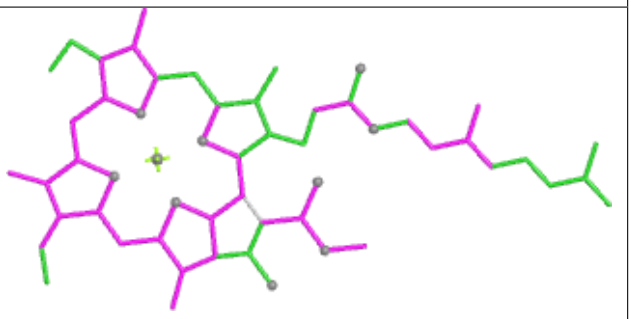
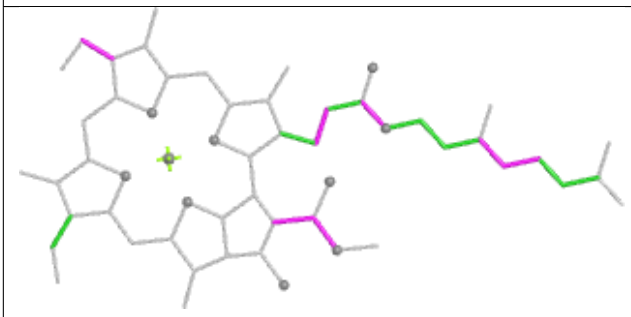


Bond angles



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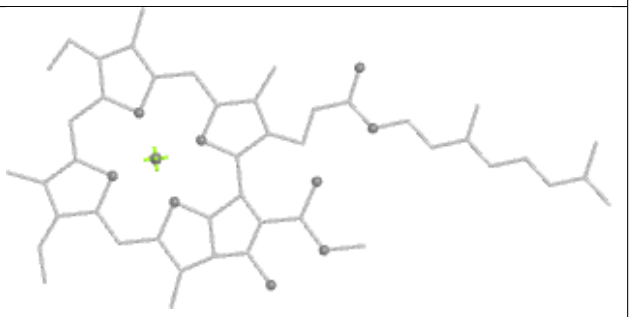
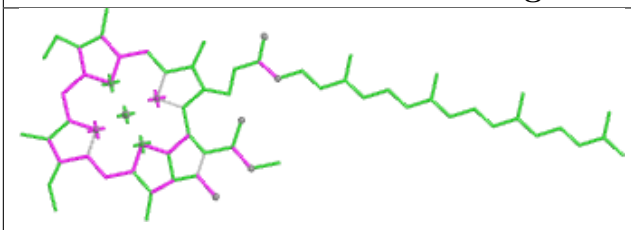


Rings

Ligand CLA B 846



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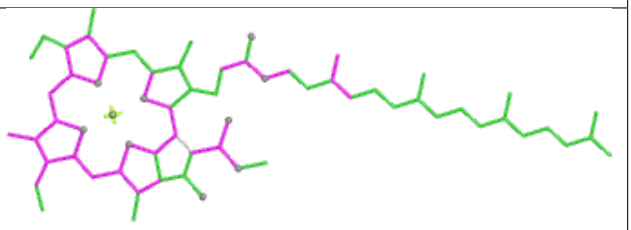
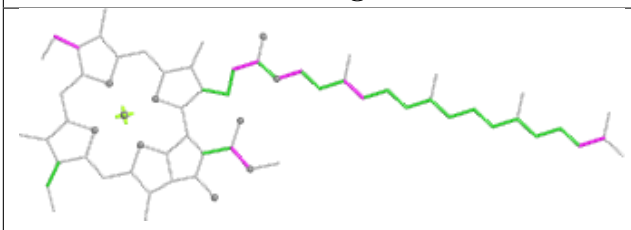


Bond angles



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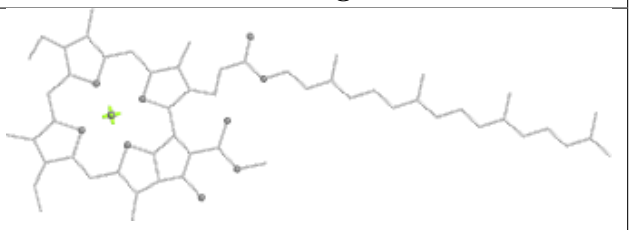
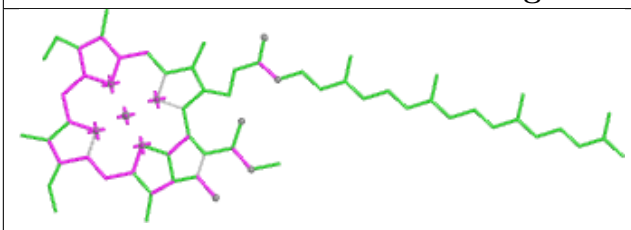


Rings

Ligand CLA A 842



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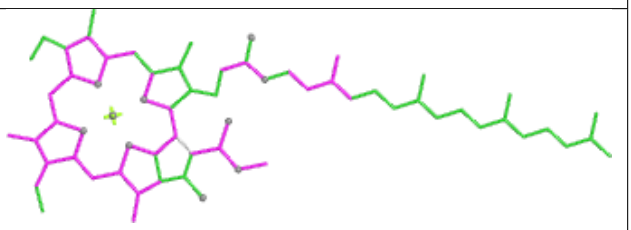
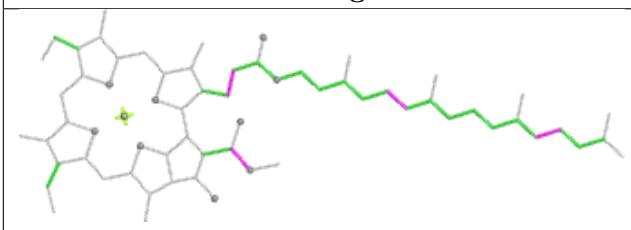


Bond angles



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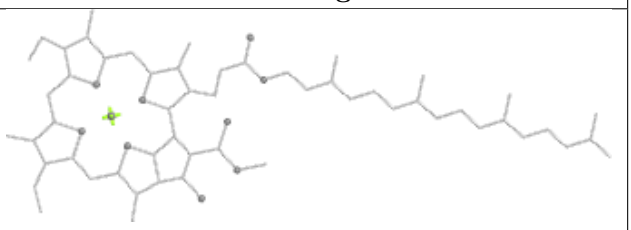
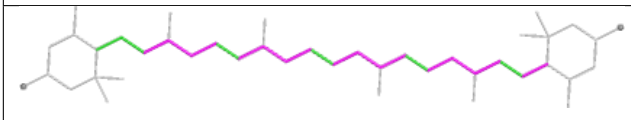


Rings

Ligand LUT 8 302

Bond lengths

Bond angles



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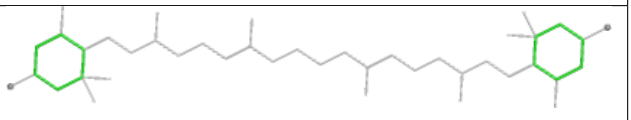
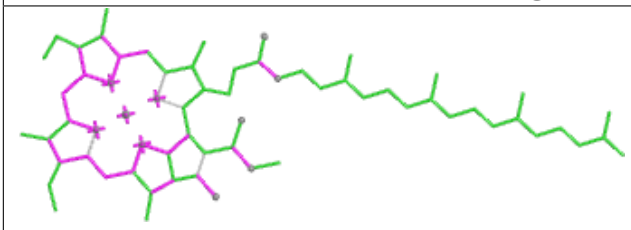
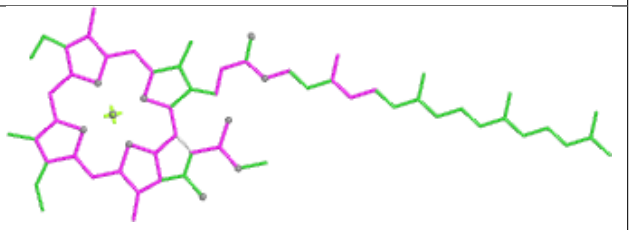
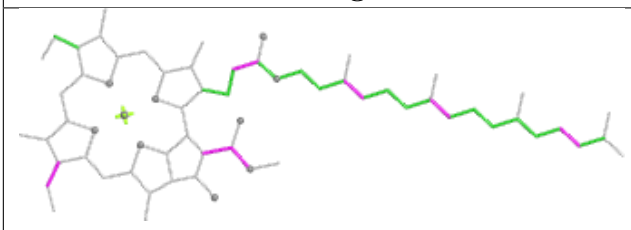
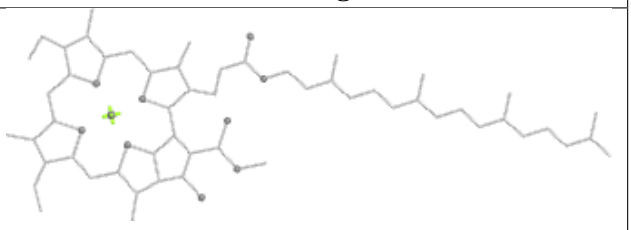
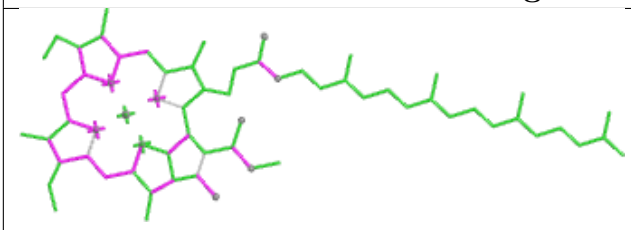
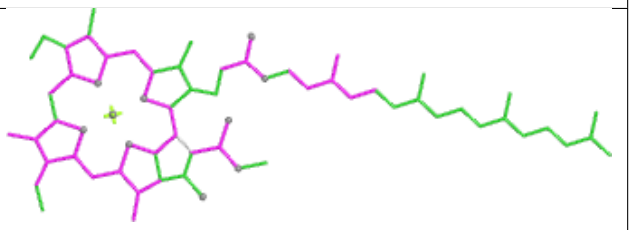
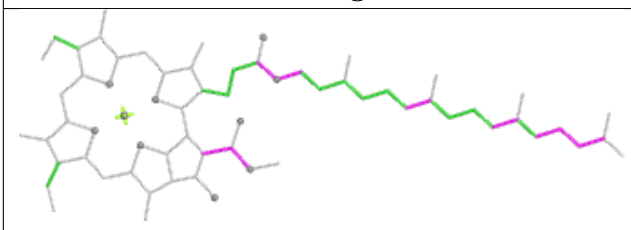
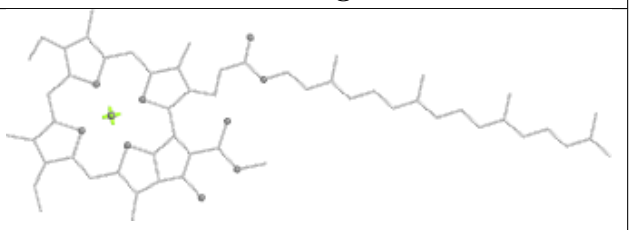
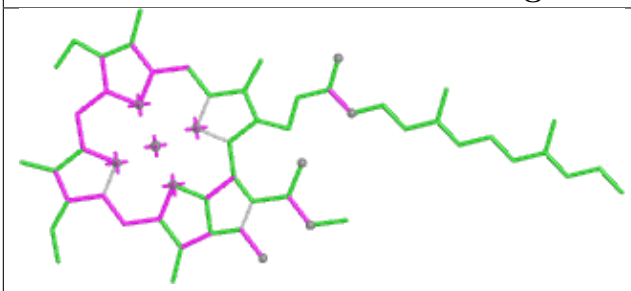


Rings

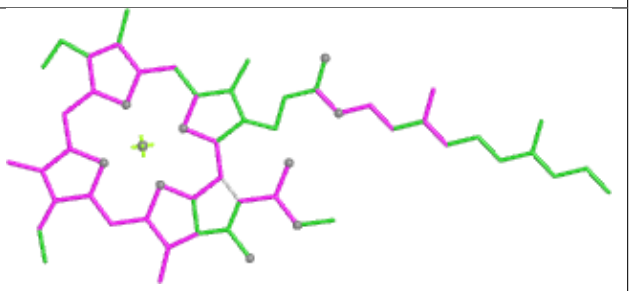
Ligand CLA 5 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

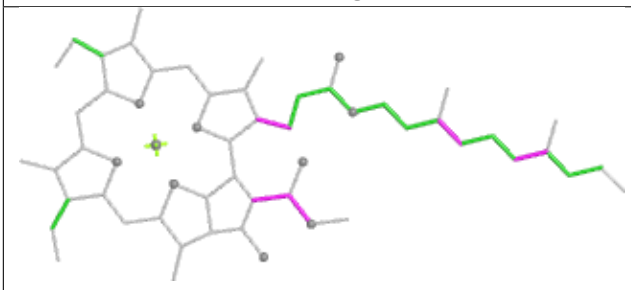
Ligand CLA B 835



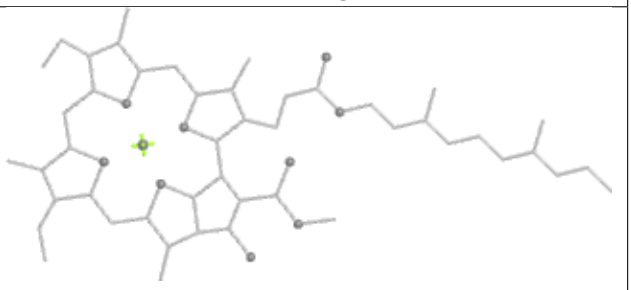
Bond lengths



Bond angles

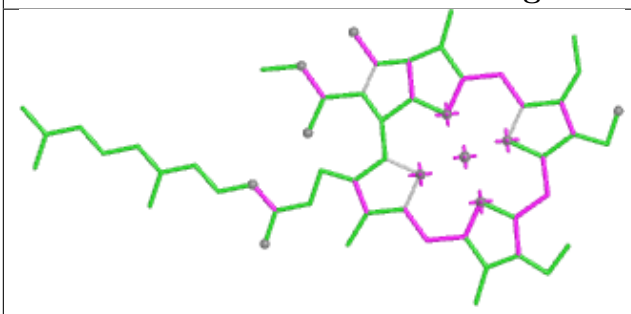


Torsions

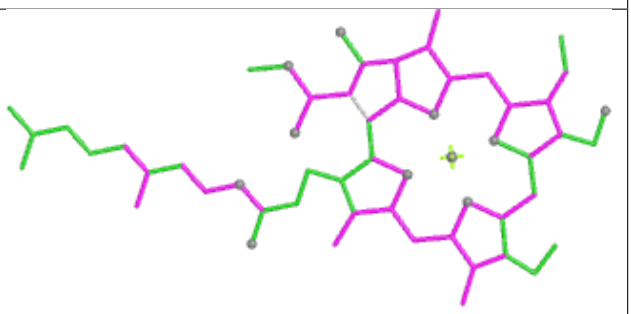


Rings

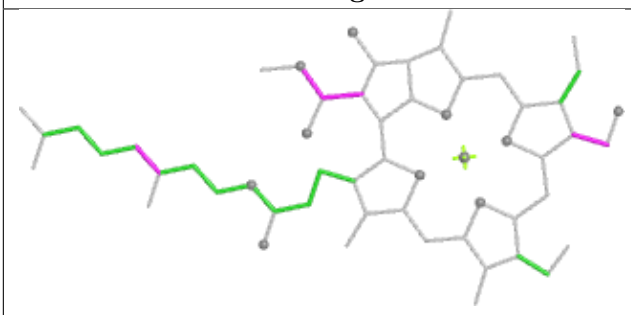
Ligand CHL A 839



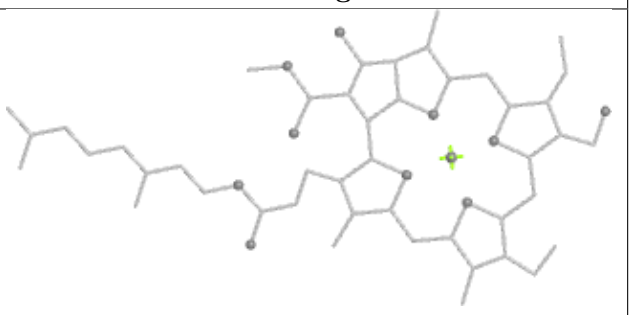
Bond lengths



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.

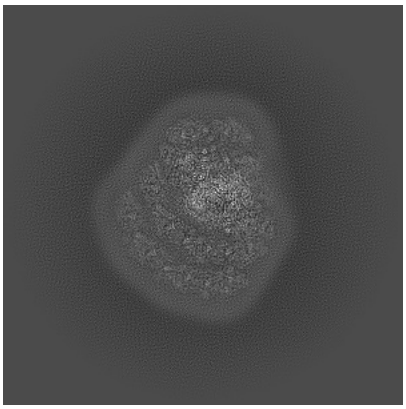
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62511. These allow visual inspection of the internal detail of the map and identification of artifacts.

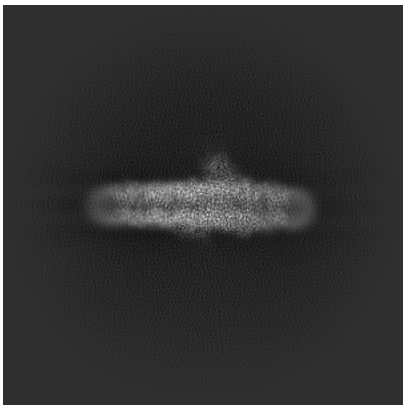
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

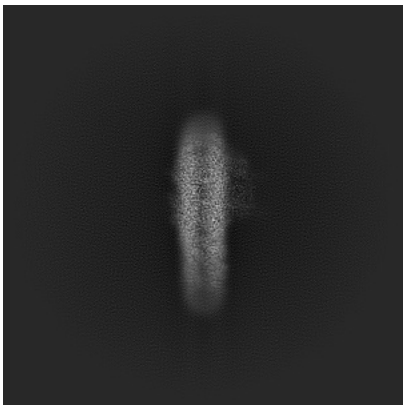
6.1.1 Primary map



X

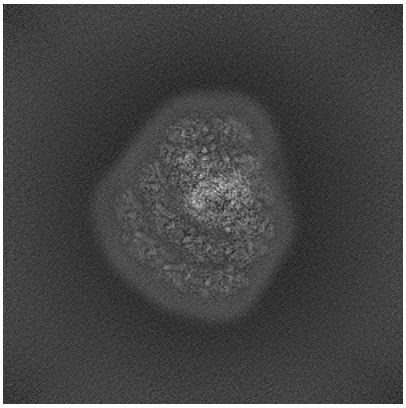


Y

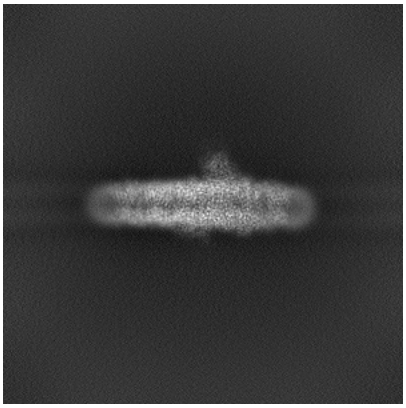


Z

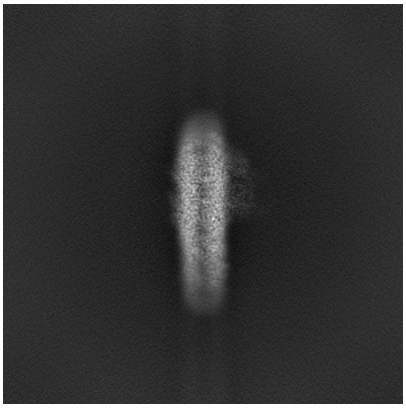
6.1.2 Raw map



X



Y

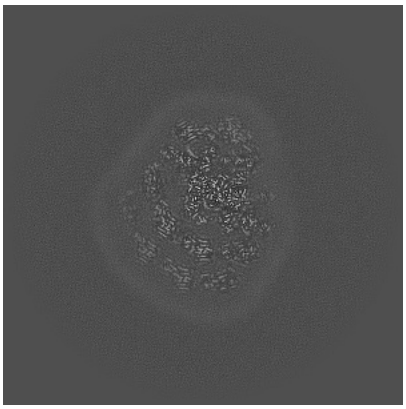


Z

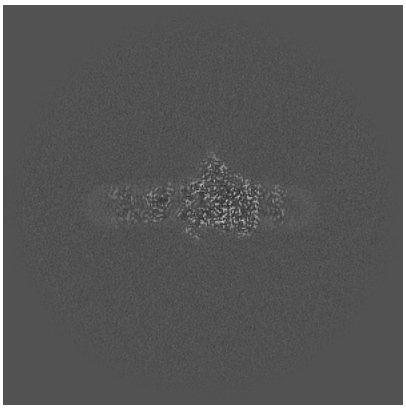
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

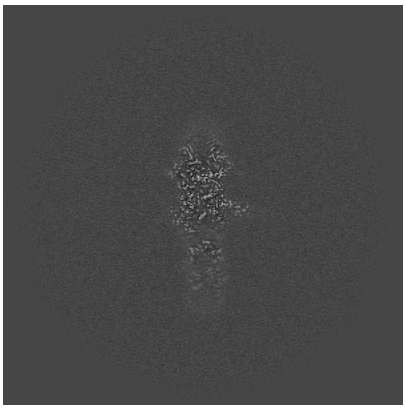
6.2.1 Primary map



X Index: 300

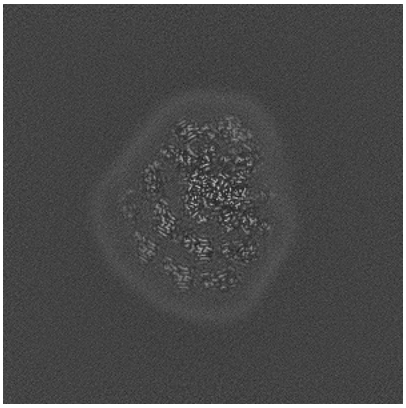


Y Index: 300

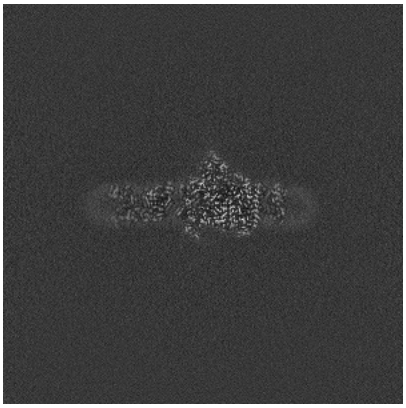


Z Index: 300

6.2.2 Raw map



X Index: 300



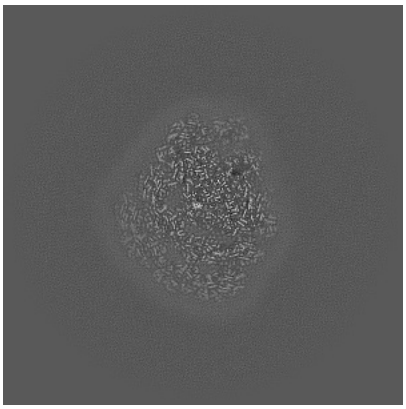
Y Index: 300

Z Index: 300

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

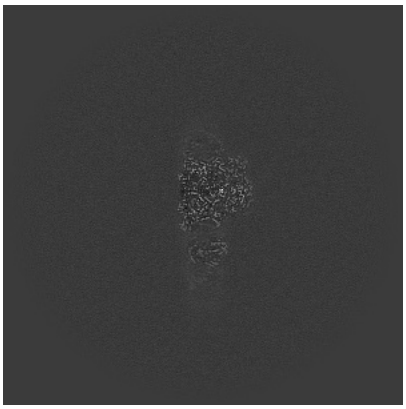
6.3 Largest variance slices (i)

6.3.1 Primary map



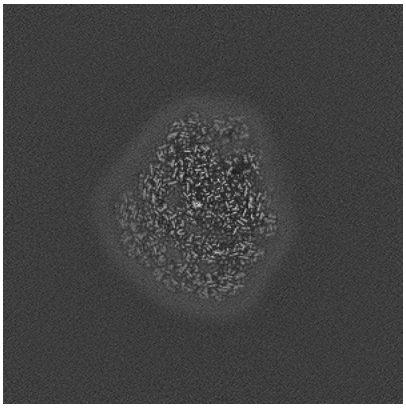
X Index: 316

Y Index: 307

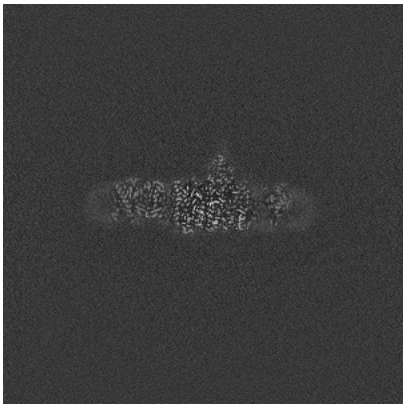


Z Index: 320

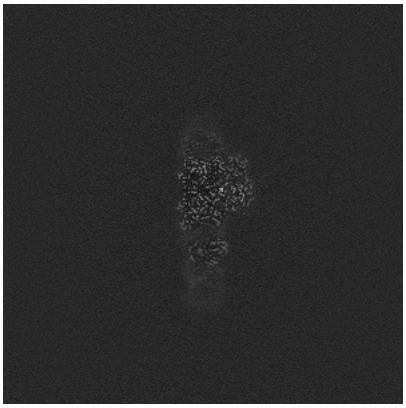
6.3.2 Raw map



X Index: 316



Y Index: 339

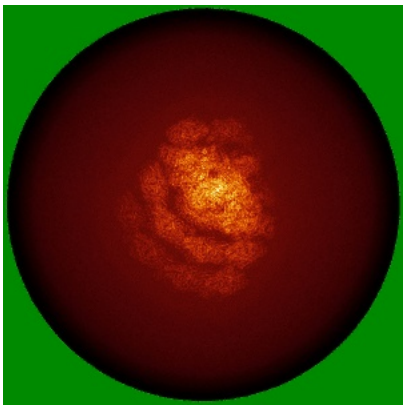


Z Index: 320

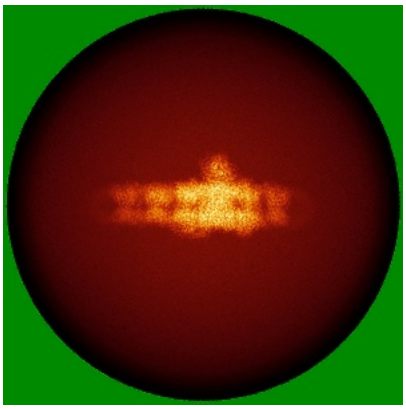
The images above show the largest variance slices of the map in three orthogonal directions.

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

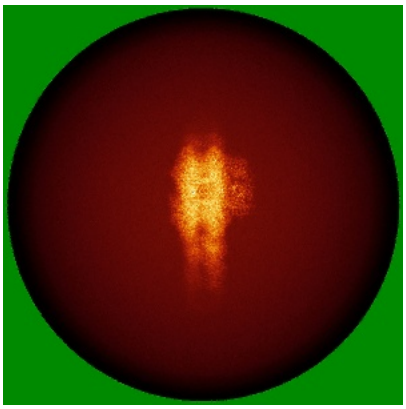
6.4.1 Primary map



X

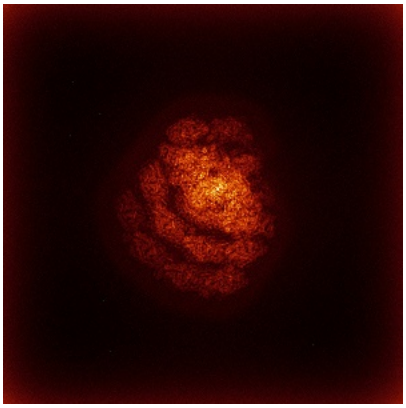


Y

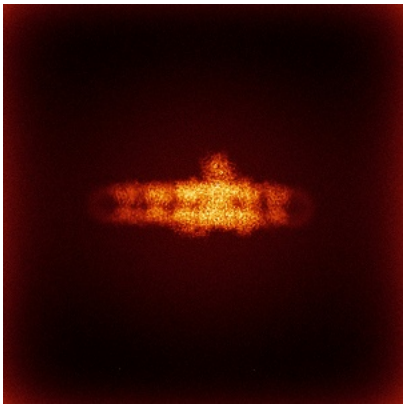


Z

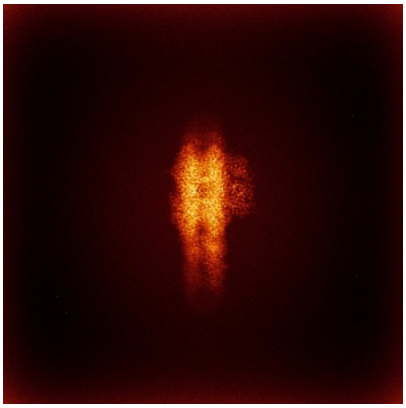
6.4.2 Raw map



X



Y

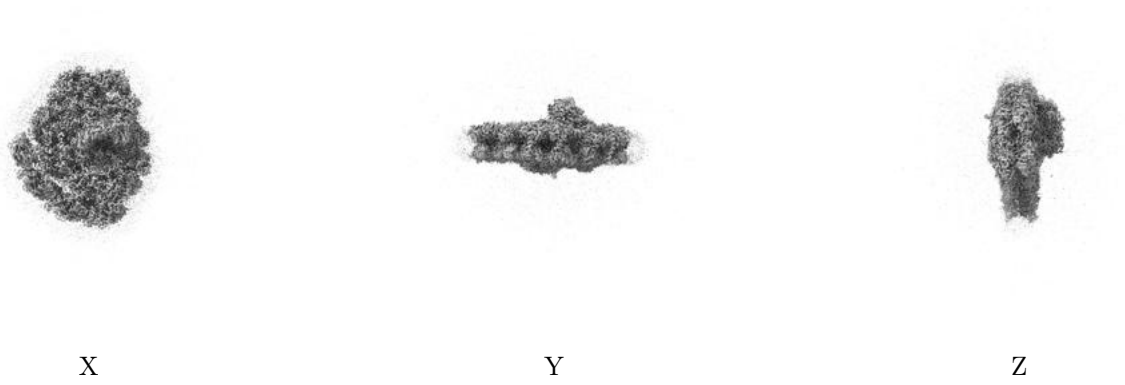


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

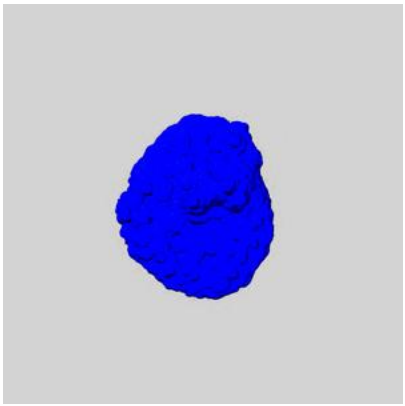
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

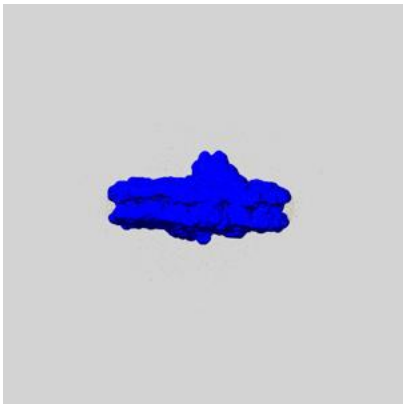
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

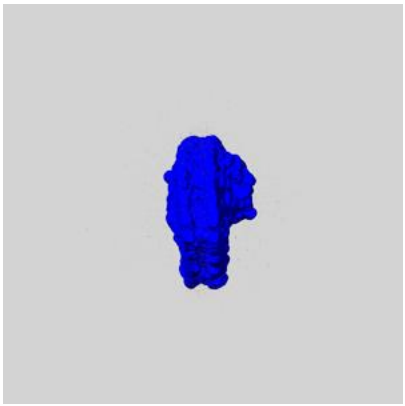
6.6.1 emd_62511_msk_1.map



X



Y

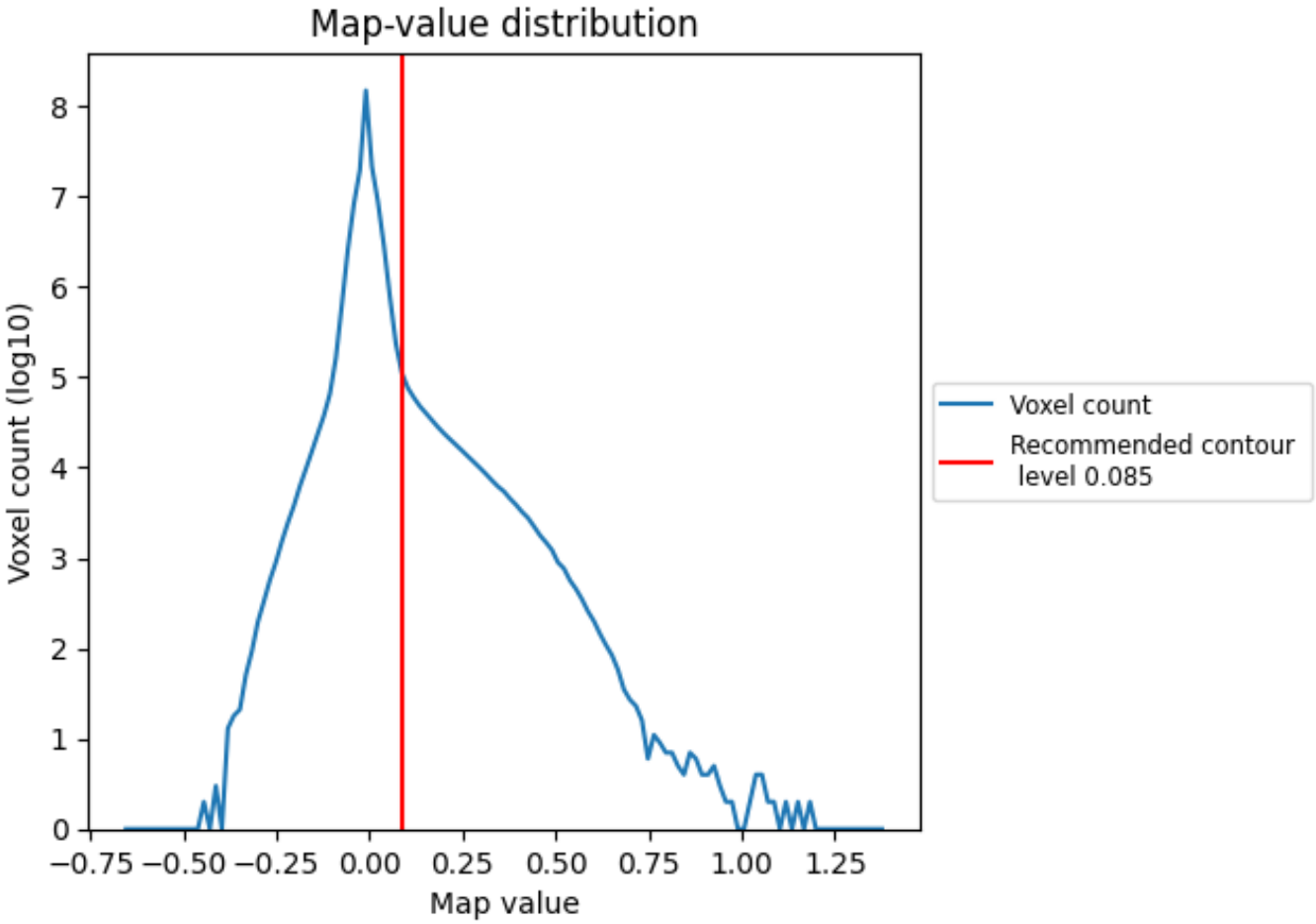


Z

7 Map analysis

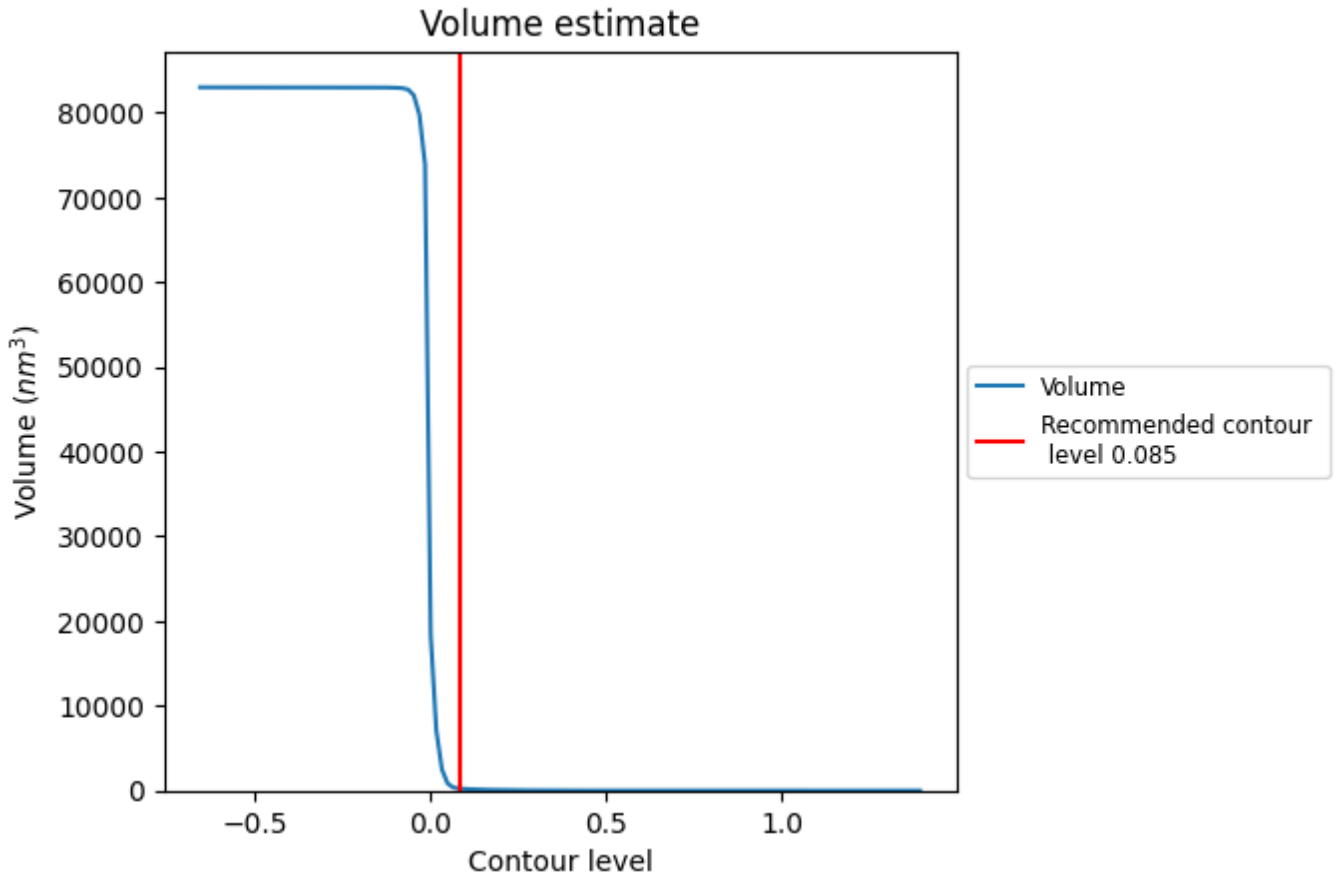
This section contains the results of statistical analysis of the map.

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.

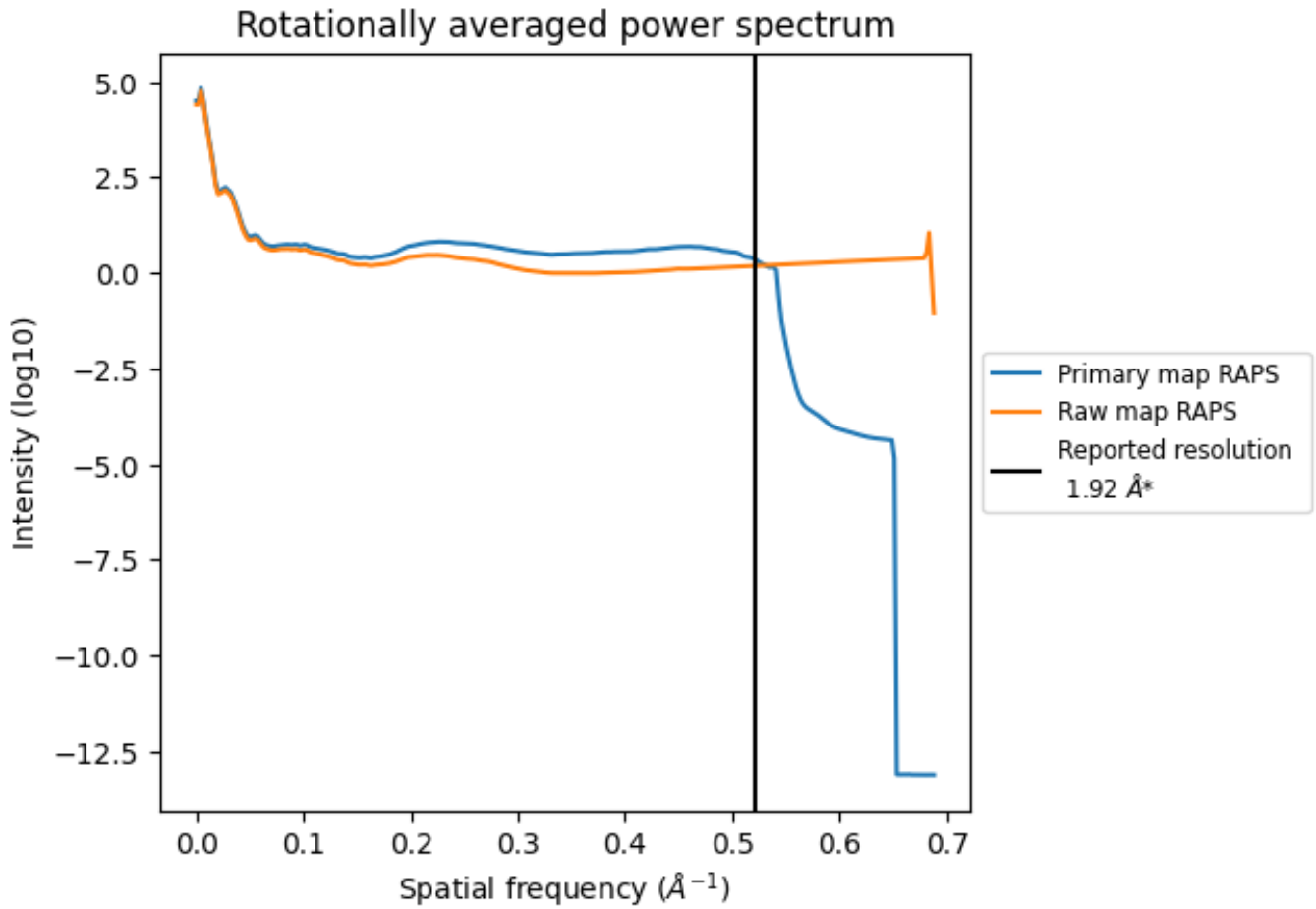
7.2 Volume estimate



The volume at the recommended contour level is 227 nm^3; this corresponds to an approximate mass of 205 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)

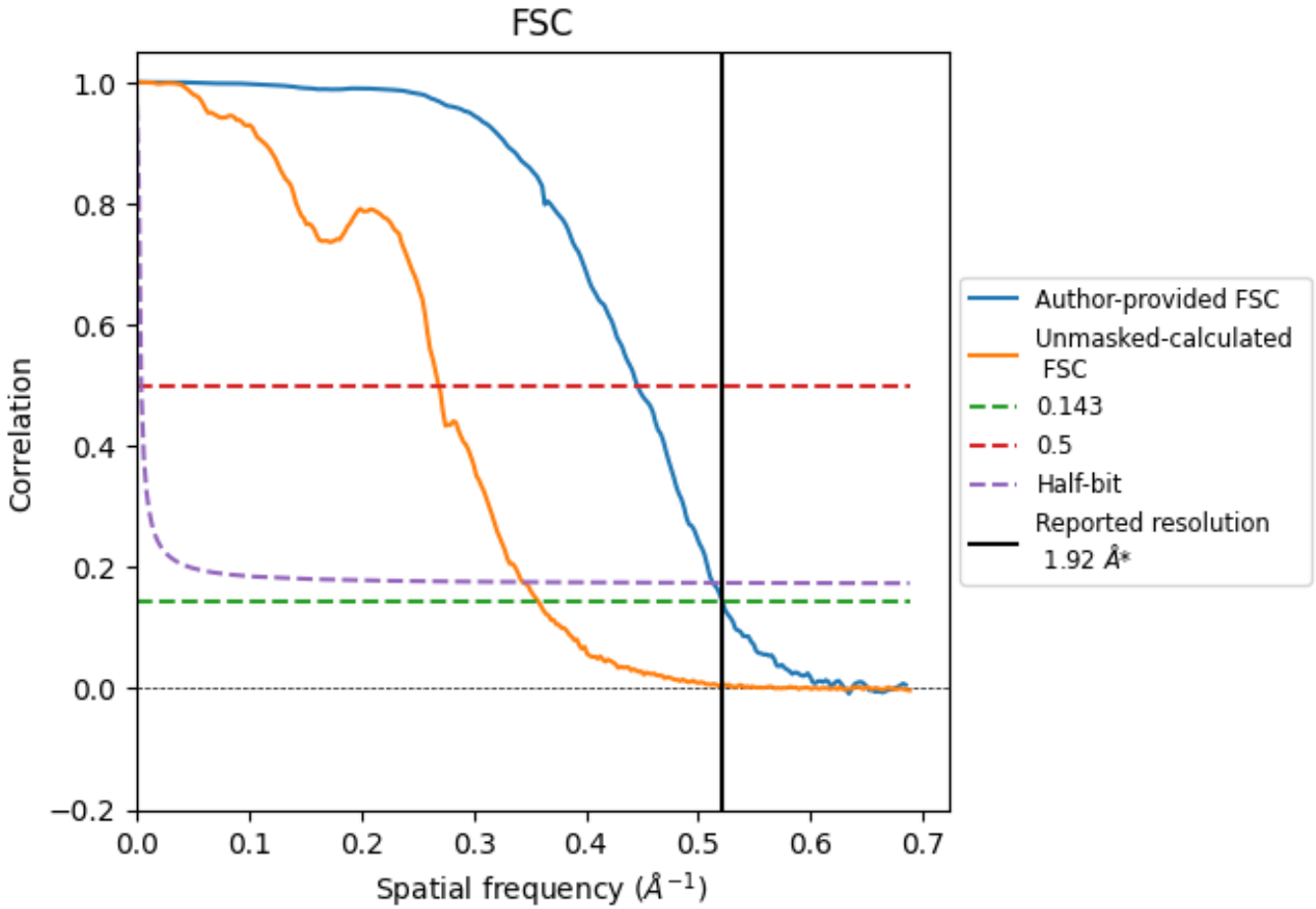


*Reported resolution corresponds to spatial frequency of 0.521 $Å^{-1}$

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 0.521 Å^{-1}

8.2 Resolution estimates (i)

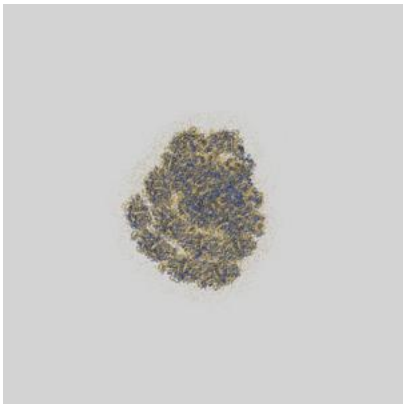
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.92	2.24	1.95
Unmasked-calculated*	2.79	3.72	2.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 1.92 by more than 10 %

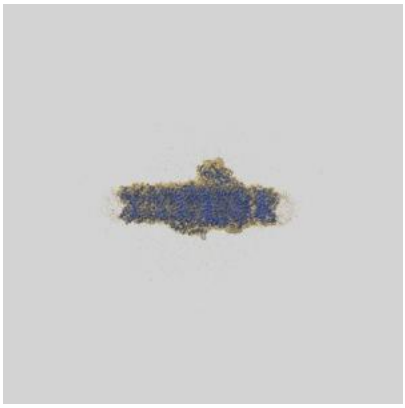
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62511 and PDB model 9KQP. Per-residue inclusion information can be found in section 3 on page 36.

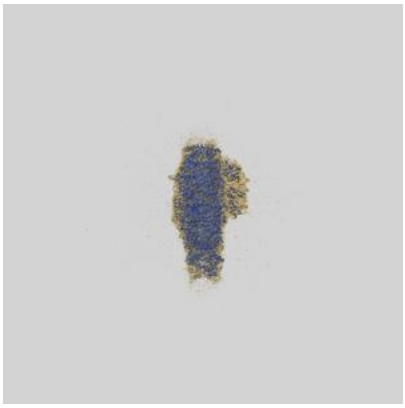
9.1 Map-model overlay



X



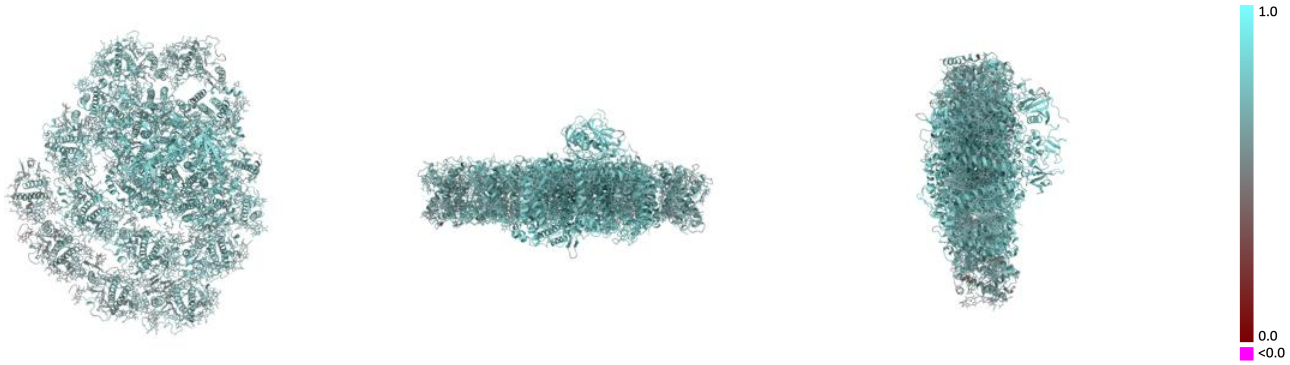
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 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.

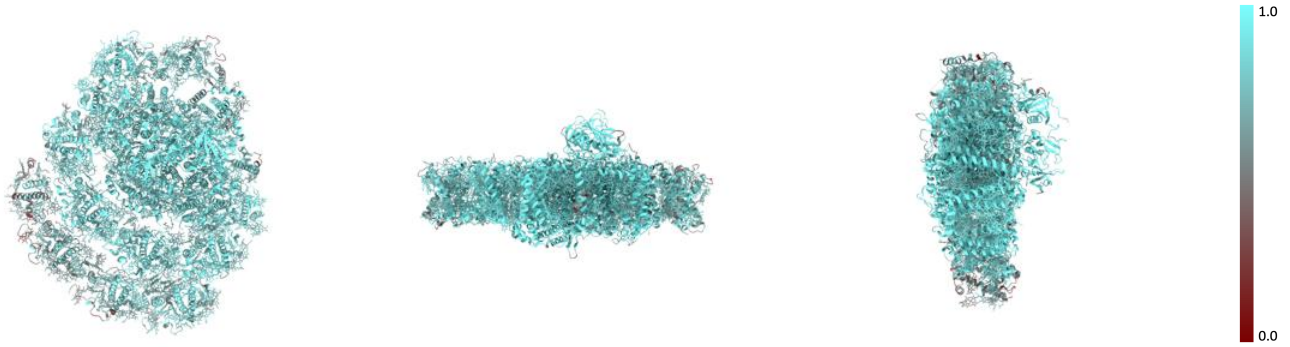
9.2 Q-score mapped to coordinate model (i)



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.

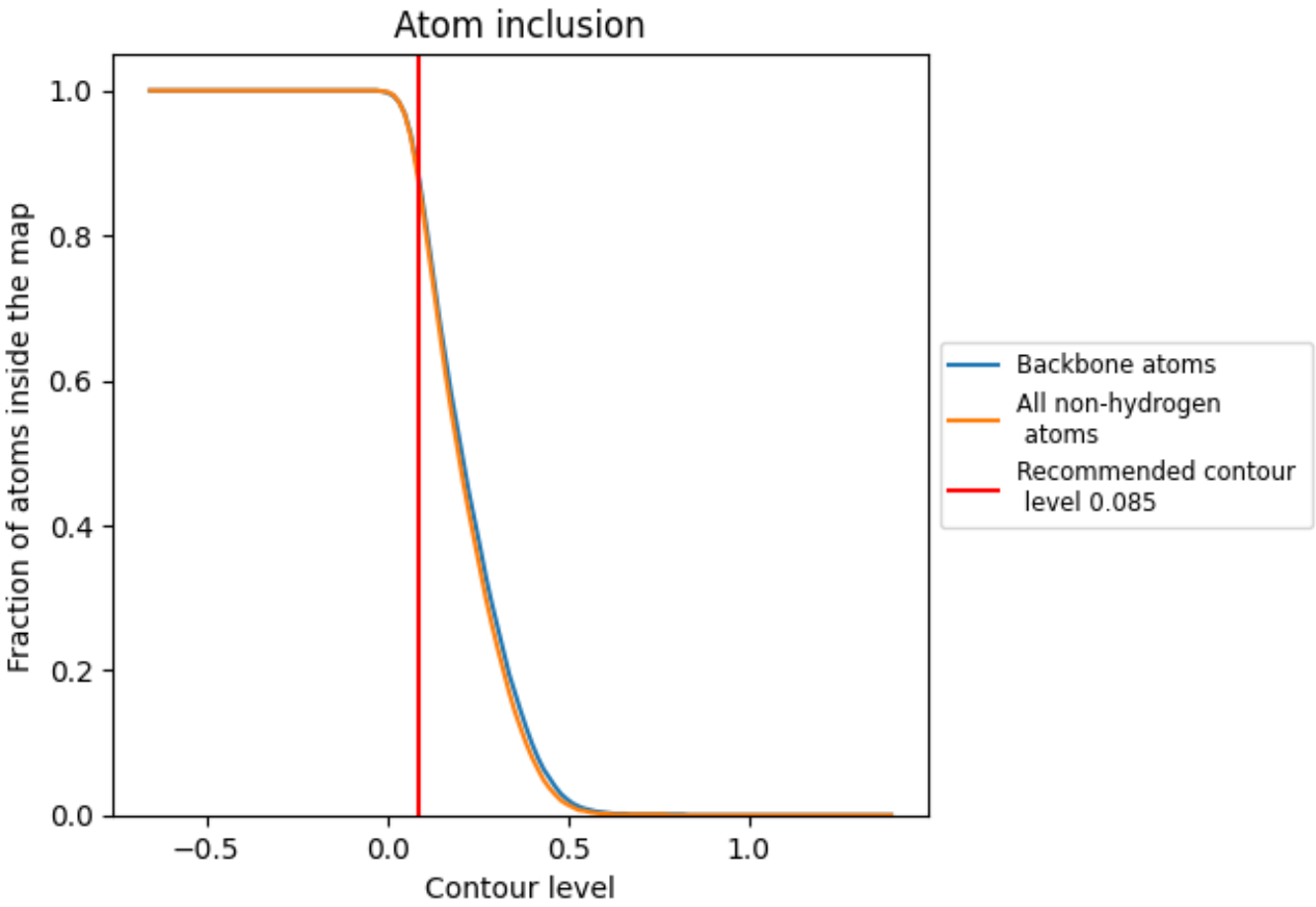
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.085).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.7230
2	0.7470	0.6320
3	0.9070	0.7070
4	0.6450	0.5770
5	0.7930	0.6420
6	0.7360	0.6210
7	0.9190	0.7280
8	0.9100	0.7290
9	0.8830	0.6910
A	0.9650	0.7910
B	0.9690	0.7950
C	0.9920	0.8120
D	0.9590	0.7800
E	0.9200	0.7700
F	0.9490	0.7810
G	0.9090	0.7300
H	0.7620	0.6860
I	0.9760	0.7770
J	0.9690	0.7790
K	0.8840	0.6980
L	0.9000	0.7320
M	0.9530	0.7720
O	0.6770	0.6560
a	0.8890	0.7080
b	0.5990	0.5800