Full wwPDB EM Validation Report

Aug 6, 2026 – 11:12 AM JST

PDB ID	:	9JZR / pdb_00009jzr
EMDB ID	:	EMD-61940
Title	:	Structure of PSI-LHCI-LHCII supercomplex from Bryopsis corticulans
Authors	:	Liu, X.Y.; Wang, W.D.
Deposited on	:	2024-10-14
Resolution	:	2.73 Å(reported)

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

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

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

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

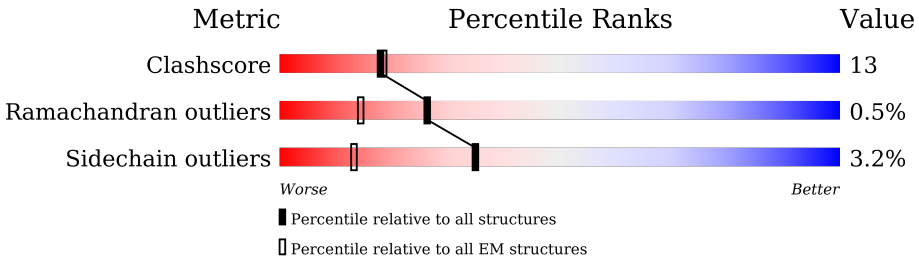
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

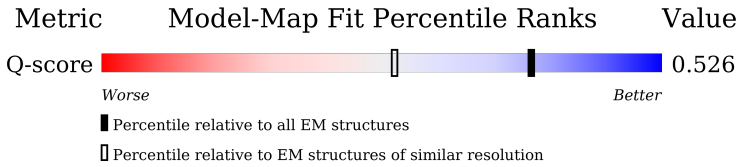
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	0	245	61% 25% • 13%
2	1	226	55% 29% • 14%
2	5	226	8% 61% 23% • 14%
3	2	256	70% 13% • 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	281	61% 20% 19%
5	6	267	69% 16% 14%
6	7	264	66% 19% 14%
7	4	248	49% 29% 6% 17%
7	8	248	58% 21% 17%
8	9	222	62% 17% 6% 15%
9	A	751	72% 26%
10	B	734	75% 23%
11	D	198	56% 16% 28%
12	E	91	60% 9% 30%
13	F	236	57% 11% 30%
14	G	167	35% 17% 44%
15	I	36	69% 28%
16	J	41	66% 32%
17	L	204	64% 15% 21%
18	C	81	74% 25%
19	K	123	57% 7% 35%
20	M	32	84% 12%
21	O	137	57% 9% 33%
22	a	250	79% 57% 22% 21%
22	h	250	80% 56% 24% 20%
23	c	254	33% 65% 20% 14%
24	b	251	38% 60% 21% 17%
25	d	280	52% 58% 19% 22%
25	g	280	71% 48% 23% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
26	f	259	17% 66% 21% 13%
27	H	133	56% 14% 29%
28	i	282	70% 54% 29% 16%
29	e	250	24% 63% 22% 14%

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
30	CHL	i	606	-	-	X	-
31	CLA	i	604	-	-	X	-
42	NEX	f	523	-	-	X	-
42	NEX	i	523	-	-	X	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 77090 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	213	Total	C	N	O	S	0	0
			1640	1063	270	296	11		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	195	Total	C	N	O	S	0	0
			1478	950	243	273	12		
2	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	216	Total	C	N	O	S	0	0
			1667	1082	269	304	12		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	228	Total	C	N	O	S	0	0
			1768	1141	288	329	10		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		
7	4	207	Total	C	N	O	S	0	0
			1569	1030	257	273	9		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	189	Total	C	N	O	S	0	0
			1453	932	245	267	9		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	746	Total	C	N	O	S	0	0
			5872	3836	998	1016	22		

- Molecule 10 is a protein called photosystem I.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	733	Total	C	N	O	S	0	0
			5824	3824	979	1002	19		

- Molecule 11 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	142	Total	C	N	O	S	0	0
			1109	709	193	202	5		

- Molecule 12 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	64	Total	C	N	O	S	0	0
			509	323	90	95	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	165	Total	C	N	O	S	0	0
			1273	810	224	235	4		

- Molecule 14 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	G	93	Total	C	N	O	0	0
			726	471	119	136		

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			262	180	37	43	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	162	Total	C	N	O	S	0	0
			1195	773	192	226	4		

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C	80	Total	C	N	O	S	0	0
			602	370	105	116	11		

- Molecule 19 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	31	Total	C	N	O	0	0
			238	158	37	43		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			728	488	116	120	4		

- Molecule 22 is a protein called Lhcb-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	198	Total	C	N	O	S	0	0
			1511	978	243	279	11		
22	h	201	Total	C	N	O	S	0	0
			1520	985	245	280	10		

- Molecule 23 is a protein called Lhcb-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	219	Total	C	N	O	S	0	0
			1680	1083	271	317	9		

- Molecule 24 is a protein called Lhcb-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	209	Total	C	N	O	S	0	0
			1609	1038	265	295	11		

- Molecule 25 is a protein called Lhcb-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	217	Total	C	N	O	S	0	0
			1634	1059	260	305	10		
25	g	199	Total	C	N	O	S	0	0
			1502	971	238	283	10		

- Molecule 26 is a protein called Lhcb-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	f	225	Total	C	N	O	P	S	0	0
			1727	1107	282	330	1	7		

- Molecule 27 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	94	Total	C	N	O	S	0	0
			717	451	126	139	1		

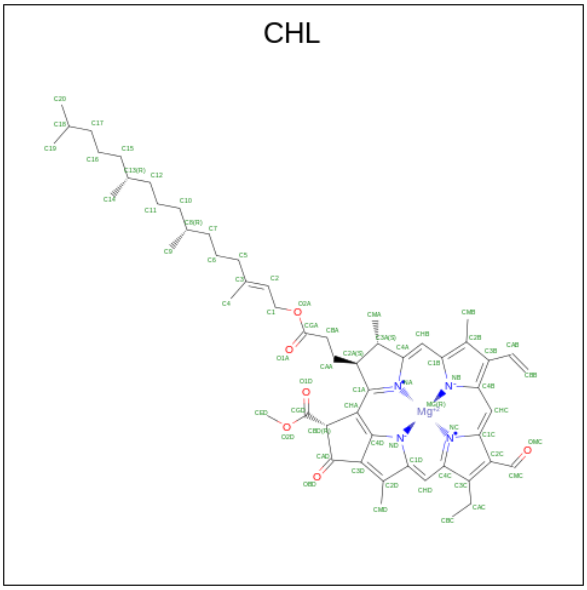
- Molecule 28 is a protein called Lhcb-i.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	i	237	Total	C	N	O	P	S	0	0
			1834	1179	305	342	1	7		

- Molecule 29 is a protein called Lhcb-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	216	Total	C	N	O	S	0	0
			1647	1066	261	310	10		

- Molecule 30 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
30	0	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	7	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	a	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			59	48	1	4	6	
30	a	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	c	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	c	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	c	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	c	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
30	c	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	c	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	f	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	f	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	g	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	g	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	h	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	h	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	h	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	h	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	h	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	h	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	h	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	h	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	i	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

Continued on next page...

Continued from previous page...

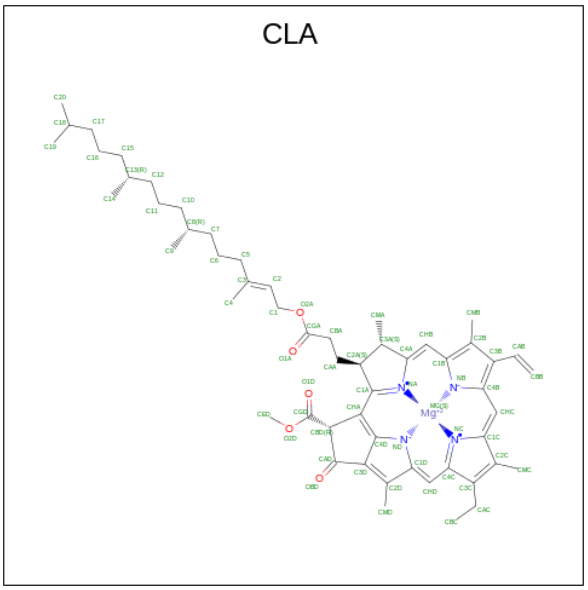
Mol	Chain	Residues	Atoms					AltConf
30	i	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	i	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	i	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	i	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	i	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	i	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	i	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	e	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	e	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	e	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	e	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	e	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	e	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	e	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	4	1	Total 54	C 43	Mg 1	N 4	O 6	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	0	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	0	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	1	1	Total 56	C 46	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			56	46	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
			60	50	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
			48	38	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
			45	35	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	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
			47	37	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
			62	52	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			45	35	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
			52	42	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			52	42	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
			60	50	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
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			45	35	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
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	7	1	Total	C	Mg	N	O	0
			52	42	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
			47	37	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	7	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	
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
			60	50	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
			46	36	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			51	41	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
			60	50	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	9	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
			55	45	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
			54	44	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
			54	44	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
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			61	51	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
			55	45	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
			49	39	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
			55	45	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
			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
			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
			46	36	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
			51	41	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			61	51	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
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			52	42	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
			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
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			62	52	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
			52	42	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
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
			59	49	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
			56	46	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
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			52	42	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
			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
			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
			56	46	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
			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
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

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
			47	37	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
			47	37	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	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
			45	35	1	4	5	
31	G	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	L	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			53	43	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
			50	40	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
31	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
31	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			53	43	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
			57	47	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
			55	45	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			55	45	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
			50	40	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
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			45	35	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
			46	36	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	h	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

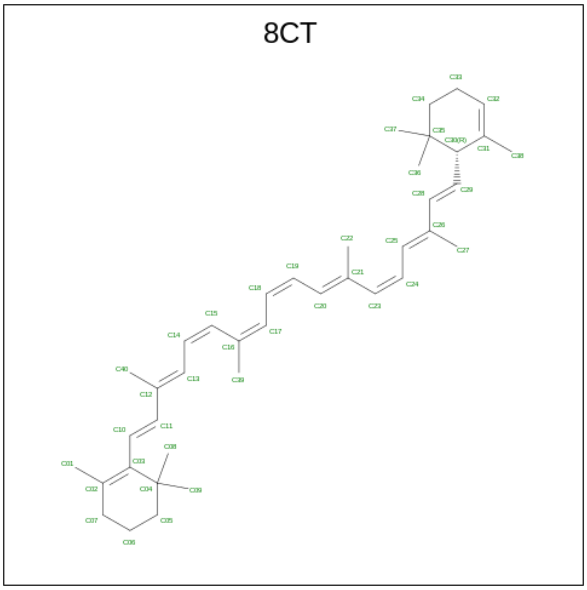
Mol	Chain	Residues	Atoms					AltConf
31	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	h	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	h	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	h	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	i	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	i	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	e	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 32 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
32	0	1	Total	C	0
			40	40	
32	1	1	Total	C	0
			40	40	
32	2	1	Total	C	0
			40	40	
32	3	1	Total	C	0
			40	40	
32	3	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

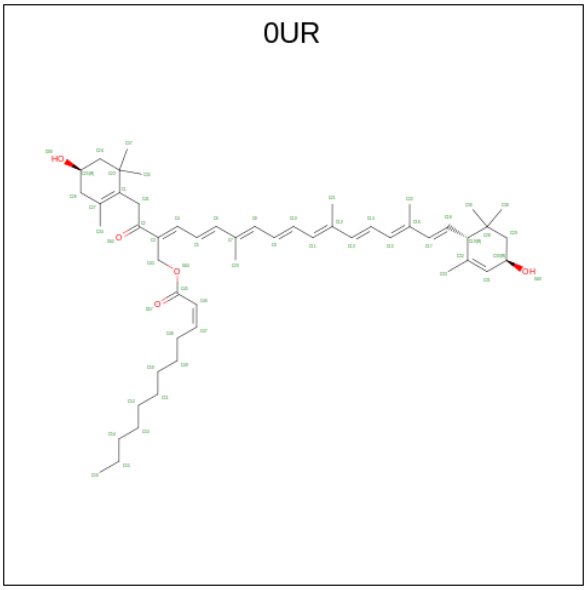
Mol	Chain	Residues	Atoms	AltConf
32	6	1	Total C 40 40	0
32	7	1	Total C 40 40	0
32	7	1	Total C 40 40	0
32	7	1	Total C 40 40	0
32	8	1	Total C 40 40	0
32	8	1	Total C 40 40	0
32	9	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
32	F	1	Total C 40 40	0
32	G	1	Total C 40 40	0
32	I	1	Total C 40 40	0
32	J	1	Total C 40 40	0
32	J	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	K	1	Total C 40 40	0
32	M	1	Total C 40 40	0
32	O	1	Total C 40 40	0
32	4	1	Total C 40 40	0

- Molecule 33 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



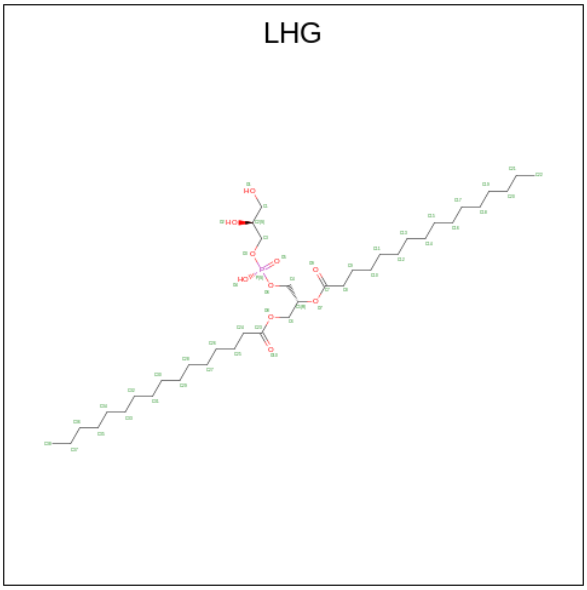
Mol	Chain	Residues	Atoms	AltConf
33	0	1	Total C O 52 47 5	0
33	0	1	Total C O 52 47 5	0
33	1	1	Total C O 52 47 5	0
33	1	1	Total C O 52 47 5	0
33	2	1	Total C O 51 46 5	0
33	2	1	Total C O 50 45 5	0
33	3	1	Total C O 51 46 5	0
33	5	1	Total C O 51 46 5	0
33	5	1	Total C O 52 47 5	0
33	6	1	Total C O 51 46 5	0
33	6	1	Total C O 52 47 5	0
33	7	1	Total C O 51 46 5	0
33	8	1	Total C O 51 46 5	0
33	8	1	Total C O 52 47 5	0
33	9	1	Total C O 52 47 5	0
33	9	1	Total C O 52 47 5	0
33	O	1	Total C O 52 47 5	0
33	a	1	Total C O 47 42 5	0
33	c	1	Total C O 52 47 5	0
33	b	1	Total C O 52 47 5	0
33	d	1	Total C O 49 44 5	0
33	f	1	Total C O 49 44 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
33	g	1	Total C O 52 47 5	0
33	h	1	Total C O 52 47 5	0
33	i	1	Total C O 50 45 5	0
33	e	1	Total C O 52 47 5	0
33	4	1	Total C O 51 46 5	0
33	4	1	Total C O 50 45 5	0

- Molecule 34 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
34	0	1	Total C O P 49 38 10 1	0
34	1	1	Total C O P 49 38 10 1	0
34	2	1	Total C O P 32 21 10 1	0
34	3	1	Total C O P 36 25 10 1	0
34	3	1	Total C O P 37 26 10 1	0

Continued on next page...

Continued from previous page...

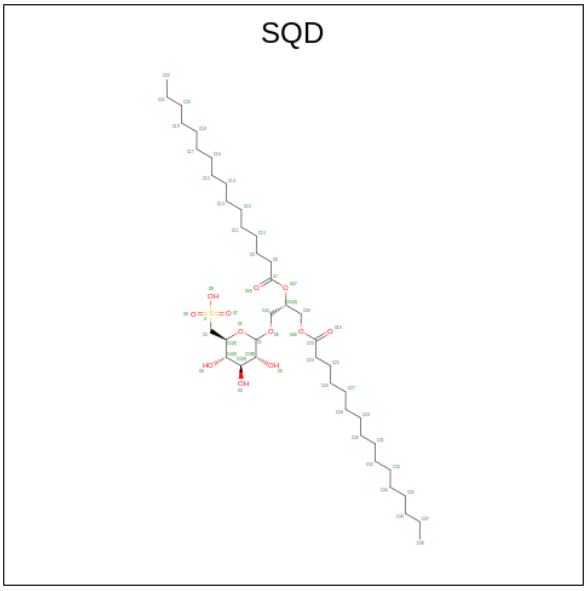
Mol	Chain	Residues	Atoms				AltConf
34	5	1	Total	C	O	P	0
			37	26	10	1	
34	6	1	Total	C	O	P	0
			37	26	10	1	
34	6	1	Total	C	O	P	0
			31	20	10	1	
34	7	1	Total	C	O	P	0
			30	19	10	1	
34	7	1	Total	C	O	P	0
			38	27	10	1	
34	7	1	Total	C	O	P	0
			39	28	10	1	
34	8	1	Total	C	O	P	0
			44	33	10	1	
34	9	1	Total	C	O	P	0
			47	36	10	1	
34	A	1	Total	C	O	P	0
			49	38	10	1	
34	A	1	Total	C	O	P	0
			27	16	10	1	
34	A	1	Total	C	O	P	0
			42	31	10	1	
34	B	1	Total	C	O	P	0
			23	12	10	1	
34	B	1	Total	C	O	P	0
			43	32	10	1	
34	G	1	Total	C	O	P	0
			38	27	10	1	
34	K	1	Total	C	O	P	0
			43	34	8	1	
34	M	1	Total	C	O	P	0
			46	35	10	1	
34	a	1	Total	C	O	P	0
			43	32	10	1	
34	c	1	Total	C	O	P	0
			40	29	10	1	
34	b	1	Total	C	O	P	0
			41	30	10	1	
34	d	1	Total	C	O	P	0
			36	25	10	1	
34	f	1	Total	C	O	P	0
			40	29	10	1	

Continued on next page...

Continued from previous page...

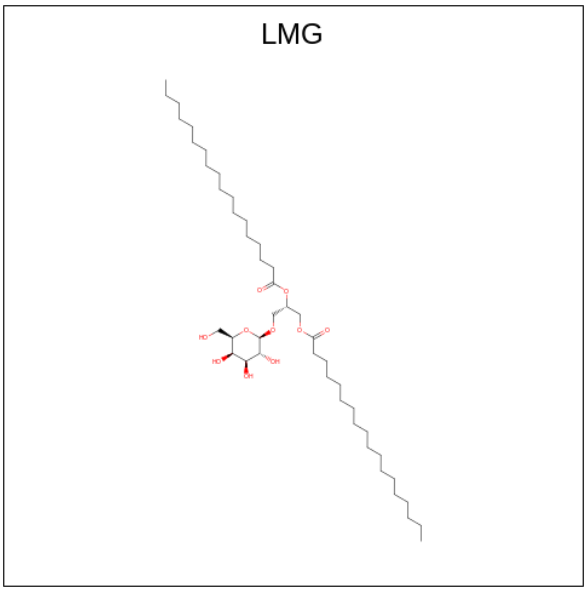
Mol	Chain	Residues	Atoms				AltConf
34	g	1	Total	C	O	P	0
			30	19	10	1	
34	h	1	Total	C	O	P	0
			39	28	10	1	
34	H	1	Total	C	O	P	0
			31	20	10	1	
34	i	1	Total	C	O	P	0
			30	19	10	1	
34	e	1	Total	C	O	P	0
			43	32	10	1	
34	4	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 35 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).



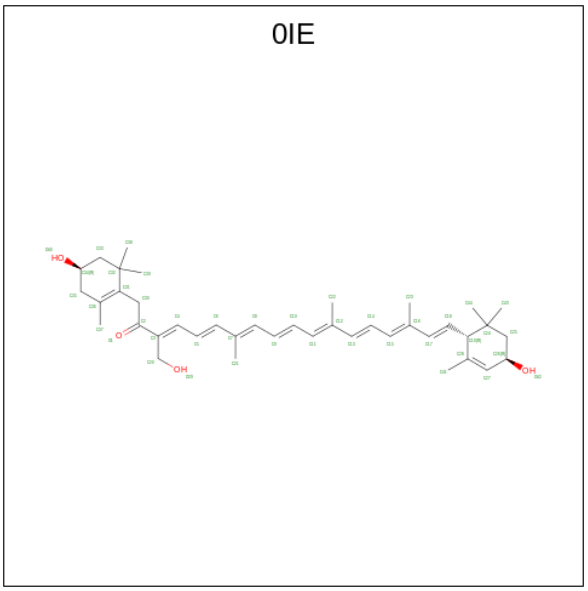
Mol	Chain	Residues	Atoms				AltConf
35	0	1	Total	C	O	S	0
			36	26	9	1	

- Molecule 36 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
36	2	1	Total C O 36 26 10	0
36	3	1	Total C O 36 26 10	0
36	9	1	Total C O 55 45 10	0
36	A	1	Total C O 36 26 10	0
36	B	1	Total C O 42 32 10	0
36	J	1	Total C O 29 19 10	0
36	J	1	Total C O 46 36 10	0
36	L	1	Total C O 31 21 10	0
36	L	1	Total C O 37 27 10	0
36	O	1	Total C O 39 29 10	0

- Molecule 37 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



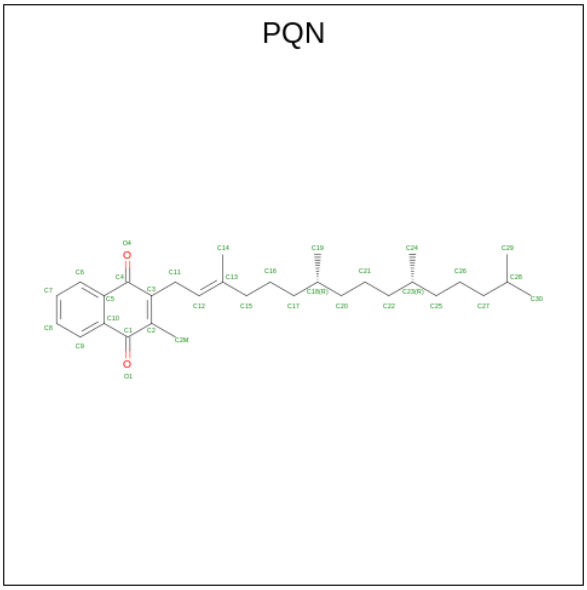
Mol	Chain	Residues	Atoms			AltConf
37	3	1	Total	C	O	0
			44	40	4	
37	7	1	Total	C	O	0
			44	40	4	
37	a	1	Total	C	O	0
			44	40	4	
37	a	1	Total	C	O	0
			44	40	4	
37	c	1	Total	C	O	0
			44	40	4	
37	c	1	Total	C	O	0
			44	40	4	
37	b	1	Total	C	O	0
			44	40	4	
37	b	1	Total	C	O	0
			44	40	4	
37	d	1	Total	C	O	0
			44	40	4	
37	d	1	Total	C	O	0
			44	40	4	
37	f	1	Total	C	O	0
			44	40	4	
37	f	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

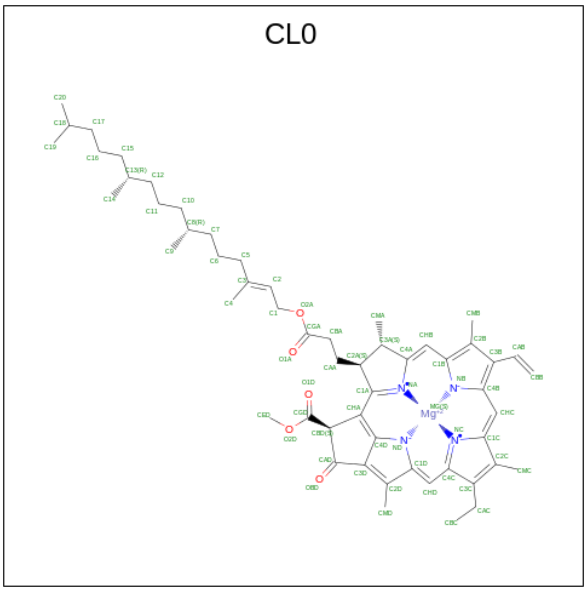
Mol	Chain	Residues	Atoms	AltConf
37	h	1	Total C O 44 40 4	0
37	h	1	Total C O 44 40 4	0
37	i	1	Total C O 44 40 4	0
37	i	1	Total C O 44 40 4	0
37	e	1	Total C O 44 40 4	0
37	e	1	Total C O 44 40 4	0

- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



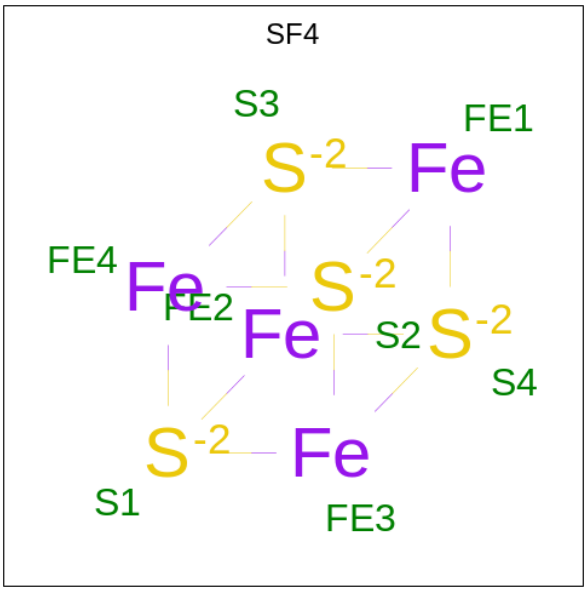
Mol	Chain	Residues	Atoms	AltConf
38	A	1	Total C O 33 31 2	0
38	B	1	Total C O 33 31 2	0

- Molecule 39 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
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



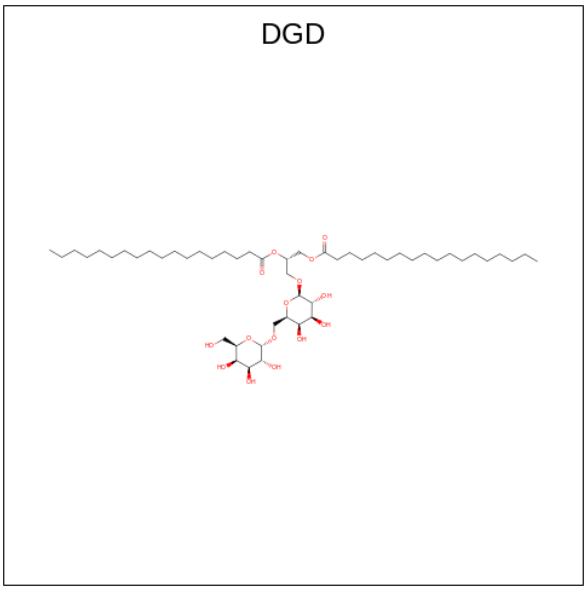
Mol	Chain	Residues	Atoms			AltConf
40	B	1	Total	Fe	S	0
			8	4	4	
40	C	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

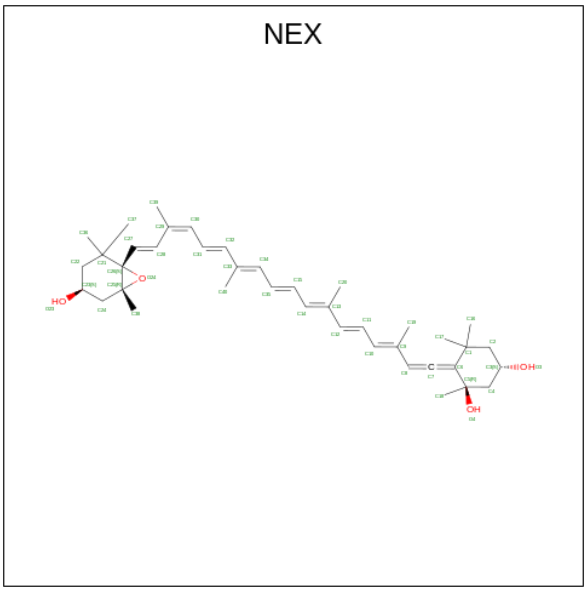
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
40	C	1	8	4	4	0

- Molecule 41 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
			Total	C	O	
41	B	1	56	41	15	0

- Molecule 42 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
42	a	1	Total	C	O	0
			44	40	4	
42	c	1	Total	C	O	0
			44	40	4	
42	b	1	Total	C	O	0
			44	40	4	
42	d	1	Total	C	O	0
			44	40	4	
42	f	1	Total	C	O	0
			44	40	4	
42	g	1	Total	C	O	0
			44	40	4	
42	h	1	Total	C	O	0
			44	40	4	
42	i	1	Total	C	O	0
			44	40	4	
42	e	1	Total	C	O	0
			44	40	4	

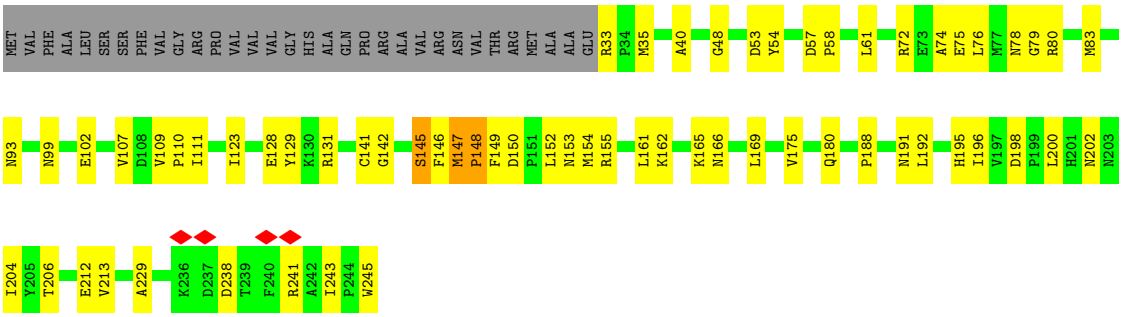
3 Residue-property plots (i)

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: Chlorophyll a-b binding protein, chloroplastic

Chain 0:

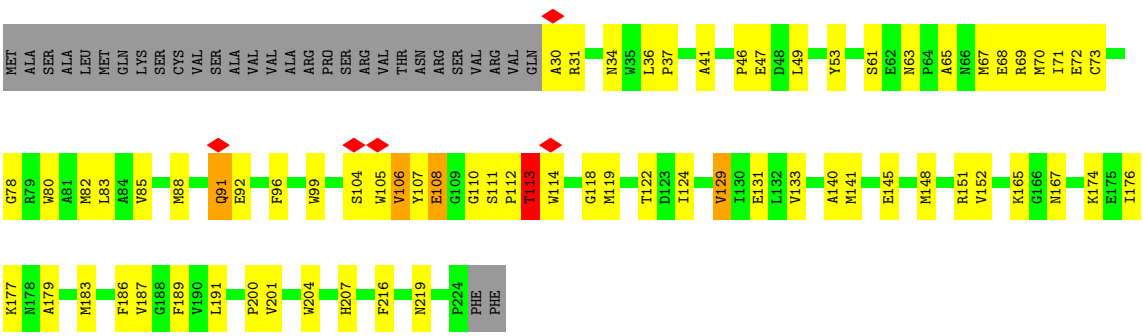




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

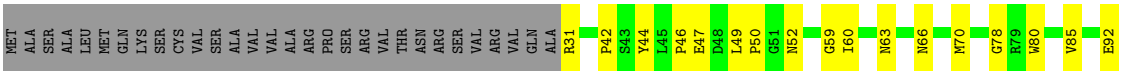


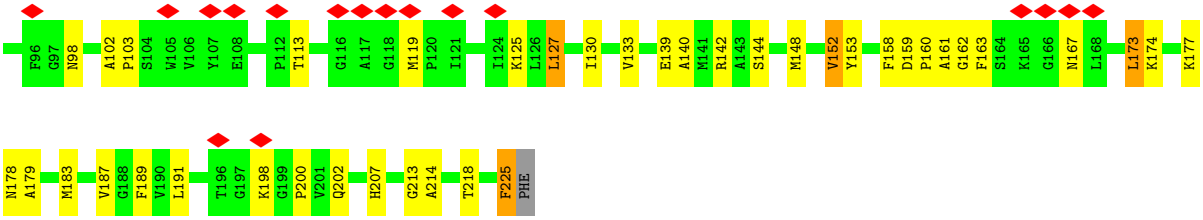


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



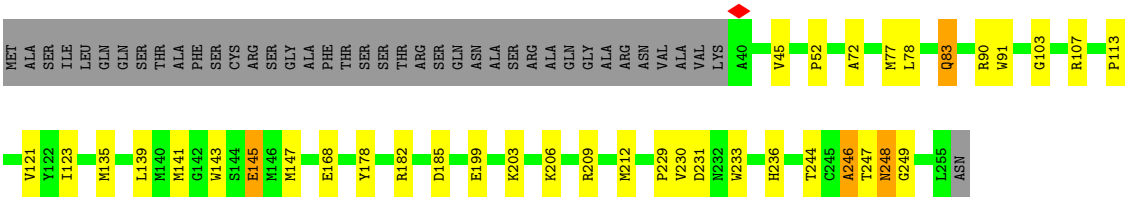




• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

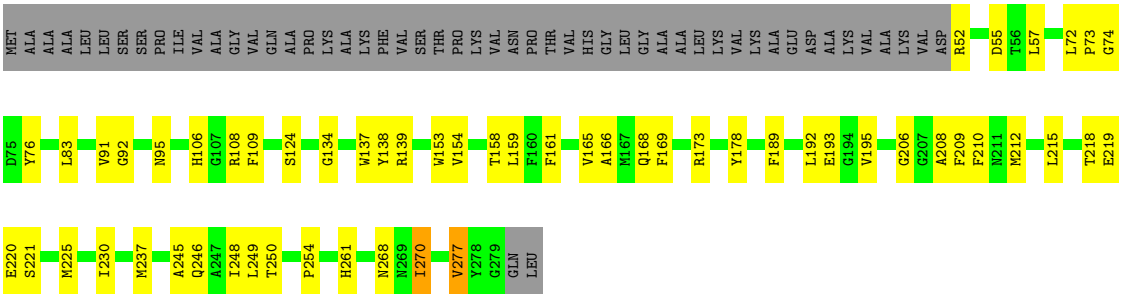




• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

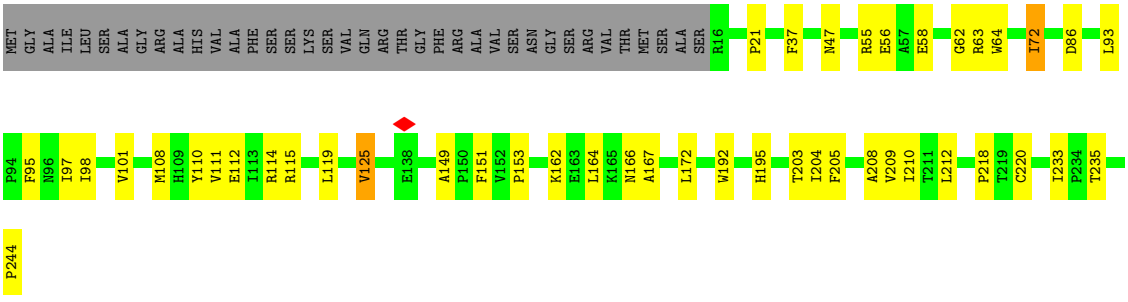




• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

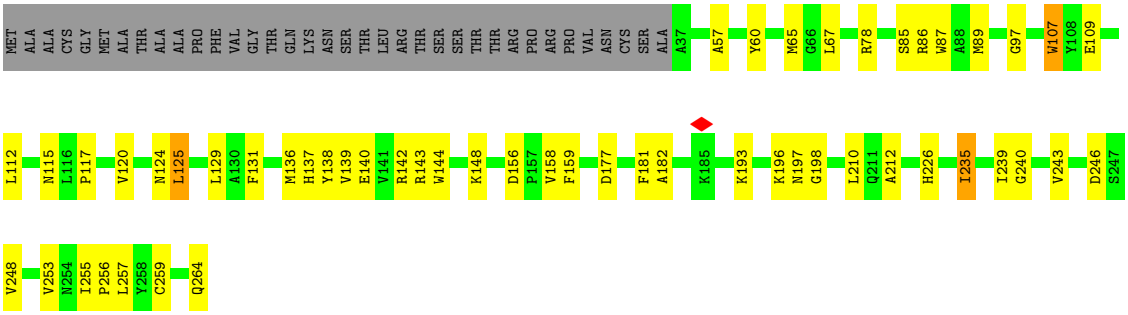




• Molecule 6: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

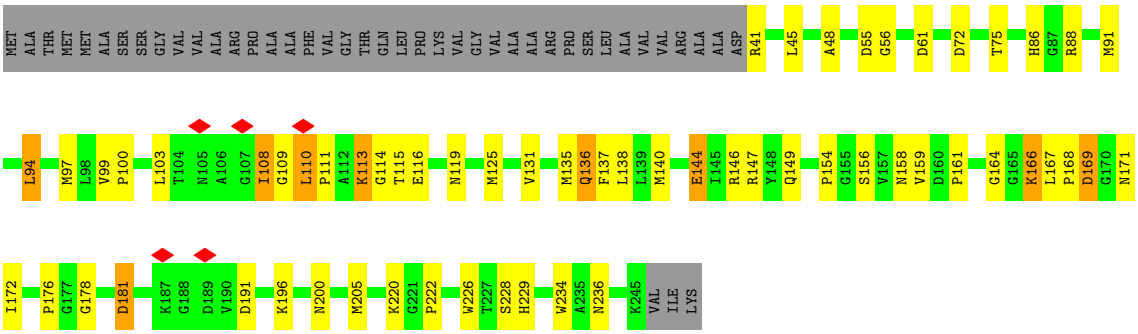




• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

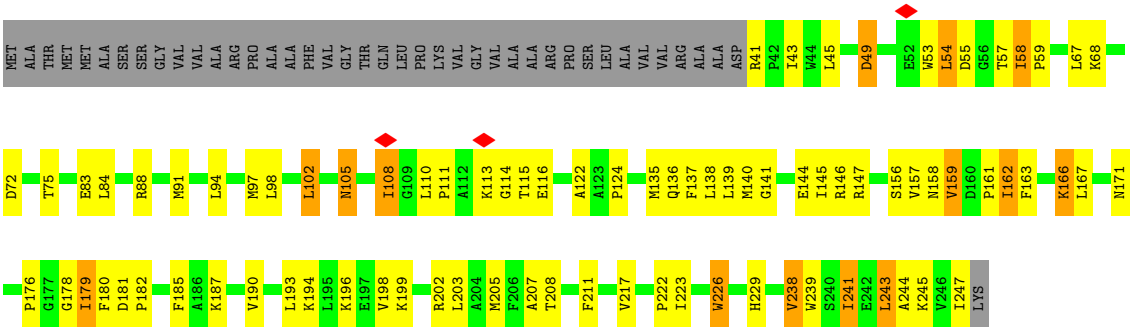




• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

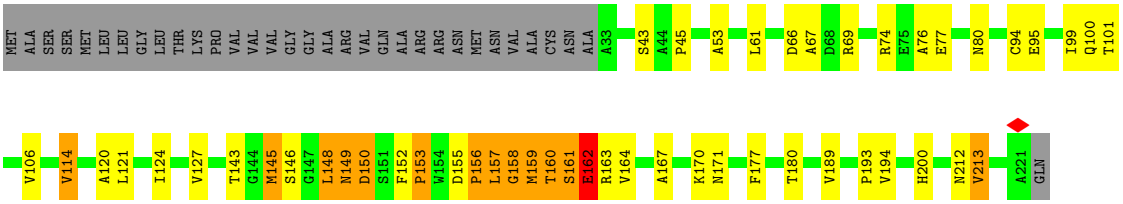




• Molecule 8: Chlorophyll a-b binding protein, chloroplastic

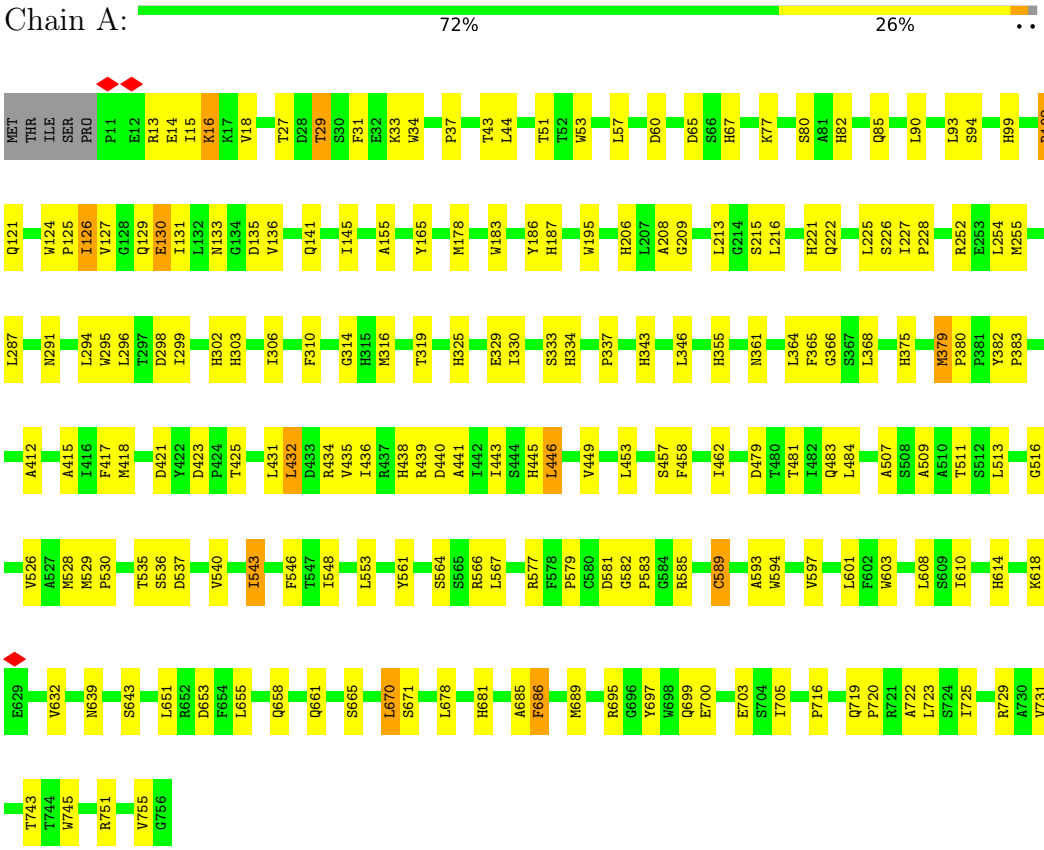
Chain 9:





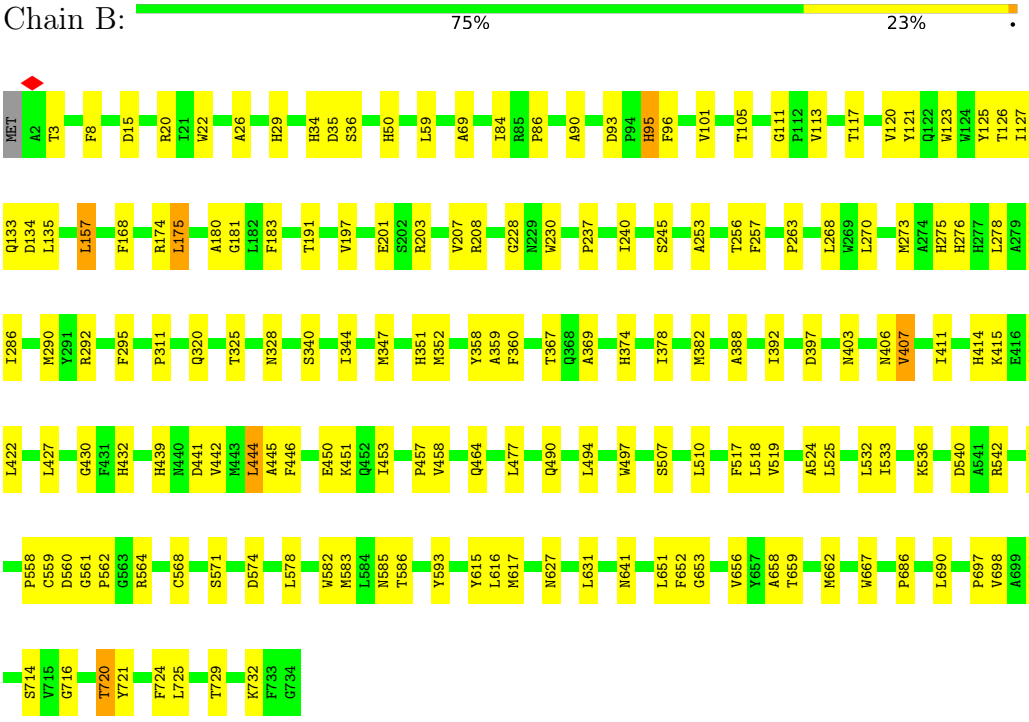
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



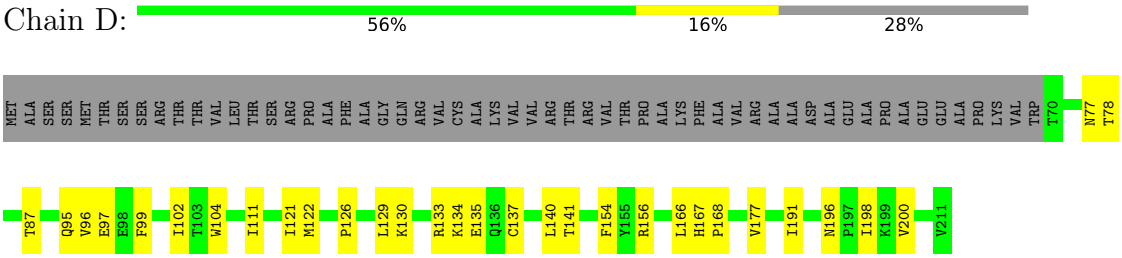
• Molecule 10: photosystem I

Chain B:



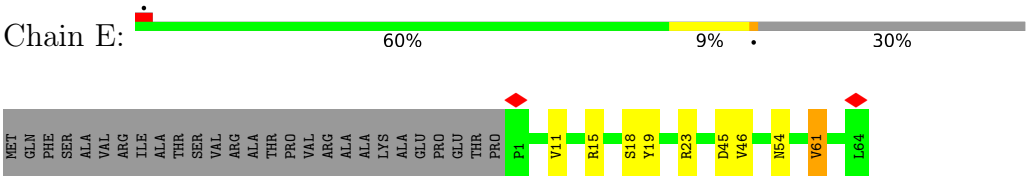
• Molecule 11: Photosystem I reaction center subunit II, chloroplastic

Chain D:



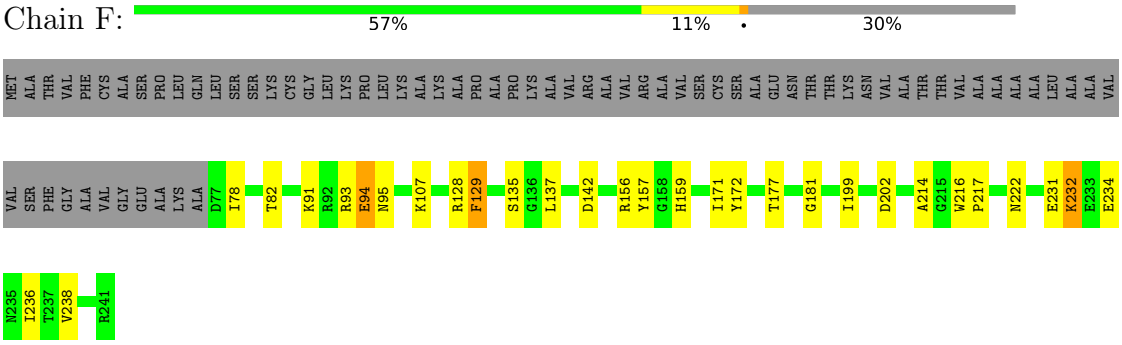
• Molecule 12: PsaE

Chain E:



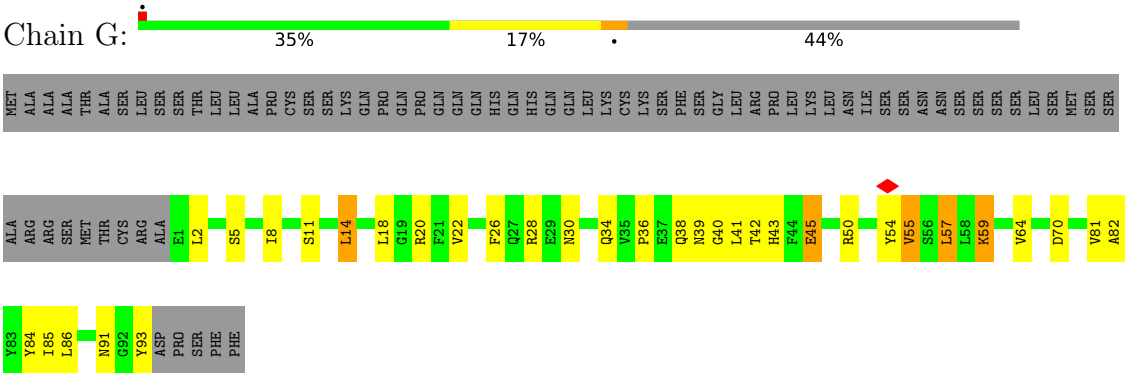
• Molecule 13: Photosystem I reaction center subunit III

Chain F:



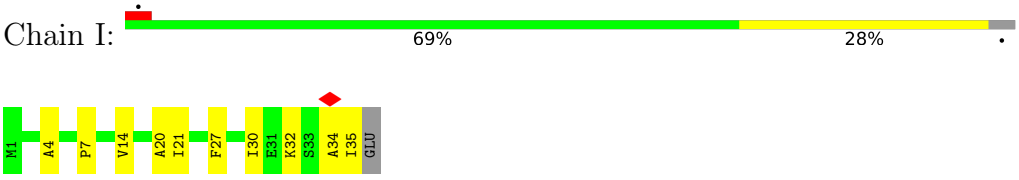
• Molecule 14: PsaG

Chain G:



• Molecule 15: Photosystem I reaction center subunit VIII

Chain I:



• Molecule 16: Photosystem I reaction center subunit IX

Chain J:

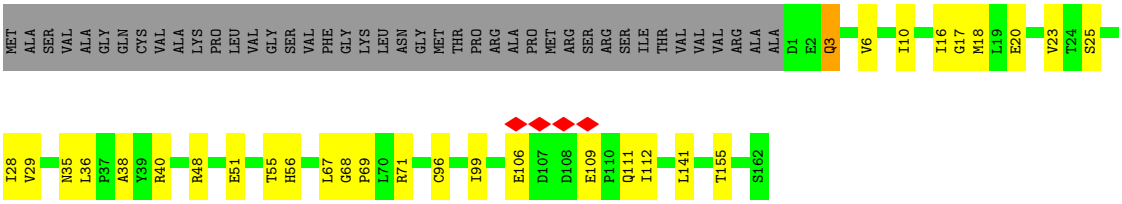




• Molecule 17: PSI subunit V

Chain L:

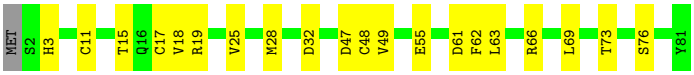




• Molecule 18: Photosystem I iron-sulfur center

Chain C:

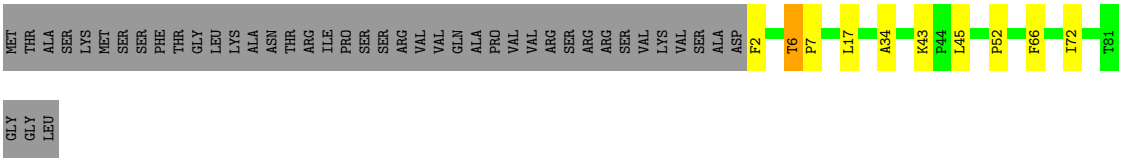




• Molecule 19: PsaK

Chain K:

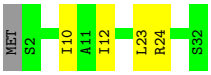




• Molecule 20: Photosystem I reaction center subunit XII

Chain M:

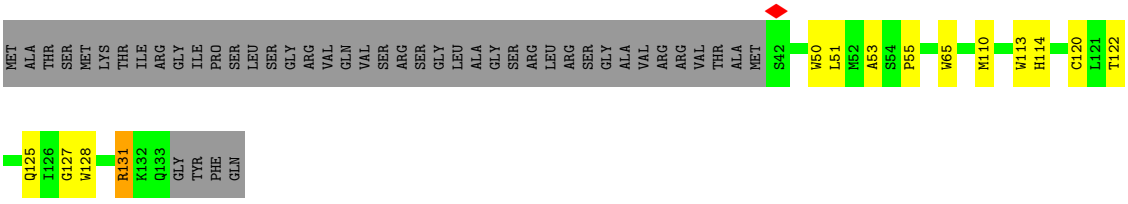




• Molecule 21: PsaO

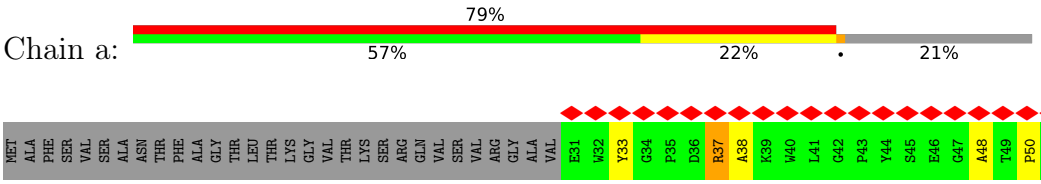
Chain O:

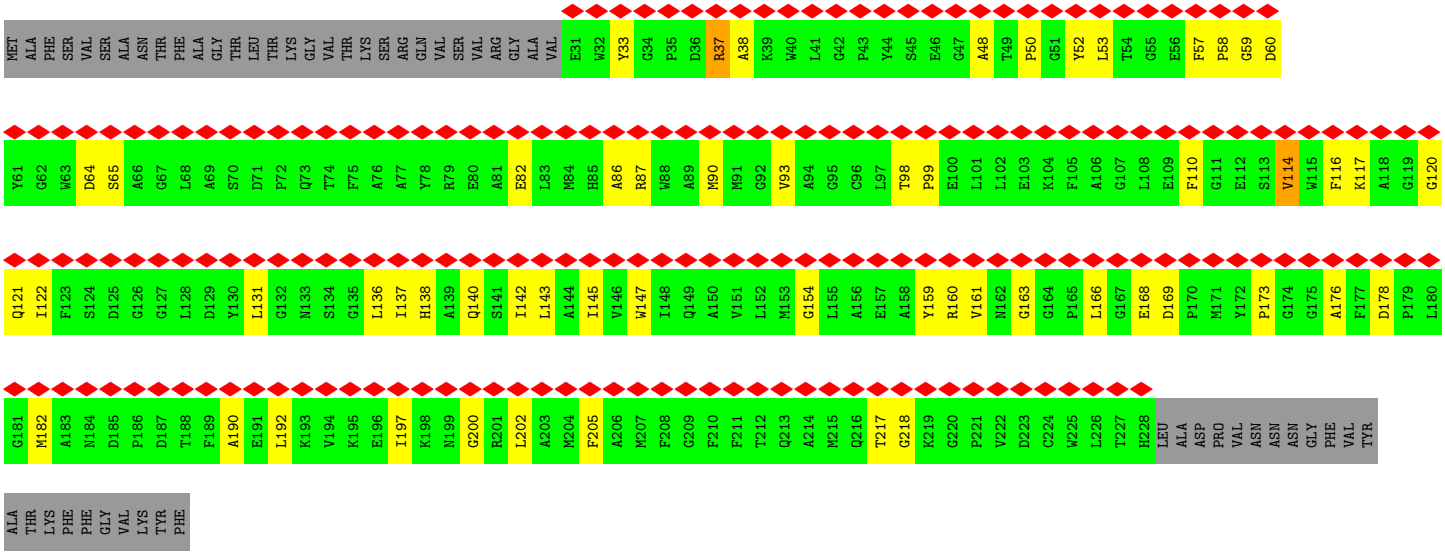




• Molecule 22: Lhcb-a

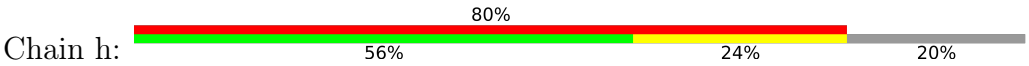
Chain a:

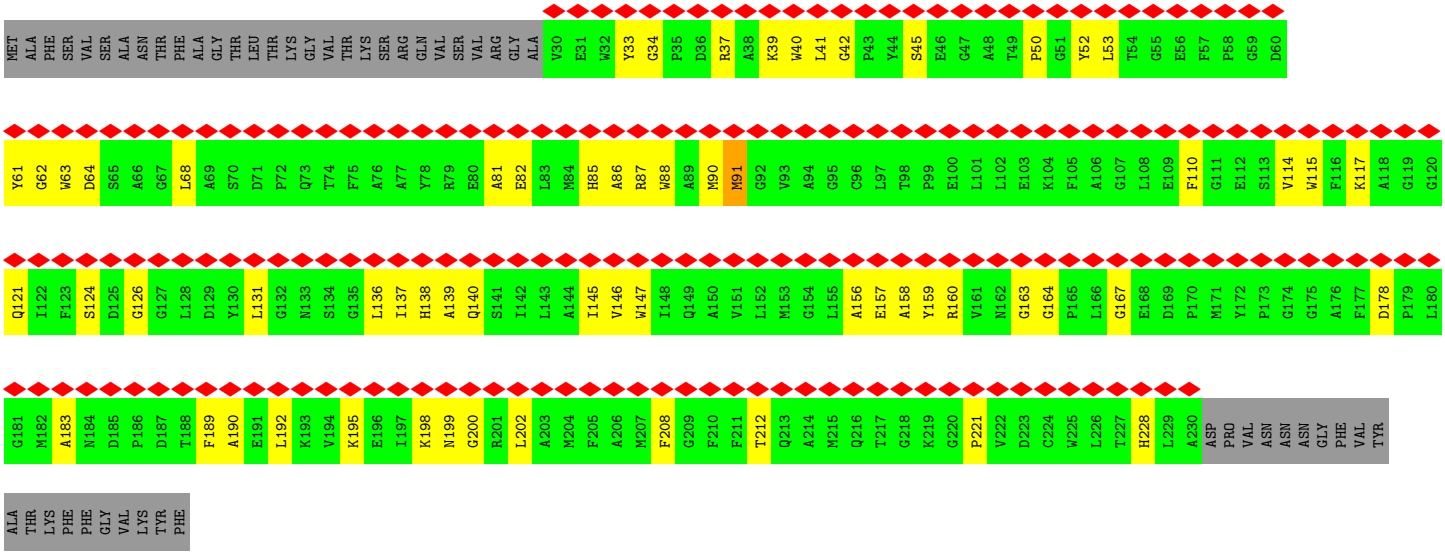




• Molecule 22: Lhcb-a

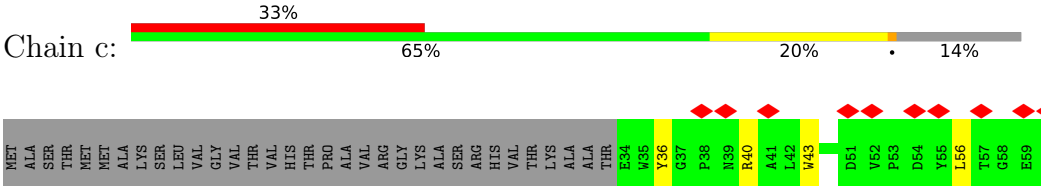
Chain h:

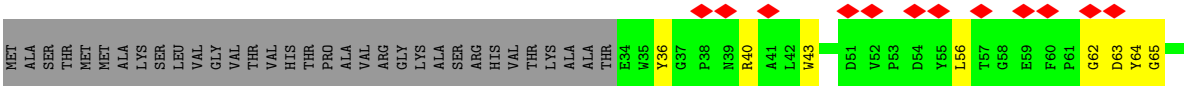


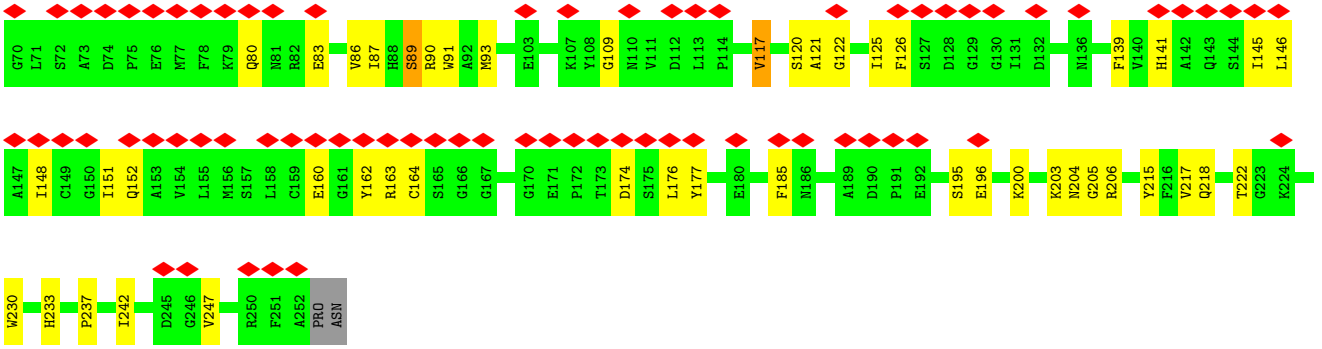


• Molecule 23: Lhcb-c

Chain c:



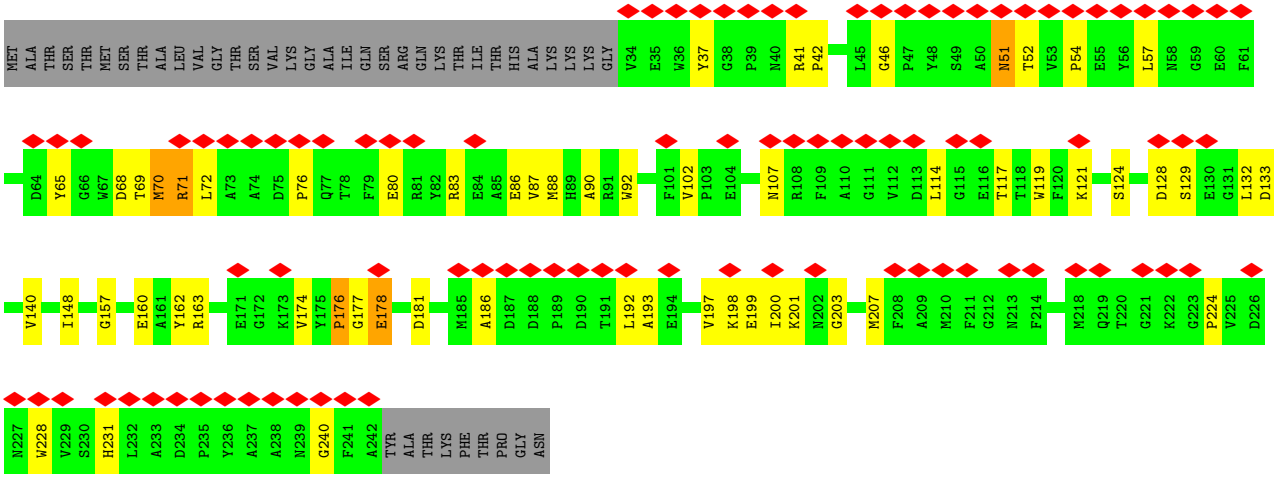




• Molecule 24: Lhcb-b

Chain b:

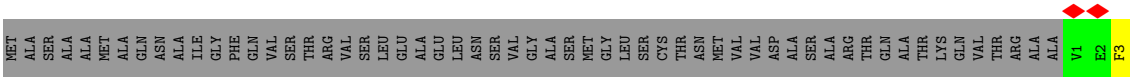


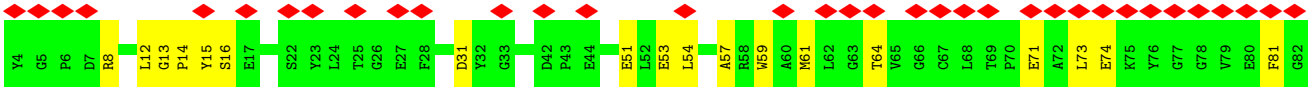


• Molecule 25: Lhcb-d

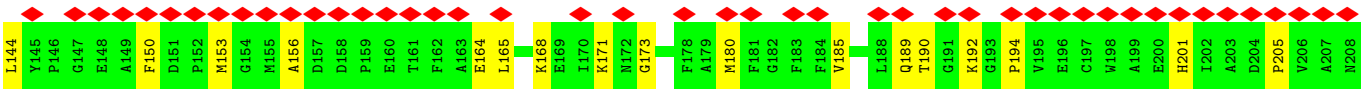
Chain d:

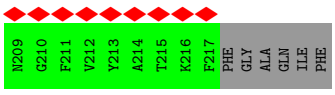






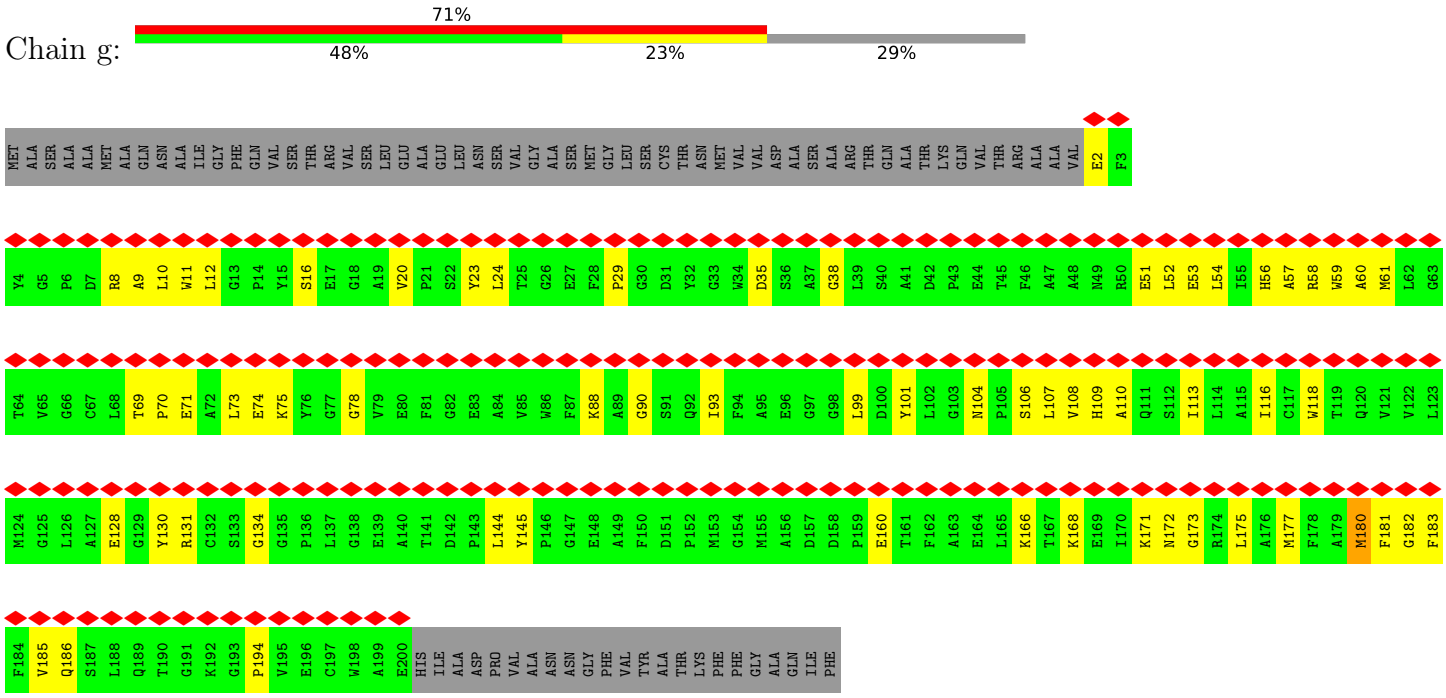






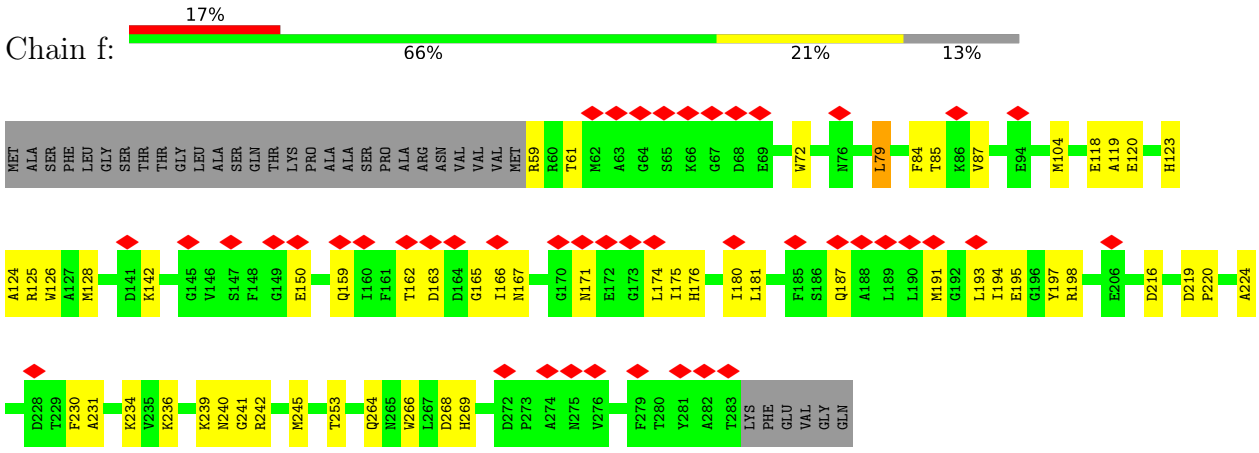
• Molecule 25: Lhcb-d

Chain g:



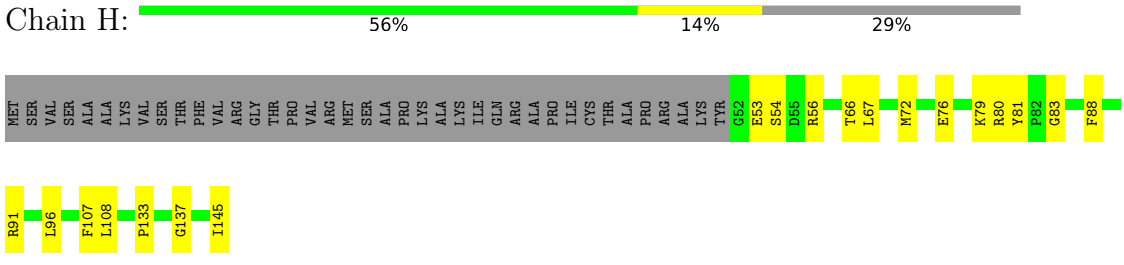
• Molecule 26: Lhcb-f

Chain f:



• Molecule 27: PsaH

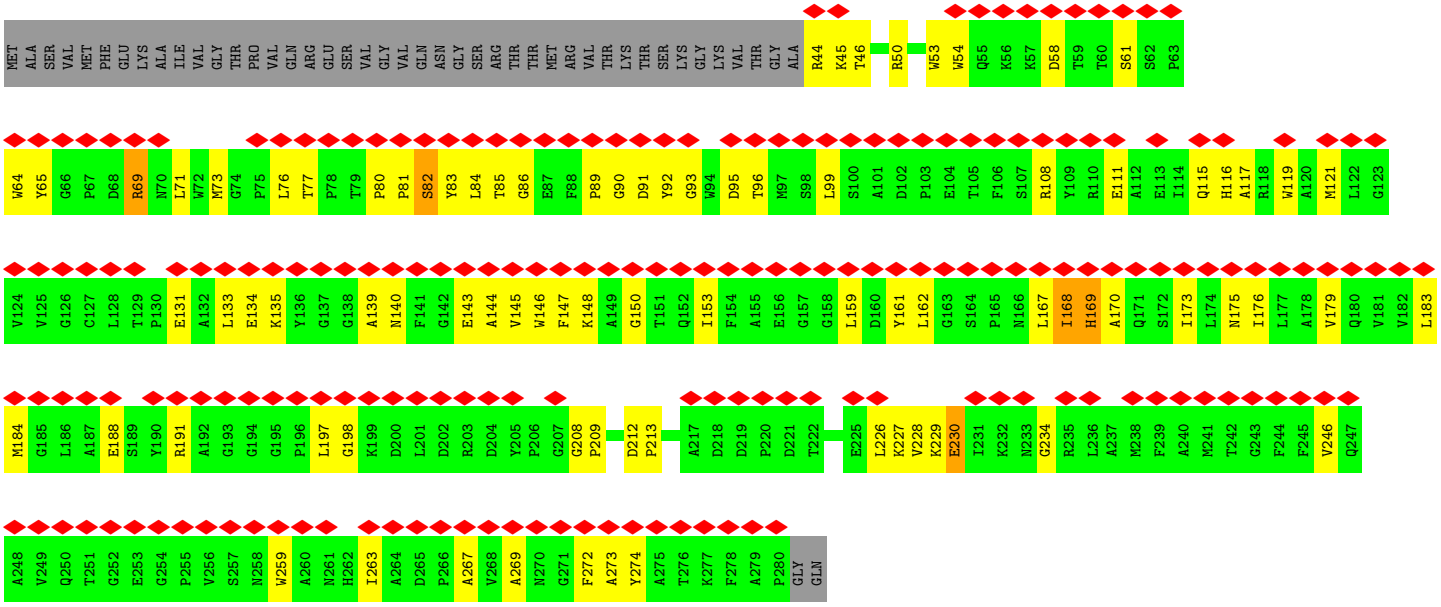
Chain H:



• Molecule 28: Lhcb-i

Chain i:

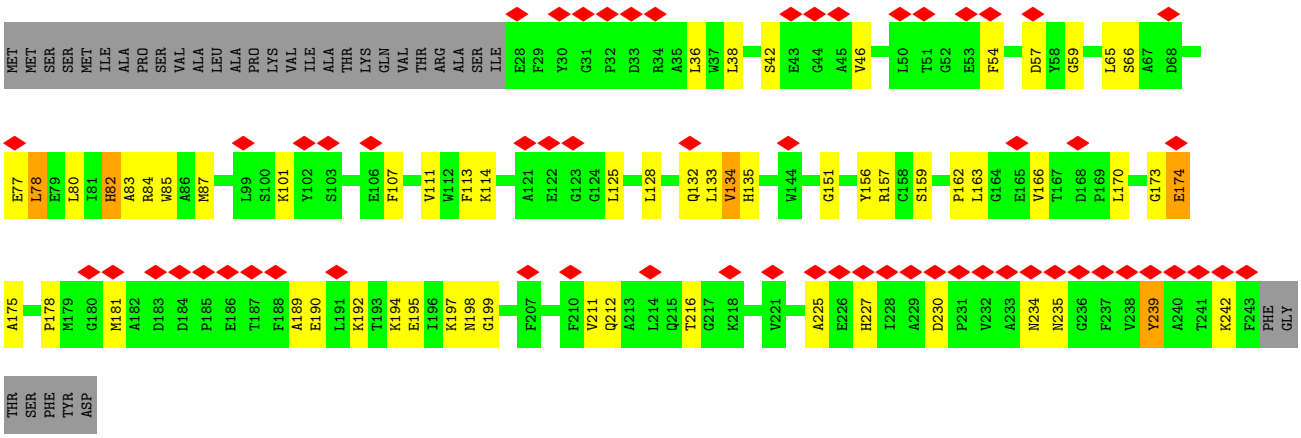




• Molecule 29: Lhcb-e

Chain e:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213217	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPHERA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.557	Depositor
Minimum map value	-0.337	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.217	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0UR, 8CT, CHL, TPO, SQD, PQN, LHG, LMG, SF4, CLA, CL0, 0IE, NEX, DGD

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	0	0.27	0/1685	0.38	0/2285
2	1	0.41	1/1523 (0.1%)	0.45	1/2073 (0.0%)
2	5	0.21	0/1530	0.41	0/2082
3	2	0.47	2/1727 (0.1%)	0.42	2/2351 (0.1%)
4	3	0.25	0/1818	0.32	0/2466
5	6	0.22	0/1862	0.29	0/2542
6	7	0.22	0/1812	0.31	0/2468
7	4	0.34	0/1619	0.62	1/2206 (0.0%)
7	8	0.20	0/1627	0.41	2/2217 (0.1%)
8	9	0.53	0/1492	0.48	1/2036 (0.0%)
9	A	0.42	1/6069 (0.0%)	0.35	1/8267 (0.0%)
10	B	0.37	0/6034	0.35	0/8239
11	D	0.21	0/1135	0.34	0/1533
12	E	0.19	0/521	0.26	0/706
13	F	0.21	0/1298	0.31	0/1748
14	G	0.25	0/743	0.41	0/1010
15	I	0.60	0/269	0.45	0/367
16	J	0.25	0/346	0.37	0/472
17	L	0.22	0/1224	0.34	0/1673
18	C	0.25	0/612	0.37	0/830
19	K	0.20	0/567	0.27	0/769
20	M	0.66	0/241	0.34	0/325
21	O	0.22	0/760	0.32	0/1042
22	a	0.12	0/1559	0.32	1/2116 (0.0%)
22	h	0.10	0/1568	0.28	0/2132
23	c	0.13	0/1733	0.30	0/2363
24	b	0.17	0/1658	0.34	0/2254
25	d	0.12	0/1685	0.29	0/2296
25	g	0.11	0/1548	0.26	0/2106
26	f	0.13	0/1765	0.27	0/2399
27	H	0.18	0/729	0.34	0/979
28	i	0.10	0/1881	0.30	0/2561

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
29	e	0.11	0/1697	0.29	0/2311
All	All	0.29	4/52337 (0.0%)	0.36	9/71224 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	246	ALA	CA-C	-5.28	1.46	1.52
9	A	689	MET	CA-C	-5.24	1.45	1.52
2	1	113	THR	CA-C	-5.19	1.45	1.53
3	2	247	THR	N-CA	-5.09	1.39	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	4	180	PHE	N-CA-C	-13.97	96.79	112.72
8	9	163	ARG	N-CA-C	-8.39	102.09	111.07
7	8	109	GLY	CA-C-N	6.66	129.49	123.10
7	8	109	GLY	C-N-CA	6.66	129.49	123.10
2	1	108	GLU	N-CA-C	-6.25	104.35	112.23
3	2	248	ASN	N-CA-C	-5.79	105.89	113.12
3	2	247	THR	N-CA-C	-5.35	104.55	111.71
9	A	686	PHE	N-CA-C	-5.27	104.95	111.33
22	a	37	ARG	CB-CA-C	-5.09	109.73	115.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1640	0	1609	50	0
2	1	1478	0	1423	56	0
2	5	1484	0	1427	42	0
3	2	1667	0	1562	27	0
4	3	1768	0	1702	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	6	1797	0	1752	37	0
6	7	1758	0	1701	48	0
7	4	1569	0	1551	65	0
7	8	1574	0	1550	51	0
8	9	1453	0	1404	42	0
9	A	5872	0	5715	162	0
10	B	5824	0	5603	149	0
11	D	1109	0	1124	26	0
12	E	509	0	506	9	0
13	F	1273	0	1290	23	0
14	G	726	0	717	32	0
15	I	262	0	279	9	0
16	J	336	0	355	13	0
17	L	1195	0	1187	25	0
18	C	602	0	591	22	0
19	K	558	0	591	7	0
20	M	238	0	248	4	0
21	O	728	0	699	16	0
22	a	1511	0	1426	44	0
22	h	1520	0	1429	56	0
23	c	1680	0	1582	47	0
24	b	1609	0	1531	51	0
25	d	1634	0	1535	49	0
25	g	1502	0	1412	51	0
26	f	1727	0	1634	62	0
27	H	717	0	684	22	0
28	i	1834	0	1741	91	0
29	e	1647	0	1559	48	0
30	0	215	0	172	13	0
30	1	291	0	262	19	0
30	2	426	0	344	21	0
30	3	179	0	166	9	0
30	4	347	0	251	22	0
30	5	304	0	228	16	0
30	6	425	0	344	22	0
30	7	334	0	280	20	0
30	8	420	0	332	20	0
30	9	193	0	132	4	0
30	a	405	0	307	21	0
30	b	390	0	341	25	0
30	c	425	0	362	32	0
30	d	415	0	331	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	e	422	0	345	24	0
30	f	430	0	364	24	0
30	g	381	0	266	15	0
30	h	386	0	280	19	0
30	i	389	0	282	32	0
31	0	478	0	426	26	0
31	1	434	0	386	18	0
31	2	389	0	356	9	0
31	3	603	0	554	23	0
31	4	371	0	324	13	0
31	5	409	0	340	13	0
31	6	527	0	456	15	0
31	7	569	0	496	26	0
31	8	364	0	314	6	0
31	9	496	0	458	19	0
31	A	2599	0	2656	135	0
31	B	2357	0	2336	146	0
31	F	45	0	33	3	0
31	G	141	0	105	2	0
31	H	200	0	160	4	0
31	J	42	0	31	2	0
31	K	209	0	176	9	0
31	L	260	0	221	11	0
31	M	46	0	33	0	0
31	O	168	0	108	7	0
31	a	315	0	266	10	0
31	b	320	0	276	11	0
31	c	303	0	244	9	0
31	d	306	0	250	11	0
31	e	317	0	270	13	0
31	f	315	0	266	12	0
31	g	280	0	208	19	0
31	h	273	0	200	11	0
31	i	292	0	228	38	0
32	0	40	0	0	0	0
32	1	40	0	0	0	0
32	2	40	0	0	0	0
32	3	80	0	0	1	0
32	4	40	0	0	1	0
32	6	40	0	0	0	0
32	7	120	0	0	1	0
32	8	80	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	9	40	0	0	0	0
32	A	240	0	0	1	0
32	B	320	0	0	2	0
32	F	40	0	0	0	0
32	G	40	0	0	0	0
32	I	40	0	0	0	0
32	J	80	0	0	1	0
32	K	40	0	0	0	0
32	L	120	0	0	1	0
32	M	40	0	0	0	0
32	O	40	0	0	0	0
33	0	104	0	0	1	0
33	1	104	0	0	1	0
33	2	101	0	0	3	0
33	3	51	0	0	1	0
33	4	101	0	0	3	0
33	5	103	0	0	4	0
33	6	103	0	0	1	0
33	7	51	0	0	2	0
33	8	103	0	0	3	0
33	9	104	0	0	3	0
33	O	52	0	0	1	0
33	a	47	0	0	2	0
33	b	52	0	0	3	0
33	c	52	0	0	1	0
33	d	49	0	0	1	0
33	e	52	0	0	0	0
33	f	49	0	0	0	0
33	g	52	0	0	0	0
33	h	52	0	0	1	0
33	i	50	0	0	2	0
34	0	49	0	74	4	0
34	1	49	0	74	6	0
34	2	32	0	34	3	0
34	3	73	0	84	4	0
34	4	32	0	34	0	0
34	5	37	0	44	1	0
34	6	68	0	76	5	0
34	7	107	0	127	4	0
34	8	44	0	58	0	0
34	9	47	0	63	5	0
34	A	118	0	152	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	66	0	75	4	0
34	G	38	0	46	2	0
34	H	31	0	32	0	0
34	K	43	0	60	4	0
34	M	46	0	65	4	0
34	a	43	0	56	4	0
34	b	41	0	52	2	0
34	c	40	0	50	5	0
34	d	36	0	42	5	0
34	e	43	0	56	5	0
34	f	40	0	50	5	0
34	g	30	0	30	3	0
34	h	39	0	48	4	0
34	i	30	0	30	4	0
35	0	36	0	41	2	0
36	2	36	0	42	0	0
36	3	36	0	42	1	0
36	9	55	0	86	4	0
36	A	36	0	42	3	0
36	B	42	0	54	1	0
36	J	75	0	93	3	0
36	L	68	0	76	3	0
36	O	39	0	48	1	0
37	3	44	0	0	0	0
37	7	44	0	0	0	0
37	a	88	0	0	0	0
37	b	88	0	0	2	0
37	c	88	0	0	1	0
37	d	88	0	0	0	0
37	e	88	0	0	0	0
37	f	88	0	0	0	0
37	g	88	0	0	0	0
37	h	88	0	0	2	0
37	i	88	0	0	4	0
38	A	33	0	46	5	0
38	B	33	0	46	1	0
39	A	65	0	72	7	0
40	B	8	0	0	1	0
40	C	16	0	0	0	0
41	B	56	0	70	3	0
42	a	44	0	56	7	0
42	b	44	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	c	44	0	56	5	0
42	d	44	0	56	10	0
42	e	44	0	56	3	0
42	f	44	0	56	26	0
42	g	44	0	56	8	0
42	h	44	0	56	15	0
42	i	44	0	56	35	0
All	All	77090	0	69459	1948	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 13.

All (1948) 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)
28:i:179:VAL:HG11	30:i:606:CHL:HED2	1.28	1.16
42:i:523:NEX:H362	31:i:604:CLA:C4B	1.79	1.11
42:a:523:NEX:H241	31:a:604:CLA:H2	1.36	1.05
1:0:147:MET:HB3	1:0:148:PRO:HD2	1.42	1.00
2:5:160:PRO:HD2	33:5:501:0UR:C30	1.90	1.00
42:i:523:NEX:H362	31:i:604:CLA:C3B	1.94	0.97
42:i:523:NEX:H383	31:i:604:CLA:C1B	1.96	0.95
42:i:523:NEX:C36	31:i:604:CLA:CHC	2.44	0.95
26:f:193:LEU:CD2	42:h:523:NEX:H172	1.99	0.93
31:A:805:CLA:H11	31:A:806:CLA:HBB1	1.51	0.92
39:A:857:CL0:H15	31:B:803:CLA:HED1	1.52	0.92
25:d:124:MET:HE1	42:d:523:NEX:H30	1.53	0.90
26:f:194:ILE:HD11	42:f:523:NEX:C34	2.01	0.89
42:i:523:NEX:H362	31:i:604:CLA:CHC	2.03	0.89
42:d:523:NEX:H241	31:d:604:CLA:H2	1.56	0.87
42:a:523:NEX:H241	31:a:604:CLA:C2	2.05	0.86
9:A:29:THR:HG21	9:A:183:TRP:HE1	1.39	0.85
8:9:145:MET:HB3	8:9:153:PRO:HD3	1.58	0.83
26:f:193:LEU:HD21	42:h:523:NEX:H172	1.61	0.82
25:d:15:TYR:CE2	42:h:523:NEX:O3	2.33	0.82
2:1:78:GLY:HA3	2:1:179:ALA:HB1	1.61	0.81
2:1:174:LYS:HD3	31:1:311:CLA:HBA1	1.64	0.80
22:a:86:ALA:HB1	22:a:200:GLY:HA3	1.64	0.79
26:f:193:LEU:HD23	42:h:523:NEX:H172	1.65	0.78
42:i:523:NEX:H363	31:i:604:CLA:CHC	2.11	0.78
31:B:803:CLA:HHB	31:B:805:CLA:H202	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:128:GLU:HG2	25:g:131:ARG:HE	1.50	0.76
31:B:824:CLA:H52	31:B:825:CLA:H142	1.67	0.76
29:e:211:VAL:HG21	31:e:613:CLA:HAC2	1.67	0.75
28:i:184:MET:HE1	42:i:523:NEX:H30	1.68	0.75
7:8:146:ARG:O	7:8:158:ASN:ND2	2.20	0.75
17:L:35:ASN:HB3	31:L:202:CLA:HAC1	1.69	0.75
8:9:152:PHE:O	8:9:153:PRO:C	2.29	0.75
28:i:159:LEU:HD13	30:i:606:CHL:CMD	2.18	0.74
30:9:306:CHL:HHC	30:9:306:CHL:HBB1	1.67	0.74
28:i:159:LEU:HD13	30:i:606:CHL:HMD2	1.70	0.74
7:4:146:ARG:NH1	30:4:319:CHL:OBD	2.20	0.74
26:f:266:TRP:HE1	30:f:614:CHL:HMC	1.52	0.74
9:A:65:ASP:OD2	9:A:355:HIS:NE2	2.20	0.73
31:A:809:CLA:HAB	31:B:833:CLA:HMD2	1.69	0.73
31:A:832:CLA:HBB2	17:L:67:LEU:HD13	1.69	0.73
30:2:319:CHL:HBB1	30:2:319:CHL:HHC	1.70	0.73
1:0:147:MET:O	1:0:148:PRO:C	2.31	0.73
30:e:602:CHL:HHC	30:e:602:CHL:HBB1	1.71	0.73
5:6:115:ARG:NH2	30:6:308:CHL:O1D	2.21	0.73
30:a:609:CHL:H2A	24:b:69:THR:HG21	1.70	0.73
23:c:43:TRP:HE1	30:c:601:CHL:HAA1	1.52	0.72
2:1:204:TRP:HE1	30:1:313:CHL:HMC	1.55	0.72
2:5:78:GLY:HA3	2:5:179:ALA:HB1	1.71	0.72
6:7:85:SER:HB2	6:7:198:GLY:HA3	1.70	0.72
7:8:88:ARG:NH1	30:8:307:CHL:OBD	2.20	0.72
9:A:252:ARG:NH1	9:A:262:PHE:O	2.22	0.72
30:4:319:CHL:HHC	30:4:319:CHL:HBB1	1.70	0.72
26:f:194:ILE:CD1	42:f:523:NEX:C34	2.67	0.72
9:A:577:ARG:NH1	34:A:844:LHG:O10	2.23	0.72
25:d:201:HIS:HD1	25:d:205:PRO:HG3	1.53	0.72
28:i:184:MET:HE1	42:i:523:NEX:H32	1.71	0.72
30:7:306:CHL:HBB1	30:7:306:CHL:HHC	1.72	0.71
30:8:305:CHL:HHC	30:8:305:CHL:HBB1	1.72	0.71
25:g:57:ALA:HB1	25:g:173:GLY:HA3	1.72	0.71
9:A:206:HIS:HB3	31:A:825:CLA:HED2	1.71	0.71
31:A:804:CLA:H61	31:A:809:CLA:H202	1.71	0.71
25:d:51:GLU:HA	25:d:144:LEU:HD21	1.71	0.71
5:6:114:ARG:NH1	30:8:301:CHL:OBD	2.22	0.71
2:1:113:THR:HG21	30:1:305:CHL:HMD3	1.71	0.71
10:B:415:LYS:HZ3	13:F:238:VAL:HG21	1.55	0.71
31:d:603:CLA:H12	29:e:65:LEU:HD11	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:601:LHG:H122	30:4:319:CHL:H2	1.73	0.71
31:A:825:CLA:HBA1	31:A:829:CLA:H203	1.73	0.71
23:c:36:TYR:HE2	23:c:195:SER:HB3	1.54	0.71
24:b:90:ALA:HB1	24:b:203:GLY:HA3	1.72	0.71
22:h:163:GLY:HA3	30:h:608:CHL:HMC	1.71	0.71
5:6:101:VAL:HG22	30:6:306:CHL:HBC1	1.73	0.70
30:c:601:CHL:H52	30:b:609:CHL:HBB1	1.71	0.70
28:i:184:MET:HE2	30:i:606:CHL:HMA1	1.73	0.70
18:C:15:THR:OG1	18:C:19:ARG:NH1	2.24	0.70
30:0:301:CHL:HBB2	30:0:302:CHL:HHD	1.71	0.70
8:9:152:PHE:CB	8:9:153:PRO:HD2	2.21	0.70
9:A:601:LEU:HD21	31:A:830:CLA:HBC1	1.71	0.70
13:F:202:ASP:HA	36:J:102:LMG:HC61	1.73	0.70
7:8:149:GLN:HB2	7:8:158:ASN:HD21	1.57	0.70
26:f:197:TYR:OH	42:f:523:NEX:C19	2.40	0.70
17:L:99:ILE:HD11	34:M:104:LHG:H111	1.74	0.69
26:f:124:ALA:HB1	26:f:241:GLY:HA3	1.71	0.69
8:9:170:LYS:NZ	34:9:601:LHG:O4	2.21	0.69
30:6:301:CHL:O1A	6:7:137:HIS:ND1	2.25	0.69
5:6:203:THR:HG22	5:6:205:PHE:H	1.56	0.69
7:4:43:ILE:HG22	7:4:45:LEU:H	1.57	0.69
28:i:69:ARG:H	28:i:69:ARG:HD3	1.57	0.69
11:D:167:HIS:HB3	11:D:168:PRO:HD3	1.75	0.69
25:d:57:ALA:HB1	25:d:173:GLY:HA3	1.72	0.69
31:8:304:CLA:H192	30:8:307:CHL:HAA2	1.75	0.69
29:e:125:LEU:HD21	31:e:604:CLA:HAA2	1.75	0.69
42:d:523:NEX:H31	30:d:606:CHL:HBA2	1.75	0.69
7:4:49:ASP:N	7:4:49:ASP:OD1	2.26	0.69
28:i:131:GLU:HA	28:i:144:ALA:HB1	1.75	0.68
30:4:306:CHL:HBB1	30:4:306:CHL:HHC	1.74	0.68
34:0:601:LHG:HC91	34:0:601:LHG:H281	1.74	0.68
7:4:226:TRP:HZ3	30:4:313:CHL:HMC	1.58	0.68
30:8:301:CHL:HHC	30:8:301:CHL:HBB1	1.74	0.68
9:A:511:THR:HG21	31:A:827:CLA:HAB	1.74	0.68
14:G:11:SER:HB3	14:G:81:VAL:HG13	1.74	0.68
9:A:13:ARG:HE	19:K:43:LYS:HE3	1.58	0.68
7:4:226:TRP:CZ3	30:4:313:CHL:HMC	2.29	0.68
26:f:193:LEU:HB2	42:f:523:NEX:C20	2.24	0.68
2:1:30:ALA:N	2:1:47:GLU:O	2.27	0.68
31:5:303:CLA:HBC1	31:5:308:CLA:HAC1	1.75	0.68
10:B:120:VAL:HG21	31:B:811:CLA:HED1	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:K:104:CLA:HAC2	30:c:601:CHL:HMC	1.75	0.68
9:A:543:ILE:HD13	39:A:857:CL0:H59	1.75	0.67
10:B:290:MET:HB2	31:B:822:CLA:HBC3	1.75	0.67
14:G:55:VAL:O	14:G:59:LYS:NZ	2.27	0.67
26:f:197:TYR:OH	42:f:523:NEX:H192	1.94	0.67
42:i:523:NEX:H222	31:i:604:CLA:C4B	2.24	0.67
13:F:137:LEU:HD21	16:J:38:ILE:HG21	1.77	0.67
28:i:259:TRP:HE1	30:i:614:CHL:HMC	1.58	0.67
25:g:8:ARG:NH2	25:g:24:LEU:O	2.28	0.67
28:i:159:LEU:CD1	30:i:606:CHL:HMD3	2.25	0.67
42:i:523:NEX:C36	31:i:604:CLA:C4B	2.62	0.67
25:d:190:THR:HG22	25:d:192:LYS:H	1.59	0.67
25:d:15:TYR:HE2	42:h:523:NEX:O3	1.74	0.67
7:8:161:PRO:HG2	7:8:166:LYS:HG3	1.76	0.67
5:6:208:ALA:HB2	5:6:218:PRO:HD3	1.77	0.67
7:4:182:PRO:HD2	33:4:501:0UR:C30	2.25	0.67
2:1:88:MET:HB3	2:1:99:TRP:HB3	1.77	0.66
9:A:77:LYS:NZ	31:A:811:CLA:OBD	2.28	0.66
23:c:242:ILE:HG22	30:c:614:CHL:HED1	1.77	0.66
26:f:193:LEU:HB2	42:f:523:NEX:H203	1.77	0.66
2:5:113:THR:OG1	2:5:119:MET:SD	2.53	0.66
29:e:197:LYS:NZ	34:e:630:LHG:O4	2.29	0.66
3:2:168:GLU:OE2	3:2:182:ARG:NH2	2.28	0.66
31:A:819:CLA:H8	31:A:819:CLA:HAB	1.76	0.66
22:h:198:LYS:NZ	34:h:630:LHG:O4	2.29	0.66
7:4:239:TRP:H	7:4:243:LEU:HD11	1.61	0.66
5:6:55:ARG:NH1	5:6:58:GLU:OE1	2.29	0.66
10:B:230:TRP:O	31:B:817:CLA:H3A	1.95	0.66
30:b:608:CHL:HBA1	30:b:608:CHL:H122	1.77	0.66
2:5:92:GLU:HB2	2:5:98:ASN:HA	1.77	0.66
9:A:209:GLY:O	9:A:213:LEU:HB2	1.95	0.65
34:i:630:LHG:HC91	34:i:630:LHG:H261	1.78	0.65
7:4:84:LEU:HD12	7:4:176:PRO:HG2	1.77	0.65
30:0:305:CHL:HHC	30:0:305:CHL:HBB1	1.77	0.65
24:b:228:TRP:HE1	30:b:614:CHL:HMC	1.60	0.65
34:d:630:LHG:H292	34:d:630:LHG:H101	1.77	0.65
1:0:33:ARG:NH2	1:0:53:ASP:O	2.30	0.65
6:7:86:ARG:NH1	30:7:307:CHL:OBD	2.24	0.65
24:b:80:GLU:OE1	24:b:83:ARG:NH2	2.29	0.65
28:i:272:PHE:O	28:i:274:TYR:N	2.30	0.65
9:A:441:ALA:O	9:A:445:HIS:ND1	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:606:CHL:HHC	30:a:606:CHL:HBB1	1.79	0.65
9:A:379:MET:HE3	31:A:818:CLA:HBD	1.79	0.65
13:F:231:GLU:HG3	13:F:232:LYS:H	1.62	0.65
2:1:216:PHE:HB3	31:1:312:CLA:H12	1.79	0.65
31:g:603:CLA:H12	22:h:68:LEU:HD11	1.78	0.65
1:0:147:MET:CB	1:0:148:PRO:HD2	2.23	0.64
30:5:301:CHL:HHC	30:5:301:CHL:HBB1	1.77	0.64
26:f:159:GLN:HB2	26:f:166:ILE:HG22	1.79	0.64
22:h:86:ALA:HB1	22:h:200:GLY:HA3	1.78	0.64
1:0:147:MET:HB3	1:0:148:PRO:CD	2.22	0.64
22:h:157:GLU:OE1	22:h:160:ARG:NH2	2.26	0.64
8:9:160:THR:HA	31:9:309:CLA:HAA2	1.78	0.64
28:i:159:LEU:CD1	30:i:606:CHL:CMD	2.75	0.64
28:i:184:MET:CE	42:i:523:NEX:H32	2.26	0.64
2:1:177:LYS:NZ	34:1:601:LHG:O4	2.31	0.64
30:2:306:CHL:HHC	30:2:306:CHL:HBB1	1.78	0.64
5:6:62:GLY:HA3	5:6:167:ALA:HB1	1.79	0.64
31:8:304:CLA:HED2	31:8:304:CLA:H2A	1.78	0.64
26:f:125:ARG:NH1	30:f:608:CHL:OBD	2.29	0.64
2:1:70:MET:HA	2:1:73:CYS:SG	2.38	0.64
30:8:307:CHL:HHC	30:8:307:CHL:HBB1	1.80	0.64
29:e:162:PRO:HG2	42:e:523:NEX:H192	1.80	0.64
4:3:124:SER:HB2	4:3:134:GLY:HA3	1.80	0.64
1:0:54:TYR:OH	1:0:165:LYS:NZ	2.31	0.64
35:0:603:SQD:H45	20:M:24:ARG:HD2	1.79	0.64
31:5:309:CLA:HAB	33:5:501:0UR:C13	2.28	0.64
6:7:97:GLY:HA3	31:7:304:CLA:HBC3	1.78	0.64
31:A:822:CLA:HAA2	19:K:34:ALA:HB3	1.79	0.64
42:i:523:NEX:H222	31:i:604:CLA:NB	2.13	0.64
24:b:160:GLU:OE1	24:b:163:ARG:NH1	2.31	0.63
42:i:523:NEX:H383	31:i:604:CLA:CHB	2.28	0.63
34:d:630:LHG:H271	34:d:630:LHG:HC62	1.80	0.63
9:A:272:LEU:HD11	19:K:72:ILE:HG23	1.80	0.63
9:A:375:HIS:ND1	31:A:818:CLA:OBD	2.27	0.63
11:D:134:LYS:NZ	18:C:47:ASP:OD2	2.30	0.63
28:i:117:ALA:HB1	28:i:234:GLY:HA3	1.81	0.63
6:7:140:GLU:OE1	6:7:143:ARG:NH2	2.28	0.63
9:A:671:SER:HB2	10:B:445:ALA:HB1	1.81	0.63
7:4:198:VAL:O	7:4:202:ARG:HG2	1.98	0.63
2:5:174:LYS:O	2:5:178:ASN:ND2	2.28	0.63
9:A:31:PHE:O	16:J:3:ASN:HB3	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:130:ARG:NH2	10:B:245:SER:OG	2.31	0.63
25:d:168:LYS:NZ	31:d:612:CLA:O1A	2.31	0.63
25:g:99:LEU:HD11	31:g:604:CLA:HAA2	1.80	0.63
29:e:163:LEU:HB2	30:e:608:CHL:HBB1	1.81	0.63
16:J:14:ILE:HD12	16:J:17:ILE:HD11	1.81	0.63
31:0:313:CLA:HBB2	8:9:120:ALA:HB1	1.81	0.63
2:1:129:VAL:HG13	14:G:14:LEU:HD22	1.80	0.63
3:2:90:ARG:NH1	30:2:307:CHL:OBD	2.28	0.63
5:6:192:TRP:HE1	30:6:313:CHL:HMC	1.63	0.63
7:8:147:ARG:NH2	30:8:308:CHL:O1D	2.32	0.62
25:g:74:GLU:HG3	25:g:75:LYS:HG3	1.81	0.62
42:g:523:NEX:O24	30:g:606:CHL:HAA1	1.98	0.62
28:i:179:VAL:HG11	30:i:606:CHL:CED	2.18	0.62
28:i:64:TRP:HZ2	31:i:611:CLA:H2A	1.62	0.62
10:B:627:ASN:OD1	10:B:732:LYS:NZ	2.32	0.62
5:6:63:ARG:NH1	30:6:307:CHL:OBD	2.27	0.62
28:i:183:LEU:HD11	30:i:606:CHL:H43	1.82	0.62
7:8:220:LYS:NZ	7:8:228:SER:OG	2.32	0.62
10:B:690:LEU:HD11	17:L:38:ALA:HB1	1.82	0.62
25:d:54:LEU:HD23	25:d:144:LEU:HD22	1.82	0.62
10:B:125:TYR:O	10:B:130:ARG:NH1	2.32	0.62
42:i:523:NEX:H362	31:i:604:CLA:CAB	2.30	0.62
29:e:83:ALA:HB1	29:e:199:GLY:HA3	1.82	0.62
1:0:93:ASN:ND2	1:0:99:ASN:OD1	2.32	0.62
26:f:193:LEU:CD1	42:f:523:NEX:H203	2.30	0.62
25:g:54:LEU:HD23	25:g:144:LEU:HD22	1.81	0.62
37:i:521:0IE:C38	30:i:606:CHL:OMC	2.47	0.62
2:1:124:ILE:HG21	14:G:91:ASN:HA	1.80	0.62
6:7:148:LYS:NZ	31:7:317:CLA:O1D	2.30	0.62
3:2:139:LEU:HB3	30:2:319:CHL:H43	1.81	0.62
30:7:307:CHL:HBB1	30:7:307:CHL:HHC	1.81	0.62
28:i:183:LEU:O	42:i:523:NEX:H201	2.00	0.62
5:6:56:GLU:HG2	5:6:119:LEU:HD22	1.81	0.61
6:7:57:ALA:O	6:7:78:ARG:NH2	2.33	0.61
26:f:266:TRP:NE1	30:f:614:CHL:HMC	2.15	0.61
2:1:165:LYS:HG3	2:1:167:ASN:H	1.66	0.61
31:A:839:CLA:HAB	31:A:839:CLA:H122	1.82	0.61
11:D:87:THR:HA	17:L:17:GLY:O	2.00	0.61
31:6:311:CLA:HHC	31:6:311:CLA:HBB1	1.81	0.61
9:A:479:ASP:O	9:A:483:GLN:NE2	2.33	0.61
5:6:162:LYS:O	5:6:166:ASN:ND2	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:9:601:LHG:H311	34:9:601:LHG:H122	1.82	0.61
26:f:193:LEU:HD21	42:h:523:NEX:H163	1.82	0.61
42:h:523:NEX:C31	30:h:606:CHL:HBA2	2.30	0.61
7:8:171:ASN:ND2	7:8:176:PRO:O	2.30	0.61
10:B:50:HIS:HE1	31:B:808:CLA:H171	1.66	0.61
42:i:523:NEX:H241	31:i:604:CLA:O2A	1.99	0.61
9:A:446:LEU:HD13	9:A:553:LEU:HA	1.83	0.61
17:L:55:THR:HG21	31:L:203:CLA:HED2	1.82	0.61
22:h:87:ARG:NH1	30:h:608:CHL:OBD	2.34	0.61
26:f:194:ILE:HD11	42:f:523:NEX:C35	2.30	0.61
5:6:244:PRO:HB3	31:6:317:CLA:HAB	1.82	0.61
42:h:523:NEX:H392	30:h:606:CHL:HHB	1.83	0.61
8:9:200:HIS:CG	31:9:312:CLA:HAA2	2.36	0.61
10:B:3:THR:HB	15:I:34:ALA:HA	1.82	0.61
28:i:183:LEU:CD1	30:i:606:CHL:H43	2.31	0.60
2:1:37:PRO:HB3	7:4:162:ILE:HG13	1.82	0.60
4:3:83:LEU:HD12	30:3:302:CHL:H11	1.83	0.60
9:A:457:SER:HB2	9:A:543:ILE:HG13	1.81	0.60
31:B:809:CLA:H2	31:B:809:CLA:HED3	1.83	0.60
31:B:817:CLA:HBD	31:B:817:CLA:HBA1	1.83	0.60
14:G:11:SER:HA	14:G:14:LEU:HD23	1.82	0.60
42:f:523:NEX:H383	31:f:604:CLA:C1B	2.31	0.60
2:1:207:HIS:CG	31:1:312:CLA:HAA2	2.36	0.60
22:h:195:LYS:O	22:h:199:ASN:ND2	2.28	0.60
30:e:602:CHL:H41	31:e:603:CLA:HBA2	1.82	0.60
7:4:53:TRP:HZ2	7:4:68:LYS:HG3	1.66	0.60
42:i:523:NEX:C22	31:i:604:CLA:C1C	2.79	0.60
42:i:523:NEX:H221	31:i:604:CLA:C1C	2.31	0.60
9:A:287:LEU:HD21	9:A:380:PRO:HD2	1.84	0.60
9:A:661:GLN:OE1	9:A:751:ARG:NH1	2.34	0.60
10:B:207:VAL:O	10:B:208:ARG:NH1	2.34	0.60
7:4:83:GLU:OE2	7:4:202:ARG:NE	2.34	0.60
7:4:156:SER:HB3	7:4:158:ASN:H	1.67	0.60
30:5:301:CHL:H42	7:8:138:LEU:HD12	1.83	0.60
28:i:93:GLY:N	30:i:602:CHL:OBD	2.34	0.60
6:7:156:ASP:OD1	6:7:159:PHE:N	2.30	0.60
29:e:157:ARG:NH2	30:e:609:CHL:O1D	2.34	0.60
31:A:828:CLA:H162	31:A:828:CLA:H101	1.84	0.60
2:5:46:PRO:HG2	2:5:49:LEU:HB2	1.84	0.59
14:G:20:ARG:HD3	31:G:103:CLA:HBB1	1.84	0.59
25:d:168:LYS:HD2	31:d:612:CLA:HBD	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:107:LEU:HD23	30:g:605:CHL:HED2	1.82	0.59
31:A:837:CLA:H141	31:L:203:CLA:H141	1.85	0.59
31:L:204:CLA:HBA2	36:L:211:LMG:H131	1.84	0.59
25:g:175:LEU:HD11	31:g:611:CLA:HHD	1.83	0.59
14:G:36:PRO:HB2	14:G:43:HIS:CD2	2.36	0.59
42:c:523:NEX:H392	30:c:606:CHL:HMB2	1.82	0.59
30:2:313:CHL:HED3	4:3:158:THR:HG23	1.85	0.59
9:A:368:LEU:HD11	31:A:819:CLA:H72	1.83	0.59
9:A:404:GLY:HA3	9:A:608:LEU:HD11	1.84	0.59
23:c:90:ARG:NH1	30:c:608:CHL:OBD	2.34	0.59
25:g:52:LEU:O	25:g:56:HIS:ND1	2.32	0.59
10:B:105:THR:HG21	27:H:133:PRO:HB3	1.83	0.59
25:d:124:MET:HE1	42:d:523:NEX:C30	2.31	0.59
22:h:50:PRO:HG2	22:h:64:ASP:HB3	1.85	0.59
22:h:195:LYS:HD3	31:h:612:CLA:HAA2	1.85	0.59
31:4:309:CLA:HAB	33:4:501:0UR:C13	2.33	0.59
1:0:129:TYR:OH	27:H:91:ARG:NH2	2.36	0.59
26:f:224:ALA:HB1	26:f:230:PHE:HD1	1.68	0.59
31:f:613:CLA:H102	34:f:630:LHG:H131	1.85	0.59
22:h:91:MET:HE1	31:h:610:CLA:HAC1	1.84	0.59
31:9:308:CLA:H43	36:9:602:LMG:H381	1.84	0.59
1:0:35:MET:HB3	1:0:40:ALA:HB3	1.84	0.59
22:h:88:TRP:CE2	30:h:608:CHL:HED2	2.37	0.59
28:i:45:LYS:O	28:i:50:ARG:NH1	2.36	0.59
28:i:69:ARG:NH1	28:i:85:THR:O	2.36	0.59
30:i:606:CHL:HMB1	30:i:609:CHL:HAC1	1.85	0.59
4:3:52:ARG:HB3	4:3:57:LEU:HD21	1.85	0.58
7:8:226:TRP:HE1	30:8:313:CHL:HMC	1.67	0.58
42:f:523:NEX:H403	30:f:606:CHL:HBA2	1.85	0.58
8:9:53:ALA:O	8:9:74:ARG:NH2	2.29	0.58
25:g:61:MET:HE1	31:g:610:CLA:HAB	1.84	0.58
2:5:139:GLU:OE1	2:5:142:ARG:NH2	2.32	0.58
9:A:82:HIS:ND1	31:A:813:CLA:OBD	2.31	0.58
28:i:198:GLY:HA3	30:i:608:CHL:HBC3	1.85	0.58
7:4:157:VAL:HG21	30:4:307:CHL:HMC	1.85	0.58
22:a:114:VAL:HG23	22:a:117:LYS:HB2	1.84	0.58
24:b:163:ARG:NH2	30:b:609:CHL:O1D	2.35	0.58
25:d:71:GLU:HA	25:d:84:ALA:HB1	1.85	0.58
28:i:111:GLU:O	28:i:115:GLN:NE2	2.35	0.58
9:A:665:SER:HB2	9:A:670:LEU:HB2	1.86	0.58
23:c:203:LYS:NZ	34:c:630:LHG:O5	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:198:ARG:NH2	30:f:609:CHL:O1D	2.36	0.58
26:f:216:ASP:OD1	28:i:44:ARG:NH1	2.36	0.58
25:g:93:ILE:HG21	25:g:113:ILE:HB	1.85	0.58
7:8:229:HIS:CG	31:8:312:CLA:HAA2	2.39	0.58
22:a:59:GLY:H	22:a:197:ILE:HG21	1.67	0.58
42:f:523:NEX:H172	28:i:76:LEU:HD11	1.84	0.58
28:i:159:LEU:HD12	30:i:606:CHL:HMD3	1.86	0.58
22:h:115:TRP:HD1	22:h:221:PRO:HD3	1.67	0.58
6:7:226:HIS:CG	31:7:312:CLA:HAA2	2.39	0.58
31:A:821:CLA:HMB2	31:A:825:CLA:HMA3	1.86	0.58
21:O:65:TRP:CD1	21:O:120:CYS:HG	2.21	0.58
25:g:171:LYS:NZ	34:g:630:LHG:O4	2.37	0.58
22:h:50:PRO:HD2	22:h:53:LEU:HD12	1.85	0.58
2:5:66:ASN:O	2:5:70:MET:HG2	2.03	0.58
9:A:566:ARG:NH2	11:D:87:THR:O	2.37	0.58
11:D:111:ILE:HG12	11:D:121:ILE:HG12	1.85	0.58
28:i:84:LEU:HD13	28:i:93:GLY:HA2	1.85	0.58
14:G:36:PRO:HB2	14:G:43:HIS:HD2	1.69	0.57
31:e:603:CLA:HAC1	30:e:607:CHL:HBB2	1.85	0.57
26:f:123:HIS:HB3	26:f:245:MET:HE3	1.86	0.57
28:i:71:LEU:HD21	28:i:80:PRO:HG3	1.86	0.57
30:2:313:CHL:HHB	34:7:602:LHG:H101	1.85	0.57
36:3:602:LMG:O3	36:A:856:LMG:O2	2.21	0.57
2:5:148:MET:O	2:5:152:VAL:HG12	2.04	0.57
10:B:406:ASN:OD1	10:B:407:VAL:N	2.36	0.57
25:g:51:GLU:HA	25:g:144:LEU:HD21	1.85	0.57
42:g:523:NEX:H362	31:g:604:CLA:C4B	2.33	0.57
42:i:523:NEX:H363	31:i:604:CLA:HHC	1.83	0.57
29:e:84:ARG:NE	29:e:195:GLU:OE2	2.35	0.57
10:B:457:PRO:HG3	10:B:517:PHE:HB2	1.86	0.57
6:7:196:LYS:NZ	34:7:601:LHG:O5	2.33	0.57
9:A:745:TRP:NE1	31:A:828:CLA:O1A	2.38	0.57
18:C:3:HIS:CE1	18:C:76:SER:HB2	2.40	0.57
9:A:627:VAL:HG22	9:A:632:VAL:HG22	1.85	0.57
10:B:311:PRO:HG2	34:B:852:LHG:HC31	1.87	0.57
34:M:104:LHG:O1	34:M:104:LHG:O9	2.23	0.57
21:O:127:GLY:O	31:O:203:CLA:HMA1	2.04	0.57
31:0:303:CLA:H42	27:H:108:LEU:HD21	1.85	0.57
7:8:168:PRO:HB3	7:8:178:GLY:HA3	1.86	0.57
30:c:601:CHL:HMA3	34:c:630:LHG:H111	1.87	0.57
4:3:178:TYR:HE2	34:3:603:LHG:HC41	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:182:ALA:HB2	31:7:309:CLA:HAA2	1.86	0.57
7:8:125:MET:HE2	30:8:305:CHL:HHD	1.85	0.57
9:A:651:LEU:HD22	10:B:651:LEU:HD21	1.87	0.57
9:A:685:ALA:HB3	31:B:801:CLA:HBB2	1.87	0.57
26:f:193:LEU:HD12	42:f:523:NEX:H203	1.87	0.57
29:e:38:LEU:HB2	29:e:42:SER:HB3	1.86	0.57
4:3:52:ARG:NH1	4:3:55:ASP:OD2	2.33	0.56
9:A:697:TYR:OH	31:B:801:CLA:OBD	2.21	0.56
31:A:839:CLA:HAA2	31:A:852:CLA:HMB1	1.87	0.56
27:H:83:GLY:N	28:i:53:TRP:O	2.24	0.56
33:i:520:0UR:C13	31:i:610:CLA:HAB	2.35	0.56
8:9:148:LEU:O	8:9:149:ASN:C	2.48	0.56
9:A:120:ALA:H	9:A:145:ILE:HG12	1.70	0.56
11:D:95:GLN:HA	27:H:67:LEU:HD13	1.87	0.56
12:E:18:SER:OG	18:C:61:ASP:OD2	2.21	0.56
12:E:54:ASN:CG	18:C:61:ASP:HB2	2.29	0.56
17:L:109:GLU:OE2	17:L:111:GLN:NE2	2.36	0.56
1:0:153:ASN:O	1:0:155:ARG:NH1	2.38	0.56
1:0:195:HIS:CG	31:0:312:CLA:HAA2	2.40	0.56
2:5:183:MET:HB2	30:5:302:CHL:HMC	1.87	0.56
31:A:832:CLA:H143	38:B:842:PQN:H191	1.87	0.56
30:a:606:CHL:HBC2	30:a:607:CHL:HHD	1.87	0.56
26:f:150:GLU:N	26:f:159:GLN:OE1	2.38	0.56
26:f:159:GLN:HE21	26:f:166:ILE:HG22	1.69	0.56
1:0:198:ASP:OD1	1:0:202:ASN:ND2	2.39	0.56
42:d:523:NEX:O24	30:d:606:CHL:HAA1	2.05	0.56
28:i:226:LEU:HD23	28:i:229:LYS:HD2	1.88	0.56
11:D:96:VAL:HG23	11:D:97:GLU:HG3	1.87	0.56
11:D:133:ARG:NH2	11:D:135:GLU:OE1	2.38	0.56
28:i:161:TYR:CD1	31:i:604:CLA:H2	2.41	0.56
1:0:229:ALA:HB2	36:9:602:LMG:H292	1.87	0.56
30:0:305:CHL:HBC2	30:0:306:CHL:HHD	1.87	0.56
3:2:45:VAL:HG11	3:2:52:PRO:HG3	1.85	0.56
3:2:233:TRP:HE1	30:2:313:CHL:HMC	1.71	0.56
8:9:66:ASP:HB3	8:9:69:ARG:HB2	1.88	0.56
24:b:46:GLY:HA3	30:b:601:CHL:HBB1	1.88	0.56
22:h:37:ARG:O	22:h:39:LYS:NZ	2.38	0.56
31:4:309:CLA:H102	31:4:311:CLA:HMB1	1.87	0.56
31:A:840:CLA:H11	31:A:840:CLA:C4D	2.36	0.56
7:4:243:LEU:HD23	31:4:314:CLA:C1D	2.36	0.56
30:2:313:CHL:HBB2	5:6:212:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:110:TYR:CZ	5:6:114:ARG:HD2	2.40	0.56
7:8:115:THR:OG1	7:8:116:GLU:N	2.39	0.56
36:9:602:LMG:H332	36:9:602:LMG:H162	1.88	0.56
31:B:823:CLA:H11	34:B:854:LHG:H242	1.88	0.56
6:7:109:GLU:O	6:7:115:ASN:ND2	2.35	0.56
9:A:516:GLY:HA2	9:A:530:PRO:HB3	1.88	0.56
26:f:236:LYS:O	26:f:240:ASN:ND2	2.31	0.56
31:B:810:CLA:HBC1	20:M:12:ILE:HA	1.88	0.56
17:L:51:GLU:OE1	27:H:81:TYR:OH	2.24	0.56
24:b:132:LEU:HD21	31:b:604:CLA:HAA2	1.88	0.56
25:g:88:LYS:HG2	30:g:607:CHL:HED2	1.88	0.56
1:0:188:PRO:O	33:0:501:0UR:O39	2.24	0.55
4:3:248:ILE:HD12	31:A:815:CLA:H62	1.87	0.55
9:A:418:MET:HE1	9:A:432:LEU:HD21	1.88	0.55
9:A:585:ARG:NH2	11:D:135:GLU:OE2	2.37	0.55
31:O:206:CLA:H11	31:f:611:CLA:H11	1.87	0.55
22:a:178:ASP:OD1	33:a:520:0UR:O40	2.24	0.55
29:e:230:ASP:O	29:e:234:ASN:ND2	2.35	0.55
31:4:309:CLA:H102	31:4:311:CLA:CMB	2.36	0.55
30:b:607:CHL:HBB1	30:b:607:CHL:HHC	1.88	0.55
25:d:189:GLN:O	25:d:190:THR:OG1	2.23	0.55
1:0:61:LEU:HD11	31:0:303:CLA:H72	1.88	0.55
2:5:50:PRO:HA	2:5:173:LEU:HD22	1.88	0.55
10:B:369:ALA:HB1	10:B:725:LEU:HD11	1.89	0.55
23:c:185:PHE:HA	29:e:178:PRO:HB2	1.87	0.55
37:i:521:0IE:C30	30:i:606:CHL:CBB	2.84	0.55
24:b:51:ASN:O	24:b:51:ASN:ND2	2.37	0.55
28:i:179:VAL:CG1	30:i:606:CHL:HED2	2.20	0.55
1:0:146:PHE:CE1	28:i:209:PRO:HB2	2.40	0.55
30:7:301:CHL:HMA3	34:7:601:LHG:H112	1.87	0.55
31:B:824:CLA:HBB1	31:B:831:CLA:HBC2	1.88	0.55
2:5:103:PRO:HG3	30:5:305:CHL:HMC	1.87	0.55
6:7:87:TRP:CE2	30:7:307:CHL:HED2	2.42	0.55
31:7:304:CLA:HMB2	30:7:305:CHL:HBB1	1.88	0.55
9:A:567:LEU:O	11:D:133:ARG:NH1	2.36	0.55
30:d:606:CHL:HMB1	30:d:609:CHL:HMC	1.88	0.55
29:e:194:LYS:O	29:e:198:ASN:ND2	2.31	0.55
4:3:91:VAL:HA	34:3:603:LHG:HC31	1.89	0.55
6:7:235:ILE:HD12	31:7:312:CLA:H42	1.89	0.55
17:L:20:GLU:OE1	17:L:25:SER:OG	2.20	0.55
42:i:523:NEX:C36	31:i:604:CLA:HHC	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:601:LHG:H282	34:1:601:LHG:HC82	1.88	0.55
2:5:31:ARG:NH2	2:5:47:GLU:OE1	2.40	0.55
8:9:66:ASP:OD1	8:9:67:ALA:N	2.38	0.55
16:J:24:SER:HB2	31:J:103:CLA:HAB	1.88	0.55
24:b:186:ALA:HB1	24:b:192:LEU:HD13	1.89	0.55
28:i:119:TRP:CE2	30:i:608:CHL:HED2	2.42	0.55
31:A:802:CLA:H151	31:H:201:CLA:HBC3	1.89	0.55
10:B:417:ALA:O	10:B:421:HIS:ND1	2.36	0.55
26:f:219:ASP:O	28:i:44:ARG:NH2	2.32	0.55
42:g:523:NEX:H383	31:g:604:CLA:C1B	2.36	0.55
4:3:108:ARG:NH1	30:3:307:CHL:OBD	2.31	0.54
6:7:117:PRO:HG2	6:7:120:VAL:HG22	1.89	0.54
22:a:192:LEU:HD21	31:a:610:CLA:H12	1.88	0.54
24:b:70:MET:O	24:b:71:ARG:C	2.49	0.54
26:f:193:LEU:HD21	42:h:523:NEX:C17	2.35	0.54
29:e:113:PHE:HD2	29:e:114:LYS:HG3	1.73	0.54
2:1:92:GLU:OE1	2:1:201:VAL:N	2.35	0.54
30:2:307:CHL:HHC	30:2:307:CHL:HBB1	1.87	0.54
25:g:168:LYS:O	25:g:172:ASN:ND2	2.34	0.54
29:e:235:ASN:O	29:e:239:TYR:N	2.40	0.54
3:2:147:MET:HA	30:2:319:CHL:HED3	1.88	0.54
9:A:228:PRO:HG3	9:A:255:MET:HE1	1.88	0.54
9:A:655:LEU:HD11	39:A:857:CL0:H43	1.88	0.54
31:A:841:CLA:H71	31:B:839:CLA:H43	1.90	0.54
21:O:110:MET:HG2	21:O:114:HIS:CE1	2.43	0.54
24:b:37:TYR:CE1	24:b:193:ALA:HB1	2.42	0.54
1:0:141:CYS:SG	1:0:142:GLY:N	2.80	0.54
31:1:303:CLA:H42	31:B:823:CLA:HMB2	1.88	0.54
9:A:537:ASP:OD1	9:A:618:LYS:NZ	2.39	0.54
10:B:191:THR:HG21	10:B:278:LEU:HB2	1.90	0.54
31:B:839:CLA:H201	15:I:20:ALA:HB2	1.90	0.54
42:a:523:NEX:O24	30:a:606:CHL:HAA1	2.06	0.54
42:i:523:NEX:H222	31:i:604:CLA:CHC	2.37	0.54
7:4:94:LEU:HD11	7:4:207:ALA:HB3	1.90	0.54
9:A:102:ARG:HD3	9:A:103:PHE:CZ	2.43	0.54
10:B:168:PHE:O	10:B:174:ARG:NH2	2.39	0.54
22:a:142:ILE:HG23	22:a:143:LEU:HD12	1.90	0.54
25:d:15:TYR:HE2	42:h:523:NEX:C3	2.20	0.54
31:d:610:CLA:H62	31:d:612:CLA:HMA3	1.90	0.54
22:h:110:PHE:HE1	22:h:131:LEU:HA	1.73	0.54
2:5:46:PRO:O	2:5:52:ASN:ND2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:177:ASP:OD1	33:7:501:0UR:O40	2.25	0.54
7:8:72:ASP:OD1	7:8:75:THR:OG1	2.23	0.54
31:9:302:CLA:HED2	31:9:302:CLA:H2A	1.90	0.54
10:B:464:GLN:NE2	31:B:836:CLA:OBD	2.35	0.54
22:a:37:ARG:NH1	22:a:60:ASP:O	2.40	0.54
22:a:161:VAL:HG12	24:b:52:THR:HG22	1.89	0.54
23:c:230:TRP:HE1	30:c:614:CHL:HMC	1.72	0.54
22:h:39:LYS:HD3	22:h:45:SER:HB2	1.90	0.54
1:0:123:ILE:HD13	30:0:305:CHL:H11	1.90	0.54
9:A:302:HIS:HB2	31:A:818:CLA:C1B	2.38	0.54
31:A:832:CLA:H41	31:A:841:CLA:HBC2	1.90	0.54
34:B:852:LHG:O3	34:B:852:LHG:O1	2.21	0.54
25:d:150:PHE:HD2	30:d:608:CHL:H2	1.72	0.54
7:4:144:GLU:OE2	7:4:147:ARG:NH2	2.40	0.54
30:1:307:CHL:HBA1	30:1:307:CHL:H13	1.90	0.54
2:5:80:TRP:CE2	30:5:307:CHL:HED2	2.43	0.54
9:A:453:LEU:HB3	9:A:546:PHE:HB2	1.90	0.54
25:g:60:ALA:HB1	25:g:180:MET:HG3	1.89	0.54
30:g:606:CHL:HBB1	30:g:606:CHL:HHC	1.89	0.54
22:h:121:GLN:O	22:h:124:SER:OG	2.26	0.54
7:4:179:ILE:C	7:4:181:ASP:H	2.15	0.54
2:1:148:MET:SD	2:1:148:MET:N	2.78	0.54
31:9:302:CLA:HAB	33:9:502:0UR:C6	2.38	0.54
10:B:50:HIS:ND1	31:B:814:CLA:OBD	2.32	0.54
10:B:542:ARG:NH2	11:D:196:ASN:OD1	2.39	0.54
30:f:601:CHL:H52	30:e:609:CHL:HBB1	1.90	0.54
22:h:147:TRP:HZ2	30:i:614:CHL:HBD	1.74	0.54
28:i:92:TYR:OH	34:i:630:LHG:O5	2.25	0.54
10:B:131:THR:HG22	10:B:133:GLN:H	1.73	0.53
10:B:237:PRO:HB3	10:B:256:THR:HG21	1.90	0.53
10:B:450:GLU:OE2	13:F:128:ARG:NH1	2.41	0.53
7:4:53:TRP:CZ2	7:4:68:LYS:HG3	2.43	0.53
31:9:302:CLA:HBC1	34:9:601:LHG:H271	1.91	0.53
10:B:347:MET:HG3	10:B:351:HIS:CE1	2.43	0.53
24:b:181:ASP:OD1	33:b:520:0UR:O40	2.25	0.53
2:1:104:SER:HG	2:1:105:TRP:CD1	2.26	0.53
5:6:37:PHE:HB2	30:6:302:CHL:HMD1	1.91	0.53
31:B:818:CLA:H41	31:B:834:CLA:HAA2	1.91	0.53
30:a:609:CHL:HED3	24:b:69:THR:HG22	1.90	0.53
25:g:182:GLY:O	25:g:186:GLN:HG2	2.07	0.53
28:i:89:PRO:HB3	28:i:227:LYS:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:3:603:LHG:HC32	34:3:603:LHG:HC62	1.89	0.53
5:6:210:ILE:HD12	31:6:317:CLA:HMC2	1.90	0.53
8:9:161:SER:HB3	8:9:164:VAL:HG22	1.89	0.53
9:A:639:ASN:O	9:A:643:SER:HB3	2.09	0.53
10:B:560:ASP:OD2	10:B:564:ARG:NH2	2.33	0.53
18:C:3:HIS:CD2	18:C:69:LEU:HA	2.43	0.53
23:c:233:HIS:CG	31:c:613:CLA:HAA2	2.44	0.53
34:6:601:LHG:H292	34:6:601:LHG:H112	1.89	0.53
42:g:523:NEX:H362	31:g:604:CLA:CHC	2.39	0.53
1:0:154:MET:HE3	31:0:309:CLA:HED1	1.90	0.53
25:g:104:ASN:ND2	25:g:106:SER:OG	2.41	0.53
7:4:108:ILE:H	7:4:108:ILE:HD13	1.74	0.53
9:A:543:ILE:CD1	39:A:857:CL0:H59	2.39	0.53
12:E:23:ARG:NH2	12:E:45:ASP:OD2	2.42	0.53
31:c:603:CLA:HAC1	30:c:607:CHL:HBB2	1.91	0.53
2:1:34:ASN:HB3	7:4:162:ILE:HD11	1.91	0.53
6:7:109:GLU:HG2	30:7:306:CHL:HED2	1.90	0.53
8:9:160:THR:O	8:9:161:SER:C	2.52	0.53
9:A:415:ALA:HB1	9:A:593:ALA:HB1	1.90	0.53
11:D:102:ILE:HD13	11:D:140:LEU:HD23	1.91	0.53
42:f:523:NEX:H362	31:f:604:CLA:CHC	2.39	0.53
30:g:601:CHL:HMD1	34:g:630:LHG:H251	1.90	0.53
27:H:88:PHE:HB2	31:H:204:CLA:HBC3	1.90	0.53
31:3:309:CLA:H191	30:7:301:CHL:H43	1.91	0.53
9:A:80:SER:OG	9:A:186:TYR:HB2	2.09	0.53
9:A:155:ALA:HB2	9:A:383:PRO:HD2	1.90	0.53
9:A:519:ILE:HG12	9:A:529:MET:HG3	1.91	0.53
25:d:171:LYS:NZ	34:d:630:LHG:O4	2.42	0.53
7:4:196:LYS:HD3	31:4:311:CLA:HAA2	1.91	0.53
31:5:304:CLA:HBA1	30:5:305:CHL:C1D	2.38	0.53
6:7:144:TRP:NE1	31:7:317:CLA:OBD	2.32	0.53
9:A:382:TYR:OH	31:A:829:CLA:OBD	2.25	0.53
21:O:128:TRP:HA	31:O:203:CLA:CMA	2.38	0.53
37:b:522:0IE:O1	37:b:522:0IE:O29	2.25	0.53
26:f:269:HIS:CG	31:f:613:CLA:HAA2	2.43	0.53
2:1:80:TRP:CE2	30:1:307:CHL:HED2	2.44	0.52
8:9:43:SER:OG	14:G:59:LYS:NZ	2.32	0.52
10:B:616:LEU:HD12	31:B:803:CLA:H11	1.91	0.52
23:c:174:ASP:OD2	23:c:177:TYR:N	2.37	0.52
31:d:612:CLA:HED2	31:d:612:CLA:H2A	1.91	0.52
25:g:131:ARG:NH2	30:g:609:CHL:O1D	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:139:ALA:HB1	22:h:145:ILE:HD11	1.91	0.52
30:0:301:CHL:HBB2	30:0:302:CHL:CHD	2.39	0.52
4:3:83:LEU:HB2	30:3:302:CHL:O1A	2.09	0.52
10:B:117:THR:HA	10:B:367:THR:HG22	1.90	0.52
10:B:276:HIS:HB2	31:B:818:CLA:C1B	2.38	0.52
7:8:161:PRO:HG3	30:8:315:CHL:C4C	2.40	0.52
9:A:294:LEU:HB2	9:A:299:ILE:HD11	1.90	0.52
31:B:810:CLA:HHB	31:B:811:CLA:HHB	1.92	0.52
21:O:51:LEU:O	21:O:53:ALA:N	2.41	0.52
30:g:608:CHL:HBD	31:g:610:CLA:HAC2	1.91	0.52
7:4:158:ASN:ND2	7:4:158:ASN:O	2.43	0.52
4:3:168:GLN:HE22	31:3:318:CLA:C1A	2.23	0.52
5:6:151:PHE:CE2	5:6:153:PRO:HG3	2.45	0.52
10:B:105:THR:HG22	10:B:111:GLY:C	2.34	0.52
31:B:801:CLA:CGA	31:B:801:CLA:H3A	2.39	0.52
24:b:54:PRO:HD2	24:b:57:LEU:HD12	1.91	0.52
25:g:71:GLU:HA	25:g:74:GLU:HG2	1.90	0.52
30:4:305:CHL:HBB1	30:4:305:CHL:HHC	1.90	0.52
2:1:106:VAL:HG23	2:1:107:TYR:CG	2.45	0.52
9:A:102:ARG:HG3	9:A:165:TYR:OH	2.09	0.52
10:B:442:VAL:HG21	31:B:833:CLA:HAC2	1.92	0.52
9:A:678:LEU:HD11	10:B:617:MET:HB2	1.90	0.52
10:B:320:GLN:O	10:B:406:ASN:ND2	2.41	0.52
31:B:829:CLA:HBB1	31:B:829:CLA:HHC	1.92	0.52
24:b:92:TRP:CE2	30:b:608:CHL:HED2	2.45	0.52
25:d:8:ARG:NE	25:d:31:ASP:O	2.33	0.52
26:f:126:TRP:CE2	30:f:608:CHL:HED2	2.45	0.52
6:7:235:ILE:HG13	31:7:312:CLA:H11	1.92	0.52
21:O:65:TRP:HH2	21:O:113:TRP:HA	1.74	0.52
37:c:522:0IE:C15	34:c:630:LHG:H112	2.40	0.52
22:h:158:ALA:HB2	28:i:73:MET:HE2	1.92	0.52
3:2:141:MET:HE2	30:2:308:CHL:C2C	2.39	0.52
2:5:173:LEU:HD12	2:5:177:LYS:HE3	1.90	0.52
10:B:26:ALA:HA	31:B:830:CLA:H43	1.92	0.52
22:a:145:ILE:HG22	30:a:605:CHL:HAC1	1.91	0.52
23:c:200:LYS:O	23:c:204:ASN:ND2	2.32	0.52
7:8:41:ARG:NH1	7:8:61:ASP:O	2.41	0.52
10:B:268:LEU:HD22	31:B:818:CLA:HBA1	1.92	0.52
31:B:824:CLA:H2A	31:B:824:CLA:HED3	1.92	0.52
24:b:201:LYS:NZ	34:b:630:LHG:O5	2.42	0.52
26:f:166:ILE:HD11	30:f:606:CHL:HMD3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:261:HIS:CG	31:3:312:CLA:HAA2	2.45	0.51
39:A:857:CL0:H14	31:B:805:CLA:NA	2.25	0.51
23:c:83:GLU:HA	23:c:176:LEU:HD21	1.91	0.51
28:i:71:LEU:HD13	28:i:77:THR:HG21	1.92	0.51
4:3:209:PHE:O	4:3:212:MET:HG3	2.10	0.51
8:9:100:GLN:HG2	8:9:106:VAL:HB	1.91	0.51
9:A:343:HIS:CE1	34:A:845:LHG:HC12	2.45	0.51
10:B:295:PHE:HA	14:G:57:LEU:HD22	1.91	0.51
7:4:245:LYS:O	7:4:247:ILE:N	2.38	0.51
30:0:305:CHL:NC	30:0:306:CHL:HBC3	2.25	0.51
31:5:309:CLA:H121	31:5:311:CLA:HBC1	1.91	0.51
7:8:196:LYS:O	7:8:200:ASN:ND2	2.26	0.51
10:B:560:ASP:OD1	18:C:66:ARG:NH1	2.39	0.51
24:b:121:LYS:HA	30:b:607:CHL:HED2	1.92	0.51
28:i:81:PRO:HD2	28:i:84:LEU:HD12	1.92	0.51
28:i:83:TYR:OH	28:i:95:ASP:OD2	2.21	0.51
38:A:842:PQN:H28	31:F:301:CLA:HBC1	1.93	0.51
10:B:411:ILE:HA	10:B:414:HIS:CE1	2.45	0.51
36:B:853:LMG:H121	20:M:10:ILE:HG21	1.92	0.51
22:a:136:LEU:HD23	30:a:605:CHL:HED2	1.92	0.51
30:0:301:CHL:H52	8:9:127:VAL:HG21	1.93	0.51
2:5:125:LYS:H	2:5:125:LYS:HD2	1.75	0.51
31:7:309:CLA:HAB	33:7:501:0UR:C13	2.41	0.51
10:B:270:LEU:HD23	10:B:273:MET:HE3	1.93	0.51
31:B:809:CLA:H151	31:B:829:CLA:HBB2	1.93	0.51
17:L:68:GLY:O	17:L:71:ARG:HG3	2.10	0.51
23:c:91:TRP:CE2	30:c:608:CHL:HED2	2.46	0.51
25:g:59:TRP:CE2	30:g:608:CHL:HED2	2.46	0.51
7:8:91:MET:SD	31:8:309:CLA:HAB	2.51	0.51
17:L:10:ILE:HG21	17:L:16:ILE:HB	1.91	0.51
30:d:607:CHL:HED1	29:e:242:LYS:HD2	1.92	0.51
26:f:193:LEU:CB	42:f:523:NEX:C20	2.89	0.51
27:H:79:LYS:HB3	28:i:54:TRP:CZ2	2.45	0.51
28:i:246:VAL:HG21	31:i:613:CLA:HAC2	1.92	0.51
7:4:110:LEU:HD12	7:4:111:PRO:HD2	1.90	0.51
1:0:238:ASP:N	1:0:238:ASP:OD1	2.44	0.51
2:1:69:ARG:HH21	34:B:854:LHG:HC5	1.74	0.51
3:2:209:ARG:HA	3:2:212:MET:HE3	1.93	0.51
30:6:301:CHL:OBD	6:7:142:ARG:NH1	2.44	0.51
9:A:643:SER:OG	9:A:653:ASP:OD2	2.22	0.51
10:B:545:LYS:NZ	12:E:18:SER:O	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:f:523:NEX:H222	31:f:604:CLA:C1C	2.40	0.51
28:i:161:TYR:HB2	28:i:168:ILE:HD13	1.93	0.51
6:7:248:VAL:HG12	6:7:255:ILE:HB	1.92	0.51
10:B:93:ASP:OD1	10:B:95:HIS:ND1	2.41	0.51
10:B:422:LEU:HD13	10:B:532:LEU:HA	1.93	0.51
31:B:808:CLA:H122	31:B:808:CLA:HBD	1.93	0.51
24:b:231:HIS:CG	31:b:613:CLA:HAA2	2.46	0.51
28:i:64:TRP:HB3	28:i:228:VAL:HG11	1.93	0.51
3:2:244:THR:HG21	4:3:158:THR:OG1	2.10	0.51
31:9:308:CLA:H43	36:9:602:LMG:H402	1.92	0.51
9:A:126:ILE:HG22	9:A:129:GLN:OE1	2.10	0.51
10:B:490:GLN:HA	10:B:494:LEU:HB3	1.93	0.51
22:h:202:LEU:HD11	31:h:611:CLA:HHD	1.93	0.51
34:6:601:LHG:O3	34:6:601:LHG:O1	2.28	0.51
9:A:222:GLN:O	9:A:227:ILE:HG12	2.11	0.51
9:A:507:ALA:O	9:A:509:ALA:N	2.43	0.51
18:C:3:HIS:HD2	18:C:69:LEU:HA	1.76	0.51
9:A:29:THR:HG23	36:A:856:LMG:O4	2.11	0.50
11:D:191:ILE:HG21	18:C:62:PHE:HD2	1.75	0.50
24:b:70:MET:O	24:b:72:LEU:N	2.45	0.50
25:d:74:GLU:HB2	25:d:81:PHE:HD2	1.74	0.50
26:f:193:LEU:CB	42:f:523:NEX:H203	2.40	0.50
22:h:40:TRP:NE1	22:h:62:GLY:O	2.44	0.50
28:i:82:SER:OG	28:i:83:TYR:N	2.44	0.50
29:e:77:GLU:HA	29:e:170:LEU:HD21	1.92	0.50
2:1:61:SER:OG	2:1:67:MET:SD	2.53	0.50
31:3:320:CLA:HBC3	31:3:320:CLA:HHD	1.94	0.50
2:5:49:LEU:HD22	30:5:302:CHL:HED2	1.93	0.50
8:9:124:ILE:HG21	30:9:305:CHL:HED2	1.93	0.50
8:9:167:ALA:O	8:9:171:ASN:ND2	2.29	0.50
10:B:126:THR:HG21	10:B:358:TYR:HD1	1.76	0.50
22:a:52:TYR:OH	22:a:64:ASP:OD2	2.22	0.50
28:i:159:LEU:HB2	28:i:170:ALA:HB2	1.93	0.50
7:4:202:ARG:HD2	30:4:302:CHL:C4C	2.41	0.50
4:3:109:PHE:CE1	31:3:308:CLA:HBC3	2.46	0.50
10:B:560:ASP:CG	18:C:66:ARG:HH12	2.19	0.50
11:D:130:LYS:NZ	27:H:66:THR:O	2.33	0.50
14:G:18:LEU:HD23	14:G:22:VAL:HG21	1.93	0.50
23:c:126:PHE:HE1	23:c:145:ILE:HG21	1.76	0.50
22:h:156:ALA:O	22:h:160:ARG:HG3	2.12	0.50
7:4:205:MET:HB2	30:4:302:CHL:HMC	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:310:CLA:HED2	31:4:310:CLA:H2A	1.92	0.50
3:2:72:ALA:HB1	3:2:78:LEU:HD13	1.92	0.50
11:D:154:PHE:CZ	11:D:167:HIS:HB2	2.47	0.50
23:c:120:SER:O	23:c:122:GLY:N	2.44	0.50
42:i:523:NEX:H31	30:i:606:CHL:HBA2	1.93	0.50
4:3:221:SER:O	4:3:225:MET:HG2	2.11	0.50
30:6:301:CHL:H2	6:7:138:TYR:HB2	1.92	0.50
9:A:37:PRO:HB2	9:A:53:TRP:HH2	1.77	0.50
10:B:174:ARG:HB2	31:B:814:CLA:HBC2	1.92	0.50
10:B:347:MET:HE1	31:B:819:CLA:H13	1.94	0.50
25:d:107:LEU:O	25:d:109:HIS:N	2.45	0.50
3:2:141:MET:O	3:2:145:GLU:HB2	2.11	0.50
6:7:107:TRP:CZ3	6:7:212:ALA:HB2	2.47	0.50
31:B:806:CLA:H3A	31:B:806:CLA:CGA	2.42	0.50
13:F:91:LYS:HE3	13:F:95:ASN:HD21	1.75	0.50
18:C:17:CYS:SG	18:C:18:VAL:N	2.85	0.50
42:a:523:NEX:H31	30:a:606:CHL:HBA2	1.93	0.50
28:i:229:LYS:HD3	31:i:612:CLA:HAA2	1.93	0.50
2:1:191:LEU:HD12	31:1:312:CLA:HAC2	1.94	0.50
5:6:114:ARG:HE	30:6:307:CHL:CMC	2.25	0.50
9:A:579:PRO:HB3	9:A:725:ILE:HB	1.94	0.50
10:B:292:ARG:NH1	14:G:34:GLN:O	2.45	0.50
30:h:608:CHL:HHC	30:h:608:CHL:HBB1	1.92	0.50
7:8:131:VAL:HG12	7:8:135:MET:HE2	1.93	0.50
31:B:817:CLA:H8	14:G:84:TYR:CE1	2.47	0.50
31:B:827:CLA:HMB2	31:B:834:CLA:HBA1	1.94	0.50
28:i:267:ALA:O	28:i:269:ALA:N	2.45	0.50
2:1:36:LEU:HD13	30:4:319:CHL:HMA3	1.93	0.50
31:A:803:CLA:H93	31:A:808:CLA:H172	1.93	0.50
22:a:160:ARG:HA	30:a:608:CHL:C3C	2.41	0.50
30:c:608:CHL:H171	30:c:608:CHL:HBA1	1.94	0.50
7:4:238:VAL:HG22	7:4:243:LEU:HD21	1.93	0.50
3:2:91:TRP:CE2	30:2:307:CHL:HED2	2.47	0.49
4:3:106:HIS:HB3	4:3:237:MET:HE3	1.94	0.49
8:9:156:PRO:HG2	33:9:501:0UR:C30	2.42	0.49
31:A:808:CLA:H2	31:A:828:CLA:H43	1.94	0.49
31:A:830:CLA:H93	31:A:840:CLA:HED3	1.93	0.49
11:D:99:PHE:CE1	27:H:67:LEU:HD21	2.47	0.49
26:f:239:LYS:NZ	34:f:630:LHG:O4	2.35	0.49
29:e:181:MET:HE3	31:e:610:CLA:H11	1.94	0.49
30:1:302:CHL:H42	31:B:841:CLA:HBB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:158:PHE:O	2:5:160:PRO:HD3	2.13	0.49
5:6:112:GLU:OE1	5:6:115:ARG:NH1	2.30	0.49
10:B:477:LEU:HD13	31:B:834:CLA:HMD1	1.93	0.49
10:B:721:TYR:HB2	31:B:805:CLA:HED3	1.93	0.49
13:F:214:ALA:HB3	7:4:67:LEU:HD22	1.94	0.49
25:d:201:HIS:CD2	31:d:613:CLA:H3A	2.47	0.49
42:i:523:NEX:H222	31:i:604:CLA:C1C	2.42	0.49
31:2:309:CLA:HAB	33:2:501:0UR:C13	2.42	0.49
2:5:159:ASP:OD1	33:5:501:0UR:O40	2.30	0.49
10:B:344:ILE:HG23	31:B:819:CLA:H61	1.93	0.49
31:B:811:CLA:O1A	31:B:828:CLA:HBD	2.12	0.49
12:E:54:ASN:OD1	18:C:61:ASP:N	2.45	0.49
13:F:78:ILE:HD11	13:F:157:TYR:HB2	1.93	0.49
19:K:6:THR:HG23	19:K:7:PRO:HD3	1.93	0.49
42:f:523:NEX:H31	30:f:606:CHL:HBA2	1.93	0.49
7:4:238:VAL:HB	31:4:312:CLA:H11	1.94	0.49
31:A:840:CLA:H202	31:F:301:CLA:HBB1	1.93	0.49
10:B:559:CYS:SG	10:B:561:GLY:N	2.75	0.49
29:e:84:ARG:NH1	30:e:608:CHL:OBD	2.34	0.49
9:A:131:ILE:HG21	10:B:446:PHE:HA	1.95	0.49
11:D:191:ILE:HG21	18:C:62:PHE:CD2	2.48	0.49
22:a:120:GLY:O	22:a:122:ILE:N	2.45	0.49
23:c:196:GLU:HG2	23:c:200:LYS:HE3	1.94	0.49
25:d:85:VAL:HG23	25:d:88:LYS:HB2	1.93	0.49
26:f:163:ASP:O	26:f:165:GLY:N	2.45	0.49
42:h:523:NEX:C29	30:h:606:CHL:HHB	2.42	0.49
2:1:165:LYS:HE3	2:1:167:ASN:HB2	1.94	0.49
31:A:803:CLA:HBB2	31:A:811:CLA:H121	1.95	0.49
23:c:148:ILE:HG12	30:c:605:CHL:HAC1	1.95	0.49
25:g:11:TRP:CE2	25:g:12:LEU:HG	2.48	0.49
25:g:58:ARG:HD3	31:g:610:CLA:C3C	2.43	0.49
22:h:81:ALA:O	22:h:85:HIS:ND1	2.34	0.49
28:i:119:TRP:O	37:i:521:0IE:O29	2.31	0.49
4:3:166:ALA:HB1	32:3:402:8CT:C18	2.42	0.49
31:A:853:CLA:HHC	31:A:853:CLA:HBB1	1.94	0.49
10:B:631:LEU:HD22	10:B:724:PHE:HA	1.94	0.49
24:b:224:PRO:O	33:b:520:0UR:O39	2.31	0.49
30:b:602:CHL:H41	31:b:603:CLA:HBA1	1.94	0.49
31:d:603:CLA:H71	31:e:603:CLA:H92	1.95	0.49
34:h:630:LHG:H291	34:h:630:LHG:HC91	1.93	0.49
28:i:143:GLU:HG3	28:i:148:LYS:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:128:GLU:OE1	1:0:131:ARG:NH2	2.39	0.49
31:0:311:CLA:H2A	31:0:311:CLA:O1A	2.13	0.49
2:1:31:ARG:NH1	2:1:41:ALA:HB2	2.28	0.49
9:A:583:PRO:HD3	10:B:561:GLY:HA2	1.94	0.49
14:G:20:ARG:HG3	14:G:64:VAL:HG11	1.95	0.49
19:K:52:PRO:HG2	31:K:104:CLA:HBC2	1.94	0.49
23:c:93:MET:SD	31:c:610:CLA:HAB	2.52	0.49
25:g:116:ILE:HG12	30:g:605:CHL:HAC1	1.93	0.49
7:4:88:ARG:NH1	30:4:307:CHL:OBD	2.33	0.49
3:2:244:THR:HG23	3:2:246:ALA:H	1.77	0.49
4:3:245:ALA:HA	31:A:815:CLA:H61	1.94	0.49
31:L:201:CLA:H51	31:L:203:CLA:H43	1.94	0.49
24:b:162:TYR:HB3	30:b:608:CHL:CMC	2.43	0.49
25:d:124:MET:HE2	30:d:606:CHL:HMA1	1.95	0.49
7:4:105:ASN:O	7:4:105:ASN:ND2	2.42	0.49
1:0:111:ILE:HG13	28:i:162:LEU:HD22	1.94	0.49
30:2:319:CHL:H62	30:2:319:CHL:H41	1.57	0.49
31:3:306:CLA:HBC2	34:3:601:LHG:H251	1.95	0.49
9:A:85:GLN:HE21	31:A:805:CLA:HMB3	1.78	0.49
9:A:221:HIS:CE1	9:A:225:LEU:HD12	2.48	0.49
10:B:197:VAL:O	10:B:201:GLU:HB2	2.12	0.49
10:B:422:LEU:HG	31:B:838:CLA:HBB1	1.94	0.49
31:B:850:CLA:OBD	13:F:156:ARG:NH1	2.44	0.49
11:D:77:ASN:O	27:H:56:ARG:NH1	2.46	0.49
14:G:18:LEU:O	14:G:22:VAL:HB	2.12	0.49
26:f:119:ALA:O	26:f:123:HIS:ND1	2.44	0.49
29:e:77:GLU:HA	29:e:170:LEU:HD11	1.94	0.49
2:1:200:PRO:O	33:1:501:0UR:O39	2.32	0.48
7:8:119:ASN:HA	30:8:306:CHL:HED2	1.94	0.48
9:A:581:ASP:OD2	9:A:585:ARG:NH1	2.44	0.48
13:F:94:GLU:HG2	13:F:129:PHE:HB3	1.95	0.48
22:a:50:PRO:HG2	22:a:64:ASP:HB3	1.95	0.48
22:a:143:LEU:HG	30:b:614:CHL:HED3	1.95	0.48
23:c:162:TYR:HB3	30:c:608:CHL:CMC	2.42	0.48
24:b:87:VAL:HB	24:b:174:VAL:HG21	1.95	0.48
2:1:106:VAL:HG23	2:1:107:TYR:CD1	2.48	0.48
31:1:304:CLA:H43	30:1:305:CHL:HBD	1.96	0.48
9:A:723:LEU:HD21	38:A:842:PQN:H151	1.96	0.48
10:B:228:GLY:HA3	14:G:86:LEU:HD13	1.94	0.48
31:B:803:CLA:HMB1	31:B:803:CLA:HBB1	1.94	0.48
21:O:127:GLY:O	31:O:203:CLA:CMA	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:167:ASN:HD22	26:f:176:HIS:HA	1.78	0.48
29:e:173:GLY:C	29:e:174:GLU:HG3	2.38	0.48
30:0:306:CHL:HHC	30:0:306:CHL:HBB1	1.95	0.48
10:B:714:SER:HB2	41:B:849:DGD:HBH1	1.95	0.48
25:d:14:PRO:HG3	42:h:523:NEX:H41	1.95	0.48
25:d:130:TYR:HB3	30:d:608:CHL:CMC	2.44	0.48
26:f:180:ILE:HG23	26:f:181:LEU:HD22	1.94	0.48
42:g:523:NEX:C36	31:g:604:CLA:CHC	2.91	0.48
28:i:153:ILE:HD13	28:i:173:ILE:HG22	1.95	0.48
29:e:189:ALA:HA	29:e:192:LYS:HE2	1.95	0.48
3:2:77:MET:HE1	16:J:5:LYS:HD3	1.95	0.48
2:5:98:ASN:HB2	2:5:200:PRO:HD2	1.96	0.48
31:A:853:CLA:H121	16:J:18:TRP:CD1	2.49	0.48
13:F:93:ARG:NH2	13:F:142:ASP:O	2.42	0.48
22:a:154:GLY:HA2	30:a:609:CHL:HAB	1.94	0.48
24:b:114:LEU:HB2	24:b:117:THR:HG22	1.95	0.48
42:i:523:NEX:C36	31:i:604:CLA:HAB	2.43	0.48
1:0:48:GLY:N	1:0:53:ASP:OD2	2.43	0.48
2:1:70:MET:HE2	31:B:841:CLA:HAB	1.95	0.48
31:1:312:CLA:NC	31:1:312:CLA:H43	2.28	0.48
2:5:207:HIS:HA	2:5:214:ALA:HB3	1.96	0.48
30:8:301:CHL:H62	30:8:313:CHL:H2	1.96	0.48
10:B:328:ASN:ND2	14:G:39:ASN:OD1	2.35	0.48
10:B:653:GLY:HA3	10:B:720:THR:HG23	1.95	0.48
31:B:817:CLA:HBC3	31:B:817:CLA:HHD	1.95	0.48
24:b:177:GLY:O	24:b:178:GLU:HB2	2.12	0.48
22:h:42:GLY:HA3	30:h:601:CHL:HBB1	1.94	0.48
28:i:69:ARG:HD2	28:i:86:GLY:HA3	1.95	0.48
30:e:601:CHL:H3A	30:e:601:CHL:HBA1	1.61	0.48
1:0:79:GLY:O	1:0:83:MET:HG3	2.14	0.48
4:3:74:GLY:HA3	4:3:230:ILE:HG21	1.95	0.48
8:9:143:THR:HB	8:9:145:MET:HE3	1.96	0.48
31:A:814:CLA:H8	31:A:816:CLA:HAB	1.94	0.48
10:B:524:ALA:HB2	31:B:837:CLA:HMA1	1.95	0.48
11:D:102:ILE:HG23	11:D:129:LEU:HB3	1.95	0.48
24:b:121:LYS:O	24:b:124:SER:OG	2.24	0.48
28:i:61:SER:HG	28:i:65:TYR:HB2	1.78	0.48
28:i:90:GLY:H	28:i:228:VAL:HG22	1.78	0.48
2:1:91:GLN:HE22	2:1:96:PHE:HD2	1.62	0.48
10:B:134:ASP:N	10:B:134:ASP:OD1	2.47	0.48
15:I:32:LYS:HD2	15:I:35:ILE:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:159:TYR:HB3	30:a:608:CHL:CMC	2.44	0.48
23:c:56:LEU:HD13	23:c:65:GLY:HA2	1.94	0.48
26:f:194:ILE:CD1	42:f:523:NEX:H34	2.43	0.48
42:f:523:NEX:C17	28:i:76:LEU:HD11	2.43	0.48
28:i:116:HIS:HE1	31:i:603:CLA:NA	2.11	0.48
34:1:601:LHG:HC91	32:4:402:8CT:C05	2.44	0.48
5:6:114:ARG:NH2	5:6:125:VAL:HG12	2.28	0.48
9:A:34:TRP:HE1	31:A:811:CLA:CHB	2.26	0.48
10:B:290:MET:HE1	31:B:820:CLA:CAD	2.44	0.48
21:O:65:TRP:CH2	21:O:113:TRP:HA	2.48	0.48
23:c:215:TYR:OH	33:c:520:0UR:O42	2.26	0.48
24:b:42:PRO:HB3	30:b:601:CHL:HBC1	1.94	0.48
25:g:58:ARG:NH1	30:g:608:CHL:OBD	2.46	0.48
30:2:301:CHL:C1C	34:2:601:LHG:HC81	2.43	0.48
31:2:310:CLA:H91	31:2:310:CLA:H111	1.68	0.48
31:2:310:CLA:HED2	31:2:310:CLA:H2A	1.96	0.48
9:A:436:ILE:O	9:A:439:ARG:HG3	2.14	0.48
9:A:695:ARG:NH1	9:A:722:ALA:O	2.47	0.48
11:D:154:PHE:CE2	11:D:167:HIS:HB2	2.49	0.48
17:L:141:LEU:HD23	27:H:96:LEU:HD13	1.96	0.48
30:c:601:CHL:H61	30:c:601:CHL:H41	1.51	0.48
25:d:12:LEU:O	30:d:601:CHL:HBB1	2.14	0.48
26:f:253:THR:HG21	31:f:613:CLA:HAC2	1.95	0.48
5:6:114:ARG:CZ	5:6:125:VAL:HG12	2.44	0.48
10:B:123:TRP:O	10:B:127:ILE:HG12	2.13	0.48
31:B:806:CLA:HBC2	31:B:806:CLA:HHD	1.95	0.48
31:B:823:CLA:H41	31:B:823:CLA:H62	1.55	0.48
13:F:199:ILE:O	16:J:11:ALA:N	2.47	0.48
19:K:66:PHE:CE2	31:K:105:CLA:HAB	2.49	0.48
26:f:104:MET:SD	29:e:78:LEU:HD13	2.54	0.48
42:i:523:NEX:C22	31:i:604:CLA:CHC	2.91	0.48
5:6:64:TRP:CE2	30:6:307:CHL:HED2	2.48	0.47
9:A:310:PHE:HE1	31:A:821:CLA:HAB	1.78	0.47
9:A:658:GLN:HB3	9:A:751:ARG:HD2	1.95	0.47
10:B:415:LYS:O	10:B:419:ILE:HG12	2.14	0.47
31:B:824:CLA:HHB	31:B:841:CLA:O1D	2.14	0.47
25:g:118:TRP:HZ2	30:h:614:CHL:HBD	1.79	0.47
29:e:83:ALA:O	29:e:87:MET:HG3	2.13	0.47
29:e:85:TRP:CE2	30:e:608:CHL:HED2	2.49	0.47
29:e:156:TYR:HB3	30:e:608:CHL:CMC	2.44	0.47
30:4:319:CHL:H62	30:4:319:CHL:H41	1.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:114:TRP:CD1	2:1:119:MET:HG2	2.49	0.47
31:7:318:CLA:H3A	31:7:318:CLA:HBA1	1.60	0.47
9:A:686:PHE:HZ	31:A:840:CLA:HBC2	1.79	0.47
13:F:172:TYR:OH	13:F:214:ALA:O	2.25	0.47
18:C:3:HIS:HE1	18:C:76:SER:HB2	1.79	0.47
22:a:57:PHE:HB3	22:a:58:PRO:HD2	1.96	0.47
23:c:83:GLU:HA	23:c:176:LEU:HD11	1.96	0.47
24:b:41:ARG:NH2	24:b:57:LEU:O	2.47	0.47
25:d:164:GLU:O	25:d:168:LYS:HG2	2.13	0.47
42:h:523:NEX:C39	30:h:606:CHL:HHB	2.44	0.47
7:4:145:ILE:HG21	30:4:319:CHL:HBA1	1.96	0.47
1:0:58:PRO:O	1:0:241:ARG:NH1	2.38	0.47
2:1:46:PRO:HD2	2:1:49:LEU:HD11	1.96	0.47
31:2:304:CLA:H111	31:2:304:CLA:H142	1.73	0.47
6:7:210:LEU:HD12	31:7:312:CLA:HAC2	1.96	0.47
31:9:308:CLA:H203	31:9:308:CLA:H141	1.95	0.47
9:A:60:ASP:O	9:A:67:HIS:NE2	2.36	0.47
10:B:519:VAL:HG21	10:B:593:TYR:HB2	1.96	0.47
25:g:2:GLU:O	25:g:9:ALA:N	2.48	0.47
22:h:34:GLY:O	22:h:37:ARG:NE	2.47	0.47
22:h:189:PHE:HE1	31:h:610:CLA:H2A	1.79	0.47
4:3:55:ASP:OD1	4:3:55:ASP:N	2.47	0.47
4:3:192:LEU:HD21	6:7:65:MET:HE3	1.95	0.47
8:9:155:ASP:O	8:9:156:PRO:C	2.58	0.47
31:A:807:CLA:HMB1	31:A:807:CLA:HBB1	1.96	0.47
31:A:828:CLA:H41	31:A:828:CLA:H61	1.55	0.47
31:A:831:CLA:HAB	31:A:838:CLA:HBB2	1.95	0.47
10:B:29:HIS:ND1	31:B:809:CLA:O1A	2.31	0.47
10:B:359:ALA:O	10:B:360:PHE:HB2	2.15	0.47
31:B:836:CLA:HMB1	31:B:836:CLA:HBB1	1.97	0.47
24:b:133:ASP:N	24:b:133:ASP:OD1	2.47	0.47
30:b:601:CHL:H122	30:b:601:CHL:H162	1.46	0.47
42:h:523:NEX:H31	30:h:606:CHL:HBA2	1.97	0.47
1:0:150:ASP:O	1:0:152:LEU:N	2.48	0.47
4:3:246:GLN:O	4:3:250:THR:OG1	2.26	0.47
31:A:840:CLA:H101	31:A:840:CLA:H61	1.50	0.47
31:B:823:CLA:HHC	31:B:841:CLA:HED1	1.97	0.47
31:B:832:CLA:H12	13:F:177:THR:HB	1.97	0.47
17:L:10:ILE:HA	17:L:20:GLU:HG2	1.97	0.47
25:g:110:ALA:HB1	25:g:116:ILE:HD11	1.96	0.47
22:h:82:GLU:HB2	30:h:602:CHL:C1B	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:i:64:TRP:CZ2	31:i:611:CLA:H2A	2.47	0.47
28:i:175:ASN:HB3	30:i:605:CHL:HBC3	1.96	0.47
31:1:309:CLA:H41	31:1:309:CLA:H62	1.68	0.47
31:7:304:CLA:H62	31:7:304:CLA:H41	1.68	0.47
7:8:108:ILE:C	7:8:110:LEU:H	2.22	0.47
9:A:333:SER:OG	31:A:823:CLA:O1D	2.30	0.47
9:A:443:ILE:HG13	9:A:561:TYR:HE1	1.79	0.47
10:B:382:MET:HE3	31:B:809:CLA:HMB1	1.96	0.47
31:B:839:CLA:H122	31:B:840:CLA:H13	1.97	0.47
14:G:11:SER:HB2	14:G:82:ALA:HB2	1.97	0.47
30:f:601:CHL:H162	30:f:601:CHL:H121	1.65	0.47
31:g:612:CLA:HED2	31:g:612:CLA:H2A	1.97	0.47
22:h:114:VAL:HB	22:h:117:LYS:HB2	1.96	0.47
22:h:126:GLY:O	22:h:140:GLN:NE2	2.48	0.47
22:h:159:TYR:HB3	30:h:608:CHL:CMC	2.44	0.47
1:0:180:GLN:HB3	1:0:191:ASN:ND2	2.30	0.47
1:0:243:ILE:O	1:0:245:TRP:N	2.47	0.47
30:3:307:CHL:HBA1	32:7:404:8CT:C24	2.45	0.47
5:6:97:ILE:HG13	5:6:98:ILE:HD12	1.96	0.47
7:8:166:LYS:O	7:8:168:PRO:HD3	2.14	0.47
8:9:76:ALA:O	8:9:80:ASN:ND2	2.37	0.47
9:A:366:GLY:HA2	9:A:403:GLY:HA2	1.96	0.47
9:A:435:VAL:HA	9:A:438:HIS:CE1	2.50	0.47
9:A:700:GLU:OE2	10:B:550:LYS:NZ	2.45	0.47
10:B:441:ASP:OD1	10:B:616:LEU:N	2.41	0.47
22:a:166:LEU:HG	22:a:176:ALA:HB3	1.97	0.47
23:c:87:ILE:HG22	30:c:609:CHL:HMD2	1.97	0.47
24:b:197:VAL:HA	24:b:200:ILE:HG22	1.97	0.47
30:b:606:CHL:HBC2	30:b:607:CHL:HHD	1.96	0.47
26:f:191:MET:HE2	30:f:606:CHL:HMA1	1.96	0.47
25:g:51:GLU:HG3	25:g:144:LEU:HD21	1.97	0.47
22:h:178:ASP:OD1	33:h:520:0UR:O40	2.32	0.47
37:i:521:0IE:C30	30:i:606:CHL:HBB2	2.45	0.47
29:e:82:HIS:HD2	30:e:602:CHL:HBB2	1.79	0.47
31:4:304:CLA:H51	30:4:305:CHL:HBD	1.96	0.47
1:0:76:LEU:O	1:0:80:ARG:HG3	2.15	0.47
1:0:192:LEU:O	1:0:196:ILE:HG12	2.15	0.47
31:0:321:CLA:HMA3	34:M:104:LHG:H241	1.97	0.47
3:2:229:PRO:O	33:2:501:0UR:O39	2.33	0.47
4:3:153:TRP:CD1	4:3:153:TRP:H	2.32	0.47
31:3:303:CLA:H2	31:3:303:CLA:H61	1.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:302:CHL:HBC1	34:6:601:LHG:H282	1.97	0.47
7:8:159:VAL:HG22	7:8:168:PRO:HD2	1.96	0.47
8:9:161:SER:OG	8:9:162:GLU:N	2.48	0.47
31:9:308:CLA:H62	31:9:308:CLA:H2	1.59	0.47
31:A:808:CLA:CHC	31:A:809:CLA:HMD2	2.45	0.47
31:A:853:CLA:H93	31:A:853:CLA:H61	1.65	0.47
10:B:283:LEU:HD22	31:B:818:CLA:HMC1	1.97	0.47
10:B:571:SER:OG	10:B:574:ASP:OD2	2.32	0.47
30:c:607:CHL:HHC	30:c:607:CHL:HBB1	1.95	0.47
26:f:84:PHE:HA	29:e:159:SER:HB3	1.97	0.47
42:i:523:NEX:H241	31:i:604:CLA:C1	2.45	0.47
4:3:169:PHE:O	4:3:173:ARG:HB2	2.15	0.47
2:5:127:LEU:HD11	30:5:305:CHL:C2D	2.45	0.47
30:5:301:CHL:HED3	7:8:146:ARG:HD2	1.97	0.47
31:7:308:CLA:H11	31:7:317:CLA:HBC2	1.95	0.47
31:9:308:CLA:H142	31:9:308:CLA:H111	1.63	0.47
9:A:215:SER:OG	9:A:303:HIS:O	2.33	0.47
26:f:194:ILE:HD12	42:f:523:NEX:H34	1.97	0.47
25:g:10:LEU:HD13	25:g:20:VAL:HG21	1.96	0.47
29:e:59:GLY:N	30:e:602:CHL:OBD	2.48	0.47
7:4:88:ARG:HA	7:4:91:MET:HE3	1.96	0.47
4:3:189:PHE:N	4:3:193:GLU:OE1	2.39	0.47
5:6:95:PHE:HB3	7:8:234:TRP:CG	2.50	0.47
9:A:178:MET:HE1	31:A:813:CLA:H71	1.96	0.47
9:A:302:HIS:CE1	9:A:306:ILE:HD13	2.50	0.47
9:A:361:ASN:O	9:A:365:PHE:HB2	2.15	0.47
23:c:160:GLU:OE1	23:c:163:ARG:NH2	2.48	0.47
25:d:59:TRP:CE2	30:d:608:CHL:HED2	2.50	0.47
22:h:195:LYS:HD3	31:h:612:CLA:HBD	1.97	0.47
1:0:204:ILE:HD11	1:0:213:VAL:HG21	1.97	0.46
3:2:236:HIS:CG	31:2:312:CLA:HAA2	2.50	0.46
30:5:306:CHL:HHC	30:5:306:CHL:HBB1	1.97	0.46
31:5:314:CLA:H3A	31:5:314:CLA:HBA1	1.58	0.46
6:7:89:MET:HE3	6:7:198:GLY:N	2.30	0.46
7:8:144:GLU:HG3	7:8:147:ARG:NH1	2.30	0.46
9:A:44:LEU:HD13	9:A:57:LEU:HA	1.97	0.46
31:A:818:CLA:HBA2	31:A:818:CLA:H3A	1.66	0.46
10:B:716:GLY:O	10:B:720:THR:OG1	2.30	0.46
18:C:25:VAL:HG21	18:C:48:CYS:HA	1.97	0.46
25:d:92:GLN:HB2	25:d:99:LEU:HD23	1.96	0.46
25:d:156:ALA:HB2	25:d:165:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:f:523:NEX:H35	42:f:523:NEX:H401	1.58	0.46
29:e:212:GLN:O	29:e:216:THR:OG1	2.20	0.46
1:0:102:GLU:HA	30:0:306:CHL:HED1	1.96	0.46
31:7:312:CLA:H92	31:7:312:CLA:H61	1.73	0.46
9:A:589:CYS:HB2	10:B:667:TRP:HB3	1.97	0.46
31:A:840:CLA:H62	31:A:840:CLA:H41	1.46	0.46
31:B:806:CLA:H72	31:B:806:CLA:H112	1.73	0.46
22:a:110:PHE:HE1	22:a:131:LEU:H	1.64	0.46
22:h:131:LEU:HD21	31:h:604:CLA:HMD3	1.97	0.46
31:0:309:CLA:H92	31:0:309:CLA:H61	1.78	0.46
2:5:198:LYS:HE2	2:5:202:GLN:HG3	1.97	0.46
7:8:97:MET:O	7:8:100:PRO:HD2	2.15	0.46
9:A:206:HIS:ND1	31:A:825:CLA:OBD	2.48	0.46
31:A:841:CLA:H62	31:A:841:CLA:H41	1.60	0.46
31:B:809:CLA:HED1	31:B:830:CLA:H2	1.98	0.46
31:B:831:CLA:HBB2	31:B:838:CLA:HMC1	1.97	0.46
31:L:202:CLA:HBA2	31:L:202:CLA:H3A	1.60	0.46
22:a:136:LEU:O	22:a:138:HIS:N	2.48	0.46
30:f:609:CHL:H91	30:f:609:CHL:H112	1.77	0.46
7:4:190:VAL:HG12	7:4:194:LYS:HE3	1.98	0.46
2:1:88:MET:HE1	2:1:186:PHE:CD1	2.50	0.46
3:2:248:ASN:OD1	3:2:249:GLY:N	2.48	0.46
31:3:309:CLA:HBA2	31:3:309:CLA:H3A	1.50	0.46
8:9:95:GLU:HG3	8:9:101:THR:HA	1.96	0.46
8:9:145:MET:SD	8:9:153:PRO:HG3	2.55	0.46
10:B:128:GLY:HA2	10:B:130:ARG:NH1	2.30	0.46
10:B:558:PRO:HB3	10:B:702:ILE:HB	1.97	0.46
31:B:834:CLA:HBC2	31:B:835:CLA:HAB	1.97	0.46
14:G:81:VAL:O	14:G:85:ILE:HG12	2.15	0.46
22:a:90:MET:SD	31:a:610:CLA:HAB	2.55	0.46
25:d:61:MET:HE3	25:d:173:GLY:N	2.31	0.46
25:g:61:MET:HE1	31:g:610:CLA:HHC	1.97	0.46
7:4:54:LEU:HD12	7:4:54:LEU:HA	1.80	0.46
31:0:312:CLA:H121	34:0:601:LHG:H101	1.96	0.46
30:1:305:CHL:HMB1	31:1:308:CLA:HBC2	1.97	0.46
30:2:313:CHL:H12	30:3:305:CHL:H42	1.96	0.46
30:6:301:CHL:H12	34:6:601:LHG:H131	1.97	0.46
30:6:302:CHL:H93	30:6:302:CHL:H61	1.74	0.46
31:6:312:CLA:H101	34:6:601:LHG:H142	1.96	0.46
6:7:87:TRP:CE2	31:7:308:CLA:HBC3	2.50	0.46
7:8:86:HIS:HB3	7:8:205:MET:HE3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:374:HIS:HB2	31:B:828:CLA:C1B	2.46	0.46
31:B:810:CLA:HHD	31:B:810:CLA:HBC2	1.97	0.46
14:G:38:GLN:N	14:G:41:LEU:O	2.44	0.46
16:J:2:GLN:O	16:J:6:ILE:HG13	2.16	0.46
17:L:38:ALA:O	17:L:48:ARG:NH2	2.48	0.46
22:a:53:LEU:HD11	22:a:64:ASP:HB2	1.97	0.46
30:b:602:CHL:H91	30:b:602:CHL:H111	1.70	0.46
7:4:146:ARG:HA	30:4:319:CHL:HED3	1.98	0.46
31:1:312:CLA:H41	31:1:312:CLA:H61	1.46	0.46
7:8:144:GLU:HG3	7:8:147:ARG:HH12	1.79	0.46
30:8:307:CHL:HBA2	30:8:307:CHL:H3A	1.64	0.46
24:b:198:LYS:HD3	31:b:612:CLA:HAA2	1.97	0.46
22:h:164:GLY:N	22:h:167:GLY:O	2.48	0.46
29:e:174:GLU:CD	29:e:175:ALA:H	2.23	0.46
7:4:88:ARG:HB3	31:4:309:CLA:CAC	2.46	0.46
2:1:104:SER:HA	2:1:108:GLU:OE1	2.15	0.46
7:8:191:ASP:N	7:8:191:ASP:OD1	2.46	0.46
7:8:196:LYS:HD3	31:8:311:CLA:HBD	1.97	0.46
30:8:313:CHL:H62	30:8:313:CHL:H41	1.57	0.46
34:A:855:LHG:H242	34:A:855:LHG:HC61	1.76	0.46
10:B:15:ASP:HB3	10:B:20:ARG:HB2	1.97	0.46
10:B:84:ILE:HD13	27:H:145:ILE:HB	1.97	0.46
28:i:61:SER:OG	28:i:65:TYR:HB2	2.16	0.46
28:i:146:TRP:CE2	28:i:147:PHE:HD1	2.34	0.46
31:i:603:CLA:HED2	31:i:603:CLA:H2A	1.98	0.46
29:e:133:LEU:HD23	30:e:605:CHL:HED2	1.98	0.46
7:4:136:GLN:O	7:4:140:MET:HB2	2.15	0.46
31:0:309:CLA:H62	31:0:309:CLA:H41	1.61	0.46
31:5:303:CLA:H42	7:4:166:LYS:HG3	1.96	0.46
6:7:259:CYS:O	34:7:602:LHG:HC62	2.16	0.46
9:A:697:TYR:CE2	10:B:536:LYS:HD2	2.51	0.46
31:B:828:CLA:HBA2	31:B:828:CLA:H3A	1.39	0.46
16:J:24:SER:CB	31:J:103:CLA:HAB	2.45	0.46
21:O:127:GLY:C	31:O:203:CLA:HMA3	2.40	0.46
22:a:182:MET:HB2	31:a:610:CLA:O1A	2.16	0.46
30:a:601:CHL:H3A	30:a:601:CHL:HBA1	1.34	0.46
25:g:52:LEU:HD23	31:g:603:CLA:HAA2	1.98	0.46
25:g:145:TYR:CZ	25:g:166:LYS:HD2	2.50	0.46
22:h:146:VAL:HB	30:h:607:CHL:HBC1	1.97	0.46
42:i:523:NEX:C22	31:i:604:CLA:NC	2.78	0.46
7:4:114:GLY:O	7:4:116:GLU:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:431:LEU:HD13	31:A:824:CLA:C1C	2.45	0.46
31:A:806:CLA:H41	34:A:844:LHG:H271	1.97	0.46
11:D:78:THR:HG23	11:D:126:PRO:HB2	1.98	0.46
42:a:523:NEX:H201	42:a:523:NEX:H15	1.62	0.46
25:d:12:LEU:HB2	25:d:16:SER:HB3	1.97	0.46
25:g:173:GLY:O	25:g:177:MET:HG2	2.16	0.46
6:7:240:GLY:O	6:7:264:GLN:N	2.49	0.46
7:8:55:ASP:N	7:8:55:ASP:OD1	2.47	0.46
7:8:56:GLY:HA2	7:8:61:ASP:HB3	1.98	0.46
34:9:601:LHG:O3	34:9:601:LHG:O1	2.26	0.46
9:A:15:ILE:HG13	9:A:16:LYS:H	1.80	0.46
25:d:194:PRO:O	33:d:520:0UR:O39	2.34	0.46
29:e:85:TRP:CD1	30:e:609:CHL:HMD3	2.51	0.46
7:4:122:ALA:C	7:4:124:PRO:HD3	2.40	0.46
2:1:148:MET:O	2:1:152:VAL:HG23	2.15	0.45
31:7:308:CLA:H42	31:7:317:CLA:HBC1	1.97	0.45
30:9:306:CHL:H3A	30:9:306:CHL:HBA1	1.64	0.45
9:A:699:GLN:O	9:A:703:GLU:HG3	2.17	0.45
10:B:22:TRP:CG	10:B:704:GLN:HE22	2.34	0.45
10:B:585:ASN:HB2	31:B:803:CLA:HBC2	1.98	0.45
24:b:207:MET:HE2	30:b:602:CHL:OMC	2.16	0.45
25:d:73:LEU:HD23	25:d:81:PHE:HZ	1.81	0.45
25:g:128:GLU:HA	25:g:131:ARG:HG2	1.97	0.45
1:0:150:ASP:OD2	1:0:154:MET:HB2	2.16	0.45
1:0:162:LYS:HD3	31:0:311:CLA:HBA1	1.99	0.45
30:0:301:CHL:H51	30:0:301:CHL:H12	1.78	0.45
2:1:49:LEU:HD22	2:1:71:ILE:HD11	1.97	0.45
2:1:61:SER:OG	2:1:61:SER:O	2.33	0.45
2:5:63:ASN:HB3	2:5:66:ASN:HB2	1.98	0.45
31:A:830:CLA:H42	34:A:844:LHG:H241	1.98	0.45
10:B:203:ARG:NH2	10:B:253:ALA:O	2.43	0.45
31:B:806:CLA:H142	31:B:806:CLA:H111	1.64	0.45
12:E:11:VAL:HB	12:E:61:VAL:HG13	1.98	0.45
17:L:6:VAL:HG13	21:O:50:TRP:HB2	1.97	0.45
42:d:523:NEX:H11	42:d:523:NEX:H191	1.82	0.45
30:f:609:CHL:HHC	30:f:609:CHL:HBB1	1.97	0.45
22:h:91:MET:HB3	31:h:604:CLA:HBB2	1.97	0.45
28:i:64:TRP:NE1	31:i:611:CLA:O1D	2.49	0.45
31:4:310:CLA:H92	31:4:310:CLA:H61	1.77	0.45
2:5:127:LEU:HD21	30:5:305:CHL:C4D	2.46	0.45
31:7:304:CLA:H71	30:7:305:CHL:HBD	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:124:TRP:CD2	31:A:809:CLA:HED3	2.51	0.45
9:A:439:ARG:NH1	9:A:564:SER:O	2.49	0.45
31:A:825:CLA:H203	31:A:825:CLA:H162	1.75	0.45
31:A:832:CLA:H141	31:A:832:CLA:H161	1.77	0.45
10:B:340:SER:O	10:B:344:ILE:HG12	2.17	0.45
22:a:65:SER:O	23:c:80:GLN:NE2	2.49	0.45
31:i:604:CLA:C4	30:i:606:CHL:O1A	2.65	0.45
7:4:97:MET:HE1	7:4:208:THR:HG23	1.97	0.45
7:4:179:ILE:HG23	7:4:179:ILE:O	2.15	0.45
3:2:206:LYS:NZ	34:2:601:LHG:O4	2.32	0.45
31:6:303:CLA:H61	31:6:303:CLA:H41	1.57	0.45
31:6:304:CLA:HMB1	30:6:305:CHL:HBB1	1.98	0.45
30:6:308:CHL:H2	30:6:308:CHL:H62	1.73	0.45
31:9:300:CLA:HBA2	14:G:50:ARG:HD3	1.97	0.45
31:9:309:CLA:HMB3	31:9:311:CLA:HAA1	1.98	0.45
9:A:18:VAL:HG21	9:A:319:THR:HB	1.98	0.45
31:A:809:CLA:H91	31:A:809:CLA:H111	1.67	0.45
10:B:415:LYS:NZ	10:B:540:ASP:OD1	2.38	0.45
10:B:415:LYS:NZ	13:F:238:VAL:HG21	2.29	0.45
31:B:839:CLA:H2A	15:I:27:PHE:HE2	1.82	0.45
26:f:187:GLN:OE1	30:f:607:CHL:HMC	2.17	0.45
28:i:145:VAL:HB	28:i:148:LYS:HE2	1.98	0.45
30:1:313:CHL:HAA2	7:4:135:MET:HE2	1.98	0.45
30:2:319:CHL:H112	30:2:319:CHL:H91	1.60	0.45
8:9:157:LEU:O	8:9:158:GLY:C	2.59	0.45
9:A:685:ALA:O	9:A:686:PHE:C	2.57	0.45
31:A:810:CLA:HBB2	31:A:813:CLA:HMA3	1.99	0.45
38:A:842:PQN:H161	38:A:842:PQN:H141	1.72	0.45
22:a:82:GLU:HB2	30:a:602:CHL:CHB	2.47	0.45
30:a:607:CHL:H3A	30:a:607:CHL:HBA1	1.42	0.45
28:i:69:ARG:NH2	28:i:91:ASP:O	2.50	0.45
28:i:135:LYS:HE3	28:i:135:LYS:HB3	1.86	0.45
29:e:107:PHE:CE2	29:e:128:LEU:HA	2.52	0.45
7:4:159:VAL:HG13	7:4:162:ILE:HB	1.99	0.45
7:4:217:VAL:HG11	7:4:241:ILE:HD13	1.98	0.45
1:0:110:PRO:HB2	28:i:162:LEU:HD23	1.99	0.45
2:5:160:PRO:HD2	33:5:501:0UR:O40	2.13	0.45
30:7:307:CHL:CBB	31:7:315:CLA:HMC2	2.47	0.45
7:8:161:PRO:HB3	30:8:315:CHL:C1C	2.46	0.45
10:B:101:VAL:O	10:B:105:THR:HG23	2.17	0.45
10:B:286:ILE:O	31:B:822:CLA:HBC1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:809:CLA:HHB	31:B:830:CLA:HAB	1.98	0.45
31:B:822:CLA:H143	14:G:81:VAL:HB	1.99	0.45
14:G:54:TYR:CG	14:G:55:VAL:N	2.85	0.45
23:c:40:ARG:NE	23:c:63:ASP:O	2.36	0.45
42:c:523:NEX:H222	31:c:604:CLA:CHC	2.47	0.45
24:b:65:TYR:HB2	30:b:602:CHL:HMD3	1.98	0.45
30:d:606:CHL:HBC2	30:d:607:CHL:HHD	1.99	0.45
22:h:228:HIS:CG	31:h:613:CLA:HAA2	2.52	0.45
31:4:310:CLA:H43	31:4:311:CLA:HMD2	1.97	0.45
30:1:306:CHL:HHC	30:1:306:CHL:HBB1	1.99	0.45
31:3:313:CLA:HBA2	31:3:313:CLA:H3A	1.57	0.45
9:A:594:TRP:NE1	31:A:830:CLA:HMD3	2.31	0.45
31:A:831:CLA:HAB	31:A:838:CLA:CBB	2.47	0.45
23:c:89:SER:HB2	23:c:205:GLY:HA3	1.99	0.45
30:b:608:CHL:H143	30:b:608:CHL:H162	1.70	0.45
30:e:608:CHL:H62	30:e:608:CHL:H101	1.64	0.45
1:0:72:ARG:NH1	1:0:75:GLU:OE1	2.50	0.45
2:1:85:VAL:HG13	2:1:189:PHE:CE2	2.52	0.45
30:2:302:CHL:H93	30:2:302:CHL:H111	1.70	0.45
4:3:215:LEU:HB2	31:3:309:CLA:HBA1	1.98	0.45
7:8:103:LEU:HD13	7:8:111:PRO:HG2	1.99	0.45
7:8:149:GLN:CB	7:8:158:ASN:HD21	2.29	0.45
9:A:119:SER:HB2	9:A:136:VAL:HG11	1.99	0.45
9:A:121:GLN:NE2	31:A:809:CLA:OBD	2.47	0.45
9:A:603:TRP:HE1	31:B:806:CLA:C1D	2.30	0.45
9:A:610:ILE:HD12	39:A:857:CL0:H53	1.98	0.45
9:A:665:SER:O	9:A:671:SER:HA	2.17	0.45
31:A:817:CLA:H41	31:A:817:CLA:H61	1.71	0.45
31:A:837:CLA:HBB1	31:A:838:CLA:CHD	2.47	0.45
31:B:819:CLA:H61	31:B:819:CLA:H93	1.84	0.45
42:g:523:NEX:H35	42:g:523:NEX:H401	1.57	0.45
22:h:158:ALA:HB1	28:i:76:LEU:HB3	1.98	0.45
22:h:183:ALA:HB2	22:h:192:LEU:HD12	1.99	0.45
22:h:212:THR:HG21	31:h:613:CLA:HAC2	1.99	0.45
28:i:134:GLU:HA	28:i:139:ALA:HB2	1.98	0.45
42:e:523:NEX:H35	42:e:523:NEX:H401	1.75	0.45
4:3:168:GLN:NE2	31:3:318:CLA:O1D	2.50	0.45
4:3:230:ILE:HD12	4:3:230:ILE:HA	1.87	0.45
9:A:133:ASN:HB3	9:A:141:GLN:HB3	1.99	0.45
9:A:295:TRP:HB2	9:A:298:ASP:OD2	2.17	0.45
9:A:434:ARG:O	9:A:438:HIS:ND1	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:842:PQN:H141	31:A:853:CLA:HBB2	1.99	0.45
10:B:658:ALA:HB3	31:B:806:CLA:HBB2	1.99	0.45
34:2:601:LHG:H272	34:2:601:LHG:H242	1.79	0.45
9:A:440:ASP:OD1	9:A:561:TYR:OH	2.29	0.45
31:A:826:CLA:H62	31:A:826:CLA:H101	1.60	0.45
31:A:843:CLA:HBA2	21:O:122:THR:HG23	1.98	0.45
31:B:819:CLA:H62	31:B:819:CLA:H41	1.57	0.45
22:a:33:TYR:CE2	22:a:190:ALA:HB1	2.52	0.45
22:a:159:TYR:HB3	30:a:608:CHL:OMC	2.17	0.45
23:c:152:GLN:HE22	30:c:607:CHL:HAC1	1.82	0.45
24:b:107:ASN:HB2	24:b:117:THR:HG21	1.99	0.45
24:b:176:PRO:HD2	31:b:610:CLA:OBD	2.16	0.45
29:e:227:HIS:CG	31:e:613:CLA:HAA2	2.52	0.45
1:0:200:LEU:HD21	8:9:114:VAL:HG23	1.99	0.44
2:5:161:ALA:O	2:5:163:PHE:N	2.50	0.44
9:A:703:GLU:CD	10:B:545:LYS:HB2	2.41	0.44
9:A:705:ILE:HD13	31:A:839:CLA:HMD1	1.99	0.44
31:A:822:CLA:HBA2	31:A:822:CLA:H3A	1.21	0.44
31:A:839:CLA:H172	13:F:181:GLY:HA2	1.99	0.44
29:e:54:PHE:O	29:e:57:ASP:HB2	2.16	0.44
2:5:167:ASN:OD1	2:5:167:ASN:N	2.50	0.44
5:6:203:THR:HG22	5:6:205:PHE:N	2.26	0.44
8:9:95:GLU:CD	8:9:194:VAL:HG12	2.42	0.44
9:A:225:LEU:C	9:A:228:PRO:HD2	2.43	0.44
31:A:831:CLA:HBA2	34:A:845:LHG:HC92	1.98	0.44
31:B:831:CLA:HBA2	31:B:831:CLA:H3A	1.34	0.44
22:a:116:PHE:CD2	22:a:117:LYS:HG3	2.52	0.44
30:c:601:CHL:H3A	30:c:601:CHL:HBA1	1.59	0.44
37:b:521:0IE:C19	30:b:602:CHL:H2	2.47	0.44
30:f:601:CHL:HBA1	30:f:601:CHL:H3A	1.73	0.44
31:g:613:CLA:H3A	31:g:613:CLA:HBA2	1.72	0.44
31:e:610:CLA:HMB3	31:e:612:CLA:HAA1	1.98	0.44
7:4:229:HIS:CG	31:4:312:CLA:HAA2	2.52	0.44
31:5:303:CLA:H111	31:5:303:CLA:H91	1.76	0.44
31:6:310:CLA:HED2	31:6:310:CLA:H2A	1.97	0.44
9:A:33:LYS:HB2	31:A:811:CLA:HAA2	1.99	0.44
9:A:401:TRP:CD1	31:A:828:CLA:HAB	2.53	0.44
9:A:458:PHE:O	9:A:462:ILE:HG12	2.18	0.44
9:A:484:LEU:H	9:A:535:THR:HG22	1.81	0.44
31:B:808:CLA:HBB1	31:B:808:CLA:HMB1	2.00	0.44
31:B:825:CLA:H111	31:B:825:CLA:H151	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:608:CHL:H43	30:c:608:CHL:H203	2.00	0.44
25:d:64:THR:HG23	25:d:180:MET:HG2	1.99	0.44
30:f:601:CHL:H12	30:f:601:CHL:H51	1.74	0.44
1:0:241:ARG:HH22	35:0:603:SQD:H5	1.83	0.44
30:0:301:CHL:HBA2	30:0:301:CHL:H3A	1.70	0.44
2:5:130:ILE:HA	2:5:133:VAL:HG12	1.99	0.44
5:6:212:LEU:O	6:7:256:PRO:HD3	2.17	0.44
8:9:145:MET:HE3	8:9:145:MET:HB2	1.62	0.44
9:A:337:PRO:HB2	17:L:6:VAL:HG23	1.99	0.44
31:A:819:CLA:HBA2	31:A:819:CLA:H3A	1.42	0.44
31:A:822:CLA:H12	31:K:105:CLA:HMB2	1.98	0.44
31:A:832:CLA:H62	31:A:832:CLA:H93	1.70	0.44
31:A:852:CLA:HMC1	31:B:838:CLA:HAC1	2.00	0.44
12:E:54:ASN:ND2	18:C:61:ASP:HB2	2.32	0.44
14:G:26:PHE:O	14:G:30:ASN:ND2	2.31	0.44
16:J:26:ILE:HG21	32:J:104:8CT:C29	2.48	0.44
17:L:40:ARG:HD2	27:H:80:ARG:HH11	1.82	0.44
42:d:523:NEX:H401	42:d:523:NEX:H35	1.57	0.44
26:f:128:MET:SD	31:f:610:CLA:HAB	2.58	0.44
26:f:220:PRO:O	28:i:50:ARG:NH2	2.42	0.44
28:i:259:TRP:CE2	28:i:263:ILE:HD11	2.51	0.44
29:e:194:LYS:NZ	31:e:612:CLA:O1D	2.41	0.44
30:e:608:CHL:H143	30:e:608:CHL:H161	1.77	0.44
7:4:243:LEU:HD22	7:4:244:ALA:N	2.33	0.44
1:0:161:LEU:HD23	31:0:310:CLA:HED2	1.99	0.44
2:1:133:VAL:HG22	14:G:14:LEU:HD13	1.99	0.44
4:3:218:THR:C	4:3:220:GLU:H	2.25	0.44
31:7:315:CLA:H11	31:7:315:CLA:HBA1	1.78	0.44
31:A:803:CLA:H193	31:B:803:CLA:H192	2.00	0.44
31:A:826:CLA:HBA2	31:A:826:CLA:H3A	1.78	0.44
10:B:430:GLY:HA2	10:B:525:LEU:HD22	1.99	0.44
31:B:801:CLA:H111	31:B:801:CLA:H143	1.65	0.44
25:d:120:GLN:HE22	30:d:607:CHL:CMC	2.31	0.44
26:f:264:GLN:NE2	26:f:268:ASP:OD1	2.50	0.44
30:f:601:CHL:H202	30:f:601:CHL:H161	1.71	0.44
30:h:602:CHL:H91	30:h:602:CHL:H111	1.79	0.44
27:H:76:GLU:OE1	27:H:76:GLU:N	2.49	0.44
28:i:184:MET:CE	42:i:523:NEX:H30	2.40	0.44
29:e:101:LYS:NZ	29:e:225:ALA:HB2	2.32	0.44
7:4:98:LEU:HD13	7:4:211:PHE:HZ	1.82	0.44
4:3:168:GLN:HE22	31:3:318:CLA:CHA	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:309:CLA:H102	31:5:311:CLA:HBC1	2.00	0.44
31:A:803:CLA:H72	31:A:803:CLA:H112	1.75	0.44
31:B:806:CLA:H92	31:B:806:CLA:H62	1.84	0.44
31:B:818:CLA:H3A	31:B:818:CLA:HBA2	1.27	0.44
22:a:217:THR:OG1	22:a:218:GLY:N	2.50	0.44
31:c:613:CLA:H2	31:c:613:CLA:H61	1.55	0.44
34:d:630:LHG:O3	34:d:630:LHG:O1	2.31	0.44
25:g:101:TYR:HD2	25:g:107:LEU:HD13	1.82	0.44
22:h:208:PHE:HD2	31:h:613:CLA:HMC1	1.83	0.44
29:e:66:SER:O	29:e:66:SER:OG	2.27	0.44
1:0:109:VAL:HG12	1:0:111:ILE:H	1.82	0.44
2:1:114:TRP:HD1	2:1:118:GLY:O	2.01	0.44
3:2:83:GLN:HE21	3:2:83:GLN:HB2	1.57	0.44
31:6:317:CLA:HMB1	31:6:317:CLA:HBB1	2.00	0.44
30:8:305:CHL:HBA1	32:8:402:8CT:C15	2.48	0.44
8:9:213:VAL:HG11	34:G:105:LHG:H251	2.00	0.44
10:B:86:PRO:HB3	10:B:121:TYR:CG	2.53	0.44
23:c:109:GLY:HA2	29:e:132:GLN:HG3	2.00	0.44
42:c:523:NEX:H11	42:c:523:NEX:H191	1.82	0.44
24:b:140:VAL:HG21	24:b:148:ILE:HD12	1.99	0.44
26:f:197:TYR:HB3	30:f:608:CHL:CMC	2.47	0.44
42:f:523:NEX:H11	42:f:523:NEX:H191	1.82	0.44
30:f:607:CHL:HHC	30:f:607:CHL:HBB1	1.99	0.44
28:i:69:ARG:H	28:i:69:ARG:CD	2.28	0.44
28:i:140:ASN:ND2	28:i:162:LEU:O	2.45	0.44
28:i:230:GLU:HB3	31:i:610:CLA:C1B	2.48	0.44
3:2:103:GLY:C	3:2:230:VAL:HG11	2.43	0.44
30:2:319:CHL:HBB1	30:2:319:CHL:CHC	2.45	0.44
31:A:821:CLA:H192	31:A:821:CLA:H162	1.84	0.44
31:A:841:CLA:H112	31:A:841:CLA:H72	1.60	0.44
10:B:397:ASP:HA	11:D:198:ILE:HD13	2.00	0.44
10:B:582:TRP:O	10:B:586:THR:HG22	2.17	0.44
31:B:820:CLA:HBC2	31:B:824:CLA:H72	2.00	0.44
31:B:830:CLA:H42	41:B:849:DGD:HB42	1.99	0.44
22:a:116:PHE:HD2	22:a:117:LYS:HG3	1.82	0.44
25:d:119:THR:HG21	30:d:605:CHL:HBC1	1.99	0.44
26:f:197:TYR:OH	42:f:523:NEX:H191	2.17	0.44
22:h:52:TYR:OH	22:h:64:ASP:OD2	2.26	0.44
7:4:98:LEU:O	7:4:102:LEU:N	2.43	0.44
7:4:222:PRO:O	33:4:501:0UR:O39	2.36	0.44
1:0:128:GLU:HG3	31:0:308:CLA:NB	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:219:ASN:ND2	31:1:312:CLA:OBD	2.50	0.44
31:1:311:CLA:H41	31:1:311:CLA:H61	1.83	0.44
3:2:185:ASP:OD1	33:2:501:0UR:O40	2.36	0.44
8:9:45:PRO:HG3	14:G:54:TYR:HE1	1.83	0.44
9:A:302:HIS:HB2	31:A:818:CLA:CHB	2.48	0.44
10:B:352:MET:HE2	10:B:352:MET:HB3	1.87	0.44
31:B:825:CLA:H18	31:B:825:CLA:H152	1.84	0.44
24:b:88:MET:HE2	24:b:163:ARG:NH1	2.32	0.44
30:g:609:CHL:HHC	30:g:609:CHL:HBB1	2.00	0.44
2:5:158:PHE:HE1	30:5:307:CHL:HBA2	1.83	0.43
30:8:315:CHL:HHC	30:8:315:CHL:HBB1	2.00	0.43
8:9:159:MET:HG3	31:9:309:CLA:O1A	2.18	0.43
9:A:519:ILE:HD13	9:A:632:VAL:HG21	1.99	0.43
31:A:813:CLA:H93	31:A:813:CLA:H111	1.73	0.43
10:B:174:ARG:HH11	31:B:808:CLA:H141	1.82	0.43
10:B:325:THR:HG21	10:B:403:ASN:OD1	2.18	0.43
10:B:378:ILE:O	10:B:382:MET:HG3	2.18	0.43
31:B:811:CLA:CGA	31:B:811:CLA:C1A	2.97	0.43
31:B:816:CLA:H51	31:B:816:CLA:H11	1.73	0.43
31:B:826:CLA:HMA1	32:B:847:8CT:C17	2.47	0.43
23:c:218:GLN:O	23:c:222:THR:N	2.52	0.43
24:b:70:MET:HB3	24:b:72:LEU:HG	1.99	0.43
33:b:520:0UR:C13	31:b:610:CLA:HAB	2.48	0.43
42:b:523:NEX:H401	42:b:523:NEX:H35	1.58	0.43
30:d:601:CHL:HBB1	30:d:601:CHL:HHC	1.99	0.43
31:d:603:CLA:HBB1	30:d:609:CHL:H161	2.00	0.43
42:f:523:NEX:H201	42:f:523:NEX:H15	1.62	0.43
30:f:606:CHL:HMB1	30:f:609:CHL:HMC	1.99	0.43
22:h:195:LYS:NZ	31:h:612:CLA:O1D	2.44	0.43
29:e:151:GLY:HA2	30:e:609:CHL:HAB	2.00	0.43
1:0:145:SER:OG	28:i:213:PRO:HA	2.18	0.43
34:1:601:LHG:H151	34:1:601:LHG:H322	1.98	0.43
4:3:76:TYR:HD2	30:3:302:CHL:HMD2	1.83	0.43
2:5:44:TYR:OH	2:5:59:GLY:HA2	2.18	0.43
7:8:222:PRO:O	33:8:501:0UR:O39	2.36	0.43
9:A:700:GLU:OE1	10:B:536:LYS:NZ	2.48	0.43
31:A:811:CLA:H202	31:A:811:CLA:H162	1.77	0.43
31:A:828:CLA:H93	31:A:828:CLA:H62	1.77	0.43
10:B:134:ASP:OD2	10:B:208:ARG:NE	2.49	0.43
10:B:290:MET:CB	31:B:822:CLA:HBC3	2.46	0.43
10:B:700:LEU:HD22	10:B:704:GLN:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:43:TRP:N	23:c:64:TYR:O	2.51	0.43
25:g:185:VAL:HG11	31:g:613:CLA:HAC2	1.99	0.43
42:g:523:NEX:H201	42:g:523:NEX:H15	1.62	0.43
42:i:523:NEX:H383	31:i:604:CLA:C2B	2.46	0.43
7:4:159:VAL:HG22	7:4:161:PRO:HD2	2.00	0.43
7:4:171:ASN:HB2	7:4:178:GLY:HA2	1.99	0.43
2:1:112:PRO:HG2	2:1:114:TRP:CZ2	2.53	0.43
8:9:61:LEU:O	31:B:813:CLA:HBA1	2.18	0.43
9:A:343:HIS:HB3	9:A:346:LEU:HD12	2.00	0.43
10:B:347:MET:O	10:B:351:HIS:ND1	2.51	0.43
31:B:825:CLA:H143	31:B:825:CLA:H161	1.80	0.43
17:L:23:VAL:O	17:L:29:VAL:HG11	2.18	0.43
31:K:102:CLA:C1D	34:K:106:LHG:H262	2.48	0.43
24:b:148:ILE:HD13	30:b:606:CHL:HMD2	2.00	0.43
25:g:160:GLU:CD	25:g:160:GLU:H	2.26	0.43
22:h:33:TYR:CZ	22:h:190:ALA:HB1	2.53	0.43
7:4:162:ILE:HD13	7:4:162:ILE:HA	1.87	0.43
2:1:72:GLU:HG3	2:1:152:VAL:HG22	1.98	0.43
30:6:315:CHL:HBB1	30:6:315:CHL:HHC	2.00	0.43
6:7:246:ASP:OD1	6:7:246:ASP:N	2.52	0.43
30:7:301:CHL:HHC	30:7:301:CHL:HBB1	1.99	0.43
7:8:45:LEU:HB3	7:8:48:ALA:HB2	1.99	0.43
7:8:136:GLN:HG3	7:8:137:PHE:N	2.33	0.43
30:8:301:CHL:HBB2	30:8:302:CHL:HBC2	2.01	0.43
10:B:128:GLY:O	10:B:208:ARG:NH2	2.51	0.43
10:B:451:LYS:HB3	31:B:833:CLA:HED3	2.00	0.43
10:B:697:PRO:HB3	31:B:839:CLA:C1C	2.49	0.43
14:G:2:LEU:HD23	14:G:2:LEU:HA	1.92	0.43
17:L:28:ILE:H	17:L:28:ILE:HD12	1.83	0.43
17:L:69:PRO:HG3	31:H:201:CLA:HBA2	1.99	0.43
23:c:91:TRP:CD1	30:c:609:CHL:HMD2	2.54	0.43
26:f:241:GLY:O	26:f:245:MET:HG3	2.18	0.43
25:g:51:GLU:HA	25:g:144:LEU:HD11	2.01	0.43
31:3:306:CLA:H3A	31:3:306:CLA:HBA2	1.65	0.43
2:5:225:PHE:HD1	2:5:225:PHE:H	1.66	0.43
31:6:310:CLA:HAB	6:7:158:VAL:HG12	2.00	0.43
6:7:136:MET:HA	6:7:139:VAL:HG22	2.00	0.43
8:9:77:GLU:HB2	31:9:302:CLA:C1B	2.48	0.43
31:9:303:CLA:HED2	31:9:303:CLA:H12	1.99	0.43
9:A:540:VAL:HG11	9:A:614:HIS:CG	2.54	0.43
10:B:282:VAL:HG21	31:B:817:CLA:HAB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:652:PHE:O	10:B:656:VAL:HG23	2.19	0.43
31:L:203:CLA:H143	31:L:203:CLA:H162	1.74	0.43
42:g:523:NEX:H362	31:g:604:CLA:C3B	2.49	0.43
7:4:58:ILE:HG22	7:4:59:PRO:HD2	2.00	0.43
30:2:302:CHL:H161	30:2:302:CHL:H122	1.45	0.43
4:3:195:VAL:HG23	4:3:208:ALA:HB3	1.99	0.43
5:6:47:ASN:OD1	5:6:47:ASN:N	2.48	0.43
5:6:204:ILE:HD13	31:6:312:CLA:HMD3	2.00	0.43
9:A:458:PHE:CE1	31:A:802:CLA:HHB	2.54	0.43
31:A:808:CLA:HBA2	31:A:808:CLA:H3A	1.38	0.43
25:d:53:GLU:HB2	30:d:602:CHL:C1B	2.48	0.43
22:h:110:PHE:CE1	22:h:131:LEU:HD23	2.54	0.43
28:i:188:GLU:OE1	28:i:191:ARG:NE	2.39	0.43
42:i:523:NEX:H222	31:i:604:CLA:NC	2.34	0.43
30:0:302:CHL:H161	30:0:302:CHL:H122	1.54	0.43
3:2:113:PRO:HG3	3:2:121:VAL:HG21	1.99	0.43
3:2:135:MET:HB2	30:4:313:CHL:HED1	2.00	0.43
4:3:137:TRP:C	4:3:139:ARG:H	2.27	0.43
4:3:189:PHE:CZ	30:3:307:CHL:HBB2	2.54	0.43
31:3:308:CLA:H3A	31:3:308:CLA:HBA2	1.32	0.43
30:6:313:CHL:HAA2	6:7:131:PHE:HA	2.00	0.43
6:7:142:ARG:NE	30:7:307:CHL:OMC	2.46	0.43
9:A:145:ILE:HD12	31:A:808:CLA:CAD	2.48	0.43
9:A:513:LEU:HB2	9:A:528:MET:HG3	1.99	0.43
9:A:731:VAL:O	9:A:735:HIS:ND1	2.52	0.43
10:B:275:HIS:HB3	31:B:818:CLA:HMB2	2.00	0.43
10:B:290:MET:HE1	31:B:820:CLA:C3D	2.48	0.43
17:L:40:ARG:HD2	27:H:80:ARG:NH1	2.33	0.43
31:K:102:CLA:C4B	34:K:106:LHG:H311	2.49	0.43
34:K:106:LHG:H172	34:K:106:LHG:H141	1.75	0.43
30:a:602:CHL:HBC1	34:a:630:LHG:H262	2.00	0.43
23:c:139:PHE:O	23:c:141:HIS:N	2.49	0.43
26:f:59:ARG:N	27:H:72:MET:O	2.52	0.43
22:h:40:TRP:HB3	22:h:61:TYR:HB3	2.00	0.43
29:e:194:LYS:NZ	31:e:612:CLA:O1A	2.39	0.43
2:5:42:PRO:HB2	2:5:44:TYR:CE2	2.53	0.43
2:5:213:GLY:HA2	2:5:218:THR:HG21	1.98	0.43
30:5:301:CHL:OBD	7:8:146:ARG:NH1	2.52	0.43
7:8:181:ASP:OD1	33:8:501:0UR:O40	2.37	0.43
8:9:152:PHE:CB	8:9:153:PRO:CD	2.95	0.43
9:A:135:ASP:OD2	13:F:107:LYS:NZ	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:601:LEU:HB3	9:A:737:ILE:HD11	1.99	0.43
10:B:378:ILE:HD13	31:B:829:CLA:CBB	2.48	0.43
10:B:444:LEU:HD22	10:B:615:TYR:CZ	2.54	0.43
10:B:686:PRO:HD2	31:L:201:CLA:HBA1	1.99	0.43
18:C:55:GLU:HB3	18:C:63:LEU:HD13	2.01	0.43
24:b:119:TRP:HD1	24:b:224:PRO:HD3	1.84	0.43
25:d:110:ALA:HA	30:d:605:CHL:HHC	2.01	0.43
25:g:53:GLU:HB2	30:g:602:CHL:CHB	2.49	0.43
30:e:608:CHL:C4A	30:e:608:CHL:HBA2	2.49	0.43
30:e:609:CHL:H91	30:e:609:CHL:H111	1.80	0.43
7:4:137:PHE:CD2	30:4:308:CHL:HBB2	2.53	0.43
31:1:303:CLA:H62	31:1:303:CLA:H41	1.59	0.43
31:1:312:CLA:H42	30:1:313:CHL:HMD1	2.01	0.43
3:2:107:ARG:NH1	3:2:231:ASP:OD1	2.49	0.43
30:6:308:CHL:H111	30:6:308:CHL:H91	1.75	0.43
8:9:94:CYS:HB3	8:9:99:ILE:O	2.19	0.43
9:A:125:PRO:HA	9:A:130:GLU:HG3	2.01	0.43
9:A:126:ILE:HG12	9:A:127:VAL:H	1.83	0.43
9:A:183:TRP:HB2	31:A:811:CLA:HMC2	2.00	0.43
9:A:729:ARG:NH2	40:B:802:SF4:S4	2.92	0.43
31:A:826:CLA:H141	31:A:826:CLA:H161	1.70	0.43
31:A:839:CLA:C4C	31:A:839:CLA:H51	2.48	0.43
36:L:211:LMG:H111	36:L:211:LMG:H142	1.72	0.43
25:d:125:GLY:HA2	30:d:609:CHL:HAB	2.01	0.43
26:f:167:ASN:HB3	26:f:171:ASN:O	2.19	0.43
25:g:130:TYR:O	25:g:134:GLY:N	2.52	0.43
22:h:40:TRP:CE2	22:h:41:LEU:HG	2.53	0.43
22:h:86:ALA:O	22:h:90:MET:HG2	2.19	0.43
34:e:630:LHG:H292	34:e:630:LHG:HC92	1.99	0.43
7:4:116:GLU:CD	7:4:116:GLU:H	2.25	0.43
30:0:301:CHL:H43	31:0:312:CLA:H52	2.01	0.43
2:1:145:GLU:HB3	2:1:151:ARG:HG3	2.00	0.43
31:3:304:CLA:H112	31:3:304:CLA:H72	1.87	0.43
31:6:318:CLA:HBA1	31:6:318:CLA:H3A	1.34	0.43
9:A:716:PRO:HG2	9:A:720:PRO:HD3	2.00	0.43
31:A:818:CLA:H122	31:A:818:CLA:H161	1.72	0.43
39:A:857:CL0:H14	31:B:805:CLA:C1A	2.48	0.43
24:b:199:GLU:HB2	31:b:610:CLA:C1B	2.49	0.43
31:b:603:CLA:HED2	31:b:603:CLA:H2A	2.00	0.43
25:d:131:ARG:HG3	30:d:608:CHL:C1D	2.49	0.43
28:i:167:LEU:O	28:i:169:HIS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:193:LEU:HD13	31:4:309:CLA:O1A	2.19	0.43
4:3:92:GLY:O	4:3:95:ASN:ND2	2.52	0.42
31:3:308:CLA:H92	31:3:308:CLA:H62	1.72	0.42
5:6:235:THR:HA	30:6:306:CHL:O1A	2.19	0.42
6:7:144:TRP:HB2	31:7:308:CLA:CMA	2.48	0.42
31:7:308:CLA:H162	31:7:308:CLA:H121	1.41	0.42
31:9:311:CLA:HBB1	31:9:311:CLA:HHC	2.01	0.42
9:A:291:ASN:HB3	9:A:383:PRO:HA	2.01	0.42
9:A:536:SER:O	9:A:540:VAL:HG23	2.18	0.42
9:A:719:GLN:NE2	12:E:19:TYR:OH	2.52	0.42
31:A:809:CLA:H62	31:A:809:CLA:H101	1.65	0.42
10:B:240:ILE:HA	10:B:263:PRO:HG2	2.00	0.42
31:B:812:CLA:HBA2	31:B:812:CLA:H3A	1.87	0.42
14:G:41:LEU:HD12	14:G:45:GLU:HB3	2.01	0.42
17:L:3:GLN:OE1	21:O:131:ARG:HB2	2.18	0.42
20:M:23:LEU:HD11	34:M:104:LHG:H371	2.00	0.42
22:a:48:ALA:HB2	23:c:164:CYS:HB3	2.01	0.42
22:a:98:THR:HB	22:a:99:PRO:HD3	2.01	0.42
22:a:169:ASP:HB3	22:a:173:PRO:HA	2.01	0.42
22:a:202:LEU:HA	34:a:630:LHG:H272	2.01	0.42
23:c:86:VAL:HG21	23:c:176:LEU:HD13	2.01	0.42
26:f:174:LEU:O	26:f:176:HIS:N	2.52	0.42
26:f:191:MET:HE1	42:f:523:NEX:H30	2.01	0.42
30:h:609:CHL:H2A	28:i:96:THR:HG21	2.01	0.42
29:e:133:LEU:O	29:e:135:HIS:N	2.52	0.42
1:0:74:ALA:O	1:0:78:ASN:ND2	2.37	0.42
2:1:80:TRP:CD1	31:1:308:CLA:HMD3	2.54	0.42
9:A:120:ALA:N	9:A:145:ILE:HG12	2.34	0.42
10:B:583:MET:HG2	31:B:826:CLA:HBC1	2.00	0.42
31:B:832:CLA:H62	31:B:832:CLA:H2	1.70	0.42
18:C:73:THR:N	18:C:76:SER:OG	2.44	0.42
24:b:157:GLY:CA	30:b:609:CHL:HAB	2.49	0.42
34:b:630:LHG:H242	34:b:630:LHG:HC62	1.68	0.42
28:i:121:MET:HB2	33:i:520:0UR:C10	2.48	0.42
28:i:208:GLY:O	28:i:212:ASP:N	2.41	0.42
29:e:111:VAL:HG23	29:e:113:PHE:O	2.19	0.42
4:3:189:PHE:CE2	30:3:307:CHL:HBB2	2.53	0.42
2:5:85:VAL:HG13	2:5:189:PHE:CE2	2.53	0.42
9:A:27:THR:O	9:A:187:HIS:ND1	2.42	0.42
9:A:296:LEU:HD23	9:A:299:ILE:HD12	2.00	0.42
9:A:548:ILE:HD11	31:A:836:CLA:HBB1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:818:CLA:H203	31:A:818:CLA:H162	1.81	0.42
32:B:804:8CT:C20	31:B:832:CLA:H3A	2.49	0.42
15:I:4:ALA:O	15:I:7:PRO:HD2	2.20	0.42
31:a:603:CLA:HAC2	30:a:607:CHL:H152	2.01	0.42
42:c:523:NEX:C39	30:c:606:CHL:HMB2	2.47	0.42
30:c:609:CHL:H61	30:c:609:CHL:H92	1.81	0.42
26:f:79:LEU:HD23	26:f:85:THR:HB	2.01	0.42
30:e:601:CHL:H12	34:e:630:LHG:H161	2.00	0.42
1:0:175:VAL:HG12	31:0:312:CLA:HAC1	2.01	0.42
2:5:60:ILE:HB	30:5:302:CHL:O1A	2.19	0.42
6:7:142:ARG:HE	30:7:307:CHL:CMC	2.29	0.42
34:A:844:LHG:O3	34:A:844:LHG:O1	2.28	0.42
31:B:811:CLA:H91	31:B:811:CLA:H112	1.72	0.42
13:F:216:TRP:CG	13:F:217:PRO:HD3	2.54	0.42
14:G:5:SER:HA	31:G:102:CLA:OBD	2.20	0.42
22:a:163:GLY:HA3	22:a:168:GLU:HG2	2.02	0.42
30:c:608:CHL:C4A	30:c:608:CHL:HBA2	2.49	0.42
24:b:76:PRO:O	24:b:80:GLU:HG2	2.20	0.42
30:d:602:CHL:H143	30:d:602:CHL:H112	1.66	0.42
31:f:613:CLA:H2	31:f:613:CLA:H61	1.74	0.42
28:i:119:TRP:CD1	30:i:609:CHL:HMD3	2.53	0.42
28:i:183:LEU:HB3	42:i:523:NEX:C15	2.50	0.42
1:0:169:LEU:HD13	31:0:310:CLA:HBC1	2.02	0.42
2:5:139:GLU:HG3	31:5:308:CLA:NB	2.34	0.42
8:9:212:ASN:ND2	31:9:312:CLA:OBD	2.51	0.42
31:A:815:CLA:H161	31:A:815:CLA:H141	1.60	0.42
31:A:832:CLA:H151	31:A:832:CLA:H112	1.83	0.42
10:B:280:ILE:HD13	10:B:280:ILE:HA	1.90	0.42
10:B:662:MET:HB2	31:B:806:CLA:C1C	2.49	0.42
31:B:810:CLA:HMA1	31:B:811:CLA:CHB	2.49	0.42
31:B:811:CLA:H111	31:B:811:CLA:H142	1.77	0.42
31:B:833:CLA:H92	16:J:25:LEU:HD21	2.02	0.42
13:F:222:ASN:HB3	7:4:75:THR:HG21	2.00	0.42
24:b:86:GLU:HB2	30:b:602:CHL:CHB	2.49	0.42
25:g:183:PHE:CE1	25:g:194:PRO:HB3	2.54	0.42
31:2:312:CLA:H2	30:2:313:CHL:HMD1	2.01	0.42
31:3:303:CLA:H42	31:A:810:CLA:H11	2.00	0.42
31:7:309:CLA:H3A	31:7:309:CLA:HBA2	1.51	0.42
31:A:829:CLA:H91	31:A:829:CLA:H111	1.69	0.42
38:A:842:PQN:H222	31:A:853:CLA:C1B	2.50	0.42
10:B:276:HIS:HB2	31:B:818:CLA:CHB	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:817:CLA:H61	31:B:817:CLA:H41	1.77	0.42
31:B:827:CLA:H162	31:B:827:CLA:H202	1.74	0.42
31:L:204:CLA:HBA1	31:L:204:CLA:H3A	1.78	0.42
18:C:32:ASP:N	18:C:32:ASP:OD1	2.51	0.42
23:c:222:THR:HA	23:c:247:VAL:HG13	2.01	0.42
25:g:12:LEU:HB2	25:g:16:SER:HA	2.00	0.42
28:i:117:ALA:O	28:i:121:MET:HG2	2.18	0.42
2:1:88:MET:HE1	2:1:186:PHE:HD1	1.85	0.42
4:3:249:LEU:O	4:3:277:VAL:HA	2.19	0.42
31:7:317:CLA:CGD	31:7:317:CLA:HBA2	2.49	0.42
7:8:138:LEU:HD13	7:8:138:LEU:HA	1.93	0.42
31:A:843:CLA:CHC	34:A:845:LHG:HC32	2.49	0.42
10:B:181:GLY:HA3	31:B:814:CLA:HBB1	2.00	0.42
10:B:257:PHE:HZ	31:B:818:CLA:H71	1.83	0.42
42:a:523:NEX:H401	42:a:523:NEX:H35	1.58	0.42
24:b:83:ARG:O	24:b:87:VAL:HG23	2.18	0.42
26:f:72:TRP:HH2	31:f:611:CLA:HMA3	1.84	0.42
22:h:115:TRP:CD1	22:h:221:PRO:HD3	2.51	0.42
22:h:202:LEU:HD23	34:h:630:LHG:H271	2.01	0.42
7:4:72:ASP:HB2	7:4:75:THR:OG1	2.20	0.42
31:0:321:CLA:HAB	15:I:21:ILE:CG2	2.49	0.42
2:1:82:MET:SD	31:1:309:CLA:HAB	2.60	0.42
31:2:314:CLA:HBC1	4:3:161:PHE:HB2	2.02	0.42
8:9:157:LEU:O	8:9:159:MET:HG2	2.19	0.42
9:A:325:HIS:HB3	9:A:330:ILE:HD11	2.02	0.42
9:A:330:ILE:O	9:A:334:HIS:ND1	2.52	0.42
31:A:828:CLA:H3A	31:A:828:CLA:HBA2	1.88	0.42
31:A:840:CLA:H142	31:A:840:CLA:H111	1.71	0.42
31:A:843:CLA:HED2	21:O:125:GLN:NE2	2.35	0.42
10:B:427:LEU:HD23	31:B:801:CLA:HBA2	2.02	0.42
10:B:507:SER:HA	10:B:510:LEU:HD21	2.02	0.42
13:F:232:LYS:HG3	13:F:234:GLU:OE1	2.20	0.42
19:K:2:PHE:CD2	34:K:106:LHG:HC61	2.55	0.42
34:a:630:LHG:H291	34:a:630:LHG:H261	1.87	0.42
24:b:68:ASP:O	24:b:69:THR:C	2.63	0.42
42:i:523:NEX:H201	42:i:523:NEX:H15	1.62	0.42
30:i:602:CHL:H92	30:i:602:CHL:H62	1.71	0.42
30:e:602:CHL:H92	30:e:602:CHL:H62	1.77	0.42
30:4:308:CHL:H3A	30:4:308:CHL:HBA1	1.78	0.42
1:0:107:VAL:HG22	31:0:304:CLA:HED3	2.02	0.42
30:1:302:CHL:H143	30:1:302:CHL:H162	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:310:CLA:H61	31:2:310:CLA:H92	1.62	0.42
4:3:254:PRO:O	33:3:501:0UR:O39	2.37	0.42
7:8:172:ILE:HD13	7:8:172:ILE:HA	1.88	0.42
9:A:364:LEU:HD21	31:A:821:CLA:H71	2.01	0.42
9:A:681:HIS:HB3	31:B:803:CLA:HBD	2.02	0.42
10:B:175:LEU:HD21	31:B:820:CLA:HMA2	2.02	0.42
31:B:819:CLA:HBA2	31:B:819:CLA:H3A	1.48	0.42
31:B:826:CLA:HMB3	31:B:827:CLA:H193	2.01	0.42
31:B:833:CLA:HMA2	36:J:105:LMG:H332	2.01	0.42
13:F:135:SER:HB2	16:J:38:ILE:HD11	2.01	0.42
14:G:28:ARG:NH2	14:G:70:ASP:OD2	2.43	0.42
17:L:10:ILE:HB	17:L:18:MET:HB3	2.02	0.42
22:a:142:ILE:HA	22:a:145:ILE:HG12	2.02	0.42
23:c:146:LEU:H	23:c:146:LEU:HD12	1.85	0.42
24:b:240:GLY:N	31:b:613:CLA:O1A	2.53	0.42
25:d:87:PHE:HE1	25:d:88:LYS:HE3	1.85	0.42
42:d:523:NEX:H31	30:d:606:CHL:CBA	2.47	0.42
42:i:523:NEX:H11	42:i:523:NEX:H191	1.82	0.42
31:i:604:CLA:H43	30:i:606:CHL:O1A	2.20	0.42
30:i:606:CHL:CMB	30:i:609:CHL:HAC1	2.48	0.42
7:4:181:ASP:OD1	7:4:185:PHE:HB2	2.20	0.42
1:0:198:ASP:OD1	1:0:198:ASP:N	2.53	0.42
2:1:113:THR:HG21	30:1:305:CHL:CMD	2.47	0.42
3:2:143:TRP:O	3:2:147:MET:HG3	2.20	0.42
3:2:178:TYR:HB3	31:2:309:CLA:HED2	2.01	0.42
30:5:301:CHL:HBB2	30:5:302:CHL:HHD	2.01	0.42
6:7:129:LEU:HD13	30:7:306:CHL:HBC3	2.02	0.42
30:7:302:CHL:H101	30:7:302:CHL:H62	1.86	0.42
7:8:167:LEU:HD23	7:8:169:ASP:H	1.85	0.42
7:8:229:HIS:ND1	7:8:236:ASN:O	2.37	0.42
30:9:301:CHL:CGA	34:9:601:LHG:H142	2.50	0.42
31:A:820:CLA:H92	31:A:820:CLA:H61	1.82	0.42
31:A:837:CLA:H62	31:A:837:CLA:H41	1.66	0.42
31:A:843:CLA:HBD	21:O:125:GLN:HG3	2.01	0.42
10:B:105:THR:OG1	27:H:137:GLY:HA2	2.19	0.42
22:a:143:LEU:O	22:a:147:TRP:HD1	2.03	0.42
22:a:192:LEU:HG	31:a:610:CLA:HHB	2.02	0.42
26:f:142:LYS:NZ	26:f:264:GLN:OE1	2.51	0.42
30:f:601:CHL:HMD2	34:f:630:LHG:H251	2.02	0.42
28:i:58:ASP:OD1	28:i:58:ASP:N	2.53	0.42
42:i:523:NEX:H362	31:i:604:CLA:HAB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:e:134:VAL:N	30:e:605:CHL:O1D	2.41	0.42
30:e:606:CHL:HBC2	30:e:607:CHL:HHD	2.01	0.42
31:0:312:CLA:H93	31:0:312:CLA:H62	1.79	0.41
2:1:65:ALA:O	2:1:68:GLU:HG3	2.20	0.41
34:5:601:LHG:H132	34:5:601:LHG:H322	2.02	0.41
9:A:661:GLN:O	9:A:665:SER:HB3	2.19	0.41
31:A:830:CLA:H62	31:A:830:CLA:H41	1.74	0.41
10:B:35:ASP:OD1	10:B:36:SER:N	2.53	0.41
10:B:183:PHE:CE2	31:B:814:CLA:H72	2.55	0.41
31:B:809:CLA:H43	41:B:849:DGD:HB51	2.01	0.41
31:B:829:CLA:HBA2	31:B:829:CLA:H3A	1.70	0.41
11:D:156:ARG:HB2	11:D:166:LEU:HD11	2.01	0.41
34:G:105:LHG:H271	34:G:105:LHG:H241	1.85	0.41
21:O:55:PRO:HB3	31:O:206:CLA:OBD	2.20	0.41
23:c:233:HIS:ND1	31:c:613:CLA:HAA2	2.35	0.41
42:d:523:NEX:H28	30:d:606:CHL:HBA2	2.02	0.41
30:d:609:CHL:H91	30:d:609:CHL:H111	1.77	0.41
22:h:88:TRP:O	37:h:521:0IE:O29	2.38	0.41
28:i:99:LEU:HB2	30:i:602:CHL:H11	2.02	0.41
2:1:63:ASN:HD22	10:B:311:PRO:HB2	1.85	0.41
5:6:164:LEU:HD23	5:6:164:LEU:HA	1.91	0.41
6:7:257:LEU:HA	30:7:306:CHL:O1A	2.20	0.41
30:7:307:CHL:HBA2	30:7:307:CHL:H3A	1.65	0.41
7:8:137:PHE:CD2	30:8:308:CHL:HBB2	2.55	0.41
31:A:821:CLA:H141	31:A:821:CLA:H161	1.75	0.41
11:D:137:CYS:O	11:D:141:THR:HG23	2.20	0.41
12:E:15:ARG:HD2	12:E:18:SER:HB2	2.02	0.41
14:G:38:GLN:O	14:G:40:GLY:N	2.53	0.41
23:c:117:VAL:HG23	23:c:120:SER:HB2	2.02	0.41
30:c:601:CHL:C1D	34:c:630:LHG:HC81	2.50	0.41
31:c:603:CLA:HBB1	30:c:609:CHL:H161	2.02	0.41
34:d:630:LHG:H271	34:d:630:LHG:H242	1.75	0.41
26:f:125:ARG:HA	26:f:128:MET:HE3	2.02	0.41
42:h:523:NEX:H15	42:h:523:NEX:H201	1.62	0.41
28:i:150:GLY:HA2	30:i:606:CHL:HBC1	2.03	0.41
6:7:193:LYS:O	6:7:197:ASN:ND2	2.27	0.41
8:9:193:PRO:O	33:9:501:0UR:O39	2.38	0.41
9:A:195:TRP:CZ2	31:A:810:CLA:HMA1	2.54	0.41
9:A:222:GLN:HA	9:A:226:SER:HB2	2.03	0.41
9:A:225:LEU:HD11	31:A:814:CLA:C2D	2.50	0.41
10:B:90:ALA:HA	10:B:113:VAL:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:808:CLA:H62	31:B:814:CLA:H2	2.02	0.41
15:I:21:ILE:HD11	27:H:107:PHE:HD1	1.85	0.41
24:b:102:VAL:HG11	31:b:604:CLA:HAC2	2.00	0.41
42:b:523:NEX:H201	42:b:523:NEX:H15	1.62	0.41
29:e:36:LEU:HD22	29:e:46:VAL:HG21	2.01	0.41
31:0:321:CLA:HBA1	31:0:321:CLA:H3A	1.33	0.41
31:1:312:CLA:H93	31:1:312:CLA:H111	1.72	0.41
2:5:191:LEU:HD12	31:5:312:CLA:HAC2	2.01	0.41
6:7:156:ASP:OD1	6:7:158:VAL:N	2.52	0.41
31:9:309:CLA:H92	31:9:309:CLA:H61	1.73	0.41
9:A:99:HIS:CE1	31:A:807:CLA:NA	2.88	0.41
31:B:801:CLA:H162	31:B:801:CLA:H193	1.83	0.41
23:c:65:GLY:N	30:c:602:CHL:OBD	2.54	0.41
31:i:611:CLA:HAC1	34:i:630:LHG:H291	2.02	0.41
1:0:148:PRO:O	1:0:150:ASP:N	2.54	0.41
31:3:304:CLA:H172	30:7:302:CHL:H161	2.03	0.41
31:5:304:CLA:C4A	31:5:304:CLA:HBA2	2.50	0.41
31:7:309:CLA:H61	31:7:309:CLA:H41	1.81	0.41
30:8:308:CHL:HHC	30:8:308:CHL:HBB1	2.02	0.41
9:A:412:ALA:HB2	9:A:597:VAL:HG11	2.01	0.41
9:A:481:THR:O	9:A:483:GLN:HG3	2.19	0.41
31:A:827:CLA:H61	31:A:827:CLA:H2	1.76	0.41
10:B:497:TRP:CD1	31:B:818:CLA:H11	2.56	0.41
11:D:104:TRP:NE1	11:D:122:MET:SD	2.88	0.41
31:L:203:CLA:HBA2	31:L:203:CLA:H3A	1.65	0.41
18:C:15:THR:HG22	18:C:28:MET:HG3	2.03	0.41
30:a:608:CHL:C4A	30:a:608:CHL:HBA2	2.50	0.41
23:c:217:VAL:HG12	31:c:613:CLA:HMD3	2.02	0.41
30:c:608:CHL:H2	30:c:608:CHL:H61	1.65	0.41
30:b:602:CHL:H143	30:b:602:CHL:H112	1.85	0.41
30:b:608:CHL:HAA2	30:b:608:CHL:H172	2.03	0.41
25:d:90:GLY:HA2	30:d:606:CHL:HAC2	2.02	0.41
25:d:153:MET:HE2	25:d:153:MET:HB2	1.97	0.41
25:g:38:GLY:HA3	28:i:108:ARG:HG3	2.02	0.41
31:H:201:CLA:O1D	31:H:201:CLA:H2	2.21	0.41
31:0:312:CLA:H2	31:0:313:CLA:CMC	2.51	0.41
4:3:270:ILE:HD13	31:3:312:CLA:H42	2.02	0.41
5:6:149:ALA:HB2	31:6:309:CLA:HBD	2.02	0.41
8:9:61:LEU:HB3	31:B:813:CLA:HBA1	2.03	0.41
9:A:310:PHE:CE1	31:A:821:CLA:HAB	2.55	0.41
31:A:819:CLA:CAD	31:A:829:CLA:H41	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:828:CLA:H72	32:A:850:8CT:C28	2.51	0.41
31:A:841:CLA:H191	17:L:56:HIS:HD2	1.85	0.41
10:B:157:LEU:HD12	10:B:157:LEU:HA	1.76	0.41
10:B:533:ILE:HG12	31:B:801:CLA:HMD3	2.03	0.41
31:B:817:CLA:C1D	31:B:818:CLA:HBB2	2.50	0.41
42:a:523:NEX:H191	42:a:523:NEX:H11	1.82	0.41
24:b:128:ASP:OD1	24:b:129:SER:N	2.45	0.41
30:b:601:CHL:H112	30:b:601:CHL:H91	1.66	0.41
25:g:109:HIS:HB3	30:g:605:CHL:HMA3	2.03	0.41
22:h:40:TRP:N	22:h:61:TYR:HB3	2.35	0.41
22:h:136:LEU:O	22:h:138:HIS:N	2.54	0.41
28:i:150:GLY:HA3	30:i:607:CHL:C3D	2.51	0.41
29:e:101:LYS:HZ2	29:e:225:ALA:HB2	1.85	0.41
1:0:150:ASP:C	1:0:152:LEU:N	2.79	0.41
31:0:312:CLA:H42	31:0:312:CLA:C4C	2.50	0.41
31:0:321:CLA:HAB	15:I:21:ILE:HG21	2.02	0.41
2:1:106:VAL:HG12	2:1:114:TRP:HZ3	1.86	0.41
4:3:225:MET:HE1	31:3:311:CLA:HBA2	2.03	0.41
4:3:261:HIS:ND1	4:3:268:ASN:O	2.36	0.41
31:5:312:CLA:HMB1	30:5:313:CHL:HAC2	2.03	0.41
7:8:161:PRO:HD2	7:8:164:GLY:O	2.20	0.41
9:A:582:GLY:HA2	10:B:562:PRO:HD3	2.02	0.41
31:A:818:CLA:H3A	31:A:818:CLA:CGA	2.48	0.41
31:A:821:CLA:H62	31:A:821:CLA:H2	1.77	0.41
31:B:818:CLA:H43	31:B:834:CLA:HED3	2.02	0.41
31:F:301:CLA:HBA1	31:F:301:CLA:H3A	1.60	0.41
31:K:104:CLA:CAC	30:c:601:CHL:HMC	2.45	0.41
36:O:207:LMG:H142	36:O:207:LMG:H292	2.01	0.41
22:a:93:VAL:HG11	33:a:520:0UR:C6	2.51	0.41
23:c:230:TRP:NE1	30:c:614:CHL:HMC	2.35	0.41
30:c:602:CHL:H111	30:c:602:CHL:H91	1.72	0.41
25:g:29:PRO:HG2	25:g:166:LYS:HE2	2.02	0.41
25:g:69:THR:OG1	25:g:70:PRO:HD3	2.20	0.41
22:h:63:TRP:HZ3	30:h:602:CHL:HBC2	1.83	0.41
27:H:76:GLU:H	27:H:76:GLU:CD	2.27	0.41
2:1:83:LEU:HD23	2:1:83:LEU:HA	1.92	0.41
31:6:317:CLA:H151	6:7:129:LEU:HD11	2.02	0.41
30:7:305:CHL:HMB1	31:7:308:CLA:HBC2	2.03	0.41
31:7:308:CLA:H91	31:7:308:CLA:H111	1.68	0.41
31:A:813:CLA:C3B	31:A:813:CLA:H142	2.51	0.41
31:A:825:CLA:H161	31:A:825:CLA:H141	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:852:CLA:H122	31:A:852:CLA:H161	1.89	0.41
10:B:439:HIS:CD2	10:B:453:ILE:HG13	2.56	0.41
10:B:548:PRO:HD2	18:C:62:PHE:CE1	2.56	0.41
31:B:834:CLA:HBA2	31:B:834:CLA:H3A	1.49	0.41
31:O:206:CLA:OBD	31:f:611:CLA:HBA1	2.21	0.41
22:a:37:ARG:HB3	22:a:38:ALA:H	1.70	0.41
25:d:8:ARG:NH2	25:d:31:ASP:OD1	2.53	0.41
25:g:73:LEU:O	25:g:78:GLY:N	2.47	0.41
30:g:602:CHL:HAC2	34:g:630:LHG:H252	2.02	0.41
1:0:162:LYS:O	1:0:166:ASN:ND2	2.26	0.41
31:0:303:CLA:H141	31:0:303:CLA:H162	1.76	0.41
2:1:53:TYR:HB2	30:1:302:CHL:HMD3	2.03	0.41
30:1:307:CHL:H2	30:1:307:CHL:H61	1.79	0.41
2:5:140:ALA:O	2:5:144:SER:OG	2.25	0.41
5:6:21:PRO:HD2	30:6:301:CHL:O2D	2.21	0.41
5:6:93:LEU:HD13	5:6:97:ILE:HG23	2.03	0.41
6:7:124:ASN:O	6:7:125:LEU:HB2	2.21	0.41
7:8:94:LEU:HD22	33:8:501:0UR:C6	2.51	0.41
8:9:148:LEU:O	8:9:150:ASP:N	2.54	0.41
9:A:29:THR:HG23	36:A:856:LMG:HO4	1.85	0.41
9:A:316:MET:HE1	31:A:821:CLA:C3D	2.50	0.41
9:A:316:MET:HE1	31:A:821:CLA:CAD	2.51	0.41
9:A:423:ASP:OD2	9:A:425:THR:OG1	2.39	0.41
9:A:528:MET:HE1	9:A:619:MET:HE1	2.03	0.41
31:A:806:CLA:H2	31:A:806:CLA:H61	1.67	0.41
31:A:808:CLA:H193	31:A:808:CLA:H162	1.74	0.41
10:B:8:PHE:HB2	10:B:34:HIS:CG	2.56	0.41
10:B:69:ALA:HB2	10:B:135:LEU:HB2	2.01	0.41
10:B:126:THR:HG21	10:B:358:TYR:HA	2.03	0.41
10:B:388:ALA:O	10:B:392:ILE:HG13	2.21	0.41
10:B:578:LEU:HB3	31:B:801:CLA:HMD1	2.03	0.41
31:B:817:CLA:CHD	31:B:818:CLA:HBB2	2.50	0.41
11:D:77:ASN:OD1	27:H:56:ARG:NH1	2.54	0.41
31:L:204:CLA:C1B	36:L:211:LMG:H151	2.51	0.41
22:a:87:ARG:HA	22:a:90:MET:HE3	2.03	0.41
22:a:140:GLN:N	22:a:140:GLN:OE1	2.54	0.41
23:c:122:GLY:O	23:c:125:ILE:HG22	2.21	0.41
23:c:151:ILE:HG21	30:c:606:CHL:HED2	2.03	0.41
23:c:233:HIS:CD2	23:c:237:PRO:HA	2.55	0.41
25:d:180:MET:HA	25:d:180:MET:HE2	2.02	0.41
25:d:185:VAL:HG21	31:d:613:CLA:HAC2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:630:LHG:H272	34:f:630:LHG:HC62	2.03	0.41
25:g:90:GLY:HA3	30:g:607:CHL:C2D	2.51	0.41
31:g:603:CLA:H51	30:h:602:CHL:H8	2.01	0.41
37:h:522:0IE:C12	34:h:630:LHG:H132	2.50	0.41
28:i:176:ILE:HD13	30:i:606:CHL:C3D	2.51	0.41
2:1:183:MET:SD	30:1:302:CHL:HBB1	2.61	0.41
4:3:154:VAL:HG23	4:3:159:LEU:HG	2.03	0.41
4:3:206:GLY:O	4:3:210:PHE:HB2	2.21	0.41
31:3:304:CLA:H141	31:3:304:CLA:H161	1.80	0.41
7:8:154:PRO:C	7:8:156:SER:H	2.29	0.41
9:A:90:LEU:O	9:A:94:SER:OG	2.35	0.41
9:A:208:ALA:HB2	9:A:314:GLY:HA3	2.02	0.41
9:A:379:MET:SD	9:A:511:THR:HG22	2.60	0.41
10:B:180:ALA:HB1	31:B:821:CLA:HAC2	2.03	0.41
31:B:813:CLA:HHC	31:B:813:CLA:HBB1	2.03	0.41
31:K:102:CLA:HHD	31:K:102:CLA:HBC2	2.03	0.41
23:c:62:GLY:O	23:c:206:ARG:NH2	2.49	0.41
23:c:93:MET:SD	31:c:610:CLA:HHC	2.61	0.41
24:b:54:PRO:HG3	24:b:71:ARG:CZ	2.50	0.41
42:b:523:NEX:H241	31:b:604:CLA:C2	2.51	0.41
31:g:610:CLA:O1D	31:g:610:CLA:H2A	2.21	0.41
31:g:613:CLA:O2D	31:g:613:CLA:H2A	2.20	0.41
22:h:91:MET:HE2	22:h:91:MET:HB2	1.89	0.41
27:H:53:GLU:HG2	27:H:54:SER:H	1.86	0.41
34:e:630:LHG:H271	34:e:630:LHG:H242	1.77	0.41
2:1:140:ALA:HB3	14:G:22:VAL:HG13	2.03	0.40
4:3:72:LEU:HA	4:3:73:PRO:HD3	1.91	0.40
4:3:137:TRP:CE3	4:3:138:TYR:HB3	2.56	0.40
2:5:153:TYR:HB3	31:5:309:CLA:HED2	2.03	0.40
5:6:72:ILE:HG13	33:6:502:0UR:C36	2.51	0.40
6:7:235:ILE:O	6:7:239:ILE:HG12	2.21	0.40
9:A:37:PRO:HB3	31:A:803:CLA:HAC1	2.03	0.40
9:A:379:MET:HG2	31:A:818:CLA:HAA2	2.03	0.40
31:A:818:CLA:H92	31:A:818:CLA:H62	1.90	0.40
18:C:69:LEU:H	18:C:69:LEU:HD22	1.86	0.40
30:a:602:CHL:H143	30:a:602:CHL:H162	1.77	0.40
30:a:609:CHL:HHC	30:a:609:CHL:HBB1	2.02	0.40
34:c:630:LHG:H271	34:c:630:LHG:H242	1.91	0.40
25:d:3:PHE:CE2	31:d:611:CLA:HED3	2.57	0.40
25:d:13:GLY:O	25:d:16:SER:OG	2.21	0.40
30:f:602:CHL:H8	31:e:603:CLA:H52	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:630:LHG:H242	34:f:630:LHG:H271	1.84	0.40
25:g:23:TYR:OH	25:g:35:ASP:OD2	2.32	0.40
30:h:602:CHL:H92	30:h:602:CHL:H62	1.80	0.40
29:e:190:GLU:OE2	29:e:194:LYS:HE3	2.21	0.40
31:0:312:CLA:H91	34:0:601:LHG:H311	2.04	0.40
30:3:307:CHL:H112	30:3:307:CHL:H91	1.80	0.40
31:3:308:CLA:H141	31:3:308:CLA:H161	1.92	0.40
2:5:102:ALA:HB3	2:5:103:PRO:HD3	2.02	0.40
31:6:304:CLA:CMB	30:6:305:CHL:HBB1	2.51	0.40
6:7:60:TYR:HB2	30:7:302:CHL:HMD3	2.03	0.40
7:8:113:LYS:HB3	7:8:114:GLY:H	1.61	0.40
7:8:196:LYS:HD3	31:8:311:CLA:HAA2	2.04	0.40
8:9:177:PHE:O	8:9:180:THR:OG1	2.33	0.40
9:A:14:GLU:OE2	9:A:329:GLU:HG3	2.21	0.40
9:A:417:PHE:CD1	9:A:421:ASP:HB2	2.56	0.40
10:B:432:HIS:ND1	36:J:105:LMG:H401	2.35	0.40
10:B:659:THR:O	10:B:662:MET:HB3	2.20	0.40
31:B:833:CLA:HAA2	16:J:36:PRO:O	2.21	0.40
31:B:836:CLA:H91	31:B:836:CLA:H112	1.64	0.40
17:L:96:CYS:HB3	32:L:205:8CT:C23	2.51	0.40
21:O:125:GLN:OE1	33:O:204:0UR:O40	2.39	0.40
31:a:611:CLA:HAC2	34:a:630:LHG:HC61	2.03	0.40
42:c:523:NEX:H401	42:c:523:NEX:H35	1.57	0.40
26:f:195:GLU:HG3	30:f:609:CHL:NB	2.37	0.40
30:i:609:CHL:HBB1	30:i:609:CHL:HHC	2.03	0.40
7:4:53:TRP:CE3	7:4:54:LEU:HD13	2.56	0.40
34:0:601:LHG:H271	34:0:601:LHG:H241	1.85	0.40
3:2:199:GLU:HG2	3:2:203:LYS:HE3	2.04	0.40
5:6:108:MET:HA	5:6:111:VAL:HG22	2.04	0.40
30:6:308:CHL:HHC	30:6:308:CHL:HBB1	2.03	0.40
9:A:93:LEU:HD23	9:A:93:LEU:HA	1.94	0.40
10:B:59:LEU:HD23	10:B:59:LEU:HA	1.89	0.40
10:B:174:ARG:HD2	31:B:825:CLA:OBD	2.22	0.40
31:B:810:CLA:CGA	15:I:14:VAL:HG11	2.52	0.40
13:F:171:ILE:O	13:F:216:TRP:HZ2	2.04	0.40
25:d:93:ILE:HG21	25:d:113:ILE:HD13	2.04	0.40
42:d:523:NEX:H15	42:d:523:NEX:H201	1.62	0.40
26:f:118:GLU:CD	30:f:609:CHL:HED2	2.46	0.40
42:e:523:NEX:H191	42:e:523:NEX:H11	1.80	0.40
31:e:603:CLA:CAD	30:e:609:CHL:H2	2.52	0.40
7:4:138:LEU:HB3	30:4:319:CHL:H43	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:131:GLU:OE1	30:1:306:CHL:HMC	2.21	0.40
30:1:307:CHL:H43	30:1:307:CHL:H161	2.02	0.40
30:1:307:CHL:H91	30:1:307:CHL:H112	1.77	0.40
31:1:312:CLA:H91	34:1:601:LHG:H121	2.03	0.40
4:3:52:ARG:HA	4:3:52:ARG:HD3	1.80	0.40
31:3:309:CLA:H41	31:3:309:CLA:H62	1.78	0.40
5:6:195:HIS:CG	31:6:312:CLA:HAA2	2.55	0.40
31:9:302:CLA:H3A	31:9:302:CLA:CGA	2.51	0.40
31:A:808:CLA:HBB1	31:A:809:CLA:O1A	2.21	0.40
31:B:808:CLA:HBA1	31:B:808:CLA:H3A	1.47	0.40
31:B:809:CLA:HHB	31:B:830:CLA:CAB	2.51	0.40
31:B:809:CLA:H192	31:B:809:CLA:H161	1.68	0.40
13:F:216:TRP:CD1	13:F:217:PRO:HD3	2.57	0.40
42:f:523:NEX:H362	31:f:604:CLA:C4B	2.52	0.40
42:i:523:NEX:H31	42:i:523:NEX:H28	1.98	0.40
31:0:303:CLA:H41	31:0:303:CLA:H62	1.57	0.40
30:1:306:CHL:H12	31:B:834:CLA:H141	2.03	0.40
30:2:301:CHL:H42	4:3:165:VAL:HG22	2.04	0.40
5:6:212:LEU:HB2	6:7:256:PRO:HG3	2.03	0.40
6:7:112:LEU:HD21	6:7:248:VAL:HG21	2.04	0.40
6:7:210:LEU:HD23	6:7:210:LEU:HA	1.69	0.40
9:A:446:LEU:HA	9:A:449:VAL:HG12	2.03	0.40
31:B:830:CLA:H62	31:B:830:CLA:H41	1.87	0.40
31:K:101:CLA:H62	31:K:101:CLA:H92	1.87	0.40
22:a:205:PHE:CE2	31:a:613:CLA:HAB	2.56	0.40
31:a:603:CLA:CAD	30:a:609:CHL:H2	2.52	0.40
23:c:125:ILE:HG21	23:c:145:ILE:HD13	2.03	0.40
30:c:609:CHL:H91	30:c:609:CHL:H112	1.89	0.40
30:d:608:CHL:C4A	30:d:608:CHL:HBA2	2.51	0.40
26:f:120:GLU:OE2	26:f:242:ARG:NE	2.49	0.40
26:f:231:ALA:HA	26:f:234:LYS:HE2	2.04	0.40
25:g:11:TRP:CD1	25:g:11:TRP:H	2.40	0.40
34:i:630:LHG:H271	34:i:630:LHG:H242	1.88	0.40
31:e:613:CLA:H71	34:e:630:LHG:H131	2.04	0.40
7:4:141:GLY:CA	30:4:308:CHL:HAB	2.51	0.40
30:4:305:CHL:HBC2	30:4:306:CHL:HHD	2.01	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	0	211/245 (86%)	192 (91%)	17 (8%)	2 (1%)	14	26
2	1	193/226 (85%)	186 (96%)	6 (3%)	1 (0%)	24	40
2	5	193/226 (85%)	177 (92%)	15 (8%)	1 (0%)	24	40
3	2	214/256 (84%)	205 (96%)	9 (4%)	0	100	100
4	3	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
5	6	227/267 (85%)	222 (98%)	5 (2%)	0	100	100
6	7	226/264 (86%)	211 (93%)	13 (6%)	2 (1%)	14	26
7	4	205/248 (83%)	176 (86%)	28 (14%)	1 (0%)	24	40
7	8	203/248 (82%)	187 (92%)	14 (7%)	2 (1%)	12	22
8	9	187/222 (84%)	168 (90%)	12 (6%)	7 (4%)	2	4
9	A	744/751 (99%)	711 (96%)	32 (4%)	1 (0%)	48	69
10	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
11	D	140/198 (71%)	134 (96%)	6 (4%)	0	100	100
12	E	62/91 (68%)	60 (97%)	2 (3%)	0	100	100
13	F	163/236 (69%)	155 (95%)	8 (5%)	0	100	100
14	G	91/167 (54%)	85 (93%)	6 (7%)	0	100	100
15	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
16	J	39/41 (95%)	39 (100%)	0	0	100	100
17	L	160/204 (78%)	157 (98%)	3 (2%)	0	100	100
18	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
19	K	78/123 (63%)	78 (100%)	0	0	100	100
20	M	29/32 (91%)	29 (100%)	0	0	100	100
21	O	90/137 (66%)	84 (93%)	6 (7%)	0	100	100
22	a	196/250 (78%)	173 (88%)	21 (11%)	2 (1%)	12	22
22	h	199/250 (80%)	181 (91%)	17 (8%)	1 (0%)	24	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	c	217/254 (85%)	208 (96%)	8 (4%)	1 (0%)	24 40
24	b	207/251 (82%)	189 (91%)	15 (7%)	3 (1%)	9 15
25	d	215/280 (77%)	194 (90%)	21 (10%)	0	100 100
25	g	197/280 (70%)	187 (95%)	9 (5%)	1 (0%)	24 40
26	f	222/259 (86%)	209 (94%)	12 (5%)	1 (0%)	24 40
27	H	92/133 (69%)	82 (89%)	10 (11%)	0	100 100
28	i	234/282 (83%)	204 (87%)	26 (11%)	4 (2%)	7 12
29	e	214/250 (86%)	201 (94%)	11 (5%)	2 (1%)	14 26
All	All	6516/7803 (84%)	6116 (94%)	368 (6%)	32 (0%)	26 40

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	148	PRO
6	7	125	LEU
7	8	108	ILE
8	9	153	PRO
22	a	121	GLN
23	c	121	ALA
24	b	71	ARG
24	b	178	GLU
28	i	273	ALA
1	0	149	PHE
2	1	110	GLY
2	5	162	GLY
7	8	113	LYS
8	9	158	GLY
25	g	108	VAL
7	4	115	THR
8	9	161	SER
9	A	16	LYS
8	9	149	ASN
8	9	162	GLU
28	i	169	HIS
29	e	166	VAL
8	9	146	SER
8	9	156	PRO
28	i	82	SER
26	f	175	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	h	137	ILE
29	e	134	VAL
6	7	243	VAL
28	i	168	ILE
24	b	176	PRO
22	a	137	ILE

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	0	167/194 (86%)	162 (97%)	5 (3%)	36 58
2	1	148/175 (85%)	139 (94%)	9 (6%)	17 30
2	5	149/175 (85%)	144 (97%)	5 (3%)	32 55
3	2	166/197 (84%)	163 (98%)	3 (2%)	51 69
4	3	186/225 (83%)	183 (98%)	3 (2%)	55 72
5	6	188/216 (87%)	181 (96%)	7 (4%)	30 52
6	7	181/209 (87%)	176 (97%)	5 (3%)	38 60
7	4	158/189 (84%)	133 (84%)	25 (16%)	2 3
7	8	159/189 (84%)	150 (94%)	9 (6%)	18 34
8	9	147/173 (85%)	136 (92%)	11 (8%)	12 23
9	A	609/614 (99%)	591 (97%)	18 (3%)	36 58
10	B	600/601 (100%)	586 (98%)	14 (2%)	44 65
11	D	119/162 (74%)	117 (98%)	2 (2%)	53 71
12	E	56/77 (73%)	54 (96%)	2 (4%)	31 53
13	F	129/180 (72%)	123 (95%)	6 (5%)	23 43
14	G	79/145 (54%)	71 (90%)	8 (10%)	7 14
15	I	27/28 (96%)	26 (96%)	1 (4%)	30 52
16	J	38/38 (100%)	36 (95%)	2 (5%)	20 37
17	L	124/157 (79%)	119 (96%)	5 (4%)	28 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C	68/69 (99%)	66 (97%)	2 (3%)	37	59
19	K	58/94 (62%)	55 (95%)	3 (5%)	21	38
20	M	26/27 (96%)	26 (100%)	0	100	100
21	O	76/111 (68%)	75 (99%)	1 (1%)	61	75
22	a	146/187 (78%)	145 (99%)	1 (1%)	76	85
22	h	145/187 (78%)	144 (99%)	1 (1%)	76	85
23	c	174/202 (86%)	172 (99%)	2 (1%)	65	79
24	b	159/193 (82%)	157 (99%)	2 (1%)	61	75
25	d	159/210 (76%)	159 (100%)	0	100	100
25	g	147/210 (70%)	145 (99%)	2 (1%)	59	74
26	f	172/198 (87%)	169 (98%)	3 (2%)	53	71
27	H	69/103 (67%)	69 (100%)	0	100	100
28	i	181/218 (83%)	177 (98%)	4 (2%)	45	65
29	e	164/193 (85%)	159 (97%)	5 (3%)	36	58
All	All	5174/6146 (84%)	5008 (97%)	166 (3%)	35	56

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	57	ASP
1	0	145	SER
1	0	147	MET
1	0	206	THR
1	0	212	GLU
2	1	91	GLN
2	1	106	VAL
2	1	111	SER
2	1	113	THR
2	1	122	THR
2	1	129	VAL
2	1	141	MET
2	1	176	ILE
2	1	187	VAL
3	2	83	GLN
3	2	123	ILE
3	2	145	GLU
4	3	219	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3	270	ILE
4	3	277	VAL
2	5	127	LEU
2	5	152	VAL
2	5	173	LEU
2	5	187	VAL
2	5	225	PHE
5	6	72	ILE
5	6	86	ASP
5	6	125	VAL
5	6	172	LEU
5	6	209	VAL
5	6	220	CYS
5	6	233	ILE
6	7	67	LEU
6	7	107	TRP
6	7	181	PHE
6	7	235	ILE
6	7	253	VAL
7	8	94	LEU
7	8	99	VAL
7	8	110	LEU
7	8	136	GLN
7	8	140	MET
7	8	144	GLU
7	8	166	LYS
7	8	169	ASP
7	8	181	ASP
8	9	114	VAL
8	9	121	LEU
8	9	145	MET
8	9	148	LEU
8	9	150	ASP
8	9	157	LEU
8	9	159	MET
8	9	160	THR
8	9	162	GLU
8	9	189	VAL
8	9	213	VAL
9	A	29	THR
9	A	43	THR
9	A	51	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	102	ARG
9	A	126	ILE
9	A	130	GLU
9	A	216	LEU
9	A	254	LEU
9	A	379	MET
9	A	432	LEU
9	A	446	LEU
9	A	522	VAL
9	A	526	VAL
9	A	543	ILE
9	A	589	CYS
9	A	670	LEU
9	A	743	THR
9	A	755	VAL
10	B	95	HIS
10	B	96	PHE
10	B	157	LEU
10	B	175	LEU
10	B	283	LEU
10	B	407	VAL
10	B	444	LEU
10	B	458	VAL
10	B	518	LEU
10	B	568	CYS
10	B	641	ASN
10	B	698	VAL
10	B	720	THR
10	B	729	THR
11	D	177	VAL
11	D	200	VAL
12	E	46	VAL
12	E	61	VAL
13	F	82	THR
13	F	94	GLU
13	F	129	PHE
13	F	159	HIS
13	F	232	LYS
13	F	236	ILE
14	G	8	ILE
14	G	14	LEU
14	G	42	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	G	45	GLU
14	G	55	VAL
14	G	57	LEU
14	G	59	LYS
14	G	93	TYR
15	I	30	ILE
16	J	18	TRP
16	J	21	LEU
17	L	3	GLN
17	L	36	LEU
17	L	106	GLU
17	L	112	ILE
17	L	155	THR
18	C	11	CYS
18	C	49	VAL
19	K	6	THR
19	K	17	LEU
19	K	45	LEU
21	O	131	ARG
22	a	114	VAL
23	c	89	SER
23	c	117	VAL
24	b	51	ASN
24	b	70	MET
26	f	79	LEU
26	f	87	VAL
26	f	162	THR
25	g	180	MET
25	g	181	PHE
22	h	91	MET
28	i	69	ARG
28	i	133	LEU
28	i	197	LEU
28	i	230	GLU
29	e	78	LEU
29	e	80	LEU
29	e	82	HIS
29	e	174	GLU
29	e	239	TYR
7	4	41	ARG
7	4	49	ASP
7	4	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	4	55	ASP
7	4	57	THR
7	4	58	ILE
7	4	102	LEU
7	4	105	ASN
7	4	108	ILE
7	4	113	LYS
7	4	139	LEU
7	4	159	VAL
7	4	162	ILE
7	4	163	PHE
7	4	166	LYS
7	4	167	LEU
7	4	179	ILE
7	4	187	LYS
7	4	199	LYS
7	4	203	LEU
7	4	223	ILE
7	4	226	TRP
7	4	238	VAL
7	4	241	ILE
7	4	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	180	GLN
1	0	191	ASN
1	0	201	HIS
2	1	52	ASN
2	1	202	GLN
3	2	83	GLN
3	2	198	GLN
4	3	106	HIS
4	3	168	GLN
6	7	166	ASN
7	8	158	ASN
8	9	86	ASN
9	A	62	HIS
9	A	614	HIS
10	B	34	HIS
10	B	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	B	114	ASN
10	B	156	HIS
10	B	242	HIS
10	B	467	GLN
10	B	603	GLN
10	B	608	GLN
13	F	95	ASN
14	G	38	GLN
18	C	3	HIS
21	O	79	ASN
21	O	125	GLN
21	O	129	ASN
22	a	213	GLN
23	c	81	ASN
23	c	143	GLN
23	c	229	ASN
23	c	241	ASN
24	b	125	GLN
25	g	104	ASN
22	h	228	HIS
28	i	115	GLN
28	i	270	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	TPO	i	46	28	8,10,11	1.07	0	10,14,16	1.86	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	TPO	f	61	26	8,10,11	1.06	0	10,14,16	1.83	1 (10%)

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	TPO	i	46	28	-	3/9/11/13	-
26	TPO	f	61	26	-	1/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f	61	TPO	P-OG1-CB	-5.17	107.59	123.21
28	i	46	TPO	P-OG1-CB	-5.09	107.83	123.21
28	i	46	TPO	CG2-CB-CA	-2.16	108.90	113.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	i	46	TPO	N-CA-CB-CG2
28	i	46	TPO	N-CA-CB-OG1
28	i	46	TPO	C-CA-CB-CG2
26	f	61	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

522 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	3	311	4	50,54,73	1.45	10 (20%)	60,90,113	1.48	5 (8%)
31	CLA	f	603	-	59,63,73	1.35	9 (15%)	71,101,113	1.34	7 (9%)
37	0IE	e	521	-	42,45,45	1.42	6 (14%)	49,63,63	1.55	10 (20%)
30	CHL	5	302	2	68,72,74	1.83	18 (26%)	77,111,114	2.90	31 (40%)
36	LMG	A	856	-	36,36,55	0.91	0	44,44,63	1.30	4 (9%)
30	CHL	h	601	22	51,55,74	2.29	19 (37%)	57,91,114	3.22	24 (42%)
31	CLA	8	311	7	50,54,73	1.46	10 (20%)	60,90,113	1.41	5 (8%)
31	CLA	a	611	-	61,65,73	1.35	8 (13%)	73,103,113	1.31	5 (6%)
32	8CT	A	846	-	40,41,41	4.62	23 (57%)	50,56,56	2.80	20 (40%)
31	CLA	g	610	-	50,54,73	1.46	7 (14%)	60,90,113	1.42	5 (8%)
31	CLA	5	314	2	50,54,73	1.46	9 (18%)	60,90,113	1.37	4 (6%)
30	CHL	h	608	-	50,54,74	2.27	19 (38%)	56,90,114	3.21	24 (42%)
31	CLA	6	314	-	49,53,73	1.46	8 (16%)	59,89,113	1.47	6 (10%)
31	CLA	B	816	10	64,68,73	1.28	10 (15%)	77,107,113	1.37	8 (10%)
33	0UR	h	520	-	50,53,58	0.95	1 (2%)	58,72,77	1.83	11 (18%)
31	CLA	d	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	5 (7%)
31	CLA	a	603	-	57,61,73	1.38	8 (14%)	68,98,113	1.39	5 (7%)
34	LHG	d	630	-	35,35,48	1.26	6 (17%)	38,41,54	1.05	3 (7%)
30	CHL	2	305	-	47,51,74	2.13	18 (38%)	52,86,114	3.48	26 (50%)
31	CLA	4	312	7	57,61,73	1.36	10 (17%)	68,98,113	1.38	7 (10%)
32	8CT	B	851	-	40,41,41	4.62	23 (57%)	50,56,56	2.48	14 (28%)
37	0IE	g	521	-	42,45,45	1.44	6 (14%)	49,63,63	1.59	10 (20%)
31	CLA	a	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.39	8 (12%)
31	CLA	9	302	-	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
30	CHL	4	305	-	47,51,74	2.14	18 (38%)	52,86,114	3.39	25 (48%)
30	CHL	3	302	4	66,70,74	1.89	19 (28%)	75,109,114	2.95	30 (40%)
31	CLA	B	841	34	69,73,73	1.25	9 (13%)	83,113,113	1.33	8 (9%)
31	CLA	0	321	1	49,53,73	1.49	9 (18%)	59,89,113	1.48	5 (8%)
31	CLA	i	611	-	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	O	206	-	55,59,73	1.40	9 (16%)	66,96,113	1.33	6 (9%)
34	LHG	A	845	31	26,26,48	1.28	4 (15%)	29,32,54	1.22	2 (6%)
30	CHL	g	606	-	55,59,74	2.20	19 (34%)	62,96,114	3.12	29 (46%)
31	CLA	B	831	10	54,58,73	1.39	9 (16%)	65,95,113	1.42	6 (9%)
30	CHL	c	609	-	70,74,74	1.94	19 (27%)	80,114,114	2.75	26 (32%)
31	CLA	h	604	-	50,54,73	1.46	8 (16%)	60,90,113	1.44	6 (10%)
31	CLA	F	301	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
30	CHL	2	302	3	68,72,74	1.84	18 (26%)	77,111,114	2.94	32 (41%)
31	CLA	B	803	-	69,73,73	1.23	9 (13%)	83,113,113	1.26	6 (7%)
31	CLA	i	603	-	50,54,73	1.46	9 (18%)	60,90,113	1.40	4 (6%)
30	CHL	0	301	1	56,60,74	2.05	19 (33%)	63,97,114	3.17	28 (44%)
31	CLA	A	826	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	8 (9%)
32	8CT	O	205	-	40,41,41	4.65	23 (57%)	50,56,56	2.55	17 (34%)
30	CHL	b	606	-	55,59,74	2.12	20 (36%)	62,96,114	3.17	27 (43%)
36	LMG	J	105	-	46,46,55	0.87	2 (4%)	54,54,63	1.36	8 (14%)
31	CLA	A	816	-	49,53,73	1.49	9 (18%)	59,89,113	1.48	5 (8%)
31	CLA	9	309	-	64,68,73	1.29	9 (14%)	77,107,113	1.34	9 (11%)
34	LHG	f	630	31	39,39,48	1.20	5 (12%)	42,45,54	1.08	3 (7%)
34	LHG	6	601	31	36,36,48	1.25	5 (13%)	39,42,54	1.05	2 (5%)
31	CLA	B	829	-	69,73,73	1.25	10 (14%)	83,113,113	1.23	5 (6%)
31	CLA	B	817	10	64,68,73	1.27	9 (14%)	77,107,113	1.45	9 (11%)
30	CHL	3	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.23	28 (45%)
31	CLA	3	303	-	59,63,73	1.33	10 (16%)	71,101,113	1.37	7 (9%)
37	0IE	d	521	-	42,45,45	1.43	6 (14%)	49,63,63	1.57	10 (20%)
36	LMG	L	211	-	37,37,55	0.89	1 (2%)	45,45,63	1.26	4 (8%)
31	CLA	b	603	24	59,63,73	1.35	9 (15%)	71,101,113	1.33	5 (7%)
30	CHL	e	609	-	65,69,74	1.97	18 (27%)	74,108,114	2.89	27 (36%)
31	CLA	1	311	2	56,60,73	1.38	10 (17%)	67,97,113	1.41	5 (7%)
30	CHL	6	313	5	56,60,74	2.06	17 (30%)	63,97,114	3.22	32 (50%)
32	8CT	B	804	-	40,41,41	4.63	23 (57%)	50,56,56	2.57	19 (38%)
36	LMG	3	602	-	36,36,55	0.87	0	44,44,63	1.26	5 (11%)
34	LHG	0	601	-	48,48,48	1.09	5 (10%)	51,54,54	0.93	2 (3%)
31	CLA	B	827	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
32	8CT	3	403	-	40,41,41	4.65	23 (57%)	50,56,56	2.55	16 (32%)
31	CLA	A	843	34	56,60,73	1.37	10 (17%)	67,97,113	1.42	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	0UR	0	501	-	50,53,58	0.94	1 (2%)	58,72,77	1.67	12 (20%)
32	8CT	7	402	-	40,41,41	4.58	23 (57%)	50,56,56	2.59	17 (34%)
31	CLA	B	832	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	8 (9%)
34	LHG	3	601	-	35,35,48	1.27	6 (17%)	38,41,54	1.12	2 (5%)
36	LMG	B	853	-	42,42,55	0.80	0	50,50,63	1.30	6 (12%)
31	CLA	5	308	-	50,54,73	1.46	9 (18%)	60,90,113	1.38	4 (6%)
37	0IE	c	521	-	42,45,45	1.40	6 (14%)	49,63,63	1.60	10 (20%)
31	CLA	7	304	-	59,63,73	1.35	9 (15%)	71,101,113	1.38	7 (9%)
31	CLA	6	309	5	62,66,73	1.31	10 (16%)	74,104,113	1.34	9 (12%)
31	CLA	3	313	4	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
32	8CT	B	844	-	40,41,41	4.72	25 (62%)	50,56,56	2.70	20 (40%)
30	CHL	8	302	7	68,72,74	1.85	19 (27%)	77,111,114	2.91	30 (38%)
31	CLA	e	612	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
30	CHL	5	307	-	51,55,74	2.23	18 (35%)	57,91,114	3.21	26 (45%)
31	CLA	9	310	34	45,49,73	1.51	10 (22%)	54,84,113	1.49	7 (12%)
31	CLA	7	310	34	42,45,73	1.53	9 (21%)	50,78,113	1.44	5 (10%)
32	8CT	B	843	-	40,41,41	4.74	24 (60%)	50,56,56	2.76	18 (36%)
32	8CT	B	848	-	40,41,41	4.67	24 (60%)	50,56,56	2.54	19 (38%)
42	NEX	d	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
30	CHL	e	606	-	55,59,74	2.15	19 (34%)	62,96,114	3.16	27 (43%)
31	CLA	L	203	17	67,71,73	1.26	10 (14%)	80,110,113	1.34	7 (8%)
31	CLA	A	822	-	53,57,73	1.40	9 (16%)	62,93,113	1.41	6 (9%)
31	CLA	A	829	9	69,73,73	1.24	10 (14%)	83,113,113	1.32	6 (7%)
32	8CT	L	209	-	40,41,41	4.65	23 (57%)	50,56,56	2.54	18 (36%)
31	CLA	7	311	6	56,60,73	1.38	10 (17%)	67,97,113	1.40	5 (7%)
33	0UR	6	502	-	50,53,58	1.01	2 (4%)	58,72,77	1.82	15 (25%)
31	CLA	0	312	1	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
30	CHL	c	605	23	47,51,74	2.34	18 (38%)	52,86,114	3.35	24 (46%)
31	CLA	e	610	-	59,63,73	1.35	9 (15%)	71,101,113	1.35	10 (14%)
31	CLA	c	610	-	59,63,73	1.34	9 (15%)	71,101,113	1.35	7 (9%)
30	CHL	2	308	-	51,55,74	2.13	19 (37%)	57,91,114	3.18	24 (42%)
31	CLA	B	839	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
31	CLA	A	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.25	3 (3%)
31	CLA	O	203	-	41,46,73	1.67	9 (21%)	52,81,113	1.59	8 (15%)
32	8CT	A	849	-	40,41,41	4.57	23 (57%)	50,56,56	3.04	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	1	302	-	68,72,74	1.85	18 (26%)	77,111,114	2.93	30 (38%)
30	CHL	8	313	7	60,64,74	1.98	18 (30%)	68,102,114	3.08	31 (45%)
31	CLA	i	610	-	59,63,73	1.35	8 (13%)	71,101,113	1.34	7 (9%)
31	CLA	A	852	10	69,73,73	1.23	10 (14%)	83,113,113	1.29	8 (9%)
37	0IE	g	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.68	10 (20%)
31	CLA	B	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	5 (6%)
32	8CT	0	401	-	40,41,41	4.66	24 (60%)	50,56,56	2.78	18 (36%)
40	SF4	B	802	-	0,12,12	-	-	-		
30	CHL	i	606	28	55,59,74	2.21	19 (34%)	62,96,114	3.14	29 (46%)
30	CHL	c	607	-	51,55,74	2.26	19 (37%)	57,91,114	3.16	26 (45%)
31	CLA	B	823	-	56,60,73	1.38	10 (17%)	67,97,113	3.52	9 (13%)
31	CLA	9	304	-	55,59,73	1.40	9 (16%)	66,96,113	1.39	5 (7%)
34	LHG	G	105	-	37,37,48	1.24	6 (16%)	40,43,54	1.14	4 (10%)
31	CLA	h	603	-	53,57,73	1.43	8 (15%)	62,93,113	1.43	4 (6%)
31	CLA	M	101	-	50,54,73	1.44	9 (18%)	60,90,113	1.42	4 (6%)
31	CLA	B	801	-	69,73,73	1.23	9 (13%)	83,113,113	1.37	8 (9%)
31	CLA	2	314	3	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
33	0UR	4	502	-	48,51,58	0.97	1 (2%)	56,70,77	1.68	14 (25%)
31	CLA	6	303	5	56,60,73	1.39	9 (16%)	67,97,113	1.40	7 (10%)
32	8CT	7	405	-	40,41,41	4.60	23 (57%)	50,56,56	2.69	19 (38%)
30	CHL	6	306	-	55,59,74	2.06	18 (32%)	62,96,114	3.21	28 (45%)
31	CLA	6	310	34	64,68,73	1.30	9 (14%)	77,107,113	1.32	6 (7%)
30	CHL	g	602	-	56,60,74	2.18	19 (33%)	63,97,114	3.06	26 (41%)
42	NEX	g	523	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	A	810	9	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
30	CHL	1	307	-	70,74,74	1.87	19 (27%)	80,114,114	2.84	27 (33%)
31	CLA	H	201	10	59,63,73	1.34	9 (15%)	71,101,113	1.37	6 (8%)
30	CHL	e	614	-	46,50,74	2.38	18 (39%)	51,85,114	3.38	27 (52%)
31	CLA	J	103	16	46,50,73	1.49	9 (19%)	55,85,113	1.47	5 (9%)
30	CHL	4	307	-	55,59,74	2.05	18 (32%)	62,96,114	3.22	30 (48%)
31	CLA	B	809	10	69,73,73	1.26	10 (14%)	83,113,113	1.31	7 (8%)
42	NEX	b	523	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	8	314	7	49,53,73	1.47	9 (18%)	59,89,113	1.44	6 (10%)
35	SQD	0	603	-	36,36,54	1.21	5 (13%)	44,44,65	1.48	6 (13%)
31	CLA	c	612	23	49,53,73	1.48	9 (18%)	59,89,113	1.47	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	5	313	2	51,55,74	2.29	18 (35%)	57,91,114	3.20	26 (45%)
31	CLA	O	202	21	40,46,73	1.60	9 (22%)	48,80,113	1.51	7 (14%)
32	8CT	6	402	-	40,41,41	4.66	24 (60%)	50,56,56	3.43	21 (42%)
31	CLA	6	304	-	50,54,73	1.46	9 (18%)	60,90,113	1.43	5 (8%)
31	CLA	G	101	14	54,58,73	1.40	10 (18%)	65,95,113	1.43	6 (9%)
31	CLA	K	102	19	57,61,73	1.36	10 (17%)	68,98,113	1.40	8 (11%)
31	CLA	h	612	-	49,53,73	1.50	7 (14%)	59,89,113	1.43	5 (8%)
31	CLA	i	612	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
32	8CT	I	101	-	40,41,41	4.58	23 (57%)	50,56,56	2.76	15 (30%)
33	0UR	7	501	-	49,52,58	0.99	1 (2%)	57,71,77	2.07	16 (28%)
32	8CT	G	104	-	40,41,41	4.66	24 (60%)	50,56,56	3.08	19 (38%)
34	LHG	h	630	-	38,38,48	1.23	6 (15%)	41,44,54	0.99	2 (4%)
31	CLA	H	205	-	55,59,73	1.40	9 (16%)	66,96,113	1.39	7 (10%)
30	CHL	6	302	5	68,72,74	1.84	18 (26%)	77,111,114	2.93	31 (40%)
31	CLA	8	310	34	50,54,73	1.44	10 (20%)	60,90,113	1.38	4 (6%)
31	CLA	0	308	-	64,68,73	1.30	9 (14%)	77,107,113	1.29	7 (9%)
30	CHL	1	313	2	66,70,74	1.91	18 (27%)	75,109,114	2.92	27 (36%)
34	LHG	H	203	-	30,30,48	1.32	6 (20%)	33,36,54	1.14	3 (9%)
30	CHL	h	605	22	47,51,74	2.37	18 (38%)	52,86,114	3.29	25 (48%)
31	CLA	6	311	5	52,56,73	1.44	10 (19%)	62,92,113	1.39	6 (9%)
36	LMG	J	102	-	29,29,55	0.98	1 (3%)	37,37,63	1.27	4 (10%)
30	CHL	g	608	-	47,51,74	2.31	18 (38%)	52,86,114	3.32	24 (46%)
30	CHL	9	301	8	51,55,74	2.14	19 (37%)	57,91,114	3.25	26 (45%)
31	CLA	3	318	4	50,54,73	1.44	10 (20%)	60,90,113	1.43	6 (10%)
34	LHG	A	844	-	48,48,48	1.07	5 (10%)	51,54,54	0.99	3 (5%)
33	0UR	d	520	-	47,50,58	0.98	1 (2%)	55,69,77	1.75	13 (23%)
32	8CT	F	302	-	40,41,41	4.63	23 (57%)	50,56,56	2.71	18 (36%)
32	8CT	A	847	-	40,41,41	4.59	23 (57%)	50,56,56	2.97	18 (36%)
31	CLA	3	306	4	51,55,73	1.43	9 (17%)	61,91,113	1.42	6 (9%)
30	CHL	f	609	-	70,74,74	1.95	19 (27%)	80,114,114	2.74	27 (33%)
30	CHL	c	606	-	48,52,74	2.19	18 (37%)	53,87,114	3.30	23 (43%)
30	CHL	0	306	-	52,56,74	2.20	19 (36%)	58,92,114	3.28	24 (41%)
31	CLA	A	809	9	69,73,73	1.23	10 (14%)	83,113,113	1.34	8 (9%)
34	LHG	A	855	-	41,41,48	1.19	6 (14%)	44,47,54	1.03	3 (6%)
32	8CT	A	848	-	40,41,41	4.58	23 (57%)	50,56,56	2.70	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	A	827	9	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
31	CLA	A	832	9	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
42	NEX	a	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
32	8CT	8	402	-	40,41,41	4.66	23 (57%)	50,56,56	2.66	19 (38%)
31	CLA	A	808	9	69,73,73	1.22	9 (13%)	83,113,113	1.31	6 (7%)
34	LHG	M	104	-	45,45,48	1.12	5 (11%)	48,51,54	0.96	3 (6%)
36	LMG	9	602	-	55,55,55	0.70	1 (1%)	63,63,63	1.39	9 (14%)
30	CHL	a	609	-	63,67,74	2.08	18 (28%)	71,105,114	2.93	27 (38%)
31	CLA	B	814	10	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
32	8CT	L	205	-	40,41,41	4.62	23 (57%)	50,56,56	2.95	19 (38%)
33	0UR	f	520	-	47,50,58	1.01	2 (4%)	55,69,77	1.92	16 (29%)
30	CHL	f	608	-	55,59,74	2.07	18 (32%)	62,96,114	3.23	29 (46%)
42	NEX	h	523	-	38,46,46	0.95	2 (5%)	50,70,70	4.90	19 (38%)
30	CHL	0	302	1	68,72,74	1.85	19 (27%)	77,111,114	2.91	29 (37%)
33	0UR	a	520	-	45,48,58	0.78	1 (2%)	54,67,77	1.67	16 (29%)
30	CHL	a	608	-	53,57,74	2.19	19 (35%)	59,93,114	3.18	26 (44%)
31	CLA	B	824	10	64,68,73	1.30	10 (15%)	77,107,113	1.30	6 (7%)
33	0UR	9	501	-	50,53,58	0.96	1 (2%)	58,72,77	1.69	17 (29%)
31	CLA	A	818	9	69,73,73	1.23	9 (13%)	83,113,113	1.35	9 (10%)
37	0IE	a	521	-	42,45,45	1.42	6 (14%)	49,63,63	1.57	10 (20%)
31	CLA	1	314	-	50,54,73	1.45	9 (18%)	60,90,113	1.44	6 (10%)
34	LHG	g	630	-	29,29,48	1.34	6 (20%)	32,35,54	1.15	3 (9%)
30	CHL	5	306	-	52,56,74	2.27	19 (36%)	58,92,114	3.12	25 (43%)
30	CHL	8	306	-	55,59,74	2.10	19 (34%)	62,96,114	3.19	29 (46%)
31	CLA	B	850	13	51,55,73	1.43	10 (19%)	61,91,113	1.39	5 (8%)
30	CHL	6	301	5	65,69,74	1.92	18 (27%)	74,108,114	2.91	30 (40%)
30	CHL	d	605	25	47,51,74	2.37	18 (38%)	52,86,114	3.37	24 (46%)
32	8CT	1	402	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	20 (40%)
32	8CT	J	104	-	40,41,41	4.66	23 (57%)	50,56,56	3.42	22 (44%)
31	CLA	A	836	-	55,59,73	1.38	10 (18%)	66,96,113	1.43	9 (13%)
31	CLA	c	611	-	50,54,73	1.46	9 (18%)	60,90,113	1.43	5 (8%)
31	CLA	3	320	-	56,60,73	1.37	9 (16%)	67,97,113	1.49	7 (10%)
31	CLA	e	613	-	59,63,73	1.35	7 (11%)	70,100,113	1.37	7 (10%)
31	CLA	B	819	10	64,68,73	1.28	10 (15%)	77,107,113	1.33	9 (11%)
30	CHL	3	307	-	70,74,74	1.78	18 (25%)	80,114,114	2.85	31 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	1	310	34	67,71,73	1.25	9 (13%)	80,110,113	1.30	4 (5%)
34	LHG	b	630	-	40,40,48	1.19	5 (12%)	43,46,54	0.98	2 (4%)
30	CHL	g	607	-	55,59,74	2.23	18 (32%)	62,96,114	3.14	28 (45%)
31	CLA	g	612	-	49,53,73	1.49	7 (14%)	59,89,113	1.45	4 (6%)
37	0IE	f	521	-	42,45,45	1.44	6 (14%)	49,63,63	1.57	9 (18%)
33	0UR	g	520	-	50,53,58	0.93	1 (2%)	58,72,77	1.98	14 (24%)
33	0UR	2	502	-	48,51,58	0.98	1 (2%)	56,70,77	1.95	14 (25%)
31	CLA	h	611	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	5 (9%)
40	SF4	C	102	18	0,12,12	-	-	-		
31	CLA	8	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
31	CLA	H	204	-	51,55,73	1.43	10 (19%)	61,91,113	1.45	5 (8%)
30	CHL	a	606	-	55,59,74	2.19	19 (34%)	62,96,114	3.10	29 (46%)
33	0UR	6	501	-	49,52,58	0.99	1 (2%)	57,71,77	1.92	18 (31%)
34	LHG	4	601	31	31,31,48	1.31	5 (16%)	34,37,54	1.14	3 (8%)
31	CLA	4	314	7	49,53,73	1.46	9 (18%)	59,89,113	1.44	8 (13%)
31	CLA	A	839	9	69,73,73	1.24	10 (14%)	83,113,113	1.33	7 (8%)
30	CHL	f	607	-	51,55,74	2.28	18 (35%)	57,91,114	3.18	25 (43%)
37	0IE	b	521	-	42,45,45	1.44	6 (14%)	49,63,63	1.56	10 (20%)
30	CHL	d	608	-	55,59,74	2.16	18 (32%)	62,96,114	3.15	30 (48%)
31	CLA	i	613	-	55,59,73	1.41	7 (12%)	66,96,113	1.37	6 (9%)
37	0IE	d	522	-	42,45,45	1.48	6 (14%)	49,63,63	1.74	10 (20%)
31	CLA	6	317	5	69,73,73	1.24	9 (13%)	83,113,113	1.34	9 (10%)
30	CHL	d	602	-	68,72,74	1.89	20 (29%)	77,111,114	2.86	29 (37%)
31	CLA	1	304	-	56,60,73	1.38	9 (16%)	67,97,113	1.36	7 (10%)
31	CLA	G	102	14	49,53,73	1.47	8 (16%)	59,89,113	1.47	4 (6%)
33	0UR	9	502	-	50,53,58	0.98	1 (2%)	58,72,77	1.69	16 (27%)
34	LHG	7	602	-	37,37,48	1.18	6 (16%)	40,43,54	1.04	2 (5%)
33	0UR	O	204	-	50,53,58	0.99	1 (2%)	58,72,77	1.92	16 (27%)
33	0UR	3	501	-	49,52,58	1.01	1 (2%)	57,71,77	2.10	17 (29%)
31	CLA	K	101	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	7 (9%)
33	0UR	c	520	-	50,53,58	1.00	2 (4%)	58,72,77	1.91	17 (29%)
31	CLA	9	312	8	60,64,73	1.33	10 (16%)	72,102,113	1.35	7 (9%)
31	CLA	A	823	9	55,59,73	1.41	10 (18%)	66,96,113	1.40	5 (7%)
31	CLA	d	612	25	49,53,73	1.50	9 (18%)	59,89,113	1.44	5 (8%)
31	CLA	A	813	9	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	a	610	-	59,63,73	1.36	8 (13%)	71,101,113	1.37	7 (9%)
31	CLA	1	309	2	59,63,73	1.34	10 (16%)	71,101,113	1.33	6 (8%)
31	CLA	6	318	-	50,54,73	1.45	9 (18%)	60,90,113	1.42	5 (8%)
33	0UR	2	501	-	49,52,58	1.00	1 (2%)	57,71,77	2.13	17 (29%)
31	CLA	7	316	6	52,56,73	1.41	10 (19%)	62,92,113	1.44	5 (8%)
33	0UR	8	501	-	49,52,58	0.96	1 (2%)	57,71,77	1.74	16 (28%)
31	CLA	0	313	1	50,54,73	1.45	8 (16%)	60,90,113	1.37	4 (6%)
31	CLA	5	303	2	63,67,73	1.30	9 (14%)	75,105,113	1.37	6 (8%)
31	CLA	A	834	9	50,54,73	1.42	9 (18%)	60,90,113	1.45	5 (8%)
31	CLA	1	308	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
31	CLA	c	613	-	59,63,73	1.34	9 (15%)	70,100,113	1.37	7 (10%)
30	CHL	f	614	26	46,50,74	2.34	18 (39%)	51,85,114	3.43	26 (50%)
31	CLA	A	833	9	69,73,73	1.23	10 (14%)	83,113,113	1.31	7 (8%)
31	CLA	A	811	9	69,73,73	1.23	9 (13%)	83,113,113	1.29	5 (6%)
34	LHG	e	630	31	42,42,48	1.18	6 (14%)	45,48,54	0.96	2 (4%)
34	LHG	c	630	-	39,39,48	1.20	5 (12%)	42,45,54	0.97	2 (4%)
30	CHL	h	602	-	68,72,74	2.00	19 (27%)	77,111,114	2.78	27 (35%)
30	CHL	2	307	-	55,59,74	2.02	18 (32%)	62,96,114	3.24	31 (50%)
31	CLA	4	304	-	64,68,73	1.28	9 (14%)	77,107,113	1.30	6 (7%)
31	CLA	B	836	10	64,68,73	1.29	10 (15%)	77,107,113	1.35	10 (12%)
34	LHG	6	603	-	30,30,48	1.33	6 (20%)	33,36,54	1.11	2 (6%)
31	CLA	3	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	7 (8%)
31	CLA	A	828	9	69,73,73	1.23	10 (14%)	83,113,113	1.29	7 (8%)
31	CLA	8	312	7	60,64,73	1.34	10 (16%)	72,102,113	1.35	6 (8%)
31	CLA	B	812	10	56,60,73	1.38	9 (16%)	67,97,113	1.43	7 (10%)
34	LHG	i	630	-	29,29,48	1.34	6 (20%)	32,35,54	1.12	2 (6%)
30	CHL	d	606	-	55,59,74	2.18	19 (34%)	62,96,114	3.11	27 (43%)
31	CLA	A	815	9	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
31	CLA	c	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	6 (9%)
30	CHL	2	306	-	52,56,74	2.15	19 (36%)	58,92,114	3.26	27 (46%)
30	CHL	9	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.19	28 (45%)
30	CHL	4	308	-	51,55,74	2.18	18 (35%)	57,91,114	3.17	24 (42%)
30	CHL	7	307	-	55,59,74	2.09	19 (34%)	62,96,114	3.14	26 (41%)
30	CHL	7	305	-	52,56,74	2.12	19 (36%)	58,92,114	3.27	26 (44%)
32	8CT	M	102	-	40,41,41	4.61	23 (57%)	50,56,56	2.83	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	O	201	-	45,49,73	1.50	9 (20%)	54,84,113	1.55	6 (11%)
31	CLA	A	803	9	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
31	CLA	7	308	-	69,73,73	1.24	10 (14%)	83,113,113	1.26	6 (7%)
30	CHL	7	306	-	65,69,74	1.95	19 (29%)	73,107,114	2.91	30 (41%)
31	CLA	B	840	10	69,73,73	1.25	8 (11%)	83,113,113	1.32	5 (6%)
31	CLA	g	613	25	51,55,73	1.46	7 (13%)	61,91,113	1.47	6 (9%)
30	CHL	a	607	-	53,57,74	2.24	19 (35%)	57,92,114	3.19	25 (43%)
30	CHL	f	606	-	55,59,74	2.16	18 (32%)	62,96,114	3.22	30 (48%)
32	8CT	B	845	-	40,41,41	4.62	23 (57%)	50,56,56	3.23	22 (44%)
31	CLA	K	104	19	50,54,73	1.45	10 (20%)	60,90,113	1.46	6 (10%)
31	CLA	B	806	-	69,73,73	1.24	11 (15%)	83,113,113	1.36	8 (9%)
32	8CT	A	854	-	40,41,41	4.64	23 (57%)	50,56,56	2.90	20 (40%)
31	CLA	8	309	-	64,68,73	1.29	10 (15%)	77,107,113	1.33	8 (10%)
30	CHL	i	614	-	46,50,74	2.39	19 (41%)	51,85,114	3.38	25 (49%)
42	NEX	i	523	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	B	834	10	65,69,73	1.29	10 (15%)	78,108,113	1.29	6 (7%)
36	LMG	O	207	-	39,39,55	0.82	1 (2%)	47,47,63	1.26	5 (10%)
31	CLA	K	105	19	54,58,73	1.40	9 (16%)	65,95,113	1.41	7 (10%)
31	CLA	g	604	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
30	CHL	d	609	-	70,74,74	1.95	18 (25%)	80,114,114	2.75	27 (33%)
31	CLA	A	837	9	65,69,73	1.27	10 (15%)	78,108,113	1.37	7 (8%)
31	CLA	A	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	9 (10%)
36	LMG	L	210	-	31,31,55	0.92	0	39,39,63	1.25	5 (12%)
31	CLA	9	308	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
30	CHL	h	606	-	55,59,74	2.17	18 (32%)	62,96,114	3.13	27 (43%)
30	CHL	e	608	-	70,74,74	1.87	19 (27%)	80,114,114	2.80	27 (33%)
31	CLA	g	611	-	50,54,73	1.45	8 (16%)	60,90,113	1.42	6 (10%)
30	CHL	e	601	29	55,59,74	2.12	18 (32%)	62,96,114	3.24	30 (48%)
33	0UR	1	501	-	50,53,58	0.95	1 (2%)	58,72,77	1.71	16 (27%)
32	8CT	L	206	-	40,41,41	4.65	23 (57%)	50,56,56	2.78	19 (38%)
31	CLA	7	312	6	59,63,73	1.35	9 (15%)	71,101,113	1.35	6 (8%)
37	0IE	i	521	-	42,45,45	1.46	6 (14%)	49,63,63	1.57	9 (18%)
31	CLA	h	613	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
31	CLA	A	820	9	59,63,73	1.33	10 (16%)	71,101,113	1.38	7 (9%)
30	CHL	5	305	-	50,54,74	2.24	19 (38%)	56,90,114	3.28	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	A	821	-	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
31	CLA	B	833	10	59,63,73	1.35	10 (16%)	71,101,113	1.37	9 (12%)
30	CHL	4	306	-	52,56,74	2.15	19 (36%)	58,92,114	3.24	27 (46%)
31	CLA	A	841	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
31	CLA	B	811	10	69,73,73	1.23	10 (14%)	83,113,113	1.36	9 (10%)
30	CHL	b	602	-	68,72,74	1.90	18 (26%)	77,111,114	2.86	28 (36%)
31	CLA	b	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	6 (9%)
31	CLA	7	303	6	49,53,73	1.48	10 (20%)	59,89,113	1.45	5 (8%)
31	CLA	A	831	9	54,58,73	1.39	10 (18%)	65,95,113	1.46	7 (10%)
31	CLA	1	312	2	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
31	CLA	B	807	10	49,53,73	1.46	10 (20%)	59,89,113	1.53	9 (15%)
30	CHL	b	607	-	51,55,74	2.23	18 (35%)	57,91,114	3.16	26 (45%)
31	CLA	f	611	34	59,63,73	1.35	9 (15%)	71,101,113	1.36	6 (8%)
40	SF4	C	101	-	0,12,12	-	-	-		
42	NEX	c	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
31	CLA	0	304	-	56,60,73	1.39	9 (16%)	67,97,113	1.39	7 (10%)
42	NEX	e	523	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
30	CHL	i	601	28	51,55,74	2.29	19 (37%)	57,91,114	3.19	24 (42%)
32	8CT	2	402	-	40,41,41	4.66	24 (60%)	50,56,56	3.05	20 (40%)
30	CHL	2	319	7	65,69,74	1.91	18 (27%)	74,108,114	2.94	31 (41%)
31	CLA	5	311	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	7 (11%)
31	CLA	2	304	-	64,68,73	1.29	9 (14%)	77,107,113	1.31	6 (7%)
31	CLA	5	309	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	10 (12%)
33	0UR	5	502	-	50,53,58	0.96	1 (2%)	58,72,77	2.05	15 (25%)
37	0IE	f	522	-	42,45,45	1.44	6 (14%)	49,63,63	1.65	9 (18%)
31	CLA	A	812	9	58,62,73	1.37	10 (17%)	69,99,113	1.34	7 (10%)
32	8CT	7	404	-	40,41,41	4.62	24 (60%)	50,56,56	3.57	23 (46%)
31	CLA	2	310	34	64,68,73	1.29	10 (15%)	77,107,113	1.30	6 (7%)
31	CLA	0	311	-	51,55,73	1.43	10 (19%)	61,91,113	1.49	6 (9%)
31	CLA	0	309	-	64,68,73	1.29	8 (12%)	77,107,113	1.33	7 (9%)
33	0UR	0	502	-	50,53,58	0.97	1 (2%)	58,72,77	1.89	16 (27%)
31	CLA	A	853	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
30	CHL	6	307	-	55,59,74	2.06	18 (32%)	62,96,114	3.24	31 (50%)
31	CLA	2	309	3	64,68,73	1.29	10 (15%)	77,107,113	1.32	10 (12%)
37	0IE	a	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.58	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	7	313	6	51,55,74	2.19	19 (37%)	57,91,114	3.22	24 (42%)
30	CHL	a	614	-	46,50,74	2.41	18 (39%)	51,85,114	3.42	25 (49%)
31	CLA	4	309	-	64,68,73	1.30	8 (12%)	77,107,113	1.25	8 (10%)
30	CHL	f	601	26	70,74,74	1.89	20 (28%)	80,114,114	2.80	27 (33%)
31	CLA	B	830	10	60,64,73	1.37	10 (16%)	72,102,113	1.47	10 (13%)
34	LHG	B	852	31	22,22,48	1.30	3 (13%)	25,28,54	1.07	1 (4%)
33	0UR	b	520	-	50,53,58	0.94	1 (2%)	58,72,77	1.74	15 (25%)
30	CHL	b	608	-	70,74,74	1.85	18 (25%)	80,114,114	2.81	30 (37%)
37	0IE	h	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.59	8 (16%)
31	CLA	g	603	-	55,59,73	1.41	8 (14%)	66,96,113	1.38	4 (6%)
30	CHL	h	614	-	46,50,74	2.41	19 (41%)	51,85,114	3.37	25 (49%)
30	CHL	8	315	-	47,51,74	2.27	18 (38%)	52,86,114	3.31	24 (46%)
31	CLA	L	207	-	51,55,73	1.45	9 (17%)	61,91,113	1.39	6 (9%)
30	CHL	c	608	-	70,74,74	1.88	19 (27%)	80,114,114	2.80	26 (32%)
30	CHL	4	313	7	55,59,74	2.05	18 (32%)	62,96,114	3.22	31 (50%)
31	CLA	B	826	-	53,56,73	1.45	11 (20%)	61,89,113	2.06	11 (18%)
31	CLA	A	835	9	61,65,73	1.32	9 (14%)	73,103,113	1.39	7 (9%)
30	CHL	d	607	-	51,55,74	2.31	19 (37%)	57,91,114	3.19	24 (42%)
32	8CT	K	107	-	40,41,41	4.61	23 (57%)	50,56,56	3.28	24 (48%)
33	0UR	i	520	-	48,51,58	0.96	1 (2%)	56,70,77	1.83	13 (23%)
30	CHL	i	608	-	54,58,74	2.18	18 (33%)	59,94,114	3.15	26 (44%)
31	CLA	L	204	-	50,54,73	1.44	10 (20%)	60,90,113	1.40	5 (8%)
31	CLA	f	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
30	CHL	8	307	-	55,59,74	2.06	18 (32%)	62,96,114	3.17	28 (45%)
31	CLA	B	820	-	60,64,73	1.34	9 (15%)	72,102,113	1.39	7 (9%)
31	CLA	e	611	34	59,63,73	1.36	8 (13%)	71,101,113	1.33	6 (8%)
31	CLA	b	610	-	59,63,73	1.36	9 (15%)	71,101,113	1.31	9 (12%)
30	CHL	9	313	8	51,55,74	2.17	17 (33%)	57,91,114	3.27	28 (49%)
31	CLA	A	806	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
31	CLA	B	822	10	64,68,73	1.30	9 (14%)	77,107,113	1.35	6 (7%)
31	CLA	L	202	17	50,54,73	1.44	10 (20%)	60,90,113	1.45	5 (8%)
38	PQN	B	842	-	34,34,34	1.54	2 (5%)	42,45,45	1.11	2 (4%)
32	8CT	8	406	-	40,41,41	4.70	24 (60%)	50,56,56	2.49	18 (36%)
39	CL0	A	857	9	69,73,73	1.31	8 (11%)	83,113,113	1.40	11 (13%)
34	LHG	B	854	-	42,42,48	1.17	6 (14%)	45,48,54	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	0IE	3	502	-	42,45,45	1.41	6 (14%)	49,63,63	1.53	10 (20%)
31	CLA	A	814	9	61,65,73	1.32	9 (14%)	73,103,113	1.36	5 (6%)
31	CLA	B	808	10	69,73,73	1.23	10 (14%)	83,113,113	1.35	8 (9%)
31	CLA	f	613	26	59,63,73	1.36	9 (15%)	70,100,113	1.36	6 (8%)
31	CLA	d	610	-	59,63,73	1.35	8 (13%)	71,101,113	1.34	10 (14%)
31	CLA	f	610	-	59,63,73	1.35	9 (15%)	71,101,113	1.34	7 (9%)
30	CHL	g	605	-	47,51,74	2.37	18 (38%)	52,86,114	3.34	24 (46%)
30	CHL	c	601	23	60,64,74	2.00	19 (31%)	68,102,114	3.07	30 (44%)
30	CHL	d	614	-	46,50,74	2.41	19 (41%)	51,85,114	3.44	25 (49%)
33	0UR	5	501	-	49,52,58	0.95	1 (2%)	57,71,77	1.75	12 (21%)
30	CHL	1	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.24	30 (48%)
31	CLA	a	613	22	59,63,73	1.37	8 (13%)	70,100,113	1.38	6 (8%)
30	CHL	7	301	6	67,71,74	1.91	18 (26%)	76,110,114	2.90	28 (36%)
31	CLA	B	818	10	63,67,73	1.30	10 (15%)	75,105,113	1.39	7 (9%)
30	CHL	f	602	-	68,72,74	1.88	19 (27%)	77,111,114	2.90	29 (37%)
36	LMG	2	602	-	36,36,55	0.89	1 (2%)	44,44,63	1.24	5 (11%)
32	8CT	9	401	-	40,41,41	4.66	23 (57%)	50,56,56	2.71	17 (34%)
31	CLA	d	611	-	50,54,73	1.46	7 (14%)	60,90,113	1.40	4 (6%)
31	CLA	b	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
32	8CT	4	402	-	40,41,41	4.64	24 (60%)	50,56,56	3.01	20 (40%)
34	LHG	9	601	31	45,45,48	1.13	6 (13%)	47,50,54	0.95	2 (4%)
31	CLA	A	838	9	60,64,73	1.34	10 (16%)	72,102,113	1.34	7 (9%)
41	DGD	B	849	-	57,57,67	0.88	2 (3%)	71,71,81	1.17	5 (7%)
31	CLA	4	310	34	64,68,73	1.29	10 (15%)	77,107,113	1.31	6 (7%)
34	LHG	1	601	31	48,48,48	1.09	5 (10%)	51,54,54	0.97	2 (3%)
31	CLA	b	613	-	59,63,73	1.36	8 (13%)	70,100,113	1.37	6 (8%)
31	CLA	A	804	9	59,63,73	1.32	10 (16%)	71,101,113	1.41	6 (8%)
34	LHG	a	630	-	42,42,48	1.17	6 (14%)	45,48,54	0.96	2 (4%)
31	CLA	i	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	5 (7%)
30	CHL	i	607	-	51,55,74	2.29	18 (35%)	57,91,114	3.21	26 (45%)
31	CLA	6	320	-	55,59,73	1.40	9 (16%)	66,96,113	1.34	5 (7%)
32	8CT	B	847	-	40,41,41	4.61	23 (57%)	50,56,56	3.09	22 (44%)
30	CHL	a	605	22	47,51,74	2.35	18 (38%)	52,86,114	3.33	24 (46%)
30	CHL	b	614	-	46,50,74	2.37	19 (41%)	51,85,114	3.38	25 (49%)
33	0UR	1	502	-	50,53,58	0.99	2 (4%)	58,72,77	1.90	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	6	305	-	47,51,74	2.15	19 (40%)	52,86,114	3.38	25 (48%)
31	CLA	7	309	-	63,67,73	1.29	10 (15%)	75,105,113	1.35	7 (9%)
31	CLA	A	807	9	57,61,73	1.36	10 (17%)	66,97,113	1.44	10 (15%)
30	CHL	e	607	-	51,55,74	2.25	19 (37%)	57,91,114	3.18	26 (45%)
32	8CT	A	850	-	40,41,41	4.55	23 (57%)	50,56,56	3.10	22 (44%)
31	CLA	8	303	7	50,54,73	1.46	10 (20%)	60,90,113	1.40	5 (8%)
32	8CT	B	846	-	40,41,41	4.76	24 (60%)	50,56,56	3.25	20 (40%)
31	CLA	2	312	3	64,68,73	1.28	9 (14%)	77,107,113	1.37	7 (9%)
30	CHL	h	609	-	51,55,74	2.28	19 (37%)	57,91,114	3.19	26 (45%)
31	CLA	e	603	29	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
31	CLA	c	603	-	56,60,73	1.39	9 (16%)	67,97,113	1.41	6 (8%)
34	LHG	7	601	31	29,29,48	1.35	5 (17%)	32,35,54	1.09	2 (6%)
37	0IE	b	522	-	42,45,45	1.46	6 (14%)	49,63,63	1.56	8 (16%)
30	CHL	g	614	-	46,50,74	2.42	19 (41%)	51,85,114	3.42	26 (50%)
31	CLA	9	311	8	56,60,73	1.40	10 (17%)	67,97,113	1.38	7 (10%)
37	0IE	h	521	-	42,45,45	1.46	6 (14%)	49,63,63	1.58	8 (16%)
34	LHG	5	601	31	36,36,48	1.24	5 (13%)	39,42,54	1.08	3 (7%)
34	LHG	8	601	31	43,43,48	1.16	5 (11%)	46,49,54	0.92	2 (4%)
30	CHL	e	605	29	47,51,74	2.30	18 (38%)	52,86,114	3.32	24 (46%)
30	CHL	4	319	2	58,62,74	2.02	19 (32%)	65,99,114	3.12	31 (47%)
31	CLA	B	837	-	69,73,73	1.23	9 (13%)	83,113,113	1.33	8 (9%)
30	CHL	c	602	-	65,69,74	1.93	19 (29%)	74,108,114	2.93	30 (40%)
31	CLA	3	309	4	69,73,73	1.24	10 (14%)	83,113,113	1.31	9 (10%)
31	CLA	1	303	2	60,64,73	1.34	10 (16%)	72,102,113	1.41	6 (8%)
34	LHG	3	603	-	35,35,48	1.26	6 (17%)	38,41,54	1.05	2 (5%)
31	CLA	B	813	10	59,63,73	1.35	10 (16%)	71,101,113	1.36	7 (9%)
30	CHL	i	605	28	47,51,74	2.35	18 (38%)	52,86,114	3.35	24 (46%)
34	LHG	K	106	-	42,42,48	1.15	6 (14%)	45,47,54	1.05	3 (6%)
30	CHL	1	306	-	52,56,74	2.17	18 (34%)	58,92,114	3.21	25 (43%)
30	CHL	b	601	24	70,74,74	1.95	18 (25%)	80,114,114	2.80	27 (33%)
30	CHL	8	305	-	51,55,74	2.16	18 (35%)	57,91,114	3.25	27 (47%)
31	CLA	7	318	6	64,68,73	1.28	9 (14%)	77,107,113	1.33	6 (7%)
30	CHL	6	308	5	64,68,74	1.96	18 (28%)	72,106,114	2.90	28 (38%)
31	CLA	4	311	-	52,56,73	1.42	10 (19%)	62,92,113	1.44	6 (9%)
31	CLA	A	830	9	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	NEX	f	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	B	810	10	66,70,73	1.26	10 (15%)	79,109,113	1.34	7 (8%)
37	0IE	7	502	-	42,45,45	1.41	6 (14%)	49,63,63	1.53	10 (20%)
31	CLA	B	828	-	64,68,73	1.28	10 (15%)	77,107,113	1.29	6 (7%)
31	CLA	B	838	10	51,55,73	1.41	10 (19%)	61,91,113	1.42	6 (9%)
31	CLA	0	303	1	66,70,73	1.27	9 (13%)	79,109,113	1.28	5 (6%)
30	CHL	c	614	-	46,50,74	2.35	19 (41%)	51,85,114	3.38	26 (50%)
31	CLA	5	310	34	49,53,73	1.47	9 (18%)	59,89,113	1.43	4 (6%)
31	CLA	L	201	9	62,66,73	1.30	10 (16%)	74,104,113	1.38	8 (10%)
31	CLA	2	303	3	60,64,73	1.35	10 (16%)	72,102,113	1.38	6 (8%)
34	LHG	7	603	-	38,38,48	1.22	6 (15%)	41,44,54	0.99	2 (4%)
30	CHL	5	301	2	56,60,74	2.15	19 (33%)	63,97,114	3.08	29 (46%)
31	CLA	A	824	9	59,63,73	1.34	10 (16%)	71,101,113	1.35	7 (9%)
38	PQN	A	842	-	34,34,34	1.50	2 (5%)	42,45,45	1.26	5 (11%)
37	0IE	i	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.61	9 (18%)
31	CLA	B	805	10	69,73,73	1.23	10 (14%)	83,113,113	1.27	7 (8%)
31	CLA	0	310	-	45,49,73	1.50	9 (20%)	54,84,113	1.51	7 (12%)
31	CLA	4	303	7	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
30	CHL	b	609	-	58,62,74	2.12	18 (31%)	65,99,114	3.02	26 (40%)
37	0IE	e	522	-	42,45,45	1.42	6 (14%)	49,63,63	1.67	9 (18%)
31	CLA	f	612	26	49,53,73	1.47	10 (20%)	59,89,113	1.48	4 (6%)
31	CLA	e	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	5 (7%)
31	CLA	5	312	2	60,64,73	1.33	10 (16%)	72,102,113	1.37	5 (6%)
33	0UR	e	520	-	50,53,58	0.96	1 (2%)	58,72,77	1.99	17 (29%)
30	CHL	a	602	-	68,72,74	1.95	19 (27%)	77,111,114	2.80	28 (36%)
30	CHL	9	306	-	52,56,74	2.15	18 (34%)	58,92,114	3.24	25 (43%)
30	CHL	6	315	5	47,51,74	2.21	17 (36%)	52,86,114	3.32	23 (44%)
31	CLA	3	310	-	66,70,73	1.28	9 (13%)	79,109,113	1.30	6 (7%)
30	CHL	i	602	-	65,69,74	1.98	18 (27%)	74,108,114	2.91	28 (37%)
31	CLA	H	202	27	51,55,73	1.43	10 (19%)	61,91,113	1.41	5 (8%)
31	CLA	a	612	-	49,53,73	1.48	8 (16%)	59,89,113	1.47	4 (6%)
30	CHL	f	605	26	47,51,74	2.34	18 (38%)	52,86,114	3.33	24 (46%)
31	CLA	h	610	-	50,54,73	1.46	7 (14%)	60,90,113	1.43	6 (10%)
30	CHL	0	305	-	55,59,74	2.14	18 (32%)	62,96,114	3.13	29 (46%)
30	CHL	2	313	3	55,59,74	2.07	18 (32%)	62,96,114	3.22	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	0UR	8	502	-	50,53,58	0.95	1 (2%)	58,72,77	1.86	15 (25%)
30	CHL	d	601	25	55,59,74	2.23	19 (34%)	62,96,114	3.10	28 (45%)
31	CLA	7	317	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
30	CHL	7	302	6	68,72,74	1.84	18 (26%)	77,111,114	2.93	30 (38%)
30	CHL	2	301	-	65,69,74	1.91	19 (29%)	74,108,114	2.93	28 (37%)
31	CLA	3	308	-	69,73,73	1.23	9 (13%)	83,113,113	1.30	7 (8%)
31	CLA	3	312	4	59,63,73	1.33	10 (16%)	71,101,113	1.35	6 (8%)
31	CLA	5	304	-	56,60,73	1.38	8 (14%)	67,97,113	1.35	4 (5%)
31	CLA	A	817	9	65,69,73	1.26	10 (15%)	78,108,113	1.37	7 (8%)
30	CHL	8	301	7	65,69,74	1.95	19 (29%)	74,108,114	2.99	29 (39%)
30	CHL	g	601	25	56,60,74	2.24	18 (32%)	63,97,114	3.12	27 (42%)
30	CHL	g	609	25	50,54,74	2.34	20 (40%)	53,88,114	3.22	24 (45%)
30	CHL	h	607	-	50,54,74	2.36	19 (38%)	56,90,114	3.16	24 (42%)
37	0IE	c	522	-	42,45,45	1.43	6 (14%)	49,63,63	1.67	10 (20%)
31	CLA	7	315	6	51,55,73	1.44	10 (19%)	61,91,113	1.43	5 (8%)
31	CLA	b	611	-	64,68,73	1.30	8 (12%)	77,107,113	1.30	4 (5%)
31	CLA	A	805	9	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
31	CLA	A	819	9	69,73,73	1.25	10 (14%)	83,113,113	1.32	11 (13%)
32	8CT	3	402	-	40,41,41	4.64	23 (57%)	50,56,56	3.05	16 (32%)
31	CLA	6	312	5	60,64,73	1.32	10 (16%)	72,102,113	1.35	7 (9%)
31	CLA	B	835	-	49,53,73	1.47	10 (20%)	59,89,113	1.48	5 (8%)
31	CLA	G	103	14	50,54,73	1.45	9 (18%)	60,90,113	1.41	5 (8%)
31	CLA	d	603	25	59,63,73	1.35	8 (13%)	71,101,113	1.35	5 (7%)
30	CHL	4	302	7	57,61,74	2.02	18 (31%)	64,98,114	3.20	33 (51%)
31	CLA	2	311	3	52,56,73	1.42	9 (17%)	62,92,113	1.47	6 (9%)
31	CLA	9	300	10	62,66,73	1.29	9 (14%)	74,104,113	1.39	7 (9%)
31	CLA	B	815	10	59,63,73	1.33	10 (16%)	71,101,113	1.37	8 (11%)
30	CHL	a	601	22	51,55,74	2.26	18 (35%)	57,91,114	3.22	25 (43%)
30	CHL	e	602	-	65,69,74	1.96	19 (29%)	74,108,114	2.92	27 (36%)
33	0UR	4	501	-	49,52,58	0.98	1 (2%)	57,71,77	2.10	19 (33%)
30	CHL	i	609	-	52,56,74	2.30	19 (36%)	58,92,114	3.14	25 (43%)
31	CLA	9	303	8	52,56,73	1.42	9 (17%)	62,92,113	1.44	6 (9%)
32	8CT	J	101	-	40,41,41	4.61	23 (57%)	50,56,56	2.81	17 (34%)
30	CHL	8	308	-	51,55,74	2.17	18 (35%)	57,91,114	3.19	24 (42%)
34	LHG	2	601	31	31,31,48	1.32	5 (16%)	34,37,54	1.12	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	d	613	-	59,63,73	1.36	8 (13%)	70,100,113	1.34	5 (7%)
31	CLA	B	821	10	54,58,73	1.39	7 (12%)	65,95,113	1.47	7 (10%)
31	CLA	A	840	9	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)

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
31	CLA	3	311	4	-	3/17/93/115	-
31	CLA	f	603	-	-	8/27/103/115	-
37	0IE	e	521	-	-	2/33/72/72	0/2/2/2
30	CHL	5	302	2	-	21/39/115/117	-
36	LMG	A	856	-	-	14/31/51/70	0/1/1/1
30	CHL	h	601	22	-	10/19/95/117	-
31	CLA	8	311	7	-	8/17/93/115	-
31	CLA	a	611	-	-	8/30/106/115	-
32	8CT	A	846	-	-	4/29/63/63	0/2/2/2
31	CLA	g	610	-	-	6/17/93/115	-
31	CLA	5	314	2	-	11/17/93/115	-
30	CHL	h	608	-	-	7/17/93/117	-
31	CLA	6	314	-	-	3/15/91/115	-
31	CLA	B	816	10	-	9/33/109/115	-
33	0UR	h	520	-	-	9/42/81/86	0/2/2/2
31	CLA	d	604	-	-	6/21/97/115	-
31	CLA	a	603	-	-	4/25/101/115	-
34	LHG	d	630	-	-	17/40/40/53	-
30	CHL	2	305	-	-	0/14/90/117	-
31	CLA	4	312	7	-	9/25/101/115	-
32	8CT	B	851	-	-	13/29/63/63	0/2/2/2
37	0IE	g	521	-	-	3/33/72/72	0/2/2/2
31	CLA	a	604	-	-	3/21/97/115	-
31	CLA	9	302	-	-	15/39/115/115	-
30	CHL	4	305	-	-	0/14/90/117	-
30	CHL	3	302	4	-	22/37/113/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	841	34	-	8/39/115/115	-
31	CLA	0	321	1	-	11/15/91/115	-
31	CLA	i	611	-	-	8/15/91/115	-
31	CLA	O	206	-	-	11/23/99/115	-
34	LHG	A	845	31	-	17/31/31/53	-
30	CHL	g	606	-	-	7/23/99/117	-
31	CLA	B	831	10	-	11/21/97/115	-
30	CHL	c	609	-	-	21/41/117/117	-
31	CLA	h	604	-	-	6/17/93/115	-
31	CLA	F	301	-	-	8/15/91/115	-
30	CHL	2	302	3	-	29/39/115/117	-
31	CLA	B	803	-	-	15/39/115/115	-
31	CLA	i	603	-	-	6/17/93/115	-
30	CHL	0	301	1	-	11/25/101/117	-
31	CLA	A	826	-	-	11/39/115/115	-
32	8CT	O	205	-	-	6/29/63/63	0/2/2/2
30	CHL	b	606	-	-	3/23/99/117	-
36	LMG	J	105	-	-	15/41/61/70	0/1/1/1
31	CLA	A	816	-	-	5/15/91/115	-
31	CLA	9	309	-	-	7/33/109/115	-
34	LHG	f	630	31	-	27/44/44/53	-
34	LHG	6	601	31	-	17/41/41/53	-
31	CLA	B	829	-	-	9/39/115/115	-
31	CLA	B	817	10	-	21/33/109/115	-
30	CHL	3	305	-	-	8/23/99/117	-
31	CLA	3	303	-	-	8/27/103/115	-
37	0IE	d	521	-	-	2/33/72/72	0/2/2/2
36	LMG	L	211	-	-	15/32/52/70	0/1/1/1
31	CLA	b	603	24	-	7/27/103/115	-
30	CHL	e	609	-	-	13/35/111/117	-
31	CLA	1	311	2	-	6/24/100/115	-
30	CHL	6	313	5	-	7/25/101/117	-
32	8CT	B	804	-	-	14/29/63/63	0/2/2/2
36	LMG	3	602	-	-	16/31/51/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	0	601	-	-	33/53/53/53	-
31	CLA	B	827	-	-	12/39/115/115	-
32	8CT	3	403	-	-	9/29/63/63	0/2/2/2
31	CLA	A	843	34	-	8/24/100/115	-
33	0UR	0	501	-	-	3/42/81/86	0/2/2/2
32	8CT	7	402	-	-	15/29/63/63	0/2/2/2
31	CLA	B	832	-	-	9/39/115/115	-
34	LHG	3	601	-	-	16/40/40/53	-
36	LMG	B	853	-	-	22/37/57/70	0/1/1/1
31	CLA	5	308	-	-	7/17/93/115	-
37	0IE	c	521	-	-	2/33/72/72	0/2/2/2
31	CLA	7	304	-	-	7/27/103/115	-
31	CLA	6	309	5	-	2/31/107/115	-
31	CLA	3	313	4	-	7/15/91/115	-
32	8CT	B	844	-	-	11/29/63/63	0/2/2/2
30	CHL	8	302	7	-	19/39/115/117	-
31	CLA	e	612	-	-	4/15/91/115	-
30	CHL	5	307	-	-	8/19/95/117	-
31	CLA	9	310	34	-	5/10/86/115	-
31	CLA	7	310	34	-	2/4/76/115	-
32	8CT	B	843	-	-	14/29/63/63	0/2/2/2
32	8CT	B	848	-	-	9/29/63/63	0/2/2/2
42	NEX	d	523	-	-	5/27/83/83	0/3/3/3
30	CHL	e	606	-	-	8/23/99/117	-
31	CLA	L	203	17	-	21/37/113/115	-
31	CLA	A	822	-	-	5/20/96/115	-
31	CLA	A	829	9	-	13/39/115/115	-
32	8CT	L	209	-	-	9/29/63/63	0/2/2/2
31	CLA	7	311	6	-	8/24/100/115	-
33	0UR	6	502	-	-	11/42/81/86	0/2/2/2
31	CLA	0	312	1	-	14/39/115/115	-
30	CHL	c	605	23	-	2/14/90/117	-
31	CLA	e	610	-	-	4/27/103/115	-
31	CLA	c	610	-	-	4/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	2	308	-	-	4/19/95/117	-
31	CLA	B	839	-	-	12/39/115/115	-
31	CLA	A	802	-	-	5/39/115/115	-
31	CLA	O	203	-	-	0/4/80/115	-
32	8CT	A	849	-	-	8/29/63/63	0/2/2/2
30	CHL	1	302	-	-	16/39/115/117	-
30	CHL	8	313	7	-	9/29/105/117	-
31	CLA	i	610	-	-	4/27/103/115	-
31	CLA	A	852	10	-	13/39/115/115	-
37	0IE	g	522	-	-	1/33/72/72	0/2/2/2
31	CLA	B	825	-	-	5/39/115/115	-
32	8CT	0	401	-	-	5/29/63/63	0/2/2/2
40	SF4	B	802	-	-	-	0/6/5/5
30	CHL	i	606	28	-	7/23/99/117	-
30	CHL	c	607	-	-	8/19/95/117	-
31	CLA	B	823	-	-	10/24/100/115	-
31	CLA	9	304	-	-	0/23/99/115	-
34	LHG	G	105	-	-	27/42/42/53	-
31	CLA	h	603	-	-	5/20/96/115	-
31	CLA	M	101	-	-	3/17/93/115	-
31	CLA	B	801	-	-	11/39/115/115	-
31	CLA	2	314	3	-	5/15/91/115	-
33	0UR	4	502	-	-	14/40/79/86	0/2/2/2
31	CLA	6	303	5	-	7/24/100/115	-
32	8CT	7	405	-	-	10/29/63/63	0/2/2/2
30	CHL	6	306	-	-	6/23/99/117	-
31	CLA	6	310	34	-	11/33/109/115	-
30	CHL	g	602	-	-	13/25/101/117	-
42	NEX	g	523	-	-	5/27/83/83	0/3/3/3
31	CLA	A	810	9	-	3/39/115/115	-
30	CHL	1	307	-	-	23/41/117/117	-
31	CLA	H	201	10	-	8/27/103/115	-
30	CHL	e	614	-	-	5/12/88/117	-
31	CLA	J	103	16	-	2/12/88/115	-
30	CHL	4	307	-	-	8/23/99/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	809	10	-	12/39/115/115	-
42	NEX	b	523	-	-	5/27/83/83	0/3/3/3
31	CLA	8	314	7	-	10/15/91/115	-
35	SQD	0	603	-	-	17/31/51/69	0/1/1/1
31	CLA	c	612	23	-	4/15/91/115	-
30	CHL	5	313	2	-	8/19/95/117	-
31	CLA	O	202	21	-	1/6/78/115	-
32	8CT	6	402	-	-	8/29/63/63	0/2/2/2
31	CLA	6	304	-	-	5/17/93/115	-
31	CLA	G	101	14	-	7/21/97/115	-
31	CLA	K	102	19	-	13/25/101/115	-
31	CLA	h	612	-	-	7/15/91/115	-
31	CLA	i	612	-	-	3/15/91/115	-
32	8CT	I	101	-	-	9/29/63/63	0/2/2/2
33	0UR	7	501	-	-	9/41/80/86	0/2/2/2
32	8CT	G	104	-	-	13/29/63/63	0/2/2/2
34	LHG	h	630	-	-	18/43/43/53	-
31	CLA	H	205	-	-	9/23/99/115	-
30	CHL	6	302	5	-	20/39/115/117	-
31	CLA	8	310	34	-	4/17/93/115	-
31	CLA	0	308	-	-	12/33/109/115	-
30	CHL	1	313	2	-	19/37/113/117	-
34	LHG	H	203	-	-	13/35/35/53	-
30	CHL	h	605	22	-	2/14/90/117	-
31	CLA	6	311	5	-	4/19/95/115	-
36	LMG	J	102	-	-	12/24/44/70	0/1/1/1
30	CHL	g	608	-	-	5/14/90/117	-
30	CHL	9	301	8	-	6/19/95/117	-
31	CLA	3	318	4	-	0/17/93/115	-
34	LHG	A	844	-	-	20/53/53/53	-
33	0UR	d	520	-	-	10/39/78/86	0/2/2/2
32	8CT	F	302	-	-	9/29/63/63	0/2/2/2
32	8CT	A	847	-	-	10/29/63/63	0/2/2/2
31	CLA	3	306	4	-	5/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	f	609	-	-	19/41/117/117	-
30	CHL	c	606	-	-	3/15/91/117	-
30	CHL	0	306	-	-	9/20/96/117	-
31	CLA	A	809	9	-	11/39/115/115	-
34	LHG	A	855	-	-	27/46/46/53	-
32	8CT	A	848	-	-	7/29/63/63	0/2/2/2
31	CLA	A	827	9	-	4/39/115/115	-
31	CLA	A	832	9	-	14/39/115/115	-
42	NEX	a	523	-	-	5/27/83/83	0/3/3/3
32	8CT	8	402	-	-	10/29/63/63	0/2/2/2
31	CLA	A	808	9	-	20/39/115/115	-
34	LHG	M	104	-	-	19/50/50/53	-
36	LMG	9	602	-	-	31/50/70/70	0/1/1/1
30	CHL	a	609	-	-	10/33/109/117	-
31	CLA	B	814	10	-	16/39/115/115	-
32	8CT	L	205	-	-	6/29/63/63	0/2/2/2
33	0UR	f	520	-	-	9/39/78/86	0/2/2/2
30	CHL	f	608	-	-	8/23/99/117	-
42	NEX	h	523	-	-	5/27/83/83	0/3/3/3
30	CHL	0	302	1	-	14/39/115/117	-
33	0UR	a	520	-	-	7/36/75/86	0/2/2/2
30	CHL	a	608	-	-	9/21/97/117	-
31	CLA	B	824	10	-	10/33/109/115	-
33	0UR	9	501	-	-	3/42/81/86	0/2/2/2
31	CLA	A	818	9	-	12/39/115/115	-
37	0IE	a	521	-	-	2/33/72/72	0/2/2/2
31	CLA	1	314	-	-	5/17/93/115	-
34	LHG	g	630	-	-	15/34/34/53	-
30	CHL	5	306	-	-	9/20/96/117	-
30	CHL	8	306	-	-	16/23/99/117	-
31	CLA	B	850	13	-	5/18/94/115	-
30	CHL	6	301	5	-	15/35/111/117	-
30	CHL	d	605	25	-	4/14/90/117	-
32	8CT	1	402	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	8CT	J	104	-	-	9/29/63/63	0/2/2/2
31	CLA	A	836	-	-	9/23/99/115	-
31	CLA	c	611	-	-	4/17/93/115	-
31	CLA	3	320	-	-	7/24/100/115	-
31	CLA	e	613	-	-	11/27/103/115	-
31	CLA	B	819	10	-	15/33/109/115	-
30	CHL	3	307	-	-	27/41/117/117	-
31	CLA	1	310	34	-	11/37/113/115	-
34	LHG	b	630	-	-	31/45/45/53	-
30	CHL	g	607	-	-	9/23/99/117	-
31	CLA	g	612	-	-	7/15/91/115	-
37	0IE	f	521	-	-	2/33/72/72	0/2/2/2
33	0UR	g	520	-	-	9/42/81/86	0/2/2/2
33	0UR	2	502	-	-	11/40/79/86	0/2/2/2
31	CLA	h	611	-	-	4/10/86/115	-
40	SF4	C	102	18	-	-	0/6/5/5
31	CLA	8	304	-	-	11/39/115/115	-
31	CLA	H	204	-	-	3/18/94/115	-
30	CHL	a	606	-	-	7/23/99/117	-
33	0UR	6	501	-	-	11/41/80/86	0/2/2/2
34	LHG	4	601	31	-	12/36/36/53	-
31	CLA	4	314	7	-	5/15/91/115	-
31	CLA	A	839	9	-	13/39/115/115	-
30	CHL	f	607	-	-	5/19/95/117	-
37	0IE	b	521	-	-	2/33/72/72	0/2/2/2
30	CHL	d	608	-	-	5/23/99/117	-
31	CLA	i	613	-	-	5/23/99/115	-
37	0IE	d	522	-	-	4/33/72/72	0/2/2/2
31	CLA	6	317	5	-	17/39/115/115	-
30	CHL	d	602	-	-	18/39/115/117	-
31	CLA	1	304	-	-	4/24/100/115	-
31	CLA	G	102	14	-	4/15/91/115	-
33	0UR	9	502	-	-	8/42/81/86	0/2/2/2
34	LHG	7	602	-	-	21/42/42/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	0UR	O	204	-	-	5/42/81/86	0/2/2/2
33	0UR	3	501	-	-	9/41/80/86	0/2/2/2
31	CLA	K	101	-	-	12/33/109/115	-
33	0UR	c	520	-	-	9/42/81/86	0/2/2/2
31	CLA	9	312	8	-	6/29/105/115	-
31	CLA	A	823	9	-	4/23/99/115	-
31	CLA	d	612	25	-	7/15/91/115	-
31	CLA	A	813	9	-	8/39/115/115	-
31	CLA	a	610	-	-	5/27/103/115	-
31	CLA	1	309	2	-	6/27/103/115	-
31	CLA	6	318	-	-	14/17/93/115	-
33	0UR	2	501	-	-	7/41/80/86	0/2/2/2
31	CLA	7	316	6	-	3/15/91/115	-
33	0UR	8	501	-	-	7/41/80/86	0/2/2/2
31	CLA	0	313	1	-	11/17/93/115	-
31	CLA	5	303	2	-	11/32/108/115	-
31	CLA	A	834	9	-	2/17/93/115	-
31	CLA	1	308	-	-	7/15/91/115	-
31	CLA	c	613	-	-	8/27/103/115	-
30	CHL	f	614	26	-	8/12/88/117	-
31	CLA	A	833	9	-	12/39/115/115	-
31	CLA	A	811	9	-	13/39/115/115	-
34	LHG	e	630	31	-	22/47/47/53	-
34	LHG	c	630	-	-	20/44/44/53	-
30	CHL	h	602	-	-	17/39/115/117	-
30	CHL	2	307	-	-	5/23/99/117	-
31	CLA	4	304	-	-	8/33/109/115	-
31	CLA	B	836	10	-	11/33/109/115	-
34	LHG	6	603	-	-	13/35/35/53	-
31	CLA	3	304	-	-	6/39/115/115	-
31	CLA	A	828	9	-	19/39/115/115	-
31	CLA	8	312	7	-	10/29/105/115	-
31	CLA	B	812	10	-	6/24/100/115	-
34	LHG	i	630	-	-	9/34/34/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	d	606	-	-	8/23/99/117	-
31	CLA	A	815	9	-	11/39/115/115	-
31	CLA	c	604	-	-	5/21/97/115	-
30	CHL	2	306	-	-	5/20/96/117	-
30	CHL	9	305	-	-	8/23/99/117	-
30	CHL	4	308	-	-	5/19/95/117	-
30	CHL	7	307	-	-	6/23/99/117	-
30	CHL	7	305	-	-	9/20/96/117	-
32	8CT	M	102	-	-	7/29/63/63	0/2/2/2
31	CLA	O	201	-	-	7/10/86/115	-
31	CLA	A	803	9	-	10/39/115/115	-
31	CLA	7	308	-	-	16/39/115/115	-
30	CHL	7	306	-	-	17/35/111/117	-
31	CLA	B	840	10	-	11/39/115/115	-
31	CLA	g	613	25	-	5/18/94/115	-
30	CHL	a	607	-	-	7/19/95/117	-
30	CHL	f	606	-	-	8/23/99/117	-
32	8CT	B	845	-	-	10/29/63/63	0/2/2/2
31	CLA	K	104	19	-	6/17/93/115	-
31	CLA	B	806	-	-	11/39/115/115	-
32	8CT	A	854	-	-	10/29/63/63	0/2/2/2
31	CLA	8	309	-	-	7/33/109/115	-
30	CHL	i	614	-	-	6/12/88/117	-
42	NEX	i	523	-	-	5/27/83/83	0/3/3/3
31	CLA	B	834	10	-	16/35/111/115	-
36	LMG	O	207	-	-	10/34/54/70	0/1/1/1
31	CLA	K	105	19	-	12/21/97/115	-
31	CLA	g	604	-	-	7/15/91/115	-
30	CHL	d	609	-	-	18/41/117/117	-
31	CLA	A	837	9	-	12/35/111/115	-
31	CLA	A	825	-	-	8/39/115/115	-
36	LMG	L	210	-	-	12/26/46/70	0/1/1/1
31	CLA	9	308	-	-	13/39/115/115	-
30	CHL	h	606	-	-	6/23/99/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	e	608	-	-	18/41/117/117	-
31	CLA	g	611	-	-	2/17/93/115	-
30	CHL	e	601	29	-	5/23/99/117	-
33	0UR	1	501	-	-	3/42/81/86	0/2/2/2
32	8CT	L	206	-	-	8/29/63/63	0/2/2/2
31	CLA	7	312	6	-	13/27/103/115	-
37	0IE	i	521	-	-	4/33/72/72	0/2/2/2
31	CLA	h	613	-	-	5/15/91/115	-
31	CLA	A	820	9	-	9/27/103/115	-
30	CHL	5	305	-	-	7/17/93/117	-
31	CLA	A	821	-	-	10/39/115/115	-
31	CLA	B	833	10	-	9/27/103/115	-
30	CHL	4	306	-	-	6/20/96/117	-
31	CLA	A	841	-	-	11/39/115/115	-
31	CLA	B	811	10	-	10/39/115/115	-
30	CHL	b	602	-	-	21/39/115/117	-
31	CLA	b	604	-	-	7/21/97/115	-
31	CLA	7	303	6	-	7/15/91/115	-
31	CLA	A	831	9	-	4/21/97/115	-
31	CLA	1	312	2	-	14/39/115/115	-
31	CLA	B	807	10	-	5/15/91/115	-
30	CHL	b	607	-	-	5/19/95/117	-
31	CLA	f	611	34	-	5/27/103/115	-
42	NEX	c	523	-	-	5/27/83/83	0/3/3/3
42	NEX	e	523	-	-	4/27/83/83	0/3/3/3
31	CLA	0	304	-	-	5/24/100/115	-
40	SF4	C	101	-	-	-	0/6/5/5
30	CHL	i	601	28	-	5/19/95/117	-
32	8CT	2	402	-	-	12/29/63/63	0/2/2/2
30	CHL	2	319	7	-	18/35/111/117	-
31	CLA	5	311	-	-	9/15/91/115	-
31	CLA	2	304	-	-	11/33/109/115	-
31	CLA	5	309	-	-	9/33/109/115	-
33	0UR	5	502	-	-	10/42/81/86	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	0IE	f	522	-	-	0/33/72/72	0/2/2/2
31	CLA	A	812	9	-	3/26/102/115	-
32	8CT	7	404	-	-	7/29/63/63	0/2/2/2
31	CLA	2	310	34	-	12/33/109/115	-
31	CLA	0	311	-	-	9/18/94/115	-
31	CLA	0	309	-	-	11/33/109/115	-
33	0UR	0	502	-	-	12/42/81/86	0/2/2/2
31	CLA	A	853	-	-	15/39/115/115	-
30	CHL	6	307	-	-	12/23/99/117	-
31	CLA	2	309	3	-	3/33/109/115	-
37	0IE	a	522	-	-	0/33/72/72	0/2/2/2
30	CHL	7	313	6	-	7/19/95/117	-
30	CHL	a	614	-	-	0/12/88/117	-
31	CLA	4	309	-	-	5/33/109/115	-
30	CHL	f	601	26	-	14/41/117/117	-
31	CLA	B	830	10	-	8/29/105/115	-
34	LHG	B	852	31	-	17/26/26/53	-
33	0UR	b	520	-	-	11/42/81/86	0/2/2/2
30	CHL	b	608	-	-	20/41/117/117	-
37	0IE	h	522	-	-	0/33/72/72	0/2/2/2
31	CLA	g	603	-	-	5/23/99/115	-
30	CHL	h	614	-	-	5/12/88/117	-
30	CHL	8	315	-	-	4/14/90/117	-
31	CLA	L	207	-	-	7/18/94/115	-
30	CHL	c	608	-	-	20/41/117/117	-
30	CHL	4	313	7	-	5/23/99/117	-
31	CLA	B	826	-	-	2/23/87/115	-
31	CLA	A	835	9	-	14/30/106/115	-
30	CHL	d	607	-	-	9/19/95/117	-
32	8CT	K	107	-	-	12/29/63/63	0/2/2/2
33	0UR	i	520	-	-	5/40/79/86	0/2/2/2
30	CHL	i	608	-	-	9/22/98/117	-
31	CLA	L	204	-	-	7/17/93/115	-
31	CLA	f	604	-	-	7/21/97/115	-
30	CHL	8	307	-	-	11/23/99/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	820	-	-	10/29/105/115	-
31	CLA	e	611	34	-	7/27/103/115	-
31	CLA	b	610	-	-	4/27/103/115	-
30	CHL	9	313	8	-	9/19/95/117	-
31	CLA	A	806	-	-	19/39/115/115	-
31	CLA	B	822	10	-	13/33/109/115	-
31	CLA	L	202	17	-	6/17/93/115	-
38	PQN	B	842	-	-	6/23/43/43	0/2/2/2
32	8CT	8	406	-	-	12/29/63/63	0/2/2/2
39	CL0	A	857	9	-	10/39/115/115	-
34	LHG	B	854	-	-	17/47/47/53	-
37	0IE	3	502	-	-	2/33/72/72	0/2/2/2
31	CLA	A	814	9	-	10/30/106/115	-
31	CLA	B	808	10	-	11/39/115/115	-
31	CLA	f	613	26	-	9/27/103/115	-
31	CLA	d	610	-	-	5/27/103/115	-
31	CLA	f	610	-	-	4/27/103/115	-
30	CHL	g	605	-	-	2/14/90/117	-
30	CHL	c	601	23	-	11/29/105/117	-
30	CHL	d	614	-	-	1/12/88/117	-
33	0UR	5	501	-	-	11/41/80/86	0/2/2/2
30	CHL	1	305	-	-	9/23/99/117	-
31	CLA	a	613	22	-	12/27/103/115	-
30	CHL	7	301	6	-	14/38/114/117	-
31	CLA	B	818	10	-	9/32/108/115	-
30	CHL	f	602	-	-	21/39/115/117	-
36	LMG	2	602	-	-	13/31/51/70	0/1/1/1
32	8CT	9	401	-	-	11/29/63/63	0/2/2/2
31	CLA	d	611	-	-	7/17/93/115	-
31	CLA	b	612	-	-	3/15/91/115	-
32	8CT	4	402	-	-	8/29/63/63	0/2/2/2
34	LHG	9	601	31	-	19/48/48/53	-
31	CLA	A	838	9	-	5/29/105/115	-
41	DGD	B	849	-	-	28/45/85/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	4	310	34	-	13/33/109/115	-
34	LHG	1	601	31	-	21/53/53/53	-
31	CLA	b	613	-	-	8/27/103/115	-
31	CLA	A	804	9	-	8/27/103/115	-
34	LHG	a	630	-	-	29/47/47/53	-
31	CLA	i	604	-	-	8/21/97/115	-
30	CHL	i	607	-	-	11/19/95/117	-
31	CLA	6	320	-	-	11/23/99/115	-
32	8CT	B	847	-	-	9/29/63/63	0/2/2/2
30	CHL	a	605	22	-	2/14/90/117	-
30	CHL	b	614	-	-	4/12/88/117	-
33	0UR	1	502	-	-	10/42/81/86	0/2/2/2
30	CHL	6	305	-	-	0/14/90/117	-
31	CLA	7	309	-	-	11/32/108/115	-
31	CLA	A	807	9	-	5/23/99/115	-
30	CHL	e	607	-	-	4/19/95/117	-
32	8CT	A	850	-	-	10/29/63/63	0/2/2/2
31	CLA	8	303	7	-	7/17/93/115	-
32	8CT	B	846	-	-	12/29/63/63	0/2/2/2
31	CLA	2	312	3	-	12/33/109/115	-
30	CHL	h	609	-	-	3/19/95/117	-
31	CLA	e	603	29	-	6/30/106/115	-
31	CLA	c	603	-	-	5/24/100/115	-
34	LHG	7	601	31	-	10/34/34/53	-
37	0IE	b	522	-	-	3/33/72/72	0/2/2/2
30	CHL	g	614	-	-	2/12/88/117	-
31	CLA	9	311	8	-	6/24/100/115	-
37	0IE	h	521	-	-	4/33/72/72	0/2/2/2
34	LHG	5	601	31	-	13/41/41/53	-
34	LHG	8	601	31	-	30/48/48/53	-
30	CHL	e	605	29	-	4/14/90/117	-
30	CHL	4	319	2	-	9/27/103/117	-
31	CLA	B	837	-	-	4/39/115/115	-
30	CHL	c	602	-	-	20/35/111/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	3	309	4	-	12/39/115/115	-
31	CLA	1	303	2	-	14/29/105/115	-
34	LHG	3	603	-	-	18/40/40/53	-
31	CLA	B	813	10	-	9/27/103/115	-
30	CHL	i	605	28	-	2/14/90/117	-
34	LHG	K	106	-	-	23/46/46/53	-
30	CHL	1	306	-	-	7/20/96/117	-
30	CHL	b	601	24	-	19/41/117/117	-
30	CHL	8	305	-	-	8/19/95/117	-
31	CLA	7	318	6	-	9/33/109/115	-
30	CHL	6	308	5	-	10/34/110/117	-
31	CLA	4	311	-	-	6/19/95/115	-
31	CLA	A	830	9	-	14/39/115/115	-
42	NEX	f	523	-	-	5/27/83/83	0/3/3/3
31	CLA	B	810	10	-	8/36/112/115	-
37	0IE	7	502	-	-	2/33/72/72	0/2/2/2
31	CLA	B	828	-	-	8/33/109/115	-
31	CLA	B	838	10	-	3/18/94/115	-
31	CLA	0	303	1	-	11/36/112/115	-
30	CHL	c	614	-	-	7/12/88/117	-
31	CLA	5	310	34	-	6/15/91/115	-
31	CLA	L	201	9	-	8/31/107/115	-
31	CLA	2	303	3	-	10/29/105/115	-
34	LHG	7	603	-	-	21/43/43/53	-
30	CHL	5	301	2	-	12/25/101/117	-
31	CLA	A	824	9	-	10/27/103/115	-
38	PQN	A	842	-	-	7/23/43/43	0/2/2/2
37	0IE	i	522	-	-	1/33/72/72	0/2/2/2
31	CLA	B	805	10	-	11/39/115/115	-
31	CLA	0	310	-	-	3/10/86/115	-
31	CLA	4	303	7	-	4/15/91/115	-
30	CHL	b	609	-	-	11/27/103/117	-
37	0IE	e	522	-	-	0/33/72/72	0/2/2/2
31	CLA	f	612	26	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	e	604	-	-	7/21/97/115	-
31	CLA	5	312	2	-	11/29/105/115	-
33	0UR	e	520	-	-	10/42/81/86	0/2/2/2
30	CHL	a	602	-	-	20/39/115/117	-
30	CHL	9	306	-	-	6/20/96/117	-
30	CHL	6	315	5	-	4/14/90/117	-
31	CLA	3	310	-	-	15/36/112/115	-
30	CHL	i	602	-	-	22/35/111/117	-
31	CLA	H	202	27	-	8/18/94/115	-
31	CLA	a	612	-	-	2/15/91/115	-
30	CHL	f	605	26	-	2/14/90/117	-
31	CLA	h	610	-	-	5/17/93/115	-
30	CHL	0	305	-	-	7/23/99/117	-
30	CHL	2	313	3	-	5/23/99/117	-
33	0UR	8	502	-	-	8/42/81/86	0/2/2/2
30	CHL	d	601	25	-	3/23/99/117	-
31	CLA	7	317	-	-	13/15/91/115	-
30	CHL	7	302	6	-	18/39/115/117	-
30	CHL	2	301	-	-	10/35/111/117	-
31	CLA	3	308	-	-	18/39/115/115	-
31	CLA	3	312	4	-	8/27/103/115	-
31	CLA	5	304	-	-	12/24/100/115	-
31	CLA	A	817	9	-	16/35/111/115	-
30	CHL	8	301	7	-	6/35/111/117	-
30	CHL	g	601	25	-	6/25/101/117	-
30	CHL	g	609	25	-	3/14/90/117	-
30	CHL	h	607	-	-	3/17/93/117	-
37	0IE	c	522	-	-	12/33/72/72	0/2/2/2
31	CLA	7	315	6	-	9/18/94/115	-
31	CLA	b	611	-	-	4/33/109/115	-
31	CLA	A	805	9	-	14/39/115/115	-
31	CLA	A	819	9	-	18/39/115/115	-
32	8CT	3	402	-	-	9/29/63/63	0/2/2/2
31	CLA	6	312	5	-	10/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	835	-	-	0/15/91/115	-
31	CLA	G	103	14	-	5/17/93/115	-
31	CLA	d	603	25	-	9/27/103/115	-
30	CHL	4	302	7	-	15/26/102/117	-
31	CLA	2	311	3	-	5/19/95/115	-
31	CLA	9	300	10	-	13/31/107/115	-
31	CLA	B	815	10	-	4/27/103/115	-
30	CHL	a	601	22	-	6/19/95/117	-
30	CHL	e	602	-	-	19/35/111/117	-
33	0UR	4	501	-	-	9/41/80/86	0/2/2/2
30	CHL	i	609	-	-	3/20/96/117	-
31	CLA	9	303	8	-	4/19/95/115	-
32	8CT	J	101	-	-	11/29/63/63	0/2/2/2
30	CHL	8	308	-	-	2/19/95/117	-
34	LHG	2	601	31	-	18/36/36/53	-
31	CLA	d	613	-	-	8/27/103/115	-
31	CLA	B	821	10	-	2/21/97/115	-
31	CLA	A	840	9	-	17/39/115/115	-

All (5939) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	844	8CT	C02-C03	14.48	1.59	1.34
32	J	104	8CT	C02-C03	14.47	1.59	1.34
32	8	406	8CT	C02-C03	14.39	1.59	1.34
32	B	848	8CT	C02-C03	14.35	1.59	1.34
32	A	846	8CT	C02-C03	14.35	1.59	1.34
32	G	104	8CT	C02-C03	14.31	1.59	1.34
32	A	849	8CT	C02-C03	14.31	1.59	1.34
32	F	302	8CT	C02-C03	14.29	1.59	1.34
32	B	804	8CT	C02-C03	14.27	1.59	1.34
32	O	205	8CT	C02-C03	14.27	1.59	1.34
32	1	402	8CT	C02-C03	14.25	1.59	1.34
32	7	404	8CT	C02-C03	14.21	1.59	1.34
32	6	402	8CT	C02-C03	14.20	1.59	1.34
32	8	402	8CT	C02-C03	14.20	1.59	1.34
32	B	843	8CT	C02-C03	14.19	1.59	1.34
32	M	102	8CT	C02-C03	14.19	1.59	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	209	8CT	C02-C03	14.18	1.59	1.34
32	2	402	8CT	C02-C03	14.17	1.59	1.34
32	A	854	8CT	C02-C03	14.16	1.59	1.34
32	7	405	8CT	C02-C03	14.14	1.58	1.34
32	L	206	8CT	C02-C03	14.14	1.58	1.34
32	A	847	8CT	C02-C03	14.13	1.58	1.34
32	A	848	8CT	C02-C03	14.12	1.58	1.34
32	B	847	8CT	C02-C03	14.11	1.58	1.34
32	K	107	8CT	C02-C03	14.11	1.58	1.34
32	I	101	8CT	C02-C03	14.06	1.58	1.34
32	B	851	8CT	C02-C03	14.05	1.58	1.34
32	B	846	8CT	C02-C03	14.04	1.58	1.34
32	L	205	8CT	C02-C03	14.04	1.58	1.34
32	3	403	8CT	C02-C03	14.04	1.58	1.34
32	3	402	8CT	C02-C03	14.04	1.58	1.34
32	9	401	8CT	C02-C03	14.03	1.58	1.34
32	4	402	8CT	C02-C03	14.02	1.58	1.34
32	B	845	8CT	C02-C03	14.00	1.58	1.34
32	0	401	8CT	C02-C03	14.00	1.58	1.34
32	J	101	8CT	C02-C03	13.97	1.58	1.34
32	7	402	8CT	C02-C03	13.90	1.58	1.34
32	A	850	8CT	C02-C03	13.88	1.58	1.34
32	1	402	8CT	C32-C31	13.85	1.60	1.32
32	B	843	8CT	C32-C31	13.84	1.59	1.32
32	3	403	8CT	C32-C31	13.84	1.59	1.32
32	B	846	8CT	C32-C31	13.83	1.59	1.32
32	8	406	8CT	C32-C31	13.82	1.59	1.32
32	9	401	8CT	C32-C31	13.81	1.59	1.32
32	7	402	8CT	C32-C31	13.81	1.59	1.32
32	L	206	8CT	C32-C31	13.81	1.59	1.32
32	O	205	8CT	C32-C31	13.80	1.59	1.32
32	B	804	8CT	C32-C31	13.79	1.59	1.32
32	6	402	8CT	C32-C31	13.79	1.59	1.32
32	8	402	8CT	C32-C31	13.70	1.59	1.32
32	B	851	8CT	C32-C31	13.70	1.59	1.32
32	B	848	8CT	C32-C31	13.69	1.59	1.32
32	7	405	8CT	C32-C31	13.69	1.59	1.32
32	L	209	8CT	C32-C31	13.68	1.59	1.32
32	F	302	8CT	C32-C31	13.64	1.59	1.32
32	A	846	8CT	C32-C31	13.61	1.59	1.32
32	0	401	8CT	C32-C31	13.61	1.59	1.32
32	3	402	8CT	C32-C31	13.61	1.59	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	847	8CT	C32-C31	13.60	1.59	1.32
32	A	848	8CT	C32-C31	13.58	1.59	1.32
32	7	404	8CT	C32-C31	13.57	1.59	1.32
32	J	101	8CT	C32-C31	13.56	1.59	1.32
32	L	205	8CT	C32-C31	13.55	1.59	1.32
32	A	850	8CT	C32-C31	13.53	1.59	1.32
32	G	104	8CT	C32-C31	13.53	1.59	1.32
32	J	104	8CT	C32-C31	13.50	1.59	1.32
32	M	102	8CT	C32-C31	13.50	1.59	1.32
32	A	854	8CT	C32-C31	13.49	1.59	1.32
32	A	849	8CT	C32-C31	13.47	1.59	1.32
32	A	847	8CT	C32-C31	13.47	1.59	1.32
32	I	101	8CT	C32-C31	13.45	1.59	1.32
32	B	844	8CT	C32-C31	13.44	1.59	1.32
32	B	845	8CT	C32-C31	13.44	1.59	1.32
32	K	107	8CT	C32-C31	13.40	1.59	1.32
32	2	402	8CT	C32-C31	13.40	1.59	1.32
32	4	402	8CT	C32-C31	13.34	1.59	1.32
32	A	848	8CT	C34-C35	-8.41	1.36	1.54
32	B	804	8CT	C34-C35	-8.30	1.37	1.54
32	B	848	8CT	C34-C35	-8.24	1.37	1.54
32	B	846	8CT	C34-C35	-8.20	1.37	1.54
32	L	209	8CT	C34-C35	-8.20	1.37	1.54
32	B	851	8CT	C34-C35	-8.17	1.37	1.54
32	3	403	8CT	C34-C35	-8.17	1.37	1.54
32	8	406	8CT	C34-C35	-8.16	1.37	1.54
32	A	850	8CT	C34-C35	-8.14	1.37	1.54
32	B	843	8CT	C34-C35	-8.14	1.37	1.54
32	A	854	8CT	C34-C35	-8.12	1.37	1.54
32	F	302	8CT	C34-C35	-8.10	1.37	1.54
32	O	205	8CT	C34-C35	-8.09	1.37	1.54
32	7	405	8CT	C34-C35	-8.09	1.37	1.54
32	1	402	8CT	C34-C35	-8.08	1.37	1.54
32	7	404	8CT	C34-C35	-8.06	1.37	1.54
32	6	402	8CT	C34-C35	-8.05	1.37	1.54
32	8	402	8CT	C34-C35	-8.05	1.37	1.54
32	A	846	8CT	C34-C35	-8.05	1.37	1.54
32	J	104	8CT	C34-C35	-8.04	1.37	1.54
32	A	847	8CT	C34-C35	-8.02	1.37	1.54
32	B	847	8CT	C34-C35	-8.02	1.37	1.54
32	7	402	8CT	C34-C35	-8.00	1.37	1.54
32	L	206	8CT	C34-C35	-7.96	1.37	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	102	8CT	C34-C35	-7.95	1.37	1.54
32	L	205	8CT	C34-C35	-7.95	1.37	1.54
32	B	844	8CT	C34-C35	-7.94	1.37	1.54
32	9	401	8CT	C34-C35	-7.93	1.37	1.54
32	B	845	8CT	C34-C35	-7.90	1.37	1.54
32	A	849	8CT	C34-C35	-7.86	1.38	1.54
32	I	101	8CT	C34-C35	-7.86	1.38	1.54
32	2	402	8CT	C34-C35	-7.82	1.38	1.54
32	3	402	8CT	C34-C35	-7.81	1.38	1.54
32	K	107	8CT	C34-C35	-7.80	1.38	1.54
32	J	101	8CT	C34-C35	-7.75	1.38	1.54
32	G	104	8CT	C34-C35	-7.71	1.38	1.54
32	0	401	8CT	C34-C35	-7.62	1.38	1.54
38	B	842	PQN	C3-C2	7.56	1.49	1.35
32	4	402	8CT	C34-C35	-7.43	1.38	1.54
38	A	842	PQN	C3-C2	7.21	1.48	1.35
32	B	846	8CT	C15-C16	6.93	1.60	1.45
32	B	844	8CT	C15-C16	6.88	1.60	1.45
32	B	843	8CT	C15-C16	6.70	1.60	1.45
32	J	104	8CT	C05-C06	-6.69	1.36	1.52
32	B	848	8CT	C05-C06	-6.69	1.36	1.52
32	B	804	8CT	C05-C06	-6.68	1.36	1.52
32	G	104	8CT	C05-C06	-6.66	1.36	1.52
32	A	849	8CT	C05-C06	-6.62	1.36	1.52
32	F	302	8CT	C05-C06	-6.62	1.36	1.52
32	6	402	8CT	C05-C06	-6.61	1.36	1.52
32	M	102	8CT	C05-C06	-6.60	1.36	1.52
32	8	406	8CT	C05-C06	-6.59	1.36	1.52
32	7	404	8CT	C05-C06	-6.59	1.36	1.52
32	B	851	8CT	C05-C06	-6.59	1.36	1.52
32	1	402	8CT	C05-C06	-6.59	1.36	1.52
32	A	854	8CT	C05-C06	-6.59	1.36	1.52
32	B	847	8CT	C05-C06	-6.58	1.36	1.52
32	3	402	8CT	C05-C06	-6.57	1.36	1.52
32	B	845	8CT	C15-C16	6.57	1.60	1.45
32	B	843	8CT	C05-C06	-6.57	1.36	1.52
32	7	405	8CT	C05-C06	-6.56	1.36	1.52
32	I	101	8CT	C05-C06	-6.55	1.36	1.52
32	7	402	8CT	C05-C06	-6.55	1.36	1.52
32	8	402	8CT	C05-C06	-6.54	1.36	1.52
32	O	205	8CT	C05-C06	-6.53	1.36	1.52
32	L	206	8CT	C05-C06	-6.53	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	205	8CT	C05-C06	-6.53	1.36	1.52
32	9	401	8CT	C05-C06	-6.51	1.36	1.52
32	B	844	8CT	C05-C06	-6.51	1.36	1.52
32	J	101	8CT	C05-C06	-6.50	1.36	1.52
32	A	847	8CT	C05-C06	-6.50	1.36	1.52
32	L	209	8CT	C05-C06	-6.50	1.36	1.52
32	4	402	8CT	C05-C06	-6.49	1.36	1.52
32	A	846	8CT	C05-C06	-6.48	1.36	1.52
32	0	401	8CT	C05-C06	-6.48	1.36	1.52
32	3	403	8CT	C05-C06	-6.47	1.36	1.52
32	B	845	8CT	C05-C06	-6.47	1.36	1.52
32	2	402	8CT	C05-C06	-6.45	1.36	1.52
32	A	850	8CT	C05-C06	-6.45	1.36	1.52
32	3	402	8CT	C15-C16	6.43	1.59	1.45
32	2	402	8CT	C28-C26	6.42	1.59	1.45
32	4	402	8CT	C28-C26	6.42	1.59	1.45
32	B	846	8CT	C05-C06	-6.41	1.36	1.52
32	B	846	8CT	C28-C26	6.40	1.59	1.45
32	K	107	8CT	C05-C06	-6.40	1.36	1.52
32	G	104	8CT	C15-C16	6.38	1.59	1.45
32	4	402	8CT	C15-C16	6.37	1.59	1.45
32	A	848	8CT	C05-C06	-6.37	1.36	1.52
32	B	848	8CT	C15-C16	6.37	1.59	1.45
32	A	854	8CT	C15-C16	6.35	1.59	1.45
32	8	402	8CT	C15-C16	6.34	1.59	1.45
32	0	401	8CT	C28-C26	6.34	1.59	1.45
32	8	406	8CT	C15-C16	6.32	1.59	1.45
32	B	843	8CT	C28-C26	6.32	1.59	1.45
32	L	209	8CT	C15-C16	6.31	1.59	1.45
32	0	401	8CT	C15-C16	6.31	1.59	1.45
32	K	107	8CT	C15-C16	6.30	1.59	1.45
32	2	402	8CT	C15-C16	6.29	1.59	1.45
32	3	403	8CT	C15-C16	6.28	1.59	1.45
32	8	406	8CT	C28-C26	6.27	1.59	1.45
32	L	206	8CT	C15-C16	6.27	1.59	1.45
32	9	401	8CT	C15-C16	6.26	1.59	1.45
32	A	846	8CT	C15-C16	6.26	1.59	1.45
32	1	402	8CT	C15-C16	6.26	1.59	1.45
32	B	844	8CT	C23-C21	6.26	1.59	1.45
32	6	402	8CT	C15-C16	6.25	1.59	1.45
32	7	404	8CT	C15-C16	6.25	1.59	1.45
32	O	205	8CT	C15-C16	6.24	1.59	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	J	104	8CT	C15-C16	6.23	1.59	1.45
32	1	402	8CT	C28-C26	6.23	1.59	1.45
32	9	401	8CT	C28-C26	6.22	1.59	1.45
32	I	101	8CT	C15-C16	6.21	1.59	1.45
32	G	104	8CT	C28-C26	6.21	1.59	1.45
32	F	302	8CT	C15-C16	6.20	1.59	1.45
32	A	847	8CT	C15-C16	6.19	1.59	1.45
32	A	854	8CT	C28-C26	6.18	1.59	1.45
32	B	804	8CT	C15-C16	6.16	1.59	1.45
32	B	847	8CT	C15-C16	6.16	1.59	1.45
32	8	402	8CT	C28-C26	6.14	1.59	1.45
32	M	102	8CT	C15-C16	6.14	1.59	1.45
32	L	209	8CT	C28-C26	6.14	1.59	1.45
32	L	205	8CT	C15-C16	6.13	1.59	1.45
32	J	104	8CT	C28-C26	6.13	1.59	1.45
32	B	844	8CT	C28-C26	6.12	1.59	1.45
32	F	302	8CT	C28-C26	6.11	1.59	1.45
32	O	205	8CT	C28-C26	6.09	1.59	1.45
32	3	402	8CT	C28-C26	6.09	1.59	1.45
32	L	206	8CT	C28-C26	6.09	1.59	1.45
32	K	107	8CT	C28-C26	6.08	1.59	1.45
32	B	851	8CT	C15-C16	6.06	1.59	1.45
32	3	403	8CT	C28-C26	6.06	1.59	1.45
32	J	101	8CT	C15-C16	6.04	1.58	1.45
32	J	101	8CT	C28-C26	6.03	1.58	1.45
32	7	405	8CT	C15-C16	6.03	1.58	1.45
32	M	102	8CT	C28-C26	6.02	1.58	1.45
32	A	850	8CT	C04-C03	-6.02	1.45	1.53
32	6	402	8CT	C28-C26	6.02	1.58	1.45
32	B	843	8CT	C23-C21	6.01	1.58	1.45
32	B	851	8CT	C28-C26	6.00	1.58	1.45
32	L	205	8CT	C28-C26	5.99	1.58	1.45
32	7	402	8CT	C15-C16	5.99	1.58	1.45
32	B	848	8CT	C28-C26	5.97	1.58	1.45
32	A	849	8CT	C15-C16	5.97	1.58	1.45
32	B	804	8CT	C28-C26	5.96	1.58	1.45
32	A	850	8CT	C15-C16	5.95	1.58	1.45
32	A	848	8CT	C15-C16	5.94	1.58	1.45
32	B	846	8CT	C23-C21	5.94	1.58	1.45
32	2	402	8CT	C23-C21	5.94	1.58	1.45
32	7	405	8CT	C28-C26	5.93	1.58	1.45
32	I	101	8CT	C28-C26	5.90	1.58	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	402	8CT	C23-C21	5.89	1.58	1.45
32	7	402	8CT	C28-C26	5.89	1.58	1.45
32	B	847	8CT	C28-C26	5.88	1.58	1.45
32	A	846	8CT	C28-C26	5.86	1.58	1.45
32	0	401	8CT	C23-C21	5.86	1.58	1.45
32	A	847	8CT	C28-C26	5.85	1.58	1.45
32	7	404	8CT	C28-C26	5.85	1.58	1.45
32	A	848	8CT	C28-C26	5.84	1.58	1.45
32	A	849	8CT	C28-C26	5.84	1.58	1.45
32	6	402	8CT	C23-C21	5.81	1.58	1.45
32	J	104	8CT	C23-C21	5.81	1.58	1.45
32	B	845	8CT	C28-C26	5.79	1.58	1.45
32	J	101	8CT	C04-C03	-5.78	1.45	1.53
32	G	104	8CT	C23-C21	5.78	1.58	1.45
32	8	406	8CT	C23-C21	5.78	1.58	1.45
32	B	845	8CT	C23-C21	5.76	1.58	1.45
32	9	401	8CT	C23-C21	5.76	1.58	1.45
32	7	402	8CT	C04-C03	-5.75	1.45	1.53
32	L	206	8CT	C23-C21	5.74	1.58	1.45
32	3	402	8CT	C23-C21	5.73	1.58	1.45
32	A	854	8CT	C23-C21	5.72	1.58	1.45
32	1	402	8CT	C23-C21	5.71	1.58	1.45
32	B	847	8CT	C23-C21	5.71	1.58	1.45
32	A	847	8CT	C04-C03	-5.70	1.45	1.53
32	9	401	8CT	C04-C03	-5.70	1.45	1.53
32	B	848	8CT	C23-C21	5.69	1.58	1.45
32	4	402	8CT	C34-C33	5.66	1.65	1.52
32	B	845	8CT	C04-C03	-5.65	1.46	1.53
32	I	101	8CT	C04-C03	-5.64	1.46	1.53
32	8	402	8CT	C23-C21	5.64	1.58	1.45
32	A	850	8CT	C28-C26	5.63	1.58	1.45
32	B	851	8CT	C04-C03	-5.62	1.46	1.53
32	F	302	8CT	C23-C21	5.62	1.58	1.45
32	A	849	8CT	C04-C03	-5.62	1.46	1.53
32	3	403	8CT	C04-C03	-5.62	1.46	1.53
32	O	205	8CT	C23-C21	5.62	1.58	1.45
32	0	401	8CT	C04-C03	-5.62	1.46	1.53
32	7	405	8CT	C23-C21	5.61	1.58	1.45
32	J	101	8CT	C23-C21	5.60	1.58	1.45
32	L	209	8CT	C23-C21	5.60	1.58	1.45
32	B	846	8CT	C04-C03	-5.59	1.46	1.53
32	0	401	8CT	C34-C33	5.59	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	K	107	8CT	C23-C21	5.59	1.57	1.45
32	B	851	8CT	C23-C21	5.58	1.57	1.45
32	M	102	8CT	C04-C03	-5.57	1.46	1.53
32	A	848	8CT	C04-C03	-5.57	1.46	1.53
32	2	402	8CT	C34-C33	5.56	1.65	1.52
32	7	404	8CT	C23-C21	5.56	1.57	1.45
32	I	101	8CT	C23-C21	5.55	1.57	1.45
32	L	205	8CT	C23-C21	5.54	1.57	1.45
32	3	403	8CT	C23-C21	5.54	1.57	1.45
32	J	101	8CT	C34-C33	5.54	1.65	1.52
32	M	102	8CT	C23-C21	5.53	1.57	1.45
32	A	854	8CT	C34-C33	5.53	1.65	1.52
32	I	101	8CT	C34-C33	5.53	1.65	1.52
32	B	844	8CT	C34-C33	5.52	1.65	1.52
32	3	402	8CT	C34-C33	5.52	1.65	1.52
32	B	843	8CT	C04-C03	-5.52	1.46	1.53
32	B	804	8CT	C04-C03	-5.49	1.46	1.53
32	4	402	8CT	C04-C03	-5.49	1.46	1.53
32	7	402	8CT	C23-C21	5.49	1.57	1.45
32	9	401	8CT	C34-C33	5.49	1.65	1.52
32	A	846	8CT	C04-C03	-5.48	1.46	1.53
32	O	205	8CT	C04-C03	-5.47	1.46	1.53
32	L	206	8CT	C04-C03	-5.47	1.46	1.53
32	7	402	8CT	C34-C33	5.47	1.65	1.52
32	A	854	8CT	C04-C03	-5.46	1.46	1.53
32	2	402	8CT	C04-C03	-5.46	1.46	1.53
32	L	205	8CT	C04-C03	-5.46	1.46	1.53
32	A	846	8CT	C23-C21	5.45	1.57	1.45
32	A	849	8CT	C34-C33	5.44	1.65	1.52
32	B	804	8CT	C23-C21	5.43	1.57	1.45
32	J	104	8CT	C34-C33	5.41	1.65	1.52
32	1	402	8CT	C04-C03	-5.41	1.46	1.53
32	6	402	8CT	C04-C03	-5.40	1.46	1.53
32	O	205	8CT	C34-C33	5.40	1.65	1.52
32	8	402	8CT	C34-C33	5.40	1.65	1.52
32	8	402	8CT	C04-C03	-5.39	1.46	1.53
32	7	405	8CT	C04-C03	-5.39	1.46	1.53
32	L	206	8CT	C34-C33	5.38	1.65	1.52
32	3	402	8CT	C04-C03	-5.37	1.46	1.53
32	B	847	8CT	C04-C03	-5.36	1.46	1.53
32	K	107	8CT	C34-C33	5.35	1.65	1.52
32	A	847	8CT	C23-C21	5.35	1.57	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	849	8CT	C23-C21	5.35	1.57	1.45
32	G	104	8CT	C34-C33	5.35	1.65	1.52
32	M	102	8CT	C34-C33	5.34	1.65	1.52
32	8	406	8CT	C34-C33	5.34	1.65	1.52
32	F	302	8CT	C34-C33	5.34	1.65	1.52
32	A	848	8CT	C23-C21	5.33	1.57	1.45
32	B	846	8CT	C34-C33	5.32	1.65	1.52
32	6	402	8CT	C34-C33	5.31	1.65	1.52
32	L	209	8CT	C04-C03	-5.31	1.46	1.53
32	A	846	8CT	C34-C33	5.31	1.65	1.52
32	7	404	8CT	C04-C03	-5.31	1.46	1.53
32	7	404	8CT	C34-C33	5.31	1.65	1.52
32	A	847	8CT	C34-C33	5.30	1.65	1.52
32	F	302	8CT	C04-C03	-5.30	1.46	1.53
32	B	845	8CT	C34-C33	5.30	1.65	1.52
32	B	851	8CT	C34-C33	5.29	1.65	1.52
32	1	402	8CT	C34-C33	5.29	1.65	1.52
32	B	848	8CT	C34-C33	5.29	1.65	1.52
32	B	844	8CT	C04-C03	-5.28	1.46	1.53
32	L	205	8CT	C34-C33	5.28	1.65	1.52
32	K	107	8CT	C04-C03	-5.26	1.46	1.53
32	A	850	8CT	C23-C21	5.25	1.57	1.45
32	B	847	8CT	C34-C33	5.24	1.64	1.52
30	h	614	CHL	O2D-CGD	5.24	1.46	1.33
32	3	403	8CT	C34-C33	5.24	1.64	1.52
32	B	804	8CT	C34-C33	5.23	1.64	1.52
32	B	843	8CT	C34-C33	5.22	1.64	1.52
30	e	614	CHL	O2D-CGD	5.22	1.45	1.33
32	7	405	8CT	C34-C33	5.21	1.64	1.52
30	g	605	CHL	O2D-CGD	5.21	1.45	1.33
30	h	606	CHL	O2D-CGD	5.20	1.45	1.33
32	L	209	8CT	C34-C33	5.20	1.64	1.52
30	g	614	CHL	O2D-CGD	5.20	1.45	1.33
30	f	605	CHL	O2D-CGD	5.20	1.45	1.33
30	a	614	CHL	O2D-CGD	5.20	1.45	1.33
32	K	107	8CT	C05-C04	5.20	1.66	1.54
30	f	607	CHL	O2D-CGD	5.19	1.45	1.33
30	e	601	CHL	O2D-CGD	5.19	1.45	1.33
32	G	104	8CT	C04-C03	-5.19	1.46	1.53
30	i	605	CHL	O2D-CGD	5.18	1.45	1.33
30	i	609	CHL	O2D-CGD	5.18	1.45	1.33
30	g	608	CHL	O2D-CGD	5.18	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	607	CHL	O2D-CGD	5.18	1.45	1.33
30	i	606	CHL	O2D-CGD	5.18	1.45	1.33
30	5	306	CHL	O2D-CGD	5.18	1.45	1.33
30	d	602	CHL	O2D-CGD	5.18	1.45	1.33
30	d	614	CHL	O2D-CGD	5.17	1.45	1.33
30	b	609	CHL	O2D-CGD	5.17	1.45	1.33
30	g	601	CHL	O2D-CGD	5.17	1.45	1.33
30	g	607	CHL	O2D-CGD	5.17	1.45	1.33
30	i	607	CHL	O2D-CGD	5.17	1.45	1.33
30	h	602	CHL	O2D-CGD	5.17	1.45	1.33
30	a	607	CHL	O2D-CGD	5.16	1.45	1.33
30	h	601	CHL	O2D-CGD	5.16	1.45	1.33
30	e	602	CHL	O2D-CGD	5.16	1.45	1.33
30	a	605	CHL	O2D-CGD	5.16	1.45	1.33
30	a	602	CHL	O2D-CGD	5.16	1.45	1.33
30	d	605	CHL	O2D-CGD	5.16	1.45	1.33
30	g	602	CHL	O2D-CGD	5.15	1.45	1.33
30	c	606	CHL	O2D-CGD	5.15	1.45	1.33
30	d	608	CHL	O2D-CGD	5.15	1.45	1.33
30	g	606	CHL	O2D-CGD	5.15	1.45	1.33
32	L	205	8CT	C05-C04	5.14	1.66	1.54
30	a	609	CHL	O2D-CGD	5.14	1.45	1.33
30	e	605	CHL	O2D-CGD	5.14	1.45	1.33
30	h	607	CHL	O2D-CGD	5.14	1.45	1.33
32	A	848	8CT	C05-C04	5.14	1.66	1.54
30	c	605	CHL	O2D-CGD	5.14	1.45	1.33
30	d	606	CHL	O2D-CGD	5.14	1.45	1.33
30	d	601	CHL	O2D-CGD	5.13	1.45	1.33
32	2	402	8CT	C05-C04	5.13	1.66	1.54
30	h	605	CHL	O2D-CGD	5.13	1.45	1.33
30	i	601	CHL	O2D-CGD	5.13	1.45	1.33
30	i	614	CHL	O2D-CGD	5.13	1.45	1.33
30	d	609	CHL	O2D-CGD	5.13	1.45	1.33
30	i	608	CHL	O2D-CGD	5.13	1.45	1.33
30	i	602	CHL	O2D-CGD	5.13	1.45	1.33
30	5	305	CHL	O2D-CGD	5.12	1.45	1.33
32	O	205	8CT	C05-C04	5.12	1.65	1.54
30	b	601	CHL	O2D-CGD	5.12	1.45	1.33
30	h	605	CHL	C2C-C3C	5.12	1.47	1.36
32	L	209	8CT	C05-C04	5.11	1.65	1.54
32	A	850	8CT	C34-C33	5.11	1.64	1.52
30	b	606	CHL	O2D-CGD	5.11	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	608	CHL	O2D-CGD	5.11	1.45	1.33
30	d	605	CHL	C2C-C3C	5.11	1.47	1.36
30	0	305	CHL	O2D-CGD	5.11	1.45	1.33
32	A	848	8CT	C34-C33	5.11	1.64	1.52
30	h	609	CHL	O2D-CGD	5.11	1.45	1.33
30	f	609	CHL	O2D-CGD	5.11	1.45	1.33
30	f	606	CHL	O2D-CGD	5.10	1.45	1.33
30	a	606	CHL	O2D-CGD	5.10	1.45	1.33
30	c	607	CHL	O2D-CGD	5.10	1.45	1.33
32	8	406	8CT	C04-C03	-5.10	1.46	1.53
30	c	608	CHL	O2D-CGD	5.10	1.45	1.33
30	g	605	CHL	C2C-C3C	5.10	1.47	1.36
30	e	607	CHL	O2D-CGD	5.10	1.45	1.33
30	f	602	CHL	O2D-CGD	5.10	1.45	1.33
30	e	608	CHL	O2D-CGD	5.10	1.45	1.33
30	g	609	CHL	O2D-CGD	5.09	1.45	1.33
30	6	315	CHL	O2D-CGD	5.09	1.45	1.33
30	e	609	CHL	O2D-CGD	5.08	1.45	1.33
30	c	602	CHL	O2D-CGD	5.08	1.45	1.33
30	b	608	CHL	O2D-CGD	5.08	1.45	1.33
32	J	104	8CT	C04-C03	-5.08	1.46	1.53
30	h	614	CHL	C2C-C3C	5.08	1.47	1.36
30	b	607	CHL	O2D-CGD	5.08	1.45	1.33
32	L	206	8CT	C05-C04	5.08	1.65	1.54
30	d	605	CHL	CHD-C1D	5.08	1.48	1.38
30	g	614	CHL	CHD-C1D	5.07	1.48	1.38
30	d	614	CHL	C2C-C3C	5.07	1.47	1.36
30	e	606	CHL	O2D-CGD	5.07	1.45	1.33
30	f	614	CHL	O2D-CGD	5.07	1.45	1.33
30	8	315	CHL	O2D-CGD	5.07	1.45	1.33
30	f	608	CHL	O2D-CGD	5.07	1.45	1.33
30	g	609	CHL	C2C-C3C	5.07	1.47	1.36
30	8	305	CHL	O2D-CGD	5.07	1.45	1.33
30	9	313	CHL	O2D-CGD	5.07	1.45	1.33
30	f	601	CHL	O2D-CGD	5.06	1.45	1.33
30	c	609	CHL	O2D-CGD	5.06	1.45	1.33
30	a	601	CHL	O2D-CGD	5.06	1.45	1.33
30	b	602	CHL	O2D-CGD	5.06	1.45	1.33
30	i	605	CHL	C2C-C3C	5.06	1.47	1.36
30	a	614	CHL	C2C-C3C	5.05	1.47	1.36
32	1	402	8CT	C05-C04	5.05	1.65	1.54
32	9	401	8CT	C05-C04	5.05	1.65	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	607	CHL	C2C-C3C	5.05	1.47	1.36
30	1	305	CHL	O2D-CGD	5.05	1.45	1.33
30	6	305	CHL	O2D-CGD	5.05	1.45	1.33
30	h	605	CHL	CHD-C1D	5.05	1.48	1.38
30	g	605	CHL	CHD-C1D	5.04	1.48	1.38
30	a	605	CHL	C2C-C3C	5.04	1.47	1.36
30	g	614	CHL	C2C-C3C	5.04	1.47	1.36
30	b	614	CHL	O2D-CGD	5.04	1.45	1.33
30	i	614	CHL	C2C-C3C	5.04	1.47	1.36
30	i	605	CHL	CHD-C1D	5.04	1.48	1.38
30	4	302	CHL	O2D-CGD	5.04	1.45	1.33
30	c	605	CHL	C2C-C3C	5.04	1.47	1.36
30	a	608	CHL	O2D-CGD	5.03	1.45	1.33
30	8	313	CHL	O2D-CGD	5.03	1.45	1.33
32	7	405	8CT	C05-C04	5.03	1.65	1.54
30	g	601	CHL	C2C-C3C	5.03	1.47	1.36
30	0	301	CHL	O2D-CGD	5.03	1.45	1.33
30	9	305	CHL	O2D-CGD	5.02	1.45	1.33
30	6	306	CHL	O2D-CGD	5.02	1.45	1.33
30	1	313	CHL	O2D-CGD	5.02	1.45	1.33
30	c	601	CHL	O2D-CGD	5.02	1.45	1.33
30	4	306	CHL	O2D-CGD	5.01	1.45	1.33
30	h	609	CHL	C2C-C3C	5.01	1.47	1.36
30	a	605	CHL	CHD-C1D	5.01	1.48	1.38
30	4	305	CHL	O2D-CGD	5.01	1.45	1.33
32	J	101	8CT	C05-C04	5.01	1.65	1.54
30	6	313	CHL	O2D-CGD	5.01	1.45	1.33
30	f	605	CHL	C2C-C3C	5.00	1.47	1.36
30	g	601	CHL	CHD-C1D	5.00	1.48	1.38
30	i	609	CHL	C2C-C3C	5.00	1.47	1.36
30	a	614	CHL	CHD-C1D	5.00	1.48	1.38
30	5	313	CHL	O2D-CGD	5.00	1.45	1.33
32	0	401	8CT	C05-C04	5.00	1.65	1.54
30	9	306	CHL	O2D-CGD	5.00	1.45	1.33
30	7	313	CHL	O2D-CGD	5.00	1.45	1.33
30	c	605	CHL	CHD-C1D	4.99	1.48	1.38
30	f	605	CHL	CHD-C1D	4.99	1.48	1.38
30	5	307	CHL	O2D-CGD	4.99	1.45	1.33
30	6	307	CHL	O2D-CGD	4.99	1.45	1.33
32	8	406	8CT	C05-C04	4.99	1.65	1.54
30	9	301	CHL	O2D-CGD	4.98	1.45	1.33
30	0	302	CHL	O2D-CGD	4.98	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	104	8CT	C05-C04	4.98	1.65	1.54
32	B	846	8CT	C05-C04	4.98	1.65	1.54
30	2	306	CHL	O2D-CGD	4.98	1.45	1.33
30	7	307	CHL	O2D-CGD	4.98	1.45	1.33
30	8	306	CHL	O2D-CGD	4.98	1.45	1.33
32	8	402	8CT	C05-C04	4.97	1.65	1.54
30	h	601	CHL	C2C-C3C	4.97	1.47	1.36
30	7	301	CHL	O2D-CGD	4.97	1.45	1.33
32	B	848	8CT	C04-C03	-4.97	1.46	1.53
30	3	305	CHL	O2D-CGD	4.97	1.45	1.33
30	1	307	CHL	O2D-CGD	4.97	1.45	1.33
30	5	301	CHL	O2D-CGD	4.97	1.45	1.33
32	B	847	8CT	C05-C04	4.97	1.65	1.54
30	3	302	CHL	O2D-CGD	4.97	1.45	1.33
30	i	609	CHL	CHD-C1D	4.97	1.48	1.38
30	2	313	CHL	O2D-CGD	4.97	1.45	1.33
30	d	614	CHL	CHD-C1D	4.97	1.48	1.38
30	2	305	CHL	O2D-CGD	4.97	1.45	1.33
30	7	305	CHL	O2D-CGD	4.96	1.45	1.33
30	e	614	CHL	C2C-C3C	4.96	1.47	1.36
30	g	609	CHL	CHD-C1D	4.96	1.48	1.38
30	3	307	CHL	O2D-CGD	4.96	1.45	1.33
30	2	307	CHL	O2D-CGD	4.96	1.45	1.33
30	h	614	CHL	CHD-C1D	4.96	1.48	1.38
30	4	307	CHL	O2D-CGD	4.96	1.45	1.33
32	7	404	8CT	C05-C04	4.95	1.65	1.54
32	M	102	8CT	C05-C04	4.95	1.65	1.54
30	0	306	CHL	C2C-C3C	4.95	1.47	1.36
32	6	402	8CT	C05-C04	4.95	1.65	1.54
32	B	844	8CT	C05-C04	4.95	1.65	1.54
30	a	609	CHL	CHD-C1D	4.95	1.48	1.38
30	2	302	CHL	O2D-CGD	4.95	1.45	1.33
30	7	306	CHL	O2D-CGD	4.95	1.45	1.33
30	i	607	CHL	C2C-C3C	4.94	1.47	1.36
30	h	602	CHL	C2C-C3C	4.94	1.47	1.36
30	5	313	CHL	C2C-C3C	4.94	1.47	1.36
30	g	607	CHL	CHD-C1D	4.94	1.48	1.38
32	B	848	8CT	C05-C04	4.94	1.65	1.54
30	i	614	CHL	CHD-C1D	4.93	1.48	1.38
30	8	308	CHL	O2D-CGD	4.93	1.45	1.33
32	A	847	8CT	C05-C04	4.93	1.65	1.54
30	h	609	CHL	CHD-C1D	4.92	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	313	CHL	O2D-CGD	4.92	1.45	1.33
30	4	308	CHL	O2D-CGD	4.92	1.45	1.33
32	3	403	8CT	C05-C04	4.92	1.65	1.54
30	g	608	CHL	C2C-C3C	4.92	1.47	1.36
30	c	609	CHL	CHD-C1D	4.92	1.47	1.38
30	a	601	CHL	C2C-C3C	4.92	1.47	1.36
30	a	609	CHL	C2C-C3C	4.92	1.47	1.36
30	g	607	CHL	C2C-C3C	4.91	1.47	1.36
30	a	607	CHL	C2C-C3C	4.91	1.47	1.36
30	8	302	CHL	O2D-CGD	4.91	1.45	1.33
32	B	843	8CT	C05-C04	4.91	1.65	1.54
30	1	302	CHL	O2D-CGD	4.91	1.45	1.33
30	5	306	CHL	C2C-C3C	4.91	1.47	1.36
30	5	302	CHL	O2D-CGD	4.91	1.45	1.33
30	c	614	CHL	O2D-CGD	4.91	1.45	1.33
32	A	854	8CT	C05-C04	4.91	1.65	1.54
32	4	402	8CT	C05-C04	4.91	1.65	1.54
32	3	402	8CT	C05-C04	4.90	1.65	1.54
30	i	601	CHL	C2C-C3C	4.90	1.47	1.36
30	2	308	CHL	O2D-CGD	4.90	1.45	1.33
30	d	607	CHL	C2C-C3C	4.90	1.47	1.36
30	h	601	CHL	CHD-C1D	4.90	1.47	1.38
30	i	606	CHL	CHD-C1D	4.90	1.47	1.38
32	B	845	8CT	C05-C04	4.90	1.65	1.54
30	1	306	CHL	O2D-CGD	4.90	1.45	1.33
30	e	614	CHL	CHD-C1D	4.90	1.47	1.38
30	6	308	CHL	O2D-CGD	4.90	1.45	1.33
30	i	606	CHL	C2C-C3C	4.89	1.47	1.36
30	a	607	CHL	CHD-C1D	4.89	1.47	1.38
30	d	609	CHL	CHD-C1D	4.89	1.47	1.38
30	g	608	CHL	CHD-C1D	4.89	1.47	1.38
30	8	301	CHL	O2D-CGD	4.89	1.45	1.33
30	6	301	CHL	O2D-CGD	4.89	1.45	1.33
30	8	307	CHL	O2D-CGD	4.89	1.45	1.33
30	e	605	CHL	C2C-C3C	4.88	1.47	1.36
30	b	614	CHL	C2C-C3C	4.88	1.47	1.36
32	B	851	8CT	C05-C04	4.88	1.65	1.54
32	J	104	8CT	C05-C04	4.88	1.65	1.54
30	2	319	CHL	O2D-CGD	4.88	1.45	1.33
30	i	607	CHL	CHD-C1D	4.88	1.47	1.38
30	c	609	CHL	C2C-C3C	4.87	1.47	1.36
30	d	609	CHL	C2C-C3C	4.87	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	I	101	8CT	C05-C04	4.87	1.65	1.54
30	5	313	CHL	CHD-C1D	4.87	1.47	1.38
30	h	607	CHL	CHD-C1D	4.87	1.47	1.38
30	d	607	CHL	CHD-C1D	4.87	1.47	1.38
30	a	606	CHL	C2C-C3C	4.87	1.47	1.36
30	d	601	CHL	C2C-C3C	4.87	1.47	1.36
30	b	601	CHL	C2C-C3C	4.87	1.47	1.36
30	i	601	CHL	CHD-C1D	4.87	1.47	1.38
30	g	606	CHL	C2C-C3C	4.86	1.47	1.36
30	4	319	CHL	O2D-CGD	4.86	1.45	1.33
32	A	846	8CT	C05-C04	4.86	1.65	1.54
30	d	601	CHL	CHD-C1D	4.86	1.47	1.38
30	c	607	CHL	C2C-C3C	4.86	1.47	1.36
32	7	402	8CT	C05-C04	4.85	1.65	1.54
30	f	609	CHL	C2C-C3C	4.85	1.47	1.36
32	B	804	8CT	C05-C04	4.85	1.65	1.54
30	f	607	CHL	CHD-C1D	4.84	1.47	1.38
32	F	302	8CT	C05-C04	4.84	1.65	1.54
30	7	302	CHL	O2D-CGD	4.83	1.45	1.33
30	e	607	CHL	C2C-C3C	4.83	1.47	1.36
30	0	306	CHL	O2D-CGD	4.83	1.45	1.33
30	5	307	CHL	C2C-C3C	4.83	1.47	1.36
30	5	306	CHL	CHD-C1D	4.82	1.47	1.38
30	5	301	CHL	C2C-C3C	4.82	1.47	1.36
30	h	608	CHL	C2C-C3C	4.82	1.47	1.36
33	d	520	0UR	O44-C45	4.82	1.45	1.34
30	f	607	CHL	C2C-C3C	4.82	1.47	1.36
30	f	609	CHL	CHD-C1D	4.81	1.47	1.38
30	e	605	CHL	CHD-C1D	4.81	1.47	1.38
30	a	606	CHL	CHD-C1D	4.81	1.47	1.38
33	3	501	0UR	O44-C45	4.81	1.45	1.34
30	b	614	CHL	CHD-C1D	4.80	1.47	1.38
30	f	606	CHL	C2C-C3C	4.80	1.47	1.36
32	A	850	8CT	C05-C04	4.80	1.65	1.54
30	f	614	CHL	C2C-C3C	4.80	1.47	1.36
33	h	520	0UR	O44-C45	4.80	1.45	1.34
33	2	501	0UR	O44-C45	4.80	1.45	1.34
30	h	602	CHL	CHD-C1D	4.80	1.47	1.38
30	b	609	CHL	CHD-C1D	4.80	1.47	1.38
33	0	501	0UR	O44-C45	4.79	1.45	1.34
30	2	301	CHL	O2D-CGD	4.79	1.44	1.33
30	b	601	CHL	CHD-C1D	4.79	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	O	204	0UR	O44-C45	4.79	1.45	1.34
33	7	501	0UR	O44-C45	4.79	1.45	1.34
32	A	849	8CT	C05-C04	4.79	1.65	1.54
30	d	608	CHL	C2C-C3C	4.79	1.47	1.36
30	d	606	CHL	C2C-C3C	4.79	1.47	1.36
30	a	601	CHL	CHD-C1D	4.78	1.47	1.38
30	g	602	CHL	C2C-C3C	4.78	1.47	1.36
30	e	607	CHL	CHD-C1D	4.77	1.47	1.38
30	b	609	CHL	C2C-C3C	4.77	1.47	1.36
30	h	606	CHL	C2C-C3C	4.77	1.47	1.36
30	c	614	CHL	C2C-C3C	4.77	1.47	1.36
30	i	602	CHL	C2C-C3C	4.76	1.47	1.36
30	f	614	CHL	CHD-C1D	4.76	1.47	1.38
30	f	606	CHL	CHD-C1D	4.76	1.47	1.38
30	g	606	CHL	CHD-C1D	4.76	1.47	1.38
30	f	601	CHL	C2C-C3C	4.76	1.46	1.36
30	e	609	CHL	C2C-C3C	4.76	1.46	1.36
30	b	607	CHL	C2C-C3C	4.76	1.46	1.36
30	h	606	CHL	CHD-C1D	4.75	1.47	1.38
33	5	501	0UR	O44-C45	4.75	1.45	1.34
30	8	315	CHL	C2C-C3C	4.75	1.46	1.36
30	e	606	CHL	C2C-C3C	4.75	1.46	1.36
30	i	608	CHL	C2C-C3C	4.74	1.46	1.36
30	i	608	CHL	CHD-C1D	4.74	1.47	1.38
33	g	520	0UR	O44-C45	4.74	1.45	1.34
30	a	608	CHL	C2C-C3C	4.74	1.46	1.36
33	i	520	0UR	O44-C45	4.74	1.45	1.34
30	c	607	CHL	CHD-C1D	4.73	1.47	1.38
30	a	602	CHL	C2C-C3C	4.73	1.46	1.36
30	h	608	CHL	CHD-C1D	4.73	1.47	1.38
30	d	606	CHL	CHD-C1D	4.73	1.47	1.38
30	g	602	CHL	CHD-C1D	4.73	1.47	1.38
33	c	520	0UR	O44-C45	4.72	1.45	1.34
30	5	307	CHL	CHD-C1D	4.72	1.47	1.38
30	c	608	CHL	C2C-C3C	4.72	1.46	1.36
33	0	502	0UR	O44-C45	4.72	1.45	1.34
33	9	501	0UR	O44-C45	4.71	1.45	1.34
33	e	520	0UR	O44-C45	4.71	1.45	1.34
30	5	305	CHL	C2C-C3C	4.71	1.46	1.36
30	8	315	CHL	CHD-C1D	4.71	1.47	1.38
30	5	305	CHL	CHD-C1D	4.70	1.47	1.38
30	e	601	CHL	C2C-C3C	4.70	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	502	0UR	O44-C45	4.69	1.45	1.34
30	0	305	CHL	C2C-C3C	4.69	1.46	1.36
30	c	614	CHL	CHD-C1D	4.69	1.47	1.38
30	c	601	CHL	C2C-C3C	4.69	1.46	1.36
33	f	520	0UR	O44-C45	4.69	1.45	1.34
33	8	501	0UR	O44-C45	4.67	1.45	1.34
30	1	307	CHL	C2C-C3C	4.67	1.46	1.36
30	9	313	CHL	C2C-C3C	4.67	1.46	1.36
33	b	520	0UR	O44-C45	4.67	1.45	1.34
33	2	502	0UR	O44-C45	4.66	1.45	1.34
30	d	605	CHL	CHC-C1C	4.66	1.48	1.38
32	A	850	8CT	C06-C07	4.66	1.67	1.52
30	8	301	CHL	C2C-C3C	4.66	1.46	1.36
30	a	602	CHL	CHD-C1D	4.66	1.47	1.38
33	8	502	0UR	O44-C45	4.66	1.45	1.34
32	B	846	8CT	C06-C07	4.66	1.67	1.52
33	1	501	0UR	O44-C45	4.65	1.45	1.34
30	6	302	CHL	O2D-CGD	4.65	1.44	1.33
30	h	602	CHL	CHC-C1C	4.65	1.48	1.38
33	4	501	0UR	O44-C45	4.65	1.45	1.34
33	6	502	0UR	O44-C45	4.65	1.45	1.34
30	i	602	CHL	CHD-C1D	4.65	1.47	1.38
30	d	608	CHL	CHD-C1D	4.65	1.47	1.38
30	b	607	CHL	CHD-C1D	4.64	1.47	1.38
30	a	608	CHL	CHD-C1D	4.64	1.47	1.38
30	7	301	CHL	C2C-C3C	4.63	1.46	1.36
32	3	403	8CT	C06-C07	4.63	1.67	1.52
30	8	308	CHL	C2C-C3C	4.63	1.46	1.36
30	b	606	CHL	C2C-C3C	4.62	1.46	1.36
32	B	848	8CT	C19-C20	4.62	1.57	1.43
30	7	306	CHL	C2C-C3C	4.62	1.46	1.36
33	1	502	0UR	O44-C45	4.62	1.45	1.34
30	h	605	CHL	CHC-C1C	4.62	1.47	1.38
30	f	608	CHL	C2C-C3C	4.62	1.46	1.36
30	h	614	CHL	CHC-C1C	4.61	1.47	1.38
30	7	313	CHL	C2C-C3C	4.61	1.46	1.36
30	e	609	CHL	CHD-C1D	4.61	1.47	1.38
30	g	605	CHL	CHC-C1C	4.61	1.47	1.38
30	2	301	CHL	C2C-C3C	4.61	1.46	1.36
30	e	602	CHL	C2C-C3C	4.61	1.46	1.36
32	0	401	8CT	C06-C07	4.61	1.67	1.52
30	1	306	CHL	C2C-C3C	4.60	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	J	101	8CT	C06-C07	4.60	1.67	1.52
37	d	522	0IE	C15-C16	4.60	1.41	1.35
30	e	602	CHL	CHD-C1D	4.60	1.47	1.38
32	A	847	8CT	C06-C07	4.60	1.67	1.52
30	c	606	CHL	C2C-C3C	4.59	1.46	1.36
30	a	605	CHL	CHC-C1C	4.59	1.47	1.38
30	e	608	CHL	C2C-C3C	4.59	1.46	1.36
30	6	315	CHL	C2C-C3C	4.59	1.46	1.36
30	8	305	CHL	C2C-C3C	4.59	1.46	1.36
32	K	107	8CT	C06-C07	4.59	1.66	1.52
30	g	608	CHL	CHC-C1C	4.59	1.47	1.38
30	c	608	CHL	CHD-C1D	4.59	1.47	1.38
30	f	601	CHL	CHD-C1D	4.59	1.47	1.38
30	i	605	CHL	CHC-C1C	4.58	1.47	1.38
30	a	614	CHL	CHC-C1C	4.58	1.47	1.38
30	g	614	CHL	CHC-C1C	4.58	1.47	1.38
32	7	402	8CT	C06-C07	4.58	1.66	1.52
32	B	845	8CT	C06-C07	4.58	1.66	1.52
30	4	306	CHL	C2C-C3C	4.58	1.46	1.36
32	A	848	8CT	C06-C07	4.58	1.66	1.52
30	e	601	CHL	CHD-C1D	4.58	1.47	1.38
33	9	502	0UR	O44-C45	4.57	1.45	1.34
30	d	614	CHL	CHC-C1C	4.57	1.47	1.38
30	d	602	CHL	C2C-C3C	4.57	1.46	1.36
33	4	502	0UR	O44-C45	4.57	1.45	1.34
30	2	308	CHL	C2C-C3C	4.56	1.46	1.36
32	A	846	8CT	C06-C07	4.56	1.66	1.52
30	8	306	CHL	C2C-C3C	4.56	1.46	1.36
30	4	308	CHL	C2C-C3C	4.56	1.46	1.36
30	9	301	CHL	C2C-C3C	4.56	1.46	1.36
30	4	319	CHL	C2C-C3C	4.56	1.46	1.36
30	h	607	CHL	CHC-C1C	4.56	1.47	1.38
32	B	844	8CT	C06-C07	4.56	1.66	1.52
30	c	601	CHL	CHD-C1D	4.56	1.47	1.38
33	6	501	0UR	O44-C45	4.55	1.45	1.34
30	0	305	CHL	CHD-C1D	4.55	1.47	1.38
30	2	306	CHL	C2C-C3C	4.55	1.46	1.36
30	0	301	CHL	C2C-C3C	4.55	1.46	1.36
32	4	402	8CT	C06-C07	4.55	1.66	1.52
32	I	101	8CT	C06-C07	4.55	1.66	1.52
30	e	608	CHL	CHD-C1D	4.55	1.47	1.38
30	d	607	CHL	CHC-C1C	4.54	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	306	CHL	CHD-C1D	4.54	1.47	1.38
32	L	209	8CT	C06-C07	4.54	1.66	1.52
30	8	306	CHL	CHD-C1D	4.54	1.47	1.38
30	f	605	CHL	CHC-C1C	4.54	1.47	1.38
30	d	601	CHL	CHC-C1C	4.54	1.47	1.38
30	6	301	CHL	C2C-C3C	4.54	1.46	1.36
30	5	301	CHL	CHD-C1D	4.53	1.47	1.38
30	9	306	CHL	C2C-C3C	4.53	1.46	1.36
30	c	606	CHL	CHD-C1D	4.53	1.47	1.38
30	e	606	CHL	CHD-C1D	4.53	1.47	1.38
32	7	405	8CT	C06-C07	4.53	1.66	1.52
30	1	313	CHL	C2C-C3C	4.53	1.46	1.36
30	c	605	CHL	CHC-C1C	4.53	1.47	1.38
32	9	401	8CT	C06-C07	4.53	1.66	1.52
30	6	313	CHL	C2C-C3C	4.52	1.46	1.36
30	g	601	CHL	CHC-C1C	4.52	1.47	1.38
30	h	608	CHL	O2A-CGA	4.52	1.45	1.30
38	A	842	PQN	C10-C5	4.52	1.48	1.40
30	i	601	CHL	CHC-C1C	4.52	1.47	1.38
30	6	315	CHL	CHD-C1D	4.52	1.47	1.38
30	b	602	CHL	C2C-C3C	4.52	1.46	1.36
30	2	313	CHL	C2C-C3C	4.51	1.46	1.36
30	2	319	CHL	C2C-C3C	4.51	1.46	1.36
30	4	308	CHL	CHD-C1D	4.51	1.47	1.38
30	6	308	CHL	C2C-C3C	4.51	1.46	1.36
30	e	605	CHL	CHC-C1C	4.51	1.47	1.38
32	B	843	8CT	C06-C07	4.51	1.66	1.52
32	O	205	8CT	C06-C07	4.51	1.66	1.52
30	7	306	CHL	CHD-C1D	4.50	1.47	1.38
32	3	402	8CT	C06-C07	4.50	1.66	1.52
30	g	602	CHL	CHC-C1C	4.50	1.47	1.38
30	i	609	CHL	CHC-C1C	4.50	1.47	1.38
30	4	307	CHL	C2C-C3C	4.50	1.46	1.36
30	h	607	CHL	O2A-CGA	4.50	1.45	1.30
30	1	305	CHL	C2C-C3C	4.49	1.46	1.36
32	L	206	8CT	C06-C07	4.49	1.66	1.52
32	A	854	8CT	C06-C07	4.49	1.66	1.52
30	8	308	CHL	CHD-C1D	4.49	1.47	1.38
30	8	313	CHL	C2C-C3C	4.49	1.46	1.36
30	g	609	CHL	CHC-C1C	4.49	1.47	1.38
32	L	205	8CT	C06-C07	4.49	1.66	1.52
32	7	404	8CT	C06-C07	4.48	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	402	8CT	C19-C20	4.48	1.57	1.43
30	b	608	CHL	C2C-C3C	4.48	1.46	1.36
30	b	608	CHL	CHD-C1D	4.48	1.47	1.38
30	1	307	CHL	CHD-C1D	4.48	1.47	1.38
32	7	404	8CT	C19-C20	4.48	1.57	1.43
30	4	313	CHL	C2C-C3C	4.48	1.46	1.36
32	B	843	8CT	C19-C20	4.48	1.57	1.43
30	8	305	CHL	CHD-C1D	4.48	1.47	1.38
30	h	601	CHL	CHC-C1C	4.48	1.47	1.38
32	2	402	8CT	C06-C07	4.48	1.66	1.52
30	6	305	CHL	C2C-C3C	4.48	1.46	1.36
32	0	401	8CT	C19-C20	4.48	1.57	1.43
30	i	614	CHL	CHC-C1C	4.48	1.47	1.38
32	B	847	8CT	C06-C07	4.47	1.66	1.52
30	i	606	CHL	CHC-C1C	4.47	1.47	1.38
32	M	102	8CT	C06-C07	4.47	1.66	1.52
32	G	104	8CT	C19-C20	4.47	1.57	1.43
30	0	306	CHL	CHD-C1D	4.47	1.47	1.38
30	b	614	CHL	CHC-C1C	4.47	1.47	1.38
32	B	851	8CT	C06-C07	4.47	1.66	1.52
32	8	406	8CT	C19-C20	4.47	1.57	1.43
32	B	844	8CT	C19-C20	4.47	1.57	1.43
32	8	402	8CT	C06-C07	4.47	1.66	1.52
30	e	614	CHL	CHC-C1C	4.46	1.47	1.38
30	5	305	CHL	O2A-CGA	4.46	1.45	1.30
32	B	845	8CT	C19-C20	4.46	1.57	1.43
30	6	306	CHL	C2C-C3C	4.46	1.46	1.36
32	6	402	8CT	C06-C07	4.45	1.66	1.52
32	1	402	8CT	C06-C07	4.45	1.66	1.52
30	7	313	CHL	CHD-C1D	4.45	1.47	1.38
38	B	842	PQN	C10-C5	4.45	1.48	1.40
32	J	104	8CT	C06-C07	4.45	1.66	1.52
30	8	301	CHL	CHD-C1D	4.45	1.47	1.38
30	b	602	CHL	CHD-C1D	4.45	1.47	1.38
30	4	305	CHL	C2C-C3C	4.45	1.46	1.36
30	5	313	CHL	CHC-C1C	4.44	1.47	1.38
30	b	606	CHL	CHD-C1D	4.44	1.47	1.38
32	9	401	8CT	C19-C20	4.44	1.57	1.43
30	8	307	CHL	C2C-C3C	4.44	1.46	1.36
32	8	406	8CT	C06-C07	4.44	1.66	1.52
30	d	602	CHL	CHD-C1D	4.44	1.47	1.38
32	A	849	8CT	C06-C07	4.43	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	804	8CT	C06-C07	4.43	1.66	1.52
30	a	609	CHL	CHC-C1C	4.43	1.47	1.38
30	g	607	CHL	CHC-C1C	4.43	1.47	1.38
32	F	302	8CT	C06-C07	4.43	1.66	1.52
30	7	301	CHL	CHD-C1D	4.43	1.47	1.38
30	a	607	CHL	CHC-C1C	4.43	1.47	1.38
32	A	850	8CT	C19-C20	4.42	1.57	1.43
30	i	607	CHL	CHC-C1C	4.42	1.47	1.38
30	3	305	CHL	C2C-C3C	4.42	1.46	1.36
30	2	319	CHL	CHD-C1D	4.42	1.47	1.38
32	G	104	8CT	C06-C07	4.41	1.66	1.52
32	B	848	8CT	C06-C07	4.41	1.66	1.52
30	g	606	CHL	CHC-C1C	4.41	1.47	1.38
30	9	301	CHL	CHD-C1D	4.41	1.47	1.38
30	d	609	CHL	CHC-C1C	4.41	1.47	1.38
30	6	308	CHL	CHD-C1D	4.40	1.46	1.38
30	9	306	CHL	CHD-C1D	4.40	1.46	1.38
32	B	846	8CT	C19-C20	4.40	1.57	1.43
30	9	305	CHL	C2C-C3C	4.40	1.46	1.36
30	2	305	CHL	C2C-C3C	4.40	1.46	1.36
30	c	602	CHL	C2C-C3C	4.40	1.46	1.36
30	b	601	CHL	CHC-C1C	4.39	1.47	1.38
32	6	402	8CT	C19-C20	4.39	1.57	1.43
30	6	307	CHL	C2C-C3C	4.39	1.46	1.36
32	8	402	8CT	C19-C20	4.39	1.57	1.43
30	f	609	CHL	CHC-C1C	4.39	1.47	1.38
30	9	313	CHL	CHD-C1D	4.39	1.46	1.38
30	h	609	CHL	CHC-C1C	4.38	1.47	1.38
30	f	608	CHL	CHD-C1D	4.38	1.46	1.38
30	f	606	CHL	CHC-C1C	4.38	1.47	1.38
30	1	305	CHL	CHD-C1D	4.38	1.46	1.38
30	4	306	CHL	CHD-C1D	4.38	1.46	1.38
30	5	301	CHL	CHC-C1C	4.37	1.47	1.38
30	f	607	CHL	CHC-C1C	4.37	1.47	1.38
30	8	313	CHL	CHD-C1D	4.37	1.46	1.38
30	2	306	CHL	CHD-C1D	4.37	1.46	1.38
32	A	854	8CT	C19-C20	4.37	1.57	1.43
30	e	606	CHL	CHC-C1C	4.37	1.47	1.38
30	c	602	CHL	CHD-C1D	4.37	1.46	1.38
32	3	402	8CT	C19-C20	4.36	1.57	1.43
30	f	602	CHL	C2C-C3C	4.36	1.46	1.36
32	O	205	8CT	C19-C20	4.36	1.57	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	305	CHL	C2C-C3C	4.36	1.46	1.36
30	c	614	CHL	CHC-C1C	4.36	1.47	1.38
30	d	606	CHL	CHC-C1C	4.36	1.47	1.38
32	K	107	8CT	C19-C20	4.36	1.57	1.43
30	5	306	CHL	CHC-C1C	4.36	1.47	1.38
30	1	313	CHL	CHD-C1D	4.36	1.46	1.38
32	L	209	8CT	C19-C20	4.36	1.56	1.43
30	3	307	CHL	C2C-C3C	4.36	1.46	1.36
30	a	606	CHL	CHC-C1C	4.35	1.47	1.38
32	B	846	8CT	C24-C25	4.35	1.56	1.43
30	4	302	CHL	C2C-C3C	4.35	1.46	1.36
30	5	302	CHL	C2C-C3C	4.35	1.46	1.36
30	b	602	CHL	CHC-C1C	4.35	1.47	1.38
30	0	302	CHL	C2C-C3C	4.34	1.46	1.36
30	f	602	CHL	CHC-C1C	4.34	1.47	1.38
32	J	104	8CT	C19-C20	4.34	1.56	1.43
32	L	205	8CT	C19-C20	4.34	1.56	1.43
30	a	606	CHL	O2A-CGA	4.34	1.46	1.33
30	f	614	CHL	CHC-C1C	4.34	1.47	1.38
32	B	847	8CT	C19-C20	4.34	1.56	1.43
30	3	302	CHL	C2C-C3C	4.34	1.46	1.36
32	M	102	8CT	C19-C20	4.34	1.56	1.43
30	7	307	CHL	CHC-C1C	4.34	1.47	1.38
30	7	307	CHL	CHD-C1D	4.34	1.46	1.38
30	3	302	CHL	CHC-C1C	4.34	1.47	1.38
30	4	306	CHL	O2A-CGA	4.34	1.46	1.33
30	7	307	CHL	C2C-C3C	4.33	1.46	1.36
32	B	804	8CT	C19-C20	4.33	1.56	1.43
32	L	206	8CT	C19-C20	4.33	1.56	1.43
30	6	302	CHL	C2C-C3C	4.33	1.46	1.36
30	i	606	CHL	O2A-CGA	4.33	1.46	1.33
30	2	301	CHL	O2A-CGA	4.33	1.46	1.33
30	g	606	CHL	O2A-CGA	4.33	1.46	1.33
30	9	305	CHL	O2A-CGA	4.32	1.46	1.33
30	5	306	CHL	O2A-CGA	4.32	1.46	1.33
32	3	403	8CT	C19-C20	4.32	1.56	1.43
30	2	306	CHL	O2A-CGA	4.32	1.46	1.33
30	a	601	CHL	CHC-C1C	4.32	1.47	1.38
30	g	601	CHL	O2A-CGA	4.32	1.46	1.33
30	6	301	CHL	CHD-C1D	4.32	1.46	1.38
30	6	305	CHL	CHD-C1D	4.32	1.46	1.38
30	6	308	CHL	O2A-CGA	4.32	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	e	602	CHL	O2A-CGA	4.31	1.45	1.33
30	8	315	CHL	CHC-C1C	4.31	1.47	1.38
30	0	301	CHL	O2A-CGA	4.31	1.45	1.33
30	b	609	CHL	O2A-CGA	4.31	1.45	1.33
30	e	607	CHL	CHC-C1C	4.31	1.47	1.38
30	d	606	CHL	O2A-CGA	4.31	1.45	1.33
30	d	608	CHL	CHC-C1C	4.31	1.47	1.38
30	5	302	CHL	O2A-CGA	4.31	1.45	1.33
30	6	306	CHL	O2A-CGA	4.31	1.45	1.33
30	5	307	CHL	CHC-C1C	4.31	1.47	1.38
30	a	609	CHL	O2A-CGA	4.30	1.45	1.33
30	c	609	CHL	CHC-C1C	4.30	1.47	1.38
30	7	305	CHL	O2A-CGA	4.30	1.45	1.33
32	4	402	8CT	C19-C20	4.30	1.56	1.43
32	7	405	8CT	C19-C20	4.30	1.56	1.43
30	8	306	CHL	O2A-CGA	4.30	1.45	1.33
32	A	846	8CT	C19-C20	4.30	1.56	1.43
30	b	601	CHL	O2A-CGA	4.30	1.45	1.33
30	a	608	CHL	CHC-C1C	4.30	1.47	1.38
30	2	302	CHL	C2C-C3C	4.30	1.46	1.36
30	f	606	CHL	O2A-CGA	4.30	1.45	1.33
30	h	608	CHL	CHC-C1C	4.30	1.47	1.38
30	b	606	CHL	O2A-CGA	4.30	1.45	1.33
30	i	608	CHL	O2A-CGA	4.30	1.45	1.33
30	8	307	CHL	CHD-C1D	4.29	1.46	1.38
30	g	602	CHL	O2A-CGA	4.29	1.45	1.33
30	7	302	CHL	C2C-C3C	4.29	1.46	1.36
30	6	306	CHL	CHD-C1D	4.29	1.46	1.38
30	1	306	CHL	O2A-CGA	4.29	1.45	1.33
30	6	313	CHL	CHD-C1D	4.29	1.46	1.38
30	f	609	CHL	O2A-CGA	4.29	1.45	1.33
30	7	301	CHL	O2A-CGA	4.29	1.45	1.33
30	3	305	CHL	CHD-C1D	4.29	1.46	1.38
30	i	608	CHL	CHC-C1C	4.29	1.47	1.38
32	B	851	8CT	C19-C20	4.29	1.56	1.43
30	7	305	CHL	CHD-C1D	4.29	1.46	1.38
30	h	606	CHL	CHC-C1C	4.28	1.47	1.38
32	J	101	8CT	C19-C20	4.28	1.56	1.43
32	B	843	8CT	C24-C25	4.28	1.56	1.43
30	c	602	CHL	CHC-C1C	4.28	1.47	1.38
30	d	609	CHL	O2A-CGA	4.28	1.45	1.33
30	1	305	CHL	O2A-CGA	4.28	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	522	0IE	C15-C16	4.28	1.41	1.35
30	e	608	CHL	O2A-CGA	4.28	1.45	1.33
32	I	101	8CT	C19-C20	4.28	1.56	1.43
30	g	607	CHL	O2A-CGA	4.28	1.45	1.33
30	0	306	CHL	O2A-CGA	4.28	1.45	1.33
32	F	302	8CT	C19-C20	4.28	1.56	1.43
30	e	606	CHL	O2A-CGA	4.28	1.45	1.33
30	d	608	CHL	O2A-CGA	4.28	1.45	1.33
30	2	301	CHL	CHD-C1D	4.28	1.46	1.38
30	i	602	CHL	O2A-CGA	4.27	1.45	1.33
30	c	607	CHL	CHC-C1C	4.27	1.47	1.38
30	c	602	CHL	O2A-CGA	4.27	1.45	1.33
30	c	608	CHL	O2A-CGA	4.27	1.45	1.33
30	8	302	CHL	CHC-C1C	4.27	1.47	1.38
30	d	601	CHL	O2A-CGA	4.27	1.45	1.33
30	b	608	CHL	O2A-CGA	4.27	1.45	1.33
30	2	308	CHL	CHD-C1D	4.27	1.46	1.38
37	i	521	0IE	C11-C12	4.27	1.41	1.35
30	a	602	CHL	CHC-C1C	4.27	1.47	1.38
30	3	305	CHL	O2A-CGA	4.27	1.45	1.33
30	0	301	CHL	CHD-C1D	4.27	1.46	1.38
30	1	313	CHL	O2A-CGA	4.27	1.45	1.33
30	3	307	CHL	O2A-CGA	4.27	1.45	1.33
30	4	305	CHL	CHD-C1D	4.26	1.46	1.38
30	5	301	CHL	O2A-CGA	4.26	1.45	1.33
30	h	602	CHL	O2A-CGA	4.26	1.45	1.33
32	A	847	8CT	C19-C20	4.26	1.56	1.43
30	f	601	CHL	O2A-CGA	4.26	1.45	1.33
30	i	609	CHL	O2A-CGA	4.26	1.45	1.33
30	2	307	CHL	C2C-C3C	4.26	1.45	1.36
30	8	313	CHL	O2A-CGA	4.26	1.45	1.33
30	0	305	CHL	O2A-CGA	4.26	1.45	1.33
30	f	602	CHL	CHD-C1D	4.26	1.46	1.38
37	i	521	0IE	C8-C7	4.25	1.41	1.35
30	f	602	CHL	O2A-CGA	4.25	1.45	1.33
30	a	602	CHL	O2A-CGA	4.25	1.45	1.33
30	e	609	CHL	O2A-CGA	4.25	1.45	1.33
30	4	302	CHL	CHD-C1D	4.25	1.46	1.38
30	1	302	CHL	C2C-C3C	4.25	1.45	1.36
37	b	522	0IE	C8-C7	4.25	1.41	1.35
30	c	601	CHL	O2A-CGA	4.25	1.45	1.33
30	h	606	CHL	O2A-CGA	4.25	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	402	8CT	C19-C20	4.25	1.56	1.43
30	d	602	CHL	CHC-C1C	4.24	1.47	1.38
30	9	306	CHL	O2A-CGA	4.24	1.45	1.33
30	b	607	CHL	CHC-C1C	4.24	1.47	1.38
30	c	609	CHL	O2A-CGA	4.24	1.45	1.33
30	c	608	CHL	CHC-C1C	4.24	1.47	1.38
30	8	302	CHL	C2C-C3C	4.24	1.45	1.36
30	2	302	CHL	CHD-C1D	4.24	1.46	1.38
30	2	305	CHL	CHD-C1D	4.24	1.46	1.38
30	f	608	CHL	O2A-CGA	4.24	1.45	1.33
30	6	302	CHL	O2A-CGA	4.24	1.45	1.33
30	6	307	CHL	O2A-CGA	4.24	1.45	1.33
30	6	313	CHL	O2A-CGA	4.24	1.45	1.33
32	4	402	8CT	C24-C25	4.24	1.56	1.43
30	b	602	CHL	O2A-CGA	4.24	1.45	1.33
30	7	306	CHL	O2A-CGA	4.23	1.45	1.33
30	2	313	CHL	O2A-CGA	4.23	1.45	1.33
30	4	319	CHL	CHD-C1D	4.23	1.46	1.38
30	7	313	CHL	CHC-C1C	4.23	1.47	1.38
30	8	307	CHL	O2A-CGA	4.23	1.45	1.33
30	a	608	CHL	O2A-CGA	4.23	1.45	1.33
30	0	302	CHL	CHD-C1D	4.23	1.46	1.38
30	9	305	CHL	CHD-C1D	4.23	1.46	1.38
30	d	602	CHL	O2A-CGA	4.22	1.45	1.33
32	2	402	8CT	C24-C25	4.22	1.56	1.43
30	i	602	CHL	CHC-C1C	4.22	1.47	1.38
30	4	319	CHL	O2A-CGA	4.22	1.45	1.33
30	6	307	CHL	CHD-C1D	4.22	1.46	1.38
30	e	601	CHL	O2A-CGA	4.22	1.45	1.33
30	4	307	CHL	O2A-CGA	4.22	1.45	1.33
37	b	522	0IE	C11-C12	4.22	1.41	1.35
30	5	302	CHL	CHD-C1D	4.22	1.46	1.38
30	e	609	CHL	CHC-C1C	4.22	1.47	1.38
30	0	302	CHL	O2A-CGA	4.21	1.45	1.33
37	h	521	0IE	C11-C12	4.21	1.41	1.35
32	7	402	8CT	C19-C20	4.21	1.56	1.43
30	b	606	CHL	CHC-C1C	4.21	1.47	1.38
30	b	609	CHL	CHC-C1C	4.21	1.47	1.38
30	e	602	CHL	CHC-C1C	4.21	1.47	1.38
30	c	606	CHL	CHC-C1C	4.21	1.47	1.38
30	2	313	CHL	CHD-C1D	4.21	1.46	1.38
30	8	302	CHL	O2A-CGA	4.21	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	319	CHL	O2A-CGA	4.20	1.45	1.33
37	d	522	0IE	C8-C7	4.20	1.41	1.35
37	a	522	0IE	C15-C16	4.20	1.41	1.35
30	1	307	CHL	O2A-CGA	4.20	1.45	1.33
30	4	313	CHL	O2A-CGA	4.20	1.45	1.33
30	3	305	CHL	CHC-C1C	4.20	1.47	1.38
30	4	302	CHL	O2A-CGA	4.20	1.45	1.33
30	4	313	CHL	CHD-C1D	4.19	1.46	1.38
30	8	302	CHL	CHD-C1D	4.19	1.46	1.38
37	c	522	0IE	C11-C12	4.19	1.41	1.35
37	h	522	0IE	C11-C12	4.19	1.41	1.35
37	g	522	0IE	C11-C12	4.19	1.41	1.35
30	3	302	CHL	O2A-CGA	4.18	1.45	1.33
30	7	307	CHL	O2A-CGA	4.18	1.45	1.33
37	h	521	0IE	C8-C7	4.18	1.41	1.35
30	7	302	CHL	CHD-C1D	4.18	1.46	1.38
30	0	306	CHL	CHC-C1C	4.18	1.47	1.38
37	a	522	0IE	C8-C7	4.18	1.41	1.35
30	7	305	CHL	CHC-C1C	4.18	1.47	1.38
30	1	302	CHL	CHD-C1D	4.17	1.46	1.38
30	6	302	CHL	CHD-C1D	4.17	1.46	1.38
30	7	302	CHL	CHC-C1C	4.17	1.47	1.38
30	1	302	CHL	CHC-C1C	4.17	1.47	1.38
30	f	601	CHL	CHC-C1C	4.17	1.47	1.38
30	2	307	CHL	O2A-CGA	4.17	1.45	1.33
37	g	522	0IE	C15-C16	4.16	1.41	1.35
30	8	301	CHL	CHC-C1C	4.16	1.47	1.38
30	0	305	CHL	CHC-C1C	4.16	1.47	1.38
30	6	301	CHL	O2A-CGA	4.15	1.45	1.33
30	7	302	CHL	O2A-CGA	4.15	1.45	1.33
30	6	307	CHL	CHC-C1C	4.15	1.47	1.38
37	g	522	0IE	C8-C7	4.15	1.41	1.35
30	5	305	CHL	CHC-C1C	4.15	1.46	1.38
30	1	307	CHL	CHC-C1C	4.15	1.46	1.38
32	A	848	8CT	C19-C20	4.15	1.56	1.43
30	2	302	CHL	O2A-CGA	4.14	1.45	1.33
30	9	305	CHL	CHC-C1C	4.14	1.46	1.38
32	B	844	8CT	C24-C25	4.14	1.56	1.43
30	6	315	CHL	CHC-C1C	4.14	1.46	1.38
37	i	522	0IE	C8-C7	4.14	1.41	1.35
32	A	849	8CT	C19-C20	4.14	1.56	1.43
37	h	521	0IE	C15-C16	4.13	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	845	8CT	C24-C25	4.13	1.56	1.43
32	B	848	8CT	C24-C25	4.13	1.56	1.43
30	7	306	CHL	CHC-C1C	4.13	1.46	1.38
37	d	522	0IE	C11-C12	4.13	1.41	1.35
37	a	522	0IE	C11-C12	4.13	1.41	1.35
37	i	522	0IE	C15-C16	4.12	1.41	1.35
32	0	401	8CT	C24-C25	4.12	1.56	1.43
30	3	302	CHL	CHD-C1D	4.12	1.46	1.38
30	e	608	CHL	CHC-C1C	4.12	1.46	1.38
30	4	307	CHL	CHD-C1D	4.12	1.46	1.38
30	1	313	CHL	CHC-C1C	4.11	1.46	1.38
37	f	522	0IE	C11-C12	4.11	1.41	1.35
32	9	401	8CT	C24-C25	4.11	1.56	1.43
32	G	104	8CT	C24-C25	4.11	1.56	1.43
32	L	209	8CT	C24-C25	4.10	1.56	1.43
37	h	522	0IE	C8-C7	4.10	1.41	1.35
37	f	521	0IE	C11-C12	4.09	1.41	1.35
37	f	522	0IE	C8-C7	4.09	1.41	1.35
32	1	402	8CT	C24-C25	4.09	1.56	1.43
30	7	301	CHL	CHC-C1C	4.09	1.46	1.38
30	1	302	CHL	O2A-CGA	4.09	1.45	1.33
30	1	305	CHL	CHC-C1C	4.09	1.46	1.38
32	8	406	8CT	C24-C25	4.09	1.56	1.43
30	8	308	CHL	CHC-C1C	4.09	1.46	1.38
32	J	104	8CT	C24-C25	4.09	1.56	1.43
30	0	302	CHL	CHC-C1C	4.08	1.46	1.38
30	e	601	CHL	CHC-C1C	4.08	1.46	1.38
30	8	301	CHL	O2A-CGA	4.08	1.45	1.33
30	1	306	CHL	CHC-C1C	4.08	1.46	1.38
30	c	614	CHL	C3A-C2A	-4.07	1.50	1.54
30	8	306	CHL	CHC-C1C	4.07	1.46	1.38
32	A	854	8CT	C24-C25	4.07	1.56	1.43
32	L	206	8CT	C24-C25	4.07	1.56	1.43
30	6	302	CHL	CHC-C1C	4.07	1.46	1.38
37	i	521	0IE	C15-C16	4.06	1.41	1.35
30	6	308	CHL	CHC-C1C	4.06	1.46	1.38
32	3	402	8CT	C24-C25	4.06	1.56	1.43
30	2	301	CHL	CHC-C1C	4.06	1.46	1.38
30	9	313	CHL	O2A-CGA	4.06	1.45	1.33
30	a	601	CHL	O2A-CGA	4.06	1.45	1.33
32	K	107	8CT	C24-C25	4.06	1.56	1.43
30	d	607	CHL	O2A-CGA	4.05	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	607	CHL	O2A-CGA	4.05	1.45	1.33
37	e	522	0IE	C15-C16	4.05	1.41	1.35
37	g	521	0IE	C8-C7	4.05	1.41	1.35
30	9	313	CHL	CHC-C1C	4.05	1.46	1.38
30	c	607	CHL	O2A-CGA	4.04	1.45	1.33
30	4	308	CHL	CHC-C1C	4.04	1.46	1.38
30	5	313	CHL	O2A-CGA	4.04	1.45	1.33
30	9	301	CHL	O2A-CGA	4.04	1.45	1.33
30	2	302	CHL	CHC-C1C	4.04	1.46	1.38
30	d	614	CHL	CHC-C4B	4.04	1.48	1.39
30	3	307	CHL	CHD-C1D	4.04	1.46	1.38
30	h	601	CHL	O2A-CGA	4.04	1.45	1.33
30	4	319	CHL	CHC-C1C	4.04	1.46	1.38
30	5	307	CHL	O2A-CGA	4.04	1.45	1.33
30	4	302	CHL	CHC-C1C	4.03	1.46	1.38
30	h	602	CHL	CHC-C4B	4.03	1.48	1.39
30	h	614	CHL	CHC-C4B	4.03	1.48	1.39
30	7	313	CHL	O2A-CGA	4.03	1.45	1.33
37	i	522	0IE	C11-C12	4.03	1.41	1.35
37	g	521	0IE	C11-C12	4.03	1.41	1.35
30	g	605	CHL	CHC-C4B	4.03	1.48	1.39
30	d	605	CHL	CHC-C4B	4.03	1.48	1.39
30	i	607	CHL	O2A-CGA	4.02	1.45	1.33
30	6	301	CHL	CHC-C1C	4.02	1.46	1.38
37	b	521	0IE	C11-C12	4.02	1.41	1.35
32	B	847	8CT	C24-C25	4.02	1.55	1.43
30	8	308	CHL	O2A-CGA	4.02	1.45	1.33
30	h	609	CHL	O2A-CGA	4.02	1.45	1.33
30	2	307	CHL	CHC-C1C	4.02	1.46	1.38
30	4	308	CHL	O2A-CGA	4.02	1.45	1.33
30	e	607	CHL	O2A-CGA	4.02	1.45	1.33
30	h	607	CHL	CHC-C4B	4.01	1.48	1.39
30	f	607	CHL	O2A-CGA	4.01	1.45	1.33
31	g	613	CLA	C1D-ND	4.01	1.42	1.37
32	L	205	8CT	C24-C25	4.01	1.55	1.43
30	f	608	CHL	CHC-C1C	4.01	1.46	1.38
37	h	522	0IE	C15-C16	4.01	1.41	1.35
32	B	844	8CT	C14-C13	4.00	1.55	1.43
30	2	319	CHL	CHC-C1C	4.00	1.46	1.38
32	7	405	8CT	C24-C25	4.00	1.55	1.43
30	9	301	CHL	CHC-C1C	4.00	1.46	1.38
30	b	607	CHL	O2A-CGA	4.00	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	306	CHL	CHC-C1C	4.00	1.46	1.38
32	3	403	8CT	C24-C25	4.00	1.55	1.43
37	f	522	0IE	C15-C16	4.00	1.41	1.35
30	g	614	CHL	CHC-C4B	3.99	1.48	1.39
30	8	307	CHL	CHC-C1C	3.99	1.46	1.38
32	O	205	8CT	C24-C25	3.99	1.55	1.43
30	5	302	CHL	CHC-C1C	3.99	1.46	1.38
30	8	305	CHL	O2A-CGA	3.99	1.45	1.33
30	i	601	CHL	O2A-CGA	3.99	1.45	1.33
30	2	308	CHL	O2A-CGA	3.99	1.45	1.33
30	i	607	CHL	CHC-C4B	3.99	1.48	1.39
37	c	522	0IE	C15-C16	3.99	1.41	1.35
30	6	313	CHL	CHC-C1C	3.98	1.46	1.38
37	e	522	0IE	C8-C7	3.98	1.41	1.35
31	h	611	CLA	C1D-ND	3.98	1.42	1.37
30	g	602	CHL	CHC-C4B	3.98	1.48	1.39
32	M	102	8CT	C24-C25	3.98	1.55	1.43
37	d	521	0IE	C8-C7	3.98	1.41	1.35
30	a	605	CHL	CHC-C4B	3.98	1.48	1.39
30	g	601	CHL	CHC-C4B	3.98	1.48	1.39
32	8	402	8CT	C24-C25	3.98	1.55	1.43
37	d	521	0IE	C11-C12	3.97	1.41	1.35
32	B	851	8CT	C24-C25	3.97	1.55	1.43
30	e	614	CHL	CHC-C4B	3.97	1.48	1.39
30	h	605	CHL	CHC-C4B	3.97	1.48	1.39
37	b	521	0IE	C8-C7	3.97	1.41	1.35
30	a	614	CHL	CHC-C4B	3.97	1.48	1.39
32	6	402	8CT	C24-C25	3.97	1.55	1.43
30	0	301	CHL	CHC-C1C	3.97	1.46	1.38
30	2	308	CHL	CHC-C1C	3.97	1.46	1.38
30	i	605	CHL	CHC-C4B	3.97	1.48	1.39
32	F	302	8CT	C24-C25	3.97	1.55	1.43
30	2	313	CHL	CHC-C1C	3.97	1.46	1.38
30	h	614	CHL	CHD-C4C	3.97	1.48	1.39
30	2	307	CHL	CHD-C1D	3.96	1.46	1.38
30	8	305	CHL	CHC-C1C	3.96	1.46	1.38
32	J	101	8CT	C24-C25	3.96	1.55	1.43
30	g	605	CHL	CHD-C4C	3.96	1.48	1.39
30	2	305	CHL	CHC-C1C	3.96	1.46	1.38
30	b	608	CHL	CHC-C1C	3.96	1.46	1.38
37	a	521	0IE	C11-C12	3.96	1.41	1.35
30	2	306	CHL	CHC-C1C	3.96	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	404	8CT	C24-C25	3.96	1.55	1.43
30	d	601	CHL	CHC-C4B	3.96	1.48	1.39
30	g	609	CHL	CHC-C4B	3.95	1.48	1.39
30	i	614	CHL	CHC-C4B	3.95	1.48	1.39
32	B	804	8CT	C24-C25	3.95	1.55	1.43
30	d	605	CHL	CHD-C4C	3.95	1.48	1.39
37	a	521	0IE	C8-C7	3.95	1.41	1.35
30	i	601	CHL	CHC-C4B	3.95	1.48	1.39
30	c	601	CHL	CHC-C1C	3.95	1.46	1.38
30	h	605	CHL	CHD-C4C	3.95	1.48	1.39
30	4	305	CHL	CHC-C1C	3.95	1.46	1.38
41	B	849	DGD	O2G-C1B	3.94	1.45	1.34
30	9	306	CHL	CHC-C1C	3.94	1.46	1.38
30	g	608	CHL	CHC-C4B	3.94	1.48	1.39
37	f	521	0IE	C8-C7	3.94	1.41	1.35
37	c	522	0IE	C8-C7	3.93	1.41	1.35
37	e	522	0IE	C11-C12	3.93	1.41	1.35
30	6	305	CHL	CHC-C1C	3.93	1.46	1.38
30	d	607	CHL	CHC-C4B	3.93	1.48	1.39
30	g	609	CHL	CHD-C4C	3.93	1.48	1.39
30	g	614	CHL	CHD-C4C	3.93	1.48	1.39
30	g	606	CHL	CHC-C4B	3.92	1.48	1.39
32	B	845	8CT	C14-C13	3.92	1.55	1.43
30	4	313	CHL	CHC-C1C	3.92	1.46	1.38
30	a	614	CHL	CHD-C4C	3.92	1.48	1.39
30	a	606	CHL	CHC-C4B	3.92	1.48	1.39
30	a	607	CHL	CHC-C4B	3.91	1.48	1.39
30	5	301	CHL	CHC-C4B	3.91	1.48	1.39
32	G	104	8CT	C14-C13	3.91	1.55	1.43
30	4	307	CHL	CHC-C1C	3.91	1.46	1.38
30	6	306	CHL	CHC-C1C	3.90	1.46	1.38
31	0	321	CLA	C1D-ND	3.90	1.42	1.37
31	a	611	CLA	C1D-ND	3.90	1.42	1.37
32	I	101	8CT	C24-C25	3.90	1.55	1.43
32	8	402	8CT	C14-C13	3.90	1.55	1.43
31	g	611	CLA	C1D-ND	3.90	1.42	1.37
30	e	605	CHL	CHC-C4B	3.90	1.48	1.39
30	c	605	CHL	CHD-C4C	3.90	1.48	1.39
37	e	521	0IE	C8-C7	3.90	1.40	1.35
30	f	605	CHL	CHD-C4C	3.90	1.48	1.39
37	e	521	0IE	C15-C16	3.89	1.40	1.35
32	7	402	8CT	C24-C25	3.89	1.55	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	521	0IE	C15-C16	3.89	1.40	1.35
30	a	605	CHL	CHD-C4C	3.89	1.48	1.39
30	i	609	CHL	CHD-C4C	3.89	1.48	1.39
32	A	846	8CT	C24-C25	3.89	1.55	1.43
30	f	605	CHL	CHC-C4B	3.88	1.48	1.39
30	g	607	CHL	CHC-C4B	3.88	1.48	1.39
30	g	607	CHL	CHD-C4C	3.88	1.48	1.39
30	i	609	CHL	CHC-C4B	3.88	1.48	1.39
30	c	605	CHL	CHC-C4B	3.88	1.48	1.39
32	B	843	8CT	C14-C13	3.88	1.55	1.43
30	b	614	CHL	CHC-C4B	3.87	1.48	1.39
37	b	521	0IE	C15-C16	3.87	1.40	1.35
30	3	307	CHL	CHC-C1C	3.87	1.46	1.38
30	d	614	CHL	CHD-C4C	3.87	1.48	1.39
30	8	313	CHL	CHC-C1C	3.87	1.46	1.38
30	i	606	CHL	CHC-C4B	3.87	1.48	1.39
31	a	613	CLA	C1D-ND	3.87	1.42	1.37
30	g	601	CHL	CHD-C4C	3.87	1.48	1.39
37	f	521	0IE	C15-C16	3.86	1.40	1.35
30	i	605	CHL	CHD-C4C	3.86	1.48	1.39
32	B	846	8CT	C30-C29	3.86	1.56	1.50
30	5	306	CHL	CHC-C4B	3.86	1.48	1.39
31	d	613	CLA	C1D-ND	3.86	1.42	1.37
31	O	203	CLA	C1D-ND	3.86	1.42	1.37
31	i	613	CLA	C1D-ND	3.85	1.42	1.37
30	h	601	CHL	CHC-C4B	3.85	1.48	1.39
37	a	521	0IE	C15-C16	3.85	1.40	1.35
30	5	313	CHL	CHC-C4B	3.84	1.48	1.39
31	i	604	CLA	C1D-ND	3.84	1.42	1.37
37	e	521	0IE	C11-C12	3.84	1.40	1.35
30	f	602	CHL	CHC-C4B	3.84	1.48	1.39
30	h	601	CHL	CHD-C4C	3.84	1.48	1.39
31	5	311	CLA	C1D-ND	3.84	1.42	1.37
30	e	606	CHL	CHC-C4B	3.84	1.48	1.39
30	5	307	CHL	CHC-C4B	3.84	1.48	1.39
30	h	607	CHL	CHD-C4C	3.84	1.48	1.39
32	A	847	8CT	C24-C25	3.84	1.55	1.43
30	c	607	CHL	CHC-C4B	3.83	1.48	1.39
32	A	850	8CT	C24-C25	3.83	1.55	1.43
30	f	609	CHL	CHC-C4B	3.83	1.48	1.39
31	h	603	CLA	C1D-ND	3.83	1.42	1.37
31	d	611	CLA	C1D-ND	3.83	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	614	CHL	CHD-C4C	3.83	1.48	1.39
32	B	846	8CT	C28-C29	3.83	1.41	1.32
30	a	609	CHL	CHD-C4C	3.82	1.48	1.39
31	a	603	CLA	C1D-ND	3.82	1.42	1.37
30	b	601	CHL	CHC-C4B	3.82	1.48	1.39
30	c	614	CHL	CHC-C4B	3.82	1.48	1.39
30	b	606	CHL	CHC-C4B	3.82	1.48	1.39
31	c	603	CLA	C1D-ND	3.82	1.42	1.37
32	B	848	8CT	C14-C13	3.82	1.55	1.43
30	h	609	CHL	CHD-C4C	3.82	1.48	1.39
30	i	606	CHL	CHD-C4C	3.82	1.48	1.39
31	i	612	CLA	C1D-ND	3.82	1.42	1.37
31	h	612	CLA	C1D-ND	3.81	1.42	1.37
30	i	607	CHL	CHD-C4C	3.81	1.47	1.39
31	g	612	CLA	C1D-ND	3.81	1.42	1.37
32	B	846	8CT	C14-C13	3.81	1.55	1.43
31	5	308	CLA	C1D-ND	3.81	1.42	1.37
31	a	612	CLA	C1D-ND	3.81	1.42	1.37
30	a	609	CHL	CHC-C4B	3.81	1.48	1.39
30	b	607	CHL	CHC-C4B	3.81	1.48	1.39
30	f	607	CHL	CHC-C4B	3.81	1.48	1.39
30	g	605	CHL	OBD-CAD	3.81	1.29	1.22
32	4	402	8CT	C14-C13	3.81	1.55	1.43
31	g	604	CLA	C1D-ND	3.81	1.42	1.37
30	7	307	CHL	CHC-C4B	3.81	1.47	1.39
32	8	406	8CT	C14-C13	3.80	1.55	1.43
31	g	603	CLA	C1D-ND	3.80	1.42	1.37
31	h	610	CLA	C1D-ND	3.80	1.42	1.37
31	g	610	CLA	C1D-ND	3.80	1.42	1.37
32	A	849	8CT	C24-C25	3.80	1.55	1.43
31	b	611	CLA	C1D-ND	3.80	1.42	1.37
30	a	605	CHL	OBD-CAD	3.80	1.29	1.22
30	d	606	CHL	CHC-C4B	3.80	1.47	1.39
32	L	206	8CT	C14-C13	3.80	1.55	1.43
30	3	302	CHL	CHC-C4B	3.80	1.47	1.39
30	i	601	CHL	CHD-C4C	3.80	1.47	1.39
31	1	308	CLA	C1D-ND	3.80	1.42	1.37
31	d	612	CLA	C1D-ND	3.80	1.42	1.37
30	h	602	CHL	CHD-C4C	3.80	1.47	1.39
30	e	607	CHL	CHC-C4B	3.79	1.47	1.39
32	6	402	8CT	C14-C13	3.79	1.55	1.43
32	K	107	8CT	C14-C13	3.79	1.55	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	607	CHL	CHD-C4C	3.79	1.47	1.39
30	f	614	CHL	CHC-C4B	3.79	1.47	1.39
31	i	603	CLA	C1D-ND	3.79	1.42	1.37
30	c	602	CHL	CHC-C4B	3.79	1.47	1.39
37	c	521	0IE	C8-C7	3.78	1.40	1.35
30	b	614	CHL	CHD-C4C	3.78	1.47	1.39
32	A	848	8CT	C24-C25	3.78	1.55	1.43
30	d	601	CHL	CHD-C4C	3.78	1.47	1.39
31	i	610	CLA	C1D-ND	3.78	1.42	1.37
30	c	609	CHL	CHD-C4C	3.78	1.47	1.39
30	f	606	CHL	CHC-C4B	3.78	1.47	1.39
32	7	404	8CT	C14-C13	3.78	1.55	1.43
30	a	602	CHL	CHC-C4B	3.78	1.47	1.39
31	f	603	CLA	C1D-ND	3.78	1.42	1.37
30	d	609	CHL	CHD-C4C	3.78	1.47	1.39
30	d	607	CHL	CHD-C4C	3.78	1.47	1.39
30	h	614	CHL	OBD-CAD	3.78	1.29	1.22
30	0	305	CHL	CHC-C4B	3.78	1.47	1.39
30	d	606	CHL	OBD-CAD	3.78	1.29	1.22
30	h	609	CHL	CHC-C4B	3.78	1.47	1.39
30	e	605	CHL	CHD-C4C	3.78	1.47	1.39
31	c	612	CLA	C1D-ND	3.77	1.42	1.37
30	5	313	CHL	CHD-C4C	3.77	1.47	1.39
31	h	613	CLA	C1D-ND	3.77	1.42	1.37
30	d	614	CHL	OBD-CAD	3.77	1.29	1.22
31	b	612	CLA	C1D-ND	3.77	1.42	1.37
30	i	602	CHL	CHC-C4B	3.77	1.47	1.39
30	f	609	CHL	CHD-C4C	3.77	1.47	1.39
32	8	402	8CT	C11-C12	3.77	1.54	1.45
31	d	603	CLA	C1D-ND	3.77	1.42	1.37
30	a	601	CHL	CHC-C4B	3.77	1.47	1.39
37	d	521	0IE	C15-C16	3.77	1.40	1.35
32	1	402	8CT	C14-C13	3.77	1.55	1.43
31	a	610	CLA	C1D-ND	3.77	1.42	1.37
31	e	612	CLA	C1D-ND	3.77	1.42	1.37
37	c	521	0IE	C11-C12	3.77	1.40	1.35
30	8	302	CHL	CHC-C4B	3.77	1.47	1.39
30	b	601	CHL	CHD-C4C	3.76	1.47	1.39
30	b	602	CHL	CHC-C4B	3.76	1.47	1.39
31	e	611	CLA	C1D-ND	3.76	1.42	1.37
30	a	606	CHL	CHD-C4C	3.76	1.47	1.39
30	g	608	CHL	CHD-C4C	3.76	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	313	CHL	CHC-C4B	3.76	1.47	1.39
30	e	614	CHL	CHD-C4C	3.76	1.47	1.39
30	e	602	CHL	CHC-C4B	3.76	1.47	1.39
31	i	611	CLA	C1D-ND	3.76	1.42	1.37
31	c	611	CLA	C1D-ND	3.76	1.42	1.37
32	0	401	8CT	C14-C13	3.76	1.55	1.43
32	2	402	8CT	C14-C13	3.75	1.55	1.43
30	1	302	CHL	CHC-C4B	3.75	1.47	1.39
30	f	607	CHL	CHD-C4C	3.75	1.47	1.39
30	c	605	CHL	OBD-CAD	3.75	1.28	1.22
30	8	315	CHL	CHC-C4B	3.75	1.47	1.39
30	5	306	CHL	CHD-C4C	3.75	1.47	1.39
31	5	304	CLA	C1D-ND	3.75	1.42	1.37
30	h	605	CHL	CHB-C1B	3.75	1.47	1.39
30	a	608	CHL	CHC-C4B	3.75	1.47	1.39
31	5	312	CLA	C1D-ND	3.75	1.42	1.37
30	g	614	CHL	OBD-CAD	3.75	1.28	1.22
30	8	301	CHL	CHC-C4B	3.75	1.47	1.39
30	d	609	CHL	CHC-C4B	3.75	1.47	1.39
30	6	308	CHL	C1D-ND	-3.74	1.33	1.37
30	a	601	CHL	CHD-C4C	3.74	1.47	1.39
30	g	606	CHL	CHD-C4C	3.74	1.47	1.39
31	d	604	CLA	C1D-ND	3.74	1.42	1.37
30	d	605	CHL	OBD-CAD	3.74	1.28	1.22
30	c	607	CHL	CHD-C4C	3.74	1.47	1.39
30	h	614	CHL	CHB-C1B	3.74	1.47	1.39
31	G	103	CLA	C1D-ND	3.73	1.42	1.37
30	h	608	CHL	CHC-C4B	3.73	1.47	1.39
30	f	606	CHL	CHD-C4C	3.73	1.47	1.39
31	e	603	CLA	C1D-ND	3.73	1.42	1.37
30	f	607	CHL	OBD-CAD	3.73	1.28	1.22
30	a	606	CHL	OBD-CAD	3.73	1.28	1.22
31	a	604	CLA	C1D-ND	3.73	1.42	1.37
30	g	606	CHL	OBD-CAD	3.73	1.28	1.22
30	h	605	CHL	OBD-CAD	3.73	1.28	1.22
30	g	607	CHL	OBD-CAD	3.73	1.28	1.22
32	J	104	8CT	C14-C13	3.73	1.55	1.43
31	f	613	CLA	C1D-ND	3.73	1.42	1.37
31	e	613	CLA	C1D-ND	3.73	1.42	1.37
30	h	608	CHL	OBD-CAD	3.73	1.28	1.22
31	f	611	CLA	C1D-ND	3.73	1.42	1.37
30	e	609	CHL	CHC-C4B	3.73	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	9	401	8CT	C14-C13	3.73	1.55	1.43
30	b	609	CHL	CHD-C4C	3.73	1.47	1.39
30	a	614	CHL	OBD-CAD	3.73	1.28	1.22
30	g	601	CHL	OBD-CAD	3.73	1.28	1.22
32	7	404	8CT	C28-C29	3.72	1.41	1.32
30	5	305	CHL	OBD-CAD	3.72	1.28	1.22
30	d	607	CHL	OBD-CAD	3.72	1.28	1.22
32	B	843	8CT	C28-C29	3.72	1.41	1.32
30	g	602	CHL	CHD-C4C	3.72	1.47	1.39
31	b	610	CLA	C1D-ND	3.72	1.42	1.37
30	i	606	CHL	OBD-CAD	3.72	1.28	1.22
32	B	843	8CT	C11-C12	3.72	1.53	1.45
30	b	614	CHL	OBD-CAD	3.72	1.28	1.22
32	B	845	8CT	C11-C12	3.72	1.53	1.45
30	h	607	CHL	OBD-CAD	3.72	1.28	1.22
30	i	608	CHL	CHC-C4B	3.72	1.47	1.39
31	9	304	CLA	C1D-ND	3.71	1.42	1.37
31	4	309	CLA	C1D-ND	3.71	1.42	1.37
30	6	315	CHL	CHC-C4B	3.71	1.47	1.39
30	h	606	CHL	CHC-C4B	3.71	1.47	1.39
30	8	315	CHL	OBD-CAD	3.71	1.28	1.22
30	g	602	CHL	OBD-CAD	3.71	1.28	1.22
30	i	607	CHL	OBD-CAD	3.71	1.28	1.22
30	9	305	CHL	CHC-C4B	3.71	1.47	1.39
30	0	305	CHL	OBD-CAD	3.71	1.28	1.22
31	8	303	CLA	C1D-ND	3.71	1.42	1.37
31	h	604	CLA	C1D-ND	3.71	1.42	1.37
31	f	604	CLA	C1D-ND	3.71	1.42	1.37
31	H	204	CLA	C1D-ND	3.71	1.42	1.37
30	c	609	CHL	CHC-C4B	3.71	1.47	1.39
30	i	605	CHL	OBD-CAD	3.71	1.28	1.22
31	c	610	CLA	C1D-ND	3.71	1.42	1.37
30	d	606	CHL	CHD-C4C	3.70	1.47	1.39
30	6	307	CHL	CHC-C4B	3.70	1.47	1.39
30	a	602	CHL	CHD-C4C	3.70	1.47	1.39
31	e	604	CLA	C1D-ND	3.70	1.42	1.37
30	g	614	CHL	CHB-C1B	3.70	1.47	1.39
31	0	308	CLA	C1D-ND	3.70	1.42	1.37
32	A	854	8CT	C14-C13	3.70	1.54	1.43
31	7	317	CLA	C1D-ND	3.70	1.42	1.37
30	i	614	CHL	OBD-CAD	3.70	1.28	1.22
32	4	402	8CT	C28-C29	3.70	1.41	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	e	608	CHL	CHC-C4B	3.70	1.47	1.39
30	a	607	CHL	OBD-CAD	3.70	1.28	1.22
30	d	605	CHL	CHB-C1B	3.70	1.47	1.39
30	d	608	CHL	CHC-C4B	3.70	1.47	1.39
31	c	604	CLA	C1D-ND	3.70	1.42	1.37
30	c	602	CHL	OBD-CAD	3.70	1.28	1.22
30	c	607	CHL	OBD-CAD	3.70	1.28	1.22
32	8	406	8CT	C11-C12	3.70	1.53	1.45
30	e	614	CHL	OBD-CAD	3.70	1.28	1.22
32	B	844	8CT	C11-C12	3.69	1.53	1.45
30	c	614	CHL	OBD-CAD	3.69	1.28	1.22
32	3	403	8CT	C14-C13	3.69	1.54	1.43
30	h	606	CHL	OBD-CAD	3.69	1.28	1.22
30	i	601	CHL	OBD-CAD	3.69	1.28	1.22
31	b	613	CLA	C1D-ND	3.69	1.42	1.37
32	A	847	8CT	C14-C13	3.69	1.54	1.43
32	A	846	8CT	C14-C13	3.69	1.54	1.43
30	d	602	CHL	CHC-C4B	3.69	1.47	1.39
30	h	601	CHL	OBD-CAD	3.69	1.28	1.22
31	c	613	CLA	C1D-ND	3.69	1.42	1.37
30	i	609	CHL	CHB-C1B	3.69	1.47	1.39
31	7	312	CLA	C1D-ND	3.68	1.42	1.37
30	f	614	CHL	CHD-C4C	3.68	1.47	1.39
31	e	610	CLA	C1D-ND	3.68	1.42	1.37
30	e	605	CHL	OBD-CAD	3.68	1.28	1.22
30	5	301	CHL	C1D-ND	-3.68	1.33	1.37
32	O	205	8CT	C14-C13	3.68	1.54	1.43
30	f	605	CHL	OBD-CAD	3.68	1.28	1.22
30	4	306	CHL	CHC-C4B	3.68	1.47	1.39
30	e	606	CHL	OBD-CAD	3.68	1.28	1.22
30	8	315	CHL	CHD-C4C	3.68	1.47	1.39
30	i	609	CHL	OBD-CAD	3.68	1.28	1.22
30	d	607	CHL	CHB-C1B	3.68	1.47	1.39
31	B	840	CLA	C1D-ND	3.68	1.42	1.37
42	e	523	NEX	C7-C8	-3.68	1.25	1.32
30	d	601	CHL	OBD-CAD	3.67	1.28	1.22
31	b	603	CLA	C1D-ND	3.67	1.42	1.37
32	0	401	8CT	C11-C12	3.67	1.53	1.45
30	6	315	CHL	OBD-CAD	3.67	1.28	1.22
31	0	309	CLA	C1D-ND	3.67	1.42	1.37
31	d	610	CLA	C1D-ND	3.67	1.42	1.37
30	e	607	CHL	CHD-C4C	3.67	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	614	CHL	CHB-C1B	3.67	1.47	1.39
31	f	610	CLA	C1D-ND	3.67	1.42	1.37
37	c	521	0IE	C15-C16	3.67	1.40	1.35
32	L	209	8CT	C14-C13	3.67	1.54	1.43
30	5	306	CHL	OBD-CAD	3.67	1.28	1.22
30	2	302	CHL	CHC-C4B	3.67	1.47	1.39
32	F	302	8CT	C14-C13	3.67	1.54	1.43
30	a	601	CHL	OBD-CAD	3.67	1.28	1.22
30	5	301	CHL	CHD-C4C	3.67	1.47	1.39
30	6	302	CHL	C1D-ND	-3.67	1.33	1.37
31	b	604	CLA	C1D-ND	3.67	1.42	1.37
30	h	602	CHL	OBD-CAD	3.67	1.28	1.22
32	J	101	8CT	C14-C13	3.67	1.54	1.43
30	c	606	CHL	CHC-C4B	3.66	1.47	1.39
32	L	205	8CT	C14-C13	3.66	1.54	1.43
32	4	402	8CT	C11-C12	3.66	1.53	1.45
30	7	305	CHL	CHC-C4B	3.66	1.47	1.39
30	2	307	CHL	CHC-C4B	3.66	1.47	1.39
32	B	844	8CT	C28-C29	3.66	1.41	1.32
30	g	609	CHL	OBD-CAD	3.66	1.28	1.22
32	1	402	8CT	C11-C12	3.66	1.53	1.45
30	i	601	CHL	CHB-C1B	3.66	1.47	1.39
41	B	849	DGD	O1G-C1A	3.66	1.44	1.33
30	4	319	CHL	CHC-C4B	3.66	1.47	1.39
32	2	402	8CT	C28-C29	3.66	1.40	1.32
30	f	601	CHL	CHC-C4B	3.66	1.47	1.39
30	h	608	CHL	CHD-C4C	3.66	1.47	1.39
30	8	308	CHL	CHC-C4B	3.66	1.47	1.39
30	c	614	CHL	CHD-C4C	3.66	1.47	1.39
30	a	605	CHL	CHB-C1B	3.66	1.47	1.39
30	c	608	CHL	CHC-C4B	3.66	1.47	1.39
30	b	601	CHL	OBD-CAD	3.66	1.28	1.22
32	3	402	8CT	C11-C12	3.66	1.53	1.45
32	B	846	8CT	C11-C12	3.66	1.53	1.45
30	b	609	CHL	CHC-C4B	3.66	1.47	1.39
30	7	301	CHL	CHC-C4B	3.66	1.47	1.39
30	c	606	CHL	OBD-CAD	3.65	1.28	1.22
30	5	305	CHL	CHC-C4B	3.65	1.47	1.39
30	f	614	CHL	OBD-CAD	3.65	1.28	1.22
31	J	103	CLA	C1D-ND	3.65	1.42	1.37
30	0	306	CHL	CHC-C4B	3.65	1.47	1.39
30	g	608	CHL	OBD-CAD	3.65	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	313	CHL	CHC-C4B	3.65	1.47	1.39
31	0	313	CLA	C1D-ND	3.65	1.42	1.37
37	7	502	0IE	C8-C7	3.65	1.40	1.35
30	b	608	CHL	OBD-CAD	3.65	1.28	1.22
30	e	607	CHL	OBD-CAD	3.65	1.28	1.22
30	f	606	CHL	OBD-CAD	3.65	1.28	1.22
30	9	313	CHL	CHC-C4B	3.65	1.47	1.39
31	H	202	CLA	C1D-ND	3.65	1.42	1.37
30	a	614	CHL	CHB-C1B	3.65	1.47	1.39
30	d	601	CHL	CHB-C1B	3.65	1.47	1.39
30	1	307	CHL	CHC-C4B	3.64	1.47	1.39
31	5	310	CLA	C1D-ND	3.64	1.42	1.37
31	B	826	CLA	C4D-ND	-3.64	1.33	1.37
31	F	301	CLA	C1D-ND	3.64	1.42	1.37
30	i	608	CHL	CHD-C4C	3.64	1.47	1.39
31	9	310	CLA	C1D-ND	3.64	1.42	1.37
30	2	313	CHL	CHC-C4B	3.64	1.47	1.39
30	c	605	CHL	CHB-C1B	3.64	1.47	1.39
30	h	607	CHL	CHB-C1B	3.64	1.47	1.39
31	O	206	CLA	C1D-ND	3.64	1.42	1.37
30	4	308	CHL	CHC-C4B	3.64	1.47	1.39
32	B	851	8CT	C14-C13	3.64	1.54	1.43
30	h	606	CHL	CHD-C4C	3.64	1.47	1.39
31	8	309	CLA	C1D-ND	3.64	1.42	1.37
31	8	312	CLA	C1D-ND	3.64	1.42	1.37
31	A	835	CLA	C1D-ND	3.64	1.42	1.37
32	B	847	8CT	C14-C13	3.64	1.54	1.43
30	2	306	CHL	CHC-C4B	3.64	1.47	1.39
30	a	609	CHL	OBD-CAD	3.64	1.28	1.22
30	d	608	CHL	CHD-C4C	3.64	1.47	1.39
31	6	310	CLA	C1D-ND	3.64	1.42	1.37
31	8	314	CLA	C1D-ND	3.64	1.42	1.37
32	B	848	8CT	C11-C12	3.64	1.53	1.45
30	f	601	CHL	OBD-CAD	3.64	1.28	1.22
30	e	601	CHL	OBD-CAD	3.64	1.28	1.22
30	4	308	CHL	C1D-ND	-3.64	1.33	1.37
31	1	310	CLA	C1D-ND	3.63	1.42	1.37
30	1	306	CHL	CHC-C4B	3.63	1.47	1.39
32	7	405	8CT	C14-C13	3.63	1.54	1.43
30	3	302	CHL	C1D-ND	-3.63	1.33	1.37
32	M	102	8CT	C14-C13	3.63	1.54	1.43
30	i	605	CHL	CHB-C1B	3.63	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	602	CHL	CHD-C4C	3.63	1.47	1.39
30	e	609	CHL	CHD-C4C	3.63	1.47	1.39
30	9	301	CHL	OBD-CAD	3.63	1.28	1.22
30	e	601	CHL	CHC-C4B	3.63	1.47	1.39
30	8	305	CHL	OBD-CAD	3.63	1.28	1.22
31	L	207	CLA	C1D-ND	3.63	1.42	1.37
30	g	601	CHL	CHB-C1B	3.63	1.47	1.39
30	0	306	CHL	OBD-CAD	3.63	1.28	1.22
30	4	306	CHL	OBD-CAD	3.63	1.28	1.22
30	2	319	CHL	CHC-C4B	3.63	1.47	1.39
30	1	305	CHL	CHC-C4B	3.62	1.47	1.39
30	i	608	CHL	OBD-CAD	3.62	1.28	1.22
30	2	301	CHL	C1D-ND	-3.62	1.33	1.37
31	7	304	CLA	C1D-ND	3.62	1.42	1.37
30	2	305	CHL	CHC-C4B	3.62	1.47	1.39
32	I	101	8CT	C14-C13	3.62	1.54	1.43
31	H	205	CLA	C1D-ND	3.62	1.42	1.37
30	8	307	CHL	CHC-C4B	3.62	1.47	1.39
37	3	502	0IE	C11-C12	3.62	1.40	1.35
30	d	608	CHL	OBD-CAD	3.62	1.28	1.22
31	A	833	CLA	C1D-ND	3.62	1.42	1.37
30	6	305	CHL	CHC-C4B	3.62	1.47	1.39
31	7	315	CLA	C1D-ND	3.62	1.42	1.37
31	G	101	CLA	C1D-ND	3.62	1.42	1.37
31	L	204	CLA	C1D-ND	3.62	1.42	1.37
30	6	308	CHL	CHC-C4B	3.62	1.47	1.39
32	B	804	8CT	C14-C13	3.62	1.54	1.43
31	A	824	CLA	C1D-ND	3.62	1.42	1.37
30	0	302	CHL	OBD-CAD	3.62	1.28	1.22
31	1	309	CLA	C1D-ND	3.61	1.42	1.37
31	4	310	CLA	C1D-ND	3.61	1.42	1.37
30	7	302	CHL	CHC-C4B	3.61	1.47	1.39
32	K	107	8CT	C11-C12	3.61	1.53	1.45
30	4	302	CHL	CHC-C4B	3.61	1.47	1.39
31	1	311	CLA	C1D-ND	3.61	1.42	1.37
31	5	314	CLA	C1D-ND	3.61	1.42	1.37
32	1	402	8CT	C28-C29	3.61	1.40	1.32
30	8	306	CHL	OBD-CAD	3.61	1.28	1.22
30	d	609	CHL	OBD-CAD	3.61	1.28	1.22
30	5	307	CHL	CHD-C4C	3.61	1.47	1.39
31	K	104	CLA	C1D-ND	3.61	1.42	1.37
30	e	602	CHL	OBD-CAD	3.61	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	609	CHL	CHB-C1B	3.61	1.47	1.39
30	2	308	CHL	CHC-C4B	3.61	1.47	1.39
30	3	305	CHL	CHC-C4B	3.61	1.47	1.39
30	9	306	CHL	CHC-C4B	3.61	1.47	1.39
32	L	209	8CT	C11-C12	3.61	1.53	1.45
31	A	815	CLA	C1D-ND	3.61	1.42	1.37
31	B	822	CLA	C1D-ND	3.61	1.42	1.37
30	a	608	CHL	CHD-C4C	3.61	1.47	1.39
30	h	609	CHL	OBD-CAD	3.61	1.28	1.22
32	B	848	8CT	C28-C29	3.61	1.40	1.32
30	6	301	CHL	CHC-C4B	3.61	1.47	1.39
31	9	308	CLA	C1D-ND	3.61	1.42	1.37
30	9	313	CHL	OBD-CAD	3.61	1.28	1.22
30	b	607	CHL	OBD-CAD	3.61	1.28	1.22
30	i	602	CHL	OBD-CAD	3.61	1.28	1.22
31	B	821	CLA	C1D-ND	3.61	1.42	1.37
37	3	502	0IE	C8-C7	3.61	1.40	1.35
32	J	104	8CT	C11-C12	3.61	1.53	1.45
31	G	102	CLA	C1D-ND	3.61	1.42	1.37
30	2	301	CHL	CHC-C4B	3.61	1.47	1.39
30	i	606	CHL	CHB-C1B	3.61	1.47	1.39
31	0	304	CLA	C1D-ND	3.60	1.42	1.37
31	A	825	CLA	C1D-ND	3.60	1.42	1.37
30	e	606	CHL	CHD-C4C	3.60	1.47	1.39
30	g	605	CHL	CHB-C1B	3.60	1.47	1.39
31	0	310	CLA	C1D-ND	3.60	1.42	1.37
30	6	313	CHL	CHC-C4B	3.60	1.47	1.39
30	a	602	CHL	OBD-CAD	3.60	1.28	1.22
31	2	303	CLA	C1D-ND	3.60	1.42	1.37
30	f	608	CHL	CHC-C4B	3.60	1.47	1.39
30	e	614	CHL	CHB-C1B	3.60	1.47	1.39
31	3	313	CLA	C1D-ND	3.60	1.42	1.37
31	1	312	CLA	C1D-ND	3.60	1.42	1.37
31	6	320	CLA	C1D-ND	3.60	1.42	1.37
30	c	601	CHL	OBD-CAD	3.60	1.28	1.22
30	3	305	CHL	OBD-CAD	3.60	1.28	1.22
30	a	601	CHL	CHB-C1B	3.60	1.47	1.39
32	2	402	8CT	C11-C12	3.60	1.53	1.45
30	i	614	CHL	CHB-C1B	3.60	1.47	1.39
30	4	305	CHL	CHC-C4B	3.60	1.47	1.39
30	4	305	CHL	OBD-CAD	3.60	1.28	1.22
30	f	614	CHL	C3A-C2A	-3.60	1.51	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	306	CHL	CHC-C4B	3.59	1.47	1.39
30	e	602	CHL	CHD-C4C	3.59	1.47	1.39
30	6	302	CHL	CHC-C4B	3.59	1.47	1.39
31	3	311	CLA	C1D-ND	3.59	1.42	1.37
31	5	303	CLA	C1D-ND	3.59	1.42	1.37
30	0	305	CHL	CHD-C4C	3.59	1.47	1.39
30	b	607	CHL	CHD-C4C	3.59	1.47	1.39
30	7	302	CHL	C1D-ND	-3.59	1.33	1.37
31	6	309	CLA	C1D-ND	3.59	1.42	1.37
31	f	612	CLA	C1D-ND	3.59	1.42	1.37
30	5	305	CHL	CHD-C4C	3.59	1.47	1.39
30	g	602	CHL	CHB-C1B	3.59	1.47	1.39
31	4	312	CLA	C1D-ND	3.59	1.42	1.37
30	g	609	CHL	CHB-C1B	3.59	1.47	1.39
30	6	302	CHL	OBD-CAD	3.59	1.28	1.22
30	h	602	CHL	CHB-C1B	3.59	1.47	1.39
31	6	314	CLA	C1D-ND	3.59	1.42	1.37
30	8	305	CHL	CHC-C4B	3.59	1.47	1.39
32	G	104	8CT	C28-C29	3.59	1.40	1.32
37	7	502	0IE	C11-C12	3.59	1.40	1.35
30	6	305	CHL	OBD-CAD	3.58	1.28	1.22
30	6	301	CHL	OBD-CAD	3.58	1.28	1.22
31	A	814	CLA	C1D-ND	3.58	1.42	1.37
30	b	614	CHL	CHB-C1B	3.58	1.47	1.39
30	e	601	CHL	CHD-C4C	3.58	1.47	1.39
31	8	310	CLA	C1D-ND	3.58	1.42	1.37
30	0	302	CHL	C1D-ND	-3.58	1.33	1.37
32	7	402	8CT	C14-C13	3.58	1.54	1.43
30	a	608	CHL	OBD-CAD	3.58	1.28	1.22
30	7	305	CHL	OBD-CAD	3.58	1.28	1.22
31	1	304	CLA	C1D-ND	3.58	1.42	1.37
30	1	305	CHL	OBD-CAD	3.58	1.28	1.22
30	5	313	CHL	OBD-CAD	3.58	1.28	1.22
30	b	608	CHL	CHC-C4B	3.58	1.47	1.39
30	c	608	CHL	CHD-C4C	3.58	1.47	1.39
31	B	816	CLA	C1D-ND	3.58	1.42	1.37
30	g	607	CHL	CHB-C1B	3.58	1.47	1.39
30	5	313	CHL	C1D-ND	-3.58	1.33	1.37
32	0	401	8CT	C28-C29	3.58	1.40	1.32
30	h	609	CHL	CHB-C1B	3.58	1.47	1.39
30	5	302	CHL	CHC-C4B	3.57	1.47	1.39
32	J	101	8CT	C11-C12	3.57	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	302	CHL	CHC-C4B	3.57	1.47	1.39
30	1	313	CHL	OBD-CAD	3.57	1.28	1.22
31	6	304	CLA	C1D-ND	3.57	1.42	1.37
30	8	315	CHL	CHB-C1B	3.57	1.47	1.39
30	c	609	CHL	OBD-CAD	3.57	1.28	1.22
31	5	309	CLA	C1D-ND	3.57	1.42	1.37
30	d	609	CHL	CHB-C1B	3.57	1.47	1.39
30	f	609	CHL	CHB-C1B	3.57	1.47	1.39
30	7	306	CHL	C1D-ND	-3.57	1.33	1.37
31	2	311	CLA	C1D-ND	3.57	1.42	1.37
30	2	306	CHL	OBD-CAD	3.57	1.28	1.22
30	h	602	CHL	C1D-ND	-3.57	1.33	1.37
31	9	312	CLA	C1D-ND	3.57	1.42	1.37
30	b	602	CHL	OBD-CAD	3.57	1.28	1.22
30	5	302	CHL	OBD-CAD	3.57	1.28	1.22
30	7	301	CHL	OBD-CAD	3.56	1.28	1.22
31	1	314	CLA	C1D-ND	3.56	1.42	1.37
30	f	601	CHL	CHD-C4C	3.56	1.47	1.39
30	c	608	CHL	OBD-CAD	3.56	1.28	1.22
31	A	837	CLA	C1D-ND	3.56	1.42	1.37
30	i	607	CHL	CHB-C1B	3.56	1.47	1.39
30	f	607	CHL	CHB-C1B	3.56	1.47	1.39
31	3	308	CLA	C1D-ND	3.56	1.42	1.37
31	B	835	CLA	C1D-ND	3.56	1.42	1.37
30	5	301	CHL	OBD-CAD	3.56	1.28	1.22
31	3	310	CLA	C1D-ND	3.56	1.42	1.37
31	A	803	CLA	C1D-ND	3.56	1.42	1.37
30	c	607	CHL	CHB-C1B	3.56	1.47	1.39
31	9	311	CLA	C1D-ND	3.56	1.42	1.37
30	4	313	CHL	OBD-CAD	3.55	1.28	1.22
30	b	609	CHL	CHB-C1B	3.55	1.47	1.39
31	B	825	CLA	C1D-ND	3.55	1.42	1.37
30	0	301	CHL	CHC-C4B	3.55	1.47	1.39
31	8	311	CLA	C1D-ND	3.55	1.42	1.37
31	A	832	CLA	C1D-ND	3.55	1.42	1.37
30	1	306	CHL	OBD-CAD	3.55	1.28	1.22
30	8	315	CHL	C1D-ND	-3.55	1.33	1.37
31	B	833	CLA	C1D-ND	3.55	1.42	1.37
31	B	836	CLA	C1D-ND	3.55	1.42	1.37
31	B	832	CLA	C1D-ND	3.55	1.42	1.37
31	O	202	CLA	C1D-ND	3.55	1.42	1.37
31	7	310	CLA	C1D-ND	3.55	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	854	8CT	C28-C29	3.55	1.40	1.32
30	e	605	CHL	CHB-C1B	3.55	1.47	1.39
30	6	308	CHL	OBD-CAD	3.55	1.28	1.22
32	3	403	8CT	C28-C29	3.55	1.40	1.32
32	9	401	8CT	C11-C12	3.55	1.53	1.45
30	a	607	CHL	CHB-C1B	3.55	1.47	1.39
30	d	606	CHL	CHB-C1B	3.54	1.47	1.39
31	K	105	CLA	C1D-ND	3.54	1.42	1.37
30	4	302	CHL	OBD-CAD	3.54	1.28	1.22
30	6	305	CHL	C1D-ND	-3.54	1.33	1.37
32	G	104	8CT	C11-C12	3.54	1.53	1.45
30	8	301	CHL	OBD-CAD	3.54	1.28	1.22
30	3	305	CHL	C1D-ND	-3.54	1.33	1.37
31	B	827	CLA	C1D-ND	3.54	1.42	1.37
31	7	318	CLA	C1D-ND	3.54	1.42	1.37
31	0	312	CLA	C1D-ND	3.54	1.42	1.37
31	7	311	CLA	C1D-ND	3.54	1.42	1.37
30	4	302	CHL	C1D-ND	-3.54	1.33	1.37
30	h	601	CHL	CHB-C1B	3.54	1.47	1.39
30	7	313	CHL	OBD-CAD	3.54	1.28	1.22
30	8	306	CHL	CHC-C4B	3.54	1.47	1.39
32	9	401	8CT	C28-C29	3.54	1.40	1.32
30	2	305	CHL	OBD-CAD	3.54	1.28	1.22
30	2	307	CHL	C1D-ND	-3.54	1.33	1.37
31	O	201	CLA	C1D-ND	3.54	1.42	1.37
30	6	301	CHL	C1D-ND	-3.54	1.33	1.37
31	0	311	CLA	C1D-ND	3.54	1.42	1.37
30	5	306	CHL	C1D-ND	-3.54	1.33	1.37
30	6	315	CHL	C1D-ND	-3.53	1.33	1.37
30	b	609	CHL	C1D-ND	-3.53	1.33	1.37
31	A	816	CLA	C1D-ND	3.53	1.42	1.37
30	8	306	CHL	CHD-C4C	3.53	1.47	1.39
30	g	608	CHL	CHB-C1B	3.53	1.47	1.39
32	8	402	8CT	C28-C29	3.53	1.40	1.32
30	f	605	CHL	CHB-C1B	3.53	1.47	1.39
30	2	305	CHL	C1D-ND	-3.53	1.33	1.37
31	4	304	CLA	C1D-ND	3.53	1.42	1.37
30	f	602	CHL	OBD-CAD	3.53	1.28	1.22
30	1	313	CHL	C1D-ND	-3.53	1.33	1.37
31	A	838	CLA	C1D-ND	3.53	1.42	1.37
31	4	311	CLA	C1D-ND	3.53	1.42	1.37
30	8	313	CHL	OBD-CAD	3.53	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	314	CLA	C1D-ND	3.53	1.42	1.37
31	3	304	CLA	C1D-ND	3.53	1.42	1.37
30	1	302	CHL	C1D-ND	-3.53	1.33	1.37
32	3	402	8CT	C14-C13	3.53	1.54	1.43
30	9	301	CHL	CHC-C4B	3.53	1.47	1.39
31	3	306	CLA	C1D-ND	3.52	1.42	1.37
32	J	104	8CT	C28-C29	3.52	1.40	1.32
30	7	305	CHL	C1D-ND	-3.52	1.33	1.37
30	7	306	CHL	CHD-C4C	3.52	1.47	1.39
30	2	319	CHL	OBD-CAD	3.52	1.28	1.22
30	f	602	CHL	C1D-ND	-3.52	1.33	1.37
30	h	607	CHL	C1D-ND	-3.52	1.33	1.37
30	4	307	CHL	C1D-ND	-3.52	1.33	1.37
30	d	601	CHL	C1D-ND	-3.52	1.33	1.37
31	B	841	CLA	C1D-ND	3.52	1.42	1.37
30	c	601	CHL	CHC-C4B	3.52	1.47	1.39
30	6	306	CHL	OBD-CAD	3.52	1.28	1.22
30	c	606	CHL	CHD-C4C	3.52	1.47	1.39
30	g	606	CHL	CHB-C1B	3.52	1.47	1.39
30	6	315	CHL	CHD-C4C	3.52	1.47	1.39
31	6	303	CLA	C1D-ND	3.52	1.42	1.37
31	A	810	CLA	C1D-ND	3.52	1.42	1.37
32	8	406	8CT	C28-C29	3.52	1.40	1.32
32	L	205	8CT	C28-C29	3.52	1.40	1.32
31	B	815	CLA	C1D-ND	3.52	1.42	1.37
30	b	614	CHL	C3A-C2A	-3.52	1.51	1.54
30	e	608	CHL	OBD-CAD	3.52	1.28	1.22
32	A	847	8CT	C11-C12	3.52	1.53	1.45
30	b	607	CHL	C1D-ND	-3.52	1.33	1.37
31	A	819	CLA	C1D-ND	3.52	1.42	1.37
31	A	843	CLA	C1D-ND	3.52	1.42	1.37
31	B	813	CLA	C1D-ND	3.52	1.42	1.37
31	4	314	CLA	C1D-ND	3.52	1.42	1.37
31	4	303	CLA	C1D-ND	3.52	1.42	1.37
30	5	306	CHL	CHB-C1B	3.51	1.47	1.39
30	6	306	CHL	CHC-C4B	3.51	1.47	1.39
30	8	301	CHL	C1D-ND	-3.51	1.33	1.37
30	8	308	CHL	C1D-ND	-3.51	1.33	1.37
30	b	602	CHL	CHD-C4C	3.51	1.47	1.39
30	9	313	CHL	CHD-C4C	3.51	1.47	1.39
32	6	402	8CT	C28-C29	3.51	1.40	1.32
32	A	848	8CT	C14-C13	3.51	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	607	CHL	C3D-C2D	3.51	1.48	1.39
32	B	847	8CT	C11-C12	3.51	1.53	1.45
31	0	303	CLA	C1D-ND	3.51	1.42	1.37
31	3	303	CLA	C1D-ND	3.51	1.42	1.37
31	B	820	CLA	C1D-ND	3.51	1.42	1.37
30	7	313	CHL	CHD-C4C	3.51	1.47	1.39
30	h	605	CHL	C3D-C2D	3.51	1.48	1.39
30	d	602	CHL	CHD-C4C	3.51	1.47	1.39
31	8	304	CLA	C1D-ND	3.51	1.42	1.37
31	7	303	CLA	C1D-ND	3.51	1.42	1.37
30	g	609	CHL	C3D-C2D	3.51	1.48	1.39
30	9	306	CHL	OBD-CAD	3.51	1.28	1.22
30	2	308	CHL	C1D-ND	-3.50	1.33	1.37
30	6	306	CHL	C1D-ND	-3.50	1.33	1.37
30	7	313	CHL	C1D-ND	-3.50	1.33	1.37
30	6	313	CHL	OBD-CAD	3.50	1.28	1.22
30	1	306	CHL	CHD-C4C	3.50	1.47	1.39
30	g	605	CHL	C3D-C2D	3.50	1.48	1.39
30	0	306	CHL	CHD-C4C	3.50	1.47	1.39
32	A	854	8CT	C11-C12	3.50	1.53	1.45
30	f	608	CHL	OBD-CAD	3.50	1.28	1.22
30	e	608	CHL	CHD-C4C	3.50	1.47	1.39
31	9	302	CLA	C1D-ND	3.50	1.42	1.37
32	A	846	8CT	C11-C12	3.50	1.53	1.45
30	d	602	CHL	OBD-CAD	3.50	1.28	1.22
32	3	402	8CT	C28-C29	3.50	1.40	1.32
30	8	302	CHL	C1D-ND	-3.50	1.33	1.37
30	2	313	CHL	C1D-ND	-3.50	1.33	1.37
32	A	849	8CT	C14-C13	3.50	1.54	1.43
30	8	313	CHL	CHC-C4B	3.49	1.47	1.39
30	8	305	CHL	CHD-C4C	3.49	1.47	1.39
32	7	405	8CT	C11-C12	3.49	1.53	1.45
32	3	402	8CT	C30-C29	3.49	1.55	1.50
30	7	307	CHL	C1D-ND	-3.49	1.33	1.37
30	c	605	CHL	C1D-ND	-3.49	1.33	1.37
31	A	802	CLA	C1D-ND	3.49	1.42	1.37
30	5	307	CHL	CHB-C1B	3.49	1.47	1.39
30	a	605	CHL	C3D-C2D	3.49	1.48	1.39
30	b	606	CHL	CHD-C4C	3.49	1.47	1.39
30	2	306	CHL	C1D-ND	-3.49	1.33	1.37
30	7	301	CHL	C1D-ND	-3.49	1.33	1.37
31	3	318	CLA	C1D-ND	3.49	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	839	CLA	C1D-ND	3.49	1.42	1.37
30	g	602	CHL	C1D-ND	-3.49	1.33	1.37
32	A	850	8CT	C14-C13	3.49	1.54	1.43
30	4	313	CHL	CHC-C4B	3.49	1.47	1.39
30	a	609	CHL	C1D-ND	-3.49	1.33	1.37
30	9	306	CHL	C1D-ND	-3.49	1.33	1.37
31	9	300	CLA	C1D-ND	3.49	1.42	1.37
32	J	101	8CT	C28-C29	3.49	1.40	1.32
30	b	606	CHL	OBD-CAD	3.49	1.28	1.22
31	9	309	CLA	C1D-ND	3.49	1.42	1.37
30	d	605	CHL	C3D-C2D	3.48	1.48	1.39
30	3	307	CHL	C1D-ND	-3.48	1.33	1.37
31	A	827	CLA	C1D-ND	3.48	1.42	1.37
30	7	302	CHL	OBD-CAD	3.48	1.28	1.22
30	h	606	CHL	CHB-C1B	3.48	1.47	1.39
30	e	606	CHL	C1D-ND	-3.48	1.33	1.37
30	6	307	CHL	C1D-ND	-3.48	1.33	1.37
30	g	601	CHL	C1D-ND	-3.48	1.33	1.37
30	8	308	CHL	CHD-C4C	3.48	1.47	1.39
32	3	403	8CT	C11-C12	3.48	1.53	1.45
31	2	312	CLA	C1D-ND	3.48	1.42	1.37
30	a	606	CHL	CHB-C1B	3.48	1.47	1.39
30	e	607	CHL	CHB-C1B	3.48	1.47	1.39
32	L	205	8CT	C30-C29	3.48	1.55	1.50
30	h	605	CHL	C1D-ND	-3.48	1.33	1.37
30	1	302	CHL	OBD-CAD	3.48	1.28	1.22
30	4	308	CHL	CHD-C4C	3.48	1.47	1.39
30	i	605	CHL	C3D-C2D	3.48	1.48	1.39
31	B	850	CLA	C1D-ND	3.47	1.42	1.37
30	f	614	CHL	CHB-C1B	3.47	1.47	1.39
30	f	609	CHL	OBD-CAD	3.47	1.28	1.22
31	2	309	CLA	C1D-ND	3.47	1.42	1.37
37	3	502	0IE	C15-C16	3.47	1.40	1.35
31	A	812	CLA	C1D-ND	3.47	1.42	1.37
30	a	614	CHL	C3D-C2D	3.47	1.48	1.39
30	7	307	CHL	OBD-CAD	3.47	1.28	1.22
30	h	602	CHL	C3D-C2D	3.47	1.48	1.39
30	3	302	CHL	OBD-CAD	3.47	1.28	1.22
32	K	107	8CT	C28-C29	3.47	1.40	1.32
30	8	307	CHL	C1D-ND	-3.47	1.33	1.37
30	3	307	CHL	CHC-C4B	3.47	1.47	1.39
32	O	205	8CT	C11-C12	3.47	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	307	CHL	OBD-CAD	3.47	1.28	1.22
32	F	302	8CT	C28-C29	3.47	1.40	1.32
31	A	811	CLA	C1D-ND	3.47	1.42	1.37
31	A	828	CLA	C1D-ND	3.47	1.42	1.37
32	6	402	8CT	C11-C12	3.47	1.53	1.45
32	L	206	8CT	C11-C12	3.47	1.53	1.45
30	4	305	CHL	C1D-ND	-3.47	1.33	1.37
31	6	317	CLA	C1D-ND	3.47	1.42	1.37
30	d	607	CHL	C1D-ND	-3.47	1.33	1.37
30	g	614	CHL	C3D-C2D	3.47	1.48	1.39
30	g	607	CHL	C3D-C2D	3.47	1.48	1.39
30	8	301	CHL	CHD-C4C	3.46	1.47	1.39
30	9	305	CHL	C1D-ND	-3.46	1.33	1.37
31	1	303	CLA	C1D-ND	3.46	1.42	1.37
30	i	609	CHL	C3D-C2D	3.46	1.48	1.39
30	c	601	CHL	CHD-C4C	3.46	1.47	1.39
31	A	808	CLA	C1D-ND	3.46	1.42	1.37
31	A	840	CLA	C1D-ND	3.46	1.42	1.37
30	4	319	CHL	C1D-ND	-3.46	1.33	1.37
31	B	834	CLA	C1D-ND	3.46	1.42	1.37
30	4	307	CHL	CHC-C4B	3.46	1.47	1.39
30	i	601	CHL	C3D-C2D	3.46	1.48	1.39
30	b	609	CHL	OBD-CAD	3.46	1.28	1.22
31	B	807	CLA	C1D-ND	3.46	1.42	1.37
30	0	306	CHL	CHB-C1B	3.46	1.47	1.39
30	c	609	CHL	CHB-C1B	3.46	1.47	1.39
30	5	307	CHL	OBD-CAD	3.46	1.28	1.22
30	e	609	CHL	CHB-C1B	3.46	1.47	1.39
30	b	601	CHL	CHB-C1B	3.45	1.47	1.39
30	4	319	CHL	OBD-CAD	3.45	1.28	1.22
30	d	607	CHL	C3D-C2D	3.45	1.48	1.39
30	1	307	CHL	OBD-CAD	3.45	1.28	1.22
31	6	311	CLA	C1D-ND	3.45	1.42	1.37
31	B	818	CLA	C1D-ND	3.45	1.42	1.37
30	g	601	CHL	C3D-C2D	3.45	1.48	1.39
30	f	607	CHL	C3D-C2D	3.45	1.48	1.39
30	8	302	CHL	OBD-CAD	3.45	1.28	1.22
32	L	206	8CT	C28-C29	3.45	1.40	1.32
30	6	313	CHL	C1D-ND	-3.45	1.33	1.37
30	9	313	CHL	C1D-ND	-3.45	1.33	1.37
31	A	853	CLA	C1D-ND	3.45	1.42	1.37
30	e	609	CHL	OBD-CAD	3.45	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	605	CHL	C1D-ND	-3.45	1.33	1.37
31	7	316	CLA	C1D-ND	3.45	1.42	1.37
30	2	302	CHL	OBD-CAD	3.45	1.28	1.22
32	L	209	8CT	C28-C29	3.45	1.40	1.32
30	5	313	CHL	C3D-C2D	3.45	1.48	1.39
31	6	318	CLA	C1D-ND	3.44	1.42	1.37
30	b	608	CHL	CHD-C4C	3.44	1.47	1.39
30	0	306	CHL	C1D-ND	-3.44	1.33	1.37
31	3	312	CLA	C1D-ND	3.44	1.42	1.37
30	2	313	CHL	OBD-CAD	3.44	1.28	1.22
31	B	823	CLA	C1D-ND	3.44	1.42	1.37
31	B	839	CLA	C1D-ND	3.44	1.42	1.37
30	f	607	CHL	C1D-ND	-3.44	1.33	1.37
31	7	308	CLA	C1D-ND	3.44	1.42	1.37
31	9	303	CLA	C1D-ND	3.44	1.42	1.37
31	2	304	CLA	C1D-ND	3.44	1.42	1.37
31	B	819	CLA	C1D-ND	3.44	1.42	1.37
31	A	805	CLA	C4D-ND	-3.44	1.33	1.37
30	i	614	CHL	C3D-C2D	3.44	1.48	1.39
30	g	602	CHL	C3D-C2D	3.44	1.48	1.39
31	3	309	CLA	C1D-ND	3.44	1.42	1.37
30	c	605	CHL	C3D-C2D	3.44	1.48	1.39
30	2	319	CHL	C1D-ND	-3.44	1.33	1.37
30	8	308	CHL	OBD-CAD	3.44	1.28	1.22
30	c	606	CHL	C1D-ND	-3.43	1.33	1.37
31	A	852	CLA	C1D-ND	3.43	1.42	1.37
31	A	805	CLA	C1D-ND	3.43	1.42	1.37
32	M	102	8CT	C28-C29	3.43	1.40	1.32
30	0	305	CHL	C1D-ND	-3.43	1.33	1.37
30	4	313	CHL	C1D-ND	-3.43	1.33	1.37
31	B	838	CLA	C1D-ND	3.43	1.42	1.37
30	2	301	CHL	OBD-CAD	3.43	1.28	1.22
30	5	313	CHL	CHB-C1B	3.43	1.47	1.39
30	c	602	CHL	CHD-C4C	3.43	1.47	1.39
30	b	602	CHL	C1D-ND	-3.43	1.33	1.37
30	d	601	CHL	C3D-C2D	3.43	1.48	1.39
30	i	607	CHL	C3D-C2D	3.43	1.48	1.39
31	L	203	CLA	C1D-ND	3.43	1.42	1.37
30	e	614	CHL	C3D-C2D	3.43	1.48	1.39
30	d	614	CHL	C3D-C2D	3.43	1.48	1.39
30	1	306	CHL	C1D-ND	-3.43	1.33	1.37
31	B	828	CLA	C1D-ND	3.43	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	202	CLA	C1D-ND	3.43	1.42	1.37
32	B	846	8CT	C35-C30	3.43	1.65	1.56
30	5	307	CHL	C1D-ND	-3.43	1.33	1.37
31	B	837	CLA	C1D-ND	3.43	1.42	1.37
30	1	305	CHL	CHD-C4C	3.43	1.47	1.39
30	4	307	CHL	OBD-CAD	3.43	1.28	1.22
30	5	301	CHL	CHB-C1B	3.43	1.47	1.39
30	6	301	CHL	CHD-C4C	3.43	1.47	1.39
31	A	806	CLA	C1D-ND	3.43	1.42	1.37
32	7	402	8CT	C11-C12	3.43	1.53	1.45
31	A	818	CLA	C1D-ND	3.43	1.42	1.37
31	B	811	CLA	C1D-ND	3.43	1.42	1.37
32	O	205	8CT	C28-C29	3.43	1.40	1.32
30	b	614	CHL	C3D-C2D	3.43	1.48	1.39
30	d	609	CHL	C1D-ND	-3.42	1.33	1.37
30	4	308	CHL	OBD-CAD	3.42	1.28	1.22
30	e	614	CHL	C1D-ND	-3.42	1.33	1.37
30	0	301	CHL	C1D-ND	-3.42	1.33	1.37
30	e	605	CHL	C1D-ND	-3.42	1.33	1.37
31	7	309	CLA	C1D-ND	3.42	1.42	1.37
30	6	307	CHL	OBD-CAD	3.42	1.28	1.22
30	4	306	CHL	CHD-C4C	3.42	1.47	1.39
32	L	205	8CT	C35-C30	3.42	1.65	1.56
31	B	808	CLA	C1D-ND	3.42	1.42	1.37
30	c	614	CHL	CHB-C1B	3.42	1.47	1.39
30	2	302	CHL	C1D-ND	-3.42	1.33	1.37
31	A	813	CLA	C1D-ND	3.42	1.42	1.37
30	0	301	CHL	OBD-CAD	3.42	1.28	1.22
30	8	305	CHL	C1D-ND	-3.42	1.33	1.37
32	B	804	8CT	C11-C12	3.42	1.53	1.45
31	K	102	CLA	C1D-ND	3.42	1.42	1.37
30	i	609	CHL	C1D-ND	-3.42	1.33	1.37
30	a	602	CHL	CHB-C1B	3.42	1.47	1.39
31	A	826	CLA	C4D-ND	-3.42	1.33	1.37
30	h	608	CHL	CHB-C1B	3.42	1.47	1.39
32	F	302	8CT	C11-C12	3.42	1.53	1.45
30	9	301	CHL	CHD-C4C	3.42	1.47	1.39
30	4	302	CHL	CHD-C4C	3.41	1.47	1.39
30	5	302	CHL	C1D-ND	-3.41	1.33	1.37
30	d	605	CHL	C1D-ND	-3.41	1.33	1.37
32	B	851	8CT	C28-C29	3.41	1.40	1.32
37	7	502	0IE	C15-C16	3.41	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	614	CHL	C1D-ND	-3.41	1.33	1.37
30	1	307	CHL	CHD-C4C	3.41	1.47	1.39
30	b	607	CHL	CHB-C1B	3.41	1.47	1.39
30	g	606	CHL	C1D-ND	-3.41	1.33	1.37
30	e	607	CHL	C1D-ND	-3.41	1.33	1.37
31	H	201	CLA	C1D-ND	3.41	1.42	1.37
30	f	605	CHL	C3D-C2D	3.41	1.48	1.39
30	7	307	CHL	CHD-C4C	3.41	1.47	1.39
30	2	301	CHL	CHD-C4C	3.41	1.47	1.39
30	c	607	CHL	C1D-ND	-3.41	1.33	1.37
31	6	311	CLA	C4B-NB	3.41	1.42	1.37
31	6	312	CLA	C1D-ND	3.41	1.42	1.37
31	M	101	CLA	C1D-ND	3.41	1.42	1.37
30	8	313	CHL	C1D-ND	-3.40	1.33	1.37
31	A	821	CLA	C1D-ND	3.40	1.42	1.37
30	i	602	CHL	CHB-C1B	3.40	1.47	1.39
30	2	306	CHL	CHD-C4C	3.40	1.47	1.39
30	7	301	CHL	CHD-C4C	3.40	1.47	1.39
31	A	813	CLA	C4D-ND	-3.40	1.33	1.37
32	B	844	8CT	C01-C02	3.40	1.56	1.50
30	i	605	CHL	C1D-ND	-3.40	1.33	1.37
30	a	609	CHL	C3D-C2D	3.40	1.48	1.39
30	5	306	CHL	C3D-C2D	3.40	1.48	1.39
30	f	606	CHL	CHB-C1B	3.40	1.47	1.39
30	c	602	CHL	C1D-ND	-3.40	1.33	1.37
30	h	614	CHL	C1D-ND	-3.40	1.33	1.37
30	c	607	CHL	C3D-C2D	3.40	1.48	1.39
30	6	313	CHL	CHD-C4C	3.40	1.47	1.39
31	A	827	CLA	C4D-ND	-3.40	1.33	1.37
30	h	601	CHL	C3D-C2D	3.40	1.48	1.39
32	G	104	8CT	C35-C30	3.40	1.65	1.56
30	f	609	CHL	C1D-ND	-3.40	1.33	1.37
32	J	101	8CT	C35-C30	3.40	1.65	1.56
31	B	818	CLA	C4D-ND	-3.40	1.33	1.37
31	g	610	CLA	C4B-NB	3.40	1.42	1.37
30	3	307	CHL	OBD-CAD	3.40	1.28	1.22
30	2	319	CHL	CHD-C4C	3.40	1.47	1.39
30	e	605	CHL	C3D-C2D	3.40	1.48	1.39
31	3	320	CLA	C1D-ND	3.39	1.42	1.37
31	A	831	CLA	C1D-ND	3.39	1.42	1.37
31	2	310	CLA	C1D-ND	3.39	1.42	1.37
30	h	609	CHL	C3D-C2D	3.39	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	609	CHL	C1D-ND	-3.39	1.33	1.37
32	A	848	8CT	C11-C12	3.39	1.53	1.45
32	L	205	8CT	C11-C12	3.39	1.53	1.45
30	d	606	CHL	C3D-C2D	3.39	1.48	1.39
30	8	306	CHL	C1D-ND	-3.39	1.33	1.37
30	b	606	CHL	C1D-ND	-3.39	1.33	1.37
30	i	606	CHL	C1D-ND	-3.39	1.33	1.37
31	h	612	CLA	C4B-NB	3.39	1.42	1.37
31	B	803	CLA	C1D-ND	3.39	1.42	1.37
31	B	812	CLA	C1D-ND	3.39	1.42	1.37
30	h	614	CHL	C3D-C2D	3.39	1.48	1.39
32	I	101	8CT	C11-C12	3.39	1.53	1.45
30	4	306	CHL	C1D-ND	-3.39	1.33	1.37
30	8	313	CHL	CHD-C4C	3.39	1.47	1.39
31	A	820	CLA	C1D-ND	3.39	1.41	1.37
30	4	319	CHL	CHD-C4C	3.39	1.47	1.39
31	9	311	CLA	C4B-NB	3.39	1.41	1.37
31	B	809	CLA	C1D-ND	3.39	1.41	1.37
32	A	850	8CT	C11-C12	3.39	1.53	1.45
32	7	404	8CT	C11-C12	3.39	1.53	1.45
30	d	609	CHL	C3D-C2D	3.39	1.48	1.39
30	f	602	CHL	CHD-C4C	3.39	1.47	1.39
30	e	606	CHL	CHB-C1B	3.39	1.47	1.39
32	B	851	8CT	C11-C12	3.39	1.53	1.45
30	f	608	CHL	CHD-C4C	3.39	1.47	1.39
30	a	602	CHL	C1D-ND	-3.39	1.33	1.37
30	6	308	CHL	CHD-C4C	3.38	1.47	1.39
42	f	523	NEX	C7-C8	-3.38	1.26	1.32
30	d	606	CHL	C1D-ND	-3.38	1.33	1.37
32	A	850	8CT	C28-C29	3.38	1.40	1.32
31	B	814	CLA	C4D-ND	-3.38	1.33	1.37
31	B	829	CLA	C1D-ND	3.38	1.41	1.37
30	1	313	CHL	CHD-C4C	3.38	1.46	1.39
30	1	307	CHL	C1D-ND	-3.38	1.33	1.37
31	A	822	CLA	C1D-ND	3.38	1.41	1.37
30	c	606	CHL	CHB-C1B	3.38	1.47	1.39
30	d	608	CHL	CHB-C1B	3.38	1.47	1.39
31	a	604	CLA	C4B-NB	3.38	1.41	1.37
30	c	614	CHL	C3D-C2D	3.38	1.48	1.39
30	h	606	CHL	C3D-C2D	3.37	1.48	1.39
30	a	607	CHL	C3D-C2D	3.37	1.48	1.39
30	a	605	CHL	C1D-ND	-3.37	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	c	523	NEX	C7-C8	-3.37	1.26	1.32
30	b	609	CHL	C3D-C2D	3.37	1.48	1.39
30	h	609	CHL	C1D-ND	-3.37	1.33	1.37
31	A	836	CLA	C1D-ND	3.37	1.41	1.37
30	6	308	CHL	CHB-C1B	3.37	1.47	1.39
31	B	824	CLA	C1D-ND	3.37	1.41	1.37
30	6	315	CHL	CHB-C1B	3.37	1.47	1.39
31	A	807	CLA	C1D-ND	3.37	1.41	1.37
42	b	523	NEX	C7-C8	-3.37	1.26	1.32
31	B	814	CLA	C1D-ND	3.37	1.41	1.37
32	B	845	8CT	C28-C29	3.36	1.40	1.32
31	b	604	CLA	C4B-NB	3.36	1.41	1.37
30	g	608	CHL	C3D-C2D	3.36	1.48	1.39
30	f	614	CHL	C1D-ND	-3.36	1.33	1.37
31	a	613	CLA	C4B-NB	3.36	1.41	1.37
30	2	307	CHL	OBD-CAD	3.36	1.28	1.22
30	4	308	CHL	CHB-C1B	3.36	1.46	1.39
30	d	614	CHL	C1D-ND	-3.36	1.33	1.37
30	e	609	CHL	C1D-ND	-3.36	1.33	1.37
31	A	823	CLA	C1D-ND	3.36	1.41	1.37
30	8	301	CHL	CHB-C1B	3.36	1.46	1.39
30	f	609	CHL	C3D-C2D	3.36	1.48	1.39
30	b	614	CHL	C1D-ND	-3.36	1.33	1.37
30	i	606	CHL	C3D-C2D	3.36	1.48	1.39
32	A	849	8CT	C28-C29	3.36	1.40	1.32
30	1	306	CHL	CHB-C1B	3.36	1.46	1.39
30	a	607	CHL	C1D-ND	-3.36	1.33	1.37
42	i	523	NEX	C7-C8	-3.35	1.26	1.32
30	2	305	CHL	CHD-C4C	3.35	1.46	1.39
30	d	602	CHL	C1D-ND	-3.35	1.33	1.37
31	A	817	CLA	C1D-ND	3.35	1.41	1.37
30	9	305	CHL	OBD-CAD	3.35	1.28	1.22
30	i	602	CHL	C1D-ND	-3.35	1.33	1.37
30	2	308	CHL	OBD-CAD	3.35	1.28	1.22
31	g	603	CLA	C4B-NB	3.35	1.41	1.37
31	B	836	CLA	C4D-ND	-3.35	1.33	1.37
32	A	848	8CT	C01-C02	3.35	1.56	1.50
30	g	609	CHL	C1D-ND	-3.35	1.33	1.37
31	d	611	CLA	C4B-NB	3.35	1.41	1.37
31	h	613	CLA	C4B-NB	3.35	1.41	1.37
30	a	608	CHL	CHB-C1B	3.35	1.46	1.39
32	G	104	8CT	C30-C29	3.35	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	305	CHL	C1D-ND	-3.35	1.33	1.37
31	B	817	CLA	C1D-ND	3.35	1.41	1.37
30	a	606	CHL	C3D-C2D	3.35	1.48	1.39
31	A	809	CLA	C1D-ND	3.35	1.41	1.37
30	0	305	CHL	CHB-C1B	3.35	1.46	1.39
30	8	302	CHL	CHD-C4C	3.35	1.46	1.39
31	L	201	CLA	C1D-ND	3.35	1.41	1.37
32	G	104	8CT	C01-C02	3.35	1.56	1.50
42	a	523	NEX	C7-C8	-3.34	1.26	1.32
30	a	606	CHL	C1D-ND	-3.34	1.33	1.37
30	7	313	CHL	CHB-C1B	3.34	1.46	1.39
31	g	613	CLA	C4B-NB	3.34	1.41	1.37
31	B	827	CLA	C4D-ND	-3.34	1.33	1.37
42	g	523	NEX	C7-C8	-3.34	1.26	1.32
32	3	402	8CT	C35-C30	3.34	1.65	1.56
30	2	302	CHL	CHD-C4C	3.34	1.46	1.39
30	i	607	CHL	C1D-ND	-3.34	1.33	1.37
31	A	840	CLA	C4D-ND	-3.34	1.33	1.37
30	c	609	CHL	C3D-C2D	3.34	1.48	1.39
30	e	607	CHL	C3D-C2D	3.34	1.48	1.39
30	0	302	CHL	CHD-C4C	3.34	1.46	1.39
30	i	608	CHL	CHB-C1B	3.34	1.46	1.39
30	b	608	CHL	C1D-ND	-3.34	1.33	1.37
30	8	315	CHL	C3D-C2D	3.34	1.48	1.39
30	8	308	CHL	CHB-C1B	3.34	1.46	1.39
30	g	606	CHL	C3D-C2D	3.34	1.48	1.39
31	A	841	CLA	C1D-ND	3.34	1.41	1.37
31	a	611	CLA	C4B-NB	3.34	1.41	1.37
31	A	816	CLA	C4B-NB	3.33	1.41	1.37
30	b	607	CHL	C3D-C2D	3.33	1.48	1.39
30	a	601	CHL	C3D-C2D	3.33	1.48	1.39
31	i	611	CLA	C4B-NB	3.33	1.41	1.37
31	A	821	CLA	C4D-ND	-3.33	1.33	1.37
30	6	306	CHL	CHD-C4C	3.33	1.46	1.39
31	B	826	CLA	C1D-ND	3.33	1.41	1.37
30	2	308	CHL	CHD-C4C	3.33	1.46	1.39
31	i	603	CLA	C4B-NB	3.33	1.41	1.37
30	9	313	CHL	CHB-C1B	3.33	1.46	1.39
32	7	402	8CT	C28-C29	3.33	1.40	1.32
30	0	301	CHL	CHD-C4C	3.33	1.46	1.39
32	B	843	8CT	C30-C29	3.33	1.55	1.50
30	i	601	CHL	C1D-ND	-3.33	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	203	CLA	C4B-NB	3.33	1.41	1.37
30	g	605	CHL	C1D-ND	-3.33	1.33	1.37
31	A	830	CLA	C1D-ND	3.33	1.41	1.37
32	3	403	8CT	C35-C30	3.33	1.65	1.56
30	a	602	CHL	C3D-C2D	3.32	1.48	1.39
42	h	523	NEX	C7-C8	-3.32	1.26	1.32
32	I	101	8CT	C28-C29	3.32	1.40	1.32
31	B	810	CLA	C4D-ND	-3.32	1.33	1.37
30	9	306	CHL	CHD-C4C	3.32	1.46	1.39
30	6	301	CHL	CHB-C1B	3.32	1.46	1.39
30	6	307	CHL	CHD-C4C	3.32	1.46	1.39
32	A	847	8CT	C28-C29	3.32	1.40	1.32
31	B	839	CLA	C4D-ND	-3.32	1.33	1.37
31	i	613	CLA	C4B-NB	3.32	1.41	1.37
30	4	305	CHL	CHD-C4C	3.32	1.46	1.39
31	g	612	CLA	C4B-NB	3.32	1.41	1.37
31	K	101	CLA	C1D-ND	3.32	1.41	1.37
31	H	201	CLA	C4D-ND	-3.32	1.33	1.37
30	6	313	CHL	CHB-C1B	3.31	1.46	1.39
30	9	301	CHL	C1D-ND	-3.31	1.33	1.37
30	6	302	CHL	CHD-C4C	3.31	1.46	1.39
32	6	402	8CT	C35-C30	3.31	1.65	1.56
30	a	614	CHL	C1D-ND	-3.31	1.33	1.37
32	B	804	8CT	C28-C29	3.31	1.40	1.32
32	8	406	8CT	C30-C29	3.31	1.55	1.50
30	a	608	CHL	C1D-ND	-3.31	1.33	1.37
30	g	614	CHL	C1D-ND	-3.31	1.33	1.37
31	A	836	CLA	C4D-ND	-3.31	1.33	1.37
30	f	601	CHL	C1D-ND	-3.31	1.33	1.37
30	3	305	CHL	CHD-C4C	3.31	1.46	1.39
30	d	608	CHL	C1D-ND	-3.31	1.33	1.37
30	7	302	CHL	CHD-C4C	3.31	1.46	1.39
32	A	846	8CT	C01-C02	3.31	1.56	1.50
31	A	804	CLA	C1D-ND	3.31	1.41	1.37
30	g	608	CHL	C1D-ND	-3.31	1.33	1.37
30	f	606	CHL	C1D-ND	-3.31	1.33	1.37
30	b	601	CHL	C1D-ND	-3.31	1.33	1.37
30	b	601	CHL	C3D-C2D	3.31	1.48	1.39
32	M	102	8CT	C11-C12	3.31	1.53	1.45
30	5	305	CHL	CHB-C1B	3.30	1.46	1.39
32	B	846	8CT	C01-C02	3.30	1.56	1.50
30	h	601	CHL	C1D-ND	-3.30	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	602	CHL	CHB-C1B	3.30	1.46	1.39
30	1	302	CHL	CHD-C4C	3.30	1.46	1.39
32	J	101	8CT	C30-C29	3.30	1.55	1.50
30	g	607	CHL	C1D-ND	-3.30	1.33	1.37
30	6	305	CHL	CHD-C4C	3.30	1.46	1.39
30	9	305	CHL	CHD-C4C	3.30	1.46	1.39
31	B	806	CLA	C4D-ND	-3.30	1.33	1.37
30	i	608	CHL	C3D-C2D	3.30	1.48	1.39
31	B	809	CLA	C4D-ND	-3.30	1.33	1.37
31	h	611	CLA	C4B-NB	3.30	1.41	1.37
30	8	305	CHL	CHB-C1B	3.30	1.46	1.39
30	3	302	CHL	CHD-C4C	3.30	1.46	1.39
30	e	602	CHL	C1D-ND	-3.30	1.33	1.37
30	h	605	CHL	MG-NA	-3.30	1.98	2.06
32	1	402	8CT	C35-C30	3.30	1.65	1.56
31	O	206	CLA	C4B-NB	3.30	1.41	1.37
31	i	604	CLA	C4B-NB	3.30	1.41	1.37
30	4	313	CHL	CHD-C4C	3.30	1.46	1.39
30	f	601	CHL	CHB-C1B	3.30	1.46	1.39
31	6	304	CLA	C4B-NB	3.30	1.41	1.37
31	d	604	CLA	C4B-NB	3.30	1.41	1.37
30	8	307	CHL	CHD-C4C	3.29	1.46	1.39
31	8	311	CLA	C4B-NB	3.29	1.41	1.37
30	a	601	CHL	C1D-ND	-3.29	1.33	1.37
32	K	107	8CT	C01-C02	3.29	1.56	1.50
30	d	605	CHL	MG-NA	-3.29	1.98	2.06
30	i	614	CHL	C1D-ND	-3.29	1.33	1.37
32	8	406	8CT	C01-C02	3.29	1.56	1.50
30	5	302	CHL	CHD-C4C	3.29	1.46	1.39
31	A	812	CLA	C4D-ND	-3.29	1.33	1.37
31	5	314	CLA	C4B-NB	3.29	1.41	1.37
30	1	307	CHL	CHB-C1B	3.29	1.46	1.39
30	i	602	CHL	C3D-C2D	3.29	1.48	1.39
30	e	614	CHL	C3A-C2A	-3.29	1.51	1.54
39	A	857	CL0	CMD-C2D	-3.29	1.43	1.50
42	d	523	NEX	C7-C8	-3.29	1.26	1.32
32	A	849	8CT	C35-C30	3.29	1.65	1.56
31	B	837	CLA	C4D-ND	-3.29	1.33	1.37
32	A	850	8CT	C35-C30	3.28	1.65	1.56
30	h	614	CHL	MG-NA	-3.28	1.98	2.06
31	A	808	CLA	C4D-ND	-3.28	1.33	1.37
31	h	603	CLA	C4B-NB	3.28	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	h	610	CLA	C4B-NB	3.28	1.41	1.37
31	A	834	CLA	C1D-ND	3.28	1.41	1.37
32	A	849	8CT	C01-C02	3.28	1.56	1.50
30	h	608	CHL	C3D-C2D	3.28	1.48	1.39
31	F	301	CLA	C4D-ND	-3.28	1.33	1.37
32	M	102	8CT	C35-C30	3.28	1.65	1.56
30	7	306	CHL	OBD-CAD	3.28	1.28	1.22
30	1	305	CHL	C1D-ND	-3.28	1.33	1.37
30	e	608	CHL	CHB-C1B	3.28	1.46	1.39
32	7	405	8CT	C28-C29	3.28	1.40	1.32
30	i	605	CHL	MG-NA	-3.28	1.98	2.06
32	4	402	8CT	C01-C02	3.28	1.56	1.50
30	g	614	CHL	MG-NA	-3.28	1.98	2.06
31	A	815	CLA	C4D-ND	-3.28	1.33	1.37
32	A	847	8CT	C01-C02	3.28	1.56	1.50
31	H	205	CLA	C4B-NB	3.27	1.41	1.37
30	5	305	CHL	C3D-C2D	3.27	1.48	1.39
30	f	614	CHL	C3D-C2D	3.27	1.48	1.39
30	g	601	CHL	MG-NA	-3.27	1.98	2.06
31	g	604	CLA	C4B-NB	3.27	1.41	1.37
30	c	608	CHL	CHB-C1B	3.27	1.46	1.39
30	e	602	CHL	C3D-C2D	3.27	1.48	1.39
31	i	612	CLA	C4B-NB	3.27	1.41	1.37
31	A	841	CLA	C4D-ND	-3.27	1.33	1.37
32	A	846	8CT	C28-C29	3.27	1.40	1.32
30	a	605	CHL	MG-NA	-3.27	1.98	2.06
30	i	608	CHL	C1D-ND	-3.27	1.33	1.37
32	3	403	8CT	C01-C02	3.27	1.56	1.50
30	b	608	CHL	CHB-C1B	3.27	1.46	1.39
30	6	315	CHL	C3D-C2D	3.27	1.48	1.39
30	h	607	CHL	MG-NA	-3.27	1.98	2.06
30	7	305	CHL	CHD-C4C	3.27	1.46	1.39
30	g	609	CHL	C3A-C2A	-3.26	1.51	1.54
31	A	826	CLA	C1D-ND	3.26	1.41	1.37
30	d	608	CHL	C3D-C2D	3.26	1.48	1.39
31	A	839	CLA	C4D-ND	-3.26	1.33	1.37
32	L	209	8CT	C35-C30	3.26	1.65	1.56
30	e	601	CHL	CHB-C1B	3.26	1.46	1.39
31	2	311	CLA	C4D-ND	-3.26	1.33	1.37
32	4	402	8CT	C35-C30	3.26	1.65	1.56
30	5	301	CHL	C3D-C2D	3.26	1.48	1.39
31	d	612	CLA	C4B-NB	3.26	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	602	CHL	C3D-C2D	3.26	1.48	1.39
31	A	837	CLA	C4D-ND	-3.26	1.33	1.37
31	B	834	CLA	C4D-ND	-3.26	1.33	1.37
31	B	805	CLA	C1D-ND	3.26	1.41	1.37
31	A	822	CLA	C4D-ND	-3.26	1.33	1.37
31	A	833	CLA	C4D-ND	-3.26	1.33	1.37
31	M	101	CLA	C4D-ND	-3.26	1.33	1.37
31	A	829	CLA	C1D-ND	3.26	1.41	1.37
32	B	847	8CT	C28-C29	3.26	1.40	1.32
31	2	303	CLA	C4D-ND	-3.26	1.33	1.37
31	A	818	CLA	C4D-ND	-3.25	1.33	1.37
30	3	307	CHL	CHD-C4C	3.25	1.46	1.39
31	A	811	CLA	C4D-ND	-3.25	1.33	1.37
30	d	614	CHL	MG-NA	-3.25	1.98	2.06
30	2	313	CHL	CHD-C4C	3.25	1.46	1.39
31	B	828	CLA	C4D-ND	-3.25	1.33	1.37
31	K	102	CLA	C4D-ND	-3.25	1.33	1.37
30	4	308	CHL	C3D-C2D	3.25	1.48	1.39
32	4	402	8CT	C18-C17	3.25	1.53	1.43
30	d	602	CHL	C3D-C2D	3.25	1.48	1.39
31	B	830	CLA	C4D-ND	-3.25	1.33	1.37
31	L	207	CLA	C4B-NB	3.25	1.41	1.37
31	B	833	CLA	C4D-ND	-3.25	1.33	1.37
31	b	613	CLA	C4B-NB	3.25	1.41	1.37
30	a	614	CHL	MG-NA	-3.24	1.98	2.06
31	f	604	CLA	C4B-NB	3.24	1.41	1.37
30	g	605	CHL	MG-NA	-3.24	1.98	2.06
31	a	610	CLA	C4B-NB	3.24	1.41	1.37
31	B	812	CLA	C4D-ND	-3.24	1.33	1.37
31	4	303	CLA	C4D-ND	-3.24	1.33	1.37
32	M	102	8CT	C01-C02	3.24	1.56	1.50
31	0	321	CLA	C4B-NB	3.24	1.41	1.37
32	0	401	8CT	C35-C30	3.24	1.65	1.56
31	d	613	CLA	C4B-NB	3.24	1.41	1.37
31	h	604	CLA	C4B-NB	3.24	1.41	1.37
31	A	819	CLA	C4D-ND	-3.24	1.33	1.37
32	8	406	8CT	C35-C30	3.24	1.65	1.56
30	i	614	CHL	C3A-C2A	-3.24	1.51	1.54
32	A	850	8CT	C01-C02	3.24	1.56	1.50
31	A	803	CLA	C4D-ND	-3.24	1.33	1.37
31	f	603	CLA	C4B-NB	3.24	1.41	1.37
32	B	843	8CT	C35-C30	3.24	1.65	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	306	CHL	C3D-C2D	3.24	1.48	1.39
30	7	313	CHL	C3D-C2D	3.24	1.48	1.39
31	K	101	CLA	C4D-ND	-3.24	1.33	1.37
30	c	605	CHL	MG-NA	-3.24	1.98	2.06
32	I	101	8CT	C01-C02	3.24	1.56	1.50
30	c	602	CHL	C3D-C2D	3.24	1.48	1.39
31	4	314	CLA	C4D-ND	-3.24	1.33	1.37
30	h	606	CHL	C1D-ND	-3.24	1.33	1.37
31	B	838	CLA	C4D-ND	-3.24	1.33	1.37
31	B	841	CLA	C4D-ND	-3.24	1.33	1.37
31	1	314	CLA	C4D-ND	-3.23	1.33	1.37
30	f	608	CHL	C1D-ND	-3.23	1.33	1.37
32	7	404	8CT	C35-C30	3.23	1.65	1.56
32	A	849	8CT	C11-C12	3.23	1.52	1.45
30	8	307	CHL	CHB-C1B	3.23	1.46	1.39
30	h	608	CHL	C1D-ND	-3.23	1.33	1.37
30	7	306	CHL	CHB-C1B	3.23	1.46	1.39
32	2	402	8CT	C18-C17	3.23	1.53	1.43
39	A	857	CL0	C4D-ND	-3.23	1.33	1.37
31	A	830	CLA	C4D-ND	-3.23	1.33	1.37
31	B	820	CLA	C4D-ND	-3.23	1.33	1.37
32	O	205	8CT	C01-C02	3.23	1.56	1.50
31	A	802	CLA	C4D-ND	-3.23	1.33	1.37
32	F	302	8CT	C01-C02	3.23	1.56	1.50
30	9	306	CHL	C3D-C2D	3.23	1.47	1.39
31	O	202	CLA	C4D-ND	-3.23	1.33	1.37
30	7	306	CHL	C3D-C2D	3.23	1.47	1.39
30	b	606	CHL	CHB-C1B	3.23	1.46	1.39
31	7	315	CLA	C4D-ND	-3.23	1.33	1.37
31	A	807	CLA	C4D-ND	-3.23	1.33	1.37
31	2	309	CLA	C4D-ND	-3.23	1.33	1.37
32	J	104	8CT	C30-C29	3.22	1.55	1.50
31	b	610	CLA	C4B-NB	3.22	1.41	1.37
30	f	605	CHL	MG-NA	-3.22	1.98	2.06
30	f	608	CHL	CHB-C1B	3.22	1.46	1.39
31	b	603	CLA	C4B-NB	3.22	1.41	1.37
31	9	312	CLA	C4D-ND	-3.22	1.33	1.37
31	K	101	CLA	C4B-NB	3.22	1.41	1.37
30	c	606	CHL	C3D-C2D	3.22	1.47	1.39
30	8	306	CHL	C3D-C2D	3.22	1.47	1.39
31	B	810	CLA	C1D-ND	3.22	1.41	1.37
32	7	402	8CT	C01-C02	3.22	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	606	CHL	C3D-C2D	3.22	1.47	1.39
31	B	819	CLA	C4D-ND	-3.22	1.33	1.37
30	g	609	CHL	O2A-CGA	3.22	1.45	1.33
30	e	609	CHL	C3D-C2D	3.22	1.47	1.39
31	B	829	CLA	C4D-ND	-3.22	1.33	1.37
32	B	847	8CT	C01-C02	3.22	1.56	1.50
32	L	205	8CT	C01-C02	3.22	1.56	1.50
30	4	307	CHL	CHD-C4C	3.22	1.46	1.39
30	c	608	CHL	C1D-ND	-3.22	1.33	1.37
31	6	309	CLA	C4D-ND	-3.22	1.33	1.37
31	A	824	CLA	C4D-ND	-3.22	1.33	1.37
30	2	306	CHL	CHB-C1B	3.22	1.46	1.39
30	d	607	CHL	MG-NA	-3.22	1.98	2.06
31	A	805	CLA	C4B-NB	3.22	1.41	1.37
30	7	301	CHL	CHB-C1B	3.22	1.46	1.39
31	A	806	CLA	C4D-ND	-3.22	1.33	1.37
31	B	811	CLA	C4D-ND	-3.22	1.33	1.37
31	L	203	CLA	C4D-ND	-3.22	1.33	1.37
32	2	402	8CT	C35-C30	3.22	1.65	1.56
31	c	603	CLA	C4B-NB	3.22	1.41	1.37
30	a	608	CHL	C3D-C2D	3.22	1.47	1.39
30	2	308	CHL	CHB-C1B	3.21	1.46	1.39
30	f	602	CHL	C3D-C2D	3.21	1.47	1.39
31	9	303	CLA	C4B-NB	3.21	1.41	1.37
31	A	825	CLA	C4D-ND	-3.21	1.33	1.37
30	5	307	CHL	C3D-C2D	3.21	1.47	1.39
31	6	303	CLA	C4D-ND	-3.21	1.33	1.37
31	e	611	CLA	C4B-NB	3.21	1.41	1.37
31	3	318	CLA	C4D-ND	-3.21	1.33	1.37
31	a	612	CLA	C4B-NB	3.21	1.41	1.37
32	B	851	8CT	C01-C02	3.21	1.56	1.50
30	c	608	CHL	C3D-C2D	3.21	1.47	1.39
32	A	848	8CT	C28-C29	3.21	1.39	1.32
31	1	304	CLA	C4D-ND	-3.21	1.33	1.37
30	6	301	CHL	C3D-C2D	3.21	1.47	1.39
30	c	601	CHL	C3D-C2D	3.21	1.47	1.39
31	B	830	CLA	C1D-ND	3.21	1.41	1.37
30	1	313	CHL	CHB-C1B	3.21	1.46	1.39
30	e	606	CHL	C3D-C2D	3.20	1.47	1.39
31	B	817	CLA	C4D-ND	-3.20	1.33	1.37
30	e	608	CHL	C1D-ND	-3.20	1.33	1.37
30	c	602	CHL	CHB-C1B	3.20	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	601	CHL	C3D-C2D	3.20	1.47	1.39
31	7	308	CLA	C4D-ND	-3.20	1.33	1.37
31	A	823	CLA	C4D-ND	-3.20	1.33	1.37
31	c	604	CLA	C4B-NB	3.20	1.41	1.37
32	0	401	8CT	C01-C02	3.20	1.56	1.50
31	B	807	CLA	C4D-ND	-3.20	1.33	1.37
31	B	831	CLA	C4D-ND	-3.20	1.33	1.37
31	B	831	CLA	C1D-ND	3.20	1.41	1.37
30	9	301	CHL	CHB-C1B	3.20	1.46	1.39
31	B	801	CLA	C4D-ND	-3.20	1.33	1.37
31	g	611	CLA	C4B-NB	3.20	1.41	1.37
31	b	612	CLA	C4B-NB	3.20	1.41	1.37
32	L	209	8CT	C01-C02	3.19	1.56	1.50
30	i	609	CHL	MG-NA	-3.19	1.98	2.06
31	e	613	CLA	C4B-NB	3.19	1.41	1.37
30	9	306	CHL	CHB-C1B	3.19	1.46	1.39
35	0	603	SQD	O48-C23	3.19	1.42	1.33
31	3	304	CLA	C4D-ND	-3.19	1.33	1.37
31	A	843	CLA	C4D-ND	-3.19	1.33	1.37
31	b	611	CLA	C4B-NB	3.19	1.41	1.37
31	7	303	CLA	C4D-ND	-3.19	1.33	1.37
32	A	854	8CT	C01-C02	3.19	1.56	1.50
31	8	303	CLA	C4B-NB	3.19	1.41	1.37
31	A	835	CLA	C4D-ND	-3.19	1.33	1.37
32	B	843	8CT	C01-C02	3.19	1.56	1.50
31	2	310	CLA	C4D-ND	-3.19	1.33	1.37
31	L	204	CLA	C4D-ND	-3.19	1.33	1.37
30	d	602	CHL	CHB-C1B	3.19	1.46	1.39
31	3	310	CLA	C4D-ND	-3.19	1.33	1.37
31	9	309	CLA	C4D-ND	-3.19	1.33	1.37
32	L	206	8CT	C01-C02	3.18	1.56	1.50
31	4	310	CLA	C4D-ND	-3.18	1.33	1.37
32	J	104	8CT	C01-C02	3.18	1.56	1.50
30	6	308	CHL	C3D-C2D	3.18	1.47	1.39
31	A	814	CLA	C4D-ND	-3.18	1.33	1.37
30	2	302	CHL	C3D-C2D	3.18	1.47	1.39
31	7	304	CLA	C4D-ND	-3.18	1.33	1.37
31	7	318	CLA	C4D-ND	-3.18	1.33	1.37
31	9	304	CLA	C4D-ND	-3.18	1.33	1.37
31	c	611	CLA	C4B-NB	3.18	1.41	1.37
31	f	611	CLA	C4B-NB	3.18	1.41	1.37
30	2	306	CHL	C3D-C2D	3.18	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	313	CHL	C3D-C2D	3.18	1.47	1.39
30	a	614	CHL	C3A-C2A	-3.18	1.51	1.54
31	6	318	CLA	C4D-ND	-3.18	1.33	1.37
30	2	313	CHL	CHB-C1B	3.18	1.46	1.39
32	1	402	8CT	C01-C02	3.18	1.56	1.50
32	G	104	8CT	C18-C17	3.18	1.53	1.43
30	8	308	CHL	C3D-C2D	3.17	1.47	1.39
31	5	308	CLA	C4B-NB	3.17	1.41	1.37
32	7	404	8CT	C18-C17	3.17	1.53	1.43
30	4	306	CHL	CHB-C1B	3.17	1.46	1.39
31	d	603	CLA	C4B-NB	3.17	1.41	1.37
30	6	302	CHL	C3D-C2D	3.17	1.47	1.39
31	A	831	CLA	C4D-ND	-3.17	1.33	1.37
31	L	207	CLA	C4D-ND	-3.17	1.33	1.37
31	9	308	CLA	C4D-ND	-3.17	1.33	1.37
31	4	304	CLA	C4D-ND	-3.17	1.33	1.37
31	9	310	CLA	C4B-NB	3.17	1.41	1.37
39	A	857	CL0	C1D-ND	3.17	1.41	1.37
31	A	852	CLA	C4D-ND	-3.17	1.33	1.37
30	5	313	CHL	MG-NA	-3.17	1.98	2.06
30	0	305	CHL	C3D-C2D	3.17	1.47	1.39
31	0	303	CLA	C4B-NB	3.17	1.41	1.37
31	8	309	CLA	C4D-ND	-3.17	1.33	1.37
32	9	401	8CT	C01-C02	3.17	1.56	1.50
31	0	313	CLA	C4D-ND	-3.17	1.33	1.37
30	7	301	CHL	C3D-C2D	3.17	1.47	1.39
30	1	302	CHL	C3D-C2D	3.17	1.47	1.39
30	2	308	CHL	C3D-C2D	3.17	1.47	1.39
31	7	310	CLA	C4B-NB	3.17	1.41	1.37
31	A	810	CLA	C4D-ND	-3.17	1.33	1.37
30	8	306	CHL	CHB-C1B	3.17	1.46	1.39
30	c	601	CHL	C1D-ND	-3.17	1.33	1.37
31	4	309	CLA	C4B-NB	3.17	1.41	1.37
32	B	847	8CT	C35-C30	3.16	1.65	1.56
30	e	601	CHL	C1D-ND	-3.16	1.33	1.37
32	B	804	8CT	C01-C02	3.16	1.56	1.50
31	0	308	CLA	C4B-NB	3.16	1.41	1.37
31	8	304	CLA	C4B-NB	3.16	1.41	1.37
31	B	822	CLA	C4B-NB	3.16	1.41	1.37
31	e	610	CLA	C4B-NB	3.16	1.41	1.37
31	B	821	CLA	C4D-ND	-3.16	1.33	1.37
31	1	303	CLA	C4B-NB	3.16	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	609	CHL	MG-NA	-3.16	1.98	2.06
30	0	306	CHL	C3D-C2D	3.16	1.47	1.39
30	8	302	CHL	C3D-C2D	3.16	1.47	1.39
32	7	404	8CT	C01-C02	3.16	1.56	1.50
32	B	848	8CT	C18-C17	3.16	1.53	1.43
31	A	820	CLA	C4D-ND	-3.16	1.33	1.37
31	B	805	CLA	C4D-ND	-3.16	1.33	1.37
31	B	815	CLA	C4D-ND	-3.16	1.33	1.37
31	B	803	CLA	C4D-ND	-3.16	1.33	1.37
31	B	822	CLA	C4D-ND	-3.16	1.33	1.37
31	2	314	CLA	C4B-NB	3.16	1.41	1.37
31	6	318	CLA	C4B-NB	3.16	1.41	1.37
31	7	315	CLA	C4B-NB	3.16	1.41	1.37
30	g	607	CHL	MG-NA	-3.16	1.98	2.06
31	A	853	CLA	C4B-NB	3.16	1.41	1.37
31	B	806	CLA	C1D-ND	3.16	1.41	1.37
31	B	808	CLA	C4D-ND	-3.15	1.33	1.37
31	B	824	CLA	C4D-ND	-3.15	1.33	1.37
30	0	302	CHL	C3D-C2D	3.15	1.47	1.39
31	A	834	CLA	C4D-ND	-3.15	1.33	1.37
31	0	311	CLA	C4D-ND	-3.15	1.33	1.37
30	6	307	CHL	CHB-C1B	3.15	1.46	1.39
30	i	614	CHL	MG-NA	-3.15	1.98	2.06
30	4	307	CHL	CHB-C1B	3.15	1.46	1.39
32	I	101	8CT	C35-C30	3.15	1.65	1.56
30	2	307	CHL	CHB-C1B	3.15	1.46	1.39
31	A	810	CLA	C3B-C4B	3.15	1.50	1.42
31	7	309	CLA	C4D-ND	-3.15	1.33	1.37
30	8	313	CHL	CHB-C1B	3.15	1.46	1.39
32	8	402	8CT	C35-C30	3.15	1.65	1.56
32	1	402	8CT	C30-C29	3.15	1.54	1.50
31	c	612	CLA	C4B-NB	3.15	1.41	1.37
30	0	301	CHL	CHB-C1B	3.15	1.46	1.39
31	6	317	CLA	C4D-ND	-3.15	1.33	1.37
30	2	307	CHL	CHD-C4C	3.15	1.46	1.39
31	9	302	CLA	C4D-ND	-3.15	1.33	1.37
31	B	835	CLA	C4D-ND	-3.15	1.33	1.37
30	6	305	CHL	CHB-C1B	3.15	1.46	1.39
30	f	607	CHL	MG-NA	-3.15	1.98	2.06
31	A	804	CLA	C4D-ND	-3.15	1.33	1.37
31	e	604	CLA	C4B-NB	3.15	1.41	1.37
30	3	302	CHL	C3D-C2D	3.15	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	201	CLA	C4B-NB	3.15	1.41	1.37
31	8	312	CLA	C4D-ND	-3.15	1.33	1.37
31	5	304	CLA	C4B-NB	3.14	1.41	1.37
31	2	314	CLA	C4D-ND	-3.14	1.33	1.37
31	f	612	CLA	C4B-NB	3.14	1.41	1.37
31	3	309	CLA	C4D-ND	-3.14	1.33	1.37
31	5	309	CLA	C4B-NB	3.14	1.41	1.37
30	9	301	CHL	C3D-C2D	3.14	1.47	1.39
31	A	829	CLA	C4D-ND	-3.14	1.33	1.37
30	e	608	CHL	C3D-C2D	3.14	1.47	1.39
31	a	603	CLA	C4B-NB	3.14	1.41	1.37
30	7	307	CHL	CHB-C1B	3.14	1.46	1.39
32	A	846	8CT	C35-C30	3.14	1.65	1.56
31	B	832	CLA	C4D-ND	-3.14	1.33	1.37
31	B	850	CLA	C4D-ND	-3.14	1.33	1.37
30	4	305	CHL	CHB-C1B	3.14	1.46	1.39
32	B	845	8CT	C18-C17	3.14	1.53	1.43
32	K	107	8CT	C35-C30	3.14	1.65	1.56
31	3	308	CLA	C4D-ND	-3.14	1.33	1.37
31	6	320	CLA	C4B-NB	3.14	1.41	1.37
31	B	809	CLA	C4B-NB	3.14	1.41	1.37
31	e	603	CLA	C4B-NB	3.14	1.41	1.37
32	7	405	8CT	C35-C30	3.14	1.65	1.56
31	9	311	CLA	C4D-ND	-3.14	1.33	1.37
31	f	613	CLA	C4B-NB	3.14	1.41	1.37
31	i	610	CLA	C4B-NB	3.14	1.41	1.37
30	2	301	CHL	C3D-C2D	3.14	1.47	1.39
32	B	845	8CT	C01-C02	3.14	1.56	1.50
31	L	201	CLA	C4D-ND	-3.13	1.33	1.37
31	B	829	CLA	C4B-NB	3.13	1.41	1.37
31	1	312	CLA	C4D-ND	-3.13	1.33	1.37
30	b	614	CHL	MG-NA	-3.13	1.98	2.06
32	L	206	8CT	C35-C30	3.13	1.65	1.56
32	B	848	8CT	C01-C02	3.13	1.56	1.50
31	0	309	CLA	C4D-ND	-3.13	1.33	1.37
30	4	302	CHL	C3D-C2D	3.13	1.47	1.39
31	1	308	CLA	C4B-NB	3.13	1.41	1.37
31	7	312	CLA	C4D-ND	-3.13	1.33	1.37
31	7	317	CLA	C4B-NB	3.13	1.41	1.37
31	e	612	CLA	C4B-NB	3.13	1.41	1.37
31	7	311	CLA	C4D-ND	-3.13	1.33	1.37
30	1	313	CHL	C3D-C2D	3.13	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	823	CLA	C4B-NB	3.13	1.41	1.37
30	8	301	CHL	C3D-C2D	3.13	1.47	1.39
30	9	313	CHL	C3D-C2D	3.13	1.47	1.39
31	A	838	CLA	C4D-ND	-3.13	1.33	1.37
30	a	609	CHL	MG-NA	-3.13	1.98	2.06
32	J	101	8CT	C01-C02	3.13	1.56	1.50
31	B	816	CLA	C4D-ND	-3.13	1.33	1.37
30	2	301	CHL	CHB-C1B	3.13	1.46	1.39
31	5	303	CLA	C4B-NB	3.13	1.41	1.37
31	B	850	CLA	C4B-NB	3.13	1.41	1.37
32	3	403	8CT	C30-C29	3.13	1.54	1.50
31	A	853	CLA	C4D-ND	-3.13	1.33	1.37
31	8	312	CLA	C4B-NB	3.13	1.41	1.37
30	i	607	CHL	MG-NA	-3.13	1.98	2.06
31	M	101	CLA	C4B-NB	3.13	1.41	1.37
31	G	102	CLA	C4D-ND	-3.12	1.33	1.37
30	6	306	CHL	CHB-C1B	3.12	1.46	1.39
30	8	305	CHL	C3D-C2D	3.12	1.47	1.39
31	6	311	CLA	C4D-ND	-3.12	1.33	1.37
31	1	304	CLA	C4B-NB	3.12	1.41	1.37
31	G	101	CLA	C4B-NB	3.12	1.41	1.37
31	c	610	CLA	C4B-NB	3.12	1.41	1.37
31	J	103	CLA	C4D-ND	-3.12	1.33	1.37
31	A	812	CLA	C4B-NB	3.12	1.41	1.37
32	0	401	8CT	C18-C17	3.12	1.53	1.43
31	d	610	CLA	C4B-NB	3.12	1.41	1.37
31	A	853	CLA	C3B-C4B	3.12	1.50	1.42
31	4	311	CLA	C4D-ND	-3.12	1.33	1.37
31	3	320	CLA	C4D-ND	-3.12	1.33	1.37
31	0	310	CLA	C4D-ND	-3.12	1.33	1.37
31	3	306	CLA	C4D-ND	-3.12	1.33	1.37
31	4	312	CLA	C4D-ND	-3.12	1.33	1.37
31	3	312	CLA	C4D-ND	-3.11	1.33	1.37
31	7	316	CLA	C4D-ND	-3.11	1.33	1.37
31	2	312	CLA	C4D-ND	-3.11	1.33	1.37
31	6	314	CLA	C4D-ND	-3.11	1.33	1.37
31	L	202	CLA	C4D-ND	-3.11	1.33	1.37
32	B	848	8CT	C35-C30	3.11	1.65	1.56
31	1	311	CLA	C4D-ND	-3.11	1.33	1.37
31	K	105	CLA	C4D-ND	-3.11	1.33	1.37
31	0	304	CLA	C4B-NB	3.11	1.41	1.37
31	2	304	CLA	C4D-ND	-3.11	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	825	CLA	C4D-ND	-3.11	1.33	1.37
31	A	828	CLA	C4D-ND	-3.11	1.33	1.37
31	3	313	CLA	C4B-NB	3.11	1.41	1.37
31	6	310	CLA	C4B-NB	3.11	1.41	1.37
30	g	608	CHL	MG-NA	-3.11	1.98	2.06
31	8	311	CLA	C4D-ND	-3.11	1.33	1.37
32	B	847	8CT	C30-C29	3.11	1.54	1.50
30	4	306	CHL	C3D-C2D	3.11	1.47	1.39
31	0	312	CLA	C4B-NB	3.11	1.41	1.37
31	A	805	CLA	C3B-C4B	3.11	1.50	1.42
31	B	801	CLA	C1D-ND	3.11	1.41	1.37
31	B	835	CLA	C4B-NB	3.11	1.41	1.37
31	H	202	CLA	C4B-NB	3.11	1.41	1.37
32	A	847	8CT	C35-C30	3.11	1.65	1.56
31	A	816	CLA	C4D-ND	-3.10	1.33	1.37
30	3	305	CHL	C3D-C2D	3.10	1.47	1.39
32	9	401	8CT	C18-C17	3.10	1.53	1.43
31	0	308	CLA	C4D-ND	-3.10	1.33	1.37
31	8	303	CLA	C4D-ND	-3.10	1.33	1.37
31	A	832	CLA	C4D-ND	-3.10	1.33	1.37
32	6	402	8CT	C18-C17	3.10	1.53	1.43
30	d	614	CHL	C3A-C2A	-3.10	1.51	1.54
30	2	319	CHL	CHB-C1B	3.10	1.46	1.39
31	3	313	CLA	C4D-ND	-3.10	1.33	1.37
30	6	302	CHL	CHB-C1B	3.10	1.46	1.39
30	b	608	CHL	C3D-C2D	3.10	1.47	1.39
32	7	405	8CT	C01-C02	3.10	1.56	1.50
30	0	301	CHL	C3D-C2D	3.10	1.47	1.39
31	8	310	CLA	C4D-ND	-3.10	1.33	1.37
32	8	406	8CT	C18-C17	3.10	1.53	1.43
32	J	104	8CT	C18-C17	3.10	1.53	1.43
31	B	829	CLA	C3B-C4B	3.10	1.50	1.42
30	f	606	CHL	C3D-C2D	3.09	1.47	1.39
31	5	309	CLA	C4D-ND	-3.09	1.33	1.37
30	9	305	CHL	C3D-C2D	3.09	1.47	1.39
31	c	613	CLA	C4B-NB	3.09	1.41	1.37
30	3	307	CHL	CHB-C1B	3.09	1.46	1.39
30	6	305	CHL	C3D-C2D	3.09	1.47	1.39
30	b	601	CHL	MG-NA	-3.09	1.98	2.06
31	0	304	CLA	C4D-ND	-3.09	1.33	1.37
30	8	315	CHL	MG-NA	-3.09	1.98	2.06
31	7	312	CLA	C4B-NB	3.09	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	319	CHL	CHB-C1B	3.09	1.46	1.39
30	e	605	CHL	MG-NA	-3.09	1.98	2.06
30	a	601	CHL	MG-NA	-3.09	1.98	2.06
30	7	305	CHL	C3D-C2D	3.09	1.47	1.39
31	K	104	CLA	C4D-ND	-3.09	1.33	1.37
30	c	601	CHL	CHB-C1B	3.09	1.46	1.39
32	1	402	8CT	C18-C17	3.09	1.53	1.43
31	H	205	CLA	C4D-ND	-3.09	1.33	1.37
32	F	302	8CT	C35-C30	3.09	1.65	1.56
30	h	601	CHL	MG-NA	-3.09	1.98	2.06
30	h	602	CHL	MG-NA	-3.09	1.98	2.06
32	A	848	8CT	C35-C30	3.09	1.65	1.56
31	5	314	CLA	C4D-ND	-3.09	1.33	1.37
31	9	310	CLA	C4D-ND	-3.09	1.33	1.37
31	B	813	CLA	C4D-ND	-3.09	1.33	1.37
30	7	302	CHL	CHB-C1B	3.08	1.46	1.39
32	6	402	8CT	C01-C02	3.08	1.56	1.50
31	G	103	CLA	C4B-NB	3.08	1.41	1.37
31	A	810	CLA	C4B-NB	3.08	1.41	1.37
31	3	303	CLA	C4D-ND	-3.08	1.33	1.37
30	5	302	CHL	CHB-C1B	3.08	1.46	1.39
30	e	601	CHL	C3D-C2D	3.08	1.47	1.39
30	i	601	CHL	MG-NA	-3.08	1.98	2.06
30	2	305	CHL	CHB-C1B	3.08	1.46	1.39
31	A	802	CLA	C4B-NB	3.08	1.41	1.37
30	d	601	CHL	MG-NA	-3.08	1.99	2.06
30	4	313	CHL	CHB-C1B	3.08	1.46	1.39
31	f	610	CLA	C4B-NB	3.08	1.41	1.37
31	B	813	CLA	C3B-C4B	3.08	1.50	1.42
30	e	614	CHL	MG-NA	-3.08	1.99	2.06
31	c	611	CLA	C4D-ND	-3.08	1.33	1.37
30	2	302	CHL	CHB-C1B	3.08	1.46	1.39
32	3	402	8CT	C01-C02	3.08	1.56	1.50
30	5	302	CHL	C3D-C2D	3.08	1.47	1.39
31	B	823	CLA	C4B-NB	3.08	1.41	1.37
31	B	840	CLA	C4D-ND	-3.07	1.33	1.37
30	e	602	CHL	CHB-C1B	3.07	1.46	1.39
31	A	817	CLA	C4D-ND	-3.07	1.33	1.37
30	4	319	CHL	C3D-C2D	3.07	1.47	1.39
31	B	834	CLA	C4B-NB	3.07	1.41	1.37
32	B	851	8CT	C35-C30	3.07	1.64	1.56
31	B	813	CLA	C4B-NB	3.07	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	302	CHL	CHB-C1B	3.07	1.46	1.39
31	6	312	CLA	C4D-ND	-3.07	1.33	1.37
30	f	609	CHL	MG-NA	-3.07	1.99	2.06
31	B	823	CLA	C4D-ND	-3.07	1.33	1.37
31	5	312	CLA	C4D-ND	-3.07	1.33	1.37
30	8	302	CHL	CHB-C1B	3.07	1.46	1.39
30	8	313	CHL	C3D-C2D	3.07	1.47	1.39
32	L	206	8CT	C18-C17	3.06	1.52	1.43
31	9	311	CLA	C3B-C4B	3.06	1.49	1.42
30	2	313	CHL	C3D-C2D	3.06	1.47	1.39
30	3	305	CHL	CHB-C1B	3.06	1.46	1.39
31	6	303	CLA	C4B-NB	3.06	1.41	1.37
30	7	307	CHL	C3D-C2D	3.06	1.47	1.39
30	1	305	CHL	C3D-C2D	3.06	1.47	1.39
30	2	319	CHL	C3D-C2D	3.06	1.47	1.39
31	3	311	CLA	C4D-ND	-3.06	1.33	1.37
30	g	614	CHL	C3A-C2A	-3.06	1.51	1.54
31	8	304	CLA	C4D-ND	-3.06	1.33	1.37
30	4	305	CHL	C3D-C2D	3.06	1.47	1.39
30	f	602	CHL	CHB-C1B	3.06	1.46	1.39
30	0	302	CHL	CHB-C1B	3.06	1.46	1.39
31	A	838	CLA	C4B-NB	3.06	1.41	1.37
31	5	310	CLA	C4B-NB	3.06	1.41	1.37
31	6	311	CLA	C3B-C4B	3.05	1.49	1.42
30	a	607	CHL	MG-NA	-3.05	1.99	2.06
31	B	825	CLA	C4B-NB	3.05	1.41	1.37
31	6	304	CLA	C4D-ND	-3.05	1.33	1.37
31	O	202	CLA	C4B-NB	3.05	1.41	1.37
30	5	306	CHL	MG-NA	-3.05	1.99	2.06
30	6	306	CHL	C3D-C2D	3.05	1.47	1.39
31	1	310	CLA	C4D-ND	-3.05	1.33	1.37
31	8	314	CLA	C4D-ND	-3.05	1.33	1.37
30	7	305	CHL	CHB-C1B	3.05	1.46	1.39
31	3	312	CLA	C4B-NB	3.05	1.41	1.37
31	G	101	CLA	C4D-ND	-3.05	1.33	1.37
31	6	310	CLA	C4D-ND	-3.05	1.33	1.37
32	2	402	8CT	C01-C02	3.05	1.55	1.50
31	L	202	CLA	C4B-NB	3.05	1.41	1.37
32	A	854	8CT	C30-C29	3.05	1.54	1.50
30	i	606	CHL	MG-NA	-3.04	1.99	2.06
32	K	107	8CT	C18-C17	3.04	1.52	1.43
31	9	302	CLA	C4B-NB	3.04	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	K	107	8CT	C30-C29	3.04	1.54	1.50
30	8	307	CHL	C3D-C2D	3.04	1.47	1.39
30	7	306	CHL	MG-NA	-3.04	1.99	2.06
31	G	103	CLA	C4D-ND	-3.04	1.33	1.37
31	6	320	CLA	C4D-ND	-3.04	1.33	1.37
30	f	608	CHL	C3D-C2D	3.04	1.47	1.39
31	2	304	CLA	C4B-NB	3.04	1.41	1.37
31	H	204	CLA	C4D-ND	-3.04	1.33	1.37
31	7	311	CLA	C4B-NB	3.04	1.41	1.37
31	4	310	CLA	C4B-NB	3.04	1.41	1.37
31	0	303	CLA	C4D-ND	-3.04	1.33	1.37
31	7	303	CLA	C4B-NB	3.04	1.41	1.37
31	B	824	CLA	C4B-NB	3.04	1.41	1.37
30	1	305	CHL	CHB-C1B	3.03	1.46	1.39
31	0	310	CLA	C4B-NB	3.03	1.41	1.37
32	8	402	8CT	C30-C29	3.03	1.54	1.50
31	2	303	CLA	C4B-NB	3.03	1.41	1.37
31	A	852	CLA	C4B-NB	3.03	1.41	1.37
32	B	846	8CT	C18-C17	3.03	1.52	1.43
31	A	806	CLA	C4B-NB	3.03	1.41	1.37
31	9	303	CLA	C4D-ND	-3.03	1.33	1.37
31	5	311	CLA	C4B-NB	3.03	1.41	1.37
31	B	832	CLA	C4B-NB	3.03	1.41	1.37
31	1	303	CLA	C4D-ND	-3.03	1.33	1.37
32	L	209	8CT	C18-C17	3.03	1.52	1.43
32	B	843	8CT	C10-C03	3.03	1.55	1.45
32	B	844	8CT	C10-C03	3.03	1.55	1.45
31	e	604	CLA	C4D-ND	-3.03	1.33	1.37
32	A	849	8CT	C30-C29	3.03	1.54	1.50
31	L	203	CLA	C4B-NB	3.03	1.41	1.37
31	i	610	CLA	C4D-ND	-3.03	1.33	1.37
32	A	854	8CT	C18-C17	3.03	1.52	1.43
31	H	202	CLA	C4D-ND	-3.03	1.33	1.37
32	F	302	8CT	C18-C17	3.03	1.52	1.43
31	K	105	CLA	C4B-NB	3.02	1.41	1.37
31	1	309	CLA	C4D-ND	-3.02	1.33	1.37
31	1	311	CLA	C4B-NB	3.02	1.41	1.37
31	H	204	CLA	C4B-NB	3.02	1.41	1.37
30	4	302	CHL	CHB-C1B	3.02	1.46	1.39
31	O	203	CLA	CAB-C3B	-3.02	1.44	1.50
31	4	303	CLA	C4B-NB	3.02	1.41	1.37
30	g	602	CHL	MG-NA	-3.02	1.99	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	610	CLA	C3B-C4B	3.02	1.49	1.42
31	b	610	CLA	C3B-C4B	3.02	1.49	1.42
31	7	317	CLA	C4D-ND	-3.02	1.33	1.37
32	9	401	8CT	C35-C30	3.02	1.64	1.56
31	0	313	CLA	C4B-NB	3.02	1.41	1.37
31	B	833	CLA	C4B-NB	3.02	1.41	1.37
32	4	402	8CT	C10-C03	3.01	1.55	1.45
31	3	306	CLA	C4B-NB	3.01	1.41	1.37
32	M	102	8CT	C18-C17	3.01	1.52	1.43
31	J	103	CLA	C4B-NB	3.01	1.41	1.37
30	1	302	CHL	CHB-C1B	3.01	1.46	1.39
31	2	310	CLA	C4B-NB	3.01	1.41	1.37
30	4	307	CHL	C3D-C2D	3.01	1.47	1.39
30	c	607	CHL	MG-NA	-3.01	1.99	2.06
31	9	300	CLA	C4D-ND	-3.01	1.33	1.37
30	6	307	CHL	C3D-C2D	3.01	1.47	1.39
31	5	310	CLA	C4D-ND	-3.01	1.33	1.37
31	9	304	CLA	C4B-NB	3.01	1.41	1.37
32	J	104	8CT	C10-C03	3.01	1.55	1.45
31	b	610	CLA	C4D-ND	-3.01	1.33	1.37
31	f	613	CLA	C4D-ND	-3.01	1.33	1.37
32	8	402	8CT	C18-C17	3.01	1.52	1.43
31	c	612	CLA	C4D-ND	-3.01	1.33	1.37
31	f	610	CLA	C4D-ND	-3.00	1.33	1.37
31	1	314	CLA	C4B-NB	3.00	1.41	1.37
31	K	104	CLA	C4B-NB	3.00	1.41	1.37
32	B	844	8CT	C18-C17	3.00	1.52	1.43
31	A	809	CLA	C4D-ND	-3.00	1.33	1.37
31	O	206	CLA	C4D-ND	-3.00	1.33	1.37
31	d	610	CLA	C4D-ND	-3.00	1.33	1.37
31	3	320	CLA	C4B-NB	3.00	1.41	1.37
31	c	610	CLA	C4D-ND	-3.00	1.33	1.37
31	6	312	CLA	C4B-NB	3.00	1.41	1.37
32	B	845	8CT	C10-C03	3.00	1.55	1.45
31	A	822	CLA	C4B-NB	3.00	1.41	1.37
31	5	312	CLA	C4B-NB	3.00	1.41	1.37
30	h	609	CHL	MG-NA	-3.00	1.99	2.06
32	2	402	8CT	C07-C02	-3.00	1.45	1.51
30	6	313	CHL	C3D-C2D	3.00	1.47	1.39
31	f	611	CLA	C4D-ND	-3.00	1.33	1.37
31	B	841	CLA	C4B-NB	3.00	1.41	1.37
31	8	310	CLA	C4B-NB	2.99	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	844	8CT	C35-C30	2.99	1.64	1.56
31	a	610	CLA	C4D-ND	-2.99	1.33	1.37
31	A	812	CLA	C3B-C4B	2.99	1.49	1.42
30	c	614	CHL	MG-NA	-2.99	1.99	2.06
31	3	310	CLA	C4B-NB	2.99	1.41	1.37
31	0	311	CLA	C4B-NB	2.99	1.41	1.37
31	3	311	CLA	C4B-NB	2.99	1.41	1.37
31	G	102	CLA	C4B-NB	2.99	1.41	1.37
31	4	311	CLA	C4B-NB	2.99	1.41	1.37
32	O	205	8CT	C18-C17	2.99	1.52	1.43
31	d	612	CLA	C4D-ND	-2.99	1.33	1.37
31	B	837	CLA	C4B-NB	2.99	1.41	1.37
31	1	308	CLA	C4D-ND	-2.99	1.33	1.37
32	F	302	8CT	C30-C29	2.98	1.54	1.50
32	2	402	8CT	C10-C03	2.98	1.55	1.45
30	5	301	CHL	MG-NA	-2.98	1.99	2.06
31	i	613	CLA	C4D-ND	-2.98	1.33	1.37
31	5	311	CLA	C4D-ND	-2.98	1.33	1.37
31	8	314	CLA	C4B-NB	2.98	1.41	1.37
31	7	304	CLA	C4B-NB	2.98	1.41	1.37
32	B	843	8CT	C18-C17	2.98	1.52	1.43
32	B	847	8CT	C07-C02	-2.98	1.45	1.51
31	B	812	CLA	C4B-NB	2.98	1.41	1.37
31	B	828	CLA	C4B-NB	2.98	1.41	1.37
30	d	609	CHL	MG-NA	-2.98	1.99	2.06
31	d	610	CLA	C3B-C4B	2.98	1.49	1.42
31	5	304	CLA	C4D-ND	-2.98	1.33	1.37
31	5	308	CLA	C3B-C4B	2.98	1.49	1.42
31	6	314	CLA	C4B-NB	2.98	1.41	1.37
31	f	603	CLA	C4D-ND	-2.97	1.33	1.37
31	d	603	CLA	C4D-ND	-2.97	1.33	1.37
30	7	302	CHL	C3D-C2D	2.97	1.47	1.39
32	3	403	8CT	C18-C17	2.97	1.52	1.43
31	e	610	CLA	C4D-ND	-2.97	1.33	1.37
32	8	406	8CT	C10-C03	2.97	1.55	1.45
31	1	310	CLA	C4B-NB	2.97	1.41	1.37
31	5	303	CLA	C4D-ND	-2.97	1.33	1.37
31	f	604	CLA	C4D-ND	-2.97	1.33	1.37
31	B	830	CLA	CMB-C2B	-2.97	1.44	1.50
31	B	808	CLA	C4B-NB	2.97	1.41	1.37
31	A	835	CLA	C4B-NB	2.97	1.41	1.37
31	4	314	CLA	C4B-NB	2.97	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	851	8CT	C30-C29	2.97	1.54	1.50
31	3	318	CLA	C4B-NB	2.97	1.41	1.37
31	A	826	CLA	C4B-NB	2.97	1.41	1.37
32	8	402	8CT	C01-C02	2.97	1.55	1.50
32	A	846	8CT	C18-C17	2.96	1.52	1.43
31	0	308	CLA	C3B-C4B	2.96	1.49	1.42
32	B	846	8CT	C10-C03	2.96	1.55	1.45
31	a	603	CLA	C4D-ND	-2.96	1.33	1.37
31	b	611	CLA	C4D-ND	-2.96	1.33	1.37
32	3	402	8CT	C10-C03	2.96	1.55	1.45
31	0	309	CLA	C4B-NB	2.96	1.41	1.37
31	O	201	CLA	C4D-ND	-2.96	1.33	1.37
31	a	611	CLA	C3B-C4B	2.96	1.49	1.42
31	B	830	CLA	C4B-NB	2.96	1.41	1.37
31	L	204	CLA	C4B-NB	2.96	1.41	1.37
32	8	402	8CT	C10-C03	2.96	1.55	1.45
31	9	308	CLA	C4B-NB	2.96	1.41	1.37
31	A	820	CLA	C4B-NB	2.96	1.41	1.37
31	c	604	CLA	C4D-ND	-2.96	1.33	1.37
31	4	309	CLA	C3B-C4B	2.96	1.49	1.42
30	f	614	CHL	MG-NA	-2.96	1.99	2.06
31	0	312	CLA	C4D-ND	-2.96	1.33	1.37
32	B	848	8CT	C10-C03	2.96	1.55	1.45
31	e	613	CLA	C4D-ND	-2.95	1.33	1.37
31	A	841	CLA	C4B-NB	2.95	1.41	1.37
31	B	821	CLA	C4B-NB	2.95	1.41	1.37
31	i	604	CLA	C4D-ND	-2.95	1.33	1.37
31	9	312	CLA	C4B-NB	2.95	1.41	1.37
30	a	608	CHL	MG-NA	-2.95	1.99	2.06
32	J	101	8CT	C18-C17	2.95	1.52	1.43
31	7	310	CLA	C4D-ND	-2.95	1.33	1.37
30	2	307	CHL	C3D-C2D	2.95	1.47	1.39
32	0	401	8CT	C30-C29	2.95	1.54	1.50
31	3	303	CLA	C4B-NB	2.95	1.41	1.37
32	O	205	8CT	C35-C30	2.95	1.64	1.56
32	B	851	8CT	C07-C02	-2.95	1.45	1.51
31	e	612	CLA	C4D-ND	-2.95	1.33	1.37
31	d	613	CLA	C4D-ND	-2.95	1.33	1.37
31	A	814	CLA	C4B-NB	2.94	1.41	1.37
32	L	209	8CT	C30-C29	2.94	1.54	1.50
31	b	612	CLA	C4D-ND	-2.94	1.33	1.37
31	4	312	CLA	C4B-NB	2.94	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	851	8CT	C18-C17	2.94	1.52	1.43
32	7	405	8CT	C18-C17	2.94	1.52	1.43
32	I	101	8CT	C18-C17	2.94	1.52	1.43
32	L	205	8CT	C18-C17	2.94	1.52	1.43
30	1	307	CHL	C3D-C2D	2.94	1.47	1.39
32	B	847	8CT	C18-C17	2.94	1.52	1.43
31	a	611	CLA	C4D-ND	-2.94	1.33	1.37
31	A	834	CLA	C4B-NB	2.94	1.41	1.37
32	3	402	8CT	C18-C17	2.94	1.52	1.43
32	B	845	8CT	C35-C30	2.94	1.64	1.56
31	f	612	CLA	C4D-ND	-2.94	1.33	1.37
31	A	830	CLA	CMB-C2B	-2.94	1.44	1.50
31	A	838	CLA	C3B-C4B	2.94	1.49	1.42
31	i	611	CLA	C4D-ND	-2.94	1.33	1.37
31	i	612	CLA	C4D-ND	-2.94	1.33	1.37
31	d	604	CLA	C4D-ND	-2.93	1.33	1.37
32	J	104	8CT	C35-C30	2.93	1.64	1.56
32	A	847	8CT	C10-C03	2.93	1.55	1.45
32	L	206	8CT	C07-C02	-2.93	1.45	1.51
31	8	309	CLA	C4B-NB	2.93	1.41	1.37
31	a	604	CLA	C4D-ND	-2.93	1.33	1.37
32	K	107	8CT	C10-C03	2.93	1.55	1.45
32	B	804	8CT	C18-C17	2.93	1.52	1.43
31	B	820	CLA	C4B-NB	2.93	1.41	1.37
32	A	847	8CT	C18-C17	2.93	1.52	1.43
31	a	613	CLA	C3B-C4B	2.93	1.49	1.42
31	e	610	CLA	C3B-C4B	2.93	1.49	1.42
31	b	604	CLA	C4D-ND	-2.93	1.33	1.37
31	b	603	CLA	C4D-ND	-2.93	1.33	1.37
31	B	807	CLA	C3B-C4B	2.93	1.49	1.42
31	h	613	CLA	C3B-C4B	2.93	1.49	1.42
31	B	840	CLA	C4B-NB	2.92	1.41	1.37
31	7	316	CLA	C4B-NB	2.92	1.41	1.37
31	d	611	CLA	C3B-C4B	2.92	1.49	1.42
32	0	401	8CT	C10-C03	2.92	1.55	1.45
31	5	309	CLA	C3B-C4B	2.92	1.49	1.42
31	1	303	CLA	C3B-C4B	2.92	1.49	1.42
30	9	305	CHL	CHB-C1B	2.92	1.46	1.39
31	c	603	CLA	C4D-ND	-2.92	1.33	1.37
31	7	308	CLA	C4B-NB	2.92	1.41	1.37
31	A	843	CLA	C4B-NB	2.92	1.41	1.37
31	A	817	CLA	C4B-NB	2.92	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	831	CLA	C4B-NB	2.92	1.41	1.37
31	4	304	CLA	C4B-NB	2.92	1.41	1.37
30	3	307	CHL	C3D-C2D	2.92	1.47	1.39
30	d	606	CHL	MG-NA	-2.91	1.99	2.06
31	2	311	CLA	C4B-NB	2.91	1.41	1.37
31	B	838	CLA	C4B-NB	2.91	1.41	1.37
31	e	611	CLA	C4D-ND	-2.91	1.33	1.37
31	h	604	CLA	C3B-C4B	2.91	1.49	1.42
31	h	610	CLA	C3B-C4B	2.91	1.49	1.42
31	a	604	CLA	C3B-C4B	2.91	1.49	1.42
31	c	613	CLA	C4D-ND	-2.91	1.33	1.37
31	g	612	CLA	C4D-ND	-2.91	1.33	1.37
32	A	854	8CT	C35-C30	2.91	1.64	1.56
31	b	613	CLA	C4D-ND	-2.91	1.33	1.37
31	4	309	CLA	C4D-ND	-2.91	1.33	1.37
31	3	309	CLA	C3B-C4B	2.91	1.49	1.42
31	H	205	CLA	C3B-C4B	2.91	1.49	1.42
31	A	840	CLA	C4B-NB	2.91	1.41	1.37
32	3	403	8CT	C10-C03	2.91	1.55	1.45
31	9	310	CLA	C3B-C4B	2.91	1.49	1.42
31	B	839	CLA	C4B-NB	2.91	1.41	1.37
31	8	311	CLA	C3B-C4B	2.91	1.49	1.42
31	c	610	CLA	C3B-C4B	2.91	1.49	1.42
32	J	101	8CT	C10-C03	2.91	1.55	1.45
32	L	205	8CT	C07-C02	-2.90	1.45	1.51
31	B	816	CLA	C4B-NB	2.90	1.41	1.37
31	B	826	CLA	C4B-NB	2.90	1.41	1.37
31	A	811	CLA	C4B-NB	2.90	1.41	1.37
31	e	603	CLA	C4D-ND	-2.90	1.33	1.37
32	B	848	8CT	C07-C02	-2.90	1.45	1.51
31	F	301	CLA	C4B-NB	2.90	1.41	1.37
31	a	610	CLA	C3B-C4B	2.90	1.49	1.42
31	5	308	CLA	C4D-ND	-2.90	1.33	1.37
32	A	854	8CT	C10-C03	2.90	1.55	1.45
31	1	312	CLA	C4B-NB	2.90	1.41	1.37
31	A	827	CLA	C4B-NB	2.90	1.41	1.37
31	B	814	CLA	C4B-NB	2.90	1.41	1.37
31	h	610	CLA	C4D-ND	-2.90	1.33	1.37
31	A	832	CLA	C4B-NB	2.90	1.41	1.37
31	B	811	CLA	C4B-NB	2.90	1.41	1.37
31	i	603	CLA	C4D-ND	-2.90	1.33	1.37
31	h	612	CLA	C4D-ND	-2.89	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	206	CLA	C3B-C4B	2.89	1.49	1.42
32	B	844	8CT	C30-C29	2.89	1.54	1.50
32	1	402	8CT	C10-C03	2.89	1.55	1.45
30	i	608	CHL	MG-NA	-2.89	1.99	2.06
30	h	614	CHL	C3A-C2A	-2.89	1.51	1.54
31	L	207	CLA	C3B-C4B	2.89	1.49	1.42
31	h	612	CLA	C3B-C4B	2.89	1.49	1.42
30	6	315	CHL	MG-NA	-2.89	1.99	2.06
30	h	608	CHL	MG-NA	-2.89	1.99	2.06
31	A	819	CLA	C4B-NB	2.89	1.41	1.37
31	B	819	CLA	C4B-NB	2.89	1.41	1.37
31	5	314	CLA	C3B-C4B	2.89	1.49	1.42
31	e	613	CLA	C3B-C4B	2.89	1.49	1.42
32	G	104	8CT	C10-C03	2.89	1.55	1.45
32	O	205	8CT	C10-C03	2.88	1.55	1.45
30	g	606	CHL	MG-NA	-2.88	1.99	2.06
30	a	606	CHL	MG-NA	-2.88	1.99	2.06
31	1	309	CLA	C4B-NB	2.88	1.41	1.37
31	3	304	CLA	C4B-NB	2.88	1.41	1.37
31	7	318	CLA	C4B-NB	2.88	1.41	1.37
31	f	610	CLA	C3B-C4B	2.88	1.49	1.42
30	d	608	CHL	MG-NA	-2.88	1.99	2.06
31	B	803	CLA	C4B-NB	2.88	1.41	1.37
31	B	817	CLA	C4B-NB	2.88	1.41	1.37
31	B	822	CLA	C3B-C4B	2.88	1.49	1.42
31	K	101	CLA	C3B-C4B	2.88	1.49	1.42
32	7	402	8CT	C10-C03	2.88	1.55	1.45
31	1	309	CLA	C3B-C4B	2.88	1.49	1.42
31	B	805	CLA	C4B-NB	2.88	1.41	1.37
31	A	821	CLA	C4B-NB	2.88	1.41	1.37
32	A	846	8CT	C10-C03	2.88	1.55	1.45
31	A	803	CLA	C4B-NB	2.88	1.41	1.37
32	L	209	8CT	C10-C03	2.88	1.55	1.45
31	g	603	CLA	C3B-C4B	2.88	1.49	1.42
32	L	206	8CT	C10-C03	2.88	1.55	1.45
32	B	804	8CT	C35-C30	2.88	1.64	1.56
30	5	307	CHL	MG-NA	-2.87	1.99	2.06
30	e	602	CHL	C3B-C4B	2.87	1.49	1.42
31	A	804	CLA	C3B-C4B	2.87	1.49	1.42
30	c	609	CHL	MG-NA	-2.87	1.99	2.06
31	B	815	CLA	C4B-NB	2.87	1.41	1.37
30	8	301	CHL	MG-NA	-2.87	1.99	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	602	CHL	MG-NA	-2.87	1.99	2.06
31	K	102	CLA	C4B-NB	2.87	1.41	1.37
32	F	302	8CT	C10-C03	2.87	1.55	1.45
32	3	402	8CT	C07-C02	-2.87	1.45	1.51
32	6	402	8CT	C30-C29	2.87	1.54	1.50
32	M	102	8CT	C07-C02	-2.87	1.45	1.51
30	b	609	CHL	MG-NA	-2.87	1.99	2.06
31	g	611	CLA	C3B-C4B	2.87	1.49	1.42
31	d	612	CLA	C3B-C4B	2.87	1.49	1.42
35	0	603	SQD	O47-C7	2.87	1.42	1.34
30	7	307	CHL	MG-NA	-2.87	1.99	2.06
31	e	611	CLA	C3B-C4B	2.87	1.49	1.42
31	h	604	CLA	C4D-ND	-2.87	1.33	1.37
32	4	402	8CT	C07-C02	-2.87	1.45	1.51
31	g	610	CLA	C4D-ND	-2.87	1.33	1.37
31	e	612	CLA	C3B-C4B	2.87	1.49	1.42
31	B	801	CLA	C4B-NB	2.87	1.41	1.37
31	d	611	CLA	C4D-ND	-2.87	1.33	1.37
31	i	610	CLA	C3B-C4B	2.87	1.49	1.42
31	i	604	CLA	C3B-C4B	2.87	1.49	1.42
31	A	809	CLA	C4B-NB	2.87	1.41	1.37
31	B	850	CLA	C3B-C4B	2.86	1.49	1.42
31	7	309	CLA	C4B-NB	2.86	1.41	1.37
31	9	309	CLA	C4B-NB	2.86	1.41	1.37
31	7	312	CLA	C3B-C4B	2.86	1.49	1.42
32	B	848	8CT	C30-C29	2.86	1.54	1.50
32	B	847	8CT	C10-C03	2.86	1.55	1.45
31	A	804	CLA	C4B-NB	2.86	1.41	1.37
32	7	402	8CT	C18-C17	2.86	1.52	1.43
30	e	607	CHL	MG-NA	-2.86	1.99	2.06
34	7	601	LHG	C26-C25	-2.86	1.35	1.51
31	9	309	CLA	C3B-C4B	2.86	1.49	1.42
31	A	830	CLA	C4B-NB	2.86	1.41	1.37
31	g	612	CLA	C3B-C4B	2.86	1.49	1.42
31	g	604	CLA	C3B-C4B	2.86	1.49	1.42
32	6	402	8CT	C10-C03	2.86	1.55	1.45
31	6	318	CLA	C3B-C4B	2.86	1.49	1.42
34	1	601	LHG	C26-C25	-2.86	1.35	1.51
34	3	601	LHG	C26-C25	-2.86	1.35	1.51
31	f	603	CLA	C3B-C4B	2.86	1.49	1.42
31	h	611	CLA	C3B-C4B	2.86	1.49	1.42
31	6	309	CLA	C4B-NB	2.86	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	206	8CT	C30-C29	2.85	1.54	1.50
31	H	202	CLA	C3B-C4B	2.85	1.49	1.42
30	6	308	CHL	MG-NA	-2.85	1.99	2.06
31	2	312	CLA	C4B-NB	2.85	1.41	1.37
32	K	107	8CT	C07-C02	-2.85	1.45	1.51
31	A	825	CLA	C4B-NB	2.85	1.41	1.37
31	g	603	CLA	C4D-ND	-2.85	1.33	1.37
31	A	831	CLA	C4B-NB	2.85	1.41	1.37
32	A	850	8CT	C18-C17	2.85	1.52	1.43
34	A	844	LHG	C26-C25	-2.85	1.35	1.51
31	0	303	CLA	C3B-C4B	2.85	1.49	1.42
31	7	303	CLA	C3B-C4B	2.85	1.49	1.42
31	7	315	CLA	C3B-C4B	2.85	1.49	1.42
31	d	604	CLA	C3B-C4B	2.85	1.49	1.42
32	7	402	8CT	C35-C30	2.85	1.64	1.56
31	B	810	CLA	C4B-NB	2.85	1.41	1.37
31	B	807	CLA	C4B-NB	2.85	1.41	1.37
30	c	608	CHL	MG-NA	-2.84	1.99	2.06
31	A	837	CLA	C4B-NB	2.84	1.41	1.37
32	7	404	8CT	C10-C03	2.84	1.55	1.45
30	b	607	CHL	MG-NA	-2.84	1.99	2.06
34	3	603	LHG	C26-C25	-2.84	1.35	1.51
31	7	309	CLA	C3B-C4B	2.84	1.49	1.42
31	h	613	CLA	C4D-ND	-2.84	1.33	1.37
31	B	809	CLA	C3B-C4B	2.84	1.49	1.42
31	A	807	CLA	C4B-NB	2.84	1.41	1.37
31	i	612	CLA	C3B-C4B	2.84	1.49	1.42
32	9	401	8CT	C30-C29	2.84	1.54	1.50
31	B	814	CLA	C3B-C4B	2.84	1.49	1.42
32	A	849	8CT	C07-C02	-2.84	1.45	1.51
31	6	310	CLA	C3B-C4B	2.84	1.49	1.42
31	O	203	CLA	C4D-ND	-2.84	1.33	1.37
31	L	201	CLA	C4B-NB	2.84	1.41	1.37
34	8	601	LHG	C26-C25	-2.84	1.35	1.51
32	G	104	8CT	C07-C02	-2.84	1.45	1.51
31	9	300	CLA	C4B-NB	2.83	1.41	1.37
31	3	306	CLA	C3B-C4B	2.83	1.49	1.42
32	B	804	8CT	C07-C02	-2.83	1.45	1.51
34	7	603	LHG	C26-C25	-2.83	1.35	1.51
31	3	309	CLA	C4B-NB	2.83	1.41	1.37
31	f	613	CLA	C3B-C4B	2.83	1.49	1.42
31	i	611	CLA	C3B-C4B	2.83	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	630	LHG	C26-C25	-2.83	1.35	1.51
32	I	101	8CT	C10-C03	2.83	1.55	1.45
31	h	603	CLA	C4D-ND	-2.83	1.33	1.37
31	8	304	CLA	C3B-C4B	2.83	1.49	1.42
31	A	823	CLA	C3B-C4B	2.83	1.49	1.42
31	B	818	CLA	C4B-NB	2.83	1.41	1.37
34	K	106	LHG	C26-C25	-2.83	1.35	1.51
31	8	312	CLA	C3B-C4B	2.83	1.49	1.42
30	6	301	CHL	MG-NA	-2.83	1.99	2.06
34	M	104	LHG	C26-C25	-2.83	1.35	1.51
34	e	630	LHG	C26-C25	-2.83	1.35	1.51
31	0	309	CLA	C3B-C4B	2.83	1.49	1.42
31	B	815	CLA	C3B-C4B	2.83	1.49	1.42
34	9	601	LHG	C26-C25	-2.83	1.35	1.51
32	9	401	8CT	C10-C03	2.83	1.55	1.45
30	2	305	CHL	C3D-C2D	2.83	1.46	1.39
31	b	613	CLA	C3B-C4B	2.83	1.49	1.42
31	2	310	CLA	C3B-C4B	2.83	1.49	1.42
31	b	611	CLA	C3B-C4B	2.83	1.49	1.42
31	O	202	CLA	C3B-C4B	2.83	1.49	1.42
34	c	630	LHG	C26-C25	-2.83	1.35	1.51
31	A	833	CLA	C4B-NB	2.82	1.41	1.37
30	a	606	CHL	C3B-C4B	2.82	1.49	1.42
34	b	630	LHG	C26-C25	-2.82	1.35	1.51
34	6	601	LHG	C26-C25	-2.82	1.35	1.51
32	A	849	8CT	C18-C17	2.82	1.52	1.43
34	2	601	LHG	C26-C25	-2.82	1.35	1.51
34	5	601	LHG	C26-C25	-2.82	1.35	1.51
32	1	402	8CT	C07-C02	-2.82	1.45	1.51
31	8	309	CLA	C3B-C4B	2.82	1.49	1.42
32	M	102	8CT	C30-C29	2.82	1.54	1.50
32	A	848	8CT	C18-C17	2.82	1.52	1.43
31	A	819	CLA	C3B-C4B	2.82	1.49	1.42
32	A	848	8CT	C10-C03	2.82	1.55	1.45
31	g	604	CLA	C4D-ND	-2.82	1.33	1.37
32	9	401	8CT	C07-C02	-2.82	1.45	1.51
34	0	601	LHG	C26-C25	-2.82	1.35	1.51
31	B	841	CLA	C3B-C4B	2.82	1.49	1.42
34	6	603	LHG	C26-C25	-2.82	1.35	1.51
34	B	854	LHG	C26-C25	-2.82	1.35	1.51
32	A	848	8CT	C07-C02	-2.82	1.45	1.51
31	d	613	CLA	C3B-C4B	2.82	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	h	630	LHG	C26-C25	-2.82	1.35	1.51
31	A	840	CLA	C3B-C4B	2.82	1.49	1.42
32	L	205	8CT	C10-C03	2.82	1.55	1.45
31	7	310	CLA	C3B-C4B	2.82	1.49	1.42
30	5	301	CHL	C3B-C4B	2.81	1.49	1.42
31	B	806	CLA	C3B-C4B	2.81	1.49	1.42
32	B	843	8CT	C07-C02	-2.81	1.45	1.51
31	i	613	CLA	C3B-C4B	2.81	1.49	1.42
30	d	605	CHL	C4D-CHA	2.81	1.48	1.38
31	B	824	CLA	C3B-C4B	2.81	1.49	1.42
32	A	847	8CT	C30-C29	2.81	1.54	1.50
31	0	312	CLA	C3B-C4B	2.81	1.49	1.42
30	g	614	CHL	C4D-CHA	2.81	1.48	1.38
31	0	321	CLA	C3B-C4B	2.81	1.49	1.42
32	J	101	8CT	C07-C02	-2.81	1.45	1.51
31	A	807	CLA	C3B-C4B	2.81	1.49	1.42
39	A	857	CL0	CMB-C2B	-2.81	1.44	1.50
32	B	804	8CT	C30-C29	2.81	1.54	1.50
31	8	310	CLA	C3B-C4B	2.81	1.49	1.42
31	A	813	CLA	C3B-C4B	2.81	1.49	1.42
31	3	308	CLA	C4B-NB	2.81	1.41	1.37
34	H	203	LHG	C26-C25	-2.81	1.35	1.51
31	1	304	CLA	C3B-C4B	2.81	1.49	1.42
34	G	105	LHG	C26-C25	-2.81	1.35	1.51
31	6	317	CLA	C4B-NB	2.81	1.41	1.37
31	4	310	CLA	C3B-C4B	2.81	1.49	1.42
34	a	630	LHG	C26-C25	-2.81	1.35	1.51
34	d	630	LHG	C26-C25	-2.81	1.35	1.51
34	i	630	LHG	C26-C25	-2.80	1.35	1.51
31	2	309	CLA	C4B-NB	2.80	1.41	1.37
32	A	846	8CT	C07-C02	-2.80	1.45	1.51
30	i	605	CHL	C4D-CHA	2.80	1.48	1.38
31	O	201	CLA	C3B-C4B	2.80	1.49	1.42
31	5	304	CLA	C3B-C4B	2.80	1.49	1.42
31	i	603	CLA	C3B-C4B	2.80	1.49	1.42
31	H	201	CLA	C4B-NB	2.80	1.41	1.37
31	9	303	CLA	C3B-C4B	2.80	1.49	1.42
31	J	103	CLA	C3B-C4B	2.80	1.49	1.42
31	c	613	CLA	C3B-C4B	2.80	1.49	1.42
31	a	612	CLA	C4D-ND	-2.80	1.33	1.37
31	a	613	CLA	C4D-ND	-2.80	1.33	1.37
31	1	311	CLA	C3B-C4B	2.80	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	606	CHL	MG-NA	-2.80	1.99	2.06
31	B	801	CLA	C3B-C4B	2.80	1.49	1.42
32	7	405	8CT	C10-C03	2.80	1.55	1.45
31	g	611	CLA	C4D-ND	-2.80	1.33	1.37
30	7	313	CHL	MG-NA	-2.80	1.99	2.06
31	c	612	CLA	C3B-C4B	2.80	1.49	1.42
30	1	306	CHL	MG-NA	-2.80	1.99	2.06
31	a	612	CLA	C3B-C4B	2.80	1.49	1.42
31	B	806	CLA	C4B-NB	2.80	1.41	1.37
30	e	609	CHL	MG-NA	-2.80	1.99	2.06
32	A	854	8CT	C07-C02	-2.80	1.45	1.51
31	h	603	CLA	C3B-C4B	2.80	1.49	1.42
34	4	601	LHG	C26-C25	-2.80	1.35	1.51
31	A	813	CLA	C4B-NB	2.80	1.41	1.37
31	3	313	CLA	C3B-C4B	2.80	1.49	1.42
31	h	611	CLA	C4D-ND	-2.80	1.33	1.37
31	A	839	CLA	C4B-NB	2.79	1.41	1.37
32	8	402	8CT	C07-C02	-2.79	1.45	1.51
31	8	303	CLA	C3B-C4B	2.79	1.49	1.42
31	b	604	CLA	C3B-C4B	2.79	1.49	1.42
30	d	614	CHL	C4D-CHA	2.79	1.48	1.38
31	b	612	CLA	C3B-C4B	2.79	1.49	1.42
30	a	614	CHL	C4D-CHA	2.79	1.48	1.38
31	3	310	CLA	C3B-C4B	2.79	1.49	1.42
31	G	103	CLA	C3B-C4B	2.79	1.49	1.42
31	g	613	CLA	C3B-C4B	2.79	1.49	1.42
31	A	829	CLA	C4B-NB	2.79	1.41	1.37
30	g	601	CHL	C4D-CHA	2.79	1.48	1.38
30	h	608	CHL	C3B-C4B	2.79	1.49	1.42
32	A	850	8CT	C07-C02	-2.79	1.45	1.51
31	7	311	CLA	C3B-C4B	2.79	1.49	1.42
32	M	102	8CT	C10-C03	2.79	1.55	1.45
31	A	828	CLA	C4B-NB	2.79	1.41	1.37
31	c	603	CLA	C3B-C4B	2.79	1.49	1.42
31	g	613	CLA	C4D-ND	-2.79	1.33	1.37
30	g	608	CHL	C4D-CHA	2.79	1.48	1.38
30	a	602	CHL	C3B-C4B	2.79	1.49	1.42
31	4	314	CLA	C3B-C4B	2.79	1.49	1.42
30	g	606	CHL	C3B-C4B	2.79	1.49	1.42
31	c	611	CLA	C3B-C4B	2.79	1.49	1.42
30	4	308	CHL	MG-NA	-2.79	1.99	2.06
32	O	205	8CT	C07-C02	-2.78	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	804	8CT	C10-C03	2.78	1.55	1.45
31	3	312	CLA	C3B-C4B	2.78	1.49	1.42
31	6	309	CLA	C3B-C4B	2.78	1.49	1.42
31	A	826	CLA	C3B-C4B	2.78	1.49	1.42
30	9	313	CHL	MG-NA	-2.78	1.99	2.06
32	F	302	8CT	C07-C02	-2.78	1.45	1.51
34	A	855	LHG	C26-C25	-2.78	1.36	1.51
32	B	851	8CT	C10-C03	2.78	1.55	1.45
32	7	405	8CT	C07-C02	-2.78	1.45	1.51
30	h	602	CHL	C3B-C4B	2.78	1.49	1.42
30	g	605	CHL	C3B-C4B	2.78	1.49	1.42
30	e	614	CHL	C4D-CHA	2.78	1.48	1.38
30	6	307	CHL	MG-NA	-2.78	1.99	2.06
31	c	604	CLA	C3B-C4B	2.78	1.49	1.42
32	8	406	8CT	C07-C02	-2.78	1.45	1.51
30	g	605	CHL	C4D-CHA	2.78	1.48	1.38
32	L	209	8CT	C07-C02	-2.77	1.45	1.51
31	2	309	CLA	C3B-C4B	2.77	1.49	1.42
31	f	604	CLA	C3B-C4B	2.77	1.49	1.42
30	g	607	CHL	C4D-CHA	2.77	1.48	1.38
31	0	310	CLA	C3B-C4B	2.77	1.49	1.42
30	e	606	CHL	MG-NA	-2.77	1.99	2.06
31	A	835	CLA	C3B-C4B	2.77	1.49	1.42
31	1	308	CLA	C3B-C4B	2.77	1.49	1.42
31	5	310	CLA	C3B-C4B	2.77	1.49	1.42
30	a	605	CHL	C4D-CHA	2.77	1.48	1.38
32	6	402	8CT	C07-C02	-2.77	1.45	1.51
31	A	806	CLA	C3B-C4B	2.77	1.49	1.42
30	0	306	CHL	MG-NA	-2.77	1.99	2.06
34	g	630	LHG	C26-C25	-2.77	1.36	1.51
31	2	303	CLA	C3B-C4B	2.77	1.49	1.42
30	c	605	CHL	C4D-CHA	2.76	1.48	1.38
31	0	321	CLA	C4D-ND	-2.76	1.33	1.37
31	f	611	CLA	C3B-C4B	2.76	1.49	1.42
31	B	837	CLA	C3B-C4B	2.76	1.49	1.42
30	4	307	CHL	MG-NA	-2.76	1.99	2.06
30	i	602	CHL	MG-NA	-2.76	1.99	2.06
31	7	304	CLA	C3B-C4B	2.76	1.49	1.42
32	7	404	8CT	C07-C02	-2.76	1.45	1.51
31	2	314	CLA	C3B-C4B	2.76	1.49	1.42
31	A	824	CLA	C4B-NB	2.76	1.41	1.37
31	A	803	CLA	C3B-C4B	2.76	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	826	CLA	C3B-C4B	2.76	1.49	1.42
30	1	307	CHL	MG-NA	-2.76	1.99	2.06
30	g	608	CHL	C3B-C4B	2.76	1.49	1.42
30	7	301	CHL	MG-NA	-2.75	1.99	2.06
31	3	318	CLA	C3B-C4B	2.75	1.49	1.42
31	A	816	CLA	C3B-C4B	2.75	1.49	1.42
30	f	605	CHL	C4D-CHA	2.75	1.48	1.38
31	3	311	CLA	C3B-C4B	2.75	1.49	1.42
31	6	317	CLA	C3B-C4B	2.75	1.49	1.42
30	1	302	CHL	C3B-C4B	2.75	1.49	1.42
31	f	612	CLA	C3B-C4B	2.75	1.49	1.42
31	h	603	CLA	C1B-C2B	2.75	1.49	1.43
31	F	301	CLA	C3B-C4B	2.75	1.49	1.42
32	O	205	8CT	C30-C29	2.75	1.54	1.50
31	A	827	CLA	C3B-C4B	2.75	1.49	1.42
32	J	104	8CT	C07-C02	-2.75	1.45	1.51
30	8	308	CHL	MG-NA	-2.75	1.99	2.06
31	G	101	CLA	C3B-C4B	2.75	1.49	1.42
31	9	302	CLA	C3B-C4B	2.75	1.49	1.42
31	A	824	CLA	C3B-C4B	2.75	1.49	1.42
31	d	603	CLA	C3B-C4B	2.75	1.49	1.42
30	g	614	CHL	C3B-C4B	2.74	1.49	1.42
31	e	603	CLA	C3B-C4B	2.74	1.49	1.42
31	K	105	CLA	C3B-C4B	2.74	1.49	1.42
32	A	850	8CT	C10-C03	2.74	1.54	1.45
31	6	320	CLA	C3B-C4B	2.74	1.49	1.42
31	a	603	CLA	C3B-C4B	2.74	1.49	1.42
30	i	614	CHL	C4D-CHA	2.74	1.48	1.38
31	B	825	CLA	C3B-C4B	2.74	1.49	1.42
30	e	608	CHL	MG-NA	-2.74	1.99	2.06
30	d	605	CHL	C3B-C4B	2.74	1.49	1.42
30	e	614	CHL	C3B-C4B	2.74	1.49	1.42
32	A	846	8CT	C30-C29	2.74	1.54	1.50
31	B	833	CLA	C3B-C4B	2.74	1.49	1.42
31	A	836	CLA	C4B-NB	2.74	1.41	1.37
32	B	845	8CT	C07-C02	-2.73	1.45	1.51
31	A	828	CLA	C3B-C4B	2.73	1.49	1.42
31	M	101	CLA	C3B-C4B	2.73	1.49	1.42
30	d	614	CHL	C3B-C4B	2.73	1.49	1.42
31	A	843	CLA	C3B-C4B	2.73	1.49	1.42
30	0	305	CHL	MG-NA	-2.73	1.99	2.06
31	6	304	CLA	C3B-C4B	2.73	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	611	CLA	C1B-C2B	2.73	1.49	1.43
31	K	102	CLA	C3B-C4B	2.73	1.49	1.42
31	B	839	CLA	C3B-C4B	2.73	1.49	1.42
31	B	832	CLA	C3B-C4B	2.73	1.49	1.42
31	B	811	CLA	C3B-C4B	2.73	1.49	1.42
31	B	834	CLA	C3B-C4B	2.73	1.49	1.42
30	h	601	CHL	C4D-CHA	2.73	1.48	1.38
30	i	608	CHL	C3B-C4B	2.73	1.49	1.42
30	6	313	CHL	MG-NA	-2.73	1.99	2.06
31	B	828	CLA	C3B-C4B	2.73	1.49	1.42
31	A	818	CLA	C4B-NB	2.72	1.41	1.37
30	5	305	CHL	MG-NA	-2.72	1.99	2.06
31	e	604	CLA	C3B-C4B	2.72	1.49	1.42
30	g	609	CHL	C3B-C4B	2.72	1.49	1.42
31	A	829	CLA	C3B-C4B	2.72	1.49	1.42
31	4	304	CLA	C3B-C4B	2.72	1.49	1.42
31	A	852	CLA	C3B-C4B	2.72	1.49	1.42
30	0	305	CHL	C3B-C4B	2.72	1.49	1.42
31	K	104	CLA	C3B-C4B	2.72	1.49	1.42
31	h	613	CLA	C1B-C2B	2.72	1.49	1.43
32	3	403	8CT	C07-C02	-2.72	1.45	1.51
30	c	606	CHL	MG-NA	-2.72	1.99	2.06
31	5	312	CLA	C3B-C4B	2.72	1.49	1.42
30	6	302	CHL	MG-NA	-2.72	1.99	2.06
30	4	306	CHL	C3B-C4B	2.72	1.49	1.42
31	A	821	CLA	C3B-C4B	2.72	1.49	1.42
31	G	102	CLA	C3B-C4B	2.72	1.49	1.42
30	a	605	CHL	C3B-C4B	2.72	1.49	1.42
31	1	314	CLA	C3B-C4B	2.72	1.49	1.42
31	8	314	CLA	C3B-C4B	2.72	1.49	1.42
31	L	204	CLA	C3B-C4B	2.72	1.49	1.42
30	f	606	CHL	MG-NA	-2.72	1.99	2.06
31	B	803	CLA	C3B-C4B	2.72	1.49	1.42
31	A	833	CLA	C3B-C4B	2.72	1.49	1.42
31	L	203	CLA	C3B-C4B	2.72	1.49	1.42
39	A	857	CL0	MG-NB	-2.72	2.00	2.05
32	7	402	8CT	C07-C02	-2.72	1.45	1.51
31	g	603	CLA	C1B-C2B	2.71	1.49	1.43
31	B	816	CLA	C3B-C4B	2.71	1.49	1.42
31	A	815	CLA	C4B-NB	2.71	1.41	1.37
31	B	827	CLA	C4B-NB	2.71	1.41	1.37
30	b	614	CHL	C4D-CHA	2.71	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	808	CLA	C3B-C4B	2.71	1.49	1.42
30	b	606	CHL	C3B-C4B	2.71	1.49	1.42
30	9	306	CHL	MG-NA	-2.71	1.99	2.06
31	9	304	CLA	C3B-C4B	2.71	1.49	1.42
31	A	822	CLA	C3B-C4B	2.71	1.49	1.42
31	b	603	CLA	C3B-C4B	2.71	1.49	1.42
30	a	614	CHL	C3B-C4B	2.71	1.49	1.42
30	e	605	CHL	C4D-CHA	2.71	1.48	1.38
30	a	601	CHL	C4D-CHA	2.71	1.48	1.38
31	A	825	CLA	C3B-C4B	2.70	1.49	1.42
39	A	857	CL0	C4B-NB	2.70	1.41	1.37
30	7	307	CHL	C3B-C4B	2.70	1.49	1.42
30	e	606	CHL	C3B-C4B	2.70	1.49	1.42
31	B	817	CLA	C3B-C4B	2.70	1.49	1.42
31	4	303	CLA	C3B-C4B	2.70	1.49	1.42
37	7	502	0IE	C13-C12	-2.70	1.40	1.45
31	A	817	CLA	C3B-C4B	2.70	1.49	1.42
30	1	313	CHL	MG-NA	-2.70	1.99	2.06
30	e	602	CHL	MG-NA	-2.70	1.99	2.06
37	3	502	0IE	C13-C12	-2.70	1.40	1.45
31	A	820	CLA	C3B-C4B	2.70	1.49	1.42
31	A	832	CLA	C3B-C4B	2.70	1.49	1.42
31	L	201	CLA	C3B-C4B	2.70	1.49	1.42
31	h	612	CLA	C1B-C2B	2.70	1.49	1.43
31	e	603	CLA	C1B-C2B	2.70	1.49	1.43
30	b	601	CHL	C4D-CHA	2.70	1.48	1.38
30	2	307	CHL	MG-NA	-2.70	1.99	2.06
31	L	202	CLA	C3B-C4B	2.70	1.49	1.42
32	I	101	8CT	C07-C02	-2.70	1.45	1.51
30	h	607	CHL	C3B-C4B	2.69	1.49	1.42
31	c	603	CLA	C1B-C2B	2.69	1.49	1.43
30	b	602	CHL	MG-NA	-2.69	1.99	2.06
30	h	614	CHL	C4D-CHA	2.69	1.48	1.38
31	a	612	CLA	C1B-C2B	2.69	1.49	1.43
30	i	607	CHL	C4D-CHA	2.69	1.48	1.38
31	g	613	CLA	C1B-C2B	2.69	1.49	1.43
31	A	831	CLA	C3B-C4B	2.69	1.49	1.42
31	i	603	CLA	C1B-C2B	2.69	1.49	1.43
31	9	312	CLA	C3B-C4B	2.69	1.49	1.42
32	A	849	8CT	C10-C03	2.69	1.54	1.45
30	i	614	CHL	C3B-C4B	2.69	1.49	1.42
31	A	808	CLA	C4B-NB	2.69	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	836	CLA	C4B-NB	2.69	1.41	1.37
32	A	847	8CT	C07-C02	-2.69	1.45	1.51
30	2	306	CHL	MG-NA	-2.69	1.99	2.06
30	d	608	CHL	C3B-C4B	2.69	1.49	1.42
31	B	836	CLA	C3B-C4B	2.69	1.49	1.42
32	0	401	8CT	C07-C02	-2.69	1.45	1.51
30	g	607	CHL	C3B-C4B	2.69	1.49	1.42
31	g	612	CLA	C1B-C2B	2.69	1.49	1.43
30	e	601	CHL	MG-NA	-2.69	1.99	2.06
31	e	611	CLA	C1B-C2B	2.69	1.49	1.43
31	h	611	CLA	C1B-C2B	2.69	1.49	1.43
31	i	612	CLA	C1B-C2B	2.69	1.49	1.43
31	9	300	CLA	C3B-C4B	2.69	1.49	1.42
31	B	823	CLA	C3B-C4B	2.69	1.49	1.42
30	4	313	CHL	MG-NA	-2.68	1.99	2.06
31	5	304	CLA	C1B-C2B	2.68	1.49	1.43
31	a	611	CLA	C1B-C2B	2.68	1.49	1.43
30	8	313	CHL	MG-NA	-2.68	1.99	2.06
30	d	601	CHL	C3B-C4B	2.68	1.49	1.42
31	5	311	CLA	C3B-C4B	2.68	1.49	1.42
31	3	304	CLA	C3B-C4B	2.68	1.49	1.42
31	B	820	CLA	C3B-C4B	2.68	1.49	1.42
30	f	614	CHL	C4D-CHA	2.68	1.47	1.38
31	3	303	CLA	C3B-C4B	2.68	1.49	1.42
31	6	312	CLA	C3B-C4B	2.68	1.49	1.42
30	a	607	CHL	C3B-C4B	2.68	1.49	1.42
31	1	312	CLA	C3B-C4B	2.68	1.49	1.42
31	7	317	CLA	C1B-C2B	2.68	1.49	1.43
30	g	601	CHL	C3B-C4B	2.67	1.49	1.42
30	4	319	CHL	C3B-C4B	2.67	1.49	1.42
30	i	601	CHL	C3B-C4B	2.67	1.49	1.42
31	i	611	CLA	C1B-C2B	2.67	1.49	1.43
31	0	311	CLA	C3B-C4B	2.67	1.49	1.42
30	a	609	CHL	C4D-CHA	2.67	1.47	1.38
31	4	311	CLA	C3B-C4B	2.67	1.49	1.42
30	i	607	CHL	C3B-C4B	2.67	1.49	1.42
31	B	835	CLA	C3B-C4B	2.67	1.49	1.42
30	b	607	CHL	C3B-C4B	2.67	1.49	1.42
30	h	605	CHL	C3B-C4B	2.67	1.49	1.42
31	0	304	CLA	C3B-C4B	2.67	1.49	1.42
31	i	613	CLA	C1B-C2B	2.67	1.49	1.43
31	a	603	CLA	C1B-C2B	2.66	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	840	CLA	C3B-C4B	2.66	1.49	1.42
31	d	613	CLA	C1B-C2B	2.66	1.49	1.43
30	9	305	CHL	C3B-C4B	2.66	1.49	1.42
30	4	305	CHL	C3B-C4B	2.66	1.49	1.42
30	d	607	CHL	C4D-CHA	2.66	1.47	1.38
30	8	307	CHL	C3B-C4B	2.66	1.49	1.42
30	h	605	CHL	C4D-CHA	2.66	1.47	1.38
31	2	312	CLA	C3B-C4B	2.66	1.49	1.42
30	i	609	CHL	C3B-C4B	2.66	1.49	1.42
30	3	302	CHL	MG-NA	-2.66	2.00	2.06
30	7	302	CHL	MG-NA	-2.66	2.00	2.06
31	g	604	CLA	C1B-C2B	2.66	1.49	1.43
31	B	805	CLA	C1B-C2B	2.66	1.49	1.43
31	e	612	CLA	C1B-C2B	2.66	1.49	1.43
30	b	614	CHL	C3B-C4B	2.66	1.49	1.42
30	i	606	CHL	C3B-C4B	2.65	1.49	1.42
31	1	310	CLA	C3B-C4B	2.65	1.49	1.42
30	7	301	CHL	C3B-C4B	2.65	1.49	1.42
30	f	601	CHL	MG-NA	-2.65	2.00	2.06
30	8	301	CHL	C3B-C4B	2.65	1.49	1.42
30	b	608	CHL	MG-NA	-2.65	2.00	2.06
30	4	302	CHL	MG-NA	-2.65	2.00	2.06
30	h	601	CHL	C3B-C4B	2.65	1.49	1.42
31	7	308	CLA	C3B-C4B	2.65	1.49	1.42
30	2	308	CHL	MG-NA	-2.65	2.00	2.06
31	O	203	CLA	C1B-C2B	2.65	1.49	1.43
31	A	836	CLA	C3B-C4B	2.65	1.49	1.42
37	3	502	0IE	C17-C16	-2.65	1.40	1.45
30	f	605	CHL	C3B-C4B	2.65	1.49	1.42
31	g	611	CLA	C1B-C2B	2.65	1.49	1.43
30	8	306	CHL	MG-NA	-2.65	2.00	2.06
31	9	308	CLA	C3B-C4B	2.65	1.49	1.42
32	B	846	8CT	C07-C02	-2.65	1.45	1.51
30	8	305	CHL	C3B-C4B	2.65	1.49	1.42
30	h	606	CHL	C4D-CHA	2.65	1.47	1.38
31	c	604	CLA	C1B-C2B	2.65	1.49	1.43
30	i	605	CHL	C3B-C4B	2.65	1.49	1.42
31	H	204	CLA	C3B-C4B	2.65	1.49	1.42
31	O	203	CLA	C4B-C3B	2.64	1.49	1.43
31	B	827	CLA	C3B-C4B	2.64	1.49	1.42
31	b	603	CLA	C1B-C2B	2.64	1.49	1.43
30	h	614	CHL	C3B-C4B	2.64	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	306	CHL	C3B-C4B	2.64	1.49	1.42
31	i	604	CLA	C1B-C2B	2.64	1.49	1.43
30	a	608	CHL	C4D-CHA	2.64	1.47	1.38
31	h	610	CLA	C1B-C2B	2.64	1.49	1.43
32	7	405	8CT	C30-C29	2.64	1.54	1.50
30	f	602	CHL	C3B-C4B	2.64	1.48	1.42
30	e	608	CHL	C3B-C4B	2.64	1.48	1.42
30	e	605	CHL	C3B-C4B	2.64	1.48	1.42
30	b	606	CHL	MG-NA	-2.64	2.00	2.06
31	3	320	CLA	C3B-C4B	2.64	1.48	1.42
30	a	608	CHL	C3B-C4B	2.64	1.48	1.42
31	H	204	CLA	C1B-C2B	2.64	1.49	1.43
30	8	302	CHL	MG-NA	-2.64	2.00	2.06
30	i	602	CHL	C3B-C4B	2.64	1.48	1.42
31	B	818	CLA	C3B-C4B	2.64	1.48	1.42
30	h	608	CHL	C4D-CHA	2.64	1.47	1.38
31	d	611	CLA	C1B-C2B	2.64	1.49	1.43
30	d	601	CHL	C4D-CHA	2.64	1.47	1.38
30	d	608	CHL	C4D-CHA	2.64	1.47	1.38
30	g	602	CHL	C3B-C4B	2.64	1.48	1.42
31	B	821	CLA	C3B-C4B	2.64	1.48	1.42
31	a	613	CLA	C1B-C2B	2.64	1.49	1.43
31	b	613	CLA	C1B-C2B	2.64	1.49	1.43
30	2	319	CHL	C3B-C4B	2.64	1.48	1.42
31	0	313	CLA	C3B-C4B	2.64	1.48	1.42
30	3	302	CHL	C3B-C4B	2.64	1.48	1.42
30	c	607	CHL	C3B-C4B	2.64	1.48	1.42
31	c	612	CLA	C1B-C2B	2.63	1.49	1.43
30	h	609	CHL	C4D-CHA	2.63	1.47	1.38
31	7	317	CLA	C3B-C4B	2.63	1.48	1.42
30	i	609	CHL	C4D-CHA	2.63	1.47	1.38
31	b	612	CLA	C1B-C2B	2.63	1.49	1.43
30	d	606	CHL	C3B-C4B	2.63	1.48	1.42
31	d	604	CLA	C1B-C2B	2.63	1.49	1.43
30	7	306	CHL	C3B-C4B	2.63	1.48	1.42
30	8	302	CHL	C3B-C4B	2.63	1.48	1.42
31	H	201	CLA	C3B-C4B	2.63	1.48	1.42
30	8	305	CHL	MG-NA	-2.63	2.00	2.06
31	2	304	CLA	C3B-C4B	2.63	1.48	1.42
31	e	604	CLA	C1B-C2B	2.63	1.49	1.43
30	c	614	CHL	C4D-CHA	2.62	1.47	1.38
30	c	614	CHL	C3B-C4B	2.62	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	608	CHL	C4D-CHA	2.62	1.47	1.38
31	5	303	CLA	C3B-C4B	2.62	1.48	1.42
30	5	306	CHL	C3B-C4B	2.62	1.48	1.42
31	d	603	CLA	C1B-C2B	2.62	1.49	1.43
31	a	610	CLA	C1B-C2B	2.62	1.49	1.43
31	d	612	CLA	C1B-C2B	2.62	1.49	1.43
30	d	607	CHL	C3B-C4B	2.62	1.48	1.42
30	a	607	CHL	C4D-CHA	2.62	1.47	1.38
30	3	305	CHL	MG-NA	-2.62	2.00	2.06
32	B	844	8CT	C07-C02	-2.62	1.45	1.51
31	A	839	CLA	C3B-C4B	2.62	1.48	1.42
31	1	310	CLA	C1B-C2B	2.62	1.49	1.43
30	f	614	CHL	C3B-C4B	2.61	1.48	1.42
31	A	837	CLA	C3B-C4B	2.61	1.48	1.42
30	c	605	CHL	C3B-C4B	2.61	1.48	1.42
31	h	604	CLA	C1B-C2B	2.61	1.49	1.43
30	h	605	CHL	C1B-C2B	2.61	1.49	1.43
31	7	318	CLA	C3B-C4B	2.61	1.48	1.42
31	4	312	CLA	C3B-C4B	2.61	1.48	1.42
31	f	603	CLA	C1B-C2B	2.61	1.49	1.43
37	7	502	0IE	C17-C16	-2.61	1.40	1.45
31	7	316	CLA	C3B-C4B	2.61	1.48	1.42
31	2	311	CLA	C3B-C4B	2.61	1.48	1.42
30	i	601	CHL	C4D-CHA	2.61	1.47	1.38
30	b	601	CHL	C3B-C4B	2.61	1.48	1.42
31	A	815	CLA	C3B-C4B	2.60	1.48	1.42
31	6	303	CLA	C1B-C2B	2.60	1.49	1.43
31	B	819	CLA	C3B-C4B	2.60	1.48	1.42
30	h	607	CHL	C4D-CHA	2.60	1.47	1.38
31	B	812	CLA	C3B-C4B	2.60	1.48	1.42
30	4	306	CHL	MG-NA	-2.60	2.00	2.06
31	A	808	CLA	C3B-C4B	2.60	1.48	1.42
31	5	314	CLA	C1B-C2B	2.60	1.49	1.43
31	f	612	CLA	C1B-C2B	2.60	1.49	1.43
30	g	609	CHL	C4D-CHA	2.60	1.47	1.38
30	h	606	CHL	C3B-C4B	2.60	1.48	1.42
31	3	308	CLA	C3B-C4B	2.60	1.48	1.42
31	A	834	CLA	C3B-C4B	2.60	1.48	1.42
30	2	302	CHL	MG-NA	-2.60	2.00	2.06
30	f	607	CHL	C4D-CHA	2.60	1.47	1.38
31	G	102	CLA	C1B-C2B	2.60	1.49	1.43
31	e	613	CLA	C1B-C2B	2.60	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	809	CLA	C3B-C4B	2.60	1.48	1.42
30	c	606	CHL	C4D-CHA	2.60	1.47	1.38
31	c	613	CLA	C1B-C2B	2.60	1.49	1.43
31	6	314	CLA	C1B-C2B	2.59	1.49	1.43
32	4	402	8CT	C30-C29	2.59	1.54	1.50
31	5	310	CLA	C1B-C2B	2.59	1.49	1.43
30	a	601	CHL	C1B-C2B	2.59	1.49	1.43
30	c	608	CHL	C3B-C4B	2.59	1.48	1.42
34	1	601	LHG	O8-C6	-2.59	1.39	1.45
31	L	202	CLA	C1B-C2B	2.59	1.49	1.43
30	b	602	CHL	C3B-C4B	2.59	1.48	1.42
30	9	306	CHL	C3B-C4B	2.59	1.48	1.42
30	2	313	CHL	MG-NA	-2.59	2.00	2.06
32	2	402	8CT	C30-C29	2.59	1.54	1.50
30	0	301	CHL	MG-NA	-2.59	2.00	2.06
31	6	314	CLA	C3B-C4B	2.59	1.48	1.42
31	L	204	CLA	C1B-C2B	2.59	1.49	1.43
30	2	307	CHL	C3B-C4B	2.59	1.48	1.42
30	b	608	CHL	C3B-C4B	2.59	1.48	1.42
31	A	841	CLA	C3B-C4B	2.59	1.48	1.42
30	2	319	CHL	MG-NA	-2.59	2.00	2.06
31	f	604	CLA	C1B-C2B	2.59	1.49	1.43
32	A	848	8CT	C30-C29	2.59	1.54	1.50
31	B	826	CLA	C4D-CHA	2.59	1.43	1.39
30	1	302	CHL	MG-NA	-2.59	2.00	2.06
31	0	321	CLA	C1B-C2B	2.58	1.49	1.43
31	M	101	CLA	C1B-C2B	2.58	1.49	1.43
30	b	607	CHL	C4D-CHA	2.58	1.47	1.38
32	I	101	8CT	C30-C29	2.58	1.54	1.50
30	0	306	CHL	C4D-CHA	2.58	1.47	1.38
30	5	313	CHL	C4D-CHA	2.58	1.47	1.38
30	c	606	CHL	C3B-C4B	2.58	1.48	1.42
30	e	607	CHL	C3B-C4B	2.58	1.48	1.42
31	8	314	CLA	C1B-C2B	2.58	1.49	1.43
30	c	608	CHL	C4D-CHA	2.58	1.47	1.38
31	7	315	CLA	C1B-C2B	2.58	1.49	1.43
31	A	811	CLA	C3B-C4B	2.58	1.48	1.42
30	d	602	CHL	MG-NA	-2.58	2.00	2.06
31	i	610	CLA	C1B-C2B	2.58	1.49	1.43
30	2	305	CHL	MG-NA	-2.58	2.00	2.06
31	4	304	CLA	C1B-C2B	2.58	1.49	1.43
30	f	601	CHL	C3B-C4B	2.58	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	308	CLA	C1B-C2B	2.58	1.49	1.43
31	B	821	CLA	C1B-C2B	2.58	1.49	1.43
31	f	611	CLA	C1B-C2B	2.58	1.49	1.43
31	B	810	CLA	C3B-C4B	2.58	1.48	1.42
30	i	614	CHL	C1B-C2B	2.58	1.49	1.43
31	0	304	CLA	C1B-C2B	2.58	1.49	1.43
30	c	601	CHL	MG-NA	-2.58	2.00	2.06
30	5	305	CHL	C3B-C4B	2.58	1.48	1.42
31	9	308	CLA	C1B-C2B	2.58	1.49	1.43
31	B	830	CLA	MG-NB	-2.57	2.00	2.05
30	c	602	CHL	MG-NA	-2.57	2.00	2.06
30	g	607	CHL	C1B-C2B	2.57	1.49	1.43
30	f	602	CHL	MG-NA	-2.57	2.00	2.06
30	e	608	CHL	C4D-CHA	2.57	1.47	1.38
30	f	609	CHL	C3B-C4B	2.57	1.48	1.42
30	2	301	CHL	MG-NA	-2.57	2.00	2.06
30	d	602	CHL	C3B-C4B	2.57	1.48	1.42
30	e	601	CHL	C3B-C4B	2.57	1.48	1.42
30	f	609	CHL	C4D-CHA	2.57	1.47	1.38
30	i	606	CHL	C4D-CHA	2.57	1.47	1.38
31	g	610	CLA	C1B-C2B	2.57	1.49	1.43
31	A	814	CLA	C3B-C4B	2.57	1.48	1.42
30	c	607	CHL	C4D-CHA	2.57	1.47	1.38
30	2	305	CHL	C3B-C4B	2.57	1.48	1.42
30	7	313	CHL	C4D-CHA	2.56	1.47	1.38
31	6	320	CLA	C1B-C2B	2.56	1.49	1.43
30	a	614	CHL	C1B-C2B	2.56	1.49	1.43
30	f	606	CHL	C3B-C4B	2.56	1.48	1.42
31	B	831	CLA	C3B-C4B	2.56	1.48	1.42
31	L	207	CLA	C1B-C2B	2.56	1.49	1.43
30	a	606	CHL	C4D-CHA	2.56	1.47	1.38
30	h	607	CHL	C1B-C2B	2.56	1.49	1.43
31	5	312	CLA	C1B-C2B	2.56	1.49	1.43
30	6	305	CHL	C3B-C4B	2.56	1.48	1.42
31	B	805	CLA	C3B-C4B	2.56	1.48	1.42
30	a	609	CHL	C1B-C2B	2.56	1.49	1.43
30	i	607	CHL	C1B-C2B	2.56	1.49	1.43
30	1	307	CHL	C3B-C4B	2.56	1.48	1.42
30	5	302	CHL	MG-NA	-2.56	2.00	2.06
31	K	104	CLA	C1B-C2B	2.56	1.49	1.43
30	h	602	CHL	C4D-CHA	2.56	1.47	1.38
30	i	602	CHL	C4D-CHA	2.56	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	404	8CT	C30-C29	2.56	1.54	1.50
30	a	609	CHL	C3B-C4B	2.56	1.48	1.42
30	9	301	CHL	MG-NA	-2.56	2.00	2.06
30	f	607	CHL	C3B-C4B	2.55	1.48	1.42
31	A	802	CLA	C3B-C4B	2.55	1.48	1.42
30	5	306	CHL	C4D-CHA	2.55	1.47	1.38
30	g	602	CHL	C4D-CHA	2.55	1.47	1.38
30	i	605	CHL	C1B-C2B	2.55	1.49	1.43
30	i	606	CHL	C1B-C2B	2.55	1.49	1.43
30	d	609	CHL	C3B-C4B	2.55	1.48	1.42
31	3	320	CLA	C1B-C2B	2.55	1.49	1.43
30	7	313	CHL	C3B-C4B	2.55	1.48	1.42
30	5	313	CHL	C3B-C4B	2.55	1.48	1.42
30	8	307	CHL	MG-NA	-2.55	2.00	2.06
30	f	607	CHL	C1B-C2B	2.55	1.49	1.43
30	f	608	CHL	C3B-C4B	2.55	1.48	1.42
31	B	835	CLA	C1B-C2B	2.55	1.49	1.43
31	0	312	CLA	C1B-C2B	2.55	1.49	1.43
30	i	609	CHL	C1B-C2B	2.55	1.49	1.43
31	f	613	CLA	C1B-C2B	2.55	1.49	1.43
30	g	614	CHL	C1B-C2B	2.54	1.49	1.43
30	h	606	CHL	C1B-C2B	2.54	1.49	1.43
30	0	306	CHL	C3B-C4B	2.54	1.48	1.42
30	4	319	CHL	MG-NA	-2.54	2.00	2.06
30	8	315	CHL	C1B-C2B	2.54	1.49	1.43
30	a	605	CHL	C1B-C2B	2.54	1.49	1.43
31	5	311	CLA	C1B-C2B	2.54	1.49	1.43
31	0	313	CLA	C1B-C2B	2.54	1.49	1.43
30	b	609	CHL	C4D-CHA	2.54	1.47	1.38
30	8	315	CHL	C3B-C4B	2.54	1.48	1.42
31	8	304	CLA	C1B-C2B	2.54	1.49	1.43
31	9	302	CLA	C1B-C2B	2.54	1.49	1.43
30	d	609	CHL	C4D-CHA	2.54	1.47	1.38
32	B	843	8CT	C25-C26	2.54	1.39	1.35
31	B	830	CLA	C3B-C4B	2.54	1.48	1.42
31	a	604	CLA	C1B-C2B	2.54	1.49	1.43
30	d	605	CHL	C1B-C2B	2.54	1.49	1.43
30	7	306	CHL	C1C-NC	-2.53	1.34	1.37
30	0	302	CHL	MG-NA	-2.53	2.00	2.06
30	c	609	CHL	C4D-CHA	2.53	1.47	1.38
30	8	315	CHL	C4D-CHA	2.53	1.47	1.38
31	2	304	CLA	C1B-C2B	2.53	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	306	CHL	C3B-C4B	2.53	1.48	1.42
39	A	857	CL0	MG-ND	-2.53	2.00	2.05
37	7	502	0IE	C6-C7	-2.53	1.40	1.45
30	6	305	CHL	MG-NA	-2.53	2.00	2.06
30	g	602	CHL	C1B-C2B	2.53	1.49	1.43
30	g	605	CHL	C1B-C2B	2.53	1.49	1.43
30	1	306	CHL	C4D-CHA	2.53	1.47	1.38
30	a	607	CHL	C1B-C2B	2.53	1.49	1.43
31	5	303	CLA	C1B-C2B	2.53	1.49	1.43
31	H	202	CLA	C1B-C2B	2.53	1.49	1.43
31	B	840	CLA	C1B-C2B	2.53	1.49	1.43
30	d	606	CHL	C4D-CHA	2.53	1.47	1.38
30	e	614	CHL	C1B-C2B	2.53	1.49	1.43
30	7	307	CHL	C4D-CHA	2.53	1.47	1.38
31	0	309	CLA	C1B-C2B	2.52	1.49	1.43
30	5	307	CHL	C3B-C4B	2.52	1.48	1.42
30	c	602	CHL	C3B-C4B	2.52	1.48	1.42
31	A	834	CLA	C1B-C2B	2.52	1.49	1.43
31	4	311	CLA	C1B-C2B	2.52	1.49	1.43
31	6	310	CLA	C1B-C2B	2.52	1.49	1.43
31	A	830	CLA	C3B-C4B	2.52	1.48	1.42
31	1	314	CLA	C1B-C2B	2.52	1.49	1.43
30	g	606	CHL	C4D-CHA	2.52	1.47	1.38
31	1	308	CLA	C1B-C2B	2.52	1.49	1.43
30	3	307	CHL	MG-NA	-2.52	2.00	2.06
31	2	314	CLA	C1B-C2B	2.52	1.49	1.43
30	g	601	CHL	C1B-C2B	2.52	1.49	1.43
31	B	830	CLA	CMD-C2D	-2.52	1.45	1.50
30	8	306	CHL	C3B-C4B	2.52	1.48	1.42
30	g	607	CHL	C4C-C3C	2.52	1.49	1.45
30	a	601	CHL	C3B-C4B	2.52	1.48	1.42
31	9	304	CLA	C1B-C2B	2.52	1.49	1.43
31	3	306	CLA	C1B-C2B	2.52	1.49	1.43
31	G	101	CLA	C1B-C2B	2.52	1.49	1.43
30	1	307	CHL	C4D-CHA	2.52	1.47	1.38
30	d	601	CHL	C1B-C2B	2.52	1.49	1.43
33	a	520	0UR	O44-C45	2.52	1.45	1.33
30	h	614	CHL	C1B-C2B	2.52	1.49	1.43
31	3	308	CLA	C1B-C2B	2.52	1.49	1.43
30	c	605	CHL	C1B-C2B	2.51	1.49	1.43
30	e	607	CHL	C4D-CHA	2.51	1.47	1.38
31	c	610	CLA	C1B-C2B	2.51	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	307	CHL	C1B-C2B	2.51	1.49	1.43
31	6	303	CLA	C3B-C4B	2.51	1.48	1.42
30	e	605	CHL	C1B-C2B	2.51	1.49	1.43
31	7	311	CLA	C1B-C2B	2.51	1.49	1.43
30	g	601	CHL	C4C-C3C	2.51	1.49	1.45
31	O	202	CLA	C1B-C2B	2.51	1.49	1.43
31	4	314	CLA	C1B-C2B	2.51	1.49	1.43
30	8	301	CHL	C4D-CHA	2.51	1.47	1.38
34	A	845	LHG	O8-C6	-2.51	1.39	1.45
30	d	614	CHL	C1B-C2B	2.51	1.49	1.43
30	f	601	CHL	C4D-CHA	2.51	1.47	1.38
31	B	838	CLA	C1B-C2B	2.51	1.49	1.43
31	d	610	CLA	C1B-C2B	2.51	1.49	1.43
31	2	312	CLA	C1B-C2B	2.51	1.49	1.43
30	5	305	CHL	C4D-CHA	2.51	1.47	1.38
30	6	306	CHL	MG-NA	-2.51	2.00	2.06
30	1	305	CHL	C3B-C4B	2.51	1.48	1.42
34	K	106	LHG	O8-C6	-2.50	1.39	1.45
30	i	601	CHL	C1B-C2B	2.50	1.49	1.43
30	e	609	CHL	C4D-CHA	2.50	1.47	1.38
31	B	810	CLA	C1B-C2B	2.50	1.49	1.43
31	f	610	CLA	C1B-C2B	2.50	1.49	1.43
30	c	607	CHL	C1B-C2B	2.50	1.49	1.43
30	d	608	CHL	C1B-C2B	2.50	1.49	1.43
30	1	313	CHL	C3B-C4B	2.50	1.48	1.42
31	0	310	CLA	C1B-C2B	2.50	1.49	1.43
31	2	311	CLA	C1B-C2B	2.50	1.49	1.43
31	A	837	CLA	C1B-C2B	2.50	1.49	1.43
31	A	814	CLA	C1B-C2B	2.50	1.49	1.43
31	O	201	CLA	C1B-C2B	2.50	1.49	1.43
30	c	609	CHL	C3B-C4B	2.50	1.48	1.42
31	8	303	CLA	C1B-C2B	2.50	1.49	1.43
30	6	313	CHL	C1B-C2B	2.50	1.49	1.43
30	h	601	CHL	C1B-C2B	2.50	1.49	1.43
30	h	609	CHL	C3B-C4B	2.50	1.48	1.42
30	b	608	CHL	C4D-CHA	2.50	1.47	1.38
31	K	102	CLA	C1B-C2B	2.50	1.49	1.43
30	1	305	CHL	MG-NA	-2.50	2.00	2.06
30	2	313	CHL	C4D-CHA	2.50	1.47	1.38
30	d	609	CHL	C1B-C2B	2.50	1.49	1.43
31	7	316	CLA	C1B-C2B	2.50	1.49	1.43
30	7	306	CHL	C1B-NB	-2.50	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	307	CHL	C4D-CHA	2.50	1.47	1.38
30	c	601	CHL	C4D-CHA	2.50	1.47	1.38
30	e	607	CHL	C1B-C2B	2.50	1.49	1.43
30	b	614	CHL	C1B-C2B	2.50	1.49	1.43
34	B	852	LHG	O8-C6	-2.50	1.39	1.45
30	7	305	CHL	MG-NA	-2.49	2.00	2.06
30	4	307	CHL	C1C-NC	-2.49	1.34	1.37
31	6	318	CLA	C1B-C2B	2.49	1.49	1.43
32	A	850	8CT	C33-C32	-2.49	1.43	1.50
30	a	608	CHL	C1B-C2B	2.49	1.49	1.43
31	B	834	CLA	C1B-C2B	2.49	1.49	1.43
30	f	605	CHL	C1B-C2B	2.49	1.49	1.43
30	g	609	CHL	C1B-C2B	2.49	1.49	1.43
31	0	303	CLA	C1B-C2B	2.49	1.49	1.43
31	8	311	CLA	C1B-C2B	2.49	1.49	1.43
30	0	301	CHL	C3B-C4B	2.49	1.48	1.42
31	1	311	CLA	C1B-C2B	2.49	1.49	1.43
31	A	822	CLA	C1B-C2B	2.49	1.49	1.43
31	1	304	CLA	C1B-C2B	2.49	1.49	1.43
32	B	845	8CT	C30-C29	2.49	1.54	1.50
31	A	808	CLA	C1B-C2B	2.49	1.49	1.43
31	b	604	CLA	C1B-C2B	2.49	1.49	1.43
30	6	315	CHL	C3B-C4B	2.49	1.48	1.42
30	f	614	CHL	C1B-C2B	2.49	1.49	1.43
31	3	313	CLA	C1B-C2B	2.49	1.49	1.43
30	f	608	CHL	C1B-C2B	2.49	1.49	1.43
34	A	844	LHG	O8-C6	-2.49	1.39	1.45
30	2	301	CHL	C1B-NB	-2.48	1.34	1.37
31	J	103	CLA	C1B-C2B	2.48	1.49	1.43
30	d	606	CHL	C1B-C2B	2.48	1.49	1.43
30	i	602	CHL	C1B-C2B	2.48	1.49	1.43
30	a	602	CHL	C4D-CHA	2.48	1.47	1.38
30	4	305	CHL	MG-NA	-2.48	2.00	2.06
30	b	609	CHL	C1B-C2B	2.48	1.49	1.43
32	7	402	8CT	C30-C29	2.48	1.53	1.50
30	e	601	CHL	C4D-CHA	2.48	1.47	1.38
37	c	521	0IE	C6-C7	-2.48	1.40	1.45
31	7	310	CLA	C1B-C2B	2.48	1.49	1.43
31	A	817	CLA	C1B-C2B	2.48	1.49	1.43
30	e	602	CHL	C4D-CHA	2.48	1.47	1.38
31	4	310	CLA	C1B-C2B	2.48	1.49	1.43
30	9	301	CHL	C3B-C4B	2.48	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	306	CHL	C1B-C2B	2.48	1.49	1.43
30	e	601	CHL	C1B-C2B	2.48	1.49	1.43
31	1	312	CLA	C1B-C2B	2.48	1.49	1.43
37	3	502	0IE	C6-C7	-2.48	1.40	1.45
30	b	606	CHL	C4D-CHA	2.48	1.47	1.38
30	b	602	CHL	C1B-C2B	2.48	1.49	1.43
31	6	309	CLA	C1B-C2B	2.47	1.49	1.43
30	g	606	CHL	C1B-C2B	2.47	1.49	1.43
31	B	838	CLA	C3B-C4B	2.47	1.48	1.42
31	4	312	CLA	C1B-C2B	2.47	1.49	1.43
30	e	609	CHL	C1B-C2B	2.47	1.49	1.43
30	d	607	CHL	C1B-C2B	2.47	1.49	1.43
31	H	201	CLA	C1B-C2B	2.47	1.49	1.43
30	h	602	CHL	C1B-C2B	2.47	1.49	1.43
30	c	601	CHL	C3B-C4B	2.47	1.48	1.42
30	i	608	CHL	C1B-C2B	2.47	1.49	1.43
31	8	312	CLA	C1B-C2B	2.47	1.49	1.43
30	7	301	CHL	C4D-CHA	2.47	1.47	1.38
30	9	305	CHL	MG-NA	-2.47	2.00	2.06
31	A	816	CLA	C1B-C2B	2.47	1.49	1.43
34	2	601	LHG	O8-C6	-2.47	1.39	1.45
37	d	521	0IE	C13-C12	-2.47	1.40	1.45
30	f	609	CHL	C1B-C2B	2.46	1.49	1.43
31	B	808	CLA	C1B-C2B	2.46	1.49	1.43
30	8	306	CHL	C4D-CHA	2.46	1.47	1.38
30	1	313	CHL	C4D-CHA	2.46	1.47	1.38
31	H	205	CLA	C1B-C2B	2.46	1.49	1.43
31	A	828	CLA	C1B-C2B	2.46	1.49	1.43
31	A	819	CLA	MG-NB	-2.46	2.00	2.05
30	4	307	CHL	C3B-C4B	2.46	1.48	1.42
31	A	818	CLA	C1B-C2B	2.46	1.49	1.43
31	A	830	CLA	MG-NB	-2.46	2.00	2.05
30	0	301	CHL	C4D-CHA	2.46	1.47	1.38
31	9	310	CLA	C1B-C2B	2.46	1.49	1.43
30	5	301	CHL	C4D-CHA	2.46	1.47	1.38
31	7	312	CLA	C1B-C2B	2.46	1.49	1.43
30	9	301	CHL	C4D-CHA	2.46	1.47	1.38
31	3	311	CLA	C1B-C2B	2.46	1.49	1.43
30	9	313	CHL	C3B-C4B	2.46	1.48	1.42
30	g	614	CHL	C4C-C3C	2.46	1.49	1.45
32	2	402	8CT	C25-C26	2.46	1.39	1.35
30	4	302	CHL	C3B-C4B	2.46	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	7	602	LHG	O7-C5	-2.46	1.40	1.46
31	8	310	CLA	C1B-C2B	2.45	1.49	1.43
30	7	305	CHL	C3B-C4B	2.45	1.48	1.42
37	c	521	0IE	C13-C12	-2.45	1.40	1.45
30	f	605	CHL	C4C-C3C	2.45	1.49	1.45
30	e	606	CHL	C4D-CHA	2.45	1.47	1.38
30	8	313	CHL	C4D-CHA	2.45	1.47	1.38
30	h	609	CHL	C1B-C2B	2.45	1.49	1.43
30	6	307	CHL	C3B-C4B	2.45	1.48	1.42
30	4	308	CHL	C4D-CHA	2.45	1.47	1.38
31	3	310	CLA	C1B-C2B	2.45	1.49	1.43
30	7	302	CHL	C3B-C4B	2.45	1.48	1.42
31	9	309	CLA	C1B-C2B	2.45	1.49	1.43
31	B	850	CLA	C1B-C2B	2.45	1.49	1.43
30	6	315	CHL	C4D-CHA	2.45	1.47	1.38
30	1	307	CHL	C1B-C2B	2.45	1.49	1.43
31	c	611	CLA	C1B-C2B	2.45	1.49	1.43
30	f	606	CHL	C4D-CHA	2.45	1.47	1.38
30	f	608	CHL	MG-NA	-2.45	2.00	2.06
31	B	837	CLA	C1B-C2B	2.45	1.49	1.43
30	b	601	CHL	C1B-C2B	2.45	1.49	1.43
30	e	609	CHL	C3B-C4B	2.44	1.48	1.42
31	6	304	CLA	CMB-C2B	-2.44	1.45	1.50
30	c	614	CHL	C1B-NB	-2.44	1.34	1.37
30	f	606	CHL	C1B-C2B	2.44	1.49	1.43
30	f	608	CHL	C4D-CHA	2.44	1.47	1.38
31	A	811	CLA	C1B-C2B	2.44	1.49	1.43
31	9	312	CLA	C1B-C2B	2.44	1.49	1.43
31	A	843	CLA	C1B-C2B	2.44	1.49	1.43
30	1	306	CHL	C1B-C2B	2.44	1.49	1.43
31	4	309	CLA	C1B-C2B	2.44	1.49	1.43
31	B	831	CLA	MG-NB	-2.44	2.01	2.05
30	2	308	CHL	C3B-C4B	2.44	1.48	1.42
31	A	829	CLA	C1B-C2B	2.44	1.49	1.43
31	7	308	CLA	C1B-C2B	2.44	1.49	1.43
31	7	304	CLA	C1B-C2B	2.44	1.49	1.43
31	G	103	CLA	C1B-C2B	2.44	1.49	1.43
32	4	402	8CT	C25-C26	2.44	1.39	1.35
30	g	609	CHL	C4C-C3C	2.43	1.49	1.45
31	B	801	CLA	MG-NB	-2.43	2.01	2.05
37	b	521	0IE	C6-C7	-2.43	1.40	1.45
30	6	308	CHL	C3B-C4B	2.43	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	313	CHL	C1B-C2B	2.43	1.49	1.43
31	B	824	CLA	C1B-C2B	2.43	1.49	1.43
31	6	311	CLA	C1B-C2B	2.43	1.49	1.43
31	A	833	CLA	C1B-C2B	2.43	1.49	1.43
30	9	306	CHL	C1C-NC	-2.43	1.34	1.37
30	c	606	CHL	C1B-C2B	2.43	1.49	1.43
30	a	606	CHL	C1B-C2B	2.43	1.49	1.43
31	L	203	CLA	C1B-C2B	2.43	1.49	1.43
30	a	614	CHL	C4C-C3C	2.43	1.49	1.45
34	B	854	LHG	O8-C6	-2.43	1.39	1.45
30	5	313	CHL	C1B-C2B	2.43	1.49	1.43
31	0	311	CLA	C1B-C2B	2.43	1.49	1.43
34	9	601	LHG	O8-C6	-2.43	1.39	1.45
34	6	601	LHG	O8-C6	-2.43	1.39	1.45
30	g	605	CHL	C4C-C3C	2.43	1.49	1.45
30	6	307	CHL	C4D-CHA	2.43	1.47	1.38
31	A	818	CLA	C3B-C4B	2.43	1.48	1.42
31	2	303	CLA	C1B-C2B	2.43	1.49	1.43
30	0	305	CHL	C4D-CHA	2.43	1.47	1.38
31	B	823	CLA	C1B-C2B	2.43	1.49	1.43
30	8	308	CHL	C4D-CHA	2.43	1.47	1.38
30	3	305	CHL	C3B-C4B	2.43	1.48	1.42
31	A	821	CLA	MG-NB	-2.43	2.01	2.05
30	e	608	CHL	C1B-C2B	2.43	1.49	1.43
31	A	820	CLA	C1B-C2B	2.43	1.49	1.43
30	6	308	CHL	C4D-CHA	2.43	1.47	1.38
30	h	605	CHL	C4C-C3C	2.43	1.49	1.45
31	K	105	CLA	C1B-C2B	2.43	1.49	1.43
30	c	602	CHL	C4D-CHA	2.43	1.47	1.38
31	B	825	CLA	C1B-C2B	2.43	1.49	1.43
30	3	305	CHL	C4D-CHA	2.42	1.47	1.38
34	5	601	LHG	O8-C6	-2.42	1.39	1.45
34	G	105	LHG	O8-C23	2.42	1.40	1.33
30	d	605	CHL	C4C-C3C	2.42	1.49	1.45
30	f	601	CHL	C1B-C2B	2.42	1.49	1.43
32	B	846	8CT	C25-C26	2.42	1.39	1.35
31	A	826	CLA	C1B-C2B	2.42	1.49	1.43
30	2	302	CHL	C3B-C4B	2.42	1.48	1.42
31	0	308	CLA	C1B-C2B	2.42	1.49	1.43
31	A	841	CLA	C1B-C2B	2.42	1.49	1.43
30	a	609	CHL	C4C-C3C	2.42	1.49	1.45
30	h	609	CHL	C4C-C3C	2.42	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	601	CHL	C1B-C2B	2.42	1.49	1.43
30	4	313	CHL	C1C-NC	-2.42	1.34	1.37
34	0	601	LHG	O8-C6	-2.42	1.39	1.45
31	B	803	CLA	C1B-C2B	2.42	1.48	1.43
31	6	312	CLA	C1B-C2B	2.42	1.48	1.43
30	2	301	CHL	C3B-C4B	2.42	1.48	1.42
31	A	839	CLA	C1B-C2B	2.42	1.48	1.43
34	4	601	LHG	O8-C6	-2.42	1.39	1.45
30	6	313	CHL	C4D-CHA	2.41	1.47	1.38
37	f	521	0IE	C13-C12	-2.41	1.40	1.45
30	g	608	CHL	C1B-C2B	2.41	1.48	1.43
30	h	608	CHL	C1B-C2B	2.41	1.48	1.43
31	B	841	CLA	C1B-C2B	2.41	1.48	1.43
31	B	831	CLA	CMD-C2D	-2.41	1.45	1.50
31	A	809	CLA	C1B-C2B	2.41	1.48	1.43
30	9	306	CHL	C4D-CHA	2.41	1.47	1.38
30	b	602	CHL	C4D-CHA	2.41	1.47	1.38
31	3	303	CLA	C1B-C2B	2.41	1.48	1.43
31	B	827	CLA	C1B-C2B	2.41	1.48	1.43
31	3	312	CLA	C1B-C2B	2.41	1.48	1.43
30	8	307	CHL	C4D-CHA	2.41	1.47	1.38
31	3	304	CLA	C1B-C2B	2.41	1.48	1.43
30	2	308	CHL	C4D-CHA	2.41	1.47	1.38
31	7	318	CLA	C1B-C2B	2.41	1.48	1.43
30	9	306	CHL	C1B-NB	-2.41	1.34	1.37
30	2	301	CHL	C4D-CHA	2.41	1.47	1.38
31	4	303	CLA	C1B-C2B	2.41	1.48	1.43
34	7	601	LHG	O8-C6	-2.41	1.39	1.45
31	A	835	CLA	C1B-C2B	2.41	1.48	1.43
31	A	836	CLA	MG-NB	-2.41	2.01	2.05
31	B	832	CLA	C1B-C2B	2.41	1.48	1.43
30	7	306	CHL	C4D-CHA	2.41	1.47	1.38
30	2	313	CHL	C3B-C4B	2.41	1.48	1.42
30	4	313	CHL	C3B-C4B	2.41	1.48	1.42
37	c	521	0IE	C17-C16	-2.41	1.40	1.45
31	A	818	CLA	MG-NB	-2.41	2.01	2.05
30	3	307	CHL	C1B-NB	-2.41	1.34	1.37
31	6	304	CLA	C1B-C2B	2.41	1.48	1.43
31	B	817	CLA	C1B-C2B	2.41	1.48	1.43
32	A	850	8CT	C30-C29	2.41	1.53	1.50
30	9	313	CHL	C4D-CHA	2.41	1.47	1.38
31	O	206	CLA	C1B-C2B	2.41	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	306	CHL	C1C-NC	-2.41	1.34	1.37
34	7	602	LHG	O8-C6	-2.40	1.39	1.45
31	A	840	CLA	C1B-C2B	2.40	1.48	1.43
30	c	605	CHL	C4C-C3C	2.40	1.49	1.45
30	8	305	CHL	C1B-C2B	2.40	1.48	1.43
30	h	601	CHL	C4C-C3C	2.40	1.49	1.45
30	b	608	CHL	C1B-C2B	2.40	1.48	1.43
31	B	811	CLA	C1B-C2B	2.40	1.48	1.43
30	c	609	CHL	C4C-C3C	2.40	1.49	1.45
30	8	308	CHL	C3B-C4B	2.40	1.48	1.42
31	A	809	CLA	MG-NB	-2.40	2.01	2.05
30	2	319	CHL	C4D-CHA	2.40	1.46	1.38
30	b	609	CHL	C3B-C4B	2.40	1.48	1.42
31	A	836	CLA	C1B-C2B	2.40	1.48	1.43
30	f	602	CHL	C4D-CHA	2.40	1.46	1.38
31	7	303	CLA	C1B-C2B	2.40	1.48	1.43
31	b	610	CLA	C1B-C2B	2.40	1.48	1.43
31	B	819	CLA	MG-NB	-2.40	2.01	2.05
31	2	310	CLA	C1B-C2B	2.40	1.48	1.43
31	B	816	CLA	C1B-C2B	2.40	1.48	1.43
30	2	306	CHL	C4D-CHA	2.40	1.46	1.38
31	A	803	CLA	C1B-C2B	2.40	1.48	1.43
32	A	848	8CT	C33-C32	-2.40	1.43	1.50
30	0	301	CHL	C1B-C2B	2.40	1.48	1.43
31	B	833	CLA	C1B-C2B	2.40	1.48	1.43
31	1	303	CLA	C1B-C2B	2.39	1.48	1.43
31	B	819	CLA	C1B-C2B	2.39	1.48	1.43
31	K	101	CLA	C1B-C2B	2.39	1.48	1.43
30	0	302	CHL	C4D-CHA	2.39	1.46	1.38
31	B	814	CLA	C1B-C2B	2.39	1.48	1.43
30	9	305	CHL	C4D-CHA	2.39	1.46	1.38
31	A	816	CLA	CMB-C2B	-2.39	1.45	1.50
30	a	602	CHL	C1B-C2B	2.39	1.48	1.43
30	d	602	CHL	C4D-CHA	2.39	1.46	1.38
30	4	306	CHL	C4D-CHA	2.39	1.46	1.38
31	L	201	CLA	MG-NB	-2.39	2.01	2.05
34	f	630	LHG	O8-C6	-2.39	1.39	1.45
37	g	521	0IE	C13-C12	-2.39	1.40	1.45
30	c	614	CHL	C1B-C2B	2.39	1.48	1.43
30	4	302	CHL	C4D-CHA	2.39	1.46	1.38
30	d	614	CHL	C4C-C3C	2.39	1.49	1.45
30	5	306	CHL	C1B-C2B	2.39	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	812	CLA	C1B-C2B	2.39	1.48	1.43
31	A	823	CLA	C1B-C2B	2.39	1.48	1.43
30	4	307	CHL	C1B-NB	-2.39	1.34	1.37
34	4	601	LHG	O7-C5	-2.39	1.40	1.46
30	i	609	CHL	C4C-C3C	2.39	1.49	1.45
30	6	315	CHL	C1B-C2B	2.39	1.48	1.43
30	4	305	CHL	C4D-CHA	2.39	1.46	1.38
30	1	305	CHL	C4D-CHA	2.39	1.46	1.38
30	0	302	CHL	C3B-C4B	2.38	1.48	1.42
37	e	521	0IE	C13-C12	-2.38	1.40	1.45
31	8	309	CLA	C1B-C2B	2.38	1.48	1.43
31	A	815	CLA	C1B-C2B	2.38	1.48	1.43
30	6	306	CHL	C4D-CHA	2.38	1.46	1.38
31	B	815	CLA	C1B-C2B	2.38	1.48	1.43
30	h	606	CHL	C4C-C3C	2.38	1.49	1.45
37	b	521	0IE	C13-C12	-2.38	1.40	1.45
30	6	301	CHL	C3B-C4B	2.38	1.48	1.42
30	6	305	CHL	C4D-CHA	2.38	1.46	1.38
31	2	309	CLA	C1B-C2B	2.38	1.48	1.43
31	e	610	CLA	C1B-C2B	2.38	1.48	1.43
34	e	630	LHG	O8-C6	-2.38	1.39	1.45
30	c	608	CHL	C1B-C2B	2.38	1.48	1.43
31	9	303	CLA	C1B-C2B	2.38	1.48	1.43
37	b	521	0IE	C17-C16	-2.38	1.40	1.45
30	8	305	CHL	C4D-CHA	2.38	1.46	1.38
30	b	607	CHL	C1B-C2B	2.38	1.48	1.43
34	8	601	LHG	O8-C6	-2.38	1.39	1.45
34	d	630	LHG	O8-C23	2.38	1.40	1.33
31	9	300	CLA	C1B-C2B	2.38	1.48	1.43
31	A	841	CLA	MG-NB	-2.38	2.01	2.05
30	8	313	CHL	C1B-C2B	2.38	1.48	1.43
31	B	812	CLA	CMB-C2B	-2.38	1.45	1.50
34	1	601	LHG	O7-C5	-2.38	1.40	1.46
30	6	313	CHL	C3B-C4B	2.38	1.48	1.42
31	A	839	CLA	MG-NB	-2.37	2.01	2.05
31	B	836	CLA	MG-NB	-2.37	2.01	2.05
30	i	605	CHL	C4C-C3C	2.37	1.49	1.45
37	e	521	0IE	C17-C16	-2.37	1.40	1.45
30	1	313	CHL	C1B-C2B	2.37	1.48	1.43
30	1	302	CHL	C4D-CHA	2.37	1.46	1.38
30	c	609	CHL	C1B-C2B	2.37	1.48	1.43
30	7	305	CHL	C4D-CHA	2.37	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	301	CHL	C1B-C2B	2.37	1.48	1.43
30	8	306	CHL	C1B-C2B	2.37	1.48	1.43
31	A	825	CLA	C1B-C2B	2.37	1.48	1.43
37	d	521	0IE	C17-C16	-2.37	1.40	1.45
34	A	855	LHG	O7-C7	2.37	1.41	1.34
31	B	820	CLA	CMB-C2B	-2.37	1.45	1.50
31	g	610	CLA	CHC-C1C	2.37	1.43	1.38
31	6	303	CLA	MG-NB	-2.37	2.01	2.05
34	c	630	LHG	O8-C6	-2.37	1.39	1.45
31	3	318	CLA	C1B-C2B	2.37	1.48	1.43
30	5	302	CHL	C4D-CHA	2.37	1.46	1.38
30	i	607	CHL	C4C-C3C	2.37	1.49	1.45
31	B	818	CLA	C1B-C2B	2.37	1.48	1.43
31	B	828	CLA	C1B-C2B	2.37	1.48	1.43
31	1	309	CLA	C1B-C2B	2.37	1.48	1.43
31	A	802	CLA	C1B-C2B	2.37	1.48	1.43
37	f	521	0IE	C17-C16	-2.37	1.40	1.45
31	B	840	CLA	CMB-C2B	-2.37	1.45	1.50
37	e	521	0IE	C6-C7	-2.37	1.40	1.45
30	f	606	CHL	C4C-C3C	2.37	1.49	1.45
30	4	319	CHL	C1B-NB	-2.37	1.34	1.37
31	B	826	CLA	C1B-C2B	2.37	1.48	1.43
31	9	312	CLA	MG-NB	-2.36	2.01	2.05
32	7	405	8CT	C33-C32	-2.36	1.43	1.50
31	B	831	CLA	C1B-C2B	2.36	1.48	1.43
32	J	104	8CT	C33-C32	-2.36	1.43	1.50
30	6	306	CHL	C1B-C2B	2.36	1.48	1.43
30	6	301	CHL	C1B-C2B	2.36	1.48	1.43
34	A	855	LHG	O8-C6	-2.36	1.39	1.45
30	5	302	CHL	C3B-C4B	2.36	1.48	1.42
30	5	305	CHL	C1B-C2B	2.36	1.48	1.43
31	A	832	CLA	C1B-C2B	2.36	1.48	1.43
31	7	309	CLA	C1B-C2B	2.36	1.48	1.43
31	B	809	CLA	C1B-C2B	2.36	1.48	1.43
31	A	827	CLA	MG-NB	-2.36	2.01	2.05
31	A	832	CLA	MG-NB	-2.36	2.01	2.05
31	H	201	CLA	MG-NB	-2.36	2.01	2.05
31	A	827	CLA	C1B-C2B	2.36	1.48	1.43
30	c	601	CHL	C1C-NC	-2.36	1.34	1.37
30	2	319	CHL	C1B-NB	-2.36	1.34	1.37
30	d	609	CHL	C4C-C3C	2.36	1.49	1.45
31	9	311	CLA	C1B-C2B	2.36	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	313	CHL	C1B-C2B	2.36	1.48	1.43
31	A	804	CLA	C1B-C2B	2.36	1.48	1.43
30	5	313	CHL	C1B-NB	-2.36	1.34	1.37
30	e	606	CHL	C1B-C2B	2.36	1.48	1.43
31	B	818	CLA	MG-NB	-2.36	2.01	2.05
34	h	630	LHG	O8-C23	2.36	1.40	1.33
31	B	822	CLA	C1B-C2B	2.36	1.48	1.43
31	B	827	CLA	MG-NB	-2.36	2.01	2.05
34	b	630	LHG	O8-C6	-2.36	1.39	1.45
30	6	308	CHL	C1B-NB	-2.36	1.34	1.37
30	c	602	CHL	C1B-C2B	2.36	1.48	1.43
30	d	606	CHL	C4C-C3C	2.36	1.49	1.45
30	6	302	CHL	C3B-C4B	2.35	1.48	1.42
31	A	824	CLA	C1B-C2B	2.35	1.48	1.43
30	a	607	CHL	C4C-C3C	2.35	1.49	1.45
34	7	603	LHG	O8-C6	-2.35	1.39	1.45
31	2	304	CLA	CMB-C2B	-2.35	1.45	1.50
34	i	630	LHG	O8-C23	2.35	1.40	1.33
30	8	302	CHL	C1B-NB	-2.35	1.34	1.37
34	A	844	LHG	O7-C5	-2.35	1.40	1.46
31	A	823	CLA	CMB-C2B	-2.35	1.45	1.50
32	B	848	8CT	C33-C32	-2.35	1.43	1.50
31	B	836	CLA	C1B-C2B	2.35	1.48	1.43
30	2	302	CHL	C4D-CHA	2.35	1.46	1.38
34	2	601	LHG	O7-C5	-2.35	1.40	1.46
31	A	806	CLA	C1B-C2B	2.35	1.48	1.43
30	h	614	CHL	C4C-C3C	2.35	1.49	1.45
30	4	307	CHL	C4D-CHA	2.35	1.46	1.38
30	e	602	CHL	C1B-NB	-2.35	1.34	1.37
30	8	313	CHL	C3B-C4B	2.35	1.48	1.42
32	K	107	8CT	C33-C32	-2.35	1.44	1.50
31	2	311	CLA	MG-NB	-2.35	2.01	2.05
32	7	404	8CT	C33-C32	-2.35	1.44	1.50
30	a	605	CHL	C4C-C3C	2.35	1.49	1.45
34	3	603	LHG	O8-C6	-2.35	1.39	1.45
30	1	302	CHL	C1B-NB	-2.35	1.34	1.37
30	5	306	CHL	C4C-C3C	2.35	1.49	1.45
30	i	601	CHL	C4C-C3C	2.35	1.49	1.45
30	i	614	CHL	C4C-C3C	2.35	1.49	1.45
30	4	308	CHL	C1B-C2B	2.35	1.48	1.43
31	A	852	CLA	C1B-C2B	2.35	1.48	1.43
31	F	301	CLA	C1B-C2B	2.35	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	308	CHL	C1B-C2B	2.34	1.48	1.43
30	2	308	CHL	C1B-C2B	2.34	1.48	1.43
31	A	821	CLA	C1B-C2B	2.34	1.48	1.43
31	A	831	CLA	MG-NB	-2.34	2.01	2.05
31	4	303	CLA	MG-NB	-2.34	2.01	2.05
30	i	606	CHL	C4C-C3C	2.34	1.49	1.45
34	3	601	LHG	O8-C6	-2.34	1.39	1.45
30	4	307	CHL	C1B-C2B	2.34	1.48	1.43
31	B	829	CLA	CMD-C2D	-2.34	1.45	1.50
31	A	825	CLA	MG-NB	-2.34	2.01	2.05
30	e	614	CHL	C4C-C3C	2.34	1.49	1.45
31	6	312	CLA	MG-NB	-2.34	2.01	2.05
31	B	823	CLA	CMD-C2D	-2.34	1.45	1.50
34	0	601	LHG	O7-C5	-2.34	1.40	1.46
30	4	319	CHL	C4D-CHA	2.34	1.46	1.38
31	B	838	CLA	MG-NB	-2.34	2.01	2.05
30	6	306	CHL	C3B-C4B	2.34	1.48	1.42
30	d	607	CHL	C4C-C3C	2.34	1.49	1.45
34	i	630	LHG	O8-C6	-2.33	1.39	1.45
31	A	841	CLA	CMD-C2D	-2.33	1.45	1.50
31	7	318	CLA	MG-NB	-2.33	2.01	2.05
30	b	614	CHL	C4C-C3C	2.33	1.49	1.45
34	a	630	LHG	O8-C23	2.33	1.40	1.33
30	4	308	CHL	C1B-NB	-2.33	1.34	1.37
30	6	301	CHL	C1C-NC	-2.33	1.34	1.37
34	A	855	LHG	O8-C23	2.33	1.40	1.33
34	H	203	LHG	O8-C23	2.33	1.40	1.33
34	B	852	LHG	O7-C7	2.33	1.40	1.34
34	g	630	LHG	O8-C23	2.33	1.40	1.33
30	4	313	CHL	C4D-CHA	2.33	1.46	1.38
32	B	847	8CT	C33-C32	-2.33	1.44	1.50
31	A	823	CLA	CMD-C2D	-2.33	1.45	1.50
34	g	630	LHG	O8-C6	-2.33	1.39	1.45
30	9	305	CHL	C1B-NB	-2.33	1.34	1.37
32	F	302	8CT	C33-C32	-2.33	1.44	1.50
31	A	837	CLA	MG-NB	-2.33	2.01	2.05
32	2	402	8CT	C33-C32	-2.33	1.44	1.50
37	a	521	0IE	C13-C12	-2.33	1.40	1.45
30	7	302	CHL	C1B-NB	-2.33	1.34	1.37
30	8	308	CHL	C1B-C2B	2.33	1.48	1.43
31	A	831	CLA	C1B-C2B	2.33	1.48	1.43
30	a	606	CHL	C4C-C3C	2.33	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	301	CHL	C1C-NC	-2.33	1.34	1.37
31	B	810	CLA	MG-NB	-2.33	2.01	2.05
34	h	630	LHG	O8-C6	-2.33	1.39	1.45
30	f	607	CHL	C1B-NB	-2.33	1.34	1.37
30	6	301	CHL	C4D-CHA	2.33	1.46	1.38
31	B	813	CLA	C1B-C2B	2.33	1.48	1.43
32	L	209	8CT	C33-C32	-2.32	1.44	1.50
31	A	815	CLA	MG-NB	-2.32	2.01	2.05
31	B	841	CLA	MG-NB	-2.32	2.01	2.05
31	F	301	CLA	MG-NB	-2.32	2.01	2.05
31	O	202	CLA	MG-NB	-2.32	2.01	2.05
31	2	303	CLA	CMB-C2B	-2.32	1.45	1.50
31	2	314	CLA	CMD-C2D	-2.32	1.45	1.50
30	b	609	CHL	C1B-NB	-2.32	1.34	1.37
32	4	402	8CT	C33-C32	-2.32	1.44	1.50
30	0	306	CHL	C1C-NC	-2.32	1.34	1.37
34	g	630	LHG	O7-C7	2.32	1.40	1.34
30	8	302	CHL	C4D-CHA	2.32	1.46	1.38
31	7	316	CLA	MG-NB	-2.32	2.01	2.05
31	9	303	CLA	MG-NB	-2.32	2.01	2.05
30	2	313	CHL	C1B-NB	-2.32	1.34	1.37
31	B	832	CLA	MG-NB	-2.32	2.01	2.05
31	B	839	CLA	C1B-C2B	2.32	1.48	1.43
31	A	806	CLA	MG-NB	-2.32	2.01	2.05
31	B	812	CLA	MG-NB	-2.32	2.01	2.05
31	b	610	CLA	CHC-C1C	2.32	1.43	1.38
34	6	603	LHG	O8-C6	-2.32	1.39	1.45
31	6	317	CLA	MG-NB	-2.32	2.01	2.05
31	3	318	CLA	MG-NB	-2.32	2.01	2.05
31	B	820	CLA	MG-NB	-2.32	2.01	2.05
30	4	308	CHL	C3B-C4B	2.32	1.48	1.42
30	2	307	CHL	C1B-NB	-2.32	1.34	1.37
34	A	845	LHG	O7-C5	-2.32	1.40	1.46
30	6	302	CHL	C4D-CHA	2.32	1.46	1.38
31	A	807	CLA	MG-NB	-2.32	2.01	2.05
30	4	313	CHL	C1B-C2B	2.32	1.48	1.43
30	f	607	CHL	C4C-C3C	2.32	1.49	1.45
32	G	104	8CT	C33-C32	-2.32	1.44	1.50
30	1	306	CHL	C1C-NC	-2.32	1.34	1.37
30	5	306	CHL	C1B-NB	-2.32	1.34	1.37
34	e	630	LHG	O8-C23	2.32	1.40	1.33
31	A	823	CLA	MG-NB	-2.32	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	307	CHL	C1B-C2B	2.32	1.48	1.43
37	g	521	0IE	C6-C7	-2.32	1.41	1.45
30	g	601	CHL	C1B-NB	-2.32	1.34	1.37
34	h	630	LHG	O7-C7	2.32	1.40	1.34
31	B	809	CLA	MG-NB	-2.31	2.01	2.05
34	3	601	LHG	O8-C23	2.31	1.40	1.33
34	b	630	LHG	O8-C23	2.31	1.40	1.33
31	A	803	CLA	MG-NB	-2.31	2.01	2.05
30	d	602	CHL	C1B-C2B	2.31	1.48	1.43
30	9	306	CHL	C1B-C2B	2.31	1.48	1.43
31	A	813	CLA	C1B-C2B	2.31	1.48	1.43
31	2	304	CLA	MG-NB	-2.31	2.01	2.05
31	A	819	CLA	CMB-C2B	-2.31	1.45	1.50
31	6	317	CLA	C1B-C2B	2.31	1.48	1.43
31	5	309	CLA	MG-NB	-2.31	2.01	2.05
30	2	313	CHL	C1B-C2B	2.31	1.48	1.43
31	4	312	CLA	MG-NB	-2.31	2.01	2.05
30	4	306	CHL	C1C-NC	-2.31	1.34	1.37
30	2	305	CHL	C4D-CHA	2.31	1.46	1.38
32	M	102	8CT	C33-C32	-2.31	1.44	1.50
30	b	609	CHL	C4C-C3C	2.31	1.49	1.45
31	B	824	CLA	CMD-C2D	-2.31	1.45	1.50
30	h	602	CHL	C4C-C3C	2.31	1.49	1.45
30	9	301	CHL	C1B-NB	-2.31	1.34	1.37
30	d	605	CHL	C1B-NB	-2.31	1.34	1.37
31	B	807	CLA	C1B-C2B	2.31	1.48	1.43
31	7	303	CLA	MG-NB	-2.31	2.01	2.05
30	2	305	CHL	C1C-NC	-2.31	1.34	1.37
30	7	301	CHL	C1C-NC	-2.31	1.34	1.37
30	1	313	CHL	C1B-NB	-2.30	1.35	1.37
37	d	521	0IE	C6-C7	-2.30	1.41	1.45
30	6	305	CHL	C1B-C2B	2.30	1.48	1.43
31	7	304	CLA	MG-NB	-2.30	2.01	2.05
37	i	521	0IE	C17-C16	-2.30	1.41	1.45
30	a	609	CHL	C1B-NB	-2.30	1.35	1.37
31	1	314	CLA	MG-NB	-2.30	2.01	2.05
31	7	309	CLA	MG-NB	-2.30	2.01	2.05
31	B	806	CLA	C1B-C2B	2.30	1.48	1.43
32	B	844	8CT	C25-C26	2.30	1.38	1.35
30	7	301	CHL	C1B-NB	-2.30	1.35	1.37
31	K	105	CLA	MG-NB	-2.30	2.01	2.05
31	A	805	CLA	CMC-C2C	-2.30	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	601	CHL	C4C-C3C	2.30	1.49	1.45
30	i	602	CHL	C4C-C3C	2.30	1.49	1.45
34	7	603	LHG	O7-C7	2.30	1.40	1.34
30	5	313	CHL	C4C-C3C	2.30	1.49	1.45
34	H	203	LHG	O8-C6	-2.30	1.39	1.45
31	6	314	CLA	MG-NB	-2.30	2.01	2.05
30	7	305	CHL	C1B-C2B	2.30	1.48	1.43
30	2	306	CHL	C1B-C2B	2.30	1.48	1.43
30	7	302	CHL	C4D-CHA	2.30	1.46	1.38
31	L	203	CLA	MG-NB	-2.30	2.01	2.05
32	3	403	8CT	C33-C32	-2.30	1.44	1.50
31	A	829	CLA	MG-NB	-2.30	2.01	2.05
30	4	319	CHL	C1C-NC	-2.30	1.34	1.37
34	d	630	LHG	O8-C6	-2.30	1.39	1.45
31	6	303	CLA	CMB-C2B	-2.30	1.45	1.50
31	A	817	CLA	MG-NB	-2.30	2.01	2.05
30	4	308	CHL	C1C-NC	-2.30	1.34	1.37
37	a	521	0IE	C17-C16	-2.30	1.41	1.45
30	g	608	CHL	C4C-C3C	2.30	1.49	1.45
34	i	630	LHG	O7-C7	2.30	1.40	1.34
34	f	630	LHG	O7-C5	-2.30	1.40	1.46
30	i	609	CHL	C1B-NB	-2.29	1.35	1.37
31	A	838	CLA	C1B-C2B	2.29	1.48	1.43
34	a	630	LHG	O7-C7	2.29	1.40	1.34
30	5	302	CHL	C1B-C2B	2.29	1.48	1.43
36	J	105	LMG	O7-C8	-2.29	1.40	1.46
32	L	205	8CT	C33-C32	-2.29	1.44	1.50
31	A	840	CLA	MG-NB	-2.29	2.01	2.05
31	A	853	CLA	CMD-C2D	-2.29	1.45	1.50
34	M	104	LHG	O7-C5	-2.29	1.40	1.46
31	2	312	CLA	MG-NB	-2.29	2.01	2.05
31	B	806	CLA	CHC-C1C	2.29	1.43	1.38
30	2	313	CHL	C1C-NC	-2.29	1.34	1.37
31	L	201	CLA	C1B-C2B	2.29	1.48	1.43
31	2	310	CLA	MG-NB	-2.29	2.01	2.05
30	a	602	CHL	C4C-C3C	2.29	1.49	1.45
34	8	601	LHG	O8-C23	2.29	1.40	1.33
31	e	610	CLA	CHC-C1C	2.29	1.43	1.38
34	a	630	LHG	O8-C6	-2.29	1.39	1.45
31	A	814	CLA	MG-NB	-2.29	2.01	2.05
30	1	302	CHL	CHB-C4A	-2.29	1.32	1.37
30	1	306	CHL	C1B-NB	-2.29	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	303	CLA	MG-NB	-2.29	2.01	2.05
31	K	104	CLA	MG-NB	-2.29	2.01	2.05
31	A	841	CLA	CMB-C2B	-2.29	1.45	1.50
30	6	306	CHL	C1B-NB	-2.29	1.35	1.37
31	3	312	CLA	MG-NB	-2.29	2.01	2.05
31	A	827	CLA	CMC-C2C	-2.29	1.46	1.50
31	A	813	CLA	MG-NB	-2.29	2.01	2.05
31	A	808	CLA	MG-NB	-2.29	2.01	2.05
34	K	106	LHG	O8-C23	2.29	1.40	1.33
31	A	805	CLA	C1B-C2B	2.29	1.48	1.43
31	A	807	CLA	C1B-C2B	2.29	1.48	1.43
31	B	833	CLA	MG-NB	-2.29	2.01	2.05
30	3	307	CHL	C4D-CHA	2.28	1.46	1.38
34	6	603	LHG	O8-C23	2.28	1.40	1.33
31	B	831	CLA	CMB-C2B	-2.28	1.46	1.50
33	c	520	0UR	C19-C18	2.28	1.53	1.50
30	4	306	CHL	C1B-C2B	2.28	1.48	1.43
31	a	613	CLA	CHC-C1C	2.28	1.43	1.38
34	3	601	LHG	O7-C7	2.28	1.40	1.34
31	A	824	CLA	MG-NB	-2.28	2.01	2.05
31	B	839	CLA	MG-NB	-2.28	2.01	2.05
34	7	601	LHG	O7-C5	-2.28	1.40	1.46
34	d	630	LHG	O7-C7	2.28	1.40	1.34
31	A	829	CLA	CMD-C2D	-2.28	1.46	1.50
31	B	818	CLA	CMC-C2C	-2.28	1.46	1.50
31	B	824	CLA	MG-NB	-2.28	2.01	2.05
37	i	522	0IE	C17-C16	-2.28	1.41	1.45
30	6	302	CHL	C1C-NC	-2.28	1.34	1.37
30	3	302	CHL	C4D-CHA	2.28	1.46	1.38
30	6	302	CHL	C1B-C2B	2.28	1.48	1.43
30	g	606	CHL	C4C-C3C	2.28	1.49	1.45
31	A	843	CLA	MG-NB	-2.28	2.01	2.05
34	M	104	LHG	O8-C6	-2.28	1.39	1.45
30	0	302	CHL	C1B-C2B	2.28	1.48	1.43
37	a	521	0IE	C6-C7	-2.28	1.41	1.45
30	4	305	CHL	C1B-C2B	2.28	1.48	1.43
34	3	603	LHG	O7-C5	-2.28	1.40	1.46
30	c	607	CHL	C4C-C3C	2.28	1.49	1.45
31	3	308	CLA	MG-NB	-2.28	2.01	2.05
31	B	814	CLA	MG-NB	-2.28	2.01	2.05
34	7	601	LHG	O8-C23	2.28	1.40	1.33
30	2	307	CHL	C4D-CHA	2.28	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	805	CLA	CMD-C2D	-2.28	1.46	1.50
31	K	102	CLA	MG-NB	-2.28	2.01	2.05
30	f	601	CHL	C4C-C3C	2.28	1.49	1.45
31	d	610	CLA	CHC-C1C	2.28	1.43	1.38
31	i	613	CLA	CHC-C1C	2.28	1.43	1.38
31	B	806	CLA	MG-NB	-2.28	2.01	2.05
30	f	602	CHL	C1B-C2B	2.28	1.48	1.43
30	7	305	CHL	C1B-NB	-2.28	1.35	1.37
34	5	601	LHG	O7-C7	2.28	1.40	1.34
34	K	106	LHG	O7-C5	-2.27	1.40	1.46
30	9	301	CHL	C1B-C2B	2.27	1.48	1.43
31	A	807	CLA	CMB-C2B	-2.27	1.46	1.50
34	8	601	LHG	O7-C7	2.27	1.40	1.34
34	G	105	LHG	O8-C6	-2.27	1.40	1.45
31	B	820	CLA	C1B-C2B	2.27	1.48	1.43
31	b	603	CLA	CMD-C2D	-2.27	1.46	1.50
31	O	203	CLA	CHC-C1C	2.27	1.43	1.38
31	A	812	CLA	MG-NB	-2.27	2.01	2.05
31	A	852	CLA	MG-NB	-2.27	2.01	2.05
31	A	809	CLA	CMD-C2D	-2.27	1.46	1.50
31	3	309	CLA	MG-NB	-2.27	2.01	2.05
34	7	602	LHG	O8-C23	2.27	1.40	1.33
31	h	613	CLA	CHC-C1C	2.27	1.43	1.38
31	4	310	CLA	MG-NB	-2.27	2.01	2.05
31	2	311	CLA	CMC-C2C	-2.27	1.46	1.50
31	A	833	CLA	MG-NB	-2.27	2.01	2.05
34	e	630	LHG	O7-C7	2.27	1.40	1.34
34	M	104	LHG	O8-C23	2.27	1.40	1.33
30	2	305	CHL	C1B-NB	-2.27	1.35	1.37
30	4	305	CHL	C1B-NB	-2.27	1.35	1.37
31	7	303	CLA	CMD-C2D	-2.27	1.46	1.50
30	1	307	CHL	C1C-NC	-2.27	1.34	1.37
30	5	301	CHL	C1B-NB	-2.27	1.35	1.37
30	g	614	CHL	C1B-NB	-2.27	1.35	1.37
31	0	304	CLA	MG-NB	-2.27	2.01	2.05
30	2	319	CHL	C1C-NC	-2.27	1.34	1.37
31	A	835	CLA	MG-NB	-2.27	2.01	2.05
37	h	522	0IE	C17-C16	-2.27	1.41	1.45
30	d	614	CHL	C1B-NB	-2.27	1.35	1.37
31	3	310	CLA	MG-NB	-2.27	2.01	2.05
31	A	826	CLA	MG-NB	-2.27	2.01	2.05
31	a	610	CLA	CHC-C1C	2.27	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	301	CHL	C1B-C2B	2.27	1.48	1.43
31	5	303	CLA	MG-NB	-2.26	2.01	2.05
34	c	630	LHG	O7-C5	-2.26	1.40	1.46
30	0	305	CHL	C1B-C2B	2.26	1.48	1.43
30	5	307	CHL	C4C-C3C	2.26	1.48	1.45
31	3	303	CLA	CMD-C2D	-2.26	1.46	1.50
31	A	805	CLA	CHC-C1C	2.26	1.43	1.38
31	4	311	CLA	MG-NB	-2.26	2.01	2.05
31	A	810	CLA	CMB-C2B	-2.26	1.46	1.50
31	8	309	CLA	MG-NB	-2.26	2.01	2.05
30	5	305	CHL	C1B-NB	-2.26	1.35	1.37
34	5	601	LHG	O8-C23	2.26	1.39	1.33
37	h	522	0IE	C13-C12	-2.26	1.41	1.45
30	3	305	CHL	C1B-C2B	2.26	1.48	1.43
34	3	601	LHG	O7-C5	-2.26	1.40	1.46
34	7	603	LHG	O8-C23	2.26	1.39	1.33
30	f	614	CHL	C1B-NB	-2.26	1.35	1.37
31	G	102	CLA	MG-NB	-2.26	2.01	2.05
31	0	313	CLA	MG-NB	-2.26	2.01	2.05
32	A	849	8CT	C33-C32	-2.26	1.44	1.50
31	A	853	CLA	C1B-C2B	2.26	1.48	1.43
30	2	301	CHL	C1C-NC	-2.26	1.34	1.37
30	6	302	CHL	C1B-NB	-2.26	1.35	1.37
30	c	609	CHL	C1B-NB	-2.26	1.35	1.37
30	b	601	CHL	C1B-NB	-2.26	1.35	1.37
37	g	521	0IE	C17-C16	-2.26	1.41	1.45
31	6	318	CLA	MG-NB	-2.26	2.01	2.05
31	4	309	CLA	CHC-C1C	2.26	1.43	1.38
31	A	826	CLA	CMD-C2D	-2.26	1.46	1.50
32	A	846	8CT	C33-C32	-2.26	1.44	1.50
30	e	605	CHL	C4C-C3C	2.26	1.48	1.45
31	A	834	CLA	MG-NB	-2.26	2.01	2.05
31	B	811	CLA	CMD-C2D	-2.26	1.46	1.50
31	B	823	CLA	MG-NB	-2.26	2.01	2.05
30	d	601	CHL	C4C-C3C	2.26	1.48	1.45
30	8	315	CHL	C1B-NB	-2.26	1.35	1.37
30	h	609	CHL	C1B-NB	-2.26	1.35	1.37
31	G	103	CLA	MG-NB	-2.26	2.01	2.05
31	B	801	CLA	CHC-C1C	2.26	1.43	1.38
30	i	608	CHL	C4C-C3C	2.26	1.48	1.45
30	i	605	CHL	C1B-NB	-2.26	1.35	1.37
30	b	606	CHL	C1B-C2B	2.26	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	101	CLA	MG-NB	-2.26	2.01	2.05
32	B	845	8CT	C33-C32	-2.26	1.44	1.50
32	6	402	8CT	C33-C32	-2.25	1.44	1.50
30	7	307	CHL	C1B-NB	-2.25	1.35	1.37
30	a	601	CHL	C4C-C3C	2.25	1.48	1.45
34	f	630	LHG	O8-C23	2.25	1.39	1.33
31	2	303	CLA	MG-NB	-2.25	2.01	2.05
31	h	604	CLA	CHC-C1C	2.25	1.43	1.38
34	H	203	LHG	O7-C7	2.25	1.40	1.34
30	e	609	CHL	C1B-NB	-2.25	1.35	1.37
37	g	522	0IE	C17-C16	-2.25	1.41	1.45
31	A	810	CLA	C1B-C2B	2.25	1.48	1.43
32	B	844	8CT	C33-C32	-2.25	1.44	1.50
31	A	802	CLA	MG-NB	-2.25	2.01	2.05
31	B	833	CLA	CMB-C2B	-2.25	1.46	1.50
31	B	801	CLA	CMB-C2B	-2.25	1.46	1.50
30	f	609	CHL	C4C-C3C	2.25	1.48	1.45
30	e	607	CHL	C4C-C3C	2.25	1.48	1.45
30	c	605	CHL	C1B-NB	-2.25	1.35	1.37
34	8	601	LHG	O7-C5	-2.25	1.41	1.46
34	A	845	LHG	O7-C7	2.25	1.40	1.34
31	3	304	CLA	MG-NB	-2.25	2.01	2.05
30	5	301	CHL	C1B-C2B	2.25	1.48	1.43
30	6	308	CHL	C1C-NC	-2.25	1.34	1.37
31	0	311	CLA	MG-NB	-2.25	2.01	2.05
31	B	825	CLA	MG-NB	-2.25	2.01	2.05
37	e	522	0IE	C6-C7	-2.25	1.41	1.45
30	8	302	CHL	CHB-C4A	-2.25	1.32	1.37
37	f	521	0IE	C6-C7	-2.25	1.41	1.45
30	g	602	CHL	C4C-C3C	2.25	1.48	1.45
31	B	815	CLA	CMD-C2D	-2.25	1.46	1.50
34	7	601	LHG	O7-C7	2.25	1.40	1.34
31	A	831	CLA	CMB-C2B	-2.25	1.46	1.50
31	1	304	CLA	MG-NB	-2.25	2.01	2.05
31	B	826	CLA	MG-NB	-2.25	2.01	2.05
31	B	840	CLA	MG-NB	-2.25	2.01	2.05
34	6	601	LHG	O8-C23	2.25	1.39	1.33
30	5	307	CHL	C1B-NB	-2.25	1.35	1.37
34	B	854	LHG	O7-C5	-2.25	1.41	1.46
37	h	521	0IE	C17-C16	-2.25	1.41	1.45
30	b	607	CHL	C4C-C3C	2.25	1.48	1.45
31	8	311	CLA	CHC-C1C	2.25	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	e	613	CLA	CHC-C1C	2.25	1.43	1.38
31	9	300	CLA	MG-NB	-2.25	2.01	2.05
31	B	805	CLA	MG-NB	-2.25	2.01	2.05
36	2	602	LMG	O7-C8	-2.24	1.41	1.46
31	a	604	CLA	CHC-C1C	2.24	1.43	1.38
30	8	307	CHL	C1C-NC	-2.24	1.34	1.37
31	B	819	CLA	CMB-C2B	-2.24	1.46	1.50
31	B	827	CLA	CMC-C2C	-2.24	1.46	1.50
31	9	304	CLA	MG-NB	-2.24	2.01	2.05
31	B	811	CLA	MG-NB	-2.24	2.01	2.05
32	B	846	8CT	C33-C32	-2.24	1.44	1.50
31	M	101	CLA	MG-NB	-2.24	2.01	2.05
31	O	201	CLA	MG-NB	-2.24	2.01	2.05
30	h	607	CHL	C1B-NB	-2.24	1.35	1.37
30	2	302	CHL	C1C-NC	-2.24	1.34	1.37
31	6	304	CLA	MG-NB	-2.24	2.01	2.05
31	6	309	CLA	MG-NB	-2.24	2.01	2.05
31	0	310	CLA	MG-NB	-2.24	2.01	2.05
31	7	312	CLA	MG-NB	-2.24	2.01	2.05
31	B	835	CLA	MG-NB	-2.24	2.01	2.05
30	f	607	CHL	C1C-NC	-2.24	1.34	1.37
31	7	304	CLA	CMB-C2B	-2.24	1.46	1.50
34	c	630	LHG	O7-C7	2.24	1.40	1.34
34	B	854	LHG	O8-C23	2.24	1.39	1.33
30	h	607	CHL	C4C-C3C	2.24	1.48	1.45
30	2	308	CHL	C1C-NC	-2.24	1.34	1.37
30	a	605	CHL	C1B-NB	-2.24	1.35	1.37
31	2	303	CLA	CMC-C2C	-2.24	1.46	1.50
31	d	613	CLA	CHC-C1C	2.24	1.43	1.38
31	A	802	CLA	CMD-C2D	-2.24	1.46	1.50
31	A	822	CLA	MG-NB	-2.24	2.01	2.05
31	B	828	CLA	MG-NB	-2.24	2.01	2.05
30	8	301	CHL	C1B-NB	-2.24	1.35	1.37
34	c	630	LHG	O8-C23	2.24	1.39	1.33
31	L	202	CLA	MG-NB	-2.24	2.01	2.05
30	0	305	CHL	C1B-NB	-2.24	1.35	1.37
34	9	601	LHG	O8-C23	2.24	1.39	1.33
31	8	310	CLA	MG-NB	-2.24	2.01	2.05
30	6	307	CHL	C1B-C2B	2.24	1.48	1.43
31	B	824	CLA	CHC-C1C	2.24	1.43	1.38
31	B	834	CLA	MG-NB	-2.24	2.01	2.05
30	8	305	CHL	C1C-NC	-2.24	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	829	CLA	CMB-C2B	-2.24	1.46	1.50
30	2	307	CHL	C1B-C2B	2.24	1.48	1.43
31	B	808	CLA	MG-NB	-2.24	2.01	2.05
34	6	601	LHG	O7-C5	-2.24	1.41	1.46
31	A	812	CLA	C1B-C2B	2.24	1.48	1.43
31	0	303	CLA	MG-NB	-2.24	2.01	2.05
31	B	837	CLA	MG-NB	-2.24	2.01	2.05
34	H	203	LHG	O7-C5	-2.24	1.41	1.46
30	d	607	CHL	C1B-NB	-2.24	1.35	1.37
31	A	812	CLA	CMB-C2B	-2.24	1.46	1.50
32	B	851	8CT	C33-C32	-2.24	1.44	1.50
31	A	805	CLA	CMB-C2B	-2.24	1.46	1.50
34	7	602	LHG	C26-C25	-2.24	1.35	1.51
30	2	306	CHL	C1B-NB	-2.24	1.35	1.37
30	f	601	CHL	C1B-NB	-2.24	1.35	1.37
30	1	313	CHL	C1C-NC	-2.23	1.34	1.37
31	B	806	CLA	CMC-C2C	-2.23	1.46	1.50
30	0	302	CHL	CHB-C4A	-2.23	1.32	1.37
30	9	313	CHL	C1C-NC	-2.23	1.34	1.37
31	5	309	CLA	C1B-C2B	2.23	1.48	1.43
34	6	603	LHG	O7-C5	-2.23	1.41	1.46
31	h	610	CLA	CHC-C1C	2.23	1.43	1.38
30	1	305	CHL	C1B-NB	-2.23	1.35	1.37
30	5	301	CHL	C4C-C3C	2.23	1.48	1.45
30	3	302	CHL	CHB-C4A	-2.23	1.32	1.37
37	e	522	0IE	C17-C16	-2.23	1.41	1.45
30	5	301	CHL	C1C-NC	-2.23	1.34	1.37
34	9	601	LHG	O7-C5	-2.23	1.41	1.46
34	G	105	LHG	O7-C5	-2.23	1.41	1.46
37	c	522	0IE	C6-C7	-2.23	1.41	1.45
31	A	802	CLA	CMB-C2B	-2.23	1.46	1.50
31	8	303	CLA	MG-NB	-2.23	2.01	2.05
30	8	306	CHL	C4C-C3C	2.23	1.48	1.45
31	A	840	CLA	CMB-C2B	-2.23	1.46	1.50
31	3	309	CLA	CHC-C1C	2.23	1.43	1.38
31	7	308	CLA	MG-NB	-2.23	2.01	2.05
31	G	101	CLA	MG-NB	-2.23	2.01	2.05
37	f	522	0IE	C13-C12	-2.23	1.41	1.45
30	1	305	CHL	CHB-C4A	-2.23	1.32	1.37
30	6	315	CHL	C1B-NB	-2.23	1.35	1.37
31	4	314	CLA	MG-NB	-2.23	2.01	2.05
37	h	521	0IE	C13-C12	-2.23	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	306	CHL	C1B-NB	-2.23	1.35	1.37
30	f	614	CHL	C4C-C3C	2.23	1.48	1.45
31	9	302	CLA	MG-NB	-2.23	2.01	2.05
31	B	823	CLA	CMB-C2B	-2.23	1.46	1.50
32	6	402	8CT	C25-C26	2.23	1.38	1.35
30	4	306	CHL	C1B-NB	-2.23	1.35	1.37
31	f	610	CLA	CHC-C1C	2.23	1.43	1.38
31	5	311	CLA	MG-NB	-2.23	2.01	2.05
31	6	310	CLA	MG-NB	-2.23	2.01	2.05
31	L	204	CLA	MG-NB	-2.23	2.01	2.05
32	A	847	8CT	C33-C32	-2.23	1.44	1.50
31	5	310	CLA	MG-NB	-2.23	2.01	2.05
30	6	305	CHL	C1C-NC	-2.22	1.34	1.37
31	B	808	CLA	CMD-C2D	-2.22	1.46	1.50
31	0	309	CLA	MG-NB	-2.22	2.01	2.05
30	0	301	CHL	C1C-NC	-2.22	1.34	1.37
31	3	304	CLA	CMB-C2B	-2.22	1.46	1.50
30	b	609	CHL	C1C-NC	-2.22	1.34	1.37
31	7	318	CLA	CMB-C2B	-2.22	1.46	1.50
31	A	821	CLA	CMD-C2D	-2.22	1.46	1.50
34	b	630	LHG	O7-C7	2.22	1.40	1.34
30	6	313	CHL	C1B-NB	-2.22	1.35	1.37
30	a	614	CHL	C1B-NB	-2.22	1.35	1.37
31	A	816	CLA	CMD-C2D	-2.22	1.46	1.50
30	6	313	CHL	C1C-NC	-2.22	1.34	1.37
30	6	315	CHL	C1C-NC	-2.22	1.34	1.37
31	1	309	CLA	MG-NB	-2.22	2.01	2.05
30	h	608	CHL	C4C-C3C	2.22	1.48	1.45
31	3	308	CLA	CMD-C2D	-2.22	1.46	1.50
31	0	308	CLA	MG-NB	-2.22	2.01	2.05
31	1	312	CLA	MG-NB	-2.22	2.01	2.05
31	B	807	CLA	MG-NB	-2.22	2.01	2.05
30	e	608	CHL	C1B-NB	-2.22	1.35	1.37
30	9	305	CHL	CHB-C4A	-2.22	1.32	1.37
31	3	313	CLA	MG-NB	-2.22	2.01	2.05
31	A	828	CLA	MG-NB	-2.22	2.01	2.05
31	B	803	CLA	MG-NB	-2.22	2.01	2.05
31	B	829	CLA	C1B-C2B	2.22	1.48	1.43
30	6	305	CHL	C1B-NB	-2.22	1.35	1.37
30	e	605	CHL	C1B-NB	-2.22	1.35	1.37
30	8	308	CHL	C1C-NC	-2.22	1.34	1.37
31	3	311	CLA	MG-NB	-2.22	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	6	603	LHG	O7-C7	2.22	1.40	1.34
30	d	608	CHL	C4C-C3C	2.22	1.48	1.45
37	i	522	0IE	C6-C7	-2.22	1.41	1.45
30	e	601	CHL	C4C-C3C	2.22	1.48	1.45
31	3	320	CLA	MG-NB	-2.22	2.01	2.05
31	2	309	CLA	CHC-C1C	2.22	1.43	1.38
30	e	602	CHL	C4C-C3C	2.22	1.48	1.45
31	B	814	CLA	CMC-C2C	-2.22	1.46	1.50
32	I	101	8CT	C33-C32	-2.22	1.44	1.50
31	8	303	CLA	CMB-C2B	-2.22	1.46	1.50
31	A	811	CLA	CMD-C2D	-2.22	1.46	1.50
31	1	311	CLA	MG-NB	-2.22	2.01	2.05
32	8	406	8CT	C25-C26	2.22	1.38	1.35
31	B	834	CLA	CMD-C2D	-2.22	1.46	1.50
31	B	816	CLA	MG-NB	-2.21	2.01	2.05
30	4	302	CHL	C1C-NC	-2.21	1.34	1.37
31	7	310	CLA	MG-NB	-2.21	2.01	2.05
31	5	309	CLA	CHC-C1C	2.21	1.43	1.38
37	f	522	0IE	C6-C7	-2.21	1.41	1.45
31	A	841	CLA	CMC-C2C	-2.21	1.46	1.50
31	B	839	CLA	CMD-C2D	-2.21	1.46	1.50
31	A	812	CLA	CHC-C1C	2.21	1.43	1.38
30	8	313	CHL	C1C-NC	-2.21	1.34	1.37
31	9	303	CLA	CMD-C2D	-2.21	1.46	1.50
30	3	307	CHL	C3B-C4B	2.21	1.48	1.42
34	6	601	LHG	O7-C7	2.21	1.40	1.34
31	K	101	CLA	CHC-C1C	2.21	1.43	1.38
31	i	610	CLA	CHC-C1C	2.21	1.43	1.38
31	4	310	CLA	CMC-C2C	-2.21	1.46	1.50
37	i	521	0IE	C13-C12	-2.21	1.41	1.45
31	8	312	CLA	MG-NB	-2.21	2.01	2.05
34	G	105	LHG	O7-C7	2.21	1.40	1.34
34	4	601	LHG	O8-C23	2.21	1.39	1.33
31	A	834	CLA	CMB-C2B	-2.21	1.46	1.50
30	6	306	CHL	C1C-NC	-2.21	1.34	1.37
34	9	601	LHG	O7-C7	2.21	1.40	1.34
31	1	309	CLA	CHC-C1C	2.21	1.43	1.38
31	c	611	CLA	CHC-C1C	2.21	1.43	1.38
32	L	206	8CT	C33-C32	-2.21	1.44	1.50
31	3	312	CLA	CMB-C2B	-2.21	1.46	1.50
31	1	303	CLA	CMD-C2D	-2.21	1.46	1.50
31	O	206	CLA	CHC-C1C	2.21	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	f	613	CLA	CHC-C1C	2.21	1.43	1.38
30	5	302	CHL	C1C-NC	-2.21	1.34	1.37
30	5	305	CHL	C4C-C3C	2.21	1.48	1.45
31	6	320	CLA	CMD-C2D	-2.21	1.46	1.50
31	A	820	CLA	CMD-C2D	-2.21	1.46	1.50
31	h	612	CLA	CHC-C1C	2.21	1.43	1.38
31	1	303	CLA	MG-NB	-2.21	2.01	2.05
30	2	305	CHL	C1B-C2B	2.21	1.48	1.43
30	h	608	CHL	C1B-NB	-2.21	1.35	1.37
30	d	608	CHL	C1B-NB	-2.21	1.35	1.37
31	A	820	CLA	MG-NB	-2.21	2.01	2.05
31	b	613	CLA	MG-NB	-2.21	2.01	2.05
30	2	308	CHL	C1B-NB	-2.21	1.35	1.37
31	5	314	CLA	CHC-C1C	2.21	1.43	1.38
31	B	817	CLA	MG-NB	-2.21	2.01	2.05
31	9	303	CLA	CMB-C2B	-2.21	1.46	1.50
37	e	522	0IE	C13-C12	-2.21	1.41	1.45
31	2	309	CLA	MG-NB	-2.20	2.01	2.05
31	B	826	CLA	C3D-C4D	2.20	1.47	1.42
31	8	311	CLA	MG-NB	-2.20	2.01	2.05
32	8	406	8CT	C33-C32	-2.20	1.44	1.50
31	2	309	CLA	CMC-C2C	-2.20	1.46	1.50
31	B	801	CLA	CMD-C2D	-2.20	1.46	1.50
31	B	840	CLA	CMD-C2D	-2.20	1.46	1.50
31	g	612	CLA	CHC-C1C	2.20	1.43	1.38
31	6	320	CLA	MG-NB	-2.20	2.01	2.05
31	B	815	CLA	MG-NB	-2.20	2.01	2.05
30	2	301	CHL	C1B-C2B	2.20	1.48	1.43
31	a	611	CLA	CHC-C1C	2.20	1.43	1.38
34	0	601	LHG	O8-C23	2.20	1.39	1.33
30	b	607	CHL	C1B-NB	-2.20	1.35	1.37
31	g	603	CLA	CHC-C1C	2.20	1.43	1.38
34	e	630	LHG	O7-C5	-2.20	1.41	1.46
30	f	609	CHL	C1B-NB	-2.20	1.35	1.37
30	f	602	CHL	C2C-C1C	2.20	1.49	1.44
37	c	522	0IE	C17-C16	-2.20	1.41	1.45
30	f	614	CHL	C1C-NC	-2.20	1.34	1.37
31	0	304	CLA	CMB-C2B	-2.20	1.46	1.50
37	d	522	0IE	C17-C16	-2.20	1.41	1.45
31	9	310	CLA	MG-NB	-2.20	2.01	2.05
31	B	829	CLA	MG-NB	-2.20	2.01	2.05
31	L	202	CLA	CMD-C2D	-2.20	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	601	LHG	O7-C7	2.20	1.40	1.34
30	h	607	CHL	C2C-C1C	2.20	1.49	1.44
30	2	319	CHL	C1B-C2B	2.20	1.48	1.43
31	B	834	CLA	CMB-C2B	-2.20	1.46	1.50
31	B	807	CLA	CHC-C1C	2.20	1.43	1.38
30	7	307	CHL	CHB-C4A	-2.20	1.32	1.37
34	B	854	LHG	O7-C7	2.20	1.40	1.34
31	4	304	CLA	MG-NB	-2.20	2.01	2.05
31	0	303	CLA	CMD-C2D	-2.20	1.46	1.50
31	0	308	CLA	CMB-C2B	-2.20	1.46	1.50
37	i	522	0IE	C13-C12	-2.20	1.41	1.45
30	c	606	CHL	C1B-NB	-2.20	1.35	1.37
30	2	302	CHL	C1B-C2B	2.20	1.48	1.43
31	B	811	CLA	CMB-C2B	-2.20	1.46	1.50
31	7	311	CLA	MG-NB	-2.20	2.01	2.05
32	A	854	8CT	C33-C32	-2.20	1.44	1.50
31	5	303	CLA	CMD-C2D	-2.20	1.46	1.50
34	3	603	LHG	O8-C23	2.20	1.39	1.33
31	A	830	CLA	C1B-NB	-2.20	1.35	1.37
31	5	312	CLA	MG-NB	-2.20	2.01	2.05
31	A	810	CLA	CHC-C1C	2.20	1.43	1.38
31	A	826	CLA	CHC-C1C	2.20	1.43	1.38
31	0	311	CLA	CMB-C2B	-2.19	1.46	1.50
34	4	601	LHG	O7-C7	2.19	1.40	1.34
31	H	205	CLA	MG-NB	-2.19	2.01	2.05
32	0	401	8CT	C25-C26	2.19	1.38	1.35
31	b	613	CLA	CHC-C1C	2.19	1.43	1.38
31	3	310	CLA	CMB-C2B	-2.19	1.46	1.50
31	A	821	CLA	CMB-C2B	-2.19	1.46	1.50
37	a	522	0IE	C6-C7	-2.19	1.41	1.45
34	3	603	LHG	O7-C7	2.19	1.40	1.34
31	3	309	CLA	CMB-C2B	-2.19	1.46	1.50
32	B	843	8CT	C33-C32	-2.19	1.44	1.50
37	i	521	0IE	C6-C7	-2.19	1.41	1.45
31	G	101	CLA	CHC-C1C	2.19	1.43	1.38
31	B	833	CLA	CMC-C2C	-2.19	1.46	1.50
30	0	306	CHL	C4C-C3C	2.19	1.48	1.45
30	c	606	CHL	C4C-C3C	2.19	1.48	1.45
31	2	314	CLA	MG-NB	-2.19	2.01	2.05
31	O	202	CLA	CHC-C1C	2.19	1.43	1.38
31	A	834	CLA	CMD-C2D	-2.19	1.46	1.50
30	4	302	CHL	C1B-C2B	2.19	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	314	CLA	MG-NB	-2.19	2.01	2.05
31	A	840	CLA	CMD-C2D	-2.19	1.46	1.50
31	A	853	CLA	MG-NB	-2.19	2.01	2.05
30	9	301	CHL	C1C-NC	-2.19	1.34	1.37
31	c	611	CLA	MG-NB	-2.19	2.01	2.05
31	4	311	CLA	CMD-C2D	-2.19	1.46	1.50
31	f	611	CLA	MG-NB	-2.19	2.01	2.05
31	9	309	CLA	CHC-C1C	2.19	1.43	1.38
37	f	522	0IE	C17-C16	-2.19	1.41	1.45
32	B	804	8CT	C33-C32	-2.19	1.44	1.50
31	8	314	CLA	MG-NB	-2.19	2.01	2.05
31	b	604	CLA	CMB-C2B	-2.19	1.46	1.50
30	8	308	CHL	C1B-NB	-2.19	1.35	1.37
32	0	401	8CT	C33-C32	-2.19	1.44	1.50
34	M	104	LHG	O7-C7	2.19	1.40	1.34
31	A	817	CLA	CMD-C2D	-2.19	1.46	1.50
30	i	614	CHL	C1B-NB	-2.19	1.35	1.37
30	e	609	CHL	C1C-NC	-2.19	1.34	1.37
31	4	303	CLA	CMD-C2D	-2.19	1.46	1.50
31	1	304	CLA	CHC-C1C	2.19	1.43	1.38
31	B	822	CLA	MG-NB	-2.19	2.01	2.05
30	c	601	CHL	C1B-NB	-2.19	1.35	1.37
30	d	601	CHL	C1B-NB	-2.19	1.35	1.37
31	A	831	CLA	CMD-C2D	-2.19	1.46	1.50
30	e	606	CHL	C4C-C3C	2.19	1.48	1.45
34	K	106	LHG	O7-C7	2.19	1.40	1.34
31	B	829	CLA	CHC-C1C	2.19	1.43	1.38
31	9	308	CLA	MG-NB	-2.19	2.01	2.05
31	9	309	CLA	MG-NB	-2.19	2.01	2.05
30	i	608	CHL	C1C-NC	-2.19	1.34	1.37
31	J	103	CLA	MG-NB	-2.19	2.01	2.05
30	5	306	CHL	C1C-NC	-2.18	1.34	1.37
31	b	603	CLA	MG-NB	-2.18	2.01	2.05
32	8	402	8CT	C33-C32	-2.18	1.44	1.50
31	9	300	CLA	CMD-C2D	-2.18	1.46	1.50
34	5	601	LHG	O7-C5	-2.18	1.41	1.46
30	b	602	CHL	C1C-NC	-2.18	1.34	1.37
31	A	827	CLA	CMD-C2D	-2.18	1.46	1.50
34	0	601	LHG	O7-C7	2.18	1.40	1.34
31	B	850	CLA	MG-NB	-2.18	2.01	2.05
30	b	607	CHL	C1C-NC	-2.18	1.34	1.37
37	a	522	0IE	C17-C16	-2.18	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	306	CHL	CHB-C4A	-2.18	1.32	1.37
30	8	307	CHL	C1B-NB	-2.18	1.35	1.37
30	g	608	CHL	C1B-NB	-2.18	1.35	1.37
31	7	311	CLA	CMC-C2C	-2.18	1.46	1.50
31	K	101	CLA	CMD-C2D	-2.18	1.46	1.50
31	b	612	CLA	MG-NB	-2.18	2.01	2.05
30	b	602	CHL	C4C-C3C	2.18	1.48	1.45
31	5	309	CLA	CMB-C2B	-2.18	1.46	1.50
31	3	306	CLA	MG-NB	-2.18	2.01	2.05
31	e	604	CLA	MG-NB	-2.18	2.01	2.05
37	h	521	0IE	C6-C7	-2.18	1.41	1.45
30	2	305	CHL	CHB-C4A	-2.18	1.32	1.37
31	K	102	CLA	CMD-C2D	-2.18	1.46	1.50
30	7	302	CHL	C1C-NC	-2.18	1.34	1.37
30	i	602	CHL	C1C-NC	-2.18	1.34	1.37
31	0	309	CLA	CHC-C1C	2.18	1.43	1.38
31	d	611	CLA	CHC-C1C	2.18	1.43	1.38
31	A	838	CLA	CMB-C2B	-2.18	1.46	1.50
31	B	809	CLA	CMB-C2B	-2.18	1.46	1.50
31	G	102	CLA	CMD-C2D	-2.18	1.46	1.50
31	A	838	CLA	MG-NB	-2.18	2.01	2.05
31	d	604	CLA	CHC-C1C	2.18	1.43	1.38
31	2	304	CLA	CMD-C2D	-2.18	1.46	1.50
31	3	308	CLA	CMB-C2B	-2.18	1.46	1.50
31	B	803	CLA	CMD-C2D	-2.18	1.46	1.50
33	6	502	0UR	C19-C18	2.18	1.53	1.50
34	i	630	LHG	O7-C5	-2.18	1.41	1.46
31	8	304	CLA	MG-NB	-2.18	2.01	2.05
31	7	315	CLA	CMC-C2C	-2.18	1.46	1.50
31	A	803	CLA	CMC-C2C	-2.18	1.46	1.50
31	1	310	CLA	MG-NB	-2.18	2.01	2.05
31	b	604	CLA	MG-NB	-2.18	2.01	2.05
31	B	825	CLA	CMD-C2D	-2.18	1.46	1.50
31	g	611	CLA	CHC-C1C	2.18	1.42	1.38
30	7	302	CHL	C1B-C2B	2.18	1.48	1.43
31	8	309	CLA	CMD-C2D	-2.18	1.46	1.50
31	7	309	CLA	CHC-C1C	2.18	1.42	1.38
31	J	103	CLA	CHC-C1C	2.18	1.42	1.38
31	c	610	CLA	CHC-C1C	2.18	1.42	1.38
31	g	604	CLA	CHC-C1C	2.18	1.42	1.38
30	4	319	CHL	C1B-C2B	2.18	1.48	1.43
31	A	804	CLA	CHC-C1C	2.18	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	522	0IE	C6-C7	-2.18	1.41	1.45
30	7	306	CHL	C1B-C2B	2.18	1.48	1.43
31	7	304	CLA	CMD-C2D	-2.18	1.46	1.50
31	A	812	CLA	CMD-C2D	-2.18	1.46	1.50
30	b	606	CHL	C1B-NB	-2.18	1.35	1.37
30	c	614	CHL	C4C-C3C	2.17	1.48	1.45
31	i	612	CLA	CHC-C1C	2.17	1.42	1.38
30	a	601	CHL	C1B-NB	-2.17	1.35	1.37
32	1	402	8CT	C33-C32	-2.17	1.44	1.50
31	7	308	CLA	CMD-C2D	-2.17	1.46	1.50
31	B	841	CLA	CHC-C1C	2.17	1.42	1.38
30	3	305	CHL	C1B-NB	-2.17	1.35	1.37
31	L	201	CLA	CMB-C2B	-2.17	1.46	1.50
30	4	302	CHL	CHB-C4A	-2.17	1.32	1.37
31	A	803	CLA	CMD-C2D	-2.17	1.46	1.50
30	c	601	CHL	C4C-C3C	2.17	1.48	1.45
30	7	313	CHL	C1B-NB	-2.17	1.35	1.37
31	e	610	CLA	MG-NB	-2.17	2.01	2.05
30	6	307	CHL	CHB-C4A	-2.17	1.32	1.37
37	a	522	0IE	C13-C12	-2.17	1.41	1.45
30	0	302	CHL	C1B-NB	-2.17	1.35	1.37
30	h	601	CHL	C1B-NB	-2.17	1.35	1.37
30	i	601	CHL	C1B-NB	-2.17	1.35	1.37
42	i	523	NEX	O24-C25	-2.17	1.43	1.46
31	i	603	CLA	CHC-C1C	2.17	1.42	1.38
31	A	835	CLA	CMB-C2B	-2.17	1.46	1.50
31	A	810	CLA	MG-NB	-2.17	2.01	2.05
31	3	309	CLA	CMD-C2D	-2.17	1.46	1.50
31	A	814	CLA	CMB-C2B	-2.17	1.46	1.50
30	h	614	CHL	C1B-NB	-2.17	1.35	1.37
30	e	607	CHL	C1B-NB	-2.17	1.35	1.37
34	b	630	LHG	O7-C5	-2.17	1.41	1.46
31	A	824	CLA	CMB-C2B	-2.17	1.46	1.50
31	G	103	CLA	CHC-C1C	2.17	1.42	1.38
31	A	811	CLA	CMB-C2B	-2.17	1.46	1.50
31	A	813	CLA	CMC-C2C	-2.17	1.46	1.50
42	f	523	NEX	O24-C25	-2.17	1.43	1.46
31	L	207	CLA	MG-NB	-2.17	2.01	2.05
30	8	305	CHL	C4C-C3C	2.17	1.48	1.45
30	7	302	CHL	CHB-C4A	-2.17	1.32	1.37
31	A	815	CLA	CMD-C2D	-2.17	1.46	1.50
30	0	305	CHL	C4C-C3C	2.17	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	305	CHL	C1C-NC	-2.17	1.34	1.37
31	1	312	CLA	CMD-C2D	-2.17	1.46	1.50
31	6	303	CLA	CMC-C2C	-2.17	1.46	1.50
30	4	313	CHL	C1B-NB	-2.17	1.35	1.37
31	A	808	CLA	CMB-C2B	-2.17	1.46	1.50
31	4	311	CLA	CMC-C2C	-2.17	1.46	1.50
31	0	312	CLA	MG-NB	-2.17	2.01	2.05
31	7	311	CLA	CMB-C2B	-2.17	1.46	1.50
31	A	805	CLA	CMD-C2D	-2.17	1.46	1.50
34	1	601	LHG	O8-C23	2.17	1.39	1.33
31	5	314	CLA	CMD-C2D	-2.17	1.46	1.50
31	9	311	CLA	CHC-C1C	2.17	1.42	1.38
31	B	803	CLA	CHC-C1C	2.17	1.42	1.38
31	b	611	CLA	CHC-C1C	2.17	1.42	1.38
30	a	602	CHL	C1C-NC	-2.17	1.34	1.37
42	d	523	NEX	O24-C25	-2.16	1.43	1.46
31	e	611	CLA	CHC-C1C	2.16	1.42	1.38
30	e	602	CHL	CHB-C4A	-2.16	1.32	1.37
31	A	838	CLA	CMD-C2D	-2.16	1.46	1.50
31	B	826	CLA	CHC-C1C	2.16	1.42	1.38
31	c	604	CLA	MG-NB	-2.16	2.01	2.05
30	7	307	CHL	C1C-NC	-2.16	1.34	1.37
31	A	806	CLA	CHC-C1C	2.16	1.42	1.38
31	0	310	CLA	CHC-C1C	2.16	1.42	1.38
31	f	610	CLA	MG-NB	-2.16	2.01	2.05
42	a	523	NEX	O24-C25	-2.16	1.43	1.46
30	8	305	CHL	C1B-NB	-2.16	1.35	1.37
31	6	311	CLA	CMD-C2D	-2.16	1.46	1.50
30	6	307	CHL	C1C-NC	-2.16	1.34	1.37
30	d	607	CHL	C1C-NC	-2.16	1.34	1.37
31	B	832	CLA	CMB-C2B	-2.16	1.46	1.50
34	2	601	LHG	O8-C23	2.16	1.39	1.33
30	c	608	CHL	C4C-C3C	2.16	1.48	1.45
31	B	850	CLA	CHC-C1C	2.16	1.42	1.38
30	0	301	CHL	C1B-NB	-2.16	1.35	1.37
34	d	630	LHG	O7-C5	-2.16	1.41	1.46
31	O	202	CLA	CMD-C2D	-2.16	1.46	1.50
31	9	312	CLA	CHC-C1C	2.16	1.42	1.38
31	c	603	CLA	CHC-C1C	2.16	1.42	1.38
30	i	609	CHL	C1C-NC	-2.16	1.34	1.37
30	g	605	CHL	C1B-NB	-2.16	1.35	1.37
31	6	309	CLA	CMD-C2D	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	852	CLA	CMB-C2B	-2.16	1.46	1.50
31	i	611	CLA	CHC-C1C	2.16	1.42	1.38
34	h	630	LHG	O7-C5	-2.16	1.41	1.46
31	A	825	CLA	CMD-C2D	-2.16	1.46	1.50
37	b	522	0IE	C17-C16	-2.16	1.41	1.45
34	A	844	LHG	O8-C23	2.16	1.39	1.33
31	B	814	CLA	CMD-C2D	-2.16	1.46	1.50
42	g	523	NEX	O24-C25	-2.16	1.43	1.46
31	6	312	CLA	CMD-C2D	-2.16	1.46	1.50
31	A	853	CLA	CMB-C2B	-2.16	1.46	1.50
31	B	810	CLA	CMD-C2D	-2.16	1.46	1.50
31	B	838	CLA	CMD-C2D	-2.16	1.46	1.50
31	d	603	CLA	CHC-C1C	2.16	1.42	1.38
30	1	306	CHL	C4C-C3C	2.16	1.48	1.45
31	9	302	CLA	CHC-C1C	2.16	1.42	1.38
31	A	813	CLA	CMB-C2B	-2.16	1.46	1.50
31	A	839	CLA	CMB-C2B	-2.16	1.46	1.50
31	H	204	CLA	CMB-C2B	-2.16	1.46	1.50
32	J	101	8CT	C33-C32	-2.16	1.44	1.50
34	7	603	LHG	O7-C5	-2.16	1.41	1.46
31	L	204	CLA	CHC-C1C	2.16	1.42	1.38
31	0	321	CLA	CMB-C2B	-2.16	1.46	1.50
30	8	313	CHL	C1B-NB	-2.16	1.35	1.37
31	A	805	CLA	MG-NB	-2.16	2.01	2.05
31	B	821	CLA	MG-NB	-2.16	2.01	2.05
31	B	815	CLA	CHC-C1C	2.16	1.42	1.38
31	H	205	CLA	CHC-C1C	2.16	1.42	1.38
31	e	612	CLA	CHC-C1C	2.16	1.42	1.38
31	A	806	CLA	CMD-C2D	-2.16	1.46	1.50
31	K	105	CLA	CMB-C2B	-2.16	1.46	1.50
31	A	827	CLA	CHC-C1C	2.16	1.42	1.38
31	h	611	CLA	CHC-C1C	2.16	1.42	1.38
31	3	304	CLA	CMD-C2D	-2.16	1.46	1.50
30	5	307	CHL	C1C-NC	-2.16	1.34	1.37
30	e	614	CHL	C1C-NC	-2.16	1.34	1.37
42	c	523	NEX	O24-C25	-2.16	1.43	1.46
31	c	611	CLA	CMB-C2B	-2.16	1.46	1.50
31	f	603	CLA	MG-NB	-2.15	2.01	2.05
31	A	832	CLA	CMB-C2B	-2.15	1.46	1.50
31	A	832	CLA	CMD-C2D	-2.15	1.46	1.50
31	B	836	CLA	CMD-C2D	-2.15	1.46	1.50
30	5	302	CHL	C1B-NB	-2.15	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	605	CHL	C1C-NC	-2.15	1.34	1.37
30	a	606	CHL	C1B-NB	-2.15	1.35	1.37
30	h	605	CHL	C1B-NB	-2.15	1.35	1.37
31	G	101	CLA	CMC-C2C	-2.15	1.46	1.50
31	B	836	CLA	CHC-C1C	2.15	1.42	1.38
31	3	318	CLA	CMD-C2D	-2.15	1.46	1.50
32	7	404	8CT	C25-C26	2.15	1.38	1.35
30	5	313	CHL	C1C-NC	-2.15	1.34	1.37
30	a	601	CHL	C1C-NC	-2.15	1.34	1.37
30	g	608	CHL	C2C-C1C	2.15	1.49	1.44
31	A	811	CLA	MG-NB	-2.15	2.01	2.05
37	h	522	0IE	C6-C7	-2.15	1.41	1.45
31	3	311	CLA	CMD-C2D	-2.15	1.46	1.50
31	6	311	CLA	CMC-C2C	-2.15	1.46	1.50
30	d	609	CHL	C1C-NC	-2.15	1.34	1.37
31	3	310	CLA	CMD-C2D	-2.15	1.46	1.50
31	B	813	CLA	MG-NB	-2.15	2.01	2.05
30	3	305	CHL	CHB-C4A	-2.15	1.32	1.37
30	4	306	CHL	CHB-C4A	-2.15	1.32	1.37
30	g	606	CHL	C2C-C1C	2.15	1.49	1.44
30	h	606	CHL	C1B-NB	-2.15	1.35	1.37
30	i	605	CHL	C2C-C1C	2.15	1.49	1.44
30	i	602	CHL	C1B-NB	-2.15	1.35	1.37
31	O	206	CLA	MG-NB	-2.15	2.01	2.05
36	J	102	LMG	O4-C4	-2.15	1.37	1.43
31	2	309	CLA	CMD-C2D	-2.15	1.46	1.50
30	1	305	CHL	C1B-C2B	2.15	1.48	1.43
31	B	813	CLA	CMB-C2B	-2.15	1.46	1.50
31	B	832	CLA	CMD-C2D	-2.15	1.46	1.50
31	3	304	CLA	CMC-C2C	-2.15	1.46	1.50
31	3	313	CLA	CMD-C2D	-2.15	1.46	1.50
31	7	309	CLA	CMD-C2D	-2.15	1.46	1.50
31	A	837	CLA	CMD-C2D	-2.15	1.46	1.50
42	b	523	NEX	O24-C25	-2.15	1.43	1.46
31	6	309	CLA	CHC-C1C	2.15	1.42	1.38
31	B	818	CLA	CMB-C2B	-2.15	1.46	1.50
30	f	609	CHL	C1C-NC	-2.15	1.34	1.37
30	f	602	CHL	CHB-C4A	-2.15	1.32	1.37
30	g	607	CHL	C1B-NB	-2.15	1.35	1.37
30	g	605	CHL	C2C-C1C	2.15	1.49	1.44
31	5	303	CLA	CMB-C2B	-2.15	1.46	1.50
31	7	312	CLA	CMB-C2B	-2.15	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	830	CLA	CMC-C2C	-2.15	1.46	1.50
31	B	811	CLA	CMC-C2C	-2.15	1.46	1.50
34	A	845	LHG	O8-C23	2.15	1.39	1.33
30	h	602	CHL	C2C-C1C	2.15	1.49	1.44
31	B	833	CLA	CHC-C1C	2.15	1.42	1.38
31	3	311	CLA	CMC-C2C	-2.15	1.46	1.50
30	6	302	CHL	CHB-C4A	-2.15	1.32	1.37
31	8	312	CLA	CMB-C2B	-2.15	1.46	1.50
34	f	630	LHG	O7-C7	2.15	1.40	1.34
31	A	816	CLA	MG-NB	-2.15	2.01	2.05
31	7	309	CLA	CMB-C2B	-2.15	1.46	1.50
31	B	816	CLA	CMB-C2B	-2.15	1.46	1.50
31	B	819	CLA	CMD-C2D	-2.15	1.46	1.50
30	1	307	CHL	C1B-NB	-2.15	1.35	1.37
30	e	608	CHL	C4C-C3C	2.15	1.48	1.45
31	9	311	CLA	CMB-C2B	-2.15	1.46	1.50
30	d	601	CHL	C2C-C1C	2.14	1.49	1.44
31	a	603	CLA	MG-NB	-2.14	2.01	2.05
30	8	306	CHL	C1B-NB	-2.14	1.35	1.37
30	i	606	CHL	C1B-NB	-2.14	1.35	1.37
31	c	612	CLA	CHC-C1C	2.14	1.42	1.38
31	1	314	CLA	CMD-C2D	-2.14	1.46	1.50
31	f	604	CLA	MG-NB	-2.14	2.01	2.05
30	2	302	CHL	CHB-C4A	-2.14	1.32	1.37
31	A	813	CLA	CHC-C1C	2.14	1.42	1.38
30	8	306	CHL	C1C-NC	-2.14	1.34	1.37
30	e	605	CHL	C1C-NC	-2.14	1.34	1.37
30	b	606	CHL	C4C-C3C	2.14	1.48	1.45
31	A	806	CLA	CMB-C2B	-2.14	1.46	1.50
31	A	808	CLA	CMD-C2D	-2.14	1.46	1.50
31	f	611	CLA	CHC-C1C	2.14	1.42	1.38
34	g	630	LHG	O7-C5	-2.14	1.41	1.46
31	f	613	CLA	MG-NB	-2.14	2.01	2.05
31	A	818	CLA	CMD-C2D	-2.14	1.46	1.50
31	A	820	CLA	CMB-C2B	-2.14	1.46	1.50
30	3	302	CHL	C1B-NB	-2.14	1.35	1.37
31	4	312	CLA	CMD-C2D	-2.14	1.46	1.50
31	H	202	CLA	CHC-C1C	2.14	1.42	1.38
31	b	610	CLA	MG-NB	-2.14	2.01	2.05
31	9	308	CLA	CMB-C2B	-2.14	1.46	1.50
31	A	810	CLA	CMD-C2D	-2.14	1.46	1.50
31	A	819	CLA	CMD-C2D	-2.14	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	302	CHL	C1B-NB	-2.14	1.35	1.37
31	e	603	CLA	CHC-C1C	2.14	1.42	1.38
31	A	836	CLA	CMB-C2B	-2.14	1.46	1.50
32	3	402	8CT	C33-C32	-2.14	1.44	1.50
30	c	607	CHL	C1B-NB	-2.14	1.35	1.37
31	B	839	CLA	CMB-C2B	-2.14	1.46	1.50
31	9	310	CLA	CHC-C1C	2.14	1.42	1.38
31	B	824	CLA	CMB-C2B	-2.14	1.46	1.50
31	K	104	CLA	CMD-C2D	-2.14	1.46	1.50
30	a	609	CHL	C1C-NC	-2.14	1.34	1.37
30	a	602	CHL	C1B-NB	-2.14	1.35	1.37
31	H	204	CLA	MG-NB	-2.14	2.01	2.05
31	9	304	CLA	CMB-C2B	-2.14	1.46	1.50
31	B	828	CLA	CMD-C2D	-2.14	1.46	1.50
31	A	819	CLA	C1B-C2B	2.14	1.48	1.43
31	6	303	CLA	CMD-C2D	-2.14	1.46	1.50
31	6	311	CLA	CMB-C2B	-2.14	1.46	1.50
31	B	816	CLA	CMC-C2C	-2.14	1.46	1.50
31	f	613	CLA	CMD-C2D	-2.14	1.46	1.50
30	2	302	CHL	C1B-NB	-2.14	1.35	1.37
30	4	305	CHL	CHB-C4A	-2.14	1.32	1.37
31	B	814	CLA	CHC-C1C	2.14	1.42	1.38
31	A	815	CLA	CMB-C2B	-2.14	1.46	1.50
31	4	312	CLA	CMB-C2B	-2.14	1.46	1.50
30	1	302	CHL	C1B-C2B	2.14	1.48	1.43
31	1	311	CLA	CHC-C1C	2.14	1.42	1.38
31	B	830	CLA	C1B-NB	-2.14	1.35	1.37
31	5	312	CLA	CMC-C2C	-2.14	1.46	1.50
31	7	303	CLA	CMB-C2B	-2.14	1.46	1.50
31	9	308	CLA	CMD-C2D	-2.14	1.46	1.50
31	A	829	CLA	CMB-C2B	-2.14	1.46	1.50
31	b	613	CLA	CMD-C2D	-2.14	1.46	1.50
31	c	603	CLA	MG-NB	-2.14	2.01	2.05
31	0	312	CLA	CMB-C2B	-2.14	1.46	1.50
31	5	304	CLA	MG-NB	-2.14	2.01	2.05
31	9	311	CLA	MG-NB	-2.14	2.01	2.05
31	f	612	CLA	MG-NB	-2.14	2.01	2.05
30	a	607	CHL	C1B-NB	-2.14	1.35	1.37
31	2	310	CLA	CHC-C1C	2.14	1.42	1.38
31	1	310	CLA	CMD-C2D	-2.13	1.46	1.50
31	8	314	CLA	CMD-C2D	-2.13	1.46	1.50
30	c	606	CHL	C1C-NC	-2.13	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	809	CLA	CMD-C2D	-2.13	1.46	1.50
31	4	310	CLA	CMB-C2B	-2.13	1.46	1.50
31	A	803	CLA	CHC-C1C	2.13	1.42	1.38
31	F	301	CLA	CMB-C2B	-2.13	1.46	1.50
31	2	303	CLA	CMD-C2D	-2.13	1.46	1.50
31	c	613	CLA	MG-NB	-2.13	2.01	2.05
31	d	603	CLA	MG-NB	-2.13	2.01	2.05
30	2	301	CHL	CHB-C4A	-2.13	1.32	1.37
31	8	311	CLA	CMD-C2D	-2.13	1.46	1.50
31	B	806	CLA	CMD-C2D	-2.13	1.46	1.50
31	h	604	CLA	MG-NB	-2.13	2.01	2.05
31	e	611	CLA	MG-NB	-2.13	2.01	2.05
31	A	828	CLA	CHC-C1C	2.13	1.42	1.38
31	b	604	CLA	CHC-C1C	2.13	1.42	1.38
31	d	612	CLA	CHC-C1C	2.13	1.42	1.38
30	0	301	CHL	CHB-C4A	-2.13	1.32	1.37
31	3	318	CLA	CHC-C1C	2.13	1.42	1.38
31	A	833	CLA	CMD-C2D	-2.13	1.46	1.50
30	b	614	CHL	C1B-NB	-2.13	1.35	1.37
31	i	604	CLA	CHC-C1C	2.13	1.42	1.38
30	7	307	CHL	C1B-C2B	2.13	1.48	1.43
31	3	320	CLA	CMB-C2B	-2.13	1.46	1.50
31	A	853	CLA	CHC-C1C	2.13	1.42	1.38
31	g	613	CLA	CHC-C1C	2.13	1.42	1.38
30	a	607	CHL	C1C-NC	-2.13	1.34	1.37
35	0	603	SQD	O3-C3	-2.13	1.38	1.43
30	6	307	CHL	C1B-NB	-2.13	1.35	1.37
31	1	311	CLA	CMD-C2D	-2.13	1.46	1.50
31	A	822	CLA	CMD-C2D	-2.13	1.46	1.50
31	A	836	CLA	CMD-C2D	-2.13	1.46	1.50
31	8	304	CLA	CHC-C1C	2.13	1.42	1.38
30	h	614	CHL	C2C-C1C	2.13	1.49	1.44
30	3	302	CHL	C1C-NC	-2.13	1.34	1.37
30	b	608	CHL	C1C-NC	-2.13	1.34	1.37
30	d	608	CHL	C1C-NC	-2.13	1.34	1.37
31	B	822	CLA	CMB-C2B	-2.13	1.46	1.50
31	B	825	CLA	CHC-C1C	2.13	1.42	1.38
30	4	319	CHL	CHB-C4A	-2.13	1.32	1.37
31	6	314	CLA	CMD-C2D	-2.13	1.46	1.50
31	9	300	CLA	CMB-C2B	-2.13	1.46	1.50
31	A	829	CLA	CHC-C1C	2.13	1.42	1.38
30	0	305	CHL	C1C-NC	-2.13	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	614	CHL	C1C-NC	-2.13	1.34	1.37
31	A	835	CLA	CMD-C2D	-2.13	1.46	1.50
31	L	202	CLA	CMB-C2B	-2.13	1.46	1.50
31	3	310	CLA	CHC-C1C	2.13	1.42	1.38
30	8	307	CHL	CHB-C4A	-2.13	1.32	1.37
31	M	101	CLA	CMD-C2D	-2.13	1.46	1.50
31	c	610	CLA	MG-NB	-2.13	2.01	2.05
31	i	612	CLA	MG-NB	-2.13	2.01	2.05
31	6	311	CLA	CHC-C1C	2.13	1.42	1.38
30	g	602	CHL	C2C-C1C	2.13	1.49	1.44
31	5	308	CLA	CMD-C2D	-2.13	1.46	1.50
31	A	815	CLA	CMC-C2C	-2.13	1.46	1.50
31	B	850	CLA	CMB-C2B	-2.13	1.46	1.50
31	A	804	CLA	MG-NB	-2.13	2.01	2.05
32	G	104	8CT	C25-C26	2.13	1.38	1.35
31	f	604	CLA	CHC-C1C	2.13	1.42	1.38
31	A	814	CLA	CMD-C2D	-2.13	1.46	1.50
31	A	830	CLA	CMD-C2D	-2.13	1.46	1.50
31	4	314	CLA	CMD-C2D	-2.13	1.46	1.50
30	a	608	CHL	C4C-C3C	2.13	1.48	1.45
31	A	818	CLA	CMB-C2B	-2.13	1.46	1.50
31	f	604	CLA	CMB-C2B	-2.13	1.46	1.50
30	c	607	CHL	C1C-NC	-2.13	1.34	1.37
31	B	816	CLA	CMD-C2D	-2.13	1.46	1.50
31	L	201	CLA	CHC-C1C	2.12	1.42	1.38
31	d	604	CLA	MG-NB	-2.12	2.01	2.05
34	A	855	LHG	O7-C5	-2.12	1.41	1.46
30	3	307	CHL	CHB-C4A	-2.12	1.32	1.37
31	H	202	CLA	MG-NB	-2.12	2.01	2.05
30	8	315	CHL	C4C-C3C	2.12	1.48	1.45
31	H	201	CLA	CMD-C2D	-2.12	1.46	1.50
31	3	309	CLA	C1B-C2B	2.12	1.48	1.43
30	d	609	CHL	C1B-NB	-2.12	1.35	1.37
31	8	312	CLA	CHC-C1C	2.12	1.42	1.38
31	f	612	CLA	CHC-C1C	2.12	1.42	1.38
31	B	827	CLA	CMB-C2B	-2.12	1.46	1.50
34	1	601	LHG	O7-C7	2.12	1.40	1.34
31	b	603	CLA	CHC-C1C	2.12	1.42	1.38
31	e	604	CLA	CMB-C2B	-2.12	1.46	1.50
31	e	603	CLA	MG-NB	-2.12	2.01	2.05
30	d	606	CHL	C1B-NB	-2.12	1.35	1.37
30	e	606	CHL	C2C-C1C	2.12	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	608	CHL	C1C-NC	-2.12	1.34	1.37
31	0	311	CLA	CMC-C2C	-2.12	1.46	1.50
31	B	827	CLA	CMD-C2D	-2.12	1.46	1.50
31	G	103	CLA	CMB-C2B	-2.12	1.46	1.50
30	1	307	CHL	C4C-C3C	2.12	1.48	1.45
30	i	607	CHL	C1B-NB	-2.12	1.35	1.37
31	A	831	CLA	CHC-C1C	2.12	1.42	1.38
31	B	837	CLA	CMB-C2B	-2.12	1.46	1.50
30	d	602	CHL	C4C-C3C	2.12	1.48	1.45
31	8	312	CLA	CMC-C2C	-2.12	1.46	1.50
31	9	311	CLA	CMD-C2D	-2.12	1.46	1.50
30	a	606	CHL	C1C-NC	-2.12	1.34	1.37
31	L	203	CLA	CHC-C1C	2.12	1.42	1.38
31	1	312	CLA	CMC-C2C	-2.12	1.46	1.50
31	B	817	CLA	CHC-C1C	2.12	1.42	1.38
31	e	612	CLA	MG-NB	-2.12	2.01	2.05
35	0	603	SQD	O2-C2	-2.12	1.38	1.43
30	e	609	CHL	C4C-C3C	2.12	1.48	1.45
30	2	307	CHL	C1C-NC	-2.12	1.34	1.37
30	i	607	CHL	C1C-NC	-2.12	1.34	1.37
31	B	807	CLA	CMD-C2D	-2.12	1.46	1.50
31	B	828	CLA	CHC-C1C	2.12	1.42	1.38
31	h	603	CLA	CHC-C1C	2.12	1.42	1.38
31	3	306	CLA	CMD-C2D	-2.12	1.46	1.50
30	1	302	CHL	C1C-NC	-2.12	1.34	1.37
31	B	808	CLA	CHC-C1C	2.12	1.42	1.38
31	6	311	CLA	MG-NB	-2.12	2.01	2.05
30	f	608	CHL	C4C-C3C	2.12	1.48	1.45
31	B	817	CLA	CMD-C2D	-2.12	1.46	1.50
31	6	318	CLA	CHC-C1C	2.12	1.42	1.38
31	c	604	CLA	CHC-C1C	2.12	1.42	1.38
30	d	602	CHL	C1B-NB	-2.12	1.35	1.37
31	2	312	CLA	CMD-C2D	-2.12	1.46	1.50
31	B	821	CLA	CMD-C2D	-2.12	1.46	1.50
31	B	850	CLA	CMD-C2D	-2.12	1.46	1.50
31	B	818	CLA	CHC-C1C	2.12	1.42	1.38
31	B	837	CLA	CHC-C1C	2.12	1.42	1.38
34	G	105	LHG	P-O6	2.12	1.67	1.59
31	A	824	CLA	CMD-C2D	-2.12	1.46	1.50
31	e	610	CLA	CMB-C2B	-2.12	1.46	1.50
30	8	315	CHL	C1C-NC	-2.12	1.34	1.37
31	c	613	CLA	CHC-C1C	2.12	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	318	CLA	CMD-C2D	-2.12	1.46	1.50
31	B	805	CLA	CMC-C2C	-2.12	1.46	1.50
30	2	319	CHL	CHB-C4A	-2.12	1.32	1.37
30	c	602	CHL	C1B-NB	-2.12	1.35	1.37
31	0	312	CLA	CMD-C2D	-2.12	1.46	1.50
31	A	828	CLA	CMD-C2D	-2.12	1.46	1.50
37	b	522	0IE	C13-C12	-2.12	1.41	1.45
31	i	604	CLA	MG-NB	-2.12	2.01	2.05
31	B	812	CLA	CMD-C2D	-2.12	1.46	1.50
31	3	312	CLA	CMD-C2D	-2.11	1.46	1.50
31	7	311	CLA	CMD-C2D	-2.11	1.46	1.50
31	7	318	CLA	CMC-C2C	-2.11	1.46	1.50
31	B	805	CLA	CMB-C2B	-2.11	1.46	1.50
34	a	630	LHG	O7-C5	-2.11	1.41	1.46
31	7	317	CLA	MG-NB	-2.11	2.01	2.05
30	e	608	CHL	C1C-NC	-2.11	1.34	1.37
42	e	523	NEX	O24-C25	-2.11	1.43	1.46
30	6	305	CHL	CHB-C4A	-2.11	1.32	1.37
31	0	312	CLA	CHC-C1C	2.11	1.42	1.38
31	8	310	CLA	CHC-C1C	2.11	1.42	1.38
34	3	601	LHG	P-O6	2.11	1.67	1.59
31	A	825	CLA	CMB-C2B	-2.11	1.46	1.50
31	0	308	CLA	CHC-C1C	2.11	1.42	1.38
31	B	813	CLA	CMD-C2D	-2.11	1.46	1.50
31	F	301	CLA	CMD-C2D	-2.11	1.46	1.50
31	1	309	CLA	CMB-C2B	-2.11	1.46	1.50
31	3	313	CLA	CMB-C2B	-2.11	1.46	1.50
31	A	814	CLA	CMC-C2C	-2.11	1.46	1.50
31	f	603	CLA	CHC-C1C	2.11	1.42	1.38
31	9	302	CLA	CMD-C2D	-2.11	1.46	1.50
31	B	850	CLA	CMC-C2C	-2.11	1.46	1.50
31	c	612	CLA	MG-NB	-2.11	2.01	2.05
30	6	301	CHL	C1B-NB	-2.11	1.35	1.37
31	b	610	CLA	CMB-C2B	-2.11	1.46	1.50
31	i	603	CLA	MG-NB	-2.11	2.01	2.05
31	4	303	CLA	CHC-C1C	2.11	1.42	1.38
31	d	612	CLA	MG-NB	-2.11	2.01	2.05
31	A	852	CLA	CHC-C1C	2.11	1.42	1.38
31	0	311	CLA	CMD-C2D	-2.11	1.46	1.50
31	A	833	CLA	CMB-C2B	-2.11	1.46	1.50
30	3	305	CHL	C1C-NC	-2.11	1.34	1.37
31	i	611	CLA	MG-NB	-2.11	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	e	606	CHL	C1B-NB	-2.11	1.35	1.37
31	B	830	CLA	MG-ND	-2.11	2.01	2.05
30	8	306	CHL	CHB-C4A	-2.11	1.32	1.37
31	7	310	CLA	CHC-C1C	2.11	1.42	1.38
31	B	809	CLA	CHC-C1C	2.11	1.42	1.38
31	7	316	CLA	CMB-C2B	-2.11	1.46	1.50
31	e	612	CLA	CMD-C2D	-2.11	1.46	1.50
39	A	857	CL0	C1B-C2B	2.11	1.48	1.43
37	g	522	0IE	C13-C12	-2.11	1.41	1.45
31	B	810	CLA	CMB-C2B	-2.11	1.46	1.50
31	H	205	CLA	CMB-C2B	-2.11	1.46	1.50
31	4	303	CLA	CMB-C2B	-2.11	1.46	1.50
31	3	303	CLA	CMB-C2B	-2.11	1.46	1.50
31	A	826	CLA	CMB-C2B	-2.11	1.46	1.50
31	O	206	CLA	CMD-C2D	-2.11	1.46	1.50
31	4	304	CLA	CMB-C2B	-2.11	1.46	1.50
30	7	306	CHL	CHB-C4A	-2.11	1.32	1.37
30	h	605	CHL	C2C-C1C	2.11	1.49	1.44
31	A	821	CLA	CHC-C1C	2.11	1.42	1.38
31	O	201	CLA	CHC-C1C	2.11	1.42	1.38
30	b	608	CHL	C4C-C3C	2.11	1.48	1.45
30	e	614	CHL	C1B-NB	-2.11	1.35	1.37
31	a	611	CLA	MG-NB	-2.11	2.01	2.05
31	1	303	CLA	CMB-C2B	-2.11	1.46	1.50
31	8	310	CLA	CMD-C2D	-2.11	1.46	1.50
31	A	809	CLA	CMB-C2B	-2.11	1.46	1.50
31	2	310	CLA	CMB-C2B	-2.11	1.46	1.50
30	i	601	CHL	C2C-C1C	2.11	1.49	1.44
30	c	601	CHL	CHB-C4A	-2.11	1.32	1.37
30	8	302	CHL	C1B-C2B	2.11	1.48	1.43
31	1	311	CLA	CMC-C2C	-2.11	1.46	1.50
31	i	613	CLA	MG-NB	-2.11	2.01	2.05
30	a	608	CHL	C1B-NB	-2.11	1.35	1.37
31	8	309	CLA	CMB-C2B	-2.11	1.46	1.50
31	B	818	CLA	CMD-C2D	-2.11	1.46	1.50
31	6	320	CLA	CHC-C1C	2.11	1.42	1.38
31	8	309	CLA	CHC-C1C	2.11	1.42	1.38
31	A	807	CLA	CHC-C1C	2.11	1.42	1.38
30	h	609	CHL	C1C-NC	-2.11	1.34	1.37
31	7	310	CLA	CMB-C2B	-2.11	1.46	1.50
31	0	308	CLA	CMD-C2D	-2.11	1.46	1.50
31	B	801	CLA	CMC-C2C	-2.11	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	820	CLA	CHC-C1C	2.11	1.42	1.38
31	A	837	CLA	CMB-C2B	-2.11	1.46	1.50
31	9	300	CLA	CHC-C1C	2.11	1.42	1.38
31	1	310	CLA	CMB-C2B	-2.10	1.46	1.50
31	A	804	CLA	CMB-C2B	-2.10	1.46	1.50
34	A	844	LHG	O7-C7	2.10	1.40	1.34
30	b	606	CHL	C1C-NC	-2.10	1.34	1.37
31	7	317	CLA	CMB-C2B	-2.10	1.46	1.50
31	L	207	CLA	CHC-C1C	2.10	1.42	1.38
30	d	601	CHL	C1C-NC	-2.10	1.34	1.37
30	h	606	CHL	C1C-NC	-2.10	1.34	1.37
31	0	304	CLA	CMD-C2D	-2.10	1.46	1.50
31	7	309	CLA	CMC-C2C	-2.10	1.46	1.50
33	1	502	0UR	C19-C18	2.10	1.53	1.50
31	9	309	CLA	CMD-C2D	-2.10	1.46	1.50
37	d	522	0IE	C6-C7	-2.10	1.41	1.45
31	5	304	CLA	CHC-C1C	2.10	1.42	1.38
31	B	820	CLA	CHC-C1C	2.10	1.42	1.38
31	e	604	CLA	CHC-C1C	2.10	1.42	1.38
30	7	313	CHL	C1C-NC	-2.10	1.34	1.37
30	c	608	CHL	C1C-NC	-2.10	1.34	1.37
30	e	607	CHL	C1C-NC	-2.10	1.34	1.37
31	0	313	CLA	CMB-C2B	-2.10	1.46	1.50
31	1	304	CLA	CMB-C2B	-2.10	1.46	1.50
31	6	312	CLA	CMB-C2B	-2.10	1.46	1.50
31	B	837	CLA	CMD-C2D	-2.10	1.46	1.50
31	B	838	CLA	CMB-C2B	-2.10	1.46	1.50
31	G	101	CLA	CMD-C2D	-2.10	1.46	1.50
35	0	603	SQD	O4-C4	-2.10	1.38	1.43
30	f	605	CHL	C1C-NC	-2.10	1.34	1.37
31	3	311	CLA	CMB-C2B	-2.10	1.46	1.50
31	K	104	CLA	CMB-C2B	-2.10	1.46	1.50
30	5	302	CHL	CHB-C4A	-2.10	1.32	1.37
30	f	605	CHL	C1B-NB	-2.10	1.35	1.37
31	A	811	CLA	CMC-C2C	-2.10	1.46	1.50
32	7	402	8CT	C33-C32	-2.10	1.44	1.50
30	3	302	CHL	C1B-C2B	2.10	1.48	1.43
30	d	605	CHL	C1C-NC	-2.10	1.34	1.37
31	5	310	CLA	CHC-C1C	2.10	1.42	1.38
32	O	205	8CT	C33-C32	-2.10	1.44	1.50
30	9	305	CHL	C2C-C1C	2.10	1.49	1.44
31	A	803	CLA	CMB-C2B	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	607	CHL	C1C-NC	-2.10	1.34	1.37
30	e	602	CHL	C1C-NC	-2.10	1.34	1.37
30	3	307	CHL	C1B-C2B	2.10	1.48	1.43
31	A	824	CLA	CHC-C1C	2.10	1.42	1.38
31	B	834	CLA	CHC-C1C	2.10	1.42	1.38
31	0	313	CLA	CMD-C2D	-2.10	1.46	1.50
31	B	835	CLA	CMB-C2B	-2.10	1.46	1.50
36	L	211	LMG	O7-C8	-2.10	1.41	1.46
31	B	823	CLA	CHC-C1C	2.10	1.42	1.38
31	1	308	CLA	CMB-C2B	-2.10	1.46	1.50
31	6	320	CLA	CMB-C2B	-2.10	1.46	1.50
31	A	839	CLA	CMD-C2D	-2.10	1.46	1.50
31	a	604	CLA	MG-NB	-2.10	2.01	2.05
30	h	601	CHL	C1C-NC	-2.10	1.34	1.37
30	0	301	CHL	C4C-C3C	2.10	1.48	1.45
31	B	807	CLA	CMB-C2B	-2.10	1.46	1.50
30	9	305	CHL	C1C-NC	-2.10	1.34	1.37
30	g	602	CHL	C1B-NB	-2.10	1.35	1.37
31	6	310	CLA	CMB-C2B	-2.10	1.46	1.50
31	L	207	CLA	CMB-C2B	-2.10	1.46	1.50
31	7	308	CLA	CMB-C2B	-2.10	1.46	1.50
31	B	806	CLA	CMB-C2B	-2.10	1.46	1.50
31	f	610	CLA	CMD-C2D	-2.10	1.46	1.50
30	8	302	CHL	C1C-NC	-2.10	1.34	1.37
30	h	607	CHL	C1C-NC	-2.10	1.34	1.37
31	A	807	CLA	CMD-C2D	-2.10	1.46	1.50
31	B	808	CLA	CMC-C2C	-2.10	1.46	1.50
31	L	203	CLA	CMD-C2D	-2.10	1.46	1.50
31	2	310	CLA	CMD-C2D	-2.10	1.46	1.50
31	B	809	CLA	CMC-C2C	-2.10	1.46	1.50
31	f	611	CLA	CMD-C2D	-2.10	1.46	1.50
30	4	313	CHL	CHB-C4A	-2.10	1.32	1.37
31	b	611	CLA	MG-NB	-2.10	2.01	2.05
31	i	610	CLA	MG-NB	-2.10	2.01	2.05
31	3	306	CLA	CMB-C2B	-2.10	1.46	1.50
31	1	311	CLA	CMB-C2B	-2.10	1.46	1.50
31	a	604	CLA	CMB-C2B	-2.10	1.46	1.50
31	6	317	CLA	CHC-C1C	2.10	1.42	1.38
31	L	207	CLA	CMD-C2D	-2.09	1.46	1.50
31	B	813	CLA	CHC-C1C	2.09	1.42	1.38
30	0	302	CHL	C1C-NC	-2.09	1.34	1.37
31	6	304	CLA	CMD-C2D	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	303	CLA	CHC-C1C	2.09	1.42	1.38
31	B	810	CLA	CHC-C1C	2.09	1.42	1.38
31	B	831	CLA	CHC-C1C	2.09	1.42	1.38
31	2	312	CLA	CMB-C2B	-2.09	1.46	1.50
31	A	824	CLA	CMC-C2C	-2.09	1.46	1.50
31	B	826	CLA	CMB-C2B	-2.09	1.46	1.50
31	4	312	CLA	CMC-C2C	-2.09	1.46	1.50
31	7	308	CLA	CHC-C1C	2.09	1.42	1.38
31	8	314	CLA	CHC-C1C	2.09	1.42	1.38
31	9	302	CLA	CMB-C2B	-2.09	1.46	1.50
31	4	310	CLA	CMD-C2D	-2.09	1.46	1.50
31	A	822	CLA	CMB-C2B	-2.09	1.46	1.50
30	i	614	CHL	C2C-C1C	2.09	1.49	1.44
31	c	611	CLA	CMD-C2D	-2.09	1.46	1.50
30	b	606	CHL	C2C-C1C	2.09	1.49	1.44
31	A	828	CLA	CMC-C2C	-2.09	1.46	1.50
31	B	836	CLA	CMB-C2B	-2.09	1.46	1.50
31	5	309	CLA	CMD-C2D	-2.09	1.46	1.50
31	6	310	CLA	CMD-C2D	-2.09	1.46	1.50
31	4	304	CLA	CMC-C2C	-2.09	1.46	1.50
30	a	614	CHL	C2C-C1C	2.09	1.49	1.44
30	7	301	CHL	CHB-C4A	-2.09	1.32	1.37
31	3	313	CLA	CHC-C1C	2.09	1.42	1.38
31	4	310	CLA	CHC-C1C	2.09	1.42	1.38
30	c	614	CHL	C1C-NC	-2.09	1.34	1.37
30	e	606	CHL	C1C-NC	-2.09	1.34	1.37
31	0	303	CLA	CMB-C2B	-2.09	1.46	1.50
31	6	318	CLA	CMD-C2D	-2.09	1.46	1.50
31	7	312	CLA	CMD-C2D	-2.09	1.46	1.50
31	B	825	CLA	CMB-C2B	-2.09	1.46	1.50
31	B	841	CLA	CMD-C2D	-2.09	1.46	1.50
30	9	305	CHL	C1B-C2B	2.09	1.48	1.43
31	1	314	CLA	CMB-C2B	-2.09	1.46	1.50
31	a	612	CLA	CHC-C1C	2.09	1.42	1.38
34	6	603	LHG	P-O6	2.09	1.67	1.59
30	b	606	CHL	CHB-C4A	-2.09	1.32	1.37
30	4	307	CHL	CHB-C4A	-2.09	1.32	1.37
31	8	303	CLA	CMD-C2D	-2.09	1.46	1.50
31	B	814	CLA	CMB-C2B	-2.09	1.46	1.50
31	B	822	CLA	CMD-C2D	-2.09	1.46	1.50
31	B	824	CLA	CMC-C2C	-2.09	1.46	1.50
30	c	605	CHL	C2C-C1C	2.09	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	614	CHL	C2C-C1C	2.09	1.49	1.44
31	G	102	CLA	CHC-C1C	2.09	1.42	1.38
31	B	820	CLA	CMD-C2D	-2.09	1.46	1.50
31	a	610	CLA	MG-NB	-2.09	2.01	2.05
30	9	301	CHL	CHB-C4A	-2.09	1.32	1.37
30	h	608	CHL	C1C-NC	-2.09	1.34	1.37
34	h	630	LHG	P-O6	2.09	1.67	1.59
30	d	602	CHL	CHB-C4A	-2.09	1.32	1.37
31	0	321	CLA	CHC-C1C	2.09	1.42	1.38
31	b	612	CLA	CHC-C1C	2.09	1.42	1.38
37	b	522	0IE	C6-C7	-2.09	1.41	1.45
31	A	813	CLA	CMD-C2D	-2.09	1.46	1.50
30	g	608	CHL	C1C-NC	-2.09	1.34	1.37
42	h	523	NEX	O24-C25	-2.09	1.43	1.46
30	a	608	CHL	C1C-NC	-2.09	1.34	1.37
30	b	601	CHL	C1C-NC	-2.09	1.34	1.37
30	g	605	CHL	C1C-NC	-2.09	1.34	1.37
31	g	613	CLA	MG-NB	-2.09	2.01	2.05
31	3	306	CLA	CHC-C1C	2.09	1.42	1.38
31	9	308	CLA	CMC-C2C	-2.09	1.46	1.50
31	O	203	CLA	MG-NB	-2.09	2.01	2.05
31	M	101	CLA	CMC-C2C	-2.09	1.46	1.50
31	4	309	CLA	CMB-C2B	-2.09	1.46	1.50
31	5	310	CLA	CMB-C2B	-2.09	1.46	1.50
31	d	613	CLA	MG-NB	-2.09	2.01	2.05
30	3	302	CHL	C2C-C1C	2.09	1.49	1.44
31	B	835	CLA	CMD-C2D	-2.08	1.46	1.50
31	9	304	CLA	CMD-C2D	-2.08	1.46	1.50
31	B	810	CLA	CMC-C2C	-2.08	1.46	1.50
31	H	204	CLA	CMD-C2D	-2.08	1.46	1.50
30	9	313	CHL	C1B-NB	-2.08	1.35	1.37
30	7	305	CHL	CHB-C4A	-2.08	1.32	1.37
30	f	605	CHL	C2C-C1C	2.08	1.49	1.44
31	2	309	CLA	CMB-C2B	-2.08	1.46	1.50
31	6	317	CLA	CMB-C2B	-2.08	1.46	1.50
31	0	321	CLA	MG-NB	-2.08	2.01	2.05
30	2	307	CHL	CHB-C4A	-2.08	1.32	1.37
31	A	843	CLA	CMB-C2B	-2.08	1.46	1.50
34	7	602	LHG	O7-C7	2.08	1.40	1.34
30	2	306	CHL	C4C-C3C	2.08	1.48	1.45
30	h	602	CHL	C1C-NC	-2.08	1.34	1.37
31	h	613	CLA	MG-NB	-2.08	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	314	CLA	CHC-C1C	2.08	1.42	1.38
31	4	309	CLA	MG-NB	-2.08	2.01	2.05
31	K	101	CLA	CMB-C2B	-2.08	1.46	1.50
31	A	838	CLA	CHC-C1C	2.08	1.42	1.38
31	K	102	CLA	CHC-C1C	2.08	1.42	1.38
31	d	611	CLA	MG-NB	-2.08	2.01	2.05
31	2	311	CLA	CMD-C2D	-2.08	1.46	1.50
31	O	201	CLA	CMD-C2D	-2.08	1.46	1.50
31	1	303	CLA	CHC-C1C	2.08	1.42	1.38
31	B	835	CLA	CHC-C1C	2.08	1.42	1.38
31	3	312	CLA	CMC-C2C	-2.08	1.46	1.50
31	f	612	CLA	CMD-C2D	-2.08	1.46	1.50
30	c	605	CHL	C1C-NC	-2.08	1.34	1.37
30	i	605	CHL	C1C-NC	-2.08	1.34	1.37
31	1	303	CLA	CMC-C2C	-2.08	1.46	1.50
31	O	202	CLA	CMB-C2B	-2.08	1.46	1.50
31	A	817	CLA	CHC-C1C	2.08	1.42	1.38
31	A	825	CLA	CHC-C1C	2.08	1.42	1.38
37	d	522	0IE	C13-C12	-2.08	1.41	1.45
31	8	311	CLA	CMC-C2C	-2.08	1.46	1.50
31	A	843	CLA	CMD-C2D	-2.08	1.46	1.50
30	6	306	CHL	CHB-C4A	-2.08	1.32	1.37
30	b	608	CHL	C1B-NB	-2.08	1.35	1.37
30	d	614	CHL	C1C-NC	-2.08	1.34	1.37
31	1	309	CLA	CMD-C2D	-2.08	1.46	1.50
30	4	306	CHL	C4C-C3C	2.08	1.48	1.45
30	6	301	CHL	CHB-C4A	-2.08	1.32	1.37
31	8	303	CLA	CMC-C2C	-2.08	1.46	1.50
31	8	311	CLA	CMB-C2B	-2.08	1.46	1.50
30	i	608	CHL	C1B-NB	-2.08	1.35	1.37
31	9	311	CLA	CMC-C2C	-2.08	1.46	1.50
31	9	312	CLA	CMD-C2D	-2.08	1.46	1.50
31	a	603	CLA	CMD-C2D	-2.08	1.46	1.50
30	5	305	CHL	C1C-NC	-2.08	1.34	1.37
31	7	317	CLA	CMD-C2D	-2.08	1.46	1.50
31	9	310	CLA	CMB-C2B	-2.08	1.46	1.50
31	J	103	CLA	CMD-C2D	-2.08	1.46	1.50
31	K	105	CLA	CMD-C2D	-2.08	1.46	1.50
31	B	822	CLA	CHC-C1C	2.07	1.42	1.38
31	5	312	CLA	CMD-C2D	-2.07	1.46	1.50
31	c	604	CLA	CMB-C2B	-2.07	1.46	1.50
34	K	106	LHG	P-O6	2.07	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	306	CHL	C2C-C1C	2.07	1.49	1.44
30	e	607	CHL	C2C-C1C	2.07	1.49	1.44
36	9	602	LMG	O8-C9	-2.07	1.40	1.45
31	2	314	CLA	CMB-C2B	-2.07	1.46	1.50
31	1	308	CLA	CMD-C2D	-2.07	1.46	1.50
31	6	317	CLA	CMD-C2D	-2.07	1.46	1.50
31	h	603	CLA	MG-NB	-2.07	2.01	2.05
31	e	613	CLA	MG-NB	-2.07	2.01	2.05
31	L	201	CLA	CMD-C2D	-2.07	1.46	1.50
31	d	610	CLA	MG-NB	-2.07	2.01	2.05
30	7	307	CHL	C2C-C1C	2.07	1.49	1.44
31	7	303	CLA	CHC-C1C	2.07	1.42	1.38
31	A	819	CLA	CMC-C2C	-2.07	1.46	1.50
31	0	310	CLA	CMD-C2D	-2.07	1.46	1.50
31	4	311	CLA	CHC-C1C	2.07	1.42	1.38
30	7	305	CHL	C1C-NC	-2.07	1.34	1.37
31	7	315	CLA	CMB-C2B	-2.07	1.46	1.50
31	A	812	CLA	CMC-C2C	-2.07	1.46	1.50
31	J	103	CLA	CMB-C2B	-2.07	1.46	1.50
31	1	312	CLA	CMB-C2B	-2.07	1.46	1.50
31	8	312	CLA	CMD-C2D	-2.07	1.46	1.50
31	A	806	CLA	CMC-C2C	-2.07	1.46	1.50
31	3	318	CLA	CMB-C2B	-2.07	1.46	1.50
31	7	315	CLA	CMD-C2D	-2.07	1.46	1.50
31	8	309	CLA	CMC-C2C	-2.07	1.46	1.50
30	6	315	CHL	C4C-C3C	2.07	1.48	1.45
31	L	204	CLA	CMB-C2B	-2.07	1.46	1.50
31	g	612	CLA	MG-NB	-2.07	2.01	2.05
31	h	612	CLA	MG-NB	-2.07	2.01	2.05
31	0	309	CLA	CMD-C2D	-2.07	1.46	1.50
31	3	320	CLA	CMD-C2D	-2.07	1.46	1.50
30	i	601	CHL	C1C-NC	-2.07	1.34	1.37
30	1	305	CHL	C2C-C1C	2.07	1.49	1.44
31	5	308	CLA	MG-NB	-2.07	2.01	2.05
31	B	832	CLA	CMC-C2C	-2.07	1.46	1.50
31	4	303	CLA	CMC-C2C	-2.07	1.46	1.50
31	1	308	CLA	MG-NB	-2.07	2.01	2.05
31	8	310	CLA	CMB-C2B	-2.07	1.46	1.50
31	B	833	CLA	CMD-C2D	-2.07	1.46	1.50
32	1	402	8CT	C25-C26	2.07	1.38	1.35
34	e	630	LHG	P-O6	2.07	1.67	1.59
31	7	310	CLA	CMD-C2D	-2.07	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	104	CLA	CMC-C2C	-2.07	1.46	1.50
30	g	609	CHL	C1B-NB	-2.07	1.35	1.37
31	9	304	CLA	CHC-C1C	2.07	1.42	1.38
31	H	202	CLA	CMD-C2D	-2.06	1.46	1.50
30	f	601	CHL	C1C-NC	-2.06	1.34	1.37
31	9	310	CLA	CMD-C2D	-2.06	1.46	1.50
31	A	843	CLA	CMC-C2C	-2.06	1.46	1.50
30	8	308	CHL	C4C-C3C	2.06	1.48	1.45
31	H	205	CLA	CMD-C2D	-2.06	1.46	1.50
31	e	604	CLA	CMD-C2D	-2.06	1.46	1.50
31	M	101	CLA	CMB-C2B	-2.06	1.46	1.50
31	3	311	CLA	CHC-C1C	2.06	1.42	1.38
31	6	310	CLA	CHC-C1C	2.06	1.42	1.38
31	A	840	CLA	CHC-C1C	2.06	1.42	1.38
31	B	807	CLA	CMC-C2C	-2.06	1.46	1.50
31	B	830	CLA	CMC-C2C	-2.06	1.46	1.50
31	A	822	CLA	CHC-C1C	2.06	1.42	1.38
31	A	835	CLA	CHC-C1C	2.06	1.42	1.38
30	5	305	CHL	CHB-C4A	-2.06	1.32	1.37
30	d	605	CHL	C2C-C1C	2.06	1.49	1.44
30	e	602	CHL	C1B-C2B	2.06	1.48	1.43
31	3	303	CLA	CMC-C2C	-2.06	1.46	1.50
31	A	802	CLA	CMC-C2C	-2.06	1.46	1.50
31	A	827	CLA	CMB-C2B	-2.06	1.46	1.50
31	1	314	CLA	CHC-C1C	2.06	1.42	1.38
31	6	312	CLA	CHC-C1C	2.06	1.42	1.38
30	h	602	CHL	C1B-NB	-2.06	1.35	1.37
30	g	609	CHL	C1C-NC	-2.06	1.34	1.37
31	9	312	CLA	CMB-C2B	-2.06	1.46	1.50
30	8	301	CHL	CHB-C4A	-2.06	1.32	1.37
31	6	314	CLA	CMB-C2B	-2.06	1.46	1.50
30	e	601	CHL	C1C-NC	-2.06	1.34	1.37
31	b	612	CLA	CMC-C2C	-2.06	1.46	1.50
31	7	311	CLA	CHC-C1C	2.06	1.42	1.38
30	0	306	CHL	C2C-C1C	2.06	1.49	1.44
36	J	105	LMG	O6-C5	-2.06	1.39	1.44
31	A	852	CLA	CMD-C2D	-2.06	1.46	1.50
31	a	613	CLA	MG-NB	-2.06	2.01	2.05
31	A	817	CLA	CMC-C2C	-2.06	1.46	1.50
31	B	828	CLA	CMB-C2B	-2.06	1.46	1.50
31	B	828	CLA	CMC-C2C	-2.06	1.46	1.50
31	d	612	CLA	CMB-C2B	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	603	CLA	CHC-C1C	2.06	1.42	1.38
30	c	602	CHL	CHB-C4A	-2.06	1.32	1.37
30	4	308	CHL	C4C-C3C	2.06	1.48	1.45
31	F	301	CLA	CMC-C2C	-2.06	1.46	1.50
31	A	804	CLA	CMD-C2D	-2.06	1.46	1.50
31	7	308	CLA	CMC-C2C	-2.06	1.46	1.50
31	9	303	CLA	CMC-C2C	-2.06	1.46	1.50
34	H	203	LHG	P-O6	2.06	1.67	1.59
31	B	832	CLA	CHC-C1C	2.06	1.42	1.38
31	f	613	CLA	CMB-C2B	-2.06	1.46	1.50
31	7	315	CLA	MG-NB	-2.06	2.01	2.05
31	A	830	CLA	C1B-C2B	2.06	1.48	1.43
32	B	848	8CT	C25-C26	2.06	1.38	1.35
31	1	310	CLA	CHC-C1C	2.06	1.42	1.38
31	6	309	CLA	CMB-C2B	-2.06	1.46	1.50
31	0	304	CLA	CHC-C1C	2.05	1.42	1.38
31	F	301	CLA	CHC-C1C	2.05	1.42	1.38
31	3	309	CLA	CMC-C2C	-2.05	1.46	1.50
30	f	602	CHL	C1B-NB	-2.05	1.35	1.37
37	c	522	0IE	C13-C12	-2.05	1.41	1.45
31	g	610	CLA	MG-NB	-2.05	2.01	2.05
31	2	314	CLA	CHC-C1C	2.05	1.42	1.38
31	L	203	CLA	CMB-C2B	-2.05	1.46	1.50
31	1	309	CLA	CMC-C2C	-2.05	1.46	1.50
31	B	825	CLA	CMC-C2C	-2.05	1.46	1.50
34	7	602	LHG	P-O6	2.05	1.67	1.59
30	a	605	CHL	C2C-C1C	2.05	1.49	1.44
30	c	602	CHL	C4C-C3C	2.05	1.48	1.45
34	d	630	LHG	P-O6	2.05	1.67	1.59
30	9	306	CHL	CHB-C4A	-2.05	1.32	1.37
31	g	603	CLA	MG-NB	-2.05	2.01	2.05
31	1	312	CLA	CHC-C1C	2.05	1.42	1.38
31	A	819	CLA	CHC-C1C	2.05	1.42	1.38
34	g	630	LHG	P-O6	2.05	1.67	1.59
32	9	401	8CT	C33-C32	-2.05	1.44	1.50
31	7	316	CLA	CMD-C2D	-2.05	1.46	1.50
31	8	304	CLA	CMD-C2D	-2.05	1.46	1.50
31	A	840	CLA	CMC-C2C	-2.05	1.46	1.50
31	H	204	CLA	CMC-C2C	-2.05	1.46	1.50
31	K	104	CLA	CHC-C1C	2.05	1.42	1.38
30	c	609	CHL	C1C-NC	-2.05	1.34	1.37
30	h	601	CHL	C2C-C1C	2.05	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	310	CLA	CMD-C2D	-2.05	1.46	1.50
31	8	304	CLA	CMB-C2B	-2.05	1.46	1.50
31	b	603	CLA	CMB-C2B	-2.05	1.46	1.50
31	h	610	CLA	MG-NB	-2.05	2.01	2.05
31	e	611	CLA	CMD-C2D	-2.05	1.46	1.50
31	A	837	CLA	CHC-C1C	2.05	1.42	1.38
30	a	607	CHL	C2C-C1C	2.05	1.49	1.44
31	6	309	CLA	CMC-C2C	-2.05	1.46	1.50
31	c	612	CLA	CMD-C2D	-2.05	1.46	1.50
31	a	612	CLA	MG-NB	-2.05	2.01	2.05
31	g	604	CLA	MG-NB	-2.05	2.01	2.05
31	B	816	CLA	CHC-C1C	2.05	1.42	1.38
31	B	808	CLA	CMB-C2B	-2.05	1.46	1.50
31	B	841	CLA	CMB-C2B	-2.05	1.46	1.50
31	K	102	CLA	CMB-C2B	-2.05	1.46	1.50
31	5	303	CLA	CHC-C1C	2.05	1.42	1.38
30	i	614	CHL	C1C-NC	-2.05	1.34	1.37
31	5	312	CLA	CHC-C1C	2.05	1.42	1.38
34	3	603	LHG	P-O6	2.05	1.67	1.59
34	a	630	LHG	P-O6	2.05	1.67	1.59
31	5	311	CLA	CMD-C2D	-2.05	1.46	1.50
31	6	318	CLA	CMB-C2B	-2.05	1.46	1.50
31	A	809	CLA	CMC-C2C	-2.05	1.46	1.50
31	B	815	CLA	CMC-C2C	-2.05	1.46	1.50
31	i	603	CLA	CMD-C2D	-2.05	1.46	1.50
30	7	305	CHL	C2C-C1C	2.05	1.49	1.44
30	2	313	CHL	CHB-C4A	-2.04	1.32	1.37
31	A	818	CLA	CMC-C2C	-2.04	1.46	1.50
31	O	201	CLA	CMB-C2B	-2.04	1.46	1.50
31	c	613	CLA	CMD-C2D	-2.04	1.46	1.50
31	3	312	CLA	CHC-C1C	2.04	1.42	1.38
31	H	201	CLA	CMB-C2B	-2.04	1.46	1.50
34	A	855	LHG	P-O6	2.04	1.67	1.59
31	7	312	CLA	CHC-C1C	2.04	1.42	1.38
31	0	311	CLA	CHC-C1C	2.04	1.42	1.38
31	A	808	CLA	CHC-C1C	2.04	1.42	1.38
31	B	839	CLA	CHC-C1C	2.04	1.42	1.38
31	L	202	CLA	CHC-C1C	2.04	1.42	1.38
31	K	105	CLA	CHC-C1C	2.04	1.42	1.38
31	c	610	CLA	CMD-C2D	-2.04	1.46	1.50
34	7	603	LHG	P-O6	2.04	1.67	1.59
31	A	809	CLA	CHC-C1C	2.04	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	0	310	CLA	CMB-C2B	-2.04	1.46	1.50
31	B	813	CLA	CMC-C2C	-2.04	1.46	1.50
31	A	817	CLA	CMB-C2B	-2.04	1.46	1.50
31	c	610	CLA	CMB-C2B	-2.04	1.46	1.50
31	2	312	CLA	CMC-C2C	-2.04	1.46	1.50
31	A	832	CLA	CMC-C2C	-2.04	1.46	1.50
31	b	604	CLA	CMD-C2D	-2.04	1.46	1.50
30	g	606	CHL	C1B-NB	-2.04	1.35	1.37
30	a	606	CHL	C2C-C1C	2.04	1.48	1.44
31	A	821	CLA	CMC-C2C	-2.04	1.46	1.50
31	7	315	CLA	CHC-C1C	2.04	1.42	1.38
31	e	610	CLA	CMD-C2D	-2.04	1.46	1.50
30	f	606	CHL	C1B-NB	-2.04	1.35	1.37
31	B	817	CLA	CMB-C2B	-2.04	1.46	1.50
31	A	839	CLA	CHC-C1C	2.04	1.42	1.38
36	O	207	LMG	O7-C8	-2.04	1.41	1.46
30	d	602	CHL	C1C-NC	-2.04	1.34	1.37
31	A	837	CLA	CMC-C2C	-2.04	1.46	1.50
31	g	604	CLA	CMD-C2D	-2.04	1.46	1.50
31	H	201	CLA	CHC-C1C	2.04	1.42	1.38
30	1	313	CHL	CHB-C4A	-2.04	1.32	1.37
31	A	833	CLA	CHC-C1C	2.04	1.42	1.38
31	A	838	CLA	CMC-C2C	-2.04	1.46	1.50
31	B	834	CLA	CMC-C2C	-2.04	1.46	1.50
31	B	836	CLA	CMC-C2C	-2.04	1.46	1.50
31	H	202	CLA	CMC-C2C	-2.04	1.46	1.50
31	4	304	CLA	CMD-C2D	-2.04	1.46	1.50
31	B	806	CLA	MG-ND	-2.04	2.01	2.05
31	G	103	CLA	CMD-C2D	-2.04	1.46	1.50
31	A	816	CLA	CMC-C2C	-2.04	1.46	1.50
30	g	606	CHL	C1C-NC	-2.04	1.34	1.37
30	h	614	CHL	C1C-NC	-2.04	1.34	1.37
31	3	318	CLA	CMC-C2C	-2.04	1.46	1.50
31	c	603	CLA	CMD-C2D	-2.04	1.46	1.50
31	H	204	CLA	CHC-C1C	2.04	1.42	1.38
30	i	609	CHL	C2C-C1C	2.04	1.48	1.44
31	a	612	CLA	CMD-C2D	-2.03	1.46	1.50
30	g	614	CHL	C2C-C1C	2.03	1.48	1.44
34	i	630	LHG	P-O6	2.03	1.67	1.59
30	d	606	CHL	C1C-NC	-2.03	1.34	1.37
31	5	308	CLA	CHC-C1C	2.03	1.42	1.38
30	5	301	CHL	C2C-C1C	2.03	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	603	CLA	CMD-C2D	-2.03	1.46	1.50
31	g	611	CLA	MG-NB	-2.03	2.01	2.05
30	h	608	CHL	C2C-C1C	2.03	1.48	1.44
31	B	803	CLA	CMB-C2B	-2.03	1.46	1.50
31	d	604	CLA	CMB-C2B	-2.03	1.46	1.50
31	2	314	CLA	CMC-C2C	-2.03	1.46	1.50
31	A	836	CLA	CHC-C1C	2.03	1.42	1.38
31	B	811	CLA	CHC-C1C	2.03	1.42	1.38
30	a	608	CHL	C2C-C1C	2.03	1.48	1.44
31	O	206	CLA	CMB-C2B	-2.03	1.46	1.50
31	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
31	A	804	CLA	CMC-C2C	-2.03	1.46	1.50
31	i	612	CLA	CMD-C2D	-2.03	1.46	1.50
31	4	311	CLA	CMB-C2B	-2.03	1.46	1.50
30	a	605	CHL	C1C-NC	-2.03	1.34	1.37
31	7	316	CLA	CHC-C1C	2.03	1.42	1.38
31	B	826	CLA	CMC-C2C	-2.03	1.46	1.50
30	c	609	CHL	C2C-C1C	2.03	1.48	1.44
31	A	807	CLA	CMC-C2C	-2.03	1.46	1.50
31	d	610	CLA	CMD-C2D	-2.03	1.46	1.50
30	d	602	CHL	C2C-C1C	2.03	1.48	1.44
30	9	301	CHL	C4C-C3C	2.03	1.48	1.45
31	B	835	CLA	CMC-C2C	-2.03	1.46	1.50
31	0	321	CLA	CMD-C2D	-2.03	1.46	1.50
31	2	311	CLA	CMB-C2B	-2.03	1.46	1.50
31	c	604	CLA	CMD-C2D	-2.03	1.46	1.50
31	4	312	CLA	CHC-C1C	2.03	1.42	1.38
30	f	601	CHL	C2C-C1C	2.03	1.48	1.44
31	1	308	CLA	CHC-C1C	2.03	1.42	1.38
31	f	603	CLA	CMD-C2D	-2.03	1.46	1.50
31	h	603	CLA	CMD-C2D	-2.03	1.46	1.50
30	3	307	CHL	C1C-NC	-2.03	1.34	1.37
30	g	601	CHL	C2C-C1C	2.03	1.48	1.44
31	A	830	CLA	MG-ND	-2.03	2.01	2.05
31	6	312	CLA	CMC-C2C	-2.03	1.46	1.50
31	A	843	CLA	CHC-C1C	2.03	1.42	1.38
31	1	304	CLA	CMD-C2D	-2.03	1.46	1.50
31	A	825	CLA	CMC-C2C	-2.03	1.46	1.50
31	b	612	CLA	CMD-C2D	-2.03	1.46	1.50
31	H	202	CLA	CMB-C2B	-2.03	1.46	1.50
31	A	841	CLA	CHC-C1C	2.03	1.42	1.38
31	9	309	CLA	CMB-C2B	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	h	604	CLA	CMD-C2D	-2.02	1.46	1.50
31	i	603	CLA	CMB-C2B	-2.02	1.46	1.50
32	B	844	8CT	C24-C23	2.02	1.39	1.34
30	f	609	CHL	C2C-C1C	2.02	1.48	1.44
31	2	310	CLA	CMC-C2C	-2.02	1.46	1.50
31	A	831	CLA	CMC-C2C	-2.02	1.46	1.50
31	0	303	CLA	CHC-C1C	2.02	1.42	1.38
31	A	810	CLA	CMC-C2C	-2.02	1.46	1.50
31	A	829	CLA	CMC-C2C	-2.02	1.46	1.50
30	8	302	CHL	C2C-C1C	2.02	1.48	1.44
31	A	839	CLA	CMC-C2C	-2.02	1.46	1.50
31	b	611	CLA	CMD-C2D	-2.02	1.46	1.50
31	f	603	CLA	CMB-C2B	-2.02	1.46	1.50
30	8	301	CHL	C4C-C3C	2.02	1.48	1.45
30	c	607	CHL	C2C-C1C	2.02	1.48	1.44
30	d	607	CHL	C2C-C1C	2.02	1.48	1.44
30	1	307	CHL	CHB-C4A	-2.02	1.32	1.37
31	5	312	CLA	CMB-C2B	-2.02	1.46	1.50
31	B	812	CLA	CMC-C2C	-2.02	1.46	1.50
31	f	611	CLA	CMB-C2B	-2.02	1.46	1.50
30	f	606	CHL	C1C-NC	-2.02	1.34	1.37
30	6	305	CHL	C4C-C3C	2.02	1.48	1.45
30	7	306	CHL	C4C-C3C	2.02	1.48	1.45
30	a	602	CHL	CHB-C4A	-2.02	1.32	1.37
31	A	823	CLA	CHC-C1C	2.02	1.42	1.38
31	L	201	CLA	CMC-C2C	-2.02	1.46	1.50
31	c	603	CLA	CMB-C2B	-2.02	1.46	1.50
31	d	613	CLA	CMD-C2D	-2.02	1.46	1.50
31	5	304	CLA	CMD-C2D	-2.02	1.46	1.50
31	A	820	CLA	CMC-C2C	-2.02	1.46	1.50
34	B	854	LHG	P-O6	2.02	1.67	1.59
30	c	614	CHL	C2C-C1C	2.02	1.48	1.44
30	f	608	CHL	CHB-C4A	-2.02	1.32	1.37
31	A	828	CLA	CMB-C2B	-2.02	1.46	1.50
31	5	311	CLA	CMB-C2B	-2.02	1.46	1.50
30	4	319	CHL	C2C-C1C	2.02	1.48	1.44
31	5	308	CLA	CMB-C2B	-2.02	1.46	1.50
31	A	852	CLA	CMC-C2C	-2.02	1.46	1.50
31	B	838	CLA	CMC-C2C	-2.02	1.46	1.50
31	h	611	CLA	MG-NB	-2.02	2.01	2.05
30	e	601	CHL	C1B-NB	-2.02	1.35	1.37
31	B	819	CLA	CMC-C2C	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	304	CLA	CMC-C2C	-2.02	1.46	1.50
30	8	313	CHL	C4C-C3C	2.02	1.48	1.45
31	B	823	CLA	CMC-C2C	-2.02	1.46	1.50
30	g	602	CHL	C1C-NC	-2.02	1.34	1.37
30	e	605	CHL	C2C-C1C	2.02	1.48	1.44
31	A	823	CLA	CMC-C2C	-2.02	1.46	1.50
31	c	612	CLA	CMB-C2B	-2.02	1.46	1.50
31	7	316	CLA	CMC-C2C	-2.02	1.46	1.50
31	A	834	CLA	CMC-C2C	-2.02	1.46	1.50
30	c	608	CHL	CHB-C4A	-2.02	1.32	1.37
30	g	614	CHL	C1C-NC	-2.02	1.34	1.37
31	B	829	CLA	CMC-C2C	-2.01	1.46	1.50
31	L	203	CLA	CMC-C2C	-2.01	1.46	1.50
31	f	612	CLA	CMC-C2C	-2.01	1.46	1.50
30	b	602	CHL	CHB-C4A	-2.01	1.32	1.37
31	3	308	CLA	CHC-C1C	2.01	1.42	1.38
31	d	603	CLA	CMD-C2D	-2.01	1.46	1.50
33	f	520	0UR	C19-C18	2.01	1.53	1.50
31	i	611	CLA	CMD-C2D	-2.01	1.46	1.50
30	6	308	CHL	CHB-C4A	-2.01	1.32	1.37
31	9	310	CLA	CMC-C2C	-2.01	1.46	1.50
31	e	603	CLA	CMD-C2D	-2.01	1.46	1.50
30	h	609	CHL	C2C-C1C	2.01	1.48	1.44
31	a	611	CLA	CMD-C2D	-2.01	1.46	1.50
31	f	612	CLA	CMB-C2B	-2.01	1.46	1.50
31	K	102	CLA	CMC-C2C	-2.01	1.46	1.50
30	7	313	CHL	C4C-C3C	2.01	1.48	1.45
30	2	305	CHL	C4C-C3C	2.01	1.48	1.45
31	0	312	CLA	CMC-C2C	-2.01	1.46	1.50
31	9	302	CLA	CMC-C2C	-2.01	1.46	1.50
31	f	610	CLA	CMB-C2B	-2.01	1.46	1.50
30	d	606	CHL	C2C-C1C	2.01	1.48	1.44
31	8	303	CLA	CHC-C1C	2.01	1.42	1.38
31	8	314	CLA	CMB-C2B	-2.01	1.46	1.50
30	6	305	CHL	C2C-C1C	2.01	1.48	1.44
31	f	604	CLA	CMD-C2D	-2.01	1.46	1.50
30	2	308	CHL	C2C-C1C	2.01	1.48	1.44
30	i	606	CHL	C2C-C1C	2.01	1.48	1.44
31	L	204	CLA	CMC-C2C	-2.01	1.46	1.50
30	8	315	CHL	C2C-C1C	2.01	1.48	1.44
31	A	836	CLA	CMC-C2C	-2.01	1.46	1.50
31	L	204	CLA	CMD-C2D	-2.01	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	612	CLA	CMD-C2D	-2.01	1.46	1.50
30	f	602	CHL	C1C-NC	-2.01	1.34	1.37
31	B	819	CLA	CHC-C1C	2.01	1.42	1.38
31	G	101	CLA	CMB-C2B	-2.01	1.46	1.50
31	L	202	CLA	CMC-C2C	-2.01	1.46	1.50
30	2	308	CHL	CHB-C4A	-2.01	1.32	1.37
31	3	320	CLA	CMC-C2C	-2.01	1.46	1.50
31	A	833	CLA	CMC-C2C	-2.01	1.46	1.50
30	c	602	CHL	C1C-NC	-2.01	1.34	1.37
30	i	606	CHL	C1C-NC	-2.01	1.34	1.37
31	B	805	CLA	CHC-C1C	2.01	1.42	1.38
31	2	304	CLA	CMC-C2C	-2.01	1.46	1.50
31	O	203	CLA	CMD-C2D	-2.01	1.46	1.50
31	c	613	CLA	CMB-C2B	-2.01	1.46	1.50
31	8	310	CLA	CMC-C2C	-2.01	1.46	1.50
31	a	610	CLA	CMD-C2D	-2.01	1.46	1.50
30	0	302	CHL	C4C-C3C	2.01	1.48	1.45
31	5	314	CLA	CMB-C2B	-2.01	1.46	1.50
31	B	838	CLA	CHC-C1C	2.01	1.42	1.38
30	1	305	CHL	C4C-C3C	2.00	1.48	1.45
31	B	815	CLA	CMB-C2B	-2.00	1.46	1.50
31	g	604	CLA	CMB-C2B	-2.00	1.46	1.50
31	7	303	CLA	CMC-C2C	-2.00	1.46	1.50
34	9	601	LHG	P-O6	2.00	1.67	1.59
30	c	608	CHL	C1B-NB	-2.00	1.35	1.37
31	i	604	CLA	CMB-C2B	-2.00	1.46	1.50
31	i	610	CLA	CMC-C2C	-2.00	1.46	1.50
31	9	312	CLA	CMC-C2C	-2.00	1.46	1.50
30	7	313	CHL	C2C-C1C	2.00	1.48	1.44
30	b	614	CHL	C2C-C1C	2.00	1.48	1.44
34	B	852	LHG	O7-C5	-2.00	1.41	1.46
31	7	304	CLA	CHC-C1C	2.00	1.42	1.38
30	3	305	CHL	C2C-C1C	2.00	1.48	1.44
31	2	303	CLA	CHC-C1C	2.00	1.42	1.38
30	e	608	CHL	CHB-C4A	-2.00	1.32	1.37
31	g	611	CLA	CMD-C2D	-2.00	1.46	1.50
31	4	314	CLA	CMB-C2B	-2.00	1.46	1.50
30	c	606	CHL	C2C-C1C	2.00	1.48	1.44
30	g	609	CHL	C2C-C1C	2.00	1.48	1.44
30	4	305	CHL	C2C-C1C	2.00	1.48	1.44
30	f	601	CHL	CHB-C4A	-2.00	1.32	1.37
31	a	613	CLA	CMC-C2C	-2.00	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	301	CHL	C4C-C3C	2.00	1.48	1.45

All (6775) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	823	CLA	O2A-CGA-O1A	-19.76	73.72	123.59
42	a	523	NEX	O24-C25-C24	19.75	128.22	113.38
42	i	523	NEX	O24-C25-C24	19.71	128.19	113.38
42	c	523	NEX	O24-C25-C24	19.70	128.18	113.38
42	f	523	NEX	O24-C25-C24	19.70	128.18	113.38
42	d	523	NEX	O24-C25-C24	19.70	128.18	113.38
42	g	523	NEX	O24-C25-C24	19.69	128.18	113.38
42	b	523	NEX	O24-C25-C24	19.69	128.17	113.38
42	h	523	NEX	O24-C25-C24	19.67	128.16	113.38
31	B	823	CLA	O2A-CGA-CBA	14.57	157.64	111.91
42	d	523	NEX	C20-C13-C12	13.49	139.34	118.08
42	h	523	NEX	C20-C13-C12	13.49	139.33	118.08
42	f	523	NEX	C20-C13-C12	13.47	139.30	118.08
42	b	523	NEX	C20-C13-C12	13.46	139.29	118.08
42	a	523	NEX	C20-C13-C12	13.46	139.28	118.08
42	c	523	NEX	C20-C13-C12	13.46	139.28	118.08
42	i	523	NEX	C20-C13-C12	13.45	139.28	118.08
42	g	523	NEX	C20-C13-C12	13.44	139.25	118.08
42	c	523	NEX	C12-C13-C14	-12.17	100.26	118.94
42	h	523	NEX	C12-C13-C14	-12.16	100.29	118.94
42	d	523	NEX	C12-C13-C14	-12.15	100.29	118.94
42	g	523	NEX	C12-C13-C14	-12.15	100.29	118.94
42	i	523	NEX	C12-C13-C14	-12.15	100.30	118.94
42	f	523	NEX	C12-C13-C14	-12.14	100.31	118.94
42	b	523	NEX	C12-C13-C14	-12.13	100.32	118.94
42	a	523	NEX	C12-C13-C14	-12.12	100.35	118.94
32	K	107	8CT	C33-C32-C31	-11.83	113.51	124.85
32	G	104	8CT	C33-C32-C31	-11.75	113.59	124.85
31	B	826	CLA	CHA-C4D-ND	11.20	135.04	125.21
32	A	849	8CT	C33-C32-C31	-11.16	114.15	124.85
42	e	523	NEX	O24-C25-C24	11.16	121.77	113.38
32	M	102	8CT	C33-C32-C31	-11.03	114.28	124.85
30	9	305	CHL	C2B-C1B-NB	10.81	117.48	110.23
30	1	305	CHL	C2B-C1B-NB	10.81	117.48	110.23
30	1	302	CHL	C2B-C1B-NB	10.80	117.47	110.23
32	A	847	8CT	C33-C32-C31	-10.80	114.49	124.85
30	8	302	CHL	C2B-C1B-NB	10.79	117.47	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	302	CHL	C2B-C1B-NB	10.78	117.46	110.23
30	e	602	CHL	C2B-C1B-NB	10.77	117.45	110.23
32	7	404	8CT	C33-C32-C31	-10.72	114.58	124.85
32	J	104	8CT	C33-C32-C31	-10.71	114.58	124.85
30	0	302	CHL	C2B-C1B-NB	10.71	117.41	110.23
30	f	602	CHL	C2B-C1B-NB	10.67	117.39	110.23
30	2	302	CHL	C2B-C1B-NB	10.66	117.38	110.23
32	B	844	8CT	C33-C32-C31	-10.66	114.63	124.85
32	J	101	8CT	C33-C32-C31	-10.64	114.65	124.85
32	B	845	8CT	C33-C32-C31	-10.63	114.66	124.85
30	4	313	CHL	C2B-C1B-NB	10.58	117.33	110.23
30	6	306	CHL	C2B-C1B-NB	10.57	117.31	110.23
30	7	302	CHL	C2B-C1B-NB	10.55	117.30	110.23
30	6	302	CHL	C2B-C1B-NB	10.54	117.30	110.23
30	8	306	CHL	C2B-C1B-NB	10.53	117.29	110.23
30	3	302	CHL	C2B-C1B-NB	10.51	117.28	110.23
30	3	305	CHL	C2B-C1B-NB	10.51	117.28	110.23
30	2	305	CHL	C2B-C1B-NB	10.46	117.25	110.23
30	6	307	CHL	C2B-C1B-NB	10.46	117.24	110.23
30	f	608	CHL	C2B-C1B-NB	10.44	117.23	110.23
30	7	305	CHL	C2B-C1B-NB	10.43	117.23	110.23
30	4	306	CHL	C2B-C1B-NB	10.41	117.21	110.23
30	4	319	CHL	C2B-C1B-NB	10.39	117.20	110.23
30	0	301	CHL	C2B-C1B-NB	10.35	117.17	110.23
30	c	608	CHL	C2B-C1B-NB	10.34	117.16	110.23
32	3	402	8CT	C33-C32-C31	-10.34	114.94	124.85
30	c	601	CHL	C2B-C1B-NB	10.33	117.16	110.23
30	2	313	CHL	C2B-C1B-NB	10.33	117.15	110.23
30	5	302	CHL	C2B-C1B-NB	10.33	117.15	110.23
32	A	846	8CT	C33-C32-C31	-10.32	114.96	124.85
30	c	602	CHL	C2B-C1B-NB	10.31	117.14	110.23
30	2	319	CHL	C2B-C1B-NB	10.31	117.14	110.23
30	2	301	CHL	C2B-C1B-NB	10.31	117.14	110.23
30	2	307	CHL	C2B-C1B-NB	10.30	117.14	110.23
30	8	307	CHL	C2B-C1B-NB	10.29	117.13	110.23
30	4	307	CHL	C2B-C1B-NB	10.29	117.13	110.23
30	7	307	CHL	C2B-C1B-NB	10.28	117.12	110.23
30	6	305	CHL	C2B-C1B-NB	10.28	117.12	110.23
30	e	601	CHL	C2B-C1B-NB	10.27	117.12	110.23
30	9	301	CHL	C2B-C1B-NB	10.27	117.12	110.23
30	4	305	CHL	C2B-C1B-NB	10.27	117.12	110.23
30	b	606	CHL	C2B-C1B-NB	10.26	117.11	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	313	CHL	C2B-C1B-NB	10.23	117.09	110.23
30	d	602	CHL	C2B-C1B-NB	10.22	117.09	110.23
30	7	301	CHL	C2B-C1B-NB	10.21	117.08	110.23
30	2	306	CHL	C2B-C1B-NB	10.19	117.06	110.23
31	B	823	CLA	O1A-CGA-CBA	-10.19	83.98	123.73
32	2	402	8CT	C33-C32-C31	-10.17	115.09	124.85
30	b	608	CHL	C2B-C1B-NB	10.16	117.04	110.23
30	e	608	CHL	C2B-C1B-NB	10.15	117.03	110.23
30	1	313	CHL	C2B-C1B-NB	10.13	117.02	110.23
32	6	402	8CT	C14-C13-C12	-10.12	112.87	127.31
30	2	308	CHL	C2B-C1B-NB	10.06	116.97	110.23
30	9	306	CHL	C2B-C1B-NB	10.05	116.97	110.23
32	B	847	8CT	C33-C32-C31	-10.05	115.22	124.85
32	J	104	8CT	C18-C17-C16	-10.04	112.97	127.31
30	5	305	CHL	C2B-C1B-NB	10.03	116.95	110.23
30	8	301	CHL	C4D-CHA-C1A	-10.01	109.07	121.25
30	b	602	CHL	C2B-C1B-NB	10.00	116.94	110.23
30	a	608	CHL	C4D-CHA-C1A	-10.00	109.08	121.25
30	h	608	CHL	C2B-C1B-NB	9.97	116.91	110.23
32	0	401	8CT	C33-C32-C31	-9.96	115.30	124.85
30	6	313	CHL	C2B-C1B-NB	9.96	116.91	110.23
30	f	601	CHL	C2B-C1B-NB	9.96	116.91	110.23
30	0	306	CHL	C4D-CHA-C1A	-9.93	109.16	121.25
30	g	608	CHL	C4D-CHA-C1A	-9.92	109.17	121.25
30	6	301	CHL	C2B-C1B-NB	9.92	116.88	110.23
30	6	307	CHL	C4D-CHA-C1A	-9.92	109.18	121.25
30	a	614	CHL	C4D-CHA-C1A	-9.91	109.18	121.25
30	h	614	CHL	C4D-CHA-C1A	-9.91	109.19	121.25
30	f	605	CHL	C4D-CHA-C1A	-9.90	109.20	121.25
30	i	608	CHL	C2B-C1B-NB	9.90	116.87	110.23
30	7	313	CHL	C2B-C1B-NB	9.89	116.86	110.23
30	d	608	CHL	C2B-C1B-NB	9.86	116.84	110.23
30	8	315	CHL	C4D-CHA-C1A	-9.85	109.26	121.25
30	e	601	CHL	C4D-CHA-C1A	-9.85	109.27	121.25
32	L	205	8CT	C33-C32-C31	-9.84	115.41	124.85
30	1	307	CHL	C4D-CHA-C1A	-9.84	109.27	121.25
30	d	614	CHL	C4D-CHA-C1A	-9.84	109.27	121.25
32	A	850	8CT	C33-C32-C31	-9.84	115.42	124.85
30	d	605	CHL	C4D-CHA-C1A	-9.84	109.28	121.25
30	2	305	CHL	C4D-CHA-C1A	-9.83	109.28	121.25
32	8	402	8CT	C33-C32-C31	-9.83	115.43	124.85
30	2	313	CHL	C4D-CHA-C1A	-9.83	109.29	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	609	CHL	C4D-CHA-C1A	-9.81	109.31	121.25
30	1	306	CHL	C2B-C1B-NB	9.81	116.81	110.23
30	i	605	CHL	C4D-CHA-C1A	-9.81	109.31	121.25
30	a	608	CHL	C2B-C1B-NB	9.81	116.81	110.23
30	e	605	CHL	C4D-CHA-C1A	-9.81	109.31	121.25
30	1	307	CHL	C2B-C1B-NB	9.80	116.80	110.23
32	4	402	8CT	C33-C32-C31	-9.80	115.46	124.85
30	f	606	CHL	C4D-CHA-C1A	-9.77	109.36	121.25
30	6	313	CHL	C4D-CHA-C1A	-9.77	109.36	121.25
30	d	608	CHL	C4D-CHA-C1A	-9.76	109.37	121.25
30	e	606	CHL	C2B-C1B-NB	9.76	116.78	110.23
32	A	854	8CT	C33-C32-C31	-9.76	115.49	124.85
30	9	313	CHL	C2B-C1B-NB	9.76	116.77	110.23
32	I	101	8CT	C33-C32-C31	-9.76	115.50	124.85
30	g	601	CHL	C4D-CHA-C1A	-9.75	109.38	121.25
30	f	614	CHL	C4D-CHA-C1A	-9.75	109.38	121.25
30	2	307	CHL	C4D-CHA-C1A	-9.75	109.38	121.25
30	b	601	CHL	C4D-CHA-C1A	-9.75	109.38	121.25
30	e	614	CHL	C4D-CHA-C1A	-9.75	109.38	121.25
30	0	305	CHL	C2B-C1B-NB	9.74	116.76	110.23
30	8	301	CHL	C2B-C1B-NB	9.74	116.76	110.23
30	g	605	CHL	C4D-CHA-C1A	-9.74	109.40	121.25
30	i	614	CHL	C4D-CHA-C1A	-9.74	109.40	121.25
30	b	608	CHL	C4D-CHA-C1A	-9.73	109.40	121.25
30	c	606	CHL	C2B-C1B-NB	9.73	116.76	110.23
30	i	607	CHL	C4D-CHA-C1A	-9.73	109.41	121.25
30	e	608	CHL	C4D-CHA-C1A	-9.73	109.41	121.25
30	g	614	CHL	C4D-CHA-C1A	-9.73	109.41	121.25
30	8	305	CHL	C2B-C1B-NB	9.73	116.75	110.23
30	1	305	CHL	C4D-CHA-C1A	-9.72	109.42	121.25
30	c	605	CHL	C4D-CHA-C1A	-9.72	109.42	121.25
30	d	607	CHL	C4D-CHA-C1A	-9.71	109.43	121.25
30	9	313	CHL	C4D-CHA-C1A	-9.70	109.44	121.25
30	g	607	CHL	C4D-CHA-C1A	-9.70	109.44	121.25
30	e	606	CHL	C4D-CHA-C1A	-9.70	109.44	121.25
30	c	614	CHL	C2B-C1B-NB	9.70	116.73	110.23
30	8	313	CHL	C4D-CHA-C1A	-9.70	109.44	121.25
30	f	608	CHL	C4D-CHA-C1A	-9.69	109.45	121.25
30	7	307	CHL	C4D-CHA-C1A	-9.69	109.46	121.25
30	3	307	CHL	C2B-C1B-NB	9.67	116.72	110.23
30	g	602	CHL	C4D-CHA-C1A	-9.67	109.48	121.25
30	d	601	CHL	C4D-CHA-C1A	-9.67	109.48	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	305	CHL	C4D-CHA-C1A	-9.66	109.49	121.25
30	3	307	CHL	C4D-CHA-C1A	-9.66	109.49	121.25
30	6	315	CHL	C2B-C1B-NB	9.66	116.71	110.23
30	i	601	CHL	C4D-CHA-C1A	-9.66	109.50	121.25
30	a	601	CHL	C4D-CHA-C1A	-9.65	109.50	121.25
30	a	606	CHL	C4D-CHA-C1A	-9.65	109.50	121.25
30	a	607	CHL	C4D-CHA-C1A	-9.65	109.51	121.25
30	i	606	CHL	C4D-CHA-C1A	-9.64	109.51	121.25
30	i	602	CHL	C2B-C1B-NB	9.64	116.70	110.23
30	a	605	CHL	C4D-CHA-C1A	-9.64	109.52	121.25
30	i	609	CHL	C4D-CHA-C1A	-9.64	109.52	121.25
30	i	608	CHL	C4D-CHA-C1A	-9.63	109.53	121.25
30	h	608	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
30	6	308	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
30	7	313	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
30	8	305	CHL	C4D-CHA-C1A	-9.62	109.54	121.25
30	2	319	CHL	C4D-CHA-C1A	-9.62	109.55	121.25
30	g	606	CHL	C4D-CHA-C1A	-9.61	109.55	121.25
30	i	602	CHL	C4D-CHA-C1A	-9.61	109.55	121.25
30	3	305	CHL	C4D-CHA-C1A	-9.61	109.56	121.25
32	7	404	8CT	C14-C13-C12	-9.61	113.60	127.31
30	c	606	CHL	C4D-CHA-C1A	-9.61	109.56	121.25
30	c	608	CHL	C4D-CHA-C1A	-9.60	109.56	121.25
30	7	302	CHL	C4D-CHA-C1A	-9.60	109.56	121.25
30	h	605	CHL	C4D-CHA-C1A	-9.60	109.56	121.25
30	f	606	CHL	C2B-C1B-NB	9.60	116.67	110.23
30	f	614	CHL	C2B-C1B-NB	9.60	116.67	110.23
30	9	305	CHL	C4D-CHA-C1A	-9.59	109.58	121.25
30	b	606	CHL	C4D-CHA-C1A	-9.59	109.58	121.25
30	f	609	CHL	C4D-CHA-C1A	-9.58	109.59	121.25
30	4	319	CHL	C4D-CHA-C1A	-9.58	109.59	121.25
30	8	308	CHL	C2B-C1B-NB	9.58	116.65	110.23
30	h	607	CHL	C4D-CHA-C1A	-9.58	109.60	121.25
30	a	602	CHL	C2B-C1B-NB	9.58	116.65	110.23
30	h	601	CHL	C4D-CHA-C1A	-9.57	109.60	121.25
30	b	607	CHL	C2B-C1B-NB	9.57	116.65	110.23
30	d	606	CHL	C4D-CHA-C1A	-9.56	109.61	121.25
30	6	308	CHL	C2B-C1B-NB	9.56	116.64	110.23
30	h	609	CHL	C4D-CHA-C1A	-9.56	109.62	121.25
30	8	308	CHL	C4D-CHA-C1A	-9.55	109.62	121.25
30	5	306	CHL	C4D-CHA-C1A	-9.55	109.63	121.25
30	b	614	CHL	C4D-CHA-C1A	-9.55	109.63	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	606	CHL	C4D-CHA-C1A	-9.55	109.63	121.25
30	b	609	CHL	C4D-CHA-C1A	-9.54	109.64	121.25
30	b	601	CHL	C2B-C1B-NB	9.54	116.63	110.23
30	1	313	CHL	C4D-CHA-C1A	-9.54	109.64	121.25
30	c	607	CHL	C4D-CHA-C1A	-9.52	109.66	121.25
30	5	305	CHL	C4D-CHA-C1A	-9.52	109.67	121.25
30	5	301	CHL	C4D-CHA-C1A	-9.51	109.67	121.25
30	c	614	CHL	C4D-CHA-C1A	-9.51	109.67	121.25
30	f	607	CHL	C4D-CHA-C1A	-9.50	109.69	121.25
32	3	402	8CT	C14-C13-C12	-9.50	113.76	127.31
30	c	602	CHL	C4D-CHA-C1A	-9.49	109.69	121.25
30	h	602	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
30	c	609	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
30	6	315	CHL	C4D-CHA-C1A	-9.47	109.72	121.25
30	e	607	CHL	C2B-C1B-NB	9.47	116.58	110.23
30	g	609	CHL	C4D-CHA-C1A	-9.46	109.73	121.25
30	6	305	CHL	C4D-CHA-C1A	-9.46	109.74	121.25
30	e	609	CHL	C2B-C1B-NB	9.46	116.57	110.23
30	4	307	CHL	C4D-CHA-C1A	-9.46	109.74	121.25
30	e	607	CHL	C4D-CHA-C1A	-9.45	109.75	121.25
30	d	609	CHL	C4D-CHA-C1A	-9.45	109.75	121.25
30	4	308	CHL	C2B-C1B-NB	9.44	116.56	110.23
30	4	305	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
30	b	607	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
30	f	602	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
30	8	306	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
30	5	301	CHL	C2B-C1B-NB	9.43	116.55	110.23
30	0	306	CHL	C2B-C1B-NB	9.41	116.54	110.23
30	5	307	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
30	3	302	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
30	6	306	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
30	e	609	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
30	e	602	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
30	h	606	CHL	C2B-C1B-NB	9.40	116.54	110.23
30	f	601	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
30	1	306	CHL	C4D-CHA-C1A	-9.39	109.83	121.25
30	7	306	CHL	C2B-C1B-NB	9.39	116.52	110.23
30	g	606	CHL	C2B-C1B-NB	9.38	116.52	110.23
30	6	301	CHL	C4D-CHA-C1A	-9.37	109.84	121.25
30	a	602	CHL	C4D-CHA-C1A	-9.35	109.86	121.25
30	h	601	CHL	C2B-C1B-NB	9.35	116.50	110.23
30	8	307	CHL	C4D-CHA-C1A	-9.35	109.87	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	305	CHL	C4D-CHA-C1A	-9.35	109.87	121.25
30	0	301	CHL	C4D-CHA-C1A	-9.34	109.88	121.25
30	2	306	CHL	C4D-CHA-C1A	-9.34	109.88	121.25
30	a	606	CHL	C2B-C1B-NB	9.33	116.49	110.23
30	b	602	CHL	C4D-CHA-C1A	-9.33	109.89	121.25
30	4	306	CHL	C4D-CHA-C1A	-9.33	109.90	121.25
30	g	608	CHL	C2B-C1B-NB	9.31	116.48	110.23
30	7	301	CHL	C4D-CHA-C1A	-9.29	109.94	121.25
32	7	404	8CT	C10-C11-C12	-9.27	112.22	126.23
30	4	308	CHL	C4D-CHA-C1A	-9.27	109.97	121.25
30	7	306	CHL	C4D-CHA-C1A	-9.26	109.97	121.25
30	5	313	CHL	C2B-C1B-NB	9.25	116.43	110.23
30	2	302	CHL	C4D-CHA-C1A	-9.25	109.99	121.25
30	1	302	CHL	C4D-CHA-C1A	-9.24	110.00	121.25
42	c	523	NEX	C30-C31-C32	-9.24	94.38	123.22
42	i	523	NEX	C30-C31-C32	-9.24	94.39	123.22
30	c	601	CHL	C4D-CHA-C1A	-9.24	110.01	121.25
42	d	523	NEX	C30-C31-C32	-9.24	94.40	123.22
42	f	523	NEX	C30-C31-C32	-9.23	94.40	123.22
42	g	523	NEX	C30-C31-C32	-9.23	94.42	123.22
42	h	523	NEX	C30-C31-C32	-9.22	94.43	123.22
30	9	301	CHL	C4D-CHA-C1A	-9.22	110.03	121.25
30	d	609	CHL	C2B-C1B-NB	9.22	116.41	110.23
42	b	523	NEX	C30-C31-C32	-9.21	94.46	123.22
42	a	523	NEX	C30-C31-C32	-9.21	94.46	123.22
30	5	307	CHL	C2B-C1B-NB	9.21	116.41	110.23
30	4	302	CHL	C4D-CHA-C1A	-9.20	110.05	121.25
32	F	302	8CT	C33-C32-C31	-9.20	116.03	124.85
30	8	302	CHL	C4D-CHA-C1A	-9.20	110.06	121.25
30	2	301	CHL	C4D-CHA-C1A	-9.19	110.07	121.25
30	a	607	CHL	C2B-C1B-NB	9.18	116.39	110.23
30	d	602	CHL	C4D-CHA-C1A	-9.18	110.08	121.25
30	b	609	CHL	C2B-C1B-NB	9.17	116.38	110.23
30	c	609	CHL	C2B-C1B-NB	9.17	116.38	110.23
30	c	607	CHL	C2B-C1B-NB	9.17	116.38	110.23
30	0	302	CHL	C4D-CHA-C1A	-9.17	110.09	121.25
30	e	605	CHL	C2B-C1B-NB	9.16	116.37	110.23
30	5	306	CHL	C2B-C1B-NB	9.15	116.37	110.23
30	2	308	CHL	C4D-CHA-C1A	-9.13	110.13	121.25
30	g	607	CHL	C2B-C1B-NB	9.13	116.35	110.23
32	7	405	8CT	C33-C32-C31	-9.13	116.10	124.85
30	d	606	CHL	C2B-C1B-NB	9.12	116.35	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	614	CHL	C2B-C1B-NB	9.11	116.34	110.23
30	i	601	CHL	C2B-C1B-NB	9.09	116.33	110.23
30	4	313	CHL	C4D-CHA-C1A	-9.09	110.18	121.25
30	i	607	CHL	C2B-C1B-NB	9.07	116.31	110.23
30	g	602	CHL	C2B-C1B-NB	9.06	116.31	110.23
30	5	302	CHL	C4D-CHA-C1A	-9.06	110.22	121.25
30	6	302	CHL	C4D-CHA-C1A	-9.06	110.23	121.25
30	f	605	CHL	C2B-C1B-NB	9.05	116.30	110.23
30	b	614	CHL	C2B-C1B-NB	9.05	116.30	110.23
30	9	306	CHL	C4D-CHA-C1A	-9.04	110.25	121.25
30	e	614	CHL	C2B-C1B-NB	9.03	116.28	110.23
30	8	315	CHL	C2B-C1B-NB	8.98	116.25	110.23
30	f	609	CHL	C2B-C1B-NB	8.98	116.25	110.23
32	J	104	8CT	C10-C11-C12	-8.97	112.68	126.23
30	a	614	CHL	C2B-C1B-NB	8.97	116.25	110.23
30	g	609	CHL	C2B-C1B-NB	8.97	116.25	110.23
32	B	848	8CT	C33-C32-C31	-8.97	116.25	124.85
30	5	313	CHL	C4D-CHA-C1A	-8.96	110.35	121.25
30	g	605	CHL	C2B-C1B-NB	8.95	116.23	110.23
30	i	606	CHL	C2B-C1B-NB	8.94	116.22	110.23
30	h	609	CHL	C2B-C1B-NB	8.94	116.22	110.23
30	h	602	CHL	C2B-C1B-NB	8.91	116.21	110.23
30	a	609	CHL	C2B-C1B-NB	8.90	116.20	110.23
30	c	605	CHL	C2B-C1B-NB	8.90	116.20	110.23
30	a	601	CHL	C2B-C1B-NB	8.89	116.19	110.23
30	d	614	CHL	C2B-C1B-NB	8.88	116.19	110.23
30	d	605	CHL	C2B-C1B-NB	8.87	116.18	110.23
30	f	607	CHL	C2B-C1B-NB	8.85	116.17	110.23
30	a	605	CHL	C2B-C1B-NB	8.83	116.15	110.23
30	g	601	CHL	C2B-C1B-NB	8.81	116.14	110.23
30	i	605	CHL	C2B-C1B-NB	8.79	116.12	110.23
32	L	209	8CT	C33-C32-C31	-8.79	116.43	124.85
30	g	614	CHL	C2B-C1B-NB	8.78	116.12	110.23
30	d	601	CHL	C2B-C1B-NB	8.75	116.10	110.23
30	h	614	CHL	C2B-C1B-NB	8.73	116.08	110.23
30	i	609	CHL	C2B-C1B-NB	8.72	116.08	110.23
30	d	607	CHL	C2B-C1B-NB	8.71	116.07	110.23
32	6	402	8CT	C18-C17-C16	-8.70	114.89	127.31
30	h	607	CHL	C2B-C1B-NB	8.68	116.05	110.23
42	e	523	NEX	C38-C25-C26	-8.64	107.77	122.26
32	9	401	8CT	C33-C32-C31	-8.62	116.59	124.85
32	L	206	8CT	C33-C32-C31	-8.61	116.59	124.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	6	402	8CT	C10-C11-C12	-8.59	113.25	126.23
32	A	848	8CT	C33-C32-C31	-8.52	116.68	124.85
32	6	402	8CT	C33-C32-C31	-8.50	116.70	124.85
32	B	846	8CT	C33-C32-C31	-8.47	116.73	124.85
30	h	605	CHL	C2B-C1B-NB	8.44	115.89	110.23
32	7	402	8CT	C33-C32-C31	-8.33	116.86	124.85
32	B	846	8CT	C24-C25-C26	-8.32	115.44	127.31
32	O	205	8CT	C33-C32-C31	-8.15	117.03	124.85
32	B	851	8CT	C33-C32-C31	-8.10	117.09	124.85
32	B	846	8CT	C10-C11-C12	-8.09	114.01	126.23
32	K	107	8CT	C14-C13-C12	-7.94	115.98	127.31
32	A	850	8CT	C19-C18-C17	-7.91	107.27	123.47
32	B	845	8CT	C19-C18-C17	-7.86	107.38	123.47
32	G	104	8CT	C18-C17-C16	-7.82	116.15	127.31
32	L	206	8CT	C14-C13-C12	-7.79	116.19	127.31
32	1	402	8CT	C33-C32-C31	-7.69	117.47	124.85
32	K	107	8CT	C18-C17-C16	-7.63	116.42	127.31
32	A	854	8CT	C24-C25-C26	-7.52	116.58	127.31
32	8	406	8CT	C33-C32-C31	-7.52	117.64	124.85
32	B	846	8CT	C04-C03-C02	-7.49	112.06	122.61
32	B	843	8CT	C18-C17-C16	-7.46	116.66	127.31
30	f	606	CHL	CMD-C2D-C1D	7.45	137.84	124.71
32	4	402	8CT	C30-C31-C32	-7.44	112.31	121.47
32	3	403	8CT	C33-C32-C31	-7.39	117.76	124.85
32	6	402	8CT	C24-C25-C26	-7.39	116.76	127.31
32	A	849	8CT	C10-C11-C12	-7.37	115.10	126.23
32	B	804	8CT	C33-C32-C31	-7.36	117.80	124.85
30	2	302	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
32	B	847	8CT	C30-C31-C32	-7.31	112.47	121.47
32	7	404	8CT	C18-C17-C16	-7.30	116.89	127.31
32	3	402	8CT	C30-C31-C32	-7.27	112.52	121.47
30	c	601	CHL	C2C-C3C-C4C	-7.17	101.38	106.49
30	1	307	CHL	CMD-C2D-C1D	7.16	137.33	124.71
30	2	305	CHL	CMD-C2D-C1D	7.16	137.33	124.71
30	1	302	CHL	C2C-C3C-C4C	-7.14	101.40	106.49
42	c	523	NEX	C27-C28-C29	7.12	136.58	125.53
32	J	101	8CT	C30-C31-C32	-7.12	112.71	121.47
30	0	306	CHL	C2C-C3C-C4C	-7.12	101.42	106.49
32	B	847	8CT	C14-C13-C12	-7.11	117.16	127.31
42	b	523	NEX	C27-C28-C29	7.11	136.56	125.53
42	g	523	NEX	C27-C28-C29	7.10	136.55	125.53
31	3	304	CLA	C4A-NA-C1A	7.10	109.90	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	h	523	NEX	C27-C28-C29	7.09	136.53	125.53
30	3	307	CHL	CMD-C2D-C1D	7.09	137.21	124.71
42	d	523	NEX	C27-C28-C29	7.08	136.52	125.53
30	6	313	CHL	CMD-C2D-C1D	7.08	137.20	124.71
30	e	601	CHL	CMD-C2D-C1D	7.08	137.19	124.71
42	i	523	NEX	C27-C28-C29	7.08	136.51	125.53
30	4	302	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
31	g	613	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	7	306	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
42	f	523	NEX	C27-C28-C29	7.07	136.51	125.53
42	a	523	NEX	C27-C28-C29	7.07	136.50	125.53
30	4	313	CHL	C2C-C3C-C4C	-7.06	101.45	106.49
30	5	307	CHL	CMD-C2D-C1D	7.06	137.15	124.71
30	1	305	CHL	CMD-C2D-C1D	7.06	137.15	124.71
30	8	305	CHL	CMD-C2D-C1D	7.05	137.14	124.71
31	H	204	CLA	C4A-NA-C1A	7.04	109.87	106.71
30	5	302	CHL	C2C-C3C-C4C	-7.03	101.48	106.49
30	f	608	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
31	f	612	CLA	C4A-NA-C1A	7.02	109.86	106.71
30	0	301	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
30	3	302	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
31	7	317	CLA	C4A-NA-C1A	7.00	109.85	106.71
30	2	313	CHL	C2C-C3C-C4C	-6.99	101.51	106.49
31	A	817	CLA	C4A-NA-C1A	6.99	109.85	106.71
31	A	816	CLA	C4A-NA-C1A	6.98	109.85	106.71
31	B	835	CLA	C4A-NA-C1A	6.98	109.84	106.71
31	B	821	CLA	C4A-NA-C1A	6.98	109.84	106.71
30	c	609	CHL	CMD-C2D-C1D	6.95	136.97	124.71
30	8	302	CHL	C2C-C3C-C4C	-6.95	101.54	106.49
30	2	306	CHL	C2C-C3C-C4C	-6.94	101.54	106.49
42	i	523	NEX	C35-C34-C33	-6.94	117.41	127.31
42	g	523	NEX	C35-C34-C33	-6.93	117.42	127.31
42	b	523	NEX	C35-C34-C33	-6.93	117.43	127.31
42	f	523	NEX	C35-C34-C33	-6.92	117.43	127.31
42	a	523	NEX	C35-C34-C33	-6.92	117.43	127.31
31	5	312	CLA	C4A-NA-C1A	6.92	109.82	106.71
30	9	313	CHL	CMD-C2D-C1D	6.92	136.91	124.71
42	d	523	NEX	C35-C34-C33	-6.92	117.44	127.31
30	i	606	CHL	CMD-C2D-C1D	6.91	136.90	124.71
30	6	302	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
31	9	308	CLA	C4A-NA-C1A	6.91	109.81	106.71
31	5	303	CLA	C4A-NA-C1A	6.91	109.81	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	c	523	NEX	C35-C34-C33	-6.91	117.45	127.31
42	h	523	NEX	C35-C34-C33	-6.90	117.46	127.31
30	b	606	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
31	0	311	CLA	C4A-NA-C1A	6.90	109.81	106.71
31	a	612	CLA	C4A-NA-C1A	6.90	109.81	106.71
31	A	837	CLA	C4A-NA-C1A	6.90	109.81	106.71
31	B	832	CLA	C4A-NA-C1A	6.89	109.80	106.71
30	f	602	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
30	e	608	CHL	CMD-C2D-C1D	6.89	136.85	124.71
31	e	612	CLA	C4A-NA-C1A	6.89	109.80	106.71
30	0	302	CHL	C2C-C3C-C4C	-6.88	101.58	106.49
31	3	311	CLA	C4A-NA-C1A	6.87	109.80	106.71
30	h	614	CHL	CMD-C2D-C1D	6.87	136.82	124.71
31	2	311	CLA	C4A-NA-C1A	6.87	109.80	106.71
30	e	609	CHL	CMD-C2D-C1D	6.87	136.82	124.71
30	6	307	CHL	C2C-C3C-C4C	-6.87	101.59	106.49
31	1	311	CLA	C4A-NA-C1A	6.86	109.79	106.71
32	B	843	8CT	C33-C32-C31	-6.86	118.28	124.85
30	4	306	CHL	C2C-C3C-C4C	-6.85	101.60	106.49
31	B	808	CLA	C4A-NA-C1A	6.85	109.79	106.71
31	B	837	CLA	C4A-NA-C1A	6.85	109.78	106.71
32	O	205	8CT	C14-C13-C12	-6.85	117.54	127.31
30	h	609	CHL	CMD-C2D-C1D	6.84	136.77	124.71
30	d	602	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
30	b	602	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
30	f	608	CHL	CMD-C2D-C1D	6.83	136.76	124.71
32	L	205	8CT	C30-C31-C32	-6.83	113.06	121.47
30	4	319	CHL	C2C-C3C-C4C	-6.83	101.62	106.49
30	h	608	CHL	CMD-C2D-C1D	6.83	136.75	124.71
31	1	303	CLA	C4A-NA-C1A	6.83	109.78	106.71
42	d	523	NEX	C35-C15-C14	6.83	137.46	123.47
31	9	303	CLA	C4A-NA-C1A	6.82	109.77	106.71
31	A	809	CLA	C4A-NA-C1A	6.82	109.77	106.71
31	c	612	CLA	C4A-NA-C1A	6.82	109.77	106.71
42	i	523	NEX	C35-C15-C14	6.82	137.45	123.47
42	a	523	NEX	C35-C15-C14	6.82	137.44	123.47
31	1	310	CLA	C4A-NA-C1A	6.81	109.77	106.71
31	L	203	CLA	C4A-NA-C1A	6.81	109.77	106.71
30	1	307	CHL	C2C-C3C-C4C	-6.81	101.63	106.49
42	g	523	NEX	C35-C15-C14	6.81	137.42	123.47
30	8	307	CHL	C2C-C3C-C4C	-6.81	101.64	106.49
42	b	523	NEX	C35-C15-C14	6.80	137.41	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	843	8CT	C19-C20-C21	-6.80	117.60	127.31
30	8	313	CHL	CMD-C2D-C1D	6.80	136.69	124.71
32	A	854	8CT	C14-C13-C12	-6.80	117.61	127.31
42	f	523	NEX	C35-C15-C14	6.80	137.40	123.47
31	M	101	CLA	C4A-NA-C1A	6.80	109.76	106.71
42	c	523	NEX	C35-C15-C14	6.79	137.38	123.47
30	4	307	CHL	C2C-C3C-C4C	-6.79	101.65	106.49
31	6	303	CLA	C4A-NA-C1A	6.79	109.76	106.71
31	A	820	CLA	C4A-NA-C1A	6.79	109.76	106.71
31	i	611	CLA	C4A-NA-C1A	6.79	109.76	106.71
30	d	614	CHL	CMD-C2D-C1D	6.78	136.67	124.71
30	6	307	CHL	CMD-C2D-C1D	6.78	136.67	124.71
31	7	311	CLA	C4A-NA-C1A	6.78	109.75	106.71
30	7	302	CHL	C2C-C3C-C4C	-6.78	101.66	106.49
31	B	840	CLA	C4A-NA-C1A	6.78	109.75	106.71
31	A	804	CLA	C4A-NA-C1A	6.78	109.75	106.71
31	B	827	CLA	C4A-NA-C1A	6.78	109.75	106.71
30	9	306	CHL	C2C-C3C-C4C	-6.78	101.66	106.49
31	A	808	CLA	C4A-NA-C1A	6.78	109.75	106.71
30	c	608	CHL	CMD-C2D-C1D	6.77	136.65	124.71
32	A	846	8CT	C14-C13-C12	-6.77	117.64	127.31
32	2	402	8CT	C30-C31-C32	-6.77	113.13	121.47
30	i	602	CHL	CMD-C2D-C1D	6.77	136.65	124.71
31	A	830	CLA	C4A-NA-C1A	6.77	109.75	106.71
42	h	523	NEX	C35-C15-C14	6.77	137.35	123.47
30	a	601	CHL	CMD-C2D-C1D	6.77	136.65	124.71
30	f	609	CHL	CMD-C2D-C1D	6.77	136.65	124.71
30	d	608	CHL	CMD-C2D-C1D	6.77	136.64	124.71
32	L	209	8CT	C10-C11-C12	-6.77	116.01	126.23
31	3	320	CLA	C4A-NA-C1A	6.77	109.75	106.71
30	9	305	CHL	C2C-C3C-C4C	-6.77	101.67	106.49
33	2	502	0UR	C14-C15-C16	-6.76	117.66	127.31
30	0	306	CHL	O2D-CGD-CBD	6.76	123.28	111.27
31	b	611	CLA	C4A-NA-C1A	6.76	109.75	106.71
31	B	807	CLA	C4A-NA-C1A	6.76	109.74	106.71
31	A	834	CLA	C4A-NA-C1A	6.76	109.74	106.71
30	2	301	CHL	C2C-C3C-C4C	-6.75	101.67	106.49
30	b	607	CHL	C2C-C3C-C4C	-6.75	101.68	106.49
31	h	603	CLA	C4A-NA-C1A	6.75	109.74	106.71
31	b	612	CLA	C4A-NA-C1A	6.74	109.74	106.71
30	1	313	CHL	C2C-C3C-C4C	-6.74	101.68	106.49
30	2	319	CHL	CMD-C2D-C1D	6.74	136.59	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	609	CHL	CMD-C2D-C1D	6.74	136.59	124.71
31	A	843	CLA	C4A-NA-C1A	6.74	109.74	106.71
30	c	602	CHL	C2C-C3C-C4C	-6.74	101.69	106.49
31	7	309	CLA	C4A-NA-C1A	6.74	109.73	106.71
31	B	838	CLA	C4A-NA-C1A	6.74	109.73	106.71
31	3	308	CLA	C4A-NA-C1A	6.74	109.73	106.71
30	2	305	CHL	C2C-C3C-C4C	-6.73	101.69	106.49
30	a	609	CHL	CMD-C2D-C1D	6.73	136.58	124.71
31	B	818	CLA	C4A-NA-C1A	6.73	109.73	106.71
30	5	305	CHL	CMD-C2D-C1D	6.73	136.57	124.71
30	g	608	CHL	CMD-C2D-C1D	6.73	136.57	124.71
30	0	305	CHL	CMD-C2D-C1D	6.72	136.56	124.71
31	B	811	CLA	C4A-NA-C1A	6.72	109.73	106.71
31	c	604	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	f	601	CHL	CMD-C2D-C1D	6.72	136.56	124.71
30	7	305	CHL	C2C-C3C-C4C	-6.71	101.70	106.49
30	2	307	CHL	CMD-C2D-C1D	6.71	136.54	124.71
31	B	817	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	3	305	CHL	C2C-C3C-C4C	-6.71	101.71	106.49
30	8	306	CHL	C2C-C3C-C4C	-6.71	101.71	106.49
30	b	614	CHL	CMD-C2D-C1D	6.70	136.53	124.71
31	B	816	CLA	C4A-NA-C1A	6.70	109.72	106.71
30	i	602	CHL	C2C-C3C-C4C	-6.70	101.71	106.49
30	c	601	CHL	CMD-C2D-C1D	6.70	136.52	124.71
32	A	847	8CT	C30-C31-C32	-6.70	113.22	121.47
31	K	104	CLA	C4A-NA-C1A	6.70	109.72	106.71
31	B	812	CLA	C4A-NA-C1A	6.70	109.72	106.71
30	4	307	CHL	CMD-C2D-C1D	6.69	136.51	124.71
31	1	312	CLA	C4A-NA-C1A	6.69	109.72	106.71
31	2	303	CLA	C4A-NA-C1A	6.69	109.72	106.71
31	4	310	CLA	C4A-NA-C1A	6.69	109.72	106.71
30	5	301	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
30	g	614	CHL	CMD-C2D-C1D	6.69	136.50	124.71
33	2	501	0UR	C4-C3-C2	-6.69	114.34	120.08
30	c	606	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
30	e	606	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
30	2	306	CHL	CMD-C2D-C1D	6.69	136.50	124.71
30	b	608	CHL	CMD-C2D-C1D	6.69	136.50	124.71
30	d	606	CHL	CMD-C2D-C1D	6.68	136.49	124.71
31	7	304	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	b	609	CHL	CMD-C2D-C1D	6.68	136.49	124.71
30	b	601	CHL	CMD-C2D-C1D	6.68	136.49	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	605	CHL	CMD-C2D-C1D	6.68	136.49	124.71
30	8	301	CHL	CMD-C2D-C1D	6.68	136.49	124.71
32	G	104	8CT	C10-C11-C12	-6.68	116.14	126.23
30	a	608	CHL	CMD-C2D-C1D	6.68	136.48	124.71
30	8	307	CHL	CMD-C2D-C1D	6.68	136.48	124.71
30	4	305	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
30	h	601	CHL	CMD-C2D-C1D	6.68	136.48	124.71
31	a	603	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	0	301	CHL	CMD-C2D-C1D	6.67	136.48	124.71
30	e	606	CHL	CMD-C2D-C1D	6.67	136.47	124.71
31	A	818	CLA	C4A-NA-C1A	6.67	109.71	106.71
31	A	833	CLA	C4A-NA-C1A	6.67	109.70	106.71
30	b	608	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
30	f	605	CHL	CMD-C2D-C1D	6.67	136.46	124.71
30	1	306	CHL	C2C-C3C-C4C	-6.67	101.74	106.49
30	i	609	CHL	CMD-C2D-C1D	6.67	136.46	124.71
30	f	614	CHL	CMD-C2D-C1D	6.66	136.46	124.71
30	a	614	CHL	CMD-C2D-C1D	6.66	136.46	124.71
31	7	315	CLA	C4A-NA-C1A	6.66	109.70	106.71
31	B	810	CLA	C4A-NA-C1A	6.66	109.70	106.71
30	a	605	CHL	CMD-C2D-C1D	6.66	136.45	124.71
31	h	610	CLA	C4A-NA-C1A	6.66	109.70	106.71
30	7	307	CHL	CMD-C2D-C1D	6.66	136.44	124.71
30	9	301	CHL	CMD-C2D-C1D	6.65	136.44	124.71
30	i	608	CHL	CMD-C2D-C1D	6.65	136.44	124.71
31	8	312	CLA	C4A-NA-C1A	6.65	109.70	106.71
30	0	306	CHL	CMD-C2D-C1D	6.65	136.44	124.71
31	e	604	CLA	C4A-NA-C1A	6.65	109.69	106.71
30	8	305	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
30	8	306	CHL	CMD-C2D-C1D	6.65	136.43	124.71
31	B	822	CLA	C4A-NA-C1A	6.65	109.69	106.71
31	c	603	CLA	C4A-NA-C1A	6.65	109.69	106.71
31	d	603	CLA	C4A-NA-C1A	6.65	109.69	106.71
30	h	606	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
32	A	850	8CT	C04-C03-C02	-6.64	113.26	122.61
31	5	311	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	a	606	CHL	CMD-C2D-C1D	6.64	136.41	124.71
30	g	605	CHL	CMD-C2D-C1D	6.64	136.41	124.71
30	e	602	CHL	CMD-C2D-C1D	6.64	136.41	124.71
30	8	315	CHL	CMD-C2D-C1D	6.64	136.41	124.71
31	L	202	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	6	305	CHL	C2C-C3C-C4C	-6.63	101.76	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	313	CHL	CMD-C2D-C1D	6.63	136.40	124.71
30	6	306	CHL	C2C-C3C-C4C	-6.63	101.76	106.49
30	4	305	CHL	CMD-C2D-C1D	6.63	136.40	124.71
30	2	301	CHL	CMD-C2D-C1D	6.63	136.40	124.71
30	7	305	CHL	CMD-C2D-C1D	6.63	136.39	124.71
30	6	315	CHL	CMD-C2D-C1D	6.62	136.39	124.71
30	h	605	CHL	CMD-C2D-C1D	6.62	136.38	124.71
30	2	319	CHL	C2C-C3C-C4C	-6.62	101.77	106.49
31	2	312	CLA	C4A-NA-C1A	6.62	109.68	106.71
31	7	316	CLA	C4A-NA-C1A	6.62	109.68	106.71
31	A	827	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	i	614	CHL	CMD-C2D-C1D	6.62	136.38	124.71
30	e	607	CHL	CMD-C2D-C1D	6.62	136.37	124.71
30	a	607	CHL	CMD-C2D-C1D	6.62	136.37	124.71
30	1	306	CHL	CMD-C2D-C1D	6.61	136.37	124.71
30	5	301	CHL	CMD-C2D-C1D	6.61	136.36	124.71
30	7	301	CHL	C2C-C3C-C4C	-6.61	101.78	106.49
30	e	614	CHL	C2C-C3C-C4C	-6.61	101.78	106.49
30	e	605	CHL	CMD-C2D-C1D	6.61	136.36	124.71
31	0	312	CLA	C4A-NA-C1A	6.61	109.68	106.71
30	d	607	CHL	CMD-C2D-C1D	6.60	136.35	124.71
31	1	308	CLA	C4A-NA-C1A	6.60	109.67	106.71
31	6	320	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	h	602	CHL	C2C-C3C-C4C	-6.60	101.78	106.49
30	g	607	CHL	CMD-C2D-C1D	6.60	136.34	124.71
30	4	319	CHL	CMD-C2D-C1D	6.60	136.34	124.71
32	A	847	8CT	C18-C17-C16	-6.60	117.89	127.31
30	c	605	CHL	CMD-C2D-C1D	6.60	136.34	124.71
31	h	613	CLA	C4A-NA-C1A	6.59	109.67	106.71
31	e	603	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	7	313	CHL	CMD-C2D-C1D	6.59	136.33	124.71
30	d	608	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
30	3	305	CHL	CMD-C2D-C1D	6.59	136.32	124.71
30	b	606	CHL	CMD-C2D-C1D	6.59	136.32	124.71
30	i	601	CHL	CMD-C2D-C1D	6.59	136.32	124.71
31	0	309	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	9	301	CHL	C2C-C3C-C4C	-6.58	101.80	106.49
30	9	313	CHL	C2C-C3C-C4C	-6.58	101.80	106.49
31	A	840	CLA	C4A-NA-C1A	6.58	109.67	106.71
30	2	313	CHL	CMD-C2D-C1D	6.58	136.31	124.71
30	h	607	CHL	CMD-C2D-C1D	6.58	136.31	124.71
31	A	831	CLA	C4A-NA-C1A	6.58	109.67	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	301	CHL	CMD-C2D-C1D	6.58	136.31	124.71
31	G	102	CLA	C4A-NA-C1A	6.58	109.66	106.71
30	7	307	CHL	C2C-C3C-C4C	-6.58	101.80	106.49
31	a	613	CLA	C4A-NA-C1A	6.58	109.66	106.71
31	6	304	CLA	C4A-NA-C1A	6.58	109.66	106.71
31	6	314	CLA	C4A-NA-C1A	6.58	109.66	106.71
31	B	823	CLA	C4A-NA-C1A	6.58	109.66	106.71
31	H	202	CLA	C4A-NA-C1A	6.58	109.66	106.71
31	B	806	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	f	614	CHL	C2C-C3C-C4C	-6.57	101.80	106.49
32	2	402	8CT	C18-C17-C16	-6.57	117.93	127.31
30	i	605	CHL	CMD-C2D-C1D	6.57	136.29	124.71
30	h	606	CHL	CMD-C2D-C1D	6.57	136.29	124.71
31	A	815	CLA	C4A-NA-C1A	6.57	109.66	106.71
31	i	604	CLA	C4A-NA-C1A	6.57	109.66	106.71
31	a	610	CLA	C4A-NA-C1A	6.56	109.66	106.71
30	f	606	CHL	C2C-C3C-C4C	-6.56	101.81	106.49
30	a	606	CHL	C2C-C3C-C4C	-6.56	101.81	106.49
31	d	612	CLA	C4A-NA-C1A	6.56	109.65	106.71
31	H	205	CLA	C4A-NA-C1A	6.56	109.65	106.71
30	7	313	CHL	C2C-C3C-C4C	-6.56	101.81	106.49
30	i	608	CHL	C2C-C3C-C4C	-6.56	101.81	106.49
30	2	308	CHL	C2C-C3C-C4C	-6.56	101.82	106.49
30	g	606	CHL	CMD-C2D-C1D	6.55	136.26	124.71
31	g	612	CLA	C4A-NA-C1A	6.55	109.65	106.71
31	4	311	CLA	C4A-NA-C1A	6.55	109.65	106.71
30	5	302	CHL	CMD-C2D-C1D	6.55	136.26	124.71
30	0	305	CHL	C2C-C3C-C4C	-6.55	101.82	106.49
30	5	307	CHL	C2C-C3C-C4C	-6.55	101.82	106.49
30	4	306	CHL	CMD-C2D-C1D	6.55	136.26	124.71
30	a	602	CHL	CMD-C2D-C1D	6.55	136.25	124.71
31	B	805	CLA	C4A-NA-C1A	6.54	109.65	106.71
32	4	402	8CT	C18-C17-C16	-6.54	117.97	127.31
30	6	305	CHL	CMD-C2D-C1D	6.54	136.24	124.71
31	A	814	CLA	C4A-NA-C1A	6.54	109.65	106.71
31	G	101	CLA	C4A-NA-C1A	6.54	109.65	106.71
30	g	601	CHL	CMD-C2D-C1D	6.54	136.24	124.71
31	f	604	CLA	C4A-NA-C1A	6.54	109.64	106.71
31	e	611	CLA	C4A-NA-C1A	6.53	109.64	106.71
30	8	301	CHL	C2C-C3C-C4C	-6.53	101.83	106.49
31	A	839	CLA	C4A-NA-C1A	6.53	109.64	106.71
31	f	611	CLA	C4A-NA-C1A	6.53	109.64	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	302	CHL	CMD-C2D-C1D	6.53	136.22	124.71
30	6	301	CHL	C2C-C3C-C4C	-6.53	101.83	106.49
31	A	811	CLA	C4A-NA-C1A	6.53	109.64	106.71
30	8	308	CHL	CMD-C2D-C1D	6.53	136.22	124.71
31	0	321	CLA	C4A-NA-C1A	6.53	109.64	106.71
31	8	314	CLA	C4A-NA-C1A	6.53	109.64	106.71
31	b	613	CLA	C4A-NA-C1A	6.53	109.64	106.71
30	e	602	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
30	e	614	CHL	CMD-C2D-C1D	6.52	136.21	124.71
31	c	613	CLA	C4A-NA-C1A	6.52	109.64	106.71
31	d	613	CLA	C4A-NA-C1A	6.52	109.64	106.71
31	6	311	CLA	C4A-NA-C1A	6.51	109.64	106.71
31	g	604	CLA	C4A-NA-C1A	6.51	109.64	106.71
30	6	313	CHL	C2C-C3C-C4C	-6.51	101.84	106.49
30	g	609	CHL	CMD-C2D-C1D	6.51	136.19	124.71
30	e	607	CHL	C2C-C3C-C4C	-6.51	101.85	106.49
30	8	308	CHL	C2C-C3C-C4C	-6.51	101.85	106.49
31	A	841	CLA	C4A-NA-C1A	6.50	109.63	106.71
31	4	312	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	1	313	CHL	CMD-C2D-C1D	6.50	136.18	124.71
30	d	601	CHL	CMD-C2D-C1D	6.50	136.18	124.71
30	4	308	CHL	C2C-C3C-C4C	-6.50	101.85	106.49
31	A	822	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	g	606	CHL	C2C-C3C-C4C	-6.50	101.86	106.49
30	2	308	CHL	CMD-C2D-C1D	6.49	136.16	124.71
30	c	606	CHL	CMD-C2D-C1D	6.49	136.16	124.71
31	9	311	CLA	C4A-NA-C1A	6.49	109.62	106.71
31	d	611	CLA	C4A-NA-C1A	6.49	109.62	106.71
30	8	313	CHL	C2C-C3C-C4C	-6.48	101.87	106.49
30	c	607	CHL	CMD-C2D-C1D	6.48	136.14	124.71
31	A	823	CLA	C4A-NA-C1A	6.48	109.62	106.71
31	b	604	CLA	C4A-NA-C1A	6.48	109.62	106.71
31	i	603	CLA	C4A-NA-C1A	6.48	109.62	106.71
30	e	608	CHL	C2C-C3C-C4C	-6.48	101.87	106.49
31	i	612	CLA	C4A-NA-C1A	6.47	109.62	106.71
30	f	601	CHL	C2C-C3C-C4C	-6.47	101.88	106.49
30	9	306	CHL	CMD-C2D-C1D	6.47	136.12	124.71
31	9	309	CLA	C4A-NA-C1A	6.47	109.61	106.71
31	A	829	CLA	C4A-NA-C1A	6.47	109.61	106.71
30	i	607	CHL	CMD-C2D-C1D	6.47	136.11	124.71
32	A	847	8CT	C14-C13-C12	-6.47	118.08	127.31
30	6	301	CHL	CMD-C2D-C1D	6.47	136.11	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	J	103	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	i	607	CHL	C2C-C3C-C4C	-6.46	101.88	106.49
31	7	308	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	6	306	CHL	CMD-C2D-C1D	6.46	136.10	124.71
30	c	608	CHL	C2C-C3C-C4C	-6.46	101.89	106.49
30	e	609	CHL	C2C-C3C-C4C	-6.46	101.89	106.49
30	4	308	CHL	CMD-C2D-C1D	6.46	136.09	124.71
30	5	306	CHL	CMD-C2D-C1D	6.46	136.09	124.71
31	2	304	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	7	306	CHL	CMD-C2D-C1D	6.46	136.09	124.71
31	3	306	CLA	C4A-NA-C1A	6.45	109.61	106.71
31	g	603	CLA	C4A-NA-C1A	6.45	109.61	106.71
31	6	310	CLA	C4A-NA-C1A	6.45	109.61	106.71
31	7	318	CLA	C4A-NA-C1A	6.45	109.61	106.71
31	g	611	CLA	C4A-NA-C1A	6.45	109.61	106.71
31	i	613	CLA	C4A-NA-C1A	6.45	109.61	106.71
30	0	302	CHL	CMD-C2D-C1D	6.45	136.08	124.71
31	h	604	CLA	C4A-NA-C1A	6.45	109.60	106.71
31	b	603	CLA	C4A-NA-C1A	6.44	109.60	106.71
30	f	607	CHL	CMD-C2D-C1D	6.44	136.07	124.71
31	6	318	CLA	C4A-NA-C1A	6.44	109.60	106.71
30	5	305	CHL	C2C-C3C-C4C	-6.44	101.90	106.49
31	A	805	CLA	C4A-NA-C1A	6.44	109.60	106.71
30	9	305	CHL	CMD-C2D-C1D	6.44	136.06	124.71
31	1	314	CLA	C4A-NA-C1A	6.43	109.60	106.71
30	a	602	CHL	C2C-C3C-C4C	-6.43	101.90	106.49
31	O	201	CLA	C4A-NA-C1A	6.43	109.60	106.71
30	3	302	CHL	CMD-C2D-C1D	6.43	136.05	124.71
30	8	301	CHL	O2D-CGD-CBD	6.43	122.69	111.27
31	A	835	CLA	C4A-NA-C1A	6.43	109.59	106.71
31	f	613	CLA	C4A-NA-C1A	6.43	109.59	106.71
30	b	601	CHL	C2C-C3C-C4C	-6.42	101.91	106.49
30	4	302	CHL	CMD-C2D-C1D	6.42	136.03	124.71
31	8	303	CLA	C4A-NA-C1A	6.42	109.59	106.71
30	c	614	CHL	C2C-C3C-C4C	-6.42	101.91	106.49
31	B	825	CLA	C4A-NA-C1A	6.42	109.59	106.71
30	d	602	CHL	CMD-C2D-C1D	6.42	136.02	124.71
30	d	606	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
30	i	606	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
30	c	614	CHL	CMD-C2D-C1D	6.41	136.01	124.71
31	h	612	CLA	C4A-NA-C1A	6.41	109.59	106.71
30	b	607	CHL	CMD-C2D-C1D	6.41	136.01	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	302	CHL	CMD-C2D-C1D	6.41	136.01	124.71
31	5	310	CLA	C4A-NA-C1A	6.40	109.58	106.71
31	h	611	CLA	C4A-NA-C1A	6.40	109.58	106.71
30	g	602	CHL	CMD-C2D-C1D	6.40	136.00	124.71
30	h	602	CHL	CMD-C2D-C1D	6.40	136.00	124.71
31	B	850	CLA	C4A-NA-C1A	6.40	109.58	106.71
31	g	610	CLA	C4A-NA-C1A	6.40	109.58	106.71
30	5	306	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
31	5	304	CLA	C4A-NA-C1A	6.39	109.58	106.71
31	A	852	CLA	C4A-NA-C1A	6.39	109.58	106.71
31	B	809	CLA	C4A-NA-C1A	6.39	109.58	106.71
31	0	304	CLA	C4A-NA-C1A	6.39	109.58	106.71
30	g	602	CHL	C2C-C3C-C4C	-6.39	101.93	106.49
31	e	613	CLA	C4A-NA-C1A	6.39	109.58	106.71
30	c	602	CHL	CMD-C2D-C1D	6.38	135.96	124.71
31	B	815	CLA	C4A-NA-C1A	6.38	109.58	106.71
30	b	602	CHL	CMD-C2D-C1D	6.38	135.96	124.71
31	0	303	CLA	C4A-NA-C1A	6.38	109.58	106.71
31	6	312	CLA	C4A-NA-C1A	6.38	109.58	106.71
30	2	307	CHL	CHD-C4C-C3C	-6.38	115.46	124.84
31	B	814	CLA	C4A-NA-C1A	6.38	109.57	106.71
30	g	607	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
30	e	601	CHL	C2C-C3C-C4C	-6.37	101.94	106.49
31	9	312	CLA	C4A-NA-C1A	6.37	109.57	106.71
31	A	803	CLA	C4A-NA-C1A	6.37	109.57	106.71
31	c	610	CLA	C4A-NA-C1A	6.37	109.57	106.71
31	c	611	CLA	C4A-NA-C1A	6.37	109.57	106.71
31	A	832	CLA	C4A-NA-C1A	6.37	109.57	106.71
31	7	312	CLA	C4A-NA-C1A	6.36	109.57	106.71
31	O	203	CLA	C4A-NA-C1A	6.36	109.57	106.71
31	f	603	CLA	C4A-NA-C1A	6.36	109.57	106.71
31	B	834	CLA	C4A-NA-C1A	6.36	109.57	106.71
30	4	313	CHL	CMD-C2D-C1D	6.36	135.92	124.71
31	B	820	CLA	C4A-NA-C1A	6.36	109.56	106.71
31	3	312	CLA	C4A-NA-C1A	6.35	109.56	106.71
31	B	833	CLA	C4A-NA-C1A	6.35	109.56	106.71
31	9	302	CLA	C4A-NA-C1A	6.35	109.56	106.71
31	a	611	CLA	C4A-NA-C1A	6.35	109.56	106.71
31	8	311	CLA	C4A-NA-C1A	6.35	109.56	106.71
42	i	523	NEX	C11-C12-C13	-6.35	108.59	126.42
31	4	314	CLA	C4A-NA-C1A	6.34	109.56	106.71
31	0	308	CLA	C4A-NA-C1A	6.34	109.56	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	310	CLA	C4A-NA-C1A	6.34	109.56	106.71
31	B	828	CLA	C4A-NA-C1A	6.34	109.56	106.71
31	B	839	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	1	305	CHL	C2C-C3C-C4C	-6.34	101.97	106.49
31	9	304	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	2	302	CHL	CMD-C2D-C1D	6.34	135.88	124.71
30	b	614	CHL	C2C-C3C-C4C	-6.34	101.97	106.49
42	c	523	NEX	C11-C12-C13	-6.33	108.62	126.42
42	b	523	NEX	C11-C12-C13	-6.33	108.63	126.42
31	7	303	CLA	C4A-NA-C1A	6.33	109.55	106.71
31	K	105	CLA	C4A-NA-C1A	6.33	109.55	106.71
42	d	523	NEX	C11-C12-C13	-6.33	108.64	126.42
42	h	523	NEX	C11-C12-C13	-6.33	108.64	126.42
31	A	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
30	f	602	CHL	CMD-C2D-C1D	6.33	135.86	124.71
30	h	608	CHL	C2C-C3C-C4C	-6.33	101.98	106.49
31	A	810	CLA	C4A-NA-C1A	6.32	109.55	106.71
31	d	604	CLA	C4A-NA-C1A	6.32	109.55	106.71
30	6	308	CHL	CMD-C2D-C1D	6.32	135.86	124.71
30	g	608	CHL	C2C-C3C-C4C	-6.32	101.98	106.49
31	L	207	CLA	C4A-NA-C1A	6.32	109.55	106.71
42	f	523	NEX	C11-C12-C13	-6.32	108.66	126.42
30	6	315	CHL	C2C-C3C-C4C	-6.32	101.99	106.49
31	2	310	CLA	C4A-NA-C1A	6.32	109.55	106.71
42	a	523	NEX	C11-C12-C13	-6.32	108.67	126.42
42	g	523	NEX	C11-C12-C13	-6.31	108.68	126.42
31	5	314	CLA	C4A-NA-C1A	6.31	109.54	106.71
30	f	607	CHL	C2C-C3C-C4C	-6.31	101.99	106.49
32	B	846	8CT	C19-C20-C21	-6.31	118.31	127.31
32	F	302	8CT	C14-C13-C12	-6.31	118.31	127.31
31	8	309	CLA	C4A-NA-C1A	6.30	109.54	106.71
31	6	309	CLA	C4A-NA-C1A	6.30	109.54	106.71
31	B	831	CLA	C4A-NA-C1A	6.30	109.54	106.71
31	0	310	CLA	C4A-NA-C1A	6.29	109.54	106.71
31	2	314	CLA	C4A-NA-C1A	6.29	109.53	106.71
31	K	102	CLA	C4A-NA-C1A	6.29	109.53	106.71
30	d	609	CHL	C2C-C3C-C4C	-6.29	102.00	106.49
31	a	604	CLA	C4A-NA-C1A	6.29	109.53	106.71
30	d	601	CHL	C2C-C3C-C4C	-6.29	102.01	106.49
31	K	101	CLA	C4A-NA-C1A	6.29	109.53	106.71
32	M	102	8CT	C10-C11-C12	-6.29	116.73	126.23
30	a	607	CHL	C2C-C3C-C4C	-6.28	102.01	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	601	CHL	C2C-C3C-C4C	-6.28	102.01	106.49
33	5	502	0UR	C14-C15-C16	-6.28	118.35	127.31
31	3	303	CLA	C4A-NA-C1A	6.27	109.53	106.71
30	b	609	CHL	C2C-C3C-C4C	-6.27	102.02	106.49
33	3	501	0UR	C4-C3-C2	-6.27	114.70	120.08
30	i	601	CHL	C2C-C3C-C4C	-6.27	102.02	106.49
32	B	804	8CT	C18-C17-C16	-6.27	118.36	127.31
31	1	309	CLA	C4A-NA-C1A	6.27	109.53	106.71
31	A	806	CLA	C4A-NA-C1A	6.27	109.53	106.71
31	L	201	CLA	C4A-NA-C1A	6.27	109.52	106.71
32	1	402	8CT	C24-C25-C26	-6.26	118.37	127.31
31	5	308	CLA	C4A-NA-C1A	6.26	109.52	106.71
31	1	304	CLA	C4A-NA-C1A	6.26	109.52	106.71
30	a	608	CHL	C2C-C3C-C4C	-6.26	102.03	106.49
30	6	308	CHL	C2C-C3C-C4C	-6.26	102.03	106.49
30	e	605	CHL	C2C-C3C-C4C	-6.26	102.03	106.49
30	d	607	CHL	C2C-C3C-C4C	-6.25	102.03	106.49
31	9	300	CLA	C4A-NA-C1A	6.25	109.52	106.71
31	B	813	CLA	C4A-NA-C1A	6.25	109.52	106.71
32	B	804	8CT	C14-C13-C12	-6.25	118.39	127.31
30	c	607	CHL	C2C-C3C-C4C	-6.25	102.03	106.49
31	9	310	CLA	C4A-NA-C1A	6.25	109.52	106.71
31	B	819	CLA	C4A-NA-C1A	6.25	109.52	106.71
32	1	402	8CT	C18-C17-C16	-6.25	118.39	127.31
31	G	103	CLA	C4A-NA-C1A	6.24	109.51	106.71
30	a	601	CHL	C2C-C3C-C4C	-6.24	102.04	106.49
33	7	501	0UR	C4-C3-C2	-6.24	114.72	120.08
31	A	807	CLA	C4A-NA-C1A	6.24	109.51	106.71
31	A	836	CLA	C4A-NA-C1A	6.24	109.51	106.71
31	L	204	CLA	C4A-NA-C1A	6.24	109.51	106.71
30	g	614	CHL	CHB-C1B-NB	-6.24	117.66	124.26
31	7	310	CLA	C4A-NA-C1A	6.22	109.50	106.71
31	A	813	CLA	C4A-NA-C1A	6.21	109.50	106.71
31	2	309	CLA	C4A-NA-C1A	6.21	109.50	106.71
31	H	201	CLA	C4A-NA-C1A	6.21	109.50	106.71
30	h	609	CHL	C2C-C3C-C4C	-6.20	102.07	106.49
30	g	601	CHL	C2C-C3C-C4C	-6.19	102.07	106.49
32	O	205	8CT	C10-C11-C12	-6.19	116.88	126.23
31	A	826	CLA	C4A-NA-C1A	6.19	109.49	106.71
30	a	605	CHL	CHB-C1B-NB	-6.19	117.70	124.26
30	5	313	CHL	C2C-C3C-C4C	-6.19	102.08	106.49
30	d	614	CHL	CHB-C1B-NB	-6.19	117.71	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	836	CLA	C4A-NA-C1A	6.18	109.48	106.71
30	a	609	CHL	C2C-C3C-C4C	-6.18	102.08	106.49
30	f	609	CHL	C2C-C3C-C4C	-6.18	102.08	106.49
30	a	614	CHL	C2C-C3C-C4C	-6.18	102.09	106.49
31	A	838	CLA	C4A-NA-C1A	6.17	109.48	106.71
31	A	853	CLA	C4A-NA-C1A	6.17	109.48	106.71
32	6	402	8CT	C01-C02-C03	-6.16	117.61	124.53
31	4	303	CLA	C4A-NA-C1A	6.15	109.47	106.71
31	F	301	CLA	C4A-NA-C1A	6.15	109.47	106.71
30	i	605	CHL	C2C-C3C-C4C	-6.14	102.11	106.49
30	d	614	CHL	C2C-C3C-C4C	-6.14	102.11	106.49
42	c	523	NEX	C38-C25-C26	-6.13	111.98	122.26
30	c	605	CHL	CHB-C1B-NB	-6.13	117.77	124.26
30	d	605	CHL	CHB-C1B-NB	-6.13	117.77	124.26
31	A	821	CLA	C4A-NA-C1A	6.13	109.46	106.71
31	A	825	CLA	C4A-NA-C1A	6.13	109.46	106.71
30	c	605	CHL	C2C-C3C-C4C	-6.12	102.12	106.49
32	A	846	8CT	C18-C17-C16	-6.12	118.58	127.31
30	i	605	CHL	CHB-C1B-NB	-6.11	117.79	124.26
32	A	849	8CT	C18-C17-C16	-6.11	118.59	127.31
30	1	302	CHL	CMD-C2D-C1D	6.11	135.47	124.71
31	4	304	CLA	C4A-NA-C1A	6.10	109.45	106.71
30	g	614	CHL	C2C-C3C-C4C	-6.10	102.14	106.49
30	h	605	CHL	C2C-C3C-C4C	-6.10	102.14	106.49
31	f	610	CLA	C4A-NA-C1A	6.10	109.45	106.71
30	f	605	CHL	C2C-C3C-C4C	-6.09	102.14	106.49
30	i	614	CHL	C2C-C3C-C4C	-6.09	102.15	106.49
42	i	523	NEX	C38-C25-C26	-6.09	112.05	122.26
42	d	523	NEX	C38-C25-C26	-6.09	112.05	122.26
31	0	313	CLA	C4A-NA-C1A	6.09	109.44	106.71
32	B	848	8CT	C10-C11-C12	-6.09	117.03	126.23
42	h	523	NEX	C38-C25-C26	-6.09	112.06	122.26
42	f	523	NEX	C38-C25-C26	-6.09	112.06	122.26
32	B	843	8CT	C14-C13-C12	-6.08	118.63	127.31
42	b	523	NEX	C38-C25-C26	-6.08	112.07	122.26
42	g	523	NEX	C38-C25-C26	-6.08	112.07	122.26
30	i	609	CHL	C2C-C3C-C4C	-6.08	102.15	106.49
31	i	610	CLA	C4A-NA-C1A	6.08	109.44	106.71
30	d	605	CHL	C2C-C3C-C4C	-6.08	102.16	106.49
31	3	318	CLA	C4A-NA-C1A	6.08	109.44	106.71
42	a	523	NEX	C38-C25-C26	-6.08	112.08	122.26
30	g	605	CHL	C2C-C3C-C4C	-6.07	102.16	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	614	CHL	C2C-C3C-C4C	-6.07	102.16	106.49
30	g	605	CHL	CHB-C1B-NB	-6.07	117.83	124.26
31	O	206	CLA	C4A-NA-C1A	6.06	109.43	106.71
30	c	609	CHL	C2C-C3C-C4C	-6.06	102.17	106.49
30	d	614	CHL	C1D-ND-C4D	6.06	110.64	106.33
30	d	605	CHL	C1D-ND-C4D	6.06	110.64	106.33
31	6	317	CLA	C4A-NA-C1A	6.06	109.43	106.71
31	B	824	CLA	C4A-NA-C1A	6.06	109.43	106.71
30	6	302	CHL	O2D-CGD-CBD	6.05	122.02	111.27
31	8	310	CLA	C4A-NA-C1A	6.05	109.42	106.71
30	a	614	CHL	CHB-C1B-NB	-6.04	117.86	124.26
30	2	307	CHL	C2C-C3C-C4C	-6.04	102.18	106.49
32	9	401	8CT	C19-C20-C21	-6.04	118.69	127.31
31	3	309	CLA	C4A-NA-C1A	6.03	109.42	106.71
30	g	601	CHL	CHB-C1B-NB	-6.03	117.87	124.26
30	g	609	CHL	C2C-C3C-C4C	-6.03	102.19	106.49
31	A	824	CLA	C4A-NA-C1A	6.02	109.41	106.71
31	e	610	CLA	C4A-NA-C1A	6.02	109.41	106.71
30	i	605	CHL	C1D-ND-C4D	6.01	110.61	106.33
32	B	804	8CT	C10-C11-C12	-6.00	117.17	126.23
33	0	502	0UR	C4-C3-C2	-6.00	114.93	120.08
30	6	302	CHL	CMD-C2D-C1D	6.00	135.29	124.71
31	3	313	CLA	C4A-NA-C1A	6.00	109.40	106.71
30	a	605	CHL	C2C-C3C-C4C	-6.00	102.21	106.49
30	g	614	CHL	C1D-ND-C4D	6.00	110.59	106.33
31	d	610	CLA	C4A-NA-C1A	5.99	109.40	106.71
30	c	605	CHL	C1D-ND-C4D	5.99	110.59	106.33
30	8	315	CHL	C2C-C3C-C4C	-5.98	102.22	106.49
31	A	819	CLA	C4A-NA-C1A	5.98	109.39	106.71
31	8	304	CLA	C4A-NA-C1A	5.97	109.39	106.71
32	A	849	8CT	C30-C31-C32	-5.95	114.15	121.47
32	A	848	8CT	C04-C03-C02	-5.95	114.23	122.61
31	B	801	CLA	C4A-NA-C1A	5.95	109.38	106.71
30	3	302	CHL	CHD-C4C-C3C	-5.95	116.10	124.84
30	3	307	CHL	CHD-C4C-C3C	-5.94	116.10	124.84
32	9	401	8CT	C10-C11-C12	-5.94	117.25	126.23
30	f	605	CHL	CHB-C1B-NB	-5.94	117.97	124.26
31	B	841	CLA	C4A-NA-C1A	5.93	109.37	106.71
32	F	302	8CT	C18-C17-C16	-5.92	118.86	127.31
30	5	313	CHL	CHB-C1B-NB	-5.91	118.00	124.26
31	O	202	CLA	C4A-NA-C1A	5.91	109.36	106.71
30	h	607	CHL	C2C-C3C-C4C	-5.90	102.29	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	L	205	8CT	C24-C25-C26	-5.89	118.90	127.31
32	7	404	8CT	C19-C20-C21	-5.88	118.91	127.31
31	A	812	CLA	C4A-NA-C1A	5.88	109.35	106.71
30	3	307	CHL	C2C-C3C-C4C	-5.87	102.30	106.49
32	1	402	8CT	C14-C13-C12	-5.87	118.93	127.31
32	J	101	8CT	C19-C20-C21	-5.87	118.93	127.31
31	B	829	CLA	C4A-NA-C1A	5.86	109.34	106.71
30	g	601	CHL	C1D-ND-C4D	5.86	110.50	106.33
30	9	306	CHL	O2D-CGD-CBD	5.85	121.66	111.27
30	a	614	CHL	C1D-ND-C4D	5.84	110.48	106.33
33	g	520	0UR	C10-C11-C12	-5.83	118.98	127.31
32	M	102	8CT	C14-C13-C12	-5.83	118.99	127.31
30	a	601	CHL	CHB-C1B-NB	-5.83	118.09	124.26
30	7	302	CHL	CHD-C4C-C3C	-5.82	116.29	124.84
30	g	607	CHL	CHB-C1B-NB	-5.81	118.10	124.26
33	g	520	0UR	C14-C15-C16	-5.81	119.02	127.31
32	B	847	8CT	C24-C25-C26	-5.80	119.04	127.31
30	i	614	CHL	CHB-C1B-NB	-5.79	118.12	124.26
32	F	302	8CT	C24-C25-C26	-5.79	119.05	127.31
30	8	307	CHL	CHD-C4C-C3C	-5.78	116.34	124.84
33	4	501	0UR	C4-C3-C2	-5.78	115.12	120.08
30	g	605	CHL	C1D-ND-C4D	5.78	110.44	106.33
32	0	401	8CT	C19-C20-C21	-5.78	119.07	127.31
32	F	302	8CT	C19-C20-C21	-5.77	119.07	127.31
32	1	402	8CT	C19-C20-C21	-5.77	119.08	127.31
31	A	802	CLA	C4A-NA-C1A	5.77	109.30	106.71
33	4	501	0UR	C43-C3-C4	-5.76	118.05	125.02
31	4	309	CLA	C4A-NA-C1A	5.76	109.29	106.71
33	c	520	0UR	C14-C15-C16	-5.76	119.09	127.31
30	b	614	CHL	CHB-C1B-NB	-5.75	118.17	124.26
30	9	305	CHL	CHD-C4C-C3C	-5.74	116.40	124.84
30	f	602	CHL	CHD-C4C-C3C	-5.74	116.40	124.84
30	6	307	CHL	CHD-C4C-C3C	-5.74	116.41	124.84
31	B	826	CLA	C4A-NA-C1A	5.74	109.28	106.71
31	B	830	CLA	C4A-NA-C1A	5.74	109.28	106.71
32	2	402	8CT	C07-C02-C03	-5.73	114.41	122.73
32	L	206	8CT	C18-C17-C16	-5.72	119.15	127.31
30	1	302	CHL	CHD-C4C-C3C	-5.71	116.44	124.84
30	8	302	CHL	CHD-C4C-C3C	-5.71	116.44	124.84
30	h	605	CHL	CHB-C1B-NB	-5.71	118.21	124.26
33	8	502	0UR	C14-C15-C16	-5.71	119.16	127.31
30	5	302	CHL	CHD-C4C-C3C	-5.71	116.45	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	601	CHL	CHB-C1B-NB	-5.70	118.22	124.26
30	a	605	CHL	C1D-ND-C4D	5.70	110.39	106.33
30	h	614	CHL	CHB-C1B-NB	-5.70	118.22	124.26
32	B	847	8CT	C18-C17-C16	-5.70	119.18	127.31
30	4	307	CHL	CHD-C4C-C3C	-5.68	116.49	124.84
30	e	614	CHL	CHB-C1B-NB	-5.68	118.25	124.26
30	f	605	CHL	C1D-ND-C4D	5.67	110.37	106.33
31	5	309	CLA	C4A-NA-C1A	5.67	109.26	106.71
30	2	307	CHL	C2A-C1A-CHA	-5.67	113.94	123.86
30	f	608	CHL	CHD-C4C-C3C	-5.67	116.50	124.84
30	7	305	CHL	CHD-C4C-C3C	-5.66	116.52	124.84
32	J	104	8CT	C11-C12-C13	5.65	127.61	118.94
30	4	313	CHL	O2D-CGD-CBD	5.65	121.31	111.27
30	i	614	CHL	C1D-ND-C4D	5.64	110.34	106.33
30	0	302	CHL	C3B-C2B-C1B	-5.64	100.36	107.16
30	e	605	CHL	CHB-C1B-NB	-5.64	118.29	124.26
32	2	402	8CT	C01-C02-C03	-5.63	118.20	124.53
30	h	614	CHL	C1D-ND-C4D	5.63	110.34	106.33
30	2	313	CHL	CHD-C4C-C3C	-5.63	116.57	124.84
31	B	803	CLA	C4A-NA-C1A	5.63	109.24	106.71
30	6	301	CHL	O2D-CGD-CBD	5.63	121.27	111.27
30	0	302	CHL	CHD-C4C-C3C	-5.61	116.60	124.84
32	3	403	8CT	C24-C25-C26	-5.60	119.31	127.31
32	L	205	8CT	C18-C17-C16	-5.60	119.32	127.31
30	g	607	CHL	C1D-ND-C4D	5.60	110.31	106.33
30	2	319	CHL	O2D-CGD-CBD	5.60	121.22	111.27
30	4	319	CHL	CHD-C4C-C3C	-5.59	116.62	124.84
30	i	607	CHL	CHB-C1B-NB	-5.59	118.34	124.26
30	h	605	CHL	C1D-ND-C4D	5.59	110.30	106.33
30	4	305	CHL	CHD-C4C-C3C	-5.58	116.63	124.84
32	8	402	8CT	C30-C31-C32	-5.58	114.60	121.47
30	d	607	CHL	C1D-ND-C4D	5.58	110.30	106.33
30	2	302	CHL	CHD-C4C-C3C	-5.57	116.65	124.84
30	4	302	CHL	C3B-C2B-C1B	-5.56	100.44	107.16
30	7	307	CHL	CHD-C4C-C3C	-5.56	116.67	124.84
30	6	307	CHL	C3B-C2B-C1B	-5.56	100.45	107.16
32	7	404	8CT	C28-C26-C25	5.56	127.47	118.94
30	6	306	CHL	CHD-C4C-C3C	-5.56	116.67	124.84
30	6	302	CHL	CHD-C4C-C3C	-5.55	116.68	124.84
30	7	302	CHL	C2A-C1A-CHA	-5.55	114.15	123.86
30	6	302	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
30	a	601	CHL	C1D-ND-C4D	5.54	110.27	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	302	CHL	CHD-C4C-C3C	-5.53	116.70	124.84
32	B	846	8CT	C39-C16-C17	-5.53	115.17	122.92
30	f	607	CHL	C1D-ND-C4D	5.53	110.27	106.33
32	7	405	8CT	C01-C02-C03	-5.53	118.32	124.53
30	3	302	CHL	C2A-C1A-CHA	-5.53	114.20	123.86
30	2	308	CHL	CHD-C4C-C3C	-5.52	116.73	124.84
30	2	305	CHL	C2A-C1A-CHA	-5.52	114.21	123.86
30	h	601	CHL	C1D-ND-C4D	5.52	110.25	106.33
30	4	313	CHL	CHD-C4C-C3C	-5.51	116.73	124.84
30	f	602	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
30	5	313	CHL	O2D-CGD-CBD	5.51	121.06	111.27
32	A	850	8CT	C07-C02-C03	-5.51	114.73	122.73
32	8	402	8CT	C18-C17-C16	-5.51	119.45	127.31
32	7	405	8CT	C14-C13-C12	-5.50	119.45	127.31
33	f	520	0UR	C14-C15-C16	-5.50	119.46	127.31
30	3	305	CHL	C3B-C2B-C1B	-5.50	100.52	107.16
32	B	845	8CT	C39-C16-C17	-5.49	115.23	122.92
30	1	305	CHL	CHD-C4C-C3C	-5.49	116.77	124.84
31	b	610	CLA	C4A-NA-C1A	5.49	109.17	106.71
30	7	301	CHL	O2D-CGD-CBD	5.49	121.02	111.27
30	7	305	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
30	6	305	CHL	CHD-C4C-C3C	-5.49	116.78	124.84
30	a	609	CHL	C1D-ND-C4D	5.49	110.23	106.33
32	2	402	8CT	C14-C13-C12	-5.49	119.48	127.31
30	g	608	CHL	C1D-ND-C4D	5.48	110.23	106.33
32	B	845	8CT	C04-C03-C02	-5.48	114.90	122.61
30	e	614	CHL	C1D-ND-C4D	5.48	110.22	106.33
30	3	307	CHL	C2A-C1A-CHA	-5.47	114.29	123.86
30	2	306	CHL	O2D-CGD-CBD	5.47	120.99	111.27
32	I	101	8CT	C14-C13-C12	-5.47	119.50	127.31
30	2	302	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
30	5	313	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
30	d	607	CHL	CHB-C1B-NB	-5.47	118.47	124.26
30	3	305	CHL	CHD-C4C-C3C	-5.46	116.81	124.84
30	2	313	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
32	B	847	8CT	C35-C30-C29	-5.46	105.81	112.70
30	6	306	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
32	M	102	8CT	C19-C20-C21	-5.45	119.53	127.31
30	9	305	CHL	C2A-C1A-CHA	-5.45	114.33	123.86
30	7	306	CHL	O2D-CGD-CBD	5.45	120.95	111.27
30	c	608	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
32	1	402	8CT	C01-C02-C03	-5.45	118.41	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	607	CHL	CHB-C1B-NB	-5.45	118.49	124.26
30	1	305	CHL	C2A-C1A-CHA	-5.44	114.34	123.86
30	h	607	CHL	CHB-C1B-NB	-5.44	118.50	124.26
32	B	845	8CT	C14-C13-C12	-5.44	119.55	127.31
32	L	205	8CT	C14-C13-C12	-5.44	119.55	127.31
30	0	301	CHL	CHD-C4C-C3C	-5.44	116.85	124.84
30	2	305	CHL	CHD-C4C-C3C	-5.44	116.85	124.84
30	8	302	CHL	C2A-C1A-CHA	-5.44	114.35	123.86
30	9	313	CHL	O2D-CGD-CBD	5.43	120.92	111.27
32	7	402	8CT	C35-C30-C29	-5.43	105.84	112.70
30	d	605	CHL	C3B-C2B-C1B	-5.42	100.61	107.16
30	8	306	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
30	i	609	CHL	C1D-ND-C4D	5.42	110.19	106.33
30	c	602	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
30	i	614	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
30	i	605	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
32	7	405	8CT	C10-C11-C12	-5.41	118.06	126.23
30	1	313	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
30	b	601	CHL	CHB-C1B-NB	-5.41	118.53	124.26
30	c	614	CHL	C3B-C2B-C1B	-5.41	100.64	107.16
30	f	605	CHL	C3B-C2B-C1B	-5.41	100.64	107.16
30	c	602	CHL	CHD-C4C-C3C	-5.40	116.90	124.84
30	c	605	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
30	8	313	CHL	CHD-C4C-C3C	-5.40	116.90	124.84
32	A	850	8CT	C01-C02-C03	-5.40	118.47	124.53
30	7	313	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
30	f	614	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
30	e	605	CHL	C3B-C2B-C1B	-5.40	100.65	107.16
30	8	302	CHL	C3B-C2B-C1B	-5.40	100.65	107.16
30	6	301	CHL	C3B-C2B-C1B	-5.39	100.65	107.16
32	J	104	8CT	C40-C12-C13	-5.39	115.37	122.92
30	h	609	CHL	O2D-CGD-CBD	5.39	120.84	111.27
30	b	601	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
30	7	307	CHL	C3B-C2B-C1B	-5.38	100.66	107.16
30	e	609	CHL	C3B-C2B-C1B	-5.38	100.66	107.16
30	d	602	CHL	C2A-C1A-CHA	-5.38	114.45	123.86
30	4	313	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
30	0	305	CHL	O2D-CGD-CBD	5.38	120.83	111.27
30	f	614	CHL	CHB-C1B-NB	-5.38	118.56	124.26
30	1	302	CHL	C2A-C1A-CHA	-5.38	114.46	123.86
32	A	849	8CT	C14-C13-C12	-5.38	119.64	127.31
30	b	601	CHL	C1D-ND-C4D	5.38	110.15	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	854	8CT	C19-C20-C21	-5.38	119.64	127.31
30	0	301	CHL	C3B-C2B-C1B	-5.37	100.67	107.16
30	d	602	CHL	CHD-C4C-C3C	-5.37	116.94	124.84
30	g	606	CHL	O2D-CGD-CBD	5.37	120.81	111.27
30	f	608	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
30	5	302	CHL	C2A-C1A-CHA	-5.37	114.47	123.86
30	a	614	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
30	1	305	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
30	2	319	CHL	CHD-C4C-C3C	-5.37	116.95	124.84
32	B	851	8CT	C10-C11-C12	-5.36	118.13	126.23
30	5	313	CHL	C1D-ND-C4D	5.36	110.14	106.33
30	b	614	CHL	C1D-ND-C4D	5.36	110.14	106.33
30	g	608	CHL	CHB-C1B-NB	-5.36	118.58	124.26
30	e	605	CHL	C1D-ND-C4D	5.36	110.14	106.33
30	h	601	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
32	0	401	8CT	C04-C03-C02	-5.36	115.06	122.61
30	i	601	CHL	CHB-C1B-NB	-5.36	118.59	124.26
30	f	606	CHL	O2D-CGD-CBD	5.36	120.78	111.27
30	a	608	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
32	8	406	8CT	C10-C11-C12	-5.35	118.15	126.23
30	2	301	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
30	i	601	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
30	d	614	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
32	7	405	8CT	C24-C25-C26	-5.35	119.68	127.31
33	3	501	0UR	C43-C3-C4	-5.35	118.56	125.02
32	0	401	8CT	C30-C31-C32	-5.35	114.89	121.47
30	6	306	CHL	C2A-C1A-CHA	-5.34	114.52	123.86
30	7	302	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
30	5	302	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
32	7	402	8CT	C18-C17-C16	-5.34	119.69	127.31
30	f	602	CHL	C2A-C1A-CHA	-5.34	114.53	123.86
30	3	302	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
30	g	605	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
30	6	313	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
30	g	607	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
30	e	607	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
33	6	501	0UR	C10-C11-C12	-5.33	119.70	127.31
30	a	607	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
30	d	608	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
30	e	601	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
30	6	315	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
30	4	305	CHL	O2D-CGD-CBD	5.33	120.73	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	602	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
30	1	313	CHL	CHD-C4C-C3C	-5.32	117.01	124.84
33	f	520	0UR	C10-C11-C12	-5.32	119.71	127.31
30	4	313	CHL	C2A-C1A-CHA	-5.32	114.56	123.86
30	d	609	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
30	d	601	CHL	O2D-CGD-CBD	5.32	120.72	111.27
30	4	308	CHL	O2D-CGD-CBD	5.32	120.72	111.27
30	2	308	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
30	5	307	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
30	6	305	CHL	C2A-C1A-CHA	-5.31	114.57	123.86
30	1	306	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
30	i	608	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
30	a	605	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
30	c	614	CHL	O2D-CGD-CBD	5.31	120.71	111.27
30	i	607	CHL	C3B-C2B-C1B	-5.31	100.76	107.16
30	i	609	CHL	CHB-C1B-NB	-5.30	118.64	124.26
30	h	614	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
32	3	402	8CT	C01-C02-C03	-5.30	118.57	124.53
30	2	302	CHL	C2A-C1A-CHA	-5.30	114.58	123.86
30	b	606	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
32	B	843	8CT	C24-C25-C26	-5.30	119.74	127.31
30	6	301	CHL	CHD-C4C-C3C	-5.30	117.05	124.84
30	g	608	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
30	8	313	CHL	C3B-C2B-C1B	-5.30	100.77	107.16
30	b	602	CHL	O2D-CGD-CBD	5.30	120.68	111.27
30	a	609	CHL	CHB-C1B-NB	-5.30	118.65	124.26
30	i	607	CHL	C1D-ND-C4D	5.30	110.10	106.33
30	9	313	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
30	f	607	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
30	h	609	CHL	C1D-ND-C4D	5.29	110.09	106.33
30	6	305	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
30	g	614	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
30	6	313	CHL	CHD-C4C-C3C	-5.29	117.07	124.84
30	f	608	CHL	C2A-C1A-CHA	-5.28	114.62	123.86
30	2	301	CHL	O2D-CGD-CBD	5.28	120.66	111.27
30	1	307	CHL	C3B-C2B-C1B	-5.28	100.78	107.16
30	4	308	CHL	C3B-C2B-C1B	-5.28	100.78	107.16
33	O	204	0UR	C9-C8-C7	-5.28	119.77	127.31
32	9	401	8CT	C01-C02-C03	-5.28	118.60	124.53
32	8	406	8CT	C28-C26-C25	5.28	127.04	118.94
32	L	209	8CT	C01-C02-C03	-5.28	118.60	124.53
30	c	606	CHL	C3B-C2B-C1B	-5.28	100.79	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	305	CHL	O2D-CGD-CBD	5.28	120.65	111.27
30	b	608	CHL	CHD-C4C-C3C	-5.28	117.08	124.84
30	f	606	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
30	3	305	CHL	O2D-CGD-CBD	5.28	120.64	111.27
30	9	313	CHL	CHD-C4C-C3C	-5.27	117.09	124.84
30	g	602	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
30	9	301	CHL	O2D-CGD-CBD	5.27	120.64	111.27
30	9	305	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
30	b	606	CHL	CHD-C4C-C3C	-5.27	117.09	124.84
30	d	602	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
32	G	104	8CT	C30-C31-C32	-5.27	114.99	121.47
30	7	301	CHL	CHD-C4C-C3C	-5.26	117.10	124.84
30	8	306	CHL	O2D-CGD-CBD	5.26	120.62	111.27
30	8	305	CHL	C2A-C1A-CHA	-5.26	114.66	123.86
30	b	614	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
30	6	302	CHL	C2A-C1A-CHA	-5.26	114.66	123.86
30	8	315	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
30	e	606	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
30	1	302	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
30	h	607	CHL	C3B-C2B-C1B	-5.26	100.82	107.16
30	a	609	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
30	e	608	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
32	7	402	8CT	C19-C20-C21	-5.25	119.81	127.31
30	f	601	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
30	2	301	CHL	CHD-C4C-C3C	-5.25	117.12	124.84
30	2	306	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
30	h	607	CHL	C1D-ND-C4D	5.24	110.06	106.33
30	4	306	CHL	CHD-C4C-C3C	-5.24	117.13	124.84
30	g	601	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
33	i	520	0UR	C48-C47-C46	-5.24	119.89	125.84
32	8	402	8CT	C01-C02-C03	-5.24	118.64	124.53
32	K	107	8CT	C30-C31-C32	-5.24	115.02	121.47
32	A	854	8CT	C30-C31-C32	-5.24	115.02	121.47
30	h	602	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
30	i	606	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
30	7	302	CHL	O2D-CGD-CBD	5.24	120.58	111.27
30	c	601	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
30	7	301	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
30	e	614	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
30	9	306	CHL	CHD-C4C-C3C	-5.23	117.15	124.84
30	b	607	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
30	i	602	CHL	O2D-CGD-CBD	5.23	120.56	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	305	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
30	9	301	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
30	7	313	CHL	O2D-CGD-CBD	5.23	120.56	111.27
30	2	302	CHL	O2D-CGD-CBD	5.23	120.56	111.27
30	h	605	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
30	h	608	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
30	a	607	CHL	CHB-C1B-NB	-5.23	118.72	124.26
30	8	308	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
30	f	609	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
30	e	607	CHL	O2D-CGD-CBD	5.22	120.54	111.27
30	d	601	CHL	C1D-ND-C4D	5.22	110.04	106.33
30	a	602	CHL	O2D-CGD-CBD	5.22	120.54	111.27
30	a	601	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
30	i	602	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
32	B	845	8CT	C18-C19-C20	5.21	134.16	123.47
30	c	607	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
30	b	609	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
30	c	601	CHL	CHD-C4C-C3C	-5.21	117.19	124.84
30	i	609	CHL	C3B-C2B-C1B	-5.21	100.88	107.16
30	4	307	CHL	C3B-C2B-C1B	-5.21	100.88	107.16
30	h	609	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
30	5	306	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
30	0	306	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
30	8	301	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
30	d	607	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
30	c	602	CHL	C2A-C1A-CHA	-5.20	114.77	123.86
33	7	501	0UR	C43-C3-C4	-5.19	118.74	125.02
30	8	313	CHL	C2A-C1A-CHA	-5.19	114.78	123.86
30	5	305	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
30	h	606	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
30	a	606	CHL	O2D-CGD-CBD	5.19	120.49	111.27
30	c	607	CHL	O2D-CGD-CBD	5.19	120.49	111.27
30	c	602	CHL	O2D-CGD-CBD	5.19	120.49	111.27
30	9	306	CHL	C3B-C2B-C1B	-5.19	100.90	107.16
30	d	601	CHL	C3B-C2B-C1B	-5.19	100.90	107.16
30	g	609	CHL	C3B-C2B-C1B	-5.19	100.90	107.16
30	h	601	CHL	O2D-CGD-CBD	5.18	120.48	111.27
30	g	609	CHL	C1D-ND-C4D	5.18	110.01	106.33
30	9	301	CHL	CHD-C4C-C3C	-5.17	117.24	124.84
30	6	308	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
30	4	306	CHL	O2D-CGD-CBD	5.16	120.45	111.27
30	d	601	CHL	CHB-C1B-NB	-5.16	118.79	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	e	520	0UR	C43-C3-C4	-5.16	118.78	125.02
30	8	307	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
30	g	606	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
30	4	306	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
32	3	403	8CT	C14-C13-C12	-5.16	119.95	127.31
30	f	609	CHL	C1D-ND-C4D	5.16	110.00	106.33
30	2	319	CHL	C3B-C2B-C1B	-5.16	100.94	107.16
33	5	502	0UR	C9-C8-C7	-5.16	119.95	127.31
30	e	601	CHL	CHD-C4C-C3C	-5.15	117.26	124.84
30	4	302	CHL	C2A-C1A-CHA	-5.15	114.85	123.86
30	g	601	CHL	O2D-CGD-CBD	5.15	120.42	111.27
32	9	401	8CT	C18-C17-C16	-5.15	119.96	127.31
30	i	601	CHL	O2D-CGD-CBD	5.15	120.41	111.27
30	1	313	CHL	O2D-CGD-CBD	5.14	120.40	111.27
32	0	401	8CT	C01-C02-C03	-5.14	118.76	124.53
30	6	313	CHL	C2A-C1A-CHA	-5.14	114.88	123.86
30	4	319	CHL	C2A-C1A-CHA	-5.14	114.88	123.86
32	I	101	8CT	C10-C11-C12	-5.13	118.48	126.23
30	b	608	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
30	8	315	CHL	O2D-CGD-CBD	5.13	120.38	111.27
30	e	602	CHL	O2D-CGD-CBD	5.13	120.38	111.27
30	4	305	CHL	C2A-C1A-CHA	-5.12	114.90	123.86
30	d	606	CHL	C3B-C2B-C1B	-5.12	100.98	107.16
30	2	306	CHL	CHD-C4C-C3C	-5.12	117.31	124.84
30	4	306	CHL	C2A-C1A-CHA	-5.12	114.91	123.86
30	g	614	CHL	O2D-CGD-CBD	5.12	120.36	111.27
32	4	402	8CT	C01-C02-C03	-5.11	118.78	124.53
30	i	601	CHL	C1D-ND-C4D	5.11	109.97	106.33
30	c	609	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
30	e	602	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
30	a	606	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
30	7	305	CHL	C2A-C1A-CHA	-5.11	114.93	123.86
42	d	523	NEX	C15-C35-C34	5.11	133.93	123.47
30	b	614	CHL	O2D-CGD-CBD	5.10	120.34	111.27
30	c	614	CHL	CHB-C1B-NB	-5.10	118.86	124.26
30	c	601	CHL	O2D-CGD-CBD	5.10	120.33	111.27
30	9	313	CHL	C2A-C1A-CHA	-5.10	114.94	123.86
42	a	523	NEX	C15-C35-C34	5.10	133.92	123.47
30	0	302	CHL	O2D-CGD-CBD	5.09	120.32	111.27
32	3	402	8CT	C19-C20-C21	-5.09	120.04	127.31
30	6	308	CHL	CHD-C4C-C3C	-5.09	117.36	124.84
30	1	307	CHL	CHD-C4C-C3C	-5.09	117.36	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	K	107	8CT	C07-C02-C03	-5.09	115.34	122.73
30	4	307	CHL	C2A-C1A-CHA	-5.09	114.96	123.86
42	i	523	NEX	C15-C35-C34	5.09	133.90	123.47
30	2	307	CHL	C3B-C2B-C1B	-5.09	101.02	107.16
30	g	614	CHL	C4A-NA-C1A	5.08	108.99	106.71
30	4	319	CHL	O2D-CGD-CBD	5.08	120.30	111.27
30	b	602	CHL	CHD-C4C-C3C	-5.08	117.37	124.84
30	5	301	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
30	e	608	CHL	CHD-C4C-C3C	-5.08	117.38	124.84
33	5	501	0UR	C10-C11-C12	-5.08	120.06	127.31
30	8	313	CHL	O2D-CGD-CBD	5.08	120.29	111.27
33	e	520	0UR	C4-C3-C2	-5.08	115.72	120.08
30	4	319	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
42	h	523	NEX	C15-C35-C34	5.08	133.87	123.47
32	0	401	8CT	C24-C25-C26	-5.07	120.07	127.31
42	c	523	NEX	C15-C35-C34	5.07	133.87	123.47
42	b	523	NEX	C15-C35-C34	5.07	133.86	123.47
42	g	523	NEX	C15-C35-C34	5.07	133.86	123.47
30	i	606	CHL	CHB-C1B-NB	-5.07	118.89	124.26
42	f	523	NEX	C15-C35-C34	5.07	133.86	123.47
30	e	601	CHL	O2D-CGD-CBD	5.07	120.28	111.27
30	e	606	CHL	O2D-CGD-CBD	5.07	120.28	111.27
30	2	301	CHL	C2A-C1A-CHA	-5.06	115.01	123.86
30	h	609	CHL	CHB-C1B-NB	-5.06	118.90	124.26
30	4	305	CHL	C3B-C2B-C1B	-5.06	101.05	107.16
30	i	606	CHL	C1D-ND-C4D	5.06	109.93	106.33
30	h	602	CHL	O2D-CGD-CBD	5.06	120.26	111.27
32	K	107	8CT	C01-C02-C03	-5.05	118.85	124.53
30	a	601	CHL	O2D-CGD-CBD	5.05	120.25	111.27
30	f	614	CHL	C1D-ND-C4D	5.05	109.92	106.33
30	f	601	CHL	O2D-CGD-CBD	5.05	120.24	111.27
30	a	602	CHL	C3B-C2B-C1B	-5.04	101.07	107.16
30	2	306	CHL	C2A-C1A-CHA	-5.04	115.04	123.86
30	a	607	CHL	O2D-CGD-CBD	5.04	120.23	111.27
33	2	501	0UR	C43-C3-C4	-5.04	118.93	125.02
30	g	609	CHL	CHB-C1B-NB	-5.04	118.92	124.26
32	A	850	8CT	C15-C16-C17	-5.04	111.21	118.94
30	a	607	CHL	C1D-ND-C4D	5.04	109.91	106.33
30	0	302	CHL	C2A-C1A-CHA	-5.03	115.06	123.86
30	d	605	CHL	C4A-NA-C1A	5.03	108.97	106.71
30	d	614	CHL	C4A-NA-C1A	5.03	108.97	106.71
30	8	305	CHL	CHD-C4C-C3C	-5.03	117.45	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	602	CHL	O2D-CGD-CBD	5.03	120.20	111.27
30	8	315	CHL	CHB-C1B-NB	-5.03	118.94	124.26
30	b	602	CHL	C2A-C1A-CHA	-5.03	115.07	123.86
30	g	602	CHL	O2D-CGD-CBD	5.03	120.20	111.27
30	5	306	CHL	CHB-C1B-NB	-5.03	118.94	124.26
30	5	301	CHL	O2D-CGD-CBD	5.02	120.19	111.27
32	B	804	8CT	C01-C02-C03	-5.02	118.89	124.53
32	3	403	8CT	C04-C03-C02	-5.02	115.54	122.61
30	2	305	CHL	O2D-CGD-CBD	5.02	120.19	111.27
30	8	301	CHL	CHD-C4C-C3C	-5.02	117.46	124.84
30	8	306	CHL	CHD-C4C-C3C	-5.02	117.46	124.84
30	2	308	CHL	C2A-C1A-CHA	-5.02	115.08	123.86
32	4	402	8CT	C07-C02-C03	-5.01	115.45	122.73
30	c	608	CHL	CHD-C4C-C3C	-5.01	117.47	124.84
30	g	609	CHL	O2D-CGD-CBD	5.00	120.16	111.27
30	2	319	CHL	C2A-C1A-CHA	-5.00	115.11	123.86
32	A	848	8CT	C07-C02-C03	-5.00	115.47	122.73
30	a	605	CHL	C4A-NA-C1A	5.00	108.95	106.71
33	0	502	0UR	C9-C8-C7	-5.00	120.17	127.31
30	0	305	CHL	C3B-C2B-C1B	-5.00	101.13	107.16
30	7	313	CHL	CHD-C4C-C3C	-5.00	117.50	124.84
30	c	609	CHL	O2D-CGD-CBD	5.00	120.15	111.27
30	6	301	CHL	C2A-C1A-CHA	-5.00	115.12	123.86
30	6	305	CHL	O2D-CGD-CBD	4.99	120.14	111.27
30	h	605	CHL	O2D-CGD-CBD	4.99	120.14	111.27
42	e	523	NEX	C27-C28-C29	-4.99	117.78	125.53
30	6	315	CHL	O2D-CGD-CBD	4.99	120.14	111.27
32	L	206	8CT	C24-C25-C26	-4.99	120.19	127.31
33	O	204	0UR	C5-C4-C3	-4.99	121.01	127.00
30	5	306	CHL	C1D-ND-C4D	4.98	109.88	106.33
30	3	302	CHL	O2D-CGD-CBD	4.98	120.12	111.27
30	e	602	CHL	CHD-C4C-C3C	-4.98	117.52	124.84
41	B	849	DGD	O2G-C1B-C2B	4.98	122.23	111.50
30	h	602	CHL	C1D-ND-C4D	4.98	109.87	106.33
30	8	308	CHL	O2D-CGD-CBD	4.98	120.11	111.27
30	d	609	CHL	O2D-CGD-CBD	4.98	120.11	111.27
32	A	846	8CT	C30-C31-C32	-4.97	115.35	121.47
30	5	302	CHL	O2D-CGD-CBD	4.97	120.09	111.27
30	i	605	CHL	C4A-NA-C1A	4.96	108.94	106.71
30	1	306	CHL	O2D-CGD-CBD	4.96	120.08	111.27
30	d	605	CHL	O2D-CGD-CBD	4.96	120.08	111.27
32	4	402	8CT	C04-C03-C02	-4.96	115.63	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	305	CHL	O2D-CGD-CBD	4.96	120.07	111.27
30	i	606	CHL	O2D-CGD-CBD	4.96	120.07	111.27
30	d	614	CHL	O2D-CGD-CBD	4.95	120.07	111.27
30	6	313	CHL	O2D-CGD-CBD	4.95	120.07	111.27
30	8	307	CHL	C2A-C1A-CHA	-4.95	115.20	123.86
30	d	602	CHL	O2D-CGD-CBD	4.95	120.06	111.27
30	e	601	CHL	C2A-C1A-CHA	-4.95	115.21	123.86
30	1	305	CHL	O2D-CGD-CBD	4.95	120.06	111.27
32	3	403	8CT	C19-C20-C21	-4.95	120.25	127.31
30	c	607	CHL	CHB-C1B-NB	-4.94	119.02	124.26
30	0	301	CHL	C2A-C1A-CHA	-4.94	115.21	123.86
30	f	607	CHL	O2D-CGD-CBD	4.94	120.04	111.27
42	e	523	NEX	C35-C34-C33	-4.94	120.26	127.31
32	J	104	8CT	C13-C14-C15	-4.94	107.81	123.22
30	i	605	CHL	O2D-CGD-CBD	4.93	120.03	111.27
30	8	315	CHL	C1D-ND-C4D	4.93	109.84	106.33
30	0	305	CHL	CHD-C4C-C3C	-4.93	117.59	124.84
30	a	614	CHL	O2D-CGD-CBD	4.93	120.03	111.27
30	f	601	CHL	CHD-C4C-C3C	-4.93	117.60	124.84
30	0	306	CHL	CHD-C4C-C3C	-4.93	117.60	124.84
30	3	307	CHL	C3B-C2B-C1B	-4.92	101.22	107.16
30	h	606	CHL	O2D-CGD-CBD	4.92	120.02	111.27
30	d	607	CHL	O2D-CGD-CBD	4.92	120.02	111.27
30	b	606	CHL	C2A-C1A-CHA	-4.92	115.25	123.86
30	d	606	CHL	O2D-CGD-CBD	4.92	120.01	111.27
30	e	606	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
30	8	308	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
30	c	606	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
30	i	607	CHL	O2D-CGD-CBD	4.91	119.99	111.27
30	c	605	CHL	O2D-CGD-CBD	4.91	119.98	111.27
30	6	315	CHL	CHD-C4C-C3C	-4.90	117.64	124.84
33	6	501	0UR	C14-C15-C16	-4.90	120.32	127.31
32	M	102	8CT	C24-C25-C26	-4.90	120.32	127.31
30	5	307	CHL	C1D-ND-C4D	4.90	109.81	106.33
32	A	847	8CT	C04-C03-C02	-4.88	115.74	122.61
32	7	404	8CT	C01-C02-C03	-4.88	119.05	124.53
32	B	844	8CT	C30-C31-C32	-4.88	115.47	121.47
30	b	606	CHL	O2D-CGD-CBD	4.88	119.94	111.27
30	a	608	CHL	CHD-C4C-C3C	-4.88	117.67	124.84
37	g	522	0IE	C10-C9-C8	4.88	133.46	123.47
30	6	307	CHL	C2A-C1A-CHA	-4.87	115.34	123.86
32	J	104	8CT	C30-C31-C32	-4.87	115.48	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	305	CHL	C3B-C2B-C1B	-4.87	101.29	107.16
30	b	608	CHL	C2A-C1A-CHA	-4.86	115.36	123.86
42	c	523	NEX	C15-C14-C13	-4.86	120.37	127.31
32	2	402	8CT	C04-C03-C02	-4.86	115.77	122.61
30	b	609	CHL	C1D-ND-C4D	4.86	109.78	106.33
30	d	609	CHL	CHB-C1B-NB	-4.85	119.12	124.26
42	h	523	NEX	C15-C14-C13	-4.85	120.39	127.31
30	c	601	CHL	C2A-C1A-CHA	-4.85	115.38	123.86
30	8	305	CHL	O2D-CGD-CBD	4.85	119.89	111.27
30	c	606	CHL	O2D-CGD-CBD	4.85	119.88	111.27
30	f	614	CHL	O2D-CGD-CBD	4.84	119.88	111.27
30	i	614	CHL	O2D-CGD-CBD	4.84	119.88	111.27
32	B	848	8CT	C19-C18-C17	-4.84	113.55	123.47
30	a	605	CHL	O2D-CGD-CBD	4.84	119.87	111.27
32	L	206	8CT	C01-C02-C03	-4.84	119.10	124.53
30	f	609	CHL	CHB-C1B-NB	-4.84	119.14	124.26
30	f	606	CHL	C2A-C1A-CHA	-4.83	115.41	123.86
30	c	614	CHL	C1D-ND-C4D	4.83	109.77	106.33
33	c	520	0UR	C10-C11-C12	-4.83	120.41	127.31
42	g	523	NEX	C15-C14-C13	-4.83	120.42	127.31
30	9	306	CHL	C2A-C1A-CHA	-4.83	115.42	123.86
42	i	523	NEX	C15-C14-C13	-4.83	120.42	127.31
30	a	608	CHL	CHB-C1B-NB	-4.83	119.15	124.26
30	7	306	CHL	CHD-C4C-C3C	-4.82	117.75	124.84
42	f	523	NEX	C15-C14-C13	-4.82	120.43	127.31
30	5	307	CHL	CHB-C1B-NB	-4.82	119.16	124.26
32	6	402	8CT	C14-C15-C16	-4.81	112.89	126.42
30	g	605	CHL	C4A-NA-C1A	4.81	108.87	106.71
42	d	523	NEX	C15-C14-C13	-4.81	120.44	127.31
32	7	402	8CT	C01-C02-C03	-4.81	119.12	124.53
30	5	305	CHL	CHD-C4C-C3C	-4.81	117.77	124.84
30	h	606	CHL	CHB-C1B-NB	-4.80	119.17	124.26
42	b	523	NEX	C15-C14-C13	-4.80	120.46	127.31
32	8	406	8CT	C14-C13-C12	-4.80	120.46	127.31
42	a	523	NEX	C15-C14-C13	-4.80	120.46	127.31
30	d	609	CHL	C1D-ND-C4D	4.80	109.74	106.33
30	6	308	CHL	O2D-CGD-CBD	4.80	119.79	111.27
30	3	307	CHL	O2D-CGD-CBD	4.79	119.79	111.27
30	c	609	CHL	C1D-ND-C4D	4.79	109.74	106.33
30	8	308	CHL	C2A-C1A-CHA	-4.79	115.49	123.86
30	g	605	CHL	O2D-CGD-CBD	4.78	119.77	111.27
30	d	608	CHL	CHD-C4C-C3C	-4.78	117.81	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	9	401	8CT	C04-C03-C02	-4.78	115.88	122.61
32	L	205	8CT	C19-C20-C21	-4.77	120.50	127.31
30	a	609	CHL	O2D-CGD-CBD	4.77	119.75	111.27
30	h	608	CHL	CHB-C1B-NB	-4.77	119.20	124.26
30	b	607	CHL	O2D-CGD-CBD	4.77	119.75	111.27
30	4	308	CHL	CHD-C4C-C3C	-4.77	117.83	124.84
30	4	302	CHL	O2D-CGD-CBD	4.77	119.74	111.27
32	7	405	8CT	C18-C17-C16	-4.76	120.51	127.31
33	h	520	0UR	C10-C11-C12	-4.76	120.52	127.31
30	i	602	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
32	B	851	8CT	C19-C20-C21	-4.76	120.52	127.31
30	e	606	CHL	C2A-C1A-CHA	-4.76	115.54	123.86
32	8	402	8CT	C19-C20-C21	-4.75	120.53	127.31
32	A	850	8CT	C13-C14-C15	-4.75	108.39	123.22
30	e	609	CHL	CHD-C4C-C3C	-4.75	117.86	124.84
30	7	306	CHL	C3B-C2B-C1B	-4.75	101.43	107.16
32	A	854	8CT	C18-C17-C16	-4.75	120.53	127.31
33	9	502	0UR	C9-C8-C7	-4.75	120.53	127.31
42	e	523	NEX	O24-C25-C38	4.74	120.74	115.06
32	A	848	8CT	C19-C20-C21	-4.74	120.54	127.31
30	d	608	CHL	CHB-C1B-NB	-4.74	119.24	124.26
32	A	848	8CT	C10-C11-C12	-4.74	119.08	126.23
30	h	607	CHL	O2D-CGD-CBD	4.74	119.69	111.27
30	1	306	CHL	CHB-C1B-NB	-4.74	119.24	124.26
32	B	845	8CT	C30-C31-C32	-4.73	115.64	121.47
30	1	302	CHL	O2D-CGD-CBD	4.73	119.68	111.27
30	h	608	CHL	CHD-C4C-C3C	-4.73	117.89	124.84
32	J	104	8CT	C01-C02-C03	-4.73	119.22	124.53
30	d	606	CHL	CHB-C1B-NB	-4.72	119.26	124.26
30	3	305	CHL	C2A-C1A-CHA	-4.72	115.61	123.86
30	i	609	CHL	O2D-CGD-CBD	4.71	119.64	111.27
30	h	602	CHL	CHB-C1B-NB	-4.71	119.27	124.26
30	c	607	CHL	C1D-ND-C4D	4.71	109.68	106.33
32	B	844	8CT	C39-C16-C17	-4.71	116.32	122.92
32	7	404	8CT	C14-C15-C16	-4.71	113.19	126.42
30	f	605	CHL	O2D-CGD-CBD	4.71	119.63	111.27
30	9	305	CHL	O2D-CGD-CBD	4.70	119.62	111.27
30	2	313	CHL	C2A-C1A-CHA	-4.70	115.64	123.86
32	J	104	8CT	C24-C25-C26	-4.70	120.60	127.31
30	f	606	CHL	CMD-C2D-C3D	-4.70	116.81	127.61
30	1	313	CHL	C2A-C1A-CHA	-4.70	115.64	123.86
30	1	306	CHL	CHD-C4C-C3C	-4.69	117.94	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	601	CHL	C2A-C1A-CHA	-4.69	115.65	123.86
30	i	608	CHL	CHD-C4C-C3C	-4.69	117.95	124.84
30	b	607	CHL	CHD-C4C-C3C	-4.69	117.95	124.84
32	B	843	8CT	C10-C11-C12	-4.69	119.15	126.23
30	g	602	CHL	C1D-ND-C4D	4.67	109.66	106.33
32	4	402	8CT	C24-C25-C26	-4.67	120.64	127.31
30	b	601	CHL	O2D-CGD-CBD	4.67	119.57	111.27
42	c	523	NEX	C31-C30-C29	-4.67	120.65	127.31
30	0	306	CHL	CHB-C1B-NB	-4.67	119.31	124.26
32	4	402	8CT	C14-C13-C12	-4.67	120.65	127.31
32	B	845	8CT	C23-C21-C20	-4.66	111.78	118.94
30	6	308	CHL	C2A-C1A-CHA	-4.66	115.70	123.86
30	e	602	CHL	C2A-C1A-CHA	-4.66	115.70	123.86
42	d	523	NEX	C31-C30-C29	-4.66	120.66	127.31
33	1	502	0UR	C5-C4-C3	-4.66	121.41	127.00
30	f	606	CHL	CHD-C4C-C3C	-4.66	118.00	124.84
32	I	101	8CT	C19-C20-C21	-4.66	120.67	127.31
30	e	607	CHL	CHD-C4C-C3C	-4.65	118.00	124.84
30	h	606	CHL	C1D-ND-C4D	4.65	109.64	106.33
32	L	205	8CT	C10-C11-C12	-4.65	119.21	126.23
32	F	302	8CT	C01-C02-C03	-4.65	119.31	124.53
30	i	608	CHL	CHB-C1B-NB	-4.65	119.34	124.26
30	e	605	CHL	O2D-CGD-CBD	4.64	119.52	111.27
30	e	609	CHL	C1D-ND-C4D	4.64	109.63	106.33
42	a	523	NEX	C31-C30-C29	-4.64	120.69	127.31
32	A	854	8CT	C01-C02-C03	-4.64	119.32	124.53
32	7	405	8CT	C19-C20-C21	-4.64	120.69	127.31
33	1	502	0UR	C9-C8-C7	-4.64	120.69	127.31
42	f	523	NEX	C31-C30-C29	-4.63	120.70	127.31
42	i	523	NEX	C31-C30-C29	-4.63	120.70	127.31
42	a	523	NEX	C38-C25-C24	-4.63	109.07	114.28
30	a	608	CHL	C1D-ND-C4D	4.63	109.62	106.33
30	7	306	CHL	C2A-C1A-CHA	-4.63	115.77	123.86
42	g	523	NEX	C31-C30-C29	-4.62	120.71	127.31
30	8	302	CHL	O2D-CGD-CBD	4.62	119.48	111.27
33	6	502	0UR	C5-C4-C3	-4.62	121.45	127.00
30	5	307	CHL	O2D-CGD-CBD	4.62	119.47	111.27
30	c	605	CHL	C4A-NA-C1A	4.62	108.78	106.71
42	h	523	NEX	C31-C30-C29	-4.62	120.72	127.31
30	5	301	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
33	0	501	0UR	C4-C3-C2	-4.61	116.12	120.08
42	b	523	NEX	C31-C30-C29	-4.61	120.73	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	606	CHL	C1D-ND-C4D	4.61	109.61	106.33
32	8	406	8CT	C01-C02-C03	-4.61	119.35	124.53
30	d	606	CHL	C1D-ND-C4D	4.61	109.61	106.33
30	6	306	CHL	O2D-CGD-CBD	4.61	119.46	111.27
32	B	847	8CT	C01-C02-C03	-4.61	119.35	124.53
30	0	305	CHL	C2A-C1A-CHA	-4.61	115.80	123.86
30	5	307	CHL	CHD-C4C-C3C	-4.60	118.07	124.84
30	6	307	CHL	O2D-CGD-CBD	4.60	119.45	111.27
30	5	305	CHL	C2A-C1A-CHA	-4.60	115.81	123.86
42	a	523	NEX	O24-C25-C38	4.60	120.57	115.06
42	f	523	NEX	C38-C25-C24	-4.60	109.11	114.28
30	b	607	CHL	C1D-ND-C4D	4.60	109.60	106.33
32	A	848	8CT	C18-C17-C16	-4.60	120.75	127.31
30	0	306	CHL	C2A-C1A-CHA	-4.60	115.82	123.86
32	J	104	8CT	C15-C16-C17	4.60	125.99	118.94
30	d	608	CHL	C1D-ND-C4D	4.59	109.60	106.33
30	g	606	CHL	CHD-C4C-C3C	-4.59	118.09	124.84
30	5	306	CHL	O2D-CGD-CBD	4.59	119.43	111.27
42	c	523	NEX	O24-C25-C38	4.59	120.56	115.06
42	f	523	NEX	O24-C25-C38	4.59	120.56	115.06
42	g	523	NEX	O24-C25-C38	4.59	120.56	115.06
42	b	523	NEX	C38-C25-C24	-4.59	109.12	114.28
32	K	107	8CT	C10-C11-C12	-4.59	119.30	126.23
42	h	523	NEX	O24-C25-C38	4.59	120.55	115.06
30	c	614	CHL	CHD-C4C-C3C	-4.58	118.10	124.84
30	b	607	CHL	CHB-C1B-NB	-4.58	119.41	124.26
42	b	523	NEX	O24-C25-C38	4.58	120.55	115.06
30	1	307	CHL	O2D-CGD-CBD	4.58	119.41	111.27
30	g	607	CHL	O2D-CGD-CBD	4.58	119.40	111.27
32	B	846	8CT	C07-C02-C03	-4.58	116.09	122.73
30	a	602	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
42	c	523	NEX	C38-C25-C24	-4.57	109.13	114.28
30	h	606	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
30	c	606	CHL	C1D-ND-C4D	4.57	109.58	106.33
42	g	523	NEX	C38-C25-C24	-4.57	109.14	114.28
42	d	523	NEX	O24-C25-C38	4.57	120.53	115.06
42	h	523	NEX	C38-C25-C24	-4.57	109.14	114.28
30	g	606	CHL	CHB-C1B-NB	-4.57	119.42	124.26
33	g	520	0UR	C5-C4-C3	-4.57	121.52	127.00
42	d	523	NEX	C38-C25-C24	-4.57	109.14	114.28
42	i	523	NEX	C38-C25-C24	-4.56	109.14	114.28
30	4	307	CHL	O2D-CGD-CBD	4.56	119.37	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	e	607	CHL	CHB-C1B-NB	-4.56	119.43	124.26
42	i	523	NEX	O24-C25-C38	4.55	120.51	115.06
32	B	846	8CT	C19-C18-C17	-4.55	114.15	123.47
30	4	308	CHL	C1D-ND-C4D	4.55	109.57	106.33
30	h	608	CHL	C1D-ND-C4D	4.54	109.56	106.33
30	2	313	CHL	O2D-CGD-CBD	4.54	119.33	111.27
30	7	301	CHL	C2A-C1A-CHA	-4.54	115.93	123.86
30	7	313	CHL	CHB-C1B-NB	-4.54	119.46	124.26
30	i	608	CHL	C1D-ND-C4D	4.53	109.56	106.33
30	1	306	CHL	C1D-ND-C4D	4.53	109.55	106.33
32	8	406	8CT	C27-C26-C25	-4.53	116.58	122.92
30	e	614	CHL	O2D-CGD-CBD	4.52	119.31	111.27
30	1	307	CHL	C1D-ND-C4D	4.52	109.55	106.33
32	B	844	8CT	C10-C11-C12	-4.52	119.41	126.23
30	g	601	CHL	C4A-NA-C1A	4.52	108.74	106.71
30	9	301	CHL	C2A-C1A-CHA	-4.52	115.96	123.86
30	a	602	CHL	C2A-C1A-CHA	-4.51	115.97	123.86
37	e	522	0IE	C20-C3-C4	-4.51	119.03	124.83
32	B	847	8CT	C07-C02-C03	-4.51	116.19	122.73
32	G	104	8CT	C35-C30-C29	-4.51	107.00	112.70
32	J	101	8CT	C07-C02-C03	-4.50	116.19	122.73
30	b	609	CHL	O2D-CGD-CBD	4.50	119.27	111.27
30	8	315	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
30	e	609	CHL	C2A-C1A-CHA	-4.50	115.99	123.86
30	8	306	CHL	C2A-C1A-CHA	-4.50	115.99	123.86
32	I	101	8CT	C18-C17-C16	-4.50	120.89	127.31
30	4	308	CHL	C2A-C1A-CHA	-4.49	116.00	123.86
30	g	602	CHL	CHB-C1B-NB	-4.49	119.50	124.26
30	g	602	CHL	CHD-C4C-C3C	-4.49	118.24	124.84
30	a	608	CHL	O2D-CGD-CBD	4.49	119.25	111.27
30	e	609	CHL	O2D-CGD-CBD	4.49	119.25	111.27
30	b	609	CHL	CHB-C1B-NB	-4.48	119.52	124.26
30	a	606	CHL	CHD-C4C-C3C	-4.47	118.27	124.84
30	a	606	CHL	CHB-C1B-NB	-4.46	119.53	124.26
30	e	609	CHL	CHB-C1B-NB	-4.46	119.53	124.26
30	8	307	CHL	O2D-CGD-CBD	4.46	119.20	111.27
30	h	614	CHL	O2D-CGD-CBD	4.46	119.20	111.27
30	i	602	CHL	C1D-ND-C4D	4.46	109.50	106.33
30	f	609	CHL	O2D-CGD-CBD	4.45	119.18	111.27
30	2	302	CHL	CHC-C1C-NC	4.45	130.96	124.20
30	g	606	CHL	C1D-ND-C4D	4.45	109.50	106.33
33	6	501	0UR	C4-C3-C2	-4.44	116.27	120.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	605	CHL	C4A-NA-C1A	4.43	108.70	106.71
30	2	305	CHL	CMD-C2D-C3D	-4.42	117.45	127.61
30	e	607	CHL	C1D-ND-C4D	4.42	109.47	106.33
30	7	313	CHL	C1D-ND-C4D	4.41	109.47	106.33
30	c	606	CHL	CHB-C1B-NB	-4.41	119.59	124.26
32	B	851	8CT	C14-C13-C12	-4.41	121.02	127.31
32	B	848	8CT	C01-C02-C03	-4.41	119.58	124.53
30	a	614	CHL	C4A-NA-C1A	4.40	108.68	106.71
30	6	315	CHL	C2A-C1A-CHA	-4.40	116.17	123.86
32	1	402	8CT	C10-C11-C12	-4.40	119.59	126.23
30	d	606	CHL	CHD-C4C-C3C	-4.39	118.39	124.84
30	3	307	CHL	OBD-CAD-C3D	-4.39	117.95	128.52
32	I	101	8CT	C18-C19-C20	-4.39	114.48	123.47
32	G	104	8CT	C24-C25-C26	-4.39	121.05	127.31
32	B	851	8CT	C24-C25-C26	-4.39	121.05	127.31
30	4	302	CHL	CHC-C1C-NC	4.39	130.86	124.20
30	f	608	CHL	O2D-CGD-CBD	4.39	119.06	111.27
30	5	301	CHL	C1D-ND-C4D	4.38	109.45	106.33
30	h	614	CHL	C4A-NA-C1A	4.38	108.68	106.71
33	b	520	0UR	C10-C11-C12	-4.38	121.06	127.31
34	A	855	LHG	O7-C7-C8	4.38	120.93	111.50
30	2	307	CHL	O2D-CGD-CBD	4.37	119.04	111.27
32	3	403	8CT	C01-C02-C03	-4.37	119.62	124.53
30	c	607	CHL	CHD-C4C-C3C	-4.37	118.41	124.84
30	b	608	CHL	O2D-CGD-CBD	4.37	119.03	111.27
30	6	315	CHL	C1D-ND-C4D	4.37	109.44	106.33
30	8	301	CHL	C1D-ND-C4D	4.37	109.44	106.33
34	G	105	LHG	O7-C7-C8	4.36	120.91	111.50
32	B	845	8CT	C19-C20-C21	4.36	133.54	127.31
32	3	403	8CT	C07-C02-C03	-4.36	116.40	122.73
30	0	306	CHL	C1D-ND-C4D	4.36	109.43	106.33
33	h	520	0UR	C9-C8-C7	-4.36	121.09	127.31
30	f	614	CHL	CHD-C4C-C3C	-4.36	118.44	124.84
32	A	847	8CT	C10-C11-C12	-4.36	119.65	126.23
30	7	306	CHL	C1D-ND-C4D	4.36	109.43	106.33
30	g	606	CHL	C2A-C1A-CHA	-4.35	116.25	123.86
30	h	602	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
30	f	606	CHL	C1D-ND-C4D	4.35	109.42	106.33
30	e	608	CHL	C2A-C1A-CHA	-4.34	116.27	123.86
33	h	520	0UR	C14-C15-C16	-4.34	121.12	127.31
37	e	522	0IE	C10-C9-C8	4.34	132.36	123.47
30	5	302	CHL	CHC-C1C-NC	4.34	130.79	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	f	522	0IE	C10-C9-C8	4.34	132.36	123.47
30	b	601	CHL	CHD-C4C-C3C	-4.33	118.47	124.84
37	f	522	0IE	C23-C16-C15	-4.33	116.86	122.92
33	4	501	0UR	C43-C3-C2	4.33	126.83	116.66
32	I	101	8CT	C24-C25-C26	-4.33	121.14	127.31
30	c	609	CHL	CHB-C1B-NB	-4.33	119.68	124.26
30	c	609	CHL	C2A-C1A-CHA	-4.32	116.31	123.86
30	b	609	CHL	CHD-C4C-C3C	-4.32	118.50	124.84
32	B	845	8CT	C10-C11-C12	-4.31	119.72	126.23
32	3	403	8CT	C10-C11-C12	-4.31	119.73	126.23
30	1	307	CHL	CHB-C1B-NB	-4.30	119.70	124.26
30	8	301	CHL	C2A-C1A-CHA	-4.30	116.33	123.86
30	4	313	CHL	CHC-C1C-NC	4.30	130.73	124.20
30	1	307	CHL	CHA-C4D-ND	4.30	141.50	132.50
32	J	101	8CT	C01-C02-C03	-4.30	119.70	124.53
30	b	609	CHL	C2A-C1A-CHA	-4.30	116.34	123.86
30	a	607	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
33	3	501	0UR	C43-C3-C2	4.29	126.75	116.66
33	4	502	0UR	C10-C11-C12	-4.29	121.18	127.31
30	c	601	CHL	CHC-C1C-NC	4.29	130.72	124.20
37	i	522	0IE	C10-C9-C8	4.29	132.26	123.47
30	1	307	CHL	CMD-C2D-C3D	-4.29	117.75	127.61
37	h	521	0IE	C10-C9-C8	4.29	132.26	123.47
30	d	607	CHL	C4A-NA-C1A	4.29	108.63	106.71
32	B	845	8CT	C01-C02-C03	-4.28	119.72	124.53
33	1	502	0UR	C14-C15-C16	-4.28	121.20	127.31
32	B	844	8CT	C01-C02-C03	-4.28	119.72	124.53
37	h	522	0IE	C10-C9-C8	4.28	132.23	123.47
30	g	608	CHL	CHD-C4C-C3C	-4.27	118.56	124.84
33	2	501	0UR	C43-C3-C2	4.27	126.70	116.66
33	a	520	0UR	C10-C11-C12	-4.27	121.21	127.31
32	A	846	8CT	C04-C03-C02	-4.27	116.60	122.61
32	K	107	8CT	C04-C03-C02	-4.27	116.60	122.61
30	8	301	CHL	CHB-C1B-NB	-4.27	119.74	124.26
30	2	308	CHL	O2D-CGD-CBD	4.27	118.85	111.27
30	i	602	CHL	C2A-C1A-CHA	-4.27	116.40	123.86
30	c	609	CHL	CMD-C2D-C3D	-4.27	117.80	127.61
30	c	608	CHL	CHB-C1B-NB	-4.26	119.74	124.26
33	5	502	0UR	C29-C30-C31	-4.26	106.89	111.74
30	2	307	CHL	OBD-CAD-C3D	-4.26	118.27	128.52
32	J	101	8CT	C18-C19-C20	-4.26	114.75	123.47
30	i	602	CHL	CHB-C1B-NB	-4.26	119.75	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	502	0UR	C9-C8-C7	-4.26	121.23	127.31
32	B	851	8CT	C01-C02-C03	-4.26	119.75	124.53
30	2	307	CHL	CHD-C4C-NC	4.26	130.91	124.20
32	2	402	8CT	C24-C25-C26	-4.26	121.24	127.31
34	f	630	LHG	O7-C7-C8	4.25	120.66	111.50
30	e	601	CHL	CMD-C2D-C3D	-4.25	117.84	127.61
30	d	609	CHL	CHD-C4C-C3C	-4.25	118.60	124.84
30	e	607	CHL	C2A-C1A-CHA	-4.25	116.43	123.86
30	5	307	CHL	CMD-C2D-C3D	-4.24	117.85	127.61
30	d	601	CHL	CHD-C4C-C3C	-4.24	118.60	124.84
30	5	307	CHL	C2A-C1A-CHA	-4.24	116.45	123.86
32	G	104	8CT	C01-C02-C03	-4.24	119.77	124.53
30	3	307	CHL	CHA-C4D-ND	4.23	141.35	132.50
30	5	301	CHL	CHB-C1B-NB	-4.23	119.78	124.26
30	6	315	CHL	CHB-C1B-NB	-4.23	119.78	124.26
30	i	606	CHL	CMD-C2D-C3D	-4.23	117.89	127.61
32	A	849	8CT	C24-C25-C26	-4.23	121.28	127.31
32	L	205	8CT	C01-C02-C03	-4.23	119.78	124.53
30	2	313	CHL	CHA-C4D-ND	4.22	141.33	132.50
30	a	602	CHL	C1D-ND-C4D	4.22	109.33	106.33
33	i	520	0UR	C10-C11-C12	-4.22	121.29	127.31
32	3	402	8CT	C24-C25-C26	-4.22	121.29	127.31
30	2	305	CHL	CHA-C4D-ND	4.22	141.32	132.50
37	a	522	0IE	C10-C9-C8	4.22	132.11	123.47
30	e	608	CHL	O2D-CGD-CBD	4.22	118.76	111.27
33	g	520	0UR	C9-C8-C7	-4.21	121.30	127.31
32	3	402	8CT	C07-C02-C03	-4.21	116.62	122.73
30	a	601	CHL	CHD-C4C-C3C	-4.21	118.65	124.84
30	i	608	CHL	O2D-CGD-CBD	4.21	118.75	111.27
30	h	614	CHL	CMD-C2D-C3D	-4.20	117.94	127.61
30	7	307	CHL	O2D-CGD-CBD	4.20	118.73	111.27
30	f	606	CHL	CHA-C4D-ND	4.20	141.29	132.50
33	7	501	0UR	C43-C3-C2	4.20	126.53	116.66
33	1	501	0UR	C10-C11-C12	-4.20	121.32	127.31
33	2	502	0UR	C9-C8-C7	-4.20	121.32	127.31
30	i	606	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
30	1	305	CHL	CMD-C2D-C3D	-4.20	117.95	127.61
30	a	608	CHL	CHA-C4D-ND	4.20	141.28	132.50
30	c	608	CHL	O2D-CGD-CBD	4.20	118.72	111.27
30	d	608	CHL	O2D-CGD-CBD	4.19	118.72	111.27
30	b	601	CHL	CHA-C4D-ND	4.19	141.27	132.50
30	e	605	CHL	CHD-C4C-C3C	-4.19	118.68	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	601	CHL	C1D-ND-C4D	4.19	109.31	106.33
32	8	402	8CT	C14-C13-C12	-4.19	121.33	127.31
30	6	307	CHL	CHA-C4D-ND	4.19	141.26	132.50
30	6	313	CHL	CMD-C2D-C3D	-4.18	117.99	127.61
30	a	601	CHL	CHA-C4D-ND	4.18	141.25	132.50
30	d	606	CHL	C2A-C1A-CHA	-4.18	116.54	123.86
32	7	402	8CT	C04-C03-C02	-4.18	116.72	122.61
30	c	609	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
30	5	305	CHL	C1D-ND-C4D	4.18	109.31	106.33
30	c	608	CHL	C1D-ND-C4D	4.18	109.31	106.33
30	e	606	CHL	C1D-ND-C4D	4.18	109.31	106.33
30	5	306	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
33	5	501	0UR	C9-C8-C7	-4.17	121.35	127.31
30	4	307	CHL	C1-C2-C3	-4.17	120.00	126.75
30	1	307	CHL	C2A-C1A-CHA	-4.17	116.56	123.86
30	8	305	CHL	CMD-C2D-C3D	-4.17	118.02	127.61
32	3	403	8CT	C18-C17-C16	-4.17	121.36	127.31
30	4	307	CHL	CHC-C1C-NC	4.17	130.53	124.20
32	A	849	8CT	C19-C20-C21	-4.17	121.36	127.31
30	g	608	CHL	CHA-C4D-ND	4.17	141.22	132.50
37	i	522	0IE	C23-C16-C15	-4.17	117.09	122.92
32	7	404	8CT	C11-C12-C13	4.16	125.33	118.94
30	h	609	CHL	CMD-C2D-C3D	-4.16	118.03	127.61
34	5	601	LHG	O7-C7-C8	4.16	120.47	111.50
30	8	308	CHL	C1D-ND-C4D	4.16	109.29	106.33
30	e	614	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
30	e	608	CHL	CHA-C4D-ND	4.16	141.20	132.50
30	e	601	CHL	CHA-C4D-ND	4.16	141.20	132.50
30	e	608	CHL	C1D-ND-C4D	4.16	109.29	106.33
33	d	520	0UR	C10-C11-C12	-4.16	121.38	127.31
30	6	308	CHL	C1D-ND-C4D	4.15	109.28	106.33
30	8	301	CHL	CHA-C4D-ND	4.15	141.19	132.50
30	i	601	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
32	L	206	8CT	C07-C02-C03	-4.15	116.71	122.73
32	B	844	8CT	C19-C20-C21	-4.15	121.39	127.31
34	1	601	LHG	O7-C7-C8	4.15	120.44	111.50
30	5	305	CHL	CHB-C1B-NB	-4.15	119.87	124.26
30	d	614	CHL	CHA-C4D-ND	4.14	141.17	132.50
30	d	608	CHL	CHA-C4D-ND	4.14	141.17	132.50
32	8	406	8CT	C18-C17-C16	-4.14	121.40	127.31
30	a	614	CHL	CHA-C4D-ND	4.14	141.17	132.50
30	5	307	CHL	CHA-C4D-ND	4.14	141.16	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	I	101	8CT	C30-C31-C32	-4.14	116.37	121.47
34	K	106	LHG	O7-C7-C8	4.14	120.42	111.50
30	f	614	CHL	CHA-C4D-ND	4.14	141.16	132.50
32	M	102	8CT	C01-C02-C03	-4.14	119.88	124.53
30	f	609	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
30	f	608	CHL	CHA-C4D-ND	4.14	141.15	132.50
30	6	313	CHL	CHA-C4D-ND	4.14	141.15	132.50
32	M	102	8CT	C18-C17-C16	-4.13	121.41	127.31
32	B	847	8CT	C10-C11-C12	-4.13	119.99	126.23
30	1	313	CHL	CHB-C1B-NB	-4.13	119.88	124.26
30	h	608	CHL	O2D-CGD-CBD	4.13	118.61	111.27
30	a	606	CHL	C2A-C1A-CHA	-4.13	116.64	123.86
32	J	101	8CT	C04-C03-C02	-4.13	116.80	122.61
30	h	601	CHL	CHA-C4D-ND	4.13	141.13	132.50
30	h	607	CHL	C4A-NA-C1A	4.13	108.56	106.71
30	7	301	CHL	C1D-ND-C4D	4.12	109.27	106.33
30	9	306	CHL	C1D-ND-C4D	4.12	109.26	106.33
30	9	313	CHL	CMD-C2D-C3D	-4.12	118.13	127.61
30	h	601	CHL	CHD-C4C-C3C	-4.12	118.79	124.84
34	A	844	LHG	O7-C7-C8	4.12	120.37	111.50
34	9	601	LHG	O7-C7-C8	4.11	120.37	111.50
30	a	609	CHL	CMD-C2D-C3D	-4.11	118.15	127.61
34	7	602	LHG	O7-C7-C8	4.11	120.36	111.50
32	K	107	8CT	C24-C25-C26	-4.11	121.44	127.31
30	1	305	CHL	CHA-C4D-ND	4.11	141.10	132.50
30	6	308	CHL	CHB-C1B-NB	-4.11	119.90	124.26
30	e	608	CHL	CHB-C1B-NB	-4.11	119.90	124.26
32	I	101	8CT	C01-C02-C03	-4.11	119.91	124.53
32	F	302	8CT	C10-C11-C12	-4.11	120.02	126.23
33	2	502	0UR	C10-C11-C12	-4.11	121.44	127.31
32	A	849	8CT	C01-C02-C03	-4.11	119.91	124.53
30	b	614	CHL	CHD-C4C-C3C	-4.11	118.81	124.84
34	3	603	LHG	O7-C7-C8	4.11	120.35	111.50
30	c	606	CHL	CHA-C4D-ND	4.10	141.09	132.50
34	A	845	LHG	O7-C7-C8	4.10	120.35	111.50
30	d	605	CHL	CHA-C4D-ND	4.10	141.08	132.50
30	1	306	CHL	C2A-C1A-CHA	-4.10	116.69	123.86
33	8	501	0UR	C4-C3-C2	-4.10	116.56	120.08
30	c	605	CHL	CHA-C4D-ND	4.10	141.07	132.50
30	7	301	CHL	CHB-C1B-NB	-4.10	119.92	124.26
30	3	305	CHL	CHA-C4D-ND	4.10	141.07	132.50
32	I	101	8CT	C35-C30-C29	-4.10	107.52	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	313	CHL	CHA-C4D-ND	4.09	141.06	132.50
30	g	601	CHL	CHA-C4D-ND	4.09	141.06	132.50
30	f	605	CHL	CHA-C4D-ND	4.09	141.06	132.50
30	i	605	CHL	CHA-C4D-ND	4.09	141.05	132.50
30	7	313	CHL	CHA-C4D-ND	4.09	141.05	132.50
34	H	203	LHG	O7-C7-C8	4.09	120.31	111.50
30	f	609	CHL	CMD-C2D-C3D	-4.09	118.21	127.61
39	A	857	CL0	CHC-C4B-NB	4.09	128.58	124.26
30	0	301	CHL	CHA-C4D-ND	4.08	141.04	132.50
30	i	609	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
32	K	107	8CT	C35-C30-C29	-4.08	107.54	112.70
30	d	609	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
30	d	609	CHL	C2A-C1A-CHA	-4.08	116.72	123.86
30	b	608	CHL	CHA-C4D-ND	4.08	141.04	132.50
30	g	608	CHL	O2D-CGD-CBD	4.08	118.52	111.27
30	8	305	CHL	CHA-C4D-ND	4.08	141.04	132.50
30	i	608	CHL	CHA-C4D-ND	4.08	141.04	132.50
30	i	614	CHL	CHA-C4D-ND	4.08	141.03	132.50
30	1	313	CHL	C1D-ND-C4D	4.08	109.23	106.33
33	8	501	0UR	C10-C11-C12	-4.08	121.49	127.31
30	d	614	CHL	CMD-C2D-C3D	-4.08	118.23	127.61
30	9	301	CHL	CHA-C4D-ND	4.08	141.03	132.50
30	7	307	CHL	C2A-C1A-CHA	-4.08	116.73	123.86
30	e	606	CHL	CHB-C1B-NB	-4.08	119.94	124.26
30	0	301	CHL	O2D-CGD-CBD	4.08	118.51	111.27
30	f	601	CHL	CHB-C1B-NB	-4.08	119.94	124.26
30	7	307	CHL	CHA-C4D-ND	4.07	141.02	132.50
30	f	605	CHL	CMD-C2D-C3D	-4.07	118.24	127.61
30	h	607	CHL	CHD-C4C-C3C	-4.07	118.86	124.84
32	B	851	8CT	C18-C17-C16	-4.07	121.50	127.31
32	L	209	8CT	C18-C17-C16	-4.07	121.50	127.31
32	A	850	8CT	C18-C19-C20	4.07	131.81	123.47
32	O	205	8CT	C18-C17-C16	-4.07	121.50	127.31
32	M	102	8CT	C07-C02-C03	-4.07	116.82	122.73
30	e	605	CHL	CHA-C4D-ND	4.07	141.01	132.50
30	i	607	CHL	CHD-C4C-C3C	-4.07	118.86	124.84
37	c	521	0IE	C23-C16-C15	-4.07	117.23	122.92
30	h	605	CHL	CMD-C2D-C3D	-4.07	118.26	127.61
30	1	306	CHL	CHA-C4D-ND	4.07	141.00	132.50
30	h	608	CHL	CHA-C4D-ND	4.06	141.00	132.50
30	i	602	CHL	CHA-C4D-ND	4.06	141.00	132.50
33	d	520	0UR	C9-C8-C7	-4.06	121.51	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	306	CHL	CHA-C4D-ND	4.06	141.00	132.50
32	4	402	8CT	C35-C30-C29	-4.06	107.56	112.70
30	e	609	CHL	CMD-C2D-C3D	-4.06	118.27	127.61
30	c	608	CHL	CHA-C4D-ND	4.06	141.00	132.50
30	g	614	CHL	CMD-C2D-C3D	-4.06	118.27	127.61
32	A	847	8CT	C07-C02-C03	-4.06	116.84	122.73
34	3	601	LHG	O7-C7-C8	4.06	120.25	111.50
30	i	609	CHL	C4A-NA-C1A	4.06	108.53	106.71
34	6	601	LHG	O7-C7-C8	4.06	120.25	111.50
30	e	614	CHL	CHA-C4D-ND	4.06	140.99	132.50
30	e	606	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
30	f	606	CHL	CHB-C1B-NB	-4.06	119.96	124.26
37	g	522	0IE	C20-C3-C4	-4.06	119.61	124.83
30	e	609	CHL	CHA-C4D-ND	4.05	140.98	132.50
33	O	204	0UR	C43-C3-C4	-4.05	120.12	125.02
32	A	847	8CT	C01-C02-C03	-4.05	119.98	124.53
30	h	606	CHL	CHA-C4D-ND	4.05	140.97	132.50
30	7	301	CHL	CHA-C4D-ND	4.05	140.97	132.50
30	f	605	CHL	C4A-NA-C1A	4.05	108.53	106.71
30	8	313	CHL	CHA-C4D-ND	4.05	140.97	132.50
30	g	607	CHL	CHA-C4D-ND	4.05	140.97	132.50
32	L	205	8CT	C07-C02-C03	-4.05	116.86	122.73
30	e	608	CHL	CMD-C2D-C3D	-4.04	118.31	127.61
30	5	301	CHL	C2A-C1A-CHA	-4.04	116.79	123.86
30	i	614	CHL	CHD-C4C-C3C	-4.04	118.90	124.84
30	b	614	CHL	CHA-C4D-ND	4.04	140.95	132.50
30	8	306	CHL	CHC-C1C-NC	4.04	130.33	124.20
30	h	609	CHL	CHD-C4C-C3C	-4.03	118.91	124.84
30	i	614	CHL	C4A-NA-C1A	4.03	108.52	106.71
37	c	522	0IE	C23-C16-C15	-4.03	117.28	122.92
32	J	101	8CT	C24-C25-C26	-4.03	121.56	127.31
30	d	605	CHL	CMD-C2D-C3D	-4.03	118.35	127.61
30	9	301	CHL	CHC-C1C-NC	4.03	130.31	124.20
30	8	306	CHL	CHA-C4D-ND	4.03	140.93	132.50
30	8	315	CHL	CHA-C4D-ND	4.03	140.93	132.50
30	b	602	CHL	CAC-C3C-C4C	4.03	130.04	124.81
30	e	614	CHL	C4A-NA-C1A	4.03	108.52	106.71
30	d	607	CHL	CMD-C2D-C3D	-4.03	118.35	127.61
30	2	306	CHL	CHA-C4D-ND	4.03	140.92	132.50
30	9	305	CHL	CHA-C4D-ND	4.03	140.92	132.50
30	6	305	CHL	CHA-C4D-ND	4.03	140.92	132.50
32	A	848	8CT	C01-C02-C03	-4.03	120.01	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	606	CHL	CMD-C2D-C3D	-4.02	118.36	127.61
30	8	308	CHL	CHA-C4D-ND	4.02	140.91	132.50
37	f	521	0IE	C20-C3-C4	-4.02	119.66	124.83
30	i	607	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	g	605	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	h	614	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	e	606	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	e	602	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	0	305	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	f	601	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	4	305	CHL	CHA-C4D-ND	4.02	140.91	132.50
30	a	601	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
30	b	609	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
30	3	307	CHL	CMD-C2D-C3D	-4.02	118.37	127.61
30	7	307	CHL	C1D-ND-C4D	4.02	109.19	106.33
30	7	302	CHL	CHA-C4D-ND	4.02	140.90	132.50
34	g	630	LHG	O7-C7-C8	4.02	120.16	111.50
32	B	845	8CT	C07-C02-C03	-4.01	116.90	122.73
30	g	614	CHL	CHA-C4D-ND	4.01	140.90	132.50
30	5	305	CHL	CHA-C4D-ND	4.01	140.90	132.50
30	h	608	CHL	CMD-C2D-C3D	-4.01	118.38	127.61
33	9	501	0UR	C10-C11-C12	-4.01	121.58	127.31
30	g	607	CHL	C4A-NA-C1A	4.01	108.51	106.71
30	2	319	CHL	CHA-C4D-ND	4.01	140.89	132.50
32	7	402	8CT	C07-C02-C03	-4.01	116.91	122.73
30	5	313	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
30	b	606	CHL	CHA-C4D-ND	4.01	140.89	132.50
30	g	605	CHL	CMD-C2D-C3D	-4.01	118.39	127.61
30	f	607	CHL	CHA-C4D-ND	4.01	140.89	132.50
30	h	609	CHL	CHA-C4D-ND	4.01	140.88	132.50
30	a	607	CHL	CHA-C4D-ND	4.01	140.88	132.50
34	2	601	LHG	O7-C7-C8	4.01	120.14	111.50
30	b	614	CHL	CMD-C2D-C3D	-4.01	118.40	127.61
30	2	307	CHL	C1-C2-C3	-4.01	120.27	126.75
32	3	402	8CT	C39-C16-C15	4.01	124.39	118.08
32	O	205	8CT	C19-C20-C21	-4.01	121.59	127.31
30	c	614	CHL	CHA-C4D-ND	4.00	140.88	132.50
30	a	609	CHL	CHA-C4D-ND	4.00	140.87	132.50
30	2	313	CHL	C1D-ND-C4D	4.00	109.18	106.33
32	7	404	8CT	C35-C30-C29	-4.00	107.64	112.70
30	a	605	CHL	CHA-C4D-ND	4.00	140.87	132.50
34	i	630	LHG	O7-C7-C8	4.00	120.12	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	608	CHL	C2A-C1A-CHA	-4.00	116.86	123.86
30	b	607	CHL	C2A-C1A-CHA	-4.00	116.86	123.86
30	4	319	CHL	CHA-C4D-ND	4.00	140.87	132.50
30	6	306	CHL	CHC-C1C-NC	4.00	130.27	124.20
30	0	305	CHL	C1D-ND-C4D	4.00	109.18	106.33
30	i	606	CHL	CHA-C4D-ND	4.00	140.86	132.50
30	0	301	CHL	CHC-C1C-NC	4.00	130.27	124.20
30	b	601	CHL	CMD-C2D-C3D	-4.00	118.42	127.61
30	4	306	CHL	CHC-C1C-NC	4.00	130.27	124.20
30	8	307	CHL	CHA-C4D-ND	4.00	140.86	132.50
30	f	607	CHL	CHD-C4C-C3C	-4.00	118.97	124.84
32	I	101	8CT	C04-C03-C02	-4.00	116.99	122.61
30	f	609	CHL	CHA-C4D-ND	3.99	140.85	132.50
30	i	601	CHL	CMD-C2D-C3D	-3.99	118.43	127.61
30	c	601	CHL	CHA-C4D-ND	3.99	140.85	132.50
37	e	522	0IE	C23-C16-C15	-3.99	117.33	122.92
30	g	602	CHL	C2A-C1A-CHA	-3.99	116.88	123.86
30	h	601	CHL	CMD-C2D-C3D	-3.99	118.43	127.61
37	d	522	0IE	C10-C9-C8	3.99	131.65	123.47
30	i	614	CHL	CMD-C2D-C3D	-3.99	118.44	127.61
33	5	502	0UR	C5-C4-C3	-3.99	122.21	127.00
32	B	844	8CT	C22-C21-C20	-3.99	117.34	122.92
30	c	609	CHL	CHA-C4D-ND	3.99	140.84	132.50
30	6	306	CHL	CHA-C4D-ND	3.98	140.84	132.50
30	a	606	CHL	CMD-C2D-C3D	-3.98	118.45	127.61
30	8	313	CHL	CHC-C1C-NC	3.98	130.25	124.20
37	d	522	0IE	C9-C10-C11	3.98	131.63	123.47
30	a	614	CHL	CMD-C2D-C3D	-3.98	118.45	127.61
30	b	609	CHL	CHA-C4D-ND	3.98	140.83	132.50
37	h	521	0IE	C23-C16-C15	-3.98	117.34	122.92
30	a	601	CHL	C4A-NA-C1A	3.98	108.50	106.71
37	g	522	0IE	C23-C16-C15	-3.98	117.35	122.92
30	c	605	CHL	CMD-C2D-C3D	-3.98	118.46	127.61
42	g	523	NEX	C11-C10-C9	-3.98	121.63	127.31
30	b	608	CHL	CMD-C2D-C3D	-3.98	118.46	127.61
30	g	609	CHL	CMD-C2D-C3D	-3.98	118.46	127.61
30	9	313	CHL	CHA-C4D-ND	3.98	140.82	132.50
30	c	608	CHL	CMD-C2D-C3D	-3.98	118.47	127.61
30	7	305	CHL	CHA-C4D-ND	3.98	140.82	132.50
30	f	601	CHL	CMD-C2D-C3D	-3.98	118.47	127.61
30	0	305	CHL	CMD-C2D-C3D	-3.97	118.47	127.61
30	a	606	CHL	CHA-C4D-ND	3.97	140.81	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	602	CHL	CHC-C1C-NC	3.97	130.23	124.20
33	i	520	0UR	C9-C8-C7	-3.97	121.64	127.31
30	4	307	CHL	CHA-C4D-ND	3.97	140.81	132.50
32	0	401	8CT	C18-C17-C16	-3.97	121.64	127.31
30	2	307	CHL	CHA-C4D-ND	3.97	140.81	132.50
30	6	315	CHL	CHA-C4D-ND	3.97	140.81	132.50
32	7	404	8CT	C04-C03-C02	-3.97	117.02	122.61
30	8	313	CHL	CMD-C2D-C3D	-3.97	118.49	127.61
30	a	605	CHL	CMD-C2D-C3D	-3.97	118.49	127.61
30	g	606	CHL	CMD-C2D-C3D	-3.97	118.49	127.61
30	2	301	CHL	CHA-C4D-ND	3.97	140.80	132.50
42	f	523	NEX	C11-C10-C9	-3.97	121.65	127.31
30	1	302	CHL	CHC-C1C-NC	3.96	130.22	124.20
30	5	305	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
30	6	302	CHL	C1-C2-C3	-3.96	119.19	126.04
30	g	601	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
42	a	523	NEX	C11-C10-C9	-3.96	121.66	127.31
30	a	607	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
30	g	608	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
30	c	601	CHL	C3B-C4B-NB	3.96	114.19	110.52
30	9	306	CHL	CHA-C4D-ND	3.96	140.79	132.50
34	B	854	LHG	O7-C7-C8	3.96	120.04	111.50
30	f	614	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
30	d	601	CHL	CHA-C4D-ND	3.96	140.78	132.50
30	4	308	CHL	CHA-C4D-ND	3.96	140.78	132.50
30	i	602	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
30	5	305	CHL	CHC-C1C-NC	3.96	130.21	124.20
30	4	306	CHL	CHA-C4D-ND	3.96	140.78	132.50
32	8	406	8CT	C19-C20-C21	-3.96	121.66	127.31
34	a	630	LHG	O7-C7-C8	3.96	120.03	111.50
30	g	607	CHL	CMD-C2D-C3D	-3.96	118.51	127.61
30	5	313	CHL	CHA-C4D-ND	3.95	140.77	132.50
30	e	602	CHL	CMD-C2D-C3D	-3.95	118.52	127.61
30	3	307	CHL	CHD-C4C-NC	3.95	130.43	124.20
34	e	630	LHG	O7-C7-C8	3.95	120.01	111.50
42	b	523	NEX	C11-C10-C9	-3.95	121.67	127.31
30	8	315	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
30	d	608	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
37	b	522	0IE	C23-C16-C15	-3.95	117.39	122.92
32	B	846	8CT	C30-C31-C32	-3.95	116.61	121.47
37	g	521	0IE	C23-C16-C15	-3.95	117.39	122.92
42	d	523	NEX	C11-C10-C9	-3.95	121.68	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	0	601	LHG	O7-C7-C8	3.94	120.00	111.50
30	b	607	CHL	CHA-C4D-ND	3.94	140.75	132.50
37	f	521	0IE	C23-C16-C15	-3.94	117.40	122.92
32	3	402	8CT	C10-C11-C12	-3.94	120.28	126.23
30	i	605	CHL	CMD-C2D-C3D	-3.94	118.55	127.61
30	5	313	CHL	C4A-NA-C1A	3.94	108.48	106.71
37	h	522	0IE	C23-C16-C15	-3.94	117.41	122.92
37	a	522	0IE	C23-C16-C15	-3.94	117.41	122.92
42	e	523	NEX	C11-C10-C9	-3.94	121.69	127.31
33	e	520	0UR	C9-C8-C7	-3.94	121.69	127.31
42	i	523	NEX	C11-C10-C9	-3.94	121.69	127.31
30	6	308	CHL	CHA-C4D-ND	3.94	140.73	132.50
30	8	315	CHL	C2A-C1A-CHA	-3.93	116.98	123.86
30	5	306	CHL	CMD-C2D-C3D	-3.93	118.56	127.61
30	i	601	CHL	CHA-C4D-ND	3.93	140.73	132.50
42	h	523	NEX	C11-C10-C9	-3.93	121.70	127.31
30	d	607	CHL	CHA-C4D-ND	3.93	140.72	132.50
32	4	402	8CT	C10-C11-C12	-3.93	120.29	126.23
37	a	521	0IE	C23-C16-C15	-3.93	117.42	122.92
30	6	307	CHL	OBD-CAD-C3D	-3.93	119.06	128.52
30	8	306	CHL	CMD-C2D-C3D	-3.93	118.57	127.61
30	5	306	CHL	CHA-C4D-ND	3.93	140.72	132.50
30	h	607	CHL	CMD-C2D-C3D	-3.93	118.58	127.61
37	g	521	0IE	C10-C9-C8	3.93	131.52	123.47
30	d	606	CHL	CHA-C4D-ND	3.93	140.71	132.50
30	2	319	CHL	CMD-C2D-C3D	-3.93	118.58	127.61
30	e	609	CHL	OBD-CAD-C3D	-3.93	119.07	128.52
30	d	609	CHL	CHA-C4D-ND	3.92	140.71	132.50
30	6	302	CHL	CHC-C1C-NC	3.92	130.15	124.20
30	f	608	CHL	CMD-C2D-C3D	-3.92	118.59	127.61
32	9	401	8CT	C14-C13-C12	-3.92	121.71	127.31
34	h	630	LHG	O7-C7-C8	3.92	119.95	111.50
33	c	520	0UR	C34-C27-C1	-3.92	119.34	124.49
30	8	302	CHL	CHC-C1C-NC	3.92	130.15	124.20
30	e	607	CHL	CMD-C2D-C3D	-3.92	118.59	127.61
32	B	843	8CT	C07-C02-C03	-3.92	117.04	122.73
30	5	301	CHL	CHA-C4D-ND	3.92	140.70	132.50
30	7	313	CHL	C2A-C1A-CHA	-3.92	117.01	123.86
30	f	609	CHL	C2A-C1A-CHA	-3.92	117.01	123.86
30	2	306	CHL	C1D-ND-C4D	3.92	109.12	106.33
33	2	501	0UR	C10-C11-C12	-3.92	121.72	127.31
33	7	501	0UR	C10-C11-C12	-3.92	121.72	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	607	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
30	g	606	CHL	CHA-C4D-ND	3.92	140.69	132.50
42	c	523	NEX	C11-C10-C9	-3.92	121.72	127.31
30	2	306	CHL	CMD-C2D-C3D	-3.91	118.61	127.61
30	a	602	CHL	CMD-C2D-C3D	-3.91	118.61	127.61
30	g	609	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
32	A	848	8CT	C14-C13-C12	-3.91	121.73	127.31
30	5	313	CHL	CMD-C2D-C3D	-3.91	118.61	127.61
32	B	843	8CT	C01-C02-C03	-3.91	120.14	124.53
30	f	607	CHL	CMD-C2D-C3D	-3.91	118.62	127.61
32	B	848	8CT	C14-C13-C12	-3.91	121.73	127.31
30	8	313	CHL	C3B-C4B-NB	3.91	114.14	110.52
30	9	301	CHL	C1D-ND-C4D	3.91	109.11	106.33
37	f	522	0IE	C20-C3-C4	-3.91	119.80	124.83
34	7	601	LHG	O7-C7-C8	3.91	119.92	111.50
30	f	602	CHL	CHA-C4D-ND	3.91	140.67	132.50
30	6	307	CHL	CMD-C2D-C3D	-3.91	118.63	127.61
30	a	608	CHL	CMD-C2D-C3D	-3.90	118.63	127.61
30	4	302	CHL	CHA-C4D-ND	3.90	140.66	132.50
30	5	306	CHL	C2A-C1A-CHA	-3.90	117.03	123.86
30	i	609	CHL	CHA-C4D-ND	3.90	140.66	132.50
30	7	306	CHL	CHA-C4D-ND	3.90	140.66	132.50
30	e	605	CHL	CMD-C2D-C3D	-3.90	118.64	127.61
30	4	313	CHL	C3B-C4B-NB	3.90	114.13	110.52
32	6	402	8CT	C11-C12-C13	3.90	124.92	118.94
30	7	306	CHL	CHC-C1C-NC	3.90	130.12	124.20
37	c	522	0IE	C10-C9-C8	3.90	131.46	123.47
30	e	607	CHL	CHA-C4D-ND	3.90	140.65	132.50
34	d	630	LHG	O7-C7-C8	3.90	119.90	111.50
30	6	315	CHL	CMD-C2D-C3D	-3.89	118.66	127.61
30	h	606	CHL	CMD-C2D-C3D	-3.89	118.66	127.61
30	2	308	CHL	CHA-C4D-ND	3.89	140.64	132.50
30	0	302	CHL	CHA-C4D-ND	3.89	140.64	132.50
30	g	609	CHL	CHA-C4D-ND	3.89	140.64	132.50
30	e	601	CHL	CHC-C1C-NC	3.89	130.11	124.20
30	f	607	CHL	C4A-NA-C1A	3.89	108.45	106.71
32	9	401	8CT	C07-C02-C03	-3.89	117.08	122.73
33	6	501	0UR	C34-C27-C1	-3.89	119.39	124.49
32	B	846	8CT	C11-C12-C13	3.89	124.91	118.94
30	c	607	CHL	CHA-C4D-ND	3.89	140.63	132.50
30	i	606	CHL	C2A-C1A-CHA	-3.89	117.06	123.86
37	e	521	0IE	C23-C16-C15	-3.88	117.48	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	g	602	CHL	CMD-C2D-C3D	-3.88	118.68	127.61
30	e	602	CHL	CHC-C1C-NC	3.88	130.09	124.20
30	d	601	CHL	CMD-C2D-C3D	-3.88	118.68	127.61
32	2	402	8CT	C22-C21-C20	-3.88	117.49	122.92
30	7	301	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
30	h	606	CHL	C2A-C1A-CHA	-3.88	117.08	123.86
34	B	852	LHG	O7-C7-C8	3.88	119.86	111.50
30	h	614	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
30	c	607	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
32	B	851	8CT	C07-C02-C03	-3.88	117.10	122.73
37	b	522	0IE	C10-C9-C8	3.88	131.42	123.47
30	h	605	CHL	CHA-C4D-ND	3.88	140.61	132.50
30	h	602	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
30	8	307	CHL	C1-C2-C3	-3.88	120.48	126.75
30	i	608	CHL	CMD-C2D-C3D	-3.88	118.70	127.61
30	3	302	CHL	CHA-C4D-ND	3.87	140.60	132.50
33	g	520	0UR	C43-C3-C4	-3.87	120.34	125.02
30	2	302	CHL	CHA-C4D-ND	3.87	140.59	132.50
30	a	602	CHL	CHB-C1B-NB	-3.87	120.16	124.26
30	6	313	CHL	C1D-ND-C4D	3.87	109.08	106.33
30	i	607	CHL	CMD-C2D-C3D	-3.87	118.72	127.61
30	g	607	CHL	CHD-C4C-C3C	-3.86	119.16	124.84
30	4	308	CHL	CHB-C1B-NB	-3.86	120.17	124.26
30	8	301	CHL	CMD-C2D-C3D	-3.86	118.73	127.61
30	c	601	CHL	CMD-C2D-C3D	-3.86	118.74	127.61
30	4	313	CHL	CHA-C4D-ND	3.86	140.57	132.50
30	b	602	CHL	CHC-C1C-NC	3.86	130.05	124.20
30	b	606	CHL	C1D-ND-C4D	3.86	109.07	106.33
32	0	401	8CT	C10-C11-C12	-3.85	120.41	126.23
30	c	606	CHL	C2A-C1A-CHA	-3.85	117.12	123.86
34	b	630	LHG	O7-C7-C8	3.85	119.81	111.50
30	5	301	CHL	CMD-C2D-C3D	-3.85	118.75	127.61
30	1	305	CHL	CHC-C1C-NC	3.85	130.05	124.20
30	i	601	CHL	C4A-NA-C1A	3.85	108.44	106.71
30	e	614	CHL	CMD-C2D-C3D	-3.85	118.75	127.61
30	g	602	CHL	CHA-C4D-ND	3.85	140.55	132.50
30	2	306	CHL	CHC-C1C-NC	3.85	130.04	124.20
30	5	302	CHL	CHA-C4D-ND	3.85	140.55	132.50
30	a	602	CHL	CHA-C4D-ND	3.85	140.55	132.50
30	c	607	CHL	C2A-C1A-CHA	-3.85	117.13	123.86
30	h	607	CHL	CHA-C4D-ND	3.85	140.55	132.50
30	3	302	CHL	CHD-C4C-NC	3.85	130.26	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	302	CHL	CHA-C4D-ND	3.85	140.54	132.50
30	7	305	CHL	CMD-C2D-C3D	-3.84	118.77	127.61
30	e	608	CHL	CHC-C1C-NC	3.84	130.03	124.20
30	1	302	CHL	CAC-C3C-C4C	3.84	129.80	124.81
37	b	521	0IE	C23-C16-C15	-3.84	117.54	122.92
30	c	602	CHL	CHA-C4D-ND	3.84	140.54	132.50
30	2	301	CHL	CMD-C2D-C3D	-3.84	118.78	127.61
30	0	306	CHL	CMD-C2D-C3D	-3.84	118.78	127.61
32	B	846	8CT	C40-C12-C13	-3.84	117.55	122.92
32	8	402	8CT	C10-C11-C12	-3.84	120.44	126.23
30	e	602	CHL	C1D-ND-C4D	3.84	109.06	106.33
30	i	609	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
30	1	306	CHL	CMD-C2D-C3D	-3.84	118.79	127.61
32	9	401	8CT	C30-C31-C32	-3.84	116.75	121.47
30	8	302	CHL	CAC-C3C-C4C	3.84	129.79	124.81
32	7	402	8CT	C24-C25-C26	-3.83	121.84	127.31
30	8	302	CHL	CHA-C4D-ND	3.83	140.52	132.50
32	L	209	8CT	C14-C15-C16	-3.83	115.65	126.42
37	d	521	0IE	C23-C16-C15	-3.83	117.56	122.92
30	f	608	CHL	C3B-C4B-NB	3.83	114.07	110.52
30	7	313	CHL	CMD-C2D-C3D	-3.83	118.81	127.61
32	A	846	8CT	C07-C02-C03	-3.83	117.17	122.73
34	8	601	LHG	O7-C7-C8	3.83	119.75	111.50
30	9	301	CHL	CHB-C1B-NB	-3.83	120.21	124.26
30	c	606	CHL	CMD-C2D-C3D	-3.82	118.82	127.61
30	h	602	CHL	CHA-C4D-ND	3.82	140.50	132.50
30	9	301	CHL	CMD-C2D-C3D	-3.82	118.82	127.61
30	b	602	CHL	CHA-C4D-ND	3.82	140.49	132.50
30	1	313	CHL	CMD-C2D-C3D	-3.82	118.82	127.61
37	e	521	0IE	C10-C9-C8	3.82	131.30	123.47
30	8	308	CHL	CMD-C2D-C3D	-3.82	118.83	127.61
30	7	307	CHL	CMD-C2D-C3D	-3.82	118.83	127.61
30	3	302	CHL	CHC-C1C-NC	3.82	130.00	124.20
33	8	502	0UR	C5-C4-C3	-3.82	122.41	127.00
37	i	521	0IE	C23-C16-C15	-3.82	117.58	122.92
30	2	302	CHL	CAC-C3C-C4C	3.82	129.76	124.81
30	d	602	CHL	CHA-C4D-ND	3.82	140.48	132.50
33	8	501	0UR	C34-C27-C1	-3.82	119.48	124.49
30	6	307	CHL	CHC-C1C-NC	3.82	129.99	124.20
30	4	308	CHL	CMD-C2D-C3D	-3.81	118.84	127.61
30	7	302	CHL	CMD-C2D-C3D	-3.81	118.84	127.61
30	a	609	CHL	CHD-C4C-C3C	-3.81	119.24	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	302	CHL	CHC-C1C-NC	3.81	129.99	124.20
30	b	608	CHL	CHC-C1C-NC	3.81	129.99	124.20
30	8	306	CHL	C1D-ND-C4D	3.81	109.04	106.33
30	f	606	CHL	CHC-C1C-NC	3.81	129.98	124.20
30	c	614	CHL	CMD-C2D-C3D	-3.81	118.86	127.61
30	g	601	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
33	e	520	0UR	C10-C11-C12	-3.80	121.88	127.31
30	e	605	CHL	C4A-NA-C1A	3.80	108.42	106.71
30	2	301	CHL	C1D-ND-C4D	3.80	109.04	106.33
30	a	605	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
30	b	606	CHL	CMD-C2D-C3D	-3.80	118.87	127.61
30	1	306	CHL	CHC-C1C-NC	3.80	129.97	124.20
32	2	402	8CT	C35-C30-C29	-3.80	107.90	112.70
39	A	857	CL0	C2D-C1D-ND	-3.80	107.31	110.10
30	3	305	CHL	CHC-C1C-NC	3.80	129.96	124.20
30	d	614	CHL	CHD-C4C-C3C	-3.80	119.26	124.84
32	O	205	8CT	C07-C02-C03	-3.80	117.22	122.73
30	a	614	CHL	CHD-C4C-C3C	-3.79	119.26	124.84
30	4	305	CHL	CMD-C2D-C3D	-3.79	118.89	127.61
32	L	206	8CT	C19-C20-C21	-3.79	121.90	127.31
30	6	306	CHL	C3B-C4B-NB	3.79	114.03	110.52
30	4	307	CHL	C3B-C4B-NB	3.79	114.03	110.52
30	6	305	CHL	CMD-C2D-C3D	-3.79	118.89	127.61
30	d	602	CHL	CHC-C1C-NC	3.79	129.96	124.20
30	g	605	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
30	7	306	CHL	CMD-C2D-C3D	-3.79	118.90	127.61
30	f	608	CHL	CHC-C1C-NC	3.79	129.95	124.20
30	8	307	CHL	CMD-C2D-C3D	-3.79	118.91	127.61
37	c	522	0IE	C9-C10-C11	3.78	131.23	123.47
30	6	306	CHL	CMD-C2D-C3D	-3.78	118.91	127.61
30	c	602	CHL	CAC-C3C-C4C	3.78	129.72	124.81
30	3	307	CHL	CHC-C1C-NC	3.78	129.94	124.20
32	O	205	8CT	C30-C31-C32	-3.78	116.81	121.47
37	7	502	0IE	C23-C16-C15	-3.78	117.62	122.92
34	6	603	LHG	O7-C7-C8	3.78	119.65	111.50
37	a	521	0IE	C10-C9-C8	3.78	131.22	123.47
30	f	605	CHL	CHD-C4C-C3C	-3.78	119.28	124.84
30	6	301	CHL	CHA-C4D-ND	3.78	140.41	132.50
32	B	845	8CT	C35-C30-C29	-3.78	107.92	112.70
34	7	603	LHG	O7-C7-C8	3.78	119.65	111.50
30	4	306	CHL	CMD-C2D-C3D	-3.78	118.92	127.61
30	i	605	CHL	CHD-C4C-C3C	-3.78	119.29	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	L	209	8CT	C07-C02-C03	-3.78	117.25	122.73
30	7	302	CHL	CHD-C4C-NC	3.77	130.15	124.20
30	f	602	CHL	CAC-C3C-C4C	3.77	129.71	124.81
30	4	307	CHL	OBD-CAD-C3D	-3.77	119.44	128.52
32	A	847	8CT	C19-C20-C21	-3.77	121.93	127.31
30	a	609	CHL	C4A-NA-C1A	3.77	108.40	106.71
30	0	301	CHL	CMD-C2D-C3D	-3.77	118.94	127.61
30	b	608	CHL	C3B-C4B-NB	3.77	114.01	110.52
35	0	603	SQD	C44-O6-C1	3.77	121.10	113.74
34	4	601	LHG	O7-C7-C8	3.77	119.62	111.50
30	6	302	CHL	CHA-C4D-ND	3.77	140.38	132.50
30	8	305	CHL	CHC-C1C-NC	3.77	129.92	124.20
30	a	608	CHL	C2A-C1A-CHA	-3.76	117.28	123.86
32	6	402	8CT	C19-C20-C21	-3.76	121.94	127.31
30	0	301	CHL	C1D-ND-C4D	3.76	109.00	106.33
34	c	630	LHG	O7-C7-C8	3.76	119.60	111.50
30	3	305	CHL	CMD-C2D-C3D	-3.76	118.97	127.61
30	b	607	CHL	CMD-C2D-C3D	-3.76	118.97	127.61
30	8	305	CHL	CHB-C1B-NB	-3.75	120.29	124.26
30	8	305	CHL	C1D-ND-C4D	3.75	109.00	106.33
30	2	313	CHL	CHB-C1B-NB	-3.75	120.29	124.26
32	B	804	8CT	C35-C30-C29	-3.74	107.97	112.70
30	4	319	CHL	CMD-C2D-C3D	-3.74	119.01	127.61
37	3	502	0IE	C23-C16-C15	-3.74	117.68	122.92
30	5	302	CHL	CMD-C2D-C3D	-3.74	119.01	127.61
30	8	306	CHL	CHB-C1B-NB	-3.74	120.30	124.26
33	e	520	0UR	C43-C3-C2	3.74	125.44	116.66
30	c	605	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
30	0	302	CHL	CHC-C1C-NC	3.74	129.87	124.20
30	2	313	CHL	CMD-C2D-C3D	-3.74	119.02	127.61
33	5	502	0UR	C34-C27-C1	-3.74	119.58	124.49
30	e	601	CHL	C3B-C4B-NB	3.74	113.98	110.52
34	M	104	LHG	O7-C7-C8	3.73	119.55	111.50
30	d	602	CHL	CMD-C2D-C3D	-3.73	119.02	127.61
37	i	521	0IE	C10-C9-C8	3.73	131.12	123.47
30	d	601	CHL	C4A-NA-C1A	3.73	108.38	106.71
30	7	307	CHL	CHB-C1B-NB	-3.73	120.31	124.26
30	3	305	CHL	C1D-ND-C4D	3.73	108.98	106.33
30	h	605	CHL	CHD-C4C-C3C	-3.73	119.36	124.84
30	8	306	CHL	C3B-C4B-NB	3.72	113.97	110.52
30	6	301	CHL	CMD-C2D-C3D	-3.72	119.05	127.61
30	9	305	CHL	CMD-C2D-C3D	-3.72	119.05	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	602	CHL	CMD-C2D-C3D	-3.72	119.05	127.61
30	4	305	CHL	CHC-C1C-NC	3.72	129.85	124.20
30	7	307	CHL	CHD-C4C-NC	3.72	130.07	124.20
30	9	306	CHL	CHC-C1C-NC	3.72	129.85	124.20
30	4	302	CHL	CMD-C2D-C3D	-3.72	119.06	127.61
32	B	847	8CT	C18-C19-C20	-3.72	115.85	123.47
30	4	307	CHL	CMD-C2D-C3D	-3.72	119.06	127.61
32	A	846	8CT	C19-C20-C21	-3.72	122.00	127.31
37	f	521	0IE	C10-C9-C8	3.72	131.09	123.47
30	9	313	CHL	C1D-ND-C4D	3.71	108.97	106.33
30	h	609	CHL	C2A-C1A-CHA	-3.71	117.36	123.86
30	9	306	CHL	CMD-C2D-C3D	-3.71	119.08	127.61
37	d	522	0IE	C22-C12-C11	-3.71	117.73	122.92
30	1	302	CHL	C1-C2-C3	-3.71	119.63	126.04
30	8	302	CHL	CHD-C4C-NC	3.71	130.05	124.20
33	7	501	0UR	C9-C8-C7	-3.71	122.02	127.31
30	b	614	CHL	C4A-NA-C1A	3.71	108.37	106.71
30	b	608	CHL	C1D-ND-C4D	3.71	108.97	106.33
30	e	601	CHL	C1D-ND-C4D	3.71	108.97	106.33
30	2	301	CHL	CHC-C1C-NC	3.70	129.82	124.20
37	d	521	0IE	C10-C9-C8	3.70	131.06	123.47
30	i	608	CHL	C2A-C1A-CHA	-3.70	117.39	123.86
30	2	305	CHL	CHC-C1C-NC	3.70	129.82	124.20
33	1	502	0UR	C43-C3-C4	-3.70	120.55	125.02
32	L	206	8CT	C35-C30-C29	-3.70	108.02	112.70
37	g	522	0IE	C21-C7-C8	-3.70	117.74	122.92
30	8	302	CHL	C1-C2-C3	-3.70	119.65	126.04
30	6	307	CHL	CHD-C4C-NC	3.69	130.02	124.20
30	6	308	CHL	CMD-C2D-C3D	-3.69	119.12	127.61
37	c	522	0IE	C21-C7-C8	-3.69	117.75	122.92
32	I	101	8CT	C07-C02-C03	-3.69	117.37	122.73
33	1	501	0UR	C34-C27-C1	-3.69	119.65	124.49
30	e	601	CHL	CHB-C1B-NB	-3.69	120.35	124.26
32	A	846	8CT	C01-C02-C03	-3.69	120.39	124.53
33	h	520	0UR	C5-C4-C3	-3.69	122.57	127.00
30	8	307	CHL	CHC-C1C-NC	3.69	129.80	124.20
32	L	205	8CT	C01-C02-C07	3.69	120.70	113.62
33	2	502	0UR	C34-C27-C1	-3.68	119.66	124.49
33	3	501	0UR	C29-C30-C31	-3.68	107.55	111.74
30	i	608	CHL	CHC-C1C-NC	3.68	129.79	124.20
32	A	850	8CT	C39-C16-C15	3.68	123.88	118.08
30	0	302	CHL	CMD-C2D-C3D	-3.68	119.15	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	502	0UR	C34-C27-C1	-3.68	119.66	124.49
30	b	602	CHL	CMD-C2D-C3D	-3.68	119.15	127.61
30	c	601	CHL	C1D-ND-C4D	3.68	108.95	106.33
30	6	313	CHL	CHC-C1C-NC	3.68	129.78	124.20
30	1	313	CHL	CHC-C1C-NC	3.68	129.78	124.20
30	9	305	CHL	CHC-C1C-NC	3.68	129.78	124.20
30	f	614	CHL	CHC-C1C-NC	3.68	129.78	124.20
30	d	608	CHL	C2A-C1A-CHA	-3.67	117.43	123.86
30	e	601	CHL	C1-C2-C3	-3.67	120.81	126.75
32	B	844	8CT	C14-C13-C12	-3.67	122.07	127.31
30	2	307	CHL	CMD-C2D-C3D	-3.67	119.17	127.61
32	7	404	8CT	C40-C12-C13	-3.67	117.78	122.92
33	8	502	0UR	O44-C45-C46	3.67	121.31	111.55
30	d	605	CHL	CHD-C4C-C3C	-3.67	119.44	124.84
30	2	302	CHL	CMD-C2D-C3D	-3.67	119.17	127.61
30	h	608	CHL	C2A-C1A-CHA	-3.67	117.44	123.86
33	8	502	0UR	C10-C11-C12	-3.67	122.08	127.31
30	c	606	CHL	CAC-C3C-C4C	3.66	129.56	124.81
30	e	602	CHL	CAC-C3C-C4C	3.66	129.56	124.81
30	3	302	CHL	CMD-C2D-C3D	-3.66	119.19	127.61
30	2	308	CHL	C1D-ND-C4D	3.66	108.94	106.33
30	2	306	CHL	CHB-C1B-NB	-3.66	120.38	124.26
30	f	602	CHL	CHC-C1C-NC	3.66	129.75	124.20
33	2	501	0UR	C9-C8-C7	-3.66	122.09	127.31
30	f	608	CHL	OBD-CAD-C3D	-3.66	119.72	128.52
30	7	301	CHL	CHC-C1C-NC	3.66	129.75	124.20
30	7	305	CHL	CHC-C1C-NC	3.66	129.75	124.20
30	4	307	CHL	CHD-C4C-NC	3.65	129.96	124.20
30	0	305	CHL	CHB-C1B-NB	-3.65	120.39	124.26
30	4	302	CHL	CAC-C3C-C4C	3.65	129.55	124.81
30	f	602	CHL	CMD-C2D-C3D	-3.65	119.21	127.61
33	b	520	0UR	C5-C4-C3	-3.65	122.61	127.00
30	c	608	CHL	CHC-C1C-NC	3.65	129.74	124.20
32	G	104	8CT	C19-C20-C21	-3.65	122.10	127.31
33	3	501	0UR	C9-C8-C7	-3.65	122.10	127.31
32	A	850	8CT	C18-C17-C16	3.65	132.52	127.31
32	A	849	8CT	C18-C19-C20	-3.65	116.00	123.47
37	g	522	0IE	C6-C7-C8	3.65	124.54	118.94
30	b	606	CHL	CHB-C1B-NB	-3.65	120.39	124.26
30	8	302	CHL	CMD-C2D-C3D	-3.65	119.22	127.61
30	6	313	CHL	C3B-C4B-NB	3.65	113.90	110.52
37	c	521	0IE	C10-C9-C8	3.65	130.94	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	502	0UR	C9-C8-C7	-3.65	122.11	127.31
30	h	606	CHL	CHC-C1C-NC	3.64	129.73	124.20
37	d	522	0IE	C13-C12-C11	3.64	124.53	118.94
30	2	308	CHL	CMD-C2D-C3D	-3.64	119.24	127.61
30	6	313	CHL	C4-C3-C5	3.64	120.15	115.98
32	L	205	8CT	C04-C03-C02	-3.64	117.48	122.61
37	c	522	0IE	C20-C3-C4	-3.64	120.15	124.83
37	i	521	0IE	C9-C10-C11	3.63	130.92	123.47
30	a	607	CHL	C2A-C1A-CHA	-3.63	117.50	123.86
30	2	313	CHL	CHC-C1C-NC	3.63	129.72	124.20
30	h	602	CHL	C2A-C1A-CHA	-3.63	117.51	123.86
30	9	301	CHL	C3B-C4B-NB	3.63	113.88	110.52
33	O	204	0UR	C14-C15-C16	-3.63	122.13	127.31
30	b	606	CHL	CHC-C1C-NC	3.63	129.71	124.20
30	4	313	CHL	CMD-C2D-C3D	-3.63	119.26	127.61
30	a	602	CHL	CAC-C3C-C4C	3.63	129.52	124.81
33	1	502	0UR	C34-C27-C1	-3.63	119.73	124.49
32	J	101	8CT	C13-C14-C15	-3.63	111.89	123.22
30	b	602	CHL	C1D-ND-C4D	3.63	108.91	106.33
33	b	520	0UR	C9-C8-C7	-3.63	122.13	127.31
30	8	308	CHL	CHB-C1B-NB	-3.63	120.42	124.26
30	g	614	CHL	CHD-C4C-C3C	-3.62	119.52	124.84
30	6	307	CHL	C1D-ND-C4D	3.62	108.91	106.33
30	1	302	CHL	CHD-C4C-NC	3.62	129.91	124.20
30	f	602	CHL	CHD-C4C-NC	3.62	129.90	124.20
30	1	307	CHL	CHC-C1C-NC	3.62	129.69	124.20
30	9	306	CHL	CHB-C1B-NB	-3.61	120.43	124.26
30	i	601	CHL	C2A-C1A-CHA	-3.61	117.54	123.86
30	8	306	CHL	CAC-C3C-C4C	3.61	129.50	124.81
30	i	607	CHL	CHC-C1C-NC	3.61	129.68	124.20
30	8	307	CHL	CHD-C4C-NC	3.61	129.89	124.20
30	2	305	CHL	C1D-ND-C4D	3.61	108.90	106.33
33	0	501	0UR	C9-C8-C7	-3.61	122.16	127.31
30	0	302	CHL	CAC-C3C-C4C	3.61	129.49	124.81
30	c	601	CHL	CHB-C1B-NB	-3.61	120.44	124.26
30	8	305	CHL	C3B-C4B-NB	3.61	113.86	110.52
30	5	302	CHL	CHD-C4C-NC	3.61	129.88	124.20
30	h	605	CHL	CHD-C1D-ND	-3.61	121.14	124.45
30	4	319	CHL	CHC-C1C-NC	3.60	129.67	124.20
30	8	313	CHL	CHB-C1B-NB	-3.60	120.44	124.26
37	b	521	0IE	C9-C10-C11	3.60	130.85	123.47
33	h	520	0UR	C43-C3-C4	-3.60	120.67	125.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	G	104	8CT	C14-C13-C12	-3.60	122.17	127.31
32	M	102	8CT	C30-C31-C32	-3.60	117.04	121.47
30	6	313	CHL	CHB-C1B-NB	-3.60	120.45	124.26
30	0	305	CHL	CHC-C1C-NC	3.60	129.66	124.20
30	2	301	CHL	C1-C2-C3	-3.60	119.82	126.04
30	6	302	CHL	C3B-C4B-NB	3.60	113.85	110.52
33	4	502	0UR	C24-C25-C26	-3.60	105.38	110.30
33	a	520	0UR	C9-C8-C7	-3.59	122.18	127.31
30	7	306	CHL	CHB-C1B-NB	-3.59	120.46	124.26
33	b	520	0UR	C34-C27-C1	-3.59	119.78	124.49
30	3	305	CHL	C1-C2-C3	-3.59	120.95	126.75
30	8	308	CHL	CHC-C1C-NC	3.59	129.64	124.20
33	2	502	0UR	C5-C4-C3	-3.58	122.70	127.00
30	2	307	CHL	CHC-C1C-NC	3.58	129.64	124.20
37	3	502	0IE	C20-C3-C4	-3.58	120.22	124.83
32	B	848	8CT	C28-C26-C25	3.58	124.44	118.94
30	9	313	CHL	CHC-C1C-NC	3.58	129.64	124.20
32	2	402	8CT	C10-C11-C12	-3.58	120.83	126.23
32	6	402	8CT	C18-C19-C20	-3.58	116.15	123.47
30	c	614	CHL	C2A-C1A-CHA	-3.58	117.61	123.85
30	h	606	CHL	CAC-C3C-C4C	3.58	129.45	124.81
30	9	305	CHL	CHD-C4C-NC	3.57	129.83	124.20
37	e	521	0IE	C20-C3-C4	-3.57	120.24	124.83
32	B	846	8CT	C28-C26-C25	3.57	124.42	118.94
30	f	601	CHL	CHC-C1C-NC	3.57	129.62	124.20
30	c	606	CHL	CHC-C1C-NC	3.57	129.61	124.20
30	6	301	CHL	CHC-C1C-NC	3.57	129.61	124.20
30	a	602	CHL	CHC-C1C-NC	3.57	129.61	124.20
32	A	850	8CT	C11-C10-C03	-3.56	117.19	127.20
42	e	523	NEX	C15-C14-C13	-3.56	122.22	127.31
30	2	313	CHL	C1-C2-C3	-3.56	120.99	126.75
38	B	842	PQN	C14-C13-C15	3.56	121.26	115.27
33	8	502	0UR	C43-C3-C4	-3.56	120.72	125.02
30	d	606	CHL	C1-C2-C3	-3.56	120.99	126.75
32	B	843	8CT	C04-C03-C02	-3.56	117.60	122.61
30	6	302	CHL	CHD-C4C-NC	3.56	129.81	124.20
37	d	522	0IE	C21-C7-C8	-3.56	117.94	122.92
30	6	305	CHL	C1D-ND-C4D	3.56	108.86	106.33
30	4	302	CHL	CHD-C4C-NC	3.56	129.81	124.20
32	J	104	8CT	C14-C13-C12	3.56	132.38	127.31
33	6	502	0UR	C34-C27-C1	-3.55	119.83	124.49
32	7	404	8CT	C30-C31-C32	-3.55	117.10	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	305	CHL	C3B-C4B-NB	3.55	113.81	110.52
30	6	306	CHL	C1-C2-C3	-3.55	121.01	126.75
30	0	301	CHL	C3B-C4B-NB	3.55	113.81	110.52
33	3	501	0UR	O44-C45-C46	3.55	120.99	111.55
32	B	848	8CT	C05-C04-C03	3.55	115.94	110.48
30	d	602	CHL	C1-C2-C3	-3.55	119.91	126.04
37	e	522	0IE	C21-C7-C8	-3.55	117.95	122.92
30	1	305	CHL	CHD-C4C-NC	3.55	129.79	124.20
30	b	601	CHL	OBD-CAD-C3D	-3.55	119.99	128.52
30	5	302	CHL	CAC-C3C-C4C	3.55	129.41	124.81
30	h	607	CHL	CHD-C1D-ND	-3.55	121.20	124.45
37	c	521	0IE	C20-C3-C4	-3.54	120.27	124.83
37	b	521	0IE	C20-C3-C4	-3.54	120.28	124.83
30	9	305	CHL	CAC-C3C-C4C	3.54	129.40	124.81
30	b	608	CHL	CHB-C1B-NB	-3.54	120.51	124.26
30	8	301	CHL	C1-C2-C3	-3.54	119.92	126.04
30	d	608	CHL	CHC-C1C-NC	3.54	129.57	124.20
30	i	602	CHL	CHC-C1C-NC	3.54	129.57	124.20
32	B	843	8CT	C22-C21-C20	-3.54	117.97	122.92
30	6	305	CHL	C3B-C4B-NB	3.53	113.79	110.52
30	i	607	CHL	C4A-NA-C1A	3.53	108.30	106.71
32	A	847	8CT	C24-C25-C26	-3.53	122.27	127.31
33	4	501	0UR	C9-C8-C7	-3.53	122.27	127.31
30	6	301	CHL	CHB-C1B-NB	-3.53	120.52	124.26
32	6	402	8CT	C40-C12-C13	-3.53	117.97	122.92
32	B	846	8CT	C01-C02-C07	3.53	120.40	113.62
32	B	845	8CT	C25-C24-C23	-3.53	112.19	123.22
30	2	305	CHL	CAC-C3C-C4C	3.53	129.39	124.81
30	e	606	CHL	CHC-C1C-NC	3.53	129.56	124.20
30	7	305	CHL	CHD-C4C-NC	3.53	129.76	124.20
30	5	305	CHL	C3B-C4B-NB	3.52	113.78	110.52
30	7	305	CHL	C1D-ND-C4D	3.52	108.84	106.33
30	3	305	CHL	CAC-C3C-C4C	3.52	129.38	124.81
30	4	307	CHL	CHB-C1B-NB	-3.52	120.53	124.26
30	7	307	CHL	CHC-C1C-NC	3.52	129.55	124.20
30	0	302	CHL	CHD-C4C-NC	3.52	129.75	124.20
32	G	104	8CT	C39-C16-C17	-3.52	117.99	122.92
32	J	104	8CT	C39-C16-C17	-3.52	117.99	122.92
30	3	305	CHL	CHB-C1B-NB	-3.52	120.53	124.26
30	e	608	CHL	C3B-C4B-NB	3.52	113.78	110.52
33	4	502	0UR	C34-C27-C1	-3.52	119.87	124.49
30	8	307	CHL	C3B-C4B-NB	3.52	113.78	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	848	8CT	C27-C26-C25	-3.52	118.00	122.92
37	b	522	0IE	C9-C10-C11	3.52	130.68	123.47
32	A	846	8CT	C10-C11-C12	-3.52	120.92	126.23
30	d	601	CHL	C1-C2-C3	-3.51	121.06	126.75
30	h	608	CHL	CHC-C1C-NC	3.51	129.53	124.20
33	c	520	0UR	C9-C8-C7	-3.51	122.30	127.31
30	d	606	CHL	CHC-C1C-NC	3.51	129.53	124.20
30	8	305	CHL	CAC-C3C-C4C	3.51	129.37	124.81
30	2	319	CHL	C1D-ND-C4D	3.51	108.83	106.33
37	c	522	0IE	C6-C7-C8	3.51	124.33	118.94
30	2	313	CHL	C3B-C4B-NB	3.51	113.77	110.52
30	3	307	CHL	C1D-ND-C4D	3.51	108.83	106.33
30	4	313	CHL	CHD-C4C-NC	3.51	129.73	124.20
31	A	835	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
39	A	857	CL0	C4A-NA-C1A	3.51	108.28	106.71
32	0	401	8CT	C01-C02-C07	3.51	120.35	113.62
30	b	602	CHL	CHB-C1B-NB	-3.51	120.55	124.26
30	2	308	CHL	C3B-C4B-NB	3.50	113.76	110.52
31	B	811	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
30	e	614	CHL	CHC-C1C-NC	3.50	129.51	124.20
30	2	302	CHL	CHD-C4C-NC	3.50	129.72	124.20
30	f	606	CHL	CAC-C3C-C4C	3.50	129.35	124.81
30	d	608	CHL	OBD-CAD-C3D	-3.50	120.10	128.52
30	4	305	CHL	CHD-C4C-NC	3.50	129.71	124.20
32	I	101	8CT	C01-C02-C07	3.50	120.33	113.62
30	c	602	CHL	CHD-C4C-NC	3.50	129.71	124.20
30	3	307	CHL	C3B-C4B-NB	3.50	113.76	110.52
30	9	306	CHL	C1D-CHD-C4C	-3.50	118.52	126.06
30	1	305	CHL	CAC-C3C-C4C	3.50	129.34	124.81
30	4	319	CHL	CHD-C4C-NC	3.49	129.71	124.20
30	g	607	CHL	CAC-C3C-C4C	3.49	129.34	124.81
30	9	306	CHL	C3B-C4B-NB	3.49	113.75	110.52
30	4	306	CHL	C3B-C4B-NB	3.49	113.75	110.52
32	A	849	8CT	C04-C03-C02	-3.49	117.70	122.61
32	B	844	8CT	C07-C02-C03	-3.49	117.67	122.73
37	b	522	0IE	C20-C3-C4	-3.49	120.34	124.83
37	f	522	0IE	C21-C7-C8	-3.49	118.04	122.92
37	h	522	0IE	C21-C7-C8	-3.49	118.04	122.92
30	4	306	CHL	C1D-ND-C4D	3.49	108.81	106.33
30	a	608	CHL	CHC-C1C-NC	3.49	129.49	124.20
30	i	607	CHL	CAC-C3C-C4C	3.49	129.33	124.81
30	6	305	CHL	CHC-C1C-NC	3.49	129.49	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	501	0UR	C10-C11-C12	-3.49	122.34	127.31
33	g	520	0UR	C34-C27-C1	-3.48	119.92	124.49
30	b	609	CHL	CAC-C3C-C4C	3.48	129.33	124.81
30	i	606	CHL	CAC-C3C-C4C	3.48	129.33	124.81
30	6	306	CHL	CHD-C4C-NC	3.48	129.69	124.20
37	h	522	0IE	C20-C3-C4	-3.48	120.35	124.83
30	7	313	CHL	CHC-C1C-NC	3.48	129.48	124.20
30	5	313	CHL	CHD-C1D-ND	-3.48	121.26	124.45
30	e	609	CHL	CHC-C1C-NC	3.48	129.48	124.20
30	b	608	CHL	CAC-C3C-C4C	3.48	129.32	124.81
32	0	401	8CT	C19-C18-C17	-3.48	116.35	123.47
30	i	602	CHL	OBD-CAD-C3D	-3.48	120.15	128.52
30	9	313	CHL	CHB-C1B-NB	-3.48	120.58	124.26
30	a	609	CHL	CAC-C3C-C4C	3.48	129.32	124.81
30	f	607	CHL	C2A-C1A-CHA	-3.48	117.78	123.86
30	b	609	CHL	CHC-C1C-NC	3.47	129.47	124.20
30	6	301	CHL	C3B-C4B-NB	3.47	113.74	110.52
30	8	313	CHL	CHD-C4C-NC	3.47	129.67	124.20
32	A	848	8CT	C01-C02-C07	3.47	120.28	113.62
30	7	305	CHL	CAC-C3C-C4C	3.47	129.31	124.81
30	3	305	CHL	CHD-C4C-NC	3.47	129.67	124.20
30	i	606	CHL	C1-C2-C3	-3.47	121.14	126.75
30	4	319	CHL	C3B-C4B-NB	3.47	113.73	110.52
30	f	608	CHL	CHD-C4C-NC	3.47	129.67	124.20
37	i	522	0IE	C21-C7-C8	-3.47	118.07	122.92
30	a	609	CHL	C2A-C1A-CHA	-3.47	117.80	123.86
30	d	606	CHL	CAC-C3C-C4C	3.47	129.31	124.81
30	2	308	CHL	CHD-C4C-NC	3.47	129.66	124.20
30	0	301	CHL	C1-C2-C3	-3.46	120.05	126.04
30	a	606	CHL	CHC-C1C-NC	3.46	129.46	124.20
37	h	521	0IE	C21-C7-C8	-3.46	118.07	122.92
30	g	607	CHL	CHC-C1C-NC	3.46	129.46	124.20
30	6	301	CHL	CHD-C4C-NC	3.46	129.66	124.20
32	7	404	8CT	C27-C26-C25	-3.46	118.08	122.92
37	d	522	0IE	C23-C16-C15	-3.46	118.08	122.92
30	5	302	CHL	C3B-C4B-NB	3.46	113.72	110.52
30	c	607	CHL	CHC-C1C-NC	3.46	129.44	124.20
32	A	850	8CT	C35-C30-C31	3.45	117.61	111.42
30	1	305	CHL	C3B-C4B-NB	3.45	113.72	110.52
30	2	308	CHL	CHC-C1C-NC	3.45	129.44	124.20
30	2	313	CHL	CHD-C4C-NC	3.45	129.64	124.20
30	6	306	CHL	C1D-ND-C4D	3.45	108.79	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	502	0UR	C10-C11-C12	-3.45	122.38	127.31
32	B	845	8CT	C22-C21-C23	3.45	123.52	118.08
32	4	402	8CT	C19-C20-C21	-3.45	122.39	127.31
30	7	306	CHL	C1D-CHD-C4C	-3.45	118.61	126.06
30	i	602	CHL	CAC-C3C-C4C	3.45	129.28	124.81
30	1	302	CHL	CMD-C2D-C3D	-3.45	119.68	127.61
30	2	319	CHL	CHC-C1C-NC	3.44	129.43	124.20
30	b	607	CHL	CHC-C1C-NC	3.44	129.43	124.20
37	a	521	0IE	C20-C3-C4	-3.44	120.40	124.83
30	7	302	CHL	C3B-C4B-NB	3.44	113.71	110.52
32	B	846	8CT	C01-C02-C03	-3.44	120.67	124.53
30	5	307	CHL	CHC-C1C-NC	3.44	129.42	124.20
30	2	307	CHL	C3B-C4B-NB	3.44	113.70	110.52
30	2	319	CHL	C3B-C4B-NB	3.44	113.70	110.52
33	9	502	0UR	C34-C27-C26	3.44	120.72	114.36
30	8	313	CHL	C1D-ND-C4D	3.44	108.78	106.33
33	1	502	0UR	O44-C45-C46	3.44	120.69	111.55
37	d	522	0IE	C15-C14-C13	3.43	133.94	123.22
30	2	305	CHL	C3B-C4B-NB	3.43	113.70	110.52
30	7	301	CHL	C3B-C4B-NB	3.43	113.70	110.52
30	f	601	CHL	C3B-C4B-NB	3.43	113.70	110.52
30	0	306	CHL	CHC-C1C-NC	3.43	129.41	124.20
30	d	602	CHL	CAC-C3C-C4C	3.43	129.26	124.81
30	i	609	CHL	C2A-C1A-CHA	-3.43	117.86	123.86
37	3	502	0IE	C10-C9-C8	3.43	130.50	123.47
30	1	305	CHL	C1D-ND-C4D	3.43	108.77	106.33
37	a	522	0IE	C21-C7-C8	-3.43	118.12	122.92
30	d	608	CHL	C1-C2-C3	-3.43	121.21	126.75
32	7	402	8CT	C11-C10-C03	-3.43	117.58	127.20
30	b	606	CHL	C1-C2-C3	-3.43	121.21	126.75
30	1	306	CHL	CAC-C3C-C4C	3.42	129.25	124.81
33	6	502	0UR	C43-C3-C4	-3.42	120.88	125.02
32	B	845	8CT	C39-C16-C15	3.42	123.47	118.08
30	4	313	CHL	C1-C2-C3	-3.42	121.21	126.75
30	h	601	CHL	C4A-NA-C1A	3.42	108.25	106.71
30	5	302	CHL	C1-C2-C3	-3.42	120.12	126.04
30	0	306	CHL	C1D-CHD-C4C	-3.42	118.68	126.06
30	b	602	CHL	C3B-C4B-NB	3.42	113.69	110.52
30	9	306	CHL	OBD-CAD-C3D	-3.42	120.29	128.52
30	g	602	CHL	CAC-C3C-C4C	3.42	129.25	124.81
32	8	402	8CT	C04-C03-C02	-3.42	117.80	122.61
30	c	608	CHL	C3B-C4B-NB	3.42	113.69	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	305	CHL	CHD-C4C-NC	3.42	129.59	124.20
30	d	602	CHL	CHD-C4C-NC	3.41	129.58	124.20
31	A	830	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
37	b	522	0IE	C21-C7-C8	-3.41	118.14	122.92
35	0	603	SQD	O47-C7-C8	3.41	118.86	111.50
30	c	609	CHL	CHC-C1C-NC	3.41	129.38	124.20
30	4	308	CHL	CHC-C1C-NC	3.41	129.38	124.20
30	6	302	CHL	CAC-C3C-C4C	3.41	129.24	124.81
30	7	301	CHL	CHD-C4C-NC	3.41	129.58	124.20
30	f	606	CHL	C1-C2-C3	-3.41	121.23	126.75
30	2	302	CHL	C3B-C4B-NB	3.41	113.68	110.52
30	1	307	CHL	C3B-C4B-NB	3.41	113.68	110.52
30	c	609	CHL	CAC-C3C-C4C	3.41	129.23	124.81
30	9	313	CHL	C3B-C4B-NB	3.41	113.67	110.52
33	h	520	0UR	O44-C45-C46	3.40	120.61	111.55
30	g	608	CHL	C4A-NA-C1A	3.40	108.24	106.71
31	O	203	CLA	C3B-C4B-NB	-3.40	107.95	110.23
37	e	522	0IE	C22-C12-C11	-3.40	118.16	122.92
30	2	305	CHL	CHD-C4C-NC	3.40	129.56	124.20
30	h	602	CHL	CAC-C3C-C4C	3.40	129.22	124.81
30	9	313	CHL	CHD-C4C-NC	3.40	129.56	124.20
30	6	308	CHL	CHC-C1C-NC	3.40	129.36	124.20
30	h	614	CHL	CHD-C1D-ND	-3.40	121.33	124.45
30	6	302	CHL	CMD-C2D-C3D	-3.40	119.80	127.61
30	6	302	CHL	C1D-CHD-C4C	-3.40	118.73	126.06
30	6	301	CHL	C1D-ND-C4D	3.40	108.75	106.33
30	f	608	CHL	C1D-ND-C4D	3.40	108.75	106.33
30	2	302	CHL	C1-C2-C3	-3.40	120.17	126.04
30	8	308	CHL	CAC-C3C-C4C	3.40	129.22	124.81
33	0	502	0UR	O44-C45-C46	3.39	120.58	111.55
30	9	305	CHL	C1D-ND-C4D	3.39	108.75	106.33
30	f	607	CHL	CAC-C3C-C4C	3.39	129.21	124.81
32	B	848	8CT	C30-C31-C32	-3.39	117.30	121.47
30	3	302	CHL	CAC-C3C-C4C	3.39	129.21	124.81
30	4	305	CHL	C1D-ND-C4D	3.39	108.74	106.33
32	0	401	8CT	C14-C13-C12	-3.39	122.47	127.31
30	6	315	CHL	CHC-C1C-NC	3.39	129.35	124.20
32	8	406	8CT	C25-C24-C23	-3.39	112.64	123.22
30	1	306	CHL	C3B-C4B-NB	3.39	113.66	110.52
30	e	608	CHL	OBD-CAD-C3D	-3.39	120.37	128.52
33	5	502	0UR	O44-C45-C46	3.38	120.55	111.55
32	B	844	8CT	C22-C21-C23	3.38	123.41	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	302	CHL	C1D-ND-C4D	3.38	108.74	106.33
30	a	606	CHL	CAC-C3C-C4C	3.38	129.20	124.81
30	2	319	CHL	CHD-C4C-NC	3.38	129.53	124.20
30	6	306	CHL	CAC-C3C-C4C	3.38	129.19	124.81
30	e	601	CHL	CHD-C4C-NC	3.38	129.53	124.20
30	5	307	CHL	OBD-CAD-C3D	-3.38	120.39	128.52
32	7	405	8CT	C07-C02-C03	-3.38	117.83	122.73
30	d	602	CHL	C1D-ND-C4D	3.38	108.73	106.33
30	i	606	CHL	CHC-C1C-NC	3.37	129.32	124.20
32	J	101	8CT	C24-C23-C21	-3.37	116.94	126.42
32	B	844	8CT	C24-C25-C26	-3.37	122.50	127.31
33	7	501	0UR	O44-C45-C46	3.37	120.52	111.55
30	c	614	CHL	CHC-C1C-NC	3.37	129.32	124.20
33	2	501	0UR	C29-C30-C31	-3.37	107.91	111.74
30	e	606	CHL	C1-C2-C3	-3.37	121.30	126.75
30	b	606	CHL	CAC-C3C-C4C	3.37	129.18	124.81
30	2	301	CHL	C3B-C4B-NB	3.37	113.64	110.52
37	e	522	0IE	C6-C7-C8	3.37	124.11	118.94
30	8	301	CHL	CHC-C1C-NC	3.36	129.31	124.20
37	f	521	0IE	C21-C7-C8	-3.36	118.21	122.92
37	7	502	0IE	C10-C9-C8	3.36	130.37	123.47
32	K	107	8CT	C19-C20-C21	-3.36	122.51	127.31
30	8	301	CHL	OBD-CAD-C3D	-3.36	120.43	128.52
30	g	606	CHL	C1-C2-C3	-3.36	121.31	126.75
30	8	307	CHL	C1D-ND-C4D	3.36	108.72	106.33
30	g	601	CHL	C4-C3-C5	3.36	119.82	115.98
32	B	845	8CT	C01-C02-C07	3.36	120.07	113.62
30	e	608	CHL	CHD-C4C-NC	3.36	129.50	124.20
30	g	609	CHL	C2A-C1A-CHA	-3.36	117.99	123.85
30	6	302	CHL	OBD-CAD-C3D	-3.36	120.44	128.52
30	a	608	CHL	OBD-CAD-C3D	-3.36	120.44	128.52
30	f	609	CHL	CAC-C3C-C4C	3.36	129.17	124.81
30	d	602	CHL	C3B-C4B-NB	3.35	113.62	110.52
30	0	302	CHL	C1D-ND-C4D	3.35	108.72	106.33
30	i	609	CHL	CHD-C1D-ND	-3.35	121.37	124.45
32	B	846	8CT	C27-C26-C25	-3.35	118.23	122.92
30	8	305	CHL	CMB-C2B-C1B	3.35	130.47	125.37
30	i	608	CHL	CAC-C3C-C4C	3.35	129.15	124.81
32	O	205	8CT	C04-C03-C02	-3.35	117.90	122.61
30	6	313	CHL	CHD-C4C-NC	3.35	129.48	124.20
30	a	605	CHL	CHD-C1D-ND	-3.35	121.38	124.45
32	A	854	8CT	C10-C11-C12	-3.35	121.18	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	e	523	NEX	C24-C23-C22	-3.34	104.31	110.77
30	h	606	CHL	C1-C2-C3	-3.34	121.34	126.75
30	b	601	CHL	CHC-C1C-NC	3.34	129.27	124.20
30	3	305	CHL	C3B-C4B-NB	3.34	113.61	110.52
30	4	308	CHL	CAC-C3C-C4C	3.34	129.14	124.81
30	e	602	CHL	C3B-C4B-NB	3.34	113.61	110.52
30	h	607	CHL	C2A-C1A-CHA	-3.34	118.02	123.86
30	e	609	CHL	C1D-CHD-C4C	-3.34	118.86	126.06
32	2	402	8CT	C19-C20-C21	-3.34	122.55	127.31
31	B	830	CLA	CHB-C1B-NB	3.34	127.79	124.26
30	b	608	CHL	CHD-C4C-NC	3.34	129.46	124.20
30	2	308	CHL	CHB-C1B-NB	-3.34	120.72	124.26
30	4	302	CHL	C1D-ND-C4D	3.34	108.70	106.33
30	6	305	CHL	CAC-C3C-C4C	3.34	129.14	124.81
32	2	402	8CT	C14-C15-C16	-3.33	117.05	126.42
30	c	608	CHL	CHD-C4C-NC	3.33	129.46	124.20
30	g	607	CHL	C1-C2-C3	-3.33	121.36	126.75
30	g	614	CHL	CHD-C1D-ND	-3.33	121.39	124.45
30	2	306	CHL	CAC-C3C-C4C	3.33	129.13	124.81
30	b	601	CHL	CAC-C3C-C4C	3.33	129.13	124.81
30	4	306	CHL	CHD-C4C-NC	3.33	129.45	124.20
30	a	607	CHL	C4A-NA-C1A	3.33	108.20	106.71
30	6	307	CHL	CHB-C1B-NB	-3.33	120.73	124.26
30	0	302	CHL	C3B-C4B-NB	3.33	113.60	110.52
30	1	313	CHL	C3B-C4B-NB	3.33	113.60	110.52
30	1	313	CHL	CHD-C4C-NC	3.33	129.45	124.20
30	a	608	CHL	CHD-C4C-NC	3.33	129.45	124.20
30	2	308	CHL	C1D-CHD-C4C	-3.33	118.88	126.06
30	2	306	CHL	C3B-C4B-NB	3.33	113.60	110.52
33	4	502	0UR	C9-C8-C7	-3.33	122.56	127.31
32	2	402	8CT	C23-C21-C20	3.32	124.04	118.94
32	9	401	8CT	C01-C02-C07	3.32	120.00	113.62
30	a	601	CHL	CHC-C1C-NC	3.32	129.25	124.20
30	6	308	CHL	C1D-CHD-C4C	-3.32	118.89	126.06
37	e	521	0IE	C21-C7-C8	-3.32	118.27	122.92
32	L	205	8CT	C11-C10-C03	-3.32	117.87	127.20
30	1	307	CHL	OBD-CAD-C3D	-3.32	120.52	128.52
37	d	522	0IE	C6-C7-C8	3.32	124.04	118.94
30	b	606	CHL	CHD-C4C-NC	3.32	129.44	124.20
32	7	402	8CT	C14-C13-C12	-3.32	122.57	127.31
30	2	319	CHL	CAC-C3C-C4C	3.32	129.12	124.81
30	b	607	CHL	CAC-C3C-C4C	3.32	129.12	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	609	CHL	CAC-C3C-C4C	3.32	129.12	124.81
30	9	305	CHL	C3B-C4B-NB	3.32	113.59	110.52
30	g	608	CHL	OBD-CAD-C3D	-3.32	120.53	128.52
30	6	308	CHL	CHD-C4C-NC	3.32	129.43	124.20
30	0	301	CHL	CHD-C4C-NC	3.32	129.43	124.20
32	4	402	8CT	C23-C21-C20	3.32	124.03	118.94
30	c	601	CHL	OBD-CAD-C3D	-3.32	120.54	128.52
30	0	302	CHL	C1-C2-C3	-3.32	120.31	126.04
30	7	307	CHL	CAC-C3C-C4C	3.32	129.11	124.81
33	h	520	0UR	C34-C27-C1	-3.32	120.14	124.49
33	4	501	0UR	O44-C45-C46	3.32	120.37	111.55
30	c	607	CHL	CAC-C3C-C4C	3.31	129.11	124.81
30	d	607	CHL	CAC-C3C-C4C	3.31	129.11	124.81
31	A	817	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
32	B	851	8CT	C01-C02-C07	3.31	119.98	113.62
30	7	306	CHL	C1-C2-C3	-3.31	120.31	126.04
30	b	614	CHL	CHC-C1C-NC	3.31	129.23	124.20
30	7	313	CHL	CAC-C3C-C4C	3.31	129.11	124.81
30	f	607	CHL	CHC-C1C-NC	3.31	129.23	124.20
33	9	502	0UR	O44-C45-C46	3.31	120.36	111.55
30	a	601	CHL	CMB-C2B-C1B	3.31	130.41	125.37
33	3	501	0UR	C10-C11-C12	-3.31	122.58	127.31
33	5	502	0UR	C24-C25-C26	-3.31	105.77	110.30
30	d	601	CHL	C2A-C1A-CHA	-3.31	118.07	123.86
30	4	308	CHL	C3B-C4B-NB	3.31	113.58	110.52
32	L	206	8CT	C10-C11-C12	-3.31	121.23	126.23
30	e	602	CHL	CHD-C4C-NC	3.31	129.42	124.20
33	0	502	0UR	C9-C10-C11	-3.31	116.70	123.47
30	g	614	CHL	CAC-C3C-C4C	3.31	129.10	124.81
32	B	848	8CT	C25-C24-C23	-3.31	112.89	123.22
30	g	601	CHL	CAC-C3C-C4C	3.31	129.10	124.81
30	h	601	CHL	CHC-C1C-NC	3.31	129.22	124.20
30	c	606	CHL	C3B-C4B-NB	3.31	113.58	110.52
30	7	301	CHL	OBD-CAD-C3D	-3.30	120.57	128.52
30	a	609	CHL	CHC-C1C-NC	3.30	129.22	124.20
30	g	606	CHL	CAC-C3C-C4C	3.30	129.10	124.81
31	B	801	CLA	C3B-C4B-NB	-3.30	107.45	110.52
30	4	302	CHL	C1-C2-C3	-3.30	120.33	126.04
30	f	614	CHL	C4A-NA-C1A	3.30	108.19	106.71
30	e	607	CHL	CHC-C1C-NC	3.30	129.21	124.20
31	A	803	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
30	g	602	CHL	CHC-C1C-NC	3.30	129.21	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	602	CHL	C1-C2-C3	-3.30	120.33	126.04
30	9	301	CHL	CHD-C4C-NC	3.30	129.41	124.20
34	A	845	LHG	O8-C23-C24	3.30	120.04	111.38
32	4	402	8CT	C22-C21-C20	-3.30	118.30	122.92
30	g	606	CHL	CHC-C1C-NC	3.30	129.21	124.20
30	a	602	CHL	C1-C2-C3	-3.30	120.33	126.04
30	0	301	CHL	CHB-C1B-NB	-3.30	120.76	124.26
30	a	607	CHL	CHC-C1C-NC	3.30	129.21	124.20
37	g	521	0IE	C21-C7-C8	-3.30	118.30	122.92
30	e	606	CHL	CAC-C3C-C4C	3.30	129.09	124.81
32	J	104	8CT	C05-C04-C03	3.30	115.56	110.48
33	e	520	0UR	O44-C45-C46	3.30	120.33	111.55
33	b	520	0UR	C43-C3-C4	-3.30	121.03	125.02
30	5	306	CHL	CHC-C1C-NC	3.30	129.21	124.20
37	f	521	0IE	C9-C10-C11	3.30	130.23	123.47
32	J	101	8CT	C01-C02-C07	3.30	119.95	113.62
31	L	202	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
30	e	605	CHL	CHC-C1C-NC	3.30	129.20	124.20
33	2	501	0UR	C24-C25-C26	-3.30	105.79	110.30
30	5	301	CHL	C4-C3-C5	3.30	119.75	115.98
30	d	609	CHL	CHC-C1C-NC	3.30	129.20	124.20
30	8	301	CHL	CHD-C4C-NC	3.30	129.40	124.20
30	6	308	CHL	C3B-C4B-NB	3.30	113.57	110.52
33	9	502	0UR	C4-C3-C2	-3.30	117.25	120.08
31	A	808	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
30	2	307	CHL	C1D-CHD-C4C	-3.29	118.95	126.06
32	O	205	8CT	C01-C02-C03	-3.29	120.83	124.53
30	d	608	CHL	C3B-C4B-NB	3.29	113.57	110.52
30	b	602	CHL	CHD-C4C-NC	3.29	129.39	124.20
33	O	204	0UR	C28-C19-C18	-3.29	108.54	112.70
37	i	522	0IE	C22-C12-C11	-3.29	118.31	122.92
32	B	843	8CT	C39-C16-C15	3.29	123.26	118.08
31	A	804	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
30	i	601	CHL	CAC-C3C-C4C	3.29	129.08	124.81
33	O	204	0UR	C34-C27-C1	-3.29	120.17	124.49
33	d	520	0UR	C14-C15-C16	-3.29	122.61	127.31
33	2	501	0UR	O44-C45-C46	3.29	120.30	111.55
31	B	808	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
30	9	306	CHL	CHD-C4C-NC	3.29	129.39	124.20
30	d	607	CHL	C1D-CHD-C4C	-3.29	118.96	126.06
32	7	404	8CT	C39-C16-C17	-3.29	118.32	122.92
30	c	602	CHL	C1D-ND-C4D	3.29	108.67	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	313	CHL	C1D-ND-C4D	3.29	108.67	106.33
30	g	605	CHL	CHD-C1D-ND	-3.29	121.43	124.45
30	h	609	CHL	CHD-C1D-ND	-3.29	121.43	124.45
33	1	501	0UR	C9-C8-C7	-3.29	122.62	127.31
30	4	308	CHL	C1D-CHD-C4C	-3.29	118.97	126.06
37	i	521	0IE	C21-C7-C8	-3.29	118.32	122.92
30	i	606	CHL	CHD-C1D-ND	-3.29	121.44	124.45
30	9	301	CHL	C1D-CHD-C4C	-3.28	118.97	126.06
30	2	301	CHL	CHD-C4C-NC	3.28	129.38	124.20
37	d	522	0IE	C20-C3-C4	-3.28	120.61	124.83
31	A	812	CLA	C3B-C4B-NB	-3.28	107.47	110.52
32	G	104	8CT	C01-C02-C07	3.28	119.92	113.62
30	7	302	CHL	CAC-C3C-C4C	3.28	129.07	124.81
32	L	206	8CT	C40-C12-C13	-3.28	118.33	122.92
30	5	301	CHL	CAC-C3C-C4C	3.28	129.06	124.81
30	2	319	CHL	OBD-CAD-C3D	-3.28	120.63	128.52
30	2	306	CHL	C1D-CHD-C4C	-3.28	118.99	126.06
37	a	521	0IE	C21-C7-C8	-3.28	118.33	122.92
31	L	203	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
30	3	302	CHL	C1-C2-C3	-3.27	120.38	126.04
30	f	614	CHL	CAC-C3C-C4C	3.27	129.06	124.81
30	h	601	CHL	CAC-C3C-C4C	3.27	129.06	124.81
30	f	601	CHL	CAC-C3C-C4C	3.27	129.06	124.81
30	6	315	CHL	CHD-C4C-NC	3.27	129.36	124.20
33	6	502	0UR	C24-C25-C26	-3.27	105.83	110.30
30	e	602	CHL	CHB-C1B-NB	-3.27	120.79	124.26
37	f	522	0IE	C6-C7-C8	3.27	123.96	118.94
32	K	107	8CT	C14-C15-C16	-3.27	117.23	126.42
30	f	608	CHL	CAC-C3C-C4C	3.27	129.05	124.81
30	f	607	CHL	OBD-CAD-C3D	-3.27	120.65	128.52
30	4	319	CHL	O2A-CGA-CBA	3.27	122.17	111.91
30	f	607	CHL	C1D-CHD-C4C	-3.27	119.00	126.06
37	c	522	0IE	C22-C12-C11	-3.27	118.34	122.92
30	2	302	CHL	C1D-ND-C4D	3.27	108.66	106.33
30	5	313	CHL	C1D-CHD-C4C	-3.27	119.01	126.06
30	8	308	CHL	C1D-CHD-C4C	-3.27	119.01	126.06
41	B	849	DGD	O1G-C1A-C2A	3.27	122.16	111.91
31	B	810	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
30	i	608	CHL	C3B-C4B-NB	3.27	113.54	110.52
33	i	520	0UR	C34-C27-C1	-3.26	120.21	124.49
30	8	308	CHL	C3B-C4B-NB	3.26	113.54	110.52
33	8	501	0UR	C9-C8-C7	-3.26	122.66	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	307	CHL	C1D-CHD-C4C	-3.26	119.03	126.06
30	g	609	CHL	CAC-C3C-C4C	3.26	129.03	124.81
30	h	606	CHL	C3B-C4B-NB	3.26	113.53	110.52
31	B	806	CLA	C3B-C4B-NB	-3.26	107.50	110.52
30	d	609	CHL	CHD-C1D-ND	-3.25	121.46	124.45
37	c	521	0IE	C21-C7-C8	-3.25	118.36	122.92
30	e	608	CHL	CAC-C3C-C4C	3.25	129.03	124.81
31	B	803	CLA	C1-C2-C3	-3.25	120.42	126.04
30	7	305	CHL	C3B-C4B-NB	3.25	113.53	110.52
30	d	609	CHL	CAC-C3C-C4C	3.25	129.03	124.81
30	f	609	CHL	C1D-CHD-C4C	-3.25	119.04	126.06
33	9	501	0UR	C34-C27-C1	-3.25	120.22	124.49
30	6	313	CHL	C1D-CHD-C4C	-3.25	119.05	126.06
30	c	608	CHL	OBD-CAD-C3D	-3.25	120.70	128.52
30	c	602	CHL	C1-C2-C3	-3.25	120.42	126.04
30	5	301	CHL	C1-C2-C3	-3.25	120.42	126.04
37	b	522	0IE	C22-C12-C11	-3.25	118.37	122.92
30	c	601	CHL	CAC-C3C-C4C	3.25	129.02	124.81
32	B	844	8CT	C39-C16-C15	3.25	123.19	118.08
30	d	607	CHL	CHD-C1D-ND	-3.25	121.47	124.45
30	4	306	CHL	C1D-CHD-C4C	-3.25	119.06	126.06
30	f	605	CHL	CAC-C3C-C4C	3.24	129.02	124.81
37	d	521	0IE	C21-C7-C8	-3.24	118.38	122.92
30	a	608	CHL	C3B-C4B-NB	3.24	113.53	110.52
30	7	301	CHL	C1D-CHD-C4C	-3.24	119.06	126.06
30	5	313	CHL	CHC-C1C-NC	3.24	129.12	124.20
30	h	609	CHL	CHC-C1C-NC	3.24	129.12	124.20
33	9	501	0UR	O44-C45-C46	3.24	120.18	111.55
30	4	305	CHL	CAC-C3C-C4C	3.24	129.02	124.81
33	9	501	0UR	C9-C8-C7	-3.24	122.68	127.31
31	A	833	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
32	9	401	8CT	C35-C30-C29	-3.24	108.60	112.70
31	0	321	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
30	c	609	CHL	CHD-C1D-ND	-3.24	121.47	124.45
30	4	306	CHL	CAC-C3C-C4C	3.24	129.01	124.81
33	5	501	0UR	C34-C27-C1	-3.24	120.24	124.49
30	h	608	CHL	C3B-C4B-NB	3.24	113.52	110.52
30	f	609	CHL	CHD-C1D-ND	-3.24	121.48	124.45
30	a	614	CHL	CAC-C3C-C4C	3.24	129.01	124.81
37	h	522	0IE	C22-C12-C11	-3.24	118.39	122.92
30	f	601	CHL	OBD-CAD-C3D	-3.23	120.73	128.52
30	4	307	CHL	C1D-ND-C4D	3.23	108.63	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	319	CHL	OBD-CAD-C3D	-3.23	120.74	128.52
30	h	609	CHL	C4A-NA-C1A	3.23	108.16	106.71
33	O	204	0UR	C9-C10-C11	-3.23	116.85	123.47
38	A	842	PQN	C14-C13-C15	3.23	120.71	115.27
30	b	614	CHL	CAC-C3C-C4C	3.23	129.00	124.81
30	f	614	CHL	C2A-C1A-CHA	-3.23	118.21	123.85
30	8	306	CHL	CHD-C4C-NC	3.23	129.30	124.20
37	a	522	0IE	C22-C12-C11	-3.23	118.40	122.92
30	6	306	CHL	C1D-CHD-C4C	-3.23	119.09	126.06
30	1	307	CHL	CHD-C4C-NC	3.23	129.29	124.20
32	B	847	8CT	C11-C10-C03	-3.23	118.13	127.20
30	7	307	CHL	OBD-CAD-C3D	-3.23	120.75	128.52
30	i	605	CHL	CHD-C1D-ND	-3.23	121.49	124.45
31	B	827	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
30	b	609	CHL	C3B-C4B-NB	3.23	113.51	110.52
30	0	301	CHL	CAC-C3C-C4C	3.23	129.00	124.81
30	e	614	CHL	CAC-C3C-C4C	3.23	129.00	124.81
30	a	607	CHL	CAC-C3C-C4C	3.23	129.00	124.81
30	b	609	CHL	C1D-CHD-C4C	-3.23	119.10	126.06
31	B	829	CLA	C3B-C4B-NB	-3.23	107.52	110.52
30	7	313	CHL	CHD-C4C-NC	3.23	129.28	124.20
37	a	521	0IE	C9-C10-C11	3.22	130.08	123.47
33	a	520	0UR	C34-C27-C1	-3.22	120.26	124.49
32	L	209	8CT	C14-C13-C12	-3.22	122.71	127.31
30	6	308	CHL	C1-C2-C3	-3.22	120.47	126.04
30	8	313	CHL	CAC-C3C-C4C	3.22	128.99	124.81
30	2	306	CHL	CHD-C4C-NC	3.22	129.28	124.20
37	i	521	0IE	C22-C12-C11	-3.22	118.41	122.92
30	7	305	CHL	CHB-C1B-NB	-3.22	120.85	124.26
32	A	849	8CT	C01-C02-C07	3.22	119.80	113.62
33	0	501	0UR	C34-C27-C1	-3.22	120.27	124.49
30	h	607	CHL	C1D-CHD-C4C	-3.22	119.11	126.06
30	g	602	CHL	C4-C3-C5	3.22	119.66	115.98
30	5	305	CHL	CAC-C3C-C4C	3.22	128.99	124.81
32	B	847	8CT	C14-C15-C16	-3.22	117.38	126.42
30	7	302	CHL	C4-C3-C5	3.22	120.68	115.27
32	B	804	8CT	C14-C15-C16	-3.22	117.38	126.42
32	A	854	8CT	C04-C03-C02	-3.22	118.08	122.61
31	B	826	CLA	C3D-C4D-ND	3.22	111.81	109.68
30	6	302	CHL	O2D-CGD-O1D	-3.22	117.55	123.84
30	c	605	CHL	CAC-C3C-C4C	3.21	128.98	124.81
30	6	301	CHL	CMB-C2B-C1B	3.21	130.26	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	608	CHL	CHB-C1B-NB	-3.21	120.86	124.26
32	9	401	8CT	C24-C25-C26	-3.21	122.72	127.31
30	5	306	CHL	CAC-C3C-C4C	3.21	128.98	124.81
30	7	302	CHL	OBD-CAD-C3D	-3.21	120.79	128.52
30	0	301	CHL	O2A-CGA-CBA	3.21	121.99	111.91
30	8	315	CHL	C4A-NA-C1A	3.21	108.15	106.71
30	4	307	CHL	C1D-CHD-C4C	-3.21	119.13	126.06
30	4	306	CHL	CHB-C1B-NB	-3.21	120.86	124.26
32	B	847	8CT	C01-C02-C07	3.21	119.78	113.62
33	c	520	0UR	C36-C28-C19	3.21	114.41	109.55
30	g	609	CHL	CHD-C1D-ND	-3.21	121.50	124.45
30	4	302	CHL	C3B-C4B-NB	3.21	113.49	110.52
32	F	302	8CT	C01-C02-C07	3.21	119.78	113.62
31	B	818	CLA	C3B-C4B-NB	-3.21	107.54	110.52
31	B	841	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
30	0	301	CHL	C4-C3-C5	3.21	119.65	115.98
33	7	501	0UR	C28-C19-C18	-3.21	108.65	112.70
30	a	609	CHL	C1D-CHD-C4C	-3.21	119.14	126.06
30	0	306	CHL	O2D-CGD-O1D	-3.21	117.57	123.84
37	h	522	0IE	C6-C7-C8	3.21	123.86	118.94
30	i	601	CHL	CHD-C1D-ND	-3.21	121.51	124.45
31	A	818	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
32	6	402	8CT	C07-C02-C03	-3.21	118.08	122.73
30	c	602	CHL	C3B-C4B-NB	3.21	113.49	110.52
30	a	614	CHL	CHC-C1C-NC	3.21	129.07	124.20
33	f	520	0UR	C34-C27-C1	-3.20	120.28	124.49
30	7	306	CHL	C3B-C4B-NB	3.20	113.49	110.52
31	6	314	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
30	i	609	CHL	CAC-C3C-C4C	3.20	128.97	124.81
30	4	313	CHL	CAC-C3C-C4C	3.20	128.97	124.81
31	A	825	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
33	O	204	0UR	C24-C25-C26	-3.20	105.92	110.30
37	i	522	0IE	C6-C7-C8	3.20	123.85	118.94
30	d	605	CHL	CHD-C1D-ND	-3.20	121.51	124.45
33	1	501	0UR	O44-C45-C46	3.20	120.06	111.55
30	1	302	CHL	C1D-CHD-C4C	-3.20	119.15	126.06
32	B	848	8CT	C14-C15-C16	-3.20	117.42	126.42
30	c	605	CHL	CHD-C1D-ND	-3.20	121.51	124.45
33	6	502	0UR	O44-C45-C46	3.20	120.06	111.55
30	g	608	CHL	CHC-C1C-NC	3.20	129.06	124.20
32	A	850	8CT	C10-C11-C12	-3.20	121.40	126.23
32	B	851	8CT	C04-C03-C02	-3.20	118.11	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	305	CHL	CHB-C1B-NB	-3.20	120.87	124.26
30	f	605	CHL	CHC-C1C-NC	3.20	129.06	124.20
30	3	302	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
30	c	601	CHL	CHD-C4C-NC	3.20	129.24	124.20
30	d	607	CHL	CHC-C1C-NC	3.20	129.05	124.20
30	d	601	CHL	C1D-CHD-C4C	-3.20	119.16	126.06
30	d	601	CHL	CAC-C3C-C4C	3.20	128.96	124.81
30	i	602	CHL	C3B-C4B-NB	3.20	113.48	110.52
32	6	402	8CT	C39-C16-C17	-3.20	118.45	122.92
30	0	305	CHL	CHD-C4C-NC	3.20	129.24	124.20
31	B	819	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
30	f	609	CHL	CHC-C1C-NC	3.19	129.05	124.20
37	d	521	0IE	C20-C3-C4	-3.19	120.72	124.83
30	d	614	CHL	C1D-CHD-C4C	-3.19	119.17	126.06
33	d	520	0UR	C34-C27-C1	-3.19	120.30	124.49
31	B	838	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
30	7	306	CHL	CAC-C3C-C4C	3.19	128.95	124.81
37	7	502	0IE	C20-C3-C4	-3.19	120.72	124.83
30	8	313	CHL	C4-C3-C5	3.19	120.64	115.27
30	i	606	CHL	C4A-NA-C1A	3.19	108.14	106.71
30	6	307	CHL	CAC-C3C-C4C	3.19	128.95	124.81
30	e	609	CHL	CAC-C3C-C4C	3.19	128.95	124.81
30	e	606	CHL	CHD-C4C-NC	3.19	129.23	124.20
30	6	315	CHL	C3B-C4B-NB	3.19	113.47	110.52
31	B	818	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
30	3	305	CHL	CMB-C2B-C1B	3.19	130.23	125.37
31	B	809	CLA	C3B-C4B-NB	-3.19	107.56	110.52
31	B	803	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
31	O	201	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
30	1	306	CHL	C1D-CHD-C4C	-3.19	119.18	126.06
30	6	305	CHL	C1D-CHD-C4C	-3.19	119.18	126.06
31	3	320	CLA	CAC-C3C-C4C	3.19	128.94	124.81
33	5	502	0UR	C43-C3-C4	-3.19	121.17	125.02
30	g	609	CHL	CHC-C1C-NC	3.19	129.04	124.20
33	7	501	0UR	C34-C27-C1	-3.19	120.31	124.49
30	i	614	CHL	CHC-C1C-NC	3.19	129.04	124.20
30	7	302	CHL	C1D-ND-C4D	3.19	108.60	106.33
31	B	833	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
32	J	101	8CT	C11-C10-C03	-3.18	118.26	127.20
30	a	609	CHL	CHD-C1D-ND	-3.18	121.53	124.45
30	f	601	CHL	C1D-CHD-C4C	-3.18	119.19	126.06
30	4	319	CHL	C1D-ND-C4D	3.18	108.60	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	602	CHL	C1-C2-C3	-3.18	120.54	126.04
30	1	313	CHL	C1D-CHD-C4C	-3.18	119.19	126.06
33	0	502	0UR	C29-C30-C31	-3.18	108.12	111.74
30	3	307	CHL	C1D-CHD-C4C	-3.18	119.20	126.06
30	h	608	CHL	CHD-C4C-NC	3.18	129.21	124.20
33	e	520	0UR	C5-C4-C3	-3.18	123.18	127.00
30	5	301	CHL	OBD-CAD-C3D	-3.18	120.87	128.52
30	5	302	CHL	C1D-ND-C4D	3.18	108.59	106.33
30	7	307	CHL	C1D-CHD-C4C	-3.18	119.20	126.06
30	c	605	CHL	C1D-CHD-C4C	-3.18	119.20	126.06
32	9	401	8CT	C18-C19-C20	-3.18	116.97	123.47
31	a	603	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
32	B	846	8CT	C39-C16-C15	3.18	123.08	118.08
31	A	827	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
30	4	313	CHL	C1D-CHD-C4C	-3.18	119.21	126.06
30	f	601	CHL	CHD-C4C-NC	3.17	129.21	124.20
37	g	522	0IE	C22-C12-C11	-3.17	118.48	122.92
30	h	605	CHL	CAC-C3C-C4C	3.17	128.93	124.81
37	a	522	0IE	C9-C10-C11	3.17	129.97	123.47
30	f	605	CHL	CHD-C1D-ND	-3.17	121.54	124.45
30	8	307	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
32	L	209	8CT	C19-C18-C17	-3.17	116.98	123.47
30	5	306	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
32	7	404	8CT	C01-C02-C07	3.17	119.71	113.62
31	9	300	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
30	g	602	CHL	C1D-CHD-C4C	-3.17	119.22	126.06
30	8	305	CHL	CHD-C4C-NC	3.17	129.20	124.20
30	0	306	CHL	C3B-C4B-NB	3.17	113.45	110.52
30	5	302	CHL	CMB-C2B-C1B	3.17	130.19	125.37
30	d	614	CHL	CHD-C1D-ND	-3.17	121.55	124.45
37	a	522	0IE	C20-C3-C4	-3.16	120.76	124.83
30	4	302	CHL	OBD-CAD-C3D	-3.16	120.91	128.52
30	0	302	CHL	CMB-C2B-C1B	3.16	130.19	125.37
31	A	853	CLA	C3B-C4B-NB	-3.16	107.58	110.52
30	5	302	CHL	C1D-CHD-C4C	-3.16	119.23	126.06
30	5	305	CHL	CHD-C4C-NC	3.16	129.19	124.20
30	c	606	CHL	CHD-C4C-NC	3.16	129.19	124.20
33	4	501	0UR	C10-C11-C12	-3.16	122.80	127.31
30	h	601	CHL	OBD-CAD-C3D	-3.16	120.91	128.52
32	G	104	8CT	C05-C04-C03	3.16	115.35	110.48
30	5	301	CHL	CHC-C1C-NC	3.16	129.00	124.20
37	f	522	0IE	C22-C12-C11	-3.16	118.50	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	e	520	0UR	C14-C15-C16	-3.16	122.80	127.31
30	d	609	CHL	C1D-CHD-C4C	-3.16	119.24	126.06
31	A	805	CLA	C3B-C4B-NB	-3.16	107.58	110.52
31	B	830	CLA	CMB-C2B-C1B	-3.16	120.56	125.37
37	3	502	0IE	C21-C7-C8	-3.16	118.50	122.92
30	c	614	CHL	C1D-CHD-C4C	-3.16	119.25	126.06
32	A	846	8CT	C11-C10-C03	-3.16	118.33	127.20
30	f	602	CHL	C1D-ND-C4D	3.16	108.58	106.33
30	1	302	CHL	C3B-C4B-NB	3.16	113.44	110.52
30	8	301	CHL	C3B-C4B-NB	3.16	113.44	110.52
33	6	501	0UR	C43-C3-C4	-3.16	121.20	125.02
37	7	502	0IE	C21-C7-C8	-3.16	118.50	122.92
30	2	313	CHL	OBD-CAD-C3D	-3.15	120.93	128.52
33	1	502	0UR	C36-C28-C19	3.15	114.32	109.55
30	9	305	CHL	CHB-C4A-NA	3.15	128.87	124.51
30	i	605	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
30	f	602	CHL	C1-C2-C3	-3.15	120.59	126.04
30	a	605	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
31	9	300	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
31	A	819	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
37	a	522	0IE	C6-C7-C8	3.15	123.78	118.94
30	0	305	CHL	CAC-C3C-C4C	3.15	128.90	124.81
30	9	313	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
30	6	305	CHL	CHB-C1B-NB	-3.15	120.92	124.26
30	2	313	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
32	B	844	8CT	C04-C03-C02	-3.15	118.18	122.61
30	a	614	CHL	CHD-C1D-ND	-3.15	121.56	124.45
30	2	319	CHL	O2A-CGA-CBA	3.15	121.78	111.91
30	8	307	CHL	CHB-C1B-NB	-3.15	120.93	124.26
37	b	521	0IE	C10-C9-C8	3.15	129.92	123.47
30	1	307	CHL	CAC-C3C-C4C	3.15	128.89	124.81
31	3	313	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
30	7	305	CHL	C1D-CHD-C4C	-3.14	119.27	126.06
30	8	301	CHL	O2D-CGD-O1D	-3.14	117.69	123.84
31	A	838	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
32	8	406	8CT	C01-C02-C07	3.14	119.65	113.62
31	L	201	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
30	e	601	CHL	OBD-CAD-C3D	-3.14	120.96	128.52
30	1	302	CHL	C1D-ND-C4D	3.14	108.57	106.33
30	4	305	CHL	C1D-CHD-C4C	-3.14	119.28	126.06
30	a	607	CHL	C1D-CHD-C4C	-3.14	119.28	126.06
33	d	520	0UR	O44-C45-C46	3.14	119.91	111.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	K	101	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
30	8	308	CHL	CHD-C4C-NC	3.14	129.15	124.20
30	e	601	CHL	CAC-C3C-C4C	3.14	128.88	124.81
32	L	209	8CT	C01-C02-C07	3.14	119.64	113.62
30	8	302	CHL	C1D-CHD-C4C	-3.14	119.29	126.06
32	L	206	8CT	C11-C10-C03	-3.14	118.39	127.20
30	2	308	CHL	CAC-C3C-C4C	3.14	128.88	124.81
32	7	405	8CT	C35-C30-C29	-3.14	108.73	112.70
30	d	608	CHL	CHD-C4C-NC	3.14	129.15	124.20
30	9	301	CHL	CAC-C3C-C4C	3.14	128.88	124.81
30	c	601	CHL	C1D-CHD-C4C	-3.14	119.29	126.06
30	i	609	CHL	C1D-CHD-C4C	-3.14	119.29	126.06
30	1	313	CHL	C1-C2-C3	-3.13	120.62	126.04
30	7	306	CHL	CHD-C4C-NC	3.13	129.14	124.20
33	O	204	0UR	O44-C45-C46	3.13	119.89	111.55
30	d	608	CHL	CAC-C3C-C4C	3.13	128.88	124.81
37	d	521	0IE	C4-C3-C2	-3.13	117.39	120.08
30	0	305	CHL	C1-C2-C3	-3.13	121.68	126.75
30	i	606	CHL	CMB-C2B-C1B	3.13	130.14	125.37
30	a	601	CHL	C1D-CHD-C4C	-3.13	119.30	126.06
32	A	847	8CT	C18-C19-C20	-3.13	117.06	123.47
32	7	404	8CT	C07-C02-C03	-3.13	118.18	122.73
32	A	854	8CT	C11-C10-C03	-3.13	118.41	127.20
30	c	606	CHL	C1D-CHD-C4C	-3.13	119.30	126.06
32	7	402	8CT	C01-C02-C07	3.13	119.63	113.62
30	2	301	CHL	OBD-CAD-C3D	-3.13	120.99	128.52
31	A	840	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
32	O	205	8CT	C01-C02-C07	3.13	119.63	113.62
33	f	520	0UR	O44-C45-C46	3.13	119.87	111.55
37	h	521	0IE	C6-C7-C8	3.13	123.74	118.94
30	7	302	CHL	C1D-CHD-C4C	-3.13	119.31	126.06
30	4	302	CHL	C1D-CHD-C4C	-3.13	119.31	126.06
30	d	602	CHL	C1D-CHD-C4C	-3.13	119.31	126.06
30	d	601	CHL	OBD-CAD-C3D	-3.13	121.00	128.52
30	8	315	CHL	CHC-C1C-NC	3.13	128.94	124.20
31	B	825	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
30	2	301	CHL	CAC-C3C-C4C	3.13	128.87	124.81
30	i	601	CHL	C1D-CHD-C4C	-3.13	119.32	126.06
30	g	608	CHL	CAC-C3C-C4C	3.12	128.86	124.81
30	3	307	CHL	O2A-CGA-CBA	3.12	121.71	111.91
30	i	602	CHL	CMB-C2B-C1B	3.12	130.13	125.37
30	7	313	CHL	C3B-C4B-NB	3.12	113.41	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	608	CHL	C1D-CHD-C4C	-3.12	119.32	126.06
30	d	607	CHL	C2A-C1A-CHA	-3.12	118.40	123.86
30	i	608	CHL	CHD-C4C-NC	3.12	129.12	124.20
30	d	605	CHL	C1D-CHD-C4C	-3.12	119.32	126.06
30	8	315	CHL	CHD-C4C-NC	3.12	129.12	124.20
30	8	307	CHL	OBD-CAD-C3D	-3.12	121.00	128.52
32	A	848	8CT	C35-C30-C29	-3.12	108.75	112.70
37	b	522	0IE	C6-C7-C8	3.12	123.73	118.94
30	0	301	CHL	C1D-CHD-C4C	-3.12	119.33	126.06
33	1	501	0UR	C29-C30-C31	-3.12	108.19	111.74
30	h	602	CHL	C1D-CHD-C4C	-3.12	119.33	126.06
30	f	606	CHL	CHD-C4C-NC	3.12	129.12	124.20
30	e	609	CHL	CHD-C4C-NC	3.12	129.12	124.20
30	1	313	CHL	CAC-C3C-C4C	3.12	128.86	124.81
30	1	313	CHL	OBD-CAD-C3D	-3.12	121.02	128.52
30	5	307	CHL	CAC-C3C-C4C	3.12	128.85	124.81
31	6	317	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
32	A	854	8CT	C27-C26-C25	-3.12	118.56	122.92
37	a	521	0IE	C22-C12-C11	-3.12	118.56	122.92
30	3	305	CHL	C1D-CHD-C4C	-3.12	119.34	126.06
37	g	521	0IE	C22-C12-C11	-3.12	118.56	122.92
31	B	837	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
30	6	315	CHL	CAC-C3C-C4C	3.12	128.85	124.81
30	2	302	CHL	C1D-CHD-C4C	-3.11	119.34	126.06
32	A	848	8CT	C25-C24-C23	-3.11	113.50	123.22
30	f	602	CHL	C1D-CHD-C4C	-3.11	119.34	126.06
30	g	605	CHL	CAC-C3C-C4C	3.11	128.85	124.81
37	h	521	0IE	C22-C12-C11	-3.11	118.56	122.92
30	8	302	CHL	C1D-ND-C4D	3.11	108.55	106.33
30	a	602	CHL	C1D-CHD-C4C	-3.11	119.35	126.06
31	A	810	CLA	C3B-C4B-NB	-3.11	107.63	110.52
30	h	605	CHL	C2A-C1A-CHA	-3.11	118.42	123.86
30	e	614	CHL	C1D-CHD-C4C	-3.11	119.35	126.06
30	b	602	CHL	C1D-CHD-C4C	-3.11	119.36	126.06
30	c	614	CHL	CAC-C3C-C4C	3.11	128.84	124.81
37	d	521	0IE	C9-C10-C11	3.11	129.84	123.47
32	A	848	8CT	C11-C10-C03	-3.10	118.48	127.20
30	3	302	CHL	OBD-CAD-C3D	-3.10	121.05	128.52
31	B	807	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
32	A	847	8CT	C01-C02-C07	3.10	119.58	113.62
30	6	307	CHL	C3B-C4B-NB	3.10	113.39	110.52
30	h	609	CHL	C1D-CHD-C4C	-3.10	119.36	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	g	601	CHL	CHC-C1C-NC	3.10	128.91	124.20
32	L	206	8CT	C01-C02-C07	3.10	119.58	113.62
37	i	522	0IE	C20-C3-C4	-3.10	120.84	124.83
31	B	841	CLA	C3B-C4B-NB	-3.10	107.64	110.52
30	2	305	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
33	1	502	0UR	C48-C47-C46	-3.10	119.20	125.85
30	0	305	CHL	C3B-C4B-NB	3.10	113.39	110.52
30	d	614	CHL	CAC-C3C-C4C	3.10	128.83	124.81
30	b	614	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
33	5	501	0UR	C5-C4-C3	-3.10	123.28	127.00
37	h	521	0IE	C20-C3-C4	-3.10	120.84	124.83
30	h	606	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
30	e	606	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
30	g	614	CHL	CHC-C1C-NC	3.10	128.90	124.20
30	2	305	CHL	OBD-CAD-C3D	-3.10	121.07	128.52
30	b	606	CHL	C1D-CHD-C4C	-3.10	119.38	126.06
30	i	609	CHL	CHC-C1C-NC	3.10	128.90	124.20
30	6	315	CHL	OBD-CAD-C3D	-3.10	121.07	128.52
30	6	313	CHL	C1-C2-C3	-3.10	120.69	126.04
31	A	824	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
30	a	601	CHL	OBD-CAD-C3D	-3.10	121.07	128.52
30	a	601	CHL	CAC-C3C-C4C	3.10	128.83	124.81
30	7	305	CHL	CMB-C2B-C1B	3.10	130.08	125.37
30	a	605	CHL	CHC-C1C-NC	3.09	128.90	124.20
30	g	606	CHL	C1D-CHD-C4C	-3.09	119.38	126.06
30	6	313	CHL	O2A-CGA-CBA	3.09	121.62	111.91
31	A	831	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
30	4	319	CHL	CAC-C3C-C4C	3.09	128.82	124.81
30	c	609	CHL	C3B-C4B-NB	3.09	113.38	110.52
31	1	314	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
30	c	609	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
30	a	602	CHL	CHD-C4C-NC	3.09	129.07	124.20
30	b	608	CHL	OBD-CAD-C3D	-3.09	121.08	128.52
30	8	301	CHL	O2A-CGA-CBA	3.09	121.61	111.91
30	i	602	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
37	h	522	0IE	C9-C10-C11	3.09	129.80	123.47
30	d	606	CHL	CMB-C2B-C1B	3.09	130.07	125.37
30	b	607	CHL	C1D-CHD-C4C	-3.09	119.39	126.06
30	4	308	CHL	CHD-C4C-NC	3.09	129.07	124.20
30	c	605	CHL	CHC-C1C-NC	3.09	128.89	124.20
31	6	312	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
37	g	521	0IE	C4-C3-C2	-3.09	117.43	120.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	302	CHL	CHB-C4A-NA	3.09	128.78	124.51
30	9	313	CHL	OBD-CAD-C3D	-3.09	121.09	128.52
30	a	602	CHL	C3B-C4B-NB	3.09	113.38	110.52
30	f	614	CHL	C1D-CHD-C4C	-3.09	119.40	126.06
30	5	301	CHL	O2A-CGA-CBA	3.09	121.59	111.91
32	6	402	8CT	C15-C16-C17	3.09	123.68	118.94
30	i	601	CHL	CHC-C1C-NC	3.09	128.88	124.20
32	A	849	8CT	C14-C15-C16	-3.09	117.75	126.42
31	3	320	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
31	B	824	CLA	C3B-C4B-NB	-3.09	107.65	110.52
31	A	836	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
31	F	301	CLA	C3B-C4B-NB	-3.08	107.65	110.52
30	2	301	CHL	C1D-CHD-C4C	-3.08	119.41	126.06
30	h	602	CHL	CHD-C1D-ND	-3.08	121.62	124.45
30	9	305	CHL	C1D-CHD-C4C	-3.08	119.41	126.06
30	b	609	CHL	C1-C2-C3	-3.08	120.72	126.04
30	h	609	CHL	OBD-CAD-C3D	-3.08	121.11	128.52
31	A	812	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
30	6	301	CHL	CAC-C3C-C4C	3.08	128.80	124.81
32	A	850	8CT	C40-C12-C11	3.08	122.93	118.08
31	2	314	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
30	d	605	CHL	CHC-C1C-NC	3.08	128.87	124.20
33	i	520	0UR	O44-C45-C46	3.08	119.73	111.55
31	A	814	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
31	g	610	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
30	f	608	CHL	C1-C2-C3	-3.07	121.78	126.75
30	i	605	CHL	CAC-C3C-C4C	3.07	128.80	124.81
30	i	602	CHL	CHD-C4C-NC	3.07	129.05	124.20
32	0	401	8CT	C07-C02-C03	-3.07	118.27	122.73
30	c	607	CHL	C1D-CHD-C4C	-3.07	119.43	126.06
33	4	501	0UR	C48-C47-C46	-3.07	119.26	125.85
31	9	302	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
30	2	307	CHL	O2A-CGA-CBA	3.07	121.55	111.91
30	g	605	CHL	C1D-CHD-C4C	-3.07	119.43	126.06
33	1	502	0UR	C10-C11-C12	-3.07	122.93	127.31
31	h	604	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
30	6	315	CHL	C1D-CHD-C4C	-3.07	119.43	126.06
31	A	815	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
30	c	608	CHL	CAC-C3C-C4C	3.07	128.79	124.81
30	6	307	CHL	C1D-CHD-C4C	-3.07	119.43	126.06
32	A	854	8CT	C01-C02-C07	3.07	119.51	113.62
30	1	306	CHL	CHD-C4C-NC	3.07	129.04	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	806	CLA	C3B-C4B-NB	-3.07	107.67	110.52
30	c	606	CHL	OBD-CAD-C3D	-3.07	121.13	128.52
30	h	605	CHL	C1D-CHD-C4C	-3.07	119.44	126.06
30	d	601	CHL	CHD-C1D-ND	-3.07	121.64	124.45
30	4	313	CHL	CHB-C1B-NB	-3.07	121.01	124.26
33	6	501	0UR	C36-C28-C19	3.07	114.19	109.55
37	c	521	0IE	C22-C12-C11	-3.07	118.63	122.92
30	8	313	CHL	C1D-CHD-C4C	-3.07	119.44	126.06
30	9	306	CHL	CAC-C3C-C4C	3.07	128.79	124.81
30	8	302	CHL	OBD-CAD-C3D	-3.07	121.14	128.52
33	f	520	0UR	C43-C3-C4	-3.07	121.31	125.02
31	3	306	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	g	614	CHL	C1D-CHD-C4C	-3.07	119.44	126.06
31	B	821	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	h	608	CHL	CAC-C3C-C4C	3.07	128.79	124.81
30	2	301	CHL	CHB-C1B-NB	-3.06	121.01	124.26
37	g	521	0IE	C9-C10-C11	3.06	129.75	123.47
30	g	605	CHL	CHC-C1C-NC	3.06	128.85	124.20
31	B	830	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
37	b	521	0IE	C21-C7-C8	-3.06	118.63	122.92
31	A	827	CLA	C3B-C4B-NB	-3.06	107.67	110.52
31	A	839	CLA	C3B-C4B-NB	-3.06	107.67	110.52
30	5	313	CHL	C2A-C1A-CHA	-3.06	118.50	123.86
30	i	601	CHL	OBD-CAD-C3D	-3.06	121.15	128.52
37	e	521	0IE	C9-C10-C11	3.06	129.74	123.47
30	e	607	CHL	C3B-C4B-NB	3.06	113.35	110.52
31	4	303	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
30	g	602	CHL	CMB-C2B-C1B	3.06	130.03	125.37
30	0	302	CHL	C1D-CHD-C4C	-3.06	119.46	126.06
30	i	607	CHL	C1D-CHD-C4C	-3.06	119.46	126.06
30	2	306	CHL	OBD-CAD-C3D	-3.06	121.16	128.52
30	e	609	CHL	C3B-C4B-NB	3.06	113.35	110.52
32	3	402	8CT	C19-C18-C17	-3.06	117.21	123.47
37	g	521	0IE	C20-C3-C4	-3.06	120.89	124.83
30	8	301	CHL	C1D-CHD-C4C	-3.06	119.46	126.06
37	e	522	0IE	C9-C10-C11	3.06	129.74	123.47
30	i	608	CHL	OBD-CAD-C3D	-3.06	121.16	128.52
30	a	608	CHL	CAC-C3C-C4C	3.06	128.78	124.81
30	0	306	CHL	CMB-C2B-C1B	3.06	130.02	125.37
30	e	605	CHL	C1D-CHD-C4C	-3.06	119.47	126.06
37	f	521	0IE	C22-C12-C11	-3.06	118.64	122.92
30	f	609	CHL	C1-C2-C3	-3.06	120.76	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	315	CHL	OBD-CAD-C3D	-3.06	121.17	128.52
30	6	301	CHL	O2A-CGA-CBA	3.05	121.49	111.91
32	A	854	8CT	C07-C02-C03	-3.05	118.30	122.73
31	B	801	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
30	b	608	CHL	C1D-CHD-C4C	-3.05	119.47	126.06
30	i	605	CHL	CHC-C1C-NC	3.05	128.84	124.20
33	4	501	0UR	C29-C30-C31	-3.05	108.27	111.74
31	B	833	CLA	C3B-C4B-NB	-3.05	107.68	110.52
30	h	614	CHL	C1D-CHD-C4C	-3.05	119.47	126.06
30	g	606	CHL	CHD-C4C-NC	3.05	129.01	124.20
30	5	305	CHL	C1D-CHD-C4C	-3.05	119.48	126.06
30	g	607	CHL	C1D-CHD-C4C	-3.05	119.48	126.06
31	5	309	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
30	4	305	CHL	OBD-CAD-C3D	-3.05	121.18	128.52
30	0	301	CHL	OBD-CAD-C3D	-3.05	121.18	128.52
31	7	312	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
37	b	521	0IE	C4-C3-C2	-3.05	117.46	120.08
30	5	301	CHL	CHD-C4C-NC	3.05	129.01	124.20
30	h	602	CHL	CHC-C1C-NC	3.05	128.83	124.20
30	b	606	CHL	C3B-C4B-NB	3.05	113.34	110.52
30	6	301	CHL	C1D-CHD-C4C	-3.05	119.48	126.06
30	8	315	CHL	C1D-CHD-C4C	-3.05	119.48	126.06
30	2	313	CHL	CAC-C3C-C4C	3.05	128.77	124.81
30	h	614	CHL	CAC-C3C-C4C	3.05	128.77	124.81
30	i	614	CHL	CAC-C3C-C4C	3.05	128.77	124.81
30	0	305	CHL	CMB-C2B-C1B	3.05	130.01	125.37
31	A	823	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
31	A	830	CLA	CMB-C2B-C1B	-3.05	120.73	125.37
30	f	614	CHL	CAA-C2A-C3A	-3.05	108.99	116.10
30	6	306	CHL	CHB-C4A-NA	3.05	128.72	124.51
30	b	614	CHL	CHD-C1D-ND	-3.05	121.66	124.45
30	b	607	CHL	C3B-C4B-NB	3.05	113.34	110.52
37	b	521	0IE	C22-C12-C11	-3.04	118.66	122.92
30	4	319	CHL	C1D-CHD-C4C	-3.04	119.49	126.06
30	d	605	CHL	CAC-C3C-C4C	3.04	128.76	124.81
32	3	402	8CT	C04-C03-C02	-3.04	118.33	122.61
32	A	849	8CT	C07-C02-C03	-3.04	118.31	122.73
30	g	602	CHL	CHD-C4C-NC	3.04	129.00	124.20
30	e	605	CHL	CAC-C3C-C4C	3.04	128.76	124.81
33	4	501	0UR	C28-C19-C18	-3.04	108.86	112.70
31	8	311	CLA	C3B-C4B-NB	-3.04	107.69	110.52
31	B	813	CLA	O2D-CGD-O1D	-3.04	117.89	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	612	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
31	A	837	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
31	B	815	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
30	c	602	CHL	C1D-CHD-C4C	-3.04	119.50	126.06
30	7	313	CHL	C1D-CHD-C4C	-3.04	119.50	126.06
30	5	313	CHL	CAC-C3C-C4C	3.04	128.75	124.81
38	A	842	PQN	C11-C12-C13	-3.04	121.74	126.79
30	2	319	CHL	C1D-CHD-C4C	-3.04	119.51	126.06
30	3	305	CHL	OBD-CAD-C3D	-3.04	121.22	128.52
30	f	602	CHL	C3B-C4B-NB	3.04	113.33	110.52
37	7	502	0IE	C9-C10-C11	3.03	129.69	123.47
31	3	318	CLA	C3B-C4B-NB	-3.03	107.70	110.52
30	1	307	CHL	C1D-CHD-C4C	-3.03	119.51	126.06
31	A	826	CLA	C3B-C4B-NB	-3.03	107.70	110.52
31	3	312	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
33	f	520	0UR	C36-C28-C19	3.03	114.14	109.55
30	4	306	CHL	OBD-CAD-C3D	-3.03	121.22	128.52
30	d	614	CHL	CHC-C1C-NC	3.03	128.80	124.20
31	B	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
31	A	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
30	b	607	CHL	CHD-C4C-NC	3.03	128.98	124.20
32	7	405	8CT	C01-C02-C07	3.03	119.44	113.62
30	c	609	CHL	C1-C2-C3	-3.03	120.80	126.04
30	a	608	CHL	C1D-CHD-C4C	-3.03	119.52	126.06
31	B	813	CLA	C3B-C4B-NB	-3.03	107.70	110.52
30	8	305	CHL	C1D-CHD-C4C	-3.03	119.53	126.06
30	3	307	CHL	C1-C2-C3	-3.03	120.81	126.04
30	9	313	CHL	CAC-C3C-C4C	3.03	128.74	124.81
33	4	501	0UR	C5-C4-C3	-3.03	123.36	127.00
30	i	614	CHL	CHD-C1D-ND	-3.03	121.67	124.45
30	i	607	CHL	C2A-C1A-CHA	-3.03	118.57	123.86
37	e	521	0IE	C22-C12-C11	-3.03	118.68	122.92
33	8	502	0UR	C24-C25-C26	-3.03	106.16	110.30
30	h	605	CHL	CHC-C1C-NC	3.03	128.79	124.20
30	a	614	CHL	C1D-CHD-C4C	-3.03	119.53	126.06
30	e	607	CHL	C1D-CHD-C4C	-3.03	119.53	126.06
30	a	605	CHL	CAC-C3C-C4C	3.03	128.74	124.81
30	f	606	CHL	C3B-C4B-NB	3.03	113.32	110.52
30	5	307	CHL	CHD-C4C-NC	3.03	128.97	124.20
30	6	313	CHL	CMB-C2B-C1B	3.02	129.98	125.37
30	9	313	CHL	CMB-C2B-C1B	3.02	129.98	125.37
37	i	522	0IE	C9-C10-C11	3.02	129.67	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	402	8CT	C24-C23-C21	-3.02	117.92	126.42
30	c	614	CHL	CHD-C4C-NC	3.02	128.97	124.20
30	e	607	CHL	CHD-C4C-NC	3.02	128.97	124.20
32	3	403	8CT	C01-C02-C07	3.02	119.42	113.62
30	8	313	CHL	CMB-C2B-C1B	3.02	129.97	125.37
30	h	607	CHL	OBD-CAD-C3D	-3.02	121.25	128.52
31	B	832	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
33	c	520	0UR	C43-C3-C4	-3.02	121.37	125.02
32	L	209	8CT	C25-C24-C23	-3.02	113.79	123.22
30	g	601	CHL	CHD-C1D-ND	-3.02	121.68	124.45
32	8	406	8CT	C05-C04-C03	3.02	115.13	110.48
32	B	846	8CT	C22-C21-C20	-3.02	118.69	122.92
31	B	840	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
32	B	851	8CT	C18-C19-C20	-3.02	117.29	123.47
33	9	502	0UR	C9-C10-C11	-3.02	117.29	123.47
30	e	607	CHL	CAC-C3C-C4C	3.02	128.73	124.81
30	a	614	CHL	OBD-CAD-C3D	-3.02	121.25	128.52
32	A	846	8CT	C35-C30-C29	-3.02	108.89	112.70
30	d	606	CHL	OBD-CAD-C3D	-3.02	121.26	128.52
31	B	820	CLA	C3B-C4B-NB	-3.02	107.72	110.52
30	d	609	CHL	C3B-C4B-NB	3.02	113.31	110.52
30	h	602	CHL	OBD-CAD-C3D	-3.02	121.26	128.52
33	5	501	0UR	C43-C3-C4	-3.02	121.37	125.02
31	F	301	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	g	613	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
30	a	606	CHL	C1D-CHD-C4C	-3.02	119.55	126.06
30	i	614	CHL	C1D-CHD-C4C	-3.01	119.55	126.06
31	6	318	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
31	B	828	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
30	c	607	CHL	CHD-C4C-NC	3.01	128.95	124.20
32	K	107	8CT	C40-C12-C13	-3.01	118.70	122.92
31	B	814	CLA	C3B-C4B-NB	-3.01	107.72	110.52
31	2	312	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
32	G	104	8CT	C15-C16-C17	3.01	123.56	118.94
30	b	609	CHL	CHD-C1D-ND	-3.01	121.69	124.45
30	a	606	CHL	OBD-CAD-C3D	-3.01	121.27	128.52
30	f	606	CHL	C1D-CHD-C4C	-3.01	119.56	126.06
31	M	101	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
30	d	609	CHL	OBD-CAD-C3D	-3.01	121.27	128.52
32	A	850	8CT	C11-C12-C13	-3.01	114.32	118.94
30	e	605	CHL	OBD-CAD-C3D	-3.01	121.27	128.52
33	2	501	0UR	C48-C47-C46	-3.01	119.39	125.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	502	0UR	C5-C4-C3	-3.01	123.39	127.00
37	f	522	0IE	C9-C10-C11	3.01	129.64	123.47
33	0	502	0UR	C10-C11-C12	-3.01	123.01	127.31
32	K	107	8CT	C01-C02-C07	3.01	119.40	113.62
31	2	310	CLA	C3B-C4B-NB	-3.01	107.72	110.52
33	4	502	0UR	C14-C15-C16	-3.01	123.02	127.31
31	3	318	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
30	a	607	CHL	CHD-C1D-ND	-3.01	121.69	124.45
33	5	502	0UR	C48-C47-C46	-3.01	119.39	125.85
30	8	308	CHL	OBD-CAD-C3D	-3.01	121.28	128.52
30	d	606	CHL	CHD-C1D-ND	-3.01	121.69	124.45
31	A	832	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
30	1	305	CHL	C1D-CHD-C4C	-3.01	119.57	126.06
30	e	608	CHL	C1D-CHD-C4C	-3.01	119.57	126.06
33	i	520	0UR	C43-C3-C4	-3.01	121.38	125.02
30	b	602	CHL	C4-C3-C5	3.01	120.33	115.27
30	7	302	CHL	C1-C2-C3	-3.01	120.84	126.04
31	B	817	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
30	8	315	CHL	CHD-C1D-ND	-3.01	121.69	124.45
30	1	302	CHL	OBD-CAD-C3D	-3.00	121.29	128.52
33	5	501	0UR	C24-C25-C26	-3.00	106.19	110.30
30	h	608	CHL	C1D-CHD-C4C	-3.00	119.58	126.06
31	H	205	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	B	817	CLA	CHB-C4A-NA	3.00	128.66	124.51
30	d	607	CHL	OBD-CAD-C3D	-3.00	121.30	128.52
30	0	302	CHL	CHB-C1B-NB	-3.00	121.08	124.26
30	0	305	CHL	C1D-CHD-C4C	-3.00	119.58	126.06
30	i	608	CHL	C1D-CHD-C4C	-3.00	119.58	126.06
34	G	105	LHG	O8-C23-C24	3.00	121.33	111.91
31	L	204	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	d	614	CHL	OBD-CAD-C3D	-3.00	121.30	128.52
30	h	606	CHL	CHD-C4C-NC	3.00	128.93	124.20
31	O	202	CLA	C3B-C4B-NB	-3.00	107.73	110.52
30	g	609	CHL	C1D-CHD-C4C	-3.00	119.59	126.06
30	1	306	CHL	CMB-C2B-C1B	3.00	129.93	125.37
31	3	309	CLA	C3B-C4B-NB	-3.00	107.73	110.52
30	g	614	CHL	OBD-CAD-C3D	-3.00	121.31	128.52
30	h	606	CHL	OBD-CAD-C3D	-2.99	121.31	128.52
30	2	301	CHL	O2A-CGA-CBA	2.99	121.31	111.91
30	8	307	CHL	CAC-C3C-C4C	2.99	128.69	124.81
30	e	609	CHL	C1-C2-C3	-2.99	120.86	126.04
31	6	311	CLA	C3B-C4B-NB	-2.99	107.74	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	306	CHL	OBD-CAD-C3D	-2.99	121.32	128.52
31	0	309	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
30	d	606	CHL	C1D-CHD-C4C	-2.99	119.60	126.06
30	6	307	CHL	CMB-C2B-C1B	2.99	129.93	125.37
30	7	307	CHL	CMB-C2B-C1B	2.99	129.92	125.37
31	B	834	CLA	C3B-C4B-NB	-2.99	107.74	110.52
30	6	306	CHL	CHB-C1B-NB	-2.99	121.09	124.26
31	6	310	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
31	7	303	CLA	C3B-C4B-NB	-2.99	107.74	110.52
30	f	606	CHL	CMB-C2B-C1B	2.99	129.92	125.37
32	B	844	8CT	C18-C17-C16	-2.99	123.05	127.31
33	5	501	0UR	C14-C15-C16	-2.99	123.05	127.31
30	4	302	CHL	CMB-C2B-C1B	2.99	129.92	125.37
30	i	606	CHL	C1D-CHD-C4C	-2.99	119.61	126.06
31	B	820	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
30	f	601	CHL	C4-C3-C5	2.99	120.29	115.27
33	0	501	0UR	C29-C30-C31	-2.99	108.34	111.74
30	e	602	CHL	OBD-CAD-C3D	-2.98	121.34	128.52
33	a	520	0UR	C29-C30-C31	-2.98	108.34	111.74
31	G	101	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
30	h	602	CHL	CHD-C4C-NC	2.98	128.91	124.20
31	B	831	CLA	C3B-C4B-NB	-2.98	107.75	110.52
30	6	301	CHL	C1-C2-C3	-2.98	120.88	126.04
31	7	318	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	2	303	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
30	d	608	CHL	C1D-CHD-C4C	-2.98	119.62	126.06
32	1	402	8CT	C07-C02-C03	-2.98	118.40	122.73
30	4	305	CHL	CMB-C2B-C1B	2.98	129.91	125.37
31	G	102	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
33	2	501	0UR	C34-C27-C1	-2.98	120.58	124.49
30	f	614	CHL	C3B-C4B-NB	2.98	113.28	110.52
31	4	311	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	3	304	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
30	a	606	CHL	CHD-C4C-NC	2.98	128.90	124.20
30	h	614	CHL	CHC-C1C-NC	2.98	128.72	124.20
30	f	601	CHL	C1-C2-C3	-2.98	120.89	126.04
31	3	310	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
31	A	805	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
31	B	836	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
30	e	602	CHL	C1D-CHD-C4C	-2.98	119.64	126.06
30	g	608	CHL	C1D-CHD-C4C	-2.98	119.64	126.06
31	8	304	CLA	O2D-CGD-O1D	-2.98	118.02	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	820	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
30	3	302	CHL	C1D-ND-C4D	2.98	108.45	106.33
30	0	302	CHL	OBD-CAD-C3D	-2.98	121.36	128.52
31	A	843	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
30	8	302	CHL	C3B-C4B-NB	2.98	113.28	110.52
30	h	607	CHL	CHC-C1C-NC	2.97	128.72	124.20
37	3	502	0IE	C4-C3-C2	-2.97	117.53	120.08
30	f	605	CHL	C1D-CHD-C4C	-2.97	119.64	126.06
30	8	301	CHL	CAC-C3C-C4C	2.97	128.67	124.81
30	8	315	CHL	CAC-C3C-C4C	2.97	128.67	124.81
33	g	520	0UR	C48-C47-C46	-2.97	119.47	125.85
30	a	607	CHL	CHD-C4C-NC	2.97	128.89	124.20
31	9	310	CLA	C3B-C4B-NB	-2.97	107.76	110.52
30	d	614	CHL	CAA-C2A-C3A	-2.97	109.16	116.10
30	g	601	CHL	C1D-CHD-C4C	-2.97	119.65	126.06
31	A	804	CLA	CHB-C4A-NA	2.97	128.62	124.51
33	1	502	0UR	C24-C25-C26	-2.97	106.24	110.30
30	6	308	CHL	CAC-C3C-C4C	2.97	128.66	124.81
30	b	614	CHL	C2A-C1A-CHA	-2.97	118.67	123.85
30	e	601	CHL	C1D-CHD-C4C	-2.97	119.65	126.06
30	c	607	CHL	CHD-C1D-ND	-2.97	121.73	124.45
33	6	502	0UR	C28-C19-C32	-2.97	106.10	111.42
30	h	607	CHL	CHD-C4C-NC	2.97	128.88	124.20
30	2	305	CHL	CHB-C1B-NB	-2.97	121.12	124.26
30	8	302	CHL	CHB-C4A-NA	2.96	128.61	124.51
30	a	601	CHL	C3B-C4B-NB	2.96	113.27	110.52
30	2	307	CHL	CHB-C4A-NA	2.96	128.61	124.51
32	7	404	8CT	C15-C16-C17	2.96	123.49	118.94
30	2	313	CHL	O2A-CGA-CBA	2.96	121.21	111.91
31	6	318	CLA	C3B-C4B-NB	-2.96	107.77	110.52
31	A	840	CLA	C3B-C4B-NB	-2.96	107.77	110.52
30	c	607	CHL	C3B-C4B-NB	2.96	113.26	110.52
30	e	606	CHL	C3B-C4B-NB	2.96	113.26	110.52
30	h	609	CHL	C3B-C4B-NB	2.96	113.26	110.52
30	3	302	CHL	O2A-CGA-CBA	2.96	121.20	111.91
30	g	608	CHL	CHD-C4C-NC	2.96	128.87	124.20
31	9	312	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	f	606	CHL	OBD-CAD-C3D	-2.96	121.40	128.52
30	d	606	CHL	CHD-C4C-NC	2.96	128.87	124.20
30	8	306	CHL	C1D-CHD-C4C	-2.96	119.67	126.06
31	2	310	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	i	602	CHL	C1-C2-C3	-2.96	120.92	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	841	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
31	A	802	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
31	B	801	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
30	a	609	CHL	C1-C2-C3	-2.96	120.93	126.04
33	0	502	0UR	C28-C19-C18	-2.96	108.97	112.70
31	A	852	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
30	b	601	CHL	C2A-C1A-CHA	-2.95	118.69	123.86
31	B	814	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
31	B	829	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
31	a	613	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
31	K	101	CLA	C3B-C4B-NB	-2.95	107.78	110.52
30	6	313	CHL	CAC-C3C-C4C	2.95	128.64	124.81
31	d	611	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
30	c	609	CHL	OBD-CAD-C3D	-2.95	121.42	128.52
30	d	601	CHL	CHC-C1C-NC	2.95	128.68	124.20
30	3	302	CHL	CMB-C2B-C1B	2.95	129.86	125.37
30	b	602	CHL	CMB-C2B-C1B	2.95	129.86	125.37
30	d	602	CHL	CHB-C1B-NB	-2.95	121.13	124.26
31	A	829	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
33	0	501	0UR	O44-C45-C46	2.95	119.40	111.55
30	3	307	CHL	CMB-C2B-C1B	2.95	129.86	125.37
30	d	609	CHL	C1-C2-C3	-2.95	120.94	126.04
33	a	520	0UR	C14-C15-C16	-2.95	123.10	127.31
31	c	613	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
30	2	319	CHL	C4-C3-C5	2.95	120.23	115.27
37	i	521	0IE	C20-C3-C4	-2.95	121.03	124.83
37	e	522	0IE	C13-C12-C11	2.95	123.47	118.94
30	2	302	CHL	CMB-C2B-C1B	2.95	129.86	125.37
30	f	602	CHL	CMB-C2B-C1B	2.95	129.86	125.37
30	a	614	CHL	CAA-C2A-C3A	-2.95	109.22	116.10
32	L	206	8CT	C14-C15-C16	-2.95	118.14	126.42
32	B	804	8CT	C19-C20-C21	-2.95	123.10	127.31
30	f	607	CHL	CHD-C1D-ND	-2.95	121.75	124.45
30	b	601	CHL	CHD-C4C-NC	2.95	128.85	124.20
30	g	606	CHL	OBD-CAD-C3D	-2.95	121.43	128.52
31	8	310	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
30	0	305	CHL	OBD-CAD-C3D	-2.95	121.43	128.52
30	6	302	CHL	CHB-C1B-NB	-2.95	121.14	124.26
31	B	807	CLA	C3B-C4B-NB	-2.94	107.78	110.52
31	K	105	CLA	C3B-C4B-NB	-2.94	107.78	110.52
32	1	402	8CT	C04-C03-C02	-2.94	118.47	122.61
30	5	302	CHL	OBD-CAD-C3D	-2.94	121.44	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	304	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
31	8	312	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
37	f	521	0IE	C6-C7-C8	2.94	123.46	118.94
37	d	521	0IE	C22-C12-C11	-2.94	118.80	122.92
32	3	403	8CT	C11-C10-C03	-2.94	118.94	127.20
30	e	605	CHL	CHD-C1D-ND	-2.94	121.75	124.45
32	B	843	8CT	C01-C02-C07	2.94	119.27	113.62
30	i	614	CHL	CAA-C2A-C3A	-2.94	109.24	116.10
31	4	303	CLA	C3B-C4B-NB	-2.94	107.79	110.52
30	h	614	CHL	C2A-C1A-CHA	-2.94	118.72	123.85
33	2	501	0UR	C28-C19-C18	-2.94	108.98	112.70
32	O	205	8CT	C24-C25-C26	-2.94	123.11	127.31
30	e	602	CHL	C1-C2-C3	-2.94	120.96	126.04
31	3	306	CLA	C3B-C4B-NB	-2.94	107.79	110.52
30	b	601	CHL	C1D-CHD-C4C	-2.94	119.72	126.06
30	5	301	CHL	CHD-C1D-ND	-2.94	121.75	124.45
31	1	303	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	9	303	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	A	820	CLA	C3B-C4B-NB	-2.94	107.79	110.52
31	A	831	CLA	C3B-C4B-NB	-2.94	107.79	110.52
30	6	305	CHL	OBD-CAD-C3D	-2.94	121.45	128.52
30	h	614	CHL	OBD-CAD-C3D	-2.94	121.45	128.52
30	8	306	CHL	C1-C2-C3	-2.94	122.00	126.75
31	b	613	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
30	2	319	CHL	CHB-C1B-NB	-2.93	121.15	124.26
30	5	306	CHL	CHD-C1D-ND	-2.93	121.76	124.45
30	e	609	CHL	CHD-C1D-ND	-2.93	121.76	124.45
33	1	502	0UR	C9-C10-C11	-2.93	117.47	123.47
30	4	319	CHL	O2D-CGD-O1D	-2.93	118.10	123.84
31	3	313	CLA	C3B-C4B-NB	-2.93	107.79	110.52
37	e	521	0IE	C6-C7-C8	2.93	123.44	118.94
30	e	607	CHL	OBD-CAD-C3D	-2.93	121.46	128.52
30	6	305	CHL	CMB-C2B-C1B	2.93	129.84	125.37
30	f	602	CHL	CHB-C1B-NB	-2.93	121.15	124.26
30	f	609	CHL	C4A-NA-C1A	2.93	108.02	106.71
31	A	810	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
33	9	502	0UR	C29-C30-C31	-2.93	108.41	111.74
30	h	601	CHL	CHD-C1D-ND	-2.93	121.76	124.45
33	3	501	0UR	C24-C25-C26	-2.93	106.29	110.30
30	h	605	CHL	OBD-CAD-C3D	-2.93	121.47	128.52
30	c	601	CHL	CMB-C2B-C1B	2.93	129.83	125.37
37	c	521	0IE	C9-C10-C11	2.93	129.47	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	501	0UR	O44-C45-C46	2.93	119.34	111.55
31	A	809	CLA	C3B-C4B-NB	-2.93	107.80	110.52
31	9	304	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
37	i	522	0IE	C17-C16-C15	2.93	123.43	118.94
30	b	601	CHL	C4A-NA-C1A	2.93	108.02	106.71
31	0	310	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	g	605	CHL	OBD-CAD-C3D	-2.93	121.48	128.52
30	f	614	CHL	OBD-CAD-C3D	-2.93	121.48	128.52
30	6	306	CHL	CMB-C2B-C1B	2.93	129.83	125.37
30	8	315	CHL	CMB-C2B-C1B	2.93	129.83	125.37
32	G	104	8CT	C14-C15-C16	-2.93	118.20	126.42
31	A	826	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
31	7	308	CLA	C3B-C4B-NB	-2.93	107.80	110.52
30	a	607	CHL	OBD-CAD-C3D	-2.93	121.48	128.52
30	b	607	CHL	OBD-CAD-C3D	-2.92	121.48	128.52
30	g	609	CHL	C4A-NA-C1A	2.92	108.02	106.71
33	6	502	0UR	C10-C11-C12	-2.92	123.14	127.31
37	h	521	0IE	C9-C10-C11	2.92	129.47	123.47
37	7	502	0IE	C4-C3-C2	-2.92	117.57	120.08
31	f	611	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
31	B	823	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
30	1	305	CHL	CHB-C4A-NA	2.92	128.55	124.51
30	1	302	CHL	CMB-C2B-C1B	2.92	129.82	125.37
32	M	102	8CT	C01-C02-C07	2.92	119.23	113.62
32	B	851	8CT	C11-C10-C03	-2.92	119.00	127.20
31	3	310	CLA	C3B-C4B-NB	-2.92	107.81	110.52
31	A	824	CLA	C3B-C4B-NB	-2.92	107.81	110.52
31	A	841	CLA	C3B-C4B-NB	-2.92	107.81	110.52
30	4	302	CHL	CHB-C1B-NB	-2.92	121.17	124.26
30	1	306	CHL	O2A-CGA-CBA	2.92	121.07	111.91
30	1	313	CHL	O2A-CGA-CBA	2.92	121.07	111.91
33	4	501	0UR	C34-C27-C1	-2.92	120.66	124.49
32	J	104	8CT	C07-C02-C03	-2.92	118.49	122.73
31	A	821	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
30	5	306	CHL	C4A-NA-C1A	2.92	108.02	106.71
30	c	608	CHL	C1-C2-C3	-2.92	121.00	126.04
31	B	822	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
30	c	601	CHL	C1-C2-C3	-2.92	121.00	126.04
30	g	602	CHL	CHD-C1D-ND	-2.92	121.77	124.45
32	8	402	8CT	C07-C02-C03	-2.92	118.50	122.73
31	f	612	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
32	K	107	8CT	C39-C16-C17	-2.91	118.84	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	848	8CT	C04-C03-C02	-2.91	118.51	122.61
30	c	608	CHL	CMB-C2B-C1B	2.91	129.81	125.37
30	5	307	CHL	C3B-C4B-NB	2.91	113.22	110.52
31	A	807	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
33	c	520	0UR	C5-C4-C3	-2.91	123.50	127.00
30	d	606	CHL	C3B-C4B-NB	2.91	113.22	110.52
30	c	608	CHL	C1D-CHD-C4C	-2.91	119.78	126.06
30	d	605	CHL	OBD-CAD-C3D	-2.91	121.52	128.52
31	3	312	CLA	C3B-C4B-NB	-2.91	107.82	110.52
32	B	846	8CT	C22-C21-C23	2.91	122.66	118.08
30	g	607	CHL	CHD-C1D-ND	-2.91	121.78	124.45
30	g	605	CHL	CHC-C4B-NB	-2.91	121.18	124.26
31	4	310	CLA	C3B-C4B-NB	-2.91	107.82	110.52
30	0	306	CHL	CHD-C4C-NC	2.91	128.79	124.20
31	4	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	6	304	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	f	602	CHL	C4-C3-C5	2.91	120.16	115.27
30	a	607	CHL	CMB-C2B-C1B	2.91	129.80	125.37
30	g	614	CHL	CAA-C2A-C3A	-2.91	109.31	116.10
33	9	501	0UR	C29-C30-C31	-2.91	108.43	111.74
30	1	305	CHL	OBD-CAD-C3D	-2.91	121.52	128.52
30	5	307	CHL	CHD-C1D-ND	-2.91	121.78	124.45
33	6	501	0UR	C9-C8-C7	-2.91	123.16	127.31
33	c	520	0UR	C48-C47-C46	-2.91	119.61	125.85
31	7	316	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
31	7	308	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
30	8	308	CHL	CMB-C2B-C1B	2.90	129.79	125.37
33	6	502	0UR	C14-C15-C16	-2.90	123.17	127.31
30	b	601	CHL	C3B-C4B-NB	2.90	113.21	110.52
33	4	501	0UR	C24-C25-C26	-2.90	106.33	110.30
30	f	608	CHL	C3C-C4C-NC	2.90	113.83	110.57
30	c	607	CHL	OBD-CAD-C3D	-2.90	121.53	128.52
31	1	309	CLA	C3B-C4B-NB	-2.90	107.82	110.52
31	a	610	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
31	2	309	CLA	C3B-C4B-NB	-2.90	107.82	110.52
31	7	312	CLA	C3B-C4B-NB	-2.90	107.82	110.52
37	3	502	0IE	C9-C10-C11	2.90	129.42	123.47
31	B	831	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
33	2	502	0UR	C24-C25-C26	-2.90	106.33	110.30
31	1	312	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	A	823	CLA	C3B-C4B-NB	-2.90	107.83	110.52
32	A	850	8CT	C10-C03-C02	-2.90	114.44	121.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	e	607	CHL	CHD-C1D-ND	-2.90	121.79	124.45
31	9	311	CLA	C3B-C4B-NB	-2.90	107.83	110.52
30	g	606	CHL	C3B-C4B-NB	2.90	113.20	110.52
30	f	614	CHL	CHD-C4C-NC	2.90	128.77	124.20
30	5	301	CHL	C1D-CHD-C4C	-2.90	119.81	126.06
31	0	304	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
33	9	502	0UR	C10-C11-C12	-2.89	123.18	127.31
37	g	521	0IE	C6-C7-C8	2.89	123.38	118.94
33	3	501	0UR	C34-C27-C1	-2.89	120.69	124.49
30	6	302	CHL	O2A-CGA-CBA	2.89	120.98	111.91
32	A	846	8CT	C01-C02-C07	2.89	119.17	113.62
31	G	103	CLA	C3B-C4B-NB	-2.89	107.83	110.52
32	L	206	8CT	C18-C19-C20	-2.89	117.55	123.47
37	d	522	0IE	C14-C15-C16	2.89	131.44	127.31
37	i	521	0IE	C13-C12-C11	2.89	123.38	118.94
31	B	839	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
30	g	614	CHL	CHC-C4B-NB	-2.89	121.20	124.26
30	1	307	CHL	C4-C3-C5	2.89	120.13	115.27
30	c	614	CHL	C3B-C4B-NB	2.89	113.20	110.52
31	0	312	CLA	C3B-C4B-NB	-2.89	107.83	110.52
30	8	301	CHL	CMB-C2B-C1B	2.89	129.77	125.37
30	4	319	CHL	C4-C3-C5	2.89	120.13	115.27
33	i	520	0UR	C5-C4-C3	-2.89	123.53	127.00
30	e	614	CHL	CAA-C2A-C3A	-2.89	109.36	116.10
30	d	609	CHL	CHD-C4C-NC	2.89	128.75	124.20
30	h	608	CHL	OBD-CAD-C3D	-2.89	121.57	128.52
31	e	604	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
33	f	520	0UR	C10-C9-C8	-2.89	117.56	123.47
30	0	301	CHL	CMB-C2B-C1B	2.89	129.76	125.37
30	3	302	CHL	C3B-C4B-NB	2.89	113.19	110.52
34	3	601	LHG	O8-C23-C24	2.89	120.96	111.91
30	f	609	CHL	OBD-CAD-C3D	-2.89	121.58	128.52
30	b	608	CHL	CMB-C2B-C1B	2.89	129.76	125.37
33	i	520	0UR	C4-C3-C2	-2.88	117.60	120.08
30	6	313	CHL	OBD-CAD-C3D	-2.88	121.58	128.52
30	i	606	CHL	CHD-C4C-NC	2.88	128.75	124.20
31	5	310	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	h	601	CHL	C1D-CHD-C4C	-2.88	119.84	126.06
30	a	602	CHL	OBD-CAD-C3D	-2.88	121.58	128.52
30	e	605	CHL	CHD-C4C-NC	2.88	128.75	124.20
30	i	607	CHL	OBD-CAD-C3D	-2.88	121.58	128.52
31	0	308	CLA	C3B-C4B-NB	-2.88	107.84	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	835	CLA	C3B-C4B-NB	-2.88	107.84	110.52
30	6	308	CHL	O2A-CGA-CBA	2.88	120.95	111.91
33	3	501	0UR	O44-C43-C3	2.88	116.82	109.11
31	0	312	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
30	7	306	CHL	CMB-C2B-C1B	2.88	129.76	125.37
30	g	601	CHL	CMB-C2B-C1B	2.88	129.76	125.37
37	i	522	0IE	C13-C12-C11	2.88	123.36	118.94
32	B	843	8CT	C35-C30-C29	-2.88	109.06	112.70
30	h	601	CHL	C3B-C4B-NB	2.88	113.19	110.52
30	7	301	CHL	CAC-C3C-C4C	2.88	128.55	124.81
31	1	310	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	7	303	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	9	309	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	e	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	8	312	CLA	C3B-C4B-NB	-2.88	107.84	110.52
30	0	302	CHL	C4-C3-C5	2.88	120.11	115.27
31	1	304	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	c	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
30	i	606	CHL	OBD-CAD-C3D	-2.88	121.59	128.52
31	g	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
30	a	609	CHL	C3B-C4B-NB	2.88	113.18	110.52
36	J	102	LMG	O6-C1-O1	-2.88	103.16	109.97
30	f	606	CHL	CHD-C1D-ND	-2.88	121.81	124.45
31	e	612	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
32	A	848	8CT	C19-C18-C17	-2.88	117.58	123.47
31	B	812	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
31	H	202	CLA	C3B-C4B-NB	-2.87	107.85	110.52
30	8	306	CHL	CMB-C2B-C1B	2.87	129.75	125.37
31	h	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	J	104	8CT	C22-C21-C23	2.87	122.60	118.08
30	4	308	CHL	OBD-CAD-C3D	-2.87	121.61	128.52
30	i	607	CHL	CHD-C1D-ND	-2.87	121.81	124.45
30	c	607	CHL	C4A-NA-C1A	2.87	108.00	106.71
30	a	601	CHL	CHD-C4C-NC	2.87	128.73	124.20
32	L	209	8CT	C35-C30-C29	-2.87	109.07	112.70
30	1	302	CHL	C4-C3-C5	2.87	120.10	115.27
31	A	803	CLA	C3B-C4B-NB	-2.87	107.85	110.52
30	2	313	CHL	C3C-C4C-NC	2.87	113.79	110.57
31	A	813	CLA	C3B-C4B-NB	-2.87	107.85	110.52
33	0	501	0UR	C14-C15-C16	-2.87	123.22	127.31
30	8	315	CHL	C3B-C4B-NB	2.87	113.18	110.52
30	b	614	CHL	CAA-C2A-C3A	-2.87	109.41	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	308	CHL	OBD-CAD-C3D	-2.87	121.62	128.52
31	B	809	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	B	848	8CT	C18-C19-C20	2.87	129.35	123.47
32	A	846	8CT	C14-C15-C16	-2.87	118.36	126.42
30	d	601	CHL	CHD-C4C-NC	2.87	128.72	124.20
31	A	830	CLA	CHB-C1B-NB	2.87	127.29	124.26
31	2	309	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	4	402	8CT	C14-C15-C16	-2.87	118.36	126.42
30	f	605	CHL	CMB-C2B-C1B	2.87	129.73	125.37
30	7	305	CHL	OBD-CAD-C3D	-2.87	121.62	128.52
30	c	609	CHL	CHD-C4C-NC	2.87	128.72	124.20
30	b	608	CHL	C1-C2-C3	-2.87	121.09	126.04
30	f	614	CHL	CMB-C2B-C1B	2.86	129.73	125.37
30	2	305	CHL	CHB-C4A-NA	2.86	128.47	124.51
30	7	302	CHL	CMB-C2B-C1B	2.86	129.73	125.37
30	e	606	CHL	OBD-CAD-C3D	-2.86	121.63	128.52
30	a	606	CHL	CHD-C1D-ND	-2.86	121.82	124.45
30	9	305	CHL	O2A-CGA-CBA	2.86	120.89	111.91
30	d	605	CHL	CMB-C2B-C1B	2.86	129.73	125.37
30	h	601	CHL	CHD-C4C-NC	2.86	128.71	124.20
30	i	614	CHL	CHD-C4C-NC	2.86	128.71	124.20
31	J	103	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
30	h	605	CHL	CMB-C2B-C1B	2.86	129.73	125.37
30	e	602	CHL	C4-C3-C5	2.86	120.08	115.27
31	J	103	CLA	C3B-C4B-NB	-2.86	107.86	110.52
30	h	601	CHL	CMB-C2B-C1B	2.86	129.72	125.37
30	g	601	CHL	OBD-CAD-C3D	-2.86	121.64	128.52
31	A	834	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
30	h	605	CHL	CHC-C4B-NB	-2.86	121.23	124.26
31	K	105	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
32	A	848	8CT	C35-C30-C31	2.86	116.54	111.42
31	G	101	CLA	C3B-C4B-NB	-2.86	107.86	110.52
30	c	614	CHL	CAA-C2A-C3A	-2.86	109.43	116.10
35	0	603	SQD	O6-C1-C2	2.86	112.76	108.30
31	A	819	CLA	C3B-C4B-NB	-2.86	107.86	110.52
30	g	606	CHL	CHD-C1D-ND	-2.86	121.83	124.45
30	h	607	CHL	CMB-C2B-C1B	2.86	129.72	125.37
37	a	521	0IE	C6-C7-C8	2.86	123.32	118.94
30	6	301	CHL	OBD-CAD-C3D	-2.86	121.65	128.52
30	2	313	CHL	CMB-C2B-C1B	2.85	129.72	125.37
30	8	302	CHL	C4-C3-C5	2.85	120.07	115.27
30	a	601	CHL	CHD-C1D-ND	-2.85	121.83	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	305	CHL	C3C-C4C-NC	2.85	113.77	110.57
37	7	502	0IE	C22-C12-C11	-2.85	118.93	122.92
31	B	805	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
37	i	521	0IE	C6-C7-C8	2.85	123.32	118.94
39	A	857	CL0	C3B-C4B-NB	-2.85	107.87	110.52
30	6	313	CHL	CHB-C4A-NA	2.85	128.46	124.51
30	2	302	CHL	CHB-C1B-NB	-2.85	121.24	124.26
30	i	601	CHL	CHD-C4C-NC	2.85	128.70	124.20
30	h	606	CHL	CMB-C2B-C1B	2.85	129.71	125.37
30	8	307	CHL	C3C-C4C-NC	2.85	113.77	110.57
30	h	602	CHL	C4A-NA-C1A	2.85	107.99	106.71
30	c	614	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
31	O	206	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
37	g	522	0IE	C9-C10-C11	2.85	129.31	123.47
30	c	605	CHL	CMB-C2B-C1B	2.85	129.71	125.37
31	6	310	CLA	C3B-C4B-NB	-2.85	107.87	110.52
30	b	609	CHL	CHD-C4C-NC	2.85	128.69	124.20
30	c	602	CHL	CMB-C2B-C1B	2.85	129.71	125.37
31	0	303	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
33	3	501	0UR	C5-C4-C3	-2.85	123.58	127.00
30	4	313	CHL	CHB-C4A-NA	2.85	128.45	124.51
37	3	502	0IE	C22-C12-C11	-2.85	118.93	122.92
30	g	602	CHL	OBD-CAD-C3D	-2.85	121.67	128.52
30	2	305	CHL	CMB-C2B-C1B	2.85	129.71	125.37
34	6	603	LHG	O8-C23-C24	2.85	120.84	111.91
31	c	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
31	c	611	CLA	C3B-C4B-NB	-2.85	107.88	110.52
30	c	602	CHL	CHB-C4A-NA	2.85	128.45	124.51
31	7	304	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
31	B	850	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
30	8	305	CHL	OBD-CAD-C3D	-2.85	121.67	128.52
30	d	605	CHL	CHC-C4B-NB	-2.85	121.25	124.26
31	a	613	CLA	C3B-C4B-NB	-2.84	107.88	110.52
30	h	602	CHL	CMB-C2B-C1B	2.84	129.70	125.37
42	h	523	NEX	C26-C27-C28	2.84	132.01	125.99
31	A	811	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
30	i	605	CHL	CMB-C2B-C1B	2.84	129.70	125.37
31	9	312	CLA	C3B-C4B-NB	-2.84	107.88	110.52
31	O	201	CLA	C3B-C4B-NB	-2.84	107.88	110.52
30	a	605	CHL	CMB-C2B-C1B	2.84	129.70	125.37
30	d	614	CHL	CHC-C4B-NB	-2.84	121.25	124.26
30	2	308	CHL	CHB-C4A-NA	2.84	128.44	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	602	CHL	C4-C3-C5	2.84	120.05	115.27
31	2	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
31	B	801	CLA	CHB-C1B-NB	2.84	127.26	124.26
30	f	609	CHL	C3B-C4B-NB	2.84	113.15	110.52
31	6	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
30	7	307	CHL	C1-C2-C3	-2.84	122.16	126.75
30	b	614	CHL	CHD-C4C-NC	2.84	128.68	124.20
31	B	811	CLA	C3B-C4B-NB	-2.84	107.88	110.52
30	i	607	CHL	CMB-C2B-C1B	2.84	129.69	125.37
30	a	602	CHL	CHD-C1D-ND	-2.84	121.85	124.45
31	b	604	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
31	B	835	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
31	c	610	CLA	C3B-C4B-NB	-2.84	107.88	110.52
33	e	520	0UR	C34-C27-C1	-2.84	120.77	124.49
33	9	502	0UR	C15-C14-C13	-2.84	114.37	123.22
30	f	607	CHL	CMB-C2B-C1B	2.84	129.69	125.37
31	A	839	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
31	L	207	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
31	a	612	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
31	7	310	CLA	C3B-C4B-NB	-2.83	107.89	110.52
31	L	207	CLA	C3B-C4B-NB	-2.83	107.89	110.52
31	g	610	CLA	C3B-C4B-NB	-2.83	107.89	110.52
42	g	523	NEX	C26-C27-C28	2.83	131.99	125.99
31	a	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	i	614	CHL	CMB-C2B-C1B	2.83	129.68	125.37
42	b	523	NEX	C26-C27-C28	2.83	131.98	125.99
33	2	502	0UR	C17-C16-C15	2.83	123.29	118.94
30	2	306	CHL	CMB-C2B-C1B	2.83	129.68	125.37
30	c	614	CHL	OBD-CAD-C3D	-2.83	121.71	128.52
31	7	311	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
31	B	850	CLA	C3B-C4B-NB	-2.83	107.89	110.52
30	7	302	CHL	CHB-C4A-NA	2.83	128.43	124.51
31	2	304	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	e	613	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
33	8	502	0UR	C9-C10-C11	-2.83	117.68	123.47
42	d	523	NEX	C26-C27-C28	2.83	131.97	125.99
31	5	314	CLA	C3B-C4B-NB	-2.83	107.89	110.52
30	g	609	CHL	CHD-C4C-NC	2.83	128.66	124.20
31	A	806	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	e	607	CHL	CMB-C2B-C1B	2.83	129.68	125.37
42	c	523	NEX	C26-C27-C28	2.83	131.97	125.99
30	i	601	CHL	CMB-C2B-C1B	2.83	129.67	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	313	CHL	CMB-C2B-C1B	2.83	129.67	125.37
30	4	307	CHL	O2A-CGA-CBA	2.83	120.78	111.91
31	c	603	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	e	602	CHL	O2A-CGA-CBA	2.83	120.78	111.91
30	6	306	CHL	O2A-CGA-CBA	2.83	120.77	111.91
31	A	809	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
31	A	813	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
31	h	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
32	7	402	8CT	C25-C24-C23	-2.82	114.41	123.22
42	f	523	NEX	C26-C27-C28	2.82	131.96	125.99
31	a	611	CLA	C3B-C4B-NB	-2.82	107.90	110.52
31	5	312	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
42	i	523	NEX	C26-C27-C28	2.82	131.96	125.99
37	c	521	0IE	C6-C7-C8	2.82	123.27	118.94
31	b	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
30	7	313	CHL	CMB-C2B-C1B	2.82	129.67	125.37
31	h	612	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
31	A	828	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
30	7	301	CHL	CMB-C2B-C1B	2.82	129.66	125.37
31	A	815	CLA	C3B-C4B-NB	-2.82	107.90	110.52
30	7	301	CHL	O2A-CGA-CBA	2.82	120.76	111.91
30	g	607	CHL	CMB-C2B-C1B	2.82	129.66	125.37
42	a	523	NEX	C26-C27-C28	2.82	131.95	125.99
30	7	302	CHL	O2A-CGA-CBA	2.82	120.75	111.91
30	a	601	CHL	C2A-C1A-CHA	-2.82	118.93	123.86
30	f	609	CHL	CHD-C4C-NC	2.82	128.65	124.20
31	c	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
33	g	520	0UR	O44-C45-C46	2.82	119.05	111.55
30	g	614	CHL	CMB-C2B-C1B	2.82	129.66	125.37
30	a	609	CHL	OBD-CAD-C3D	-2.82	121.74	128.52
32	L	209	8CT	C04-C03-C02	-2.82	118.65	122.61
31	H	201	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	g	609	CHL	OBD-CAD-C3D	-2.81	121.75	128.52
30	7	306	CHL	O2A-CGA-CBA	2.81	120.74	111.91
30	6	305	CHL	CHB-C4A-NA	2.81	128.40	124.51
31	b	610	CLA	C3B-C4B-NB	-2.81	107.91	110.52
30	e	614	CHL	CHD-C4C-NC	2.81	128.64	124.20
30	a	602	CHL	CMB-C2B-C1B	2.81	129.65	125.37
30	e	605	CHL	CMB-C2B-C1B	2.81	129.65	125.37
30	5	305	CHL	OBD-CAD-C3D	-2.81	121.75	128.52
31	A	832	CLA	C3B-C4B-NB	-2.81	107.91	110.52
31	f	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	522	0IE	C13-C12-C11	2.81	123.26	118.94
30	5	306	CHL	CHD-C4C-NC	2.81	128.63	124.20
30	5	302	CHL	CHB-C4A-NA	2.81	128.40	124.51
30	5	302	CHL	O2A-CGA-CBA	2.81	120.73	111.91
31	4	310	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
31	7	309	CLA	C3B-C4B-NB	-2.81	107.91	110.52
30	b	614	CHL	OBD-CAD-C3D	-2.81	121.76	128.52
31	3	303	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	I	101	8CT	C11-C10-C03	-2.81	119.31	127.20
30	7	306	CHL	CHD-C1D-ND	-2.81	121.87	124.45
30	g	606	CHL	CMB-C2B-C1B	2.81	129.65	125.37
30	4	306	CHL	CMB-C2B-C1B	2.81	129.65	125.37
30	d	609	CHL	CMB-C2B-C1B	2.81	129.65	125.37
30	f	601	CHL	CMB-C2B-C1B	2.81	129.65	125.37
30	0	301	CHL	C3C-C4C-NC	2.81	113.72	110.57
30	1	307	CHL	CMB-C2B-C1B	2.81	129.65	125.37
31	d	603	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
31	H	204	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	2	307	CHL	CMB-C2B-C1B	2.81	129.64	125.37
31	H	202	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
32	4	402	8CT	C01-C02-C07	2.81	119.01	113.62
31	B	830	CLA	C2D-C1D-ND	-2.81	108.04	110.10
30	7	305	CHL	C3C-C4C-NC	2.81	113.72	110.57
31	0	310	CLA	C3B-C4B-NB	-2.81	107.91	110.52
31	A	852	CLA	C3B-C4B-NB	-2.81	107.91	110.52
30	i	607	CHL	CHD-C4C-NC	2.81	128.62	124.20
33	7	501	0UR	C48-C47-C46	-2.81	119.83	125.85
30	d	601	CHL	CMB-C2B-C1B	2.80	129.64	125.37
31	1	308	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
34	f	630	LHG	O8-C23-C24	2.80	120.71	111.91
33	g	520	0UR	C14-C13-C12	-2.80	118.54	126.42
30	c	602	CHL	CHB-C1B-NB	-2.80	121.29	124.26
31	3	309	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
31	8	311	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
33	4	502	0UR	C43-C3-C4	-2.80	121.63	125.02
30	f	609	CHL	O2A-CGA-CBA	2.80	120.71	111.91
30	b	602	CHL	OBD-CAD-C3D	-2.80	121.77	128.52
30	g	608	CHL	CHD-C1D-ND	-2.80	121.88	124.45
33	8	501	0UR	O44-C45-C46	2.80	119.01	111.55
31	i	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	5	307	CHL	CMB-C2B-C1B	2.80	129.64	125.37
31	5	310	CLA	C3B-C4B-NB	-2.80	107.92	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	312	CLA	C3B-C4B-NB	-2.80	107.92	110.52
31	L	203	CLA	C3B-C4B-NB	-2.80	107.92	110.52
32	B	843	8CT	C22-C21-C23	2.80	122.49	118.08
30	2	302	CHL	O2A-CGA-CBA	2.80	120.70	111.91
33	2	502	0UR	O44-C45-C46	2.80	119.00	111.55
42	e	523	NEX	C39-C29-C30	-2.80	119.00	122.92
31	d	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
31	g	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
31	O	201	CLA	CAA-C2A-C3A	-2.80	109.56	116.10
33	9	501	0UR	C48-C47-C46	-2.80	119.84	125.85
30	8	313	CHL	C1-C2-C3	-2.80	121.20	126.04
31	h	603	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
31	A	829	CLA	C1-C2-C3	-2.80	121.20	126.04
31	i	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	7	313	CHL	OBD-CAD-C3D	-2.80	121.79	128.52
31	A	822	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
32	A	847	8CT	C11-C10-C03	-2.80	119.35	127.20
31	L	201	CLA	CMB-C2B-C1B	-2.80	121.11	125.37
30	a	608	CHL	CMB-C2B-C1B	2.80	129.63	125.37
30	d	602	CHL	C4-C3-C5	2.80	119.97	115.27
31	5	314	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	9	301	CHL	OBD-CAD-C3D	-2.79	121.80	128.52
31	g	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
31	A	828	CLA	C1-C2-C3	-2.79	121.21	126.04
30	a	606	CHL	CMB-C2B-C1B	2.79	129.62	125.37
31	8	309	CLA	C3B-C4B-NB	-2.79	107.92	110.52
31	4	304	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	2	308	CHL	CMB-C2B-C1B	2.79	129.62	125.37
31	B	824	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	B	804	8CT	C04-C03-C02	-2.79	118.68	122.61
30	1	313	CHL	CMB-C2B-C1B	2.79	129.62	125.37
31	O	203	CLA	CAA-C2A-C3A	-2.79	109.59	116.10
31	K	102	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	5	313	CHL	CMB-C2B-C1B	2.79	129.62	125.37
30	b	614	CHL	CMB-C2B-C1B	2.79	129.62	125.37
30	f	608	CHL	CMB-C2B-C1B	2.79	129.62	125.37
30	g	605	CHL	CMB-C2B-C1B	2.79	129.62	125.37
31	e	610	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	8	307	CHL	O2A-CGA-CBA	2.79	120.65	111.91
31	f	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	4	313	CHL	O2A-CGA-CBA	2.79	120.65	111.91
32	A	846	8CT	C25-C24-C23	-2.79	114.52	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	g	607	CHL	C3B-C4B-NB	2.79	113.10	110.52
31	h	612	CLA	C3B-C4B-NB	-2.79	107.93	110.52
30	e	606	CHL	CMB-C2B-C1B	2.79	129.61	125.37
30	d	607	CHL	CHD-C4C-NC	2.78	128.59	124.20
30	f	607	CHL	CHD-C4C-NC	2.78	128.59	124.20
30	c	607	CHL	CMB-C2B-C1B	2.78	129.61	125.37
30	f	602	CHL	C3C-C4C-NC	2.78	113.69	110.57
32	6	402	8CT	C35-C30-C31	2.78	116.40	111.42
31	f	610	CLA	C3B-C4B-NB	-2.78	107.93	110.52
30	6	302	CHL	CHB-C4A-NA	2.78	128.36	124.51
31	B	839	CLA	C3B-C4B-NB	-2.78	107.93	110.52
32	J	104	8CT	C23-C21-C20	-2.78	114.67	118.94
30	6	315	CHL	CMB-C2B-C1B	2.78	129.60	125.37
33	1	501	0UR	C48-C47-C46	-2.78	119.88	125.85
30	8	301	CHL	C4-C3-C5	2.78	119.95	115.27
30	a	609	CHL	CMB-C2B-C1B	2.78	129.60	125.37
33	9	501	0UR	C10-C9-C8	-2.78	117.78	123.47
37	a	522	0IE	C13-C12-C11	2.78	123.21	118.94
31	1	311	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
30	f	608	CHL	CHB-C4A-NA	2.78	128.35	124.51
31	5	309	CLA	C3B-C4B-NB	-2.78	107.94	110.52
33	9	501	0UR	C4-C3-C2	-2.78	117.69	120.08
30	5	301	CHL	CHC-C4B-NB	-2.78	121.32	124.26
30	g	609	CHL	CHC-C4B-NB	-2.78	121.32	124.26
32	F	302	8CT	C11-C10-C03	-2.78	119.40	127.20
33	2	502	0UR	C43-C3-C4	-2.78	121.66	125.02
30	e	614	CHL	CMB-C2B-C1B	2.78	129.60	125.37
31	A	817	CLA	C3B-C4B-NB	-2.78	107.94	110.52
30	4	302	CHL	C4-C3-C5	2.78	119.94	115.27
30	2	319	CHL	O2D-CGD-O1D	-2.78	118.41	123.84
31	7	315	CLA	C3B-C4B-NB	-2.78	107.94	110.52
30	5	313	CHL	CHD-C4C-NC	2.78	128.58	124.20
32	A	850	8CT	C25-C24-C23	-2.78	114.56	123.22
30	c	608	CHL	O2A-CGA-CBA	2.78	120.62	111.91
32	1	402	8CT	C01-C02-C07	2.78	118.95	113.62
30	8	305	CHL	CHD-C1D-ND	-2.77	121.90	124.45
30	a	614	CHL	CMB-C2B-C1B	2.77	129.59	125.37
30	d	614	CHL	CMB-C2B-C1B	2.77	129.59	125.37
33	f	520	0UR	C9-C8-C7	-2.77	123.35	127.31
31	9	311	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
30	8	307	CHL	CMB-C2B-C1B	2.77	129.59	125.37
33	d	520	0UR	C24-C25-C26	-2.77	106.51	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	614	CHL	CHD-C1D-ND	-2.77	121.91	124.45
31	A	836	CLA	C3B-C4B-NB	-2.77	107.94	110.52
32	J	101	8CT	C10-C11-C12	-2.77	122.05	126.23
30	d	608	CHL	O2A-CGA-CBA	2.77	120.61	111.91
31	a	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	f	610	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	e	609	CHL	C4-C3-C5	2.77	119.93	115.27
31	h	610	CLA	C3B-C4B-NB	-2.77	107.94	110.52
31	3	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	e	601	CHL	CMB-C2B-C1B	2.77	129.59	125.37
31	A	807	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
30	0	305	CHL	CHD-C1D-ND	-2.77	121.91	124.45
30	0	302	CHL	CHB-C4A-NA	2.77	128.34	124.51
31	0	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	h	614	CHL	CHD-C4C-NC	2.77	128.57	124.20
30	a	606	CHL	C3B-C4B-NB	2.77	113.08	110.52
31	i	610	CLA	C3B-C4B-NB	-2.77	107.95	110.52
30	7	305	CHL	CHB-C4A-NA	2.77	128.34	124.51
37	g	522	0IE	C13-C12-C11	2.77	123.19	118.94
30	e	614	CHL	CHD-C1D-ND	-2.77	121.91	124.45
30	4	307	CHL	CMB-C2B-C1B	2.77	129.58	125.37
42	e	523	NEX	C5-C4-C3	-2.77	108.47	111.75
30	b	609	CHL	C4-C3-C5	2.77	119.92	115.27
31	B	815	CLA	C3B-C4B-NB	-2.77	107.95	110.52
31	e	610	CLA	C3B-C4B-NB	-2.77	107.95	110.52
30	8	306	CHL	OBD-CAD-C3D	-2.77	121.86	128.52
30	b	601	CHL	CMB-C2B-C1B	2.76	129.58	125.37
30	9	306	CHL	O2D-CGD-O1D	-2.76	118.43	123.84
31	5	303	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
30	d	608	CHL	CMB-C2B-C1B	2.76	129.58	125.37
30	3	307	CHL	CHB-C4A-NA	2.76	128.33	124.51
31	M	101	CLA	C3B-C4B-NB	-2.76	107.95	110.52
31	A	853	CLA	C1-C2-C3	-2.76	121.26	126.04
31	0	313	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	6	308	CHL	CMB-C2B-C1B	2.76	129.58	125.37
33	7	501	0UR	O44-C43-C3	2.76	116.50	109.11
31	2	314	CLA	C3B-C4B-NB	-2.76	107.95	110.52
30	5	306	CHL	CMB-C2B-C1B	2.76	129.58	125.37
33	2	501	0UR	O44-C43-C3	2.76	116.50	109.11
31	3	311	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	i	610	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	a	607	CHL	C3B-C4B-NB	2.76	113.08	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	605	CHL	OBD-CAD-C3D	-2.76	121.88	128.52
30	d	607	CHL	CMB-C2B-C1B	2.76	129.57	125.37
30	h	602	CHL	C4-C3-C5	2.76	119.91	115.27
32	2	402	8CT	C11-C10-C03	-2.76	119.45	127.20
30	b	609	CHL	CMB-C2B-C1B	2.76	129.57	125.37
30	i	609	CHL	CMB-C2B-C1B	2.76	129.57	125.37
33	b	520	0UR	C48-C47-C46	-2.76	119.93	125.85
30	4	319	CHL	C3C-C4C-NC	2.76	113.67	110.57
37	h	522	0IE	C13-C12-C11	2.76	123.17	118.94
32	8	402	8CT	C01-C02-C07	2.76	118.92	113.62
30	6	306	CHL	OBD-CAD-C3D	-2.76	121.88	128.52
31	1	310	CLA	C3B-C4B-NB	-2.76	107.96	110.52
31	A	837	CLA	C3B-C4B-NB	-2.76	107.96	110.52
31	8	314	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
31	7	315	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
30	h	609	CHL	CHD-C4C-NC	2.76	128.54	124.20
32	F	302	8CT	C05-C04-C03	2.75	114.72	110.48
33	2	502	0UR	C22-C16-C15	-2.75	119.06	122.92
30	f	605	CHL	OBD-CAD-C3D	-2.75	121.89	128.52
30	5	302	CHL	C3C-C4C-NC	2.75	113.66	110.57
30	9	306	CHL	O2A-CGA-CBA	2.75	120.55	111.91
30	2	307	CHL	CHB-C1B-NB	-2.75	121.34	124.26
30	e	605	CHL	C2A-C1A-CHA	-2.75	119.05	123.86
31	6	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	6	313	CHL	CHD-C1D-ND	-2.75	121.92	124.45
30	c	609	CHL	O2A-CGA-CBA	2.75	120.54	111.91
30	g	609	CHL	C3B-C4B-NB	2.75	113.07	110.52
30	1	306	CHL	OBD-CAD-C3D	-2.75	121.90	128.52
30	i	605	CHL	OBD-CAD-C3D	-2.75	121.90	128.52
36	L	211	LMG	O6-C1-O1	-2.75	103.46	109.97
31	b	603	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	4	305	CHL	C3C-C4C-NC	2.75	113.65	110.57
34	4	601	LHG	O8-C23-C24	2.75	120.53	111.91
30	g	607	CHL	OBD-CAD-C3D	-2.75	121.91	128.52
38	B	842	PQN	C11-C12-C13	-2.75	122.22	126.79
30	e	614	CHL	OBD-CAD-C3D	-2.75	121.91	128.52
33	4	502	0UR	O44-C45-C46	2.75	118.86	111.55
30	0	302	CHL	C3C-C4C-NC	2.75	113.65	110.57
30	5	305	CHL	CHD-C1D-ND	-2.75	121.93	124.45
33	8	501	0UR	C29-C30-C31	-2.75	108.61	111.74
37	7	502	0IE	C23-C16-C17	2.75	122.40	118.08
30	b	607	CHL	CMB-C2B-C1B	2.75	129.55	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	e	611	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	1	302	CHL	C3C-C4C-NC	2.75	113.65	110.57
31	G	103	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	7	302	CHL	CHB-C1B-NB	-2.75	121.35	124.26
30	g	608	CHL	CHC-C4B-NB	-2.75	121.35	124.26
33	1	501	0UR	C43-C3-C4	-2.74	121.70	125.02
30	b	609	CHL	O2A-CGA-CBA	2.74	120.52	111.91
30	e	606	CHL	CHD-C1D-ND	-2.74	121.93	124.45
30	a	602	CHL	C4-C3-C5	2.74	119.89	115.27
30	f	602	CHL	O2A-CGA-CBA	2.74	120.52	111.91
32	B	848	8CT	C01-C02-C07	2.74	118.88	113.62
31	A	821	CLA	C3B-C4B-NB	-2.74	107.97	110.52
31	f	613	CLA	C3B-C4B-NB	-2.74	107.97	110.52
30	e	608	CHL	C4-C3-C5	2.74	119.88	115.27
30	3	305	CHL	O2A-CGA-CBA	2.74	120.51	111.91
31	9	308	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
30	4	305	CHL	CHB-C4A-NA	2.74	128.30	124.51
31	B	811	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
31	h	613	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
33	c	520	0UR	C29-C30-C31	-2.74	108.62	111.74
30	3	302	CHL	CHB-C4A-NA	2.74	128.30	124.51
32	8	402	8CT	C24-C25-C26	-2.74	123.40	127.31
30	a	614	CHL	CHC-C4B-NB	-2.74	121.36	124.26
34	d	630	LHG	O8-C23-C24	2.74	120.50	111.91
30	g	601	CHL	C1-C2-C3	-2.74	121.31	126.04
30	e	609	CHL	CMB-C2B-C1B	2.74	129.54	125.37
30	f	609	CHL	CMB-C2B-C1B	2.74	129.54	125.37
30	6	307	CHL	C1-C2-C3	-2.74	122.33	126.75
31	7	309	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
31	8	310	CLA	C3B-C4B-NB	-2.74	107.98	110.52
30	6	305	CHL	C3C-C4C-NC	2.74	113.64	110.57
32	7	402	8CT	C30-C31-C32	-2.74	118.10	121.47
30	6	306	CHL	C3C-C4C-NC	2.73	113.64	110.57
30	3	302	CHL	C3C-C4C-NC	2.73	113.64	110.57
31	8	303	CLA	C3B-C4B-NB	-2.73	107.98	110.52
31	d	612	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	h	614	CHL	CMB-C2B-C1B	2.73	129.53	125.37
30	h	614	CHL	CHC-C4B-NB	-2.73	121.36	124.26
30	2	302	CHL	C3C-C4C-NC	2.73	113.63	110.57
31	A	829	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	b	614	CHL	C3B-C4B-NB	2.73	113.05	110.52
32	A	850	8CT	C28-C26-C25	-2.73	114.75	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	610	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
37	d	521	0IE	C6-C7-C8	2.73	123.13	118.94
31	2	303	CLA	C3B-C4B-NB	-2.73	107.98	110.52
32	L	206	8CT	C11-C12-C13	2.73	123.13	118.94
34	K	106	LHG	O8-C23-C24	2.73	120.47	111.91
30	2	302	CHL	CHB-C4A-NA	2.73	128.28	124.51
30	f	602	CHL	OBD-CAD-C3D	-2.73	121.96	128.52
33	5	502	0UR	C22-C16-C15	-2.73	119.10	122.92
30	h	605	CHL	CHD-C4C-NC	2.73	128.50	124.20
31	6	320	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
33	O	204	0UR	C10-C11-C12	-2.73	123.42	127.31
30	2	302	CHL	OMC-CMC-C2C	-2.73	119.52	125.69
37	c	521	0IE	C4-C3-C2	-2.73	117.74	120.08
31	3	304	CLA	CHB-C4A-NA	2.73	128.28	124.51
30	i	609	CHL	CHD-C4C-NC	2.73	128.50	124.20
31	8	309	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
31	i	603	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
31	7	316	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	K	102	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	0	311	CLA	CHB-C4A-NA	2.72	128.28	124.51
33	d	520	0UR	C29-C30-C31	-2.72	108.64	111.74
30	c	602	CHL	OBD-CAD-C3D	-2.72	121.96	128.52
31	B	805	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	f	603	CLA	C3B-C4B-NB	-2.72	107.99	110.52
30	e	608	CHL	CMB-C2B-C1B	2.72	129.52	125.37
30	2	307	CHL	C3C-C4C-NC	2.72	113.62	110.57
37	f	522	0IE	C13-C12-C11	2.72	123.12	118.94
30	5	306	CHL	C3B-C4B-NB	2.72	113.04	110.52
31	3	308	CLA	C3B-C4B-NB	-2.72	107.99	110.52
30	1	307	CHL	O2A-CGA-CBA	2.72	120.45	111.91
30	1	305	CHL	O2A-CGA-CBA	2.72	120.45	111.91
30	a	605	CHL	CHD-C4C-NC	2.72	128.49	124.20
30	2	302	CHL	OBD-CAD-C3D	-2.72	121.97	128.52
37	f	522	0IE	C17-C16-C15	2.72	123.12	118.94
31	A	812	CLA	CHB-C1B-NB	2.72	127.14	124.26
30	9	313	CHL	CHD-C1D-ND	-2.72	121.95	124.45
30	f	614	CHL	CHD-C1D-ND	-2.72	121.95	124.45
36	J	105	LMG	O6-C1-O1	-2.72	103.53	109.97
32	G	104	8CT	C18-C19-C20	-2.72	117.90	123.47
30	5	313	CHL	C3B-C4B-NB	2.72	113.04	110.52
31	6	304	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	8	314	CLA	C3B-C4B-NB	-2.72	107.99	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	e	609	CHL	O2A-CGA-CBA	2.72	120.44	111.91
31	i	613	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	e	613	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	c	612	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
32	A	854	8CT	C14-C15-C16	-2.71	118.79	126.42
30	4	302	CHL	OMC-CMC-C2C	-2.71	119.55	125.69
30	c	601	CHL	O2A-CGA-CBA	2.71	120.42	111.91
30	i	605	CHL	CHC-C4B-NB	-2.71	121.38	124.26
30	0	306	CHL	C3C-C4C-NC	2.71	113.61	110.57
33	b	520	0UR	C14-C15-C16	-2.71	123.44	127.31
33	i	520	0UR	C14-C15-C16	-2.71	123.44	127.31
30	7	301	CHL	O2D-CGD-O1D	-2.71	118.53	123.84
30	g	605	CHL	CHD-C4C-NC	2.71	128.48	124.20
31	A	804	CLA	C3B-C4B-NB	-2.71	108.00	110.52
30	4	313	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
30	i	608	CHL	CMB-C2B-C1B	2.71	129.50	125.37
30	a	609	CHL	C4-C3-C5	2.71	119.83	115.27
31	8	303	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
31	i	603	CLA	C3B-C4B-NB	-2.71	108.00	110.52
32	B	848	8CT	C07-C02-C03	-2.71	118.80	122.73
30	2	308	CHL	C3C-C4C-NC	2.71	113.61	110.57
32	F	302	8CT	C30-C31-C32	-2.71	118.13	121.47
33	e	520	0UR	C28-C19-C18	-2.71	109.28	112.70
31	i	604	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	b	606	CHL	CMB-C2B-C1B	2.71	129.50	125.37
30	c	605	CHL	OBD-CAD-C3D	-2.71	122.00	128.52
30	d	602	CHL	CHB-C4A-NA	2.71	128.26	124.51
30	2	306	CHL	O2A-CGA-CBA	2.71	120.41	111.91
34	M	104	LHG	O8-C23-C24	2.71	120.41	111.91
30	d	602	CHL	CMB-C2B-C1B	2.71	129.50	125.37
30	c	602	CHL	O2A-CGA-CBA	2.71	120.41	111.91
38	A	842	PQN	C2M-C2-C3	-2.71	119.98	124.40
30	c	602	CHL	C4-C3-C5	2.71	119.83	115.27
31	7	317	CLA	CHB-C4A-NA	2.71	128.26	124.51
32	L	209	8CT	C19-C20-C21	-2.71	123.45	127.31
31	B	834	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
31	L	201	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	i	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
33	b	520	0UR	O44-C45-C46	2.71	118.75	111.55
31	0	311	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
30	8	302	CHL	CMB-C2B-C1B	2.71	129.49	125.37
31	9	302	CLA	C3B-C4B-NB	-2.71	108.00	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	838	CLA	C3B-C4B-NB	-2.71	108.00	110.52
30	a	605	CHL	CHC-C4B-NB	-2.71	121.39	124.26
31	A	816	CLA	C3B-C4B-NB	-2.70	108.01	110.52
31	B	817	CLA	C3B-C4B-NB	-2.70	108.01	110.52
31	4	312	CLA	C3B-C4B-NB	-2.70	108.01	110.52
33	1	501	0UR	C24-C25-C26	-2.70	106.60	110.30
30	0	305	CHL	O2A-CGA-CBA	2.70	120.39	111.91
30	f	609	CHL	C4-C3-C5	2.70	119.82	115.27
30	d	609	CHL	C4-C3-C5	2.70	119.82	115.27
31	A	810	CLA	C1-C2-C3	-2.70	121.37	126.04
30	c	609	CHL	C4-C3-C5	2.70	119.82	115.27
33	0	502	0UR	C14-C15-C16	-2.70	123.45	127.31
30	h	606	CHL	O2A-CGA-CBA	2.70	120.39	111.91
31	B	806	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
30	d	606	CHL	O2A-CGA-CBA	2.70	120.39	111.91
30	f	607	CHL	C3B-C4B-NB	2.70	113.02	110.52
30	h	608	CHL	CHD-C1D-ND	-2.70	121.97	124.45
30	e	601	CHL	O2A-CGA-CBA	2.70	120.38	111.91
31	d	612	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	1	303	CLA	C3B-C4B-NB	-2.70	108.01	110.52
30	3	305	CHL	CHB-C4A-NA	2.70	128.24	124.51
31	1	308	CLA	C3B-C4B-NB	-2.70	108.01	110.52
33	b	520	0UR	C28-C19-C18	-2.70	109.29	112.70
31	B	807	CLA	CHB-C4A-NA	2.70	128.24	124.51
31	7	311	CLA	C3B-C4B-NB	-2.70	108.01	110.52
31	B	822	CLA	C3B-C4B-NB	-2.70	108.01	110.52
30	d	614	CHL	CHD-C4C-NC	2.70	128.45	124.20
30	b	602	CHL	O2A-CGA-CBA	2.70	120.37	111.91
30	f	601	CHL	CHD-C1D-ND	-2.70	121.98	124.45
31	5	308	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
30	e	614	CHL	C2A-C1A-CHA	-2.69	119.15	123.85
36	L	210	LMG	O6-C1-O1	-2.69	103.59	109.97
30	g	607	CHL	CHD-C4C-NC	2.69	128.45	124.20
31	d	613	CLA	C3B-C4B-NB	-2.69	108.02	110.52
30	i	606	CHL	O2A-CGA-CBA	2.69	120.36	111.91
31	7	317	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
32	K	107	8CT	C11-C12-C13	2.69	123.07	118.94
34	A	855	LHG	O8-C23-C24	2.69	120.36	111.91
30	i	609	CHL	O2A-CGA-CBA	2.69	120.36	111.91
30	b	606	CHL	O2A-CGA-CBA	2.69	120.36	111.91
32	A	848	8CT	C27-C26-C28	2.69	122.32	118.08
30	5	302	CHL	CHB-C1B-NB	-2.69	121.41	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	301	CHL	CMB-C2B-C1B	2.69	129.47	125.37
30	b	606	CHL	OBD-CAD-C3D	-2.69	122.05	128.52
31	A	825	CLA	C3B-C4B-NB	-2.69	108.02	110.52
30	2	305	CHL	C3C-C4C-NC	2.69	113.59	110.57
30	b	608	CHL	O2A-CGA-CBA	2.69	120.35	111.91
31	d	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
31	A	806	CLA	CHB-C4A-NA	2.69	128.23	124.51
30	i	609	CHL	OBD-CAD-C3D	-2.69	122.05	128.52
30	i	608	CHL	O2A-CGA-CBA	2.69	120.34	111.91
37	7	502	0IE	C6-C7-C8	2.69	123.06	118.94
30	g	601	CHL	C4B-CHC-C1C	-2.69	119.97	126.34
30	7	305	CHL	O2A-CGA-CBA	2.69	120.34	111.91
31	9	310	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
30	f	605	CHL	CHD-C4C-NC	2.69	128.44	124.20
30	2	307	CHL	C1D-ND-C4D	2.69	108.24	106.33
31	1	309	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
30	f	608	CHL	O2A-CGA-CBA	2.69	120.34	111.91
31	B	832	CLA	C3B-C4B-NB	-2.69	108.02	110.52
31	1	311	CLA	C3B-C4B-NB	-2.68	108.03	110.52
31	6	320	CLA	C3B-C4B-NB	-2.68	108.03	110.52
30	b	601	CHL	O2A-CGA-CBA	2.68	120.33	111.91
31	e	603	CLA	C3B-C4B-NB	-2.68	108.03	110.52
30	5	313	CHL	OBD-CAD-C3D	-2.68	122.06	128.52
31	9	310	CLA	CAA-C2A-C3A	-2.68	109.84	116.10
31	K	104	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
30	6	315	CHL	CHD-C1D-ND	-2.68	121.99	124.45
31	1	308	CLA	CHB-C4A-NA	2.68	128.22	124.51
30	5	302	CHL	C4-C3-C5	2.68	119.78	115.27
33	b	520	0UR	C29-C30-C31	-2.68	108.69	111.74
30	g	608	CHL	CMB-C2B-C1B	2.68	129.45	125.37
31	K	104	CLA	C3B-C4B-NB	-2.68	108.03	110.52
30	7	306	CHL	OBD-CAD-C3D	-2.68	122.07	128.52
30	a	609	CHL	CHD-C4C-NC	2.68	128.43	124.20
30	c	606	CHL	CMB-C2B-C1B	2.68	129.45	125.37
31	0	311	CLA	C3B-C4B-NB	-2.68	108.03	110.52
31	c	612	CLA	C3B-C4B-NB	-2.68	108.03	110.52
30	g	601	CHL	CHC-C4B-NB	-2.68	121.42	124.26
31	6	317	CLA	C3B-C4B-NB	-2.68	108.03	110.52
31	b	613	CLA	C3B-C4B-NB	-2.68	108.03	110.52
31	4	309	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
30	a	614	CHL	CHD-C4C-NC	2.68	128.42	124.20
33	8	502	0UR	C22-C16-C15	-2.68	119.17	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	501	0UR	C48-C47-C46	-2.68	120.11	125.85
31	5	311	CLA	CHB-C4A-NA	2.68	128.21	124.51
33	0	501	0UR	C4-C5-C6	-2.68	114.86	123.22
30	c	605	CHL	CHC-C4B-NB	-2.68	121.42	124.26
30	a	608	CHL	O2A-CGA-CBA	2.68	120.31	111.91
30	4	308	CHL	CHD-C1D-ND	-2.68	122.00	124.45
30	a	609	CHL	O2A-CGA-CBA	2.68	120.30	111.91
31	H	205	CLA	C3B-C4B-NB	-2.68	108.03	110.52
33	0	502	0UR	C34-C27-C1	-2.68	120.98	124.49
32	7	402	8CT	C18-C19-C20	-2.68	117.99	123.47
30	c	601	CHL	C3C-C4C-NC	2.68	113.57	110.57
30	h	607	CHL	CAC-C3C-C4C	2.67	128.28	124.81
33	e	520	0UR	C24-C25-C26	-2.67	106.64	110.30
30	g	601	CHL	CHD-C4C-NC	2.67	128.42	124.20
31	9	309	CLA	C3B-C4B-NB	-2.67	108.03	110.52
30	6	307	CHL	C3C-C4C-NC	2.67	113.57	110.57
31	B	808	CLA	C3B-C4B-NB	-2.67	108.04	110.52
31	h	604	CLA	C3B-C4B-NB	-2.67	108.04	110.52
31	g	613	CLA	CHB-C4A-NA	2.67	128.21	124.51
32	3	402	8CT	C01-C02-C07	2.67	118.75	113.62
31	8	304	CLA	C3B-C4B-NB	-2.67	108.04	110.52
34	4	601	LHG	C26-C25-C24	2.67	122.79	113.19
32	J	104	8CT	C35-C30-C29	-2.67	109.33	112.70
30	0	302	CHL	O2A-CGA-CBA	2.67	120.29	111.91
30	h	609	CHL	CMB-C2B-C1B	2.67	129.44	125.37
32	4	402	8CT	C24-C23-C21	-2.67	118.92	126.42
30	i	606	CHL	C3B-C4B-NB	2.67	112.99	110.52
31	7	304	CLA	C3B-C4B-NB	-2.67	108.04	110.52
36	3	602	LMG	O6-C1-O1	-2.67	103.66	109.97
30	4	308	CHL	CMB-C2B-C1B	2.67	129.43	125.37
30	d	605	CHL	CHD-C4C-NC	2.67	128.41	124.20
30	i	605	CHL	CHD-C4C-NC	2.67	128.41	124.20
30	7	302	CHL	C3C-C4C-NC	2.67	113.56	110.57
30	i	614	CHL	OBD-CAD-C3D	-2.67	122.10	128.52
32	B	804	8CT	C07-C02-C03	-2.67	118.86	122.73
30	e	614	CHL	C3B-C4B-NB	2.67	112.99	110.52
31	d	611	CLA	C3B-C4B-NB	-2.67	108.04	110.52
31	3	311	CLA	CHB-C4A-NA	2.67	128.20	124.51
31	d	604	CLA	C1-C2-C3	-2.66	122.44	126.75
30	i	614	CHL	CHC-C4B-NB	-2.66	121.44	124.26
30	7	306	CHL	C4-C3-C5	2.66	119.75	115.27
31	A	853	CLA	O2D-CGD-O1D	-2.66	118.63	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	843	8CT	C39-C16-C17	-2.66	119.19	122.92
30	4	302	CHL	CHB-C4A-NA	2.66	128.20	124.51
30	b	601	CHL	CHD-C1D-ND	-2.66	122.01	124.45
30	5	301	CHL	CMB-C2B-C1B	2.66	129.43	125.37
31	B	825	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	h	601	CHL	C4B-CHC-C1C	-2.66	120.02	126.34
30	i	609	CHL	C3B-C4B-NB	2.66	112.98	110.52
30	g	602	CHL	C1-C2-C3	-2.66	121.44	126.04
30	b	608	CHL	C4-C3-C5	2.66	119.75	115.27
32	B	804	8CT	C24-C25-C26	-2.66	123.51	127.31
30	i	602	CHL	CHD-C1D-ND	-2.66	122.01	124.45
30	5	301	CHL	C3B-C4B-NB	2.66	112.98	110.52
30	8	302	CHL	O2A-CGA-CBA	2.66	120.25	111.91
32	O	205	8CT	C14-C15-C16	-2.66	118.95	126.42
30	h	601	CHL	C2A-C1A-CHA	-2.66	119.21	123.86
30	f	602	CHL	CHB-C4A-NA	2.66	128.19	124.51
30	g	607	CHL	O2A-CGA-CBA	2.66	120.25	111.91
33	8	501	0UR	C28-C19-C18	-2.66	109.34	112.70
30	9	306	CHL	CMB-C2B-C1B	2.66	129.41	125.37
30	d	601	CHL	O2A-CGA-CBA	2.66	120.24	111.91
31	L	204	CLA	C3B-C4B-NB	-2.65	108.05	110.52
34	b	630	LHG	O8-C23-C24	2.65	120.24	111.91
30	e	605	CHL	C3B-C4B-NB	2.65	112.98	110.52
31	B	836	CLA	C3B-C4B-NB	-2.65	108.05	110.52
32	B	804	8CT	C01-C02-C07	2.65	118.71	113.62
30	4	307	CHL	C3C-C4C-NC	2.65	113.55	110.57
30	g	601	CHL	O2A-CGA-CBA	2.65	120.23	111.91
31	f	612	CLA	C3B-C4B-NB	-2.65	108.06	110.52
30	7	302	CHL	O2D-CGD-O1D	-2.65	118.65	123.84
31	6	317	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
34	a	630	LHG	O8-C23-C24	2.65	120.23	111.91
30	b	601	CHL	C1-C2-C3	-2.65	121.46	126.04
32	7	405	8CT	C04-C03-C02	-2.65	118.88	122.61
34	7	602	LHG	O8-C23-C24	2.65	120.22	111.91
30	g	608	CHL	C2A-C1A-CHA	-2.65	119.23	123.86
31	A	808	CLA	CHB-C4A-NA	2.65	128.17	124.51
31	1	314	CLA	C3B-C4B-NB	-2.65	108.06	110.52
31	4	311	CLA	C3B-C4B-NB	-2.65	108.06	110.52
32	B	845	8CT	C24-C25-C26	-2.65	123.53	127.31
30	3	307	CHL	C4-C3-C5	2.65	119.72	115.27
32	M	102	8CT	C04-C03-C02	-2.65	118.89	122.61
31	B	808	CLA	CHB-C4A-NA	2.65	128.17	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	7	501	0UR	C24-C25-C26	-2.65	106.68	110.30
32	8	402	8CT	C39-C16-C17	-2.64	119.22	122.92
30	8	306	CHL	O2D-CGD-O1D	-2.64	118.67	123.84
31	b	611	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
30	1	313	CHL	C3C-C4C-NC	2.64	113.54	110.57
34	5	601	LHG	O8-C23-C24	2.64	120.21	111.91
30	f	606	CHL	O2A-CGA-CBA	2.64	120.20	111.91
31	9	300	CLA	CHB-C4A-NA	2.64	128.17	124.51
31	b	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
31	6	309	CLA	C3B-C4B-NB	-2.64	108.06	110.52
31	h	613	CLA	C3B-C4B-NB	-2.64	108.06	110.52
31	6	317	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
31	A	840	CLA	O2A-C1-C2	2.64	115.58	108.64
30	i	607	CHL	C3B-C4B-NB	2.64	112.97	110.52
30	i	614	CHL	C3B-C4B-NB	2.64	112.97	110.52
32	7	404	8CT	C05-C04-C03	2.64	114.55	110.48
30	4	313	CHL	C3C-C4C-NC	2.64	113.53	110.57
31	i	611	CLA	CHB-C4A-NA	2.64	128.16	124.51
34	7	603	LHG	O8-C23-C24	2.64	120.19	111.91
30	8	313	CHL	OBD-CAD-C3D	-2.64	122.17	128.52
30	0	306	CHL	C4A-NA-C1A	2.64	107.89	106.71
30	g	606	CHL	O2A-CGA-CBA	2.64	120.19	111.91
31	A	808	CLA	C3B-C4B-NB	-2.64	108.07	110.52
33	6	501	0UR	C10-C9-C8	-2.64	118.07	123.47
34	2	601	LHG	O8-C23-C24	2.64	120.19	111.91
32	A	850	8CT	C27-C26-C28	2.64	122.23	118.08
30	1	302	CHL	O2A-CGA-CBA	2.64	120.18	111.91
30	e	606	CHL	O2A-CGA-CBA	2.64	120.18	111.91
31	f	613	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
31	A	820	CLA	CHB-C4A-NA	2.64	128.16	124.51
33	9	501	0UR	C15-C14-C13	-2.63	114.99	123.22
30	e	608	CHL	O2A-CGA-CBA	2.63	120.18	111.91
32	L	206	8CT	C05-C04-C03	2.63	114.54	110.48
30	2	302	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
30	a	606	CHL	O2A-CGA-CBA	2.63	120.17	111.91
31	6	309	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
31	d	603	CLA	C3B-C4B-NB	-2.63	108.07	110.52
30	3	305	CHL	C3C-C4C-NC	2.63	113.52	110.57
31	i	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
30	c	605	CHL	CHD-C4C-NC	2.63	128.35	124.20
30	d	606	CHL	C4A-NA-C1A	2.63	107.89	106.71
30	4	302	CHL	O2A-CGA-CBA	2.63	120.17	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	610	CLA	C3B-C4B-NB	-2.63	108.07	110.52
30	f	601	CHL	O2A-CGA-CBA	2.63	120.16	111.91
37	3	502	0IE	C23-C16-C17	2.63	122.22	118.08
42	e	523	NEX	C31-C30-C29	-2.63	123.56	127.31
32	B	844	8CT	C01-C02-C07	2.63	118.67	113.62
33	g	520	0UR	C24-C25-C26	-2.63	106.70	110.30
31	O	206	CLA	C3B-C4B-NB	-2.63	108.08	110.52
30	h	608	CHL	CMB-C2B-C1B	2.63	129.37	125.37
30	d	602	CHL	OBD-CAD-C3D	-2.63	122.19	128.52
30	b	601	CHL	C4-C3-C5	2.63	119.69	115.27
31	4	314	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
34	H	203	LHG	O8-C23-C24	2.63	120.16	111.91
31	i	604	CLA	C3B-C4B-NB	-2.63	108.08	110.52
30	2	319	CHL	C3C-C4C-NC	2.63	113.52	110.57
30	c	608	CHL	C4-C3-C5	2.63	119.69	115.27
31	0	312	CLA	CHB-C4A-NA	2.63	128.14	124.51
31	A	819	CLA	CHB-C1B-NB	2.63	127.04	124.26
30	d	607	CHL	CHC-C4B-NB	-2.62	121.48	124.26
30	4	306	CHL	CHB-C4A-NA	2.62	128.14	124.51
33	d	520	0UR	C4-C3-C2	-2.62	117.83	120.08
33	c	520	0UR	O44-C45-C46	2.62	118.53	111.55
30	2	319	CHL	CMB-C2B-C1B	2.62	129.36	125.37
30	b	609	CHL	OBD-CAD-C3D	-2.62	122.21	128.52
30	6	307	CHL	O2A-CGA-CBA	2.62	120.14	111.91
30	0	306	CHL	CHD-C1D-ND	-2.62	122.04	124.45
32	O	205	8CT	C35-C30-C29	-2.62	109.39	112.70
32	3	402	8CT	C15-C16-C17	-2.62	114.92	118.94
30	5	305	CHL	CMB-C2B-C1B	2.62	129.36	125.37
34	6	601	LHG	O8-C23-C24	2.62	120.14	111.91
30	6	302	CHL	C3C-C4C-NC	2.62	113.51	110.57
31	5	311	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
31	9	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
30	8	302	CHL	C3C-C4C-NC	2.62	113.51	110.57
31	A	833	CLA	C3B-C4B-NB	-2.62	108.08	110.52
31	B	825	CLA	C3B-C4B-NB	-2.62	108.08	110.52
31	1	311	CLA	CHB-C4A-NA	2.62	128.13	124.51
32	4	402	8CT	C11-C10-C03	-2.62	119.85	127.20
30	9	313	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
30	0	306	CHL	O1D-CGD-CBD	-2.62	119.13	124.48
31	A	834	CLA	C3B-C4B-NB	-2.62	108.09	110.52
30	7	307	CHL	C3B-C4B-NB	2.62	112.94	110.52
32	A	849	8CT	C35-C30-C29	-2.62	109.39	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	318	CLA	C3B-C4B-NB	-2.62	108.09	110.52
31	4	309	CLA	C3B-C4B-NB	-2.62	108.09	110.52
31	c	612	CLA	CHB-C4A-NA	2.61	128.13	124.51
33	0	502	0UR	C34-C27-C26	2.61	119.20	114.36
30	e	614	CHL	C4B-CHC-C1C	-2.61	120.14	126.34
30	i	607	CHL	C4B-CHC-C1C	-2.61	120.14	126.34
30	2	301	CHL	C3C-C4C-NC	2.61	113.50	110.57
30	g	608	CHL	C3B-C4B-NB	2.61	112.94	110.52
30	i	601	CHL	C3B-C4B-NB	2.61	112.94	110.52
31	A	831	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	3	302	CHL	C4-C3-C5	2.61	119.66	115.27
30	h	602	CHL	CHC-C4B-NB	-2.61	121.49	124.26
31	B	826	CLA	C3B-C4B-NB	-2.61	108.09	110.52
31	G	102	CLA	C3B-C4B-NB	-2.61	108.09	110.52
33	2	502	0UR	C29-C30-C31	-2.61	108.77	111.74
30	8	313	CHL	O2A-CGA-CBA	2.61	120.10	111.91
33	9	501	0UR	C24-C25-C26	-2.61	106.73	110.30
30	2	301	CHL	CMB-C2B-C1B	2.61	129.34	125.37
31	4	314	CLA	C3B-C4B-NB	-2.61	108.10	110.52
31	B	827	CLA	C3B-C4B-NB	-2.61	108.10	110.52
30	4	307	CHL	CHB-C4A-NA	2.61	128.12	124.51
30	6	308	CHL	CHD-C1D-ND	-2.61	122.06	124.45
34	A	844	LHG	O8-C23-C24	2.60	120.08	111.91
39	A	857	CL0	C1C-C2C-C3C	-2.60	104.22	106.96
31	B	813	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	i	601	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
32	G	104	8CT	C04-C03-C02	-2.60	118.95	122.61
31	3	308	CLA	C1-C2-C3	-2.60	121.54	126.04
30	g	614	CHL	CHD-C4C-NC	2.60	128.31	124.20
36	9	602	LMG	O1-C1-C2	-2.60	104.24	108.30
31	3	311	CLA	C3B-C4B-NB	-2.60	108.10	110.52
30	6	302	CHL	OMC-CMC-C2C	-2.60	119.80	125.69
31	O	202	CLA	O2D-CGD-O1D	-2.60	118.18	124.09
31	B	827	CLA	C1-C2-C3	-2.60	121.54	126.04
31	5	311	CLA	C3B-C4B-NB	-2.60	108.10	110.52
31	1	303	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	g	602	CHL	C3B-C4B-NB	2.60	112.93	110.52
31	c	613	CLA	C3B-C4B-NB	-2.60	108.10	110.52
33	4	502	0UR	C25-C26-C27	-2.60	106.67	111.85
30	2	301	CHL	CHD-C1D-ND	-2.60	122.06	124.45
30	1	305	CHL	CHB-C1B-NB	-2.60	121.50	124.26
30	h	601	CHL	CHC-C4B-NB	-2.60	121.50	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	804	8CT	C25-C24-C23	-2.60	115.11	123.22
30	i	609	CHL	CHC-C4B-NB	-2.60	121.51	124.26
31	2	304	CLA	C3B-C4B-NB	-2.60	108.11	110.52
30	d	601	CHL	CHC-C4B-NB	-2.60	121.51	124.26
30	e	602	CHL	CHD-C1D-ND	-2.60	122.07	124.45
30	i	614	CHL	C2A-C1A-CHA	-2.60	119.32	123.85
30	4	302	CHL	C3C-C4C-NC	2.60	113.48	110.57
32	7	404	8CT	C25-C24-C23	-2.60	115.11	123.22
31	B	816	CLA	CHB-C4A-NA	2.60	128.10	124.51
32	A	847	8CT	C27-C26-C28	2.60	122.17	118.08
30	h	607	CHL	CHC-C4B-NB	-2.60	121.51	124.26
33	f	520	0UR	C5-C4-C3	-2.60	123.88	127.00
32	O	205	8CT	C25-C24-C23	-2.60	115.12	123.22
30	g	614	CHL	C4B-CHC-C1C	-2.60	120.18	126.34
30	6	301	CHL	C4-C3-C5	2.60	119.64	115.27
32	0	401	8CT	C11-C10-C03	-2.60	119.91	127.20
30	4	319	CHL	CHB-C1B-NB	-2.59	121.51	124.26
32	A	846	8CT	C24-C25-C26	-2.59	123.61	127.31
30	8	308	CHL	CHD-C1D-ND	-2.59	122.07	124.45
33	5	501	0UR	C48-C47-C46	-2.59	120.29	125.85
31	5	303	CLA	CHB-C4A-NA	2.59	128.10	124.51
33	0	502	0UR	C15-C14-C13	-2.59	115.13	123.22
33	f	520	0UR	C24-C25-C26	-2.59	106.76	110.30
31	B	818	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	d	605	CHL	C4B-CHC-C1C	-2.59	120.19	126.34
34	e	630	LHG	O8-C23-C24	2.59	120.03	111.91
36	O	207	LMG	O6-C1-O1	-2.59	103.84	109.97
33	3	501	0UR	C28-C19-C18	-2.59	109.43	112.70
31	0	321	CLA	CHB-C4A-NA	2.59	128.09	124.51
31	a	612	CLA	CHB-C4A-NA	2.59	128.09	124.51
30	5	306	CHL	O2A-CGA-CBA	2.59	120.03	111.91
30	g	602	CHL	O2A-CGA-CBA	2.59	120.03	111.91
30	d	602	CHL	C3C-C4C-NC	2.59	113.47	110.57
31	3	309	CLA	CHB-C4A-NA	2.59	128.09	124.51
37	g	521	0IE	C13-C12-C11	2.59	122.91	118.94
30	g	607	CHL	CHC-C4B-NB	-2.59	121.52	124.26
30	b	602	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
30	4	319	CHL	CHB-C4A-NA	2.59	128.09	124.51
32	A	850	8CT	C01-C02-C07	2.59	118.58	113.62
30	b	606	CHL	C3C-C4C-NC	2.58	113.47	110.57
30	g	607	CHL	C4B-CHC-C1C	-2.58	120.21	126.34
30	6	301	CHL	O2D-CGD-O1D	-2.58	118.78	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	A	857	CL0	C2C-C1C-NC	2.58	112.39	109.97
31	5	308	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	c	603	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	g	612	CLA	C3B-C4B-NB	-2.58	108.12	110.52
30	1	307	CHL	C1-C2-C3	-2.58	121.58	126.04
30	h	606	CHL	CHD-C1D-ND	-2.58	122.08	124.45
30	3	307	CHL	C3C-C4C-NC	2.58	113.47	110.57
37	f	521	0IE	C13-C12-C11	2.58	122.90	118.94
34	g	630	LHG	O8-C23-C24	2.58	120.01	111.91
30	d	607	CHL	C3B-C4B-NB	2.58	112.91	110.52
30	h	602	CHL	O2A-CGA-CBA	2.58	120.01	111.91
33	8	501	0UR	C48-C47-C46	-2.58	120.31	125.85
34	3	603	LHG	O8-C23-C24	2.58	120.01	111.91
30	f	605	CHL	CHC-C4B-NB	-2.58	121.53	124.26
30	9	306	CHL	C3C-C4C-NC	2.58	113.46	110.57
33	6	502	0UR	C48-C47-C46	-2.58	120.31	125.85
31	B	806	CLA	CHB-C4A-NA	2.58	128.08	124.51
33	7	501	0UR	C10-C9-C8	-2.58	118.19	123.47
31	B	819	CLA	C3B-C4B-NB	-2.58	108.12	110.52
34	c	630	LHG	O8-C23-C24	2.58	120.00	111.91
32	K	107	8CT	C11-C10-C03	-2.58	119.96	127.20
33	8	501	0UR	C4-C5-C6	-2.58	115.17	123.22
31	B	820	CLA	CHB-C1B-NB	2.58	126.99	124.26
32	1	402	8CT	C05-C04-C03	2.58	114.45	110.48
37	a	521	0IE	C13-C12-C11	2.58	122.90	118.94
31	2	311	CLA	CHB-C4A-NA	2.58	128.08	124.51
30	a	602	CHL	O2A-CGA-CBA	2.58	120.00	111.91
31	9	303	CLA	CHB-C4A-NA	2.58	128.07	124.51
31	A	819	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
31	B	821	CLA	CHB-C4A-NA	2.58	128.07	124.51
33	O	204	0UR	C15-C14-C13	-2.58	115.18	123.22
32	B	804	8CT	C18-C19-C20	-2.58	118.20	123.47
30	4	308	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
33	8	502	0UR	C48-C47-C46	-2.57	120.33	125.85
30	6	313	CHL	C3C-C4C-NC	2.57	113.46	110.57
34	B	854	LHG	O8-C23-C24	2.57	119.98	111.91
30	d	601	CHL	C3B-C4B-NB	2.57	112.90	110.52
31	a	610	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	0	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
31	A	827	CLA	CHB-C4A-NA	2.57	128.07	124.51
37	h	521	0IE	C13-C12-C11	2.57	122.89	118.94
31	B	840	CLA	C3B-C4B-NB	-2.57	108.13	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	608	CHL	C3C-C4C-NC	2.57	113.45	110.57
31	3	318	CLA	CHB-C4A-NA	2.57	128.06	124.51
33	c	520	0UR	C33-C32-C31	-2.57	118.06	123.56
36	9	602	LMG	O6-C1-O1	-2.57	103.89	109.97
31	B	816	CLA	C3B-C4B-NB	-2.57	108.13	110.52
30	1	302	CHL	CHB-C1B-NB	-2.57	121.54	124.26
31	A	817	CLA	CHB-C4A-NA	2.57	128.06	124.51
32	M	102	8CT	C14-C15-C16	-2.57	119.20	126.42
30	9	306	CHL	CHD-C1D-ND	-2.57	122.09	124.45
32	8	402	8CT	C05-C04-C03	2.57	114.43	110.48
34	0	601	LHG	O8-C23-C24	2.57	119.96	111.91
30	i	608	CHL	CHD-C1D-ND	-2.56	122.10	124.45
32	A	848	8CT	C13-C14-C15	-2.56	115.21	123.22
31	H	204	CLA	CHB-C4A-NA	2.56	128.06	124.51
30	a	614	CHL	C4B-CHC-C1C	-2.56	120.26	126.34
31	5	309	CLA	CMB-C2B-C1B	-2.56	121.46	125.37
30	d	609	CHL	O2A-CGA-CBA	2.56	119.95	111.91
31	b	612	CLA	CHB-C4A-NA	2.56	128.06	124.51
32	A	854	8CT	C24-C23-C21	-2.56	119.22	126.42
31	A	840	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
34	7	601	LHG	O8-C23-C24	2.56	119.95	111.91
33	d	520	0UR	C28-C19-C18	-2.56	109.46	112.70
30	1	302	CHL	OMC-CMC-C2C	-2.56	119.89	125.69
30	2	301	CHL	CHB-C4A-NA	2.56	128.06	124.51
33	0	502	0UR	C43-C3-C2	2.56	122.68	116.66
32	7	402	8CT	C10-C11-C12	-2.56	122.36	126.23
31	a	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
31	h	610	CLA	CHB-C4A-NA	2.56	128.05	124.51
37	3	502	0IE	C6-C7-C8	2.56	122.87	118.94
30	i	602	CHL	O2A-CGA-CBA	2.56	119.94	111.91
33	5	502	0UR	C9-C10-C11	-2.56	118.23	123.47
30	5	302	CHL	OMC-CMC-C2C	-2.56	119.90	125.69
34	i	630	LHG	O8-C23-C24	2.56	119.94	111.91
32	1	402	8CT	C27-C26-C25	-2.56	119.34	122.92
30	i	605	CHL	C4B-CHC-C1C	-2.56	120.27	126.34
30	h	605	CHL	C4B-CHC-C1C	-2.56	120.27	126.34
31	A	822	CLA	C3B-C4B-NB	-2.56	108.14	110.52
30	1	305	CHL	C3C-C4C-NC	2.56	113.44	110.57
30	3	305	CHL	O2D-CGD-O1D	-2.55	118.84	123.84
32	8	402	8CT	C11-C10-C03	-2.55	120.03	127.20
32	6	402	8CT	C05-C04-C03	2.55	114.41	110.48
34	1	601	LHG	O8-C23-C24	2.55	119.92	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	606	CHL	CHD-C1D-ND	-2.55	122.11	124.45
30	g	609	CHL	CMB-C2B-C1B	2.55	129.26	125.37
30	4	313	CHL	OBD-CAD-C3D	-2.55	122.38	128.52
33	3	501	0UR	C15-C14-C13	-2.55	115.25	123.22
30	a	606	CHL	CHC-C4B-NB	-2.55	121.56	124.26
30	i	601	CHL	CHC-C4B-NB	-2.55	121.56	124.26
31	8	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
31	4	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	J	101	8CT	C39-C16-C15	2.55	122.10	118.08
33	f	520	0UR	C14-C13-C12	-2.55	119.25	126.42
31	A	807	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	7	309	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	6	302	CHL	C4-C3-C5	2.55	119.56	115.27
30	f	605	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
31	i	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
31	9	309	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	1	402	8CT	C39-C16-C17	-2.55	119.35	122.92
30	a	605	CHL	C4B-CHC-C1C	-2.55	120.30	126.34
30	2	301	CHL	O2D-CGD-O1D	-2.55	118.86	123.84
31	a	604	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	H	201	CLA	C3B-C4B-NB	-2.55	108.15	110.52
36	9	602	LMG	O1-C7-C8	-2.55	104.75	110.90
31	h	603	CLA	CHB-C4A-NA	2.55	128.03	124.51
31	A	831	CLA	C1-C2-C3	-2.55	122.63	126.75
32	1	402	8CT	C14-C15-C16	-2.54	119.27	126.42
31	9	308	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	g	603	CLA	C3B-C4B-NB	-2.54	108.16	110.52
42	e	523	NEX	C26-C27-C28	-2.54	120.61	125.99
33	f	520	0UR	C4-C3-C2	-2.54	117.90	120.08
30	8	313	CHL	C3C-C4C-NC	2.54	113.42	110.57
30	2	302	CHL	C4-C3-C5	2.54	119.55	115.27
37	c	522	0IE	C13-C12-C11	2.54	122.84	118.94
32	A	847	8CT	C39-C16-C17	-2.54	119.36	122.92
31	f	612	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	f	605	CHL	C3B-C4B-NB	2.54	112.87	110.52
30	5	306	CHL	OBD-CAD-C3D	-2.54	122.41	128.52
31	A	815	CLA	CHB-C4A-NA	2.54	128.03	124.51
31	A	810	CLA	CHB-C1B-NB	2.54	126.95	124.26
31	A	853	CLA	CHB-C1B-NB	2.54	126.95	124.26
34	9	601	LHG	O8-C23-C24	2.54	119.88	111.91
31	e	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	g	606	CHL	O2D-CGD-O1D	-2.54	118.87	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	306	CHL	C3C-C4C-NC	2.54	113.42	110.57
30	1	305	CHL	CMB-C2B-C1B	2.54	129.24	125.37
34	h	630	LHG	O8-C23-C24	2.54	119.87	111.91
31	7	315	CLA	CHB-C4A-NA	2.54	128.02	124.51
31	a	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
33	1	501	0UR	C5-C4-C3	-2.54	123.96	127.00
30	5	307	CHL	C4A-NA-C1A	2.54	107.85	106.71
31	b	604	CLA	C3B-C4B-NB	-2.54	108.16	110.52
33	0	502	0UR	C48-C47-C46	-2.53	120.41	125.85
31	B	815	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	B	827	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	0	309	CLA	C3B-C4B-NB	-2.53	108.17	110.52
33	d	520	0UR	C43-C3-C4	-2.53	121.96	125.02
30	c	608	CHL	CHD-C1D-ND	-2.53	122.13	124.45
31	5	303	CLA	C3B-C4B-NB	-2.53	108.17	110.52
36	A	856	LMG	O6-C5-C4	2.53	114.29	109.69
33	1	501	0UR	C28-C19-C18	-2.53	109.50	112.70
30	g	601	CHL	C3B-C4B-NB	2.53	112.86	110.52
30	2	306	CHL	C3C-C4C-NC	2.53	113.41	110.57
30	h	609	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
30	i	602	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
30	4	307	CHL	CHD-C1D-ND	-2.53	122.13	124.45
31	B	830	CLA	C3B-C4B-NB	-2.53	108.17	110.52
30	d	602	CHL	O2A-CGA-CBA	2.53	119.84	111.91
31	A	839	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	O	203	CLA	CMB-C2B-C3B	2.53	130.14	123.59
31	J	103	CLA	CHB-C4A-NA	2.53	128.00	124.51
34	8	601	LHG	O8-C23-C24	2.53	119.83	111.91
32	7	405	8CT	C11-C10-C03	-2.53	120.11	127.20
32	B	844	8CT	C35-C30-C29	-2.53	109.51	112.70
32	B	847	8CT	C05-C04-C03	2.52	114.37	110.48
32	L	206	8CT	C30-C31-C32	-2.52	118.36	121.47
31	6	311	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	K	102	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	4	310	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	L	202	CLA	C3B-C4B-NB	-2.52	108.17	110.52
31	a	603	CLA	C3B-C4B-NB	-2.52	108.17	110.52
37	b	521	0IE	C6-C7-C8	2.52	122.81	118.94
31	5	312	CLA	CHB-C4A-NA	2.52	128.00	124.51
33	d	520	0UR	C5-C4-C3	-2.52	123.97	127.00
31	g	610	CLA	CHB-C4A-NA	2.52	128.00	124.51
32	7	402	8CT	C13-C14-C15	-2.52	115.35	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	847	8CT	C25-C24-C23	-2.52	115.35	123.22
32	M	102	8CT	C18-C19-C20	-2.52	118.31	123.47
30	2	308	CHL	CHD-C1D-ND	-2.52	122.14	124.45
31	B	806	CLA	CAC-C3C-C4C	2.52	128.08	124.81
31	b	603	CLA	C3B-C4B-NB	-2.52	108.18	110.52
31	B	808	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
30	8	307	CHL	C5-C3-C4	2.52	120.17	114.60
30	e	614	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
31	g	604	CLA	C3B-C4B-NB	-2.52	108.18	110.52
33	6	502	0UR	C29-C30-C31	-2.52	108.87	111.74
31	A	809	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	B	820	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	K	104	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	A	843	CLA	C3B-C4B-NB	-2.52	108.18	110.52
31	c	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	i	614	CHL	C4B-CHC-C1C	-2.52	120.37	126.34
30	5	313	CHL	O2D-CGD-O1D	-2.52	118.92	123.84
30	e	601	CHL	CHD-C1D-ND	-2.52	122.14	124.45
31	O	203	CLA	CAB-C3B-C2B	2.52	130.11	123.59
30	2	319	CHL	CHB-C4A-NA	2.52	127.99	124.51
31	0	303	CLA	C3B-C4B-NB	-2.52	108.18	110.52
31	B	837	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	6	301	CHL	CHD-C1D-ND	-2.52	122.14	124.45
30	c	602	CHL	C3C-C4C-NC	2.52	113.39	110.57
33	4	501	0UR	C14-C15-C16	-2.51	123.72	127.31
30	i	606	CHL	C4B-CHC-C1C	-2.51	120.38	126.34
30	2	306	CHL	O2D-CGD-O1D	-2.51	118.92	123.84
30	0	306	CHL	O2A-CGA-CBA	2.51	119.80	111.91
30	9	305	CHL	CMB-C2B-C1B	2.51	129.20	125.37
31	9	300	CLA	C3B-C4B-NB	-2.51	108.18	110.52
30	2	307	CHL	CHD-C1D-ND	-2.51	122.14	124.45
30	d	602	CHL	CHD-C1D-ND	-2.51	122.14	124.45
30	3	307	CHL	CAC-C3C-C4C	2.51	128.07	124.81
31	B	831	CLA	C1-C2-C3	-2.51	122.69	126.75
31	B	812	CLA	C3B-C4B-NB	-2.51	108.19	110.52
30	b	607	CHL	CHD-C1D-ND	-2.51	122.15	124.45
31	A	837	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	L	201	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	A	818	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	e	614	CHL	CHC-C4B-NB	-2.51	121.60	124.26
32	6	402	8CT	C01-C02-C07	2.51	118.44	113.62
30	b	601	CHL	C4B-CHC-C1C	-2.51	120.39	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	608	CHL	CHD-C1D-ND	-2.51	122.15	124.45
30	e	601	CHL	C5-C3-C4	2.51	120.14	114.60
31	G	101	CLA	CHB-C4A-NA	2.51	127.98	124.51
33	6	501	0UR	O44-C45-C46	2.51	118.22	111.55
31	6	310	CLA	CHB-C4A-NA	2.51	127.98	124.51
33	8	501	0UR	C43-C3-C4	-2.51	121.99	125.02
30	a	614	CHL	C2A-C1A-CHA	-2.51	119.48	123.85
31	1	309	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	b	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	g	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	h	614	CHL	C4B-CHC-C1C	-2.51	120.39	126.34
30	2	306	CHL	CHD-C1D-ND	-2.51	122.15	124.45
33	4	501	0UR	C15-C14-C13	-2.51	115.40	123.22
30	b	614	CHL	CHC-C4B-NB	-2.51	121.61	124.26
31	7	311	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	B	840	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	B	841	CLA	CHB-C4A-NA	2.51	127.98	124.51
31	G	102	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	a	608	CHL	CHD-C1D-ND	-2.50	122.15	124.45
36	2	602	LMG	O6-C1-O1	-2.50	104.05	109.97
32	B	804	8CT	C05-C04-C03	2.50	114.33	110.48
30	4	306	CHL	O2A-CGA-CBA	2.50	119.76	111.91
30	c	601	CHL	C4-C3-C5	2.50	119.48	115.27
31	B	832	CLA	CAA-CBA-CGA	-2.50	105.94	113.25
33	a	520	0UR	C43-C3-C4	-2.50	121.99	125.02
33	c	520	0UR	C22-C16-C15	-2.50	119.42	122.92
30	4	306	CHL	CHD-C1D-ND	-2.50	122.15	124.45
30	4	319	CHL	CMB-C2B-C1B	2.50	129.18	125.37
31	g	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	0	321	CLA	C3B-C4B-NB	-2.50	108.19	110.52
36	J	105	LMG	C40-C39-C38	-2.50	101.73	114.42
30	f	606	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
30	g	607	CHL	C2A-C1A-CHA	-2.50	119.49	123.86
31	L	203	CLA	CHB-C4A-NA	2.50	127.97	124.51
32	B	845	8CT	C11-C10-C03	-2.50	120.18	127.20
31	7	304	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	F	301	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	h	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	3	302	CHL	CHD-C1D-ND	-2.50	122.16	124.45
30	4	305	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
31	7	310	CLA	CAA-C2A-C3A	-2.50	110.27	116.10
31	B	809	CLA	CHB-C4A-NA	2.50	127.97	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
33	6	501	0UR	C43-C3-C2	2.50	122.53	116.66
30	9	313	CHL	CHB-C4A-NA	2.50	127.97	124.51
30	c	601	CHL	CHB-C4A-NA	2.50	127.97	124.51
31	6	318	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	8	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	a	610	CLA	CHB-C4A-NA	2.50	127.97	124.51
37	b	521	0IE	C13-C12-C11	2.50	122.77	118.94
30	9	306	CHL	CHB-C4A-NA	2.50	127.97	124.51
31	A	840	CLA	CHB-C4A-NA	2.50	127.96	124.51
31	7	316	CLA	CHB-C4A-NA	2.50	127.96	124.51
31	d	603	CLA	CHB-C4A-NA	2.50	127.96	124.51
31	e	613	CLA	CHB-C4A-NA	2.50	127.96	124.51
30	8	302	CHL	CHD-C1D-ND	-2.50	122.16	124.45
31	g	612	CLA	CHB-C4A-NA	2.49	127.96	124.51
31	e	611	CLA	C3B-C4B-NB	-2.49	108.20	110.52
37	b	521	0IE	C23-C16-C17	2.49	122.01	118.08
30	f	614	CHL	C4B-CHC-C1C	-2.49	120.42	126.34
31	3	304	CLA	C3B-C4B-NB	-2.49	108.20	110.52
31	B	823	CLA	C3B-C4B-NB	-2.49	108.20	110.52
33	3	501	0UR	C48-C47-C46	-2.49	120.50	125.85
31	A	834	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	e	607	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
31	c	603	CLA	CHB-C4A-NA	2.49	127.96	124.51
31	d	612	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	a	601	CHL	C4B-CHC-C1C	-2.49	120.43	126.34
32	2	402	8CT	C24-C23-C21	-2.49	119.42	126.42
31	b	611	CLA	C3B-C4B-NB	-2.49	108.20	110.52
30	f	607	CHL	CHC-C4B-NB	-2.49	121.62	124.26
30	c	602	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
32	7	405	8CT	C35-C30-C31	2.49	115.88	111.42
32	O	205	8CT	C18-C19-C20	-2.49	118.37	123.47
31	f	604	CLA	C3B-C4B-NB	-2.49	108.20	110.52
33	e	520	0UR	C48-C47-C46	-2.49	120.51	125.85
31	d	613	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	B	835	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	H	201	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	i	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	2	308	CHL	OBD-CAD-C3D	-2.49	122.53	128.52
33	h	520	0UR	C24-C25-C26	-2.49	106.90	110.30
31	6	317	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	8	311	CLA	CHB-C4A-NA	2.49	127.95	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	854	8CT	C28-C26-C25	2.49	122.76	118.94
31	A	809	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
32	A	846	8CT	C39-C16-C17	-2.49	119.44	122.92
31	2	312	CLA	C3B-C4B-NB	-2.49	108.21	110.52
31	3	320	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	B	810	CLA	CHD-C1D-ND	-2.49	122.17	124.45
30	g	605	CHL	C4B-CHC-C1C	-2.49	120.44	126.34
32	4	402	8CT	C04-C03-C10	2.49	122.81	115.78
30	7	306	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
30	h	602	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
31	3	309	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
31	0	308	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	g	606	CHL	CHC-C4B-NB	-2.49	121.62	124.26
32	A	849	8CT	C25-C24-C23	-2.49	115.46	123.22
30	f	607	CHL	C4B-CHC-C1C	-2.49	120.44	126.34
30	8	306	CHL	O2A-CGA-CBA	2.49	119.71	111.91
31	f	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
32	A	847	8CT	C40-C12-C13	-2.48	119.44	122.92
32	L	209	8CT	C22-C21-C23	2.48	121.99	118.08
30	2	319	CHL	C1-C2-C3	-2.48	121.75	126.04
31	A	841	CLA	C1-C2-C3	-2.48	121.75	126.04
31	h	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	c	605	CHL	C3B-C4B-NB	2.48	112.82	110.52
30	8	305	CHL	C3C-C4C-NC	2.48	113.35	110.57
31	A	811	CLA	C3B-C4B-NB	-2.48	108.21	110.52
30	e	605	CHL	C4B-CHC-C1C	-2.48	120.45	126.34
30	9	301	CHL	C3C-C4C-NC	2.48	113.35	110.57
31	A	813	CLA	CHB-C4A-NA	2.48	127.94	124.51
31	d	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	a	614	CHL	C3B-C4B-NB	2.48	112.82	110.52
30	d	609	CHL	C4A-NA-C1A	2.48	107.82	106.71
30	e	602	CHL	CHC-C4B-NB	-2.48	121.63	124.26
31	B	837	CLA	C3B-C4B-NB	-2.48	108.22	110.52
30	1	306	CHL	CHD-C1D-ND	-2.48	122.18	124.45
31	f	611	CLA	C3B-C4B-NB	-2.48	108.22	110.52
30	h	608	CHL	CHC-C4B-NB	-2.48	121.63	124.26
30	b	602	CHL	CHB-C4A-NA	2.48	127.94	124.51
31	3	313	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	g	601	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
30	9	313	CHL	C3C-C4C-NC	2.48	113.35	110.57
31	O	201	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	d	601	CHL	O2D-CGD-O1D	-2.48	119.00	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	307	CHL	C3C-C4C-NC	2.48	113.35	110.57
31	3	303	CLA	C3B-C4B-NB	-2.47	108.22	110.52
32	1	402	8CT	C11-C10-C03	-2.47	120.25	127.20
32	2	402	8CT	C39-C16-C17	-2.47	119.46	122.92
31	3	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
31	b	612	CLA	C3B-C4B-NB	-2.47	108.22	110.52
31	0	311	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
30	1	306	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
33	2	501	0UR	C10-C9-C8	-2.47	118.41	123.47
32	M	102	8CT	C11-C10-C03	-2.47	120.26	127.20
31	3	306	CLA	CHB-C4A-NA	2.47	127.93	124.51
31	6	314	CLA	C3B-C4B-NB	-2.47	108.22	110.52
30	d	614	CHL	C4B-CHC-C1C	-2.47	120.48	126.34
30	3	307	CHL	CHB-C1B-NB	-2.47	121.64	124.26
33	4	501	0UR	O44-C43-C3	2.47	115.72	109.11
30	8	308	CHL	CHB-C4A-NA	2.47	127.93	124.51
31	9	311	CLA	CHB-C4A-NA	2.47	127.93	124.51
32	G	104	8CT	C07-C02-C03	-2.47	119.15	122.73
30	h	614	CHL	C3B-C4B-NB	2.47	112.81	110.52
31	e	604	CLA	C3B-C4B-NB	-2.47	108.22	110.52
31	A	805	CLA	CHB-C4A-NA	2.47	127.92	124.51
31	M	101	CLA	CHB-C4A-NA	2.47	127.92	124.51
30	i	609	CHL	C4B-CHC-C1C	-2.47	120.48	126.34
31	A	803	CLA	CHB-C4A-NA	2.47	127.92	124.51
31	1	304	CLA	C3B-C4B-NB	-2.47	108.23	110.52
31	5	309	CLA	CHB-C1B-NB	2.47	126.87	124.26
30	c	602	CHL	CHD-C1D-ND	-2.47	122.19	124.45
31	O	203	CLA	O2D-CGD-O1D	-2.47	118.49	124.09
31	A	807	CLA	CHB-C1B-NB	2.47	126.87	124.26
30	0	305	CHL	O2D-CGD-O1D	-2.47	119.02	123.84
31	A	836	CLA	C1-C2-C3	-2.47	121.78	126.04
31	2	310	CLA	CHB-C4A-NA	2.47	127.92	124.51
31	9	304	CLA	CHB-C4A-NA	2.47	127.92	124.51
30	8	315	CHL	O2D-CGD-O1D	-2.47	119.02	123.84
31	H	202	CLA	CHB-C4A-NA	2.47	127.92	124.51
31	A	818	CLA	C3B-C4B-NB	-2.47	108.23	110.52
30	g	609	CHL	C4B-CHC-C1C	-2.47	120.49	126.34
37	a	521	0IE	C4-C3-C2	-2.46	117.96	120.08
31	3	309	CLA	CHB-C1B-NB	2.46	126.87	124.26
31	7	317	CLA	C3B-C4B-NB	-2.46	108.23	110.52
30	7	313	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
30	5	305	CHL	O2D-CGD-O1D	-2.46	119.02	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	312	CLA	C3B-C4B-NB	-2.46	108.23	110.52
31	B	836	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
32	B	844	8CT	C27-C26-C25	-2.46	119.47	122.92
30	1	313	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
33	6	501	0UR	C24-C25-C26	-2.46	106.93	110.30
32	3	403	8CT	C30-C31-C32	-2.46	118.44	121.47
32	1	402	8CT	C40-C12-C13	-2.46	119.47	122.92
30	i	607	CHL	OMC-CMC-C2C	-2.46	120.12	125.69
31	2	309	CLA	CHB-C4A-NA	2.46	127.92	124.51
31	3	303	CLA	CHB-C4A-NA	2.46	127.92	124.51
31	a	604	CLA	CHB-C4A-NA	2.46	127.92	124.51
31	4	304	CLA	C3B-C4B-NB	-2.46	108.23	110.52
31	B	826	CLA	CAA-C2A-C1A	-2.46	103.91	111.97
30	d	607	CHL	C4B-CHC-C1C	-2.46	120.50	126.34
30	8	313	CHL	CHB-C4A-NA	2.46	127.91	124.51
31	7	308	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	c	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	c	614	CHL	C4A-NA-C1A	2.46	107.81	106.71
31	H	205	CLA	CHB-C4A-NA	2.46	127.91	124.51
38	A	842	PQN	C12-C11-C3	-2.46	105.42	112.05
31	h	611	CLA	CAA-C2A-C3A	-2.46	110.36	116.10
30	h	601	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
30	g	608	CHL	C4B-CHC-C1C	-2.46	120.51	126.34
30	b	601	CHL	CHC-C4B-NB	-2.46	121.66	124.26
31	d	604	CLA	C3B-C4B-NB	-2.46	108.24	110.52
31	B	811	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	h	611	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	h	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	8	302	CHL	OMC-CMC-C2C	-2.46	120.14	125.69
33	1	501	0UR	C4-C3-C2	-2.45	117.97	120.08
31	6	309	CLA	CHB-C4A-NA	2.45	127.91	124.51
30	7	301	CHL	CHD-C1D-ND	-2.45	122.20	124.45
31	c	610	CLA	CHB-C4A-NA	2.45	127.91	124.51
31	2	304	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	B	822	CLA	CHB-C4A-NA	2.45	127.90	124.51
32	A	854	8CT	C40-C12-C13	-2.45	119.49	122.92
30	4	302	CHL	C6-C5-C3	-2.45	110.61	114.62
30	7	301	CHL	C3C-C4C-NC	2.45	113.32	110.57
31	B	814	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	g	605	CHL	C3B-C4B-NB	2.45	112.79	110.52
31	9	303	CLA	C3B-C4B-NB	-2.45	108.24	110.52
31	B	835	CLA	C3B-C4B-NB	-2.45	108.24	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	807	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	h	605	CHL	C3B-C4B-NB	2.45	112.79	110.52
31	e	603	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	B	850	CLA	CHB-C4A-NA	2.45	127.90	124.51
33	8	501	0UR	C14-C15-C16	-2.45	123.82	127.31
32	O	205	8CT	C40-C12-C13	-2.45	119.50	122.92
30	i	614	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
32	K	107	8CT	C35-C30-C31	2.45	115.80	111.42
31	9	310	CLA	CHB-C4A-NA	2.45	127.89	124.51
31	B	839	CLA	CHB-C4A-NA	2.45	127.89	124.51
36	B	853	LMG	O1-C7-C8	-2.45	105.00	110.90
30	7	301	CHL	C4-C3-C5	2.45	119.39	115.27
33	9	501	0UR	C5-C4-C3	-2.45	124.06	127.00
31	4	314	CLA	CHB-C4A-NA	2.44	127.89	124.51
33	e	520	0UR	C29-C30-C31	-2.44	108.96	111.74
31	2	312	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
31	c	604	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	1	310	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	8	301	CHL	CHD-C1D-ND	-2.44	122.21	124.45
30	c	601	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
30	2	313	CHL	C5-C3-C4	2.44	120.00	114.60
30	a	606	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
31	b	613	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	1	302	CHL	C6-C5-C3	-2.44	107.06	113.45
30	c	614	CHL	CMB-C2B-C1B	2.44	129.08	125.37
31	9	304	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	2	312	CLA	CHB-C4A-NA	2.44	127.88	124.51
31	9	302	CLA	CHB-C4A-NA	2.44	127.88	124.51
30	1	307	CHL	CHD-C1D-ND	-2.44	122.21	124.45
31	6	303	CLA	C3B-C4B-NB	-2.44	108.25	110.52
36	A	856	LMG	O3-C3-C2	-2.44	104.72	110.35
32	4	402	8CT	C39-C16-C17	-2.44	119.51	122.92
31	B	801	CLA	CHB-C4A-NA	2.44	127.88	124.51
30	7	301	CHL	C1-C2-C3	-2.44	121.83	126.04
32	L	205	8CT	C14-C15-C16	-2.44	119.58	126.42
31	B	810	CLA	CHB-C4A-NA	2.43	127.88	124.51
31	K	105	CLA	CHB-C4A-NA	2.43	127.88	124.51
31	c	611	CLA	CHB-C4A-NA	2.43	127.88	124.51
30	3	302	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
30	1	302	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
37	e	521	0IE	C13-C12-C11	2.43	122.67	118.94
30	5	306	CHL	CHC-C4B-NB	-2.43	121.68	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	839	CLA	C1-C2-C3	-2.43	121.83	126.04
32	1	402	8CT	C35-C30-C29	-2.43	109.63	112.70
31	2	303	CLA	CHB-C4A-NA	2.43	127.88	124.51
31	A	816	CLA	CHB-C4A-NA	2.43	127.88	124.51
30	g	614	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
31	h	603	CLA	C3B-C4B-NB	-2.43	108.26	110.52
31	B	815	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
31	A	833	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	4	319	CHL	C1-C2-C3	-2.43	121.84	126.04
31	A	821	CLA	CHB-C4A-NA	2.43	127.87	124.51
31	B	836	CLA	CHB-C4A-NA	2.43	127.87	124.51
42	e	523	NEX	O24-C25-C26	-2.43	56.95	58.96
31	L	201	CLA	CHB-C1B-NB	2.43	126.83	124.26
31	0	310	CLA	CAA-C2A-C3A	-2.43	110.43	116.10
30	5	302	CHL	O2D-CGD-O1D	-2.43	119.09	123.84
31	A	825	CLA	CHB-C4A-NA	2.43	127.87	124.51
31	B	838	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	7	313	CHL	CHD-C1D-ND	-2.43	122.22	124.45
30	6	301	CHL	C3C-C4C-NC	2.43	113.29	110.57
31	A	811	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	f	605	CHL	C4B-CHC-C1C	-2.43	120.58	126.34
33	a	520	0UR	C4-C5-C6	-2.43	115.65	123.22
31	A	837	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
30	c	609	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
31	i	612	CLA	C3B-C4B-NB	-2.42	108.27	110.52
32	9	401	8CT	C25-C24-C23	-2.42	115.65	123.22
31	3	310	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	b	602	CHL	CHD-C1D-ND	-2.42	122.23	124.45
30	7	306	CHL	CHC-C4B-NB	-2.42	121.69	124.26
30	b	614	CHL	C4B-CHC-C1C	-2.42	120.59	126.34
32	A	848	8CT	C10-C03-C02	-2.42	115.59	121.46
31	f	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	h	607	CHL	C4B-CHC-C1C	-2.42	120.59	126.34
30	i	607	CHL	CHC-C4B-NB	-2.42	121.69	124.26
31	7	303	CLA	CHB-C1B-NB	2.42	126.82	124.26
30	g	602	CHL	C4A-NA-C1A	2.42	107.79	106.71
31	6	303	CLA	CHB-C4A-NA	2.42	127.86	124.51
31	e	613	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
31	a	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
31	B	828	CLA	C3B-C4B-NB	-2.42	108.27	110.52
31	h	611	CLA	C3B-C4B-NB	-2.42	108.27	110.52
30	5	313	CHL	C4B-CHC-C1C	-2.42	120.60	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	521	0IE	C23-C16-C17	2.42	121.89	118.08
30	g	602	CHL	C4B-CHC-C1C	-2.42	120.60	126.34
33	2	501	0UR	C15-C14-C13	-2.42	115.67	123.22
30	h	602	CHL	C4B-CHC-C1C	-2.42	120.60	126.34
33	7	501	0UR	C29-C30-C31	-2.42	108.99	111.74
31	G	103	CLA	CHB-C4A-NA	2.42	127.85	124.51
33	4	502	0UR	C15-C14-C13	-2.42	115.68	123.22
32	7	404	8CT	C22-C21-C20	-2.42	119.54	122.92
30	c	609	CHL	CMB-C2B-C1B	2.41	129.05	125.37
31	b	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
30	a	609	CHL	CHC-C4B-NB	-2.41	121.70	124.26
31	A	819	CLA	CHB-C4A-NA	2.41	127.85	124.51
33	b	520	0UR	C4-C5-C6	-2.41	115.68	123.22
30	c	605	CHL	C4B-CHC-C1C	-2.41	120.61	126.34
32	J	104	8CT	C04-C03-C02	-2.41	119.21	122.61
31	1	312	CLA	C3B-C4B-NB	-2.41	108.28	110.52
30	9	305	CHL	CHB-C1B-NB	-2.41	121.70	124.26
31	A	830	CLA	CHB-C4A-NA	2.41	127.85	124.51
30	f	601	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
33	1	501	0UR	C10-C9-C8	-2.41	118.53	123.47
30	h	607	CHL	C3B-C4B-NB	2.41	112.75	110.52
31	e	612	CLA	C3B-C4B-NB	-2.41	108.28	110.52
31	a	610	CLA	C1-C2-C3	-2.41	121.87	126.04
30	8	302	CHL	CHB-C1B-NB	-2.41	121.70	124.26
31	f	604	CLA	C1-C2-C3	-2.41	122.85	126.75
30	a	605	CHL	C3B-C4B-NB	2.41	112.75	110.52
31	e	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
37	c	521	0IE	C13-C12-C11	2.41	122.64	118.94
31	6	304	CLA	CHB-C1B-NB	2.41	126.81	124.26
33	6	502	0UR	C28-C19-C18	2.41	115.75	112.70
31	i	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	e	608	CHL	CHD-C1D-ND	-2.41	122.24	124.45
30	7	307	CHL	O2A-CGA-CBA	2.41	119.47	111.91
31	7	312	CLA	CHB-C4A-NA	2.41	127.84	124.51
31	A	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
31	3	312	CLA	CHB-C4A-NA	2.41	127.84	124.51
32	B	846	8CT	C25-C24-C23	2.41	130.73	123.22
31	A	806	CLA	C1-C2-C3	-2.41	121.88	126.04
30	a	607	CHL	CHC-C4B-NB	-2.41	121.71	124.26
32	8	402	8CT	C25-C24-C23	-2.41	115.71	123.22
30	e	602	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
30	2	307	CHL	CHA-C1A-NA	2.40	131.90	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	501	0UR	C5-C4-C3	-2.40	124.12	127.00
30	f	614	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
33	f	520	0UR	C33-C32-C31	-2.40	118.42	123.56
31	B	831	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	1	305	CHL	CHD-C1D-ND	-2.40	122.25	124.45
31	0	310	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	i	610	CLA	CHB-C4A-NA	2.40	127.83	124.51
32	B	804	8CT	C27-C26-C28	2.40	121.86	118.08
31	A	836	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	L	207	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	9	301	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
33	9	501	0UR	C43-C3-C4	-2.40	122.12	125.02
31	e	610	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
30	7	307	CHL	C3C-C4C-NC	2.40	113.26	110.57
30	5	313	CHL	CHC-C4B-NB	-2.40	121.72	124.26
30	g	602	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
31	e	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	e	606	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
31	7	310	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	g	613	CLA	C3B-C4B-NB	-2.40	108.29	110.52
30	6	302	CHL	CMB-C2B-C1B	2.40	129.02	125.37
32	3	402	8CT	C11-C10-C03	-2.40	120.47	127.20
30	a	602	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
32	3	403	8CT	C35-C30-C31	2.40	115.71	111.42
31	f	604	CLA	CHB-C4A-NA	2.40	127.82	124.51
31	A	814	CLA	CHB-C4A-NA	2.39	127.82	124.51
31	A	838	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	3	307	CHL	CHD-C1D-ND	-2.39	122.25	124.45
31	A	841	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	8	315	CHL	C4B-CHC-C1C	-2.39	120.67	126.34
30	3	302	CHL	CHB-C1B-NB	-2.39	121.72	124.26
31	A	813	CLA	CHB-C1B-NB	2.39	126.79	124.26
32	B	847	8CT	C04-C03-C02	-2.39	119.25	122.61
30	c	607	CHL	C4B-CHC-C1C	-2.39	120.67	126.34
30	g	606	CHL	C4A-NA-C1A	2.39	107.78	106.71
30	d	614	CHL	C3B-C4B-NB	2.39	112.73	110.52
33	i	520	0UR	C15-C14-C13	-2.39	115.76	123.22
30	c	607	CHL	CHC-C4B-NB	-2.39	121.73	124.26
32	J	104	8CT	C27-C26-C25	-2.39	119.57	122.92
31	f	603	CLA	CHB-C4A-NA	2.39	127.82	124.51
31	4	304	CLA	CHB-C4A-NA	2.39	127.82	124.51
31	2	314	CLA	CHB-C4A-NA	2.39	127.82	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	852	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	b	609	CHL	C4A-NA-C1A	2.39	107.78	106.71
31	G	103	CLA	CHB-C1B-NB	2.39	126.79	124.26
33	b	520	0UR	C24-C25-C26	-2.39	107.03	110.30
31	B	834	CLA	CHB-C4A-NA	2.39	127.81	124.51
36	9	602	LMG	C38-C37-C36	-2.39	102.31	114.42
31	i	610	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
31	A	835	CLA	CHB-C4A-NA	2.39	127.81	124.51
31	A	853	CLA	CHB-C4A-NA	2.39	127.81	124.51
31	4	303	CLA	CHB-C4A-NA	2.39	127.81	124.51
33	4	501	0UR	C4-C5-C6	-2.38	115.78	123.22
31	B	810	CLA	C3B-C4B-NB	-2.38	108.30	110.52
31	G	101	CLA	C1-C2-C3	-2.38	122.89	126.75
35	0	603	SQD	O48-C23-C24	2.38	119.39	111.91
30	8	301	CHL	CHC-C4B-NB	-2.38	121.73	124.26
30	8	306	CHL	C3C-C4C-NC	2.38	113.24	110.57
31	H	204	CLA	C3B-C4B-NB	-2.38	108.31	110.52
30	0	301	CHL	CHB-C4A-NA	2.38	127.81	124.51
36	9	602	LMG	C40-C39-C38	-2.38	102.33	114.42
31	A	853	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
30	4	319	CHL	CHD-C1D-ND	-2.38	122.27	124.45
33	7	501	0UR	C15-C14-C13	-2.38	115.79	123.22
31	8	309	CLA	C1-C2-C3	-2.38	121.93	126.04
30	c	607	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
31	5	308	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	b	602	CHL	C3C-C4C-NC	2.38	113.24	110.57
33	5	501	0UR	C10-C9-C8	-2.38	118.60	123.47
33	b	520	0UR	C10-C9-C8	-2.38	118.60	123.47
30	8	313	CHL	CHD-C1D-ND	-2.38	122.27	124.45
30	a	601	CHL	CHC-C4B-NB	-2.38	121.74	124.26
36	J	102	LMG	O3-C3-C2	-2.38	104.85	110.35
30	d	606	CHL	C4B-CHC-C1C	-2.38	120.69	126.34
30	8	301	CHL	O1D-CGD-CBD	-2.38	119.62	124.48
31	A	810	CLA	CHB-C4A-NA	2.38	127.80	124.51
36	J	105	LMG	O3-C3-C2	-2.38	104.85	110.35
31	8	310	CLA	CHB-C4A-NA	2.38	127.80	124.51
36	3	602	LMG	O3-C3-C2	-2.38	104.85	110.35
30	e	601	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
30	i	605	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
31	5	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
31	A	826	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	a	607	CHL	C4B-CHC-C1C	-2.38	120.70	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	602	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
30	8	308	CHL	C3C-C4C-NC	2.38	113.23	110.57
32	B	847	8CT	C19-C20-C21	-2.38	123.92	127.31
30	a	609	CHL	C4B-CHC-C1C	-2.37	120.70	126.34
31	8	309	CLA	CHB-C4A-NA	2.37	127.80	124.51
34	G	105	LHG	C26-C25-C24	2.37	121.73	113.19
31	1	312	CLA	CHB-C4A-NA	2.37	127.80	124.51
31	6	314	CLA	CHB-C4A-NA	2.37	127.80	124.51
30	8	306	CHL	C5-C3-C4	2.37	119.84	114.60
37	g	522	0IE	C4-C5-C6	2.37	130.62	123.22
31	c	611	CLA	CHB-C1B-NB	2.37	126.77	124.26
31	0	304	CLA	C3B-C4B-NB	-2.37	108.31	110.52
30	g	614	CHL	C3B-C4B-NB	2.37	112.72	110.52
33	9	502	0UR	C22-C16-C17	2.37	121.81	118.08
33	a	520	0UR	C4-C3-C2	-2.37	118.04	120.08
31	4	312	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	5	304	CLA	C3B-C4B-NB	-2.37	108.32	110.52
41	B	849	DGD	O1G-C1A-O1A	-2.37	117.61	123.59
31	1	303	CLA	CHB-C1B-NB	2.37	126.77	124.26
31	B	807	CLA	CHB-C1B-NB	2.37	126.77	124.26
31	A	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	i	610	CLA	C1-C2-C3	-2.37	121.95	126.04
30	4	306	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
31	B	832	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
31	5	309	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	6	320	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	7	318	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	A	824	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	B	821	CLA	C3B-C4B-NB	-2.37	108.32	110.52
31	6	317	CLA	CHB-C1B-NB	2.37	126.76	124.26
30	9	301	CHL	CHD-C1D-ND	-2.37	122.28	124.45
33	O	204	0UR	C29-C30-C31	-2.37	109.05	111.74
36	J	105	LMG	C38-C37-C36	-2.37	102.41	114.42
31	A	843	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	e	610	CLA	CHB-C4A-NA	2.37	127.79	124.51
32	L	209	8CT	C35-C30-C31	2.37	115.66	111.42
32	8	406	8CT	C04-C03-C02	-2.37	119.28	122.61
37	c	522	0IE	C15-C14-C13	2.37	130.60	123.22
30	b	614	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
31	6	309	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
31	d	610	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
30	h	609	CHL	C4B-CHC-C1C	-2.37	120.72	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	824	CLA	CHB-C4A-NA	2.36	127.78	124.51
31	K	101	CLA	CHB-C4A-NA	2.36	127.78	124.51
32	B	845	8CT	C40-C12-C13	-2.36	119.61	122.92
30	6	305	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
30	8	306	CHL	CHD-C1D-ND	-2.36	122.28	124.45
30	i	608	CHL	CHC-C4B-NB	-2.36	121.75	124.26
31	e	604	CLA	C1-C2-C3	-2.36	122.93	126.75
30	8	308	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
31	9	311	CLA	CHB-C1B-NB	2.36	126.76	124.26
31	4	309	CLA	CHB-C4A-NA	2.36	127.78	124.51
30	a	601	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
30	h	606	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
30	7	305	CHL	CHD-C1D-ND	-2.36	122.28	124.45
30	7	313	CHL	C3C-C4C-NC	2.36	113.22	110.57
31	1	314	CLA	CHB-C4A-NA	2.36	127.78	124.51
32	6	402	8CT	C04-C03-C02	-2.36	119.29	122.61
31	6	312	CLA	CHB-C4A-NA	2.36	127.78	124.51
32	A	846	8CT	C40-C12-C13	-2.36	119.62	122.92
30	g	609	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
32	0	401	8CT	C22-C21-C20	-2.36	119.62	122.92
31	8	303	CLA	CHB-C4A-NA	2.36	127.77	124.51
31	d	604	CLA	CHB-C4A-NA	2.36	127.77	124.51
31	B	833	CLA	CHB-C4A-NA	2.36	127.77	124.51
32	L	205	8CT	C05-C04-C03	2.36	114.11	110.48
31	e	610	CLA	CHB-C1B-NB	2.36	126.75	124.26
31	f	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
31	A	814	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	A	817	CLA	O2D-CGD-CBD	2.36	115.46	111.27
30	5	307	CHL	C4B-CHC-C1C	-2.36	120.75	126.34
30	i	601	CHL	C4B-CHC-C1C	-2.36	120.75	126.34
32	K	107	8CT	C18-C19-C20	-2.35	118.65	123.47
30	6	308	CHL	C3C-C4C-NC	2.35	113.21	110.57
36	3	602	LMG	O1-C7-C8	-2.35	105.22	110.90
30	f	606	CHL	C4B-CHC-C1C	-2.35	120.75	126.34
32	3	402	8CT	C04-C03-C10	2.35	122.44	115.78
32	L	205	8CT	C18-C19-C20	-2.35	118.65	123.47
30	h	606	CHL	C5-C3-C4	2.35	119.80	114.60
37	d	521	0IE	C13-C12-C11	2.35	122.55	118.94
30	2	305	CHL	C4D-C3D-CAD	2.35	110.87	108.10
31	d	610	CLA	CHB-C4A-NA	2.35	127.77	124.51
30	e	601	CHL	C3C-C4C-NC	2.35	113.21	110.57
32	J	101	8CT	C15-C16-C17	-2.35	115.33	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	829	CLA	CHB-C4A-NA	2.35	127.76	124.51
30	a	607	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
30	d	609	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
30	5	302	CHL	C4B-CHC-C1C	-2.35	120.76	126.34
32	J	104	8CT	C19-C18-C17	-2.35	118.66	123.47
30	d	601	CHL	C4B-CHC-C1C	-2.35	120.76	126.34
31	A	825	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
30	d	614	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
31	0	303	CLA	CHB-C4A-NA	2.35	127.76	124.51
30	a	602	CHL	CHC-C4B-NB	-2.35	121.77	124.26
31	B	812	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	O	203	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	2	311	CLA	C3B-C4B-NB	-2.35	108.34	110.52
31	8	309	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
30	6	307	CHL	CHD-C1D-ND	-2.35	122.30	124.45
31	5	310	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	9	312	CLA	CHB-C4A-NA	2.35	127.76	124.51
38	A	842	PQN	C2M-C2-C1	2.35	120.16	116.27
31	7	303	CLA	CHB-C4A-NA	2.35	127.76	124.51
30	b	606	CHL	C5-C3-C4	2.35	119.79	114.60
30	6	315	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
32	F	302	8CT	C27-C26-C25	-2.35	119.64	122.92
36	9	602	LMG	O2-C2-C1	-2.35	104.35	110.05
32	B	843	8CT	C40-C12-C13	-2.35	119.64	122.92
32	9	401	8CT	C11-C10-C03	-2.35	120.61	127.20
31	i	603	CLA	CHB-C4A-NA	2.35	127.75	124.51
31	A	830	CLA	O2D-CGD-CBD	2.34	115.43	111.27
30	5	305	CHL	C4B-CHC-C1C	-2.34	120.78	126.34
30	0	302	CHL	O2D-CGD-O1D	-2.34	119.25	123.84
31	B	817	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
30	a	614	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
31	F	301	CLA	CHB-C1B-NB	2.34	126.74	124.26
31	A	828	CLA	C3B-C4B-NB	-2.34	108.34	110.52
30	f	601	CHL	C3C-C4C-NC	2.34	113.20	110.57
30	g	606	CHL	C5-C3-C4	2.34	119.78	114.60
30	c	606	CHL	C3C-C4C-NC	2.34	113.20	110.57
31	0	304	CLA	CHB-C4A-NA	2.34	127.75	124.51
31	6	310	CLA	C1-C2-C3	-2.34	121.99	126.04
31	B	841	CLA	CHB-C1B-NB	2.34	126.74	124.26
31	5	314	CLA	CHB-C4A-NA	2.34	127.75	124.51
31	A	843	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
30	d	601	CHL	C5-C3-C4	2.34	119.77	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	614	CHL	C2A-C1A-CHA	-2.34	119.77	123.85
32	8	402	8CT	C27-C26-C28	2.34	121.76	118.08
30	c	602	CHL	C4B-CHC-C1C	-2.34	120.79	126.34
32	A	848	8CT	C24-C25-C26	-2.34	123.97	127.31
31	A	826	CLA	CAA-C2A-C1A	-2.34	104.32	111.97
30	d	608	CHL	C5-C3-C4	2.34	119.77	114.60
31	g	611	CLA	C3B-C4B-NB	-2.34	108.35	110.52
31	6	311	CLA	CHB-C1B-NB	2.34	126.73	124.26
30	i	607	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
33	0	501	0UR	C10-C9-C8	-2.33	118.69	123.47
31	9	309	CLA	C1-C2-C3	-2.33	122.01	126.04
31	A	806	CLA	CHB-C1B-NB	2.33	126.73	124.26
31	6	304	CLA	CHB-C4A-NA	2.33	127.74	124.51
31	H	205	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
30	i	606	CHL	C5-C3-C4	2.33	119.76	114.60
33	f	520	0UR	C4-C5-C6	-2.33	115.94	123.22
30	h	606	CHL	C4B-CHC-C1C	-2.33	120.81	126.34
31	B	823	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	a	605	CHL	C2A-C1A-CHA	-2.33	119.78	123.86
33	9	501	0UR	C4-C5-C6	-2.33	115.94	123.22
30	0	305	CHL	C5-C3-C4	2.33	119.75	114.60
36	9	602	LMG	O3-C3-C2	-2.33	104.96	110.35
31	B	826	CLA	CHB-C4A-NA	2.33	127.73	124.51
36	J	102	LMG	C6-C5-C4	-2.33	107.55	113.00
31	f	610	CLA	CHB-C1B-NB	2.33	126.72	124.26
31	c	604	CLA	C1-C2-C3	-2.33	122.99	126.75
30	c	605	CHL	C2A-C1A-CHA	-2.33	119.79	123.86
30	2	302	CHL	C4B-CHC-C1C	-2.33	120.82	126.34
31	3	303	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
31	B	807	CLA	CMB-C2B-C1B	-2.33	121.83	125.37
36	L	210	LMG	O1-C7-C8	-2.32	105.29	110.90
30	4	313	CHL	C5-C3-C4	2.32	119.74	114.60
31	a	612	CLA	C3B-C4B-NB	-2.32	108.36	110.52
30	c	605	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
30	d	606	CHL	C5-C3-C4	2.32	119.73	114.60
31	B	839	CLA	CHB-C1B-NB	2.32	126.72	124.26
30	4	302	CHL	C4B-CHC-C1C	-2.32	120.83	126.34
31	3	303	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
31	A	835	CLA	CHD-C1D-ND	-2.32	122.32	124.45
30	4	307	CHL	CAC-C3C-C4C	2.32	127.82	124.81
31	B	819	CLA	CHB-C4A-NA	2.32	127.72	124.51
30	1	313	CHL	C4-C3-C5	2.32	119.17	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	307	CHL	C5-C3-C4	2.32	119.73	114.60
30	f	606	CHL	C5-C3-C4	2.32	119.73	114.60
30	g	607	CHL	C5-C3-C4	2.32	119.73	114.60
31	A	808	CLA	O2D-CGD-CBD	2.32	115.39	111.27
33	b	520	0UR	C15-C14-C13	-2.32	115.98	123.22
30	d	606	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
33	7	501	0UR	C5-C4-C3	-2.32	124.22	127.00
30	6	308	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
31	K	105	CLA	C1-C2-C3	-2.32	123.00	126.75
30	1	305	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
33	8	501	0UR	C24-C25-C26	-2.32	107.13	110.30
30	0	305	CHL	C3C-C4C-NC	2.32	113.17	110.57
30	a	606	CHL	C4A-NA-C1A	2.32	107.75	106.71
31	b	603	CLA	CHB-C4A-NA	2.31	127.71	124.51
30	7	307	CHL	CHD-C1D-ND	-2.31	122.33	124.45
31	9	312	CLA	CHB-C1B-NB	2.31	126.71	124.26
33	a	520	0UR	C10-C9-C8	-2.31	118.74	123.47
30	7	305	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
37	e	521	0IE	C23-C16-C17	2.31	121.72	118.08
33	8	501	0UR	C10-C9-C8	-2.31	118.74	123.47
30	e	608	CHL	C1-C2-C3	-2.31	122.05	126.04
31	c	610	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
32	A	848	8CT	C18-C19-C20	-2.31	118.75	123.47
30	f	607	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
30	c	606	CHL	C4B-CHC-C1C	-2.31	120.87	126.34
33	9	502	0UR	C21-C12-C13	2.31	121.71	118.08
31	1	312	CLA	CHD-C1D-ND	-2.31	122.33	124.45
30	2	305	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
33	2	501	0UR	C22-C16-C17	2.31	121.71	118.08
30	e	606	CHL	C3C-C4C-NC	2.31	113.16	110.57
30	d	605	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
30	e	606	CHL	C5-C3-C4	2.31	119.69	114.60
36	L	210	LMG	O1-C1-C2	-2.30	104.70	108.30
30	h	605	CHL	O2D-CGD-O1D	-2.30	119.33	123.84
31	7	304	CLA	CHB-C1B-NB	2.30	126.69	124.26
31	A	838	CLA	CHB-C1B-NB	2.30	126.69	124.26
30	a	606	CHL	C4B-CHC-C1C	-2.30	120.88	126.34
32	M	102	8CT	C05-C04-C03	2.30	114.03	110.48
31	7	309	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
30	i	605	CHL	C3B-C4B-NB	2.30	112.65	110.52
32	G	104	8CT	C35-C30-C31	2.30	115.54	111.42
31	A	813	CLA	CMB-C2B-C1B	-2.30	121.86	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	404	8CT	C27-C26-C28	-2.30	114.45	118.08
30	i	605	CHL	C2A-C1A-CHA	-2.30	119.83	123.86
30	0	301	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
31	A	821	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
31	5	309	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
30	e	605	CHL	CHC-C4B-NB	-2.30	121.82	124.26
37	i	521	0IE	C23-C16-C17	2.30	121.70	118.08
31	A	835	CLA	O2D-CGD-CBD	2.30	115.36	111.27
32	J	104	8CT	C25-C24-C23	-2.30	116.04	123.22
30	d	602	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
31	A	839	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
31	A	852	CLA	CHB-C1B-NB	2.30	126.69	124.26
30	8	307	CHL	CHB-C4A-NA	2.30	127.69	124.51
30	a	608	CHL	C4B-CHC-C1C	-2.30	120.89	126.34
31	B	832	CLA	CHB-C4A-NA	2.30	127.69	124.51
33	0	502	0UR	C4-C5-C6	-2.30	116.05	123.22
31	A	840	CLA	CHB-C1B-NB	2.30	126.69	124.26
31	B	817	CLA	CHD-C1D-ND	-2.29	122.34	124.45
30	9	301	CHL	CHB-C4A-NA	2.29	127.69	124.51
30	8	301	CHL	C3C-C4C-NC	2.29	113.14	110.57
42	d	523	NEX	C39-C29-C30	-2.29	119.71	122.92
31	B	829	CLA	CHB-C1B-NB	2.29	126.69	124.26
30	8	313	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
30	0	305	CHL	CHC-C4B-NB	-2.29	121.83	124.26
32	6	402	8CT	C35-C30-C29	-2.29	109.80	112.70
31	A	825	CLA	C1-C2-C3	-2.29	122.08	126.04
32	A	850	8CT	C24-C23-C21	-2.29	119.98	126.42
31	A	823	CLA	CHB-C4A-NA	2.29	127.68	124.51
31	b	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
30	7	307	CHL	CHC-C4B-NB	-2.29	121.83	124.26
30	g	607	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
30	9	305	CHL	OBD-CAD-C3D	-2.29	123.01	128.52
30	b	606	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
30	1	313	CHL	CHD-C1D-ND	-2.29	122.35	124.45
31	2	309	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
35	0	603	SQD	C1-O5-C5	2.29	118.18	113.69
42	a	523	NEX	C39-C29-C30	-2.29	119.72	122.92
31	B	801	CLA	CMB-C2B-C3B	2.29	132.13	126.59
30	a	608	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
33	c	520	0UR	C14-C13-C12	-2.29	119.99	126.42
33	1	502	0UR	C20-C7-C8	-2.29	119.72	122.92
36	B	853	LMG	O3-C3-C2	-2.29	105.06	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	307	CHL	C4B-CHC-C1C	-2.29	120.92	126.34
42	c	523	NEX	C39-C29-C30	-2.29	119.72	122.92
31	A	805	CLA	CHB-C1B-NB	2.28	126.68	124.26
39	A	857	CL0	CHB-C1B-NB	2.28	126.68	124.26
31	B	826	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
31	O	206	CLA	CHB-C4A-NA	2.28	127.67	124.51
31	B	809	CLA	CHB-C1B-NB	2.28	126.67	124.26
42	e	523	NEX	C35-C15-C14	-2.28	118.80	123.47
33	8	501	0UR	C15-C14-C13	-2.28	116.10	123.22
31	9	309	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
34	K	106	LHG	C26-C25-C24	2.28	121.39	113.19
31	A	805	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	f	609	CHL	CHC-C4B-NB	-2.28	121.84	124.26
33	1	502	0UR	C33-C32-C31	-2.28	118.68	123.56
31	0	313	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	A	812	CLA	CHB-C4A-NA	2.28	127.66	124.51
31	6	312	CLA	CHB-C1B-NB	2.28	126.67	124.26
30	e	607	CHL	C4A-NA-C1A	2.28	107.73	106.71
31	B	813	CLA	CHB-C1B-NB	2.28	126.67	124.26
30	e	608	CHL	C3C-C4C-NC	2.28	113.12	110.57
30	g	601	CHL	C2A-C1A-CHA	-2.28	119.88	123.86
30	c	614	CHL	C4B-CHC-C1C	-2.28	120.94	126.34
32	J	104	8CT	C01-C02-C07	2.28	117.99	113.62
33	i	520	0UR	C10-C9-C8	-2.28	118.81	123.47
30	7	302	CHL	CHD-C1D-ND	-2.28	122.36	124.45
33	d	520	0UR	C48-C47-C46	-2.27	120.85	125.34
31	B	841	CLA	CHD-C1D-ND	-2.27	122.36	124.45
30	3	307	CHL	O2D-CGD-O1D	-2.27	119.39	123.84
30	4	302	CHL	O2D-CGD-O1D	-2.27	119.39	123.84
31	0	313	CLA	CHB-C4A-NA	2.27	127.66	124.51
31	a	610	CLA	CHD-C1D-ND	-2.27	122.36	124.45
31	3	309	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
30	9	305	CHL	CHB-C1B-C2B	-2.27	120.82	127.24
42	b	523	NEX	C39-C29-C30	-2.27	119.74	122.92
31	A	823	CLA	CHB-C1B-NB	2.27	126.66	124.26
31	O	202	CLA	CHB-C1B-NB	2.27	126.66	124.26
32	8	406	8CT	C35-C30-C31	2.27	115.49	111.42
30	1	305	CHL	CHA-C1A-NA	2.27	131.60	126.40
30	7	302	CHL	CHA-C1A-NA	2.27	131.60	126.40
30	5	302	CHL	CHD-C1D-ND	-2.27	122.37	124.45
31	b	610	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
32	8	406	8CT	C18-C19-C20	-2.27	118.82	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	836	CLA	CHB-C1B-NB	2.27	126.66	124.26
32	B	804	8CT	C30-C31-C32	-2.27	118.67	121.47
31	7	309	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
30	8	302	CHL	CHB-C1B-C2B	-2.27	120.83	127.24
31	8	311	CLA	CHB-C1B-NB	2.27	126.66	124.26
30	4	307	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
31	L	202	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	J	101	8CT	C40-C12-C11	2.27	121.65	118.08
31	H	201	CLA	C1-C2-C3	-2.27	122.12	126.04
32	M	102	8CT	C35-C30-C31	2.27	115.48	111.42
33	9	502	0UR	C4-C5-C6	-2.27	116.14	123.22
32	L	206	8CT	C04-C03-C02	-2.27	119.42	122.61
33	0	501	0UR	C24-C25-C26	-2.27	107.20	110.30
31	d	610	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
33	1	502	0UR	C5-C6-C7	-2.27	120.05	126.42
30	1	307	CHL	C4B-CHC-C1C	-2.27	120.97	126.34
42	h	523	NEX	C39-C29-C30	-2.27	119.75	122.92
30	i	602	CHL	C3C-C4C-NC	2.26	113.11	110.57
30	5	301	CHL	O2D-CGD-O1D	-2.26	119.41	123.84
30	8	305	CHL	CHB-C4A-NA	2.26	127.64	124.51
31	B	828	CLA	CHB-C4A-NA	2.26	127.64	124.51
31	L	204	CLA	CHB-C4A-NA	2.26	127.64	124.51
30	8	302	CHL	O2D-CGD-O1D	-2.26	119.41	123.84
42	f	523	NEX	C39-C29-C30	-2.26	119.75	122.92
31	7	318	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
33	i	520	0UR	C4-C5-C6	-2.26	116.15	123.22
30	b	607	CHL	CHC-C4B-NB	-2.26	121.86	124.26
30	f	608	CHL	C5-C3-C4	2.26	119.60	114.60
30	2	305	CHL	CHD-C1D-ND	-2.26	122.38	124.45
33	4	501	0UR	C22-C16-C17	2.26	121.64	118.08
32	I	101	8CT	C24-C23-C21	-2.26	120.06	126.42
33	a	520	0UR	C5-C4-C3	-2.26	124.29	127.00
31	9	303	CLA	CHB-C1B-NB	2.26	126.65	124.26
30	a	609	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
30	e	601	CHL	CHB-C4A-NA	2.26	127.64	124.51
30	b	609	CHL	C4B-CHC-C1C	-2.26	120.98	126.34
31	B	822	CLA	CHB-C1B-NB	2.26	126.65	124.26
30	e	608	CHL	C4B-CHC-C1C	-2.26	120.98	126.34
42	g	523	NEX	C39-C29-C30	-2.26	119.76	122.92
31	1	304	CLA	CHB-C4A-NA	2.26	127.64	124.51
31	3	303	CLA	CHB-C1B-NB	2.26	126.65	124.26
31	8	312	CLA	CHB-C1B-NB	2.26	126.65	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	L	211	LMG	O3-C3-C2	-2.26	105.13	110.35
32	B	804	8CT	C11-C10-C03	-2.26	120.86	127.20
32	0	401	8CT	C10-C03-C02	-2.26	115.99	121.46
30	7	306	CHL	C3C-C4C-NC	2.26	113.10	110.57
31	B	830	CLA	CHB-C4A-NA	2.26	127.63	124.51
39	A	857	CL0	CHB-C4A-NA	2.26	127.63	124.51
31	A	824	CLA	CHB-C1B-NB	2.26	126.65	124.26
30	d	605	CHL	C3B-C4B-NB	2.26	112.61	110.52
32	A	848	8CT	C40-C12-C11	2.26	121.63	118.08
32	7	405	8CT	C30-C31-C32	-2.26	118.69	121.47
31	A	814	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
30	4	302	CHL	CHD-C1D-ND	-2.26	122.38	124.45
30	c	606	CHL	O2D-CGD-O1D	-2.26	119.43	123.84
33	f	520	0UR	C29-C30-C31	-2.26	109.17	111.74
33	g	520	0UR	C29-C30-C31	-2.25	109.17	111.74
30	4	308	CHL	C3C-C4C-NC	2.25	113.10	110.57
30	h	602	CHL	C3B-C4B-NB	2.25	112.61	110.52
31	L	201	CLA	CMB-C2B-C3B	2.25	132.05	126.59
30	c	601	CHL	CHD-C1D-ND	-2.25	122.38	124.45
31	B	821	CLA	C1-C2-C3	-2.25	123.11	126.75
36	L	210	LMG	O3-C3-C2	-2.25	105.14	110.35
32	3	403	8CT	C19-C18-C17	-2.25	118.86	123.47
30	i	606	CHL	CHC-C4B-NB	-2.25	121.87	124.26
31	B	817	CLA	CBA-CAA-C2A	2.25	120.51	113.86
36	2	602	LMG	O1-C7-C8	-2.25	105.46	110.90
30	3	302	CHL	CHA-C1A-NA	2.25	131.55	126.40
33	a	520	0UR	C24-C25-C26	-2.25	107.22	110.30
32	8	402	8CT	C39-C16-C15	2.25	121.62	118.08
33	2	502	0UR	C21-C12-C11	-2.25	119.77	122.92
30	4	307	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
30	6	302	CHL	CHD-C1D-ND	-2.25	122.39	124.45
30	i	608	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
31	B	825	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
30	c	609	CHL	C4B-CHC-C1C	-2.25	121.00	126.34
32	7	405	8CT	C14-C15-C16	-2.25	120.09	126.42
31	B	814	CLA	CHB-C1B-NB	2.25	126.64	124.26
31	A	807	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
31	3	313	CLA	CHD-C1D-ND	-2.25	122.39	124.45
30	7	307	CHL	C5-C3-C4	2.25	119.57	114.60
41	B	849	DGD	C1E-O6E-C5E	-2.25	109.28	113.69
31	B	815	CLA	CHB-C1B-NB	2.25	126.64	124.26
31	6	309	CLA	C1-C2-C3	-2.25	122.16	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	i	523	NEX	C39-C29-C30	-2.25	119.78	122.92
31	8	309	CLA	CHB-C1B-NB	2.25	126.64	124.26
30	8	307	CHL	CHD-C1D-ND	-2.25	122.39	124.45
30	d	609	CHL	C4B-CHC-C1C	-2.25	121.01	126.34
33	a	520	0UR	C28-C19-C18	-2.25	109.86	112.70
31	0	309	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
30	2	307	CHL	C5-C3-C4	2.25	119.56	114.60
31	G	101	CLA	O2A-CGA-O1A	-2.25	117.93	123.59
30	2	319	CHL	CHD-C1D-ND	-2.24	122.39	124.45
32	A	849	8CT	C11-C10-C03	-2.24	120.90	127.20
30	b	601	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
30	g	605	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
37	c	522	0IE	C17-C16-C15	2.24	122.38	118.94
31	B	822	CLA	CHD-C1D-ND	-2.24	122.39	124.45
31	K	101	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
31	7	317	CLA	C2A-C1A-CHA	2.24	127.78	123.86
31	A	837	CLA	CHD-C1D-ND	-2.24	122.39	124.45
36	2	602	LMG	O3-C3-C2	-2.24	105.17	110.35
32	A	849	8CT	C10-C03-C02	-2.24	116.04	121.46
31	B	806	CLA	CHB-C1B-NB	2.24	126.63	124.26
30	f	605	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
30	8	313	CHL	CHA-C1A-NA	2.24	131.52	126.40
31	A	818	CLA	CHC-C4B-NB	2.24	126.63	124.26
31	K	101	CLA	CHB-C1B-NB	2.24	126.63	124.26
32	B	844	8CT	C11-C10-C03	-2.24	120.92	127.20
30	6	308	CHL	C4-C3-C5	2.24	119.03	115.27
30	d	608	CHL	C4B-CHC-C1C	-2.24	121.03	126.34
30	2	313	CHL	O2D-CGD-O1D	-2.24	119.47	123.84
30	7	301	CHL	C6-C5-C3	-2.24	107.59	113.45
30	9	306	CHL	O1D-CGD-CBD	-2.23	119.91	124.48
33	6	501	0UR	C4-C5-C6	-2.23	116.24	123.22
31	B	830	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
33	h	520	0UR	C29-C30-C31	-2.23	109.20	111.74
31	6	317	CLA	CMB-C2B-C3B	2.23	132.00	126.59
30	f	609	CHL	C4B-CHC-C1C	-2.23	121.04	126.34
30	4	319	CHL	O2A-CGA-O1A	-2.23	117.96	123.59
31	8	303	CLA	CHB-C1B-NB	2.23	126.62	124.26
31	9	309	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
31	A	803	CLA	C1-C2-C3	-2.23	122.18	126.04
31	O	202	CLA	CBD-CHA-C1A	2.23	131.13	128.50
30	6	306	CHL	C5-C3-C4	2.23	119.53	114.60
31	e	610	CLA	C1-C2-C3	-2.23	122.18	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	821	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
30	a	605	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
31	8	304	CLA	CHB-C4A-NA	2.23	127.60	124.51
30	3	305	CHL	CHD-C1D-ND	-2.23	122.40	124.45
30	f	602	CHL	CHD-C1D-ND	-2.23	122.40	124.45
31	B	831	CLA	CHB-C1B-NB	2.23	126.62	124.26
30	b	607	CHL	C3C-C4C-NC	2.23	113.07	110.57
31	3	320	CLA	C3B-C4B-NB	-2.23	108.45	110.52
31	B	810	CLA	O2D-CGD-CBD	2.23	115.23	111.27
33	a	520	0UR	C15-C14-C13	-2.23	116.26	123.22
37	7	502	0IE	C13-C12-C11	2.23	122.36	118.94
31	B	833	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
30	e	607	CHL	C4B-CHC-C1C	-2.23	121.06	126.34
31	b	610	CLA	CHB-C1B-NB	2.23	126.61	124.26
36	2	602	LMG	O1-C1-C2	-2.23	104.83	108.30
30	f	614	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
32	G	104	8CT	C10-C03-C02	-2.23	116.07	121.46
32	4	402	8CT	C27-C26-C25	-2.23	119.80	122.92
30	c	608	CHL	C3C-C4C-NC	2.23	113.07	110.57
30	7	313	CHL	C4B-CHC-C1C	-2.23	121.06	126.34
42	i	523	NEX	C31-C32-C33	-2.23	120.16	126.42
31	H	201	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
33	g	520	0UR	C10-C9-C8	-2.22	118.92	123.47
30	g	606	CHL	C4B-CHC-C1C	-2.22	121.07	126.34
31	A	821	CLA	CHB-C1B-NB	2.22	126.61	124.26
32	8	406	8CT	C40-C12-C13	-2.22	119.81	122.92
36	B	853	LMG	O6-C1-O1	-2.22	104.71	109.97
36	O	207	LMG	O2-C2-C1	-2.22	104.65	110.05
30	e	602	CHL	C3C-C4C-NC	2.22	113.06	110.57
30	8	306	CHL	CHB-C4A-NA	2.22	127.58	124.51
31	6	303	CLA	CHC-C4B-NB	2.22	126.61	124.26
31	B	813	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
31	B	838	CLA	C3B-C4B-NB	-2.22	108.46	110.52
41	B	849	DGD	O2G-C1B-O1B	-2.22	118.34	123.70
31	4	303	CLA	CHB-C1B-NB	2.22	126.61	124.26
30	6	301	CHL	O1D-CGD-CBD	-2.22	119.94	124.48
30	c	608	CHL	C4B-CHC-C1C	-2.22	121.08	126.34
32	A	846	8CT	C27-C26-C28	2.22	121.57	118.08
30	3	307	CHL	CHA-C1A-NA	2.22	131.48	126.40
30	6	308	CHL	CHB-C4A-NA	2.22	127.58	124.51
32	A	854	8CT	C22-C21-C20	-2.22	119.82	122.92
31	A	826	CLA	CHB-C1B-NB	2.22	126.60	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	827	CLA	C1-C2-C3	-2.22	122.21	126.04
30	1	302	CHL	CHB-C1B-C2B	-2.21	120.98	127.24
42	f	523	NEX	C31-C32-C33	-2.21	120.19	126.42
37	c	521	0IE	C25-C26-C27	-2.21	109.22	111.74
30	8	305	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
32	8	406	8CT	C10-C03-C02	-2.21	116.10	121.46
42	d	523	NEX	C31-C32-C33	-2.21	120.20	126.42
32	1	402	8CT	C35-C30-C31	2.21	115.38	111.42
39	A	857	CL0	O2A-CGA-O1A	-2.21	118.01	123.59
30	3	302	CHL	CHB-C1B-C2B	-2.21	120.99	127.24
36	3	602	LMG	O2-C2-C1	-2.21	104.67	110.05
30	b	607	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
31	1	312	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
31	A	826	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
30	2	305	CHL	CHA-C1A-NA	2.21	131.46	126.40
31	A	831	CLA	CHB-C1B-NB	2.21	126.60	124.26
42	c	523	NEX	C31-C32-C33	-2.21	120.21	126.42
30	1	306	CHL	C4B-CHC-C1C	-2.21	121.10	126.34
32	B	847	8CT	C39-C16-C17	-2.21	119.83	122.92
33	c	520	0UR	C4-C3-C2	-2.21	118.18	120.08
33	c	520	0UR	C24-C25-C26	-2.21	107.28	110.30
33	e	520	0UR	C15-C14-C13	-2.21	116.33	123.22
33	6	502	0UR	C9-C10-C11	-2.21	118.95	123.47
33	c	520	0UR	C10-C9-C8	-2.21	118.95	123.47
30	1	302	CHL	CHD-C1D-ND	-2.21	122.43	124.45
32	L	209	8CT	C04-C03-C10	2.21	122.02	115.78
42	g	523	NEX	C31-C32-C33	-2.21	120.22	126.42
30	9	301	CHL	OMC-CMC-C2C	-2.21	120.70	125.69
37	3	502	0IE	C13-C12-C11	2.21	122.33	118.94
42	h	523	NEX	C31-C32-C33	-2.21	120.22	126.42
33	9	501	0UR	C28-C19-C18	-2.21	109.91	112.70
30	6	315	CHL	C4B-CHC-C1C	-2.21	121.11	126.34
30	4	313	CHL	CHD-C1D-ND	-2.20	122.43	124.45
31	H	205	CLA	CHD-C1D-ND	-2.20	122.43	124.45
31	B	838	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
30	5	305	CHL	C3C-C4C-NC	2.20	113.04	110.57
31	B	808	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
31	1	309	CLA	CHB-C1B-NB	2.20	126.59	124.26
31	A	837	CLA	C1-C2-C3	-2.20	122.23	126.04
30	d	608	CHL	OMC-CMC-C2C	-2.20	120.70	125.69
30	d	608	CHL	C3C-C4C-NC	2.20	113.04	110.57
30	i	608	CHL	C4B-CHC-C1C	-2.20	121.11	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	405	8CT	C18-C19-C20	-2.20	118.96	123.47
36	O	207	LMG	O3-C3-C2	-2.20	105.26	110.35
30	g	614	CHL	C2A-C1A-CHA	-2.20	120.01	123.85
31	6	318	CLA	CHB-C1B-NB	2.20	126.59	124.26
30	i	602	CHL	C4B-CHC-C1C	-2.20	121.12	126.34
30	f	608	CHL	CHA-C1A-NA	2.20	131.44	126.40
30	1	305	CHL	CHB-C1B-C2B	-2.20	121.02	127.24
30	f	602	CHL	CHA-C1A-NA	2.20	131.44	126.40
31	A	825	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
30	6	305	CHL	CHD-C1D-ND	-2.20	122.43	124.45
31	K	102	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
36	9	602	LMG	O7-C10-O9	-2.20	118.39	123.70
31	7	312	CLA	CHB-C1B-NB	2.20	126.59	124.26
32	3	402	8CT	C18-C17-C16	-2.20	124.17	127.31
30	d	607	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
31	1	308	CLA	CHD-C1D-ND	-2.20	122.43	124.45
31	f	610	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
31	7	318	CLA	CHB-C1B-NB	2.20	126.58	124.26
31	A	841	CLA	CHB-C1B-NB	2.20	126.58	124.26
42	b	523	NEX	C31-C32-C33	-2.20	120.24	126.42
42	a	523	NEX	C31-C32-C33	-2.20	120.24	126.42
31	5	311	CLA	CHB-C1B-NB	2.20	126.58	124.26
32	A	847	8CT	C13-C14-C15	-2.20	116.36	123.22
30	h	607	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
31	3	304	CLA	C1-C2-C3	-2.20	122.24	126.04
30	4	307	CHL	CHA-C1A-NA	2.20	131.43	126.40
33	1	501	0UR	C15-C14-C13	-2.20	116.36	123.22
30	2	305	CHL	C3D-C4D-CHA	-2.20	107.70	112.72
31	B	828	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
31	B	829	CLA	CHB-C4A-NA	2.20	127.55	124.51
31	3	312	CLA	CHB-C1B-NB	2.20	126.58	124.26
32	B	851	8CT	C13-C14-C15	-2.20	116.36	123.22
30	6	308	CHL	C4A-NA-C1A	2.20	107.69	106.71
30	e	607	CHL	C3C-C4C-NC	2.20	113.03	110.57
31	A	818	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
31	B	833	CLA	C1-C2-C3	-2.19	122.25	126.04
30	a	606	CHL	C5-C3-C4	2.19	119.45	114.60
32	A	846	8CT	C19-C18-C17	-2.19	118.98	123.47
33	g	520	0UR	C21-C12-C11	-2.19	119.85	122.92
32	M	102	8CT	C24-C23-C21	-2.19	120.25	126.42
30	8	306	CHL	C4B-CHC-C1C	-2.19	121.14	126.34
30	1	306	CHL	C4A-NA-C1A	2.19	107.69	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	e	609	CHL	C4A-NA-C1A	2.19	107.69	106.71
33	5	501	0UR	C29-C30-C31	-2.19	109.25	111.74
30	f	607	CHL	O2A-CGA-CBA	2.19	120.90	112.23
31	B	826	CLA	CHD-C1D-ND	-2.19	122.44	124.45
36	A	856	LMG	O2-C2-C1	-2.19	104.72	110.05
32	B	845	8CT	C04-C03-C10	2.19	121.98	115.78
30	g	605	CHL	C2A-C1A-CHA	-2.19	120.03	123.86
30	e	606	CHL	C4B-CHC-C1C	-2.19	121.14	126.34
32	3	403	8CT	C27-C26-C25	-2.19	119.86	122.92
30	b	608	CHL	C4D-C3D-CAD	2.19	110.68	108.10
33	1	501	0UR	C14-C15-C16	-2.19	124.19	127.31
31	B	803	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
31	L	207	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
30	4	305	CHL	CHD-C1D-ND	-2.19	122.44	124.45
31	A	807	CLA	CHD-C1D-ND	-2.19	122.44	124.45
30	b	602	CHL	C4B-CHC-C1C	-2.19	121.15	126.34
30	b	607	CHL	C4B-CHC-C1C	-2.19	121.15	126.34
31	O	201	CLA	CHB-C1B-NB	2.19	126.57	124.26
31	2	311	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
33	3	501	0UR	C14-C15-C16	-2.19	124.19	127.31
30	6	307	CHL	C4B-CHC-C1C	-2.19	121.15	126.34
31	B	803	CLA	C3B-C4B-NB	-2.19	108.49	110.52
33	0	501	0UR	C15-C14-C13	-2.19	116.39	123.22
30	4	307	CHL	C5-C3-C4	2.19	119.43	114.60
32	B	845	8CT	C27-C26-C25	-2.19	119.86	122.92
36	L	211	LMG	O2-C2-C1	-2.19	104.73	110.05
32	K	107	8CT	C27-C26-C25	-2.19	119.86	122.92
30	e	609	CHL	C3C-C4C-NC	2.19	113.02	110.57
31	A	808	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
31	9	310	CLA	CHB-C1B-NB	2.18	126.57	124.26
30	2	301	CHL	C6-C5-C3	-2.18	107.73	113.45
30	i	609	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
33	6	501	0UR	C22-C16-C15	-2.18	119.86	122.92
31	3	308	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
33	7	501	0UR	C22-C16-C17	2.18	121.52	118.08
30	5	313	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
30	1	306	CHL	C3C-C4C-NC	2.18	113.02	110.57
36	L	210	LMG	O2-C2-C1	-2.18	104.75	110.05
30	9	313	CHL	CHA-C1A-NA	2.18	131.39	126.40
30	6	301	CHL	C4B-CHC-C1C	-2.18	121.16	126.34
32	2	402	8CT	C18-C19-C20	-2.18	119.00	123.47
33	O	204	0UR	C5-C6-C7	-2.18	120.29	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	405	8CT	C19-C18-C17	-2.18	119.01	123.47
31	7	309	CLA	CHB-C1B-NB	2.18	126.57	124.26
31	B	832	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
32	1	402	8CT	C22-C21-C20	-2.18	119.87	122.92
32	B	847	8CT	C40-C12-C13	-2.18	119.87	122.92
30	e	609	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
30	9	305	CHL	CHA-C1A-NA	2.18	131.39	126.40
30	9	305	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
32	B	843	8CT	C27-C26-C25	-2.18	119.87	122.92
31	2	303	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	1	313	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
31	O	202	CLA	CHB-C4A-NA	2.18	127.52	124.51
30	2	307	CHL	CAC-C3C-C4C	2.18	127.64	124.81
37	e	522	0IE	C4-C5-C6	2.18	130.01	123.22
30	e	601	CHL	C4B-CHC-C1C	-2.18	121.17	126.34
31	e	610	CLA	CHD-C1D-ND	-2.18	122.45	124.45
31	6	309	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
31	A	827	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
42	e	523	NEX	C28-C29-C30	2.18	122.28	118.94
31	L	203	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
31	7	310	CLA	CMA-C3A-C2A	-2.18	111.02	116.10
30	e	605	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
32	0	401	8CT	C24-C23-C21	-2.18	120.30	126.42
36	J	105	LMG	C42-C41-C40	-2.18	103.38	114.42
30	5	306	CHL	C4B-CHC-C1C	-2.18	121.18	126.34
30	h	608	CHL	C4B-CHC-C1C	-2.18	121.18	126.34
33	6	501	0UR	C33-C32-C31	-2.18	118.90	123.56
30	h	609	CHL	CHC-C4B-NB	-2.18	121.95	124.26
30	1	307	CHL	C4D-C3D-CAD	2.18	110.66	108.10
33	0	502	0UR	C43-C3-C4	-2.18	122.39	125.02
30	2	306	CHL	CHB-C4A-NA	2.18	127.52	124.51
30	2	302	CHL	CHD-C1D-ND	-2.18	122.45	124.45
31	A	830	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
31	e	610	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
32	B	804	8CT	C39-C16-C17	-2.17	119.88	122.92
31	4	309	CLA	CHD-C1D-ND	-2.17	122.46	124.45
30	6	306	CHL	CHA-C1A-NA	2.17	131.37	126.40
33	4	502	0UR	C29-C30-C31	-2.17	109.27	111.74
30	f	614	CHL	CHC-C4B-NB	-2.17	121.96	124.26
31	B	833	CLA	CHB-C1B-NB	2.17	126.56	124.26
30	2	319	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
31	3	306	CLA	CHD-C1D-ND	-2.17	122.46	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	F	302	8CT	C14-C15-C16	-2.17	120.31	126.42
30	9	301	CHL	C4B-CHC-C1C	-2.17	121.19	126.34
31	d	610	CLA	CHB-C1B-NB	2.17	126.56	124.26
33	i	520	0UR	C24-C25-C26	-2.17	107.33	110.30
32	K	107	8CT	C10-C03-C02	-2.17	116.20	121.46
31	A	813	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
30	c	606	CHL	CHD-C1D-ND	-2.17	122.46	124.45
31	f	613	CLA	CHD-C1D-ND	-2.17	122.46	124.45
31	2	310	CLA	CHB-C1B-NB	2.17	126.56	124.26
31	A	803	CLA	CHD-C1D-ND	-2.17	122.46	124.45
31	B	828	CLA	CHD-C1D-ND	-2.17	122.46	124.45
30	2	302	CHL	CHA-C1A-NA	2.17	131.37	126.40
33	4	502	0UR	C9-C10-C11	-2.17	119.03	123.47
31	B	836	CLA	C1-C2-C3	-2.17	122.29	126.04
30	e	602	CHL	CMB-C2B-C1B	2.17	128.67	125.37
31	B	817	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
31	A	826	CLA	CHD-C1D-ND	-2.17	122.46	124.45
31	A	817	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
31	2	311	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
30	c	614	CHL	CHC-C4B-NB	-2.17	121.96	124.26
31	2	303	CLA	CHB-C1B-NB	2.17	126.55	124.26
30	f	608	CHL	C4D-C3D-CAD	2.17	110.65	108.10
30	6	315	CHL	C3C-C4C-NC	2.17	113.00	110.57
33	5	502	0UR	C17-C16-C15	2.17	122.27	118.94
30	b	607	CHL	C4A-NA-C1A	2.17	107.68	106.71
32	F	302	8CT	C24-C23-C21	-2.17	120.33	126.42
31	6	303	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
30	5	307	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
31	0	308	CLA	CHB-C1B-NB	2.17	126.55	124.26
31	7	304	CLA	CMB-C2B-C1B	-2.16	122.07	125.37
30	0	302	CHL	CHD-C1D-ND	-2.16	122.47	124.45
31	3	318	CLA	CHB-C1B-NB	2.16	126.55	124.26
31	A	807	CLA	CMB-C2B-C3B	2.16	131.83	126.59
31	A	805	CLA	CHD-C1D-ND	-2.16	122.47	124.45
30	i	606	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
30	9	313	CHL	O2A-CGA-CBA	2.16	120.78	112.23
30	4	313	CHL	CHA-C1A-NA	2.16	131.35	126.40
30	9	305	CHL	C5-C3-C4	2.16	119.38	114.60
31	A	809	CLA	C1-C2-C3	-2.16	122.31	126.04
30	8	313	CHL	C4B-CHC-C1C	-2.16	121.21	126.34
31	A	836	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
36	B	853	LMG	C1-C2-C3	-2.16	105.50	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	810	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
31	B	826	CLA	CHB-C1B-NB	2.16	126.54	124.26
31	B	801	CLA	C1-C2-C3	-2.16	122.31	126.04
31	O	202	CLA	CHD-C1D-ND	-2.16	122.47	124.45
32	7	404	8CT	C10-C03-C02	-2.16	116.23	121.46
30	4	307	CHL	C4B-CHC-C1C	-2.16	121.22	126.34
33	3	501	0UR	C9-C10-C11	-2.16	119.05	123.47
31	B	805	CLA	C1-C2-C3	-2.16	122.31	126.04
30	7	306	CHL	O1D-CGD-CBD	-2.16	120.07	124.48
31	c	610	CLA	CHB-C1B-NB	2.16	126.54	124.26
30	5	313	CHL	O2A-CGA-CBA	2.16	120.75	112.23
31	B	812	CLA	C1-C2-C3	-2.16	122.31	126.04
33	5	502	0UR	C20-C7-C8	-2.16	119.90	122.92
31	A	803	CLA	CHB-C1B-NB	2.16	126.54	124.26
33	9	502	0UR	O44-C45-O57	-2.15	118.19	122.93
31	B	827	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
31	1	303	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
31	A	804	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
31	B	811	CLA	CHB-C1B-NB	2.15	126.54	124.26
36	O	207	LMG	O1-C7-C8	-2.15	105.70	110.90
31	B	833	CLA	O2D-CGD-CBD	2.15	115.09	111.27
30	7	306	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
31	B	826	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
30	g	607	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
31	7	308	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
31	B	840	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
32	A	849	8CT	C22-C21-C23	2.15	121.47	118.08
33	4	501	0UR	C10-C9-C8	-2.15	119.07	123.47
31	B	809	CLA	C1-C2-C3	-2.15	122.32	126.04
30	d	608	CHL	CHC-C4B-NB	-2.15	121.98	124.26
32	K	107	8CT	C15-C16-C17	2.15	122.24	118.94
30	4	319	CHL	CHA-C1A-NA	2.15	131.32	126.40
30	2	306	CHL	O1D-CGD-CBD	-2.15	120.08	124.48
31	b	610	CLA	C1-C2-C3	-2.15	122.32	126.04
30	6	307	CHL	CHA-C1A-NA	2.15	131.32	126.40
30	i	602	CHL	CHC-C4B-NB	-2.15	121.98	124.26
30	7	305	CHL	C4B-CHC-C1C	-2.15	121.24	126.34
30	f	606	CHL	C3D-C4D-CHA	-2.15	107.81	112.72
32	9	401	8CT	C22-C21-C20	-2.15	119.91	122.92
31	B	834	CLA	CHD-C1D-ND	-2.15	122.48	124.45
30	6	307	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
30	6	313	CHL	O1D-CGD-CBD	-2.15	120.09	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	602	CHL	OMC-CMC-C2C	-2.15	120.83	125.69
31	B	811	CLA	C1-C2-C3	-2.15	122.33	126.04
31	b	610	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
33	6	502	0UR	C15-C14-C13	-2.15	116.52	123.22
30	3	307	CHL	C4D-C3D-CAD	2.15	110.63	108.10
32	L	209	8CT	C30-C31-C32	-2.15	118.83	121.47
31	A	820	CLA	CHD-C1D-ND	-2.15	122.48	124.45
30	a	606	CHL	C1-C2-C3	-2.15	123.28	126.75
30	3	302	CHL	OMC-CMC-C2C	-2.15	120.84	125.69
30	6	307	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
32	L	206	8CT	C39-C16-C17	-2.14	119.92	122.92
31	0	311	CLA	CHB-C1B-NB	2.14	126.53	124.26
31	A	828	CLA	CHB-C4A-NA	2.14	127.48	124.51
32	K	107	8CT	C05-C04-C03	2.14	113.78	110.48
30	4	306	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
30	3	305	CHL	C4B-CHC-C1C	-2.14	121.25	126.34
42	e	523	NEX	C17-C1-C6	-2.14	108.55	110.47
30	1	305	CHL	C3D-C4D-CHA	-2.14	107.82	112.72
31	e	613	CLA	CHD-C1D-ND	-2.14	122.48	124.45
31	A	818	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
31	0	310	CLA	CHB-C1B-NB	2.14	126.53	124.26
33	9	501	0UR	C22-C16-C17	2.14	121.45	118.08
30	1	305	CHL	C4D-C3D-CAD	2.14	110.62	108.10
30	2	302	CHL	C6-C5-C3	-2.14	107.84	113.45
31	B	819	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
30	b	609	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
30	6	301	CHL	CHA-C1A-NA	2.14	131.30	126.40
31	3	310	CLA	CHB-C1B-NB	2.14	126.52	124.26
31	3	312	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
30	5	305	CHL	OMC-CMC-C2C	-2.14	120.85	125.69
31	f	613	CLA	CHB-C1B-NB	2.14	126.52	124.26
31	6	317	CLA	CHD-C1D-ND	-2.14	122.49	124.45
33	e	520	0UR	C4-C5-C6	-2.14	116.54	123.22
31	B	816	CLA	C1-C2-C3	-2.14	122.34	126.04
31	B	811	CLA	O2D-CGD-CBD	2.14	115.07	111.27
31	B	805	CLA	CHB-C4A-NA	2.14	127.47	124.51
31	3	306	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
32	8	406	8CT	C07-C02-C03	-2.14	119.63	122.73
31	B	812	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
32	A	854	8CT	C18-C19-C20	-2.14	119.10	123.47
36	L	211	LMG	O1-C7-C8	-2.14	105.74	110.90
31	B	813	CLA	CHD-C1D-ND	-2.14	122.49	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	J	103	CLA	CHB-C1B-NB	2.14	126.52	124.26
30	6	301	CHL	O2A-CGA-O1A	-2.14	118.20	123.59
31	A	812	CLA	CHD-C1D-ND	-2.14	122.49	124.45
31	f	603	CLA	CHB-C1B-NB	2.14	126.52	124.26
31	4	310	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
30	c	602	CHL	CHA-C1A-NA	2.14	131.29	126.40
36	9	602	LMG	C42-C41-C40	-2.13	103.59	114.42
31	L	207	CLA	CHB-C1B-NB	2.13	126.52	124.26
30	4	308	CHL	CHB-C4A-NA	2.13	127.46	124.51
31	A	827	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
32	F	302	8CT	C07-C02-C03	-2.13	119.63	122.73
32	K	107	8CT	C25-C24-C23	-2.13	116.56	123.22
30	d	606	CHL	CHC-C4B-NB	-2.13	122.00	124.26
31	A	815	CLA	C1-C2-C3	-2.13	122.35	126.04
31	1	309	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
31	4	309	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
31	B	807	CLA	O2A-CGA-O1A	-2.13	117.98	123.30
32	8	406	8CT	C22-C21-C23	2.13	121.44	118.08
32	0	401	8CT	C27-C26-C25	-2.13	119.94	122.92
33	g	520	0UR	C22-C16-C15	-2.13	119.94	122.92
31	B	809	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
31	B	819	CLA	CHD-C1D-ND	-2.13	122.50	124.45
31	B	837	CLA	CHD-C1D-ND	-2.13	122.50	124.45
30	h	605	CHL	CHD-C1D-C2D	2.13	129.95	125.48
30	e	607	CHL	CHC-C4B-NB	-2.13	122.00	124.26
30	6	313	CHL	CHA-C1A-NA	2.13	131.27	126.40
32	B	843	8CT	C11-C10-C03	-2.13	121.22	127.20
31	9	309	CLA	CHD-C1D-ND	-2.13	122.50	124.45
31	d	610	CLA	CHD-C1D-ND	-2.13	122.50	124.45
33	a	520	0UR	C34-C27-C26	2.13	118.30	114.36
31	A	852	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
32	B	847	8CT	C38-C31-C32	-2.13	114.76	122.33
31	A	843	CLA	CHB-C1B-NB	2.13	126.51	124.26
30	2	301	CHL	C4-C3-C5	2.13	118.85	115.27
32	6	402	8CT	C22-C21-C23	2.13	121.43	118.08
31	B	806	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
31	0	308	CLA	CHD-C1D-ND	-2.13	122.50	124.45
30	h	614	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
31	K	105	CLA	CHB-C1B-NB	2.13	126.51	124.26
33	2	502	0UR	C36-C28-C38	-2.13	104.76	107.89
30	f	606	CHL	C4D-C3D-CAD	2.13	110.60	108.10
30	i	602	CHL	OMC-CMC-C2C	-2.13	120.88	125.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	601	CHL	C4B-CHC-C1C	-2.13	121.29	126.34
31	1	314	CLA	CHB-C1B-NB	2.13	126.51	124.26
31	9	304	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
30	5	307	CHL	C3C-C4C-NC	2.13	112.95	110.57
37	g	522	0IE	C17-C16-C15	2.13	122.20	118.94
31	B	817	CLA	CAC-C3C-C4C	2.12	127.57	124.81
30	h	606	CHL	C3C-C4C-NC	2.12	112.95	110.57
31	B	818	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
33	e	520	0UR	C9-C10-C11	-2.12	119.12	123.47
30	5	301	CHL	C4B-CHC-C1C	-2.12	121.30	126.34
31	7	316	CLA	CHB-C1B-NB	2.12	126.51	124.26
30	e	601	CHL	CHA-C1A-NA	2.12	131.26	126.40
32	B	848	8CT	C23-C21-C20	-2.12	115.68	118.94
31	B	816	CLA	CHB-C1B-NB	2.12	126.50	124.26
30	c	601	CHL	CHC-C1C-C2C	-2.12	118.41	126.11
31	B	808	CLA	CMB-C2B-C3B	2.12	131.73	126.59
31	A	836	CLA	CHB-C1B-NB	2.12	126.50	124.26
30	f	601	CHL	C4B-CHC-C1C	-2.12	121.30	126.34
31	1	314	CLA	CHD-C1D-ND	-2.12	122.50	124.45
37	g	521	0IE	C23-C16-C17	2.12	121.42	118.08
30	f	608	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
32	2	402	8CT	C06-C07-C02	-2.12	110.29	114.08
30	e	614	CHL	CED-O2D-CGD	2.12	120.73	115.94
30	6	301	CHL	CHB-C4A-NA	2.12	127.44	124.51
31	b	610	CLA	CHD-C1D-ND	-2.12	122.50	124.45
30	1	305	CHL	C5-C3-C4	2.12	119.29	114.60
31	B	837	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
31	h	610	CLA	CHD-C1D-ND	-2.12	122.51	124.45
31	4	314	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
31	A	815	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
34	A	844	LHG	C5-O7-C7	-2.12	112.57	117.79
31	a	613	CLA	CHB-C1B-NB	2.12	126.50	124.26
37	e	521	0IE	C4-C3-C2	-2.12	118.26	120.08
30	0	305	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
31	L	203	CLA	CHB-C1B-NB	2.12	126.50	124.26
31	O	206	CLA	CHD-C1D-ND	-2.12	122.51	124.45
32	B	847	8CT	C27-C26-C25	-2.12	119.96	122.92
30	5	302	CHL	CHA-C1A-NA	2.12	131.25	126.40
32	9	401	8CT	C14-C15-C16	-2.12	120.47	126.42
31	A	835	CLA	CHB-C1B-NB	2.12	126.50	124.26
31	B	834	CLA	CHB-C1B-NB	2.12	126.50	124.26
30	f	608	CHL	CHD-C1D-ND	-2.12	122.51	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
31	A	843	CLA	O1D-CGD-CBD	2.12	128.81	124.48
31	A	830	CLA	C3B-C4B-NB	-2.12	108.55	110.52
32	7	405	8CT	C40-C12-C13	-2.12	119.96	122.92
30	4	313	CHL	O1D-CGD-CBD	-2.12	120.16	124.48
31	F	301	CLA	CHD-C1D-ND	-2.12	122.51	124.45
30	d	608	CHL	C4A-NA-C1A	2.12	107.66	106.71
31	A	827	CLA	CHB-C1B-NB	2.11	126.50	124.26
31	4	312	CLA	CHB-C1B-NB	2.11	126.50	124.26
31	A	831	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
33	h	520	0UR	C28-C19-C18	-2.11	110.03	112.70
30	4	313	CHL	OMC-CMC-C2C	-2.11	120.91	125.69
30	7	307	CHL	C4B-CHC-C1C	-2.11	121.32	126.34
31	A	815	CLA	CHD-C1D-ND	-2.11	122.51	124.45
31	2	309	CLA	CHB-C1B-NB	2.11	126.50	124.26
32	F	302	8CT	C40-C12-C13	-2.11	119.96	122.92
31	B	818	CLA	O2D-CGD-CBD	2.11	115.02	111.27
30	e	601	CHL	C4D-C3D-CAD	2.11	110.59	108.10
30	7	302	CHL	C3D-C4D-CHA	-2.11	107.89	112.72
31	A	813	CLA	CHD-C1D-ND	-2.11	122.51	124.45
33	1	501	0UR	C22-C16-C17	2.11	121.41	118.08
31	c	603	CLA	C1-C2-C3	-2.11	122.39	126.04
31	d	610	CLA	C1-C2-C3	-2.11	122.39	126.04
32	0	401	8CT	C35-C30-C29	-2.11	110.03	112.70
31	9	309	CLA	CHB-C1B-NB	2.11	126.49	124.26
30	6	305	CHL	CHA-C1A-NA	2.11	131.23	126.40
31	2	312	CLA	CHB-C1B-NB	2.11	126.49	124.26
31	B	838	CLA	CHC-C4B-NB	2.11	126.49	124.26
30	a	602	CHL	C4B-CHC-C1C	-2.11	121.33	126.34
33	0	502	0UR	C21-C12-C13	2.11	121.40	118.08
36	2	602	LMG	O2-C2-C1	-2.11	104.92	110.05
32	6	402	8CT	C27-C26-C25	-2.11	119.97	122.92
31	3	304	CLA	CHD-C1D-ND	-2.11	122.52	124.45
31	B	841	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
30	1	307	CHL	O2D-CGD-O1D	-2.11	119.71	123.84
31	B	820	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	F	302	8CT	C04-C03-C02	-2.11	119.64	122.61
31	B	816	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
30	d	602	CHL	C4B-CHC-C1C	-2.11	121.34	126.34
33	4	501	0UR	C9-C10-C11	-2.11	119.15	123.47
31	A	832	CLA	CHD-C1D-ND	-2.11	122.52	124.45
30	0	305	CHL	O2A-CGA-O1A	-2.11	118.27	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	802	CLA	CHD-C1D-ND	-2.11	122.52	124.45
30	1	302	CHL	CHA-C1A-NA	2.11	131.22	126.40
30	9	305	CHL	CHD-C1D-ND	-2.11	122.52	124.45
31	B	830	CLA	CHD-C1D-ND	-2.11	122.52	124.45
31	a	604	CLA	CHB-C1B-NB	2.11	126.49	124.26
31	e	613	CLA	CHB-C1B-NB	2.11	126.49	124.26
30	4	319	CHL	CHB-C1B-C2B	-2.11	121.29	127.24
32	F	302	8CT	C10-C03-C02	-2.11	116.36	121.46
30	1	313	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
31	H	202	CLA	CHB-C1B-NB	2.11	126.49	124.26
31	B	836	CLA	CMB-C2B-C3B	2.11	131.69	126.59
30	5	301	CHL	C3C-C4C-NC	2.11	112.93	110.57
30	d	602	CHL	OMC-CMC-C2C	-2.10	120.93	125.69
36	A	856	LMG	O6-C1-C2	2.10	114.80	110.35
31	2	309	CLA	CHD-C1D-ND	-2.10	122.52	124.45
30	c	614	CHL	C3C-C4C-NC	2.10	112.93	110.57
36	J	105	LMG	C1-O6-C5	-2.10	109.56	113.69
33	b	520	0UR	C22-C16-C17	2.10	121.39	118.08
33	f	520	0UR	C22-C16-C15	-2.10	119.98	122.92
31	f	611	CLA	CHB-C1B-NB	2.10	126.48	124.26
31	a	603	CLA	O2D-CGD-CBD	2.10	115.00	111.27
33	0	501	0UR	C48-C47-C46	-2.10	121.34	125.85
31	A	825	CLA	CHB-C1B-NB	2.10	126.48	124.26
36	J	102	LMG	O7-C10-O9	-2.10	118.62	123.70
30	8	305	CHL	CHA-C1A-NA	2.10	131.21	126.40
30	c	609	CHL	C4A-NA-C1A	2.10	107.65	106.71
31	1	304	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	i	608	CHL	C3C-C4C-NC	2.10	112.93	110.57
33	6	501	0UR	C23-C24-C25	-2.10	108.90	113.64
30	8	302	CHL	CHA-C1A-NA	2.10	131.21	126.40
30	e	601	CHL	C3D-C4D-CHA	-2.10	107.92	112.72
31	1	312	CLA	C1-C2-C3	-2.10	122.41	126.04
39	A	857	CL0	CHA-C4D-ND	2.10	136.89	132.50
31	5	312	CLA	CHD-C1D-ND	-2.10	122.52	124.45
30	8	307	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
31	A	843	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
31	B	808	CLA	O2D-CGD-CBD	2.10	115.00	111.27
31	0	312	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	f	601	CHL	CHB-C4A-NA	2.10	127.41	124.51
34	A	855	LHG	C26-C25-C24	2.10	120.73	113.19
30	h	606	CHL	C4A-NA-C1A	2.10	107.65	106.71
30	6	308	CHL	C4B-CHC-C1C	-2.10	121.36	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	320	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
31	0	310	CLA	CHD-C1D-ND	-2.10	122.53	124.45
31	8	312	CLA	CHD-C1D-ND	-2.10	122.53	124.45
31	A	824	CLA	CHD-C1D-ND	-2.10	122.53	124.45
33	2	501	0UR	C14-C15-C16	-2.10	124.32	127.31
30	2	307	CHL	CAA-CBA-CGA	-2.10	107.13	113.25
31	b	603	CLA	CHB-C1B-NB	2.10	126.47	124.26
30	3	307	CHL	C3D-C4D-CHA	-2.09	107.93	112.72
30	d	602	CHL	CHA-C1A-NA	2.09	131.19	126.40
31	A	829	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
30	f	609	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
30	4	313	CHL	C4B-CHC-C1C	-2.09	121.37	126.34
30	2	319	CHL	CHC-C4B-NB	-2.09	122.04	124.26
33	9	501	0UR	C20-C7-C6	2.09	121.38	118.08
30	f	606	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
31	0	312	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	B	814	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	G	105	LHG	C5-O7-C7	-2.09	112.64	117.79
42	h	523	NEX	C40-C33-C34	-2.09	119.99	122.92
30	0	301	CHL	CHD-C1D-ND	-2.09	122.53	124.45
30	a	608	CHL	CHC-C4B-NB	-2.09	122.04	124.26
31	2	304	CLA	CHB-C1B-NB	2.09	126.47	124.26
31	B	823	CLA	CHB-C1B-NB	2.09	126.47	124.26
31	5	303	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	J	101	8CT	C22-C21-C20	-2.09	119.99	122.92
32	L	205	8CT	C35-C30-C31	2.09	115.16	111.42
30	4	302	CHL	CHA-C1A-NA	2.09	131.18	126.40
31	6	309	CLA	CHB-C1B-NB	2.09	126.47	124.26
30	0	305	CHL	C4B-CHC-C1C	-2.09	121.38	126.34
31	B	839	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	B	803	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
42	e	523	NEX	C30-C31-C32	-2.09	116.69	123.22
31	B	805	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	8	315	CHL	CHC-C4B-NB	-2.09	122.05	124.26
42	c	523	NEX	C40-C33-C34	-2.09	120.00	122.92
30	i	606	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
30	h	608	CHL	C4A-NA-C1A	2.09	107.64	106.71
31	A	809	CLA	CHC-C4B-NB	2.09	126.47	124.26
31	A	839	CLA	CHB-C1B-NB	2.09	126.47	124.26
31	c	610	CLA	C1-C2-C3	-2.09	122.43	126.04
31	A	822	CLA	CHD-C1D-ND	-2.09	122.54	124.45
32	B	848	8CT	C22-C21-C23	2.09	121.36	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	313	CLA	CHB-C1B-NB	2.09	126.47	124.26
31	0	309	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
30	e	609	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
31	A	818	CLA	O2D-CGD-CBD	2.09	114.97	111.27
32	8	402	8CT	C40-C12-C13	-2.09	120.00	122.92
31	b	604	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
33	1	501	0UR	C4-C5-C6	-2.09	116.71	123.22
30	7	302	CHL	CHB-C1B-C2B	-2.09	121.35	127.24
30	9	301	CHL	O1D-CGD-CBD	-2.09	120.22	124.48
31	A	833	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
31	3	304	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
32	A	849	8CT	C35-C30-C31	2.08	115.15	111.42
31	9	311	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
32	B	844	8CT	C19-C18-C17	-2.08	119.20	123.47
31	B	819	CLA	C1-C2-C3	-2.08	122.44	126.04
31	4	309	CLA	C1-C2-C3	-2.08	122.44	126.04
36	B	853	LMG	O2-C2-C1	-2.08	104.98	110.05
31	6	312	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
33	a	520	0UR	C43-O44-C45	2.08	119.79	116.07
30	3	302	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
31	9	312	CLA	CHD-C1D-ND	-2.08	122.54	124.45
32	M	102	8CT	C35-C30-C29	-2.08	110.07	112.70
31	K	102	CLA	CAC-C3C-C4C	2.08	127.51	124.81
31	A	836	CLA	CHD-C1D-ND	-2.08	122.54	124.45
31	B	806	CLA	C1-C2-C3	-2.08	122.44	126.04
30	6	302	CHL	CHA-C1A-NA	2.08	131.16	126.40
31	e	612	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
31	e	611	CLA	C1-C2-C3	-2.08	122.44	126.04
31	A	824	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
31	B	820	CLA	CHD-C1D-ND	-2.08	122.54	124.45
31	4	312	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	8	305	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
31	3	311	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
32	O	205	8CT	C05-C04-C03	2.08	113.68	110.48
30	4	313	CHL	CHC-C1C-C2C	-2.08	118.57	126.11
42	d	523	NEX	C40-C33-C34	-2.08	120.01	122.92
30	d	605	CHL	C2A-C1A-CHA	-2.08	120.22	123.86
30	4	308	CHL	C4B-CHC-C1C	-2.08	121.41	126.34
30	c	601	CHL	C6-C5-C3	-2.08	108.01	113.45
31	7	311	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
33	8	502	0UR	O44-C45-O57	-2.08	118.36	122.93
31	L	203	CLA	CHD-C1D-ND	-2.08	122.55	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	K	102	CLA	CHD-C1D-ND	-2.08	122.55	124.45
31	A	807	CLA	C1-C2-C3	-2.08	122.45	126.04
30	g	606	CHL	C3C-C4C-NC	2.08	112.90	110.57
30	6	302	CHL	C4B-CHC-C1C	-2.08	121.41	126.34
32	A	848	8CT	C28-C26-C25	-2.08	115.75	118.94
30	7	306	CHL	CHB-C4A-NA	2.08	127.38	124.51
31	A	828	CLA	CMB-C2B-C1B	-2.08	122.21	125.37
31	H	204	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
30	c	607	CHL	O2A-CGA-CBA	2.08	120.43	112.23
31	A	815	CLA	CHB-C1B-NB	2.08	126.45	124.26
31	H	205	CLA	CHB-C1B-NB	2.08	126.45	124.26
30	8	302	CHL	C4B-CHC-C1C	-2.08	121.42	126.34
31	7	312	CLA	CHD-C1D-ND	-2.08	122.55	124.45
31	A	811	CLA	CHD-C1D-ND	-2.08	122.55	124.45
30	4	302	CHL	CHB-C1B-C2B	-2.08	121.38	127.24
31	d	603	CLA	C1-C2-C3	-2.07	122.45	126.04
31	4	309	CLA	CHB-C1B-NB	2.07	126.45	124.26
30	6	306	CHL	C4B-CHC-C1C	-2.07	121.42	126.34
31	a	610	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
42	g	523	NEX	C40-C33-C34	-2.07	120.02	122.92
33	d	520	0UR	C4-C5-C6	-2.07	116.75	123.22
31	6	311	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
30	2	306	CHL	CHC-C4B-NB	-2.07	122.06	124.26
30	2	302	CHL	CHB-C1B-C2B	-2.07	121.38	127.24
30	6	307	CHL	CHB-C4A-NA	2.07	127.38	124.51
33	e	520	0UR	C10-C9-C8	-2.07	119.23	123.47
34	2	601	LHG	C26-C25-C24	2.07	120.64	113.19
31	B	812	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
31	L	202	CLA	CHD-C1D-ND	-2.07	122.55	124.45
31	i	610	CLA	CHD-C1D-ND	-2.07	122.55	124.45
33	5	502	0UR	C34-C27-C26	2.07	118.19	114.36
31	0	303	CLA	CHB-C1B-NB	2.07	126.45	124.26
31	5	309	CLA	CMB-C2B-C3B	2.07	131.61	126.59
30	h	608	CHL	C3C-C4C-NC	2.07	112.89	110.57
32	A	848	8CT	C39-C16-C15	2.07	121.34	118.08
31	5	311	CLA	CHD-C1D-ND	-2.07	122.55	124.45
31	A	806	CLA	CHD-C1D-ND	-2.07	122.55	124.45
31	4	310	CLA	CHB-C1B-NB	2.07	126.45	124.26
36	B	853	LMG	O7-C10-O9	-2.07	118.70	123.70
30	8	301	CHL	O2A-CGA-O1A	-2.07	118.37	123.59
31	3	309	CLA	CMB-C2B-C3B	2.07	131.60	126.59
31	1	304	CLA	CHD-C1D-ND	-2.07	122.55	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	852	CLA	CHD-C1D-ND	-2.07	122.55	124.45
31	B	819	CLA	CHB-C1B-NB	2.07	126.45	124.26
31	h	604	CLA	CHB-C1B-NB	2.07	126.45	124.26
30	e	607	CHL	O2A-CGA-CBA	2.07	120.41	112.23
30	b	608	CHL	CHA-C1A-NA	2.07	131.13	126.40
32	L	205	8CT	C24-C23-C21	-2.07	120.61	126.42
42	a	523	NEX	C40-C33-C34	-2.07	120.03	122.92
30	8	307	CHL	CHA-C1A-NA	2.07	131.13	126.40
30	6	306	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
31	9	303	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
30	5	306	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
32	2	402	8CT	C27-C26-C25	-2.07	120.03	122.92
31	A	803	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
31	K	104	CLA	CHD-C1D-ND	-2.07	122.56	124.45
30	6	313	CHL	C4B-CHC-C1C	-2.06	121.44	126.34
31	9	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
31	A	818	CLA	C1-C2-C3	-2.06	122.47	126.04
31	9	312	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
30	e	608	CHL	C4D-C3D-CAD	2.06	110.53	108.10
30	f	606	CHL	C3C-C4C-NC	2.06	112.89	110.57
30	6	313	CHL	O2D-CGD-O1D	-2.06	119.80	123.84
30	f	606	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
30	h	609	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
31	8	309	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
30	7	313	CHL	OMC-CMC-C2C	-2.06	121.02	125.69
33	O	204	0UR	C21-C12-C13	2.06	121.33	118.08
31	h	612	CLA	CHB-C1B-NB	2.06	126.44	124.26
30	6	307	CHL	C4D-C3D-CAD	2.06	110.53	108.10
32	B	847	8CT	C22-C21-C23	2.06	121.33	118.08
31	A	819	CLA	C1-C2-C3	-2.06	122.48	126.04
30	e	614	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
30	b	608	CHL	CHB-C4A-NA	2.06	127.36	124.51
30	7	305	CHL	CHA-C1A-NA	2.06	131.12	126.40
33	1	502	0UR	C22-C16-C15	-2.06	120.04	122.92
31	2	309	CLA	C1-C2-C3	-2.06	122.48	126.04
31	A	828	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
31	B	815	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
31	8	304	CLA	C1-C2-C3	-2.06	122.48	126.04
30	9	313	CHL	C4B-CHC-C1C	-2.06	121.45	126.34
31	A	838	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
31	i	604	CLA	CHD-C1D-ND	-2.06	122.56	124.45
34	5	601	LHG	C26-C25-C24	2.06	120.59	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	824	CLA	CHB-C1B-NB	2.06	126.44	124.26
33	4	502	0UR	C4-C5-C6	-2.06	116.79	123.22
30	a	608	CHL	C3C-C4C-NC	2.06	112.88	110.57
42	b	523	NEX	C40-C33-C34	-2.06	120.04	122.92
30	e	608	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
32	B	851	8CT	C40-C12-C13	-2.06	120.04	122.92
33	6	501	0UR	C21-C12-C11	-2.06	120.04	122.92
31	A	819	CLA	CHD-C1D-ND	-2.06	122.56	124.45
31	f	603	CLA	CHD-C1D-ND	-2.06	122.56	124.45
31	h	613	CLA	CHD-C1D-ND	-2.06	122.56	124.45
33	4	502	0UR	C34-C27-C26	2.06	118.17	114.36
30	b	608	CHL	C4B-CHC-C1C	-2.06	121.46	126.34
31	A	822	CLA	CHB-C1B-NB	2.06	126.44	124.26
31	2	309	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
30	2	307	CHL	C4D-C3D-CAD	2.06	110.52	108.10
30	8	305	CHL	C4D-C3D-CAD	2.06	110.52	108.10
31	A	838	CLA	CHD-C1D-ND	-2.06	122.56	124.45
31	B	837	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
31	B	824	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
31	2	304	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
30	5	302	CHL	CHC-C1C-C2C	-2.06	118.66	126.11
33	8	501	0UR	C23-C24-C25	-2.06	109.00	113.64
31	A	836	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
31	5	309	CLA	CHD-C1D-ND	-2.06	122.56	124.45
33	9	502	0UR	C25-C26-C27	-2.05	107.76	111.85
33	c	520	0UR	C21-C12-C11	-2.05	120.05	122.92
31	0	321	CLA	CHB-C1B-NB	2.05	126.43	124.26
31	3	308	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	0	301	CHL	C4B-CHC-C1C	-2.05	121.47	126.34
30	5	302	CHL	CHB-C1B-C2B	-2.05	121.44	127.24
30	d	601	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
42	i	523	NEX	C40-C33-C34	-2.05	120.05	122.92
34	g	630	LHG	C26-C25-C24	2.05	120.57	113.19
31	i	612	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
30	g	608	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
31	3	310	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
30	0	302	CHL	C4B-CHC-C1C	-2.05	121.47	126.34
31	9	302	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
31	B	816	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
30	2	313	CHL	C4B-CHC-C1C	-2.05	121.47	126.34
31	7	304	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
30	8	313	CHL	C3D-C4D-CHA	-2.05	108.03	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	f	630	LHG	C5-O7-C7	-2.05	112.74	117.79
32	A	854	8CT	C05-C04-C03	2.05	113.64	110.48
31	a	611	CLA	CHB-C1B-NB	2.05	126.43	124.26
31	h	610	CLA	CHB-C1B-NB	2.05	126.43	124.26
31	4	312	CLA	CHC-C4B-NB	2.05	126.43	124.26
31	2	312	CLA	CMB-C2B-C3B	2.05	131.55	126.59
31	B	815	CLA	CMB-C2B-C3B	2.05	131.55	126.59
31	4	314	CLA	CHB-C1B-NB	2.05	126.43	124.26
31	A	832	CLA	C1-C2-C3	-2.05	122.50	126.04
31	B	819	CLA	O2D-CGD-CBD	2.05	114.91	111.27
31	c	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
31	O	203	CLA	CHB-C1B-NB	2.05	126.43	124.26
30	5	301	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
42	f	523	NEX	C40-C33-C34	-2.05	120.05	122.92
31	A	840	CLA	C1-C2-C3	2.05	129.59	126.04
31	1	311	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
31	A	841	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
30	b	608	CHL	CHD-C1D-ND	-2.05	122.57	124.45
31	A	806	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
30	8	308	CHL	C4B-CHC-C1C	-2.05	121.48	126.34
31	6	303	CLA	CHB-C1B-NB	2.05	126.42	124.26
31	9	308	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
30	f	602	CHL	CHB-C1B-C2B	-2.05	121.46	127.24
32	L	205	8CT	C27-C26-C25	-2.05	120.06	122.92
30	4	306	CHL	CHA-C1A-NA	2.05	131.08	126.40
31	4	314	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	B	839	CLA	CMB-C2B-C1B	-2.04	122.25	125.37
31	6	320	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
32	7	402	8CT	C40-C12-C11	2.04	121.30	118.08
31	1	312	CLA	CHB-C1B-NB	2.04	126.42	124.26
31	B	832	CLA	CHB-C1B-NB	2.04	126.42	124.26
30	e	602	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
31	A	820	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
30	7	302	CHL	C4B-CHC-C1C	-2.04	121.49	126.34
35	0	603	SQD	O2-C2-C3	-2.04	105.63	110.35
30	5	307	CHL	O2A-CGA-CBA	2.04	120.30	112.23
30	f	602	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
32	B	846	8CT	C37-C35-C30	2.04	112.64	109.55
31	9	302	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	1	305	CHL	C4B-CHC-C1C	-2.04	121.49	126.34
31	0	304	CLA	CHB-C1B-NB	2.04	126.42	124.26
31	A	816	CLA	CHB-C1B-NB	2.04	126.42	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	f	610	CLA	C1-C2-C3	-2.04	122.51	126.04
30	4	319	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
33	8	502	0UR	C17-C16-C15	2.04	122.07	118.94
30	8	307	CHL	C4D-C3D-CAD	2.04	110.50	108.10
30	a	601	CHL	O2A-CGA-CBA	2.04	120.30	112.23
31	8	314	CLA	CHB-C1B-NB	2.04	126.42	124.26
30	a	602	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
30	4	305	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
31	A	833	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	6	314	CLA	O2D-CGD-CBD	2.04	114.89	111.27
31	0	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
33	9	502	0UR	C34-C27-C1	-2.04	121.81	124.49
31	A	821	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
31	h	604	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
31	9	311	CLA	C1-C2-C3	-2.04	122.52	126.04
31	A	819	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
31	g	611	CLA	CHD-C1D-ND	-2.04	122.58	124.45
36	J	105	LMG	O1-C7-C8	-2.04	105.98	110.90
31	A	812	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
31	4	311	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	i	606	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
33	8	501	0UR	C43-C3-C2	2.04	121.45	116.66
33	8	502	0UR	C34-C27-C26	2.04	118.13	114.36
31	B	814	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	a	602	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
31	g	613	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	g	606	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
33	9	502	0UR	C43-C3-C4	-2.04	122.56	125.02
31	b	613	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	f	608	CHL	C3D-C4D-CHA	-2.04	108.06	112.72
30	c	608	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
30	b	608	CHL	O2D-CGD-O1D	-2.04	119.86	123.84
30	6	306	CHL	CHC-C1C-C2C	-2.04	118.73	126.11
32	7	405	8CT	C05-C04-C03	2.04	113.61	110.48
31	c	613	CLA	CHD-C1D-ND	-2.03	122.58	124.45
32	A	846	8CT	C35-C30-C31	2.03	115.06	111.42
30	4	305	CHL	CHA-C1A-NA	2.03	131.06	126.40
31	a	604	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
30	g	614	CHL	CHD-C1D-C2D	2.03	129.75	125.48
30	h	614	CHL	CHD-C1D-C2D	2.03	129.75	125.48
30	3	305	CHL	CHA-C1A-NA	2.03	131.05	126.40
31	c	604	CLA	O2A-CGA-O1A	-2.03	118.46	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	e	611	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
31	L	204	CLA	CHD-C1D-ND	-2.03	122.58	124.45
31	i	613	CLA	CHB-C1B-NB	2.03	126.41	124.26
30	b	606	CHL	CHA-C1A-NA	2.03	131.05	126.40
30	b	607	CHL	O2A-CGA-CBA	2.03	120.27	112.23
30	i	607	CHL	O2A-CGA-CBA	2.03	120.27	112.23
31	B	837	CLA	O2D-CGD-CBD	2.03	114.88	111.27
30	0	302	CHL	CHA-C1A-NA	2.03	131.05	126.40
31	d	612	CLA	CHB-C1B-NB	2.03	126.41	124.26
31	8	304	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
37	a	521	0IE	C23-C16-C17	2.03	121.28	118.08
30	2	308	CHL	O2D-CGD-O1D	-2.03	119.86	123.84
30	9	305	CHL	C3D-C4D-CHA	-2.03	108.07	112.72
32	8	402	8CT	C13-C14-C15	-2.03	116.88	123.22
39	A	857	CL0	CMC-C2C-C1C	2.03	128.13	125.04
30	c	607	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
30	i	608	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
30	8	301	CHL	C4B-CHC-C1C	-2.03	121.52	126.34
31	7	308	CLA	CHB-C1B-NB	2.03	126.41	124.26
31	B	805	CLA	CHC-C4B-NB	2.03	126.41	124.26
30	a	608	CHL	C4A-NA-C1A	2.03	107.62	106.71
31	b	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
31	B	807	CLA	CMB-C2B-C3B	2.03	131.50	126.59
30	5	305	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
31	g	611	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
31	B	836	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
31	c	613	CLA	CHB-C1B-NB	2.03	126.41	124.26
31	2	309	CLA	O2D-CGD-CBD	2.03	114.87	111.27
30	0	302	CHL	CHB-C1B-C2B	-2.03	121.51	127.24
31	5	309	CLA	C2D-C1D-ND	-2.03	108.61	110.10
30	d	609	CHL	CHC-C4B-NB	-2.03	122.11	124.26
32	L	209	8CT	C39-C16-C15	2.03	121.27	118.08
30	8	313	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
30	2	313	CHL	CHB-C4A-NA	2.03	127.32	124.51
33	h	520	0UR	C4-C3-C2	-2.03	118.34	120.08
30	2	307	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
33	O	204	0UR	C34-C27-C26	2.03	118.11	114.36
31	5	303	CLA	CHC-C4B-NB	2.03	126.40	124.26
31	7	315	CLA	CHB-C1B-NB	2.03	126.40	124.26
31	A	833	CLA	CHB-C1B-NB	2.03	126.40	124.26
30	6	313	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
31	c	613	CLA	O2A-CGA-O1A	-2.03	118.48	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	K	101	CLA	O2D-CGD-CBD	2.03	114.87	111.27
31	4	304	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
31	O	206	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
31	A	819	CLA	CMB-C2B-C3B	2.03	131.49	126.59
30	7	301	CHL	O2A-C1-C2	2.03	113.96	108.64
31	K	105	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
34	d	630	LHG	C26-C25-C24	2.02	120.47	113.19
33	6	502	0UR	C36-C28-C19	2.02	112.61	109.55
36	J	105	LMG	O2-C2-C1	-2.02	105.13	110.05
31	b	613	CLA	CHB-C1B-NB	2.02	126.40	124.26
30	6	307	CHL	C3D-C4D-CHA	-2.02	108.09	112.72
31	B	811	CLA	CHD-C1D-ND	-2.02	122.59	124.45
31	B	833	CLA	CHD-C1D-ND	-2.02	122.59	124.45
31	f	611	CLA	CHD-C1D-ND	-2.02	122.59	124.45
30	b	602	CHL	CHA-C1A-NA	2.02	131.03	126.40
30	2	307	CHL	CHB-C1B-C2B	-2.02	121.52	127.24
30	2	313	CHL	CHA-C1A-NA	2.02	131.03	126.40
31	g	613	CLA	O2D-CGD-CBD	2.02	114.86	111.27
31	0	309	CLA	CHD-C1D-ND	-2.02	122.59	124.45
31	6	312	CLA	CHD-C1D-ND	-2.02	122.59	124.45
30	4	306	CHL	O1D-CGD-CBD	-2.02	120.34	124.48
31	B	826	CLA	CMB-C2B-C3B	2.02	131.49	126.59
30	3	307	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
31	h	613	CLA	CHB-C1B-NB	2.02	126.40	124.26
31	6	309	CLA	CMB-C2B-C3B	2.02	131.49	126.59
31	B	835	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
30	2	301	CHL	C4B-CHC-C1C	-2.02	121.54	126.34
30	b	606	CHL	C4B-CHC-C1C	-2.02	121.54	126.34
34	H	203	LHG	C26-C25-C24	2.02	120.46	113.19
30	h	609	CHL	O2A-CGA-CBA	2.02	120.22	112.23
31	5	311	CLA	CHC-C4B-NB	2.02	126.40	124.26
31	4	303	CLA	CHD-C1D-ND	-2.02	122.60	124.45
31	A	825	CLA	CMB-C2B-C3B	2.02	131.48	126.59
31	8	314	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
31	2	310	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
31	g	610	CLA	CHD-C1D-ND	-2.02	122.60	124.45
31	i	613	CLA	CHD-C1D-ND	-2.02	122.60	124.45
33	6	501	0UR	C14-C13-C12	-2.02	120.74	126.42
37	f	521	0IE	C23-C16-C17	2.02	121.26	118.08
30	7	301	CHL	CHC-C4B-NB	-2.02	122.12	124.26
30	9	313	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
33	a	520	0UR	C20-C7-C6	2.02	121.26	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	319	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
30	4	319	CHL	CHC-C4B-NB	-2.02	122.12	124.26
31	B	827	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
33	8	502	0UR	C25-C26-C27	-2.02	107.83	111.85
31	B	807	CLA	CHD-C1D-ND	-2.02	122.60	124.45
30	2	302	CHL	CHC-C1C-C2C	-2.02	118.80	126.11
30	2	319	CHL	CHA-C1A-NA	2.02	131.01	126.40
30	4	302	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
31	A	817	CLA	CHB-C1B-NB	2.02	126.39	124.26
31	A	827	CLA	CMB-C2B-C3B	2.02	131.47	126.59
30	d	608	CHL	O2D-CGD-O1D	-2.02	119.90	123.84
31	1	304	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
31	A	804	CLA	CHD-C1D-ND	-2.02	122.60	124.45
30	9	313	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
31	A	834	CLA	CHB-C1B-NB	2.01	126.39	124.26
31	0	304	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
30	8	306	CHL	C3D-C4D-CHA	-2.01	108.11	112.72
30	a	607	CHL	O2A-CGA-CBA	2.01	120.19	112.23
32	B	847	8CT	C06-C07-C02	-2.01	110.48	114.08
31	4	311	CLA	CHB-C1B-NB	2.01	126.39	124.26
31	d	610	CLA	CMB-C2B-C3B	2.01	131.47	126.59
31	A	852	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
30	a	606	CHL	C3C-C4C-NC	2.01	112.83	110.57
30	6	302	CHL	CHB-C1B-C2B	-2.01	121.55	127.24
30	7	306	CHL	C4B-CHC-C1C	-2.01	121.56	126.34
32	L	205	8CT	C19-C18-C17	-2.01	119.35	123.47
30	8	306	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
33	O	204	0UR	C43-C3-C2	2.01	121.39	116.66
31	L	201	CLA	CHD-C1D-ND	-2.01	122.61	124.45
33	3	501	0UR	C10-C9-C8	-2.01	119.35	123.47
31	6	310	CLA	CHB-C1B-NB	2.01	126.39	124.26
31	3	318	CLA	CHD-C1D-ND	-2.01	122.61	124.45
31	B	836	CLA	CHD-C1D-ND	-2.01	122.61	124.45
31	3	320	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
34	M	104	LHG	C5-O7-C7	-2.01	112.84	117.79
31	B	830	CLA	CMB-C2B-C3B	2.01	131.46	126.59
30	c	602	CHL	CHB-C1B-C2B	-2.01	121.56	127.24
31	a	613	CLA	CHD-C1D-ND	-2.01	122.61	124.45
30	c	601	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
31	2	314	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
31	B	818	CLA	CHB-C1B-NB	2.01	126.38	124.26
31	K	102	CLA	CHB-C1B-NB	2.01	126.38	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	319	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
31	9	300	CLA	O2D-CGD-CBD	2.01	114.84	111.27
31	A	819	CLA	O2D-CGD-CBD	2.01	114.84	111.27
30	2	308	CHL	CHA-C1A-NA	2.01	131.00	126.40
36	3	602	LMG	O7-C10-O9	-2.01	118.85	123.70
32	B	848	8CT	C40-C12-C13	-2.01	120.11	122.92
33	5	501	0UR	C15-C14-C13	-2.01	116.95	123.22
31	f	604	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
31	B	823	CLA	C2D-C1D-ND	-2.01	108.62	110.10
31	d	613	CLA	CHD-C1D-ND	-2.01	122.61	124.45
30	6	305	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
30	4	307	CHL	CHC-C1C-C2C	-2.01	118.83	126.11
31	9	300	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	a	604	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	B	821	CLA	CHD-C1D-ND	-2.01	122.61	124.45
32	B	844	8CT	C28-C26-C25	2.01	122.02	118.94
31	A	830	CLA	CHC-C1C-NC	2.01	127.25	124.20
32	A	849	8CT	C27-C26-C28	2.01	121.24	118.08
30	8	313	CHL	CHC-C1C-C2C	-2.01	118.84	126.11
32	A	850	8CT	C24-C25-C26	-2.01	124.45	127.31
30	5	307	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
32	3	403	8CT	C24-C23-C21	-2.01	120.78	126.42
30	2	307	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
33	2	502	0UR	C48-C47-C46	-2.01	123.56	125.84
31	B	841	CLA	C1-C2-C3	-2.01	122.57	126.04
31	f	604	CLA	CHB-C1B-NB	2.01	126.38	124.26
33	9	501	0UR	C14-C15-C16	-2.01	124.45	127.31
30	d	608	CHL	C4D-C3D-CAD	2.00	110.46	108.10
30	4	302	CHL	CHC-C1C-C2C	-2.00	118.84	126.11
36	O	207	LMG	O7-C10-O9	-2.00	118.86	123.70
31	3	309	CLA	C2D-C1D-ND	-2.00	108.63	110.10
31	g	604	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
30	6	313	CHL	C4D-C3D-CAD	2.00	110.46	108.10
33	9	502	0UR	C48-C47-C46	-2.00	121.55	125.85
30	e	606	CHL	CHC-C4B-NB	-2.00	122.14	124.26
31	K	104	CLA	CHB-C1B-NB	2.00	126.38	124.26
30	2	313	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
31	4	304	CLA	CHD-C1D-ND	-2.00	122.61	124.45
32	B	848	8CT	C39-C16-C15	2.00	121.23	118.08
31	A	820	CLA	CHB-C1B-NB	2.00	126.38	124.26
31	i	611	CLA	CHB-C1B-NB	2.00	126.38	124.26
31	9	310	CLA	CHD-C1D-ND	-2.00	122.61	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	312	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	f	603	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	4	314	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
31	A	809	CLA	CHB-C1B-NB	2.00	126.38	124.26
31	B	850	CLA	CHB-C1B-NB	2.00	126.38	124.26
30	0	301	CHL	CHC-C1C-C2C	-2.00	118.85	126.11
31	e	610	CLA	CMB-C2B-C3B	2.00	131.44	126.59
31	6	314	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
31	0	304	CLA	CHD-C1D-ND	-2.00	122.61	124.45
31	e	603	CLA	CHD-C1D-ND	-2.00	122.61	124.45
30	3	305	CHL	C5-C3-C4	2.00	119.02	114.60
30	b	608	CHL	C3D-C4D-CHA	-2.00	108.14	112.72
30	8	305	CHL	O2A-CGA-CBA	2.00	120.14	112.23
30	2	306	CHL	CHA-C1A-NA	2.00	130.98	126.40
30	6	313	CHL	C3D-C4D-CHA	-2.00	108.15	112.72
30	5	301	CHL	O1D-CGD-CBD	-2.00	120.39	124.48
30	6	302	CHL	O1D-CGD-CBD	-2.00	120.39	124.48
30	a	606	CHL	OMC-CMC-C2C	-2.00	121.16	125.69

There are no chirality outliers.

All (4828) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	301	CHL	C1A-C2A-CAA-CBA
30	0	301	CHL	C3A-C2A-CAA-CBA
30	0	301	CHL	C1C-C2C-CMC-OMC
30	0	301	CHL	C3C-C2C-CMC-OMC
30	0	301	CHL	C2-C3-C5-C6
30	0	301	CHL	C4-C3-C5-C6
30	0	302	CHL	C2B-C3B-CAB-CBB
30	0	302	CHL	C4B-C3B-CAB-CBB
30	0	302	CHL	C12-C13-C15-C16
30	0	305	CHL	C1A-C2A-CAA-CBA
30	0	305	CHL	C3A-C2A-CAA-CBA
30	0	305	CHL	C3C-C2C-CMC-OMC
30	0	306	CHL	CHA-CBD-CGD-O1D
30	0	306	CHL	CHA-CBD-CGD-O2D
30	1	302	CHL	C3C-C2C-CMC-OMC
30	1	302	CHL	CHA-CBD-CGD-O2D
30	1	306	CHL	CHA-CBD-CGD-O1D
30	1	306	CHL	CHA-CBD-CGD-O2D
30	1	307	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	1	307	CHL	C11-C10-C8-C9
30	1	313	CHL	C3C-C2C-CMC-OMC
30	2	302	CHL	C1C-C2C-CMC-OMC
30	2	302	CHL	C3C-C2C-CMC-OMC
30	2	302	CHL	CHA-CBD-CGD-O1D
30	2	302	CHL	CHA-CBD-CGD-O2D
30	2	302	CHL	C6-C7-C8-C9
30	2	302	CHL	C12-C13-C15-C16
30	2	306	CHL	C3C-C2C-CMC-OMC
30	2	307	CHL	CBD-CGD-O2D-CED
30	2	313	CHL	C2A-CAA-CBA-CGA
30	2	319	CHL	CHA-CBD-CGD-O1D
30	2	319	CHL	CHA-CBD-CGD-O2D
30	2	319	CHL	CAD-CBD-CGD-O1D
30	2	319	CHL	C2-C3-C5-C6
30	2	319	CHL	C4-C3-C5-C6
30	3	302	CHL	C3C-C2C-CMC-OMC
30	3	302	CHL	CHA-CBD-CGD-O1D
30	3	302	CHL	CHA-CBD-CGD-O2D
30	3	305	CHL	C2B-C3B-CAB-CBB
30	3	305	CHL	C4B-C3B-CAB-CBB
30	5	301	CHL	C2-C3-C5-C6
30	5	301	CHL	C4-C3-C5-C6
30	5	302	CHL	C2B-C3B-CAB-CBB
30	5	302	CHL	C4B-C3B-CAB-CBB
30	5	302	CHL	C1C-C2C-CMC-OMC
30	5	302	CHL	C3C-C2C-CMC-OMC
30	5	305	CHL	C3C-C2C-CMC-OMC
30	5	307	CHL	C3C-C2C-CMC-OMC
30	6	301	CHL	CHA-CBD-CGD-O1D
30	6	301	CHL	CHA-CBD-CGD-O2D
30	6	302	CHL	C1C-C2C-CMC-OMC
30	6	302	CHL	C3C-C2C-CMC-OMC
30	6	302	CHL	C11-C10-C8-C9
30	6	306	CHL	C1A-C2A-CAA-CBA
30	6	306	CHL	C3C-C2C-CMC-OMC
30	6	307	CHL	C1A-C2A-CAA-CBA
30	6	307	CHL	C3C-C2C-CMC-OMC
30	6	313	CHL	C2-C3-C5-C6
30	6	313	CHL	C4-C3-C5-C6
30	6	315	CHL	CHA-CBD-CGD-O1D
30	6	315	CHL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	7	302	CHL	CHA-CBD-CGD-O1D
30	7	302	CHL	CHA-CBD-CGD-O2D
30	7	302	CHL	C14-C13-C15-C16
30	7	307	CHL	C1A-C2A-CAA-CBA
30	7	307	CHL	C3A-C2A-CAA-CBA
30	7	307	CHL	CBD-CGD-O2D-CED
30	8	302	CHL	C3C-C2C-CMC-OMC
30	8	302	CHL	CHA-CBD-CGD-O2D
30	8	306	CHL	C1A-C2A-CAA-CBA
30	8	306	CHL	C3C-C2C-CMC-OMC
30	8	306	CHL	CHA-CBD-CGD-O1D
30	8	306	CHL	CHA-CBD-CGD-O2D
30	8	306	CHL	CAD-CBD-CGD-O1D
30	8	307	CHL	C1A-C2A-CAA-CBA
30	8	307	CHL	C3A-C2A-CAA-CBA
30	8	313	CHL	C3C-C2C-CMC-OMC
30	8	313	CHL	C2-C3-C5-C6
30	8	313	CHL	C4-C3-C5-C6
30	8	315	CHL	CHA-CBD-CGD-O2D
30	9	301	CHL	C3C-C2C-CMC-OMC
30	9	313	CHL	C1A-C2A-CAA-CBA
30	9	313	CHL	C3A-C2A-CAA-CBA
30	a	601	CHL	C3A-C2A-CAA-CBA
30	a	602	CHL	CHA-CBD-CGD-O1D
30	a	602	CHL	CHA-CBD-CGD-O2D
30	a	607	CHL	C1A-C2A-CAA-CBA
30	a	607	CHL	C3A-C2A-CAA-CBA
30	a	608	CHL	CAD-CBD-CGD-O1D
30	a	608	CHL	CAD-CBD-CGD-O2D
30	a	608	CHL	CBD-CGD-O2D-CED
30	a	609	CHL	C6-C7-C8-C9
30	c	601	CHL	C1C-C2C-CMC-OMC
30	c	601	CHL	C3C-C2C-CMC-OMC
30	c	601	CHL	C2-C3-C5-C6
30	c	601	CHL	C4-C3-C5-C6
30	c	602	CHL	C2B-C3B-CAB-CBB
30	c	602	CHL	C4B-C3B-CAB-CBB
30	c	602	CHL	C1C-C2C-CMC-OMC
30	c	602	CHL	C3C-C2C-CMC-OMC
30	c	602	CHL	CHA-CBD-CGD-O1D
30	c	602	CHL	CHA-CBD-CGD-O2D
30	c	608	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	c	614	CHL	CHA-CBD-CGD-O1D
30	c	614	CHL	CHA-CBD-CGD-O2D
30	c	614	CHL	CAD-CBD-CGD-O1D
30	c	614	CHL	CAD-CBD-CGD-O2D
30	b	601	CHL	C2-C3-C5-C6
30	b	601	CHL	C4-C3-C5-C6
30	b	602	CHL	CHA-CBD-CGD-O1D
30	b	602	CHL	CHA-CBD-CGD-O2D
30	b	608	CHL	CBD-CGD-O2D-CED
30	d	602	CHL	CHA-CBD-CGD-O1D
30	d	602	CHL	CHA-CBD-CGD-O2D
30	d	607	CHL	C1A-C2A-CAA-CBA
30	d	608	CHL	C3C-C2C-CMC-OMC
30	d	608	CHL	CBD-CGD-O2D-CED
30	f	602	CHL	CHA-CBD-CGD-O1D
30	f	602	CHL	CHA-CBD-CGD-O2D
30	f	606	CHL	C3C-C2C-CMC-OMC
30	f	608	CHL	C1A-C2A-CAA-CBA
30	f	608	CHL	CBD-CGD-O2D-CED
30	f	609	CHL	C14-C13-C15-C16
30	f	614	CHL	C1C-C2C-CMC-OMC
30	f	614	CHL	C3C-C2C-CMC-OMC
30	f	614	CHL	CHA-CBD-CGD-O1D
30	f	614	CHL	CHA-CBD-CGD-O2D
30	f	614	CHL	CAD-CBD-CGD-O1D
30	f	614	CHL	CAD-CBD-CGD-O2D
30	g	601	CHL	C2-C3-C5-C6
30	g	601	CHL	C4-C3-C5-C6
30	g	602	CHL	CHA-CBD-CGD-O1D
30	g	602	CHL	CHA-CBD-CGD-O2D
30	g	607	CHL	C3C-C2C-CMC-OMC
30	g	608	CHL	C3A-C2A-CAA-CBA
30	g	608	CHL	CBD-CGD-O2D-CED
30	h	601	CHL	C2A-CAA-CBA-CGA
30	h	602	CHL	CHA-CBD-CGD-O1D
30	h	602	CHL	CHA-CBD-CGD-O2D
30	h	602	CHL	C6-C7-C8-C9
30	h	608	CHL	C1A-C2A-CAA-CBA
30	h	614	CHL	CHA-CBD-CGD-O1D
30	h	614	CHL	CHA-CBD-CGD-O2D
30	i	602	CHL	C3C-C2C-CMC-OMC
30	i	602	CHL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	i	606	CHL	C3C-C2C-CMC-OMC
30	i	607	CHL	C1A-C2A-CAA-CBA
30	i	607	CHL	C1C-C2C-CMC-OMC
30	i	607	CHL	C3C-C2C-CMC-OMC
30	i	608	CHL	C3C-C2C-CMC-OMC
30	i	614	CHL	CHA-CBD-CGD-O1D
30	i	614	CHL	CHA-CBD-CGD-O2D
30	i	614	CHL	CAD-CBD-CGD-O1D
30	i	614	CHL	CAD-CBD-CGD-O2D
30	e	602	CHL	CHA-CBD-CGD-O2D
30	e	608	CHL	C3C-C2C-CMC-OMC
30	e	608	CHL	C11-C10-C8-C9
30	e	609	CHL	C3C-C2C-CMC-OMC
30	e	609	CHL	CBD-CGD-O2D-CED
30	e	614	CHL	C1C-C2C-CMC-OMC
30	e	614	CHL	C3C-C2C-CMC-OMC
30	4	302	CHL	C2B-C3B-CAB-CBB
30	4	302	CHL	C4B-C3B-CAB-CBB
30	4	302	CHL	C1C-C2C-CMC-OMC
30	4	302	CHL	C3C-C2C-CMC-OMC
30	4	306	CHL	C3C-C2C-CMC-OMC
30	4	307	CHL	C1C-C2C-CMC-OMC
30	4	307	CHL	C3C-C2C-CMC-OMC
30	4	307	CHL	CBD-CGD-O2D-CED
30	4	308	CHL	C1A-C2A-CAA-CBA
30	4	313	CHL	C1C-C2C-CMC-OMC
30	4	313	CHL	C3C-C2C-CMC-OMC
30	4	319	CHL	CAD-CBD-CGD-O1D
30	4	319	CHL	CAD-CBD-CGD-O2D
30	4	319	CHL	C2-C3-C5-C6
30	4	319	CHL	C4-C3-C5-C6
31	0	303	CLA	C4-C3-C5-C6
31	0	304	CLA	C1A-C2A-CAA-CBA
31	0	304	CLA	C3A-C2A-CAA-CBA
31	0	308	CLA	C1A-C2A-CAA-CBA
31	0	308	CLA	C3A-C2A-CAA-CBA
31	0	309	CLA	CHA-CBD-CGD-O1D
31	0	309	CLA	CHA-CBD-CGD-O2D
31	0	309	CLA	C2-C3-C5-C6
31	0	309	CLA	C4-C3-C5-C6
31	0	311	CLA	C2B-C3B-CAB-CBB
31	0	311	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	0	312	CLA	CHA-CBD-CGD-O1D
31	0	312	CLA	CHA-CBD-CGD-O2D
31	0	312	CLA	C6-C7-C8-C9
31	0	313	CLA	CBA-CGA-O2A-C1
31	0	313	CLA	CHA-CBD-CGD-O1D
31	0	313	CLA	CHA-CBD-CGD-O2D
31	0	313	CLA	CBD-CGD-O2D-CED
31	0	321	CLA	C1A-C2A-CAA-CBA
31	0	321	CLA	C3A-C2A-CAA-CBA
31	0	321	CLA	CAD-CBD-CGD-O1D
31	1	303	CLA	C2-C3-C5-C6
31	1	303	CLA	C4-C3-C5-C6
31	1	311	CLA	C1A-C2A-CAA-CBA
31	1	311	CLA	C3A-C2A-CAA-CBA
31	1	312	CLA	CHA-CBD-CGD-O1D
31	1	312	CLA	CHA-CBD-CGD-O2D
31	1	312	CLA	C4-C3-C5-C6
31	2	303	CLA	C2-C3-C5-C6
31	2	303	CLA	C4-C3-C5-C6
31	2	312	CLA	CHA-CBD-CGD-O1D
31	2	312	CLA	CHA-CBD-CGD-O2D
31	3	303	CLA	C1A-C2A-CAA-CBA
31	3	306	CLA	C1A-C2A-CAA-CBA
31	3	306	CLA	C3A-C2A-CAA-CBA
31	3	308	CLA	C1A-C2A-CAA-CBA
31	3	308	CLA	C3A-C2A-CAA-CBA
31	3	309	CLA	C1A-C2A-CAA-CBA
31	3	309	CLA	C3A-C2A-CAA-CBA
31	3	309	CLA	C2-C3-C5-C6
31	3	309	CLA	C4-C3-C5-C6
31	3	320	CLA	CHA-CBD-CGD-O1D
31	3	320	CLA	CHA-CBD-CGD-O2D
31	5	304	CLA	CHA-CBD-CGD-O1D
31	5	304	CLA	CHA-CBD-CGD-O2D
31	5	304	CLA	CAD-CBD-CGD-O1D
31	5	304	CLA	CBD-CGD-O2D-CED
31	5	308	CLA	C1A-C2A-CAA-CBA
31	5	308	CLA	C3A-C2A-CAA-CBA
31	5	311	CLA	CBD-CGD-O2D-CED
31	5	312	CLA	C1A-C2A-CAA-CBA
31	5	312	CLA	C3A-C2A-CAA-CBA
31	5	312	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	5	314	CLA	CHA-CBD-CGD-O1D
31	5	314	CLA	CHA-CBD-CGD-O2D
31	6	303	CLA	C2-C3-C5-C6
31	6	303	CLA	C4-C3-C5-C6
31	6	304	CLA	CBA-CGA-O2A-C1
31	6	312	CLA	C2B-C3B-CAB-CBB
31	6	312	CLA	C4B-C3B-CAB-CBB
31	6	317	CLA	CHA-CBD-CGD-O1D
31	6	317	CLA	CHA-CBD-CGD-O2D
31	6	317	CLA	CAD-CBD-CGD-O1D
31	6	317	CLA	CAD-CBD-CGD-O2D
31	6	318	CLA	C1A-C2A-CAA-CBA
31	6	318	CLA	C3A-C2A-CAA-CBA
31	7	303	CLA	CBD-CGD-O2D-CED
31	7	308	CLA	C1A-C2A-CAA-CBA
31	7	308	CLA	C3A-C2A-CAA-CBA
31	7	309	CLA	C1A-C2A-CAA-CBA
31	7	309	CLA	C3A-C2A-CAA-CBA
31	7	309	CLA	C2-C3-C5-C6
31	7	309	CLA	C4-C3-C5-C6
31	7	312	CLA	CHA-CBD-CGD-O1D
31	7	312	CLA	CHA-CBD-CGD-O2D
31	7	315	CLA	CBD-CGD-O2D-CED
31	7	318	CLA	C3A-C2A-CAA-CBA
31	8	303	CLA	CBA-CGA-O2A-C1
31	8	304	CLA	C1A-C2A-CAA-CBA
31	8	304	CLA	C3A-C2A-CAA-CBA
31	8	312	CLA	CHA-CBD-CGD-O1D
31	8	312	CLA	CHA-CBD-CGD-O2D
31	8	314	CLA	C3A-C2A-CAA-CBA
31	9	300	CLA	C1A-C2A-CAA-CBA
31	9	311	CLA	CBD-CGD-O2D-CED
31	A	804	CLA	C1A-C2A-CAA-CBA
31	A	804	CLA	C3A-C2A-CAA-CBA
31	A	805	CLA	CHA-CBD-CGD-O1D
31	A	805	CLA	CHA-CBD-CGD-O2D
31	A	805	CLA	CAD-CBD-CGD-O1D
31	A	806	CLA	C3A-C2A-CAA-CBA
31	A	806	CLA	C4B-C3B-CAB-CBB
31	A	808	CLA	C3A-C2A-CAA-CBA
31	A	811	CLA	C1A-C2A-CAA-CBA
31	A	817	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	817	CLA	CHA-CBD-CGD-O2D
31	A	818	CLA	C3A-C2A-CAA-CBA
31	A	819	CLA	C1A-C2A-CAA-CBA
31	A	819	CLA	C3A-C2A-CAA-CBA
31	A	820	CLA	C1A-C2A-CAA-CBA
31	A	820	CLA	C3A-C2A-CAA-CBA
31	A	820	CLA	C2B-C3B-CAB-CBB
31	A	820	CLA	C4B-C3B-CAB-CBB
31	A	822	CLA	C1A-C2A-CAA-CBA
31	A	822	CLA	C3A-C2A-CAA-CBA
31	A	824	CLA	CHA-CBD-CGD-O1D
31	A	824	CLA	CHA-CBD-CGD-O2D
31	A	828	CLA	CBD-CGD-O2D-CED
31	A	830	CLA	CHA-CBD-CGD-O1D
31	A	830	CLA	CHA-CBD-CGD-O2D
31	A	833	CLA	CHA-CBD-CGD-O1D
31	A	833	CLA	CHA-CBD-CGD-O2D
31	A	835	CLA	CHA-CBD-CGD-O1D
31	A	835	CLA	CHA-CBD-CGD-O2D
31	A	837	CLA	C2-C3-C5-C6
31	A	837	CLA	C4-C3-C5-C6
31	A	840	CLA	O2A-C1-C2-C3
31	A	840	CLA	C4-C3-C5-C6
31	A	841	CLA	C4-C3-C5-C6
31	A	843	CLA	C3A-C2A-CAA-CBA
31	A	843	CLA	CBD-CGD-O2D-CED
31	A	852	CLA	C12-C13-C15-C16
31	A	853	CLA	CBD-CGD-O2D-CED
31	A	853	CLA	O1D-CGD-O2D-CED
31	B	801	CLA	CBD-CGD-O2D-CED
31	B	803	CLA	CHA-CBD-CGD-O1D
31	B	803	CLA	CHA-CBD-CGD-O2D
31	B	803	CLA	CAD-CBD-CGD-O1D
31	B	805	CLA	CHA-CBD-CGD-O1D
31	B	805	CLA	CHA-CBD-CGD-O2D
31	B	808	CLA	C1A-C2A-CAA-CBA
31	B	808	CLA	C3A-C2A-CAA-CBA
31	B	810	CLA	CHA-CBD-CGD-O1D
31	B	814	CLA	C1A-C2A-CAA-CBA
31	B	817	CLA	C1A-C2A-CAA-CBA
31	B	818	CLA	C1A-C2A-CAA-CBA
31	B	818	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	818	CLA	C2B-C3B-CAB-CBB
31	B	818	CLA	C4B-C3B-CAB-CBB
31	B	819	CLA	C1A-C2A-CAA-CBA
31	B	819	CLA	C3A-C2A-CAA-CBA
31	B	820	CLA	C1A-C2A-CAA-CBA
31	B	820	CLA	C2B-C3B-CAB-CBB
31	B	820	CLA	C4B-C3B-CAB-CBB
31	B	823	CLA	C2-C3-C5-C6
31	B	823	CLA	C4-C3-C5-C6
31	B	824	CLA	CHA-CBD-CGD-O1D
31	B	824	CLA	CHA-CBD-CGD-O2D
31	B	827	CLA	C1A-C2A-CAA-CBA
31	B	828	CLA	C3A-C2A-CAA-CBA
31	B	829	CLA	C1A-C2A-CAA-CBA
31	B	829	CLA	C3A-C2A-CAA-CBA
31	B	830	CLA	C4-C3-C5-C6
31	B	831	CLA	C1A-C2A-CAA-CBA
31	B	831	CLA	C3A-C2A-CAA-CBA
31	B	833	CLA	C1A-C2A-CAA-CBA
31	B	833	CLA	C3A-C2A-CAA-CBA
31	B	833	CLA	C4B-C3B-CAB-CBB
31	B	834	CLA	C1A-C2A-CAA-CBA
31	B	834	CLA	C3A-C2A-CAA-CBA
31	B	836	CLA	C1A-C2A-CAA-CBA
31	F	301	CLA	CHA-CBD-CGD-O1D
31	F	301	CLA	CHA-CBD-CGD-O2D
31	G	101	CLA	C1A-C2A-CAA-CBA
31	G	101	CLA	C3A-C2A-CAA-CBA
31	G	103	CLA	CBA-CGA-O2A-C1
31	L	202	CLA	C1A-C2A-CAA-CBA
31	L	203	CLA	C1A-C2A-CAA-CBA
31	L	203	CLA	CHA-CBD-CGD-O1D
31	L	203	CLA	CHA-CBD-CGD-O2D
31	L	203	CLA	CAD-CBD-CGD-O1D
31	L	204	CLA	C1A-C2A-CAA-CBA
31	L	204	CLA	C3A-C2A-CAA-CBA
31	L	204	CLA	CBA-CGA-O2A-C1
31	K	104	CLA	CBA-CGA-O2A-C1
31	K	104	CLA	O1A-CGA-O2A-C1
31	K	105	CLA	C1A-C2A-CAA-CBA
31	K	105	CLA	C3A-C2A-CAA-CBA
31	M	101	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	O	201	CLA	CAD-CBD-CGD-O1D
31	O	201	CLA	CAD-CBD-CGD-O2D
31	O	201	CLA	CBD-CGD-O2D-CED
31	O	206	CLA	CHA-CBD-CGD-O1D
31	O	206	CLA	CHA-CBD-CGD-O2D
31	O	206	CLA	CAD-CBD-CGD-O1D
31	O	206	CLA	CAD-CBD-CGD-O2D
31	O	206	CLA	CBD-CGD-O2D-CED
31	O	206	CLA	C2-C3-C5-C6
31	O	206	CLA	C4-C3-C5-C6
31	a	603	CLA	CHA-CBD-CGD-O1D
31	a	603	CLA	CHA-CBD-CGD-O2D
31	a	604	CLA	C1A-C2A-CAA-CBA
31	a	604	CLA	C3A-C2A-CAA-CBA
31	a	610	CLA	CBD-CGD-O2D-CED
31	a	613	CLA	CAD-CBD-CGD-O1D
31	a	613	CLA	CAD-CBD-CGD-O2D
31	c	603	CLA	CBD-CGD-O2D-CED
31	c	610	CLA	CBD-CGD-O2D-CED
31	c	611	CLA	C2B-C3B-CAB-CBB
31	c	611	CLA	C4B-C3B-CAB-CBB
31	c	613	CLA	CHA-CBD-CGD-O1D
31	c	613	CLA	CHA-CBD-CGD-O2D
31	b	604	CLA	C1A-C2A-CAA-CBA
31	b	613	CLA	CHA-CBD-CGD-O1D
31	b	613	CLA	CHA-CBD-CGD-O2D
31	d	603	CLA	CBD-CGD-O2D-CED
31	d	604	CLA	CHA-CBD-CGD-O1D
31	d	611	CLA	CHA-CBD-CGD-O1D
31	d	611	CLA	CHA-CBD-CGD-O2D
31	d	612	CLA	CBD-CGD-O2D-CED
31	f	604	CLA	CHA-CBD-CGD-O1D
31	f	604	CLA	CHA-CBD-CGD-O2D
31	f	610	CLA	CBD-CGD-O2D-CED
31	g	603	CLA	CBD-CGD-O2D-CED
31	g	604	CLA	C1A-C2A-CAA-CBA
31	g	604	CLA	C3A-C2A-CAA-CBA
31	g	604	CLA	CHA-CBD-CGD-O1D
31	g	604	CLA	CHA-CBD-CGD-O2D
31	g	604	CLA	CAD-CBD-CGD-O1D
31	h	604	CLA	CBD-CGD-O2D-CED
31	h	610	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	h	610	CLA	CHA-CBD-CGD-O2D
31	h	610	CLA	CBD-CGD-O2D-CED
31	h	611	CLA	CBD-CGD-O2D-CED
31	H	201	CLA	C1A-C2A-CAA-CBA
31	H	201	CLA	CHA-CBD-CGD-O1D
31	H	201	CLA	CHA-CBD-CGD-O2D
31	H	201	CLA	CAD-CBD-CGD-O1D
31	H	201	CLA	CAD-CBD-CGD-O2D
31	H	202	CLA	CHA-CBD-CGD-O1D
31	H	202	CLA	CHA-CBD-CGD-O2D
31	H	205	CLA	C2-C3-C5-C6
31	H	205	CLA	C4-C3-C5-C6
31	i	603	CLA	CBD-CGD-O2D-CED
31	i	604	CLA	CHA-CBD-CGD-O1D
31	i	604	CLA	CHA-CBD-CGD-O2D
31	i	613	CLA	CBD-CGD-O2D-CED
31	i	613	CLA	O1D-CGD-O2D-CED
31	e	604	CLA	C1A-C2A-CAA-CBA
31	e	613	CLA	CHA-CBD-CGD-O1D
31	e	613	CLA	CHA-CBD-CGD-O2D
31	4	312	CLA	CHA-CBD-CGD-O1D
31	4	312	CLA	CHA-CBD-CGD-O2D
32	0	401	8CT	C02-C03-C10-C11
32	1	402	8CT	C22-C21-C23-C24
32	1	402	8CT	C28-C29-C30-C31
32	1	402	8CT	C28-C29-C30-C35
32	2	402	8CT	C20-C21-C23-C24
32	2	402	8CT	C22-C21-C23-C24
32	3	402	8CT	C02-C03-C10-C11
32	3	402	8CT	C28-C29-C30-C31
32	3	402	8CT	C28-C29-C30-C35
32	3	403	8CT	C04-C03-C10-C11
32	3	403	8CT	C10-C11-C12-C13
32	3	403	8CT	C28-C29-C30-C31
32	6	402	8CT	C10-C11-C12-C13
32	6	402	8CT	C10-C11-C12-C40
32	6	402	8CT	C16-C17-C18-C19
32	7	402	8CT	C10-C11-C12-C40
32	7	402	8CT	C14-C15-C16-C39
32	7	402	8CT	C20-C21-C23-C24
32	7	402	8CT	C22-C21-C23-C24
32	7	402	8CT	C25-C26-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	7	402	8CT	C27-C26-C28-C29
32	7	404	8CT	C10-C11-C12-C13
32	7	404	8CT	C10-C11-C12-C40
32	7	405	8CT	C02-C03-C10-C11
32	7	405	8CT	C04-C03-C10-C11
32	7	405	8CT	C14-C15-C16-C39
32	8	402	8CT	C10-C11-C12-C13
32	8	402	8CT	C10-C11-C12-C40
32	8	402	8CT	C14-C15-C16-C17
32	8	402	8CT	C14-C15-C16-C39
32	8	402	8CT	C18-C19-C20-C21
32	8	402	8CT	C28-C29-C30-C35
32	8	406	8CT	C02-C03-C10-C11
32	8	406	8CT	C12-C13-C14-C15
32	9	401	8CT	C20-C21-C23-C24
32	9	401	8CT	C22-C21-C23-C24
32	A	847	8CT	C14-C15-C16-C17
32	A	847	8CT	C27-C26-C28-C29
32	A	848	8CT	C10-C11-C12-C13
32	A	848	8CT	C10-C11-C12-C40
32	A	848	8CT	C14-C15-C16-C17
32	A	848	8CT	C14-C15-C16-C39
32	A	849	8CT	C16-C17-C18-C19
32	A	850	8CT	C04-C03-C10-C11
32	A	850	8CT	C14-C15-C16-C17
32	A	850	8CT	C14-C15-C16-C39
32	A	850	8CT	C18-C19-C20-C21
32	A	854	8CT	C20-C21-C23-C24
32	A	854	8CT	C22-C21-C23-C24
32	B	804	8CT	C10-C11-C12-C13
32	B	804	8CT	C10-C11-C12-C40
32	B	804	8CT	C20-C21-C23-C24
32	B	804	8CT	C22-C21-C23-C24
32	B	804	8CT	C28-C29-C30-C35
32	B	843	8CT	C10-C11-C12-C13
32	B	843	8CT	C10-C11-C12-C40
32	B	843	8CT	C20-C21-C23-C24
32	B	843	8CT	C22-C21-C23-C24
32	B	843	8CT	C28-C29-C30-C35
32	B	844	8CT	C10-C11-C12-C13
32	B	844	8CT	C10-C11-C12-C40
32	B	845	8CT	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	B	845	8CT	C10-C11-C12-C40
32	B	845	8CT	C18-C19-C20-C21
32	B	846	8CT	C14-C15-C16-C17
32	B	846	8CT	C14-C15-C16-C39
32	B	846	8CT	C28-C29-C30-C31
32	B	846	8CT	C28-C29-C30-C35
32	B	847	8CT	C10-C11-C12-C13
32	B	848	8CT	C14-C15-C16-C17
32	B	848	8CT	C14-C15-C16-C39
32	B	851	8CT	C14-C15-C16-C17
32	B	851	8CT	C14-C15-C16-C39
32	B	851	8CT	C16-C17-C18-C19
32	B	851	8CT	C28-C29-C30-C31
32	B	851	8CT	C28-C29-C30-C35
32	F	302	8CT	C02-C03-C10-C11
32	F	302	8CT	C14-C15-C16-C17
32	F	302	8CT	C14-C15-C16-C39
32	F	302	8CT	C28-C29-C30-C31
32	F	302	8CT	C28-C29-C30-C35
32	G	104	8CT	C10-C11-C12-C13
32	G	104	8CT	C10-C11-C12-C40
32	G	104	8CT	C12-C13-C14-C15
32	G	104	8CT	C14-C15-C16-C17
32	G	104	8CT	C14-C15-C16-C39
32	G	104	8CT	C20-C21-C23-C24
32	G	104	8CT	C22-C21-C23-C24
32	G	104	8CT	C25-C26-C28-C29
32	G	104	8CT	C27-C26-C28-C29
32	G	104	8CT	C28-C29-C30-C31
32	I	101	8CT	C25-C26-C28-C29
32	I	101	8CT	C27-C26-C28-C29
32	J	101	8CT	C18-C19-C20-C21
32	J	101	8CT	C20-C21-C23-C24
32	J	101	8CT	C22-C21-C23-C24
32	J	101	8CT	C25-C26-C28-C29
32	J	101	8CT	C27-C26-C28-C29
32	J	101	8CT	C28-C29-C30-C31
32	J	101	8CT	C28-C29-C30-C35
32	J	104	8CT	C18-C19-C20-C21
32	J	104	8CT	C28-C29-C30-C31
32	J	104	8CT	C28-C29-C30-C35
32	L	205	8CT	C25-C26-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	L	205	8CT	C27-C26-C28-C29
32	L	205	8CT	C28-C29-C30-C31
32	L	209	8CT	C02-C03-C10-C11
32	L	209	8CT	C10-C11-C12-C13
32	K	107	8CT	C10-C11-C12-C13
32	K	107	8CT	C10-C11-C12-C40
32	K	107	8CT	C22-C21-C23-C24
32	M	102	8CT	C25-C26-C28-C29
32	M	102	8CT	C27-C26-C28-C29
32	O	205	8CT	C10-C11-C12-C13
32	O	205	8CT	C10-C11-C12-C40
32	O	205	8CT	C14-C15-C16-C17
32	O	205	8CT	C14-C15-C16-C39
32	4	402	8CT	C20-C21-C23-C24
32	4	402	8CT	C22-C21-C23-C24
33	0	502	0UR	C2-C3-C43-O44
33	0	502	0UR	C4-C3-C43-O44
33	0	502	0UR	C46-C45-O44-C43
33	0	502	0UR	O57-C45-O44-C43
33	1	502	0UR	C17-C18-C19-C28
33	1	502	0UR	C17-C18-C19-C32
33	1	502	0UR	C46-C45-O44-C43
33	1	502	0UR	O57-C45-O44-C43
33	2	501	0UR	C2-C3-C43-O44
33	2	501	0UR	C4-C3-C43-O44
33	2	501	0UR	O42-C2-C3-C4
33	2	501	0UR	C46-C45-O44-C43
33	2	501	0UR	O57-C45-O44-C43
33	2	502	0UR	C2-C3-C43-O44
33	2	502	0UR	C4-C3-C43-O44
33	2	502	0UR	C41-C2-C3-C4
33	3	501	0UR	C2-C3-C43-O44
33	3	501	0UR	C4-C3-C43-O44
33	3	501	0UR	C46-C45-O44-C43
33	3	501	0UR	O57-C45-O44-C43
33	5	501	0UR	O42-C2-C3-C43
33	5	501	0UR	C5-C6-C7-C20
33	5	501	0UR	C5-C6-C7-C8
33	5	502	0UR	C2-C3-C43-O44
33	5	502	0UR	C4-C3-C43-O44
33	5	502	0UR	C17-C18-C19-C28
33	5	502	0UR	C17-C18-C19-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	6	501	0UR	C17-C18-C19-C28
33	6	501	0UR	C17-C18-C19-C32
33	6	501	0UR	C46-C45-O44-C43
33	6	501	0UR	O57-C45-O44-C43
33	6	502	0UR	C4-C3-C43-O44
33	6	502	0UR	C17-C18-C19-C28
33	7	501	0UR	C2-C3-C43-O44
33	7	501	0UR	C4-C3-C43-O44
33	7	501	0UR	C46-C45-O44-C43
33	7	501	0UR	O57-C45-O44-C43
33	8	502	0UR	C46-C45-O44-C43
33	9	502	0UR	C2-C3-C43-O44
33	9	502	0UR	C4-C3-C43-O44
33	9	502	0UR	O42-C2-C3-C43
33	9	502	0UR	C46-C45-O44-C43
33	O	204	0UR	C46-C45-O44-C43
33	a	520	0UR	O42-C2-C3-C43
33	a	520	0UR	C5-C6-C7-C20
33	a	520	0UR	C5-C6-C7-C8
33	c	520	0UR	C17-C18-C19-C28
33	c	520	0UR	C17-C18-C19-C32
33	b	520	0UR	O42-C2-C3-C43
33	d	520	0UR	O42-C2-C3-C43
33	f	520	0UR	O42-C2-C3-C4
33	f	520	0UR	C17-C18-C19-C28
33	f	520	0UR	C17-C18-C19-C32
33	g	520	0UR	O42-C2-C3-C43
33	h	520	0UR	C46-C45-O44-C43
33	h	520	0UR	O57-C45-O44-C43
33	i	520	0UR	C46-C47-C48-C49
33	e	520	0UR	C4-C3-C43-O44
33	e	520	0UR	O42-C2-C3-C43
33	e	520	0UR	C46-C45-O44-C43
33	4	501	0UR	C2-C3-C43-O44
33	4	501	0UR	C4-C3-C43-O44
33	4	501	0UR	C46-C45-O44-C43
33	4	501	0UR	O57-C45-O44-C43
33	4	502	0UR	C2-C3-C43-O44
33	4	502	0UR	C4-C3-C43-O44
33	4	502	0UR	C11-C12-C13-C14
33	4	502	0UR	C21-C12-C13-C14
34	0	601	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	0	601	LHG	C4-O6-P-O4
34	1	601	LHG	O2-C2-C3-O3
34	2	601	LHG	O1-C1-C2-C3
34	2	601	LHG	O2-C2-C3-O3
34	2	601	LHG	C3-O3-P-O6
34	3	601	LHG	O1-C1-C2-C3
34	3	601	LHG	C3-O3-P-O4
34	3	601	LHG	C3-O3-P-O5
34	3	601	LHG	C3-O3-P-O6
34	3	601	LHG	O7-C5-C6-O8
34	3	603	LHG	O1-C1-C2-C3
34	3	603	LHG	O2-C2-C3-O3
34	3	603	LHG	C4-O6-P-O3
34	3	603	LHG	C4-O6-P-O4
34	3	603	LHG	C4-O6-P-O5
34	6	603	LHG	C4-O6-P-O5
34	6	603	LHG	C5-C4-O6-P
34	7	601	LHG	C1-C2-C3-O3
34	7	602	LHG	C3-O3-P-O5
34	7	602	LHG	C3-O3-P-O6
34	7	602	LHG	C4-O6-P-O5
34	7	602	LHG	C8-C7-O7-C5
34	7	603	LHG	C4-O6-P-O4
34	7	603	LHG	C4-O6-P-O5
34	8	601	LHG	C3-O3-P-O5
34	8	601	LHG	C4-O6-P-O5
34	9	601	LHG	C3-O3-P-O5
34	9	601	LHG	C4-O6-P-O5
34	9	601	LHG	C18-C19-C20-C21
34	A	844	LHG	C4-O6-P-O3
34	A	845	LHG	O2-C2-C3-O3
34	A	845	LHG	C3-O3-P-O4
34	A	845	LHG	C4-O6-P-O3
34	A	845	LHG	C4-O6-P-O4
34	A	845	LHG	C4-O6-P-O5
34	A	845	LHG	O6-C4-C5-O7
34	A	845	LHG	C8-C7-O7-C5
34	A	855	LHG	C3-O3-P-O5
34	A	855	LHG	O9-C7-O7-C5
34	A	855	LHG	C24-C23-O8-C6
34	B	852	LHG	C1-C2-C3-O3
34	B	852	LHG	C3-O3-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	B	852	LHG	C3-O3-P-O5
34	B	852	LHG	C4-O6-P-O4
34	B	852	LHG	C8-C7-O7-C5
34	B	854	LHG	C4-O6-P-O5
34	G	105	LHG	C1-C2-C3-O3
34	G	105	LHG	O2-C2-C3-O3
34	G	105	LHG	C3-O3-P-O5
34	G	105	LHG	C4-O6-P-O3
34	G	105	LHG	C4-O6-P-O4
34	K	106	LHG	C5-C4-O6-P
34	M	104	LHG	O1-C1-C2-C3
34	M	104	LHG	O9-C7-O7-C5
34	M	104	LHG	C8-C7-O7-C5
34	a	630	LHG	O2-C2-C3-O3
34	a	630	LHG	C4-O6-P-O4
34	a	630	LHG	C4-O6-P-O5
34	c	630	LHG	O1-C1-C2-C3
34	c	630	LHG	C4-O6-P-O4
34	c	630	LHG	C4-O6-P-O5
34	b	630	LHG	C1-C2-C3-O3
34	b	630	LHG	O2-C2-C3-O3
34	b	630	LHG	C5-C4-O6-P
34	b	630	LHG	O10-C23-O8-C6
34	b	630	LHG	C24-C23-O8-C6
34	d	630	LHG	C3-O3-P-O6
34	d	630	LHG	O10-C23-O8-C6
34	d	630	LHG	C24-C23-O8-C6
34	f	630	LHG	C3-O3-P-O6
34	g	630	LHG	C1-C2-C3-O3
34	g	630	LHG	O2-C2-C3-O3
34	g	630	LHG	C3-O3-P-O6
34	g	630	LHG	C4-O6-P-O5
34	h	630	LHG	O1-C1-C2-C3
34	h	630	LHG	C3-O3-P-O4
34	h	630	LHG	C3-O3-P-O5
34	H	203	LHG	O1-C1-C2-C3
34	i	630	LHG	O1-C1-C2-C3
34	i	630	LHG	O2-C2-C3-O3
34	e	630	LHG	C1-C2-C3-O3
34	e	630	LHG	O2-C2-C3-O3
34	4	601	LHG	C3-O3-P-O4
35	0	603	SQD	O5-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	2	602	LMG	O6-C1-O1-C7
36	3	602	LMG	C2-C1-O1-C7
36	3	602	LMG	O6-C1-O1-C7
36	3	602	LMG	O7-C8-C9-O8
36	3	602	LMG	O9-C10-O7-C8
36	A	856	LMG	C11-C10-O7-C8
36	B	853	LMG	C2-C1-O1-C7
36	B	853	LMG	O6-C1-O1-C7
36	J	102	LMG	C2-C1-O1-C7
36	J	102	LMG	O6-C1-O1-C7
36	L	211	LMG	O7-C8-C9-O8
37	c	522	0IE	O1-C2-C3-C20
37	c	522	0IE	O29-C20-C3-C4
37	c	522	0IE	O29-C20-C3-C2
37	c	522	0IE	C10-C11-C12-C13
37	c	522	0IE	C10-C11-C12-C22
37	c	522	0IE	C11-C12-C13-C14
37	c	522	0IE	C22-C12-C13-C14
37	c	522	0IE	C17-C18-C19-C24
37	c	522	0IE	C17-C18-C19-C28
37	b	522	0IE	O29-C20-C3-C4
37	b	522	0IE	O29-C20-C3-C2
39	A	857	CL0	C4B-C3B-CAB-CBB
41	B	849	DGD	O1B-C1B-O2G-C2G
41	B	849	DGD	C2D-C1D-O3G-C3G
41	B	849	DGD	O6D-C1D-O3G-C3G
42	a	523	NEX	O24-C26-C27-C28
42	c	523	NEX	O24-C26-C27-C28
42	b	523	NEX	O24-C26-C27-C28
42	d	523	NEX	O24-C26-C27-C28
42	f	523	NEX	O24-C26-C27-C28
42	g	523	NEX	O24-C26-C27-C28
42	h	523	NEX	O24-C26-C27-C28
42	i	523	NEX	O24-C26-C27-C28
42	e	523	NEX	O24-C26-C27-C28
31	0	313	CLA	O1D-CGD-O2D-CED
31	0	321	CLA	O1D-CGD-O2D-CED
31	7	316	CLA	O1D-CGD-O2D-CED
31	B	806	CLA	O1D-CGD-O2D-CED
31	a	611	CLA	O1D-CGD-O2D-CED
31	d	610	CLA	O1D-CGD-O2D-CED
31	h	610	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	e	610	CLA	O1D-CGD-O2D-CED
30	e	608	CHL	O1D-CGD-O2D-CED
31	7	303	CLA	O1D-CGD-O2D-CED
31	9	309	CLA	O1D-CGD-O2D-CED
31	A	843	CLA	O1D-CGD-O2D-CED
31	B	805	CLA	O1D-CGD-O2D-CED
31	d	603	CLA	O1D-CGD-O2D-CED
31	h	604	CLA	O1D-CGD-O2D-CED
31	h	611	CLA	O1D-CGD-O2D-CED
31	4	314	CLA	O1D-CGD-O2D-CED
30	1	307	CHL	CBD-CGD-O2D-CED
30	5	307	CHL	CBD-CGD-O2D-CED
30	6	306	CHL	CBD-CGD-O2D-CED
30	6	307	CHL	CBD-CGD-O2D-CED
30	8	307	CHL	CBD-CGD-O2D-CED
30	c	608	CHL	CBD-CGD-O2D-CED
30	f	609	CHL	CBD-CGD-O2D-CED
30	g	605	CHL	CBD-CGD-O2D-CED
30	g	607	CHL	CBD-CGD-O2D-CED
30	g	609	CHL	CBD-CGD-O2D-CED
30	h	608	CHL	CBD-CGD-O2D-CED
30	h	614	CHL	CBD-CGD-O2D-CED
30	i	608	CHL	CBD-CGD-O2D-CED
30	e	608	CHL	CBD-CGD-O2D-CED
31	0	304	CLA	CBD-CGD-O2D-CED
31	0	321	CLA	CBD-CGD-O2D-CED
31	1	308	CLA	CBD-CGD-O2D-CED
31	1	311	CLA	CBD-CGD-O2D-CED
31	1	314	CLA	CBD-CGD-O2D-CED
31	2	311	CLA	CBD-CGD-O2D-CED
31	3	303	CLA	CBD-CGD-O2D-CED
31	5	308	CLA	CBD-CGD-O2D-CED
31	6	310	CLA	CBD-CGD-O2D-CED
31	7	316	CLA	CBD-CGD-O2D-CED
31	8	303	CLA	CBD-CGD-O2D-CED
31	8	304	CLA	CBD-CGD-O2D-CED
31	8	311	CLA	CBD-CGD-O2D-CED
31	8	312	CLA	CBD-CGD-O2D-CED
31	9	302	CLA	CBD-CGD-O2D-CED
31	9	309	CLA	CBD-CGD-O2D-CED
31	B	805	CLA	CBD-CGD-O2D-CED
31	B	806	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	807	CLA	CBD-CGD-O2D-CED
31	G	102	CLA	CBD-CGD-O2D-CED
31	K	102	CLA	CBD-CGD-O2D-CED
31	a	611	CLA	CBD-CGD-O2D-CED
31	a	613	CLA	CBD-CGD-O2D-CED
31	b	603	CLA	CBD-CGD-O2D-CED
31	d	610	CLA	CBD-CGD-O2D-CED
31	d	613	CLA	CBD-CGD-O2D-CED
31	g	610	CLA	CBD-CGD-O2D-CED
31	g	613	CLA	CBD-CGD-O2D-CED
31	h	612	CLA	CBD-CGD-O2D-CED
31	h	613	CLA	CBD-CGD-O2D-CED
31	i	610	CLA	CBD-CGD-O2D-CED
31	i	611	CLA	CBD-CGD-O2D-CED
31	e	610	CLA	CBD-CGD-O2D-CED
31	e	613	CLA	CBD-CGD-O2D-CED
31	4	314	CLA	CBD-CGD-O2D-CED
31	3	309	CLA	O1A-CGA-O2A-C1
31	A	805	CLA	O1A-CGA-O2A-C1
31	A	852	CLA	O1A-CGA-O2A-C1
31	B	813	CLA	O1A-CGA-O2A-C1
31	B	823	CLA	O1A-CGA-O2A-C1
34	5	601	LHG	O10-C23-O8-C6
34	A	855	LHG	O10-C23-O8-C6
34	K	106	LHG	O10-C23-O8-C6
34	a	630	LHG	O10-C23-O8-C6
36	J	102	LMG	O10-C28-O8-C9
31	0	313	CLA	O1A-CGA-O2A-C1
31	G	103	CLA	O1A-CGA-O2A-C1
31	L	204	CLA	O1A-CGA-O2A-C1
30	c	608	CHL	O1D-CGD-O2D-CED
31	3	303	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	O1D-CGD-O2D-CED
31	d	613	CLA	O1D-CGD-O2D-CED
31	h	612	CLA	O1D-CGD-O2D-CED
31	h	613	CLA	O1D-CGD-O2D-CED
31	i	610	CLA	O1D-CGD-O2D-CED
30	2	307	CHL	O1D-CGD-O2D-CED
30	b	608	CHL	O1D-CGD-O2D-CED
30	d	608	CHL	O1D-CGD-O2D-CED
30	h	608	CHL	O1D-CGD-O2D-CED
30	i	608	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	e	609	CHL	O1D-CGD-O2D-CED
31	5	312	CLA	O1D-CGD-O2D-CED
31	A	828	CLA	O1D-CGD-O2D-CED
31	O	206	CLA	O1D-CGD-O2D-CED
31	a	610	CLA	O1D-CGD-O2D-CED
31	a	613	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	O1D-CGD-O2D-CED
31	c	610	CLA	O1D-CGD-O2D-CED
31	d	612	CLA	O1D-CGD-O2D-CED
31	f	610	CLA	O1D-CGD-O2D-CED
31	g	603	CLA	O1D-CGD-O2D-CED
31	g	613	CLA	O1D-CGD-O2D-CED
31	i	603	CLA	O1D-CGD-O2D-CED
31	B	813	CLA	CBA-CGA-O2A-C1
34	5	601	LHG	C24-C23-O8-C6
34	K	106	LHG	C24-C23-O8-C6
34	a	630	LHG	C24-C23-O8-C6
36	J	102	LMG	C29-C28-O8-C9
30	0	301	CHL	CBD-CGD-O2D-CED
30	1	306	CHL	CBD-CGD-O2D-CED
30	3	302	CHL	CBD-CGD-O2D-CED
30	3	307	CHL	CBD-CGD-O2D-CED
30	5	302	CHL	CBD-CGD-O2D-CED
30	5	306	CHL	CBD-CGD-O2D-CED
30	7	305	CHL	CBD-CGD-O2D-CED
30	a	605	CHL	CBD-CGD-O2D-CED
30	c	601	CHL	CBD-CGD-O2D-CED
30	c	609	CHL	CBD-CGD-O2D-CED
30	b	601	CHL	CBD-CGD-O2D-CED
30	b	607	CHL	CBD-CGD-O2D-CED
30	b	609	CHL	CBD-CGD-O2D-CED
30	f	614	CHL	CBD-CGD-O2D-CED
30	h	607	CHL	CBD-CGD-O2D-CED
30	i	614	CHL	CBD-CGD-O2D-CED
30	e	605	CHL	CBD-CGD-O2D-CED
30	e	614	CHL	CBD-CGD-O2D-CED
31	0	312	CLA	CBD-CGD-O2D-CED
31	2	310	CLA	CBD-CGD-O2D-CED
31	2	312	CLA	CBD-CGD-O2D-CED
31	5	309	CLA	CBD-CGD-O2D-CED
31	5	314	CLA	CBD-CGD-O2D-CED
31	6	317	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	7	312	CLA	CBD-CGD-O2D-CED
31	A	832	CLA	CBD-CGD-O2D-CED
31	A	833	CLA	CBD-CGD-O2D-CED
31	A	839	CLA	CBD-CGD-O2D-CED
31	B	815	CLA	CBD-CGD-O2D-CED
31	B	816	CLA	CBD-CGD-O2D-CED
31	B	820	CLA	CBD-CGD-O2D-CED
31	F	301	CLA	CBD-CGD-O2D-CED
31	G	101	CLA	CBD-CGD-O2D-CED
31	c	613	CLA	CBD-CGD-O2D-CED
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	610	CLA	CBD-CGD-O2D-CED
31	g	612	CLA	CBD-CGD-O2D-CED
31	h	603	CLA	CBD-CGD-O2D-CED
31	H	205	CLA	CBD-CGD-O2D-CED
31	4	310	CLA	CBD-CGD-O2D-CED
31	4	312	CLA	CBD-CGD-O2D-CED
31	2	310	CLA	O1A-CGA-O2A-C1
31	7	309	CLA	O1A-CGA-O2A-C1
31	7	315	CLA	O1A-CGA-O2A-C1
31	B	850	CLA	O1A-CGA-O2A-C1
31	L	203	CLA	O1A-CGA-O2A-C1
31	H	202	CLA	O1A-CGA-O2A-C1
34	1	601	LHG	O10-C23-O8-C6
34	M	104	LHG	O10-C23-O8-C6
34	g	630	LHG	O10-C23-O8-C6
34	e	630	LHG	O10-C23-O8-C6
36	9	602	LMG	O10-C28-O8-C9
36	B	853	LMG	O10-C28-O8-C9
31	8	303	CLA	O1A-CGA-O2A-C1
30	7	307	CHL	O1D-CGD-O2D-CED
30	a	608	CHL	O1D-CGD-O2D-CED
30	g	608	CHL	O1D-CGD-O2D-CED
31	5	311	CLA	O1D-CGD-O2D-CED
31	9	311	CLA	O1D-CGD-O2D-CED
31	O	201	CLA	O1D-CGD-O2D-CED
30	f	608	CHL	O1D-CGD-O2D-CED
30	4	307	CHL	O1D-CGD-O2D-CED
31	5	304	CLA	O1D-CGD-O2D-CED
31	8	311	CLA	O1D-CGD-O2D-CED
30	9	305	CHL	CBD-CGD-O2D-CED
30	c	605	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	609	CHL	CBD-CGD-O2D-CED
31	0	310	CLA	CBD-CGD-O2D-CED
31	6	312	CLA	CBD-CGD-O2D-CED
31	7	311	CLA	CBD-CGD-O2D-CED
31	7	318	CLA	CBD-CGD-O2D-CED
31	B	803	CLA	CBD-CGD-O2D-CED
31	B	824	CLA	CBD-CGD-O2D-CED
31	B	836	CLA	CBD-CGD-O2D-CED
31	f	604	CLA	CBD-CGD-O2D-CED
31	f	612	CLA	CBD-CGD-O2D-CED
31	5	308	CLA	O1D-CGD-O2D-CED
31	8	303	CLA	O1D-CGD-O2D-CED
31	8	312	CLA	O1D-CGD-O2D-CED
31	B	801	CLA	O1D-CGD-O2D-CED
31	G	102	CLA	O1D-CGD-O2D-CED
34	7	602	LHG	O9-C7-O7-C5
34	A	845	LHG	O9-C7-O7-C5
34	B	852	LHG	O9-C7-O7-C5
36	9	602	LMG	O9-C10-O7-C8
36	A	856	LMG	O9-C10-O7-C8
36	B	853	LMG	O9-C10-O7-C8
36	J	102	LMG	O9-C10-O7-C8
36	L	211	LMG	O9-C10-O7-C8
31	h	604	CLA	CBA-CGA-O2A-C1
31	5	314	CLA	O1A-CGA-O2A-C1
31	b	603	CLA	O1D-CGD-O2D-CED
33	8	502	0UR	O57-C45-O44-C43
33	9	502	0UR	O57-C45-O44-C43
33	O	204	0UR	O57-C45-O44-C43
33	e	520	0UR	O57-C45-O44-C43
30	2	302	CHL	C3-C5-C6-C7
31	0	303	CLA	C3-C5-C6-C7
31	2	303	CLA	C3-C5-C6-C7
31	3	303	CLA	C3-C5-C6-C7
31	5	309	CLA	C3-C5-C6-C7
31	7	308	CLA	C3-C5-C6-C7
31	9	300	CLA	C3-C5-C6-C7
31	A	806	CLA	C3-C5-C6-C7
31	A	808	CLA	C3-C5-C6-C7
31	A	821	CLA	C3-C5-C6-C7
31	A	832	CLA	C3-C5-C6-C7
31	B	811	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	822	CLA	C3-C5-C6-C7
31	B	836	CLA	C3-C5-C6-C7
31	L	201	CLA	C3-C5-C6-C7
31	d	610	CLA	C3-C5-C6-C7
31	e	611	CLA	C3-C5-C6-C7
38	B	842	PQN	C13-C15-C16-C17
31	3	309	CLA	CBA-CGA-O2A-C1
31	3	310	CLA	CBA-CGA-O2A-C1
31	5	303	CLA	CBA-CGA-O2A-C1
31	A	805	CLA	CBA-CGA-O2A-C1
31	A	808	CLA	CBA-CGA-O2A-C1
31	A	852	CLA	CBA-CGA-O2A-C1
31	B	819	CLA	CBA-CGA-O2A-C1
31	B	824	CLA	CBA-CGA-O2A-C1
34	1	601	LHG	C24-C23-O8-C6
34	g	630	LHG	C24-C23-O8-C6
34	e	630	LHG	C24-C23-O8-C6
36	9	602	LMG	C29-C28-O8-C9
36	B	853	LMG	C29-C28-O8-C9
30	0	306	CHL	C2C-C3C-CAC-CBC
30	0	306	CHL	C4C-C3C-CAC-CBC
33	5	501	0UR	C46-C45-O44-C43
33	8	501	0UR	C46-C45-O44-C43
33	d	520	0UR	C46-C45-O44-C43
33	g	520	0UR	C46-C45-O44-C43
34	A	855	LHG	C8-C7-O7-C5
35	0	603	SQD	C8-C7-O47-C45
41	B	849	DGD	C2B-C1B-O2G-C2G
30	d	607	CHL	CBD-CGD-O2D-CED
30	f	605	CHL	CBD-CGD-O2D-CED
30	i	602	CHL	CBD-CGD-O2D-CED
31	B	822	CLA	CBD-CGD-O2D-CED
31	6	304	CLA	O1A-CGA-O2A-C1
31	h	604	CLA	O1A-CGA-O2A-C1
31	5	314	CLA	CBA-CGA-O2A-C1
31	6	318	CLA	CBA-CGA-O2A-C1
31	1	309	CLA	C4-C3-C5-C6
31	7	304	CLA	C4-C3-C5-C6
38	A	842	PQN	C14-C13-C15-C16
31	0	303	CLA	C2-C3-C5-C6
31	A	840	CLA	C2-C3-C5-C6
31	A	841	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	830	CLA	C2-C3-C5-C6
30	f	607	CHL	CBD-CGD-O2D-CED
30	g	602	CHL	CBD-CGD-O2D-CED
30	h	606	CHL	CBD-CGD-O2D-CED
31	1	303	CLA	CBD-CGD-O2D-CED
31	7	317	CLA	CBD-CGD-O2D-CED
31	a	603	CLA	CBD-CGD-O2D-CED
31	H	201	CLA	CBD-CGD-O2D-CED
30	1	305	CHL	C2A-CAA-CBA-CGA
30	1	307	CHL	C2A-CAA-CBA-CGA
30	5	306	CHL	C2A-CAA-CBA-CGA
30	5	313	CHL	C2A-CAA-CBA-CGA
30	6	307	CHL	C2A-CAA-CBA-CGA
30	7	307	CHL	C2A-CAA-CBA-CGA
30	9	305	CHL	C2A-CAA-CBA-CGA
30	a	601	CHL	C2A-CAA-CBA-CGA
30	a	607	CHL	C2A-CAA-CBA-CGA
30	d	606	CHL	C2A-CAA-CBA-CGA
30	f	606	CHL	C2A-CAA-CBA-CGA
30	f	608	CHL	C2A-CAA-CBA-CGA
30	g	601	CHL	C2A-CAA-CBA-CGA
30	g	607	CHL	C2A-CAA-CBA-CGA
30	h	602	CHL	C2A-CAA-CBA-CGA
30	i	607	CHL	C2A-CAA-CBA-CGA
30	e	607	CHL	C2A-CAA-CBA-CGA
30	e	608	CHL	C2A-CAA-CBA-CGA
31	8	304	CLA	C2A-CAA-CBA-CGA
31	8	314	CLA	C2A-CAA-CBA-CGA
31	A	822	CLA	C2A-CAA-CBA-CGA
31	A	824	CLA	C2A-CAA-CBA-CGA
31	B	813	CLA	C2A-CAA-CBA-CGA
31	B	834	CLA	C2A-CAA-CBA-CGA
31	i	604	CLA	C2A-CAA-CBA-CGA
34	7	602	LHG	O10-C23-O8-C6
34	0	601	LHG	C24-C25-C26-C27
34	2	601	LHG	C24-C25-C26-C27
34	3	603	LHG	C24-C25-C26-C27
34	5	601	LHG	C24-C25-C26-C27
34	A	855	LHG	C24-C25-C26-C27
34	B	854	LHG	C24-C25-C26-C27
34	G	105	LHG	C24-C25-C26-C27
34	K	106	LHG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	a	630	LHG	C24-C25-C26-C27
34	c	630	LHG	C24-C25-C26-C27
34	b	630	LHG	C24-C25-C26-C27
34	d	630	LHG	C24-C25-C26-C27
34	f	630	LHG	C24-C25-C26-C27
34	g	630	LHG	C24-C25-C26-C27
34	h	630	LHG	C24-C25-C26-C27
34	H	203	LHG	C24-C25-C26-C27
34	i	630	LHG	C24-C25-C26-C27
34	e	630	LHG	C24-C25-C26-C27
34	4	601	LHG	C24-C25-C26-C27
31	0	309	CLA	C3-C5-C6-C7
31	9	308	CLA	C3-C5-C6-C7
31	B	803	CLA	C3-C5-C6-C7
31	c	613	CLA	C3-C5-C6-C7
31	f	611	CLA	C3-C5-C6-C7
30	5	302	CHL	CBA-CGA-O2A-C1
31	1	311	CLA	CBA-CGA-O2A-C1
31	2	310	CLA	CBA-CGA-O2A-C1
31	7	309	CLA	CBA-CGA-O2A-C1
31	7	315	CLA	CBA-CGA-O2A-C1
31	9	311	CLA	CBA-CGA-O2A-C1
31	A	806	CLA	CBA-CGA-O2A-C1
31	B	822	CLA	CBA-CGA-O2A-C1
31	B	823	CLA	CBA-CGA-O2A-C1
31	B	850	CLA	CBA-CGA-O2A-C1
31	L	203	CLA	CBA-CGA-O2A-C1
31	H	202	CLA	CBA-CGA-O2A-C1
31	4	310	CLA	CBA-CGA-O2A-C1
34	M	104	LHG	C24-C23-O8-C6
34	f	630	LHG	C24-C23-O8-C6
34	4	601	LHG	C24-C23-O8-C6
35	0	603	SQD	C24-C23-O48-C46
36	9	602	LMG	C4-C5-C6-O5
33	0	502	0UR	O44-C45-C46-C47
33	5	502	0UR	O44-C45-C46-C47
33	c	520	0UR	O44-C45-C46-C47
30	6	307	CHL	O1D-CGD-O2D-CED
31	8	304	CLA	O1D-CGD-O2D-CED
31	e	613	CLA	O1D-CGD-O2D-CED
30	d	606	CHL	CBD-CGD-O2D-CED
30	h	601	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	1	312	CLA	CBD-CGD-O2D-CED
31	4	304	CLA	CBD-CGD-O2D-CED
30	8	307	CHL	O1D-CGD-O2D-CED
30	f	609	CHL	O1D-CGD-O2D-CED
31	1	311	CLA	O1D-CGD-O2D-CED
31	2	311	CLA	O1D-CGD-O2D-CED
31	6	310	CLA	O1D-CGD-O2D-CED
35	0	603	SQD	O49-C7-O47-C45
31	1	311	CLA	O1A-CGA-O2A-C1
31	5	303	CLA	O1A-CGA-O2A-C1
31	A	808	CLA	O1A-CGA-O2A-C1
31	A	819	CLA	O1A-CGA-O2A-C1
31	B	819	CLA	O1A-CGA-O2A-C1
31	B	822	CLA	O1A-CGA-O2A-C1
31	B	824	CLA	O1A-CGA-O2A-C1
31	B	833	CLA	O1A-CGA-O2A-C1
31	4	310	CLA	O1A-CGA-O2A-C1
34	B	854	LHG	O10-C23-O8-C6
34	G	105	LHG	O10-C23-O8-C6
34	f	630	LHG	O10-C23-O8-C6
39	A	857	CL0	O1A-CGA-O2A-C1
31	0	304	CLA	O1D-CGD-O2D-CED
32	3	403	8CT	C18-C19-C20-C21
32	7	402	8CT	C16-C17-C18-C19
32	7	404	8CT	C16-C17-C18-C19
32	8	402	8CT	C12-C13-C14-C15
32	B	804	8CT	C12-C13-C14-C15
32	F	302	8CT	C12-C13-C14-C15
32	I	101	8CT	C16-C17-C18-C19
32	I	101	8CT	C18-C19-C20-C21
32	J	101	8CT	C23-C24-C25-C26
32	K	107	8CT	C12-C13-C14-C15
32	M	102	8CT	C18-C19-C20-C21
32	O	205	8CT	C18-C19-C20-C21
37	c	522	0IE	C9-C10-C11-C12
36	J	102	LMG	O6-C5-C6-O5
30	5	313	CHL	CBD-CGD-O2D-CED
30	8	302	CHL	CBD-CGD-O2D-CED
30	8	306	CHL	CBD-CGD-O2D-CED
30	c	606	CHL	CBD-CGD-O2D-CED
30	f	601	CHL	CBD-CGD-O2D-CED
30	g	601	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	g	614	CHL	CBD-CGD-O2D-CED
30	i	607	CHL	CBD-CGD-O2D-CED
30	i	609	CHL	CBD-CGD-O2D-CED
31	2	314	CLA	CBD-CGD-O2D-CED
31	A	806	CLA	CBD-CGD-O2D-CED
31	A	819	CLA	CBD-CGD-O2D-CED
31	L	207	CLA	CBD-CGD-O2D-CED
30	5	307	CHL	O1D-CGD-O2D-CED
30	g	609	CHL	O1D-CGD-O2D-CED
33	2	502	0UR	O57-C45-O44-C43
33	5	501	0UR	O57-C45-O44-C43
33	8	501	0UR	O57-C45-O44-C43
33	b	520	0UR	O57-C45-O44-C43
33	d	520	0UR	O57-C45-O44-C43
33	g	520	0UR	O57-C45-O44-C43
33	4	502	0UR	O57-C45-O44-C43
34	7	601	LHG	O2-C2-C3-O3
34	7	603	LHG	O2-C2-C3-O3
34	B	854	LHG	O2-C2-C3-O3
30	1	313	CHL	C3-C5-C6-C7
30	2	301	CHL	C3-C5-C6-C7
30	c	602	CHL	C3-C5-C6-C7
31	5	303	CLA	C3-C5-C6-C7
31	7	309	CLA	C3-C5-C6-C7
30	7	301	CHL	CBA-CGA-O2A-C1
31	A	819	CLA	CBA-CGA-O2A-C1
31	A	837	CLA	CBA-CGA-O2A-C1
31	B	833	CLA	CBA-CGA-O2A-C1
31	B	840	CLA	CBA-CGA-O2A-C1
31	K	102	CLA	CBA-CGA-O2A-C1
31	i	604	CLA	CBA-CGA-O2A-C1
31	4	304	CLA	CBA-CGA-O2A-C1
34	B	854	LHG	C24-C23-O8-C6
39	A	857	CL0	CBA-CGA-O2A-C1
31	3	310	CLA	O1A-CGA-O2A-C1
31	A	837	CLA	O1A-CGA-O2A-C1
35	0	603	SQD	O10-C23-O48-C46
36	B	853	LMG	O6-C5-C6-O5
33	2	502	0UR	C46-C45-O44-C43
33	b	520	0UR	C46-C45-O44-C43
33	4	502	0UR	C46-C45-O44-C43
30	1	307	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	614	CHL	O1D-CGD-O2D-CED
31	B	807	CLA	O1D-CGD-O2D-CED
31	K	102	CLA	O1D-CGD-O2D-CED
36	9	602	LMG	C11-C10-O7-C8
36	B	853	LMG	C11-C10-O7-C8
31	8	311	CLA	CBA-CGA-O2A-C1
31	c	611	CLA	CBA-CGA-O2A-C1
30	0	302	CHL	CBD-CGD-O2D-CED
30	5	305	CHL	CBD-CGD-O2D-CED
30	6	315	CHL	CBD-CGD-O2D-CED
30	7	306	CHL	CBD-CGD-O2D-CED
30	b	614	CHL	CBD-CGD-O2D-CED
30	d	605	CHL	CBD-CGD-O2D-CED
30	h	602	CHL	CBD-CGD-O2D-CED
30	h	605	CHL	CBD-CGD-O2D-CED
31	3	310	CLA	CBD-CGD-O2D-CED
31	3	313	CLA	CBD-CGD-O2D-CED
31	B	817	CLA	CBD-CGD-O2D-CED
31	L	204	CLA	CBD-CGD-O2D-CED
36	3	602	LMG	O6-C5-C6-O5
41	B	849	DGD	O6E-C5E-C6E-O5E
34	A	844	LHG	C12-C13-C14-C15
31	g	610	CLA	O1D-CGD-O2D-CED
31	B	840	CLA	O1A-CGA-O2A-C1
31	i	604	CLA	O1A-CGA-O2A-C1
34	4	601	LHG	O10-C23-O8-C6
33	6	501	0UR	O44-C45-C46-C47
33	7	501	0UR	O44-C45-C46-C47
33	9	502	0UR	O44-C45-C46-C47
33	O	204	0UR	O44-C45-C46-C47
33	f	520	0UR	O44-C45-C46-C47
33	i	520	0UR	O44-C45-C46-C47
34	0	601	LHG	C12-C13-C14-C15
34	A	855	LHG	C12-C13-C14-C15
36	9	602	LMG	O6-C5-C6-O5
36	L	210	LMG	O6-C5-C6-O5
36	3	602	LMG	C4-C5-C6-O5
30	g	607	CHL	O1D-CGD-O2D-CED
31	1	314	CLA	O1D-CGD-O2D-CED
34	M	104	LHG	C12-C13-C14-C15
30	a	609	CHL	CBD-CGD-O2D-CED
31	f	611	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	6	308	CHL	C3-C5-C6-C7
31	A	838	CLA	C3-C5-C6-C7
31	B	820	CLA	C3-C5-C6-C7
38	A	842	PQN	C13-C15-C16-C17
34	7	602	LHG	C24-C23-O8-C6
34	G	105	LHG	C24-C23-O8-C6
31	1	308	CLA	O1D-CGD-O2D-CED
31	9	302	CLA	O1D-CGD-O2D-CED
31	i	611	CLA	O1D-CGD-O2D-CED
36	O	207	LMG	O6-C5-C6-O5
31	3	320	CLA	C2C-C3C-CAC-CBC
34	M	104	LHG	C2-C3-O3-P
30	5	302	CHL	O1A-CGA-O2A-C1
31	9	311	CLA	O1A-CGA-O2A-C1
31	A	806	CLA	O1A-CGA-O2A-C1
31	K	102	CLA	O1A-CGA-O2A-C1
31	4	304	CLA	O1A-CGA-O2A-C1
31	A	828	CLA	C4-C3-C5-C6
31	B	819	CLA	C4-C3-C5-C6
36	B	853	LMG	C4-C5-C6-O5
31	1	312	CLA	C2-C3-C5-C6
31	A	828	CLA	C2-C3-C5-C6
31	B	819	CLA	C2-C3-C5-C6
30	a	602	CHL	C2A-CAA-CBA-CGA
30	a	606	CHL	C2A-CAA-CBA-CGA
30	a	608	CHL	C2A-CAA-CBA-CGA
30	c	608	CHL	C2A-CAA-CBA-CGA
30	b	606	CHL	C2A-CAA-CBA-CGA
30	d	602	CHL	C2A-CAA-CBA-CGA
30	d	608	CHL	C2A-CAA-CBA-CGA
30	g	606	CHL	C2A-CAA-CBA-CGA
30	h	607	CHL	C2A-CAA-CBA-CGA
30	i	602	CHL	C2A-CAA-CBA-CGA
30	e	602	CHL	C2A-CAA-CBA-CGA
31	3	306	CLA	C2A-CAA-CBA-CGA
31	3	308	CLA	C2A-CAA-CBA-CGA
31	B	823	CLA	C2A-CAA-CBA-CGA
31	L	207	CLA	C2A-CAA-CBA-CGA
31	M	101	CLA	C2A-CAA-CBA-CGA
31	O	206	CLA	C2A-CAA-CBA-CGA
31	a	613	CLA	C2A-CAA-CBA-CGA
31	e	604	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	1	601	LHG	C31-C32-C33-C34
31	B	834	CLA	O1A-CGA-O2A-C1
36	3	602	LMG	O10-C28-O8-C9
31	6	318	CLA	O1A-CGA-O2A-C1
31	2	304	CLA	CBA-CGA-O2A-C1
31	3	304	CLA	CBA-CGA-O2A-C1
31	A	807	CLA	CBA-CGA-O2A-C1
31	A	841	CLA	CBA-CGA-O2A-C1
31	B	831	CLA	CBA-CGA-O2A-C1
31	B	834	CLA	CBA-CGA-O2A-C1
34	A	855	LHG	C10-C11-C12-C13
30	a	601	CHL	CBD-CGD-O2D-CED
33	6	502	0UR	O44-C45-C46-C47
33	8	501	0UR	O44-C45-C46-C47
33	8	502	0UR	O44-C45-C46-C47
33	b	520	0UR	O44-C45-C46-C47
33	d	520	0UR	O44-C45-C46-C47
30	6	306	CHL	O1D-CGD-O2D-CED
30	b	607	CHL	O1D-CGD-O2D-CED
30	g	605	CHL	O1D-CGD-O2D-CED
30	7	301	CHL	O1A-CGA-O2A-C1
36	J	102	LMG	C11-C10-O7-C8
30	3	307	CHL	O1D-CGD-O2D-CED
30	h	607	CHL	O1D-CGD-O2D-CED
31	5	314	CLA	O1D-CGD-O2D-CED
31	b	604	CLA	O1D-CGD-O2D-CED
30	8	315	CHL	CBD-CGD-O2D-CED
34	A	855	LHG	C11-C10-C9-C8
31	B	815	CLA	O1D-CGD-O2D-CED
31	4	310	CLA	O1D-CGD-O2D-CED
34	0	601	LHG	C1-C2-C3-O3
34	2	601	LHG	C1-C2-C3-O3
34	3	603	LHG	C1-C2-C3-O3
34	7	603	LHG	C1-C2-C3-O3
34	a	630	LHG	C1-C2-C3-O3
31	2	304	CLA	O1A-CGA-O2A-C1
31	A	841	CLA	O1A-CGA-O2A-C1
34	9	601	LHG	C12-C13-C14-C15
31	B	834	CLA	C3-C5-C6-C7
31	e	603	CLA	C3-C5-C6-C7
31	e	613	CLA	C3-C5-C6-C7
31	8	310	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	e	614	CHL	O1D-CGD-O2D-CED
30	2	301	CHL	CBA-CGA-O2A-C1
30	2	307	CHL	CBA-CGA-O2A-C1
30	8	306	CHL	CBA-CGA-O2A-C1
30	8	307	CHL	CBA-CGA-O2A-C1
30	d	602	CHL	CBA-CGA-O2A-C1
30	4	307	CHL	CBA-CGA-O2A-C1
31	A	804	CLA	CBA-CGA-O2A-C1
31	A	810	CLA	CBA-CGA-O2A-C1
31	A	817	CLA	CBA-CGA-O2A-C1
31	A	831	CLA	CBA-CGA-O2A-C1
31	A	833	CLA	CBA-CGA-O2A-C1
31	a	613	CLA	CBA-CGA-O2A-C1
31	d	604	CLA	CBA-CGA-O2A-C1
31	f	604	CLA	CBA-CGA-O2A-C1
31	H	205	CLA	CBA-CGA-O2A-C1
36	3	602	LMG	C29-C28-O8-C9
36	J	105	LMG	C29-C28-O8-C9
36	J	105	LMG	O6-C5-C6-O5
31	f	603	CLA	CBD-CGD-O2D-CED
34	3	603	LHG	C28-C29-C30-C31
34	M	104	LHG	C28-C29-C30-C31
31	A	839	CLA	O1D-CGD-O2D-CED
31	F	301	CLA	O1D-CGD-O2D-CED
31	4	312	CLA	O1D-CGD-O2D-CED
32	0	401	8CT	C16-C17-C18-C19
32	0	401	8CT	C18-C19-C20-C21
32	7	402	8CT	C18-C19-C20-C21
32	G	104	8CT	C16-C17-C18-C19
32	G	104	8CT	C18-C19-C20-C21
32	J	101	8CT	C16-C17-C18-C19
32	L	209	8CT	C12-C13-C14-C15
32	L	209	8CT	C18-C19-C20-C21
34	0	601	LHG	C30-C31-C32-C33
34	2	601	LHG	C11-C10-C9-C8
34	M	104	LHG	C14-C15-C16-C17
30	7	302	CHL	C5-C6-C7-C8
30	8	306	CHL	O1A-CGA-O2A-C1
34	A	844	LHG	C28-C29-C30-C31
33	1	502	0UR	O44-C45-C46-C47
33	g	520	0UR	O44-C45-C46-C47
31	8	311	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	J	102	LMG	C4-C5-C6-O5
30	1	307	CHL	C8-C10-C11-C12
30	b	602	CHL	C5-C6-C7-C8
30	f	602	CHL	C5-C6-C7-C8
30	f	609	CHL	C15-C16-C17-C18
30	i	602	CHL	C5-C6-C7-C8
31	2	310	CLA	C5-C6-C7-C8
31	9	308	CLA	C10-C11-C12-C13
31	A	806	CLA	C8-C10-C11-C12
31	A	809	CLA	C8-C10-C11-C12
31	A	841	CLA	C5-C6-C7-C8
31	B	827	CLA	C8-C10-C11-C12
33	6	502	0UR	O57-C45-O44-C43
34	0	601	LHG	O2-C2-C3-O3
30	4	302	CHL	C3-C5-C6-C7
31	B	823	CLA	C3-C5-C6-C7
34	1	601	LHG	O7-C5-C6-O8
34	7	603	LHG	O7-C5-C6-O8
35	0	603	SQD	O47-C45-C46-O48
36	2	602	LMG	O7-C8-C9-O8
34	A	855	LHG	C14-C15-C16-C17
30	2	301	CHL	O1A-CGA-O2A-C1
30	2	307	CHL	O1A-CGA-O2A-C1
30	8	307	CHL	O1A-CGA-O2A-C1
31	A	817	CLA	O1A-CGA-O2A-C1
41	B	849	DGD	C4E-C5E-C6E-O5E
31	7	304	CLA	C2-C3-C5-C6
38	A	842	PQN	C12-C13-C15-C16
33	6	502	0UR	C46-C45-O44-C43
30	2	302	CHL	C11-C10-C8-C9
30	2	319	CHL	C6-C7-C8-C9
30	2	319	CHL	C11-C10-C8-C9
30	5	302	CHL	C14-C13-C15-C16
30	6	301	CHL	C11-C10-C8-C9
30	6	302	CHL	C6-C7-C8-C9
30	6	308	CHL	C11-C10-C8-C9
30	7	301	CHL	C14-C13-C15-C16
30	a	602	CHL	C14-C13-C15-C16
30	c	602	CHL	C6-C7-C8-C9
30	c	608	CHL	C14-C13-C15-C16
30	b	602	CHL	C11-C12-C13-C14
30	d	609	CHL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	f	601	CHL	C11-C12-C13-C14
30	f	602	CHL	C11-C12-C13-C14
30	i	602	CHL	C6-C7-C8-C9
30	e	602	CHL	C6-C7-C8-C9
31	2	303	CLA	C6-C7-C8-C9
31	2	310	CLA	C11-C10-C8-C9
31	3	309	CLA	C14-C13-C15-C16
31	3	310	CLA	C6-C7-C8-C9
31	5	309	CLA	C6-C7-C8-C9
31	6	310	CLA	C6-C7-C8-C9
31	7	308	CLA	C11-C12-C13-C14
31	7	309	CLA	C11-C10-C8-C9
31	9	308	CLA	C11-C12-C13-C14
31	9	309	CLA	C6-C7-C8-C9
31	A	839	CLA	C11-C12-C13-C14
31	A	853	CLA	C6-C7-C8-C9
31	B	806	CLA	C11-C12-C13-C14
31	B	808	CLA	C6-C7-C8-C9
31	B	814	CLA	C11-C12-C13-C14
31	B	836	CLA	C11-C10-C8-C9
31	L	201	CLA	C6-C7-C8-C9
30	0	301	CHL	O1D-CGD-O2D-CED
30	a	605	CHL	O1D-CGD-O2D-CED
30	b	601	CHL	O1D-CGD-O2D-CED
30	e	605	CHL	O1D-CGD-O2D-CED
31	g	612	CLA	O1D-CGD-O2D-CED
30	5	301	CHL	CBD-CGD-O2D-CED
30	c	602	CHL	CBD-CGD-O2D-CED
31	A	814	CLA	CBD-CGD-O2D-CED
30	h	602	CHL	C13-C15-C16-C17
31	B	806	CLA	C8-C10-C11-C12
30	0	302	CHL	C2A-CAA-CBA-CGA
30	9	306	CHL	C2A-CAA-CBA-CGA
30	f	602	CHL	C2A-CAA-CBA-CGA
31	5	304	CLA	C2A-CAA-CBA-CGA
31	5	314	CLA	C2A-CAA-CBA-CGA
31	9	300	CLA	C2A-CAA-CBA-CGA
31	B	828	CLA	C2A-CAA-CBA-CGA
31	B	829	CLA	C2A-CAA-CBA-CGA
31	G	103	CLA	C2A-CAA-CBA-CGA
32	1	402	8CT	C10-C11-C12-C40
32	2	402	8CT	C27-C26-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	6	402	8CT	C22-C21-C23-C24
32	7	405	8CT	C27-C26-C28-C29
32	9	401	8CT	C10-C11-C12-C40
32	A	846	8CT	C10-C11-C12-C40
32	A	847	8CT	C10-C11-C12-C40
32	A	847	8CT	C14-C15-C16-C39
32	A	849	8CT	C10-C11-C12-C40
32	A	850	8CT	C10-C11-C12-C40
32	A	854	8CT	C27-C26-C28-C29
32	B	804	8CT	C14-C15-C16-C39
32	B	804	8CT	C27-C26-C28-C29
32	B	843	8CT	C14-C15-C16-C39
32	B	847	8CT	C10-C11-C12-C40
32	B	851	8CT	C10-C11-C12-C40
32	I	101	8CT	C10-C11-C12-C40
32	L	206	8CT	C10-C11-C12-C40
32	L	209	8CT	C14-C15-C16-C39
32	K	107	8CT	C14-C15-C16-C39
32	M	102	8CT	C10-C11-C12-C40
32	4	402	8CT	C27-C26-C28-C29
33	1	502	0UR	C22-C16-C17-C18
33	2	502	0UR	C22-C16-C17-C18
33	5	502	0UR	C22-C16-C17-C18
33	6	501	0UR	C22-C16-C17-C18
33	6	502	0UR	C22-C16-C17-C18
33	c	520	0UR	C22-C16-C17-C18
33	b	520	0UR	C5-C6-C7-C20
33	f	520	0UR	C22-C16-C17-C18
33	5	502	0UR	O57-C45-C46-C47
33	6	501	0UR	O57-C45-C46-C47
33	7	501	0UR	O57-C45-C46-C47
33	9	502	0UR	O57-C45-C46-C47
33	O	204	0UR	O57-C45-C46-C47
33	c	520	0UR	O57-C45-C46-C47
33	f	520	0UR	O57-C45-C46-C47
33	i	520	0UR	O57-C45-C46-C47
32	1	402	8CT	C10-C11-C12-C13
32	1	402	8CT	C20-C21-C23-C24
32	2	402	8CT	C25-C26-C28-C29
32	6	402	8CT	C20-C21-C23-C24
32	7	402	8CT	C10-C11-C12-C13
32	7	402	8CT	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	8	406	8CT	C14-C15-C16-C17
32	9	401	8CT	C10-C11-C12-C13
32	A	846	8CT	C10-C11-C12-C13
32	A	847	8CT	C10-C11-C12-C13
32	A	849	8CT	C10-C11-C12-C13
32	A	850	8CT	C20-C21-C23-C24
32	A	854	8CT	C25-C26-C28-C29
32	B	804	8CT	C14-C15-C16-C17
32	B	804	8CT	C25-C26-C28-C29
32	I	101	8CT	C10-C11-C12-C13
32	L	206	8CT	C10-C11-C12-C13
32	L	209	8CT	C14-C15-C16-C17
32	K	107	8CT	C14-C15-C16-C17
32	4	402	8CT	C25-C26-C28-C29
33	1	502	0UR	C15-C16-C17-C18
33	2	502	0UR	C15-C16-C17-C18
33	5	502	0UR	C15-C16-C17-C18
33	6	501	0UR	C15-C16-C17-C18
33	c	520	0UR	C15-C16-C17-C18
33	f	520	0UR	C15-C16-C17-C18
30	f	614	CHL	O1D-CGD-O2D-CED
36	L	211	LMG	C11-C10-O7-C8
34	0	601	LHG	C23-C24-C25-C26
34	7	603	LHG	C7-C8-C9-C10
31	B	805	CLA	C8-C10-C11-C12
31	B	814	CLA	C8-C10-C11-C12
31	4	310	CLA	C5-C6-C7-C8
31	5	309	CLA	O1D-CGD-O2D-CED
31	7	312	CLA	O1D-CGD-O2D-CED
31	A	833	CLA	O1D-CGD-O2D-CED
31	i	603	CLA	CBA-CGA-O2A-C1
30	5	306	CHL	O1D-CGD-O2D-CED
31	B	820	CLA	O1D-CGD-O2D-CED
30	7	301	CHL	C3-C5-C6-C7
31	A	803	CLA	C3-C5-C6-C7
31	A	833	CLA	C3-C5-C6-C7
30	b	602	CHL	CBA-CGA-O2A-C1
30	1	307	CHL	C15-C16-C17-C18
30	1	313	CHL	C8-C10-C11-C12
30	6	302	CHL	C13-C15-C16-C17
30	8	302	CHL	C10-C11-C12-C13
30	c	609	CHL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	602	CHL	C10-C11-C12-C13
30	d	609	CHL	C15-C16-C17-C18
30	f	602	CHL	C13-C15-C16-C17
30	e	608	CHL	C5-C6-C7-C8
30	e	608	CHL	C8-C10-C11-C12
31	A	803	CLA	C8-C10-C11-C12
31	A	830	CLA	C5-C6-C7-C8
31	A	835	CLA	C5-C6-C7-C8
31	A	840	CLA	C5-C6-C7-C8
31	B	809	CLA	C5-C6-C7-C8
31	B	814	CLA	C15-C16-C17-C18
31	B	819	CLA	C5-C6-C7-C8
31	B	839	CLA	C13-C15-C16-C17
34	f	630	LHG	C7-C8-C9-C10
41	B	849	DGD	C1B-C2B-C3B-C4B
31	2	310	CLA	O1D-CGD-O2D-CED
31	h	603	CLA	O1D-CGD-O2D-CED
30	c	607	CHL	CBD-CGD-O2D-CED
34	b	630	LHG	C28-C29-C30-C31
33	0	502	0UR	O57-C45-C46-C47
33	6	502	0UR	O57-C45-C46-C47
33	8	501	0UR	O57-C45-C46-C47
33	b	520	0UR	O57-C45-C46-C47
30	2	302	CHL	C8-C10-C11-C12
30	3	302	CHL	C8-C10-C11-C12
30	3	307	CHL	C13-C15-C16-C17
30	8	302	CHL	C13-C15-C16-C17
30	c	601	CHL	C5-C6-C7-C8
30	c	608	CHL	C8-C10-C11-C12
30	c	609	CHL	C8-C10-C11-C12
30	b	601	CHL	C13-C15-C16-C17
30	b	602	CHL	C8-C10-C11-C12
30	b	602	CHL	C13-C15-C16-C17
30	b	608	CHL	C8-C10-C11-C12
30	b	608	CHL	C13-C15-C16-C17
30	f	602	CHL	C8-C10-C11-C12
30	e	608	CHL	C15-C16-C17-C18
31	A	811	CLA	C8-C10-C11-C12
31	A	811	CLA	C13-C15-C16-C17
31	A	811	CLA	C15-C16-C17-C18
31	A	826	CLA	C5-C6-C7-C8
31	A	829	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	832	CLA	C5-C6-C7-C8
31	A	852	CLA	C13-C15-C16-C17
31	B	808	CLA	C15-C16-C17-C18
31	B	827	CLA	C15-C16-C17-C18
31	B	834	CLA	C8-C10-C11-C12
31	B	836	CLA	C5-C6-C7-C8
31	B	836	CLA	C8-C10-C11-C12
31	L	203	CLA	C13-C15-C16-C17
31	d	610	CLA	C5-C6-C7-C8
34	A	855	LHG	C28-C29-C30-C31
31	6	317	CLA	O1D-CGD-O2D-CED
31	c	613	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	O1D-CGD-O2D-CED
31	f	604	CLA	O1A-CGA-O2A-C1
34	2	601	LHG	C23-C24-C25-C26
34	M	104	LHG	C7-C8-C9-C10
34	h	630	LHG	C23-C24-C25-C26
34	e	630	LHG	C7-C8-C9-C10
36	J	102	LMG	C28-C29-C30-C31
30	7	313	CHL	CBD-CGD-O2D-CED
31	0	312	CLA	O1D-CGD-O2D-CED
30	5	302	CHL	C13-C15-C16-C17
30	c	608	CHL	C15-C16-C17-C18
30	b	601	CHL	C15-C16-C17-C18
31	1	312	CLA	C13-C15-C16-C17
31	A	853	CLA	C5-C6-C7-C8
31	B	803	CLA	C13-C15-C16-C17
31	B	814	CLA	C5-C6-C7-C8
30	7	306	CHL	CBA-CGA-O2A-C1
30	d	609	CHL	CBA-CGA-O2A-C1
30	5	302	CHL	O1D-CGD-O2D-CED
30	7	305	CHL	O1D-CGD-O2D-CED
31	B	816	CLA	O1D-CGD-O2D-CED
31	A	805	CLA	C2-C1-O2A-CGA
39	A	857	CL0	C2-C1-O2A-CGA
30	2	319	CHL	C5-C6-C7-C8
30	2	319	CHL	C8-C10-C11-C12
30	b	601	CHL	C8-C10-C11-C12
31	6	317	CLA	C10-C11-C12-C13
31	A	813	CLA	C13-C15-C16-C17
31	A	818	CLA	C13-C15-C16-C17
31	B	828	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	0	601	LHG	C7-C8-C9-C10
34	K	106	LHG	C23-C24-C25-C26
36	9	602	LMG	C28-C29-C30-C31
30	c	614	CHL	CBD-CGD-O2D-CED
30	b	602	CHL	CBD-CGD-O2D-CED
30	i	601	CHL	CBD-CGD-O2D-CED
31	8	314	CLA	CBD-CGD-O2D-CED
30	7	301	CHL	C13-C15-C16-C17
30	c	606	CHL	C2A-CAA-CBA-CGA
31	L	202	CLA	CBA-CGA-O2A-C1
33	1	502	0UR	O57-C45-C46-C47
33	d	520	0UR	O57-C45-C46-C47
30	a	608	CHL	O2A-C1-C2-C3
30	c	609	CHL	C13-C15-C16-C17
30	f	609	CHL	C8-C10-C11-C12
31	1	303	CLA	C5-C6-C7-C8
31	A	829	CLA	C8-C10-C11-C12
30	c	605	CHL	O1D-CGD-O2D-CED
30	i	614	CHL	O1D-CGD-O2D-CED
31	B	836	CLA	O1D-CGD-O2D-CED
31	f	612	CLA	O1D-CGD-O2D-CED
30	2	302	CHL	C11-C10-C8-C7
30	5	302	CHL	C6-C7-C8-C10
30	7	306	CHL	C11-C10-C8-C7
30	a	602	CHL	C12-C13-C15-C16
30	c	602	CHL	C6-C7-C8-C10
30	f	601	CHL	C6-C7-C8-C10
30	f	602	CHL	C11-C12-C13-C15
31	0	308	CLA	C6-C7-C8-C10
31	7	308	CLA	C12-C13-C15-C16
31	9	302	CLA	C11-C10-C8-C7
31	A	803	CLA	C11-C10-C8-C7
31	A	806	CLA	C6-C7-C8-C10
31	A	817	CLA	C11-C12-C13-C15
31	A	818	CLA	C11-C10-C8-C7
31	A	821	CLA	C6-C7-C8-C10
31	B	808	CLA	C6-C7-C8-C10
31	B	828	CLA	C6-C7-C8-C10
30	4	307	CHL	O1A-CGA-O2A-C1
31	A	804	CLA	O1A-CGA-O2A-C1
32	6	402	8CT	C18-C19-C20-C21
32	8	406	8CT	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	854	8CT	C23-C24-C25-C26
32	B	845	8CT	C12-C13-C14-C15
32	J	104	8CT	C16-C17-C18-C19
33	4	502	0UR	C13-C14-C15-C16
31	0	309	CLA	CBA-CGA-O2A-C1
30	0	301	CHL	C2A-CAA-CBA-CGA
30	2	302	CHL	C2A-CAA-CBA-CGA
30	b	608	CHL	C2A-CAA-CBA-CGA
30	d	607	CHL	C2A-CAA-CBA-CGA
30	e	606	CHL	C2A-CAA-CBA-CGA
31	6	318	CLA	C2A-CAA-CBA-CGA
31	A	829	CLA	C2A-CAA-CBA-CGA
31	B	803	CLA	C2A-CAA-CBA-CGA
31	B	807	CLA	C2A-CAA-CBA-CGA
30	1	306	CHL	O1D-CGD-O2D-CED
30	3	302	CHL	O1D-CGD-O2D-CED
30	9	305	CHL	O1D-CGD-O2D-CED
30	c	601	CHL	O1D-CGD-O2D-CED
30	c	609	CHL	O1D-CGD-O2D-CED
30	b	609	CHL	O1D-CGD-O2D-CED
31	0	310	CLA	O1D-CGD-O2D-CED
31	2	312	CLA	O1D-CGD-O2D-CED
31	6	312	CLA	O1D-CGD-O2D-CED
31	7	311	CLA	O1D-CGD-O2D-CED
31	A	832	CLA	O1D-CGD-O2D-CED
31	G	101	CLA	O1D-CGD-O2D-CED
31	f	604	CLA	O1D-CGD-O2D-CED
31	H	205	CLA	O1D-CGD-O2D-CED
30	a	602	CHL	C8-C10-C11-C12
30	b	608	CHL	C15-C16-C17-C18
31	8	309	CLA	C5-C6-C7-C8
31	A	826	CLA	C15-C16-C17-C18
31	B	806	CLA	C10-C11-C12-C13
31	B	830	CLA	C5-C6-C7-C8
31	A	831	CLA	O1A-CGA-O2A-C1
31	a	613	CLA	O1A-CGA-O2A-C1
31	H	205	CLA	O1A-CGA-O2A-C1
30	9	301	CHL	CBD-CGD-O2D-CED
30	i	606	CHL	CBD-CGD-O2D-CED
33	8	502	0UR	O57-C45-C46-C47
30	c	602	CHL	C8-C10-C11-C12
31	3	308	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	806	CLA	C15-C16-C17-C18
31	B	803	CLA	O1D-CGD-O2D-CED
31	B	806	CLA	C2C-C3C-CAC-CBC
31	B	817	CLA	C2C-C3C-CAC-CBC
34	1	601	LHG	C7-C8-C9-C10
34	B	852	LHG	O2-C2-C3-O3
34	c	630	LHG	O2-C2-C3-O3
34	f	630	LHG	O2-C2-C3-O3
31	c	611	CLA	O1A-CGA-O2A-C1
31	9	312	CLA	C3-C5-C6-C7
30	1	302	CHL	C13-C15-C16-C17
30	e	602	CHL	C5-C6-C7-C8
30	e	609	CHL	C8-C10-C11-C12
31	3	303	CLA	C5-C6-C7-C8
31	A	808	CLA	C15-C16-C17-C18
31	A	852	CLA	C10-C11-C12-C13
31	B	814	CLA	C10-C11-C12-C13
31	B	827	CLA	C5-C6-C7-C8
38	A	842	PQN	C15-C16-C17-C18
38	B	842	PQN	C18-C20-C21-C22
30	4	319	CHL	CBA-CGA-O2A-C1
30	9	313	CHL	CBD-CGD-O2D-CED
30	d	601	CHL	CBD-CGD-O2D-CED
30	d	602	CHL	O1A-CGA-O2A-C1
31	3	304	CLA	O1A-CGA-O2A-C1
31	A	807	CLA	O1A-CGA-O2A-C1
31	A	810	CLA	O1A-CGA-O2A-C1
31	A	833	CLA	O1A-CGA-O2A-C1
31	B	831	CLA	O1A-CGA-O2A-C1
31	d	604	CLA	O1A-CGA-O2A-C1
34	A	844	LHG	C23-C24-C25-C26
33	5	501	0UR	O44-C45-C46-C47
30	2	302	CHL	C5-C6-C7-C8
30	6	302	CHL	C8-C10-C11-C12
31	2	304	CLA	C10-C11-C12-C13
31	7	308	CLA	C5-C6-C7-C8
31	B	811	CLA	C5-C6-C7-C8
30	d	607	CHL	O1D-CGD-O2D-CED
30	d	609	CHL	O1D-CGD-O2D-CED
30	f	605	CHL	O1D-CGD-O2D-CED
31	7	318	CLA	O1D-CGD-O2D-CED
31	B	824	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	g	520	0UR	O57-C45-C46-C47
30	7	301	CHL	CBD-CGD-O2D-CED
30	b	602	CHL	O1A-CGA-O2A-C1
30	d	609	CHL	O1A-CGA-O2A-C1
30	6	302	CHL	C5-C6-C7-C8
30	7	302	CHL	C13-C15-C16-C17
30	a	602	CHL	C13-C15-C16-C17
30	f	601	CHL	C13-C15-C16-C17
30	h	602	CHL	C5-C6-C7-C8
31	0	312	CLA	C5-C6-C7-C8
31	1	309	CLA	C5-C6-C7-C8
31	5	312	CLA	C5-C6-C7-C8
31	9	308	CLA	C5-C6-C7-C8
31	A	815	CLA	C13-C15-C16-C17
31	A	819	CLA	C15-C16-C17-C18
31	A	840	CLA	C13-C15-C16-C17
31	A	852	CLA	C5-C6-C7-C8
31	A	852	CLA	C8-C10-C11-C12
31	B	809	CLA	C15-C16-C17-C18
31	B	828	CLA	C10-C11-C12-C13
31	L	203	CLA	C5-C6-C7-C8
34	0	601	LHG	C4-O6-P-O3
34	1	601	LHG	C3-O3-P-O6
34	3	603	LHG	C3-O3-P-O6
34	5	601	LHG	C3-O3-P-O6
34	6	601	LHG	C3-O3-P-O6
34	6	601	LHG	C4-O6-P-O3
34	6	603	LHG	C4-O6-P-O3
34	7	602	LHG	C4-O6-P-O3
34	7	603	LHG	C4-O6-P-O3
34	8	601	LHG	C4-O6-P-O3
34	A	845	LHG	C3-O3-P-O6
34	A	855	LHG	C3-O3-P-O6
34	B	852	LHG	C3-O3-P-O6
34	B	852	LHG	C4-O6-P-O3
34	a	630	LHG	C4-O6-P-O3
34	c	630	LHG	C4-O6-P-O3
34	b	630	LHG	C3-O3-P-O6
34	b	630	LHG	C4-O6-P-O3
34	d	630	LHG	C4-O6-P-O3
34	g	630	LHG	C4-O6-P-O3
34	h	630	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	4	601	LHG	C3-O3-P-O6
31	2	312	CLA	C3-C5-C6-C7
31	3	320	CLA	C4C-C3C-CAC-CBC
30	2	319	CHL	CBA-CGA-O2A-C1
30	a	602	CHL	CBA-CGA-O2A-C1
30	f	602	CHL	CBA-CGA-O2A-C1
31	2	312	CLA	CBA-CGA-O2A-C1
31	B	822	CLA	O1D-CGD-O2D-CED
31	B	839	CLA	C15-C16-C17-C18
31	f	611	CLA	C5-C6-C7-C8
31	6	303	CLA	C3-C5-C6-C7
31	6	311	CLA	O2A-C1-C2-C3
30	i	602	CHL	O1D-CGD-O2D-CED
34	1	601	LHG	C1-C2-C3-O3
34	A	845	LHG	C1-C2-C3-O3
34	B	854	LHG	C1-C2-C3-O3
34	c	630	LHG	C1-C2-C3-O3
34	i	630	LHG	C1-C2-C3-O3
31	A	830	CLA	C4-C3-C5-C6
31	B	817	CLA	C4-C3-C5-C6
31	L	201	CLA	C5-C6-C7-C8
31	A	807	CLA	CBD-CGD-O2D-CED
30	1	302	CHL	C2A-CAA-CBA-CGA
30	7	302	CHL	C2A-CAA-CBA-CGA
30	8	307	CHL	C2A-CAA-CBA-CGA
30	c	602	CHL	C2A-CAA-CBA-CGA
30	b	602	CHL	C2A-CAA-CBA-CGA
30	g	602	CHL	C2A-CAA-CBA-CGA
30	i	606	CHL	C2A-CAA-CBA-CGA
30	i	608	CHL	C2A-CAA-CBA-CGA
31	A	808	CLA	C2A-CAA-CBA-CGA
31	A	840	CLA	C2A-CAA-CBA-CGA
31	h	613	CLA	C2A-CAA-CBA-CGA
33	h	520	0UR	O44-C45-C46-C47
31	5	312	CLA	C3-C5-C6-C7
31	B	809	CLA	C3-C5-C6-C7
30	0	302	CHL	CBA-CGA-O2A-C1
30	8	302	CHL	CBA-CGA-O2A-C1
31	1	312	CLA	CBA-CGA-O2A-C1
31	9	300	CLA	CBA-CGA-O2A-C1
31	c	604	CLA	CBA-CGA-O2A-C1
31	H	201	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	609	CHL	C8-C10-C11-C12
31	A	837	CLA	C5-C6-C7-C8
34	8	601	LHG	C30-C31-C32-C33
34	B	854	LHG	C34-C35-C36-C37
32	1	402	8CT	C18-C19-C20-C21
32	7	404	8CT	C18-C19-C20-C21
32	9	401	8CT	C18-C19-C20-C21
32	A	847	8CT	C12-C13-C14-C15
32	A	848	8CT	C16-C17-C18-C19
32	B	848	8CT	C12-C13-C14-C15
32	B	851	8CT	C18-C19-C20-C21
37	d	522	0IE	C13-C14-C15-C16
34	8	601	LHG	C11-C12-C13-C14
34	f	630	LHG	C11-C12-C13-C14
36	B	853	LMG	C16-C17-C18-C19
31	a	603	CLA	O1D-CGD-O2D-CED
30	a	607	CHL	CBD-CGD-O2D-CED
31	A	826	CLA	CBD-CGD-O2D-CED
30	2	308	CHL	CBA-CGA-O2A-C1
37	d	522	0IE	C14-C15-C16-C23
30	e	602	CHL	C3-C5-C6-C7
31	0	308	CLA	C3-C5-C6-C7
31	a	613	CLA	C6-C7-C8-C10
34	0	601	LHG	C15-C16-C17-C18
34	8	601	LHG	C14-C15-C16-C17
34	A	844	LHG	C30-C31-C32-C33
34	h	630	LHG	C12-C13-C14-C15
36	9	602	LMG	C14-C15-C16-C17
41	B	849	DGD	C2A-C3A-C4A-C5A
30	h	606	CHL	O1D-CGD-O2D-CED
31	7	317	CLA	O1D-CGD-O2D-CED
30	b	601	CHL	C16-C17-C18-C19
30	b	608	CHL	C16-C17-C18-C20
31	b	611	CLA	C11-C12-C13-C15
30	7	302	CHL	CBA-CGA-O2A-C1
30	6	308	CHL	C10-C11-C12-C13
34	K	106	LHG	C9-C10-C11-C12
34	b	630	LHG	C12-C13-C14-C15
34	f	630	LHG	C10-C11-C12-C13
36	9	602	LMG	C20-C21-C22-C23
41	B	849	DGD	C4B-C5B-C6B-C7B
35	0	603	SQD	C44-C45-O47-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	9	602	LMG	C9-C8-O7-C10
30	f	607	CHL	O1D-CGD-O2D-CED
31	1	303	CLA	O1D-CGD-O2D-CED
31	1	312	CLA	O1D-CGD-O2D-CED
30	i	602	CHL	C8-C10-C11-C12
34	7	602	LHG	C15-C16-C17-C18
34	4	601	LHG	C10-C11-C12-C13
41	B	849	DGD	C7A-C8A-C9A-CAA
33	2	502	0UR	O44-C45-C46-C47
34	B	852	LHG	C5-C4-O6-P
30	7	306	CHL	O1A-CGA-O2A-C1
34	A	844	LHG	C10-C11-C12-C13
34	B	854	LHG	C25-C26-C27-C28
34	a	630	LHG	C10-C11-C12-C13
34	a	630	LHG	C13-C14-C15-C16
35	0	603	SQD	C26-C27-C28-C29
36	9	602	LMG	C30-C31-C32-C33
30	d	606	CHL	O1D-CGD-O2D-CED
30	g	602	CHL	O1D-CGD-O2D-CED
30	b	607	CHL	CBA-CGA-O2A-C1
34	1	601	LHG	C15-C16-C17-C18
36	9	602	LMG	C33-C34-C35-C36
30	i	602	CHL	C3-C5-C6-C7
31	1	310	CLA	C3-C5-C6-C7
31	2	304	CLA	CBD-CGD-O2D-CED
41	B	849	DGD	C2E-C1E-O5D-C6D
30	e	602	CHL	CBA-CGA-O2A-C1
31	1	303	CLA	CBA-CGA-O2A-C1
31	1	310	CLA	CBA-CGA-O2A-C1
34	2	601	LHG	C24-C23-O8-C6
34	8	601	LHG	C25-C26-C27-C28
34	g	630	LHG	C26-C27-C28-C29
34	e	630	LHG	C25-C26-C27-C28
31	7	312	CLA	C5-C6-C7-C8
30	8	302	CHL	O1A-CGA-O2A-C1
30	f	602	CHL	O1A-CGA-O2A-C1
31	0	309	CLA	O1A-CGA-O2A-C1
30	1	307	CHL	C16-C17-C18-C20
30	c	609	CHL	C16-C17-C18-C19
30	f	609	CHL	C16-C17-C18-C19
31	e	611	CLA	C6-C7-C8-C10
30	g	614	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	601	CHL	O1D-CGD-O2D-CED
30	i	607	CHL	O1D-CGD-O2D-CED
30	i	609	CHL	O1D-CGD-O2D-CED
31	2	314	CLA	O1D-CGD-O2D-CED
31	A	806	CLA	O1D-CGD-O2D-CED
31	4	304	CLA	O1D-CGD-O2D-CED
34	5	601	LHG	C28-C29-C30-C31
34	A	844	LHG	C15-C16-C17-C18
34	A	844	LHG	C26-C27-C28-C29
34	a	630	LHG	C14-C15-C16-C17
36	9	602	LMG	C34-C35-C36-C37
41	B	849	DGD	C3B-C4B-C5B-C6B
31	1	309	CLA	C2-C3-C5-C6
30	2	302	CHL	C14-C13-C15-C16
30	3	302	CHL	C11-C10-C8-C9
30	b	601	CHL	C11-C10-C8-C9
30	h	602	CHL	C11-C10-C8-C9
30	e	609	CHL	C6-C7-C8-C9
31	7	318	CLA	C6-C7-C8-C9
31	A	826	CLA	C11-C12-C13-C14
31	A	828	CLA	C6-C7-C8-C9
31	A	840	CLA	C11-C10-C8-C9
31	A	852	CLA	C14-C13-C15-C16
31	B	816	CLA	C6-C7-C8-C9
31	B	832	CLA	C6-C7-C8-C9
30	c	606	CHL	O1D-CGD-O2D-CED
31	L	207	CLA	O1D-CGD-O2D-CED
34	1	601	LHG	C28-C29-C30-C31
34	3	601	LHG	C13-C14-C15-C16
34	3	603	LHG	C11-C10-C9-C8
34	K	106	LHG	C31-C32-C33-C34
36	B	853	LMG	C14-C15-C16-C17
30	0	305	CHL	C2A-CAA-CBA-CGA
30	1	313	CHL	C2A-CAA-CBA-CGA
30	2	306	CHL	C2A-CAA-CBA-CGA
30	3	307	CHL	C2A-CAA-CBA-CGA
30	8	305	CHL	C2A-CAA-CBA-CGA
30	4	306	CHL	C2A-CAA-CBA-CGA
31	5	308	CLA	C2A-CAA-CBA-CGA
31	B	816	CLA	C2A-CAA-CBA-CGA
31	L	202	CLA	C2A-CAA-CBA-CGA
31	g	604	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	H	202	CLA	C2A-CAA-CBA-CGA
30	2	319	CHL	O1A-CGA-O2A-C1
30	4	319	CHL	O1A-CGA-O2A-C1
32	3	403	8CT	C10-C11-C12-C40
32	8	406	8CT	C14-C15-C16-C39
32	9	401	8CT	C27-C26-C28-C29
32	A	850	8CT	C22-C21-C23-C24
32	A	850	8CT	C27-C26-C28-C29
32	L	209	8CT	C10-C11-C12-C40
42	c	523	NEX	C31-C32-C33-C40
42	b	523	NEX	C31-C32-C33-C40
42	h	523	NEX	C31-C32-C33-C40
34	A	844	LHG	C9-C10-C11-C12
36	J	105	LMG	C32-C33-C34-C35
34	6	601	LHG	O1-C1-C2-C3
34	6	603	LHG	O1-C1-C2-C3
34	7	603	LHG	O1-C1-C2-C3
34	A	845	LHG	O1-C1-C2-C3
34	B	852	LHG	O1-C1-C2-C3
34	g	630	LHG	O1-C1-C2-C3
34	e	630	LHG	O1-C1-C2-C3
32	9	401	8CT	C25-C26-C28-C29
32	A	850	8CT	C10-C11-C12-C13
32	A	850	8CT	C25-C26-C28-C29
32	F	302	8CT	C10-C11-C12-C13
32	M	102	8CT	C10-C11-C12-C13
31	K	102	CLA	C3-C5-C6-C7
30	8	302	CHL	C8-C10-C11-C12
30	c	608	CHL	C13-C15-C16-C17
30	d	609	CHL	C8-C10-C11-C12
34	8	601	LHG	C12-C13-C14-C15
36	J	105	LMG	C30-C31-C32-C33
34	g	630	LHG	C23-C24-C25-C26
34	i	630	LHG	C23-C24-C25-C26
36	L	210	LMG	C10-C11-C12-C13
30	8	306	CHL	O1D-CGD-O2D-CED
31	f	613	CLA	C6-C7-C8-C10
34	0	601	LHG	C28-C29-C30-C31
34	1	601	LHG	C14-C15-C16-C17
34	3	601	LHG	C14-C15-C16-C17
34	K	106	LHG	C15-C16-C17-C18
34	i	630	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	e	630	LHG	C12-C13-C14-C15
30	2	302	CHL	C4B-C3B-CAB-CBB
31	0	312	CLA	C4B-C3B-CAB-CBB
31	1	308	CLA	C4B-C3B-CAB-CBB
31	1	310	CLA	C4B-C3B-CAB-CBB
31	3	310	CLA	C4B-C3B-CAB-CBB
31	A	824	CLA	C4B-C3B-CAB-CBB
31	A	839	CLA	C4B-C3B-CAB-CBB
31	B	824	CLA	C4B-C3B-CAB-CBB
31	G	103	CLA	C4B-C3B-CAB-CBB
31	O	201	CLA	C4B-C3B-CAB-CBB
30	3	307	CHL	C16-C17-C18-C20
30	6	301	CHL	C11-C12-C13-C15
30	c	609	CHL	C16-C17-C18-C20
30	b	608	CHL	C16-C17-C18-C19
30	d	609	CHL	C16-C17-C18-C19
30	d	609	CHL	C16-C17-C18-C20
31	0	309	CLA	C11-C12-C13-C14
31	A	824	CLA	C6-C7-C8-C9
36	J	105	LMG	O6-C1-O1-C7
41	B	849	DGD	O6E-C1E-O5D-C6D
30	6	301	CHL	C8-C10-C11-C12
34	a	630	LHG	C15-C16-C17-C18
34	d	630	LHG	C25-C26-C27-C28
30	h	601	CHL	CBA-CGA-O2A-C1
30	i	601	CHL	CBA-CGA-O2A-C1
31	b	613	CLA	CBD-CGD-O2D-CED
30	5	313	CHL	O1D-CGD-O2D-CED
30	8	302	CHL	O1D-CGD-O2D-CED
31	A	819	CLA	O1D-CGD-O2D-CED
34	3	603	LHG	C9-C10-C11-C12
34	d	630	LHG	C23-C24-C25-C26
30	3	307	CHL	C8-C10-C11-C12
31	3	308	CLA	C8-C10-C11-C12
30	a	602	CHL	O1A-CGA-O2A-C1
31	2	312	CLA	O1A-CGA-O2A-C1
31	9	300	CLA	O1A-CGA-O2A-C1
33	2	502	0UR	O57-C45-C46-C47
31	7	311	CLA	CBA-CGA-O2A-C1
36	3	602	LMG	C12-C13-C14-C15
36	J	105	LMG	C34-C35-C36-C37
30	6	301	CHL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	607	CHL	C3A-C2A-CAA-CBA
30	f	607	CHL	C3A-C2A-CAA-CBA
30	i	607	CHL	C3A-C2A-CAA-CBA
31	0	303	CLA	C3A-C2A-CAA-CBA
31	0	311	CLA	C3A-C2A-CAA-CBA
31	0	313	CLA	C3A-C2A-CAA-CBA
31	3	303	CLA	C3A-C2A-CAA-CBA
31	7	317	CLA	C3A-C2A-CAA-CBA
31	9	311	CLA	C3A-C2A-CAA-CBA
31	A	803	CLA	C3A-C2A-CAA-CBA
31	A	832	CLA	C3A-C2A-CAA-CBA
31	A	836	CLA	C3A-C2A-CAA-CBA
31	B	814	CLA	C3A-C2A-CAA-CBA
31	B	817	CLA	C3A-C2A-CAA-CBA
31	B	827	CLA	C3A-C2A-CAA-CBA
31	B	836	CLA	C3A-C2A-CAA-CBA
31	L	202	CLA	C3A-C2A-CAA-CBA
31	H	201	CLA	C3A-C2A-CAA-CBA
30	b	601	CHL	C5-C6-C7-C8
30	e	608	CHL	C13-C15-C16-C17
31	A	840	CLA	C10-C11-C12-C13
31	B	817	CLA	C8-C10-C11-C12
32	9	401	8CT	C16-C17-C18-C19
33	g	520	0UR	C3-C4-C5-C6
34	B	854	LHG	C28-C29-C30-C31
34	G	105	LHG	C13-C14-C15-C16
41	B	849	DGD	C9B-CAB-CBB-CCB
30	7	313	CHL	CBA-CGA-O2A-C1
30	f	601	CHL	O1D-CGD-O2D-CED
30	c	608	CHL	C16-C17-C18-C19
30	f	609	CHL	C16-C17-C18-C20
31	A	824	CLA	C6-C7-C8-C10
34	f	630	LHG	C9-C10-C11-C12
34	f	630	LHG	C26-C27-C28-C29
34	4	601	LHG	C9-C10-C11-C12
36	9	602	LMG	C12-C13-C14-C15
34	7	601	LHG	C4-C5-C6-O8
30	f	602	CHL	CBD-CGD-O2D-CED
30	4	313	CHL	CBD-CGD-O2D-CED
31	6	303	CLA	CBD-CGD-O2D-CED
31	B	825	CLA	CBD-CGD-O2D-CED
34	1	601	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	e	630	LHG	C14-C15-C16-C17
31	A	805	CLA	O2A-C1-C2-C3
30	4	319	CHL	C3-C5-C6-C7
31	A	828	CLA	C3-C5-C6-C7
34	e	630	LHG	C15-C16-C17-C18
30	7	306	CHL	C4-C3-C5-C6
31	9	300	CLA	C4-C3-C5-C6
31	d	613	CLA	CBA-CGA-O2A-C1
41	B	849	DGD	C2A-C1A-O1G-C1G
31	8	310	CLA	O1A-CGA-O2A-C1
30	1	313	CHL	C2-C3-C5-C6
30	7	306	CHL	C2-C3-C5-C6
34	G	105	LHG	C8-C7-O7-C5
36	3	602	LMG	C11-C10-O7-C8
30	d	605	CHL	O1D-CGD-O2D-CED
30	8	302	CHL	C2A-CAA-CBA-CGA
30	h	608	CHL	C2A-CAA-CBA-CGA
34	2	601	LHG	O1-C1-C2-O2
34	3	601	LHG	O1-C1-C2-O2
34	3	603	LHG	O1-C1-C2-O2
34	M	104	LHG	O1-C1-C2-O2
34	c	630	LHG	O1-C1-C2-O2
34	h	630	LHG	O1-C1-C2-O2
34	H	203	LHG	O1-C1-C2-O2
34	5	601	LHG	C26-C27-C28-C29
35	0	603	SQD	C11-C10-C9-C8
36	9	602	LMG	C38-C39-C40-C41
31	1	312	CLA	O1A-CGA-O2A-C1
31	c	604	CLA	O1A-CGA-O2A-C1
30	b	601	CHL	C16-C17-C18-C20
30	e	608	CHL	C16-C17-C18-C19
31	b	611	CLA	C11-C12-C13-C14
34	K	106	LHG	C14-C15-C16-C17
36	L	211	LMG	C13-C14-C15-C16
30	2	302	CHL	C2B-C3B-CAB-CBB
30	f	602	CHL	C2B-C3B-CAB-CBB
31	0	312	CLA	C2B-C3B-CAB-CBB
31	0	321	CLA	C2B-C3B-CAB-CBB
31	1	308	CLA	C2B-C3B-CAB-CBB
31	1	310	CLA	C2B-C3B-CAB-CBB
31	3	310	CLA	C2B-C3B-CAB-CBB
31	5	311	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	7	317	CLA	C2B-C3B-CAB-CBB
31	A	806	CLA	C2B-C3B-CAB-CBB
31	A	824	CLA	C2B-C3B-CAB-CBB
31	A	839	CLA	C2B-C3B-CAB-CBB
31	B	824	CLA	C2B-C3B-CAB-CBB
31	B	833	CLA	C2B-C3B-CAB-CBB
31	G	103	CLA	C2B-C3B-CAB-CBB
31	O	201	CLA	C2B-C3B-CAB-CBB
39	A	857	CL0	C2B-C3B-CAB-CBB
30	i	602	CHL	CBA-CGA-O2A-C1
36	L	210	LMG	C4-C5-C6-O5
33	3	501	0UR	O44-C45-C46-C47
31	c	613	CLA	C6-C7-C8-C10
30	0	302	CHL	O1A-CGA-O2A-C1
30	7	302	CHL	O1A-CGA-O2A-C1
30	a	602	CHL	C10-C11-C12-C13
34	A	844	LHG	C1-C2-C3-O3
34	b	630	LHG	C30-C31-C32-C33
34	g	630	LHG	C25-C26-C27-C28
34	H	203	LHG	C26-C27-C28-C29
34	M	104	LHG	C25-C26-C27-C28
33	a	520	0UR	C46-C45-O44-C43
30	5	302	CHL	C8-C10-C11-C12
31	9	302	CLA	C13-C15-C16-C17
31	B	820	CLA	C5-C6-C7-C8
34	3	601	LHG	C5-C4-O6-P
31	1	303	CLA	O1A-CGA-O2A-C1
36	J	105	LMG	O10-C28-O8-C9
36	9	602	LMG	C17-C18-C19-C20
36	J	105	LMG	C14-C15-C16-C17
31	e	611	CLA	C6-C7-C8-C9
34	a	630	LHG	C23-C24-C25-C26
31	i	603	CLA	O1A-CGA-O2A-C1
30	h	602	CHL	C3-C5-C6-C7
31	B	819	CLA	C3-C5-C6-C7
32	1	402	8CT	C02-C03-C10-C11
32	2	402	8CT	C02-C03-C10-C11
32	3	402	8CT	C04-C03-C10-C11
32	6	402	8CT	C02-C03-C10-C11
32	7	402	8CT	C04-C03-C10-C11
32	7	404	8CT	C02-C03-C10-C11
32	8	402	8CT	C02-C03-C10-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	8	406	8CT	C04-C03-C10-C11
32	9	401	8CT	C02-C03-C10-C11
32	A	848	8CT	C04-C03-C10-C11
32	A	854	8CT	C02-C03-C10-C11
32	B	804	8CT	C02-C03-C10-C11
32	B	845	8CT	C02-C03-C10-C11
32	B	847	8CT	C02-C03-C10-C11
32	B	847	8CT	C04-C03-C10-C11
32	B	848	8CT	C02-C03-C10-C11
32	B	851	8CT	C02-C03-C10-C11
32	G	104	8CT	C02-C03-C10-C11
32	I	101	8CT	C02-C03-C10-C11
32	J	101	8CT	C04-C03-C10-C11
32	L	206	8CT	C02-C03-C10-C11
32	L	206	8CT	C04-C03-C10-C11
32	L	209	8CT	C04-C03-C10-C11
32	K	107	8CT	C04-C03-C10-C11
32	4	402	8CT	C02-C03-C10-C11
31	K	102	CLA	C2C-C3C-CAC-CBC
34	1	601	LHG	C10-C11-C12-C13
36	O	207	LMG	C33-C34-C35-C36
33	3	501	0UR	O57-C45-C46-C47
31	3	313	CLA	O1D-CGD-O2D-CED
30	3	307	CHL	CBA-CGA-O2A-C1
31	1	304	CLA	CBA-CGA-O2A-C1
31	4	311	CLA	CBA-CGA-O2A-C1
30	d	609	CHL	C13-C15-C16-C17
30	f	601	CHL	C15-C16-C17-C18
31	A	828	CLA	C5-C6-C7-C8
31	B	837	CLA	C5-C6-C7-C8
34	b	630	LHG	C8-C7-O7-C5
34	K	106	LHG	C27-C28-C29-C30
36	9	602	LMG	C13-C14-C15-C16
31	2	311	CLA	O2A-C1-C2-C3
30	g	601	CHL	O1D-CGD-O2D-CED
30	e	602	CHL	O1A-CGA-O2A-C1
31	1	310	CLA	O1A-CGA-O2A-C1
31	A	838	CLA	C11-C10-C8-C9
34	5	601	LHG	C23-C24-C25-C26
34	f	630	LHG	C23-C24-C25-C26
31	c	613	CLA	C11-C10-C8-C7
34	7	603	LHG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	f	609	CHL	C13-C15-C16-C17
30	b	602	CHL	C15-C16-C17-C18
35	0	603	SQD	C9-C10-C11-C12
30	1	313	CHL	C4-C3-C5-C6
30	c	608	CHL	C4-C3-C5-C6
30	b	614	CHL	O1D-CGD-O2D-CED
30	1	313	CHL	C6-C7-C8-C10
30	1	313	CHL	C11-C12-C13-C15
30	2	319	CHL	C6-C7-C8-C10
30	3	302	CHL	C11-C10-C8-C7
30	3	307	CHL	C2-C3-C5-C6
30	6	308	CHL	C6-C7-C8-C10
30	c	608	CHL	C2-C3-C5-C6
30	b	602	CHL	C11-C12-C13-C15
30	f	601	CHL	C11-C12-C13-C15
30	e	608	CHL	C6-C7-C8-C10
31	0	312	CLA	C12-C13-C15-C16
31	3	309	CLA	C12-C13-C15-C16
31	5	312	CLA	C6-C7-C8-C10
31	6	317	CLA	C11-C12-C13-C15
31	7	309	CLA	C11-C10-C8-C7
31	A	806	CLA	C12-C13-C15-C16
31	A	808	CLA	C11-C12-C13-C15
31	A	826	CLA	C11-C12-C13-C15
31	A	828	CLA	C12-C13-C15-C16
31	A	830	CLA	C12-C13-C15-C16
31	B	814	CLA	C11-C12-C13-C15
31	B	814	CLA	C12-C13-C15-C16
31	B	816	CLA	C6-C7-C8-C10
31	B	832	CLA	C6-C7-C8-C10
31	B	839	CLA	C11-C12-C13-C15
31	L	201	CLA	C6-C7-C8-C10
38	B	842	PQN	C21-C22-C23-C25
39	A	857	CL0	C12-C13-C15-C16
30	d	607	CHL	CBA-CGA-O2A-C1
31	7	311	CLA	O1A-CGA-O2A-C1
31	d	613	CLA	O1A-CGA-O2A-C1
34	2	601	LHG	O10-C23-O8-C6
41	B	849	DGD	O1A-C1A-O1G-C1G
31	b	613	CLA	C6-C7-C8-C10
30	0	302	CHL	C13-C15-C16-C17
30	7	302	CHL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	7	306	CHL	C8-C10-C11-C12
30	d	602	CHL	C13-C15-C16-C17
31	B	801	CLA	C10-C11-C12-C13
32	B	843	8CT	C18-C19-C20-C21
32	B	846	8CT	C16-C17-C18-C19
32	M	102	8CT	C16-C17-C18-C19
30	i	605	CHL	CBD-CGD-O2D-CED
31	A	817	CLA	CBD-CGD-O2D-CED
31	B	817	CLA	O1D-CGD-O2D-CED
34	G	105	LHG	O9-C7-O7-C5
34	h	630	LHG	O9-C7-O7-C5
34	G	105	LHG	C23-C24-C25-C26
30	2	302	CHL	CBA-CGA-O2A-C1
30	6	302	CHL	CBA-CGA-O2A-C1
30	a	609	CHL	CBA-CGA-O2A-C1
30	h	602	CHL	CBA-CGA-O2A-C1
30	4	302	CHL	CBA-CGA-O2A-C1
31	5	312	CLA	CBA-CGA-O2A-C1
31	6	310	CLA	CBA-CGA-O2A-C1
31	A	840	CLA	CBA-CGA-O2A-C1
34	0	601	LHG	C24-C23-O8-C6
33	5	501	0UR	O57-C45-C46-C47
33	h	520	0UR	O57-C45-C46-C47
34	9	601	LHG	C11-C10-C9-C8
34	b	630	LHG	C26-C27-C28-C29
30	3	305	CHL	C2A-CAA-CBA-CGA
30	5	302	CHL	C2A-CAA-CBA-CGA
30	5	305	CHL	C2A-CAA-CBA-CGA
30	b	601	CHL	C2A-CAA-CBA-CGA
30	4	302	CHL	C2A-CAA-CBA-CGA
31	A	841	CLA	C2A-CAA-CBA-CGA
31	B	831	CLA	C2A-CAA-CBA-CGA
31	K	104	CLA	C2A-CAA-CBA-CGA
30	h	605	CHL	O1D-CGD-O2D-CED
31	f	613	CLA	C5-C6-C7-C8
34	3	601	LHG	C15-C16-C17-C18
34	A	844	LHG	C25-C26-C27-C28
34	f	630	LHG	C12-C13-C14-C15
36	A	856	LMG	O6-C5-C6-O5
36	B	853	LMG	C31-C32-C33-C34
30	i	602	CHL	O1A-CGA-O2A-C1
30	5	305	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	7	306	CHL	O1D-CGD-O2D-CED
30	a	609	CHL	O1D-CGD-O2D-CED
31	A	838	CLA	C11-C10-C8-C7
31	L	204	CLA	O1D-CGD-O2D-CED
31	1	312	CLA	C8-C10-C11-C12
31	9	309	CLA	C5-C6-C7-C8
30	f	602	CHL	C15-C16-C17-C18
30	2	319	CHL	C3-C5-C6-C7
31	A	835	CLA	C3-C5-C6-C7
31	3	310	CLA	O1D-CGD-O2D-CED
34	7	602	LHG	C10-C11-C12-C13
31	A	823	CLA	CBD-CGD-O2D-CED
31	B	823	CLA	CBD-CGD-O2D-CED
31	K	105	CLA	CBA-CGA-O2A-C1
33	4	502	0UR	O57-C45-C46-C47
31	3	304	CLA	C15-C16-C17-C18
31	B	811	CLA	C8-C10-C11-C12
31	f	603	CLA	C5-C6-C7-C8
30	0	302	CHL	O1D-CGD-O2D-CED
30	6	315	CHL	O1D-CGD-O2D-CED
30	h	602	CHL	O1D-CGD-O2D-CED
34	7	603	LHG	C28-C29-C30-C31
34	H	203	LHG	C25-C26-C27-C28
36	A	856	LMG	C30-C31-C32-C33
34	e	630	LHG	C23-C24-C25-C26
36	B	853	LMG	C10-C11-C12-C13
34	K	106	LHG	C8-C7-O7-C5
34	f	630	LHG	C8-C7-O7-C5
34	h	630	LHG	C8-C7-O7-C5
36	L	210	LMG	C11-C10-O7-C8
36	B	853	LMG	C15-C16-C17-C18
36	B	853	LMG	C17-C18-C19-C20
30	1	307	CHL	C13-C15-C16-C17
31	3	309	CLA	C5-C6-C7-C8
30	8	305	CHL	CBD-CGD-O2D-CED
30	a	602	CHL	CBD-CGD-O2D-CED
30	e	601	CHL	CBD-CGD-O2D-CED
31	B	814	CLA	CBD-CGD-O2D-CED
34	f	630	LHG	O9-C7-O7-C5
31	3	310	CLA	C3-C5-C6-C7
35	0	603	SQD	C2-C1-O6-C44
30	i	602	CHL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	7	601	LHG	O7-C5-C6-O8
34	7	603	LHG	C26-C27-C28-C29
30	a	601	CHL	O1D-CGD-O2D-CED
31	B	817	CLA	C11-C12-C13-C14
31	7	309	CLA	C5-C6-C7-C8
31	B	840	CLA	C15-C16-C17-C18
31	A	806	CLA	C4-C3-C5-C6
30	4	308	CHL	CBA-CGA-O2A-C1
30	1	307	CHL	C2-C3-C5-C6
31	A	830	CLA	C2-C3-C5-C6
31	B	817	CLA	C2-C3-C5-C6
34	M	104	LHG	C26-C27-C28-C29
30	0	302	CHL	C14-C13-C15-C16
30	1	307	CHL	C6-C7-C8-C9
30	1	313	CHL	C6-C7-C8-C9
30	2	301	CHL	C6-C7-C8-C9
30	3	307	CHL	C6-C7-C8-C9
30	6	308	CHL	C6-C7-C8-C9
30	7	306	CHL	C11-C10-C8-C9
30	b	608	CHL	C14-C13-C15-C16
31	0	308	CLA	C6-C7-C8-C9
31	3	308	CLA	C6-C7-C8-C9
31	6	317	CLA	C11-C10-C8-C9
31	6	317	CLA	C11-C12-C13-C14
31	8	304	CLA	C11-C10-C8-C9
31	9	302	CLA	C11-C10-C8-C9
31	9	309	CLA	C11-C10-C8-C9
31	A	806	CLA	C14-C13-C15-C16
31	A	811	CLA	C11-C10-C8-C9
31	A	818	CLA	C11-C10-C8-C9
31	A	819	CLA	C11-C10-C8-C9
31	A	819	CLA	C14-C13-C15-C16
31	A	821	CLA	C6-C7-C8-C9
31	A	828	CLA	C14-C13-C15-C16
31	A	832	CLA	C6-C7-C8-C9
31	B	814	CLA	C14-C13-C15-C16
31	B	839	CLA	C11-C12-C13-C14
31	4	310	CLA	C11-C10-C8-C9
38	B	842	PQN	C21-C22-C23-C24
36	2	602	LMG	C30-C31-C32-C33
30	2	307	CHL	C2A-CAA-CBA-CGA
30	3	302	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	6	302	CHL	C2A-CAA-CBA-CGA
30	7	305	CHL	C2A-CAA-CBA-CGA
30	8	306	CHL	C2A-CAA-CBA-CGA
31	1	312	CLA	C2A-CAA-CBA-CGA
31	h	604	CLA	C2A-CAA-CBA-CGA
34	G	105	LHG	C25-C26-C27-C28
34	a	630	LHG	C25-C26-C27-C28
31	L	202	CLA	O1A-CGA-O2A-C1
32	2	402	8CT	C14-C15-C16-C39
32	F	302	8CT	C10-C11-C12-C40
32	J	104	8CT	C14-C15-C16-C39
32	L	205	8CT	C10-C11-C12-C40
42	a	523	NEX	C31-C32-C33-C40
42	d	523	NEX	C31-C32-C33-C40
42	f	523	NEX	C31-C32-C33-C40
42	g	523	NEX	C31-C32-C33-C40
42	i	523	NEX	C31-C32-C33-C40
31	f	611	CLA	O1D-CGD-O2D-CED
30	f	601	CHL	C8-C10-C11-C12
31	B	837	CLA	C15-C16-C17-C18
36	2	602	LMG	C32-C33-C34-C35
36	A	856	LMG	C29-C30-C31-C32
32	J	104	8CT	C14-C15-C16-C17
32	L	205	8CT	C10-C11-C12-C13
30	3	307	CHL	O1A-CGA-O2A-C1
31	1	304	CLA	O1A-CGA-O2A-C1
31	4	311	CLA	O1A-CGA-O2A-C1
30	5	313	CHL	C1A-C2A-CAA-CBA
30	a	601	CHL	C1A-C2A-CAA-CBA
30	b	601	CHL	C1A-C2A-CAA-CBA
30	f	607	CHL	C1A-C2A-CAA-CBA
30	4	307	CHL	C1A-C2A-CAA-CBA
31	0	303	CLA	C1A-C2A-CAA-CBA
31	0	311	CLA	C1A-C2A-CAA-CBA
31	0	313	CLA	C1A-C2A-CAA-CBA
31	1	309	CLA	C1A-C2A-CAA-CBA
31	5	309	CLA	C1A-C2A-CAA-CBA
31	7	317	CLA	C1A-C2A-CAA-CBA
31	7	318	CLA	C1A-C2A-CAA-CBA
31	8	314	CLA	C1A-C2A-CAA-CBA
31	9	308	CLA	C1A-C2A-CAA-CBA
31	9	311	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	803	CLA	C1A-C2A-CAA-CBA
31	A	806	CLA	C1A-C2A-CAA-CBA
31	A	808	CLA	C1A-C2A-CAA-CBA
31	A	818	CLA	C1A-C2A-CAA-CBA
31	A	832	CLA	C1A-C2A-CAA-CBA
31	A	836	CLA	C1A-C2A-CAA-CBA
31	A	843	CLA	C1A-C2A-CAA-CBA
31	B	828	CLA	C1A-C2A-CAA-CBA
31	K	101	CLA	C1A-C2A-CAA-CBA
31	a	610	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C1A-C2A-CAA-CBA
31	d	610	CLA	C1A-C2A-CAA-CBA
31	h	610	CLA	C1A-C2A-CAA-CBA
31	H	202	CLA	C1A-C2A-CAA-CBA
31	e	610	CLA	C1A-C2A-CAA-CBA
30	8	313	CHL	C6-C7-C8-C9
30	c	608	CHL	C16-C17-C18-C20
31	0	309	CLA	C11-C12-C13-C15
31	A	828	CLA	C16-C17-C18-C19
31	B	827	CLA	C16-C17-C18-C19
31	K	101	CLA	C11-C12-C13-C14
34	b	630	LHG	O9-C7-O7-C5
34	8	601	LHG	C10-C11-C12-C13
34	f	630	LHG	C27-C28-C29-C30
32	A	846	8CT	C18-C19-C20-C21
32	A	848	8CT	C18-C19-C20-C21
32	A	854	8CT	C18-C19-C20-C21
32	L	205	8CT	C16-C17-C18-C19
32	K	107	8CT	C16-C17-C18-C19
30	5	301	CHL	O1D-CGD-O2D-CED
30	7	301	CHL	C10-C11-C12-C13
30	c	602	CHL	C5-C6-C7-C8
30	c	609	CHL	C5-C6-C7-C8
31	1	310	CLA	C10-C11-C12-C13
31	B	816	CLA	C10-C11-C12-C13
38	B	842	PQN	C20-C21-C22-C23
34	8	601	LHG	C3-O3-P-O6
34	9	601	LHG	C4-O6-P-O3
34	G	105	LHG	C3-O3-P-O6
34	M	104	LHG	C30-C31-C32-C33
34	c	630	LHG	C29-C30-C31-C32
34	4	601	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	2	302	CHL	CBD-CGD-O2D-CED
31	A	817	CLA	C3-C5-C6-C7
31	4	310	CLA	C3-C5-C6-C7
34	7	603	LHG	C5-C4-O6-P
31	B	810	CLA	C2C-C3C-CAC-CBC
34	c	630	LHG	C9-C10-C11-C12
30	1	313	CHL	C10-C11-C12-C13
30	1	302	CHL	CBA-CGA-O2A-C1
30	g	606	CHL	CBA-CGA-O2A-C1
31	B	818	CLA	CBA-CGA-O2A-C1
34	B	852	LHG	O6-C4-C5-C6
34	d	630	LHG	O6-C4-C5-C6
34	M	104	LHG	C9-C10-C11-C12
41	B	849	DGD	CBB-CCB-CDB-CEB
33	e	520	0UR	O57-C45-C46-C47
34	A	855	LHG	C23-C24-C25-C26
34	f	630	LHG	C14-C15-C16-C17
36	3	602	LMG	C32-C33-C34-C35
34	B	854	LHG	C27-C28-C29-C30
34	a	630	LHG	C11-C10-C9-C8
30	6	301	CHL	C3-C5-C6-C7
31	0	311	CLA	CBA-CGA-O2A-C1
31	A	814	CLA	CBA-CGA-O2A-C1
30	3	307	CHL	C4-C3-C5-C6
34	G	105	LHG	C9-C10-C11-C12
34	K	106	LHG	C32-C33-C34-C35
34	b	630	LHG	C14-C15-C16-C17
36	2	602	LMG	C12-C13-C14-C15
31	f	603	CLA	O1D-CGD-O2D-CED
30	4	302	CHL	O1A-CGA-O2A-C1
31	5	312	CLA	O1A-CGA-O2A-C1
31	6	310	CLA	O1A-CGA-O2A-C1
34	0	601	LHG	O10-C23-O8-C6
34	9	601	LHG	C31-C32-C33-C34
31	0	308	CLA	C2A-CAA-CBA-CGA
31	1	304	CLA	C2A-CAA-CBA-CGA
31	7	308	CLA	C2A-CAA-CBA-CGA
31	7	317	CLA	C2A-CAA-CBA-CGA
31	A	820	CLA	C2A-CAA-CBA-CGA
30	e	602	CHL	C11-C12-C13-C15
30	8	315	CHL	O1D-CGD-O2D-CED
33	4	502	0UR	O44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	1	601	LHG	C4-C5-C6-O8
34	2	601	LHG	C4-C5-C6-O8
34	7	603	LHG	C4-C5-C6-O8
34	G	105	LHG	C4-C5-C6-O8
35	0	603	SQD	O6-C44-C45-C46
35	0	603	SQD	C44-C45-C46-O48
36	A	856	LMG	C7-C8-C9-O8
36	B	853	LMG	C18-C19-C20-C21
33	a	520	0UR	O57-C45-O44-C43
30	2	302	CHL	O1A-CGA-O2A-C1
30	6	302	CHL	O1A-CGA-O2A-C1
30	h	602	CHL	O1A-CGA-O2A-C1
31	A	840	CLA	O1A-CGA-O2A-C1
36	3	602	LMG	C8-C7-O1-C1
36	B	853	LMG	C32-C33-C34-C35
30	3	302	CHL	C14-C13-C15-C16
30	2	319	CHL	CAA-CBA-CGA-O2A
30	d	607	CHL	CAA-CBA-CGA-O2A
31	6	318	CLA	CAA-CBA-CGA-O2A
30	a	609	CHL	O1A-CGA-O2A-C1
31	K	105	CLA	O1A-CGA-O2A-C1
34	0	601	LHG	C14-C15-C16-C17
30	5	313	CHL	CBA-CGA-O2A-C1
36	9	602	LMG	O6-C1-O1-C7
34	e	630	LHG	C10-C11-C12-C13
31	A	852	CLA	CBD-CGD-O2D-CED
30	0	302	CHL	C15-C16-C17-C18
30	d	602	CHL	C15-C16-C17-C18
34	7	603	LHG	C10-C11-C12-C13
41	B	849	DGD	CAB-CBB-CCB-CDB
31	5	308	CLA	CBA-CGA-O2A-C1
31	A	814	CLA	O1D-CGD-O2D-CED
30	1	307	CHL	C4-C3-C5-C6
31	A	839	CLA	C4-C3-C5-C6
34	7	602	LHG	C11-C10-C9-C8
31	A	806	CLA	C2-C3-C5-C6
31	A	839	CLA	C2-C3-C5-C6
30	1	307	CHL	C16-C17-C18-C19
31	A	830	CLA	C16-C17-C18-C19
31	3	308	CLA	CBA-CGA-O2A-C1
31	A	815	CLA	CBA-CGA-O2A-C1
31	A	843	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	L	211	LMG	O6-C5-C6-O5
31	8	309	CLA	CBD-CGD-O2D-CED
31	A	835	CLA	CBD-CGD-O2D-CED
31	J	103	CLA	CBD-CGD-O2D-CED
30	8	313	CHL	C5-C6-C7-C8
31	3	304	CLA	C13-C15-C16-C17
31	7	308	CLA	C8-C10-C11-C12
31	9	302	CLA	C10-C11-C12-C13
31	A	804	CLA	C5-C6-C7-C8
31	B	801	CLA	C15-C16-C17-C18
31	B	805	CLA	C15-C16-C17-C18
31	4	304	CLA	C8-C10-C11-C12
30	5	302	CHL	C15-C16-C17-C18
34	H	203	LHG	C28-C29-C30-C31
36	L	211	LMG	C17-C18-C19-C20
34	B	852	LHG	C6-C5-O7-C7
36	3	602	LMG	C7-C8-O7-C10
30	c	607	CHL	C2A-CAA-CBA-CGA
31	7	303	CLA	C2A-CAA-CBA-CGA
31	A	809	CLA	C2A-CAA-CBA-CGA
34	K	106	LHG	O9-C7-O7-C5
30	3	307	CHL	C15-C16-C17-C18
31	A	839	CLA	C13-C15-C16-C17
31	K	101	CLA	C10-C11-C12-C13
30	1	302	CHL	C2-C1-O2A-CGA
30	b	602	CHL	C2-C1-O2A-CGA
36	J	105	LMG	C4-C5-C6-O5
30	7	313	CHL	O1D-CGD-O2D-CED
30	c	607	CHL	O1D-CGD-O2D-CED
30	e	606	CHL	CBD-CGD-O2D-CED
31	B	833	CLA	C3-C5-C6-C7
34	0	601	LHG	C33-C34-C35-C36
33	e	520	0UR	O44-C45-C46-C47
30	i	606	CHL	O1D-CGD-O2D-CED
30	6	308	CHL	C8-C10-C11-C12
34	H	203	LHG	C2-C3-O3-P
30	1	302	CHL	C15-C16-C17-C18
30	h	602	CHL	C15-C16-C17-C18
34	b	630	LHG	C15-C16-C17-C18
30	c	602	CHL	CBA-CGA-O2A-C1
31	B	830	CLA	CBA-CGA-O2A-C1
30	i	602	CHL	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	e	609	CHL	C11-C12-C13-C15
31	A	830	CLA	C16-C17-C18-C20
31	K	101	CLA	C11-C12-C13-C15
35	0	603	SQD	C10-C11-C12-C13
34	1	601	LHG	C27-C28-C29-C30
30	9	313	CHL	O1D-CGD-O2D-CED
30	c	602	CHL	O1D-CGD-O2D-CED
30	i	601	CHL	O1D-CGD-O2D-CED
31	8	314	CLA	O1D-CGD-O2D-CED
30	1	302	CHL	O1A-CGA-O2A-C1
36	9	602	LMG	C37-C38-C39-C40
30	h	602	CHL	C8-C10-C11-C12
31	6	309	CLA	C5-C6-C7-C8
31	A	829	CLA	C10-C11-C12-C13
31	B	819	CLA	C10-C11-C12-C13
37	d	522	0IE	C14-C15-C16-C17
30	5	306	CHL	CAA-CBA-CGA-O2A
34	A	855	LHG	O7-C5-C6-O8
30	8	302	CHL	C15-C16-C17-C18
36	A	856	LMG	C32-C33-C34-C35
31	B	839	CLA	C5-C6-C7-C8
30	g	606	CHL	O1A-CGA-O2A-C1
34	8	601	LHG	C28-C29-C30-C31
34	4	601	LHG	C12-C13-C14-C15
36	9	602	LMG	C36-C37-C38-C39
30	b	608	CHL	C4-C3-C5-C6
31	A	835	CLA	C4-C3-C5-C6
31	6	310	CLA	C5-C6-C7-C8
31	B	841	CLA	C13-C15-C16-C17
30	1	307	CHL	C6-C7-C8-C10
30	2	301	CHL	C6-C7-C8-C10
30	2	302	CHL	C6-C7-C8-C10
30	3	307	CHL	C6-C7-C8-C10
30	3	307	CHL	C12-C13-C15-C16
30	5	302	CHL	C11-C10-C8-C7
30	5	302	CHL	C11-C12-C13-C15
30	5	302	CHL	C12-C13-C15-C16
30	7	301	CHL	C12-C13-C15-C16
30	8	302	CHL	C12-C13-C15-C16
30	c	608	CHL	C12-C13-C15-C16
30	b	601	CHL	C12-C13-C15-C16
30	d	602	CHL	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	609	CHL	C12-C13-C15-C16
31	0	308	CLA	C11-C10-C8-C7
31	1	312	CLA	C6-C7-C8-C10
31	2	304	CLA	C11-C10-C8-C7
31	3	309	CLA	C11-C12-C13-C15
31	3	310	CLA	C6-C7-C8-C10
31	6	317	CLA	C11-C10-C8-C7
31	8	304	CLA	C11-C10-C8-C7
31	8	309	CLA	C11-C10-C8-C7
31	9	300	CLA	C6-C7-C8-C10
31	9	309	CLA	C11-C10-C8-C7
31	A	803	CLA	C12-C13-C15-C16
31	A	808	CLA	C11-C10-C8-C7
31	A	811	CLA	C11-C10-C8-C7
31	A	811	CLA	C11-C12-C13-C15
31	A	813	CLA	C6-C7-C8-C10
31	A	815	CLA	C6-C7-C8-C10
31	A	817	CLA	C11-C10-C8-C7
31	A	819	CLA	C6-C7-C8-C10
31	A	819	CLA	C11-C10-C8-C7
31	A	819	CLA	C11-C12-C13-C15
31	A	819	CLA	C12-C13-C15-C16
31	A	825	CLA	C11-C10-C8-C7
31	A	828	CLA	C11-C12-C13-C15
31	A	835	CLA	C2-C3-C5-C6
31	A	839	CLA	C11-C12-C13-C15
31	A	853	CLA	C6-C7-C8-C10
31	B	801	CLA	C11-C10-C8-C7
31	B	817	CLA	C11-C10-C8-C7
31	B	820	CLA	C6-C7-C8-C10
31	B	834	CLA	C6-C7-C8-C10
31	B	834	CLA	C11-C10-C8-C7
30	2	308	CHL	O1A-CGA-O2A-C1
30	6	302	CHL	C15-C16-C17-C18
31	5	303	CLA	C10-C11-C12-C13
34	K	106	LHG	C30-C31-C32-C33
30	1	313	CHL	C11-C10-C8-C9
30	3	307	CHL	C14-C13-C15-C16
30	5	302	CHL	C11-C12-C13-C14
30	c	602	CHL	C11-C10-C8-C9
30	c	608	CHL	C6-C7-C8-C9
30	c	609	CHL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	b	608	CHL	C6-C7-C8-C9
30	d	602	CHL	C6-C7-C8-C9
30	d	602	CHL	C11-C12-C13-C14
30	d	609	CHL	C11-C12-C13-C14
31	0	312	CLA	C14-C13-C15-C16
31	1	312	CLA	C6-C7-C8-C9
31	2	310	CLA	C6-C7-C8-C9
31	3	309	CLA	C11-C12-C13-C14
31	3	310	CLA	C11-C12-C13-C14
31	9	300	CLA	C6-C7-C8-C9
31	9	302	CLA	C14-C13-C15-C16
31	A	803	CLA	C14-C13-C15-C16
31	A	805	CLA	C6-C7-C8-C9
31	A	808	CLA	C11-C10-C8-C9
31	A	815	CLA	C14-C13-C15-C16
31	A	819	CLA	C6-C7-C8-C9
31	A	819	CLA	C11-C12-C13-C14
31	A	825	CLA	C11-C10-C8-C9
31	A	828	CLA	C11-C12-C13-C14
31	A	829	CLA	C11-C12-C13-C14
31	A	830	CLA	C14-C13-C15-C16
31	A	833	CLA	C6-C7-C8-C9
31	B	801	CLA	C11-C10-C8-C9
31	B	809	CLA	C11-C12-C13-C14
31	B	817	CLA	C11-C10-C8-C9
31	B	819	CLA	C11-C10-C8-C9
31	B	839	CLA	C14-C13-C15-C16
31	4	304	CLA	C11-C10-C8-C9
31	A	841	CLA	CBD-CGD-O2D-CED
30	a	602	CHL	C15-C16-C17-C18
34	9	601	LHG	C27-C28-C29-C30
36	9	602	LMG	C16-C17-C18-C19
31	2	303	CLA	CBA-CGA-O2A-C1
31	b	604	CLA	CBA-CGA-O2A-C1
31	i	613	CLA	CBA-CGA-O2A-C1
30	4	307	CHL	C2A-CAA-CBA-CGA
34	c	630	LHG	C14-C15-C16-C17
31	B	818	CLA	O1A-CGA-O2A-C1
31	9	310	CLA	CBD-CGD-O2D-CED
32	A	854	8CT	C10-C11-C12-C40
33	4	502	0UR	C22-C16-C17-C18
30	9	301	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	607	CHL	O1D-CGD-O2D-CED
30	d	601	CHL	O1D-CGD-O2D-CED
32	0	401	8CT	C25-C26-C28-C29
32	7	405	8CT	C14-C15-C16-C17
32	8	406	8CT	C25-C26-C28-C29
32	B	848	8CT	C10-C11-C12-C13
33	4	502	0UR	C15-C16-C17-C18
30	6	308	CHL	C11-C12-C13-C15
34	7	601	LHG	C25-C26-C27-C28
30	8	313	CHL	C3-C5-C6-C7
30	c	614	CHL	O1D-CGD-O2D-CED
30	1	307	CHL	C5-C6-C7-C8
31	2	310	CLA	C8-C10-C11-C12
31	9	302	CLA	C8-C10-C11-C12
36	J	105	LMG	C42-C43-C44-C45
30	3	302	CHL	CBA-CGA-O2A-C1
31	6	320	CLA	CBA-CGA-O2A-C1
31	K	101	CLA	CBA-CGA-O2A-C1
36	A	856	LMG	C29-C28-O8-C9
30	a	607	CHL	CBA-CGA-O2A-C1
31	5	304	CLA	C3-C5-C6-C7
30	b	607	CHL	O1A-CGA-O2A-C1
30	f	602	CHL	C4B-C3B-CAB-CBB
31	0	321	CLA	C4B-C3B-CAB-CBB
31	2	314	CLA	C4B-C3B-CAB-CBB
31	3	306	CLA	C4B-C3B-CAB-CBB
31	3	313	CLA	C4B-C3B-CAB-CBB
31	5	310	CLA	C4B-C3B-CAB-CBB
31	5	311	CLA	C4B-C3B-CAB-CBB
31	6	304	CLA	C4B-C3B-CAB-CBB
31	6	320	CLA	C4B-C3B-CAB-CBB
31	7	317	CLA	C4B-C3B-CAB-CBB
31	8	312	CLA	C4B-C3B-CAB-CBB
31	A	809	CLA	C4B-C3B-CAB-CBB
31	A	832	CLA	C4B-C3B-CAB-CBB
31	A	835	CLA	C4B-C3B-CAB-CBB
31	B	805	CLA	C4B-C3B-CAB-CBB
31	K	105	CLA	C4B-C3B-CAB-CBB
31	b	603	CLA	C4B-C3B-CAB-CBB
31	h	612	CLA	C4B-C3B-CAB-CBB
31	H	202	CLA	C4B-C3B-CAB-CBB
31	H	205	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	e	603	CLA	C4B-C3B-CAB-CBB
31	9	308	CLA	C13-C15-C16-C17
34	f	630	LHG	O6-C4-C5-C6
30	8	305	CHL	CBA-CGA-O2A-C1
31	3	308	CLA	O1A-CGA-O2A-C1
30	3	307	CHL	C5-C6-C7-C8
31	A	826	CLA	C13-C15-C16-C17
30	b	602	CHL	O1D-CGD-O2D-CED
36	J	105	LMG	C13-C14-C15-C16
31	A	853	CLA	C4-C3-C5-C6
31	L	201	CLA	C4-C3-C5-C6
30	b	608	CHL	C2-C3-C5-C6
31	9	300	CLA	C2-C3-C5-C6
36	L	210	LMG	C30-C31-C32-C33
31	3	308	CLA	C13-C15-C16-C17
31	A	843	CLA	O1A-CGA-O2A-C1
34	a	630	LHG	C12-C13-C14-C15
36	O	207	LMG	C32-C33-C34-C35
31	B	832	CLA	C3-C5-C6-C7
30	2	319	CHL	C11-C12-C13-C14
30	c	607	CHL	CBA-CGA-O2A-C1
31	5	303	CLA	C11-C12-C13-C15
34	d	630	LHG	C11-C10-C9-C8
36	3	602	LMG	C30-C31-C32-C33
31	A	828	CLA	C15-C16-C17-C18
31	A	807	CLA	O1D-CGD-O2D-CED
31	0	321	CLA	C2A-CAA-CBA-CGA
31	f	611	CLA	C2A-CAA-CBA-CGA
34	H	203	LHG	O8-C23-C24-C25
34	G	105	LHG	C2-C3-O3-P
31	A	814	CLA	O1A-CGA-O2A-C1
31	A	815	CLA	O1A-CGA-O2A-C1
30	6	306	CHL	C3A-C2A-CAA-CBA
30	6	307	CHL	C3A-C2A-CAA-CBA
30	c	601	CHL	C3A-C2A-CAA-CBA
30	b	601	CHL	C3A-C2A-CAA-CBA
30	f	608	CHL	C3A-C2A-CAA-CBA
30	h	608	CHL	C3A-C2A-CAA-CBA
30	4	308	CHL	C3A-C2A-CAA-CBA
31	5	314	CLA	C3A-C2A-CAA-CBA
31	6	317	CLA	C3A-C2A-CAA-CBA
31	9	308	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	816	CLA	C3A-C2A-CAA-CBA
31	B	820	CLA	C3A-C2A-CAA-CBA
31	L	203	CLA	C3A-C2A-CAA-CBA
31	a	611	CLA	C3A-C2A-CAA-CBA
31	b	604	CLA	C3A-C2A-CAA-CBA
31	e	604	CLA	C3A-C2A-CAA-CBA
30	h	601	CHL	O1A-CGA-O2A-C1
34	8	601	LHG	C26-C27-C28-C29
32	8	402	8CT	C16-C17-C18-C19
34	f	630	LHG	C28-C29-C30-C31
30	6	302	CHL	C3-C5-C6-C7
30	8	301	CHL	C3-C5-C6-C7
31	A	840	CLA	C3-C5-C6-C7
31	B	819	CLA	C8-C10-C11-C12
30	2	319	CHL	C11-C12-C13-C15
30	f	601	CHL	C16-C17-C18-C20
31	2	304	CLA	O1D-CGD-O2D-CED
30	f	606	CHL	CBA-CGA-O2A-C1
30	e	609	CHL	CBA-CGA-O2A-C1
31	A	824	CLA	CBA-CGA-O2A-C1
31	A	830	CLA	CBA-CGA-O2A-C1
31	B	829	CLA	CBA-CGA-O2A-C1
31	B	836	CLA	CBA-CGA-O2A-C1
31	e	613	CLA	CBA-CGA-O2A-C1
31	L	203	CLA	C15-C16-C17-C18
36	B	853	LMG	C11-C12-C13-C14
31	2	309	CLA	C10-C11-C12-C13
30	7	301	CHL	O1D-CGD-O2D-CED
32	9	401	8CT	C28-C29-C30-C35
34	7	602	LHG	C4-C5-C6-O8
34	8	601	LHG	C4-C5-C6-O8
34	4	601	LHG	C4-C5-C6-O8
36	2	602	LMG	C7-C8-C9-O8
36	L	211	LMG	O1-C7-C8-C9
36	J	105	LMG	C37-C38-C39-C40
34	1	601	LHG	C23-C24-C25-C26
31	0	311	CLA	O1A-CGA-O2A-C1
36	L	211	LMG	C18-C19-C20-C21
34	B	854	LHG	C26-C27-C28-C29
34	h	630	LHG	C26-C27-C28-C29
31	B	830	CLA	O1A-CGA-O2A-C1
31	3	310	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	853	CLA	C2-C3-C5-C6
31	7	309	CLA	C11-C12-C13-C14
30	8	301	CHL	C10-C11-C12-C13
30	0	306	CHL	C3C-C2C-CMC-OMC
30	1	306	CHL	C3C-C2C-CMC-OMC
30	2	313	CHL	C3C-C2C-CMC-OMC
30	6	313	CHL	C3C-C2C-CMC-OMC
30	7	301	CHL	C3C-C2C-CMC-OMC
30	7	305	CHL	C3C-C2C-CMC-OMC
30	7	306	CHL	C3C-C2C-CMC-OMC
30	7	313	CHL	C3C-C2C-CMC-OMC
30	8	305	CHL	C3C-C2C-CMC-OMC
30	8	307	CHL	C3C-C2C-CMC-OMC
30	8	308	CHL	C3C-C2C-CMC-OMC
30	9	306	CHL	C3C-C2C-CMC-OMC
30	9	313	CHL	C3C-C2C-CMC-OMC
30	a	602	CHL	C3C-C2C-CMC-OMC
30	a	606	CHL	C3C-C2C-CMC-OMC
30	c	607	CHL	C3C-C2C-CMC-OMC
30	b	601	CHL	C3C-C2C-CMC-OMC
30	b	602	CHL	C3C-C2C-CMC-OMC
30	b	606	CHL	C3C-C2C-CMC-OMC
30	b	608	CHL	C3C-C2C-CMC-OMC
30	b	609	CHL	C3C-C2C-CMC-OMC
30	b	614	CHL	C3C-C2C-CMC-OMC
30	d	605	CHL	C3C-C2C-CMC-OMC
30	d	606	CHL	C3C-C2C-CMC-OMC
30	g	602	CHL	C3C-C2C-CMC-OMC
30	g	608	CHL	C3C-C2C-CMC-OMC
30	h	606	CHL	C3C-C2C-CMC-OMC
30	h	608	CHL	C3C-C2C-CMC-OMC
30	e	601	CHL	C3C-C2C-CMC-OMC
30	e	602	CHL	C3C-C2C-CMC-OMC
30	e	605	CHL	C3C-C2C-CMC-OMC
30	e	606	CHL	C3C-C2C-CMC-OMC
30	c	602	CHL	O1A-CGA-O2A-C1
34	B	854	LHG	C31-C32-C33-C34
30	i	605	CHL	O1D-CGD-O2D-CED
31	A	826	CLA	O1D-CGD-O2D-CED
30	i	601	CHL	C2A-CAA-CBA-CGA
31	A	852	CLA	C2A-CAA-CBA-CGA
34	0	601	LHG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	i	630	LHG	O1-C1-C2-O2
34	4	601	LHG	C11-C12-C13-C14
34	c	630	LHG	O6-C4-C5-O7
34	g	630	LHG	O6-C4-C5-O7
30	5	301	CHL	CBA-CGA-O2A-C1
31	0	312	CLA	CBA-CGA-O2A-C1
31	7	304	CLA	CBA-CGA-O2A-C1
31	7	312	CLA	CBA-CGA-O2A-C1
34	K	106	LHG	C10-C11-C12-C13
30	8	313	CHL	C6-C7-C8-C10
30	e	608	CHL	C16-C17-C18-C20
31	B	827	CLA	C16-C17-C18-C20
31	A	809	CLA	C5-C6-C7-C8
31	2	314	CLA	C2B-C3B-CAB-CBB
31	3	306	CLA	C2B-C3B-CAB-CBB
31	A	832	CLA	C2B-C3B-CAB-CBB
31	B	805	CLA	C2B-C3B-CAB-CBB
31	K	105	CLA	C2B-C3B-CAB-CBB
31	h	612	CLA	C2B-C3B-CAB-CBB
31	H	205	CLA	C2B-C3B-CAB-CBB
31	e	603	CLA	C2B-C3B-CAB-CBB
30	3	302	CHL	O1A-CGA-O2A-C1
31	2	303	CLA	O1A-CGA-O2A-C1
34	0	601	LHG	C18-C19-C20-C21
31	b	613	CLA	O1D-CGD-O2D-CED
30	7	306	CHL	C12-C13-C15-C16
34	6	601	LHG	C11-C10-C9-C8
34	0	601	LHG	O7-C5-C6-O8
34	2	601	LHG	O7-C5-C6-O8
34	5	601	LHG	O7-C5-C6-O8
34	B	854	LHG	O7-C5-C6-O8
34	G	105	LHG	O7-C5-C6-O8
34	4	601	LHG	O7-C5-C6-O8
35	0	603	SQD	O6-C44-C45-O47
36	A	856	LMG	O1-C7-C8-O7
36	L	211	LMG	O1-C7-C8-O7
41	B	849	DGD	O2G-C2G-C3G-O3G
30	1	313	CHL	CBD-CGD-O2D-CED
34	f	630	LHG	O8-C23-C24-C25
33	4	501	0UR	O44-C45-C46-C47
36	O	207	LMG	C31-C32-C33-C34
31	0	309	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	7	302	CHL	C15-C16-C17-C18
31	1	312	CLA	C3-C5-C6-C7
30	1	305	CHL	C2-C1-O2A-CGA
30	3	302	CHL	C2-C1-O2A-CGA
30	5	301	CHL	C2-C1-O2A-CGA
30	6	313	CHL	C2-C1-O2A-CGA
30	7	306	CHL	C2-C1-O2A-CGA
30	8	302	CHL	C2-C1-O2A-CGA
30	9	305	CHL	C2-C1-O2A-CGA
30	a	606	CHL	C2-C1-O2A-CGA
30	f	602	CHL	C2-C1-O2A-CGA
30	4	302	CHL	C2-C1-O2A-CGA
31	7	308	CLA	C2-C1-O2A-CGA
31	K	102	CLA	C2-C1-O2A-CGA
34	9	601	LHG	C10-C11-C12-C13
30	1	307	CHL	C11-C12-C13-C14
30	3	302	CHL	C6-C7-C8-C9
30	5	302	CHL	C6-C7-C8-C9
30	5	302	CHL	C11-C10-C8-C9
30	6	301	CHL	C6-C7-C8-C9
30	c	609	CHL	C14-C13-C15-C16
30	d	609	CHL	C11-C10-C8-C9
30	d	609	CHL	C14-C13-C15-C16
31	2	304	CLA	C6-C7-C8-C9
31	2	304	CLA	C11-C10-C8-C9
31	A	813	CLA	C6-C7-C8-C9
31	A	817	CLA	C11-C10-C8-C9
31	A	818	CLA	C11-C12-C13-C14
31	A	825	CLA	C11-C12-C13-C14
31	A	826	CLA	C14-C13-C15-C16
31	A	830	CLA	C11-C10-C8-C9
31	A	832	CLA	C11-C10-C8-C9
31	A	833	CLA	C11-C10-C8-C9
31	B	801	CLA	C11-C12-C13-C14
31	B	803	CLA	C14-C13-C15-C16
31	B	809	CLA	C14-C13-C15-C16
31	B	827	CLA	C11-C12-C13-C14
31	B	832	CLA	C14-C13-C15-C16
31	B	834	CLA	C11-C10-C8-C9
38	A	842	PQN	C24-C23-C25-C26
30	2	302	CHL	C15-C16-C17-C18
34	h	630	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	8	305	CHL	O1D-CGD-O2D-CED
31	4	310	CLA	C8-C10-C11-C12
34	3	603	LHG	C5-C4-O6-P
34	7	601	LHG	C2-C3-O3-P
34	8	601	LHG	C2-C3-O3-P
34	A	855	LHG	C2-C3-O3-P
34	A	855	LHG	C5-C4-O6-P
34	B	852	LHG	C2-C3-O3-P
34	B	854	LHG	C2-C3-O3-P
31	b	604	CLA	O1A-CGA-O2A-C1
30	f	601	CHL	C16-C17-C18-C19
30	i	602	CHL	C11-C12-C13-C14
31	A	828	CLA	C16-C17-C18-C20
31	B	817	CLA	C11-C12-C13-C15
32	7	402	8CT	C02-C03-C10-C11
32	A	847	8CT	C04-C03-C10-C11
32	B	843	8CT	C04-C03-C10-C11
32	B	844	8CT	C04-C03-C10-C11
32	F	302	8CT	C04-C03-C10-C11
32	J	101	8CT	C02-C03-C10-C11
32	M	102	8CT	C02-C03-C10-C11
30	2	301	CHL	C10-C11-C12-C13
34	9	601	LHG	C34-C35-C36-C37
32	0	401	8CT	C27-C26-C28-C29
32	8	406	8CT	C27-C26-C28-C29
32	A	849	8CT	C14-C15-C16-C39
32	B	848	8CT	C10-C11-C12-C40
33	0	502	0UR	C22-C16-C17-C18
33	g	520	0UR	C46-C47-C48-C49
30	7	306	CHL	C11-C12-C13-C15
34	A	844	LHG	C27-C28-C29-C30
31	i	613	CLA	O1A-CGA-O2A-C1
31	A	817	CLA	O1D-CGD-O2D-CED
32	7	405	8CT	C25-C26-C28-C29
32	A	847	8CT	C25-C26-C28-C29
32	B	843	8CT	C14-C15-C16-C17
32	B	851	8CT	C10-C11-C12-C13
32	K	107	8CT	C20-C21-C23-C24
33	6	502	0UR	C15-C16-C17-C18
30	2	302	CHL	C13-C15-C16-C17
31	8	304	CLA	C13-C15-C16-C17
31	e	613	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	b	630	LHG	C27-C28-C29-C30
30	f	602	CHL	O1D-CGD-O2D-CED
30	i	601	CHL	O1A-CGA-O2A-C1
34	8	601	LHG	C13-C14-C15-C16
30	3	307	CHL	C16-C17-C18-C19
30	6	301	CHL	C11-C12-C13-C14
30	e	602	CHL	C11-C12-C13-C14
30	e	609	CHL	C11-C12-C13-C14
31	B	819	CLA	C11-C12-C13-C15
30	4	313	CHL	O1D-CGD-O2D-CED
33	2	502	0UR	C46-C47-C48-C49
30	a	602	CHL	O1D-CGD-O2D-CED
30	e	601	CHL	O1D-CGD-O2D-CED
31	6	303	CLA	O1D-CGD-O2D-CED
31	A	818	CLA	C15-C16-C17-C18
34	0	601	LHG	O6-C4-C5-C6
34	6	601	LHG	O6-C4-C5-C6
34	6	603	LHG	O6-C4-C5-C6
34	7	603	LHG	O6-C4-C5-C6
34	a	630	LHG	O6-C4-C5-C6
34	c	630	LHG	O6-C4-C5-C6
34	g	630	LHG	O6-C4-C5-C6
30	i	607	CHL	CAA-CBA-CGA-O2A
34	b	630	LHG	C10-C11-C12-C13
30	1	307	CHL	C11-C10-C8-C7
30	1	307	CHL	C11-C12-C13-C15
30	1	307	CHL	C12-C13-C15-C16
30	1	313	CHL	C11-C10-C8-C7
30	6	302	CHL	C6-C7-C8-C10
30	6	302	CHL	C11-C10-C8-C7
30	7	301	CHL	C11-C12-C13-C15
30	7	302	CHL	C12-C13-C15-C16
30	a	602	CHL	C11-C12-C13-C15
30	c	608	CHL	C6-C7-C8-C10
30	c	609	CHL	C12-C13-C15-C16
30	b	608	CHL	C6-C7-C8-C10
30	f	609	CHL	C11-C12-C13-C15
30	f	609	CHL	C12-C13-C15-C16
30	h	602	CHL	C6-C7-C8-C10
30	e	608	CHL	C11-C10-C8-C7
31	0	312	CLA	C6-C7-C8-C10
31	3	310	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	5	303	CLA	C6-C7-C8-C10
31	6	310	CLA	C6-C7-C8-C10
31	7	308	CLA	C11-C12-C13-C15
31	9	302	CLA	C12-C13-C15-C16
31	A	805	CLA	C6-C7-C8-C10
31	A	818	CLA	C11-C12-C13-C15
31	A	829	CLA	C11-C12-C13-C15
31	A	830	CLA	C11-C10-C8-C7
31	A	833	CLA	C6-C7-C8-C10
31	A	840	CLA	C6-C7-C8-C10
31	A	853	CLA	C12-C13-C15-C16
31	B	803	CLA	C12-C13-C15-C16
31	B	809	CLA	C11-C12-C13-C15
31	B	809	CLA	C12-C13-C15-C16
31	B	819	CLA	C11-C10-C8-C7
31	B	832	CLA	C12-C13-C15-C16
31	B	839	CLA	C12-C13-C15-C16
31	4	304	CLA	C11-C10-C8-C7
33	1	502	0UR	C46-C47-C48-C49
31	A	814	CLA	C3-C5-C6-C7
31	B	810	CLA	C3-C5-C6-C7
31	A	823	CLA	O1D-CGD-O2D-CED
41	B	849	DGD	C5A-C6A-C7A-C8A
32	3	403	8CT	C16-C17-C18-C19
32	7	402	8CT	C23-C24-C25-C26
32	7	405	8CT	C12-C13-C14-C15
32	A	846	8CT	C16-C17-C18-C19
32	A	849	8CT	C18-C19-C20-C21
32	B	848	8CT	C18-C19-C20-C21
32	L	206	8CT	C16-C17-C18-C19
32	K	107	8CT	C18-C19-C20-C21
32	O	205	8CT	C16-C17-C18-C19
33	5	502	0UR	C3-C4-C5-C6
30	c	602	CHL	C11-C12-C13-C14
34	7	602	LHG	C14-C15-C16-C17
31	B	825	CLA	O1D-CGD-O2D-CED
31	6	320	CLA	O1A-CGA-O2A-C1
31	K	101	CLA	O1A-CGA-O2A-C1
30	5	307	CHL	C2A-CAA-CBA-CGA
30	6	301	CHL	C2A-CAA-CBA-CGA
30	7	313	CHL	C2A-CAA-CBA-CGA
30	h	606	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	2	602	LMG	C13-C14-C15-C16
36	2	602	LMG	C11-C10-O7-C8
33	0	501	0UR	O42-C2-C3-C4
33	0	502	0UR	O42-C2-C3-C4
33	1	501	0UR	O42-C2-C3-C4
33	2	502	0UR	O42-C2-C3-C4
33	3	501	0UR	O42-C2-C3-C4
33	5	501	0UR	O42-C2-C3-C4
33	6	501	0UR	O42-C2-C3-C4
33	7	501	0UR	O42-C2-C3-C4
33	8	501	0UR	O42-C2-C3-C4
33	9	501	0UR	O42-C2-C3-C4
33	9	502	0UR	O42-C2-C3-C4
33	a	520	0UR	O42-C2-C3-C4
33	c	520	0UR	O42-C2-C3-C4
33	b	520	0UR	O42-C2-C3-C4
33	d	520	0UR	O42-C2-C3-C4
33	d	520	0UR	C45-C46-C47-C48
33	f	520	0UR	C45-C46-C47-C48
33	g	520	0UR	O42-C2-C3-C4
33	h	520	0UR	O42-C2-C3-C4
33	i	520	0UR	O42-C2-C3-C4
33	e	520	0UR	O42-C2-C3-C4
33	4	501	0UR	O42-C2-C3-C4
34	9	601	LHG	C30-C31-C32-C33
37	3	502	0IE	O1-C2-C3-C4
37	7	502	0IE	O1-C2-C3-C4
37	a	521	0IE	O1-C2-C3-C4
37	c	521	0IE	O1-C2-C3-C4
37	b	521	0IE	O1-C2-C3-C4
37	d	521	0IE	O1-C2-C3-C4
37	f	521	0IE	O1-C2-C3-C4
37	g	521	0IE	O1-C2-C3-C4
37	g	522	0IE	O1-C2-C30-C31
37	h	521	0IE	O1-C2-C3-C4
37	i	521	0IE	O1-C2-C3-C4
37	e	521	0IE	O1-C2-C3-C4
31	B	806	CLA	C4C-C3C-CAC-CBC
36	9	602	LMG	C41-C42-C43-C44
31	B	829	CLA	C8-C10-C11-C12
30	1	305	CHL	CBA-CGA-O2A-C1
31	7	308	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	h	630	LHG	C11-C10-C9-C8
34	7	601	LHG	C9-C10-C11-C12
34	i	630	LHG	C11-C10-C9-C8
30	i	607	CHL	CBA-CGA-O2A-C1
31	A	817	CLA	C8-C10-C11-C12
31	A	853	CLA	C13-C15-C16-C17
31	B	825	CLA	C5-C6-C7-C8
30	2	313	CHL	CAD-CBD-CGD-O2D
30	8	306	CHL	CAD-CBD-CGD-O2D
30	b	607	CHL	CAD-CBD-CGD-O2D
30	e	614	CHL	CAD-CBD-CGD-O2D
31	0	304	CLA	CAD-CBD-CGD-O2D
31	0	310	CLA	CAD-CBD-CGD-O2D
31	0	311	CLA	CAD-CBD-CGD-O2D
31	0	321	CLA	CAD-CBD-CGD-O2D
31	1	314	CLA	CAD-CBD-CGD-O2D
31	5	304	CLA	CAD-CBD-CGD-O2D
31	5	309	CLA	CAD-CBD-CGD-O2D
31	5	312	CLA	CAD-CBD-CGD-O2D
31	6	310	CLA	CAD-CBD-CGD-O2D
31	6	311	CLA	CAD-CBD-CGD-O2D
31	6	314	CLA	CAD-CBD-CGD-O2D
31	7	303	CLA	CAD-CBD-CGD-O2D
31	7	311	CLA	CAD-CBD-CGD-O2D
31	7	316	CLA	CAD-CBD-CGD-O2D
31	8	303	CLA	CAD-CBD-CGD-O2D
31	8	304	CLA	CAD-CBD-CGD-O2D
31	8	309	CLA	CAD-CBD-CGD-O2D
31	8	314	CLA	CAD-CBD-CGD-O2D
31	A	812	CLA	CAD-CBD-CGD-O2D
31	A	820	CLA	CAD-CBD-CGD-O2D
31	A	826	CLA	CAD-CBD-CGD-O2D
31	A	836	CLA	CAD-CBD-CGD-O2D
31	A	852	CLA	CAD-CBD-CGD-O2D
31	B	817	CLA	CAD-CBD-CGD-O2D
31	B	822	CLA	CAD-CBD-CGD-O2D
31	B	827	CLA	CAD-CBD-CGD-O2D
31	B	834	CLA	CAD-CBD-CGD-O2D
31	B	838	CLA	CAD-CBD-CGD-O2D
31	L	204	CLA	CAD-CBD-CGD-O2D
31	K	104	CLA	CAD-CBD-CGD-O2D
31	c	604	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	f	603	CLA	CAD-CBD-CGD-O2D
31	f	610	CLA	CAD-CBD-CGD-O2D
31	g	603	CLA	CAD-CBD-CGD-O2D
31	g	604	CLA	CAD-CBD-CGD-O2D
31	g	613	CLA	CAD-CBD-CGD-O2D
31	e	603	CLA	CAD-CBD-CGD-O2D
31	4	311	CLA	CAD-CBD-CGD-O2D
31	4	314	CLA	CAD-CBD-CGD-O2D
41	B	849	DGD	C3G-C2G-O2G-C1B
31	A	808	CLA	C8-C10-C11-C12
31	B	817	CLA	C10-C11-C12-C13
31	B	812	CLA	CBA-CGA-O2A-C1
31	B	817	CLA	CBA-CGA-O2A-C1
31	f	613	CLA	CBA-CGA-O2A-C1
31	A	825	CLA	C15-C16-C17-C18
33	d	520	0UR	C4-C3-C43-O44
34	3	601	LHG	C4-C5-C6-O8
34	a	630	LHG	C4-C5-C6-O8
34	d	630	LHG	C4-C5-C6-O8
36	3	602	LMG	C7-C8-C9-O8
36	A	856	LMG	O1-C7-C8-C9
36	J	105	LMG	C7-C8-C9-O8
36	L	210	LMG	C7-C8-C9-O8
36	O	207	LMG	C7-C8-C9-O8
31	0	303	CLA	CBD-CGD-O2D-CED
31	7	304	CLA	O1A-CGA-O2A-C1
34	0	601	LHG	O6-C4-C5-O7
34	6	601	LHG	O6-C4-C5-O7
34	6	603	LHG	O6-C4-C5-O7
34	7	603	LHG	O6-C4-C5-O7
34	8	601	LHG	O6-C4-C5-O7
34	B	852	LHG	O6-C4-C5-O7
34	G	105	LHG	O6-C4-C5-O7
34	a	630	LHG	O6-C4-C5-O7
34	d	630	LHG	O6-C4-C5-O7
34	H	203	LHG	O6-C4-C5-O7
31	A	806	CLA	C5-C6-C7-C8
30	3	307	CHL	C3-C5-C6-C7
31	4	312	CLA	C3-C5-C6-C7
30	9	313	CHL	CAA-CBA-CGA-O2A
36	L	210	LMG	O7-C10-C11-C12
34	a	630	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	3	320	CLA	C2A-CAA-CBA-CGA
31	c	604	CLA	C2A-CAA-CBA-CGA
30	c	602	CHL	C11-C12-C13-C15
36	B	853	LMG	C34-C35-C36-C37
30	1	302	CHL	CHA-CBD-CGD-O1D
30	2	301	CHL	CHA-CBD-CGD-O1D
30	2	301	CHL	CHA-CBD-CGD-O2D
30	6	302	CHL	CHA-CBD-CGD-O1D
30	8	301	CHL	CHA-CBD-CGD-O1D
30	8	301	CHL	CHA-CBD-CGD-O2D
30	8	302	CHL	CHA-CBD-CGD-O1D
30	8	315	CHL	CHA-CBD-CGD-O1D
30	i	602	CHL	CHA-CBD-CGD-O1D
30	e	602	CHL	CHA-CBD-CGD-O1D
30	4	302	CHL	CHA-CBD-CGD-O1D
30	4	302	CHL	CHA-CBD-CGD-O2D
31	3	312	CLA	CHA-CBD-CGD-O1D
31	3	312	CLA	CHA-CBD-CGD-O2D
31	7	317	CLA	CHA-CBD-CGD-O1D
31	7	317	CLA	CHA-CBD-CGD-O2D
31	9	300	CLA	CHA-CBD-CGD-O1D
31	9	300	CLA	CHA-CBD-CGD-O2D
31	A	808	CLA	CHA-CBD-CGD-O1D
31	A	808	CLA	CHA-CBD-CGD-O2D
31	A	815	CLA	CHA-CBD-CGD-O1D
31	A	816	CLA	CHA-CBD-CGD-O1D
31	A	816	CLA	CHA-CBD-CGD-O2D
31	A	827	CLA	CHA-CBD-CGD-O1D
31	A	827	CLA	CHA-CBD-CGD-O2D
31	A	838	CLA	CHA-CBD-CGD-O1D
31	A	838	CLA	CHA-CBD-CGD-O2D
31	B	810	CLA	CHA-CBD-CGD-O2D
31	B	831	CLA	CHA-CBD-CGD-O1D
31	B	833	CLA	CHA-CBD-CGD-O1D
31	B	833	CLA	CHA-CBD-CGD-O2D
31	G	101	CLA	CHA-CBD-CGD-O1D
31	G	101	CLA	CHA-CBD-CGD-O2D
31	L	207	CLA	CHA-CBD-CGD-O1D
31	L	207	CLA	CHA-CBD-CGD-O2D
31	K	105	CLA	CHA-CBD-CGD-O1D
31	M	101	CLA	CHA-CBD-CGD-O2D
31	d	604	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	f	612	CLA	CHA-CBD-CGD-O1D
31	f	612	CLA	CHA-CBD-CGD-O2D
31	g	611	CLA	CHA-CBD-CGD-O1D
31	g	611	CLA	CHA-CBD-CGD-O2D
31	g	612	CLA	CHA-CBD-CGD-O1D
31	g	612	CLA	CHA-CBD-CGD-O2D
31	h	611	CLA	CHA-CBD-CGD-O1D
31	e	612	CLA	CHA-CBD-CGD-O1D
31	e	612	CLA	CHA-CBD-CGD-O2D
33	6	502	0UR	C2-C3-C43-O44
33	d	520	0UR	C2-C3-C43-O44
33	e	520	0UR	C2-C3-C43-O44
41	B	849	DGD	C2B-C3B-C4B-C5B
30	5	301	CHL	O1A-CGA-O2A-C1
30	f	606	CHL	O1A-CGA-O2A-C1
30	e	609	CHL	O1A-CGA-O2A-C1
31	7	312	CLA	O1A-CGA-O2A-C1
31	A	830	CLA	O1A-CGA-O2A-C1
31	B	829	CLA	O1A-CGA-O2A-C1
31	B	836	CLA	O1A-CGA-O2A-C1
34	G	105	LHG	C15-C16-C17-C18
30	e	606	CHL	O1D-CGD-O2D-CED
31	3	304	CLA	C8-C10-C11-C12
34	8	601	LHG	O7-C5-C6-O8
34	a	630	LHG	O7-C5-C6-O8
36	A	856	LMG	O7-C8-C9-O8
36	J	105	LMG	O7-C8-C9-O8
30	5	307	CHL	CBA-CGA-O2A-C1
34	c	630	LHG	C31-C32-C33-C34
31	7	308	CLA	O1A-CGA-O2A-C1
31	e	613	CLA	O1A-CGA-O2A-C1
34	5	601	LHG	C12-C13-C14-C15
31	B	837	CLA	C16-C17-C18-C19
34	B	852	LHG	O1-C1-C2-O2
31	B	823	CLA	O1D-CGD-O2D-CED
31	A	819	CLA	C13-C15-C16-C17
33	h	520	0UR	C47-C48-C49-C50
31	A	805	CLA	C4-C3-C5-C6
36	2	602	LMG	C33-C34-C35-C36
31	0	312	CLA	O1A-CGA-O2A-C1
31	A	824	CLA	O1A-CGA-O2A-C1
34	A	844	LHG	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	810	CLA	C5-C6-C7-C8
31	B	824	CLA	C8-C10-C11-C12
30	1	302	CHL	C14-C13-C15-C16
30	3	302	CHL	C11-C12-C13-C14
30	7	301	CHL	C11-C12-C13-C14
30	a	602	CHL	C11-C12-C13-C14
31	2	312	CLA	C11-C10-C8-C9
31	A	837	CLA	C6-C7-C8-C9
30	1	305	CHL	O1A-CGA-O2A-C1
31	J	103	CLA	O1D-CGD-O2D-CED
31	B	810	CLA	C2A-CAA-CBA-CGA
31	d	613	CLA	C2A-CAA-CBA-CGA
34	f	630	LHG	C11-C10-C9-C8
36	B	853	LMG	C35-C36-C37-C38
30	7	313	CHL	O1A-CGA-O2A-C1
30	e	606	CHL	CBA-CGA-O2A-C1
32	3	403	8CT	C22-C21-C23-C24
32	B	847	8CT	C27-C26-C28-C29
32	B	851	8CT	C27-C26-C28-C29
33	8	502	0UR	C22-C16-C17-C18
34	9	601	LHG	C25-C26-C27-C28
36	O	207	LMG	C4-C5-C6-O5
32	2	402	8CT	C14-C15-C16-C17
32	A	849	8CT	C14-C15-C16-C17
32	A	854	8CT	C10-C11-C12-C13
32	B	847	8CT	C25-C26-C28-C29
32	B	851	8CT	C25-C26-C28-C29
33	8	502	0UR	C15-C16-C17-C18
30	6	301	CHL	C1A-C2A-CAA-CBA
30	c	601	CHL	C1A-C2A-CAA-CBA
30	f	602	CHL	C1A-C2A-CAA-CBA
30	h	609	CHL	C1A-C2A-CAA-CBA
30	e	602	CHL	C1A-C2A-CAA-CBA
31	0	309	CLA	C1A-C2A-CAA-CBA
31	2	310	CLA	C1A-C2A-CAA-CBA
31	5	314	CLA	C1A-C2A-CAA-CBA
31	6	309	CLA	C1A-C2A-CAA-CBA
31	6	317	CLA	C1A-C2A-CAA-CBA
31	8	309	CLA	C1A-C2A-CAA-CBA
31	A	824	CLA	C1A-C2A-CAA-CBA
31	a	611	CLA	C1A-C2A-CAA-CBA
31	i	610	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	4	309	CLA	C1A-C2A-CAA-CBA
30	8	301	CHL	C11-C12-C13-C15
31	9	312	CLA	C5-C6-C7-C8
31	B	817	CLA	C4C-C3C-CAC-CBC
31	B	814	CLA	O1D-CGD-O2D-CED
31	A	831	CLA	C2-C1-O2A-CGA
31	L	203	CLA	C2-C1-O2A-CGA
30	f	609	CHL	CBA-CGA-O2A-C1
34	9	601	LHG	C28-C29-C30-C31
32	A	854	8CT	C16-C17-C18-C19
32	L	209	8CT	C16-C17-C18-C19
30	2	302	CHL	O1D-CGD-O2D-CED
31	8	309	CLA	O1D-CGD-O2D-CED
34	a	630	LHG	C3-O3-P-O6
34	e	630	LHG	C3-O3-P-O6
34	0	601	LHG	C17-C18-C19-C20
31	9	310	CLA	O1D-CGD-O2D-CED
31	A	852	CLA	O1D-CGD-O2D-CED
31	3	320	CLA	C4-C3-C5-C6
31	B	813	CLA	C3-C5-C6-C7
34	c	630	LHG	C2-C3-O3-P
31	A	805	CLA	C2-C3-C5-C6
31	B	817	CLA	O1A-CGA-O2A-C1
30	3	302	CHL	C4B-C3B-CAB-CBB
30	6	307	CHL	C4B-C3B-CAB-CBB
30	7	302	CHL	C4B-C3B-CAB-CBB
30	7	305	CHL	C4B-C3B-CAB-CBB
31	2	303	CLA	C4B-C3B-CAB-CBB
31	2	310	CLA	C4B-C3B-CAB-CBB
31	3	312	CLA	C4B-C3B-CAB-CBB
31	5	314	CLA	C4B-C3B-CAB-CBB
31	6	310	CLA	C4B-C3B-CAB-CBB
31	6	318	CLA	C4B-C3B-CAB-CBB
31	7	310	CLA	C4B-C3B-CAB-CBB
31	7	311	CLA	C4B-C3B-CAB-CBB
31	7	312	CLA	C4B-C3B-CAB-CBB
31	7	315	CLA	C4B-C3B-CAB-CBB
31	8	310	CLA	C4B-C3B-CAB-CBB
31	8	311	CLA	C4B-C3B-CAB-CBB
31	9	310	CLA	C4B-C3B-CAB-CBB
31	A	823	CLA	C4B-C3B-CAB-CBB
31	A	840	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	809	CLA	C4B-C3B-CAB-CBB
31	B	811	CLA	C4B-C3B-CAB-CBB
31	B	822	CLA	C4B-C3B-CAB-CBB
31	B	834	CLA	C4B-C3B-CAB-CBB
31	B	850	CLA	C4B-C3B-CAB-CBB
31	F	301	CLA	C4B-C3B-CAB-CBB
31	L	207	CLA	C4B-C3B-CAB-CBB
31	K	101	CLA	C4B-C3B-CAB-CBB
31	O	206	CLA	C4B-C3B-CAB-CBB
31	a	611	CLA	C4B-C3B-CAB-CBB
31	d	611	CLA	C4B-C3B-CAB-CBB
31	d	612	CLA	C4B-C3B-CAB-CBB
31	f	603	CLA	C4B-C3B-CAB-CBB
31	4	303	CLA	C4B-C3B-CAB-CBB
31	4	310	CLA	C4B-C3B-CAB-CBB
34	1	601	LHG	C3-O3-P-O4
34	3	603	LHG	C3-O3-P-O4
34	3	603	LHG	C3-O3-P-O5
34	5	601	LHG	C3-O3-P-O4
34	6	601	LHG	C3-O3-P-O4
34	6	601	LHG	C4-O6-P-O4
34	6	601	LHG	C4-O6-P-O5
34	6	603	LHG	C4-O6-P-O4
34	7	602	LHG	C4-O6-P-O4
34	8	601	LHG	C3-O3-P-O4
34	9	601	LHG	C4-O6-P-O4
34	A	845	LHG	C3-O3-P-O5
34	A	855	LHG	C3-O3-P-O4
34	A	855	LHG	C4-O6-P-O4
34	B	852	LHG	C4-O6-P-O5
34	G	105	LHG	C4-O6-P-O5
34	K	106	LHG	C4-O6-P-O5
34	b	630	LHG	C3-O3-P-O4
34	b	630	LHG	C4-O6-P-O4
34	d	630	LHG	C4-O6-P-O4
34	i	630	LHG	C3-O3-P-O5
34	e	630	LHG	C4-O6-P-O4
31	B	803	CLA	C16-C17-C18-C19
34	K	106	LHG	C7-C8-C9-C10
31	B	818	CLA	C8-C10-C11-C12
34	8	601	LHG	O6-C4-C5-C6
34	A	845	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	G	105	LHG	O6-C4-C5-C6
34	H	203	LHG	O6-C4-C5-C6
34	8	601	LHG	C15-C16-C17-C18
36	9	602	LMG	C11-C12-C13-C14
30	d	607	CHL	O1A-CGA-O2A-C1
30	f	607	CHL	CAA-CBA-CGA-O2A
34	6	601	LHG	C11-C12-C13-C14
31	c	613	CLA	C2A-CAA-CBA-CGA
31	H	205	CLA	C2A-CAA-CBA-CGA
34	A	855	LHG	C27-C28-C29-C30
36	9	602	LMG	C32-C33-C34-C35
31	6	317	CLA	C16-C17-C18-C20
31	B	822	CLA	C4C-C3C-CAC-CBC
34	7	601	LHG	C26-C27-C28-C29
30	2	301	CHL	CAD-CBD-CGD-O1D
30	6	301	CHL	CAD-CBD-CGD-O1D
30	h	614	CHL	CAD-CBD-CGD-O1D
31	0	313	CLA	CAD-CBD-CGD-O1D
31	6	320	CLA	C2-C3-C5-C6
31	A	835	CLA	CAD-CBD-CGD-O1D
31	A	836	CLA	C2-C3-C5-C6
31	B	826	CLA	C2-C3-C5-C6
31	K	105	CLA	CAD-CBD-CGD-O1D
31	d	604	CLA	CAD-CBD-CGD-O1D
31	f	604	CLA	CAD-CBD-CGD-O1D
31	h	604	CLA	CAD-CBD-CGD-O1D
31	i	604	CLA	CAD-CBD-CGD-O1D
30	e	607	CHL	CBA-CGA-O2A-C1
31	A	808	CLA	C5-C6-C7-C8
34	6	601	LHG	C25-C26-C27-C28
34	B	854	LHG	C32-C33-C34-C35
31	B	812	CLA	O1A-CGA-O2A-C1
34	0	601	LHG	C10-C11-C12-C13
31	A	841	CLA	C3-C5-C6-C7
31	L	203	CLA	C3-C5-C6-C7
34	b	630	LHG	C23-C24-C25-C26
30	0	306	CHL	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	g	603	CLA	CBA-CGA-O2A-C1
31	e	611	CLA	CBA-CGA-O2A-C1
31	A	841	CLA	O1D-CGD-O2D-CED
31	3	308	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	9	302	CLA	C16-C17-C18-C20
30	1	302	CHL	C11-C12-C13-C15
30	3	302	CHL	C11-C12-C13-C15
30	3	307	CHL	C11-C12-C13-C15
30	c	608	CHL	C11-C12-C13-C15
30	c	609	CHL	C11-C12-C13-C15
30	b	601	CHL	C11-C12-C13-C15
30	b	602	CHL	C12-C13-C15-C16
30	b	608	CHL	C11-C12-C13-C15
30	d	602	CHL	C12-C13-C15-C16
30	f	602	CHL	C12-C13-C15-C16
30	h	609	CHL	C3A-C2A-CAA-CBA
30	e	602	CHL	C6-C7-C8-C10
31	1	303	CLA	C6-C7-C8-C10
31	2	303	CLA	C6-C7-C8-C10
31	2	312	CLA	C11-C10-C8-C7
31	3	308	CLA	C11-C10-C8-C7
31	5	309	CLA	C6-C7-C8-C10
31	9	308	CLA	C12-C13-C15-C16
31	9	309	CLA	C6-C7-C8-C10
31	A	826	CLA	C6-C7-C8-C10
31	A	837	CLA	C6-C7-C8-C10
31	B	808	CLA	C11-C10-C8-C7
31	B	810	CLA	C6-C7-C8-C10
31	B	817	CLA	C6-C7-C8-C10
31	B	841	CLA	C12-C13-C15-C16
31	a	611	CLA	C11-C10-C8-C7
32	7	402	8CT	C28-C29-C30-C31
32	8	402	8CT	C28-C29-C30-C31
32	B	843	8CT	C28-C29-C30-C31
32	B	847	8CT	C28-C29-C30-C31
32	I	101	8CT	C28-C29-C30-C31
32	L	206	8CT	C28-C29-C30-C31
32	K	107	8CT	C28-C29-C30-C31
33	2	501	0UR	O42-C2-C3-C43
33	6	502	0UR	C17-C18-C19-C32
33	a	520	0UR	C3-C2-C41-C1
33	f	520	0UR	O42-C2-C3-C43
34	f	630	LHG	O6-C4-C5-O7
37	b	522	0IE	C3-C2-C30-C31
37	g	521	0IE	O1-C2-C3-C20
37	g	521	0IE	C3-C2-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	h	521	0IE	O29-C20-C3-C2
37	i	521	0IE	O29-C20-C3-C2
31	A	811	CLA	C10-C11-C12-C13
32	7	402	8CT	C12-C13-C14-C15
32	B	804	8CT	C16-C17-C18-C19
31	0	311	CLA	CBD-CGD-O2D-CED
31	9	300	CLA	CAA-CBA-CGA-O2A
31	B	811	CLA	C10-C11-C12-C13
31	B	840	CLA	C13-C15-C16-C17
34	a	630	LHG	C8-C7-O7-C5
34	K	106	LHG	C26-C27-C28-C29
30	e	606	CHL	O1A-CGA-O2A-C1
31	f	613	CLA	O1A-CGA-O2A-C1
31	g	603	CLA	O1A-CGA-O2A-C1
34	A	844	LHG	O2-C2-C3-O3
30	1	305	CHL	CBD-CGD-O2D-CED
31	a	610	CLA	C2A-CAA-CBA-CGA
30	0	305	CHL	C1C-C2C-CMC-OMC
30	1	302	CHL	C1C-C2C-CMC-OMC
30	1	306	CHL	C1C-C2C-CMC-OMC
30	1	307	CHL	C1C-C2C-CMC-OMC
30	1	313	CHL	C1C-C2C-CMC-OMC
30	2	306	CHL	C1C-C2C-CMC-OMC
30	2	313	CHL	C1C-C2C-CMC-OMC
30	3	302	CHL	C1C-C2C-CMC-OMC
30	5	305	CHL	C1C-C2C-CMC-OMC
30	5	307	CHL	C1C-C2C-CMC-OMC
30	6	306	CHL	C1C-C2C-CMC-OMC
30	6	307	CHL	C1C-C2C-CMC-OMC
30	6	313	CHL	C1C-C2C-CMC-OMC
30	7	301	CHL	C1C-C2C-CMC-OMC
30	7	305	CHL	C1C-C2C-CMC-OMC
30	7	306	CHL	C1C-C2C-CMC-OMC
30	7	313	CHL	C1C-C2C-CMC-OMC
30	8	302	CHL	C1C-C2C-CMC-OMC
30	8	305	CHL	C1C-C2C-CMC-OMC
30	8	306	CHL	C1C-C2C-CMC-OMC
30	8	307	CHL	C1C-C2C-CMC-OMC
30	8	308	CHL	C1C-C2C-CMC-OMC
30	8	313	CHL	C1C-C2C-CMC-OMC
30	9	301	CHL	C1C-C2C-CMC-OMC
30	9	306	CHL	C1C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	9	313	CHL	C1C-C2C-CMC-OMC
30	a	602	CHL	C1C-C2C-CMC-OMC
30	a	606	CHL	C1C-C2C-CMC-OMC
30	c	607	CHL	C1C-C2C-CMC-OMC
30	c	608	CHL	C1C-C2C-CMC-OMC
30	b	601	CHL	C1C-C2C-CMC-OMC
30	b	602	CHL	C1C-C2C-CMC-OMC
30	b	606	CHL	C1C-C2C-CMC-OMC
30	b	608	CHL	C1C-C2C-CMC-OMC
30	b	609	CHL	C1C-C2C-CMC-OMC
30	b	614	CHL	C1C-C2C-CMC-OMC
30	d	605	CHL	C1C-C2C-CMC-OMC
30	d	606	CHL	C1C-C2C-CMC-OMC
30	d	608	CHL	C1C-C2C-CMC-OMC
30	f	606	CHL	C1C-C2C-CMC-OMC
30	g	602	CHL	C1C-C2C-CMC-OMC
30	g	607	CHL	C1C-C2C-CMC-OMC
30	g	608	CHL	C1C-C2C-CMC-OMC
30	g	609	CHL	O1A-CGA-O2A-C1
30	h	608	CHL	C1C-C2C-CMC-OMC
30	i	602	CHL	C1C-C2C-CMC-OMC
30	i	606	CHL	C1C-C2C-CMC-OMC
30	i	608	CHL	C1C-C2C-CMC-OMC
30	e	601	CHL	C1C-C2C-CMC-OMC
30	e	602	CHL	C1C-C2C-CMC-OMC
30	e	605	CHL	C1C-C2C-CMC-OMC
30	e	606	CHL	C1C-C2C-CMC-OMC
30	e	608	CHL	C1C-C2C-CMC-OMC
30	e	609	CHL	C1C-C2C-CMC-OMC
30	4	306	CHL	C1C-C2C-CMC-OMC
34	K	106	LHG	C4-C5-C6-O8
35	0	603	SQD	O5-C5-C6-S
36	2	602	LMG	O1-C7-C8-C9
36	9	602	LMG	C7-C8-C9-O8
36	B	853	LMG	C7-C8-C9-O8
36	L	210	LMG	O1-C7-C8-C9
36	L	211	LMG	C7-C8-C9-O8
30	4	308	CHL	O1A-CGA-O2A-C1
34	7	602	LHG	O7-C5-C6-O8
34	K	106	LHG	O7-C5-C6-O8
34	d	630	LHG	O7-C5-C6-O8
36	2	602	LMG	O1-C7-C8-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	9	602	LMG	O7-C8-C9-O8
36	B	853	LMG	O7-C8-C9-O8
31	0	308	CLA	C8-C10-C11-C12
31	0	308	CLA	C10-C11-C12-C13
36	9	602	LMG	C21-C22-C23-C24
30	1	305	CHL	O2A-C1-C2-C3
30	9	305	CHL	O2A-C1-C2-C3
30	4	319	CHL	CAA-CBA-CGA-O2A
31	B	805	CLA	C16-C17-C18-C19
30	c	608	CHL	C10-C11-C12-C13
34	1	601	LHG	C12-C13-C14-C15
34	M	104	LHG	C34-C35-C36-C37
34	3	601	LHG	C2-C3-O3-P
30	6	313	CHL	O1A-CGA-O2A-C1
30	f	609	CHL	O1A-CGA-O2A-C1
31	1	310	CLA	C4-C3-C5-C6
31	A	829	CLA	C4-C3-C5-C6
31	8	312	CLA	C11-C10-C8-C9
30	6	313	CHL	CBA-CGA-O2A-C1
30	9	306	CHL	CAA-CBA-CGA-O2A
34	K	106	LHG	C12-C13-C14-C15
30	1	307	CHL	C14-C13-C15-C16
30	b	601	CHL	C11-C12-C13-C14
30	b	602	CHL	C14-C13-C15-C16
30	f	602	CHL	C14-C13-C15-C16
30	f	609	CHL	C11-C12-C13-C14
30	i	602	CHL	C11-C10-C8-C9
31	0	308	CLA	C11-C10-C8-C9
31	3	310	CLA	C11-C10-C8-C9
31	5	303	CLA	C6-C7-C8-C9
31	6	312	CLA	C6-C7-C8-C9
31	7	308	CLA	C14-C13-C15-C16
31	A	803	CLA	C11-C10-C8-C9
31	A	806	CLA	C6-C7-C8-C9
31	A	811	CLA	C11-C12-C13-C14
31	A	811	CLA	C14-C13-C15-C16
31	A	817	CLA	C11-C12-C13-C14
31	A	821	CLA	C14-C13-C15-C16
31	A	853	CLA	C14-C13-C15-C16
30	1	305	CHL	O1D-CGD-O2D-CED
31	0	303	CLA	O1D-CGD-O2D-CED
31	b	613	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	e	611	CLA	O1A-CGA-O2A-C1
30	g	606	CHL	CBD-CGD-O2D-CED
34	h	630	LHG	C25-C26-C27-C28
31	3	312	CLA	C6-C7-C8-C10
36	2	602	LMG	C10-C11-C12-C13
30	0	306	CHL	O1A-CGA-O2A-C1
31	A	818	CLA	CAA-CBA-CGA-O2A
34	g	630	LHG	O1-C1-C2-O2
34	e	630	LHG	O1-C1-C2-O2
34	1	601	LHG	C35-C36-C37-C38
32	3	402	8CT	C13-C14-C15-C16
32	6	402	8CT	C21-C23-C24-C25
32	B	843	8CT	C13-C14-C15-C16
32	B	843	8CT	C21-C23-C24-C25
32	B	844	8CT	C13-C14-C15-C16
32	B	844	8CT	C21-C23-C24-C25
32	B	845	8CT	C13-C14-C15-C16
32	B	846	8CT	C13-C14-C15-C16
32	B	846	8CT	C21-C23-C24-C25
37	c	522	0IE	C12-C13-C14-C15
30	1	313	CHL	O1D-CGD-O2D-CED
32	3	402	8CT	C10-C11-C12-C40
34	M	104	LHG	C13-C14-C15-C16
34	b	630	LHG	C11-C12-C13-C14
34	G	105	LHG	C7-C8-C9-C10
33	5	501	0UR	C41-C2-C3-C4
33	b	520	0UR	C41-C2-C3-C4
33	d	520	0UR	C41-C2-C3-C4
33	g	520	0UR	C41-C2-C3-C4
33	e	520	0UR	C41-C2-C3-C4
35	0	603	SQD	C4-C5-C6-S
33	4	501	0UR	O57-C45-C46-C47
34	0	601	LHG	C31-C32-C33-C34
33	b	520	0UR	C5-C6-C7-C8
34	6	603	LHG	O8-C23-C24-C25
30	6	307	CHL	C2B-C3B-CAB-CBB
31	3	312	CLA	C2B-C3B-CAB-CBB
31	3	313	CLA	C2B-C3B-CAB-CBB
31	5	310	CLA	C2B-C3B-CAB-CBB
31	5	314	CLA	C2B-C3B-CAB-CBB
31	6	304	CLA	C2B-C3B-CAB-CBB
31	6	320	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	7	310	CLA	C2B-C3B-CAB-CBB
31	8	311	CLA	C2B-C3B-CAB-CBB
31	8	312	CLA	C2B-C3B-CAB-CBB
31	8	314	CLA	C2B-C3B-CAB-CBB
31	9	310	CLA	C2B-C3B-CAB-CBB
31	A	809	CLA	C2B-C3B-CAB-CBB
31	A	815	CLA	C2B-C3B-CAB-CBB
31	A	835	CLA	C2B-C3B-CAB-CBB
31	A	837	CLA	C2B-C3B-CAB-CBB
31	B	831	CLA	C2B-C3B-CAB-CBB
31	B	850	CLA	C2B-C3B-CAB-CBB
31	b	603	CLA	C2B-C3B-CAB-CBB
31	d	613	CLA	C2B-C3B-CAB-CBB
31	H	202	CLA	C2B-C3B-CAB-CBB
31	4	303	CLA	C2B-C3B-CAB-CBB
31	4	310	CLA	C2B-C3B-CAB-CBB
36	9	602	LMG	C15-C16-C17-C18
31	A	821	CLA	C13-C15-C16-C17
31	b	611	CLA	C8-C10-C11-C12
34	6	601	LHG	C27-C28-C29-C30
34	G	105	LHG	C12-C13-C14-C15
31	A	814	CLA	C4-C3-C5-C6
31	A	821	CLA	C4-C3-C5-C6
34	2	601	LHG	C7-C8-C9-C10
31	A	830	CLA	C13-C15-C16-C17
31	B	827	CLA	C10-C11-C12-C13
30	i	608	CHL	C1-C2-C3-C4
31	A	822	CLA	C1-C2-C3-C4
31	h	603	CLA	C1-C2-C3-C4
30	c	608	CHL	C3-C5-C6-C7
30	5	313	CHL	O1A-CGA-O2A-C1
31	5	308	CLA	O1A-CGA-O2A-C1
36	B	853	LMG	C9-C8-O7-C10
31	2	312	CLA	C2A-CAA-CBA-CGA
31	A	802	CLA	C2A-CAA-CBA-CGA
31	A	817	CLA	C2A-CAA-CBA-CGA
31	A	837	CLA	C2A-CAA-CBA-CGA
31	A	839	CLA	C2A-CAA-CBA-CGA
31	K	105	CLA	C2A-CAA-CBA-CGA
31	b	613	CLA	C2A-CAA-CBA-CGA
31	f	613	CLA	C2A-CAA-CBA-CGA
31	g	610	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	i	613	CLA	C2A-CAA-CBA-CGA
31	e	610	CLA	C2A-CAA-CBA-CGA
34	A	855	LHG	C15-C16-C17-C18
34	a	630	LHG	O9-C7-O7-C5
30	0	302	CHL	C2-C1-O2A-CGA
30	1	313	CHL	C2-C1-O2A-CGA
30	7	302	CHL	C2-C1-O2A-CGA
30	8	307	CHL	C2-C1-O2A-CGA
30	a	609	CHL	C2-C1-O2A-CGA
30	c	602	CHL	C2-C1-O2A-CGA
30	d	601	CHL	C2-C1-O2A-CGA
30	d	609	CHL	C2-C1-O2A-CGA
30	f	609	CHL	C2-C1-O2A-CGA
31	A	814	CLA	C2-C1-O2A-CGA
31	A	821	CLA	C2-C1-O2A-CGA
31	A	853	CLA	C2-C1-O2A-CGA
31	G	101	CLA	C2-C1-O2A-CGA
30	c	601	CHL	C2C-C3C-CAC-CBC
34	K	106	LHG	C29-C30-C31-C32
34	6	601	LHG	O8-C23-C24-C25
31	8	312	CLA	C3-C5-C6-C7
31	A	827	CLA	C3-C5-C6-C7
34	M	104	LHG	C15-C16-C17-C18
34	6	603	LHG	C2-C3-O3-P
34	2	601	LHG	C10-C11-C12-C13
31	B	814	CLA	C16-C17-C18-C19
31	B	822	CLA	C2C-C3C-CAC-CBC
36	L	211	LMG	C14-C15-C16-C17
34	6	603	LHG	C24-C23-O8-C6
31	B	805	CLA	CAA-CBA-CGA-O2A
31	4	304	CLA	C10-C11-C12-C13
33	0	501	0UR	C46-C47-C48-C49
30	5	301	CHL	C2A-CAA-CBA-CGA
31	3	312	CLA	C2A-CAA-CBA-CGA
36	L	210	LMG	O7-C8-C9-O8
31	B	824	CLA	C5-C6-C7-C8
34	7	603	LHG	C3-O3-P-O6
34	9	601	LHG	C3-O3-P-O6
34	A	844	LHG	C3-O3-P-O6
34	c	630	LHG	C3-O3-P-O6
34	f	630	LHG	C4-O6-P-O3
34	A	855	LHG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	2	304	CLA	C8-C10-C11-C12
31	A	803	CLA	C16-C17-C18-C20
31	d	613	CLA	C11-C10-C8-C7
31	A	853	CLA	C15-C16-C17-C18
34	A	855	LHG	C4-C5-C6-O8
41	B	849	DGD	C1G-C2G-C3G-O3G
30	6	302	CHL	C12-C13-C15-C16
30	b	608	CHL	C12-C13-C15-C16
30	d	602	CHL	C11-C12-C13-C15
31	6	312	CLA	C6-C7-C8-C10
31	A	828	CLA	C6-C7-C8-C10
31	A	832	CLA	C6-C7-C8-C10
31	B	806	CLA	C11-C12-C13-C15
31	L	203	CLA	C11-C10-C8-C7
31	A	835	CLA	O1D-CGD-O2D-CED
30	8	302	CHL	C14-C13-C15-C16
30	f	601	CHL	C6-C7-C8-C9
30	e	608	CHL	C6-C7-C8-C9
31	8	309	CLA	C11-C10-C8-C9
31	A	815	CLA	C6-C7-C8-C9
31	B	803	CLA	C11-C12-C13-C14
31	B	808	CLA	C11-C10-C8-C9
31	B	817	CLA	C6-C7-C8-C9
31	B	820	CLA	C6-C7-C8-C9
39	A	857	CL0	C14-C13-C15-C16
30	6	308	CHL	C5-C6-C7-C8
32	7	405	8CT	C16-C17-C18-C19
32	8	406	8CT	C16-C17-C18-C19
32	A	847	8CT	C18-C19-C20-C21
32	L	206	8CT	C18-C19-C20-C21
31	6	317	CLA	C16-C17-C18-C19
30	f	609	CHL	C10-C11-C12-C13
30	2	319	CHL	CAA-CBA-CGA-O1A
30	d	607	CHL	CAA-CBA-CGA-O1A
30	9	301	CHL	C2A-CAA-CBA-CGA
31	5	311	CLA	C2A-CAA-CBA-CGA
31	A	835	CLA	C2A-CAA-CBA-CGA
31	d	611	CLA	C2A-CAA-CBA-CGA
31	6	320	CLA	O1D-CGD-O2D-CED
36	O	207	LMG	C12-C13-C14-C15
32	2	402	8CT	C10-C11-C12-C40
33	4	502	0UR	C5-C6-C7-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	3	308	CLA	C16-C17-C18-C20
34	2	601	LHG	C12-C13-C14-C15
30	5	313	CHL	CAA-CBA-CGA-O2A
33	8	502	0UR	C46-C47-C48-C49
30	f	609	CHL	C5-C6-C7-C8
30	g	606	CHL	O1D-CGD-O2D-CED
33	0	502	0UR	C15-C16-C17-C18
34	3	601	LHG	C25-C26-C27-C28
31	7	312	CLA	C3-C5-C6-C7
31	0	311	CLA	O1D-CGD-O2D-CED
30	3	302	CHL	C12-C13-C15-C16
31	8	312	CLA	C11-C10-C8-C7
31	A	817	CLA	C12-C13-C15-C16
34	6	601	LHG	C23-C24-C25-C26
31	6	320	CLA	CBD-CGD-O2D-CED
31	A	821	CLA	C2-C3-C5-C6
31	L	201	CLA	C2-C3-C5-C6
31	9	302	CLA	C16-C17-C18-C19
31	B	805	CLA	C16-C17-C18-C20
34	8	601	LHG	C24-C23-O8-C6
34	c	630	LHG	C23-C24-C25-C26
36	L	211	LMG	C30-C31-C32-C33
34	e	630	LHG	C11-C12-C13-C14
31	A	816	CLA	O1D-CGD-O2D-CED
34	7	602	LHG	C13-C14-C15-C16
34	h	630	LHG	C28-C29-C30-C31
34	6	603	LHG	O10-C23-O8-C6
30	8	305	CHL	O1A-CGA-O2A-C1
30	a	607	CHL	O1A-CGA-O2A-C1
31	A	816	CLA	CBD-CGD-O2D-CED
31	5	309	CLA	CBA-CGA-O2A-C1
31	A	813	CLA	CBA-CGA-O2A-C1
34	6	601	LHG	C7-C8-C9-C10
33	6	501	0UR	C46-C47-C48-C49
33	6	502	0UR	C46-C47-C48-C49
33	8	501	0UR	C46-C47-C48-C49
33	c	520	0UR	C46-C47-C48-C49
33	b	520	0UR	C46-C47-C48-C49
33	e	520	0UR	C46-C47-C48-C49
30	8	302	CHL	C4B-C3B-CAB-CBB
30	b	602	CHL	C4B-C3B-CAB-CBB
31	1	314	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	5	303	CLA	C4B-C3B-CAB-CBB
31	8	303	CLA	C4B-C3B-CAB-CBB
31	8	314	CLA	C4B-C3B-CAB-CBB
31	A	815	CLA	C4B-C3B-CAB-CBB
31	A	837	CLA	C4B-C3B-CAB-CBB
31	B	831	CLA	C4B-C3B-CAB-CBB
31	B	840	CLA	C4B-C3B-CAB-CBB
31	L	203	CLA	C4B-C3B-CAB-CBB
31	d	613	CLA	C4B-C3B-CAB-CBB
31	i	611	CLA	C4B-C3B-CAB-CBB
31	A	818	CLA	C2A-CAA-CBA-CGA
36	O	207	LMG	O6-C1-O1-C7
32	B	846	8CT	C18-C19-C20-C21
34	b	630	LHG	O6-C4-C5-C6
31	A	813	CLA	O1A-CGA-O2A-C1
31	B	834	CLA	C10-C11-C12-C13
34	0	601	LHG	C9-C10-C11-C12
31	5	310	CLA	CBD-CGD-O2D-CED
31	9	312	CLA	C4-C3-C5-C6
31	3	308	CLA	C5-C6-C7-C8
31	f	613	CLA	C2-C3-C5-C6
34	8	601	LHG	O10-C23-O8-C6
30	c	607	CHL	O1A-CGA-O2A-C1
30	1	313	CHL	C5-C6-C7-C8
31	B	832	CLA	C15-C16-C17-C18
36	A	856	LMG	C33-C34-C35-C36
31	A	837	CLA	CBD-CGD-O2D-CED
30	e	602	CHL	C2-C1-O2A-CGA
31	6	320	CLA	C2-C1-O2A-CGA
31	A	839	CLA	C2-C1-O2A-CGA
31	B	812	CLA	C2-C1-O2A-CGA
31	K	102	CLA	C4C-C3C-CAC-CBC
31	a	611	CLA	C8-C10-C11-C12
34	2	601	LHG	C9-C10-C11-C12
36	9	602	LMG	C31-C32-C33-C34
31	A	829	CLA	C5-C6-C7-C8
30	9	313	CHL	C2A-CAA-CBA-CGA
31	1	303	CLA	C2A-CAA-CBA-CGA
31	6	312	CLA	C2A-CAA-CBA-CGA
31	7	312	CLA	C2A-CAA-CBA-CGA
31	9	312	CLA	C2A-CAA-CBA-CGA
36	O	207	LMG	O7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	829	CLA	CBA-CGA-O2A-C1
31	K	101	CLA	CBD-CGD-O2D-CED
31	6	318	CLA	CAA-CBA-CGA-O1A
31	K	102	CLA	C5-C6-C7-C8
30	3	307	CHL	C3A-C2A-CAA-CBA
30	9	306	CHL	C3A-C2A-CAA-CBA
30	i	608	CHL	C3A-C2A-CAA-CBA
31	5	304	CLA	C3A-C2A-CAA-CBA
31	A	828	CLA	C3A-C2A-CAA-CBA
31	F	301	CLA	C3A-C2A-CAA-CBA
31	A	829	CLA	C16-C17-C18-C20
30	2	308	CHL	C2C-C3C-CAC-CBC
34	9	601	LHG	C29-C30-C31-C32
30	5	306	CHL	C2C-C3C-CAC-CBC
31	B	808	CLA	C4-C3-C5-C6
31	f	613	CLA	C4-C3-C5-C6
31	B	841	CLA	CBD-CGD-O2D-CED
31	A	829	CLA	C2-C3-C5-C6
30	a	609	CHL	C11-C10-C8-C9
30	c	608	CHL	C11-C12-C13-C14
30	b	608	CHL	C11-C12-C13-C14
30	e	602	CHL	C11-C10-C8-C9
30	e	609	CHL	C11-C10-C8-C9
31	1	310	CLA	C11-C12-C13-C14
31	7	308	CLA	C11-C10-C8-C9
31	A	809	CLA	C11-C10-C8-C9
31	B	806	CLA	C14-C13-C15-C16
31	B	827	CLA	C11-C10-C8-C9
31	A	804	CLA	C6-C7-C8-C10
31	A	829	CLA	C16-C17-C18-C19
31	B	840	CLA	C16-C17-C18-C20
34	8	601	LHG	C9-C10-C11-C12
31	i	612	CLA	CAA-CBA-CGA-O2A
34	0	601	LHG	C16-C17-C18-C19
34	6	601	LHG	C28-C29-C30-C31
34	7	603	LHG	C9-C10-C11-C12
32	2	402	8CT	C19-C20-C21-C22
32	3	402	8CT	C40-C12-C13-C14
32	3	403	8CT	C28-C29-C30-C35
32	7	404	8CT	C24-C25-C26-C27
32	7	405	8CT	C24-C25-C26-C27
32	8	406	8CT	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	B	843	8CT	C39-C16-C17-C18
32	B	844	8CT	C39-C16-C17-C18
32	B	844	8CT	C19-C20-C21-C22
32	B	844	8CT	C24-C25-C26-C27
32	B	845	8CT	C39-C16-C17-C18
32	B	845	8CT	C24-C25-C26-C27
32	B	846	8CT	C40-C12-C13-C14
32	B	846	8CT	C39-C16-C17-C18
32	B	848	8CT	C24-C25-C26-C27
32	B	851	8CT	C40-C12-C13-C14
32	J	104	8CT	C40-C12-C13-C14
32	L	206	8CT	C28-C29-C30-C35
32	4	402	8CT	C19-C20-C21-C22
33	0	502	0UR	C17-C18-C19-C28
33	O	204	0UR	C17-C18-C19-C28
33	h	520	0UR	C17-C18-C19-C28
34	A	845	LHG	C4-C5-C6-O8
42	a	523	NEX	C39-C29-C30-C31
42	c	523	NEX	C39-C29-C30-C31
42	b	523	NEX	C39-C29-C30-C31
42	d	523	NEX	C39-C29-C30-C31
42	f	523	NEX	C39-C29-C30-C31
42	g	523	NEX	C39-C29-C30-C31
42	h	523	NEX	C39-C29-C30-C31
42	i	523	NEX	C39-C29-C30-C31
42	e	523	NEX	C39-C29-C30-C31
31	0	303	CLA	C10-C11-C12-C13
31	2	304	CLA	C5-C6-C7-C8
31	A	829	CLA	O1A-CGA-O2A-C1
31	8	304	CLA	C16-C17-C18-C20
30	a	606	CHL	O2A-C1-C2-C3
30	4	306	CHL	O1D-CGD-O2D-CED
31	8	314	CLA	CAA-CBA-CGA-O1A
31	i	612	CLA	CAA-CBA-CGA-O1A
34	h	630	LHG	C27-C28-C29-C30
31	7	317	CLA	CAA-CBA-CGA-O2A
36	J	102	LMG	C7-C8-O7-C10
30	6	301	CHL	C5-C6-C7-C8
31	A	840	CLA	C15-C16-C17-C18
31	B	829	CLA	C4-C3-C5-C6
31	K	102	CLA	C4-C3-C5-C6
30	3	307	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	i	608	CHL	C1A-C2A-CAA-CBA
31	5	310	CLA	C1A-C2A-CAA-CBA
31	6	310	CLA	C1A-C2A-CAA-CBA
31	A	802	CLA	C1A-C2A-CAA-CBA
31	A	828	CLA	C1A-C2A-CAA-CBA
31	B	813	CLA	C1A-C2A-CAA-CBA
31	B	816	CLA	C1A-C2A-CAA-CBA
31	c	610	CLA	C1A-C2A-CAA-CBA
31	d	604	CLA	C1A-C2A-CAA-CBA
34	2	601	LHG	C25-C26-C27-C28
34	6	601	LHG	C10-C11-C12-C13
30	2	302	CHL	C11-C12-C13-C15
30	i	602	CHL	C6-C7-C8-C10
31	1	310	CLA	C2-C3-C5-C6
31	9	308	CLA	C11-C10-C8-C7
31	9	308	CLA	C11-C12-C13-C15
31	A	818	CLA	C12-C13-C15-C16
31	A	827	CLA	C6-C7-C8-C10
31	A	832	CLA	C11-C10-C8-C7
31	B	801	CLA	C12-C13-C15-C16
31	B	806	CLA	C15-C16-C17-C18
31	h	612	CLA	CAA-CBA-CGA-O1A
31	e	612	CLA	CAA-CBA-CGA-O1A
32	A	847	8CT	C23-C24-C25-C26
32	B	804	8CT	C18-C19-C20-C21
30	a	608	CHL	C3C-C2C-CMC-OMC
30	c	614	CHL	C3C-C2C-CMC-OMC
30	f	608	CHL	C3C-C2C-CMC-OMC
30	h	601	CHL	C3C-C2C-CMC-OMC
30	4	308	CHL	C3C-C2C-CMC-OMC
34	H	203	LHG	C24-C23-O8-C6
31	5	309	CLA	O1A-CGA-O2A-C1
31	7	317	CLA	CAA-CBA-CGA-O1A
31	g	612	CLA	CAA-CBA-CGA-O2A
31	2	309	CLA	C11-C12-C13-C15
31	8	304	CLA	C16-C17-C18-C19
31	7	318	CLA	C2A-CAA-CBA-CGA
31	B	806	CLA	C2A-CAA-CBA-CGA
31	c	603	CLA	C2A-CAA-CBA-CGA
34	A	845	LHG	O1-C1-C2-O2
30	2	301	CHL	C8-C10-C11-C12
31	9	300	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	820	CLA	C5-C6-C7-C8
31	4	312	CLA	O1A-CGA-O2A-C1
34	A	855	LHG	O6-C4-C5-O7
31	B	818	CLA	C11-C12-C13-C14
31	4	309	CLA	C10-C11-C12-C13
31	B	813	CLA	C6-C7-C8-C10
31	c	612	CLA	CAA-CBA-CGA-O1A
30	a	601	CHL	CBA-CGA-O2A-C1
30	2	302	CHL	C4-C3-C5-C6
30	4	302	CHL	C4-C3-C5-C6
31	A	819	CLA	C4-C3-C5-C6
30	d	602	CHL	C5-C6-C7-C8
31	e	604	CLA	CBD-CGD-O2D-CED
30	3	302	CHL	C2B-C3B-CAB-CBB
30	3	307	CHL	C2B-C3B-CAB-CBB
30	7	302	CHL	C2B-C3B-CAB-CBB
30	7	305	CHL	C2B-C3B-CAB-CBB
30	8	302	CHL	C2B-C3B-CAB-CBB
30	b	602	CHL	C2B-C3B-CAB-CBB
30	f	606	CHL	C2B-C3B-CAB-CBB
31	1	314	CLA	C2B-C3B-CAB-CBB
31	2	303	CLA	C2B-C3B-CAB-CBB
31	2	310	CLA	C2B-C3B-CAB-CBB
31	6	310	CLA	C2B-C3B-CAB-CBB
31	6	318	CLA	C2B-C3B-CAB-CBB
31	7	311	CLA	C2B-C3B-CAB-CBB
31	7	312	CLA	C2B-C3B-CAB-CBB
31	7	315	CLA	C2B-C3B-CAB-CBB
31	8	303	CLA	C2B-C3B-CAB-CBB
31	8	310	CLA	C2B-C3B-CAB-CBB
31	A	823	CLA	C2B-C3B-CAB-CBB
31	A	840	CLA	C2B-C3B-CAB-CBB
31	B	809	CLA	C2B-C3B-CAB-CBB
31	B	811	CLA	C2B-C3B-CAB-CBB
31	B	822	CLA	C2B-C3B-CAB-CBB
31	B	834	CLA	C2B-C3B-CAB-CBB
31	B	840	CLA	C2B-C3B-CAB-CBB
31	B	841	CLA	C2B-C3B-CAB-CBB
31	F	301	CLA	C2B-C3B-CAB-CBB
31	L	207	CLA	C2B-C3B-CAB-CBB
31	K	101	CLA	C2B-C3B-CAB-CBB
31	O	206	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	611	CLA	C2B-C3B-CAB-CBB
31	d	611	CLA	C2B-C3B-CAB-CBB
31	d	612	CLA	C2B-C3B-CAB-CBB
31	f	603	CLA	C2B-C3B-CAB-CBB
31	c	612	CLA	CAA-CBA-CGA-O2A
31	g	612	CLA	CAA-CBA-CGA-O1A
30	d	602	CHL	C8-C10-C11-C12
39	A	857	CL0	C8-C10-C11-C12
31	6	318	CLA	CBD-CGD-O2D-CED
31	A	837	CLA	O1D-CGD-O2D-CED
32	2	402	8CT	C19-C20-C21-C23
32	3	402	8CT	C11-C12-C13-C14
32	7	404	8CT	C24-C25-C26-C28
32	7	405	8CT	C24-C25-C26-C28
32	8	406	8CT	C24-C25-C26-C28
32	B	843	8CT	C15-C16-C17-C18
32	B	844	8CT	C15-C16-C17-C18
32	B	844	8CT	C19-C20-C21-C23
32	B	844	8CT	C24-C25-C26-C28
32	B	845	8CT	C15-C16-C17-C18
32	B	845	8CT	C24-C25-C26-C28
32	B	846	8CT	C11-C12-C13-C14
32	B	846	8CT	C15-C16-C17-C18
32	B	848	8CT	C24-C25-C26-C28
32	B	851	8CT	C11-C12-C13-C14
32	J	104	8CT	C11-C12-C13-C14
32	4	402	8CT	C19-C20-C21-C23
42	a	523	NEX	C28-C29-C30-C31
42	c	523	NEX	C28-C29-C30-C31
42	b	523	NEX	C28-C29-C30-C31
42	d	523	NEX	C28-C29-C30-C31
42	f	523	NEX	C28-C29-C30-C31
42	g	523	NEX	C28-C29-C30-C31
42	h	523	NEX	C28-C29-C30-C31
42	i	523	NEX	C28-C29-C30-C31
42	e	523	NEX	C28-C29-C30-C31
31	B	813	CLA	C5-C6-C7-C8
31	1	309	CLA	CBA-CGA-O2A-C1
32	B	847	8CT	C23-C24-C25-C26
31	A	836	CLA	C2C-C3C-CAC-CBC
34	b	630	LHG	C25-C26-C27-C28
34	G	105	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	808	CLA	CAA-CBA-CGA-O2A
34	f	630	LHG	C1-C2-C3-O3
31	5	303	CLA	C8-C10-C11-C12
31	b	611	CLA	C10-C11-C12-C13
31	e	604	CLA	O1D-CGD-O2D-CED
30	6	302	CHL	C4-C3-C5-C6
30	f	609	CHL	C4-C3-C5-C6
30	c	609	CHL	C2-C1-O2A-CGA
30	b	609	CHL	C2-C1-O2A-CGA
30	d	602	CHL	C2-C1-O2A-CGA
30	d	606	CHL	C2-C1-O2A-CGA
30	i	606	CHL	C2-C1-O2A-CGA
31	0	308	CLA	C2-C1-O2A-CGA
31	7	311	CLA	C2-C1-O2A-CGA
30	5	305	CHL	CAA-CBA-CGA-O2A
31	8	314	CLA	CAA-CBA-CGA-O2A
34	9	601	LHG	C26-C27-C28-C29
31	0	303	CLA	C11-C12-C13-C14
31	A	853	CLA	C11-C10-C8-C9
31	B	828	CLA	C6-C7-C8-C9
31	4	309	CLA	C6-C7-C8-C9
30	5	306	CHL	CAA-CBA-CGA-O1A
31	A	825	CLA	C8-C10-C11-C12
34	H	203	LHG	O10-C23-O8-C6
31	4	314	CLA	CAA-CBA-CGA-O2A
30	g	602	CHL	C4-C3-C5-C6
31	6	320	CLA	C4-C3-C5-C6
31	A	836	CLA	C4-C3-C5-C6
30	5	307	CHL	O1A-CGA-O2A-C1
30	5	306	CHL	C2-C1-O2A-CGA
31	1	309	CLA	O1A-CGA-O2A-C1
34	3	601	LHG	C12-C13-C14-C15
34	A	855	LHG	C9-C10-C11-C12
31	A	828	CLA	C8-C10-C11-C12
31	0	312	CLA	C2A-CAA-CBA-CGA
31	8	312	CLA	C2A-CAA-CBA-CGA
31	A	836	CLA	C2A-CAA-CBA-CGA
31	B	815	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
31	4	312	CLA	C2A-CAA-CBA-CGA
31	4	303	CLA	CAA-CBA-CGA-O1A
31	4	303	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	M	104	LHG	C10-C11-C12-C13
30	0	301	CHL	O1A-CGA-O2A-C1
32	2	402	8CT	C04-C03-C10-C11
32	A	849	8CT	C04-C03-C10-C11
32	I	101	8CT	C04-C03-C10-C11
31	B	832	CLA	C13-C15-C16-C17
31	6	318	CLA	O1D-CGD-O2D-CED
30	e	602	CHL	C8-C10-C11-C12
34	b	630	LHG	O1-C1-C2-C3
31	6	312	CLA	O1A-CGA-O2A-C1
32	B	847	8CT	C12-C13-C14-C15
33	8	502	0UR	C3-C4-C5-C6
31	B	813	CLA	C4-C3-C5-C6
31	B	822	CLA	C4-C3-C5-C6
31	e	613	CLA	C4-C3-C5-C6
32	3	402	8CT	C10-C11-C12-C13
42	a	523	NEX	C31-C32-C33-C34
42	c	523	NEX	C31-C32-C33-C34
42	b	523	NEX	C31-C32-C33-C34
42	d	523	NEX	C31-C32-C33-C34
42	g	523	NEX	C31-C32-C33-C34
42	h	523	NEX	C31-C32-C33-C34
42	i	523	NEX	C31-C32-C33-C34
34	d	630	LHG	C9-C10-C11-C12
36	9	602	LMG	C35-C36-C37-C38
31	9	312	CLA	C2-C3-C5-C6
31	B	808	CLA	C2-C3-C5-C6
31	e	612	CLA	CAA-CBA-CGA-O2A
30	g	602	CHL	O1A-CGA-O2A-C1
34	a	630	LHG	C17-C18-C19-C20
31	4	312	CLA	CBA-CGA-O2A-C1
31	0	321	CLA	CAA-CBA-CGA-O2A
31	h	612	CLA	CAA-CBA-CGA-O2A
30	i	607	CHL	O1A-CGA-O2A-C1
36	L	211	LMG	C29-C30-C31-C32
31	A	808	CLA	C16-C17-C18-C19
33	3	501	0UR	C46-C47-C48-C49
33	9	501	0UR	C46-C47-C48-C49
39	A	857	CL0	C13-C15-C16-C17
30	1	313	CHL	C14-C13-C15-C16
31	B	830	CLA	C11-C10-C8-C9
30	1	306	CHL	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	0	306	CHL	C2A-CAA-CBA-CGA
30	8	313	CHL	C2A-CAA-CBA-CGA
41	B	849	DGD	C6A-C7A-C8A-C9A
31	A	836	CLA	CBD-CGD-O2D-CED
30	0	301	CHL	CBA-CGA-O2A-C1
30	3	305	CHL	CBA-CGA-O2A-C1
31	6	312	CLA	CBA-CGA-O2A-C1
34	G	105	LHG	C14-C15-C16-C17
31	G	102	CLA	CAA-CBA-CGA-O2A
30	3	307	CHL	C4B-C3B-CAB-CBB
31	A	834	CLA	C4B-C3B-CAB-CBB
31	B	839	CLA	C4B-C3B-CAB-CBB
31	B	841	CLA	C4B-C3B-CAB-CBB
31	a	613	CLA	C4B-C3B-CAB-CBB
31	d	603	CLA	C4B-C3B-CAB-CBB
31	g	612	CLA	C4B-C3B-CAB-CBB
36	L	211	LMG	O6-C1-O1-C7
31	A	828	CLA	CAA-CBA-CGA-O2A
30	7	302	CHL	C4-C3-C5-C6
30	d	609	CHL	C4-C3-C5-C6
30	e	609	CHL	C4-C3-C5-C6
31	A	817	CLA	C4-C3-C5-C6
30	d	609	CHL	C11-C12-C13-C15
30	i	602	CHL	C11-C10-C8-C7
30	e	608	CHL	C11-C12-C13-C15
31	3	310	CLA	C2-C3-C5-C6
31	3	310	CLA	C11-C10-C8-C7
31	9	312	CLA	C6-C7-C8-C10
31	6	314	CLA	CAA-CBA-CGA-O2A
31	7	303	CLA	CAA-CBA-CGA-O2A
33	5	501	0UR	C46-C47-C48-C49
34	6	603	LHG	O1-C1-C2-O2
34	b	630	LHG	O1-C1-C2-O2
30	3	305	CHL	O1A-CGA-O2A-C1
34	B	854	LHG	C35-C36-C37-C38
32	K	107	8CT	C23-C24-C25-C26
31	7	318	CLA	C11-C12-C13-C14
30	5	305	CHL	CAA-CBA-CGA-O1A
34	9	601	LHG	C5-C4-O6-P
31	B	840	CLA	C2C-C3C-CAC-CBC
36	L	210	LMG	O1-C7-C8-O7
30	e	607	CHL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	8	601	LHG	C31-C32-C33-C34
34	H	203	LHG	O10-C23-C24-C25
30	i	608	CHL	O2A-C1-C2-C3
31	K	105	CLA	CAA-CBA-CGA-O2A
30	4	313	CHL	C2A-CAA-CBA-CGA
31	1	310	CLA	C2A-CAA-CBA-CGA
31	9	302	CLA	C15-C16-C17-C18
34	b	630	LHG	C9-C10-C11-C12
31	B	813	CLA	C6-C7-C8-C9
31	b	612	CLA	CAA-CBA-CGA-O2A
30	g	602	CHL	CBA-CGA-O2A-C1
31	A	821	CLA	CBA-CGA-O2A-C1
33	1	501	0UR	C46-C47-C48-C49
33	4	501	0UR	C46-C47-C48-C49
33	4	502	0UR	O42-C2-C3-C4
37	c	522	0IE	O1-C2-C3-C4
37	d	522	0IE	O1-C2-C30-C31
31	0	313	CLA	CAA-CBA-CGA-O2A
34	7	602	LHG	O7-C7-C8-C9
34	b	630	LHG	O7-C7-C8-C9
34	5	601	LHG	C27-C28-C29-C30
30	b	609	CHL	C4-C3-C5-C6
30	f	601	CHL	C4-C3-C5-C6
30	i	602	CHL	C4-C3-C5-C6
31	A	808	CLA	C4-C3-C5-C6
31	A	809	CLA	C4-C3-C5-C6
31	A	810	CLA	C4-C3-C5-C6
31	L	203	CLA	C4-C3-C5-C6
30	3	307	CHL	C10-C11-C12-C13
31	A	808	CLA	C13-C15-C16-C17
31	i	611	CLA	CAA-CBA-CGA-O2A
30	f	609	CHL	C2-C3-C5-C6
30	4	302	CHL	C2-C3-C5-C6
31	3	320	CLA	C2-C3-C5-C6
31	e	613	CLA	C2-C3-C5-C6
30	b	609	CHL	C5-C6-C7-C8
30	i	609	CHL	C2-C1-O2A-CGA
30	4	319	CHL	C5-C6-C7-C8
34	7	602	LHG	C11-C12-C13-C14
31	d	603	CLA	C6-C7-C8-C10
30	b	602	CHL	C10-C11-C12-C13
31	A	820	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	A	845	LHG	C10-C11-C12-C13
30	1	313	CHL	C12-C13-C15-C16
31	B	830	CLA	C11-C10-C8-C7
30	1	302	CHL	C11-C12-C13-C14
30	3	307	CHL	C11-C12-C13-C14
30	a	602	CHL	C11-C10-C8-C9
30	c	609	CHL	C11-C12-C13-C14
30	d	602	CHL	C14-C13-C15-C16
30	f	609	CHL	C6-C7-C8-C9
31	0	303	CLA	C6-C7-C8-C9
31	1	303	CLA	C6-C7-C8-C9
31	3	308	CLA	C11-C10-C8-C9
31	5	312	CLA	C6-C7-C8-C9
31	A	835	CLA	C11-C10-C8-C9
31	A	853	CLA	C11-C12-C13-C14
31	B	841	CLA	C14-C13-C15-C16
31	L	203	CLA	C11-C10-C8-C9
31	L	203	CLA	C14-C13-C15-C16
38	A	842	PQN	C21-C22-C23-C24
31	K	101	CLA	O1D-CGD-O2D-CED
31	5	311	CLA	CAA-CBA-CGA-O1A
31	A	841	CLA	C8-C10-C11-C12
30	f	601	CHL	C3A-C2A-CAA-CBA
30	h	601	CHL	C3A-C2A-CAA-CBA
31	3	313	CLA	C3A-C2A-CAA-CBA
31	A	802	CLA	C3A-C2A-CAA-CBA
31	d	611	CLA	C3A-C2A-CAA-CBA
31	i	604	CLA	C3A-C2A-CAA-CBA
31	e	611	CLA	C3A-C2A-CAA-CBA
34	8	601	LHG	O2-C2-C3-O3
30	0	302	CHL	CAA-CBA-CGA-O2A
30	a	606	CHL	CAA-CBA-CGA-O2A
30	e	602	CHL	CAA-CBA-CGA-O2A
31	5	303	CLA	CAA-CBA-CGA-O2A
34	A	844	LHG	O8-C23-C24-C25
33	2	501	0UR	C46-C47-C48-C49
33	h	520	0UR	C46-C47-C48-C49
30	4	306	CHL	CBD-CGD-O2D-CED
31	B	807	CLA	CAA-CBA-CGA-O2A
31	f	612	CLA	CAA-CBA-CGA-O2A
30	2	319	CHL	CAD-CBD-CGD-O2D
30	9	305	CHL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	614	CHL	CAD-CBD-CGD-O2D
31	0	303	CLA	CAD-CBD-CGD-O2D
31	1	304	CLA	CAD-CBD-CGD-O2D
31	1	308	CLA	CAD-CBD-CGD-O2D
31	3	311	CLA	CAD-CBD-CGD-O2D
31	5	310	CLA	CAD-CBD-CGD-O2D
31	5	311	CLA	CAD-CBD-CGD-O2D
31	6	312	CLA	CAD-CBD-CGD-O2D
31	6	320	CLA	CAD-CBD-CGD-O2D
31	7	315	CLA	CAD-CBD-CGD-O2D
31	9	310	CLA	CAD-CBD-CGD-O2D
31	A	802	CLA	CAD-CBD-CGD-O2D
31	A	807	CLA	CAD-CBD-CGD-O2D
31	A	809	CLA	CAD-CBD-CGD-O2D
31	A	831	CLA	CAD-CBD-CGD-O2D
31	A	832	CLA	CAD-CBD-CGD-O2D
31	A	840	CLA	CAD-CBD-CGD-O2D
31	B	803	CLA	CAD-CBD-CGD-O2D
31	B	808	CLA	CAD-CBD-CGD-O2D
31	B	811	CLA	CAD-CBD-CGD-O2D
31	B	816	CLA	CAD-CBD-CGD-O2D
31	B	830	CLA	CAD-CBD-CGD-O2D
31	B	832	CLA	CAD-CBD-CGD-O2D
31	B	839	CLA	CAD-CBD-CGD-O2D
31	B	841	CLA	CAD-CBD-CGD-O2D
31	L	203	CLA	CAD-CBD-CGD-O2D
31	c	610	CLA	CAD-CBD-CGD-O2D
31	b	603	CLA	CAD-CBD-CGD-O2D
31	g	610	CLA	CAD-CBD-CGD-O2D
31	h	603	CLA	CAD-CBD-CGD-O2D
31	h	612	CLA	CAD-CBD-CGD-O2D
31	i	603	CLA	CAD-CBD-CGD-O2D
31	i	610	CLA	CAD-CBD-CGD-O2D
31	i	612	CLA	CAD-CBD-CGD-O2D
31	A	803	CLA	C16-C17-C18-C19
30	5	306	CHL	C4C-C3C-CAC-CBC
38	B	842	PQN	C15-C16-C17-C18
30	c	601	CHL	C4C-C3C-CAC-CBC
30	2	302	CHL	C2-C1-O2A-CGA
30	6	308	CHL	C2-C1-O2A-CGA
30	0	305	CHL	CAA-CBA-CGA-O2A
30	7	306	CHL	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	9	305	CHL	CAA-CBA-CGA-O2A
31	A	805	CLA	CAA-CBA-CGA-O2A
31	L	203	CLA	CAA-CBA-CGA-O2A
34	3	603	LHG	O8-C23-C24-C25
34	a	630	LHG	O8-C23-C24-C25
30	a	609	CHL	C4-C3-C5-C6
30	c	609	CHL	C4-C3-C5-C6
31	B	811	CLA	C4-C3-C5-C6
31	4	309	CLA	C11-C12-C13-C15
31	A	805	CLA	C3-C5-C6-C7
31	7	303	CLA	CAA-CBA-CGA-O1A
31	4	314	CLA	CAA-CBA-CGA-O1A
30	7	305	CHL	C2-C1-O2A-CGA
30	2	302	CHL	C2-C3-C5-C6
30	i	602	CHL	C2-C3-C5-C6
31	A	819	CLA	C2-C3-C5-C6
31	L	203	CLA	C2-C3-C5-C6
30	8	306	CHL	CAA-CBA-CGA-O2A
31	1	303	CLA	CAA-CBA-CGA-O2A
31	b	603	CLA	CAA-CBA-CGA-O2A
34	A	844	LHG	O7-C7-C8-C9
32	3	403	8CT	C20-C21-C23-C24
42	f	523	NEX	C31-C32-C33-C34
33	1	502	0UR	C4-C3-C43-O44
34	0	601	LHG	C4-C5-C6-O8
34	B	854	LHG	C4-C5-C6-O8
36	J	102	LMG	O1-C7-C8-C9
31	0	321	CLA	CAA-CBA-CGA-O1A
31	a	612	CLA	CAA-CBA-CGA-O2A
31	d	612	CLA	CAA-CBA-CGA-O1A
30	g	607	CHL	O1A-CGA-O2A-C1
31	A	832	CLA	C13-C15-C16-C17
30	3	307	CHL	CAA-CBA-CGA-O2A
31	A	825	CLA	CAA-CBA-CGA-O2A
31	H	204	CLA	CAA-CBA-CGA-O2A
34	7	601	LHG	O8-C23-C24-C25
34	7	603	LHG	O7-C7-C8-C9
34	8	601	LHG	O8-C23-C24-C25
34	e	630	LHG	O8-C23-C24-C25
30	b	609	CHL	C2C-C3C-CAC-CBC
34	c	630	LHG	C25-C26-C27-C28
31	h	603	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	d	612	CLA	CAA-CBA-CGA-O2A
34	8	601	LHG	C11-C10-C9-C8
34	K	106	LHG	C35-C36-C37-C38
30	6	307	CHL	O2A-C1-C2-C3
30	7	301	CHL	O2A-C1-C2-C3
30	7	307	CHL	O2A-C1-C2-C3
30	8	306	CHL	O2A-C1-C2-C3
30	f	608	CHL	O2A-C1-C2-C3
30	g	602	CHL	O2A-C1-C2-C3
30	g	607	CHL	O2A-C1-C2-C3
30	h	606	CHL	O2A-C1-C2-C3
30	e	608	CHL	O2A-C1-C2-C3
31	5	304	CLA	O2A-C1-C2-C3
31	A	835	CLA	O2A-C1-C2-C3
31	B	803	CLA	O2A-C1-C2-C3
31	B	818	CLA	O2A-C1-C2-C3
31	B	822	CLA	O2A-C1-C2-C3
31	e	603	CLA	O2A-C1-C2-C3
31	B	840	CLA	C4C-C3C-CAC-CBC
30	c	609	CHL	CBA-CGA-O2A-C1
30	g	607	CHL	CBA-CGA-O2A-C1
31	e	604	CLA	CBA-CGA-O2A-C1
31	B	801	CLA	C2A-CAA-CBA-CGA
31	a	604	CLA	C2A-CAA-CBA-CGA
31	b	610	CLA	C2A-CAA-CBA-CGA
31	4	309	CLA	C2A-CAA-CBA-CGA
31	7	315	CLA	CAA-CBA-CGA-O2A
31	7	304	CLA	C3-C5-C6-C7
31	a	612	CLA	CAA-CBA-CGA-O1A
31	b	612	CLA	CAA-CBA-CGA-O1A
33	0	502	0UR	C46-C47-C48-C49
33	5	502	0UR	C46-C47-C48-C49
34	8	601	LHG	C27-C28-C29-C30
36	O	207	LMG	C28-C29-C30-C31
31	5	310	CLA	O1D-CGD-O2D-CED
30	5	301	CHL	CHA-CBD-CGD-O1D
30	a	608	CHL	CHA-CBD-CGD-O1D
30	a	608	CHL	CHA-CBD-CGD-O2D
30	h	601	CHL	CHA-CBD-CGD-O1D
30	h	601	CHL	CHA-CBD-CGD-O2D
31	1	303	CLA	CHA-CBD-CGD-O1D
31	1	303	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	3	304	CLA	CHA-CBD-CGD-O2D
31	6	304	CLA	CHA-CBD-CGD-O2D
31	6	318	CLA	CHA-CBD-CGD-O1D
31	6	318	CLA	CHA-CBD-CGD-O2D
31	7	304	CLA	CHA-CBD-CGD-O1D
31	7	304	CLA	CHA-CBD-CGD-O2D
31	9	302	CLA	CHA-CBD-CGD-O1D
31	9	302	CLA	CHA-CBD-CGD-O2D
31	A	804	CLA	CHA-CBD-CGD-O1D
31	A	804	CLA	CHA-CBD-CGD-O2D
31	A	806	CLA	CHA-CBD-CGD-O2D
31	A	815	CLA	CHA-CBD-CGD-O2D
31	A	843	CLA	CHA-CBD-CGD-O1D
31	A	843	CLA	CHA-CBD-CGD-O2D
31	B	814	CLA	CHA-CBD-CGD-O1D
31	B	821	CLA	CHA-CBD-CGD-O1D
31	B	822	CLA	CHA-CBD-CGD-O2D
31	K	102	CLA	CHA-CBD-CGD-O1D
31	K	105	CLA	CHA-CBD-CGD-O2D
31	O	201	CLA	CHA-CBD-CGD-O2D
31	a	613	CLA	CHA-CBD-CGD-O1D
31	a	613	CLA	CHA-CBD-CGD-O2D
31	c	603	CLA	CHA-CBD-CGD-O1D
31	c	603	CLA	CHA-CBD-CGD-O2D
31	c	604	CLA	CHA-CBD-CGD-O2D
31	c	612	CLA	CHA-CBD-CGD-O1D
31	b	612	CLA	CHA-CBD-CGD-O1D
31	d	603	CLA	CHA-CBD-CGD-O1D
31	d	603	CLA	CHA-CBD-CGD-O2D
31	f	613	CLA	CHA-CBD-CGD-O2D
31	h	611	CLA	CHA-CBD-CGD-O2D
31	i	611	CLA	CHA-CBD-CGD-O1D
31	i	611	CLA	CHA-CBD-CGD-O2D
31	4	310	CLA	CHA-CBD-CGD-O2D
31	B	807	CLA	CAA-CBA-CGA-O1A
31	G	102	CLA	CAA-CBA-CGA-O1A
31	h	613	CLA	CAA-CBA-CGA-O2A
31	2	311	CLA	CAA-CBA-CGA-O2A
31	3	308	CLA	CAA-CBA-CGA-O2A
31	B	809	CLA	CAA-CBA-CGA-O2A
31	f	603	CLA	CAA-CBA-CGA-O2A
31	B	811	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	e	613	CLA	C11-C10-C8-C7
36	3	602	LMG	C33-C34-C35-C36
30	1	307	CHL	C3-C5-C6-C7
34	e	630	LHG	C28-C29-C30-C31
31	5	311	CLA	CAA-CBA-CGA-O2A
31	f	612	CLA	CAA-CBA-CGA-O1A
41	B	849	DGD	C3A-C4A-C5A-C6A
31	B	819	CLA	C11-C12-C13-C14
31	A	802	CLA	C13-C15-C16-C17
31	B	839	CLA	C8-C10-C11-C12
30	2	302	CHL	CAA-CBA-CGA-O2A
31	2	312	CLA	CAA-CBA-CGA-O2A
31	B	838	CLA	CAA-CBA-CGA-O2A
34	c	630	LHG	O8-C23-C24-C25
34	f	630	LHG	O7-C7-C8-C9
36	2	602	LMG	O8-C28-C29-C30
30	c	609	CHL	C2C-C3C-CAC-CBC
31	e	604	CLA	O1A-CGA-O2A-C1
31	B	841	CLA	O1D-CGD-O2D-CED
30	f	602	CHL	CAA-CBA-CGA-O2A
31	K	104	CLA	CAA-CBA-CGA-O2A
31	d	603	CLA	CAA-CBA-CGA-O2A
34	0	601	LHG	O8-C23-C24-C25
34	A	855	LHG	O7-C7-C8-C9
34	h	630	LHG	O8-C23-C24-C25
30	2	306	CHL	O1D-CGD-O2D-CED
31	6	317	CLA	C2A-CAA-CBA-CGA
34	7	603	LHG	O1-C1-C2-O2
31	B	837	CLA	C13-C15-C16-C17
30	b	608	CHL	CBA-CGA-O2A-C1
30	3	305	CHL	O1D-CGD-O2D-CED
30	1	302	CHL	CAA-CBA-CGA-O2A
31	A	808	CLA	CAA-CBA-CGA-O2A
31	A	814	CLA	CAA-CBA-CGA-O2A
31	A	833	CLA	CAA-CBA-CGA-O2A
31	B	823	CLA	CAA-CBA-CGA-O2A
34	3	601	LHG	O8-C23-C24-C25
34	d	630	LHG	O7-C7-C8-C9
31	6	314	CLA	CAA-CBA-CGA-O1A
31	i	611	CLA	CAA-CBA-CGA-O1A
34	1	601	LHG	C16-C17-C18-C19
30	b	608	CHL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	821	CLA	O1A-CGA-O2A-C1
31	B	810	CLA	C4C-C3C-CAC-CBC
31	f	613	CLA	C11-C10-C8-C7
30	6	308	CHL	C2-C3-C5-C6
30	a	602	CHL	C11-C10-C8-C7
30	a	609	CHL	C6-C7-C8-C10
30	c	609	CHL	C2-C3-C5-C6
30	d	609	CHL	C6-C7-C8-C10
31	9	308	CLA	C6-C7-C8-C10
31	A	814	CLA	C2-C3-C5-C6
31	7	317	CLA	C2C-C3C-CAC-CBC
36	L	210	LMG	O9-C10-O7-C8
34	a	630	LHG	O7-C7-C8-C9
30	6	302	CHL	C14-C13-C15-C16
31	9	308	CLA	C14-C13-C15-C16
31	A	808	CLA	C11-C12-C13-C14
31	B	801	CLA	C14-C13-C15-C16
31	B	825	CLA	C6-C7-C8-C9
36	L	210	LMG	C28-C29-C30-C31
30	0	305	CHL	CAA-CBA-CGA-O1A
31	K	105	CLA	CAA-CBA-CGA-O1A
31	1	308	CLA	CAA-CBA-CGA-O2A
30	5	301	CHL	CAA-CBA-CGA-O2A
31	8	311	CLA	CAA-CBA-CGA-O2A
34	0	601	LHG	O7-C7-C8-C9
37	h	521	0IE	O29-C20-C3-C4
37	i	521	0IE	O29-C20-C3-C4
34	e	630	LHG	C31-C32-C33-C34
31	A	839	CLA	C15-C16-C17-C18
34	G	105	LHG	C28-C29-C30-C31
31	A	817	CLA	C14-C13-C15-C16
33	7	501	0UR	C46-C47-C48-C49
34	f	630	LHG	O10-C23-C24-C25
31	B	840	CLA	C16-C17-C18-C19
39	A	857	CL0	C16-C17-C18-C19
31	A	813	CLA	C4-C3-C5-C6
34	0	601	LHG	O1-C1-C2-C3
30	c	609	CHL	O1A-CGA-O2A-C1
31	4	311	CLA	O2A-C1-C2-C3
31	0	313	CLA	CAA-CBA-CGA-O1A
31	1	303	CLA	CAA-CBA-CGA-O1A
31	2	311	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2	402	8CT	C10-C11-C12-C13
42	e	523	NEX	C11-C12-C13-C14
31	9	303	CLA	CBA-CGA-O2A-C1
30	2	313	CHL	C1A-C2A-CAA-CBA
30	5	301	CHL	C1A-C2A-CAA-CBA
30	5	306	CHL	C1A-C2A-CAA-CBA
30	7	305	CHL	C1A-C2A-CAA-CBA
30	7	306	CHL	C1A-C2A-CAA-CBA
30	9	306	CHL	C1A-C2A-CAA-CBA
30	f	601	CHL	C1A-C2A-CAA-CBA
30	f	606	CHL	C1A-C2A-CAA-CBA
30	g	601	CHL	C1A-C2A-CAA-CBA
30	h	601	CHL	C1A-C2A-CAA-CBA
30	e	601	CHL	C1A-C2A-CAA-CBA
31	3	313	CLA	C1A-C2A-CAA-CBA
31	5	304	CLA	C1A-C2A-CAA-CBA
31	5	311	CLA	C1A-C2A-CAA-CBA
31	A	813	CLA	C1A-C2A-CAA-CBA
31	A	826	CLA	C1A-C2A-CAA-CBA
31	F	301	CLA	C1A-C2A-CAA-CBA
31	a	613	CLA	C1A-C2A-CAA-CBA
31	d	611	CLA	C1A-C2A-CAA-CBA
31	d	612	CLA	C1A-C2A-CAA-CBA
31	f	610	CLA	C1A-C2A-CAA-CBA
31	i	604	CLA	C1A-C2A-CAA-CBA
31	e	611	CLA	C1A-C2A-CAA-CBA
31	4	310	CLA	C1A-C2A-CAA-CBA
34	8	601	LHG	C1-C2-C3-O3
30	9	305	CHL	CAA-CBA-CGA-O1A
31	A	825	CLA	CAA-CBA-CGA-O1A
31	b	603	CLA	CAA-CBA-CGA-O1A
34	e	630	LHG	O10-C23-C24-C25
31	7	317	CLA	C4C-C3C-CAC-CBC
31	7	318	CLA	O1A-CGA-O2A-C1
31	5	304	CLA	C2-C1-O2A-CGA
31	B	809	CLA	C2-C1-O2A-CGA
31	B	826	CLA	C2-C1-O2A-CGA
31	B	840	CLA	C2-C1-O2A-CGA
31	A	818	CLA	C10-C11-C12-C13
30	b	609	CHL	CBA-CGA-O2A-C1
31	7	318	CLA	CBA-CGA-O2A-C1
30	9	301	CHL	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	823	CLA	CAA-CBA-CGA-O1A
34	7	601	LHG	O10-C23-C24-C25
34	A	844	LHG	O10-C23-C24-C25
34	b	630	LHG	O9-C7-C8-C9
34	f	630	LHG	O9-C7-C8-C9
36	L	211	LMG	O9-C10-C11-C12
34	5	601	LHG	C4-C5-C6-O8
36	J	105	LMG	O1-C7-C8-C9
31	B	829	CLA	C10-C11-C12-C13
31	6	320	CLA	C2A-CAA-CBA-CGA
31	H	204	CLA	C2A-CAA-CBA-CGA
34	e	630	LHG	C4-O6-P-O3
31	A	811	CLA	C16-C17-C18-C20
31	A	840	CLA	C16-C17-C18-C19
31	d	603	CLA	C6-C7-C8-C9
31	4	310	CLA	C11-C12-C13-C14
38	A	842	PQN	C26-C27-C28-C30
31	3	308	CLA	CAA-CBA-CGA-O1A
31	5	303	CLA	CAA-CBA-CGA-O1A
31	A	820	CLA	CAA-CBA-CGA-O1A
41	B	849	DGD	C7B-C8B-C9B-CAB
36	9	602	LMG	C19-C20-C21-C22
30	a	602	CHL	C3-C5-C6-C7
31	2	310	CLA	C3-C5-C6-C7
30	a	606	CHL	CAA-CBA-CGA-O1A
30	f	602	CHL	CAA-CBA-CGA-O1A
31	A	808	CLA	CAA-CBA-CGA-O1A
34	7	602	LHG	O9-C7-C8-C9
34	A	855	LHG	O9-C7-C8-C9
41	B	849	DGD	O6D-C5D-C6D-O5D
30	2	308	CHL	C4C-C3C-CAC-CBC
31	6	303	CLA	O1A-CGA-O2A-C1
31	6	317	CLA	C8-C10-C11-C12
31	A	809	CLA	C13-C15-C16-C17
30	1	305	CHL	C4B-C3B-CAB-CBB
30	5	313	CHL	C4B-C3B-CAB-CBB
30	f	606	CHL	C4B-C3B-CAB-CBB
30	g	602	CHL	C4B-C3B-CAB-CBB
31	0	308	CLA	C4B-C3B-CAB-CBB
31	7	303	CLA	C4B-C3B-CAB-CBB
31	9	303	CLA	C4B-C3B-CAB-CBB
31	A	816	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	612	CLA	C4B-C3B-CAB-CBB
31	i	603	CLA	C4B-C3B-CAB-CBB
34	0	601	LHG	C3-O3-P-O4
34	6	603	LHG	C3-O3-P-O5
31	B	832	CLA	C16-C17-C18-C20
30	i	607	CHL	CAA-CBA-CGA-O1A
31	A	814	CLA	CAA-CBA-CGA-O1A
31	B	809	CLA	CAA-CBA-CGA-O1A
34	7	603	LHG	O9-C7-C8-C9
34	8	601	LHG	O10-C23-C24-C25
31	A	822	CLA	O2A-C1-C2-C3
30	d	602	CHL	CAA-CBA-CGA-O2A
31	9	303	CLA	O1A-CGA-O2A-C1
34	7	602	LHG	O6-C4-C5-C6
30	b	609	CHL	C4C-C3C-CAC-CBC
31	3	309	CLA	C15-C16-C17-C18
31	B	811	CLA	C13-C15-C16-C17
31	A	805	CLA	CAA-CBA-CGA-O1A
34	3	603	LHG	O10-C23-C24-C25
34	a	630	LHG	O10-C23-C24-C25
30	i	606	CHL	CAA-CBA-CGA-O2A
31	B	834	CLA	CAA-CBA-CGA-O2A
34	9	601	LHG	O8-C23-C24-C25
31	h	613	CLA	CAA-CBA-CGA-O1A
31	A	812	CLA	C2A-CAA-CBA-CGA
31	B	814	CLA	C2A-CAA-CBA-CGA
30	8	306	CHL	CAA-CBA-CGA-O1A
34	c	630	LHG	O10-C23-C24-C25
31	A	836	CLA	O1D-CGD-O2D-CED
34	A	844	LHG	C17-C18-C19-C20
31	3	303	CLA	CAA-CBA-CGA-O2A
30	0	302	CHL	CAA-CBA-CGA-O1A
30	7	306	CHL	CAA-CBA-CGA-O1A
30	e	602	CHL	CAA-CBA-CGA-O1A
31	7	315	CLA	CAA-CBA-CGA-O1A
31	B	838	CLA	CAA-CBA-CGA-O1A
31	d	603	CLA	CAA-CBA-CGA-O1A
31	H	204	CLA	CAA-CBA-CGA-O1A
30	6	302	CHL	C2-C3-C5-C6
30	e	609	CHL	C2-C3-C5-C6
30	0	306	CHL	CAD-CBD-CGD-O1D
30	5	301	CHL	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	6	302	CHL	CAD-CBD-CGD-O1D
30	g	602	CHL	CAD-CBD-CGD-O1D
30	h	602	CHL	CAD-CBD-CGD-O1D
31	6	318	CLA	CAD-CBD-CGD-O1D
31	A	813	CLA	CAD-CBD-CGD-O1D
31	A	815	CLA	CAD-CBD-CGD-O1D
31	B	812	CLA	CAD-CBD-CGD-O1D
31	B	814	CLA	CAD-CBD-CGD-O1D
31	B	821	CLA	CAD-CBD-CGD-O1D
31	B	828	CLA	CAD-CBD-CGD-O1D
31	B	831	CLA	CAD-CBD-CGD-O1D
31	B	850	CLA	CAD-CBD-CGD-O1D
31	K	102	CLA	CAD-CBD-CGD-O1D
31	g	610	CLA	CAD-CBD-CGD-O1D
31	i	611	CLA	CAD-CBD-CGD-O1D
36	J	102	LMG	C9-C8-O7-C10
30	b	609	CHL	O1A-CGA-O2A-C1
30	1	302	CHL	CAA-CBA-CGA-O1A
30	2	302	CHL	CAA-CBA-CGA-O1A
30	3	307	CHL	CAA-CBA-CGA-O1A
31	2	312	CLA	CAA-CBA-CGA-O1A
31	L	203	CLA	CAA-CBA-CGA-O1A
34	A	844	LHG	O9-C7-C8-C9
34	d	630	LHG	O9-C7-C8-C9
30	7	302	CHL	CAA-CBA-CGA-O2A
30	2	302	CHL	C11-C12-C13-C14
30	8	301	CHL	C6-C7-C8-C9
30	e	608	CHL	C11-C12-C13-C14
31	3	308	CLA	C11-C12-C13-C14
31	9	308	CLA	C6-C7-C8-C9
31	A	839	CLA	C11-C10-C8-C9
31	B	819	CLA	C6-C7-C8-C9
31	B	827	CLA	C14-C13-C15-C16
31	L	201	CLA	C11-C10-C8-C9
31	1	308	CLA	CAA-CBA-CGA-O1A
31	L	201	CLA	C8-C10-C11-C12
30	9	313	CHL	CAA-CBA-CGA-O1A
31	8	311	CLA	CAA-CBA-CGA-O1A
30	2	306	CHL	C2-C1-O2A-CGA
30	6	307	CHL	CAA-CBA-CGA-O2A
31	7	308	CLA	CAA-CBA-CGA-O2A
31	7	312	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	812	CLA	CAA-CBA-CGA-O2A
31	B	817	CLA	CAA-CBA-CGA-O2A
31	a	610	CLA	CAA-CBA-CGA-O2A
31	g	613	CLA	CAA-CBA-CGA-O2A
31	4	311	CLA	CAA-CBA-CGA-O2A
31	1	310	CLA	CBD-CGD-O2D-CED
34	3	603	LHG	C26-C27-C28-C29
34	f	630	LHG	C25-C26-C27-C28
31	2	309	CLA	C2A-CAA-CBA-CGA
31	9	302	CLA	C2A-CAA-CBA-CGA
30	h	609	CHL	C2C-C3C-CAC-CBC
31	6	303	CLA	CBA-CGA-O2A-C1
30	1	305	CHL	CAA-CBA-CGA-O2A
30	g	607	CHL	CAA-CBA-CGA-O2A
30	4	302	CHL	CAA-CBA-CGA-O2A
31	2	303	CLA	CAA-CBA-CGA-O2A
31	3	311	CLA	CAA-CBA-CGA-O2A
31	6	311	CLA	CAA-CBA-CGA-O2A
31	9	303	CLA	CAA-CBA-CGA-O2A
31	K	101	CLA	CAA-CBA-CGA-O2A
31	4	312	CLA	CAA-CBA-CGA-O2A
34	b	630	LHG	O8-C23-C24-C25
31	2	314	CLA	CAA-CBA-CGA-O2A
31	A	833	CLA	CAA-CBA-CGA-O1A
31	K	104	CLA	CAA-CBA-CGA-O1A
34	0	601	LHG	O10-C23-C24-C25
34	h	630	LHG	O10-C23-C24-C25
30	1	302	CHL	C12-C13-C15-C16
30	6	301	CHL	C11-C10-C8-C7
30	7	302	CHL	C6-C7-C8-C10
30	8	306	CHL	C3A-C2A-CAA-CBA
31	A	811	CLA	C3A-C2A-CAA-CBA
31	A	811	CLA	C12-C13-C15-C16
31	A	852	CLA	C6-C7-C8-C10
31	A	853	CLA	C11-C10-C8-C7
31	B	801	CLA	C11-C12-C13-C15
31	B	803	CLA	C6-C7-C8-C10
31	B	825	CLA	C6-C7-C8-C10
31	B	829	CLA	C2-C3-C5-C6
31	B	836	CLA	C11-C10-C8-C7
31	K	102	CLA	C2-C3-C5-C6
31	O	202	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	9	401	8CT	C28-C29-C30-C31
32	A	849	8CT	C28-C29-C30-C31
32	B	804	8CT	C28-C29-C30-C31
33	0	501	0UR	O42-C2-C3-C43
33	0	502	0UR	O42-C2-C3-C43
33	1	501	0UR	O42-C2-C3-C43
33	3	501	0UR	O42-C2-C3-C43
33	5	501	0UR	C3-C2-C41-C1
33	6	501	0UR	O42-C2-C3-C43
33	7	501	0UR	O42-C2-C3-C43
33	8	501	0UR	O42-C2-C3-C43
33	9	501	0UR	O42-C2-C3-C43
33	c	520	0UR	O42-C2-C3-C43
33	b	520	0UR	C3-C2-C41-C1
33	h	520	0UR	O42-C2-C3-C43
33	i	520	0UR	O42-C2-C3-C43
33	4	501	0UR	O42-C2-C3-C43
34	5	601	LHG	O6-C4-C5-O7
34	b	630	LHG	O6-C4-C5-O7
37	3	502	0IE	O1-C2-C3-C20
37	7	502	0IE	O1-C2-C3-C20
37	a	521	0IE	O1-C2-C3-C20
37	c	521	0IE	O1-C2-C3-C20
37	b	521	0IE	O1-C2-C3-C20
37	d	521	0IE	O1-C2-C3-C20
37	f	521	0IE	O1-C2-C3-C20
37	h	521	0IE	O1-C2-C3-C20
37	i	521	0IE	O1-C2-C3-C20
37	i	522	0IE	C3-C2-C30-C31
37	e	521	0IE	O1-C2-C3-C20
31	3	311	CLA	CAA-CBA-CGA-O1A
31	f	603	CLA	CAA-CBA-CGA-O1A
30	3	302	CHL	CAA-CBA-CGA-O2A
30	3	305	CHL	CAA-CBA-CGA-O2A
30	5	302	CHL	CAA-CBA-CGA-O2A
30	5	307	CHL	CAA-CBA-CGA-O2A
30	h	606	CHL	CAA-CBA-CGA-O2A
30	e	606	CHL	CAA-CBA-CGA-O2A
31	3	312	CLA	CAA-CBA-CGA-O2A
31	A	809	CLA	CAA-CBA-CGA-O2A
31	A	841	CLA	CAA-CBA-CGA-O2A
31	B	831	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	839	CLA	CAA-CBA-CGA-O2A
31	L	202	CLA	CAA-CBA-CGA-O2A
34	d	630	LHG	C31-C32-C33-C34
30	d	606	CHL	O1A-CGA-O2A-C1
34	A	845	LHG	O8-C23-C24-C25
32	8	406	8CT	C10-C11-C12-C13
32	J	104	8CT	C20-C21-C23-C24
32	4	402	8CT	C14-C15-C16-C17
33	4	502	0UR	C5-C6-C7-C8
30	7	302	CHL	CAA-CBA-CGA-O1A
31	3	312	CLA	CAA-CBA-CGA-O1A
31	7	312	CLA	CAA-CBA-CGA-O1A
31	B	812	CLA	CAA-CBA-CGA-O1A
31	B	834	CLA	CAA-CBA-CGA-O1A
30	g	606	CHL	CAA-CBA-CGA-O2A
30	h	602	CHL	CAA-CBA-CGA-O2A
31	g	610	CLA	CAA-CBA-CGA-O2A
30	6	301	CHL	C10-C11-C12-C13
30	6	307	CHL	CAA-CBA-CGA-O1A
30	g	606	CHL	CAA-CBA-CGA-O1A
31	3	303	CLA	CAA-CBA-CGA-O1A
31	7	308	CLA	CAA-CBA-CGA-O1A
31	B	839	CLA	CAA-CBA-CGA-O1A
31	K	101	CLA	CAA-CBA-CGA-O1A
31	4	311	CLA	CAA-CBA-CGA-O1A
34	a	630	LHG	O9-C7-C8-C9
30	d	606	CHL	CBA-CGA-O2A-C1
30	4	306	CHL	C2-C1-O2A-CGA
31	A	825	CLA	C13-C15-C16-C17
30	1	307	CHL	CAA-CBA-CGA-O2A
30	8	302	CHL	CAA-CBA-CGA-O2A
30	8	305	CHL	CAA-CBA-CGA-O2A
30	c	607	CHL	CAA-CBA-CGA-O2A
30	f	608	CHL	CAA-CBA-CGA-O2A
30	i	602	CHL	CAA-CBA-CGA-O2A
31	A	812	CLA	CAA-CBA-CGA-O2A
34	1	601	LHG	O8-C23-C24-C25
34	2	601	LHG	O8-C23-C24-C25
34	A	855	LHG	O8-C23-C24-C25
30	3	302	CHL	CAA-CBA-CGA-O1A
30	3	305	CHL	CAA-CBA-CGA-O1A
30	4	302	CHL	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	809	CLA	CAA-CBA-CGA-O1A
31	B	831	CLA	CAA-CBA-CGA-O1A
31	g	613	CLA	CAA-CBA-CGA-O1A
34	0	601	LHG	O9-C7-C8-C9
34	3	601	LHG	O10-C23-C24-C25
30	c	609	CHL	C4C-C3C-CAC-CBC
31	3	308	CLA	C4C-C3C-CAC-CBC
34	7	602	LHG	C16-C17-C18-C19
30	c	609	CHL	C10-C11-C12-C13
31	B	815	CLA	CBA-CGA-O2A-C1
36	A	856	LMG	C11-C12-C13-C14
36	A	856	LMG	C12-C13-C14-C15
31	6	311	CLA	CAA-CBA-CGA-O1A
31	B	817	CLA	CAA-CBA-CGA-O1A
31	2	304	CLA	C4-C3-C5-C6
41	B	849	DGD	C6B-C7B-C8B-C9B
30	8	307	CHL	CAA-CBA-CGA-O2A
31	A	834	CLA	CAA-CBA-CGA-O2A
31	3	313	CLA	CAA-CBA-CGA-O2A
30	e	607	CHL	O1D-CGD-O2D-CED
31	e	603	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

411 monomers are involved in 1119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	3	311	CLA	1	0
30	5	302	CHL	4	0
36	A	856	LMG	3	0
30	h	601	CHL	1	0
31	8	311	CLA	2	0
31	a	611	CLA	1	0
31	g	610	CLA	5	0
31	5	314	CLA	1	0
30	h	608	CHL	5	0
31	B	816	CLA	1	0
33	h	520	0UR	1	0
31	d	604	CLA	1	0
31	a	603	CLA	2	0
34	d	630	LHG	5	0
31	4	312	CLA	2	0
31	a	604	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	9	302	CLA	5	0
30	4	305	CHL	3	0
30	3	302	CHL	3	0
31	B	841	CLA	4	0
31	0	321	CLA	4	0
31	i	611	CLA	4	0
31	O	206	CLA	3	0
34	A	845	LHG	3	0
30	g	606	CHL	2	0
31	B	831	CLA	3	0
30	c	609	CHL	5	0
31	h	604	CLA	2	0
31	F	301	CLA	3	0
30	2	302	CHL	2	0
31	B	803	CLA	7	0
31	i	603	CLA	2	0
30	0	301	CHL	6	0
31	A	826	CLA	3	0
30	b	606	CHL	2	0
36	J	105	LMG	2	0
31	A	816	CLA	1	0
31	9	309	CLA	4	0
34	f	630	LHG	5	0
34	6	601	LHG	5	0
31	B	829	CLA	4	0
31	B	817	CLA	8	0
30	3	305	CHL	1	0
31	3	303	CLA	2	0
36	L	211	LMG	3	0
31	b	603	CLA	2	0
30	e	609	CHL	6	0
31	1	311	CLA	2	0
30	6	313	CHL	2	0
32	B	804	8CT	1	0
36	3	602	LMG	1	0
34	0	601	LHG	4	0
31	B	827	CLA	3	0
31	A	843	CLA	4	0
33	0	501	0UR	1	0
31	B	832	CLA	3	0
34	3	601	LHG	1	0
36	B	853	LMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	5	308	CLA	2	0
31	7	304	CLA	4	0
31	6	309	CLA	1	0
31	3	313	CLA	1	0
30	8	302	CHL	1	0
31	e	612	CLA	3	0
30	5	307	CHL	2	0
42	d	523	NEX	10	0
30	e	606	CHL	1	0
31	L	203	CLA	5	0
31	A	822	CLA	3	0
31	A	829	CLA	4	0
33	6	502	0UR	1	0
31	0	312	CLA	8	0
30	c	605	CHL	1	0
31	e	610	CLA	2	0
31	c	610	CLA	2	0
30	2	308	CHL	1	0
31	B	839	CLA	5	0
31	A	802	CLA	2	0
31	O	203	CLA	4	0
30	1	302	CHL	4	0
30	8	313	CHL	3	0
31	i	610	CLA	2	0
31	A	852	CLA	3	0
31	B	825	CLA	5	0
40	B	802	SF4	1	0
30	i	606	CHL	21	0
30	c	607	CHL	3	0
31	B	823	CLA	4	0
34	G	105	LHG	2	0
31	B	801	CLA	8	0
31	2	314	CLA	1	0
31	6	303	CLA	1	0
30	6	306	CHL	2	0
31	6	310	CLA	2	0
30	g	602	CHL	2	0
42	g	523	NEX	8	0
31	A	810	CLA	3	0
30	1	307	CHL	5	0
31	H	201	CLA	3	0
31	J	103	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	4	307	CHL	2	0
31	B	809	CLA	9	0
42	b	523	NEX	3	0
35	0	603	SQD	2	0
30	5	313	CHL	1	0
31	6	304	CLA	2	0
31	K	102	CLA	3	0
31	h	612	CLA	3	0
31	i	612	CLA	1	0
33	7	501	0UR	2	0
34	h	630	LHG	4	0
30	6	302	CHL	3	0
31	0	308	CLA	1	0
30	1	313	CHL	3	0
31	6	311	CLA	1	0
36	J	102	LMG	1	0
30	g	608	CHL	3	0
30	9	301	CHL	1	0
31	3	318	CLA	3	0
34	A	844	LHG	4	0
33	d	520	0UR	1	0
31	3	306	CLA	2	0
30	f	609	CHL	6	0
30	c	606	CHL	3	0
30	0	306	CHL	4	0
31	A	809	CLA	8	0
34	A	855	LHG	1	0
31	A	827	CLA	2	0
31	A	832	CLA	6	0
42	a	523	NEX	7	0
32	8	402	8CT	1	0
31	A	808	CLA	7	0
34	M	104	LHG	4	0
36	9	602	LMG	4	0
30	a	609	CHL	5	0
31	B	814	CLA	5	0
32	L	205	8CT	1	0
30	f	608	CHL	3	0
42	h	523	NEX	15	0
30	0	302	CHL	3	0
33	a	520	0UR	2	0
30	a	608	CHL	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	824	CLA	5	0
33	9	501	0UR	2	0
31	A	818	CLA	10	0
34	g	630	LHG	3	0
30	5	306	CHL	1	0
30	8	306	CHL	1	0
31	B	850	CLA	1	0
30	6	301	CHL	5	0
30	d	605	CHL	2	0
32	J	104	8CT	1	0
31	A	836	CLA	1	0
31	3	320	CLA	1	0
31	e	613	CLA	3	0
31	B	819	CLA	5	0
30	3	307	CHL	5	0
34	b	630	LHG	2	0
30	g	607	CHL	2	0
31	g	612	CLA	1	0
31	h	611	CLA	1	0
31	8	304	CLA	2	0
31	H	204	CLA	1	0
30	a	606	CHL	4	0
31	4	314	CLA	1	0
31	A	839	CLA	5	0
30	f	607	CHL	2	0
37	b	521	0IE	1	0
30	d	608	CHL	5	0
31	i	613	CLA	1	0
31	6	317	CLA	4	0
30	d	602	CHL	2	0
31	1	304	CLA	1	0
31	G	102	CLA	1	0
33	9	502	0UR	1	0
34	7	602	LHG	2	0
33	O	204	0UR	1	0
33	3	501	0UR	1	0
31	K	101	CLA	1	0
33	c	520	0UR	1	0
31	9	312	CLA	2	0
31	A	823	CLA	1	0
31	d	612	CLA	4	0
31	A	813	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	610	CLA	4	0
31	1	309	CLA	2	0
31	6	318	CLA	1	0
33	2	501	0UR	3	0
33	8	501	0UR	3	0
31	0	313	CLA	2	0
31	5	303	CLA	3	0
31	1	308	CLA	2	0
31	c	613	CLA	4	0
30	f	614	CHL	2	0
31	A	811	CLA	6	0
34	e	630	LHG	5	0
34	c	630	LHG	5	0
30	h	602	CHL	5	0
30	2	307	CHL	3	0
31	4	304	CLA	1	0
31	B	836	CLA	3	0
31	3	304	CLA	3	0
31	A	828	CLA	8	0
31	8	312	CLA	1	0
31	B	812	CLA	1	0
34	i	630	LHG	4	0
30	d	606	CHL	8	0
31	A	815	CLA	3	0
31	c	604	CLA	1	0
30	2	306	CHL	1	0
30	9	305	CHL	1	0
30	4	308	CHL	3	0
30	7	307	CHL	7	0
30	7	305	CHL	3	0
31	A	803	CLA	5	0
31	7	308	CLA	7	0
30	7	306	CHL	4	0
31	B	840	CLA	1	0
31	g	613	CLA	3	0
30	a	607	CHL	3	0
30	f	606	CHL	5	0
31	K	104	CLA	3	0
31	B	806	CLA	8	0
31	8	309	CLA	1	0
30	i	614	CHL	2	0
42	i	523	NEX	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	834	CLA	7	0
36	O	207	LMG	1	0
31	K	105	CLA	2	0
31	g	604	CLA	6	0
30	d	609	CHL	4	0
31	A	837	CLA	3	0
31	A	825	CLA	6	0
31	9	308	CLA	5	0
30	h	606	CHL	5	0
30	e	608	CHL	7	0
31	g	611	CLA	1	0
30	e	601	CHL	2	0
33	1	501	0UR	1	0
31	7	312	CLA	5	0
37	i	521	0IE	4	0
31	h	613	CLA	3	0
31	A	820	CLA	1	0
30	5	305	CHL	4	0
31	A	821	CLA	9	0
31	B	833	CLA	6	0
30	4	306	CHL	2	0
31	A	841	CLA	5	0
31	B	811	CLA	7	0
30	b	602	CHL	7	0
31	b	604	CLA	3	0
31	A	831	CLA	3	0
31	1	312	CLA	9	0
30	b	607	CHL	3	0
31	f	611	CLA	3	0
42	c	523	NEX	5	0
31	0	304	CLA	1	0
42	e	523	NEX	3	0
30	2	319	CHL	6	0
31	5	311	CLA	2	0
31	2	304	CLA	1	0
31	5	309	CLA	4	0
32	7	404	8CT	1	0
31	2	310	CLA	3	0
31	0	311	CLA	2	0
31	0	309	CLA	3	0
31	A	853	CLA	5	0
30	6	307	CHL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	309	CLA	2	0
31	4	309	CLA	5	0
30	f	601	CHL	6	0
31	B	830	CLA	6	0
34	B	852	LHG	2	0
33	b	520	0UR	3	0
30	b	608	CHL	5	0
37	h	522	0IE	1	0
31	g	603	CLA	3	0
30	h	614	CHL	1	0
30	8	315	CHL	3	0
30	c	608	CHL	7	0
30	4	313	CHL	3	0
31	B	826	CLA	3	0
30	d	607	CHL	3	0
33	i	520	0UR	2	0
30	i	608	CHL	2	0
31	L	204	CLA	3	0
31	f	604	CLA	4	0
30	8	307	CHL	4	0
31	B	820	CLA	4	0
31	b	610	CLA	3	0
31	A	806	CLA	3	0
31	B	822	CLA	4	0
31	L	202	CLA	2	0
38	B	842	PQN	1	0
39	A	857	CL0	7	0
34	B	854	LHG	2	0
31	A	814	CLA	2	0
31	B	808	CLA	6	0
31	f	613	CLA	4	0
31	d	610	CLA	1	0
31	f	610	CLA	1	0
30	g	605	CHL	3	0
30	c	601	CHL	8	0
33	5	501	0UR	4	0
30	1	305	CHL	4	0
31	a	613	CLA	1	0
30	7	301	CHL	3	0
31	B	818	CLA	12	0
30	f	602	CHL	1	0
31	d	611	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	612	CLA	1	0
32	4	402	8CT	1	0
34	9	601	LHG	5	0
31	A	838	CLA	3	0
41	B	849	DGD	3	0
31	4	310	CLA	3	0
34	1	601	LHG	6	0
31	b	613	CLA	2	0
31	A	804	CLA	1	0
34	a	630	LHG	4	0
31	i	604	CLA	28	0
30	i	607	CHL	1	0
32	B	847	8CT	1	0
30	a	605	CHL	2	0
30	b	614	CHL	2	0
30	6	305	CHL	2	0
31	7	309	CLA	4	0
31	A	807	CLA	2	0
30	e	607	CHL	2	0
32	A	850	8CT	1	0
31	2	312	CLA	2	0
30	h	609	CHL	1	0
31	e	603	CLA	5	0
31	c	603	CLA	2	0
34	7	601	LHG	2	0
37	b	522	0IE	1	0
31	9	311	CLA	2	0
37	h	521	0IE	1	0
34	5	601	LHG	1	0
30	e	605	CHL	2	0
30	4	319	CHL	8	0
31	B	837	CLA	1	0
30	c	602	CHL	2	0
31	3	309	CLA	4	0
31	1	303	CLA	2	0
34	3	603	LHG	3	0
31	B	813	CLA	3	0
30	i	605	CHL	1	0
34	K	106	LHG	4	0
30	1	306	CHL	3	0
30	b	601	CHL	4	0
30	8	305	CHL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	318	CLA	1	0
30	6	308	CHL	4	0
31	4	311	CLA	4	0
31	A	830	CLA	5	0
42	f	523	NEX	26	0
31	B	810	CLA	5	0
31	B	828	CLA	3	0
31	B	838	CLA	3	0
31	0	303	CLA	4	0
30	c	614	CHL	3	0
31	L	201	CLA	2	0
30	5	301	CHL	5	0
31	A	824	CLA	1	0
38	A	842	PQN	5	0
31	B	805	CLA	4	0
31	0	310	CLA	2	0
30	b	609	CHL	3	0
31	e	604	CLA	1	0
31	5	312	CLA	2	0
30	a	602	CHL	3	0
30	9	306	CHL	2	0
30	6	315	CHL	1	0
30	i	602	CHL	3	0
31	h	610	CLA	2	0
30	0	305	CHL	4	0
30	2	313	CHL	6	0
30	d	601	CHL	2	0
31	7	317	CLA	5	0
30	7	302	CHL	3	0
30	2	301	CHL	2	0
31	3	308	CLA	4	0
31	3	312	CLA	2	0
31	5	304	CLA	2	0
31	A	817	CLA	1	0
30	8	301	CHL	4	0
30	g	601	CHL	1	0
30	g	609	CHL	2	0
30	h	607	CHL	1	0
37	c	522	0IE	1	0
31	7	315	CLA	2	0
31	A	805	CLA	2	0
31	A	819	CLA	4	0

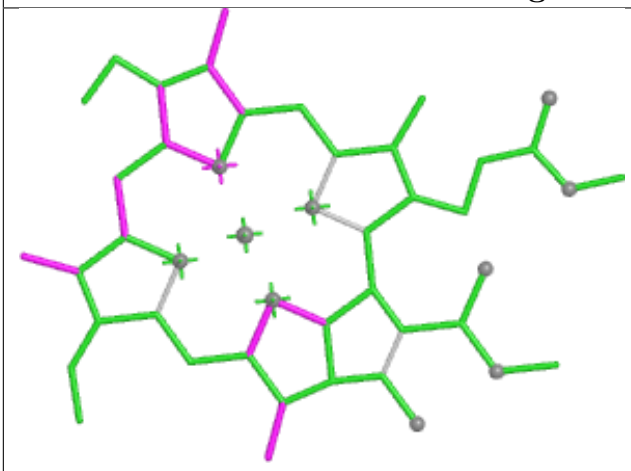
Continued on next page...

Continued from previous page...

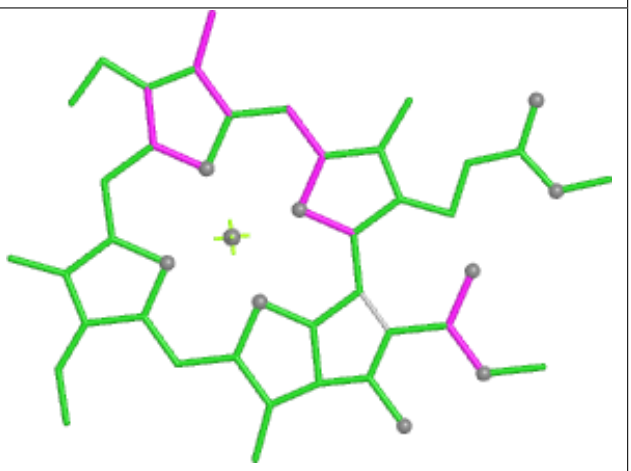
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	3	402	8CT	1	0
31	6	312	CLA	3	0
31	B	835	CLA	1	0
31	G	103	CLA	1	0
31	d	603	CLA	3	0
30	4	302	CHL	2	0
31	9	300	CLA	1	0
30	a	601	CHL	1	0
30	e	602	CHL	5	0
33	4	501	0UR	3	0
30	i	609	CHL	4	0
31	9	303	CLA	1	0
30	8	308	CHL	3	0
34	2	601	LHG	3	0
31	d	613	CLA	2	0
31	B	821	CLA	1	0
31	A	840	CLA	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

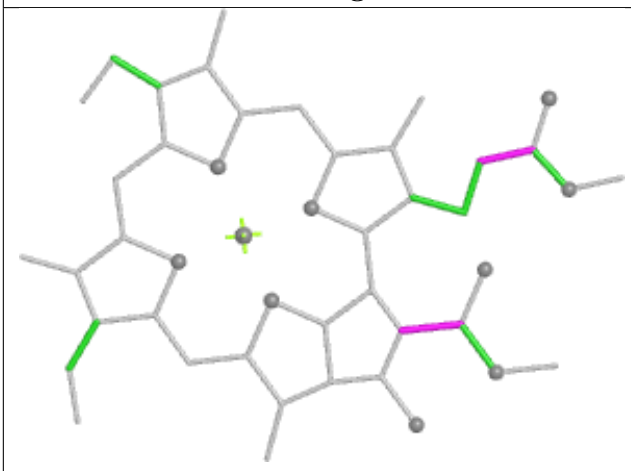
Ligand CLA 3 311



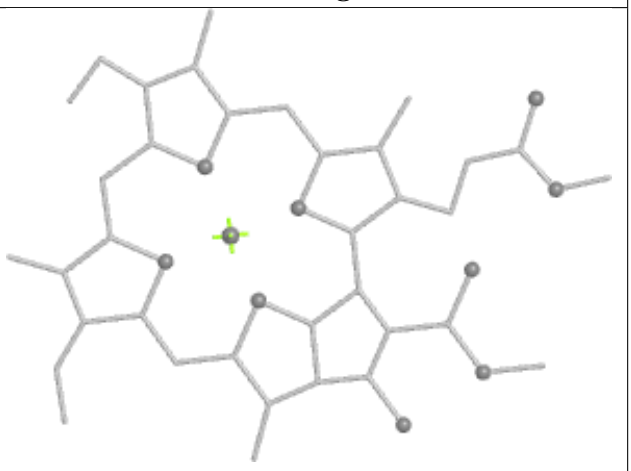
Bond lengths



Bond angles

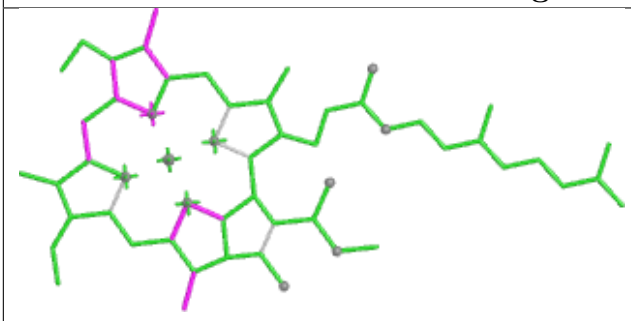


Torsions

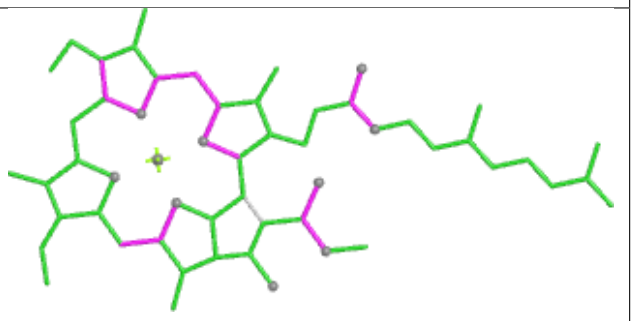


Rings

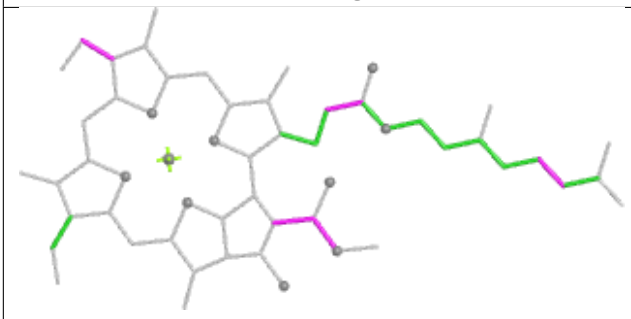
Ligand CLA f 603



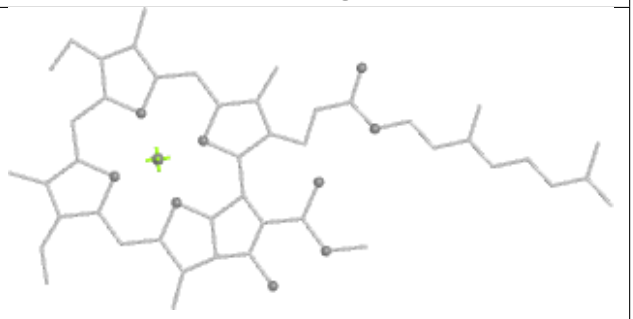
Bond lengths



Bond angles

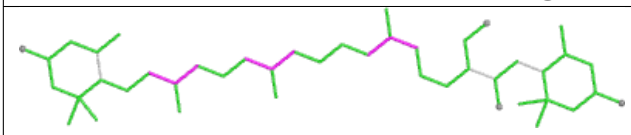


Torsions

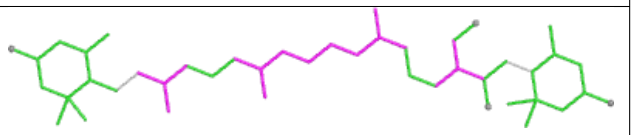


Rings

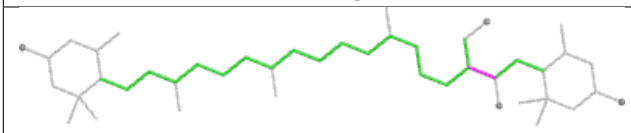
Ligand 0IE e 521



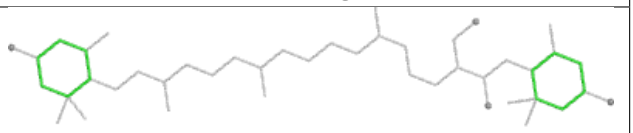
Bond lengths



Bond angles

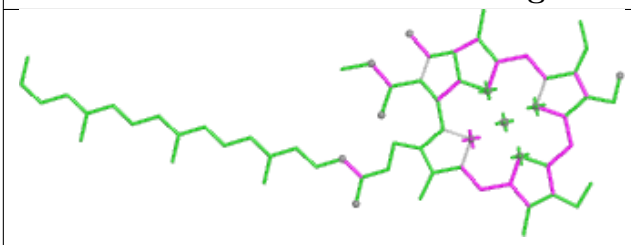


Torsions

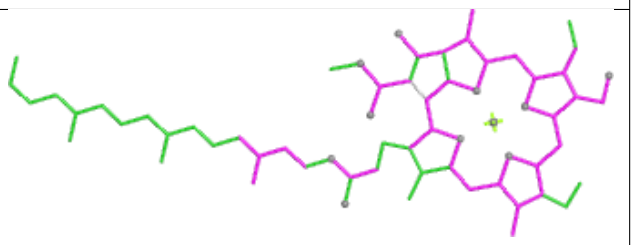


Rings

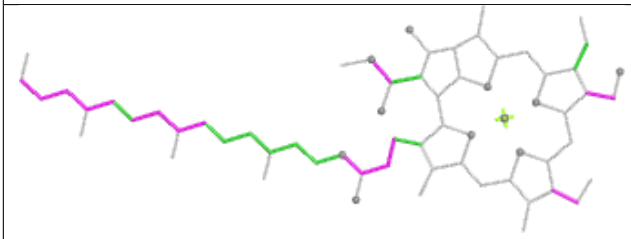
Ligand CHL 5 302



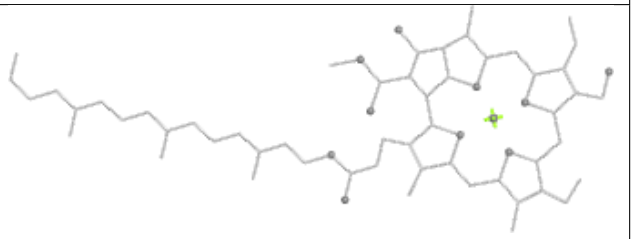
Bond lengths



Bond angles

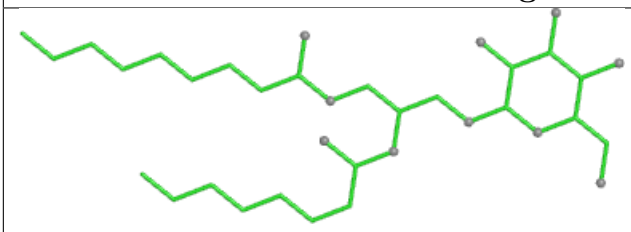


Torsions

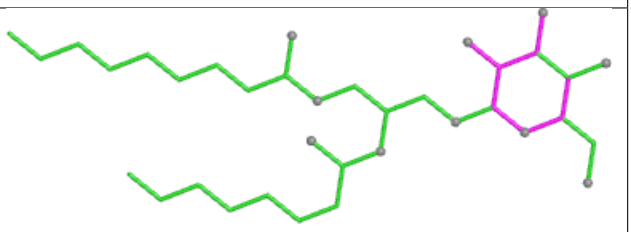


Rings

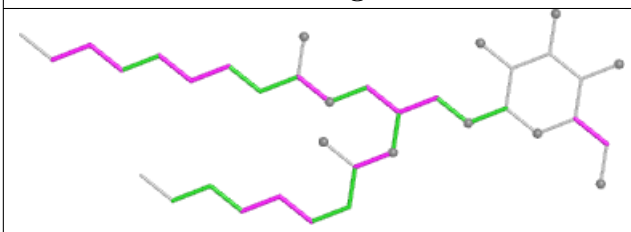
Ligand LMG A 856



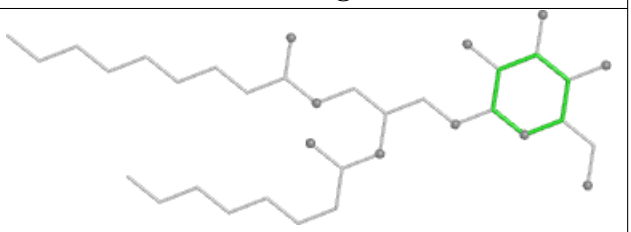
Bond lengths



Bond angles

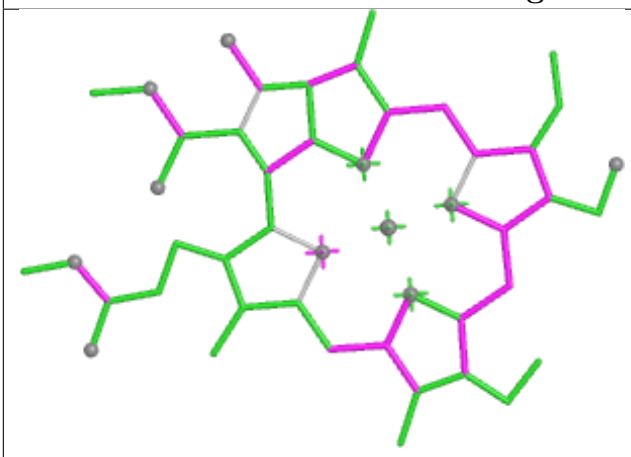


Torsions

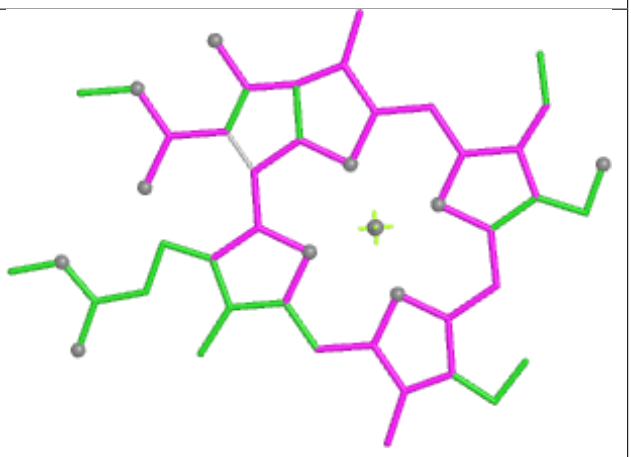


Rings

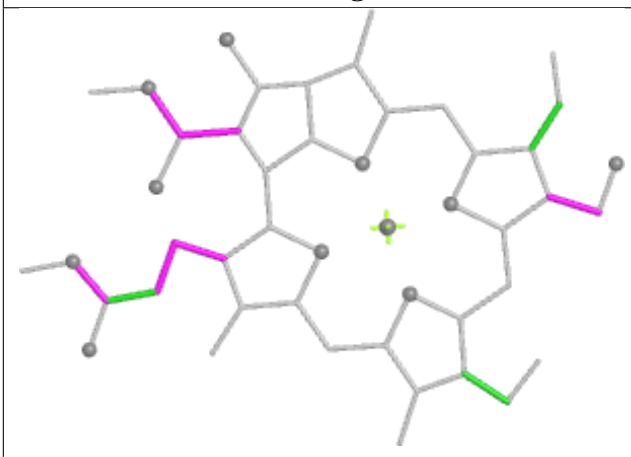
Ligand CHL h 601



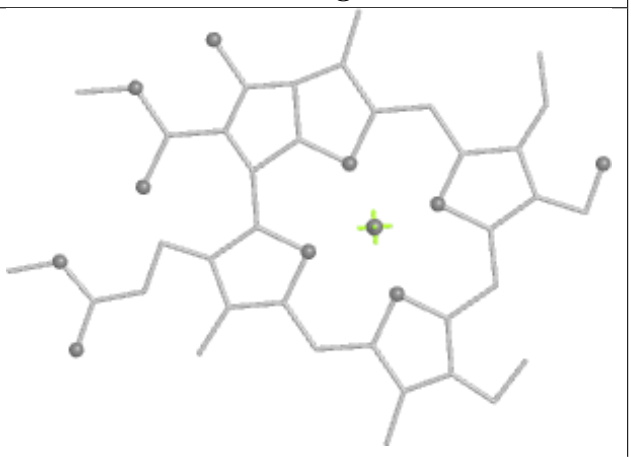
Bond lengths



Bond angles

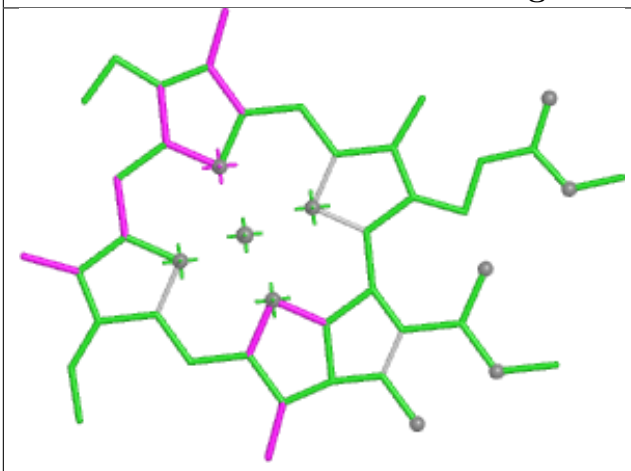


Torsions

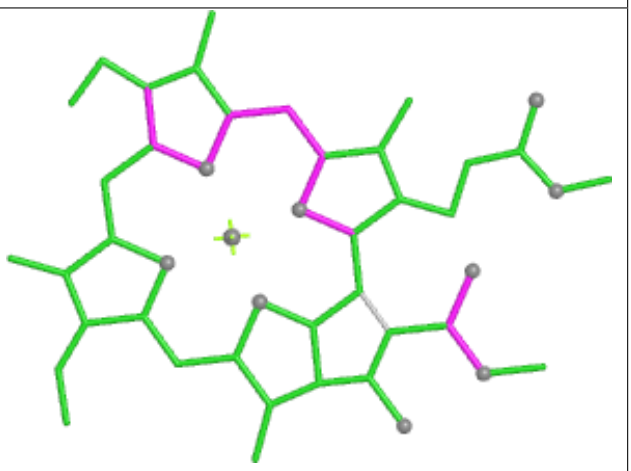


Rings

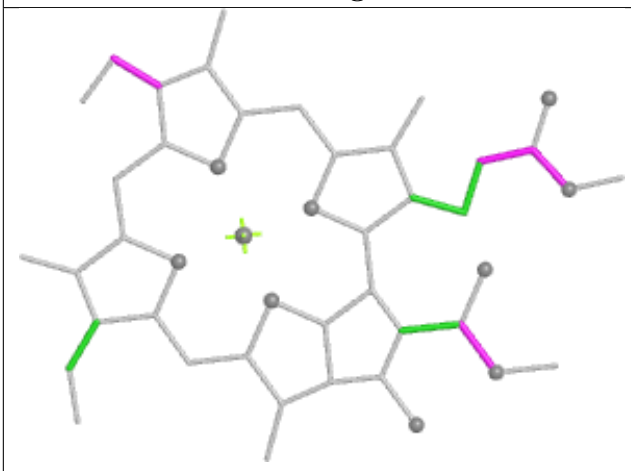
Ligand CLA 8 311



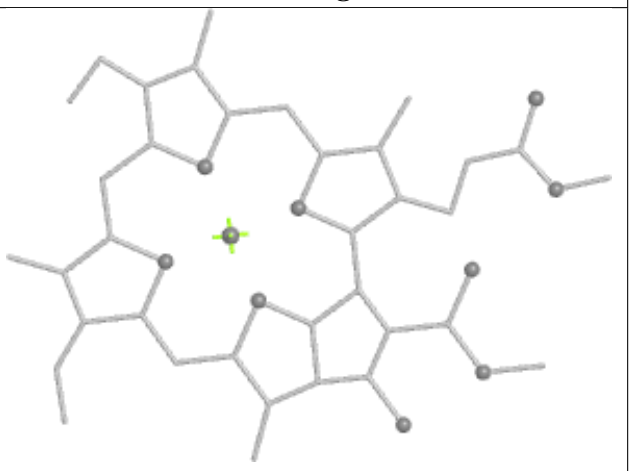
Bond lengths



Bond angles

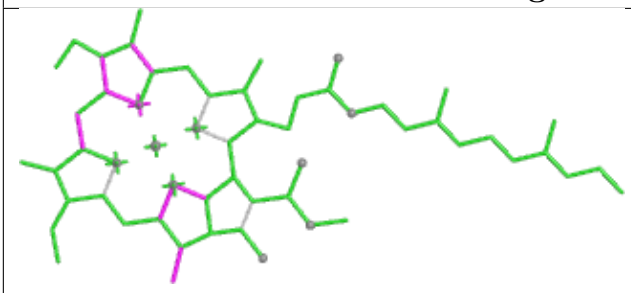


Torsions

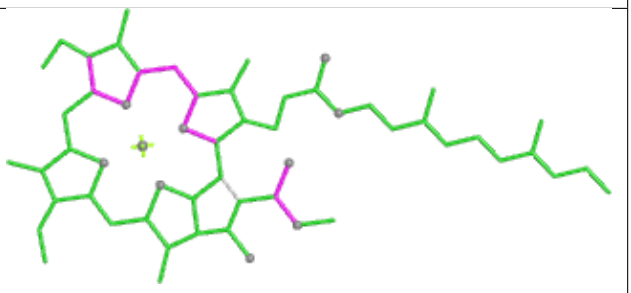


Rings

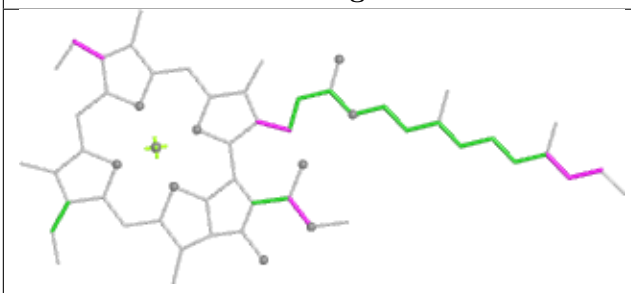
Ligand CLA a 611



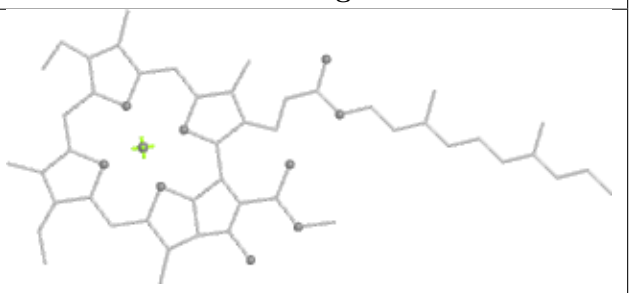
Bond lengths



Bond angles

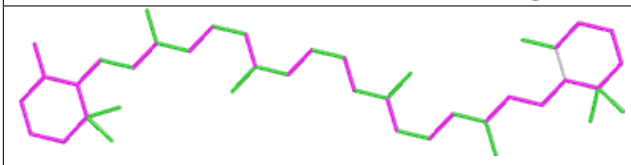


Torsions

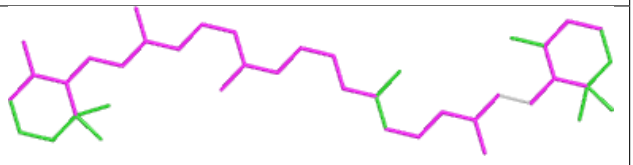


Rings

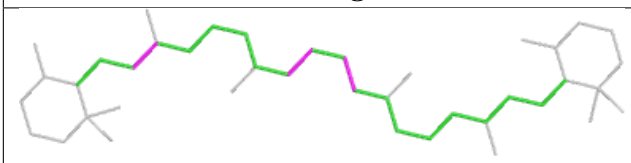
Ligand 8CT A 846



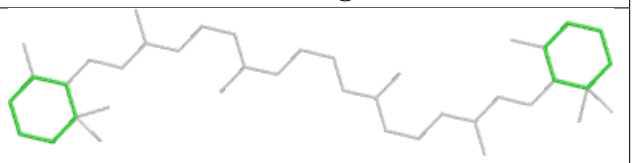
Bond lengths



Bond angles

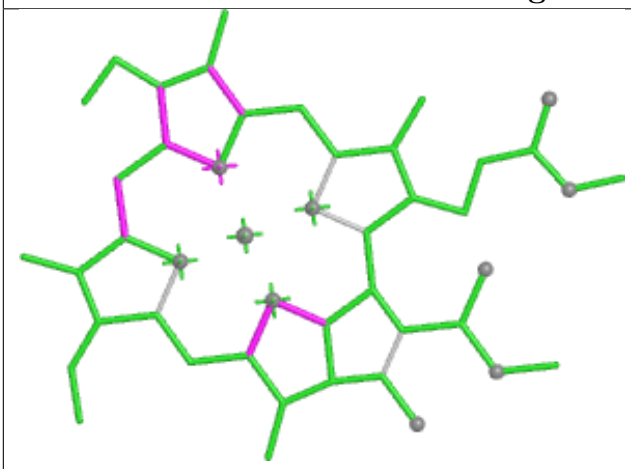


Torsions

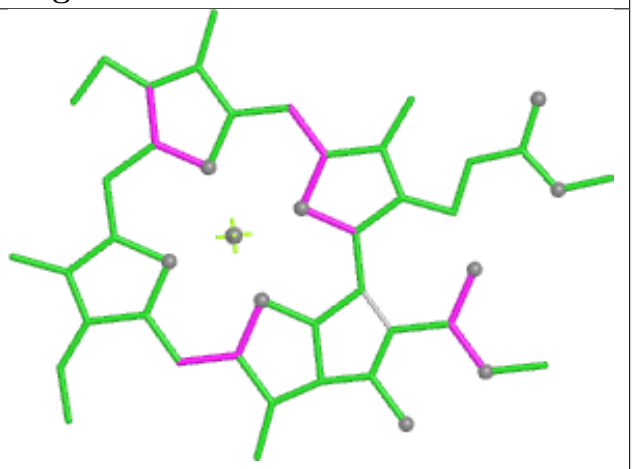


Rings

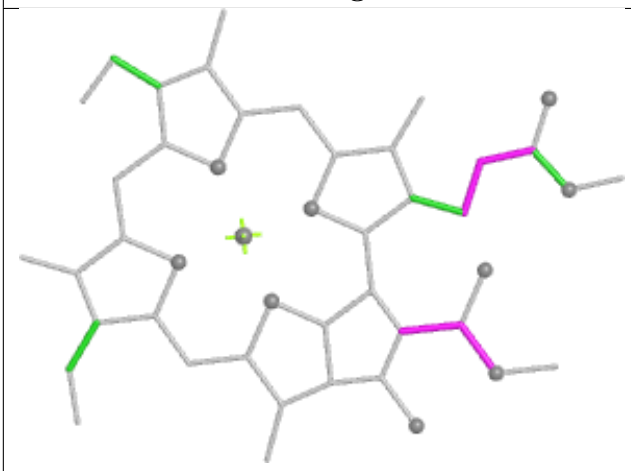
Ligand CLA g 610



Bond lengths



Bond angles

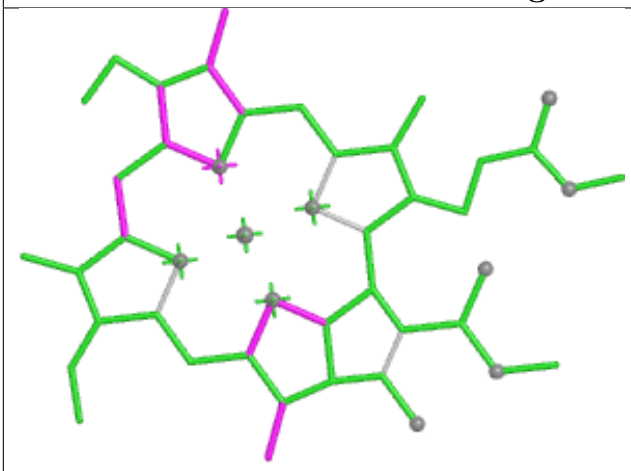


Torsions

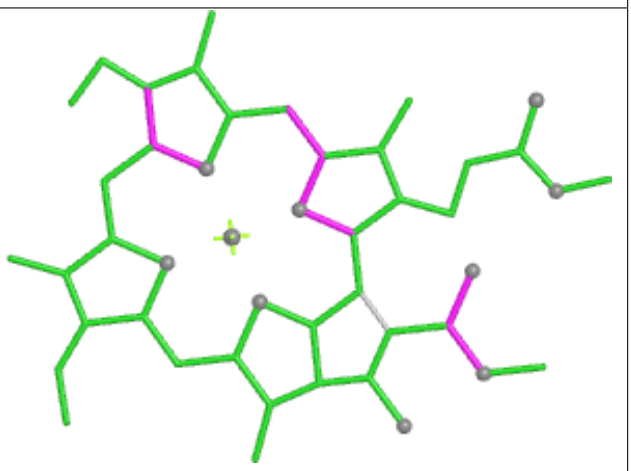


Rings

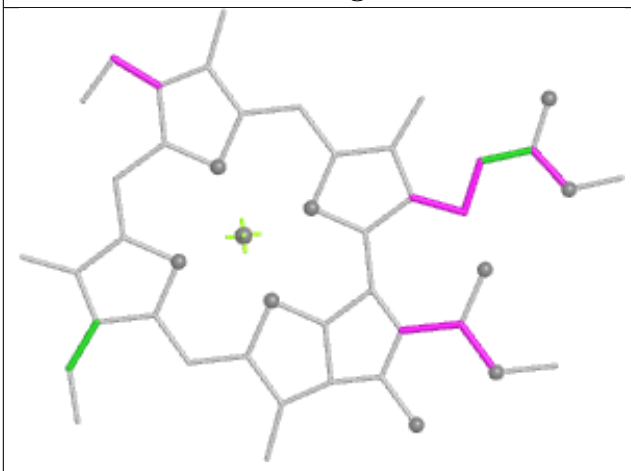
Ligand CLA 5 314



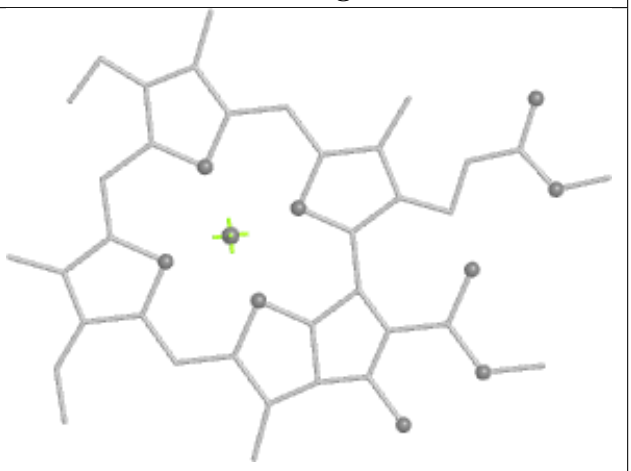
Bond lengths



Bond angles

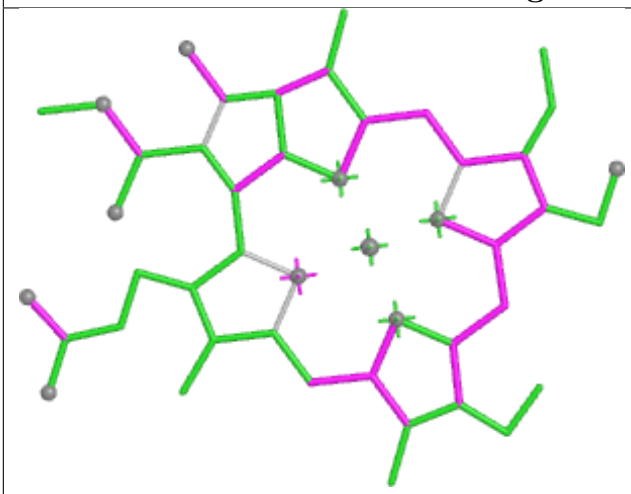


Torsions

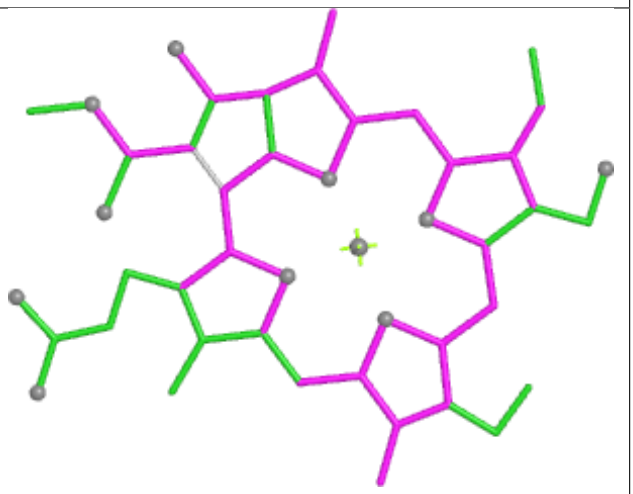


Rings

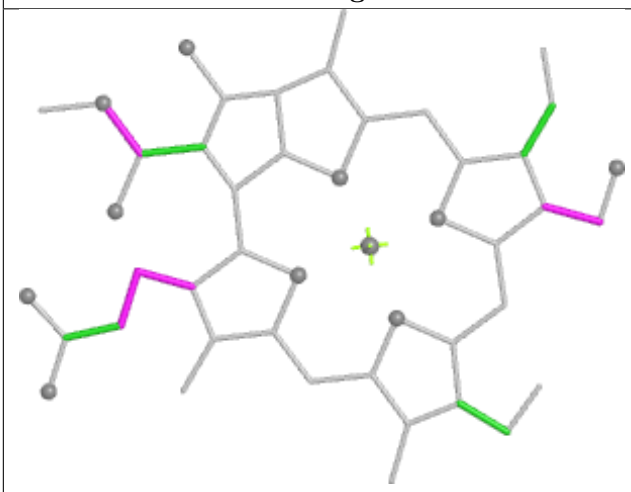
Ligand CHL h 608



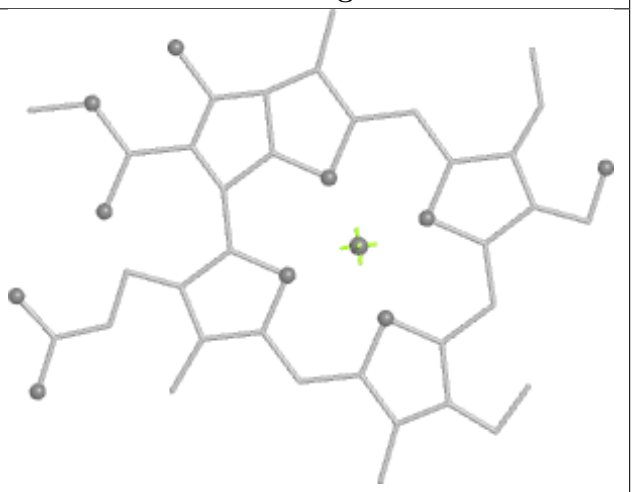
Bond lengths



Bond angles

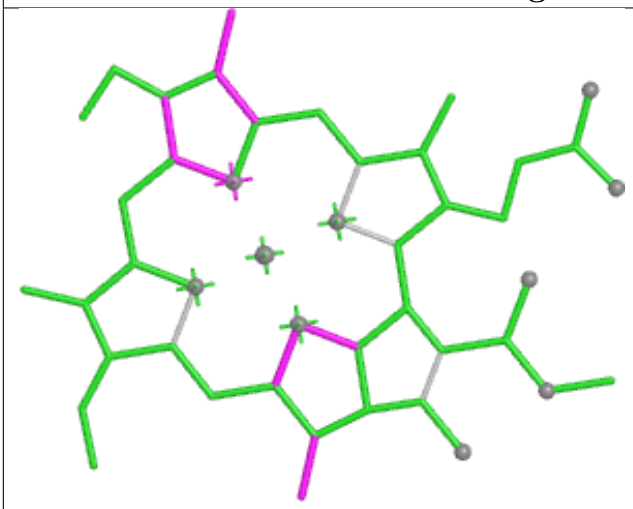


Torsions

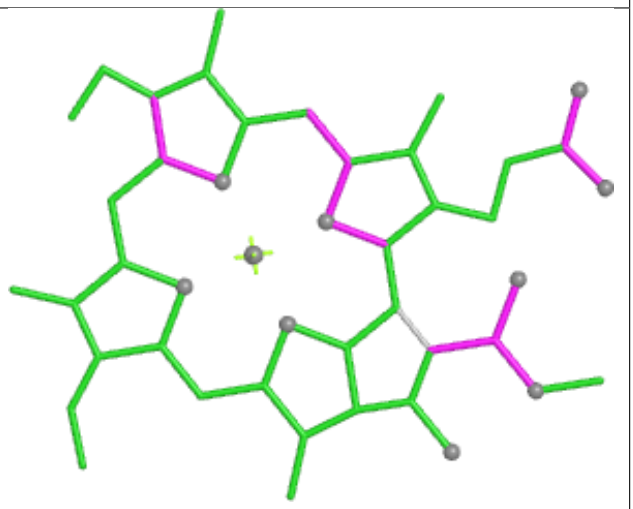


Rings

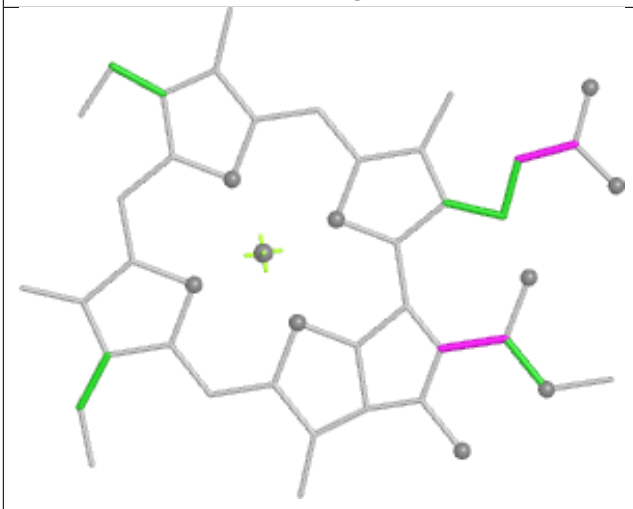
Ligand CLA 6 314



Bond lengths



Bond angles

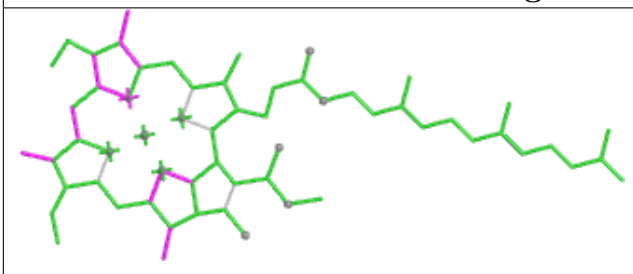


Torsions

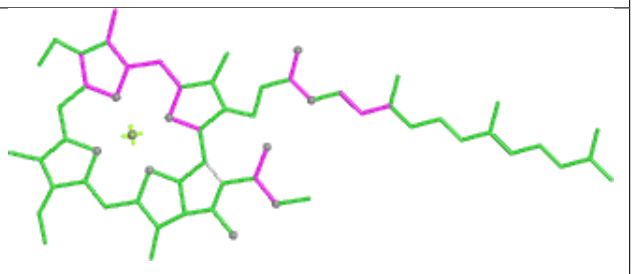


Rings

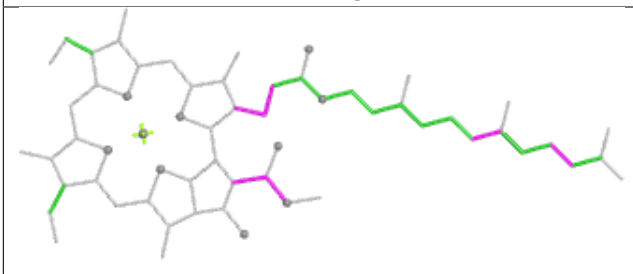
Ligand CLA B 816



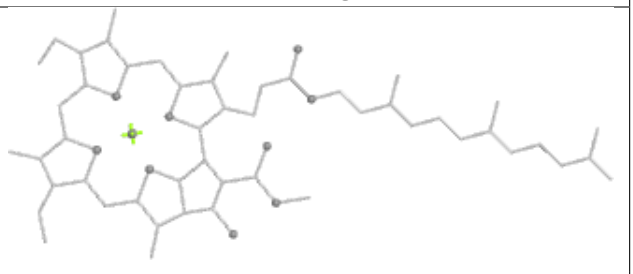
Bond lengths



Bond angles

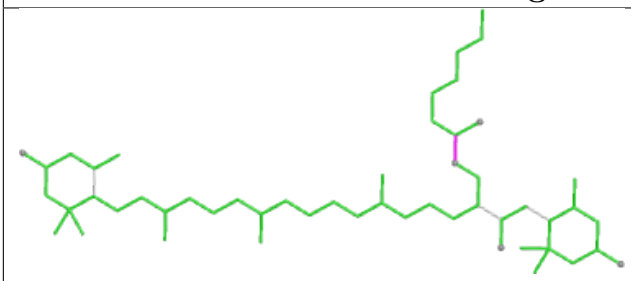


Torsions

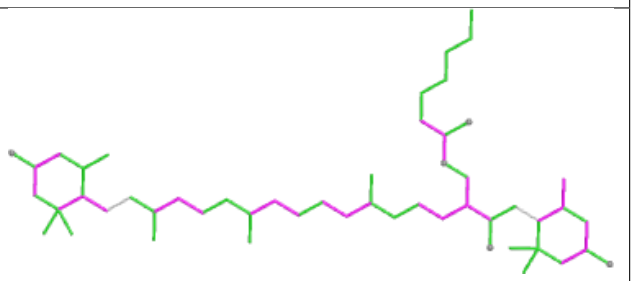


Rings

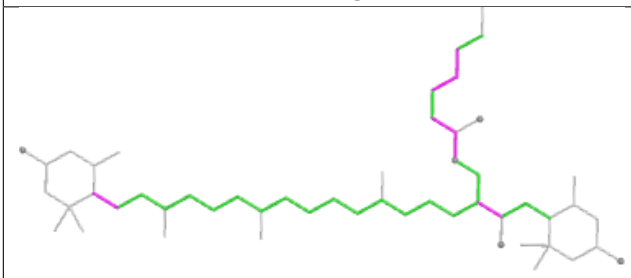
Ligand 0UR h 520



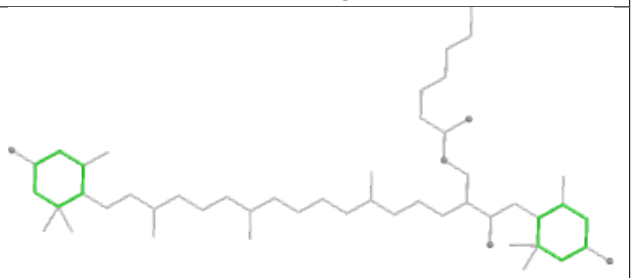
Bond lengths



Bond angles

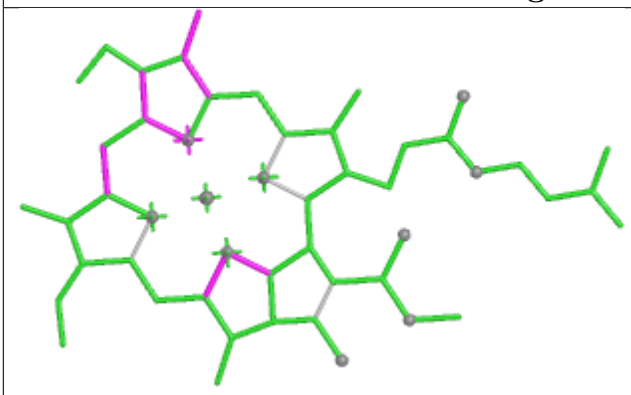


Torsions

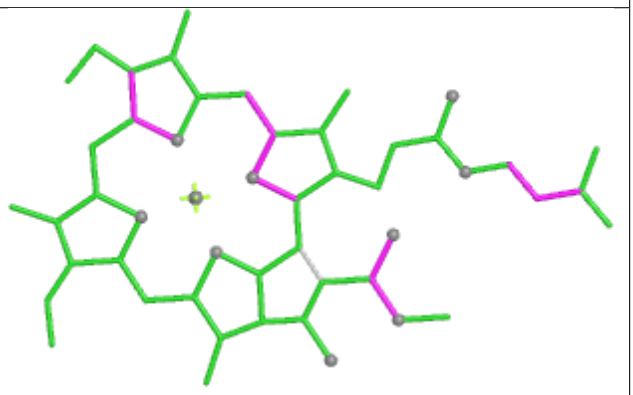


Rings

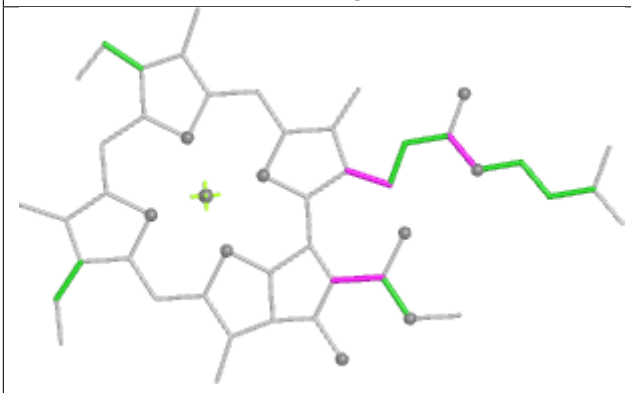
Ligand CLA d 604



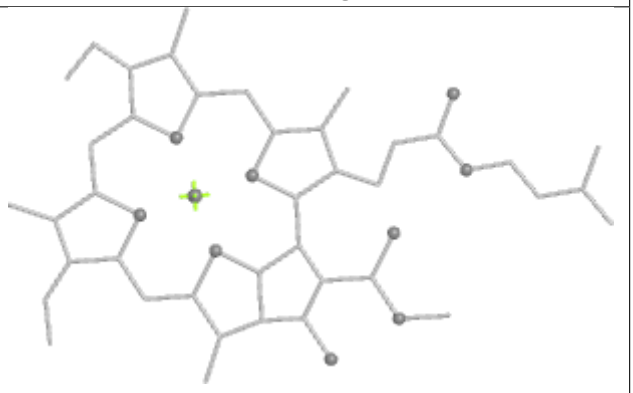
Bond lengths



Bond angles

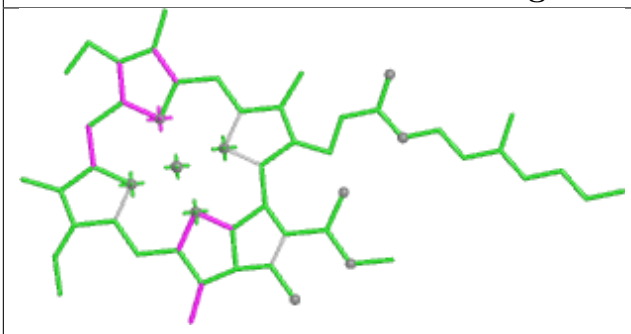


Torsions

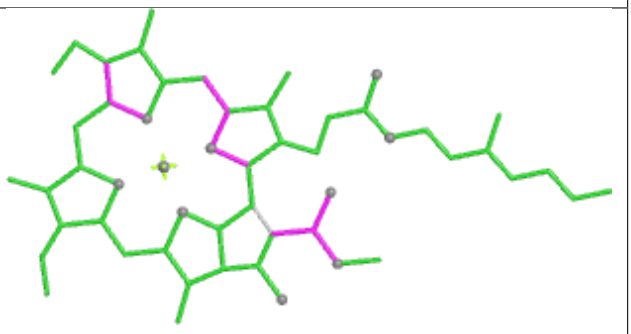


Rings

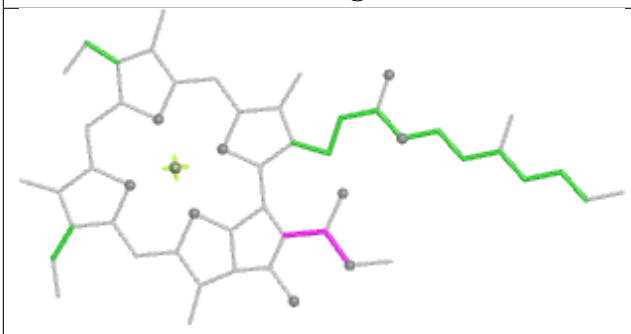
Ligand CLA a 603



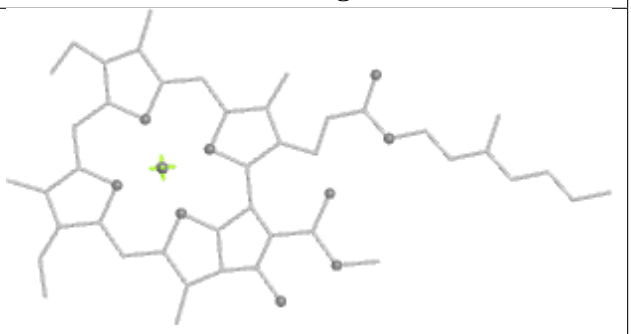
Bond lengths



Bond angles

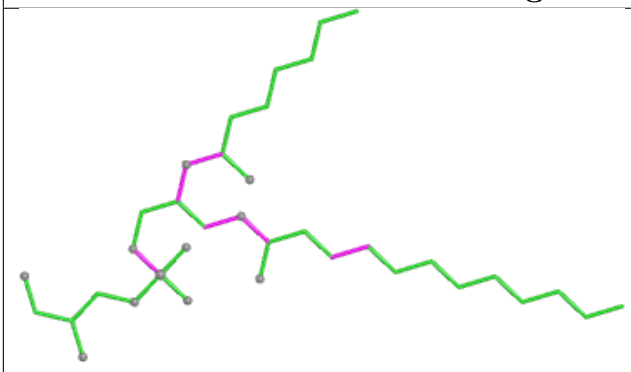


Torsions

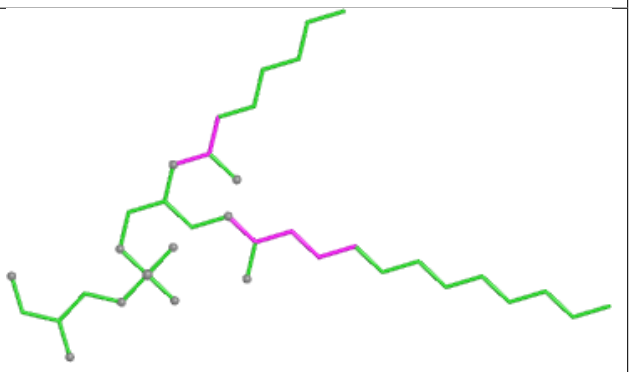


Rings

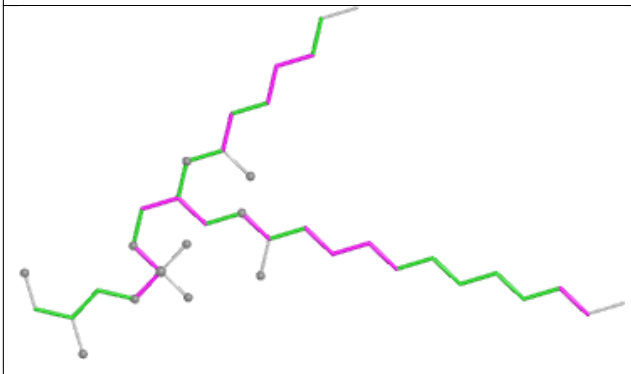
Ligand LHG d 630



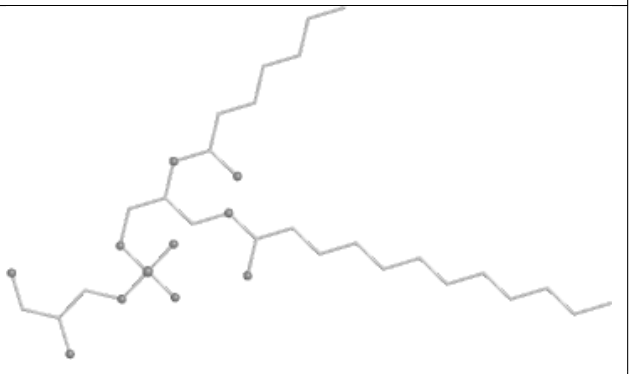
Bond lengths



Bond angles

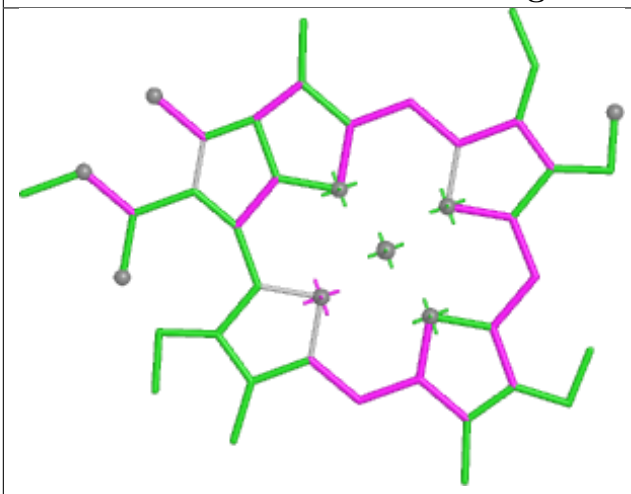


Torsions

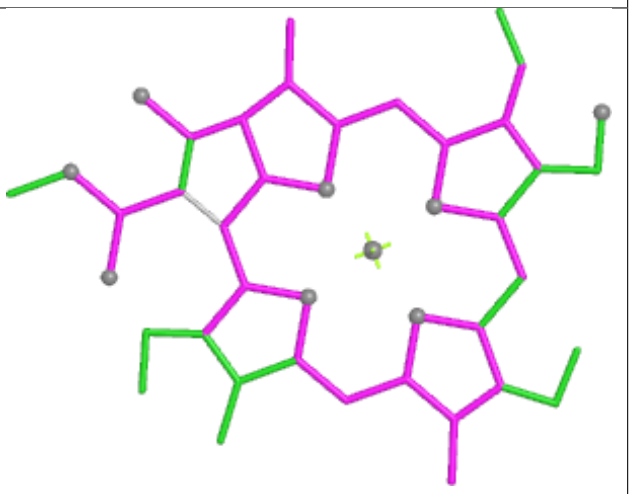


Rings

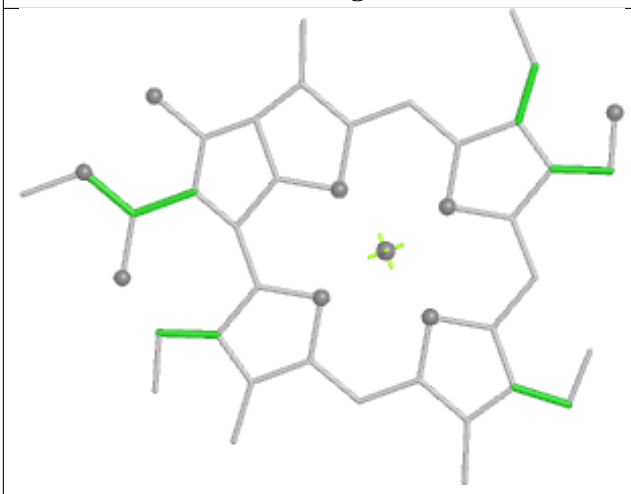
Ligand CHL 2 305



Bond lengths



Bond angles

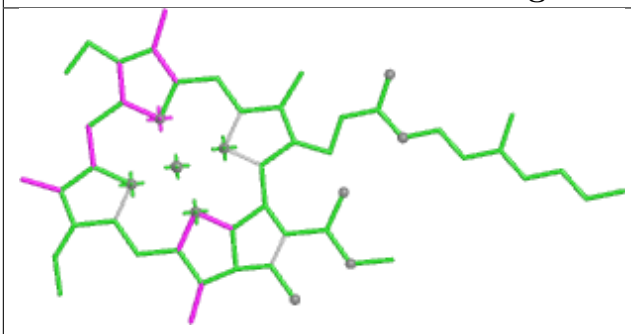


Torsions

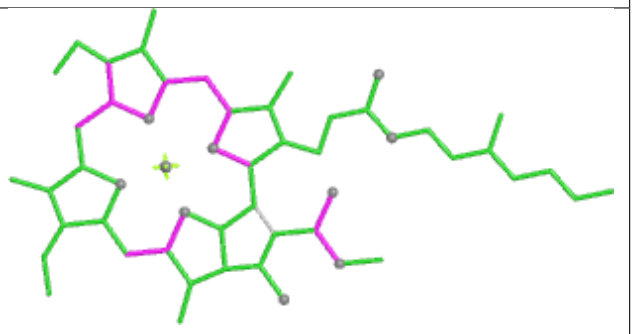


Rings

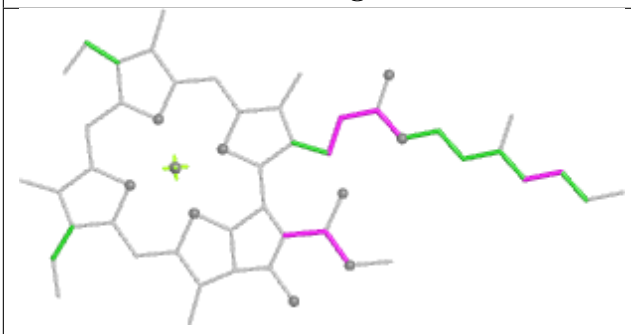
Ligand CLA 4 312



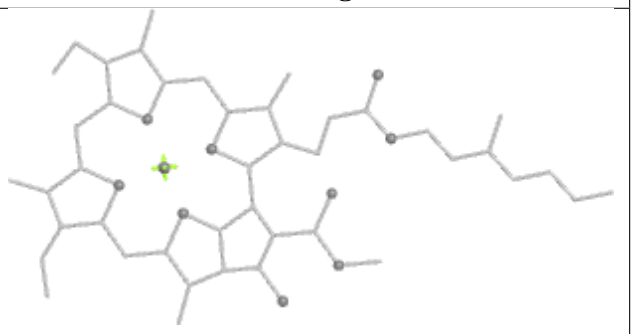
Bond lengths



Bond angles

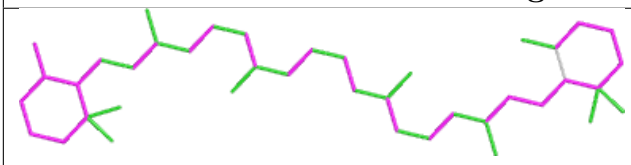


Torsions

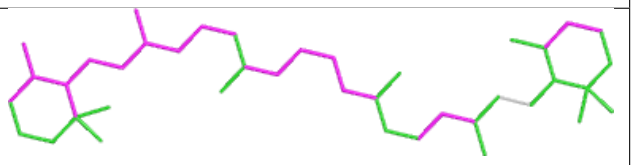


Rings

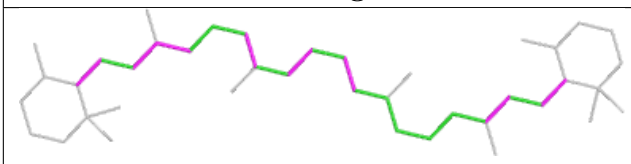
Ligand 8CT B 851



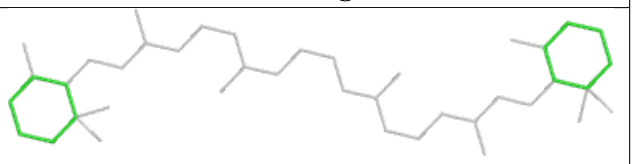
Bond lengths



Bond angles

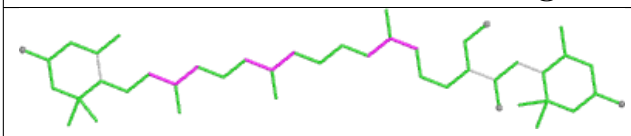


Torsions

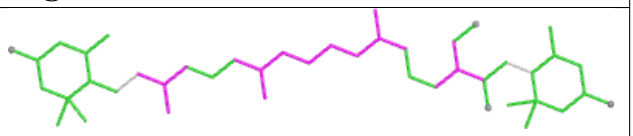


Rings

Ligand 0IE g 521



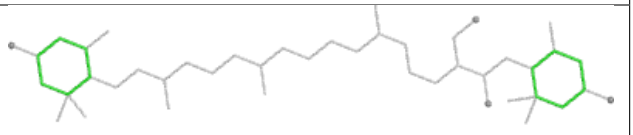
Bond lengths



Bond angles

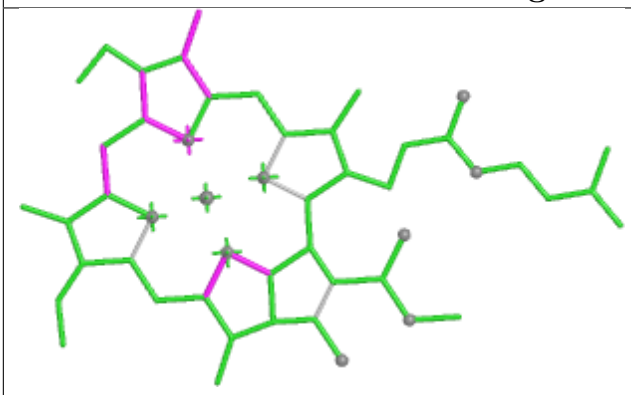


Torsions

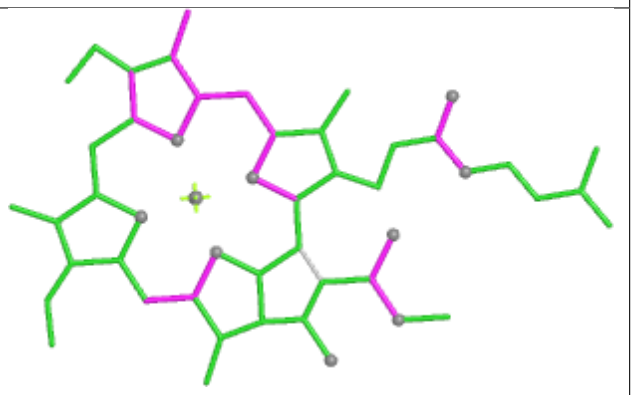


Rings

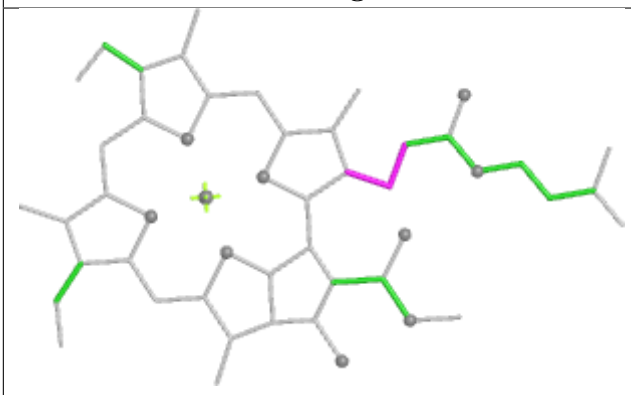
Ligand CLA a 604



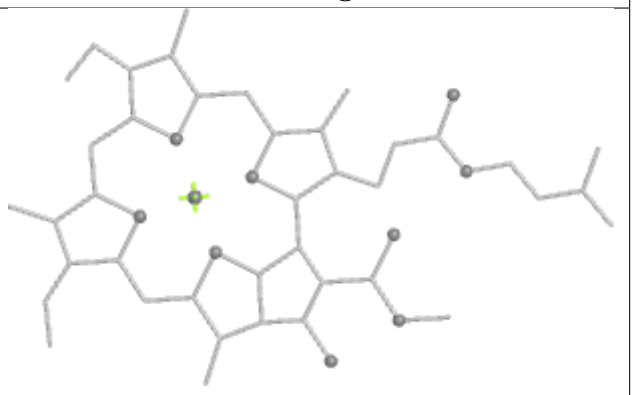
Bond lengths



Bond angles

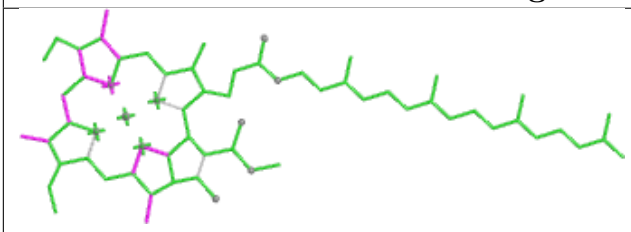


Torsions

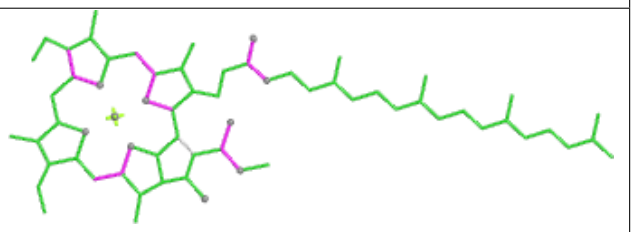


Rings

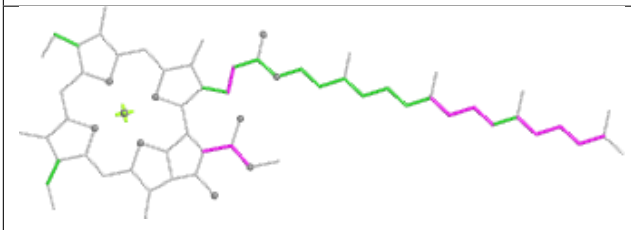
Ligand CLA 9 302



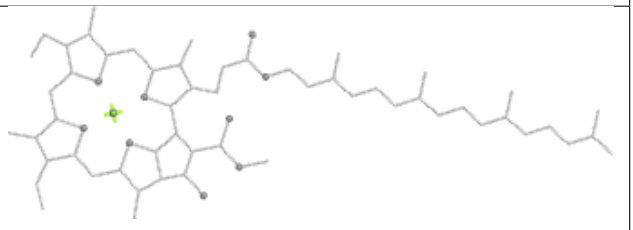
Bond lengths



Bond angles

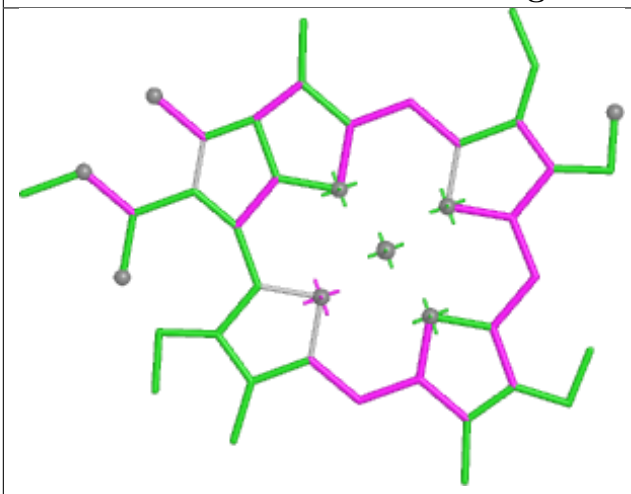


Torsions

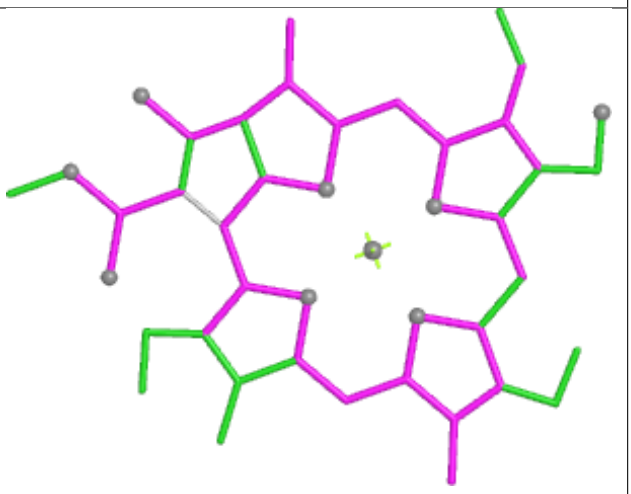


Rings

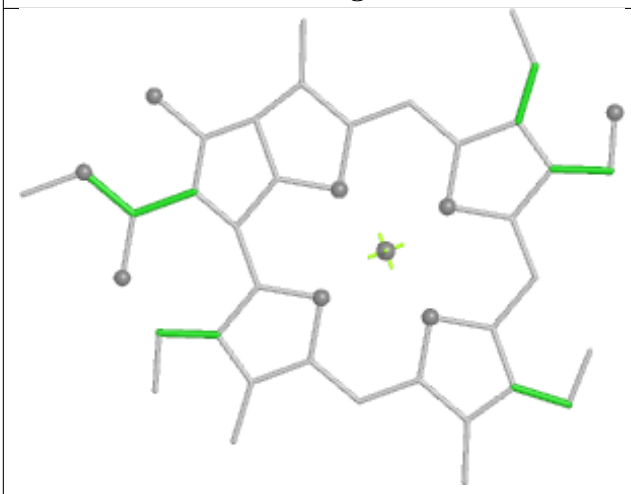
Ligand CHL 4 305



Bond lengths



Bond angles

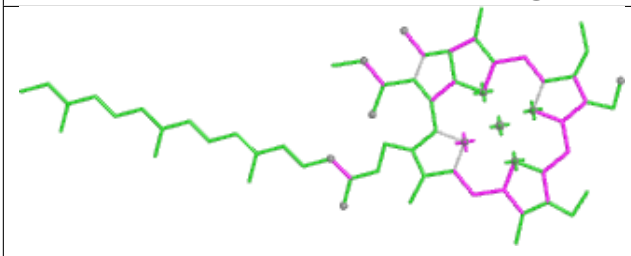


Torsions

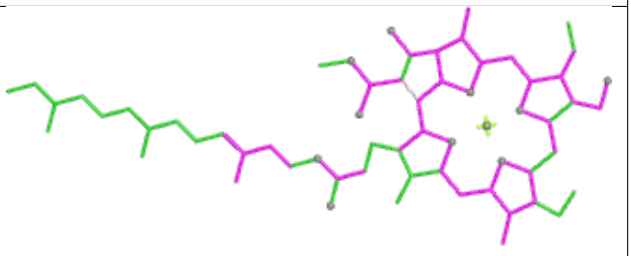


Rings

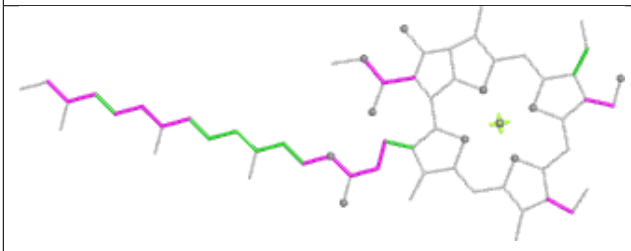
Ligand CHL 3 302



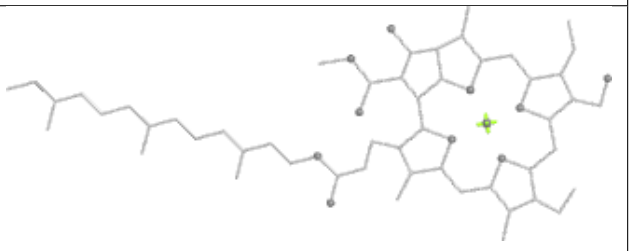
Bond lengths



Bond angles

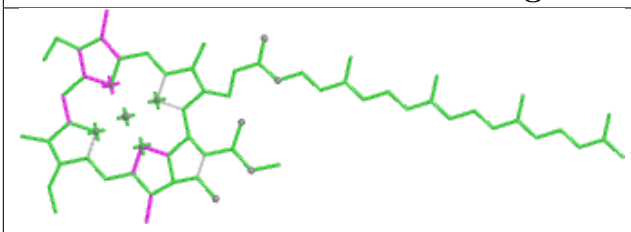


Torsions

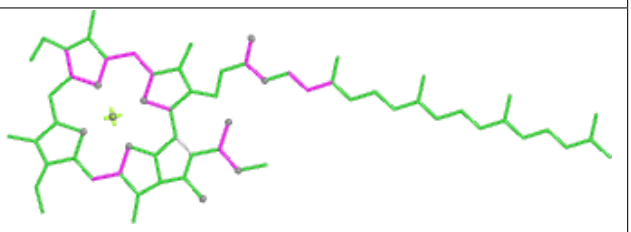


Rings

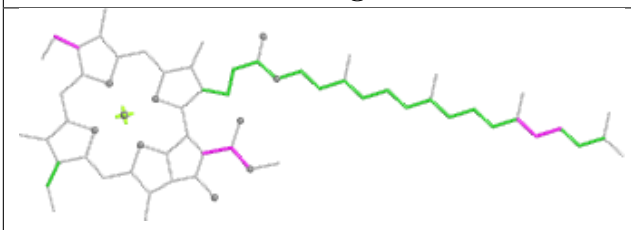
Ligand CLA B 841



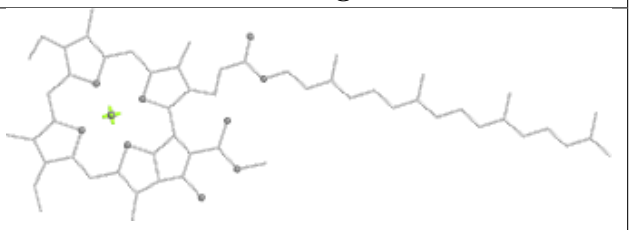
Bond lengths



Bond angles

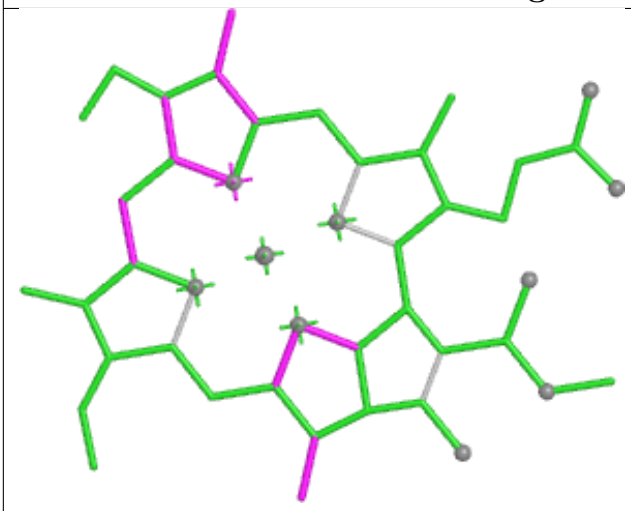


Torsions

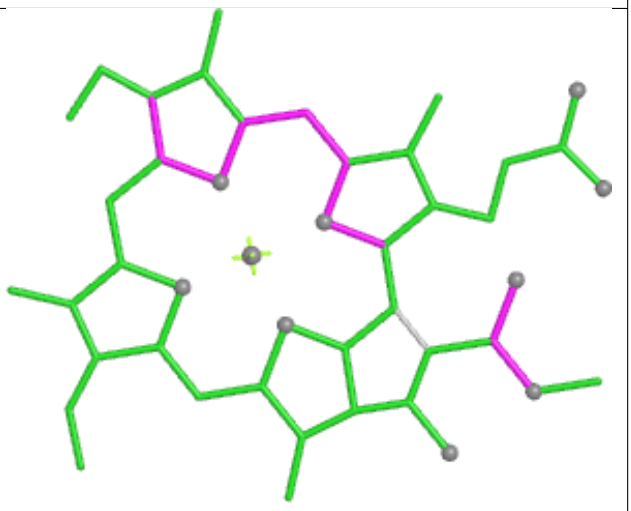


Rings

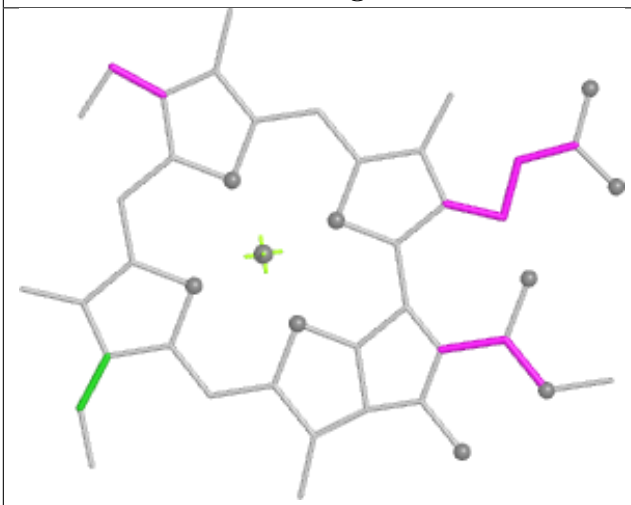
Ligand CLA 0 321



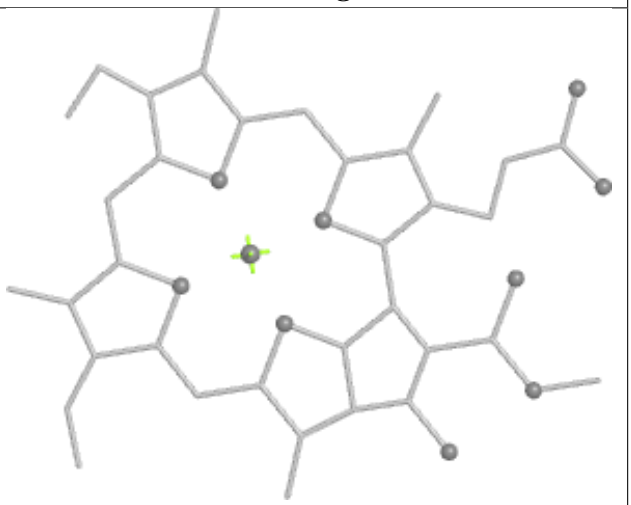
Bond lengths



Bond angles

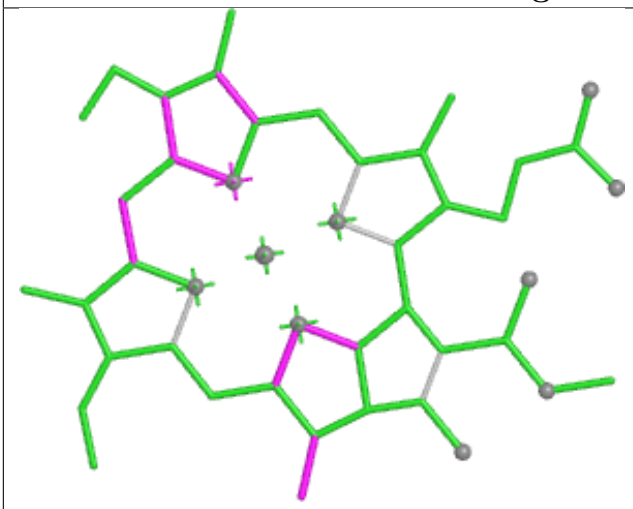


Torsions

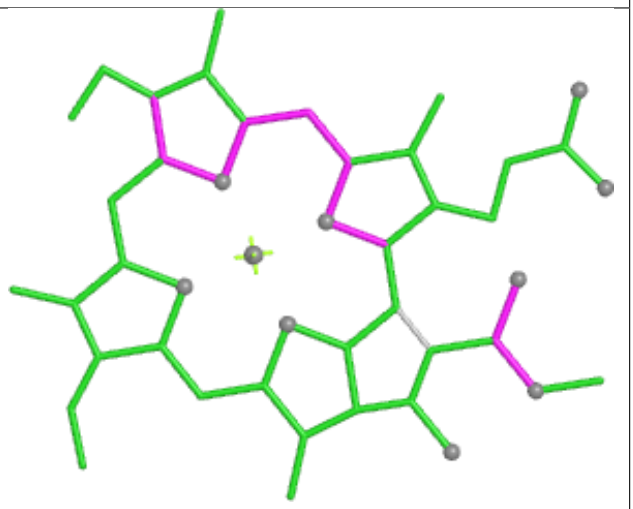


Rings

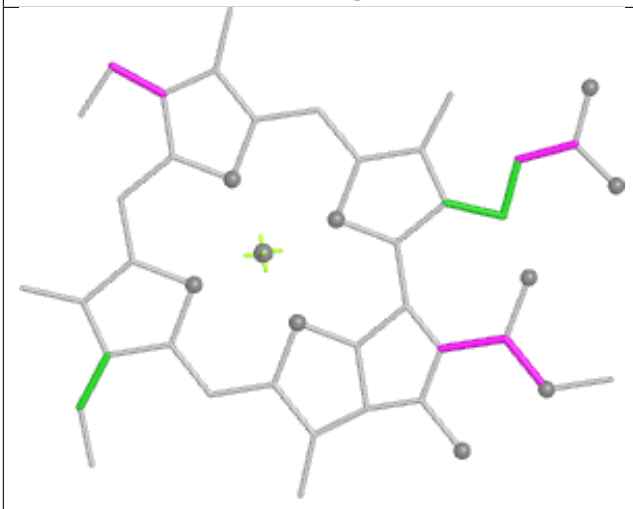
Ligand CLA i 611



Bond lengths



Bond angles

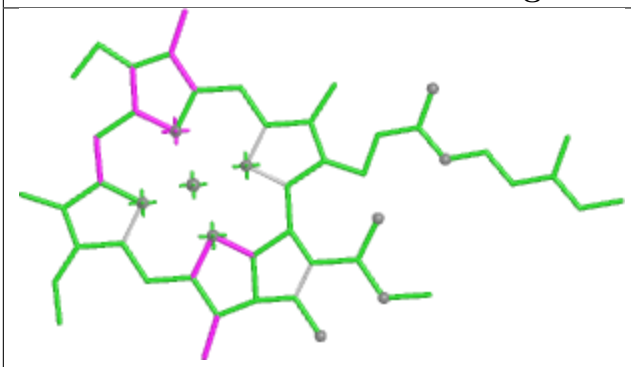


Torsions

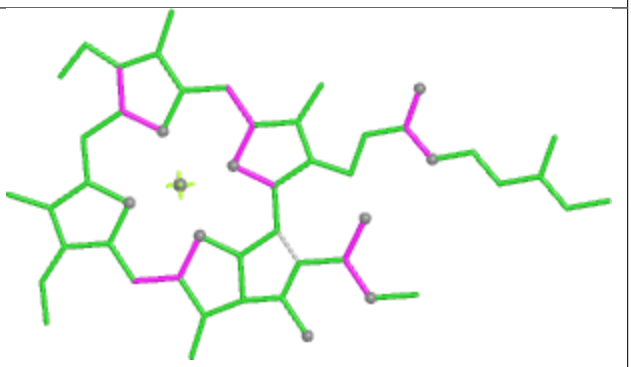


Rings

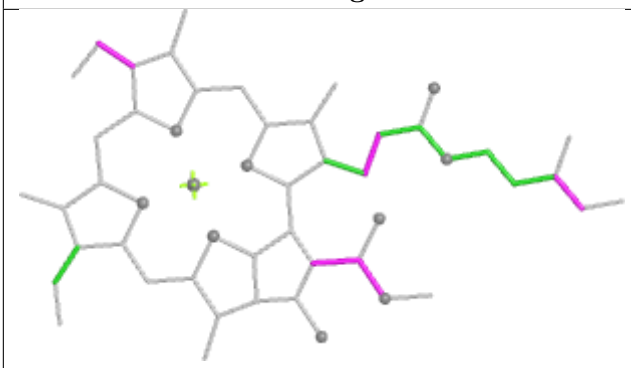
Ligand CLA O 206



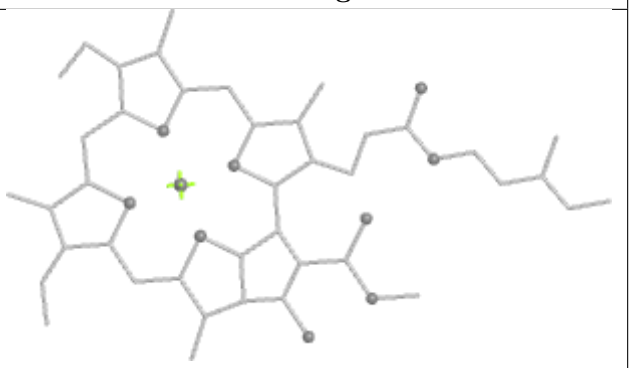
Bond lengths



Bond angles

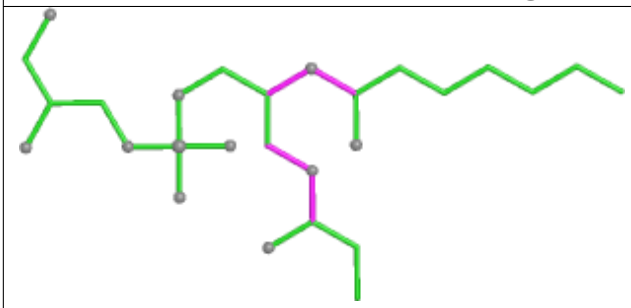


Torsions

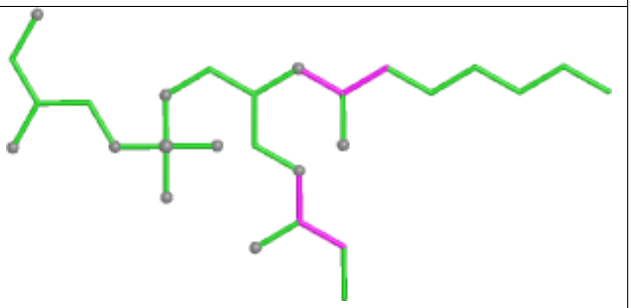


Rings

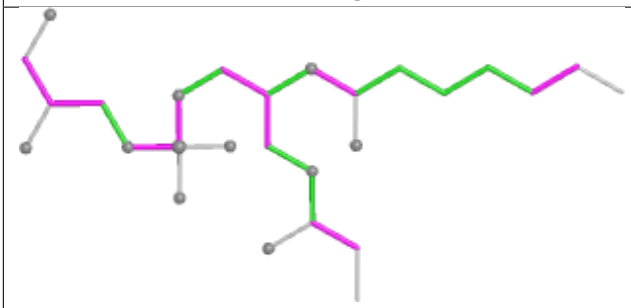
Ligand LHG A 845



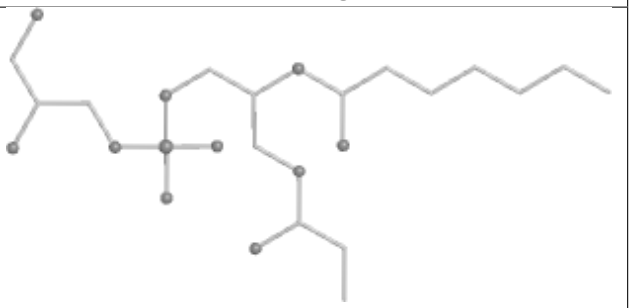
Bond lengths



Bond angles

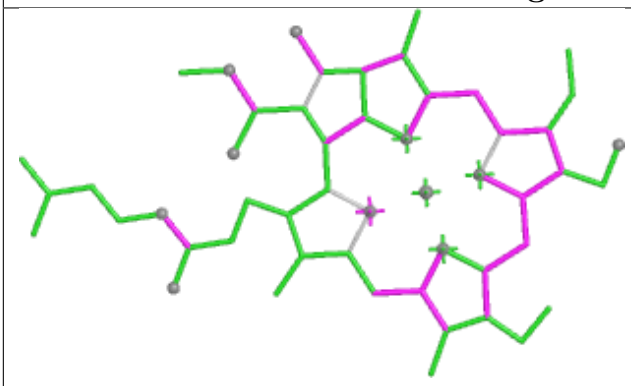


Torsions

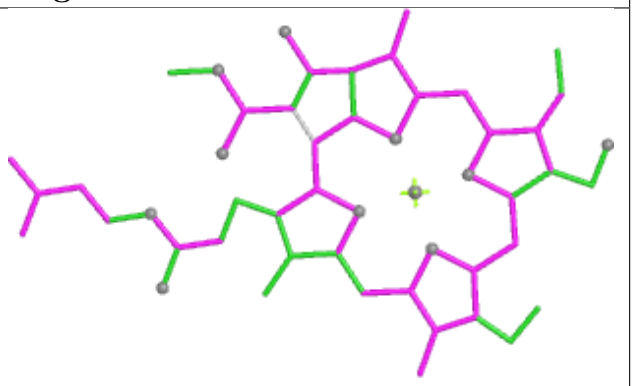


Rings

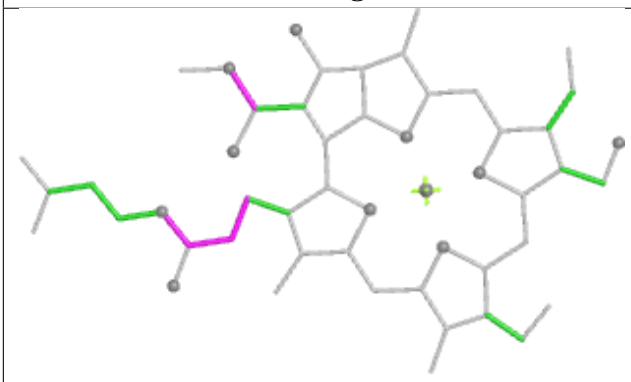
Ligand CHL g 606



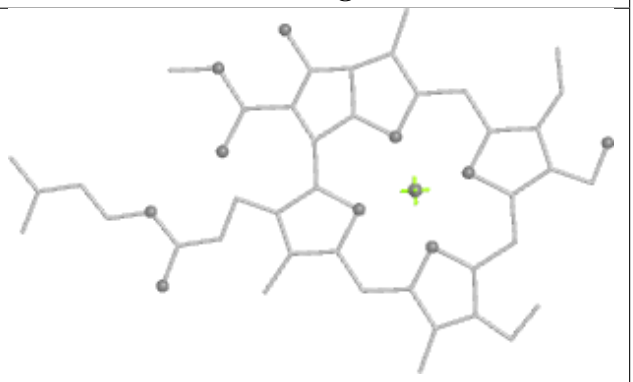
Bond lengths



Bond angles

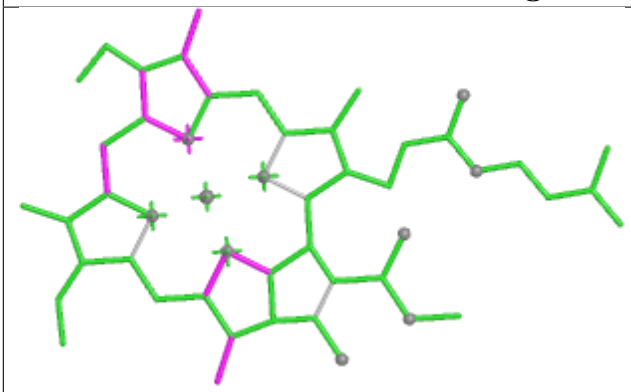


Torsions

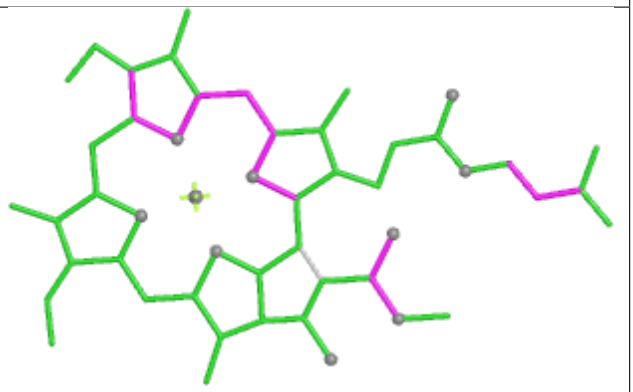


Rings

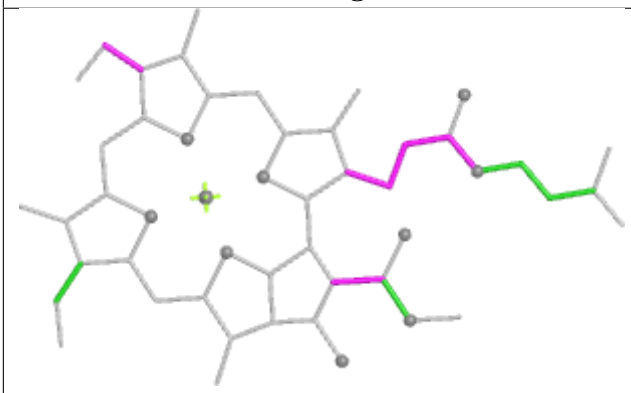
Ligand CLA B 831



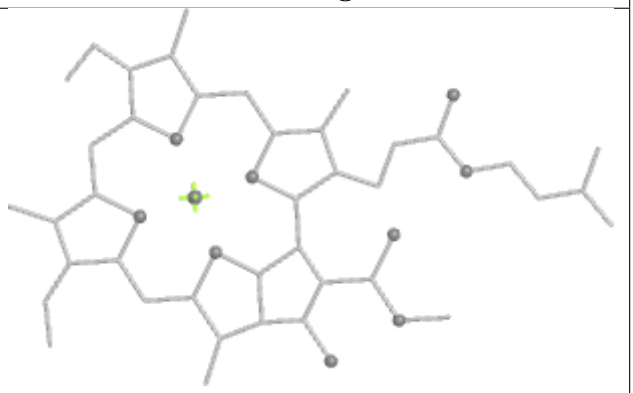
Bond lengths



Bond angles

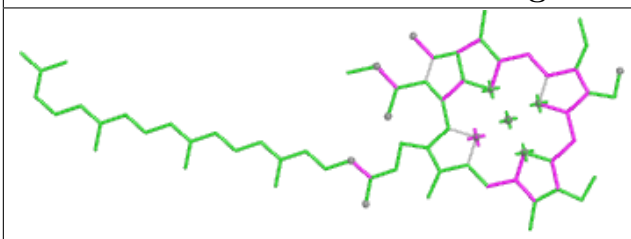


Torsions

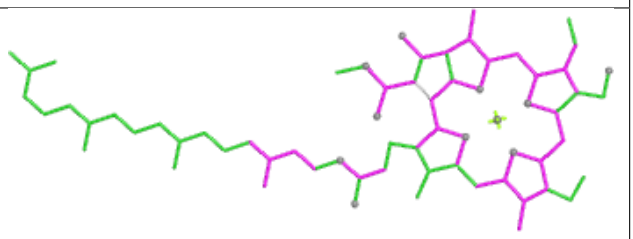


Rings

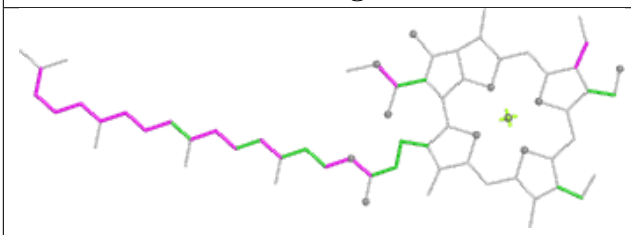
Ligand CHL c 609



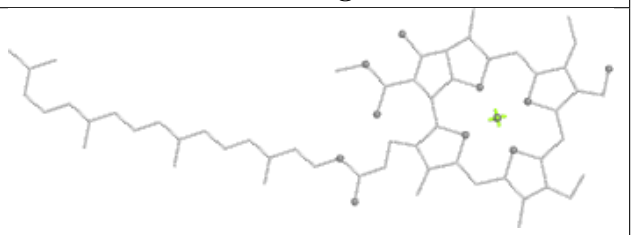
Bond lengths



Bond angles

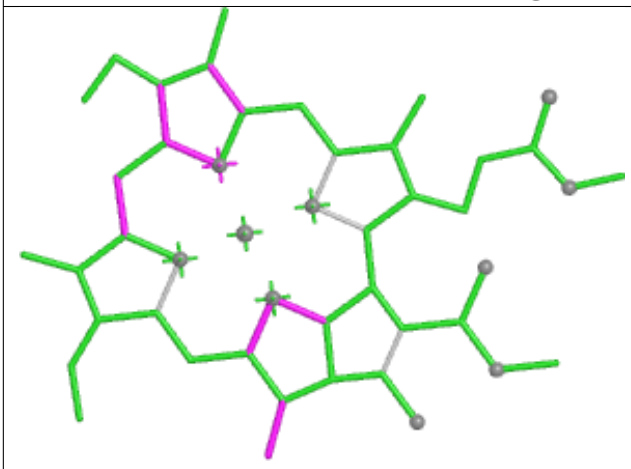


Torsions

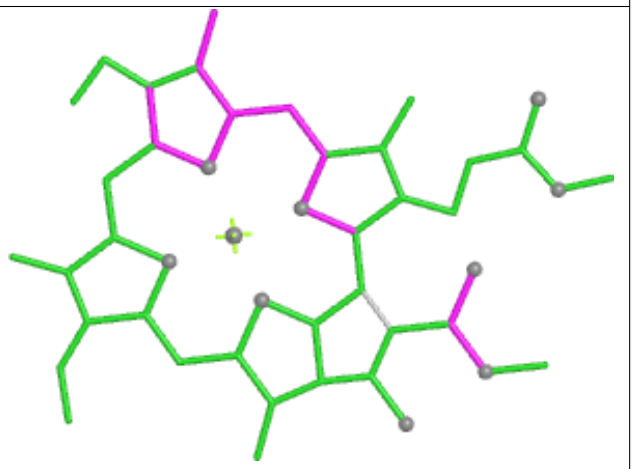


Rings

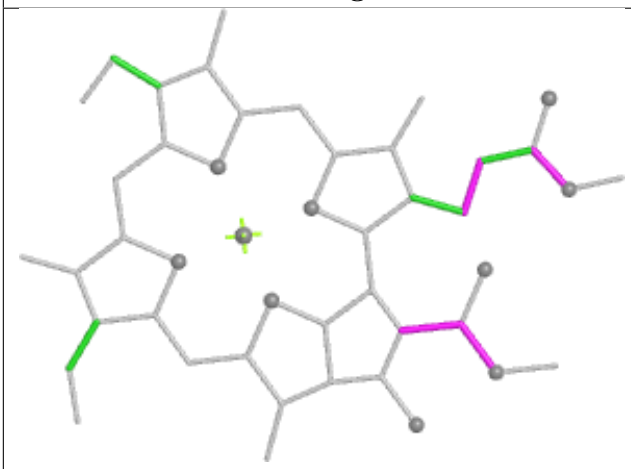
Ligand CLA h 604



Bond lengths



Bond angles

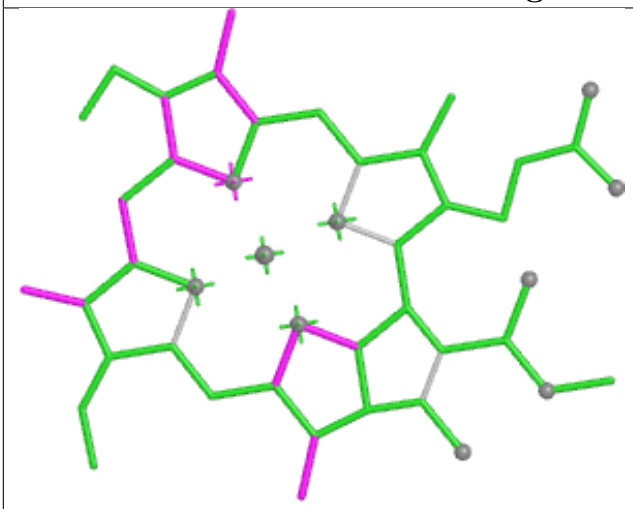


Torsions

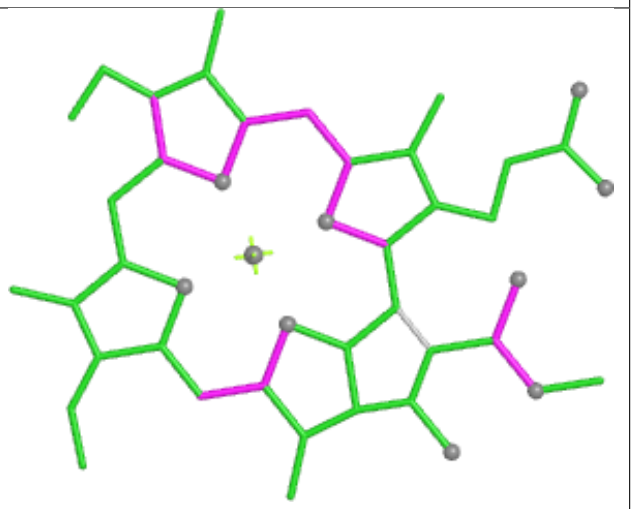


Rings

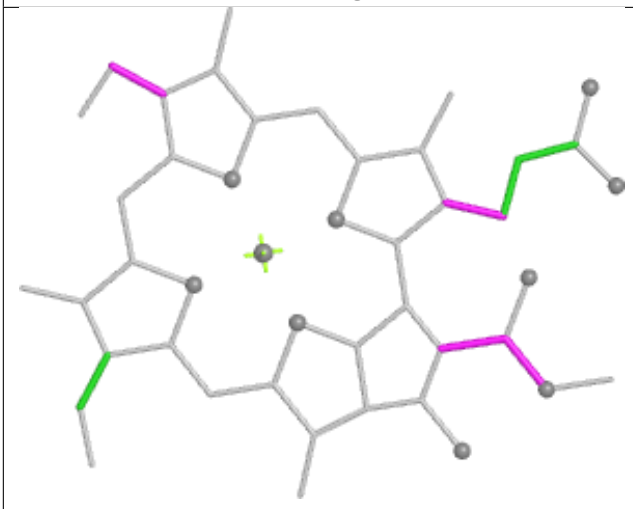
Ligand CLA F 301



Bond lengths



Bond angles

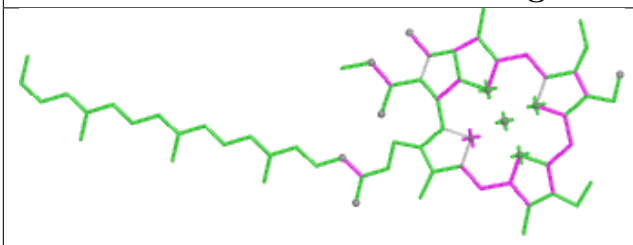


Torsions

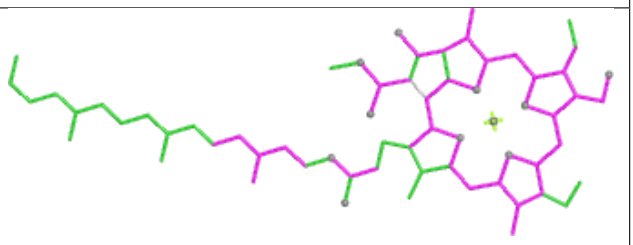


Rings

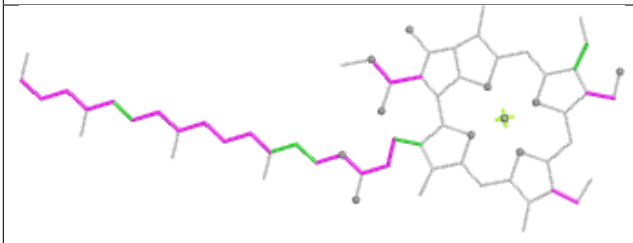
Ligand CHL 2 302



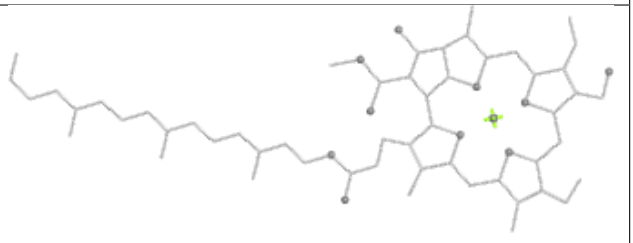
Bond lengths



Bond angles

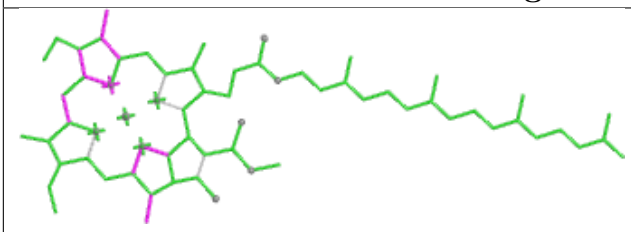


Torsions

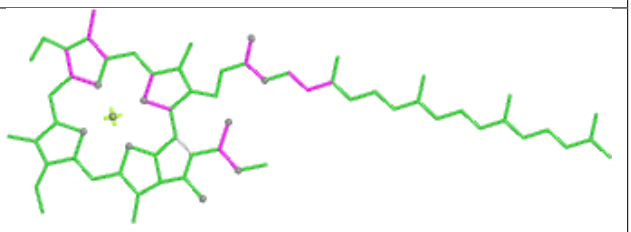


Rings

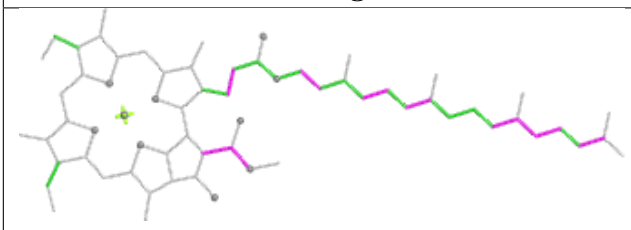
Ligand CLA B 803



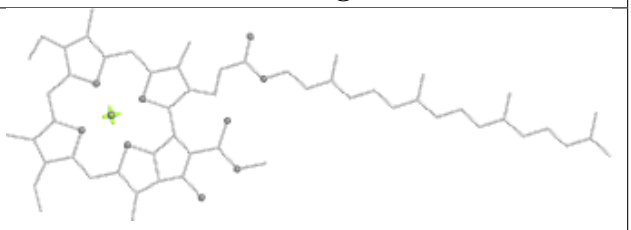
Bond lengths



Bond angles

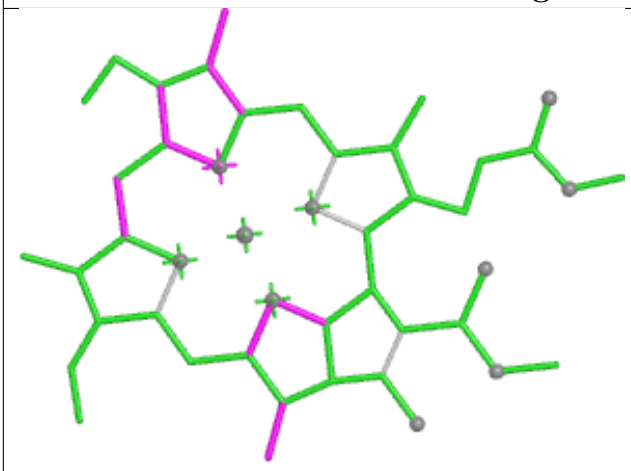


Torsions

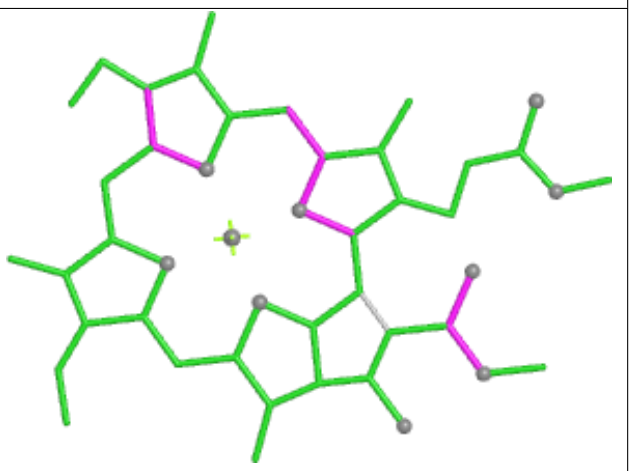


Rings

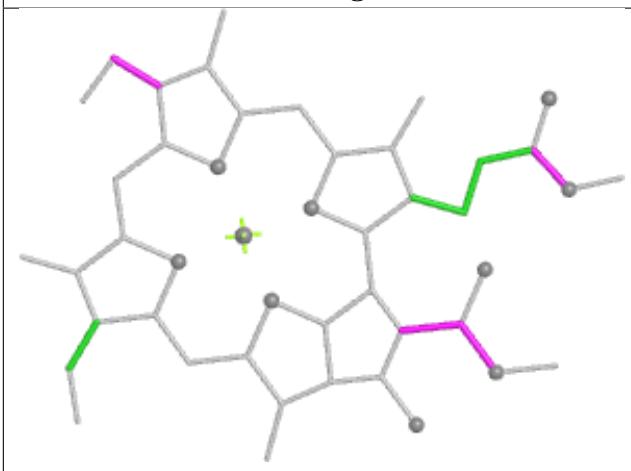
Ligand CLA i 603



Bond lengths



Bond angles

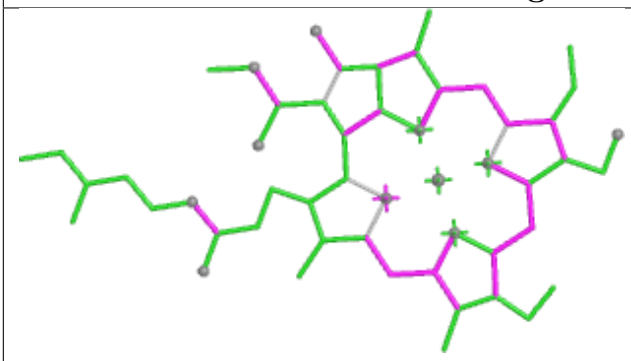


Torsions

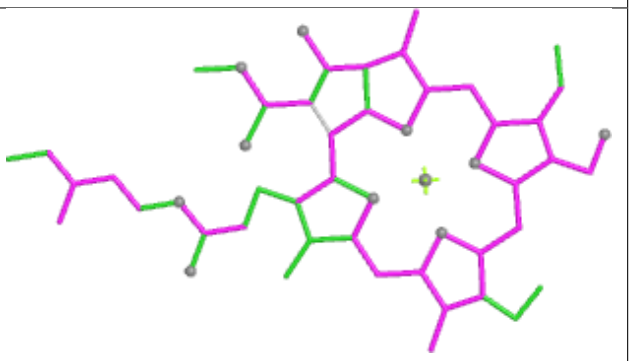


Rings

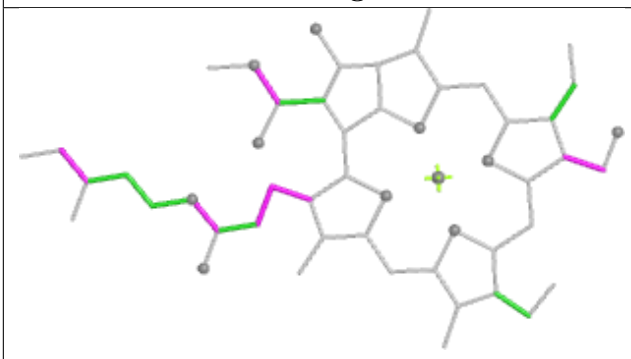
Ligand CHL 0 301



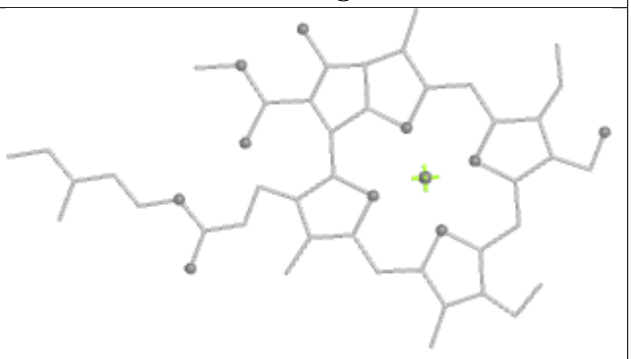
Bond lengths



Bond angles

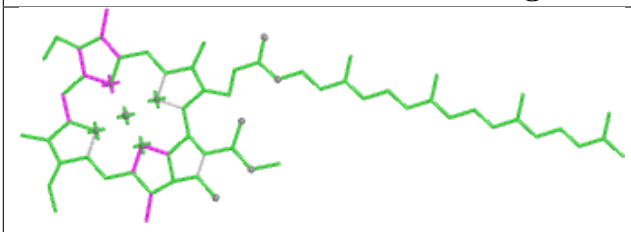


Torsions

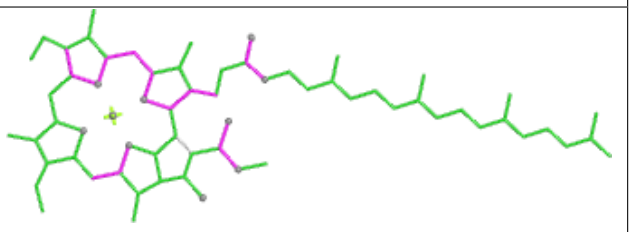


Rings

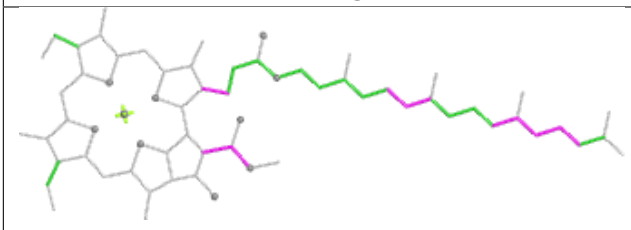
Ligand CLA A 826



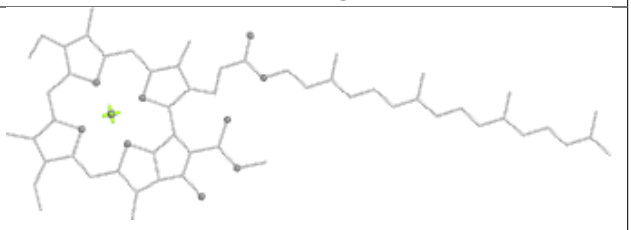
Bond lengths



Bond angles

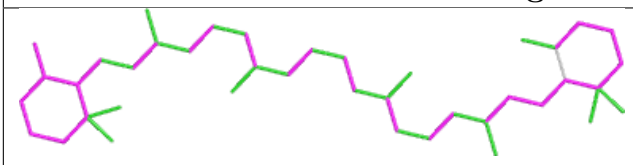


Torsions

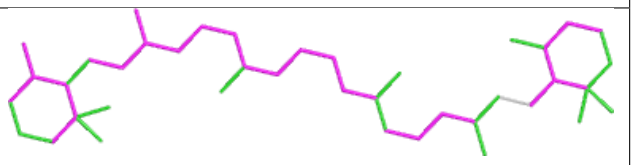


Rings

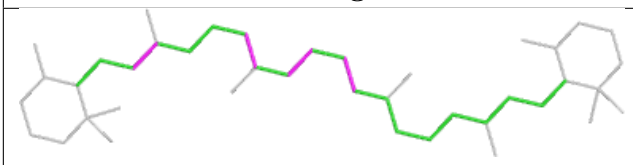
Ligand 8CT O 205



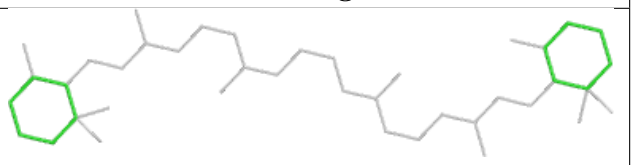
Bond lengths



Bond angles

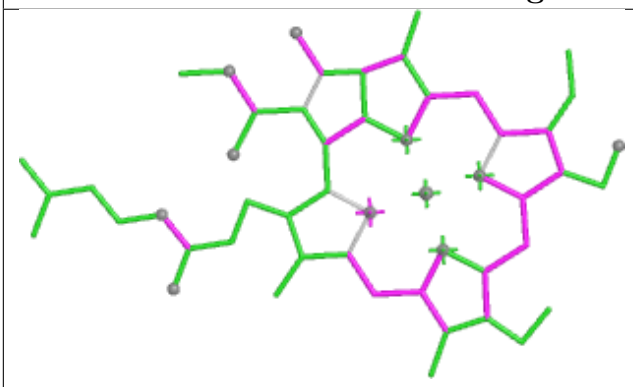


Torsions

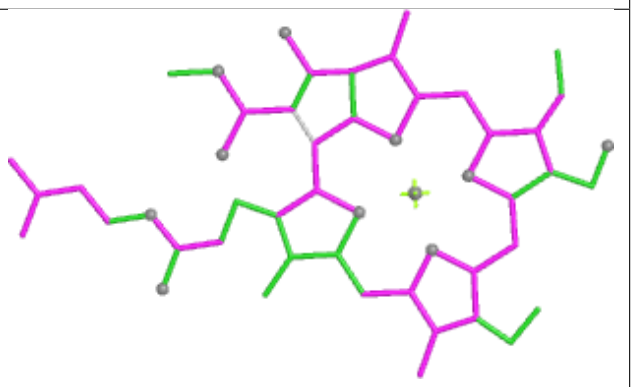


Rings

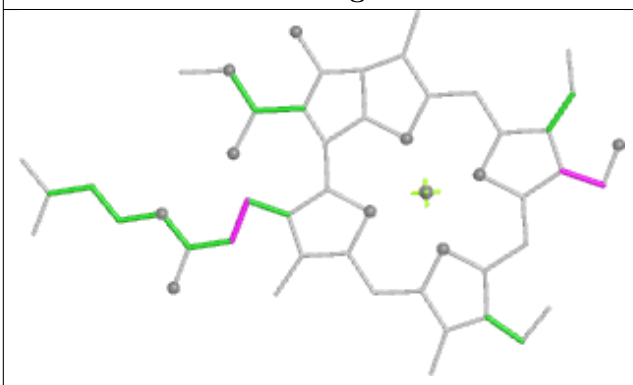
Ligand CHL b 606



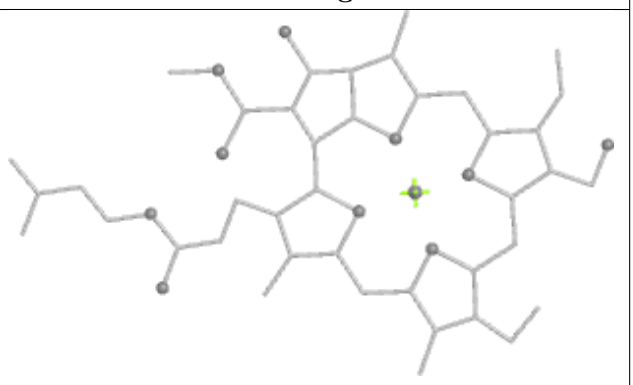
Bond lengths



Bond angles

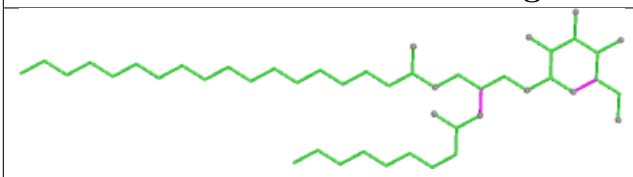


Torsions

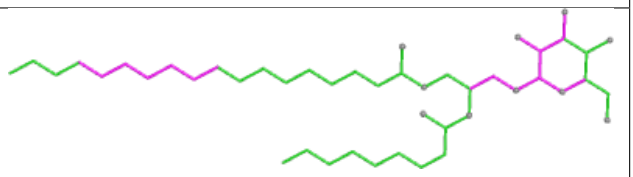


Rings

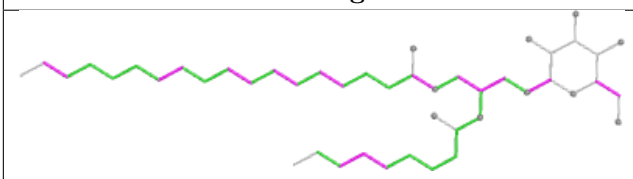
Ligand LMG J 105



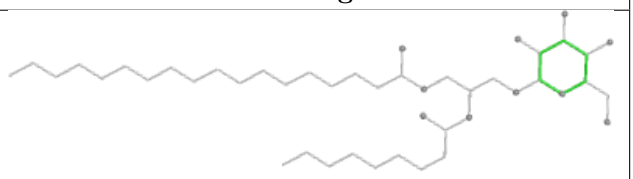
Bond lengths



Bond angles

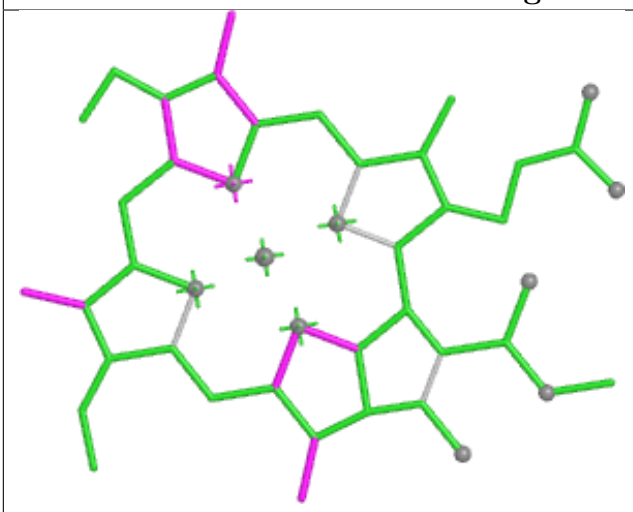


Torsions

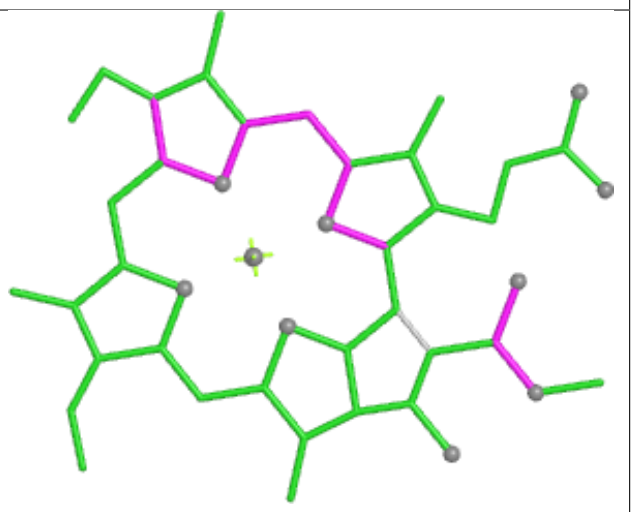


Rings

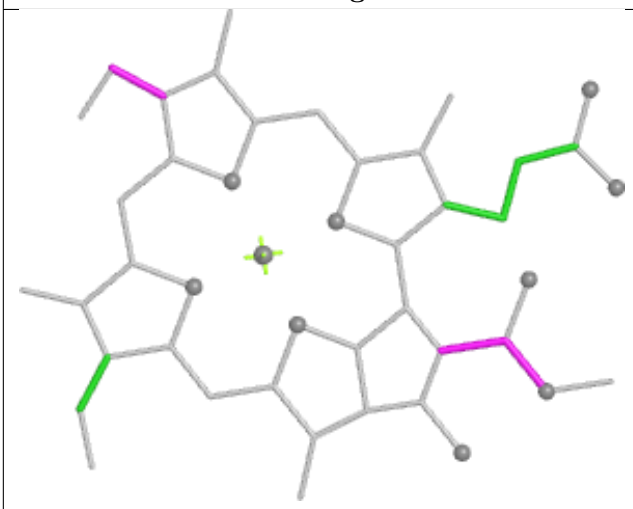
Ligand CLA A 816



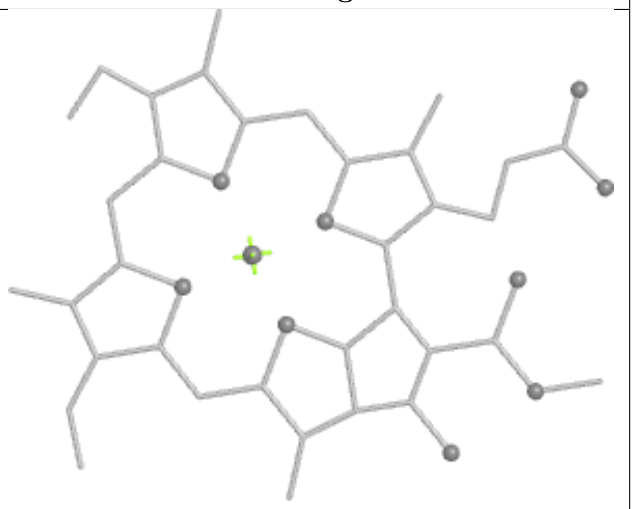
Bond lengths



Bond angles

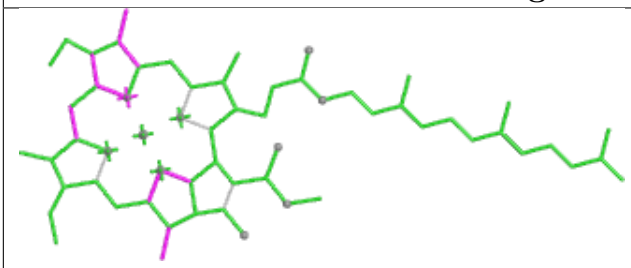


Torsions

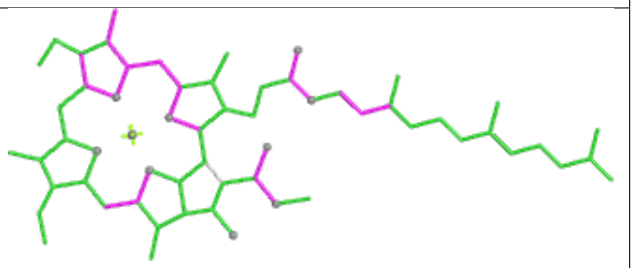


Rings

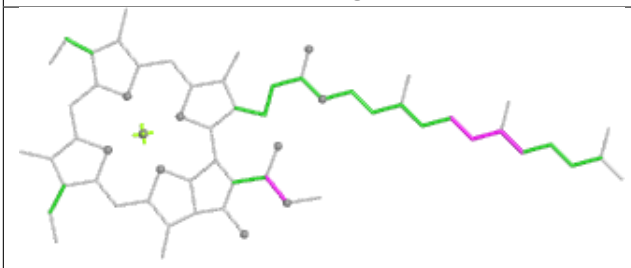
Ligand CLA 9 309



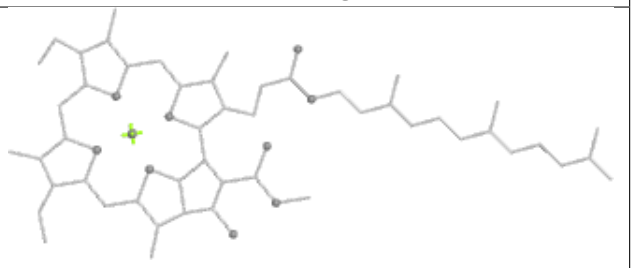
Bond lengths



Bond angles

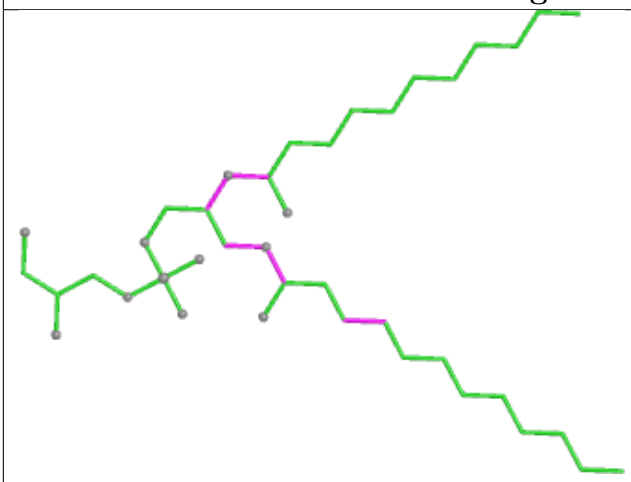


Torsions

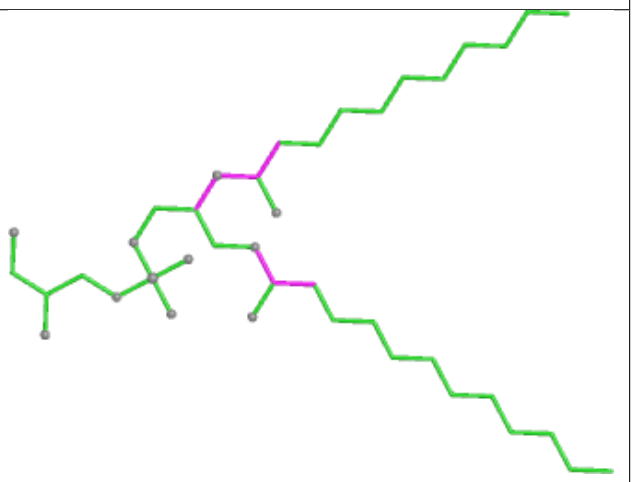


Rings

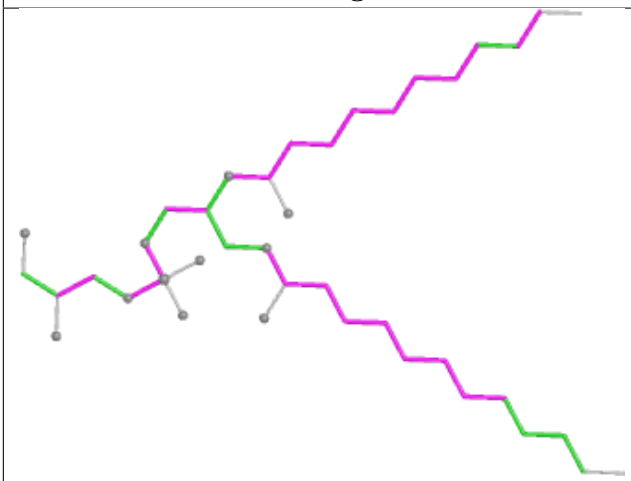
Ligand LHG f 630



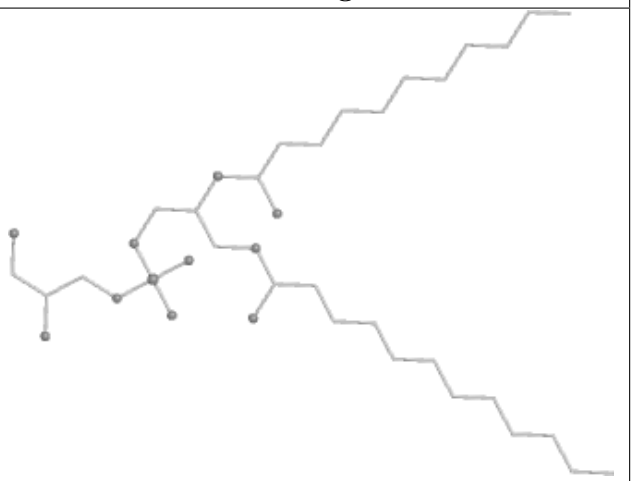
Bond lengths



Bond angles

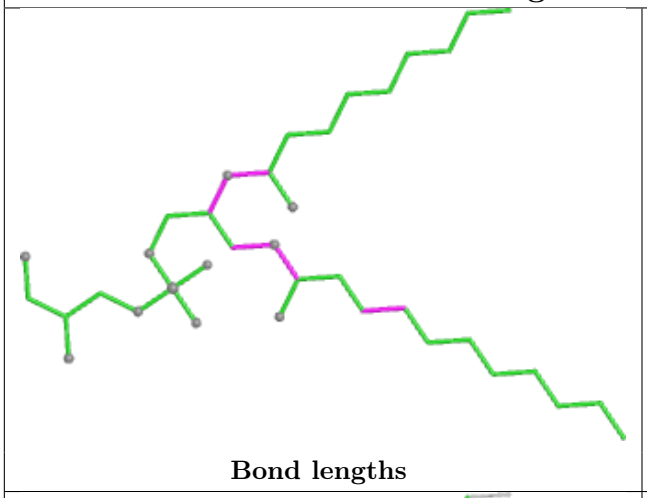


Torsions

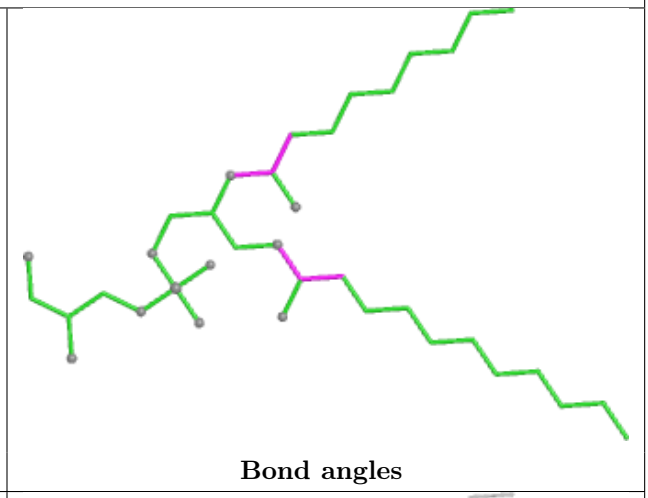


Rings

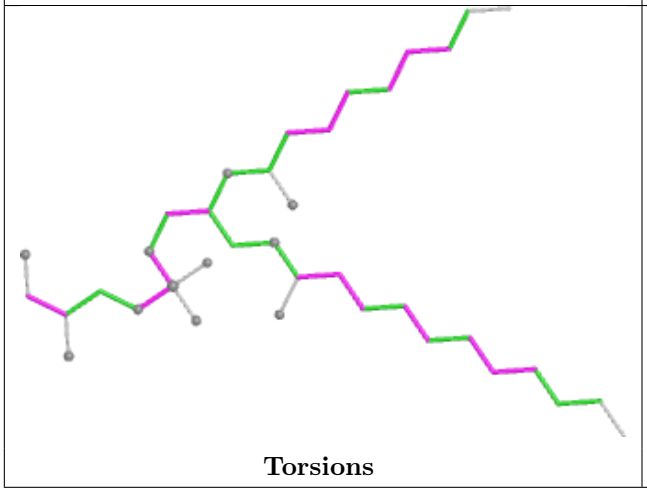
Ligand LHG 6 601



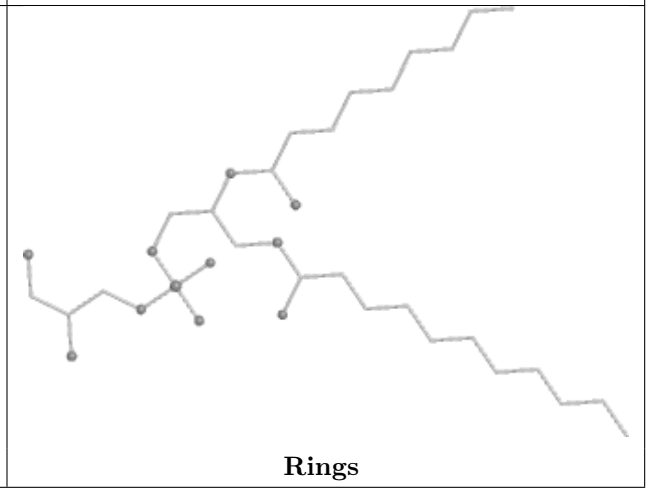
Bond lengths



Bond angles

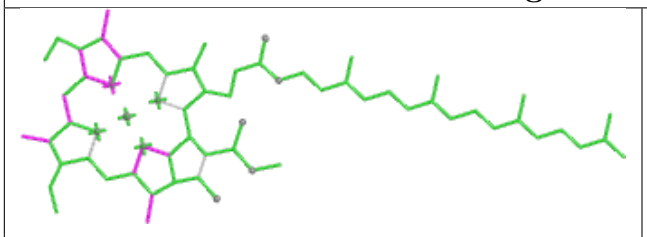


Torsions

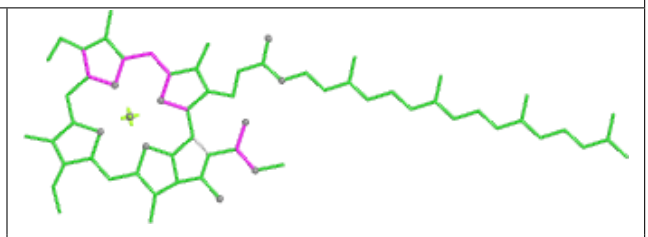


Rings

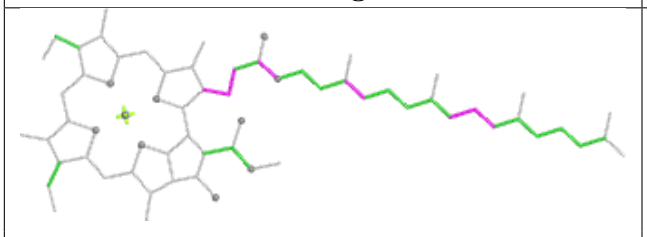
Ligand CLA B 829



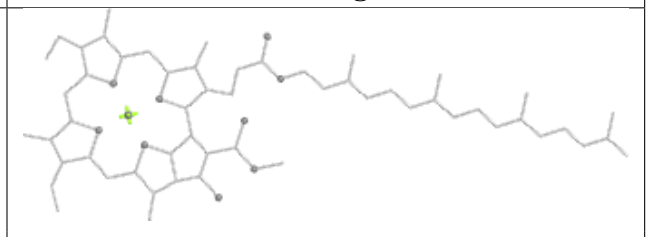
Bond lengths



Bond angles

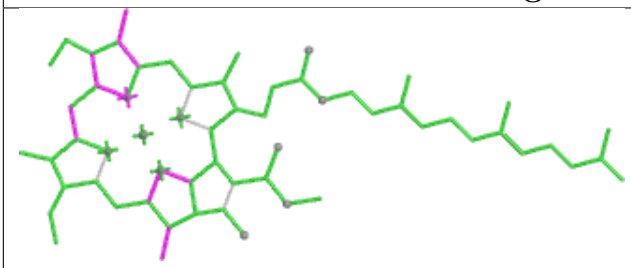


Torsions

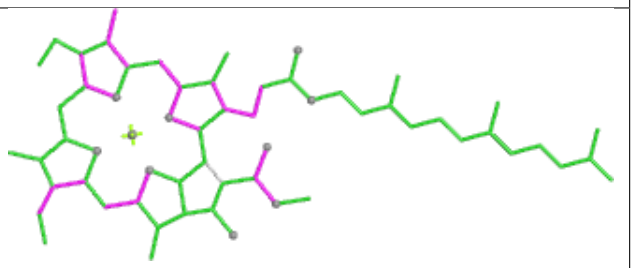


Rings

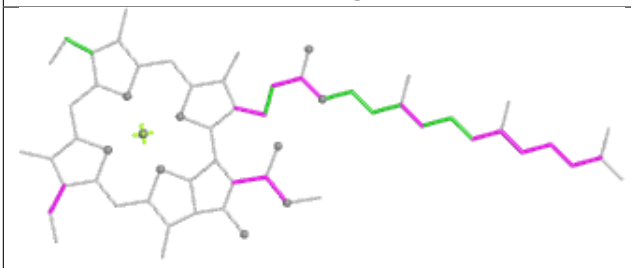
Ligand CLA B 817



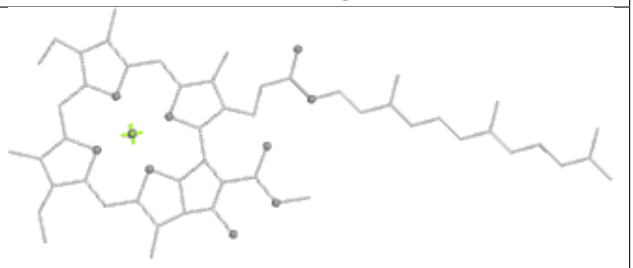
Bond lengths



Bond angles

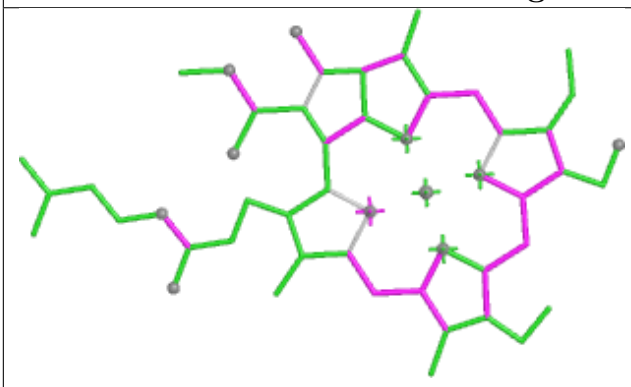


Torsions

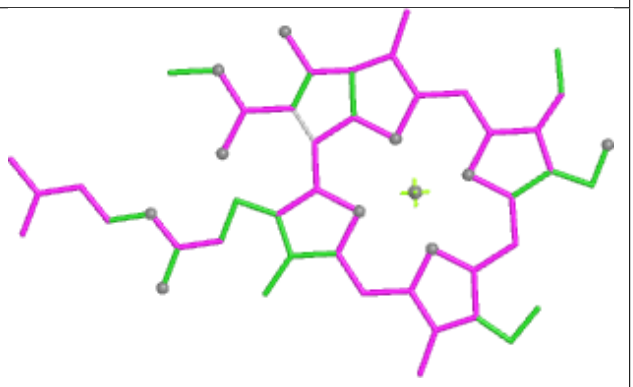


Rings

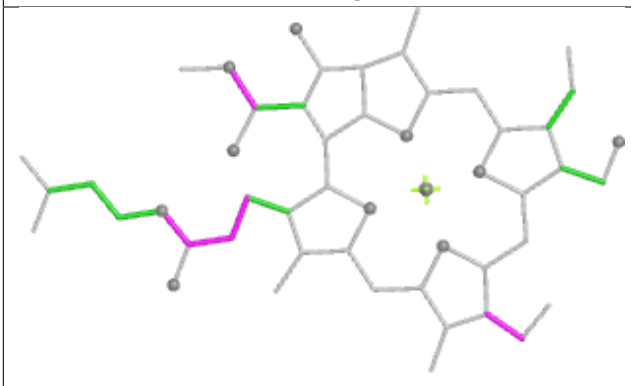
Ligand CHL 3 305



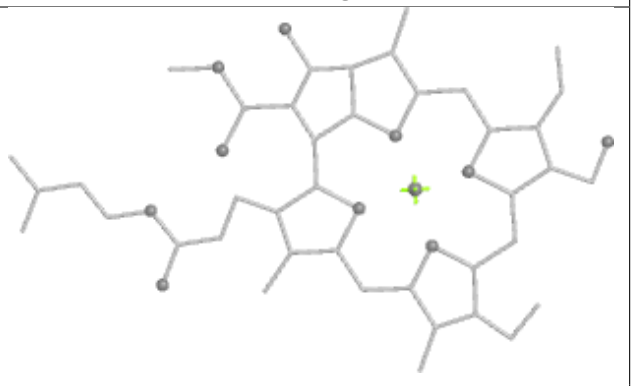
Bond lengths



Bond angles

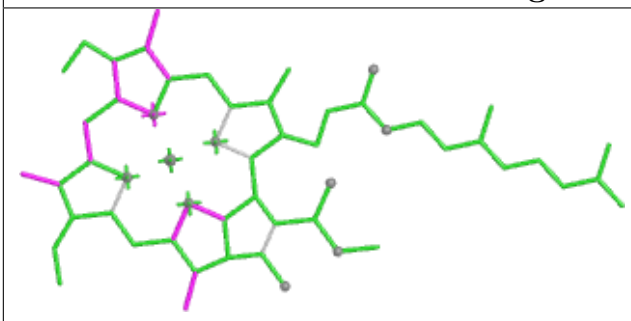


Torsions

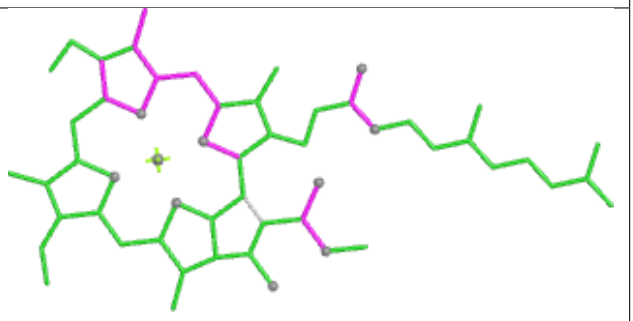


Rings

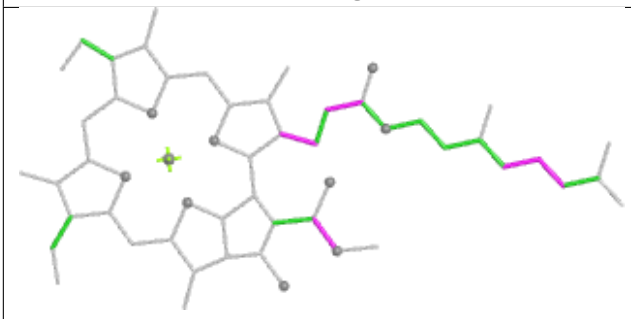
Ligand CLA 3 303



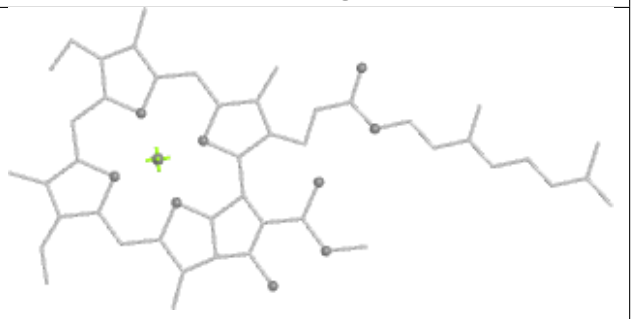
Bond lengths



Bond angles

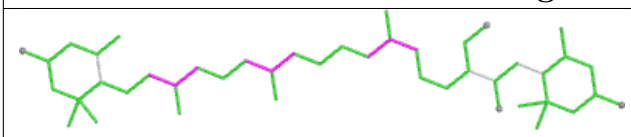


Torsions

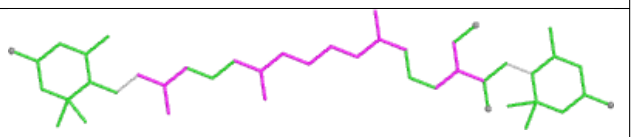


Rings

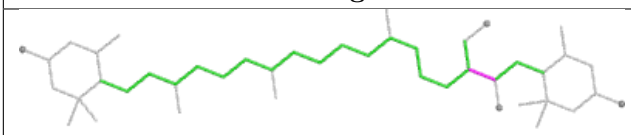
Ligand 0IE d 521



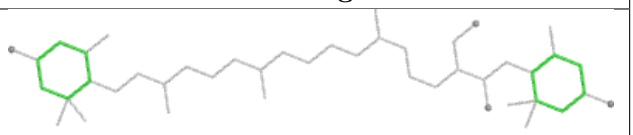
Bond lengths



Bond angles

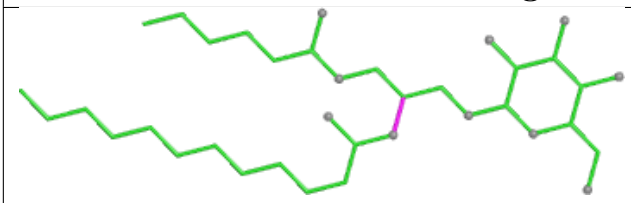


Torsions

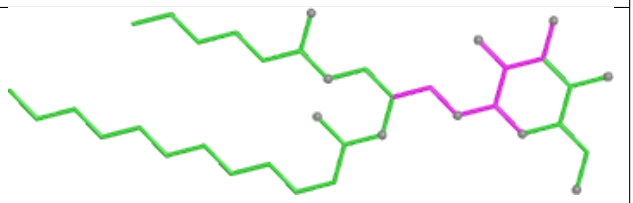


Rings

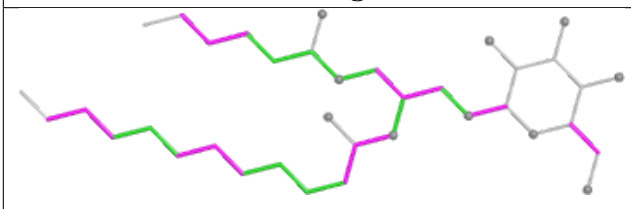
Ligand LMG L 211



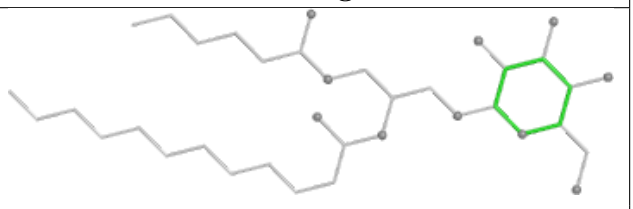
Bond lengths



Bond angles

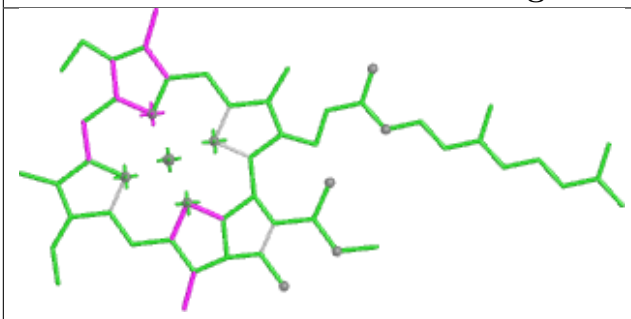


Torsions

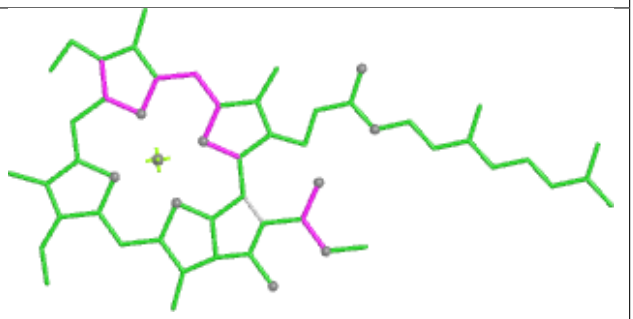


Rings

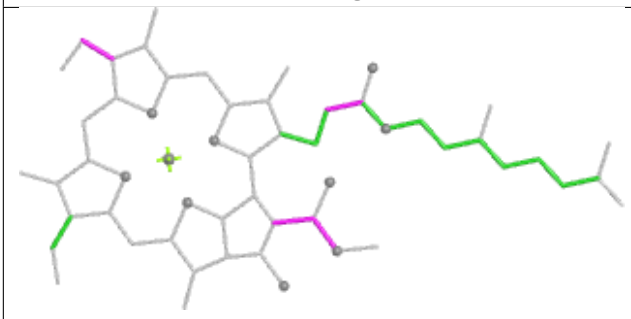
Ligand CLA b 603



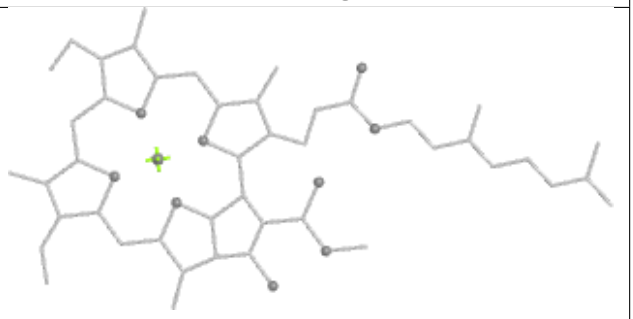
Bond lengths



Bond angles

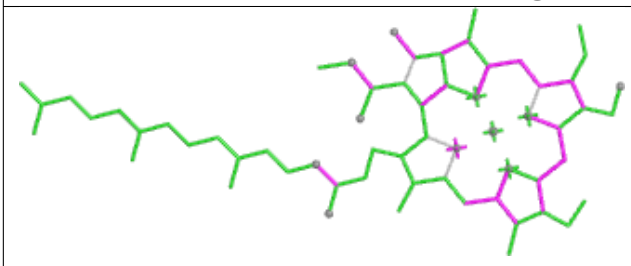


Torsions

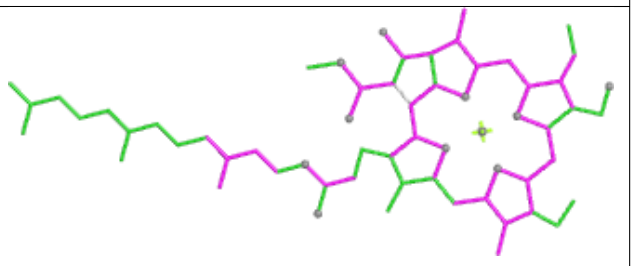


Rings

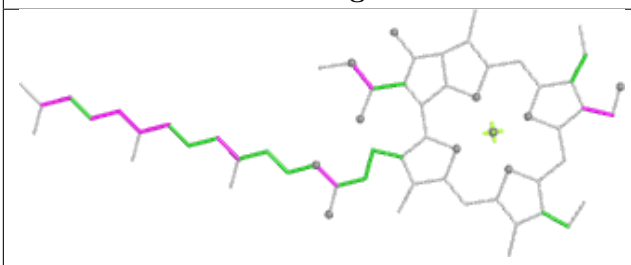
Ligand CHL e 609



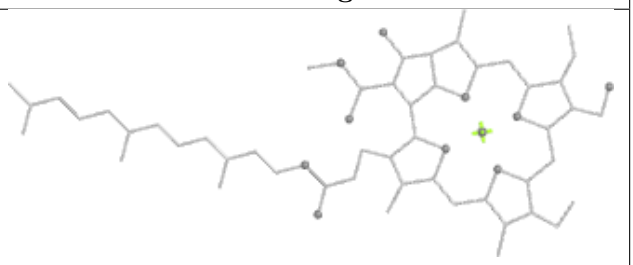
Bond lengths



Bond angles

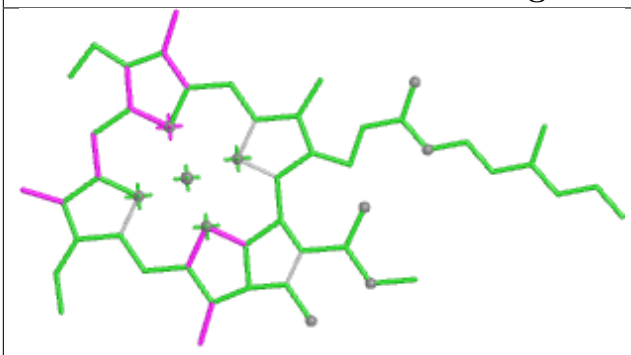


Torsions

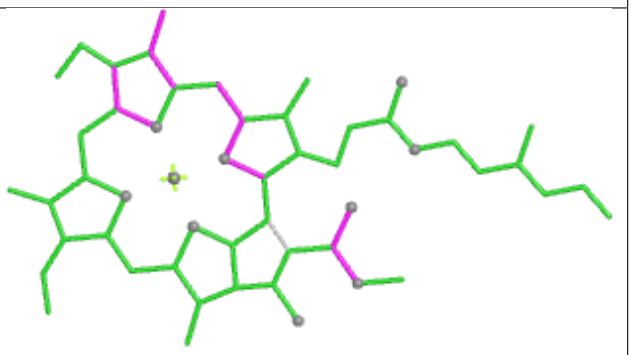


Rings

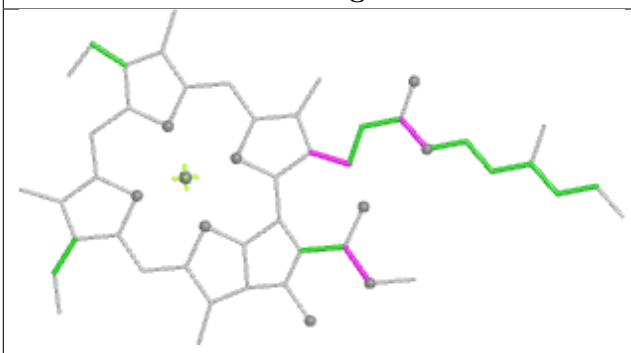
Ligand CLA 1 311



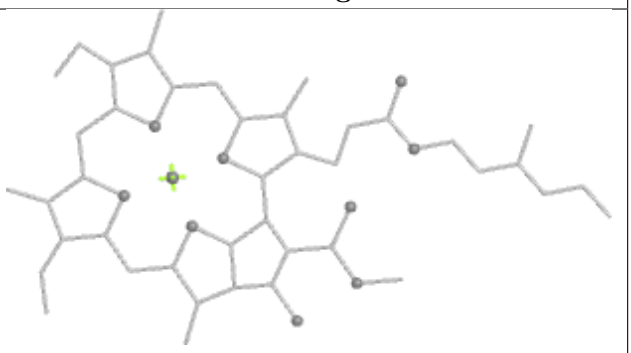
Bond lengths



Bond angles

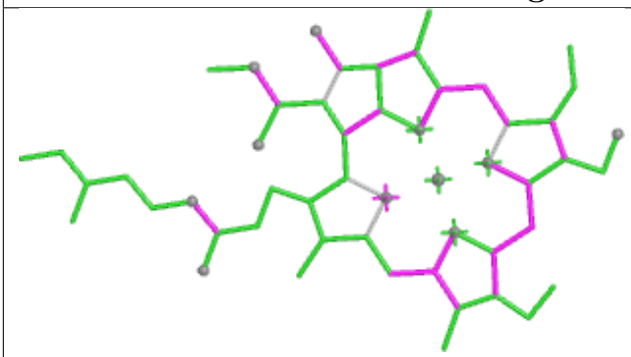


Torsions

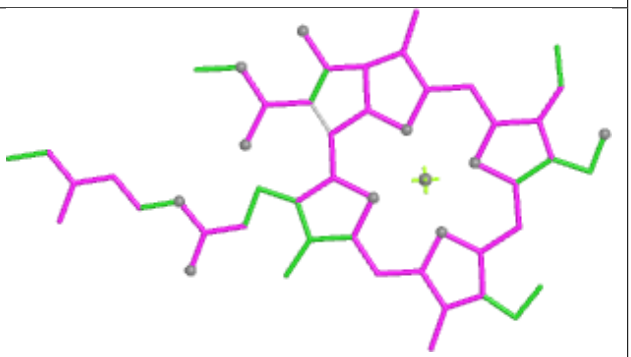


Rings

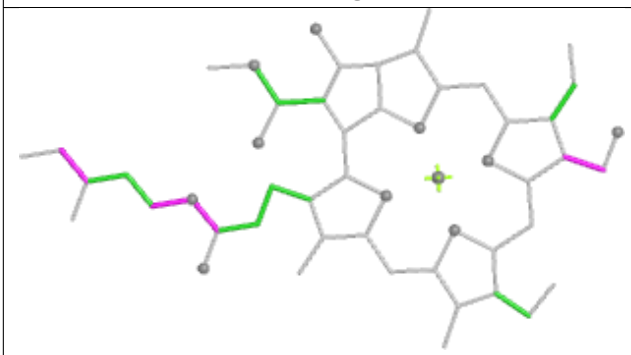
Ligand CHL 6 313



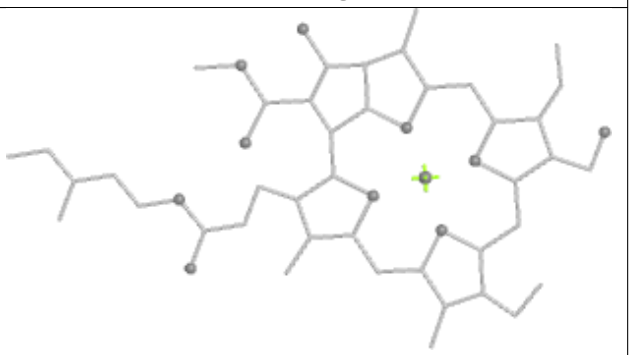
Bond lengths



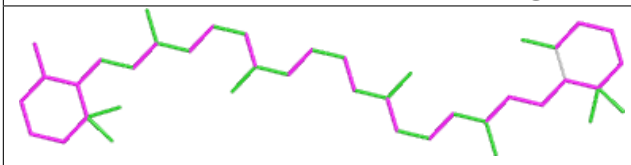
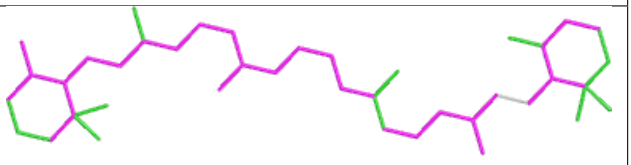
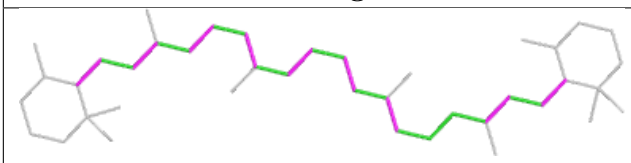
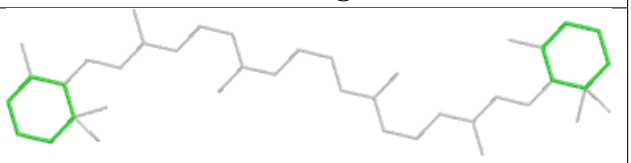
Bond angles

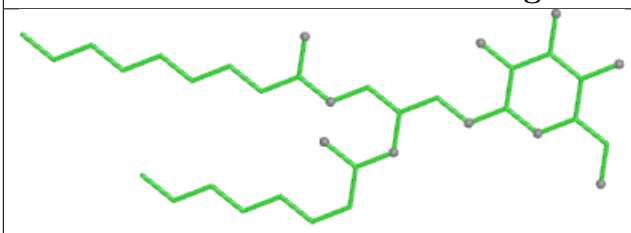
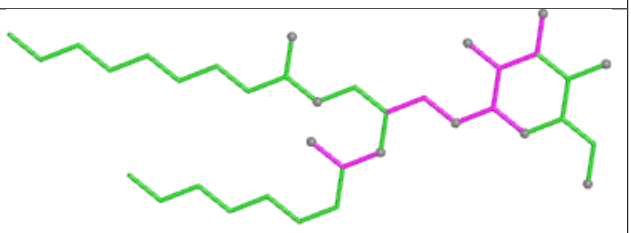
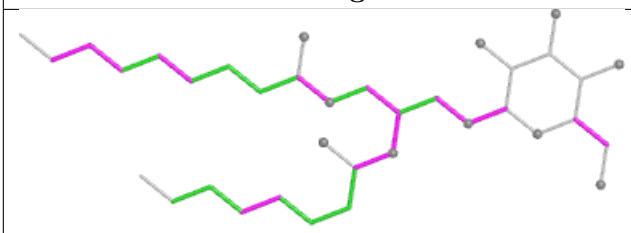
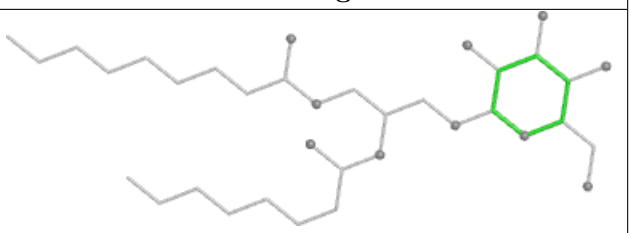


Torsions

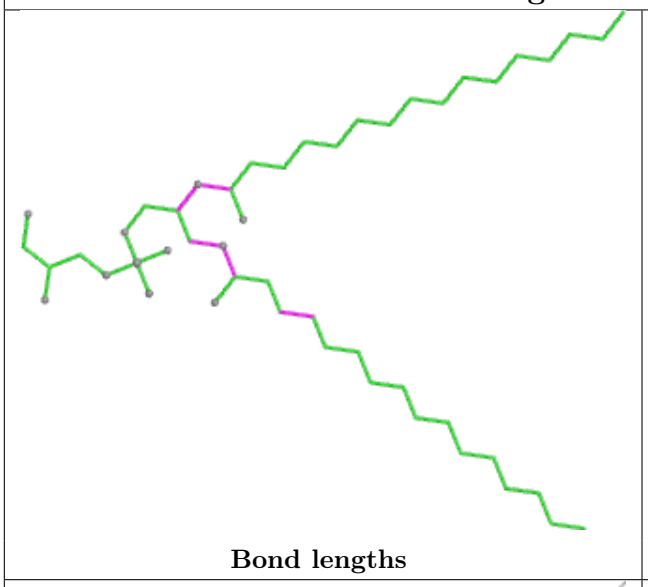


Rings

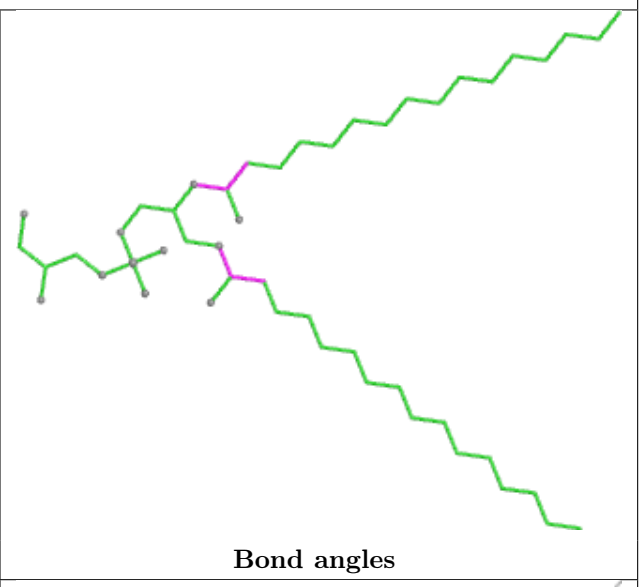
Ligand 8CT B 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG 3 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

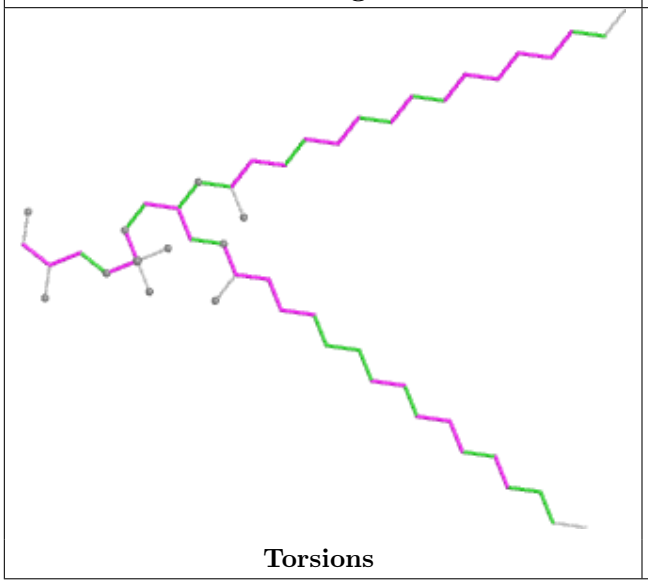
Ligand LHG 0 601



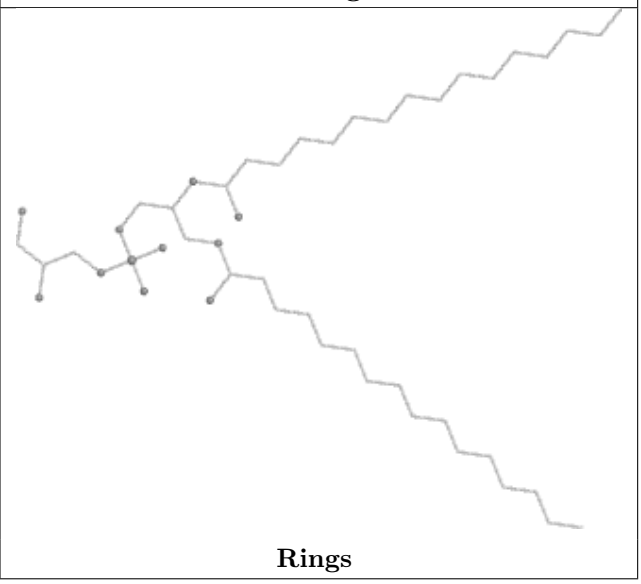
Bond lengths



Bond angles

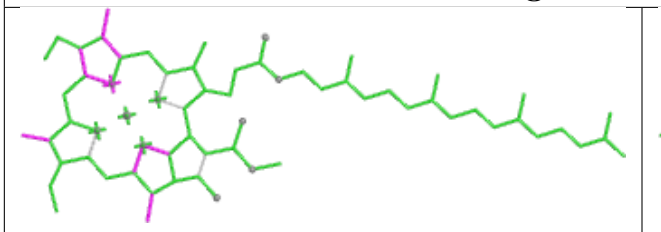


Torsions

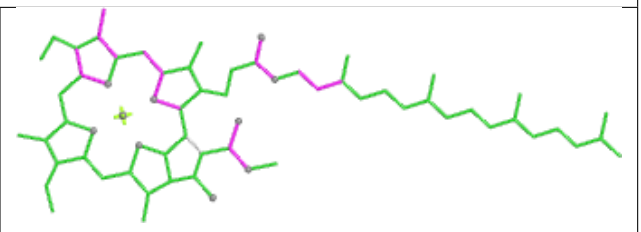


Rings

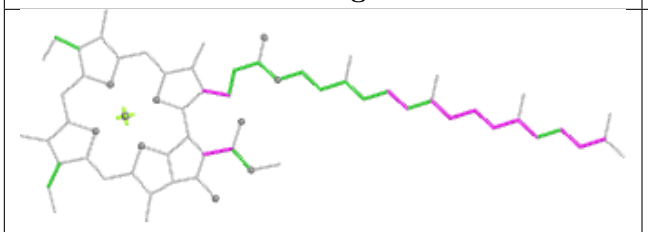
Ligand CLA B 827



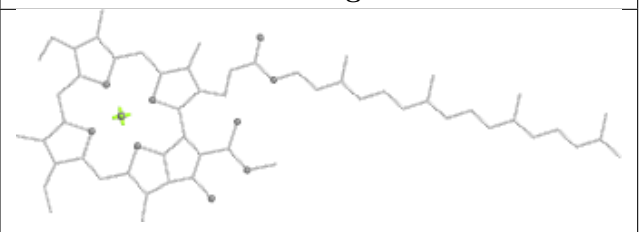
Bond lengths



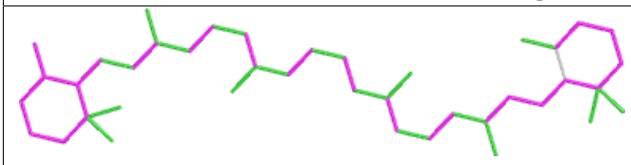
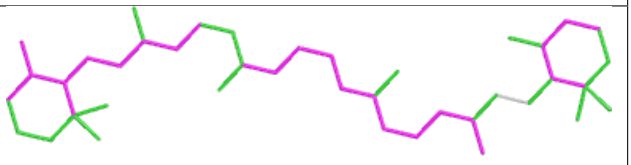
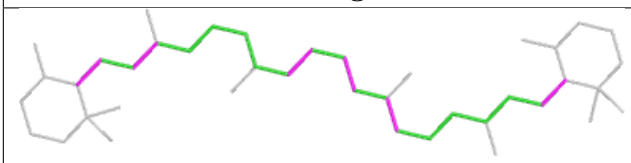
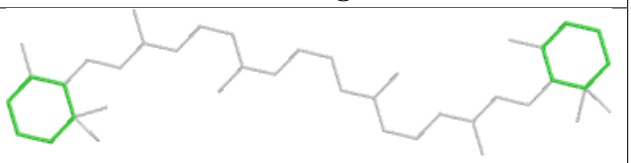
Bond angles

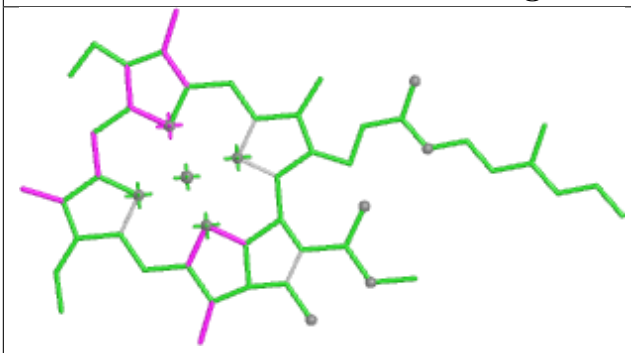
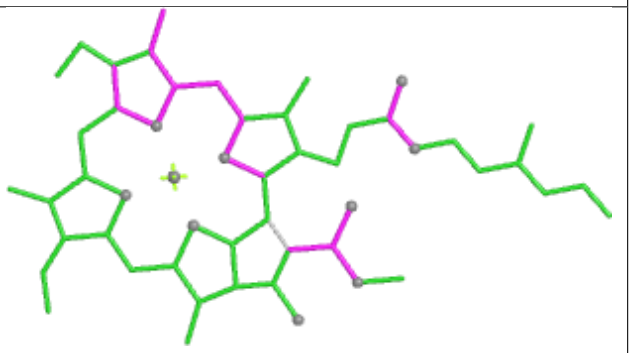
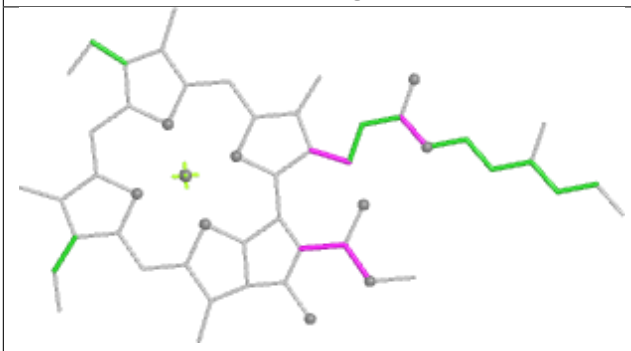
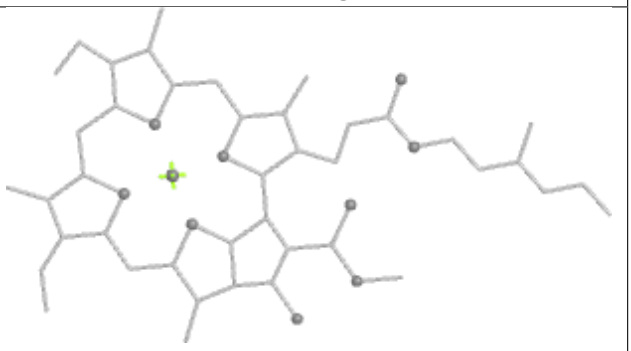


Torsions

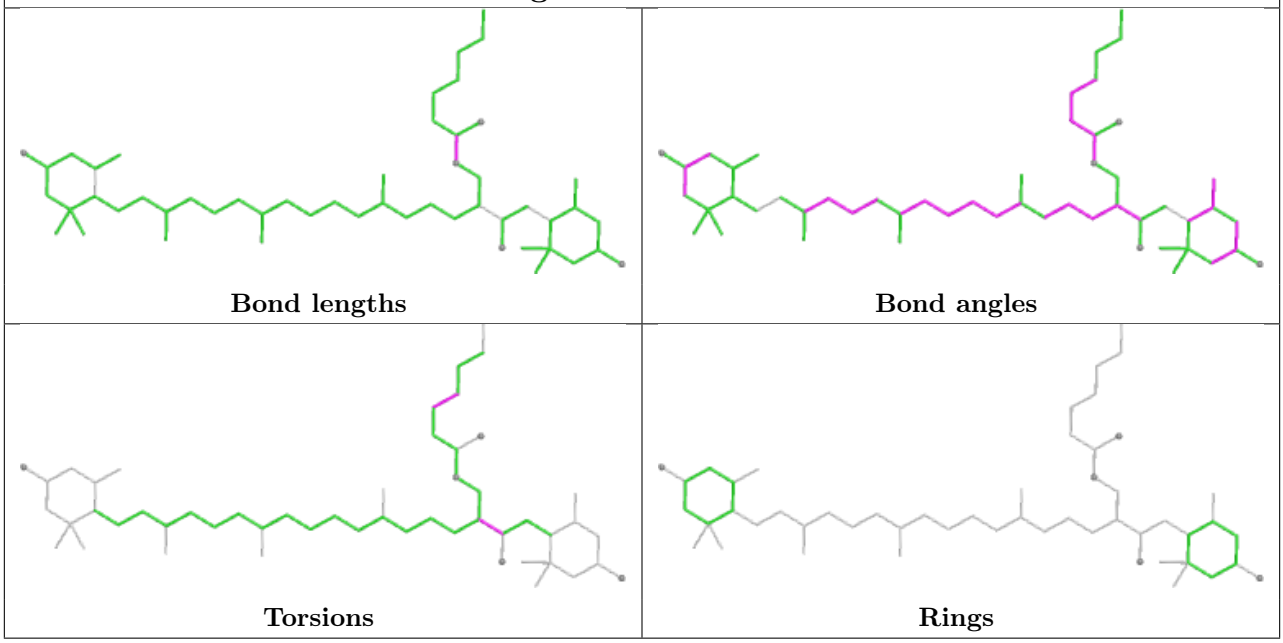


Rings

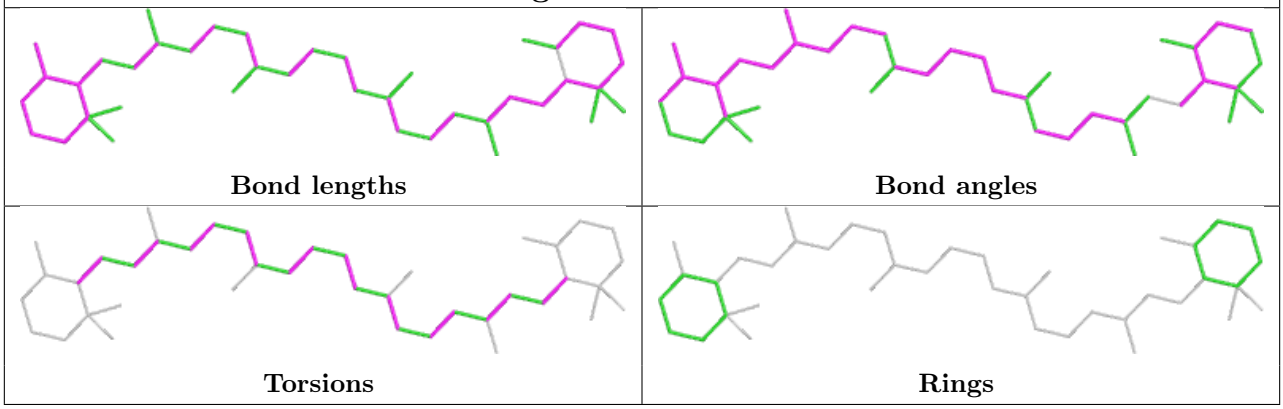
Ligand 8CT 3 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

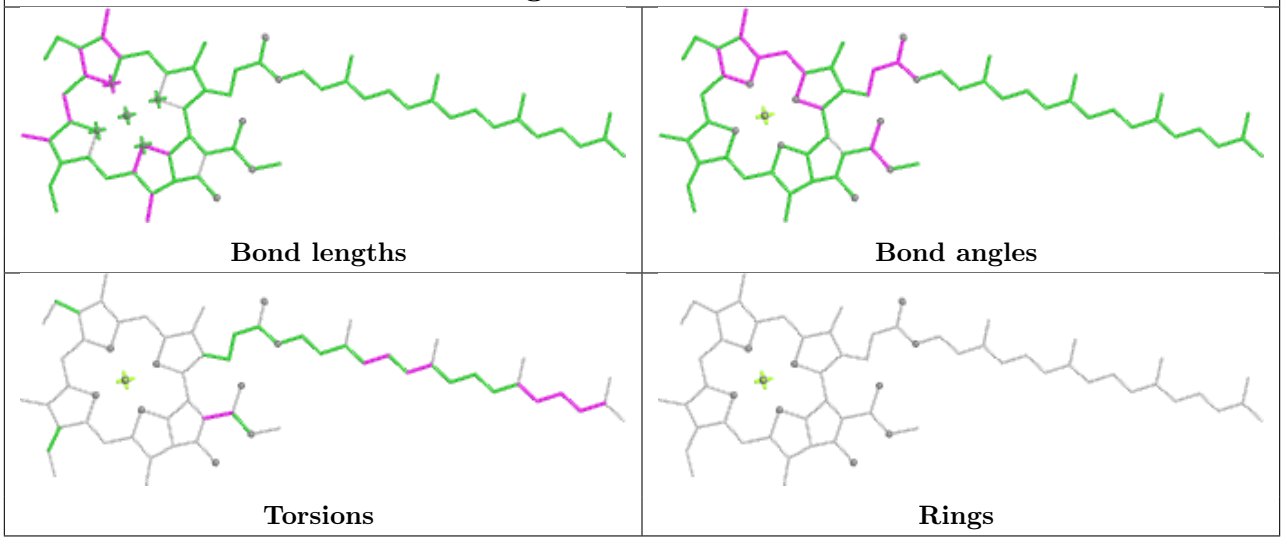
Ligand 0UR 0 501



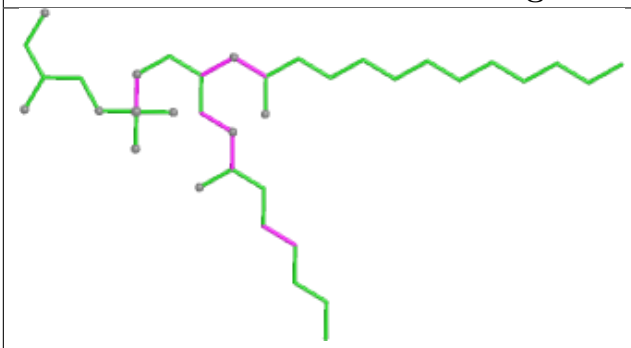
Ligand 8CT 7 402



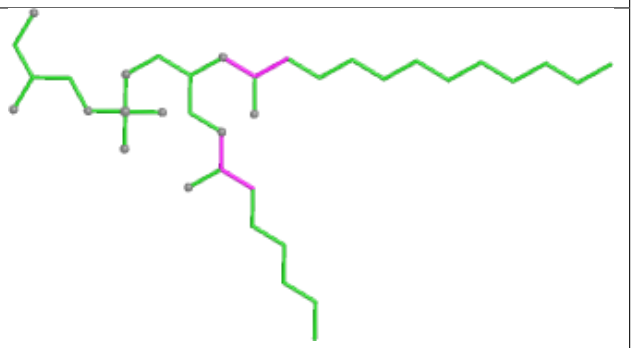
Ligand CLA B 832



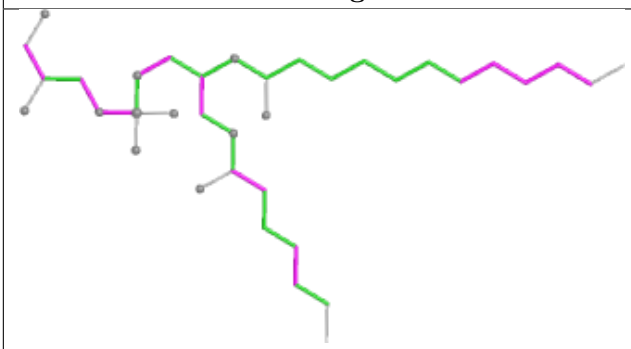
Ligand LHG 3 601



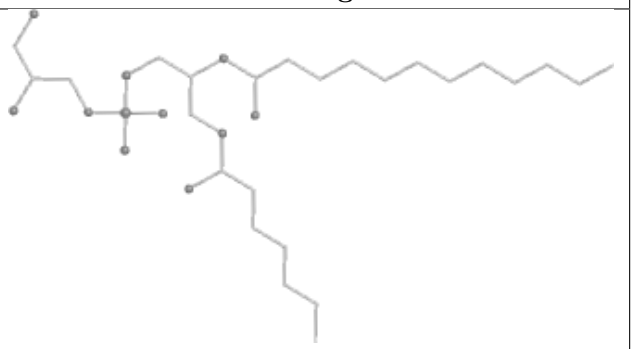
Bond lengths



Bond angles

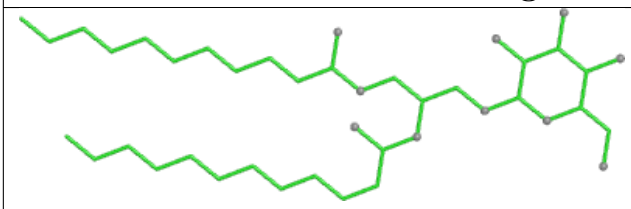


Torsions

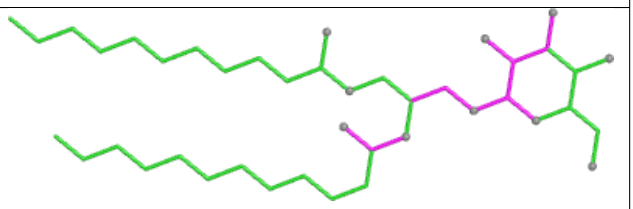


Rings

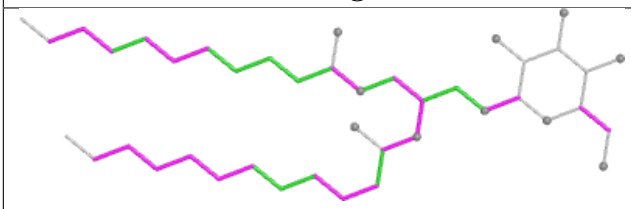
Ligand LMG B 853



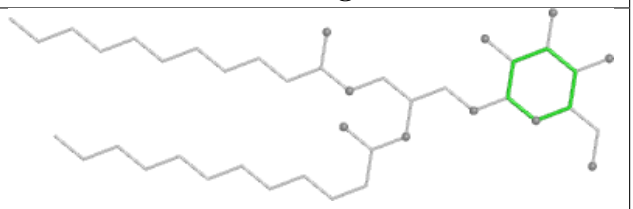
Bond lengths



Bond angles

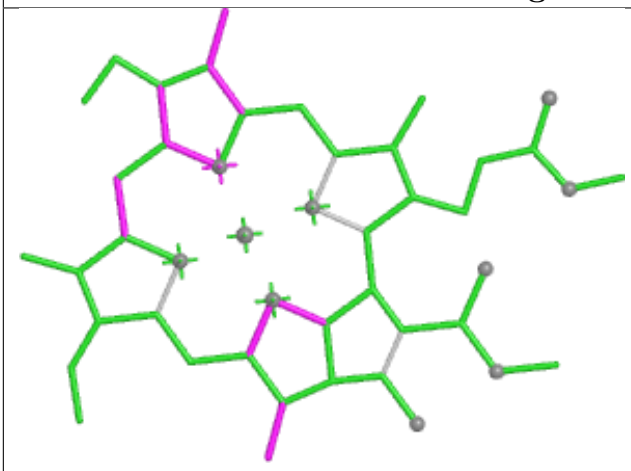


Torsions

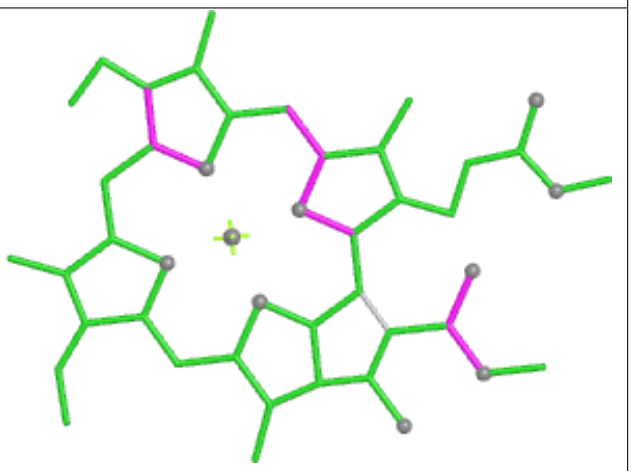


Rings

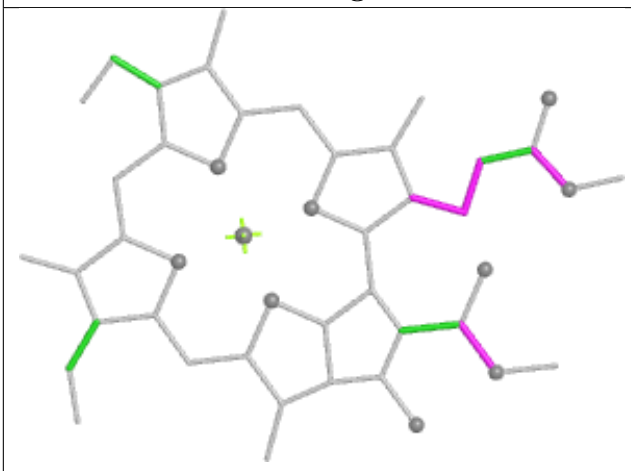
Ligand CLA 5 308



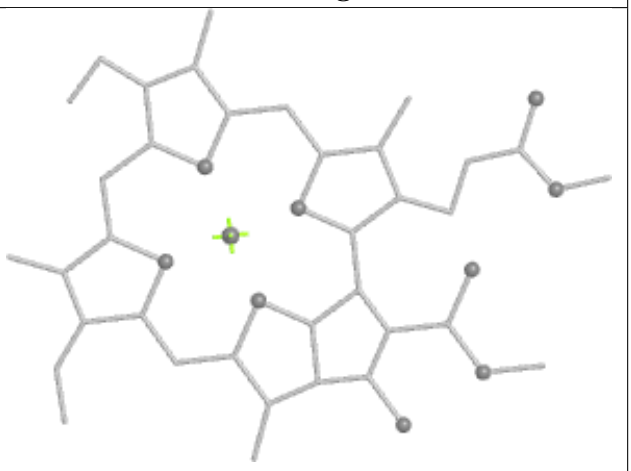
Bond lengths



Bond angles



Torsions

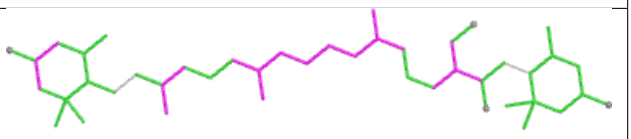


Rings

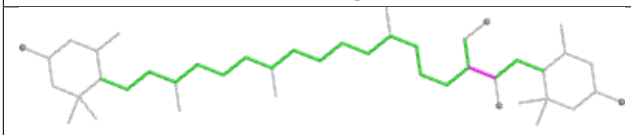
Ligand 0IE c 521



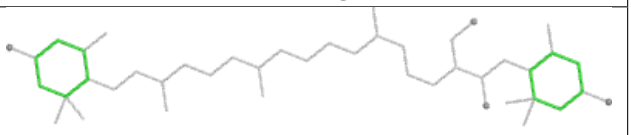
Bond lengths



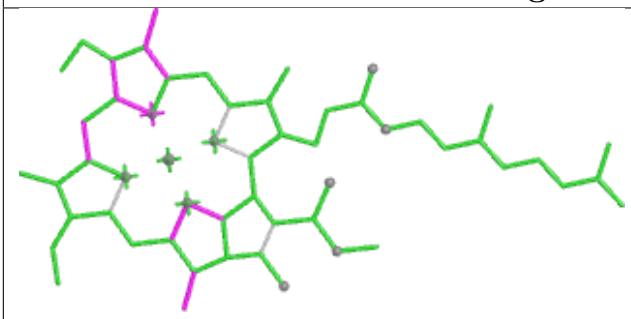
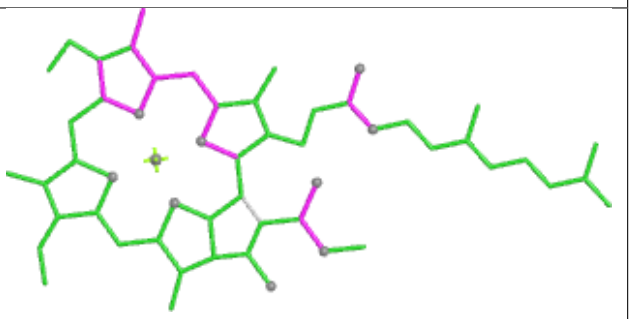
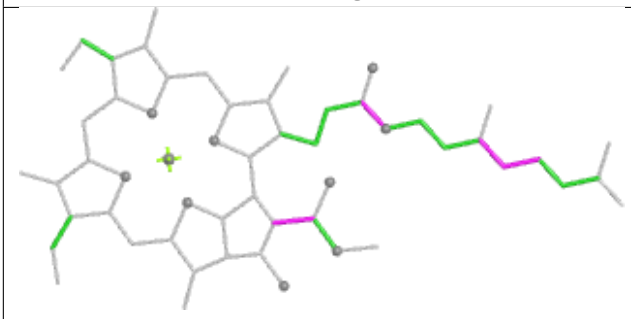
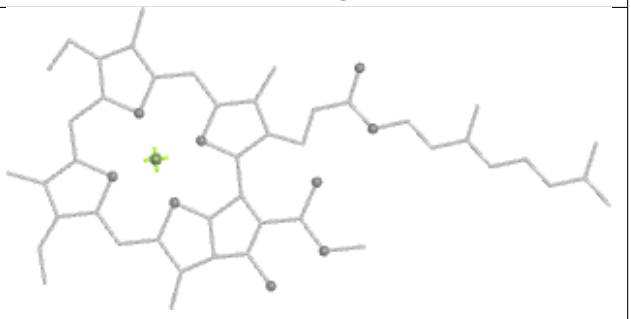
Bond angles

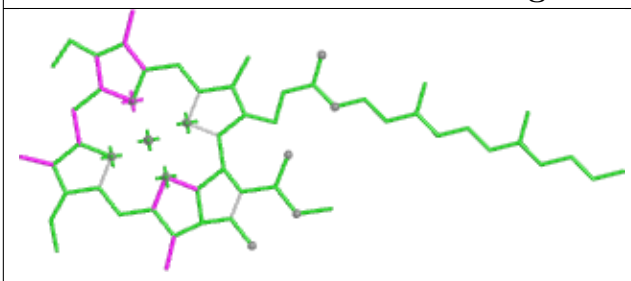
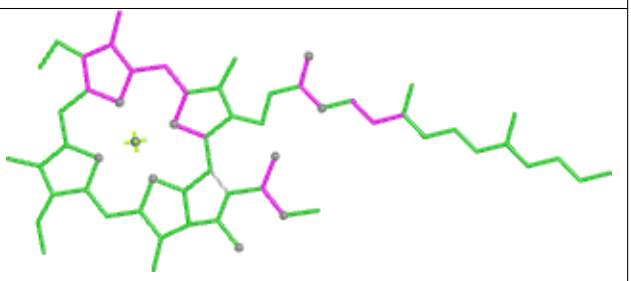
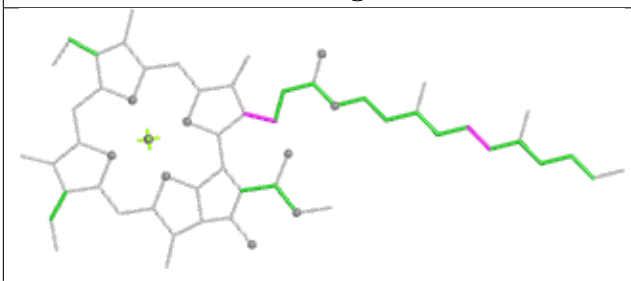
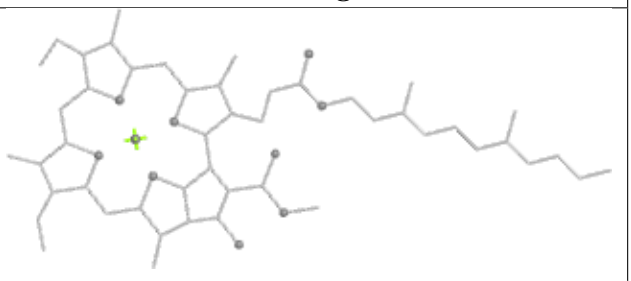


Torsions

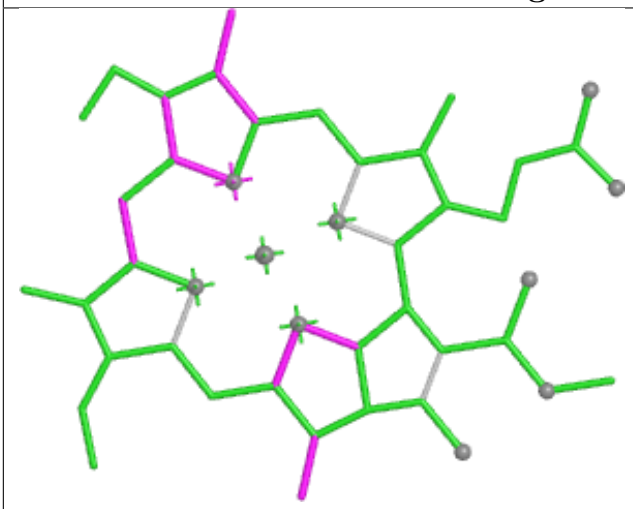


Rings

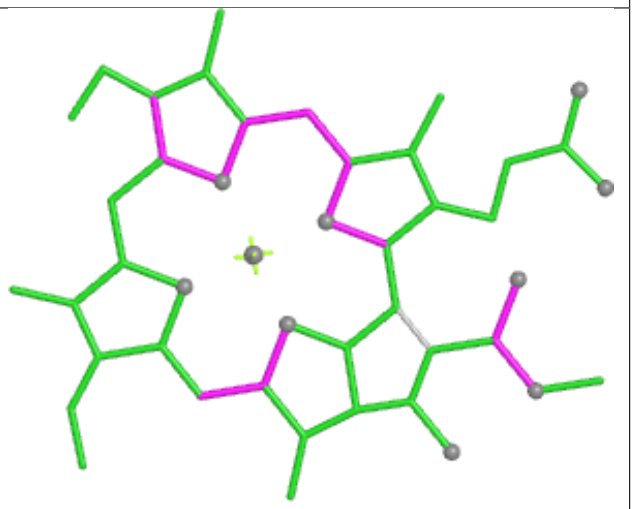
Ligand CLA 7 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

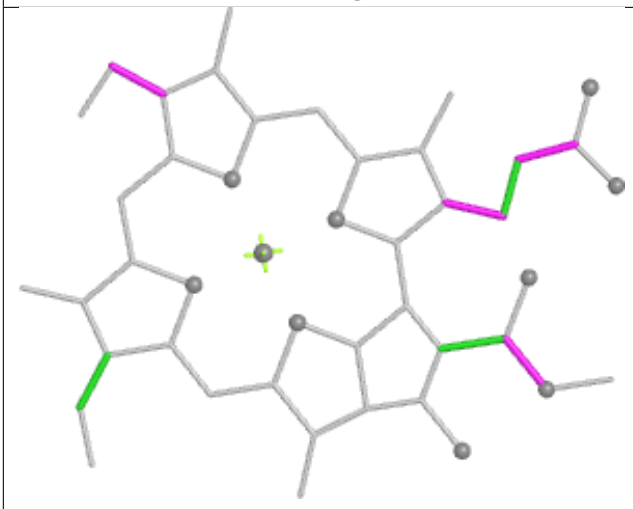
Ligand CLA 3 313



Bond lengths



Bond angles

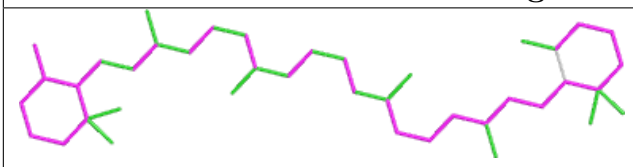


Torsions

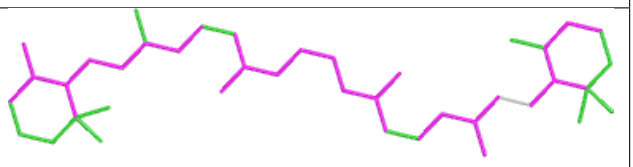


Rings

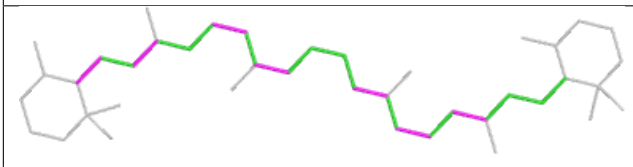
Ligand 8CT B 844



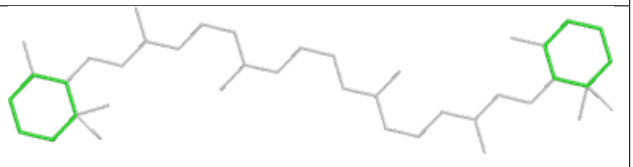
Bond lengths



Bond angles

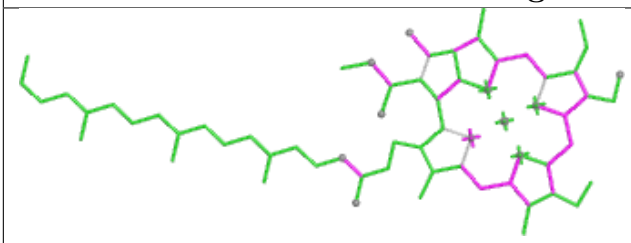


Torsions

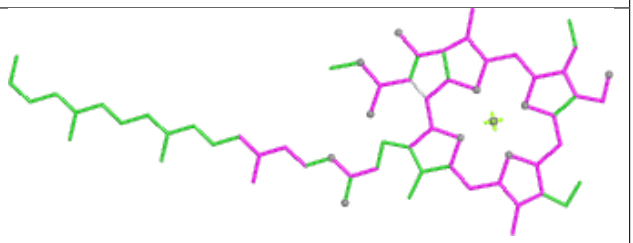


Rings

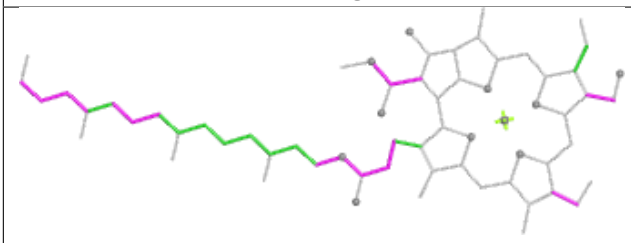
Ligand CHL 8 302



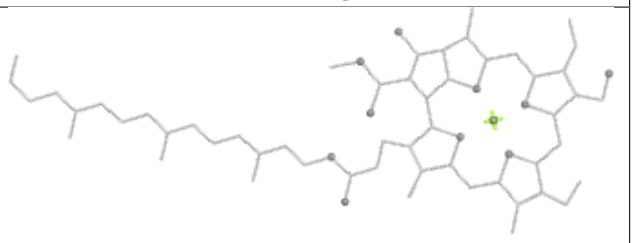
Bond lengths



Bond angles

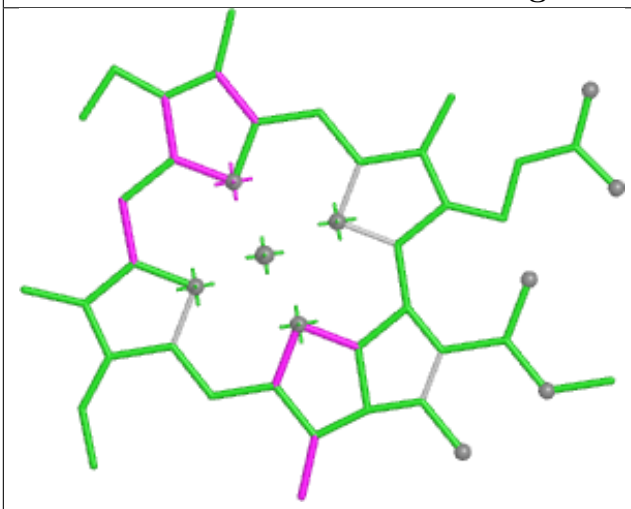


Torsions

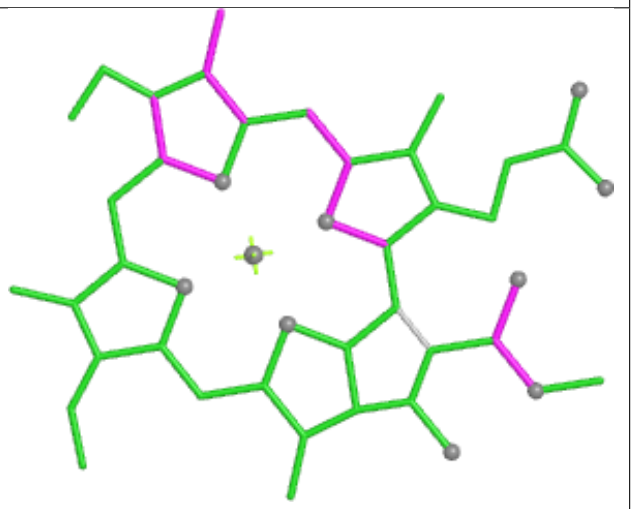


Rings

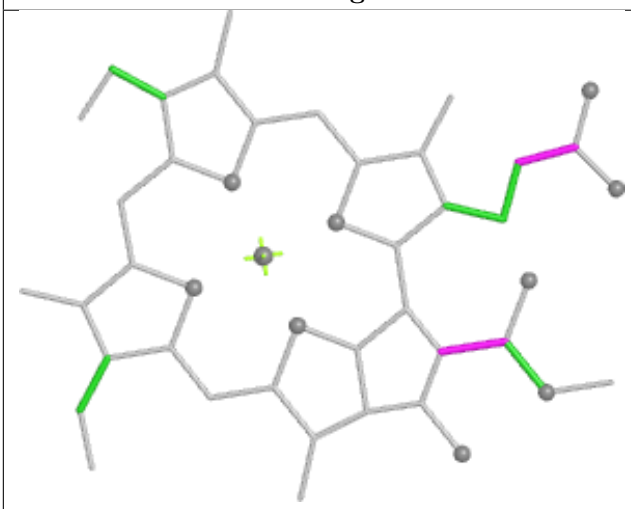
Ligand CLA e 612



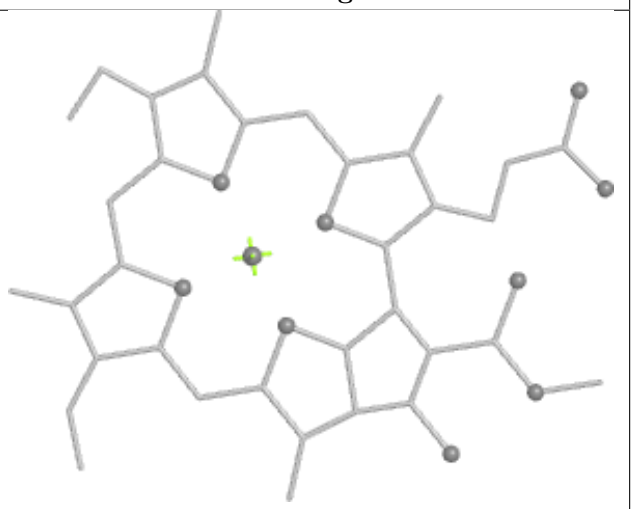
Bond lengths



Bond angles

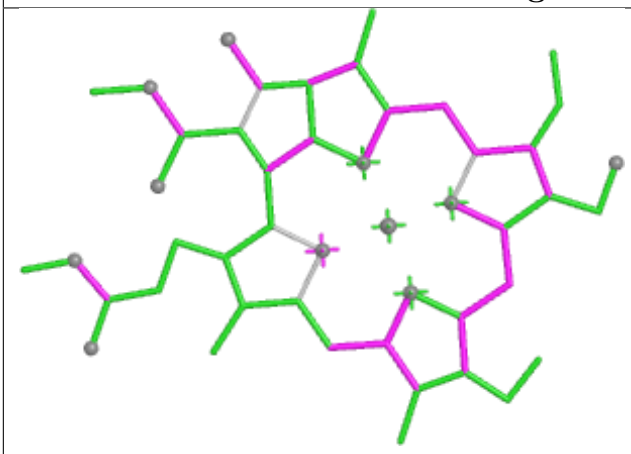


Torsions

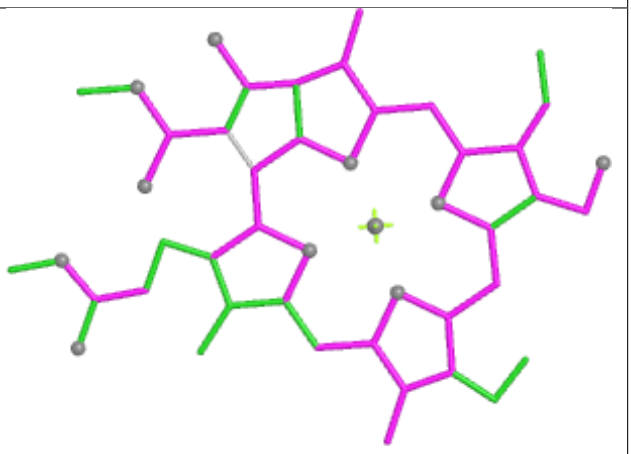


Rings

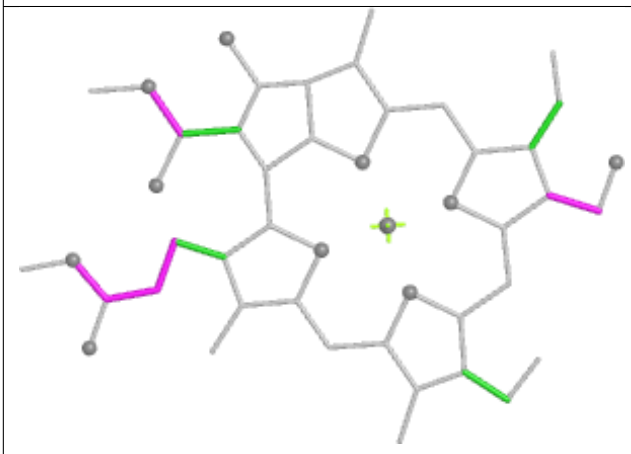
Ligand CHL 5 307



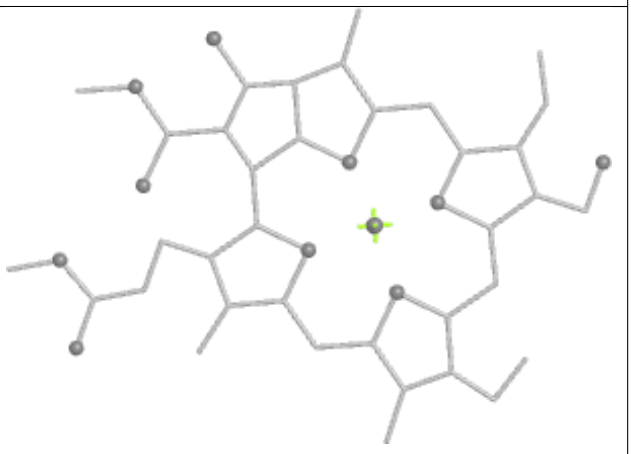
Bond lengths



Bond angles

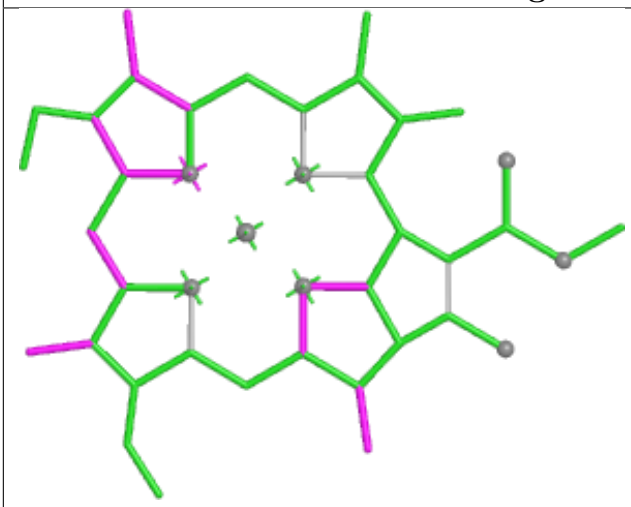


Torsions

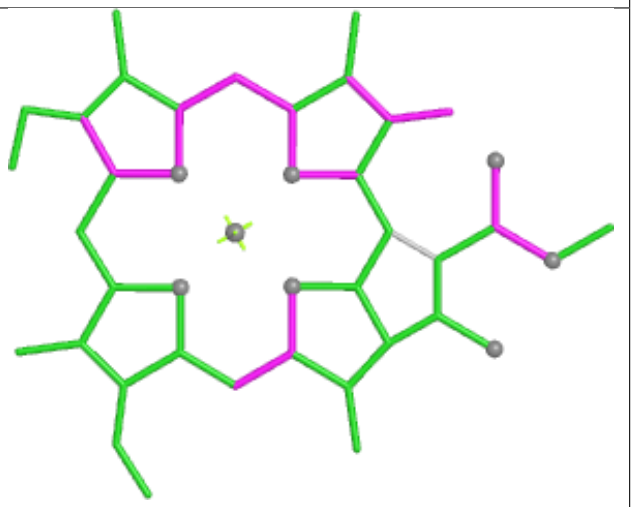


Rings

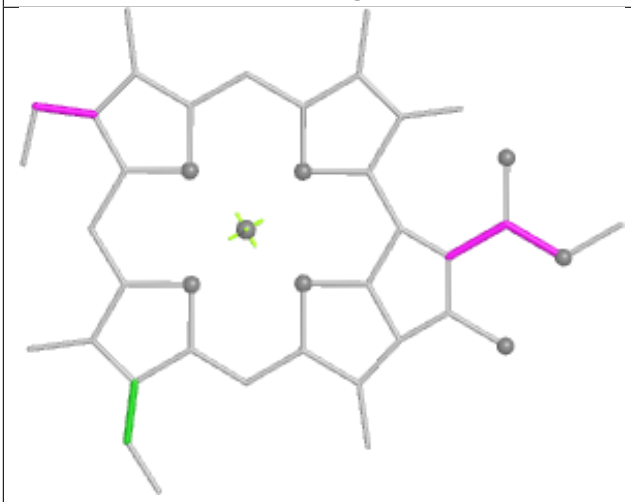
Ligand CLA 9 310



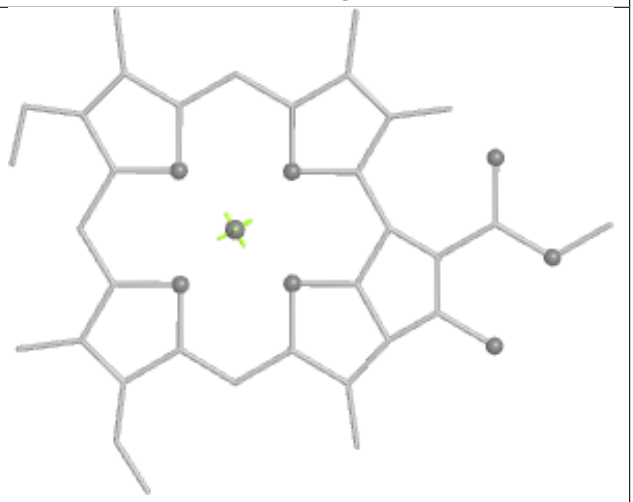
Bond lengths



Bond angles

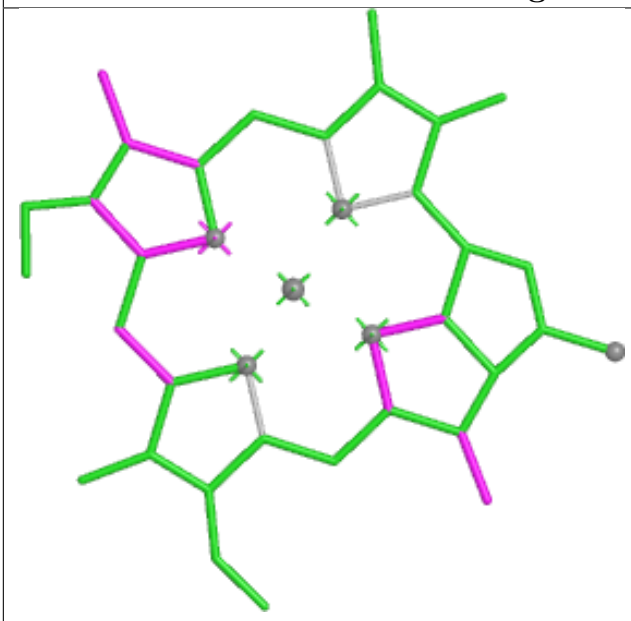


Torsions

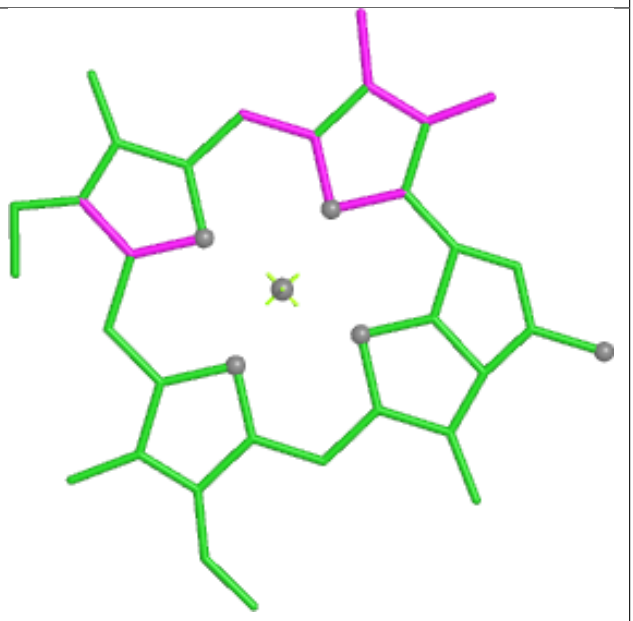


Rings

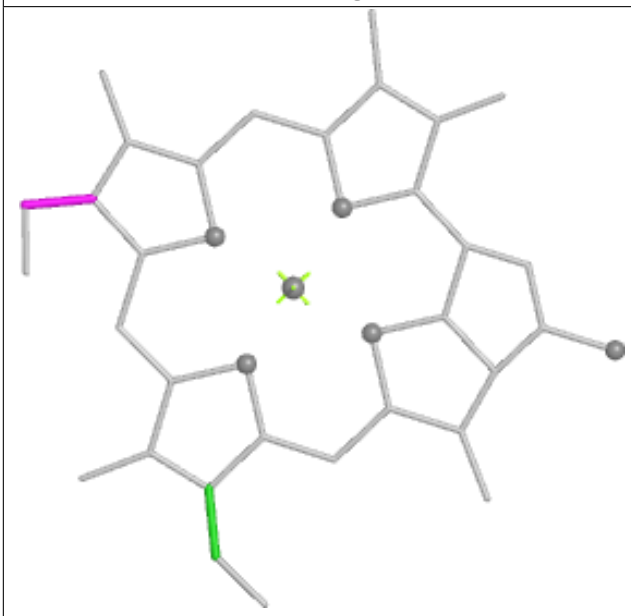
Ligand CLA 7 310



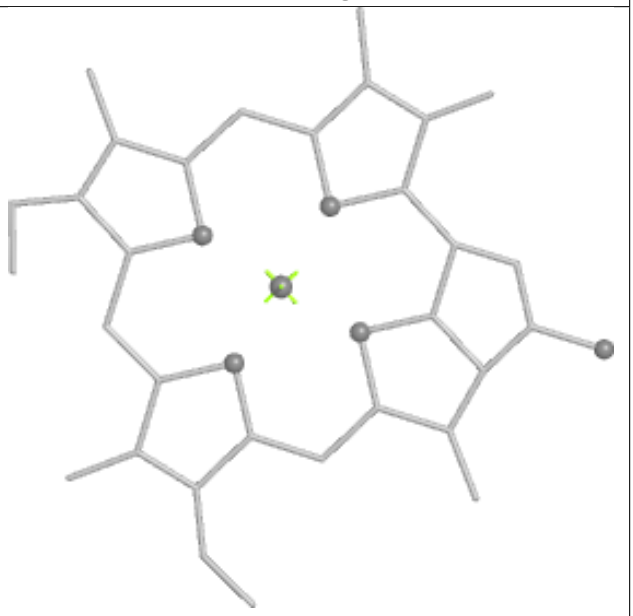
Bond lengths



Bond angles

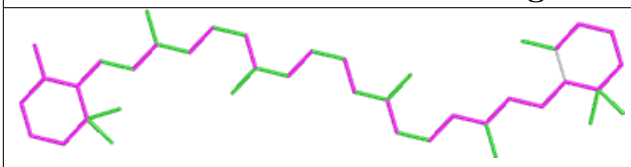


Torsions

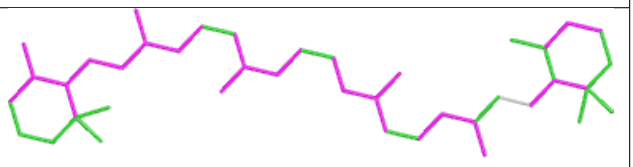


Rings

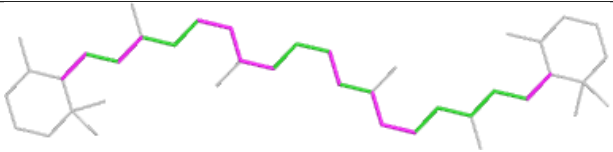
Ligand 8CT B 843



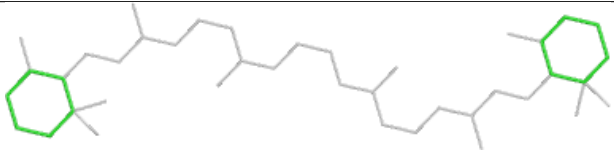
Bond lengths



Bond angles

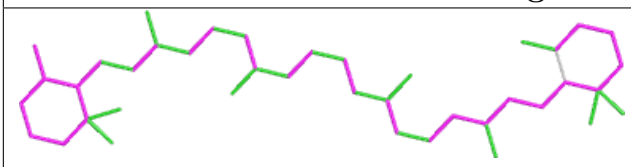


Torsions

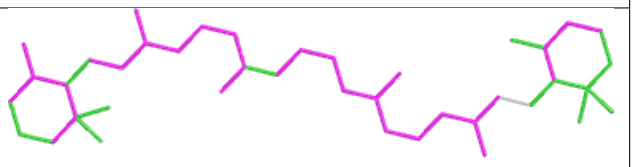


Rings

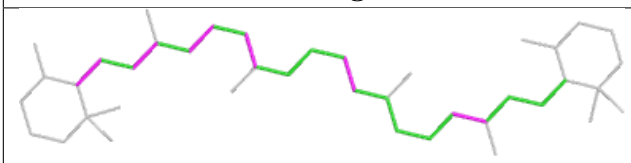
Ligand 8CT B 848



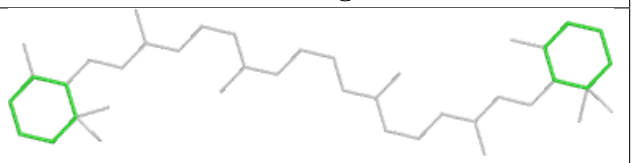
Bond lengths



Bond angles

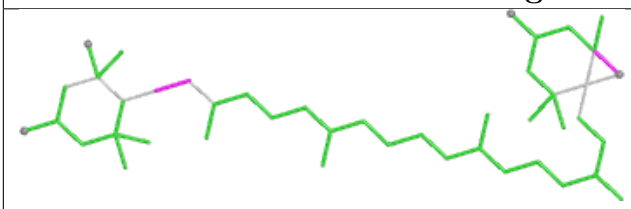


Torsions

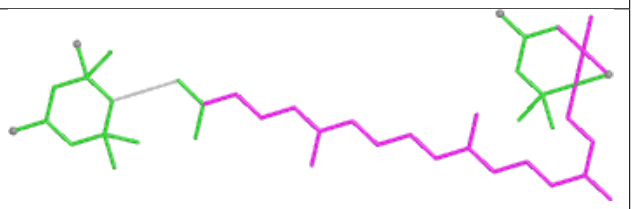


Rings

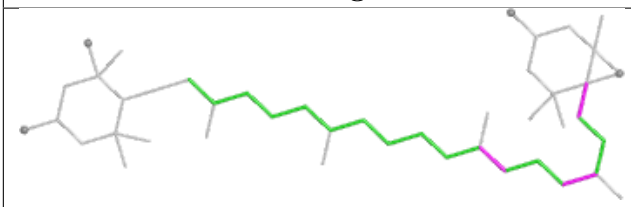
Ligand NEX d 523



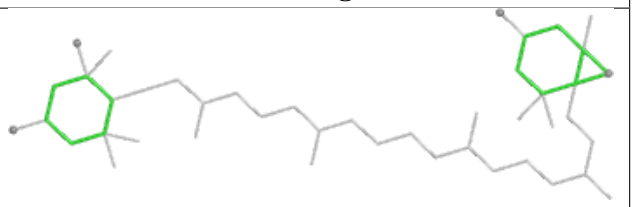
Bond lengths



Bond angles

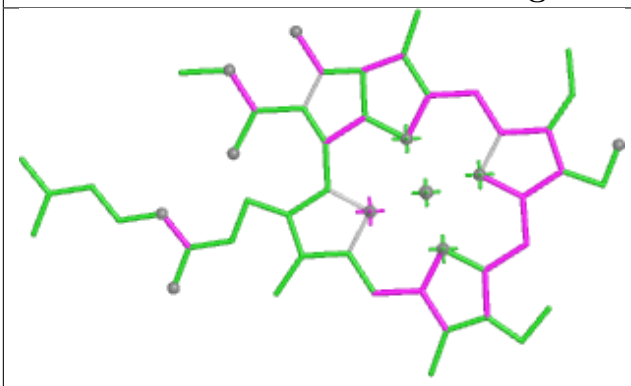


Torsions

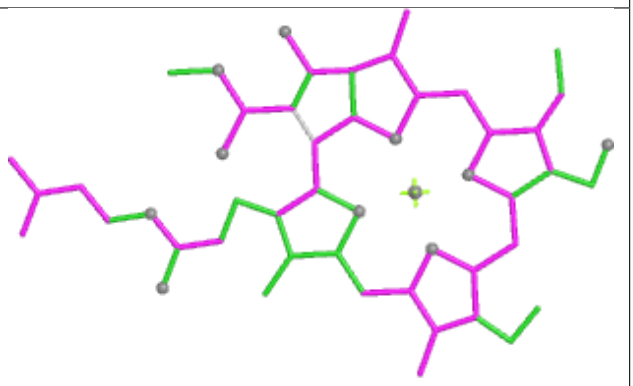


Rings

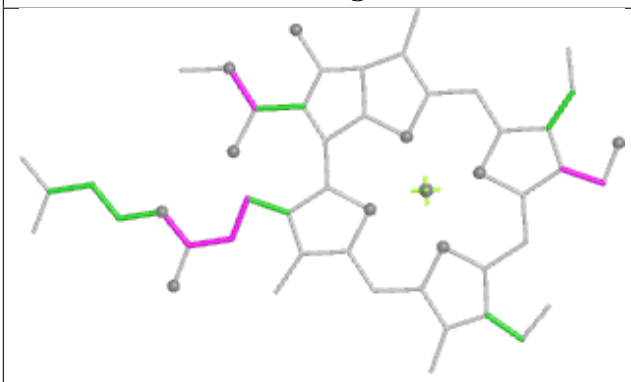
Ligand CHL e 606



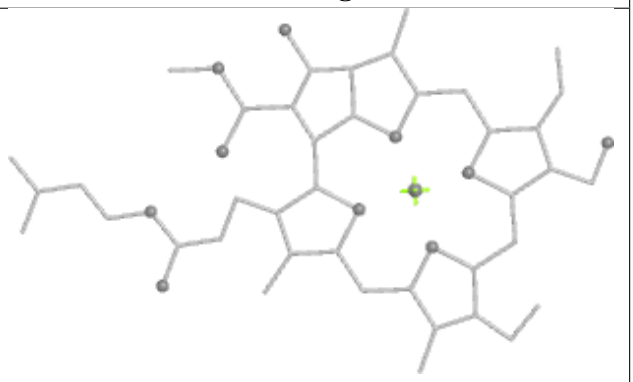
Bond lengths



Bond angles

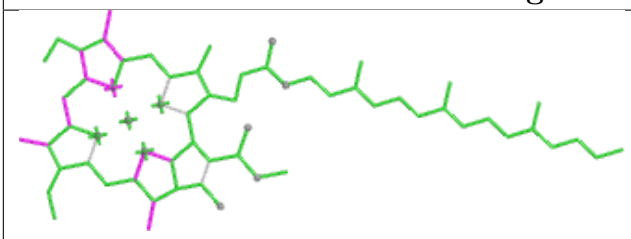


Torsions

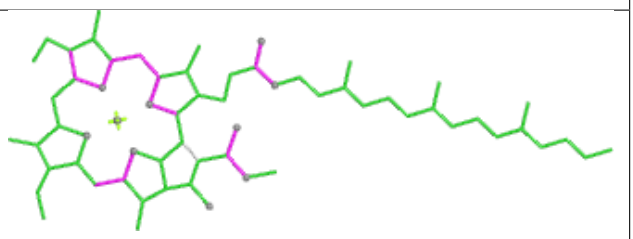


Rings

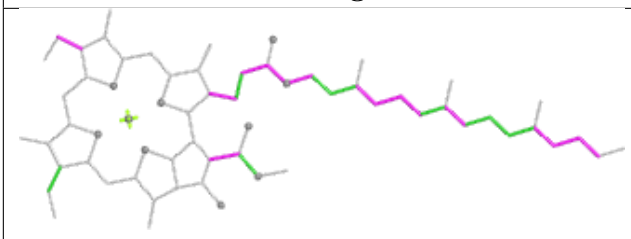
Ligand CLA L 203



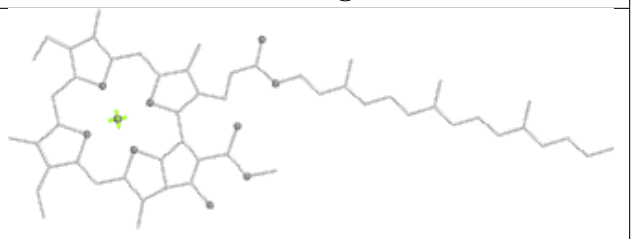
Bond lengths



Bond angles

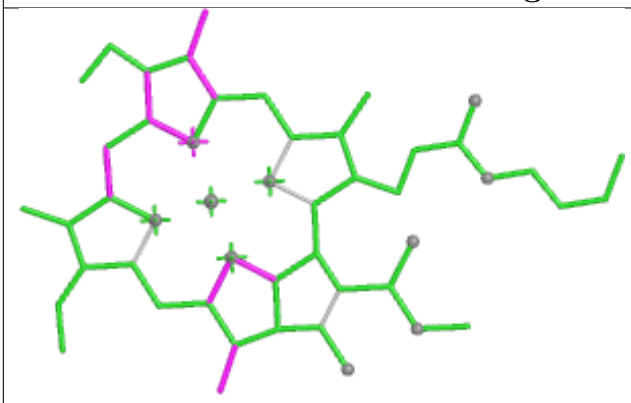


Torsions

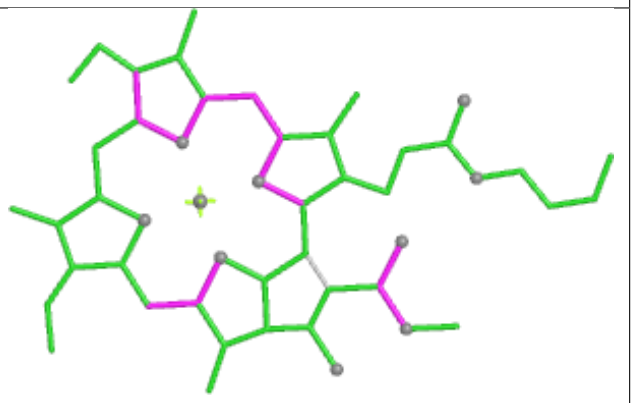


Rings

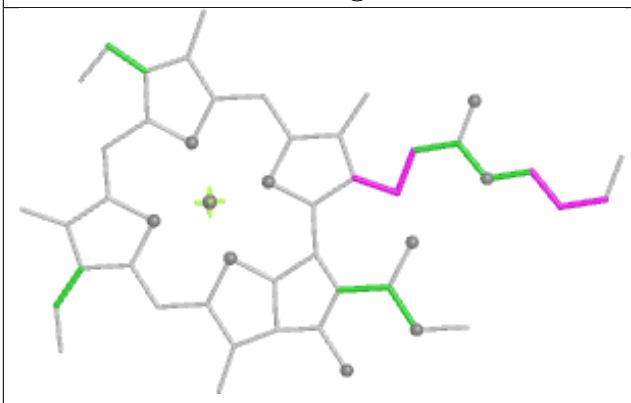
Ligand CLA A 822



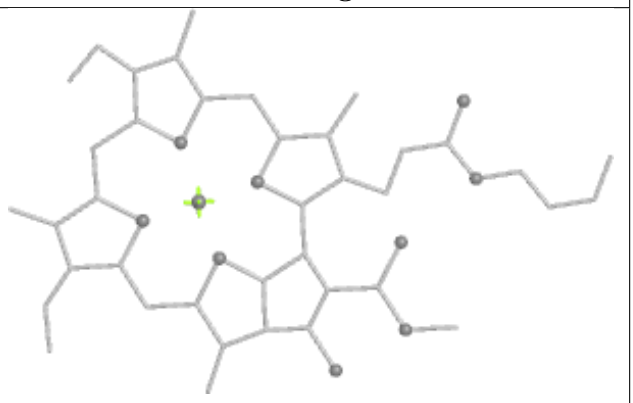
Bond lengths



Bond angles

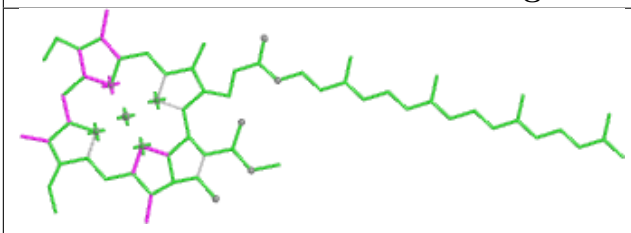


Torsions

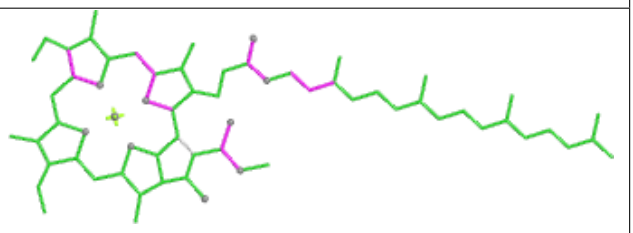


Rings

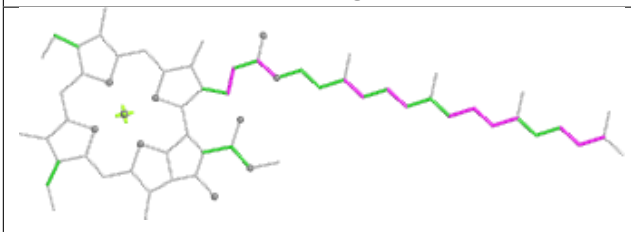
Ligand CLA A 829



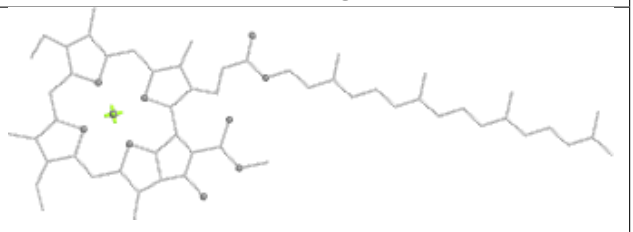
Bond lengths



Bond angles

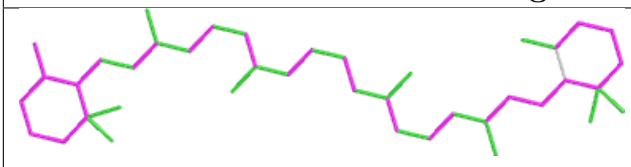


Torsions

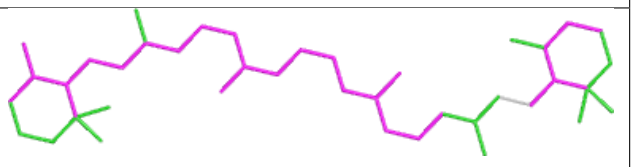


Rings

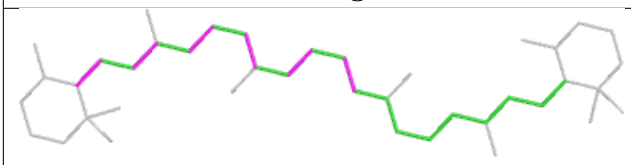
Ligand 8CT L 209



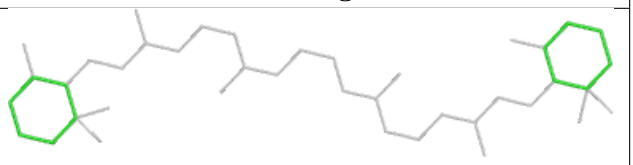
Bond lengths



Bond angles

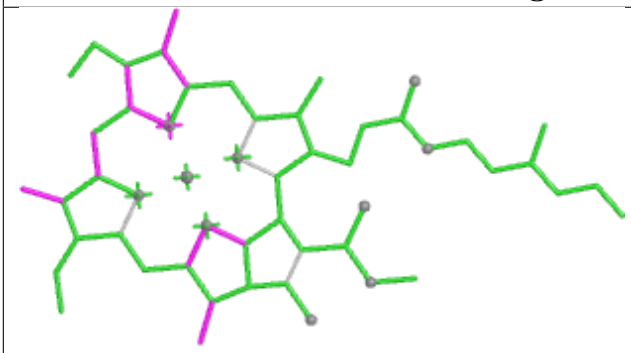


Torsions

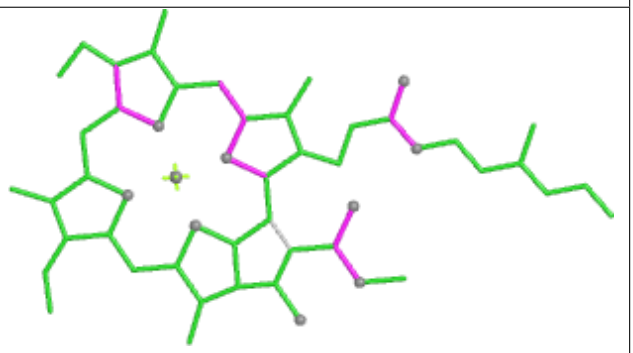


Rings

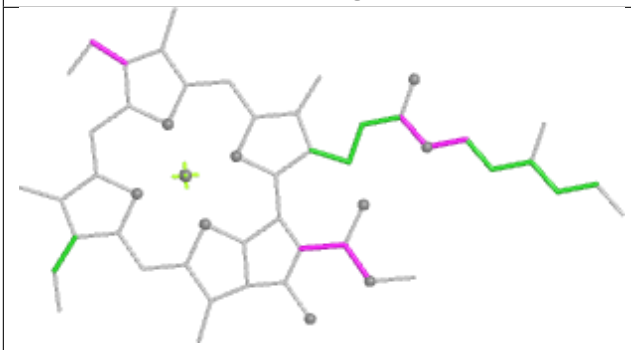
Ligand CLA 7 311



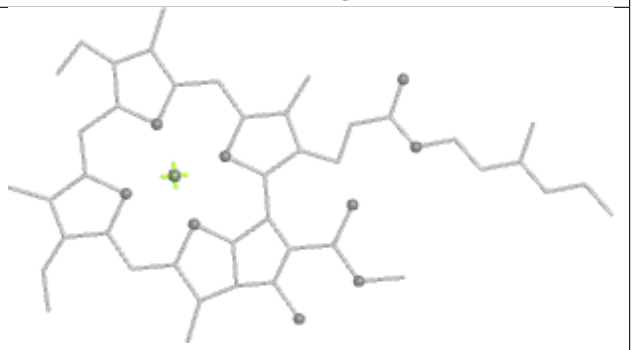
Bond lengths



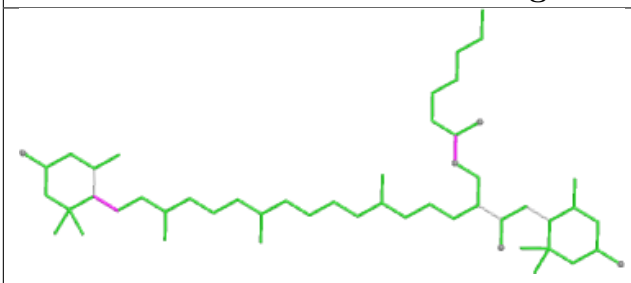
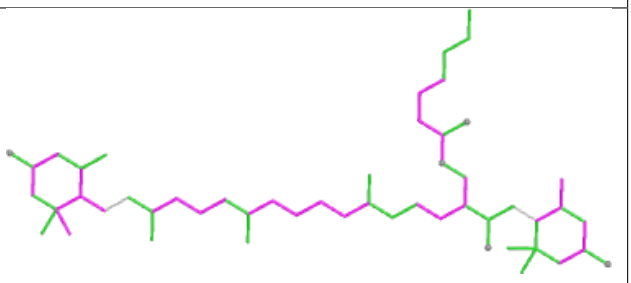
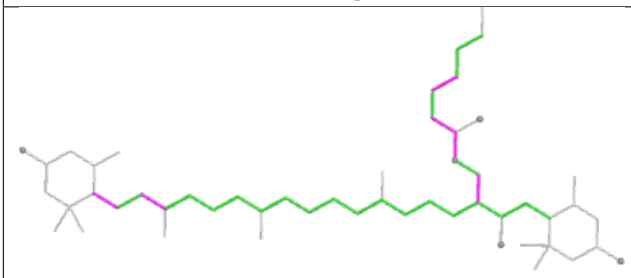
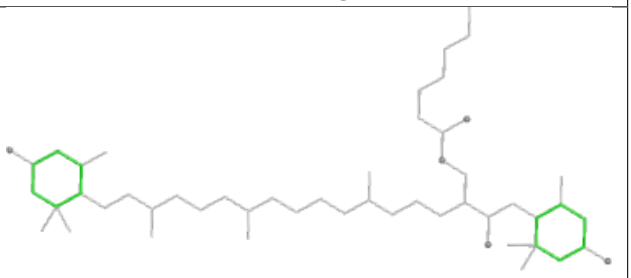
Bond angles

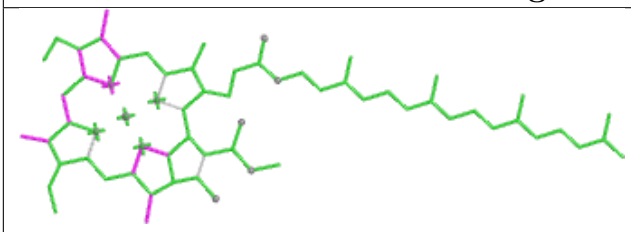
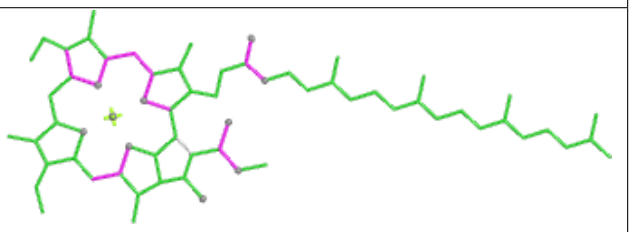
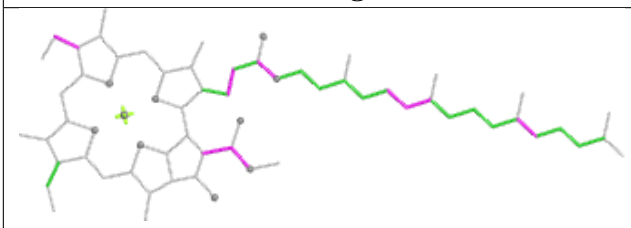
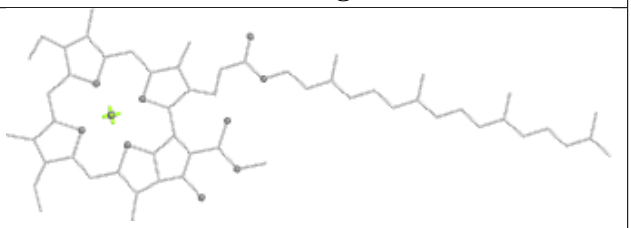


Torsions

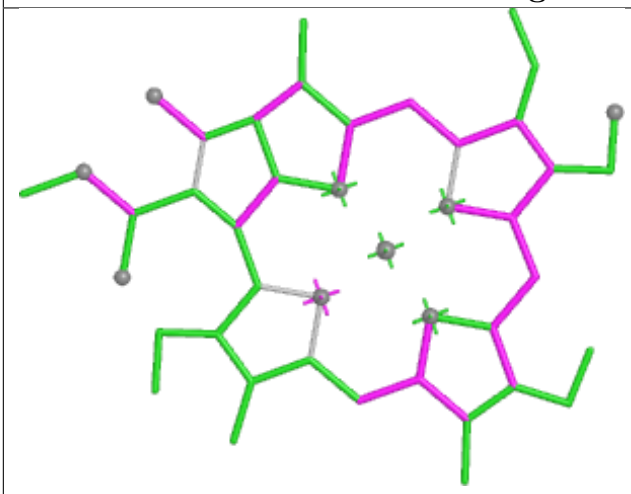


Rings

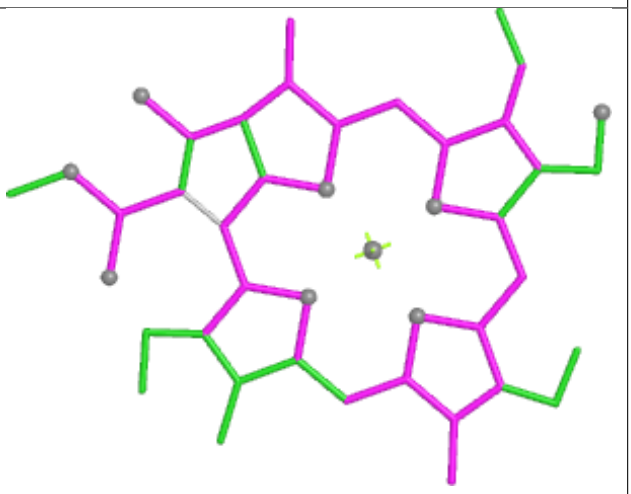
Ligand 0UR 6 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

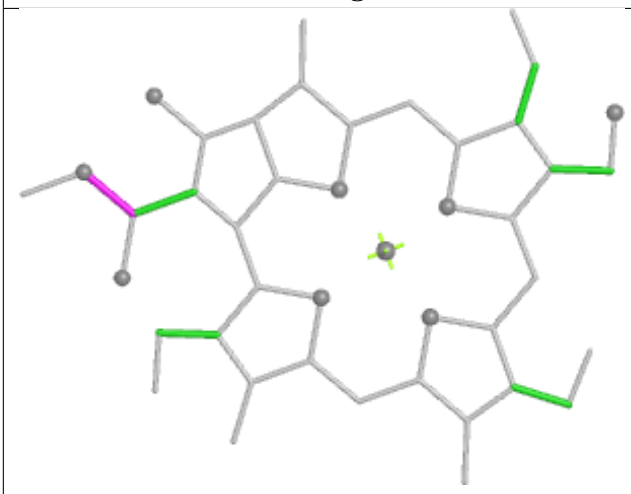
Ligand CHL c 605



Bond lengths



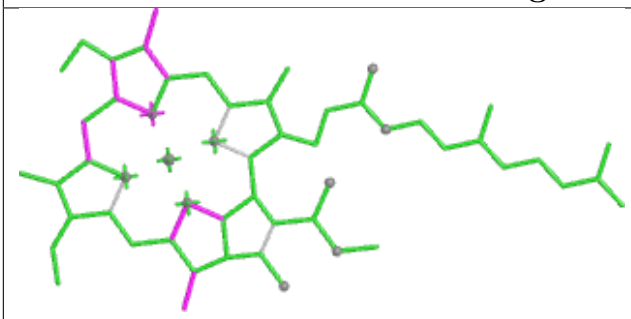
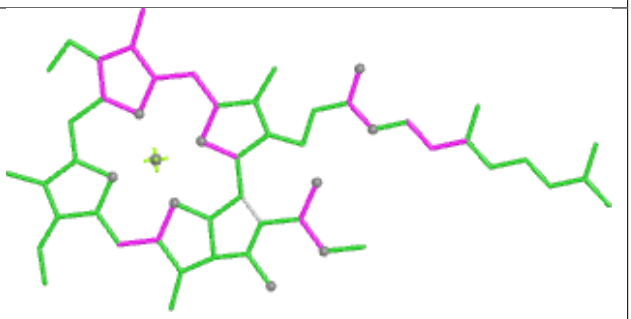
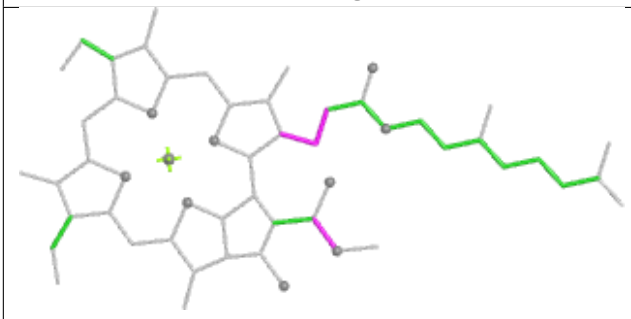
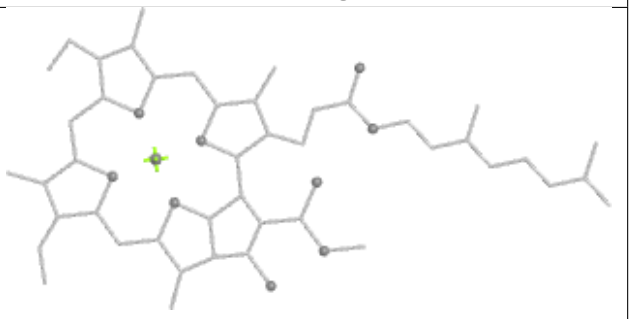
Bond angles

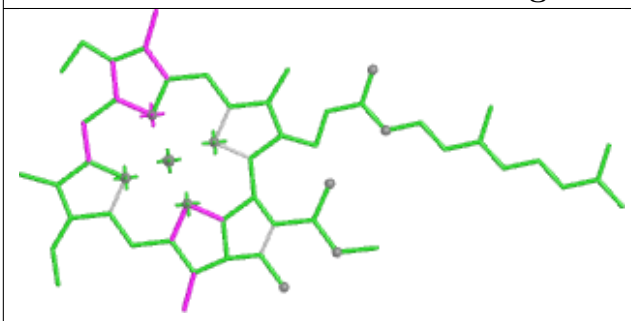
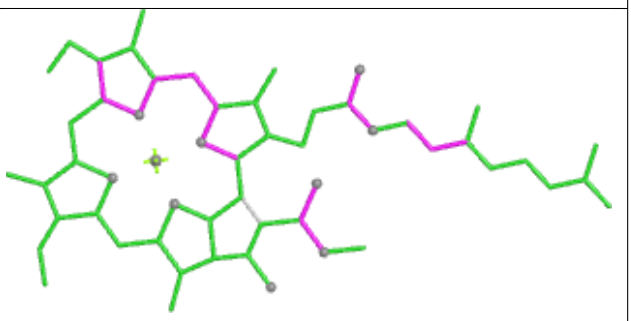
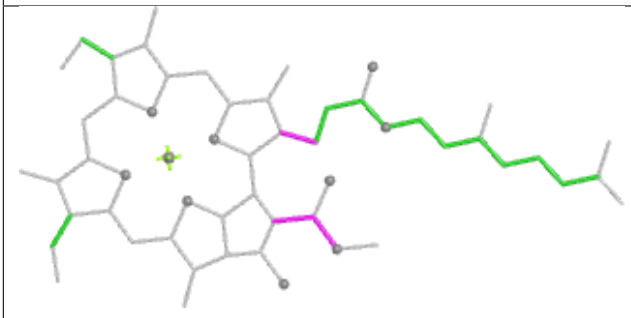
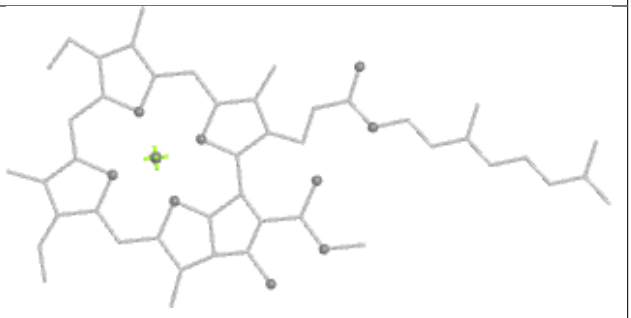


Torsions

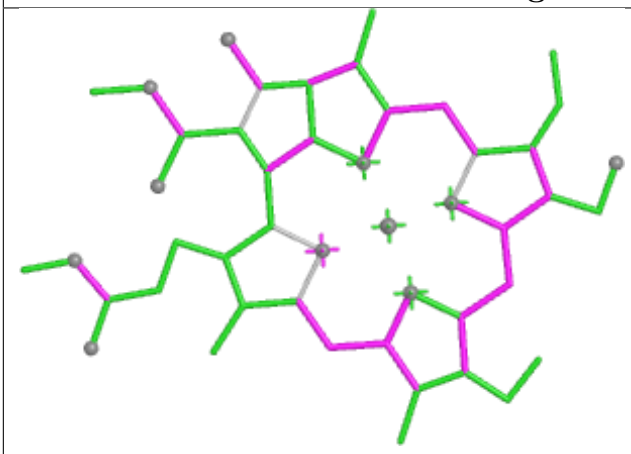


Rings

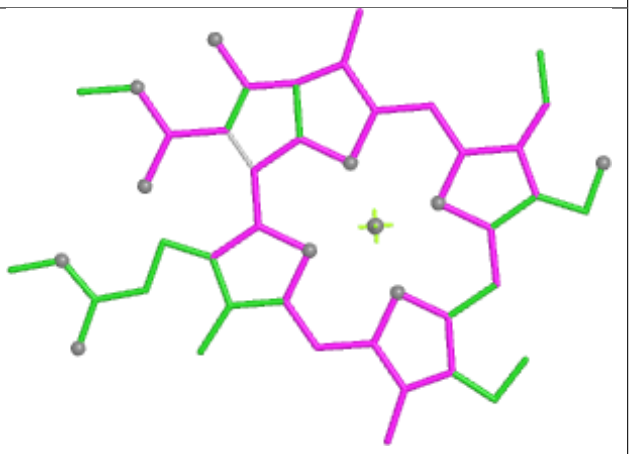
Ligand CLA e 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

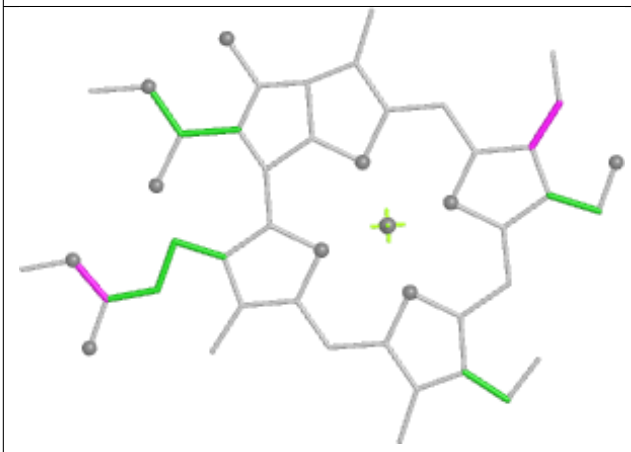
Ligand CHL 2 308



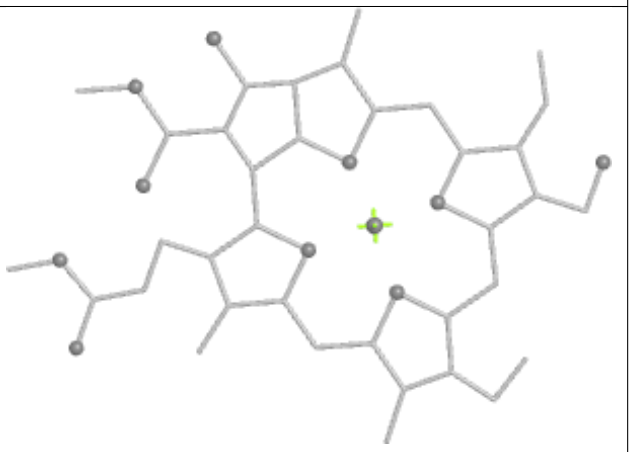
Bond lengths



Bond angles

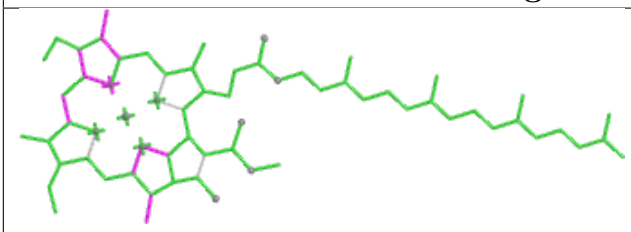


Torsions

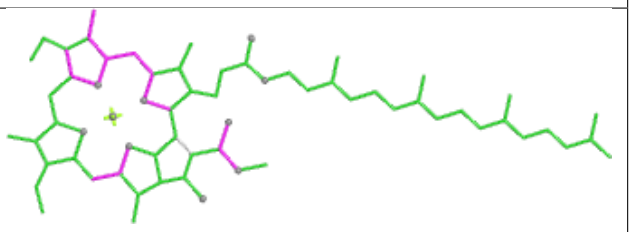


Rings

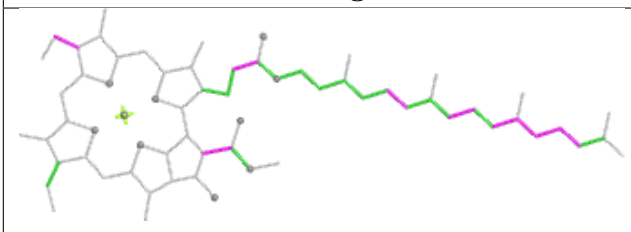
Ligand CLA B 839



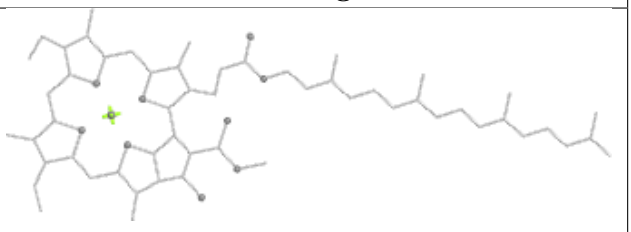
Bond lengths



Bond angles

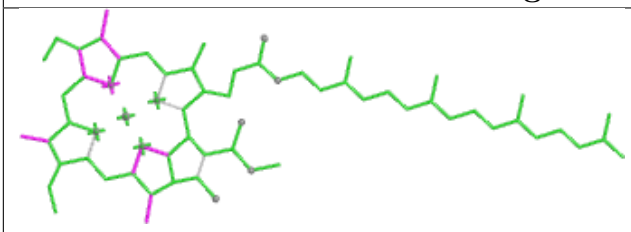


Torsions

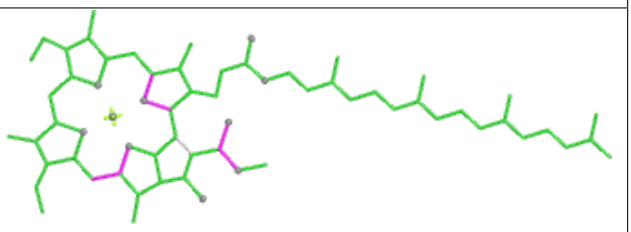


Rings

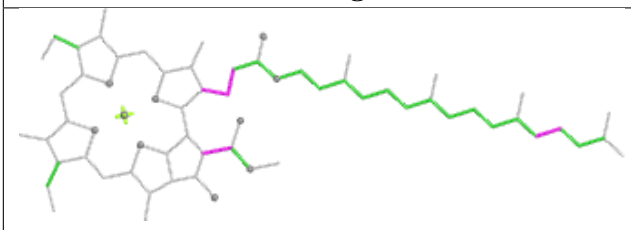
Ligand CLA A 802



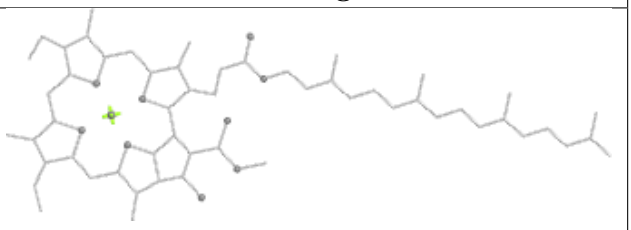
Bond lengths



Bond angles



Torsions



Rings

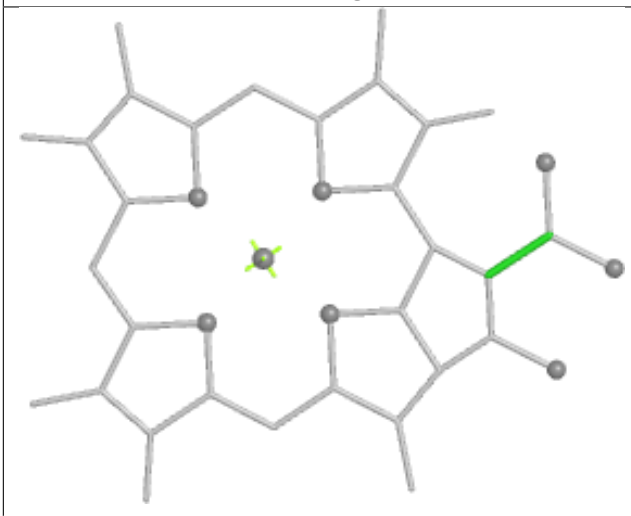
Ligand CLA O 203



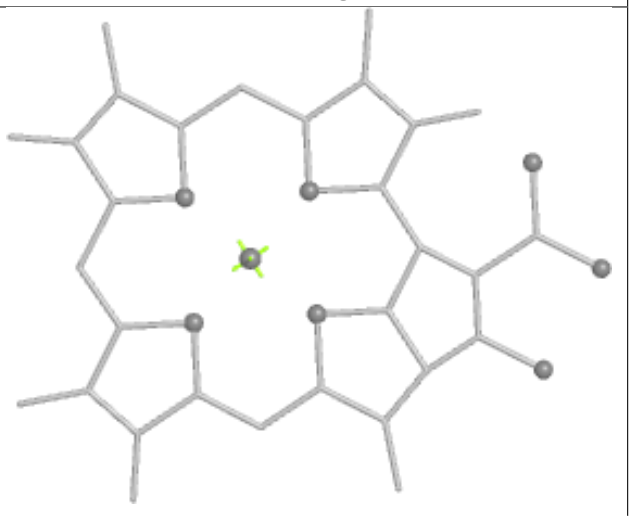
Bond lengths



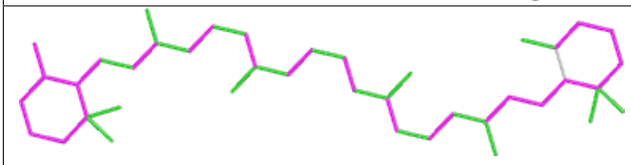
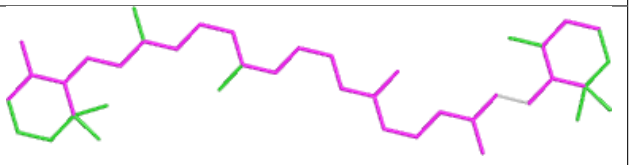
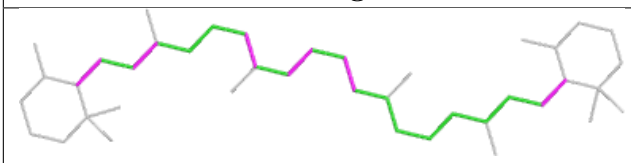
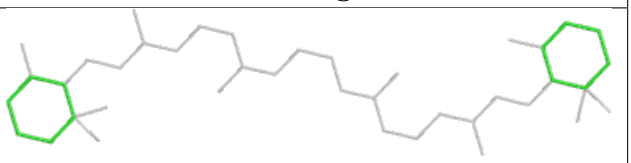
Bond angles

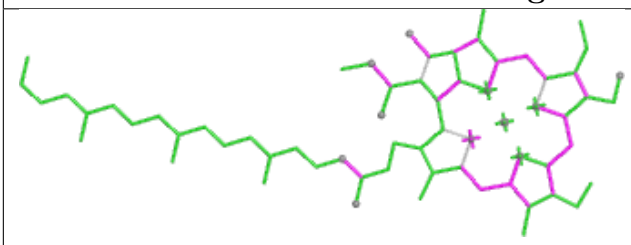
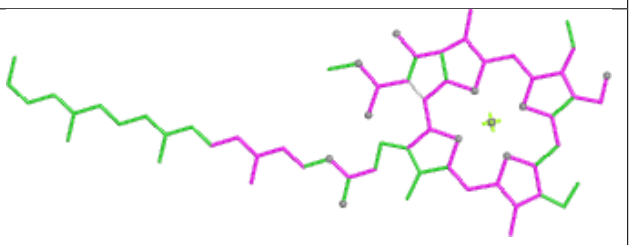
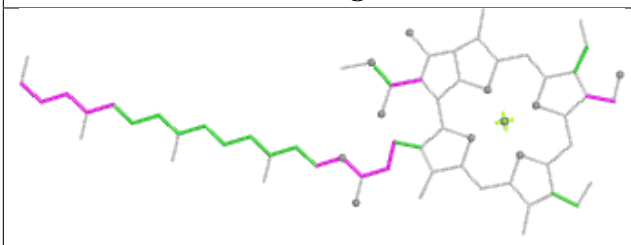
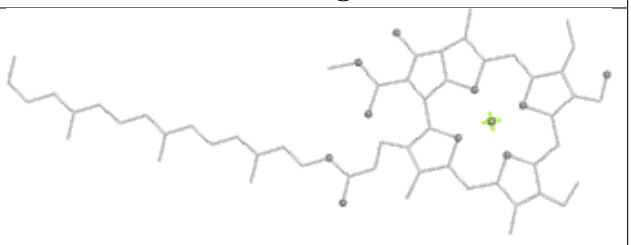


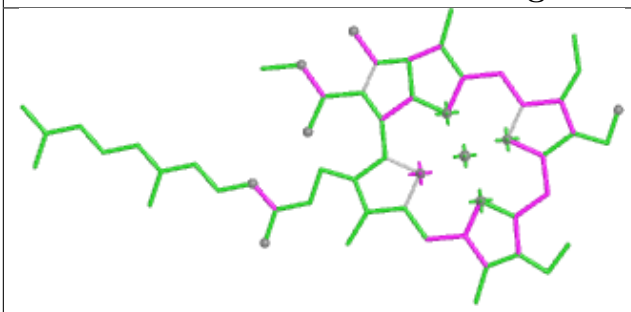
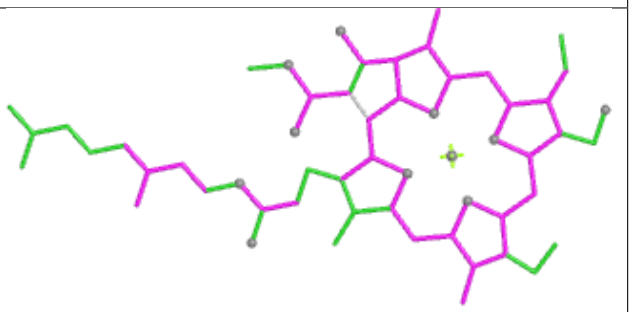
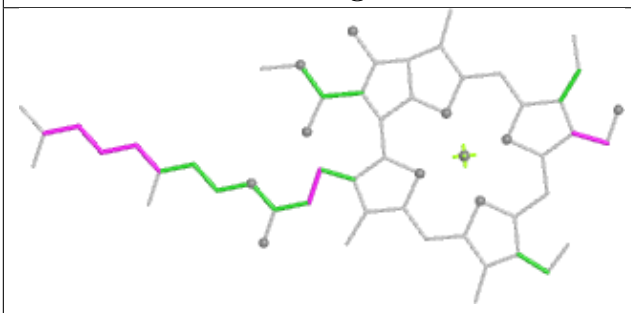
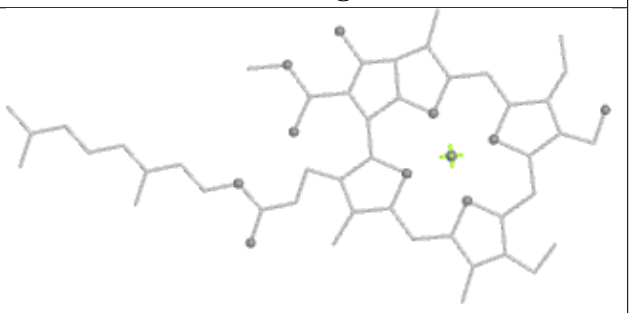
Torsions

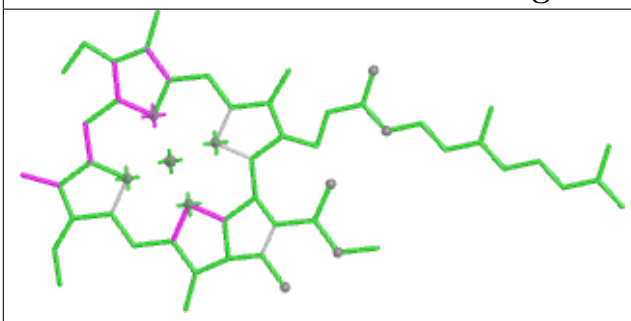
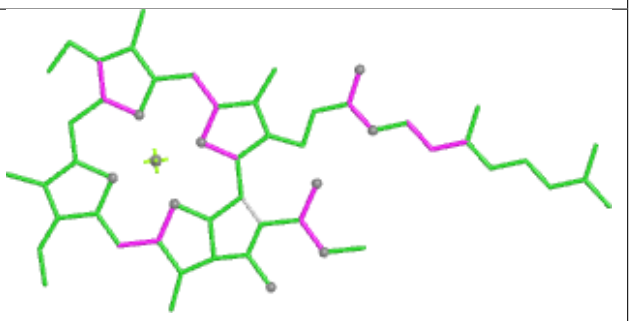
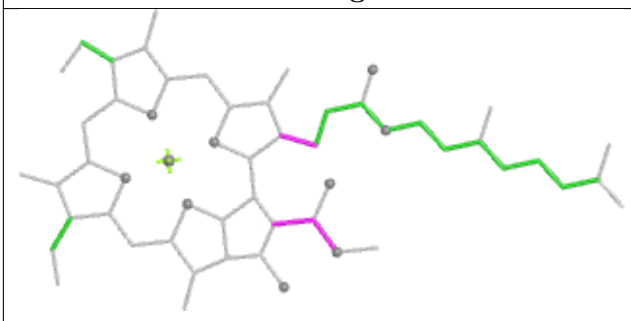
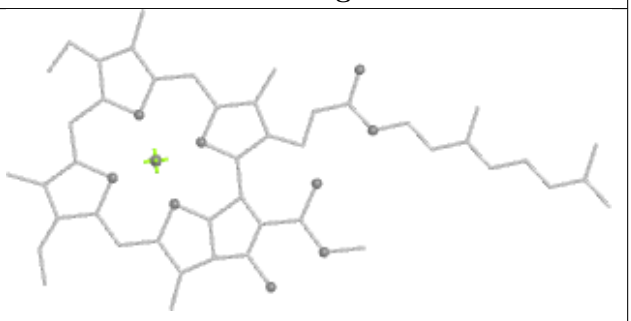


Rings

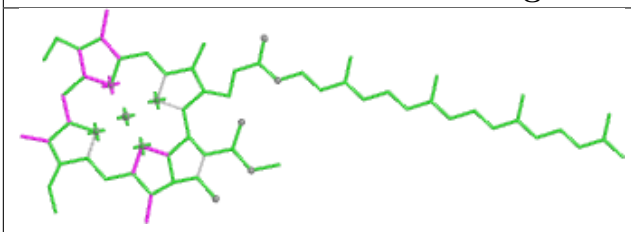
Ligand 8CT A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

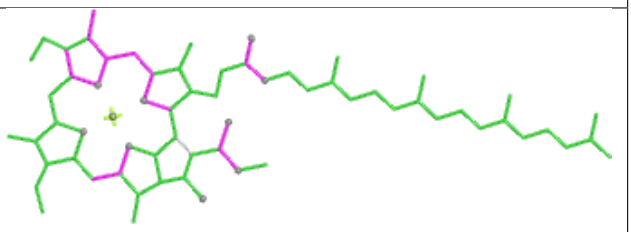
Ligand CHL 8 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA i 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

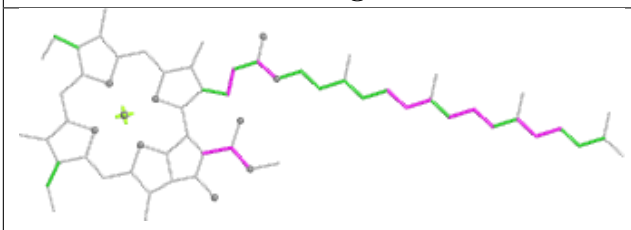
Ligand CLA A 852



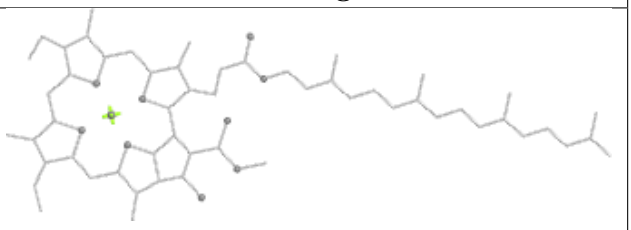
Bond lengths



Bond angles



Torsions

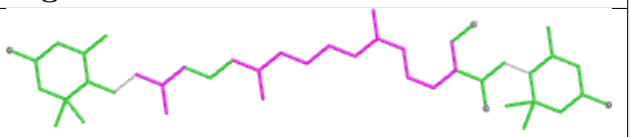


Rings

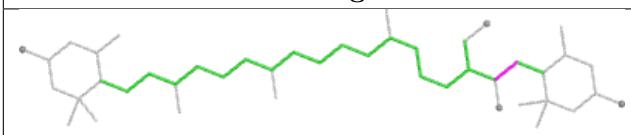
Ligand 0IE g 522



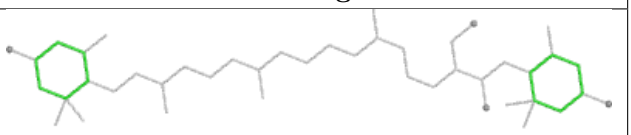
Bond lengths



Bond angles

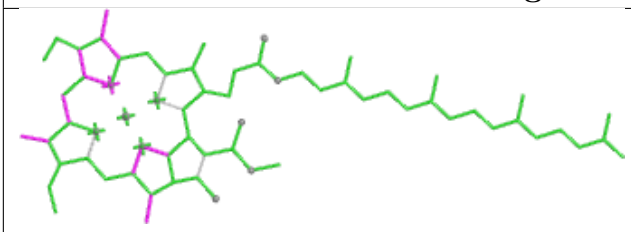


Torsions

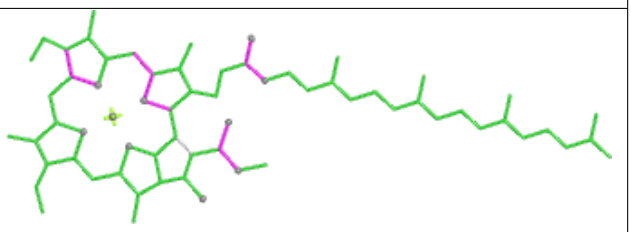


Rings

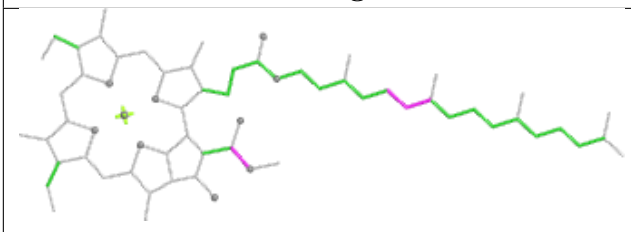
Ligand CLA B 825



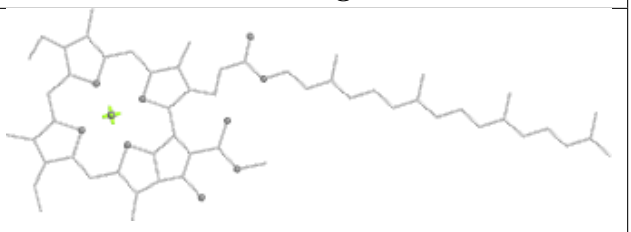
Bond lengths



Bond angles

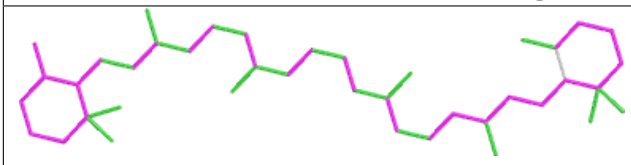


Torsions

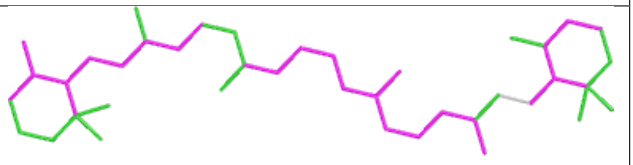


Rings

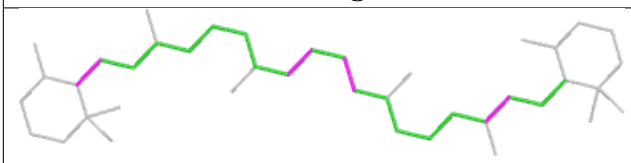
Ligand 8CT 0 401



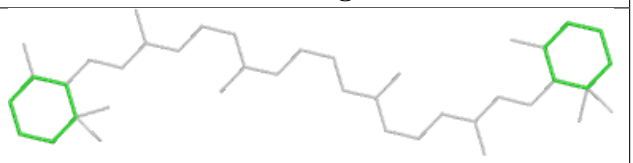
Bond lengths



Bond angles

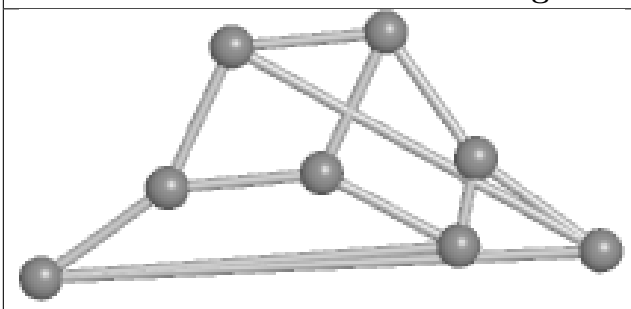


Torsions

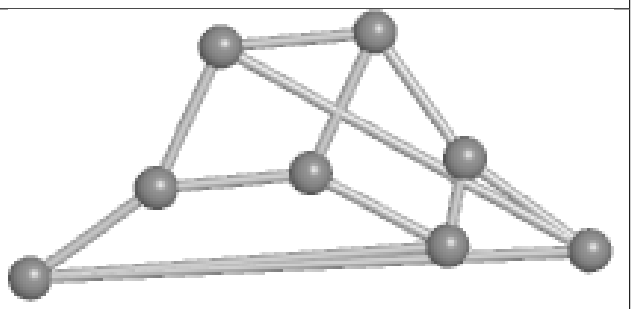


Rings

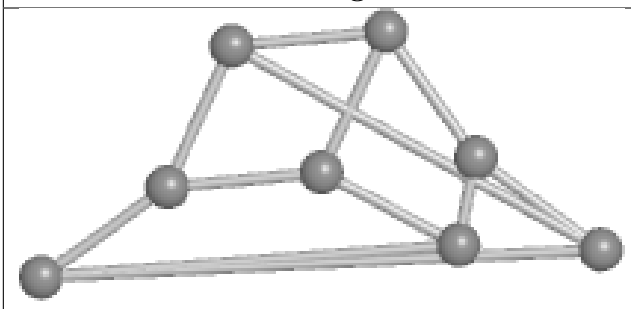
Ligand SF4 B 802



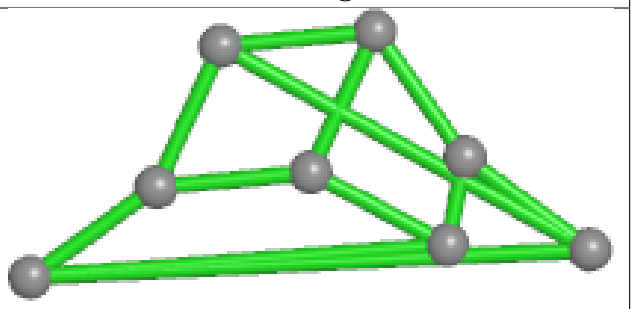
Bond lengths



Bond angles

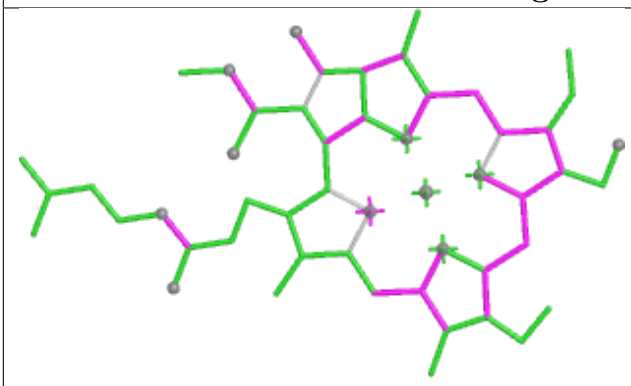


Torsions

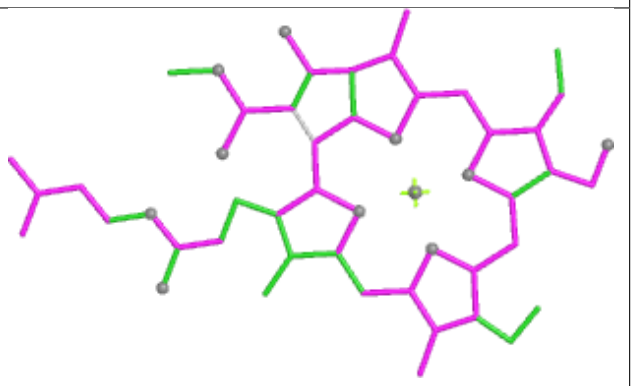


Rings

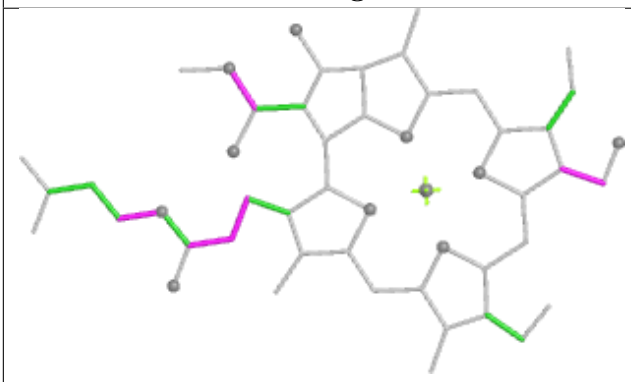
Ligand CHL i 606



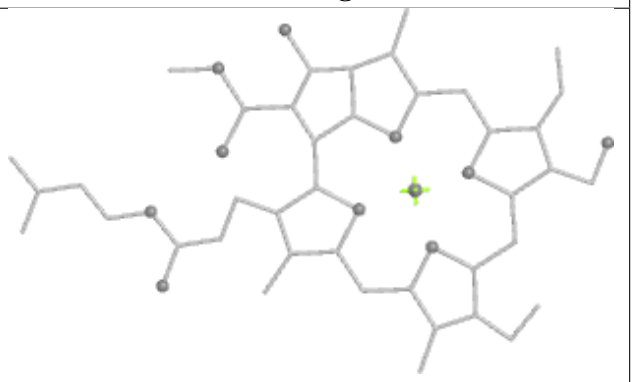
Bond lengths



Bond angles

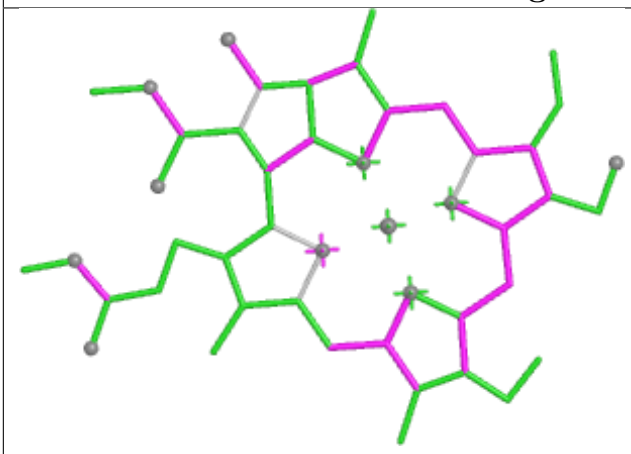


Torsions

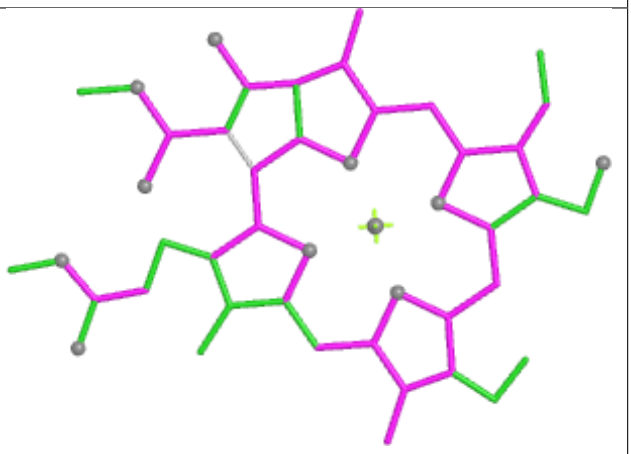


Rings

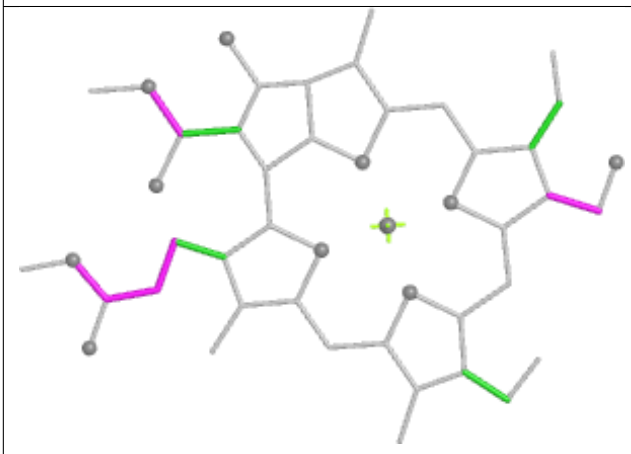
Ligand CHL c 607



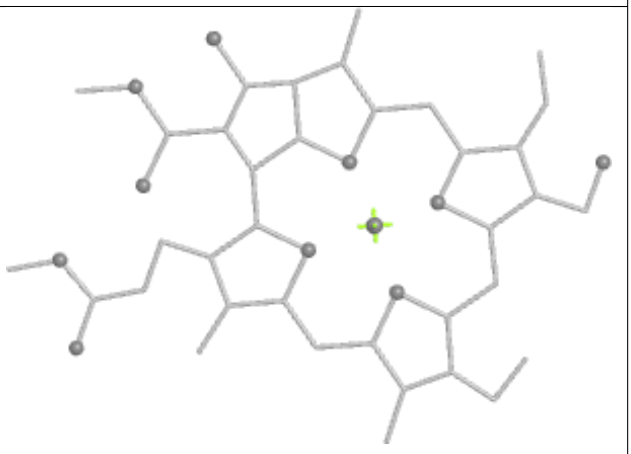
Bond lengths



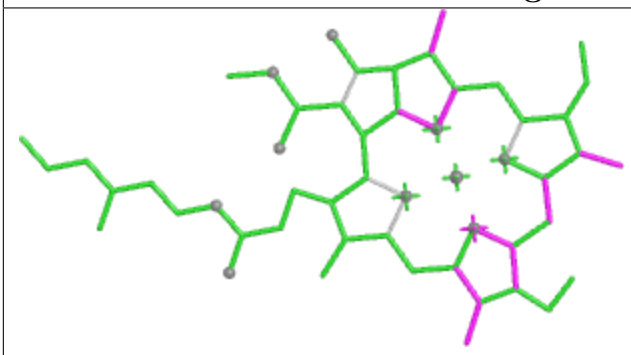
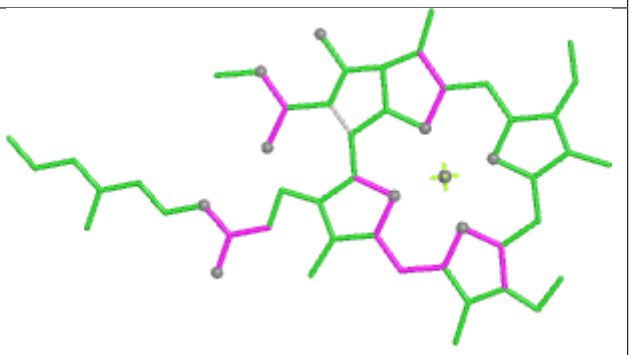
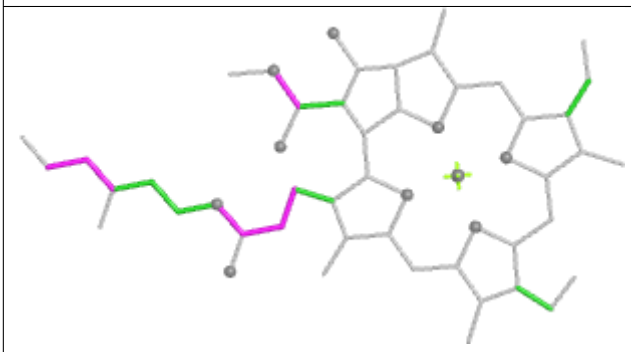
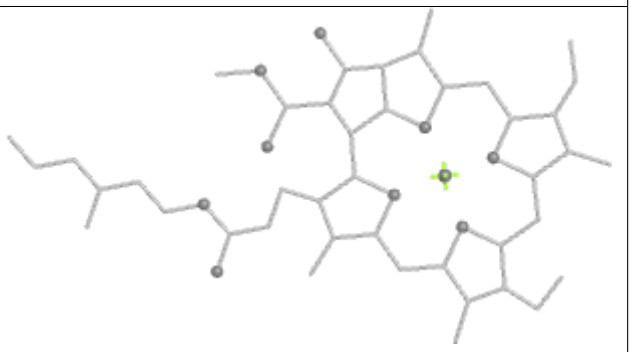
Bond angles

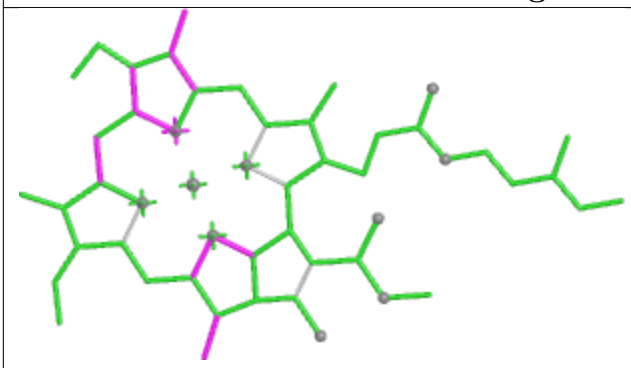
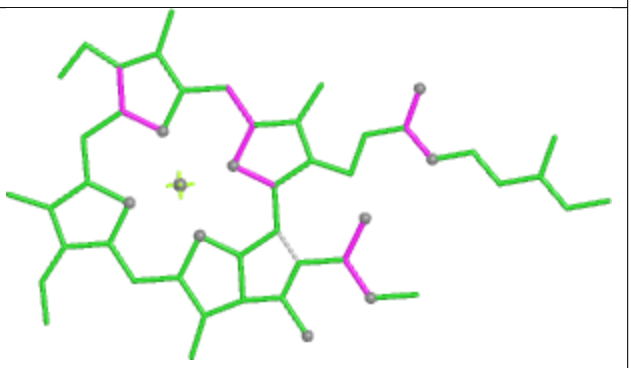
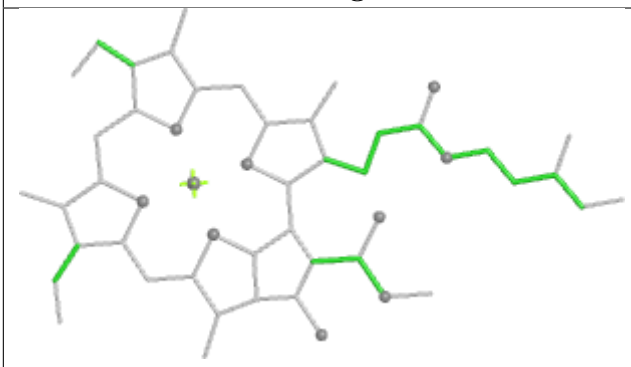
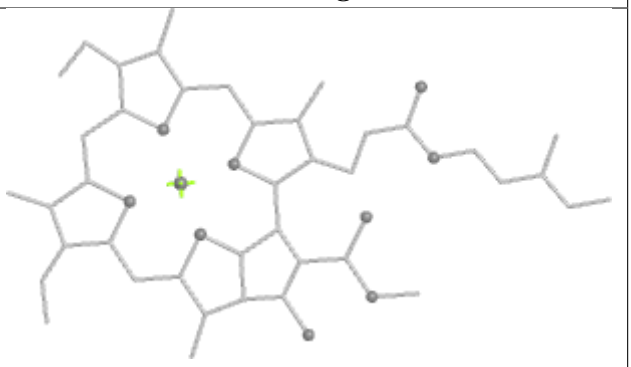


Torsions

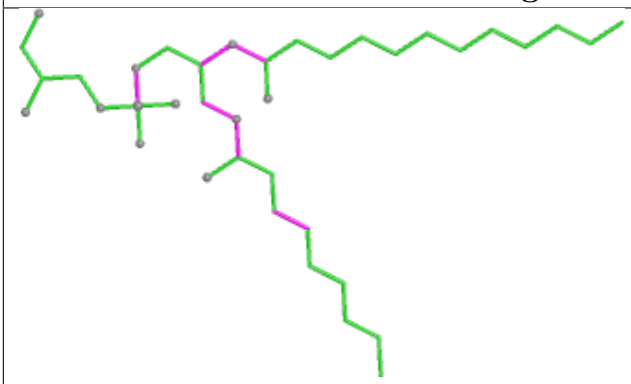


Rings

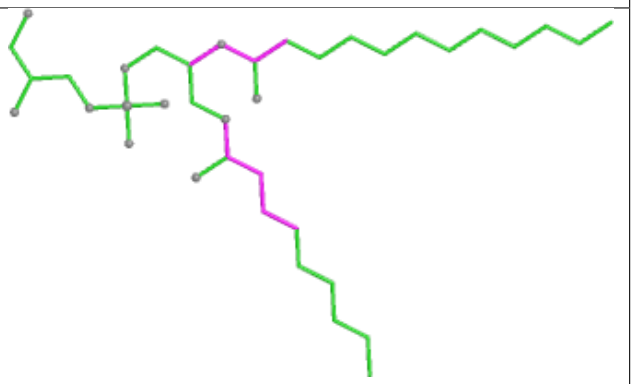
Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

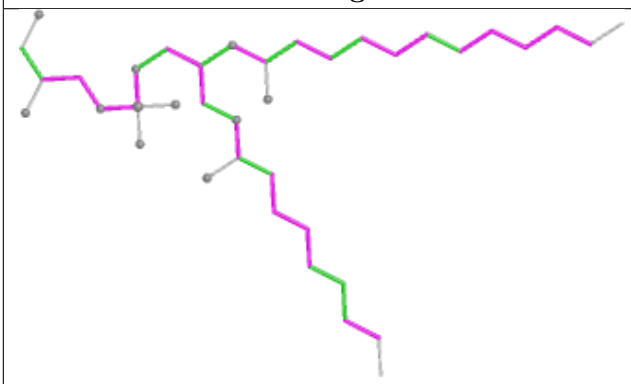
Ligand LHG G 105



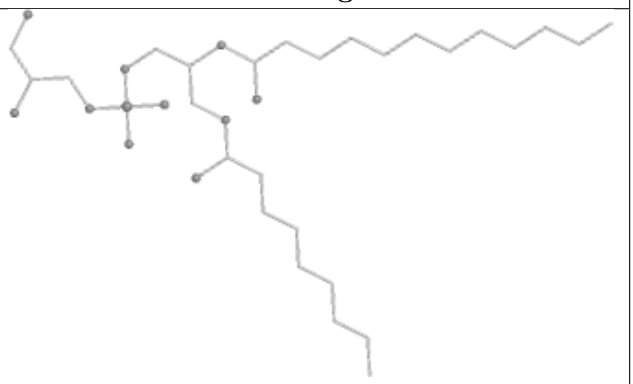
Bond lengths



Bond angles

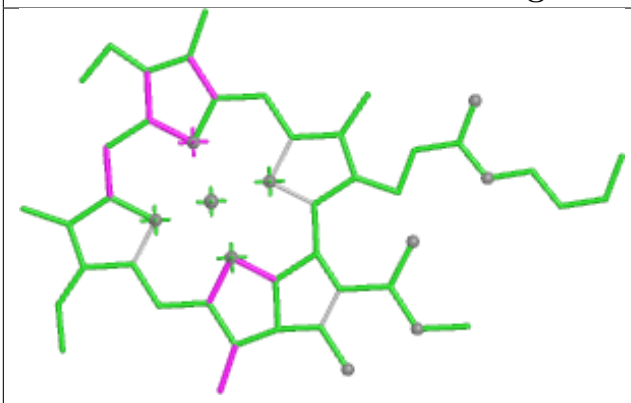


Torsions

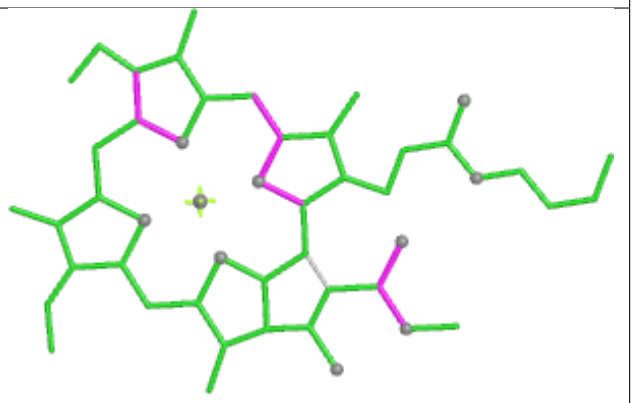


Rings

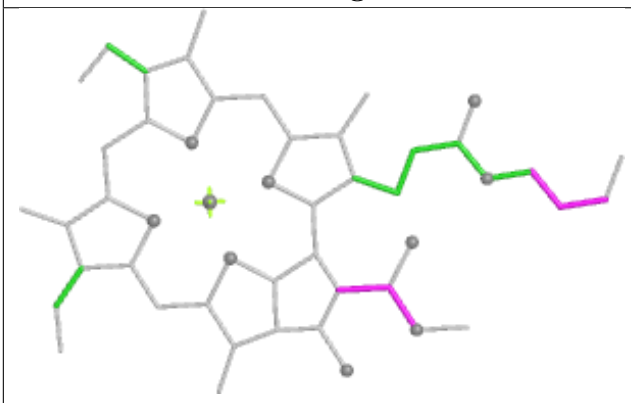
Ligand CLA h 603



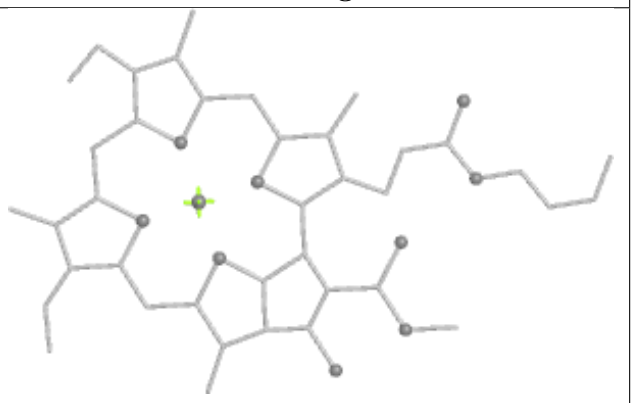
Bond lengths



Bond angles

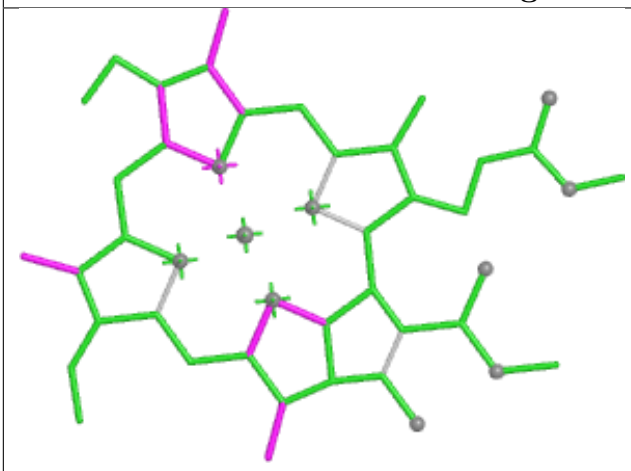


Torsions

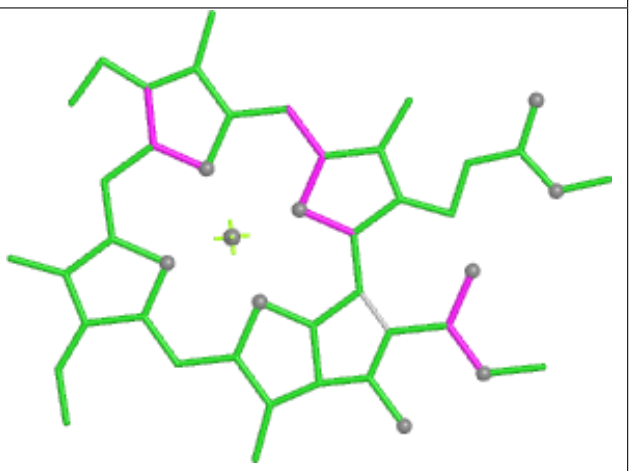


Rings

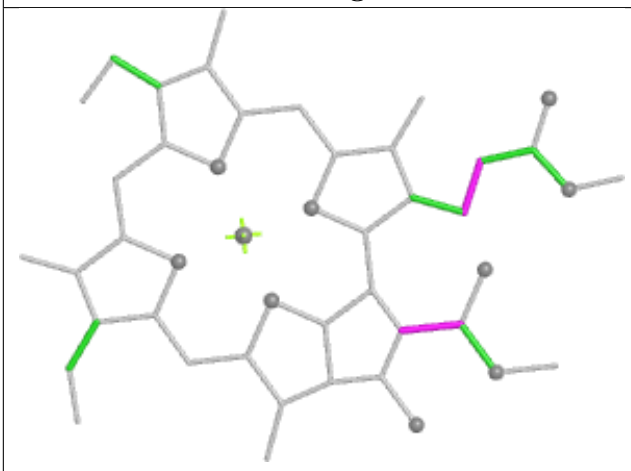
Ligand CLA M 101



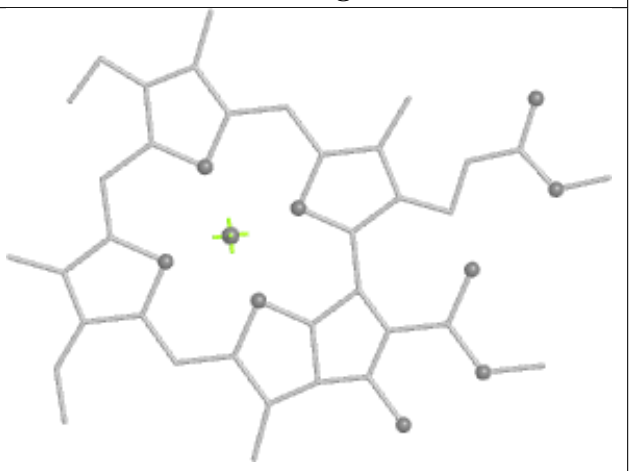
Bond lengths



Bond angles

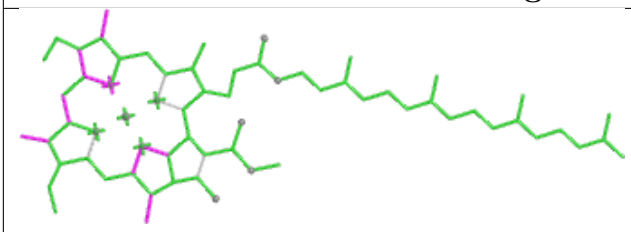


Torsions

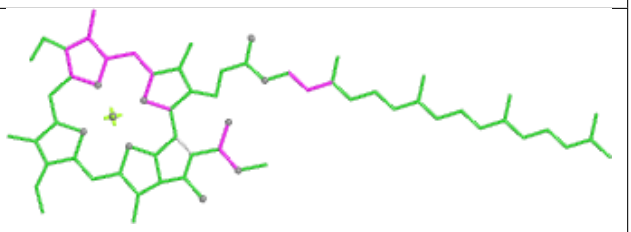


Rings

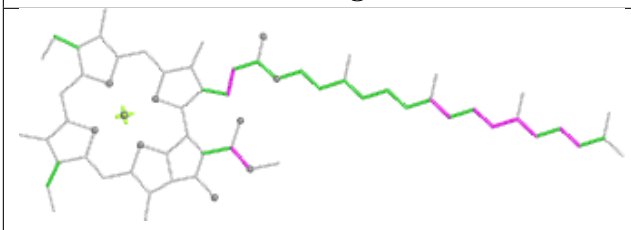
Ligand CLA B 801



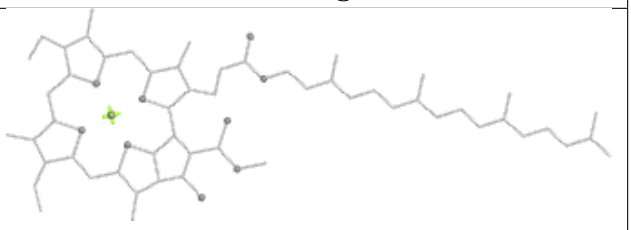
Bond lengths



Bond angles

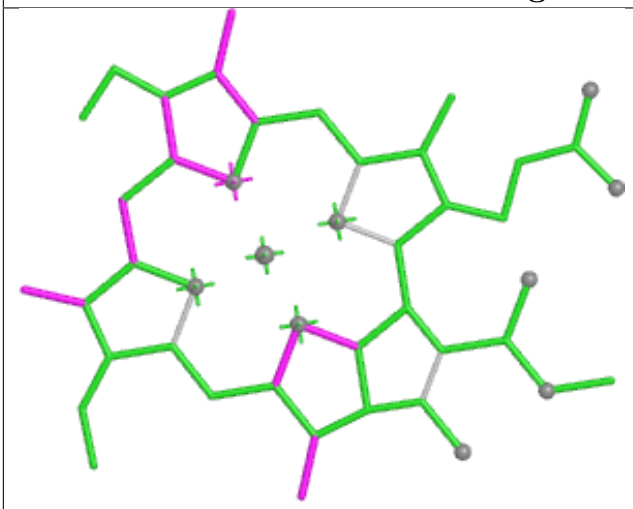


Torsions

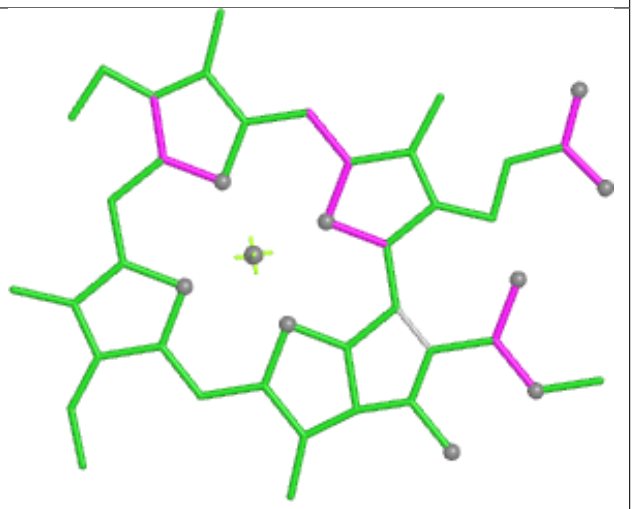


Rings

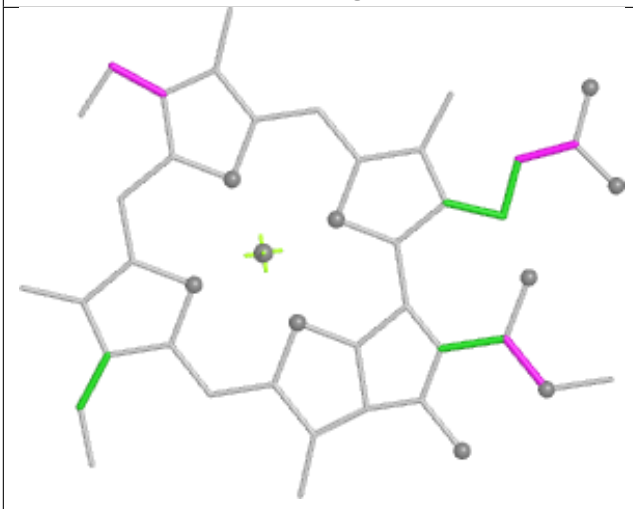
Ligand CLA 2 314



Bond lengths



Bond angles

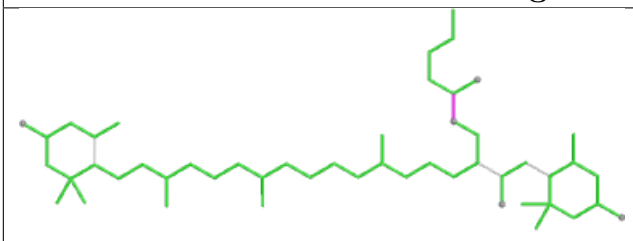


Torsions

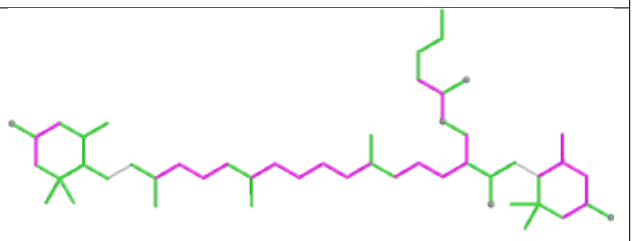


Rings

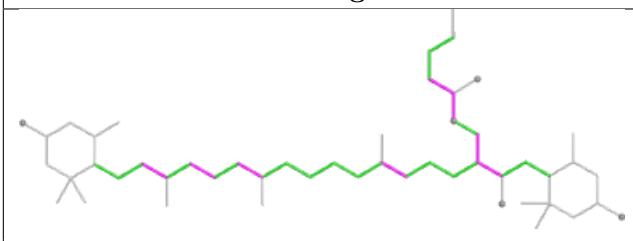
Ligand 0UR 4 502



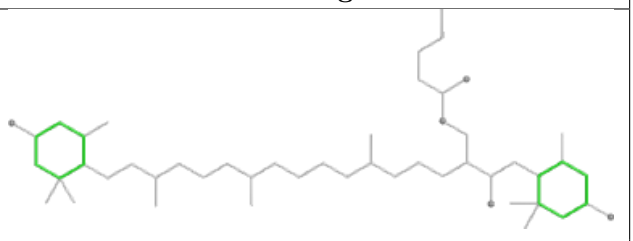
Bond lengths



Bond angles

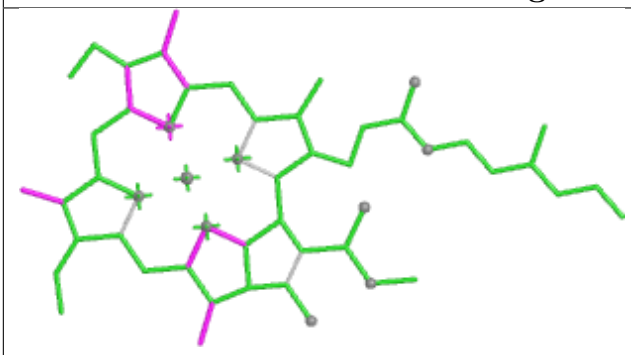


Torsions

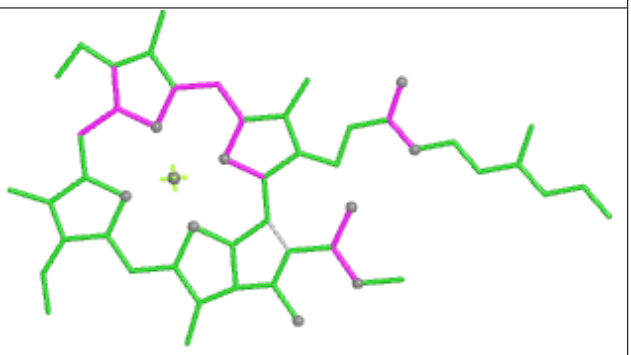


Rings

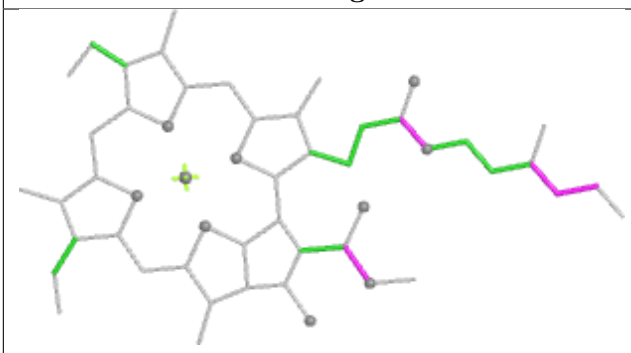
Ligand CLA 6 303



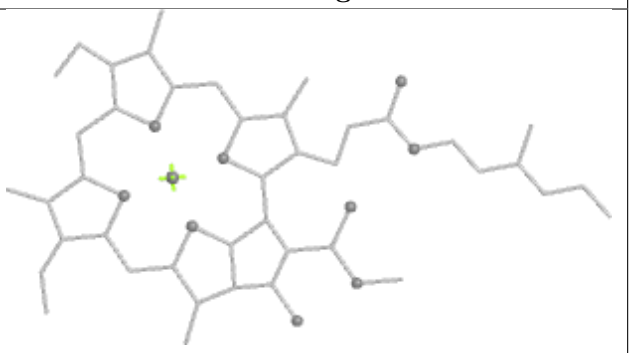
Bond lengths



Bond angles

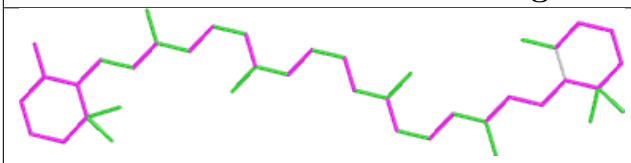


Torsions

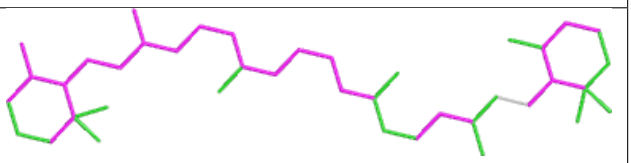


Rings

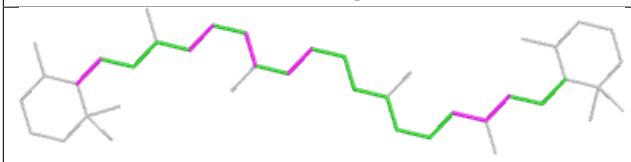
Ligand 8CT 7 405



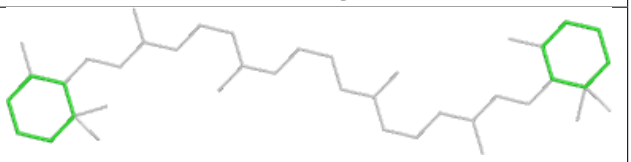
Bond lengths



Bond angles

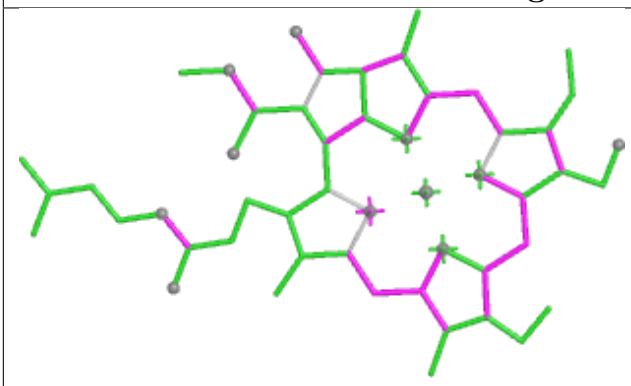


Torsions

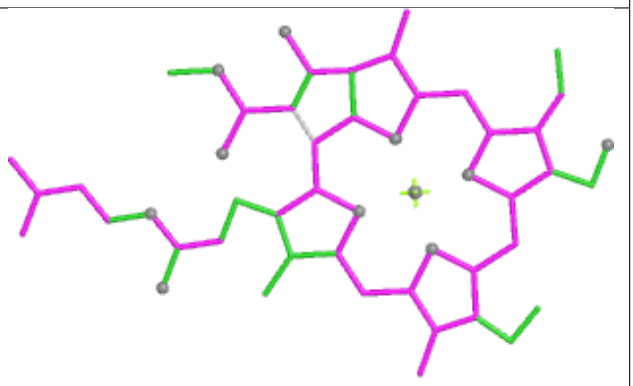


Rings

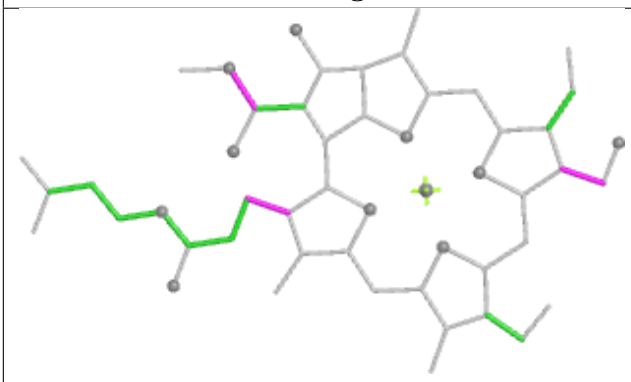
Ligand CHL 6 306



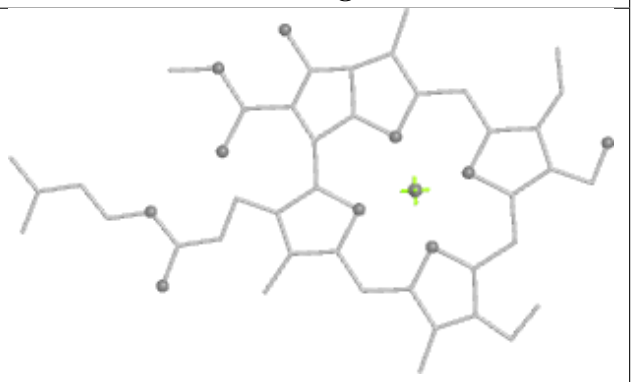
Bond lengths



Bond angles

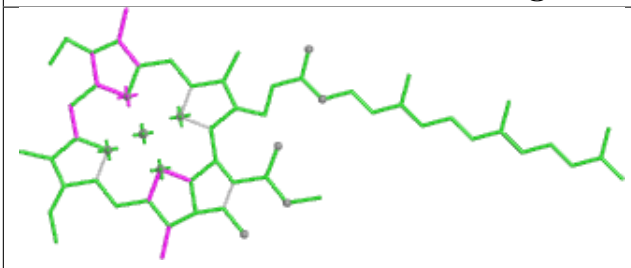


Torsions

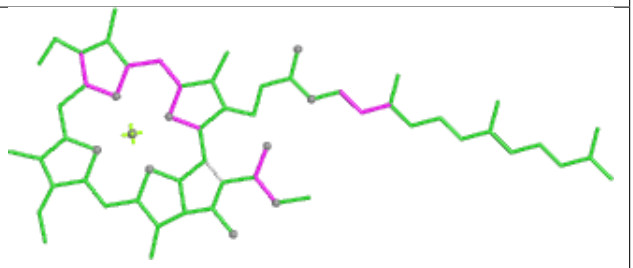


Rings

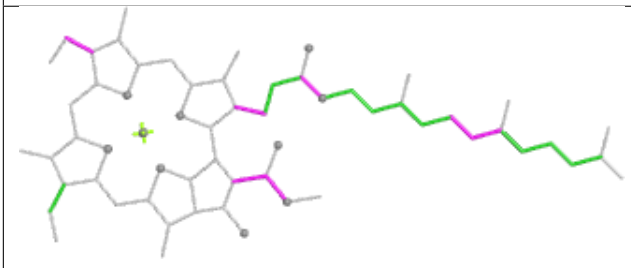
Ligand CLA 6 310



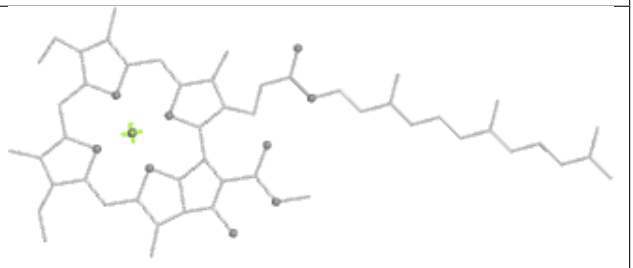
Bond lengths



Bond angles

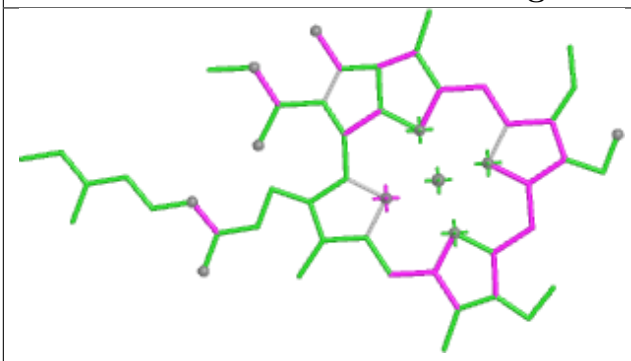


Torsions

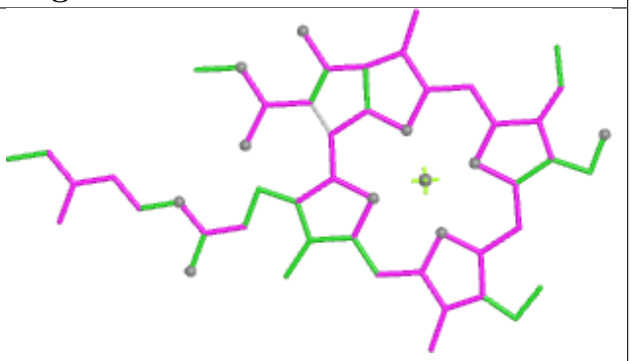


Rings

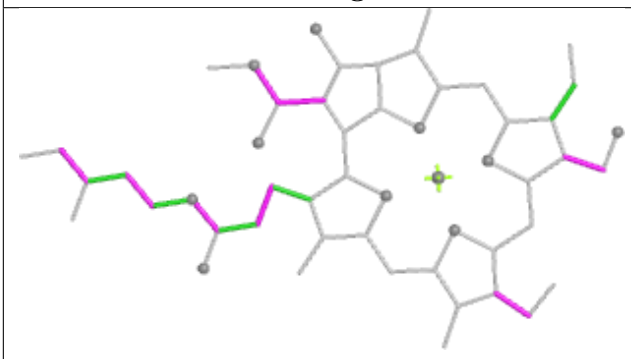
Ligand CHL g 602



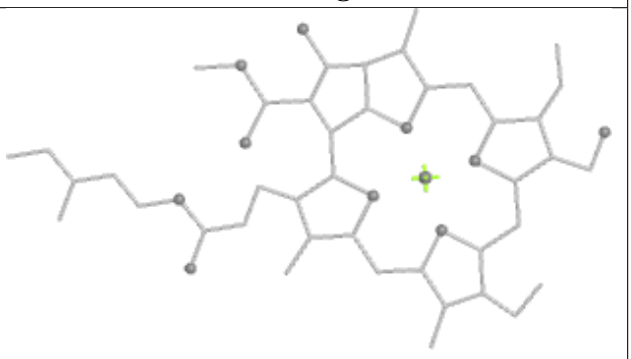
Bond lengths



Bond angles

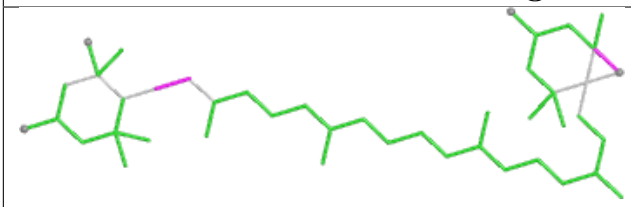


Torsions

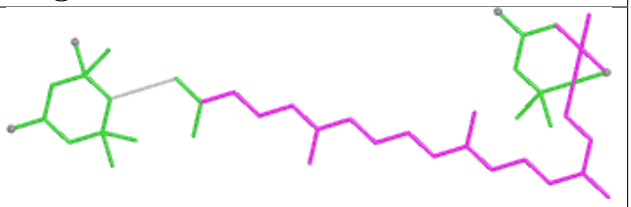


Rings

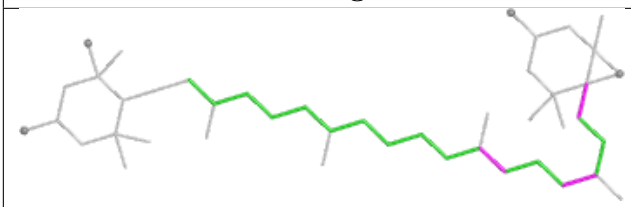
Ligand NEX g 523



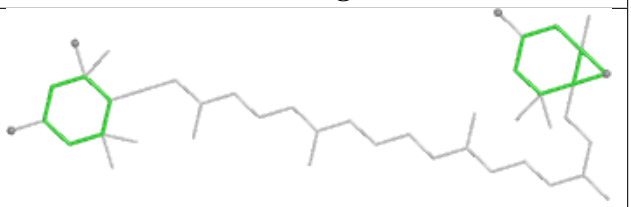
Bond lengths



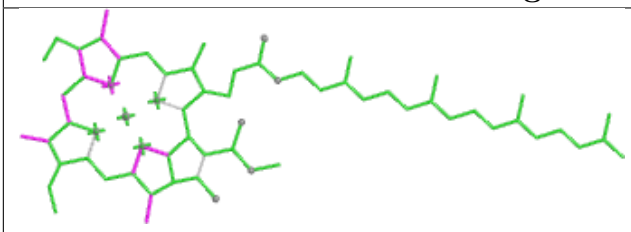
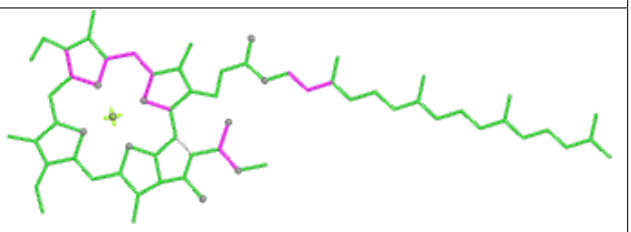
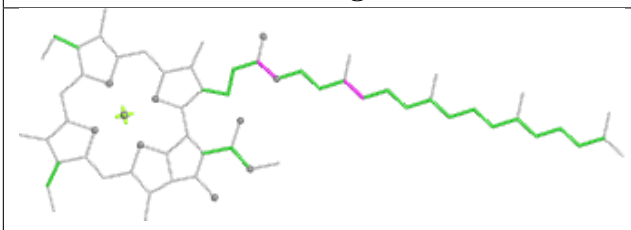
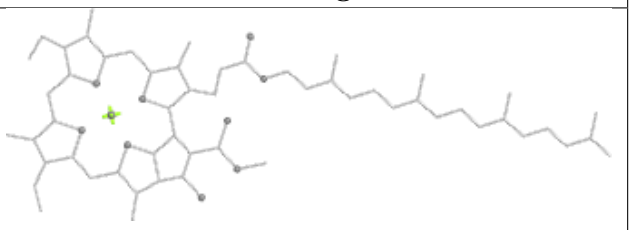
Bond angles

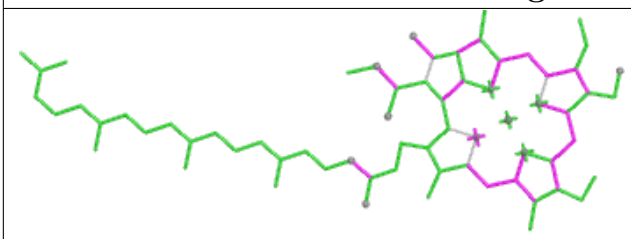
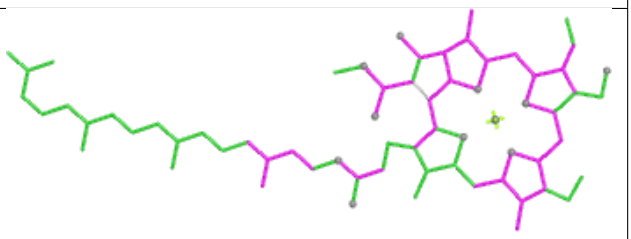
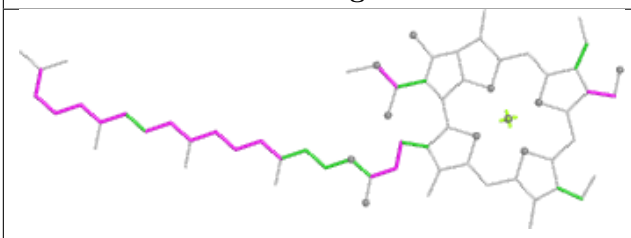
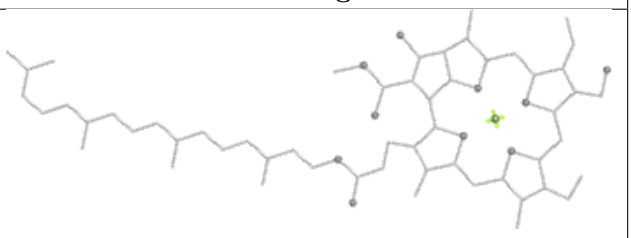


Torsions

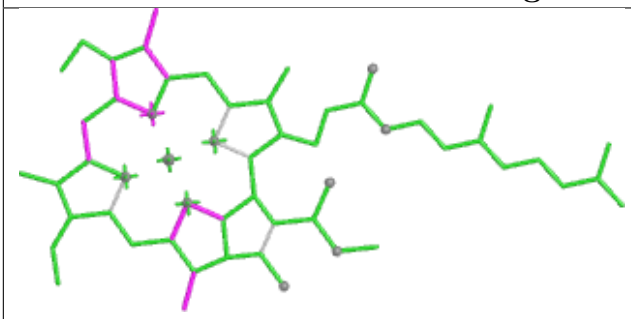


Rings

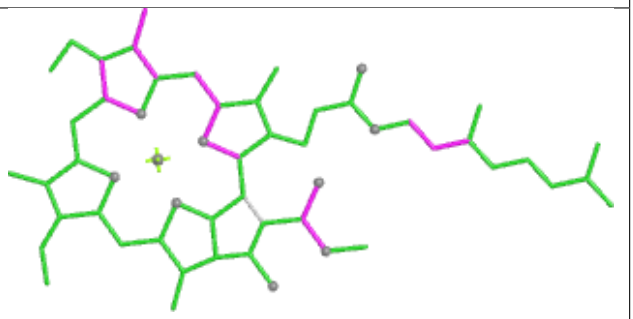
Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 1 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

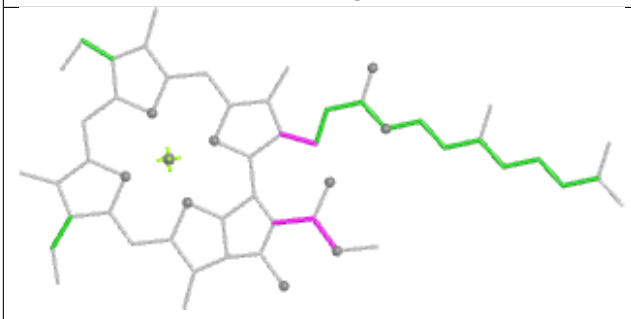
Ligand CLA H 201



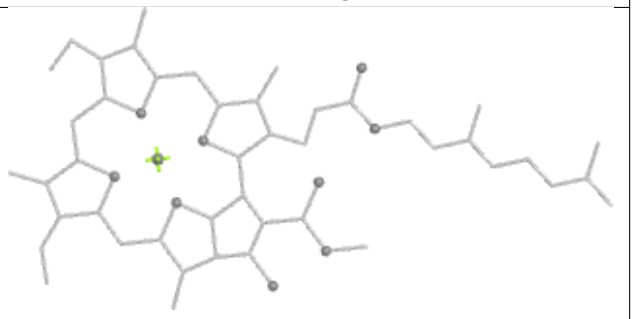
Bond lengths



Bond angles

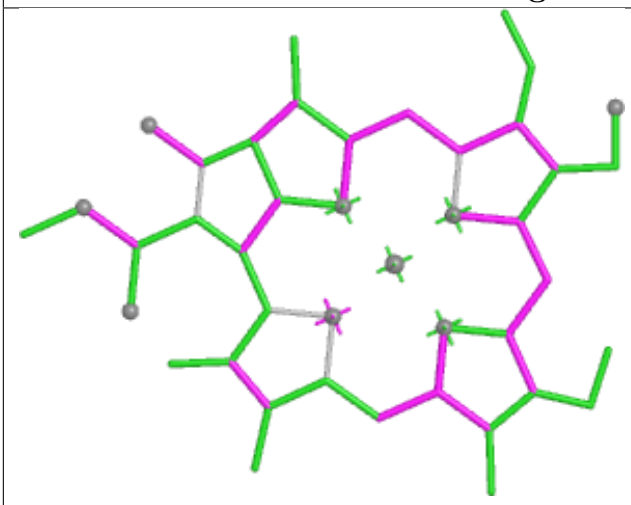


Torsions

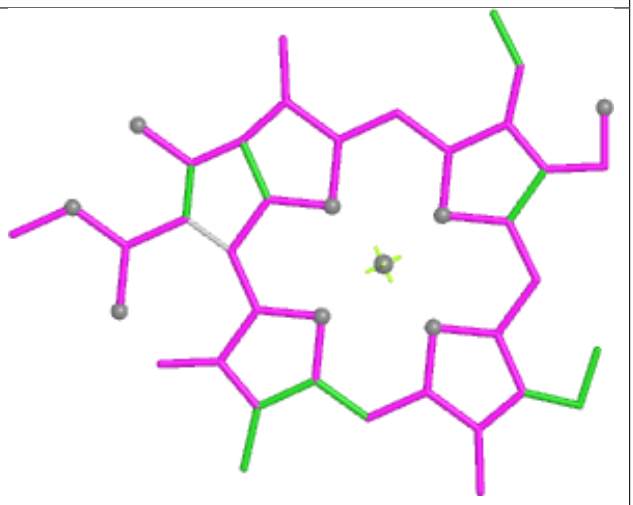


Rings

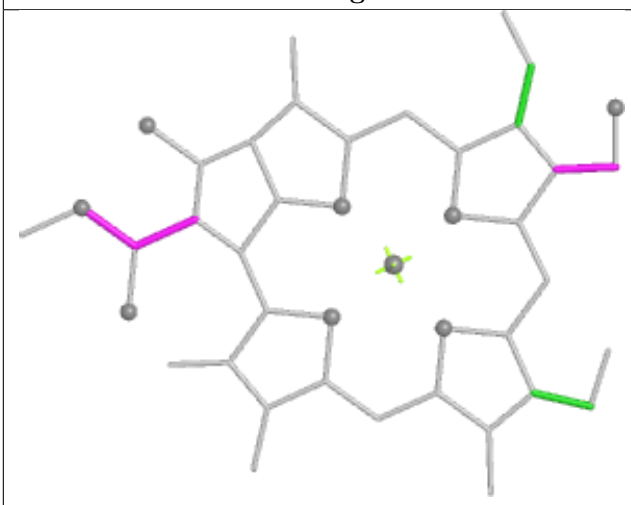
Ligand CHL e 614



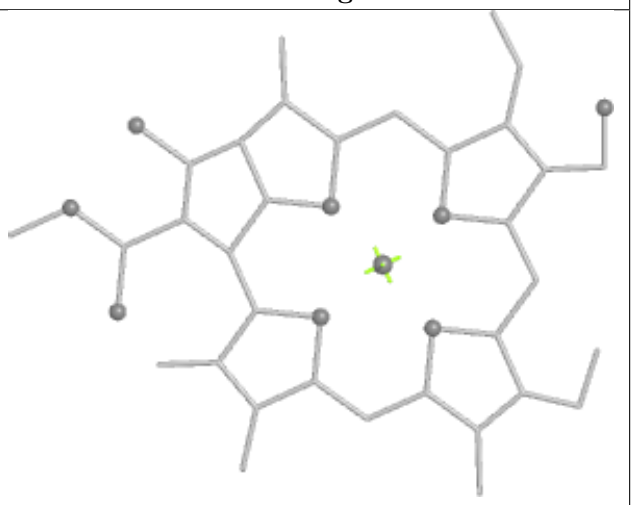
Bond lengths



Bond angles

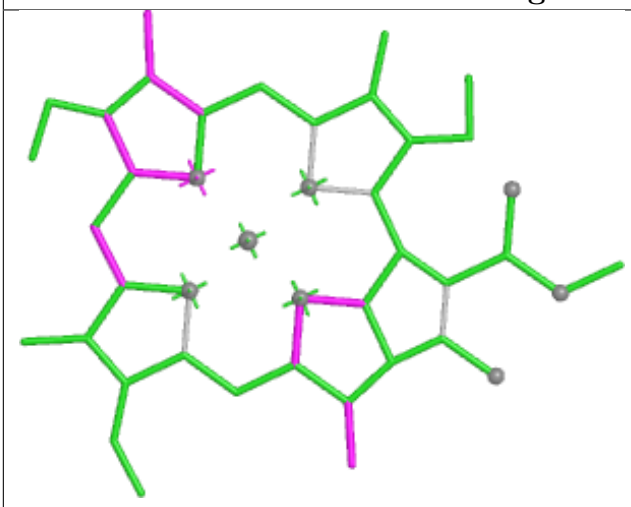


Torsions

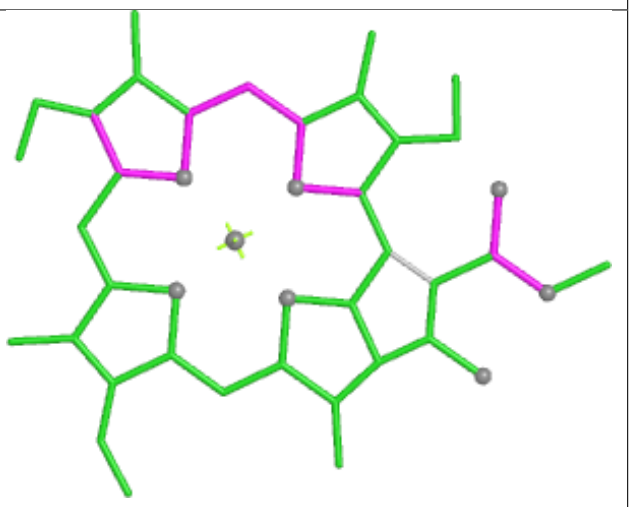


Rings

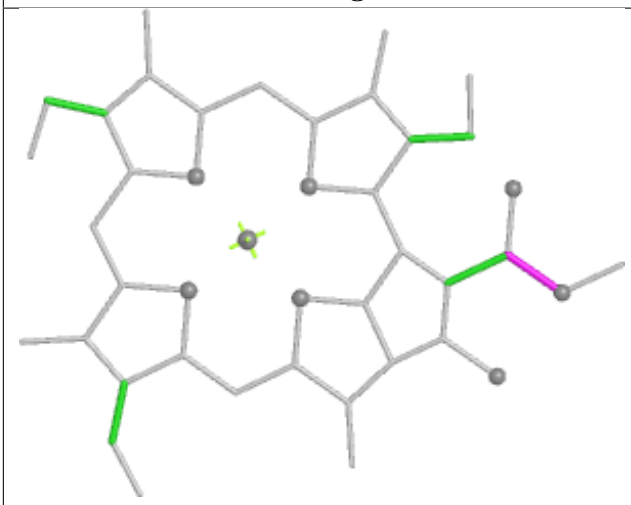
Ligand CLA J 103



Bond lengths



Bond angles

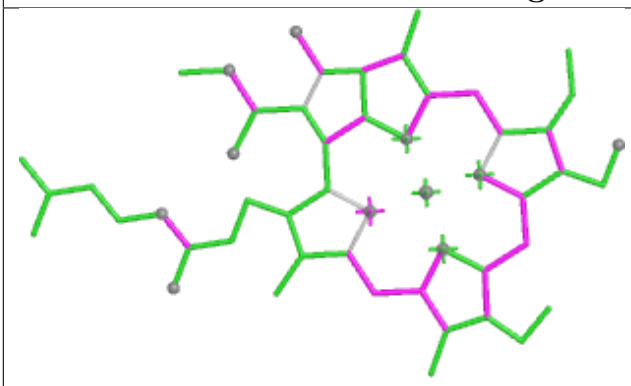


Torsions

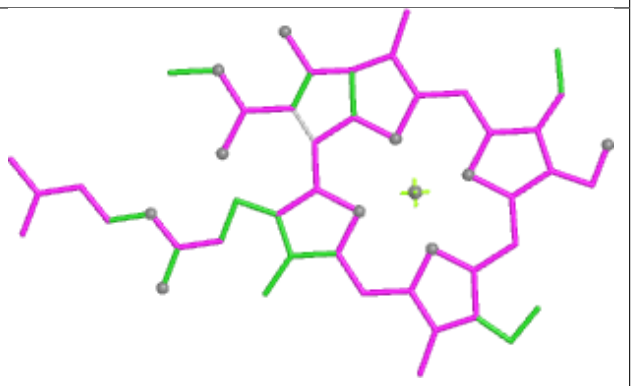


Rings

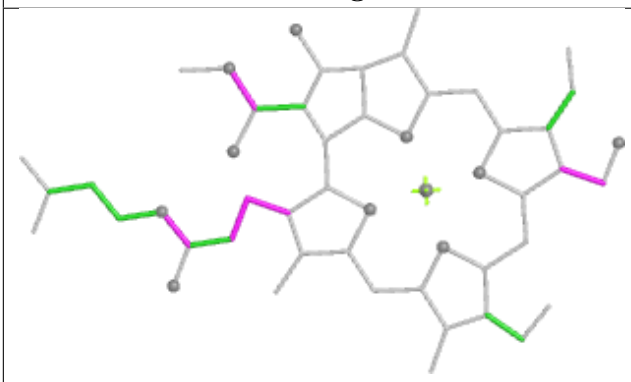
Ligand CHL 4 307



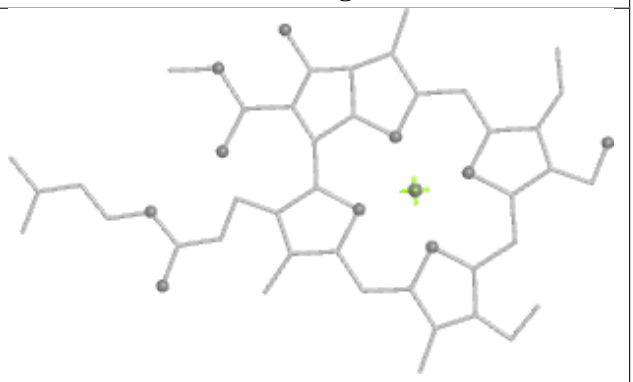
Bond lengths



Bond angles

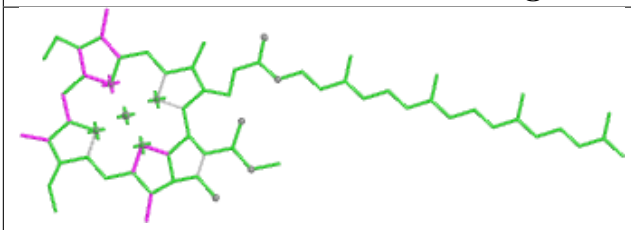


Torsions

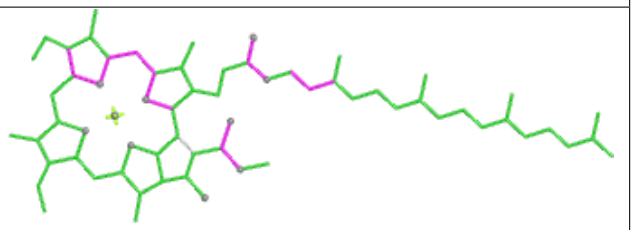


Rings

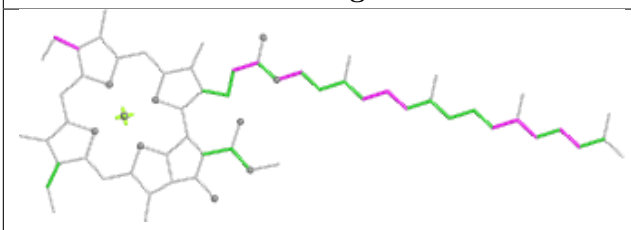
Ligand CLA B 809



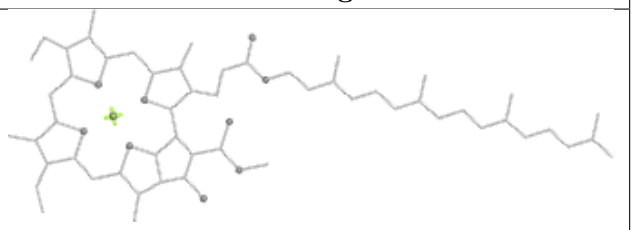
Bond lengths



Bond angles

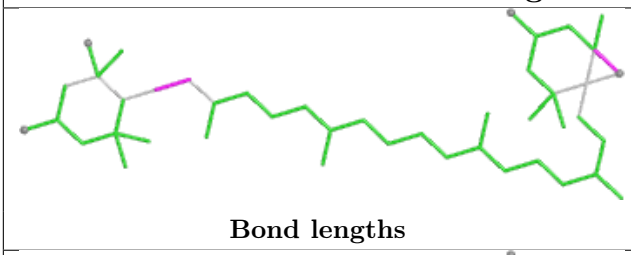


Torsions

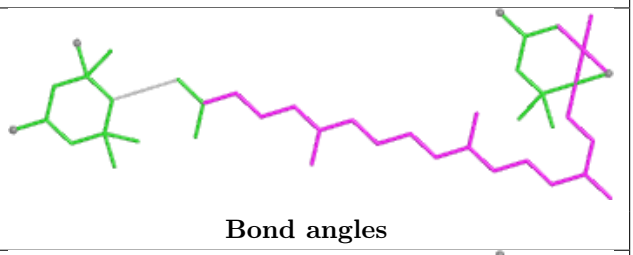


Rings

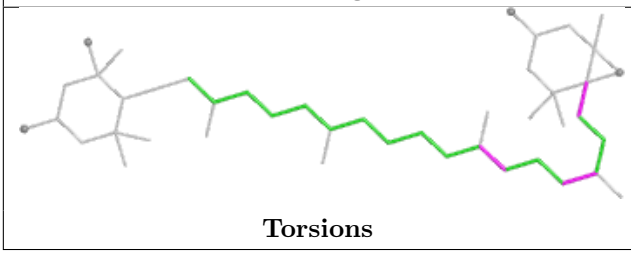
Ligand NEX b 523



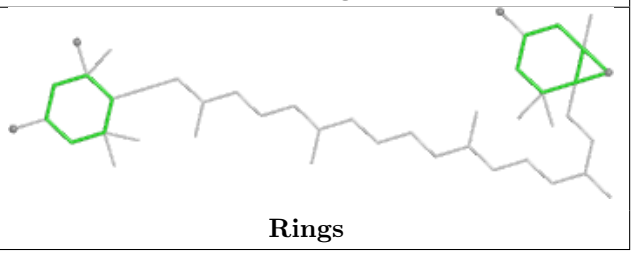
Bond lengths



Bond angles

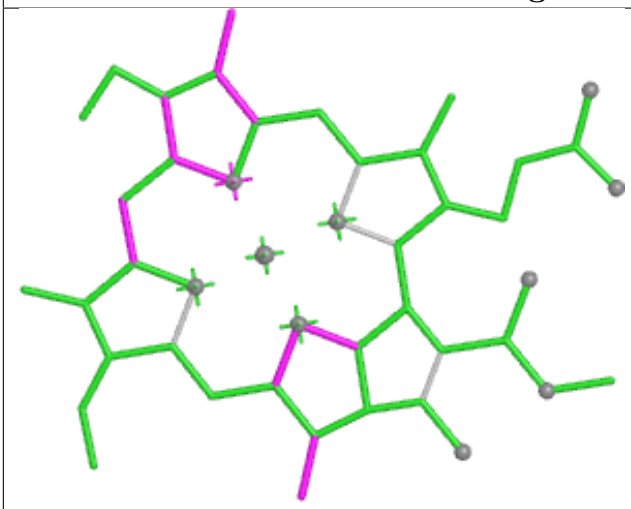


Torsions

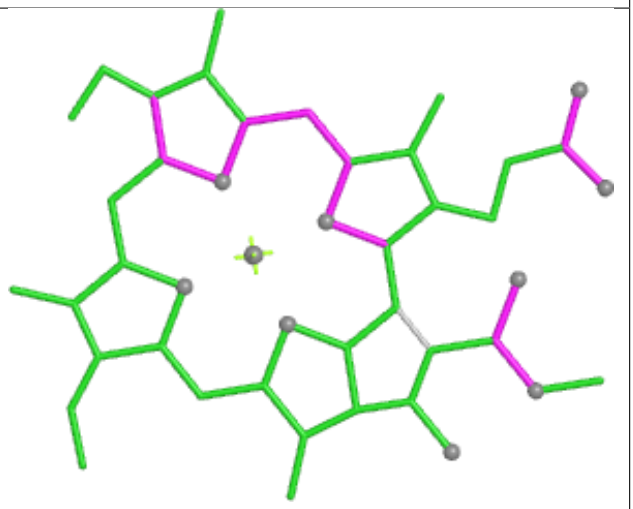


Rings

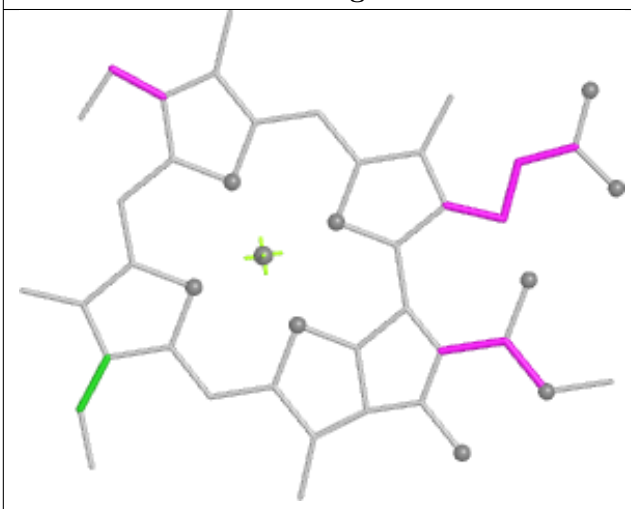
Ligand CLA 8 314



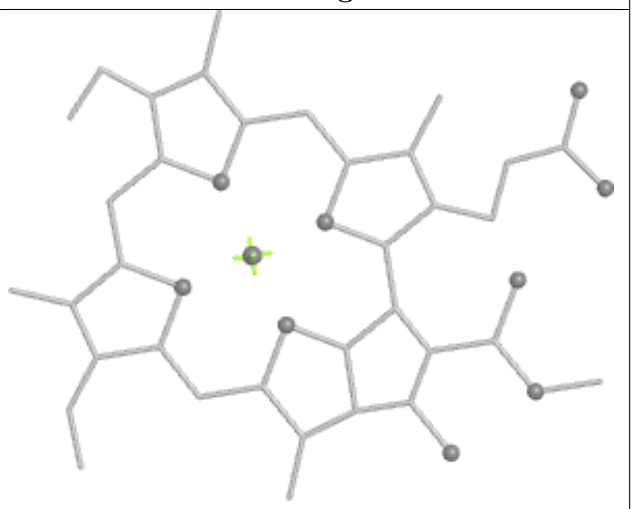
Bond lengths



Bond angles

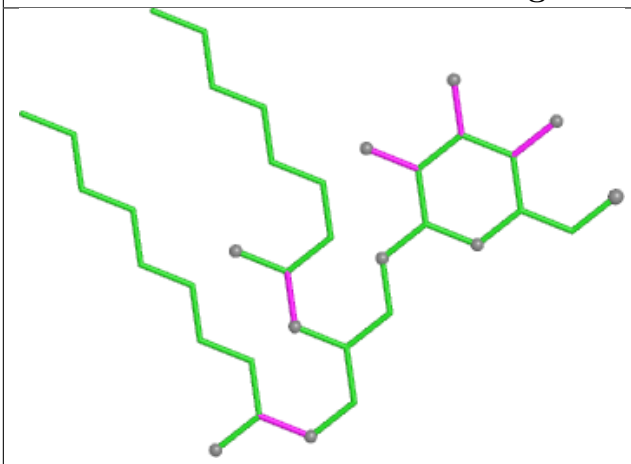


Torsions

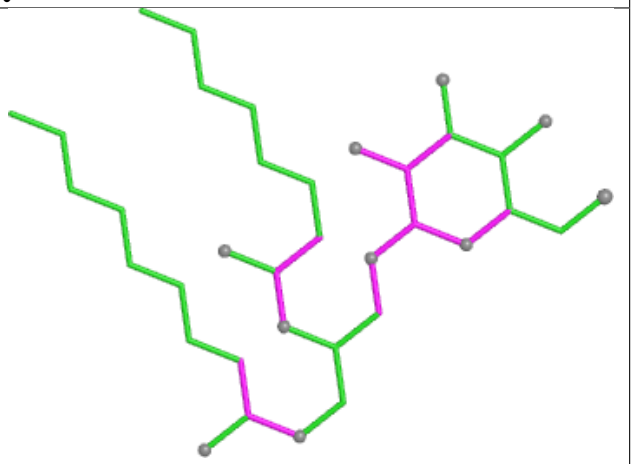


Rings

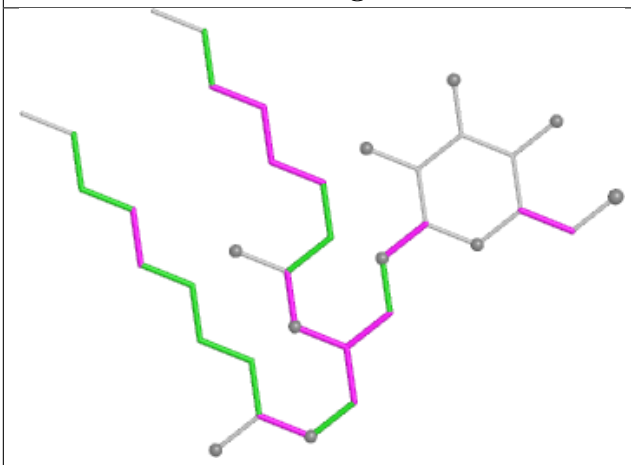
Ligand SQD 0 603



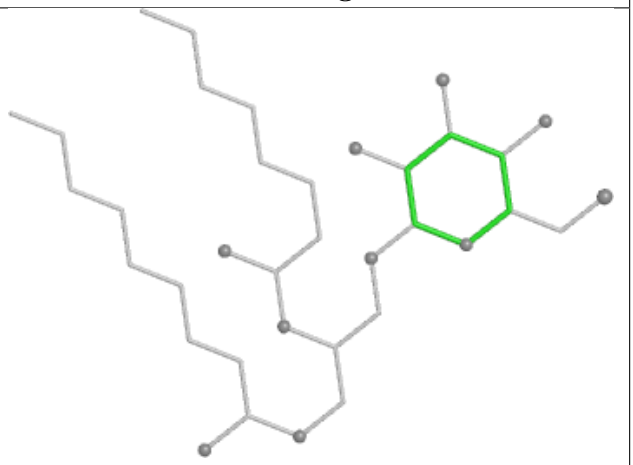
Bond lengths



Bond angles

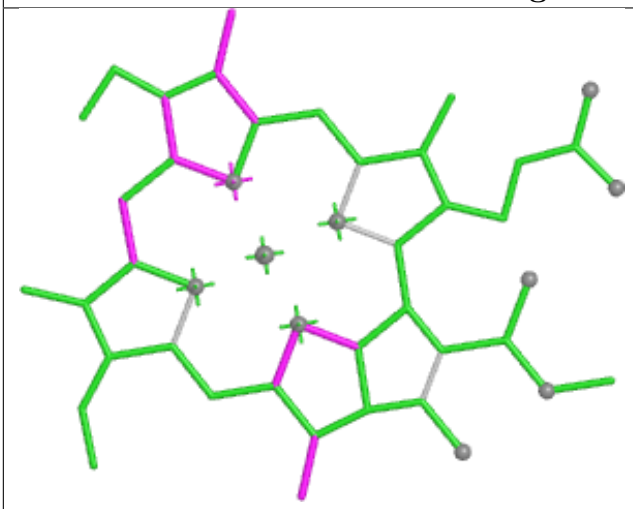


Torsions

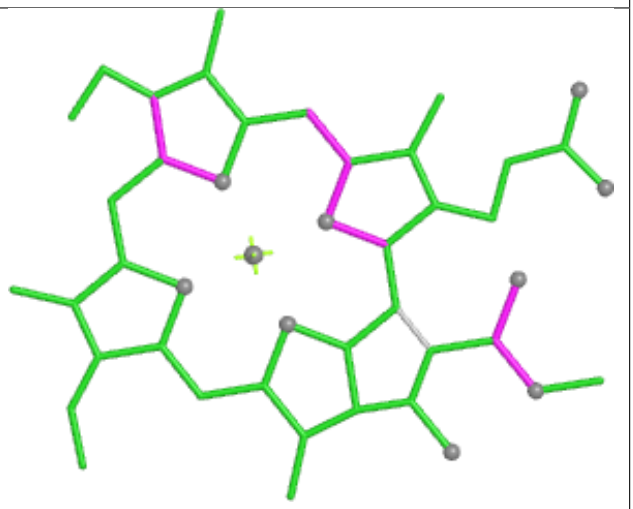


Rings

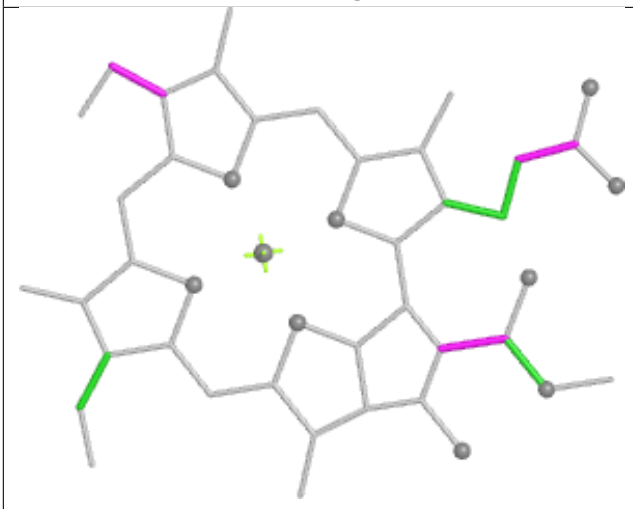
Ligand CLA c 612



Bond lengths



Bond angles

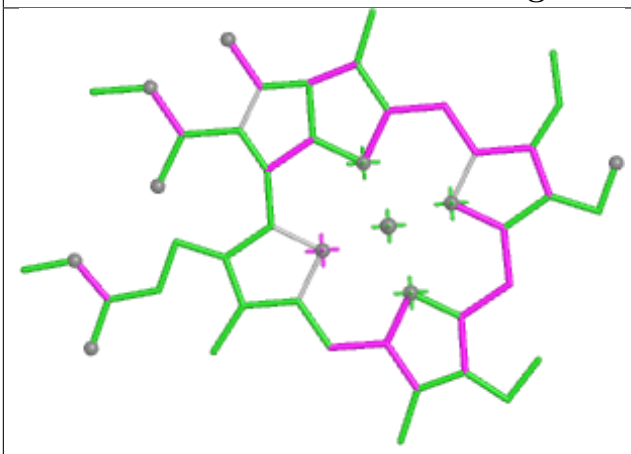


Torsions

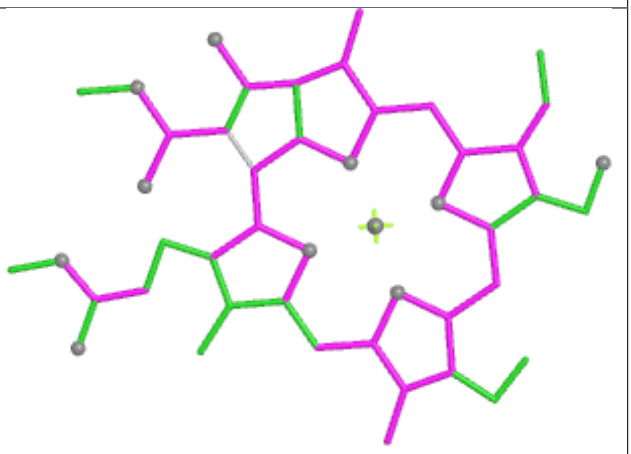


Rings

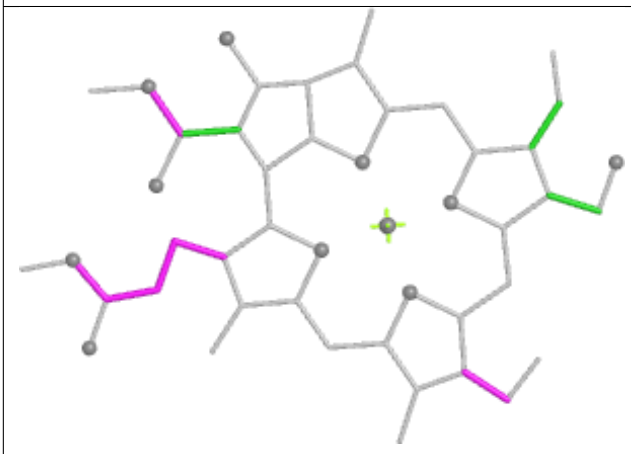
Ligand CHL 5 313



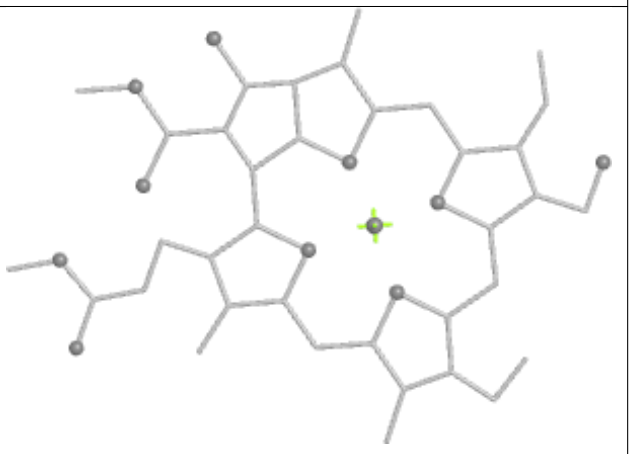
Bond lengths



Bond angles

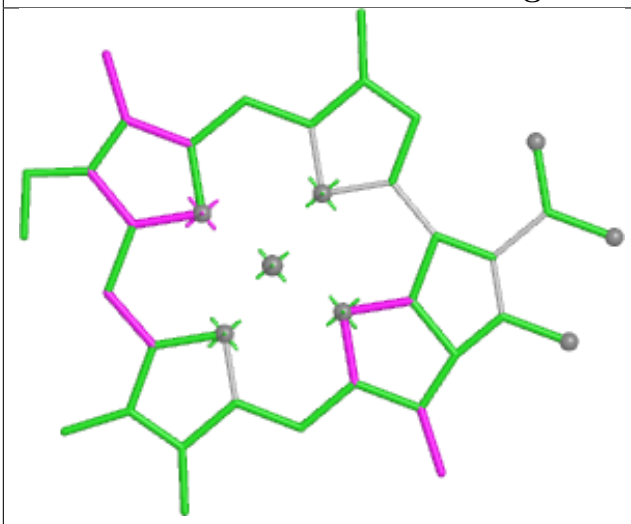


Torsions

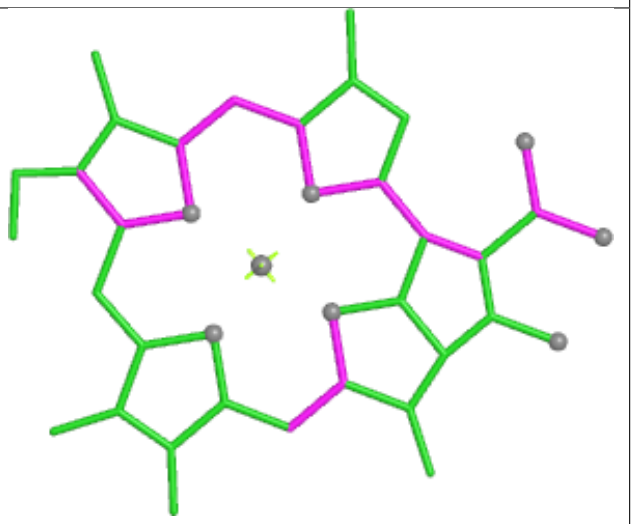


Rings

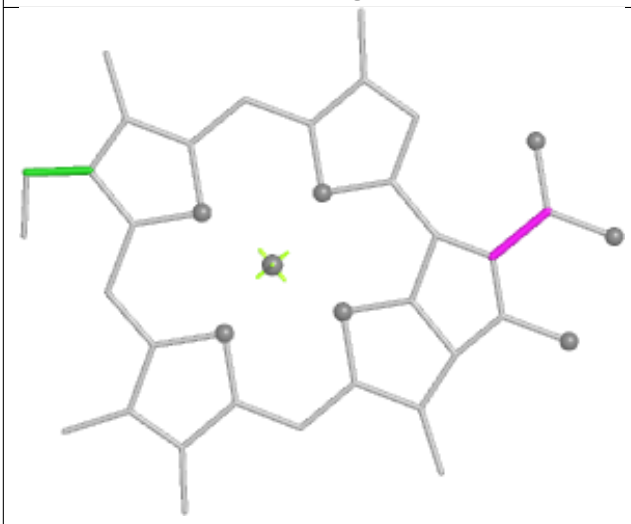
Ligand CLA O 202



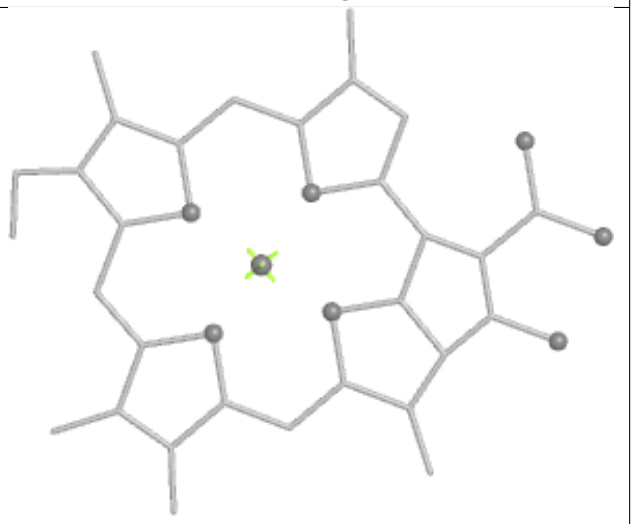
Bond lengths



Bond angles

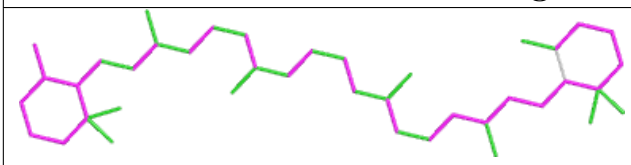


Torsions

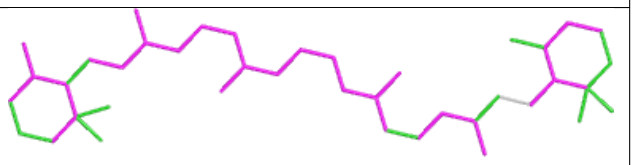


Rings

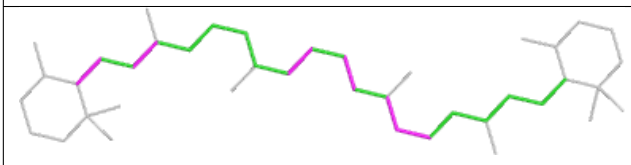
Ligand 8CT 6 402



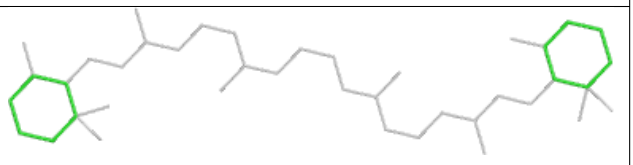
Bond lengths



Bond angles

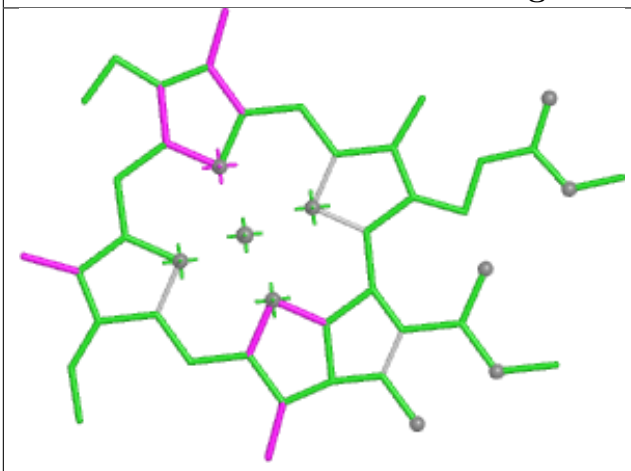


Torsions

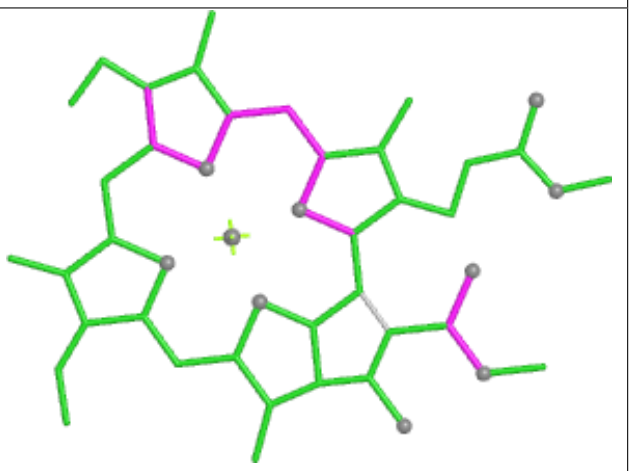


Rings

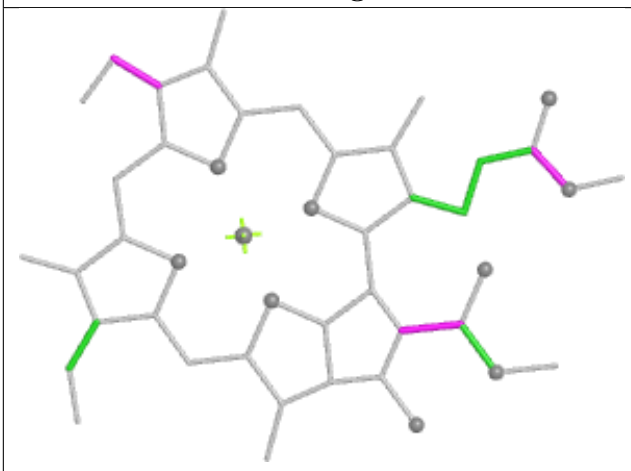
Ligand CLA 6 304



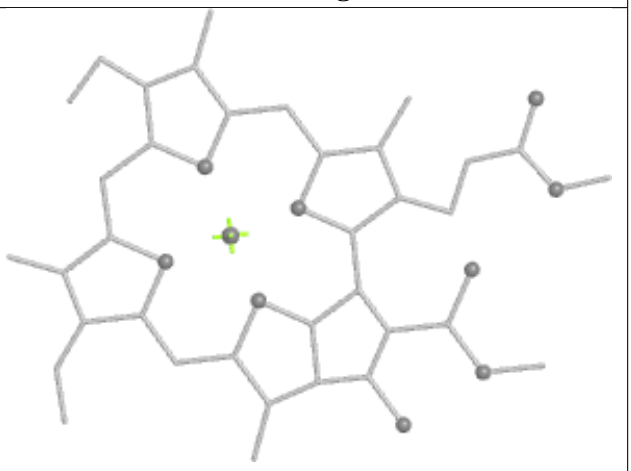
Bond lengths



Bond angles

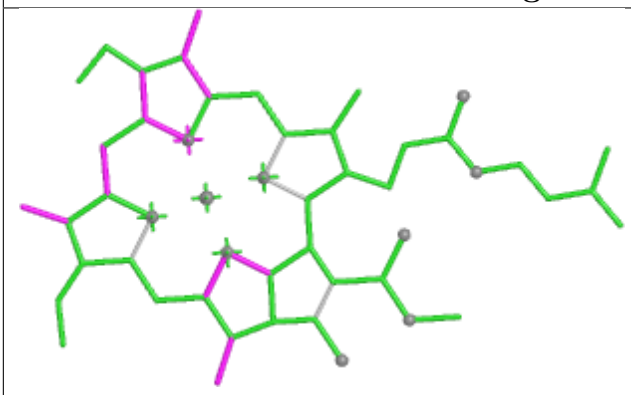


Torsions

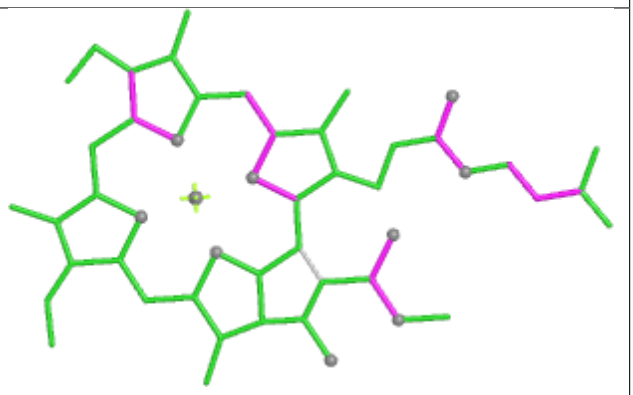


Rings

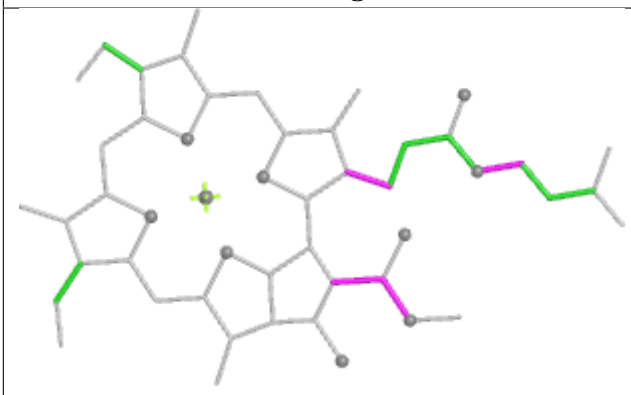
Ligand CLA G 101



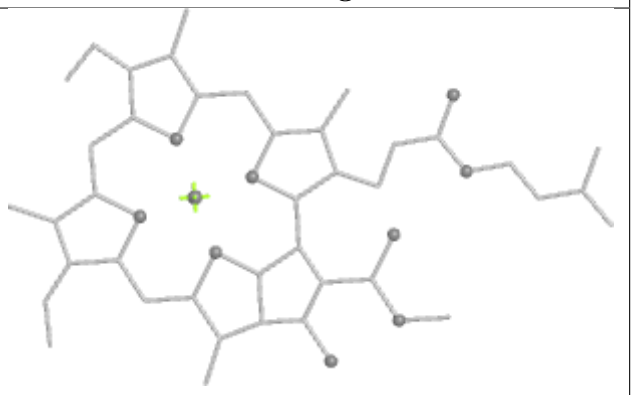
Bond lengths



Bond angles

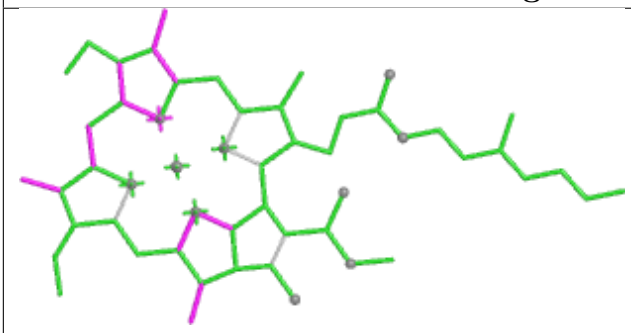


Torsions

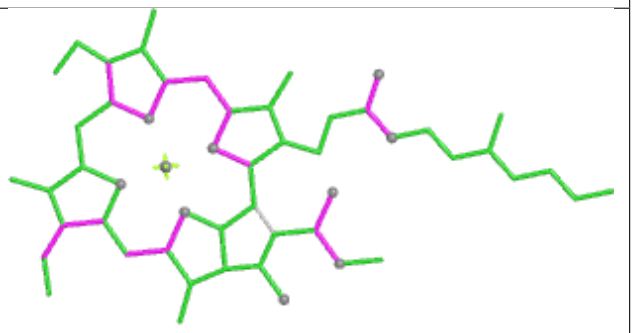


Rings

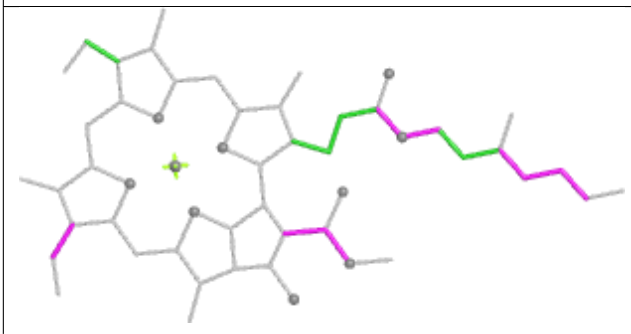
Ligand CLA K 102



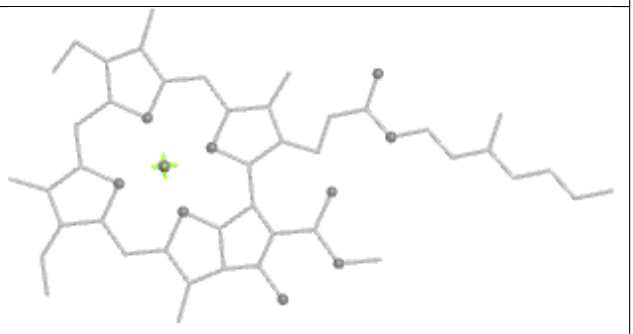
Bond lengths



Bond angles

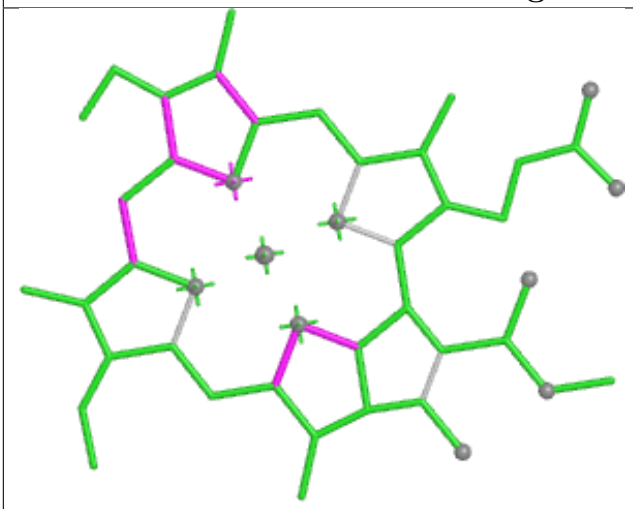


Torsions

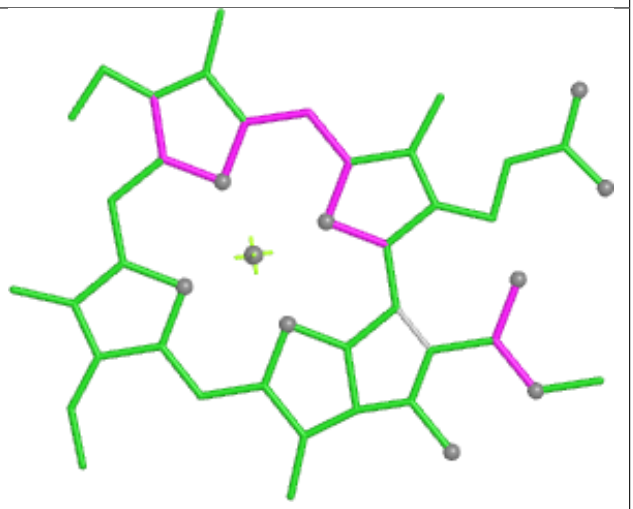


Rings

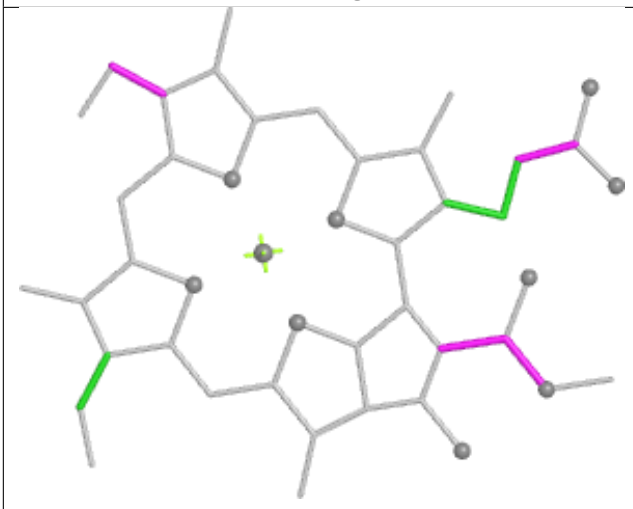
Ligand CLA h 612



Bond lengths



Bond angles

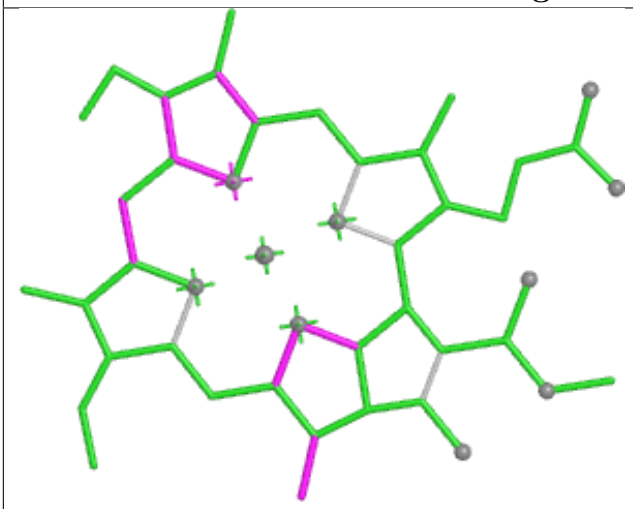


Torsions

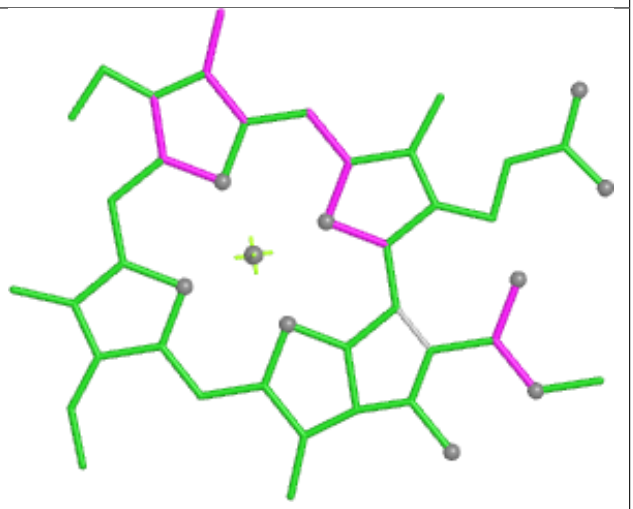


Rings

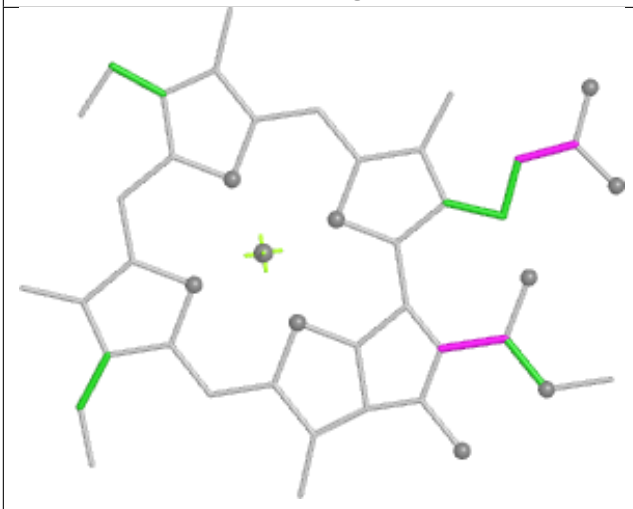
Ligand CLA i 612



Bond lengths



Bond angles

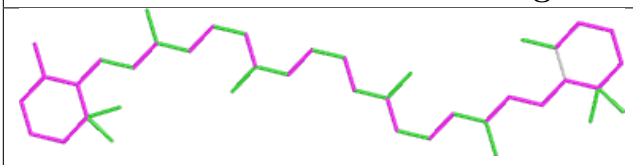


Torsions

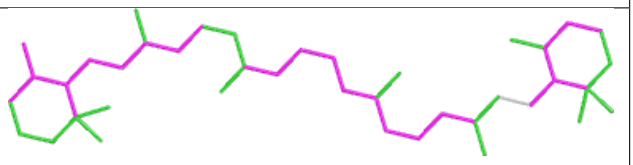


Rings

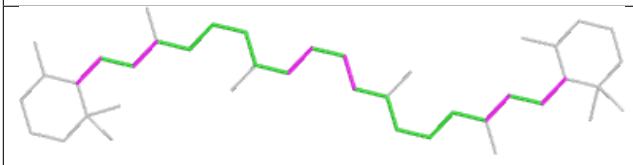
Ligand 8CT I 101



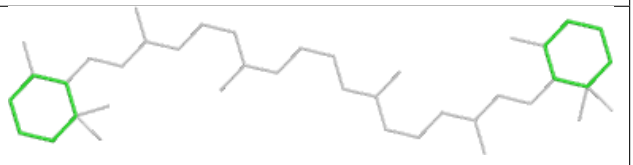
Bond lengths



Bond angles

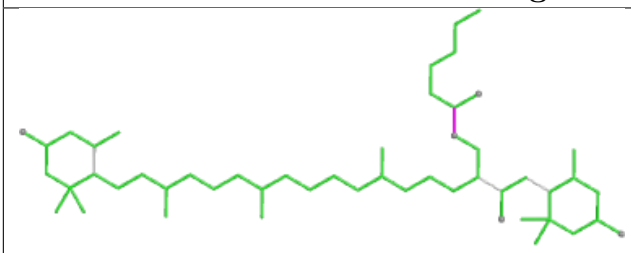


Torsions

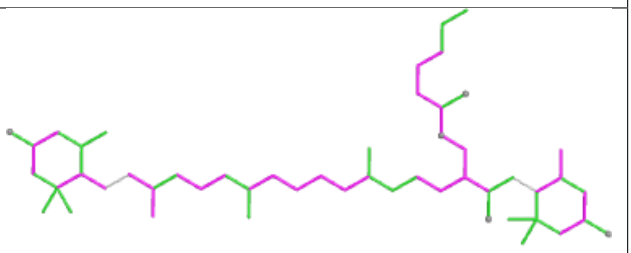


Rings

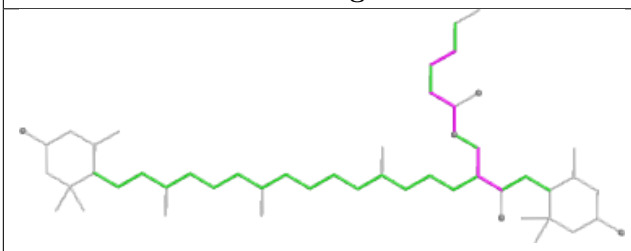
Ligand 0UR 7 501



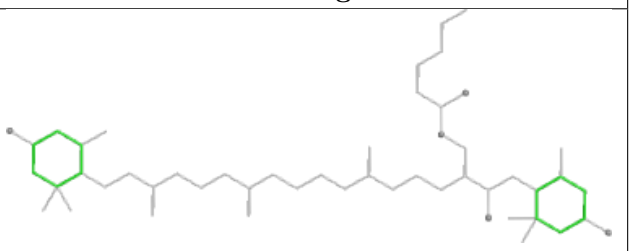
Bond lengths



Bond angles

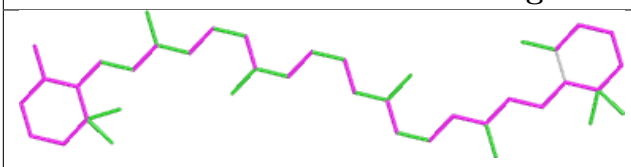


Torsions

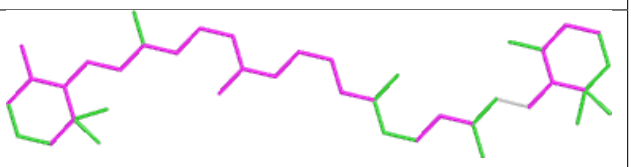


Rings

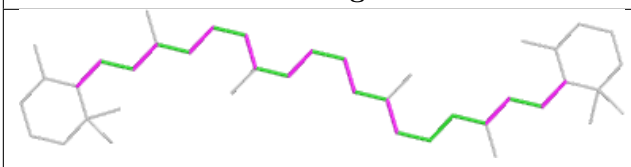
Ligand 8CT G 104



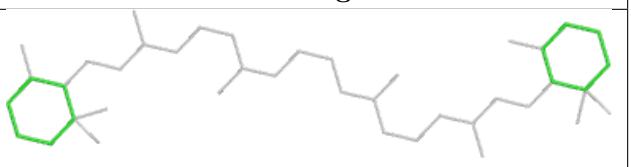
Bond lengths



Bond angles

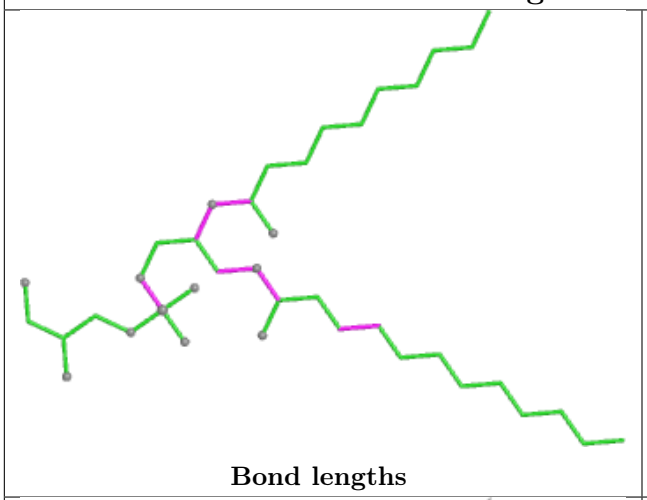


Torsions

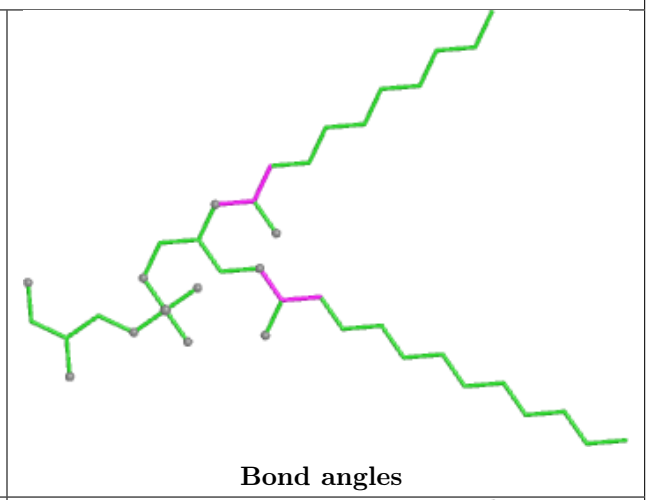


Rings

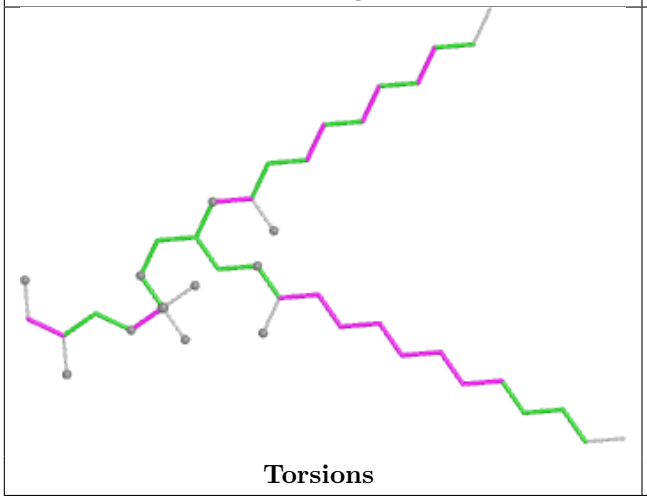
Ligand LHG h 630



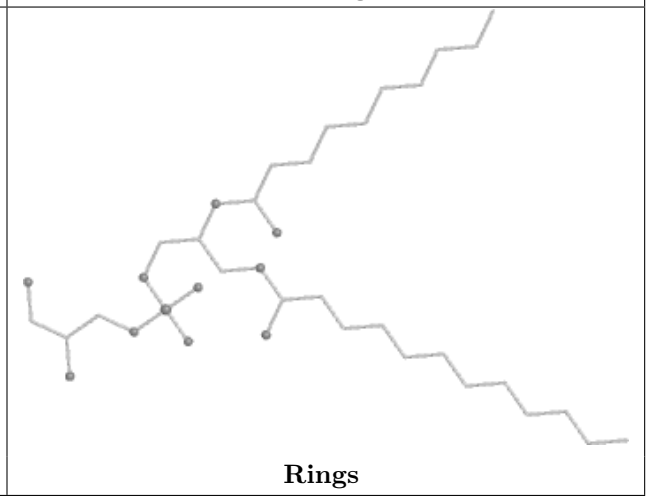
Bond lengths



Bond angles

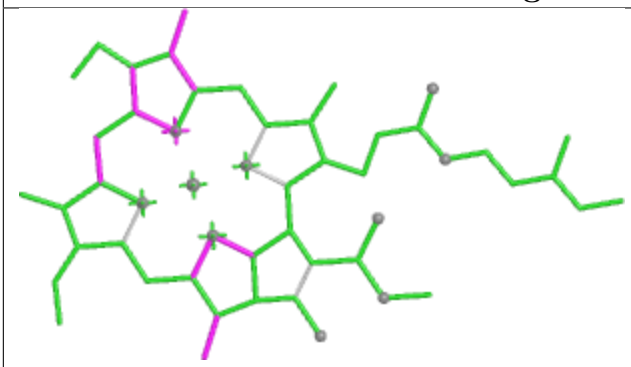


Torsions

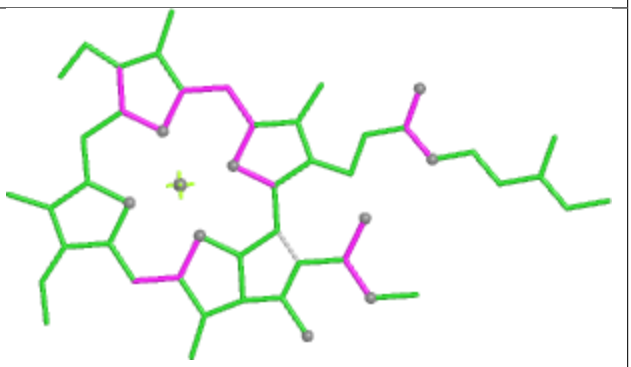


Rings

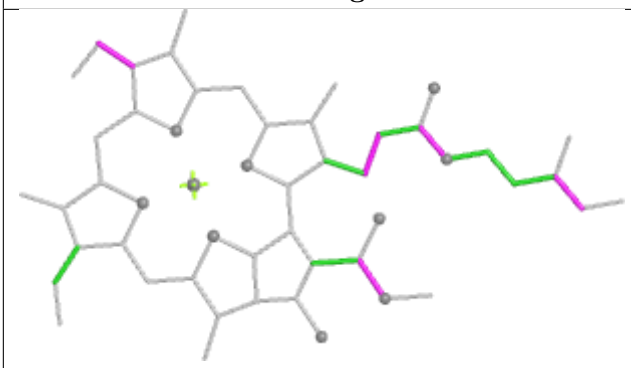
Ligand CLA H 205



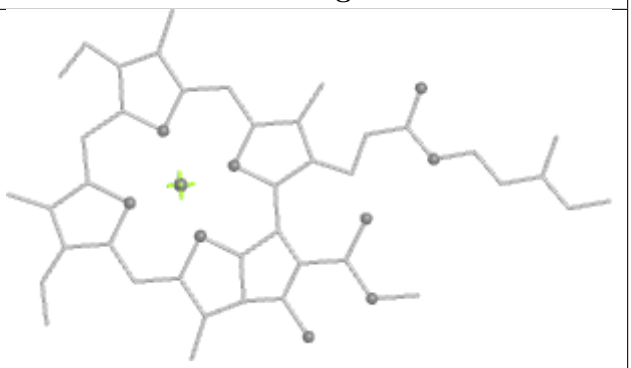
Bond lengths



Bond angles

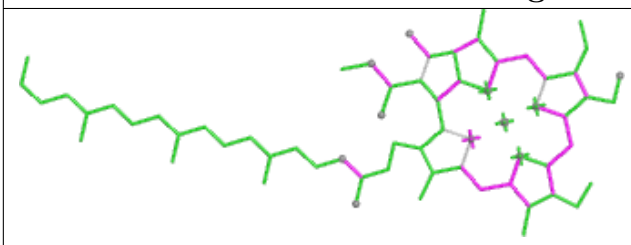


Torsions

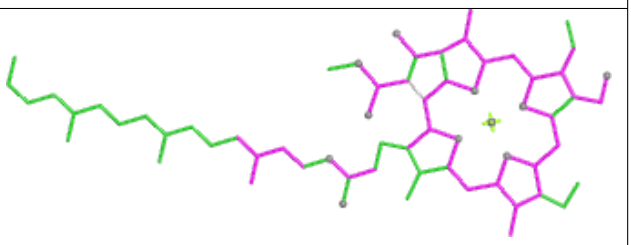


Rings

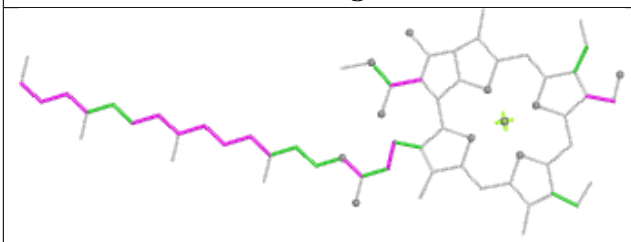
Ligand CHL 6 302



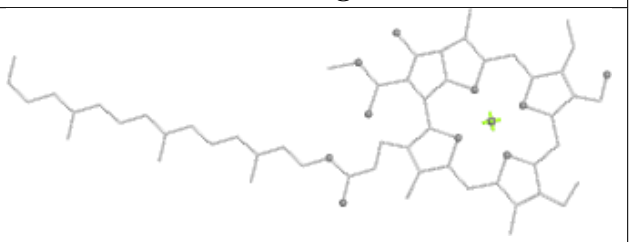
Bond lengths



Bond angles

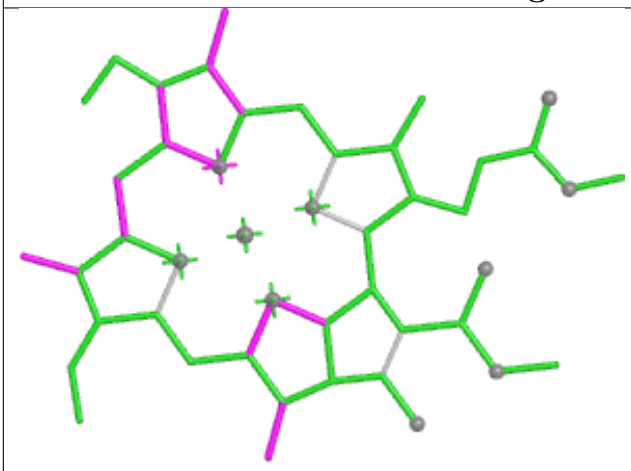


Torsions

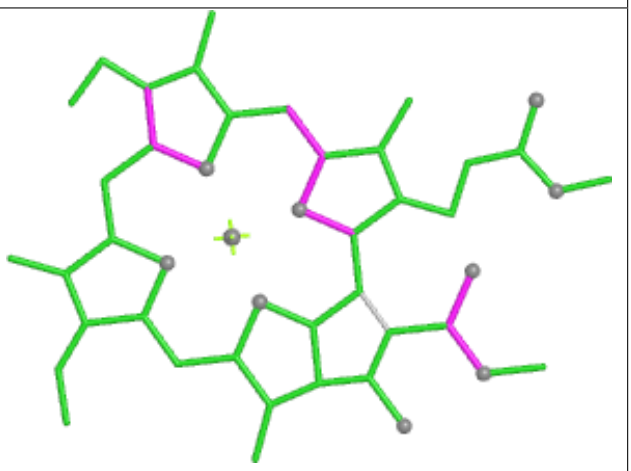


Rings

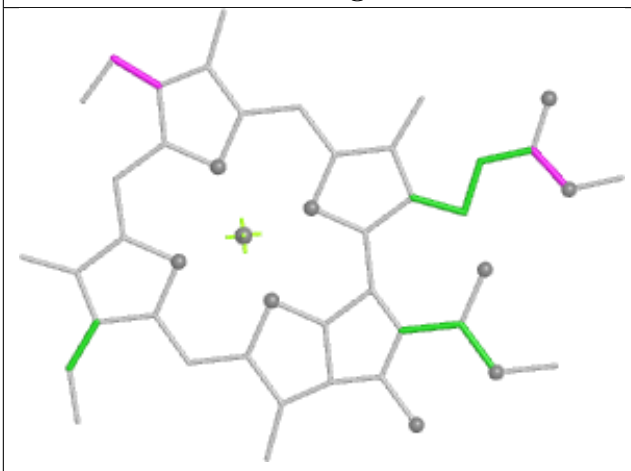
Ligand CLA 8 310



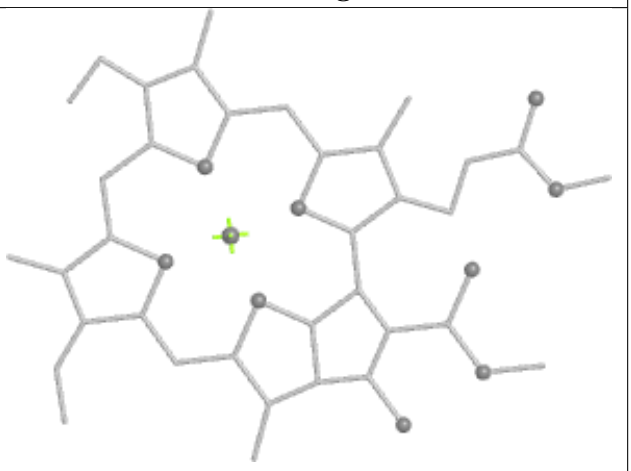
Bond lengths



Bond angles

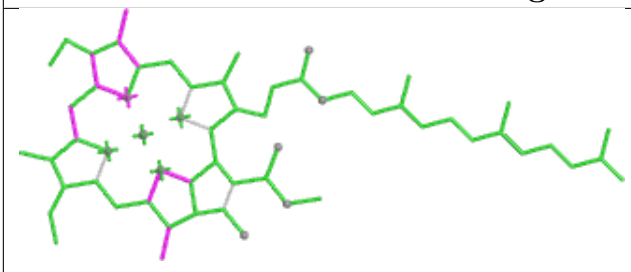


Torsions

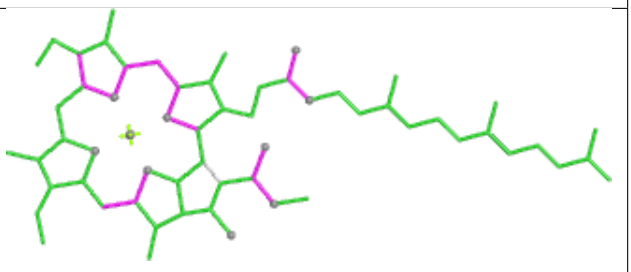


Rings

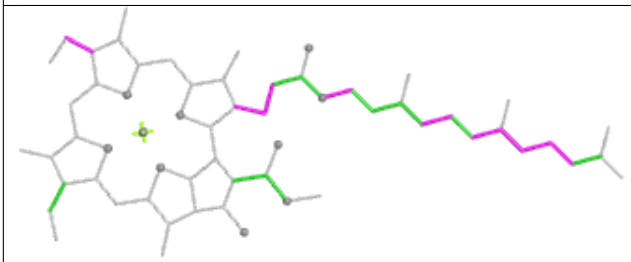
Ligand CLA 0 308



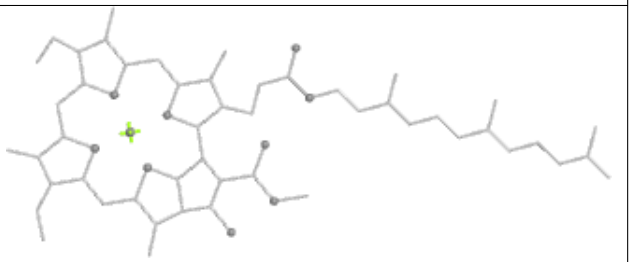
Bond lengths



Bond angles

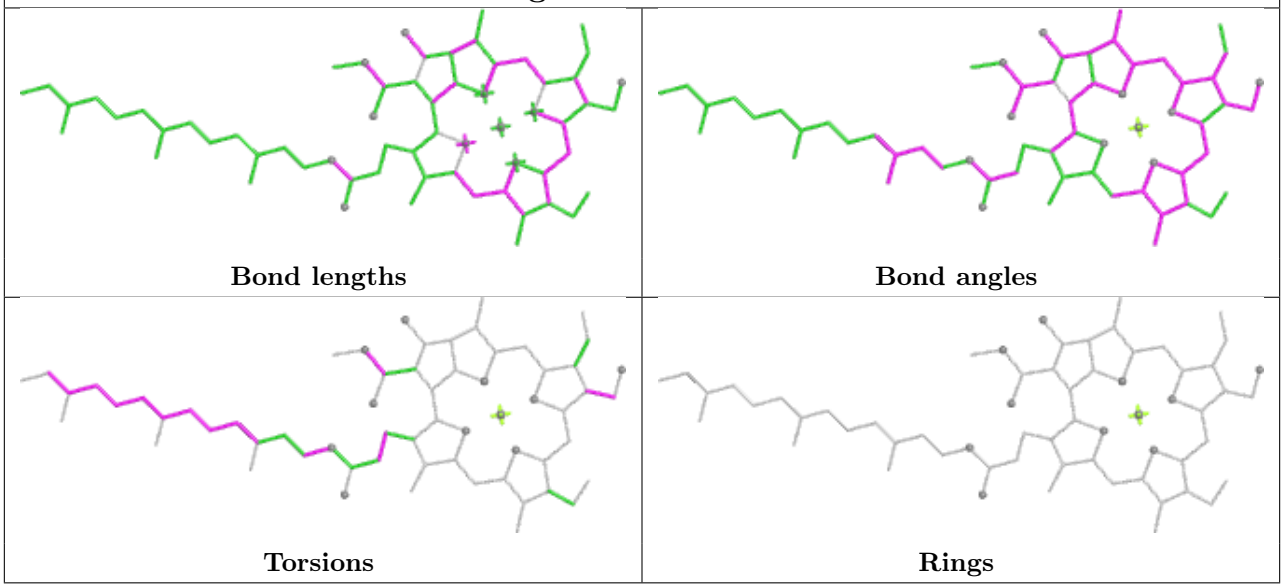


Torsions

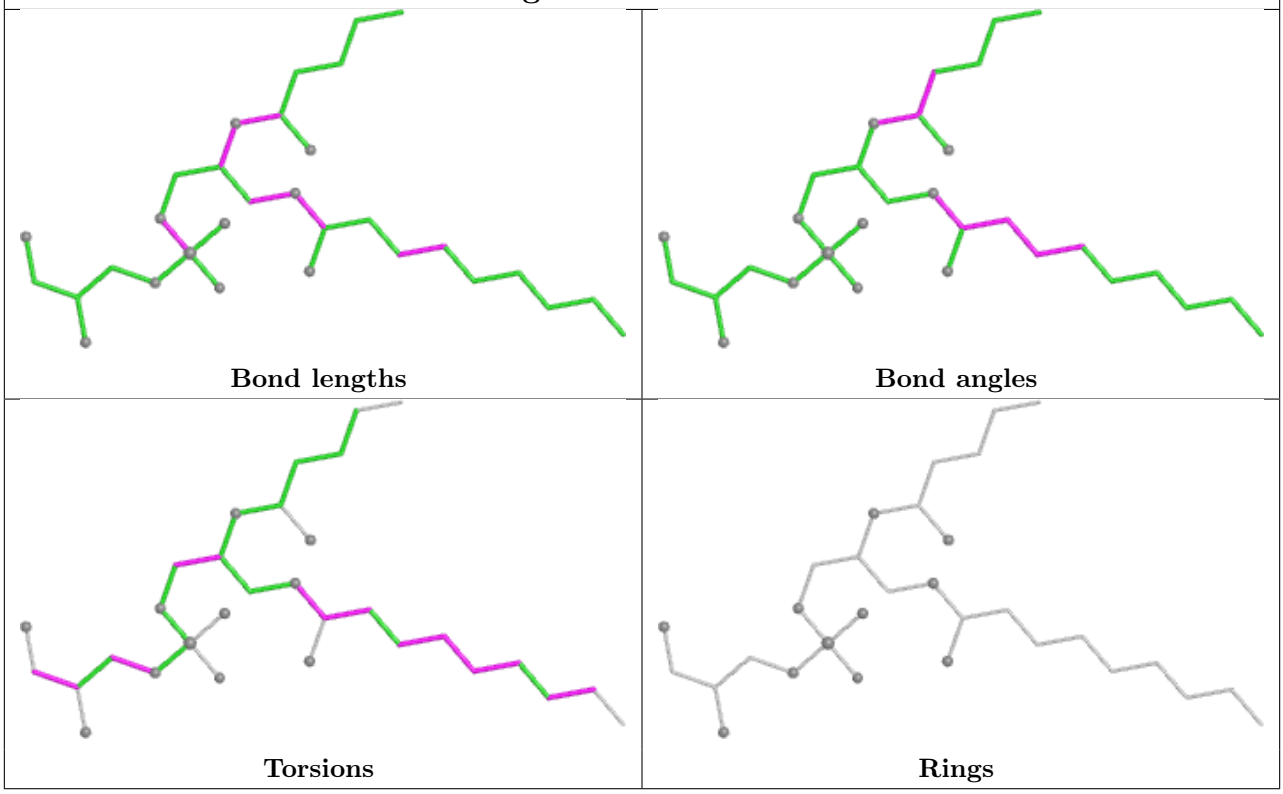


Rings

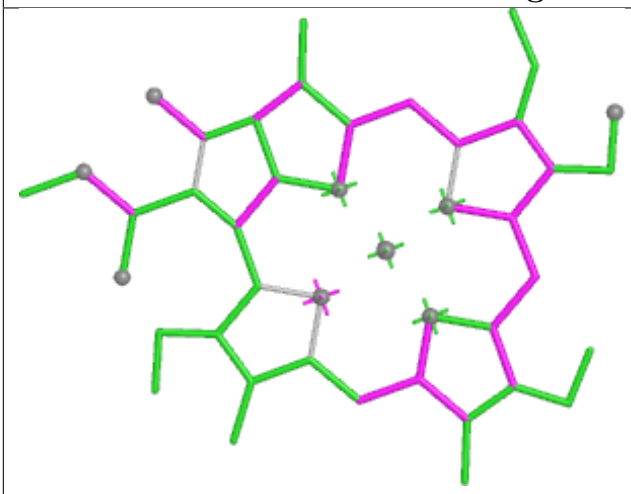
Ligand CHL 1 313



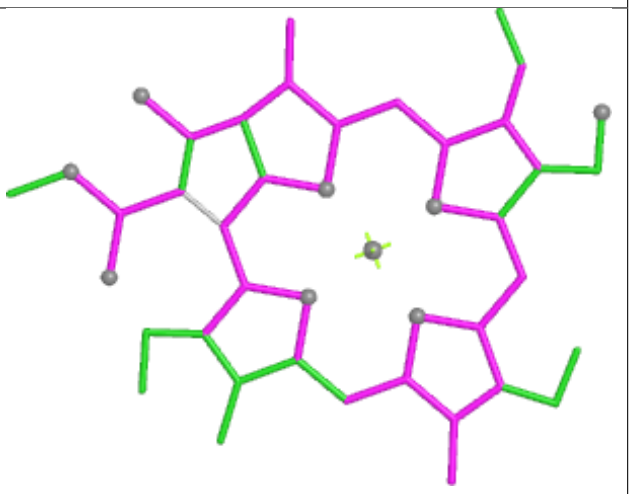
Ligand LHG H 203



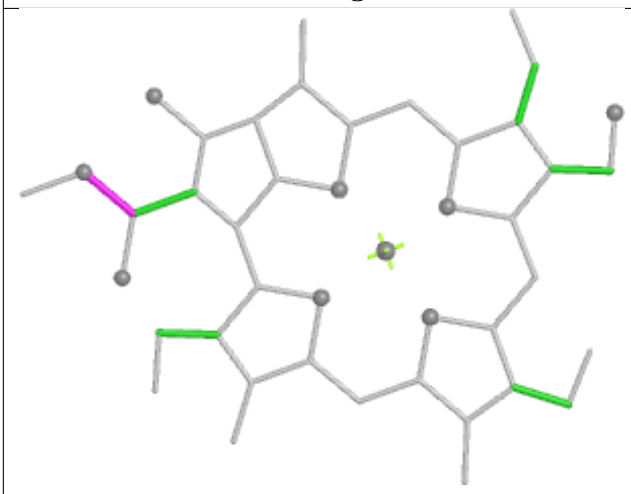
Ligand CHL h 605



Bond lengths



Bond angles

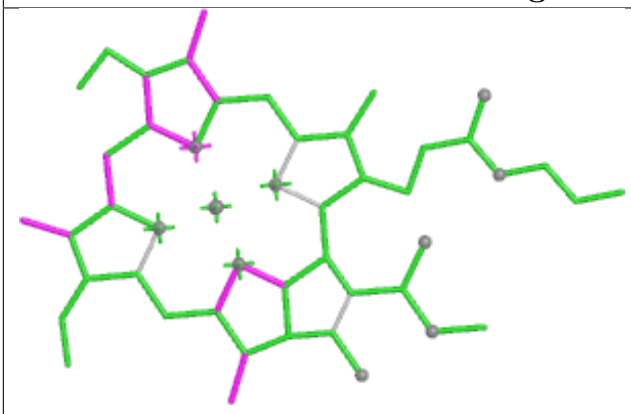


Torsions

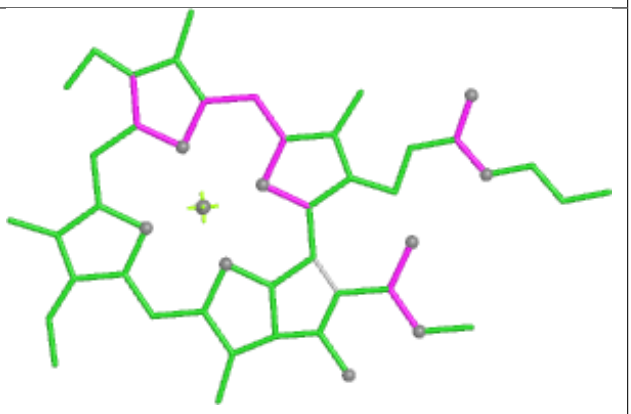


Rings

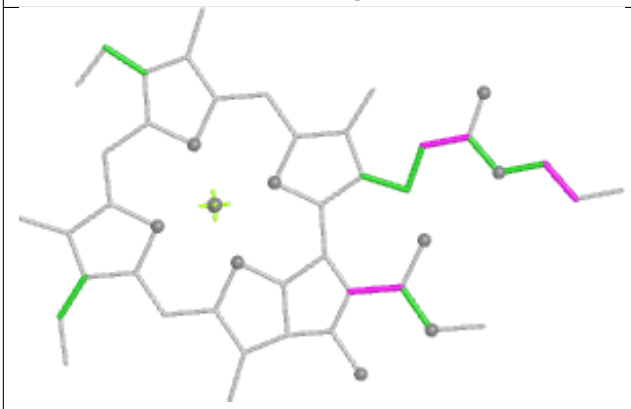
Ligand CLA 6 311



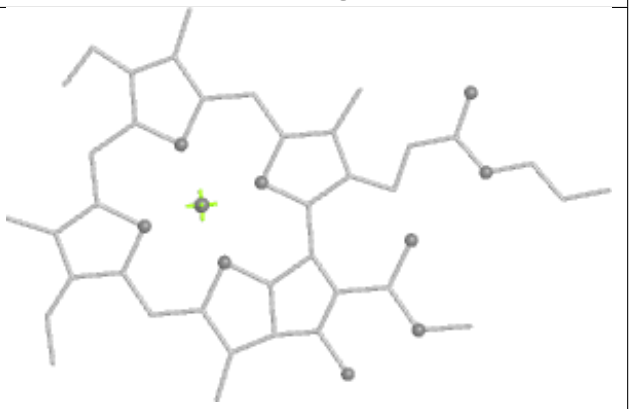
Bond lengths



Bond angles

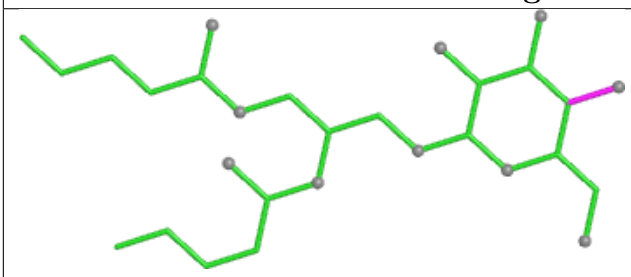


Torsions

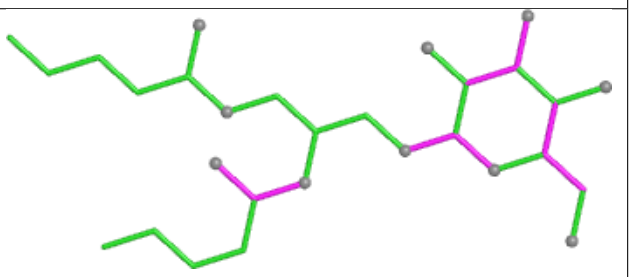


Rings

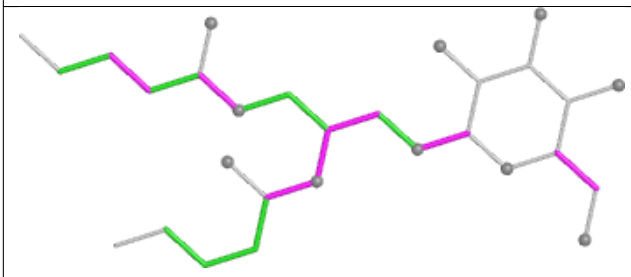
Ligand LMG J 102



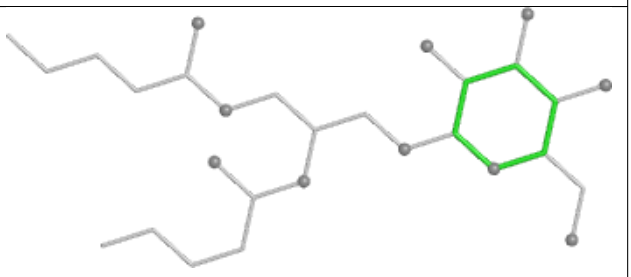
Bond lengths



Bond angles

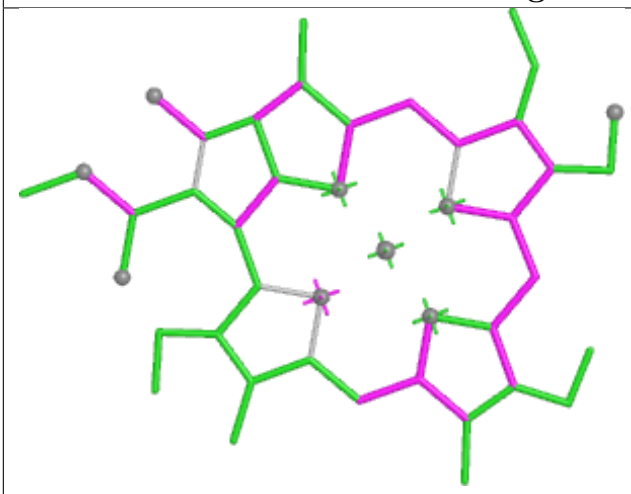


Torsions

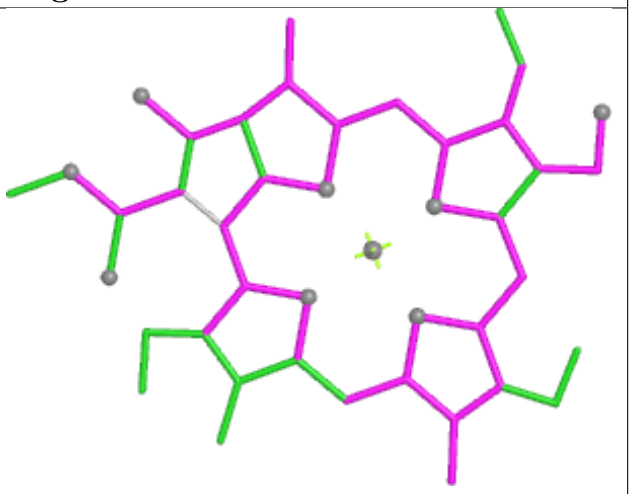


Rings

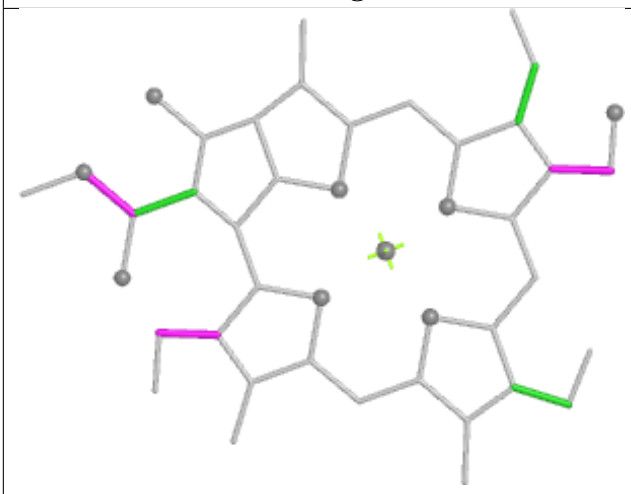
Ligand CHL g 608



Bond lengths



Bond angles

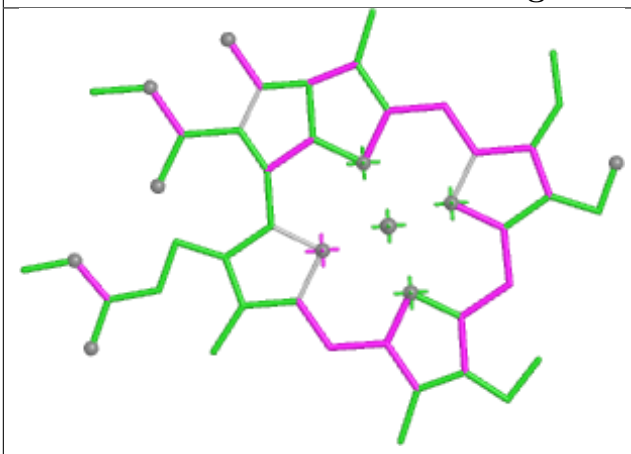


Torsions

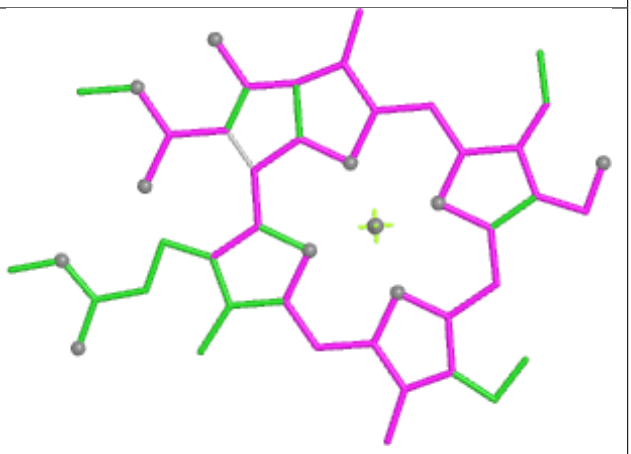


Rings

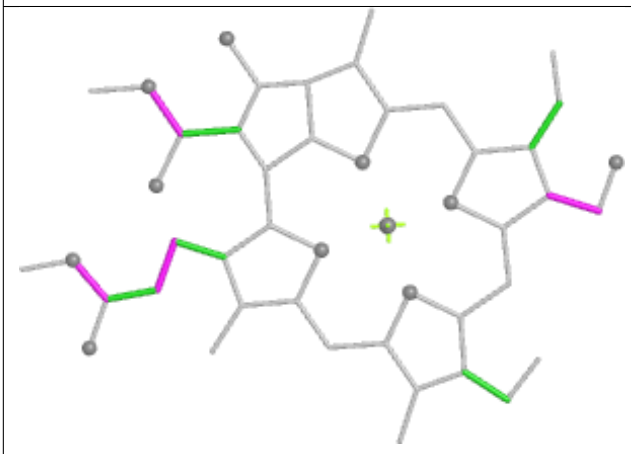
Ligand CHL 9 301



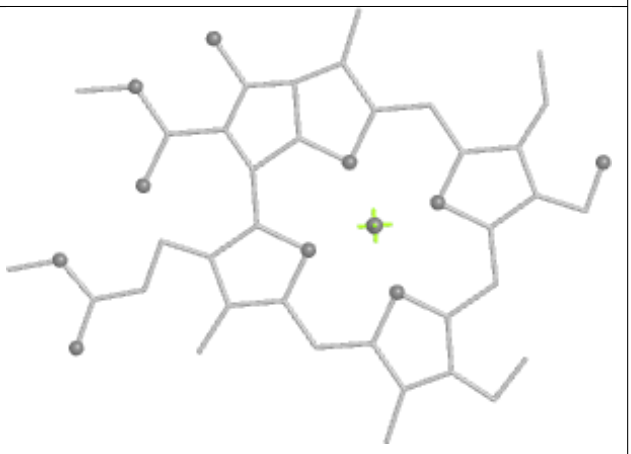
Bond lengths



Bond angles

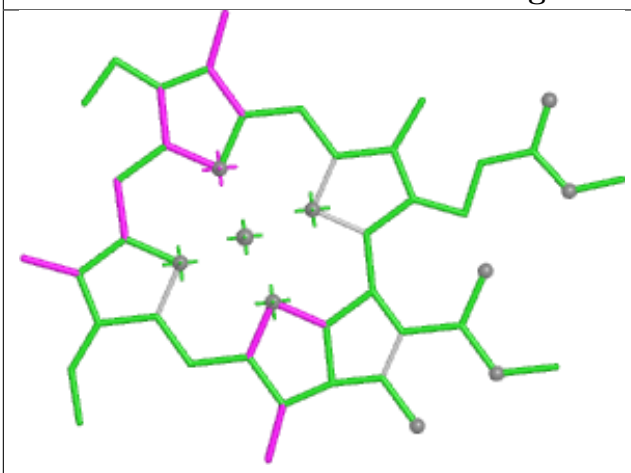


Torsions

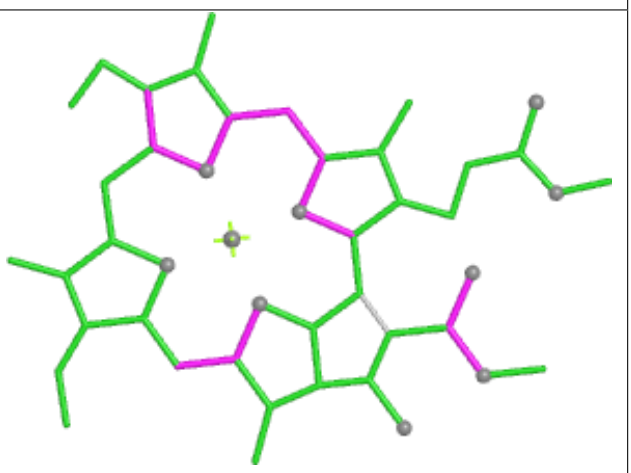


Rings

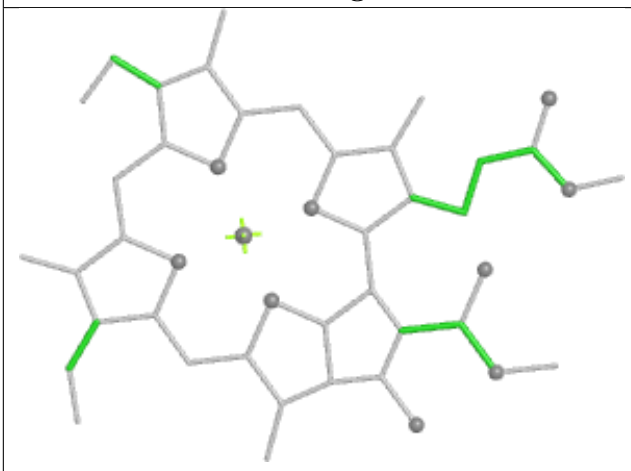
Ligand CLA 3 318



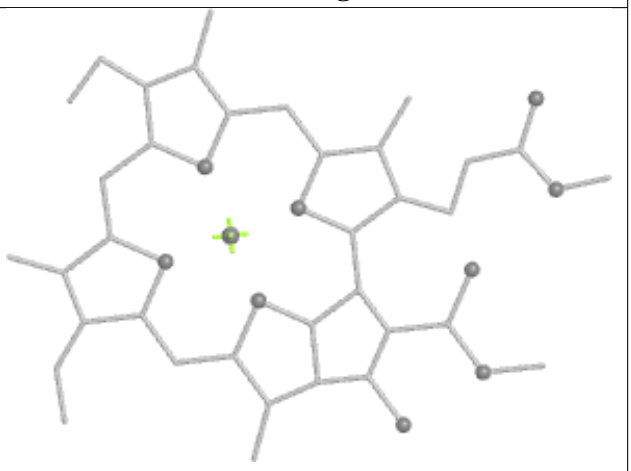
Bond lengths



Bond angles

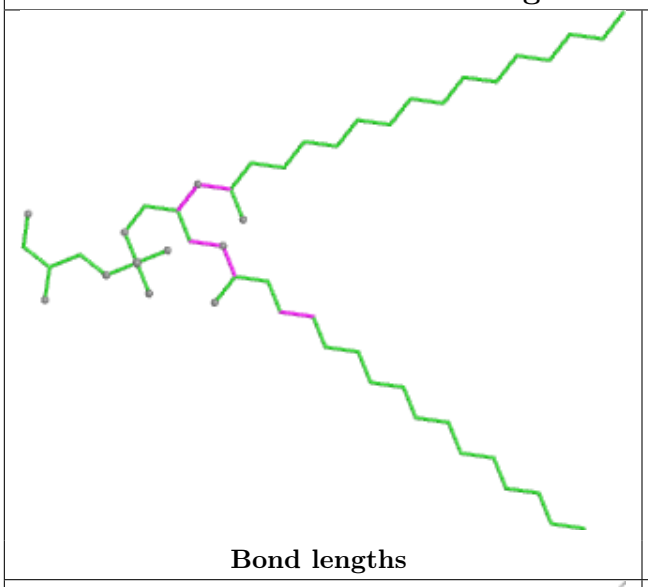


Torsions

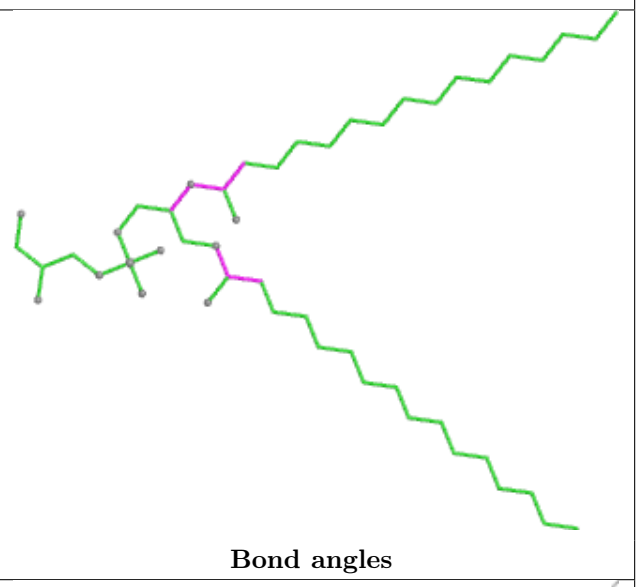


Rings

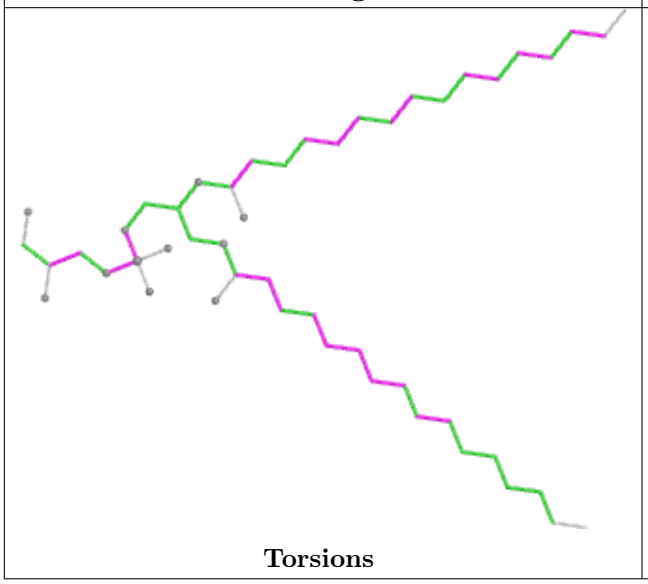
Ligand LHG A 844



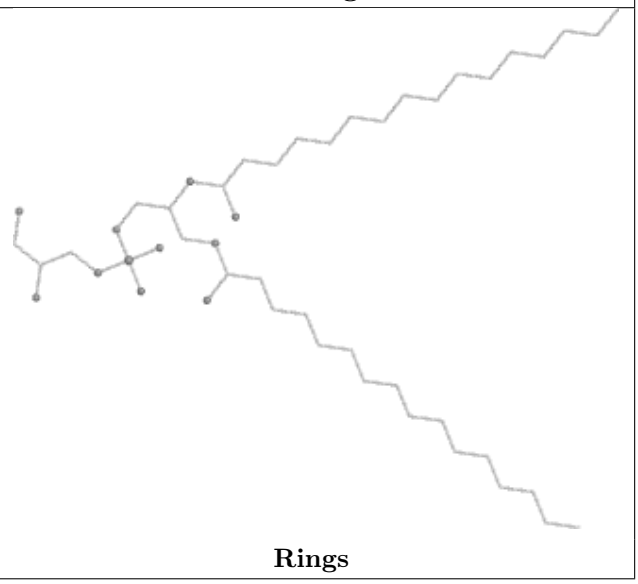
Bond lengths



Bond angles

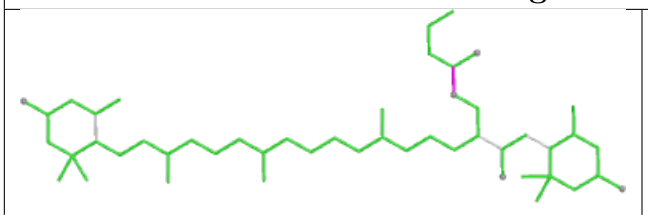


Torsions

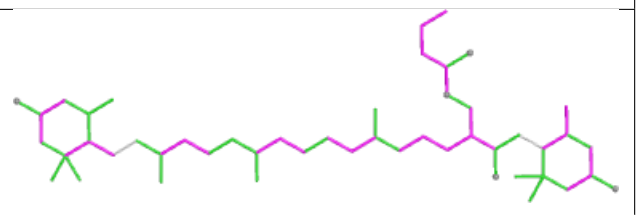


Rings

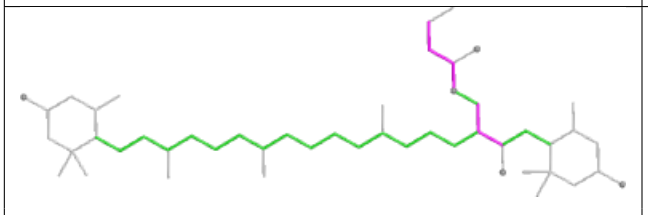
Ligand 0UR d 520



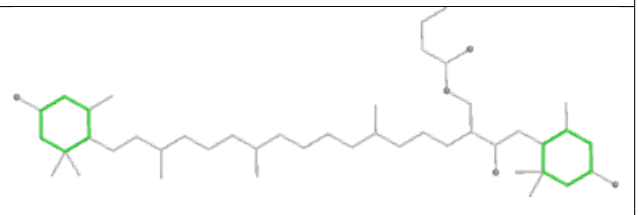
Bond lengths



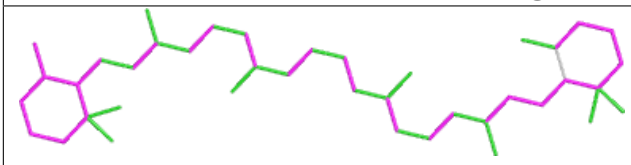
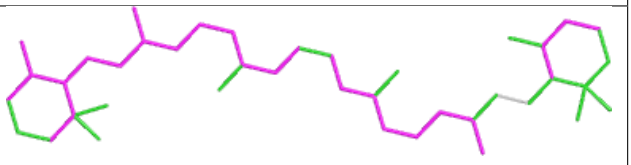
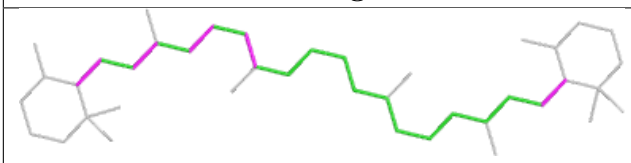
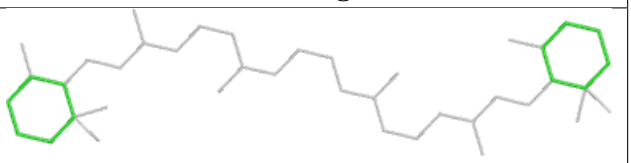
Bond angles

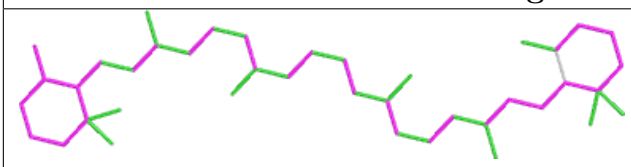
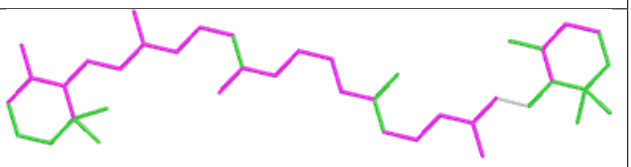
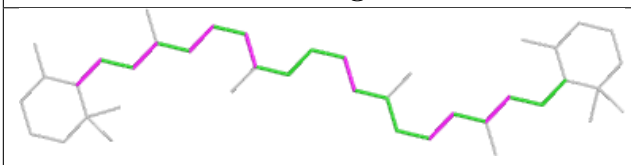
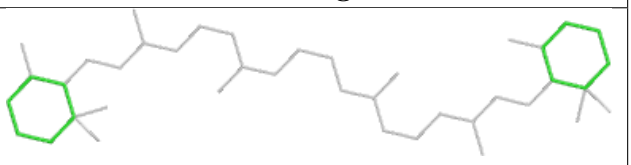


Torsions

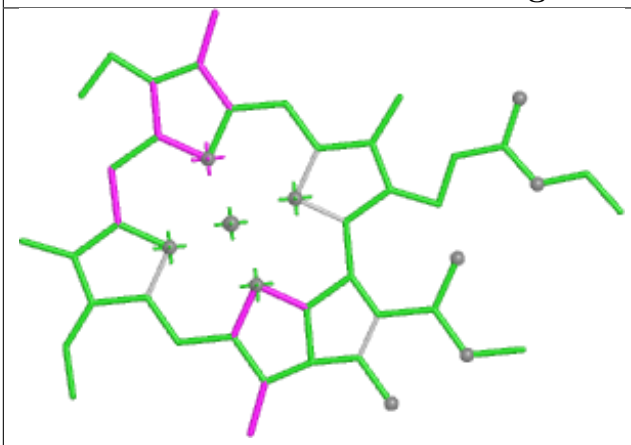


Rings

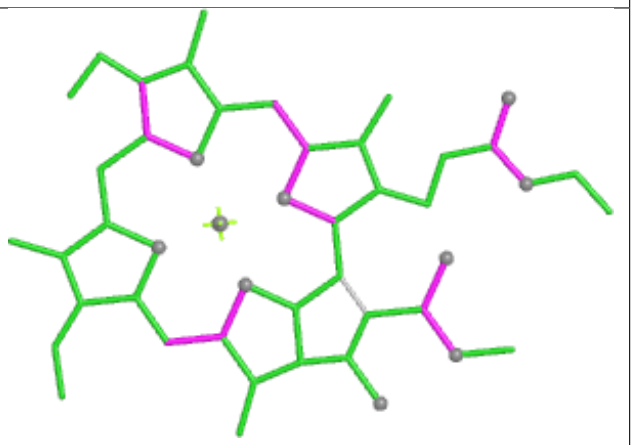
Ligand 8CT F 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

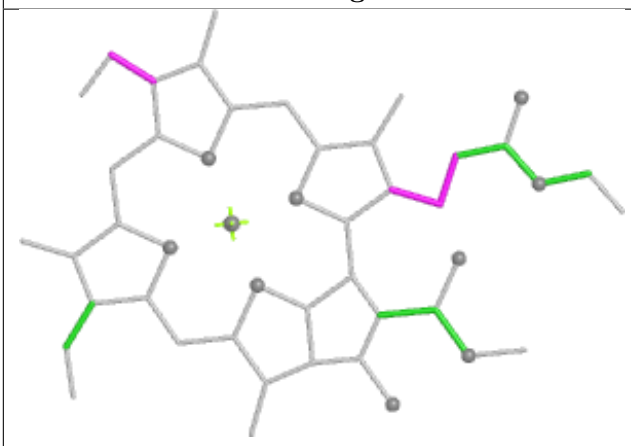
Ligand CLA 3 306



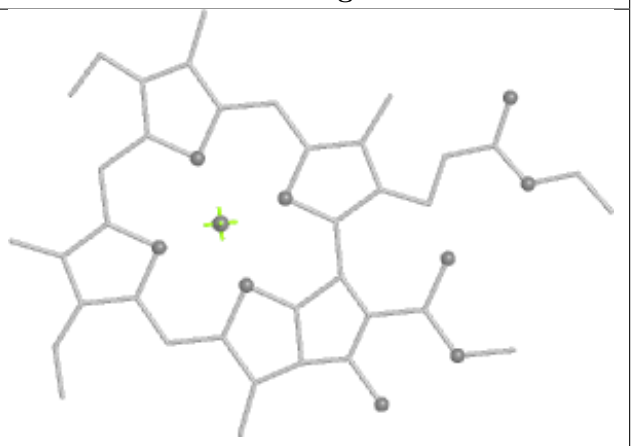
Bond lengths



Bond angles

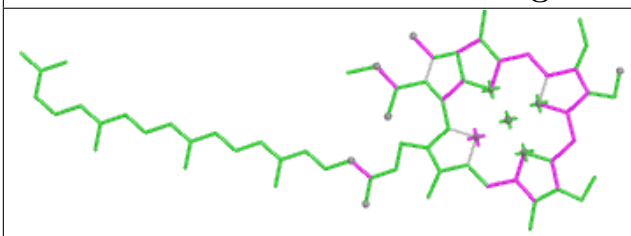


Torsions

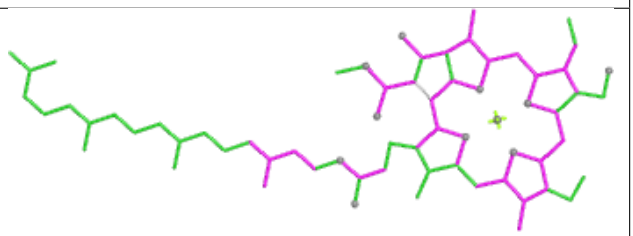


Rings

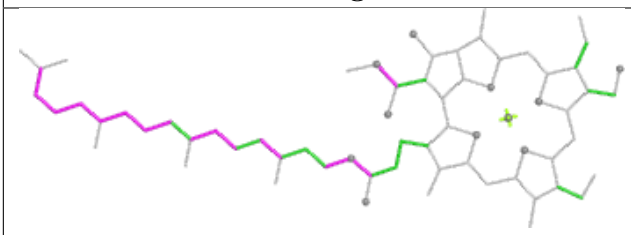
Ligand CHL f 609



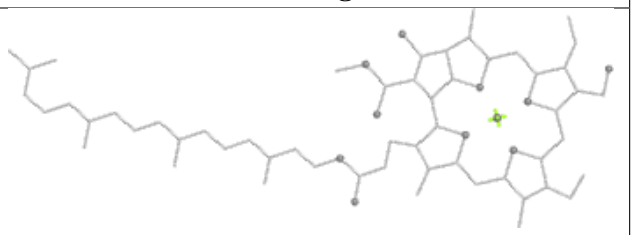
Bond lengths



Bond angles

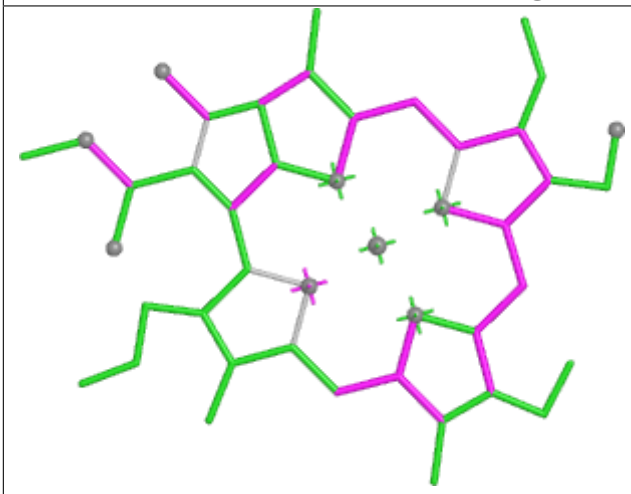


Torsions

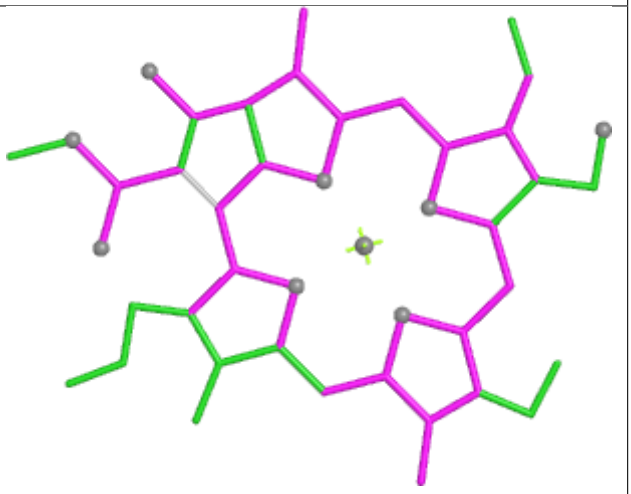


Rings

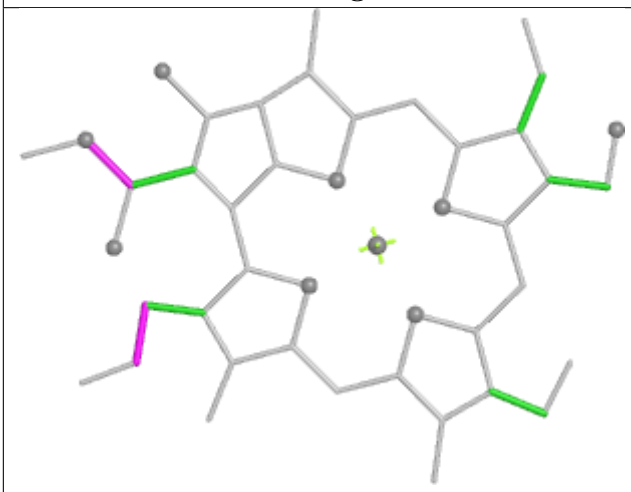
Ligand CHL c 606



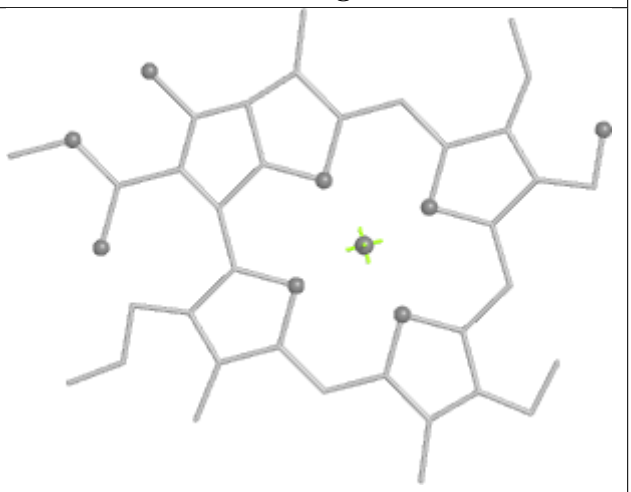
Bond lengths



Bond angles

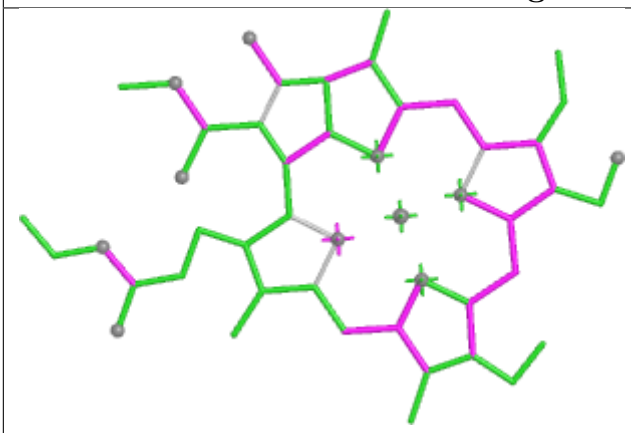


Torsions

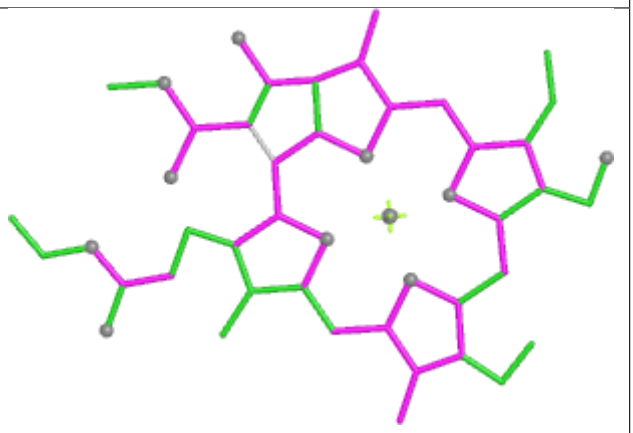


Rings

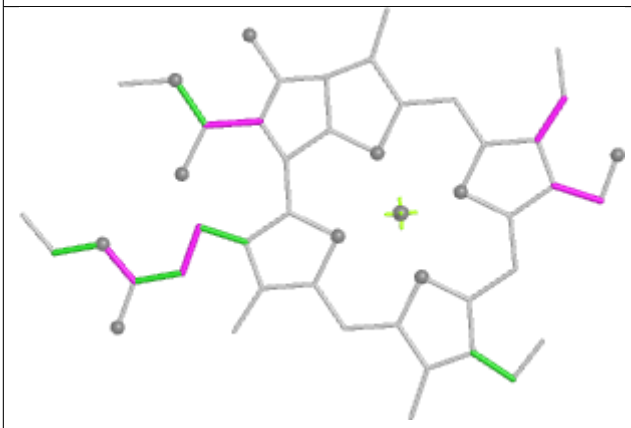
Ligand CHL 0 306



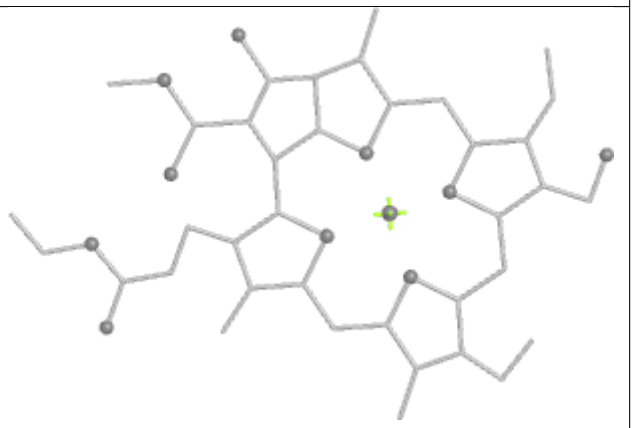
Bond lengths



Bond angles

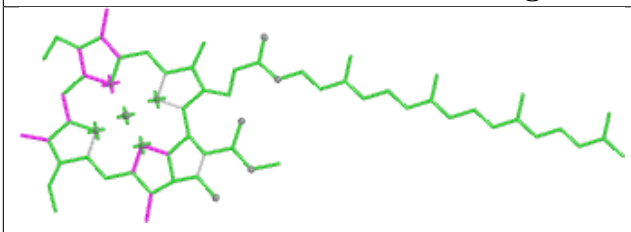


Torsions

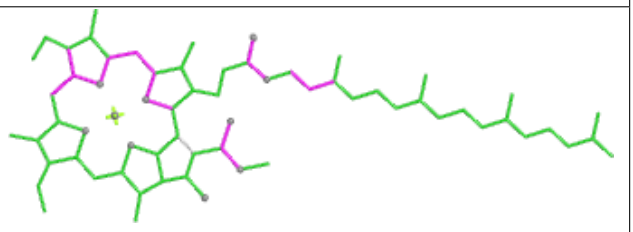


Rings

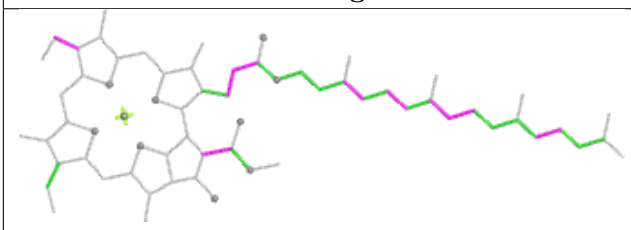
Ligand CLA A 809



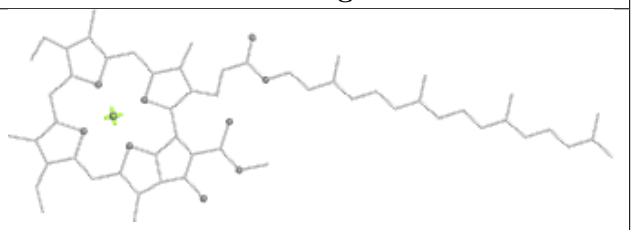
Bond lengths



Bond angles

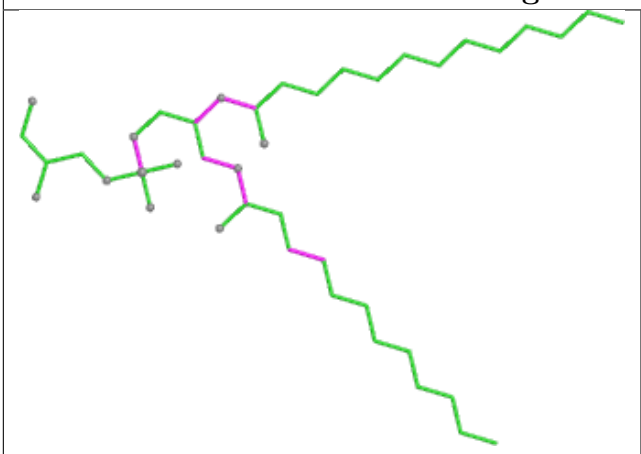


Torsions

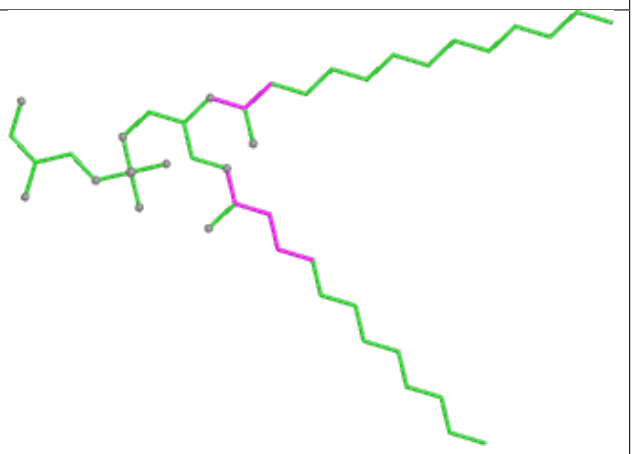


Rings

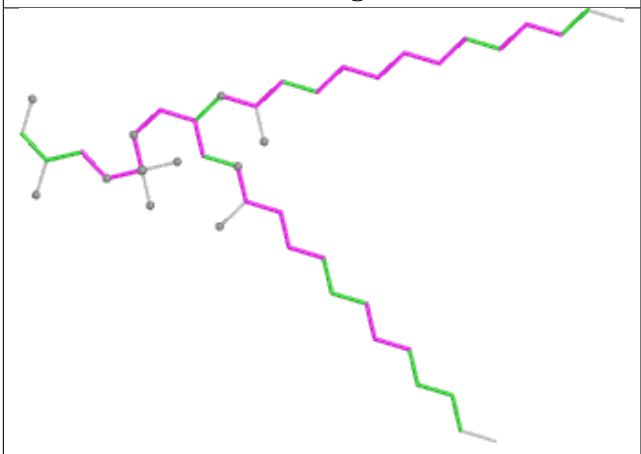
Ligand LHG A 855



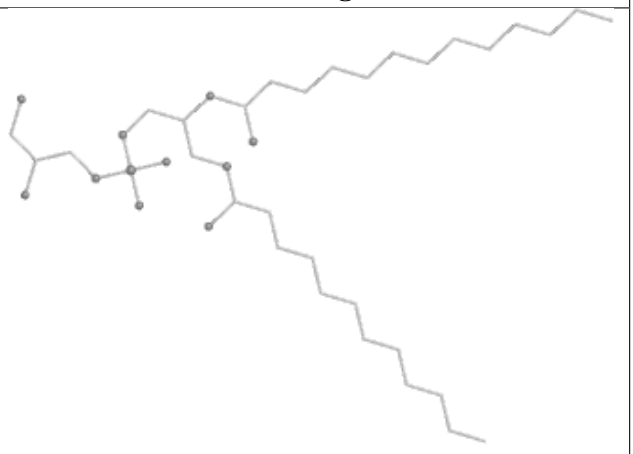
Bond lengths



Bond angles

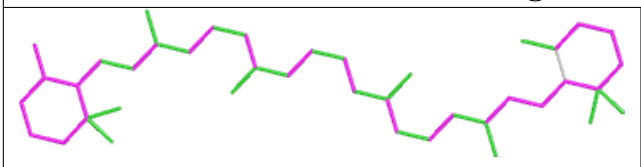


Torsions

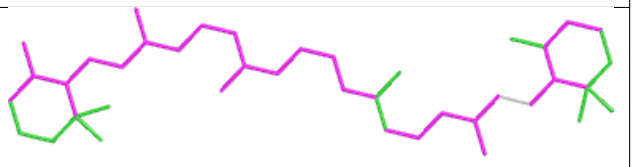


Rings

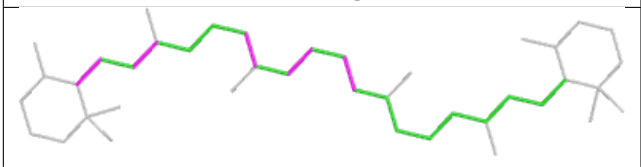
Ligand 8CT A 848



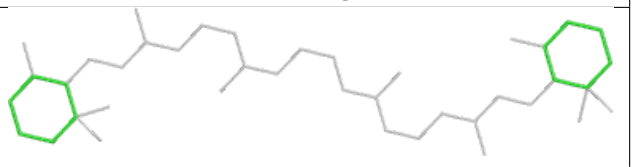
Bond lengths



Bond angles

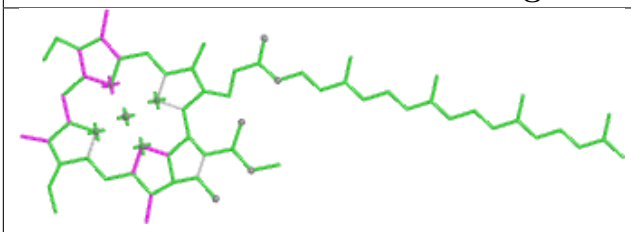


Torsions

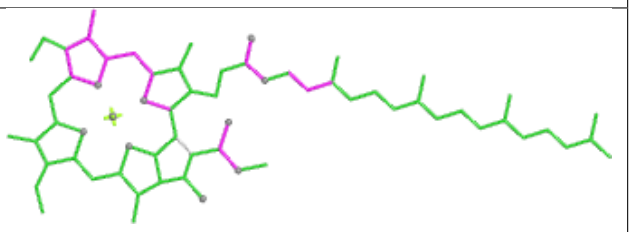


Rings

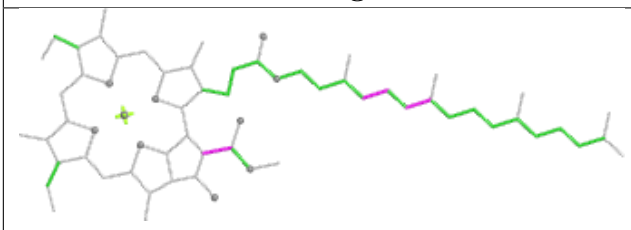
Ligand CLA A 827



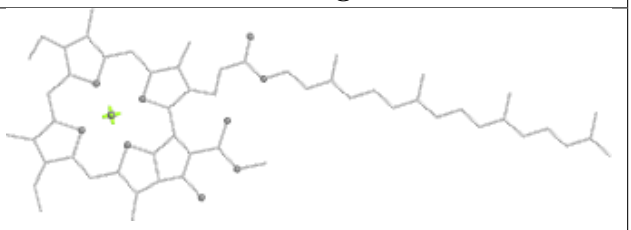
Bond lengths



Bond angles

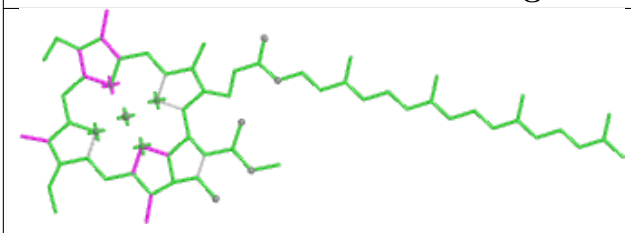


Torsions

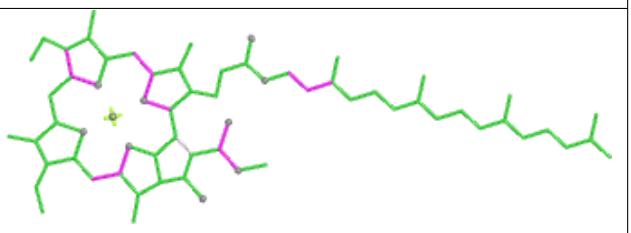


Rings

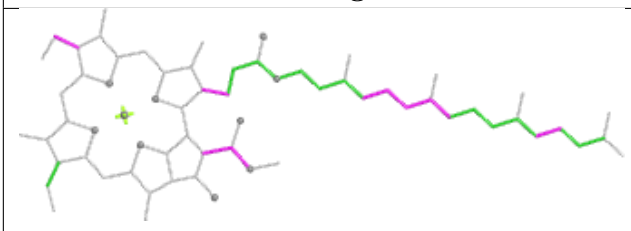
Ligand CLA A 832



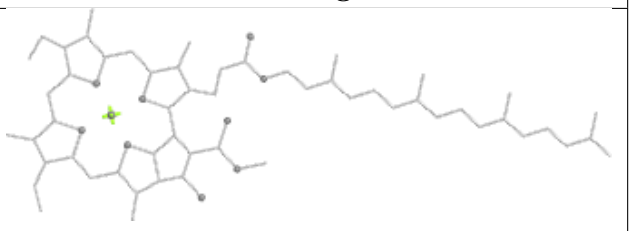
Bond lengths



Bond angles

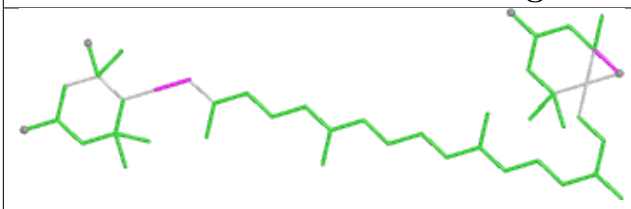


Torsions

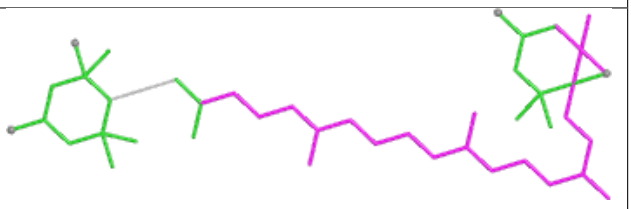


Rings

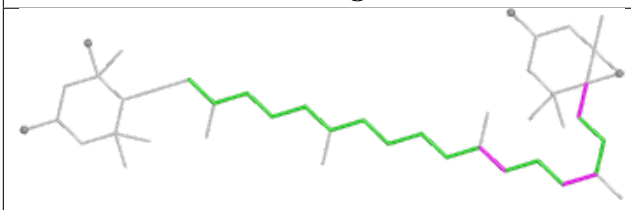
Ligand NEX a 523



Bond lengths



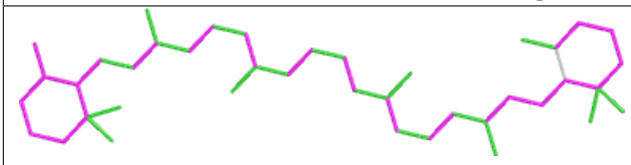
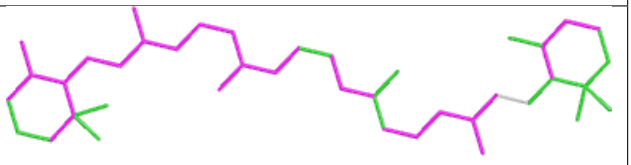
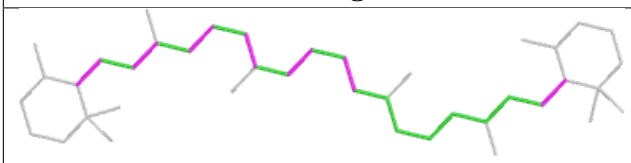
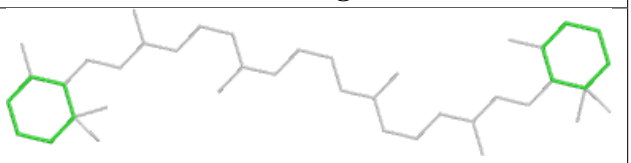
Bond angles

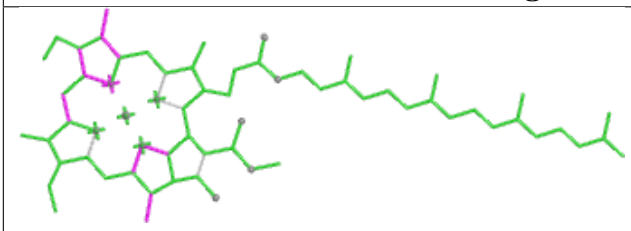
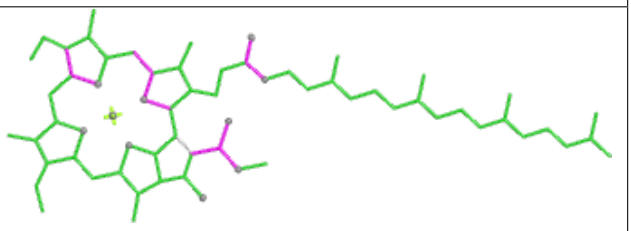
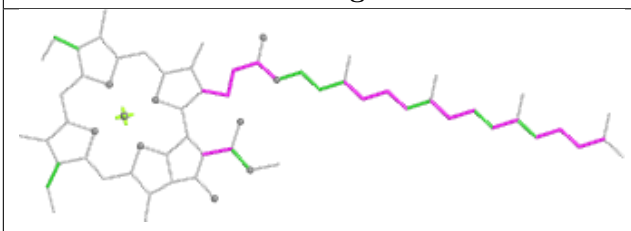
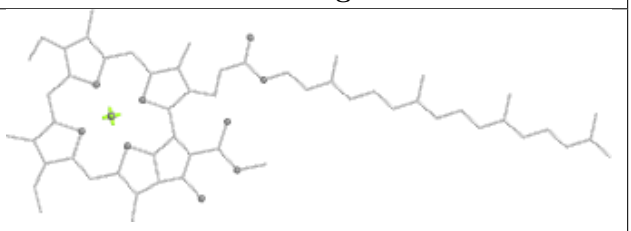


Torsions

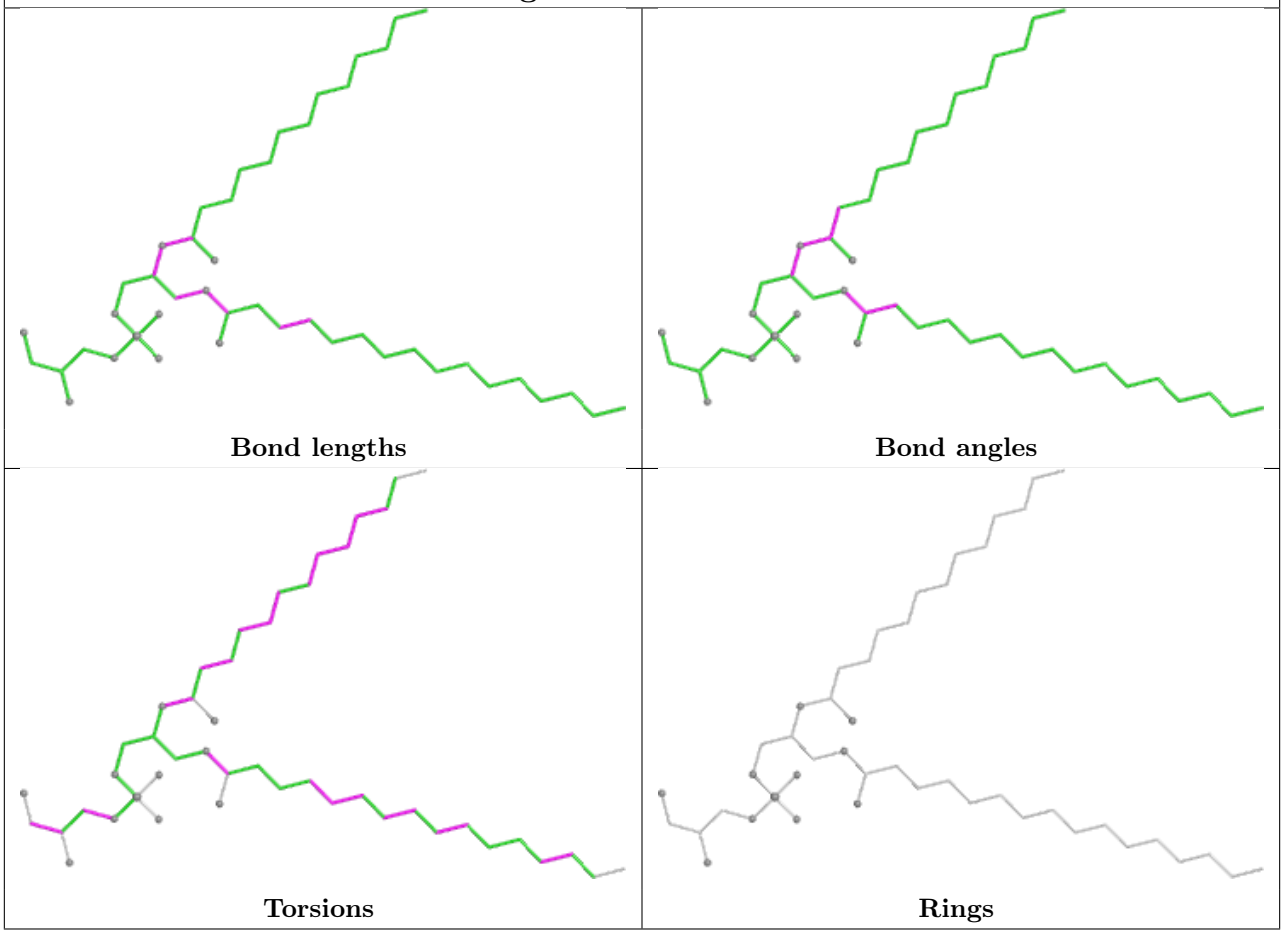


Rings

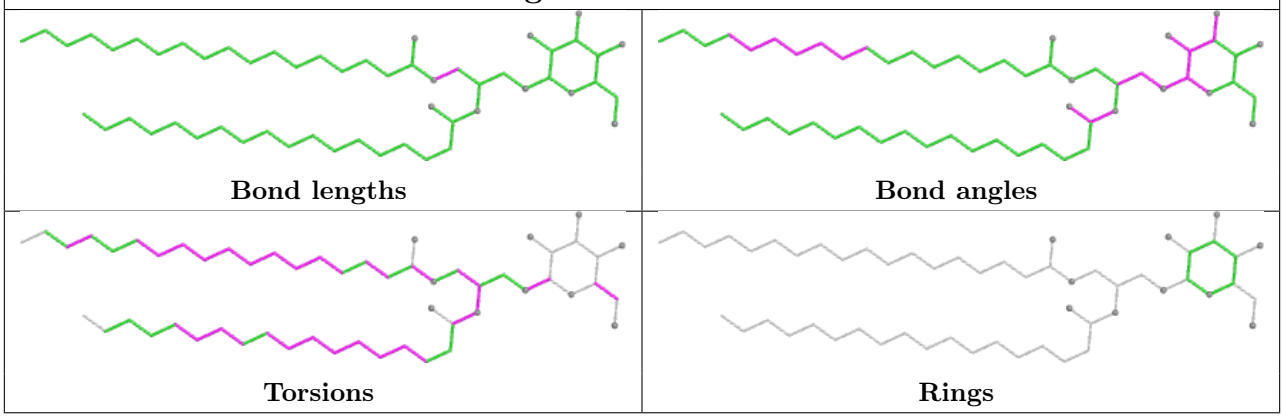
Ligand 8CT 8 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

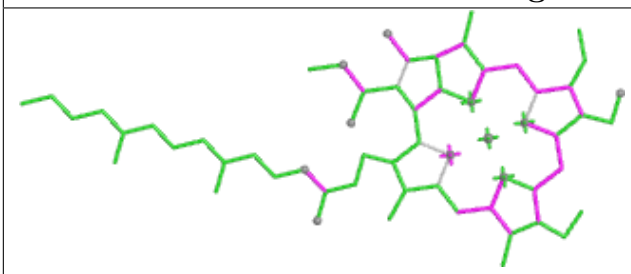
Ligand LHG M 104



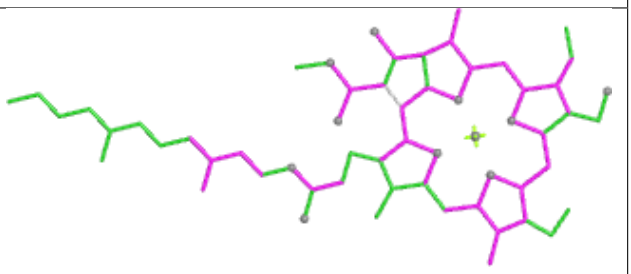
Ligand LMG 9 602



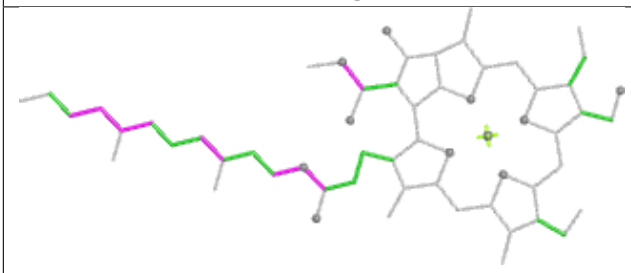
Ligand CHL a 609



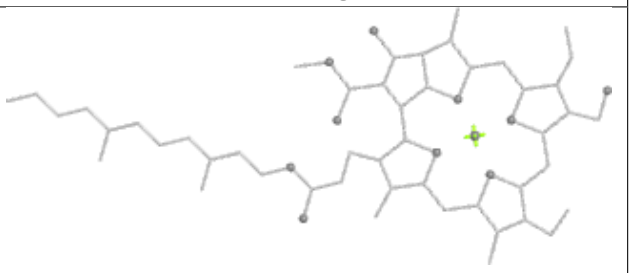
Bond lengths



Bond angles

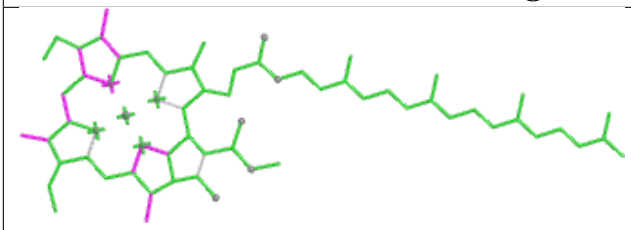


Torsions

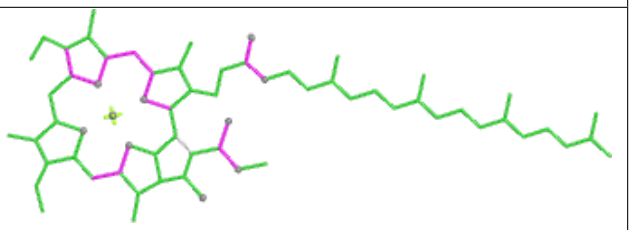


Rings

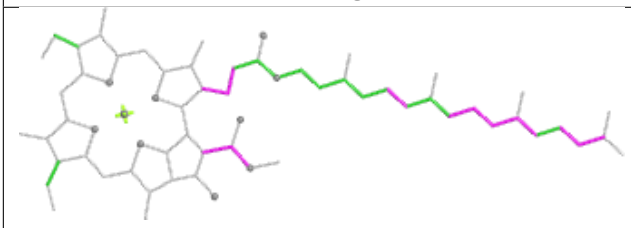
Ligand CLA B 814



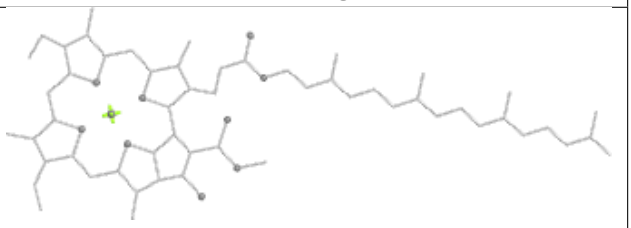
Bond lengths



Bond angles

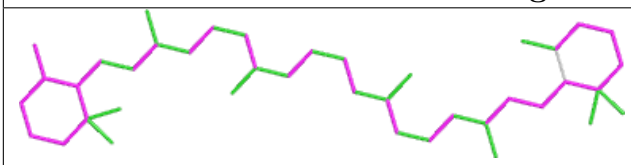


Torsions

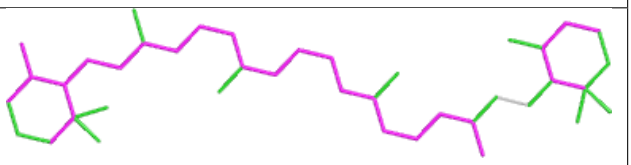


Rings

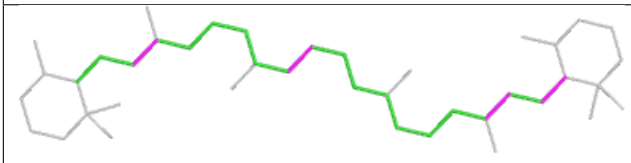
Ligand 8CT L 205



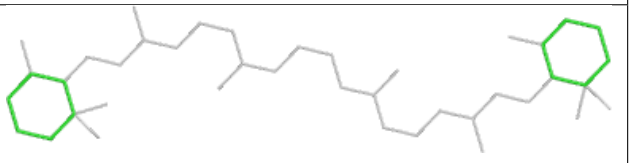
Bond lengths



Bond angles

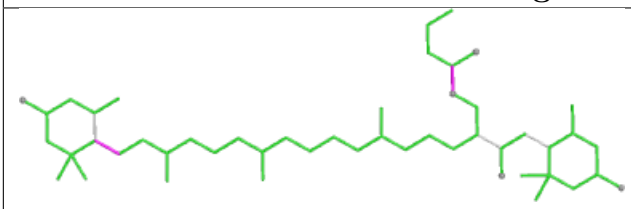


Torsions

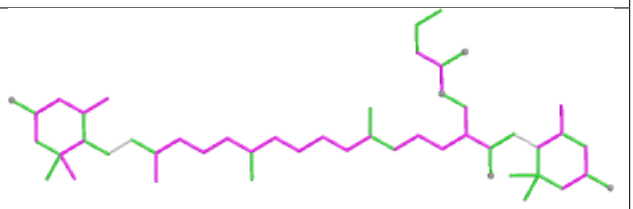


Rings

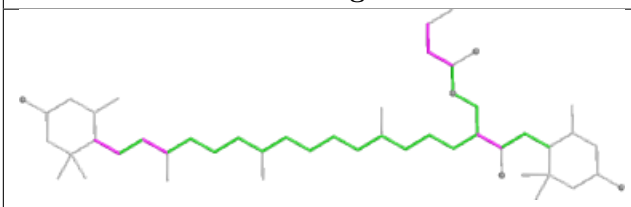
Ligand 0UR f 520



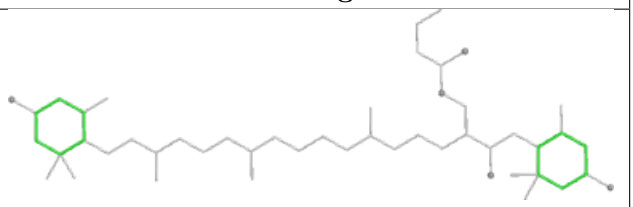
Bond lengths



Bond angles

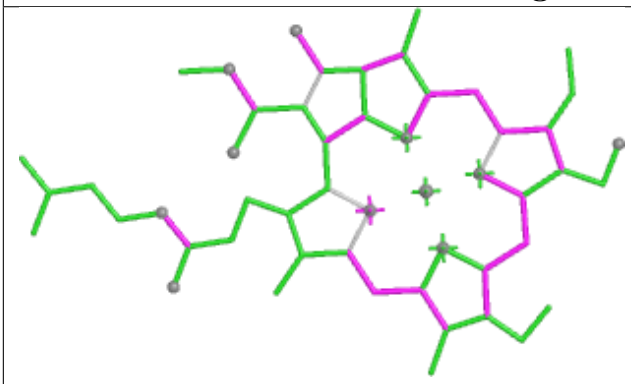


Torsions

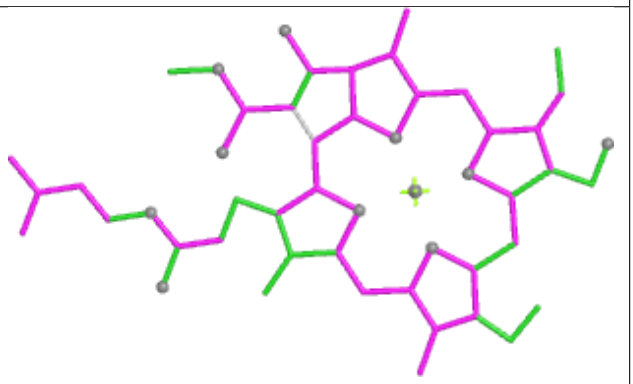


Rings

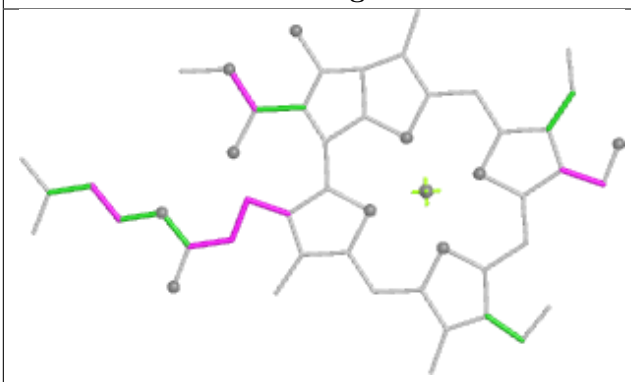
Ligand CHL f 608



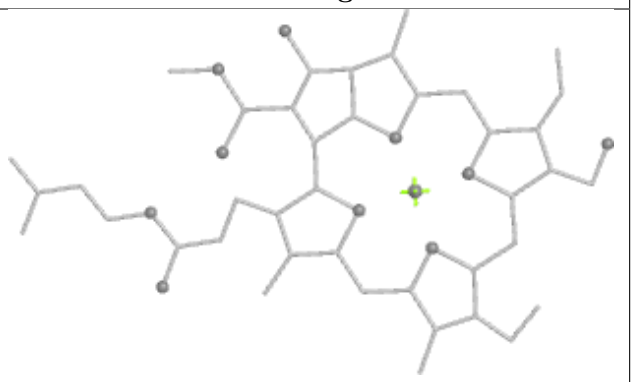
Bond lengths



Bond angles

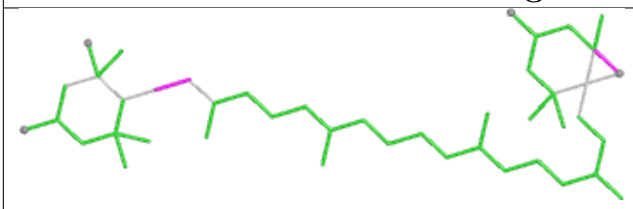


Torsions

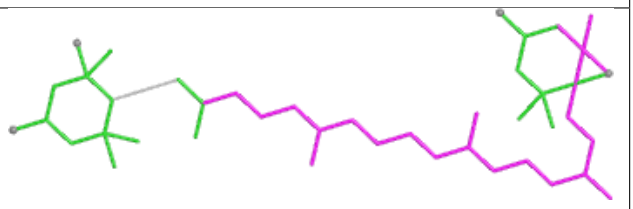


Rings

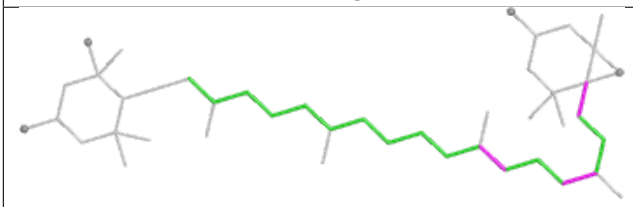
Ligand NEX h 523



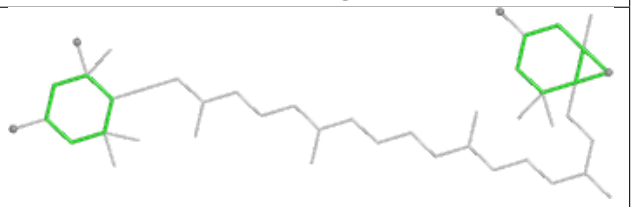
Bond lengths



Bond angles

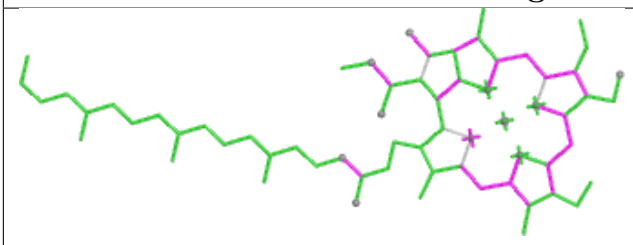


Torsions

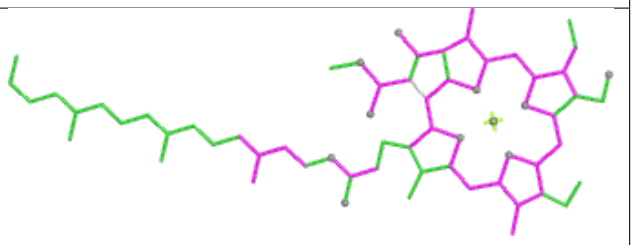


Rings

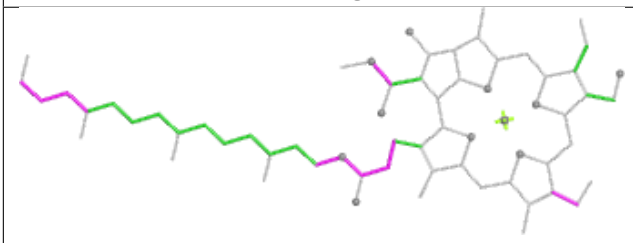
Ligand CHL 0 302



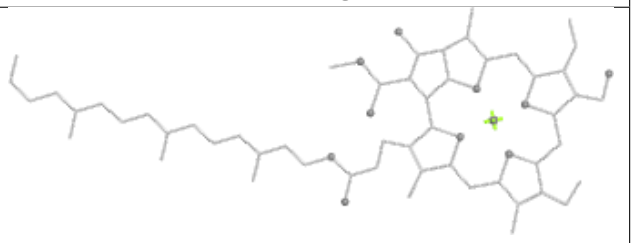
Bond lengths



Bond angles

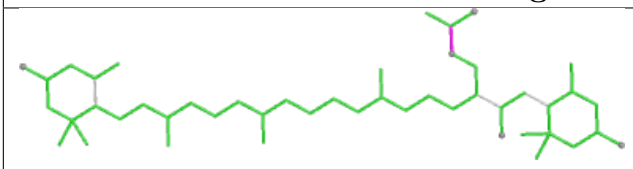


Torsions

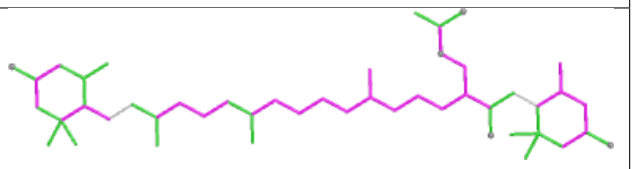


Rings

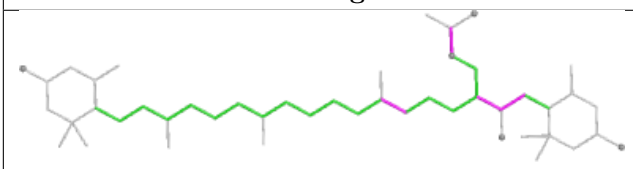
Ligand 0UR a 520



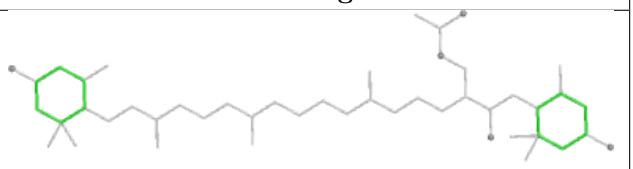
Bond lengths



Bond angles

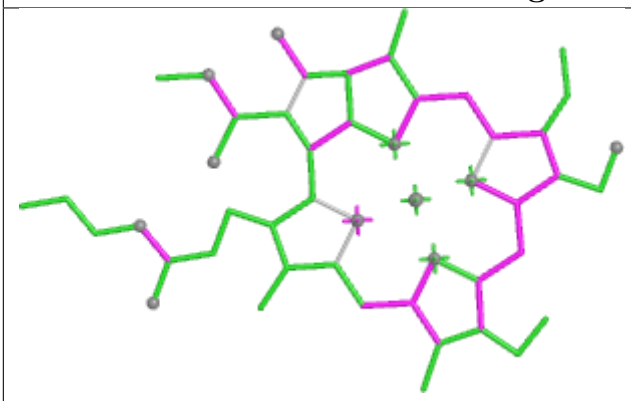


Torsions

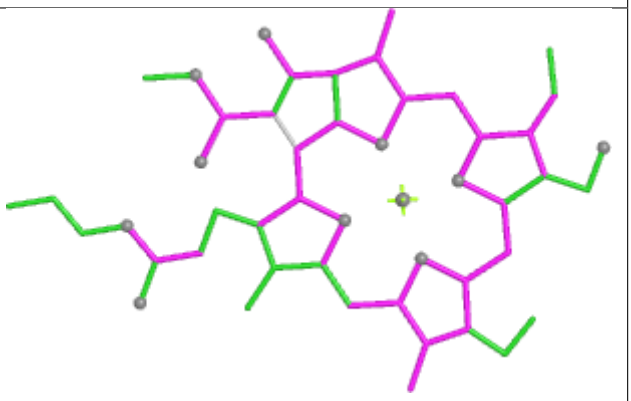


Rings

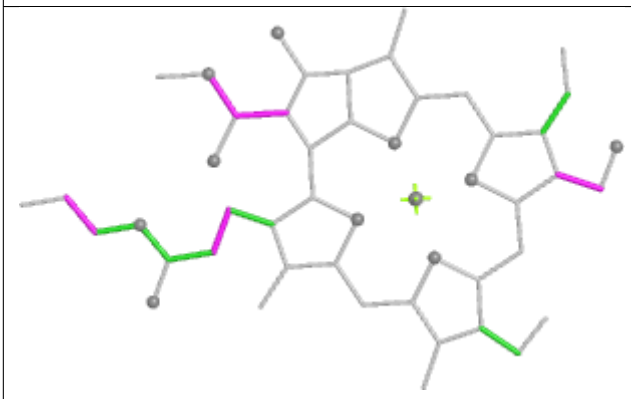
Ligand CHL a 608



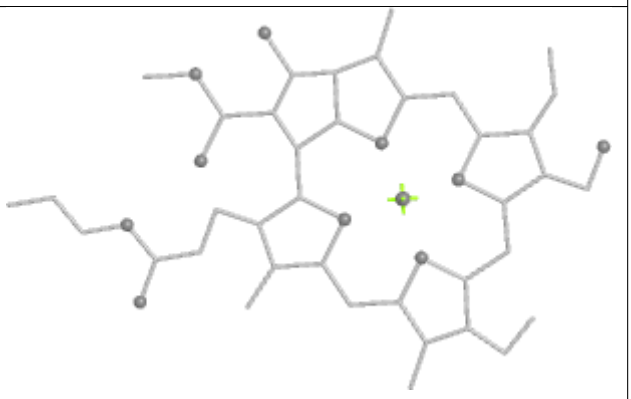
Bond lengths



Bond angles

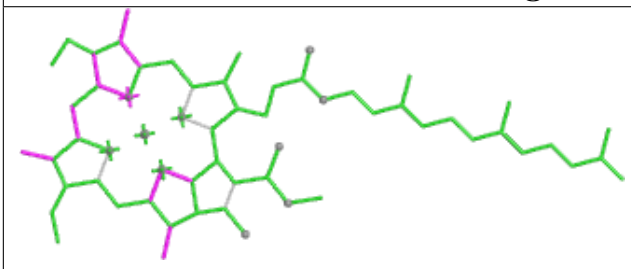


Torsions

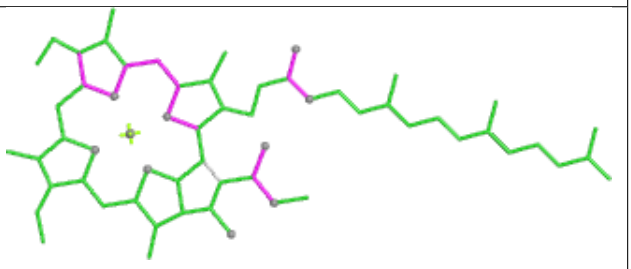


Rings

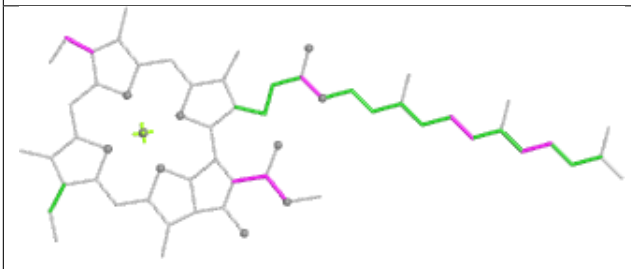
Ligand CLA B 824



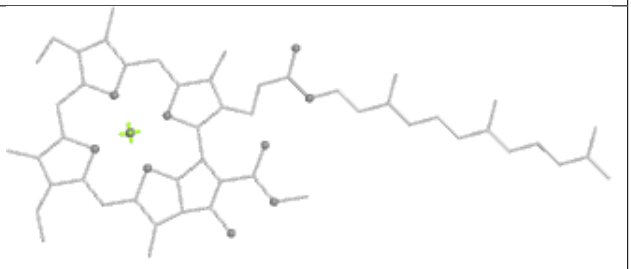
Bond lengths



Bond angles

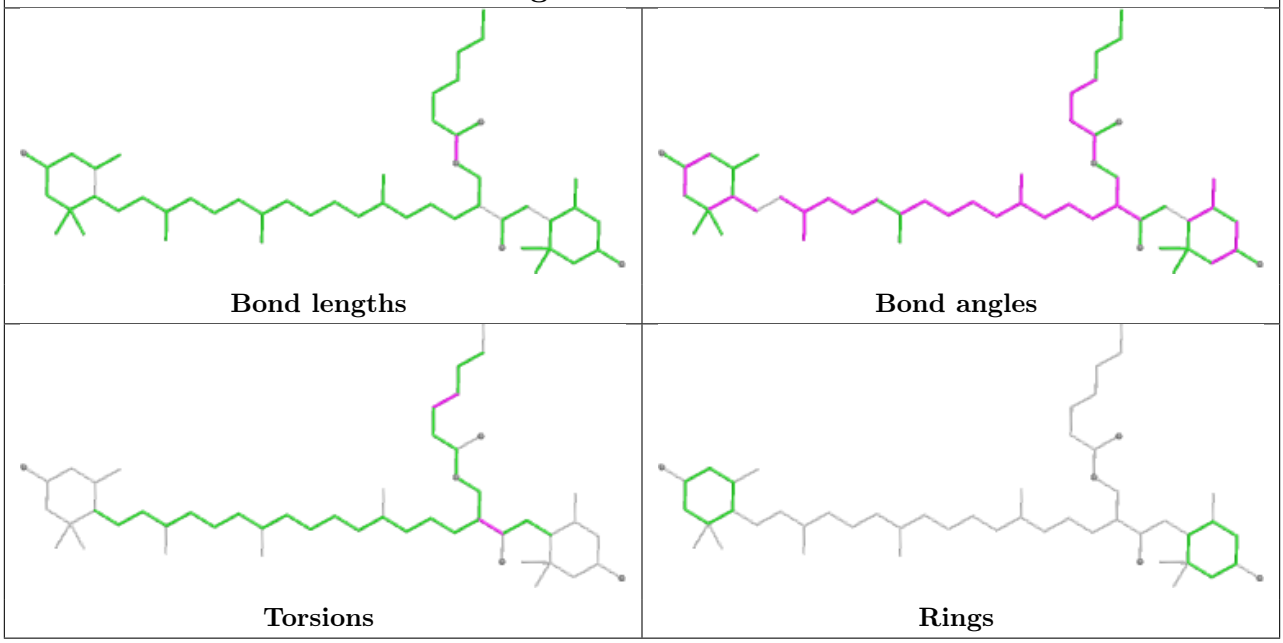


Torsions

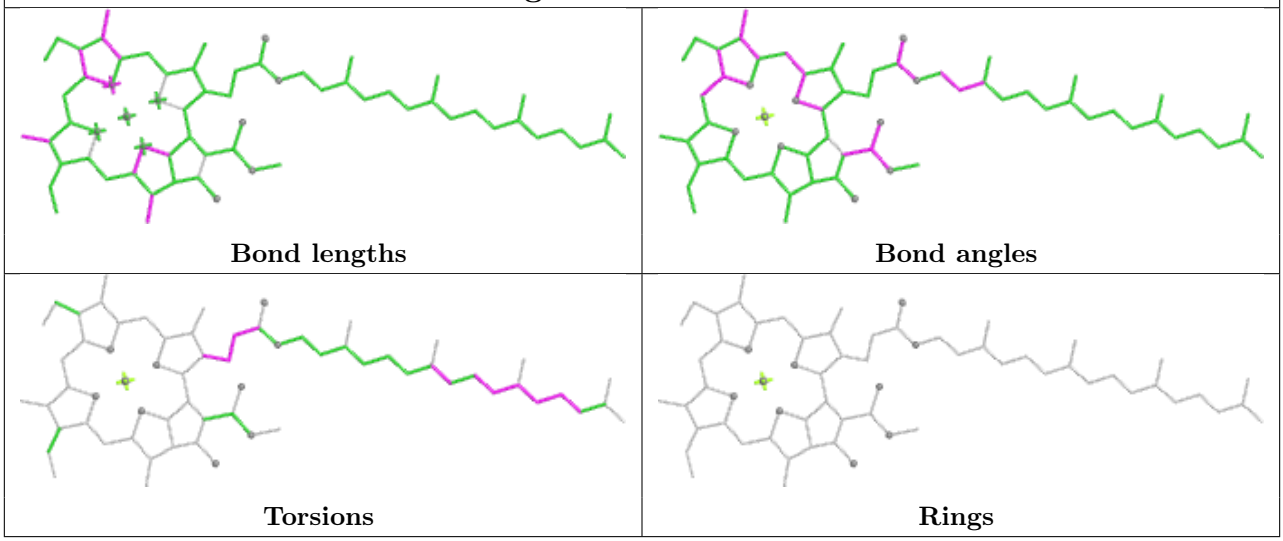


Rings

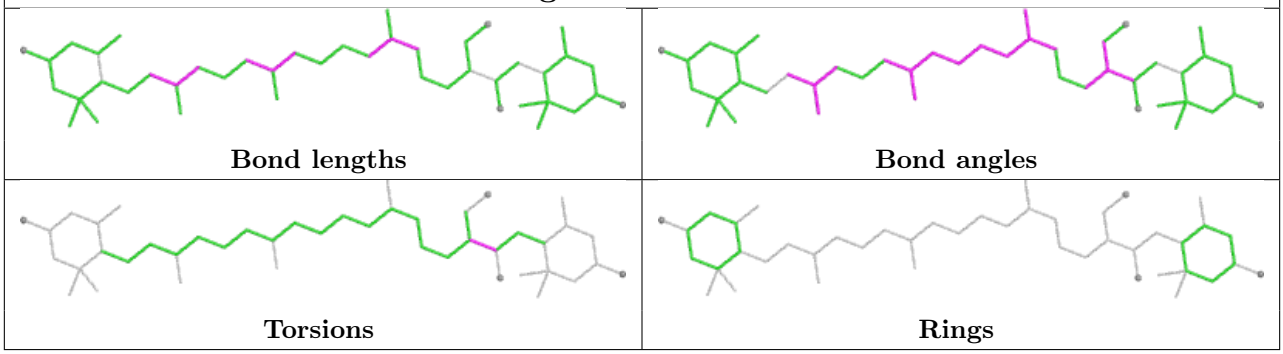
Ligand 0UR 9 501



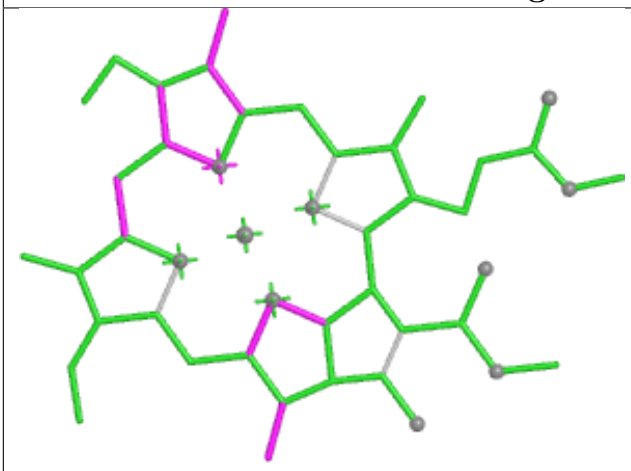
Ligand CLA A 818



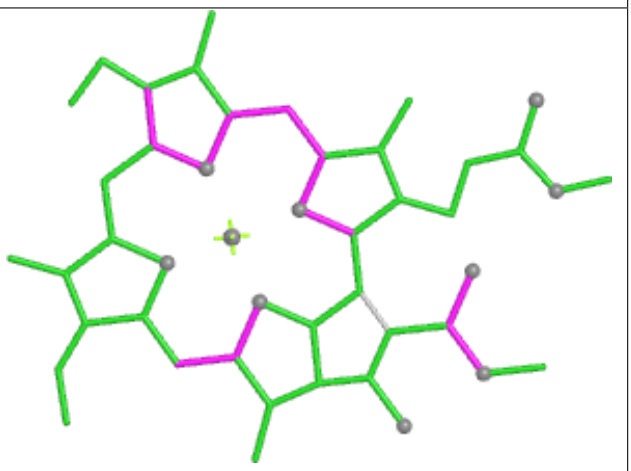
Ligand 0IE a 521



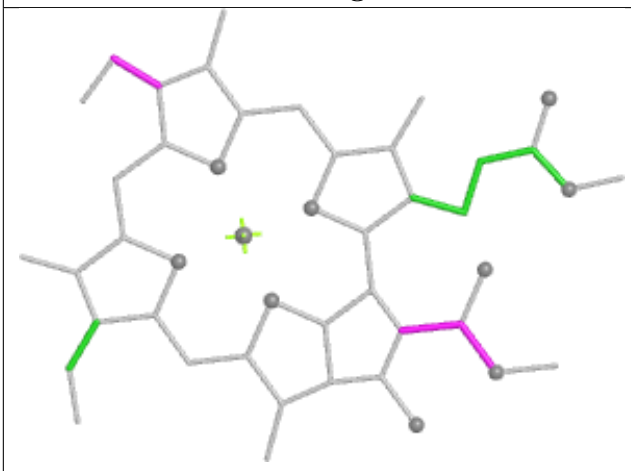
Ligand CLA 1 314



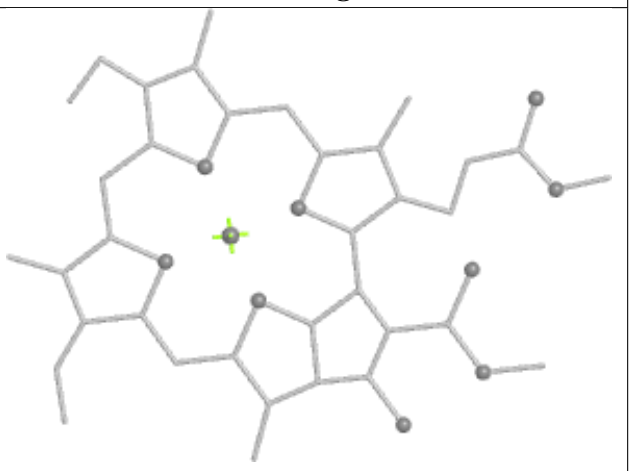
Bond lengths



Bond angles

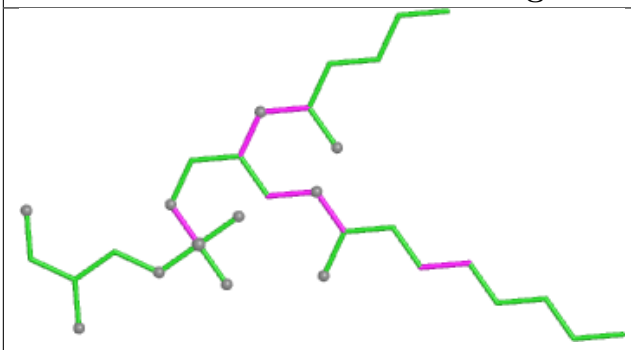


Torsions

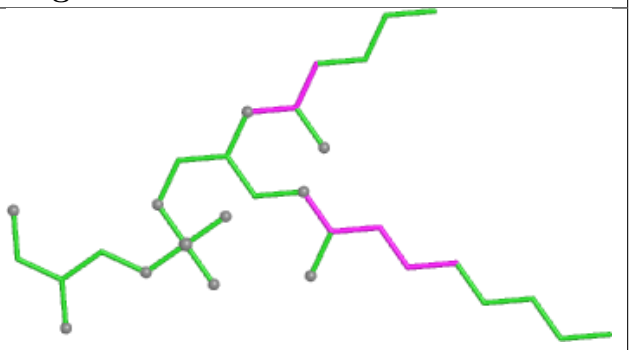


Rings

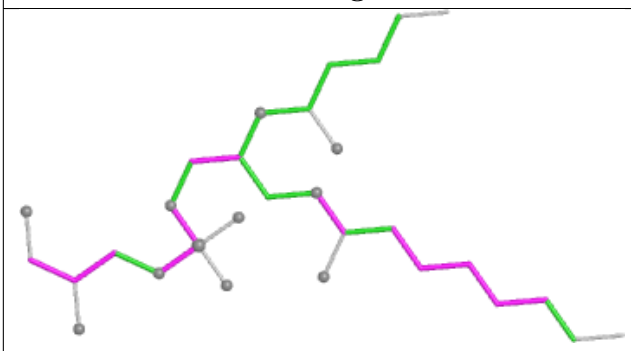
Ligand LHG g 630



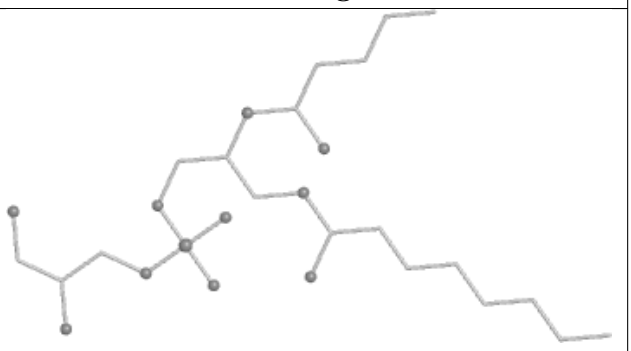
Bond lengths



Bond angles

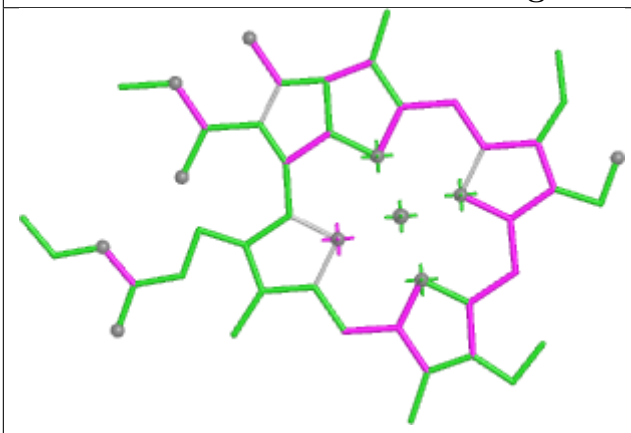


Torsions

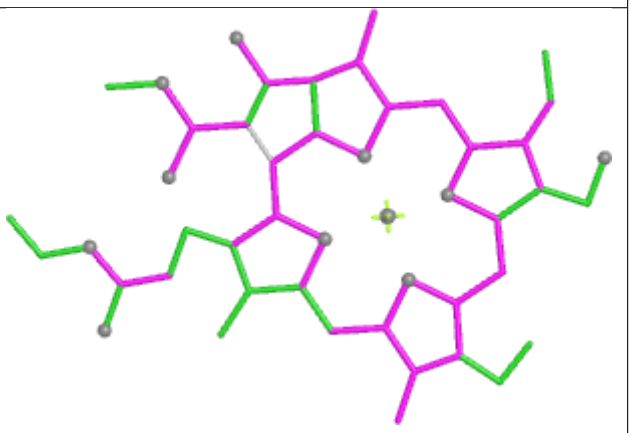


Rings

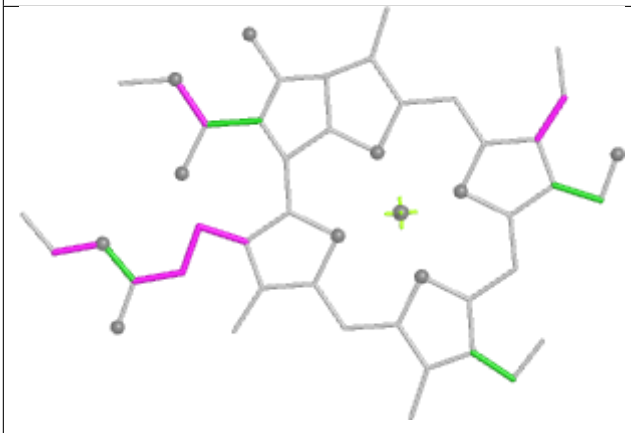
Ligand CHL 5 306



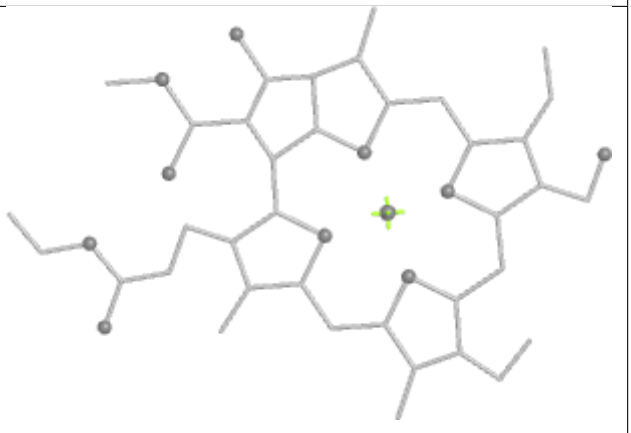
Bond lengths



Bond angles

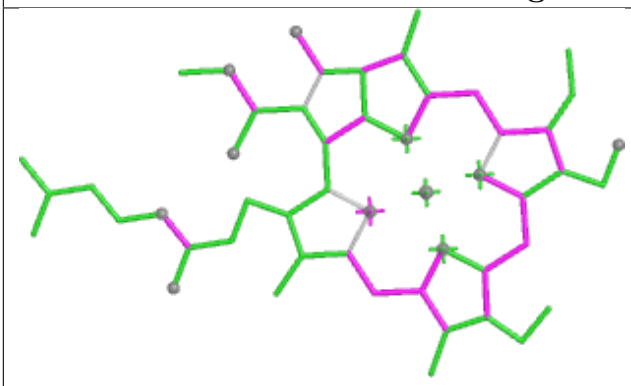


Torsions

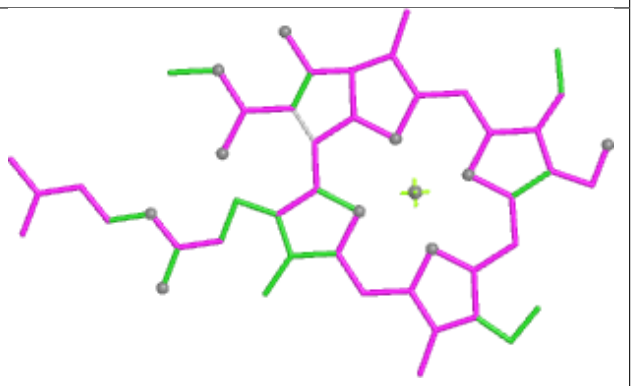


Rings

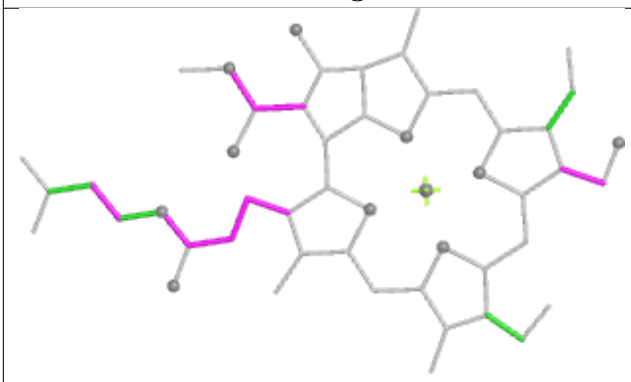
Ligand CHL 8 306



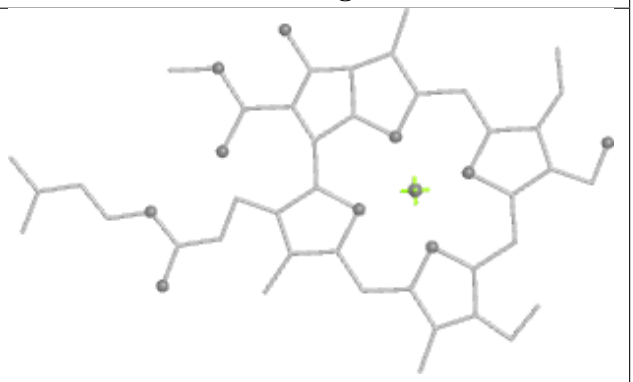
Bond lengths



Bond angles

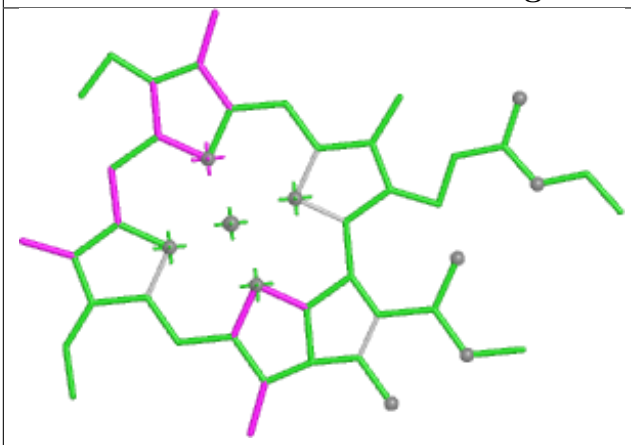


Torsions

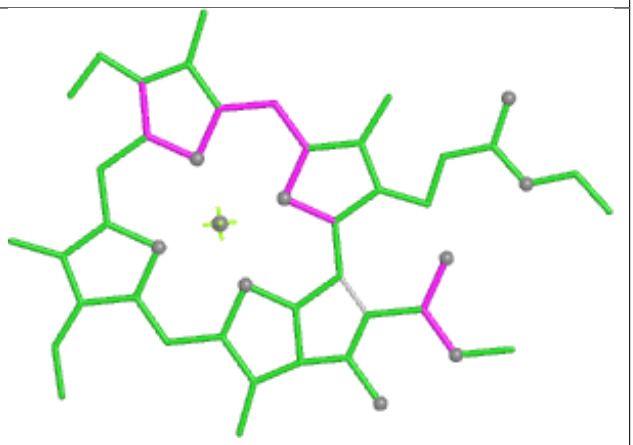


Rings

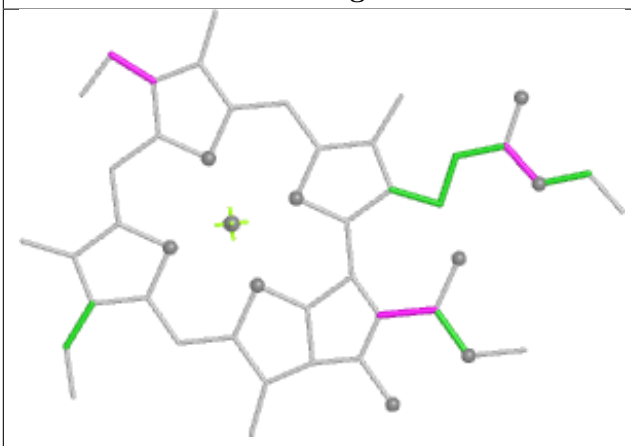
Ligand CLA B 850



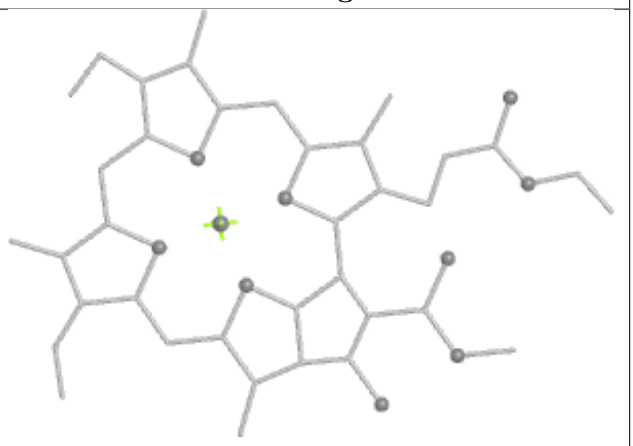
Bond lengths



Bond angles

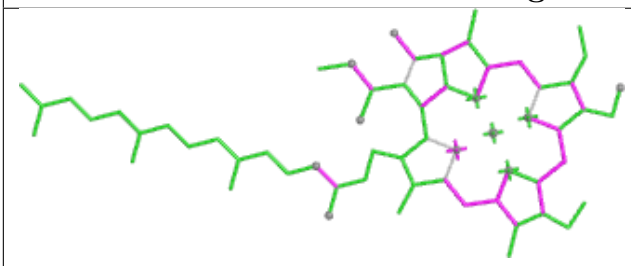


Torsions

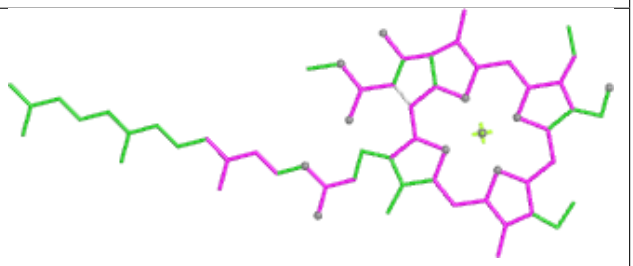


Rings

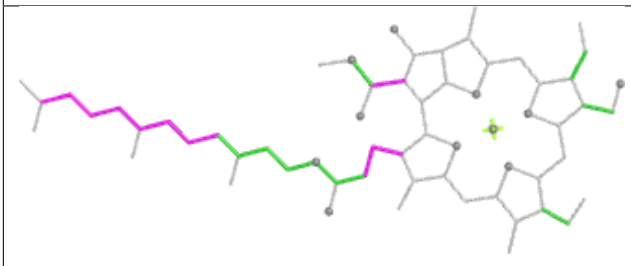
Ligand CHL 6 301



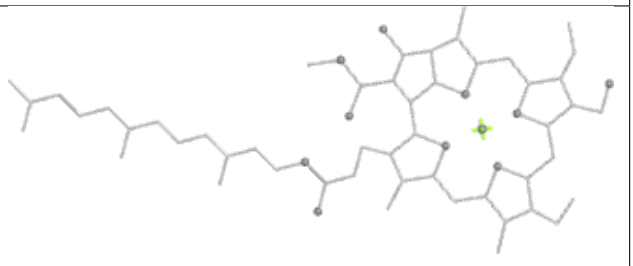
Bond lengths



Bond angles

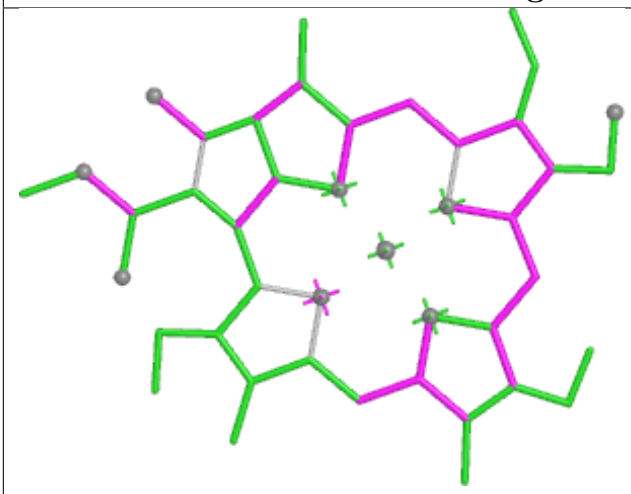


Torsions

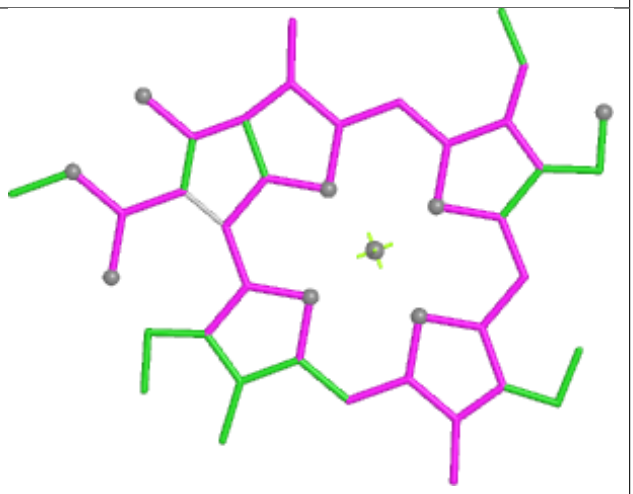


Rings

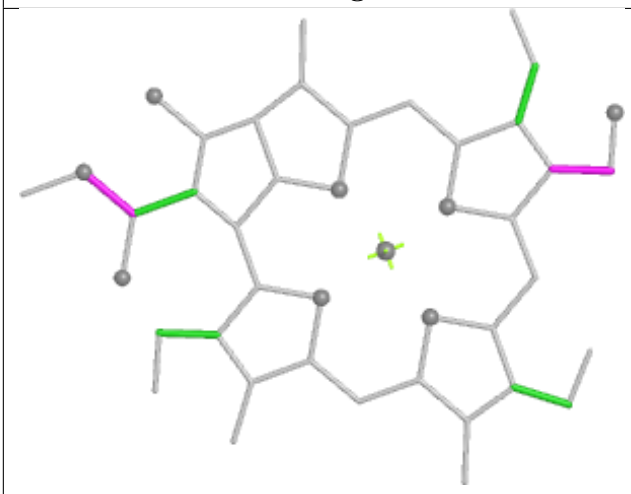
Ligand CHL d 605



Bond lengths



Bond angles

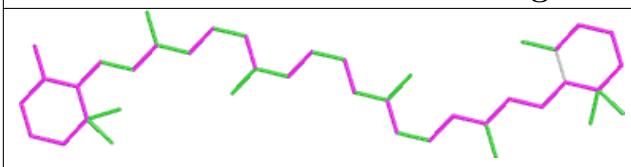


Torsions

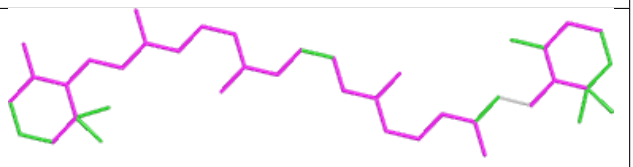


Rings

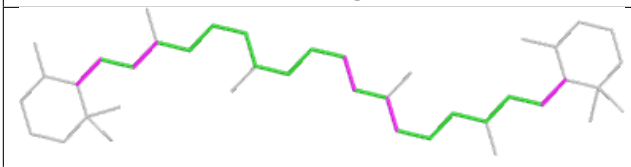
Ligand 8CT 1 402



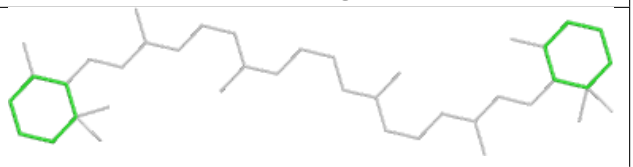
Bond lengths



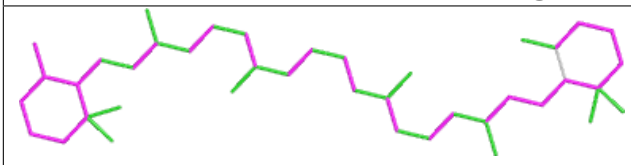
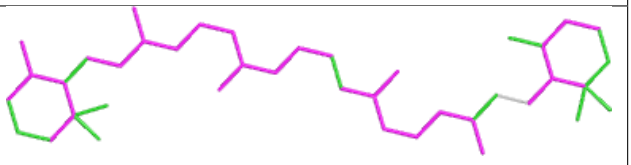
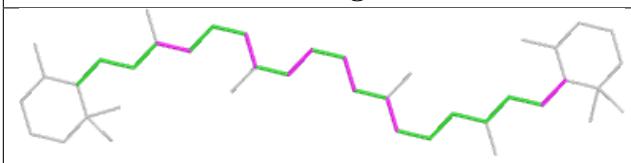
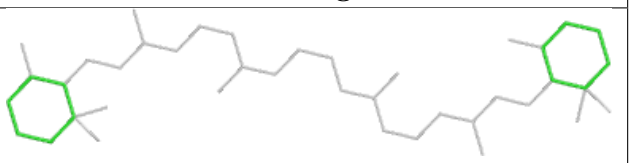
Bond angles

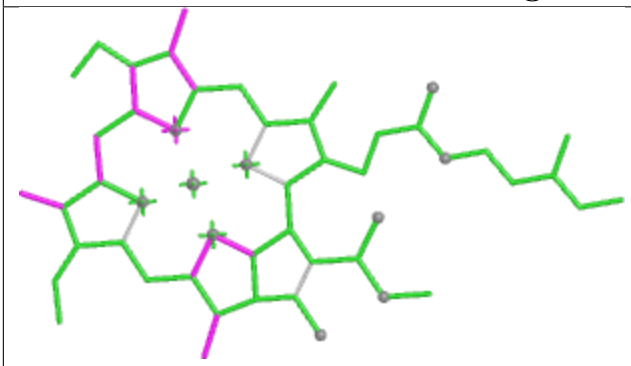
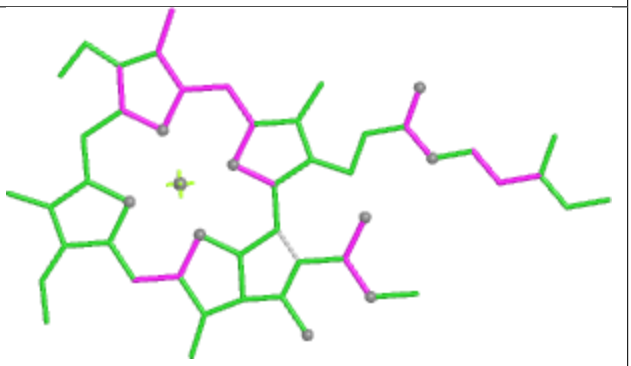
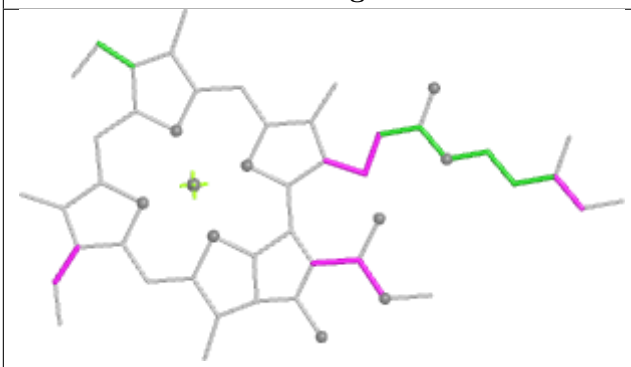
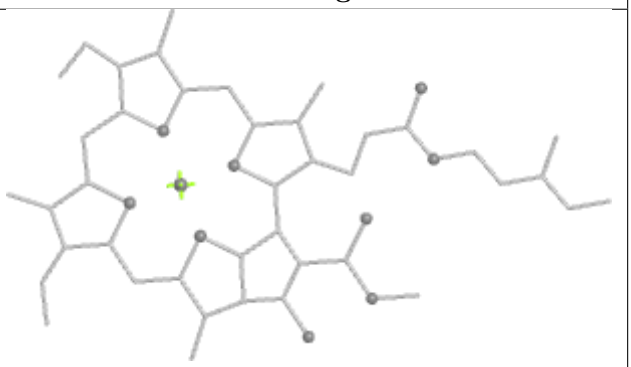


Torsions

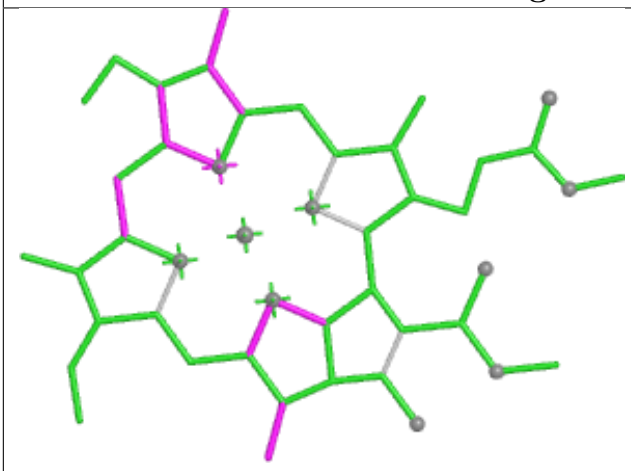


Rings

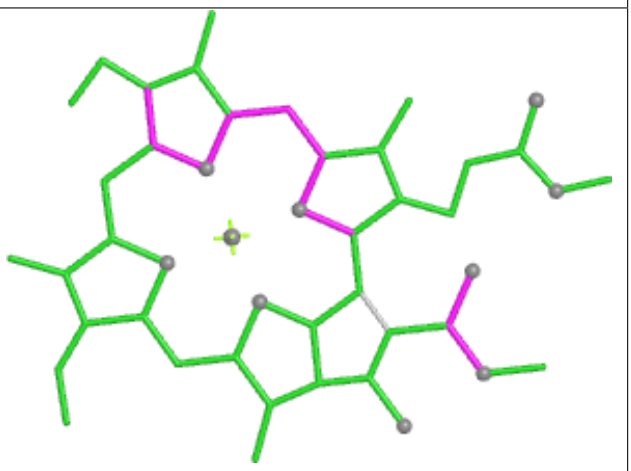
Ligand 8CT J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

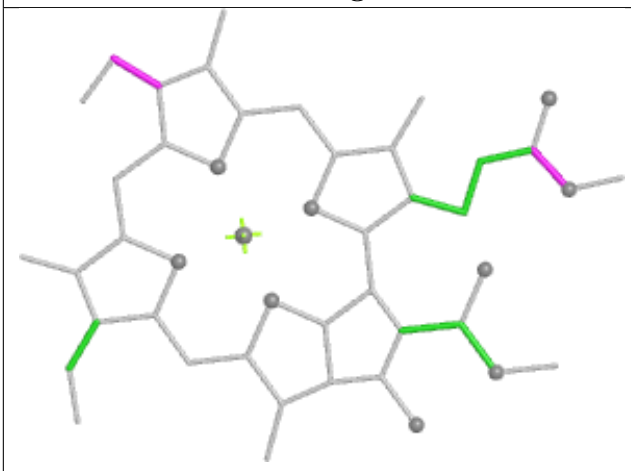
Ligand CLA c 611



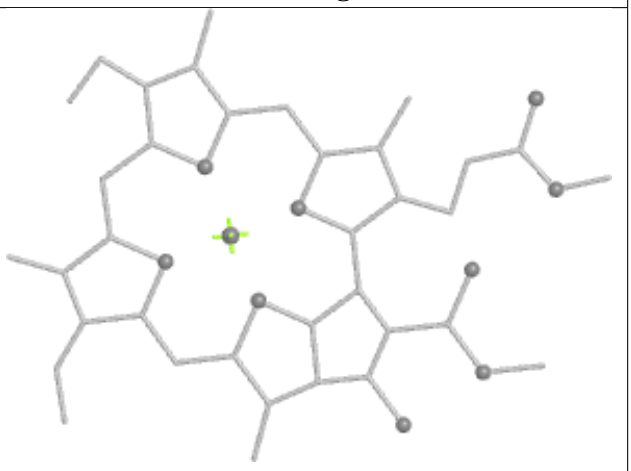
Bond lengths



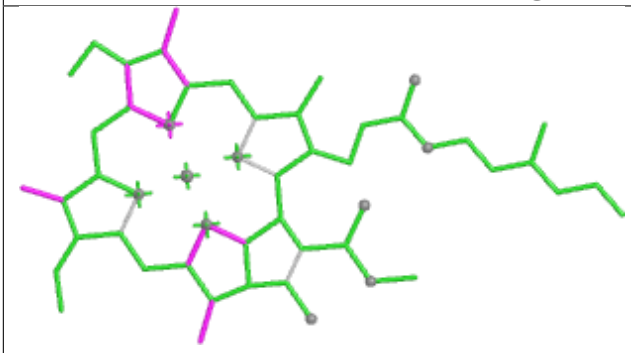
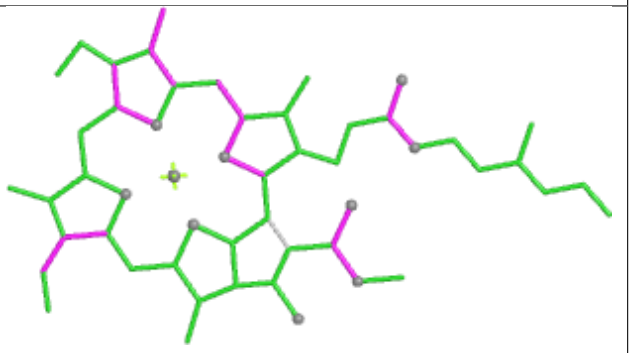
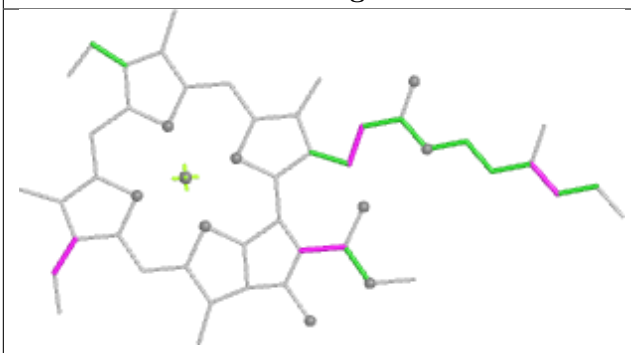
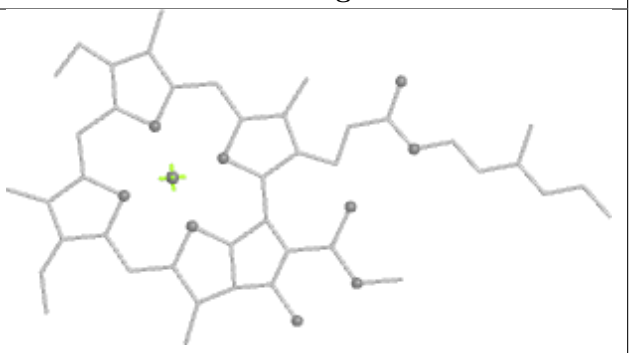
Bond angles

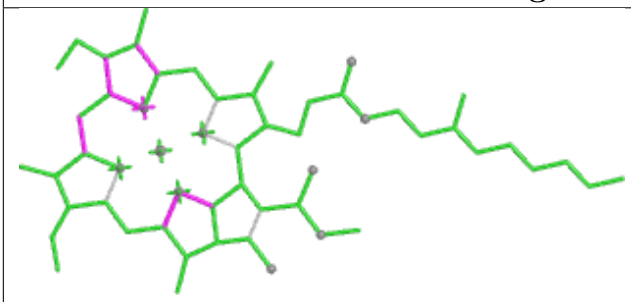
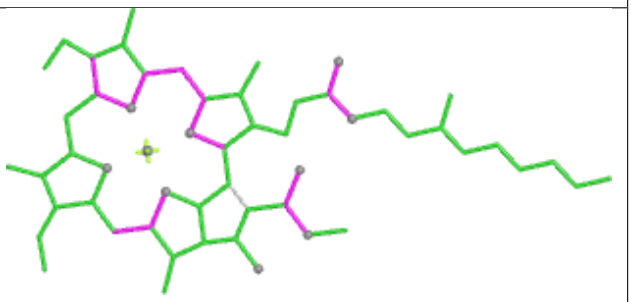
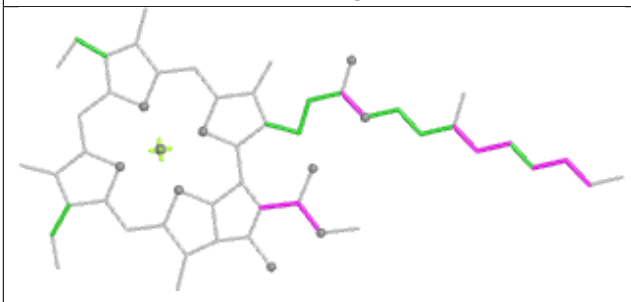
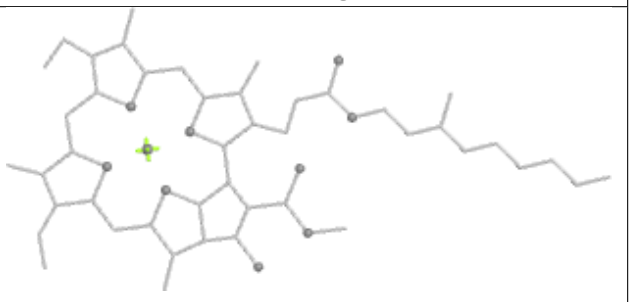


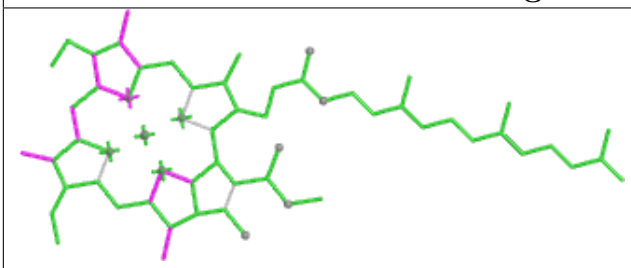
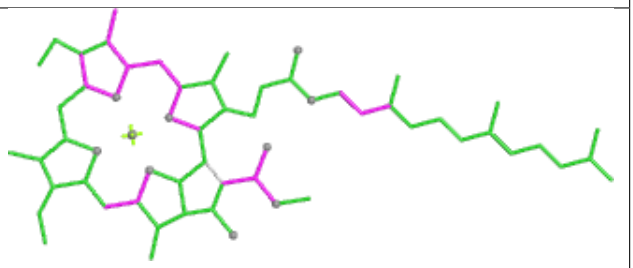
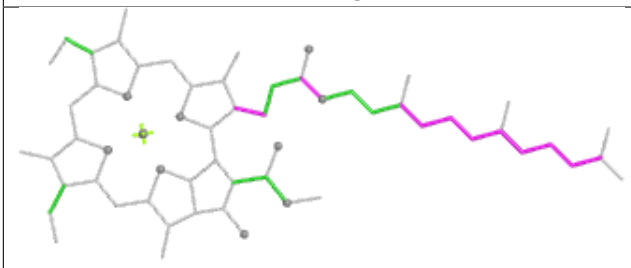
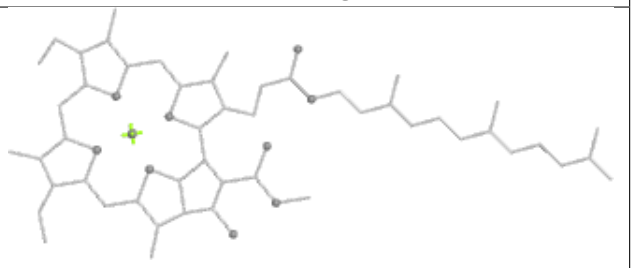
Torsions

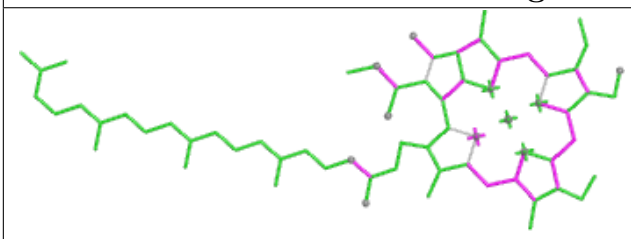
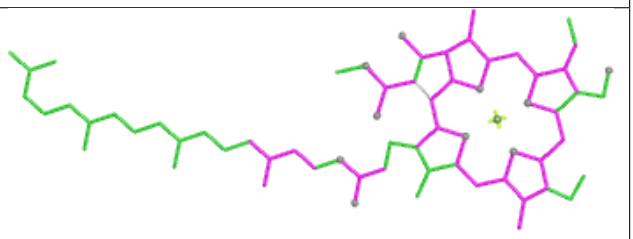
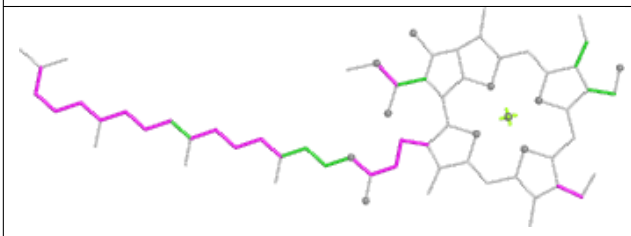
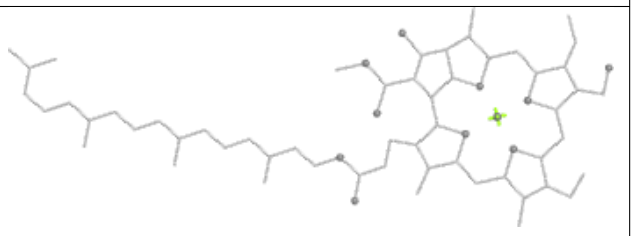


Rings

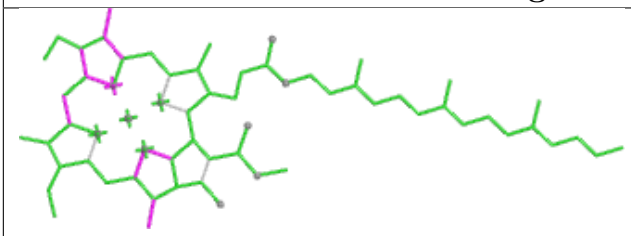
Ligand CLA 3 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

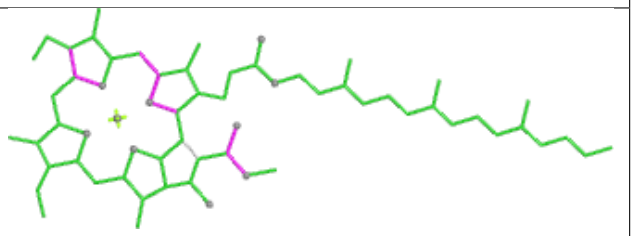
Ligand CLA B 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 3 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

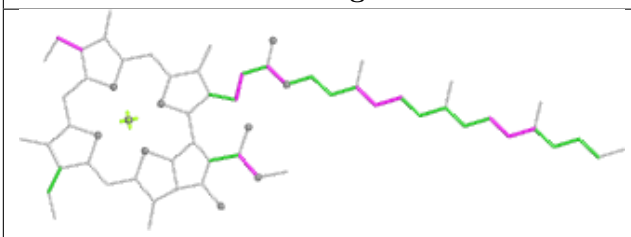
Ligand CLA 1 310



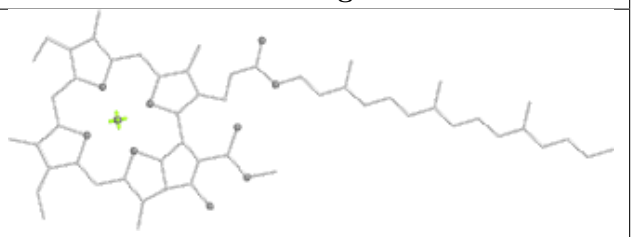
Bond lengths



Bond angles

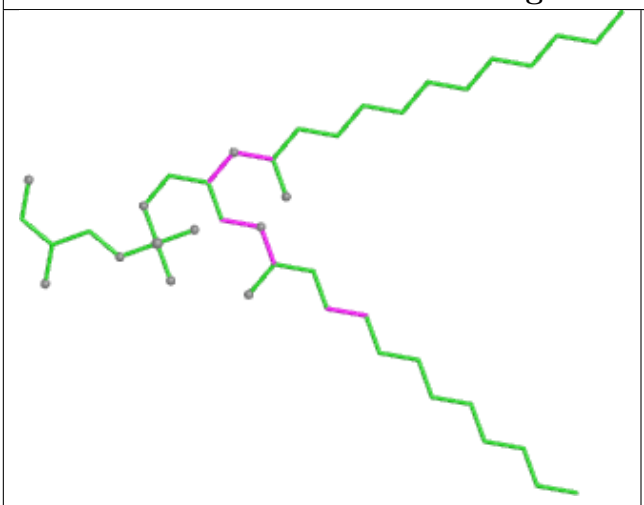


Torsions

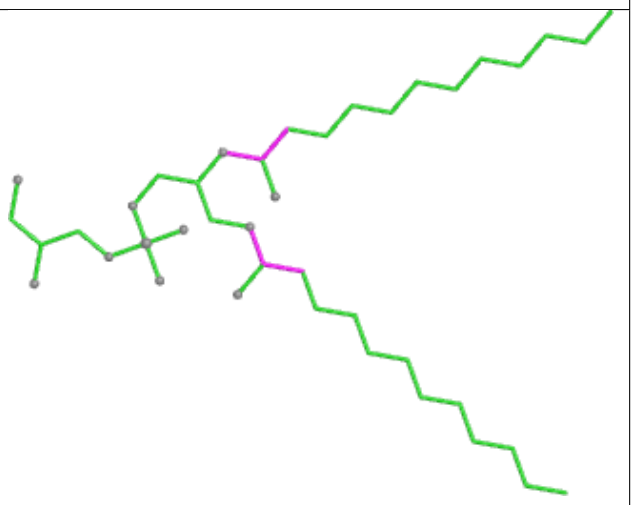


Rings

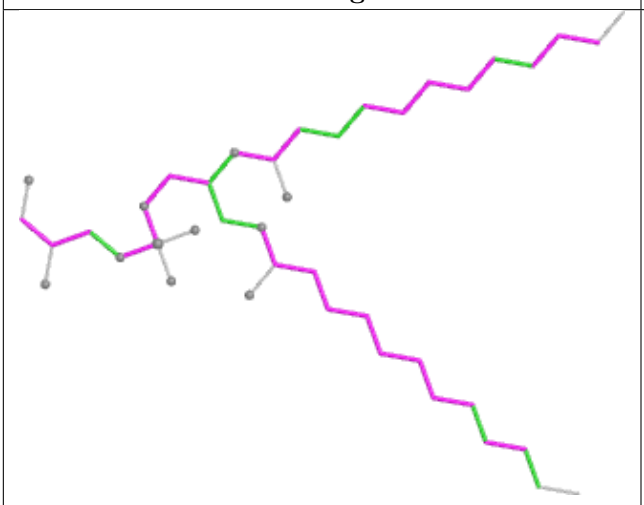
Ligand LHG b 630



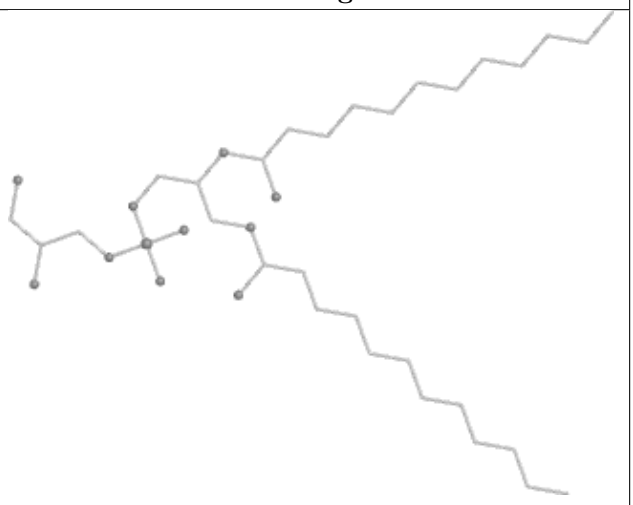
Bond lengths



Bond angles

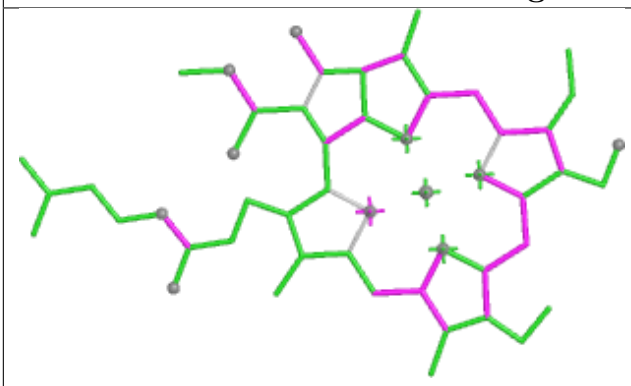


Torsions

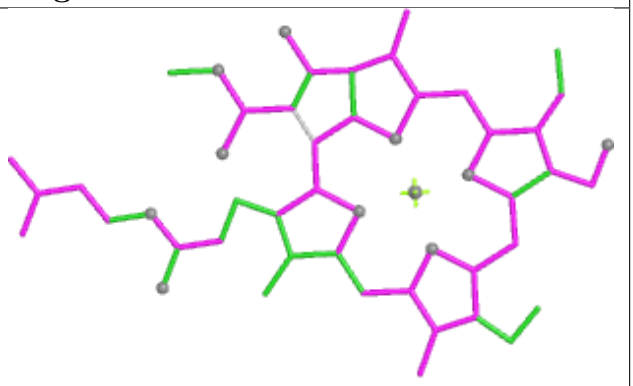


Rings

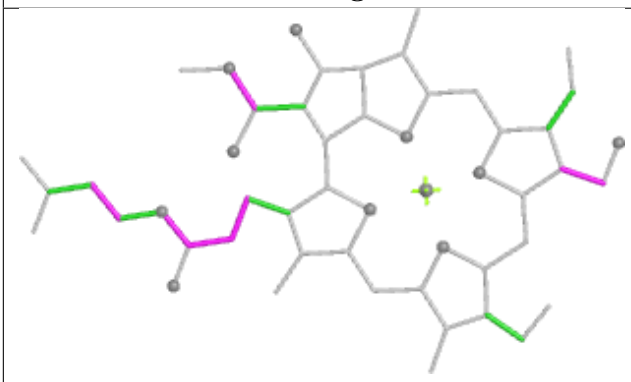
Ligand CHL g 607



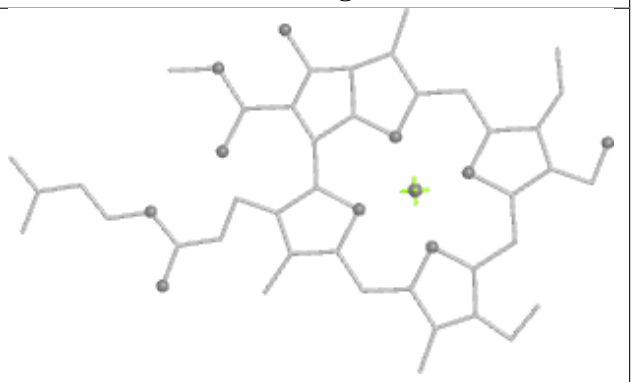
Bond lengths



Bond angles

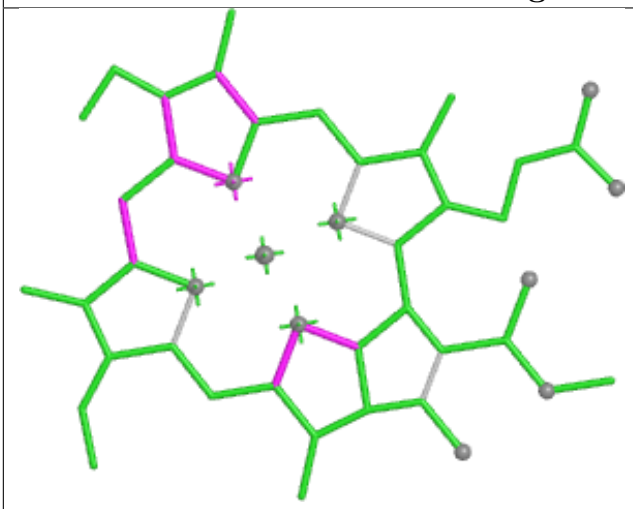


Torsions

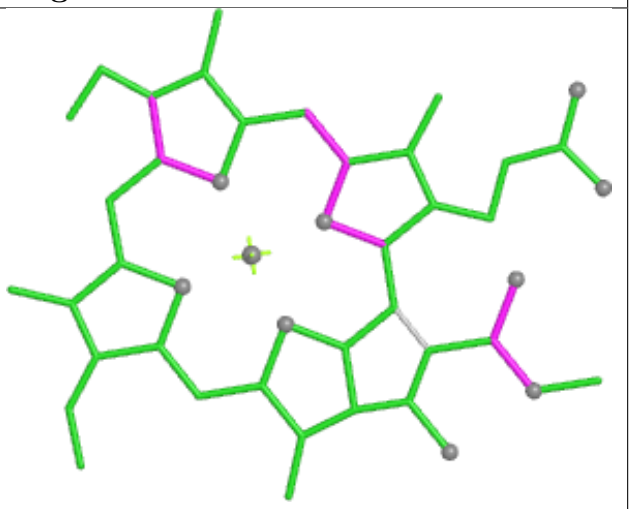


Rings

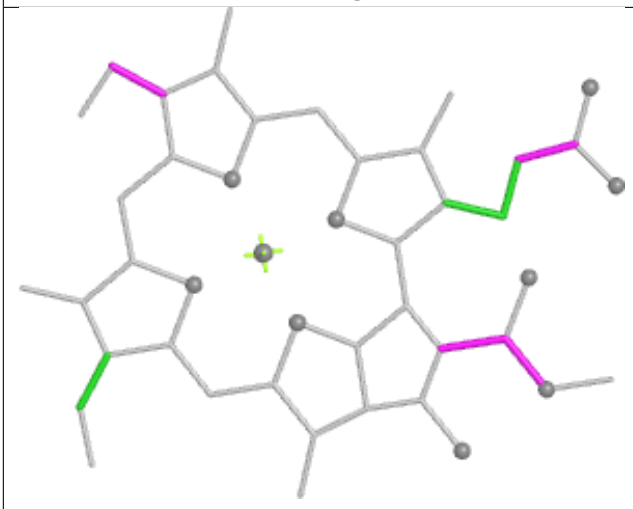
Ligand CLA g 612



Bond lengths



Bond angles

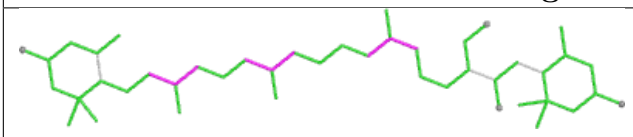


Torsions

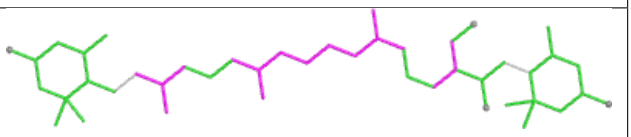


Rings

Ligand 0IE f 521



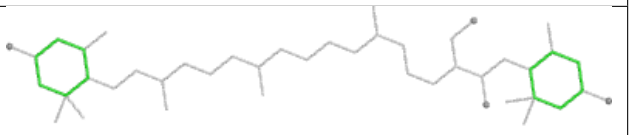
Bond lengths



Bond angles

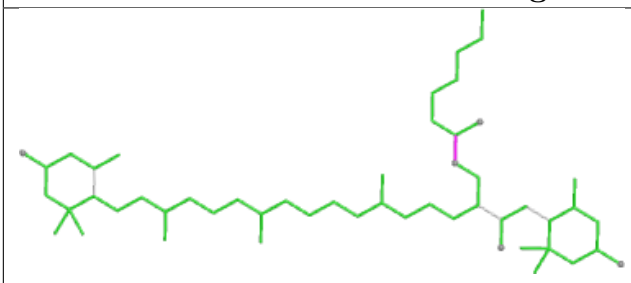


Torsions

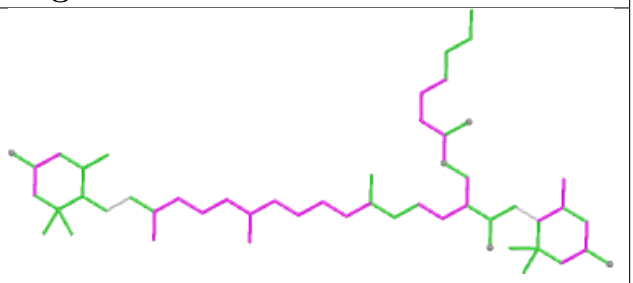


Rings

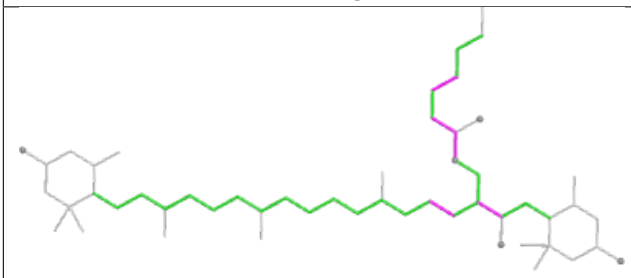
Ligand 0UR g 520



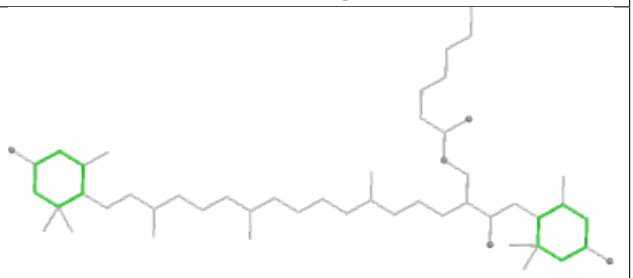
Bond lengths



Bond angles

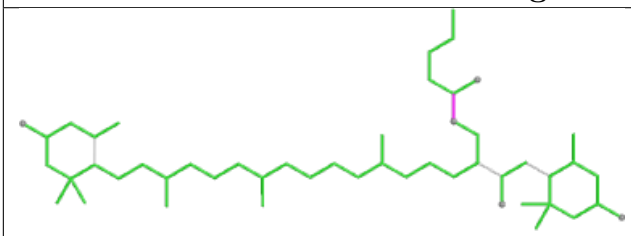


Torsions

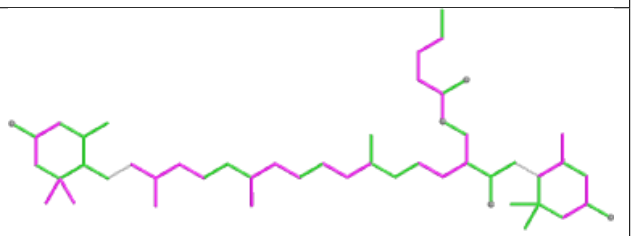


Rings

Ligand 0UR 2 502



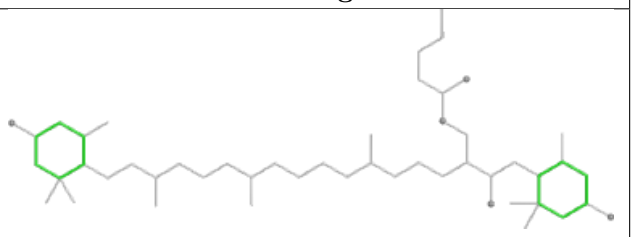
Bond lengths



Bond angles

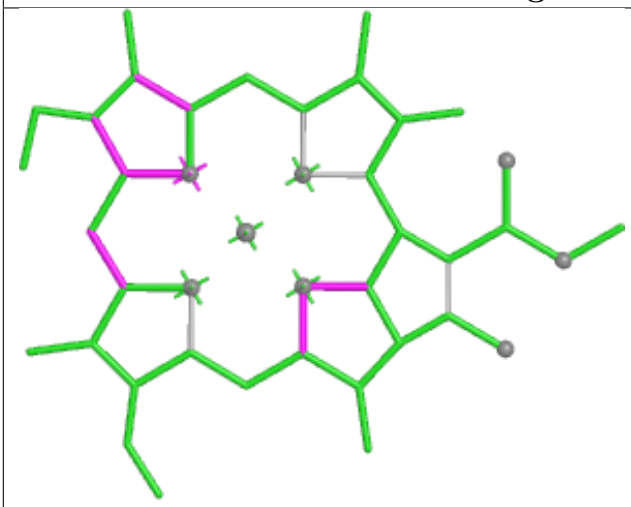


Torsions

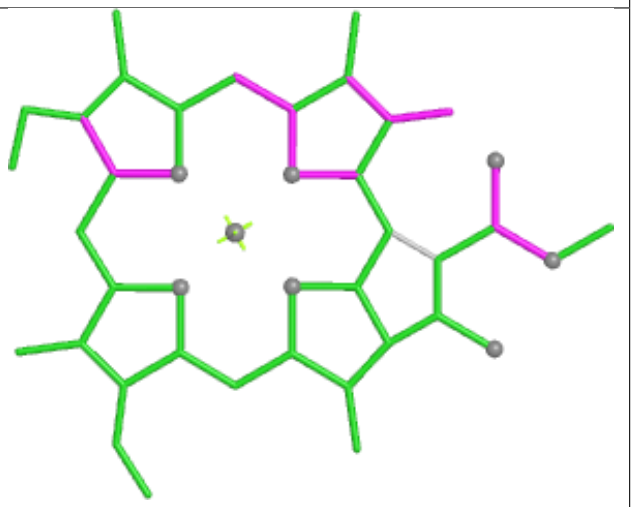


Rings

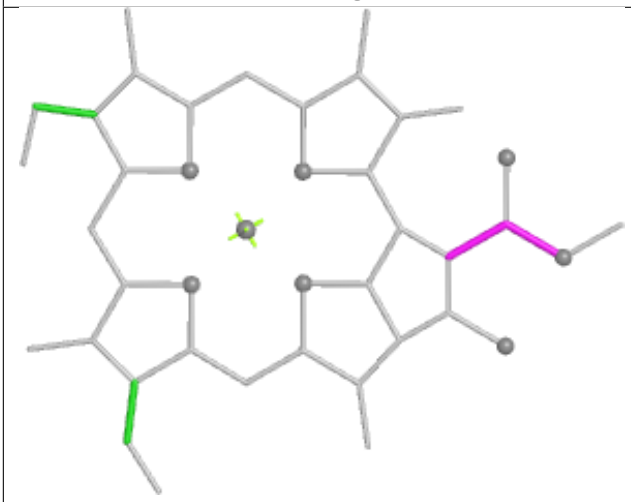
Ligand CLA h 611



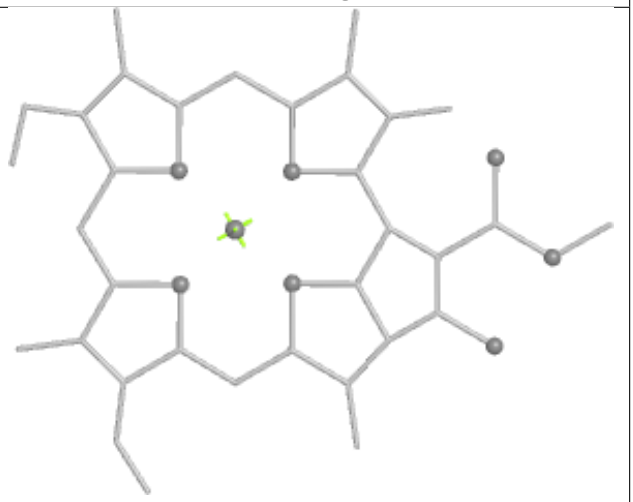
Bond lengths



Bond angles

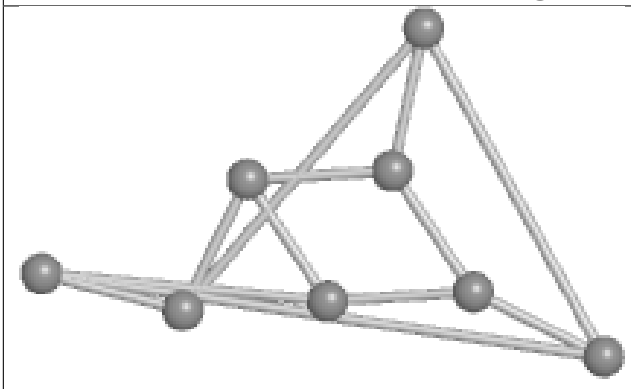


Torsions

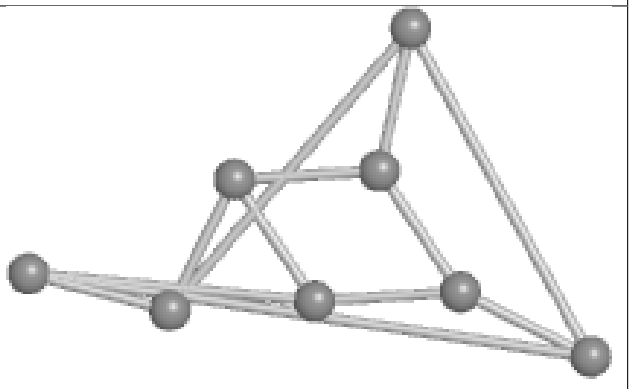


Rings

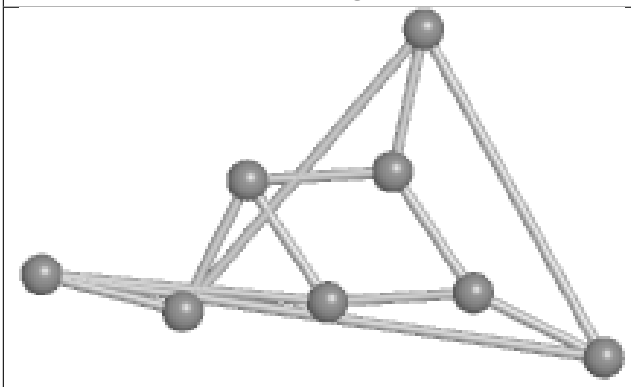
Ligand SF4 C 102



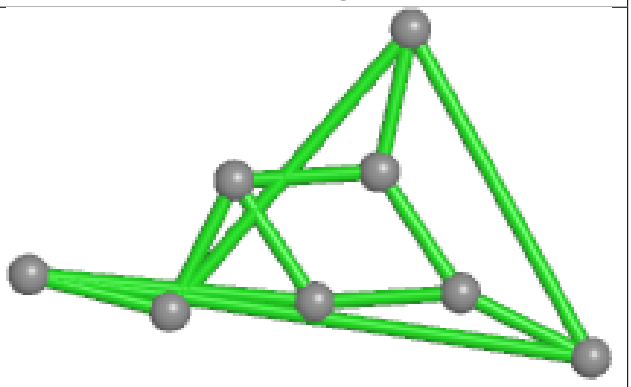
Bond lengths



Bond angles

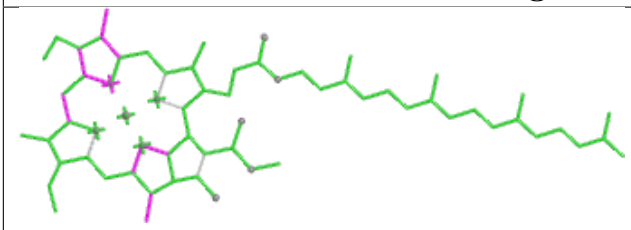


Torsions

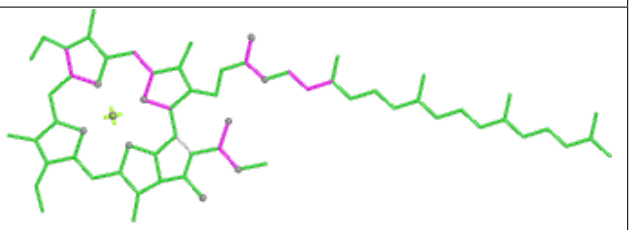


Rings

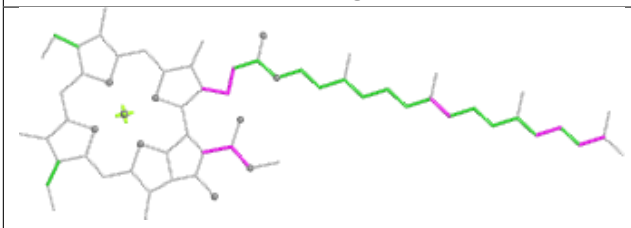
Ligand CLA 8 304



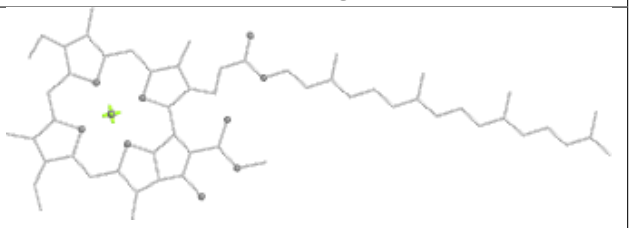
Bond lengths



Bond angles

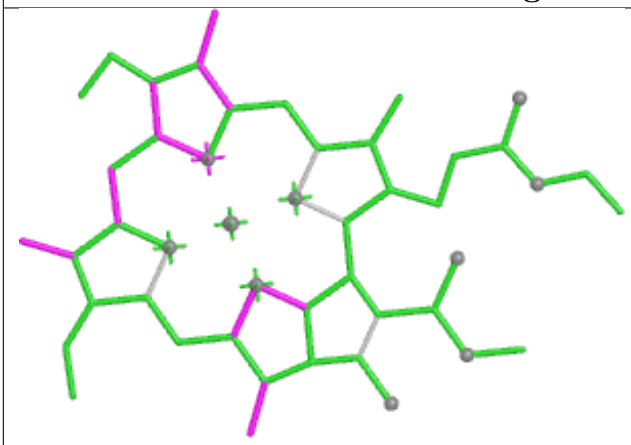


Torsions

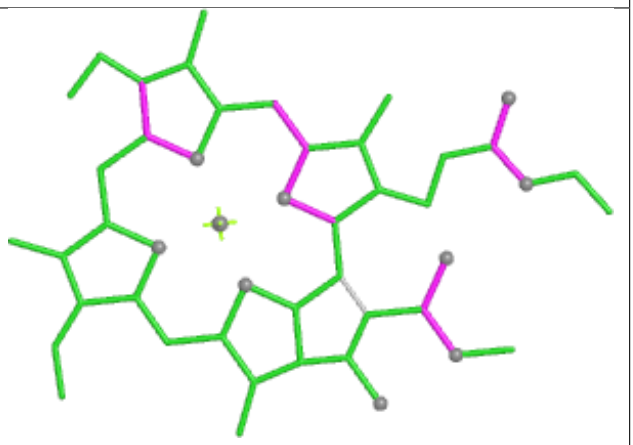


Rings

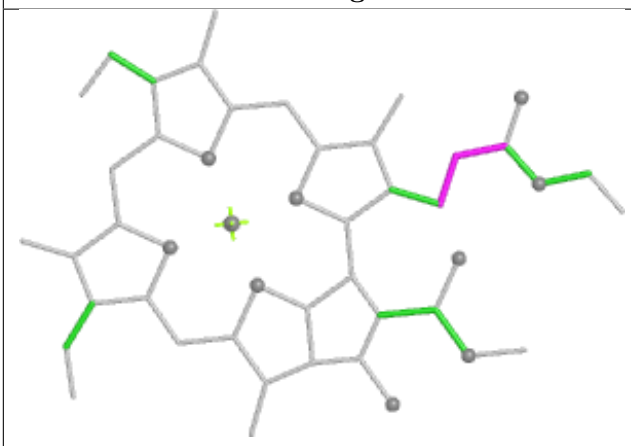
Ligand CLA H 204



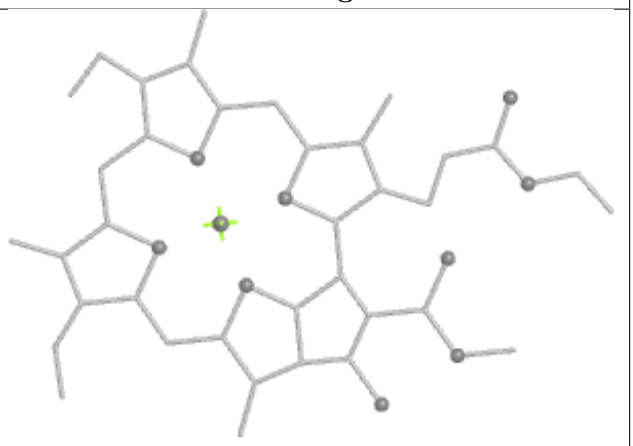
Bond lengths



Bond angles

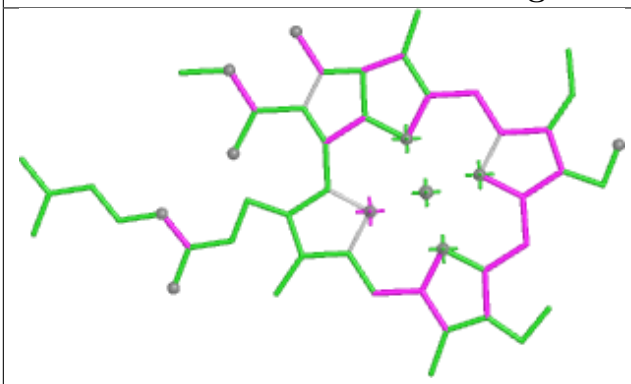


Torsions

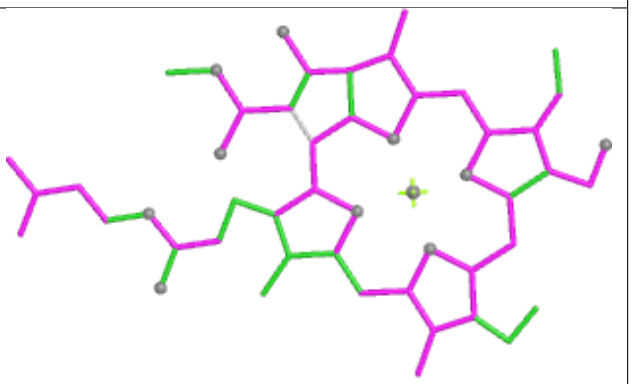


Rings

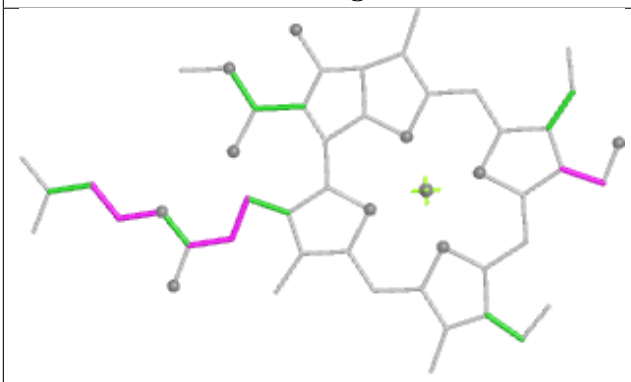
Ligand CHL a 606



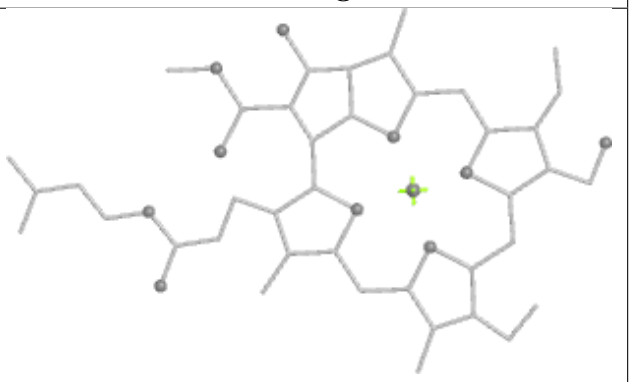
Bond lengths



Bond angles

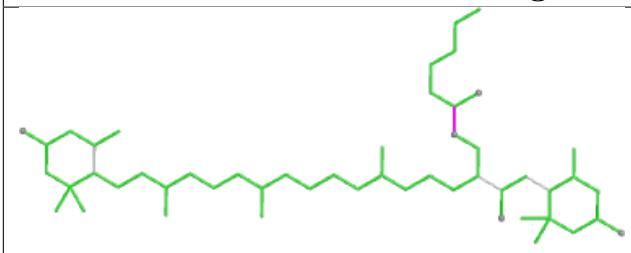


Torsions

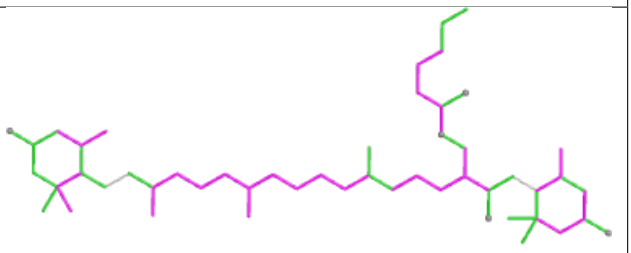


Rings

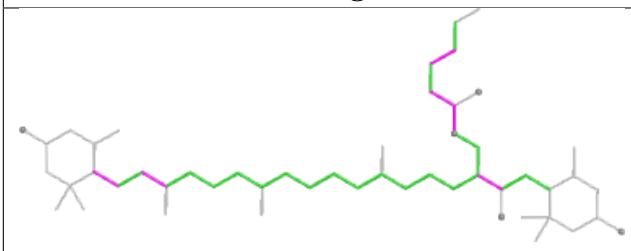
Ligand 0UR 6 501



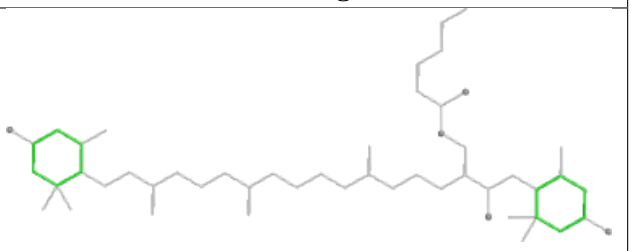
Bond lengths



Bond angles

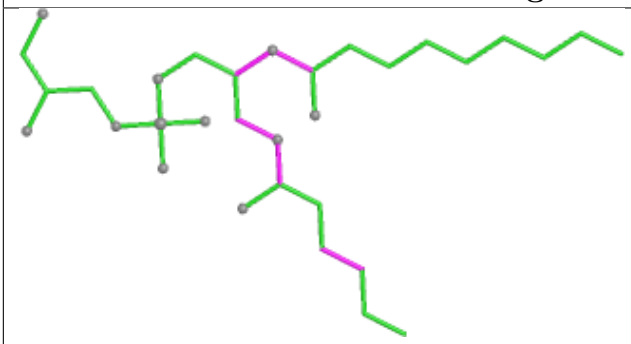


Torsions

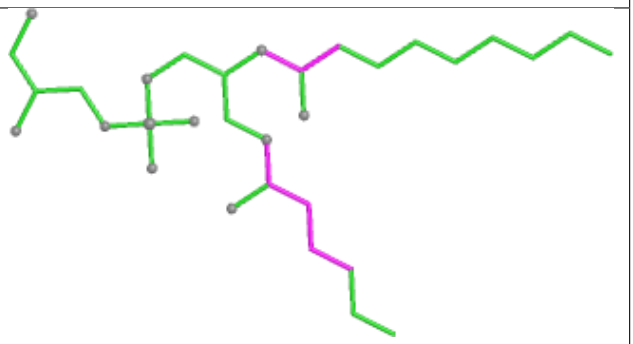


Rings

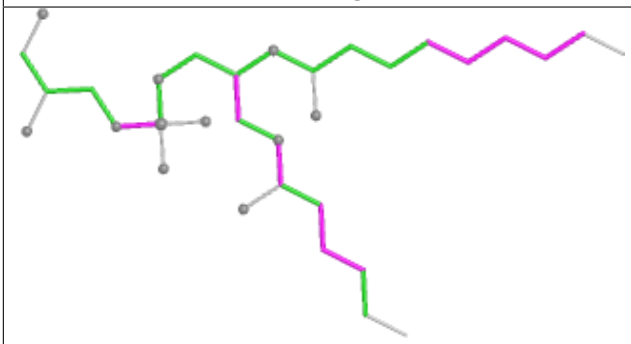
Ligand LHG 4 601



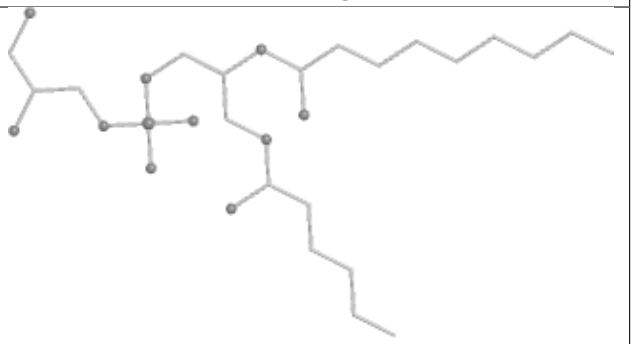
Bond lengths



Bond angles

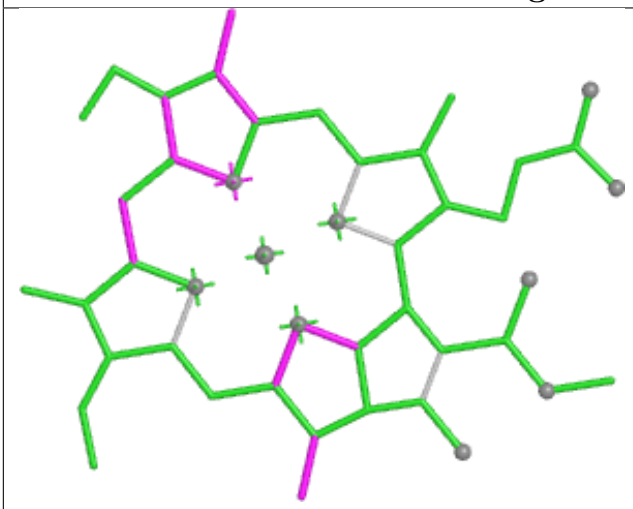


Torsions

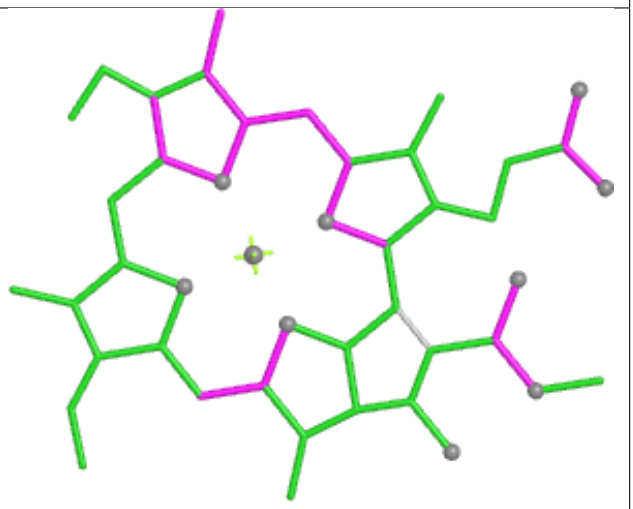


Rings

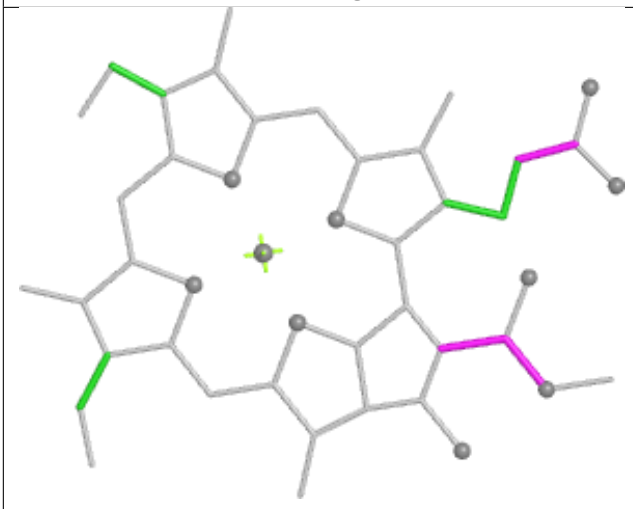
Ligand CLA 4 314



Bond lengths



Bond angles

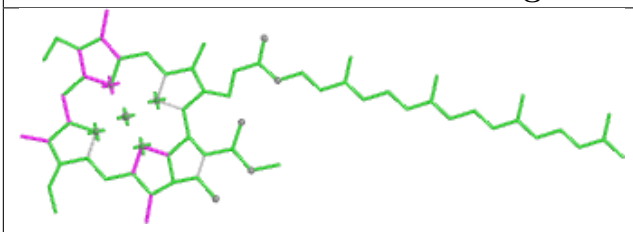


Torsions

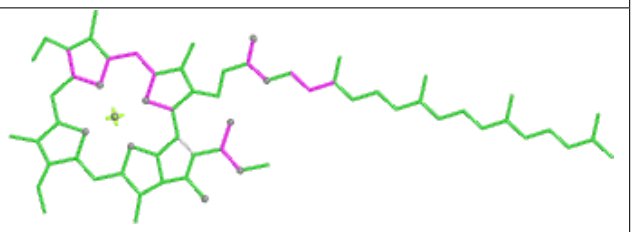


Rings

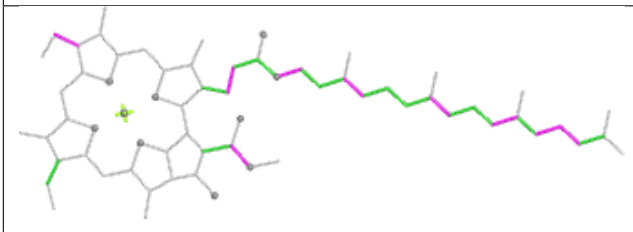
Ligand CLA A 839



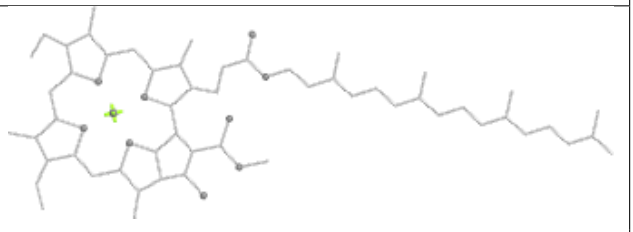
Bond lengths



Bond angles

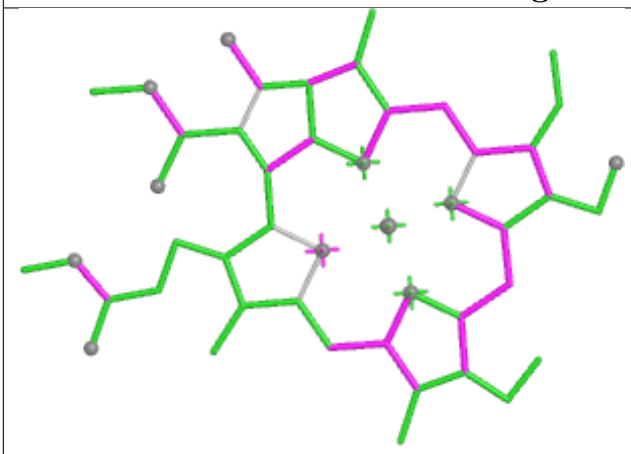


Torsions

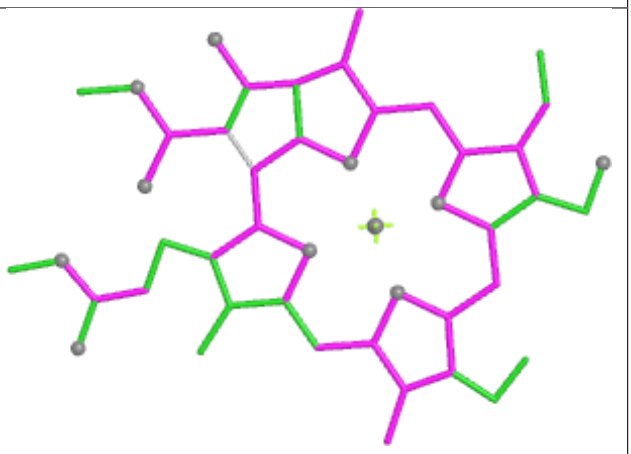


Rings

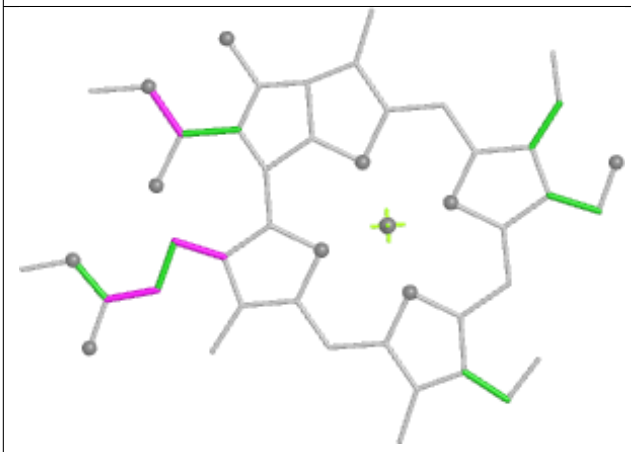
Ligand CHL f 607



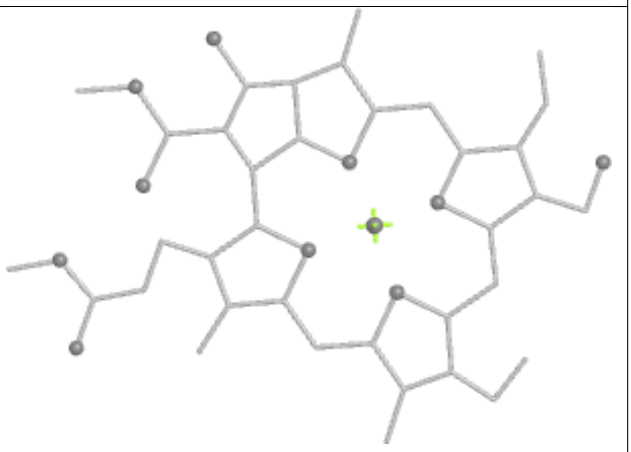
Bond lengths



Bond angles

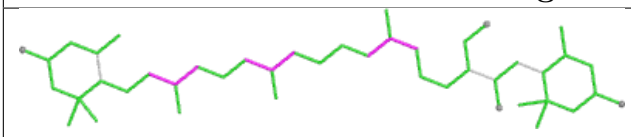


Torsions

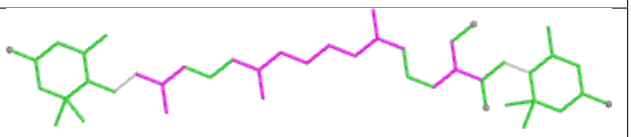


Rings

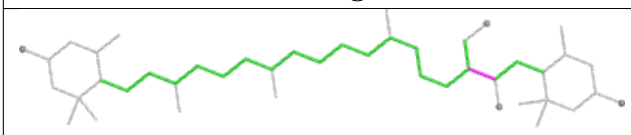
Ligand 0IE b 521



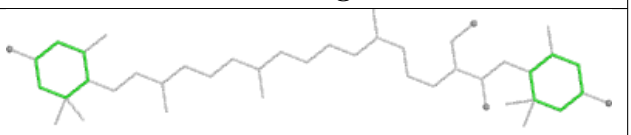
Bond lengths



Bond angles

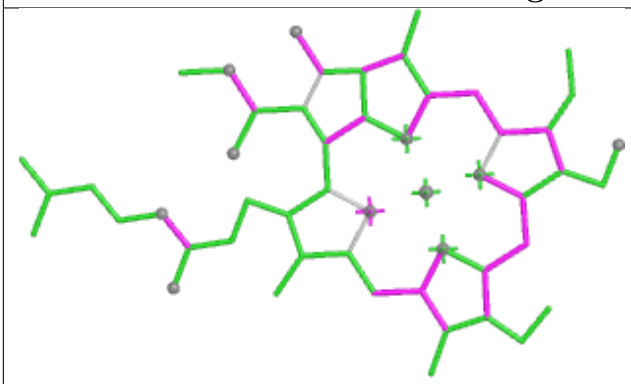


Torsions

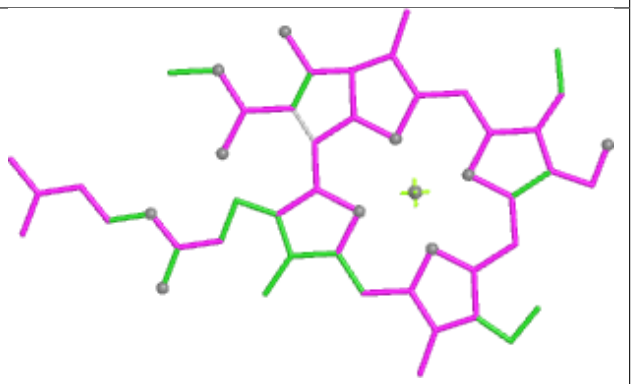


Rings

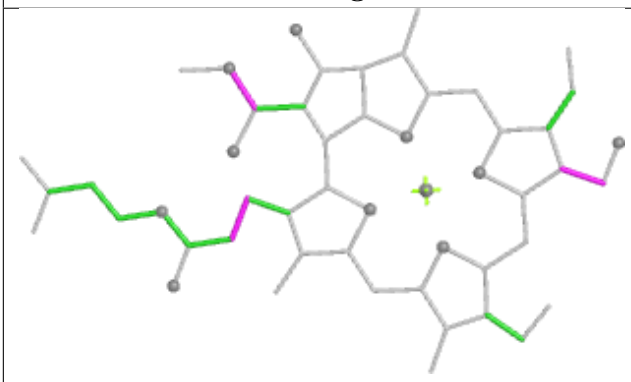
Ligand CHL d 608



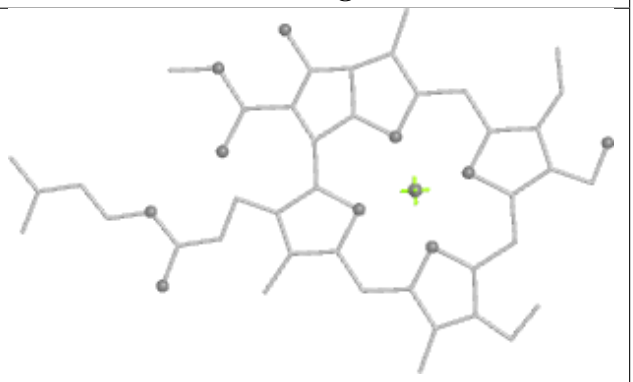
Bond lengths



Bond angles

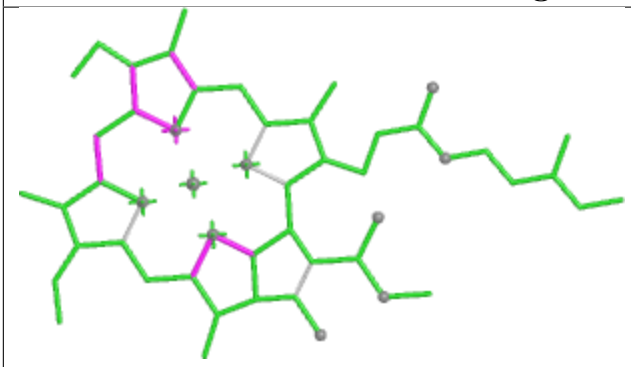


Torsions

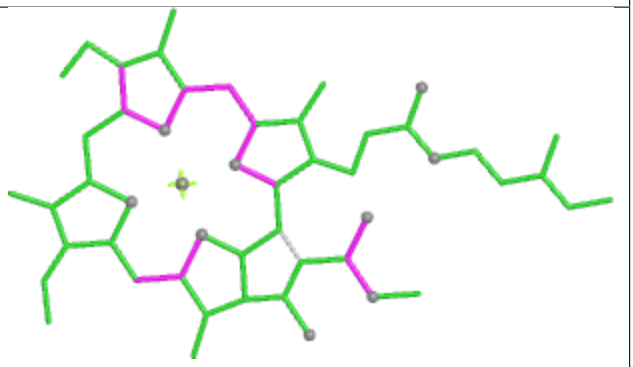


Rings

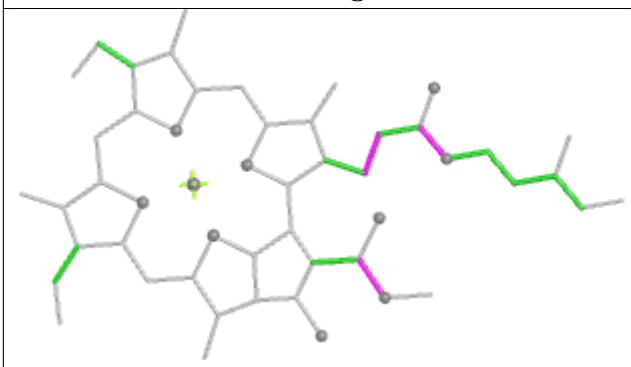
Ligand CLA i 613



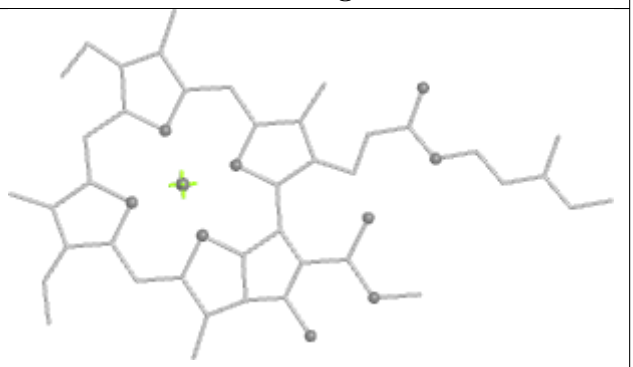
Bond lengths



Bond angles

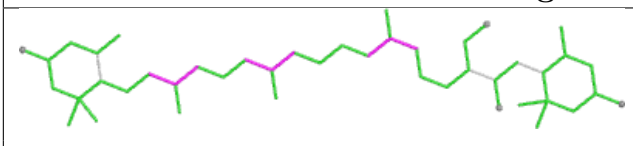


Torsions

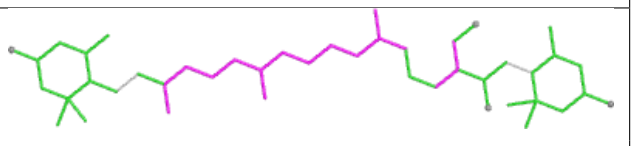


Rings

Ligand 0IE d 522



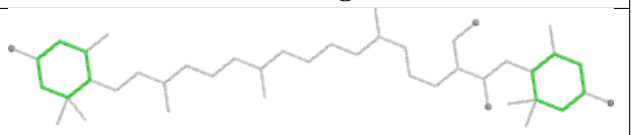
Bond lengths



Bond angles

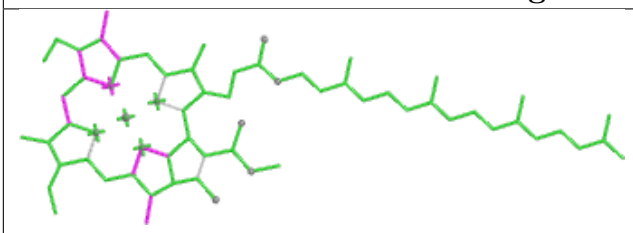


Torsions

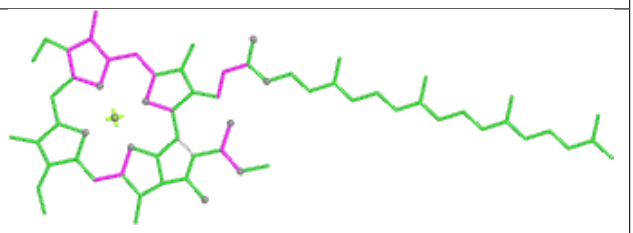


Rings

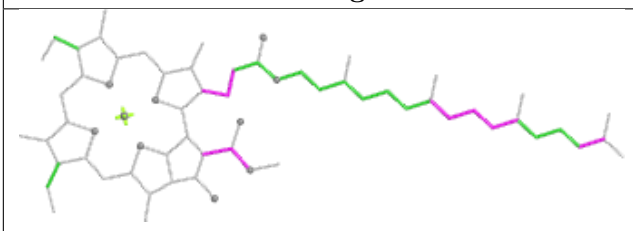
Ligand CLA 6 317



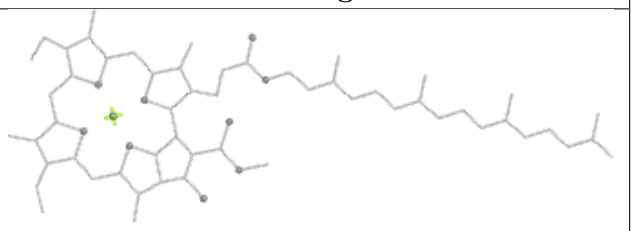
Bond lengths



Bond angles

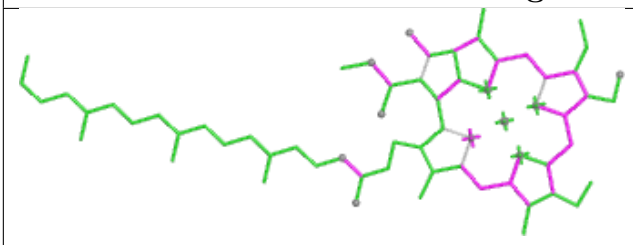


Torsions

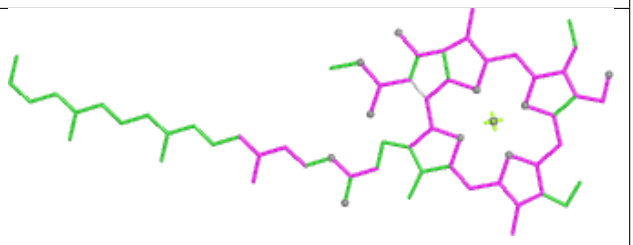


Rings

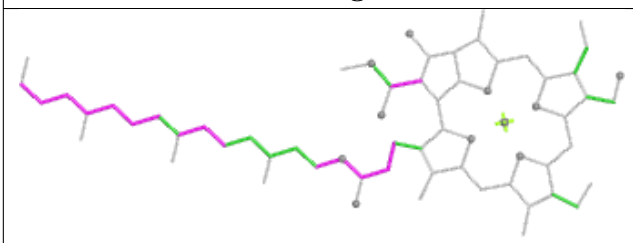
Ligand CHL d 602



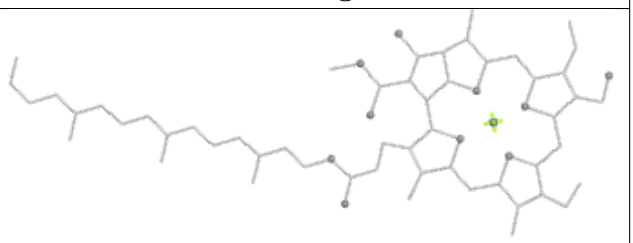
Bond lengths



Bond angles

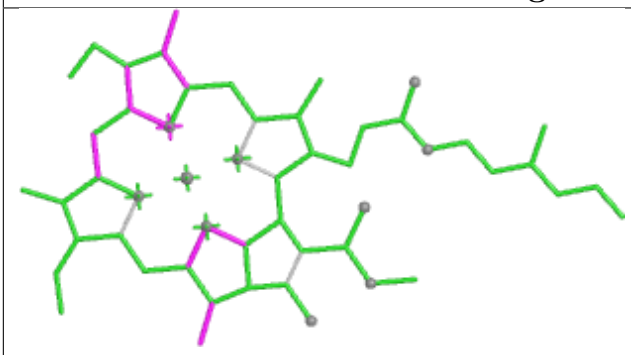


Torsions

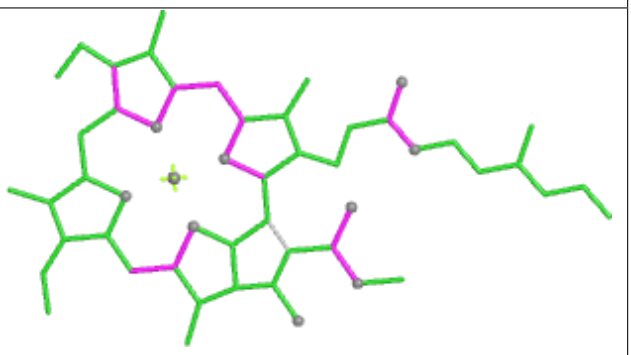


Rings

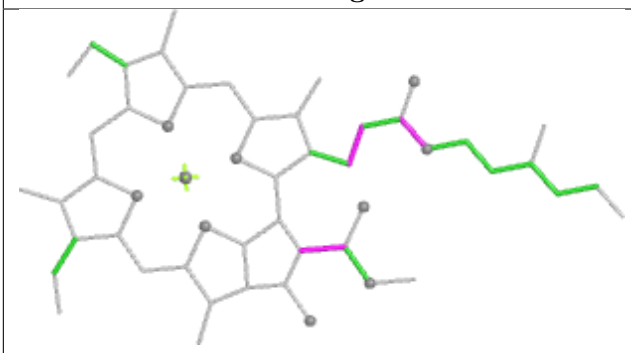
Ligand CLA 1 304



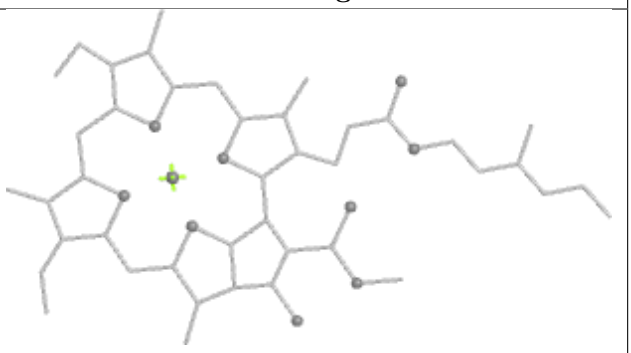
Bond lengths



Bond angles

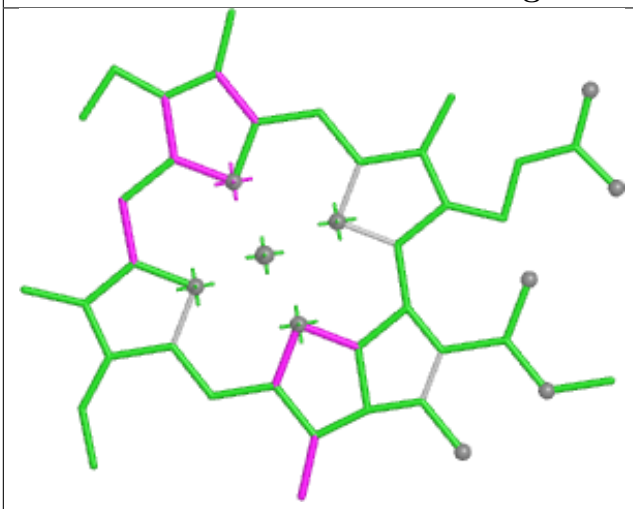


Torsions

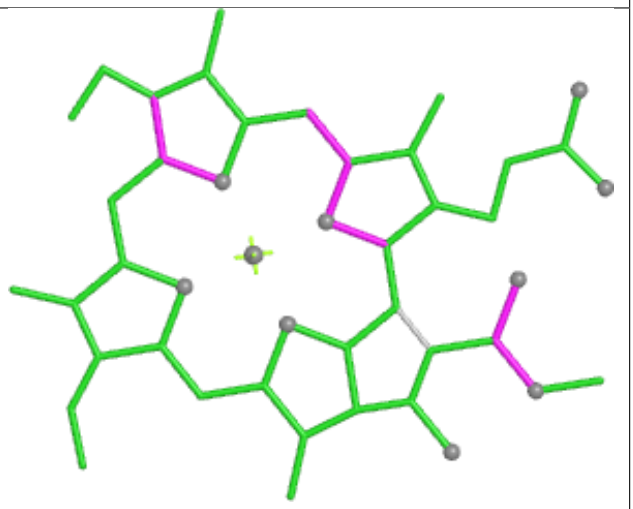


Rings

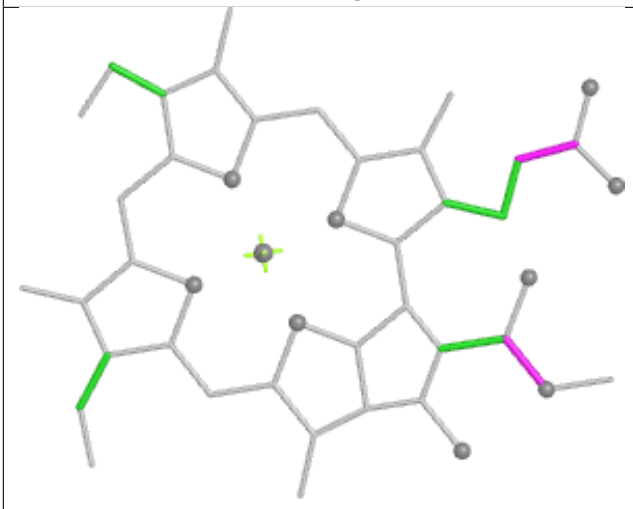
Ligand CLA G 102



Bond lengths



Bond angles

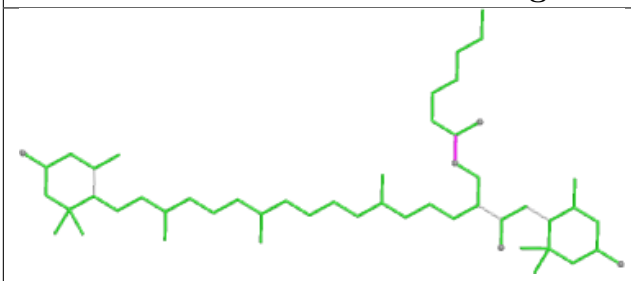


Torsions

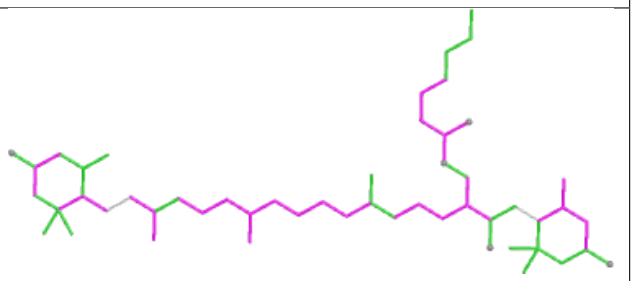


Rings

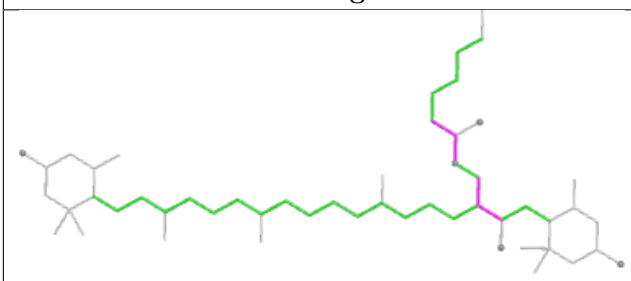
Ligand 0UR 9 502



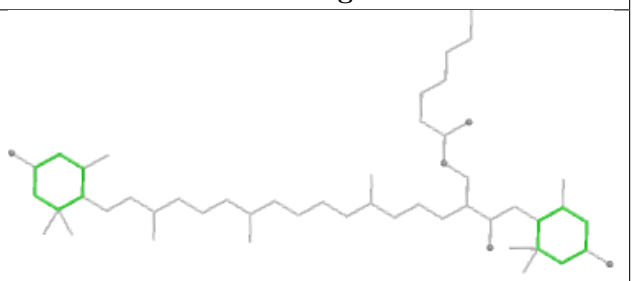
Bond lengths



Bond angles

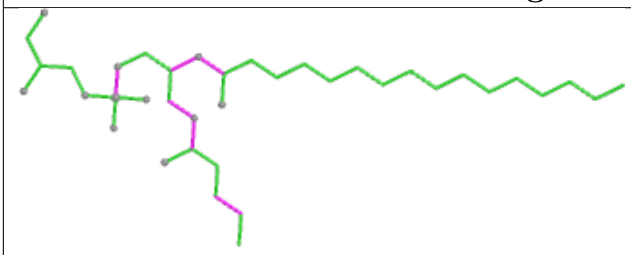


Torsions

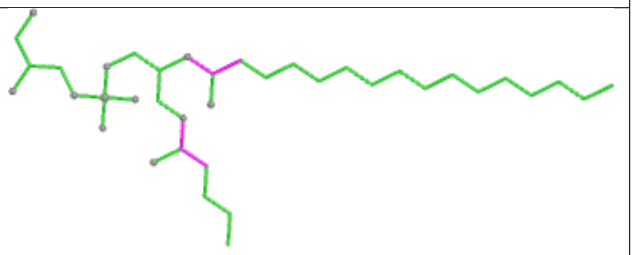


Rings

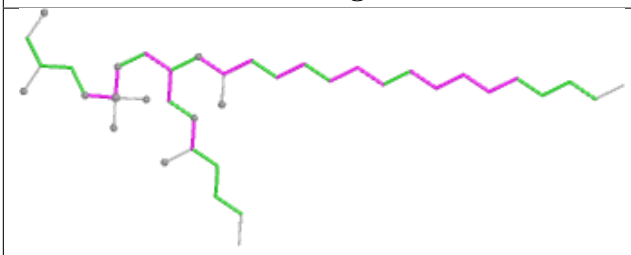
Ligand LHG 7 602



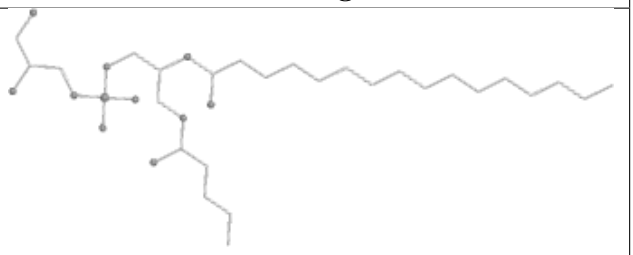
Bond lengths



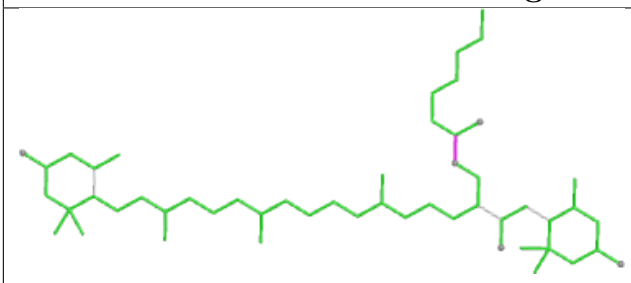
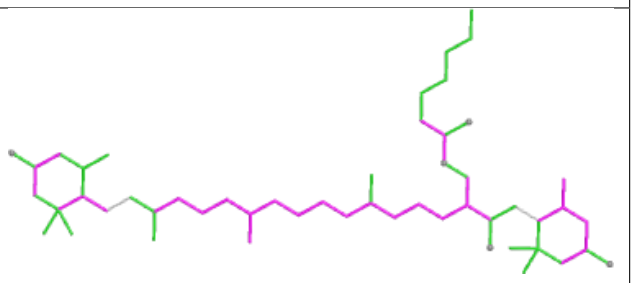
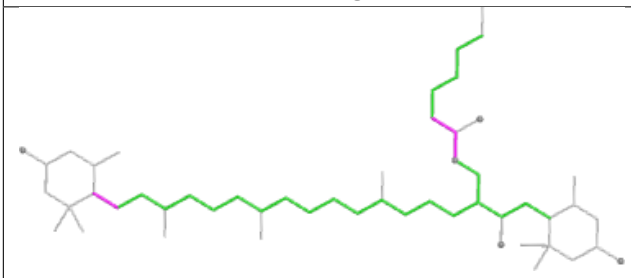
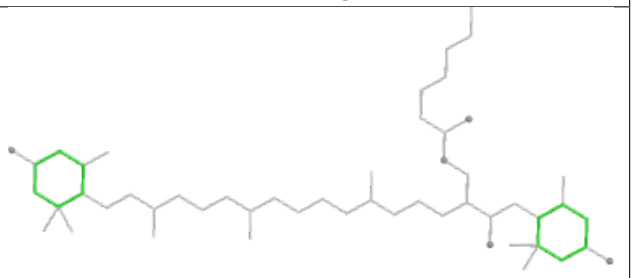
Bond angles

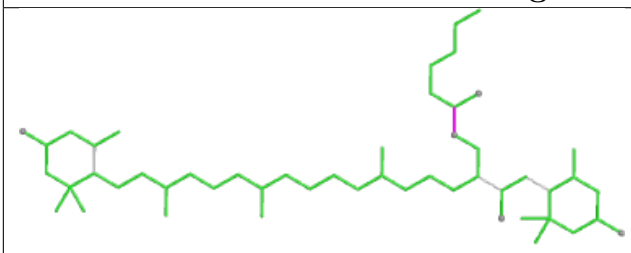
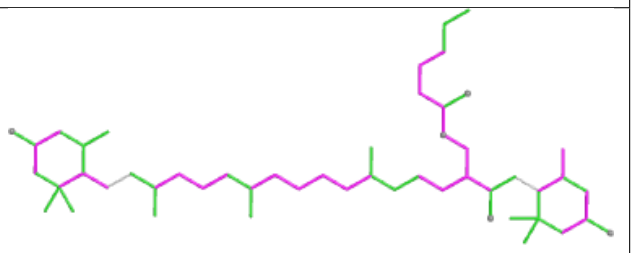
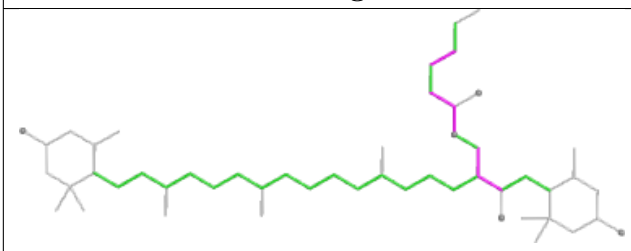
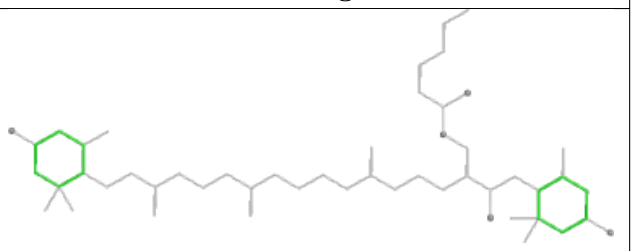


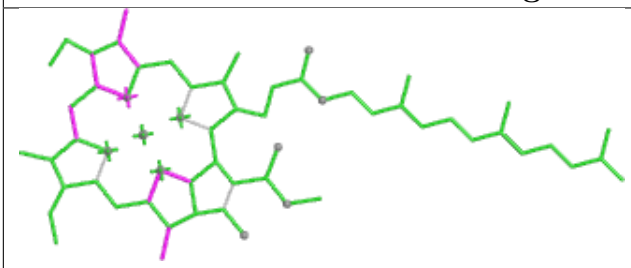
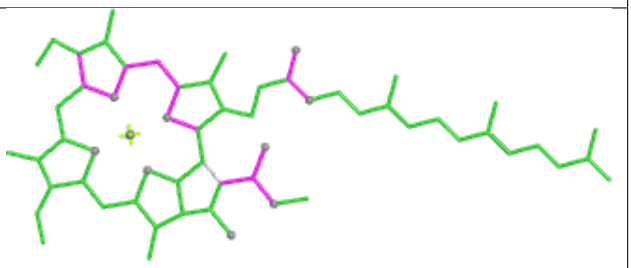
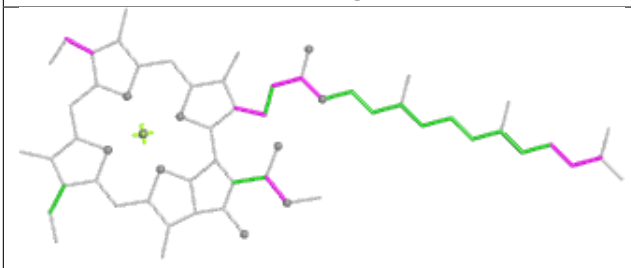
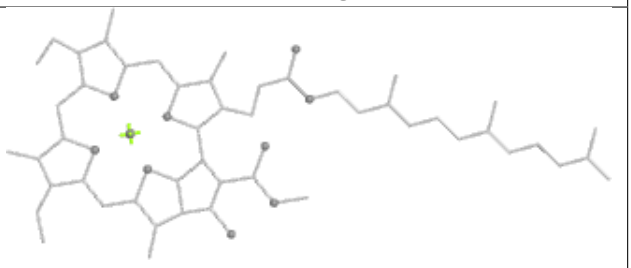
Torsions

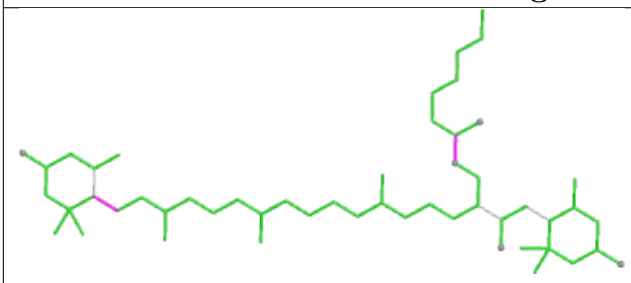
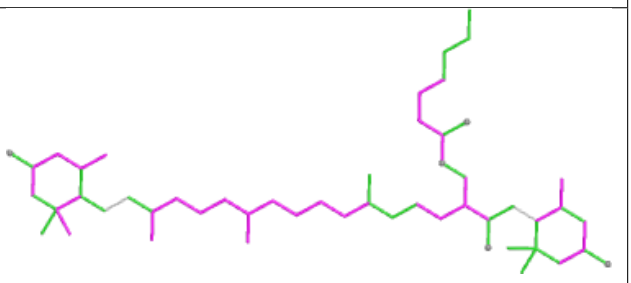
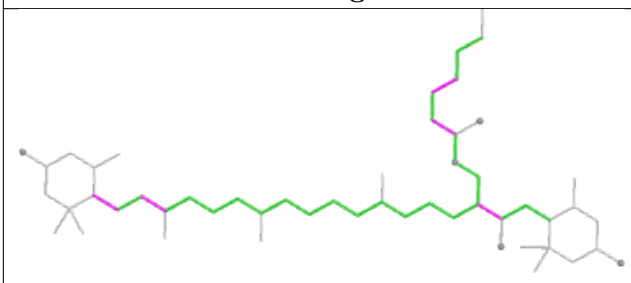
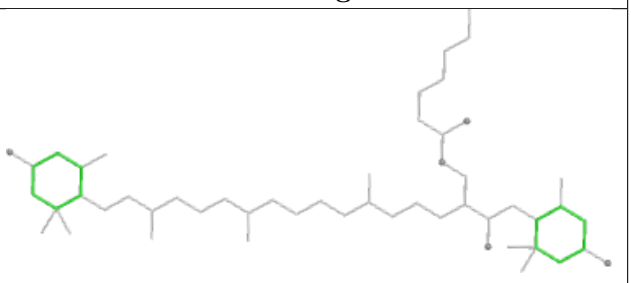


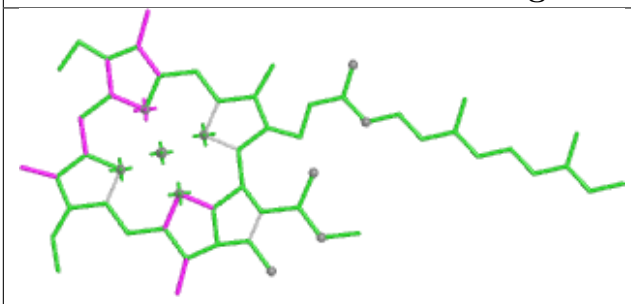
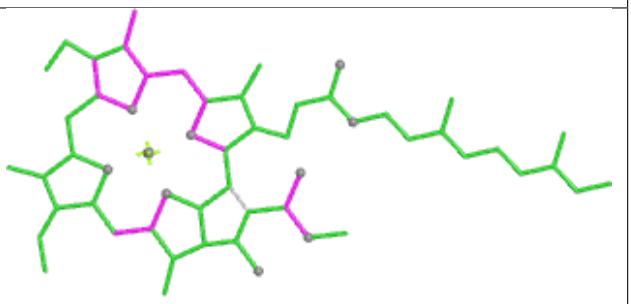
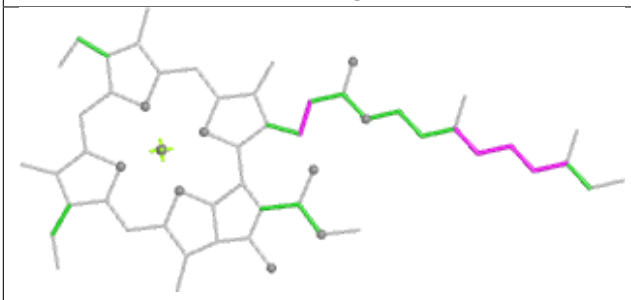
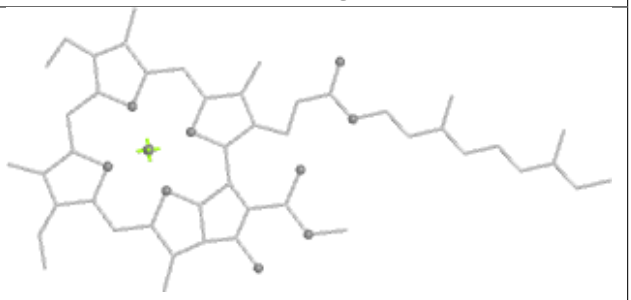
Rings

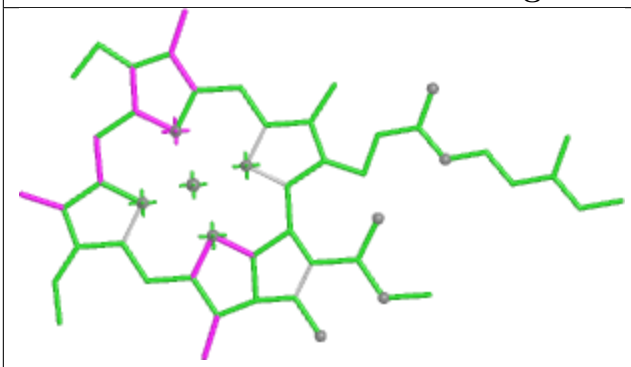
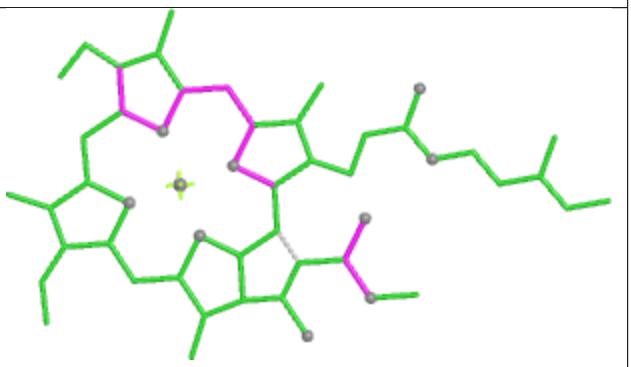
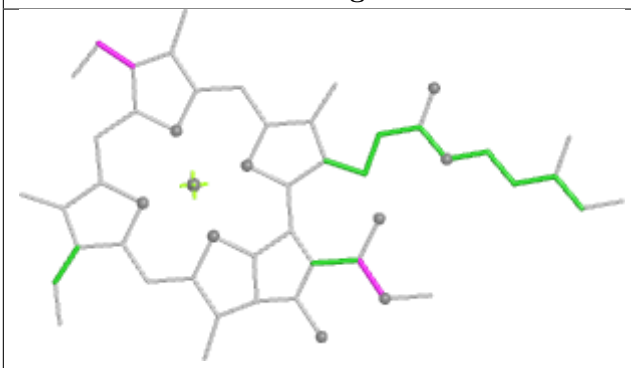
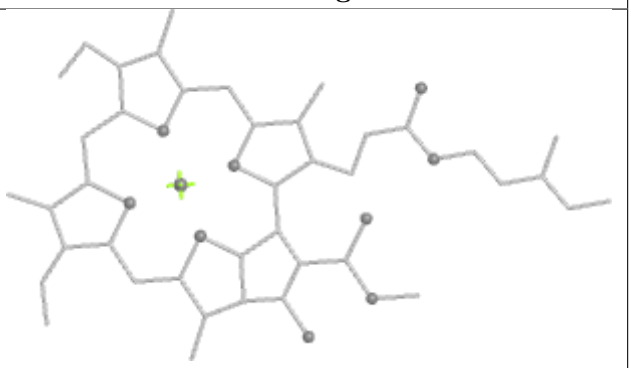
Ligand 0UR O 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 0UR 3 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

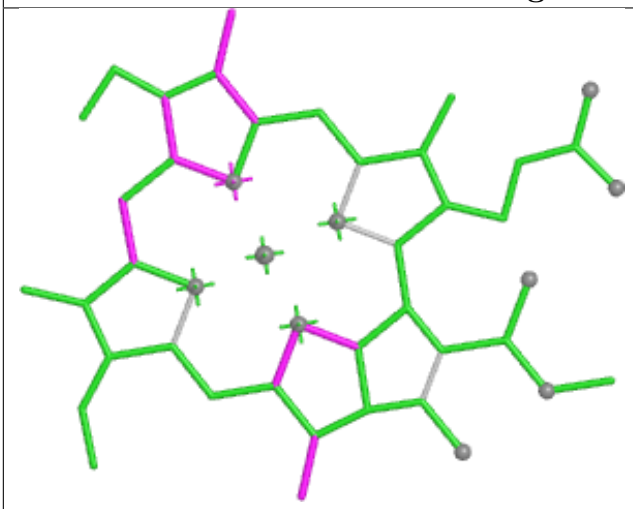
Ligand CLA K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 0UR c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

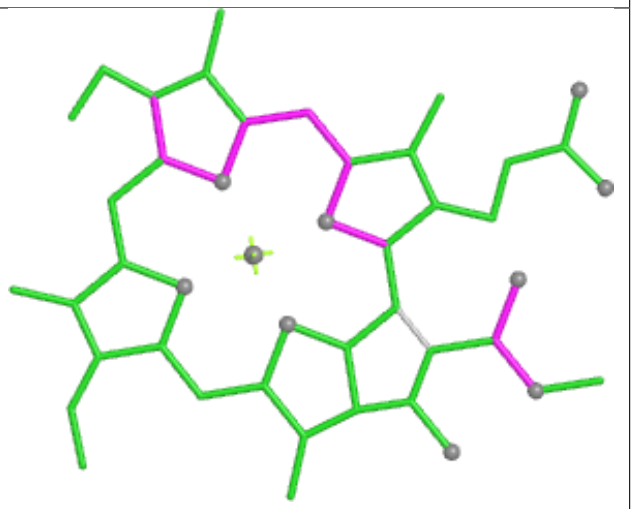
Ligand CLA 9 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

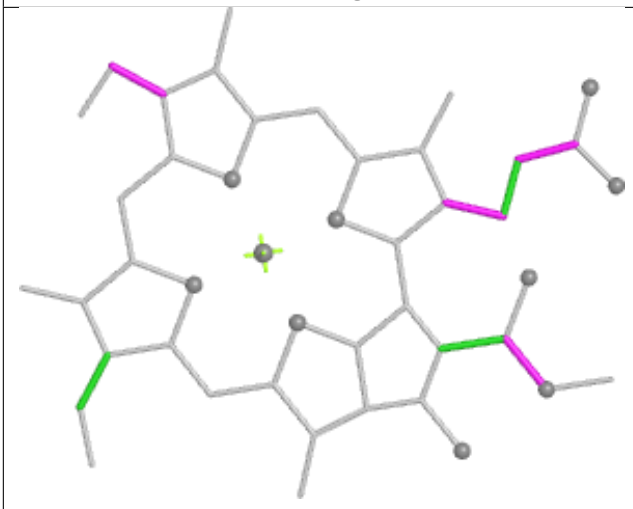
Ligand CLA d 612



Bond lengths



Bond angles

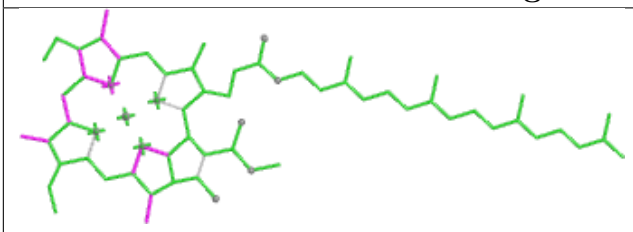


Torsions

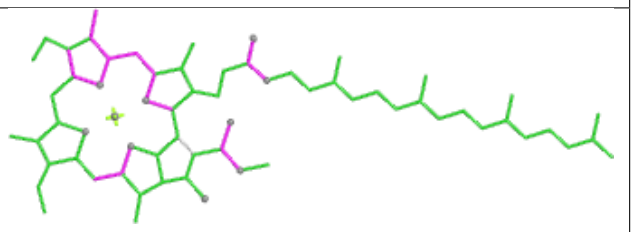


Rings

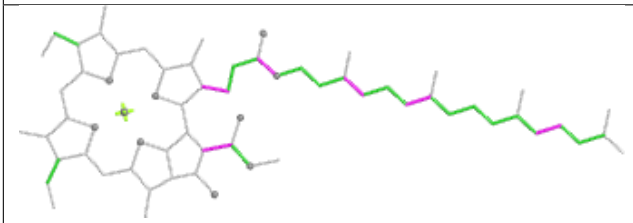
Ligand CLA A 813



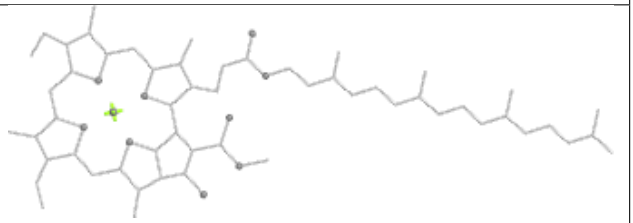
Bond lengths



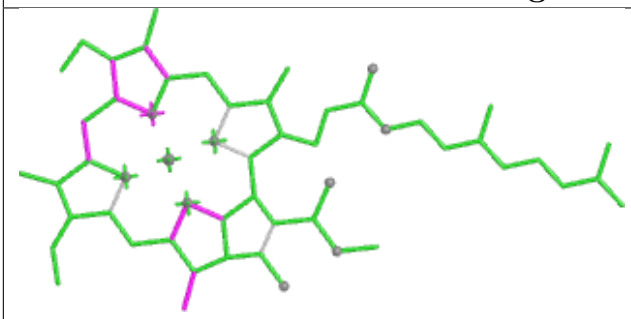
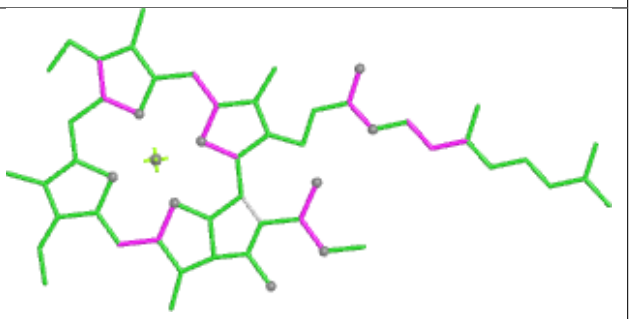
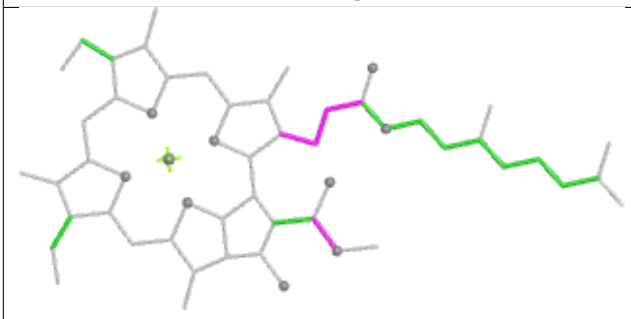
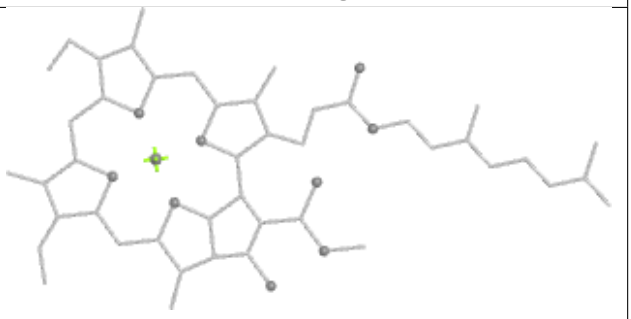
Bond angles

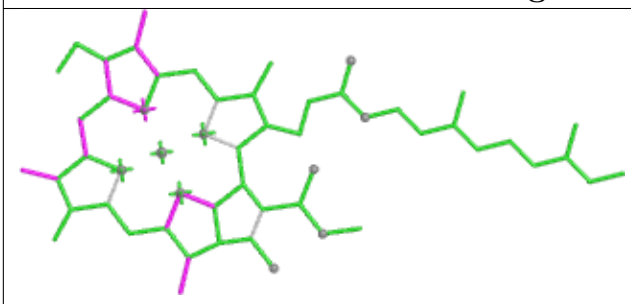
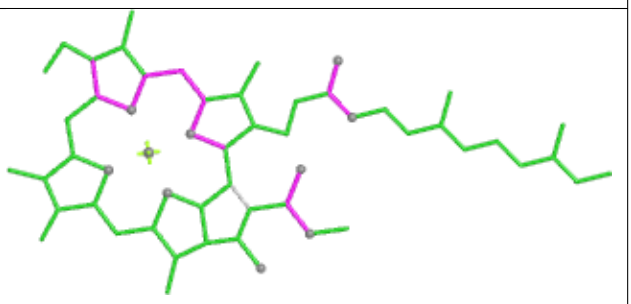
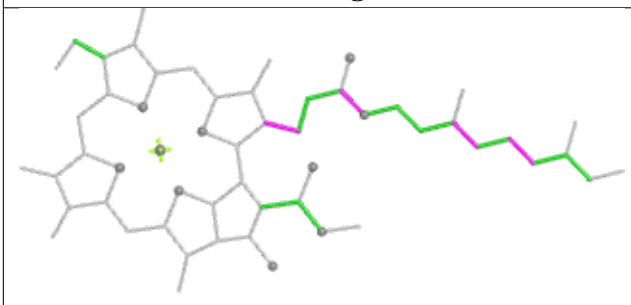
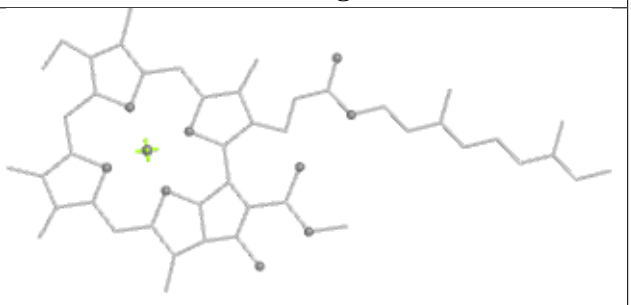


Torsions

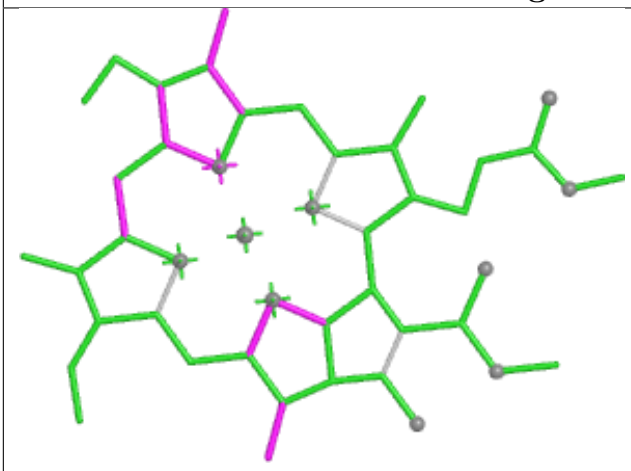


Rings

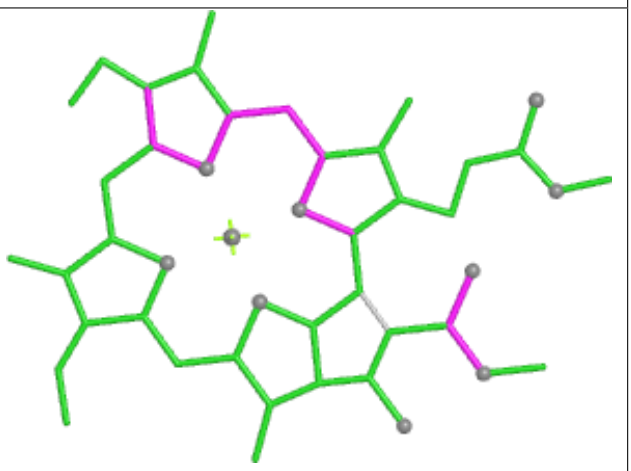
Ligand CLA a 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

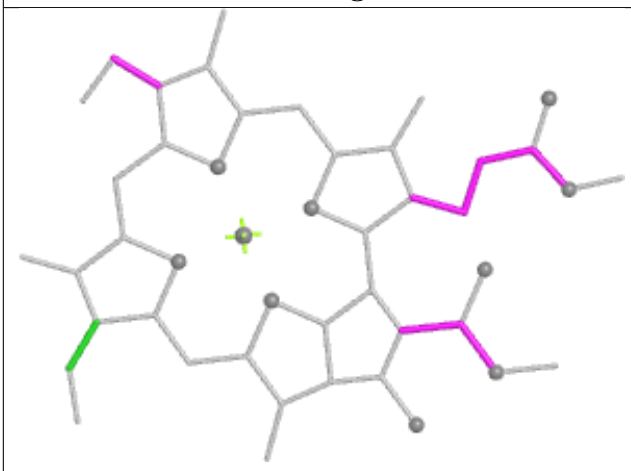
Ligand CLA 6 318



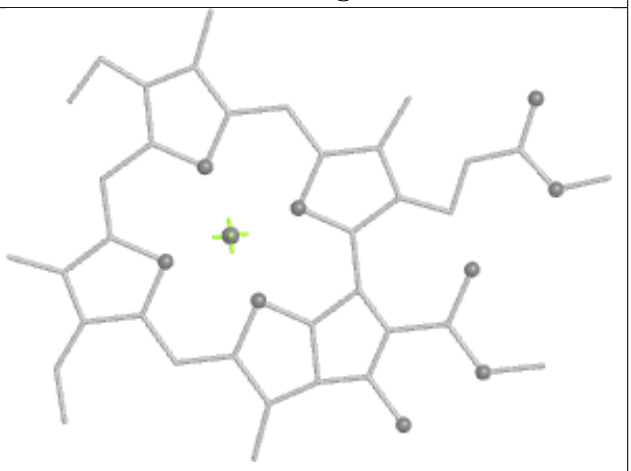
Bond lengths



Bond angles

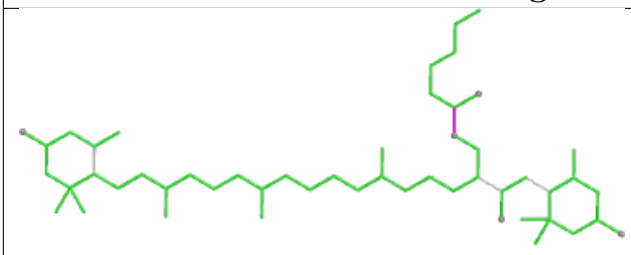


Torsions

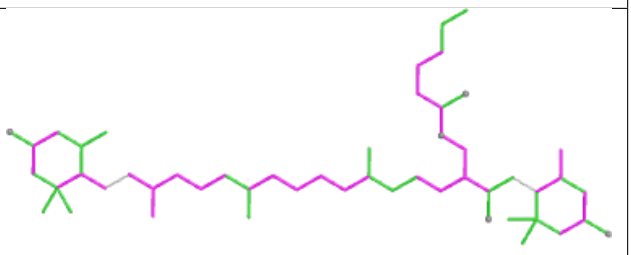


Rings

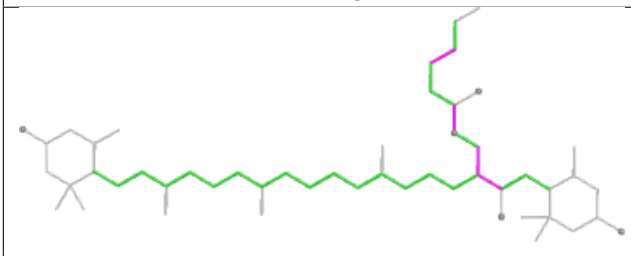
Ligand 0UR 2 501



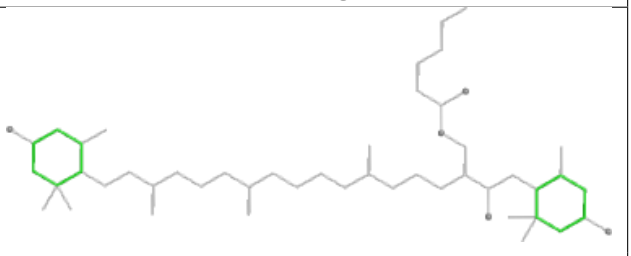
Bond lengths



Bond angles

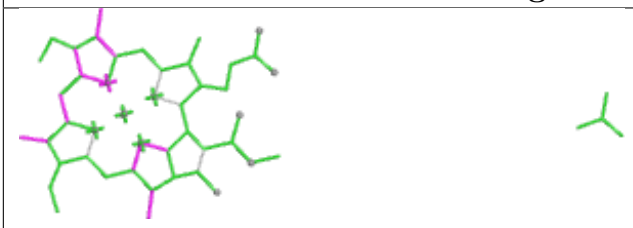


Torsions

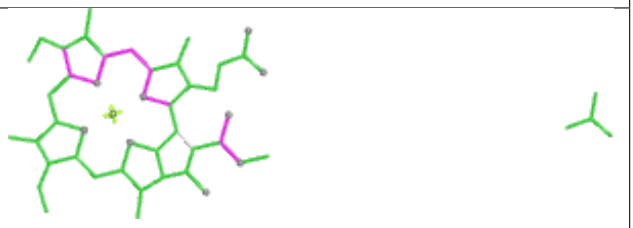


Rings

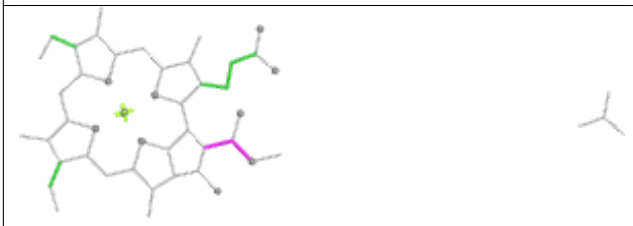
Ligand CLA 7 316



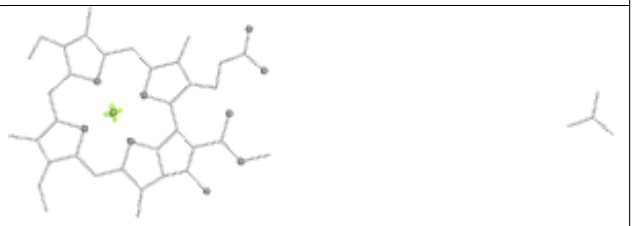
Bond lengths



Bond angles

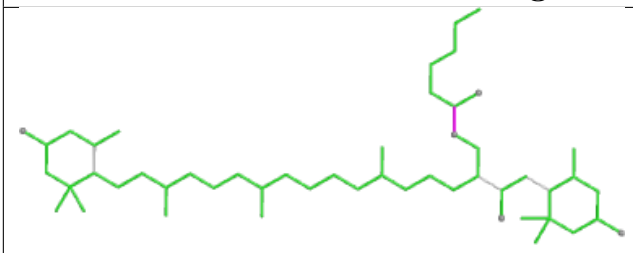


Torsions

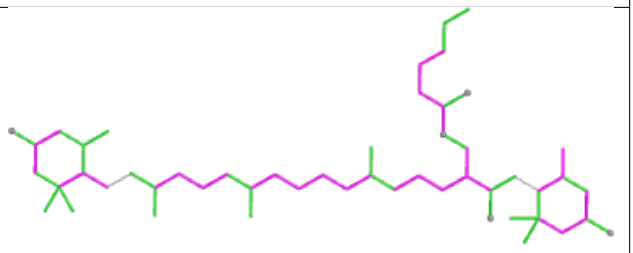


Rings

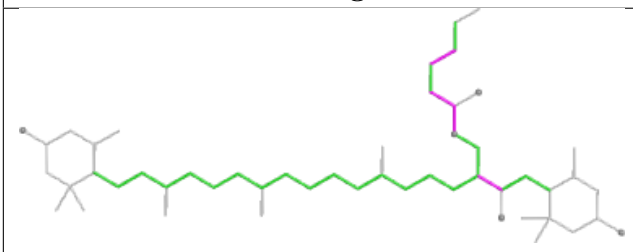
Ligand 0UR 8 501



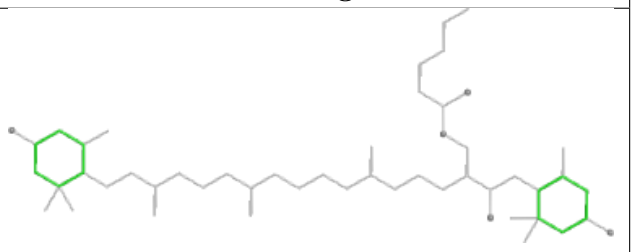
Bond lengths



Bond angles

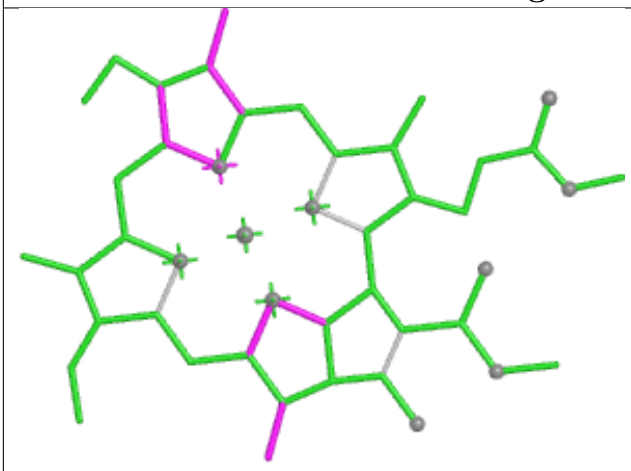


Torsions

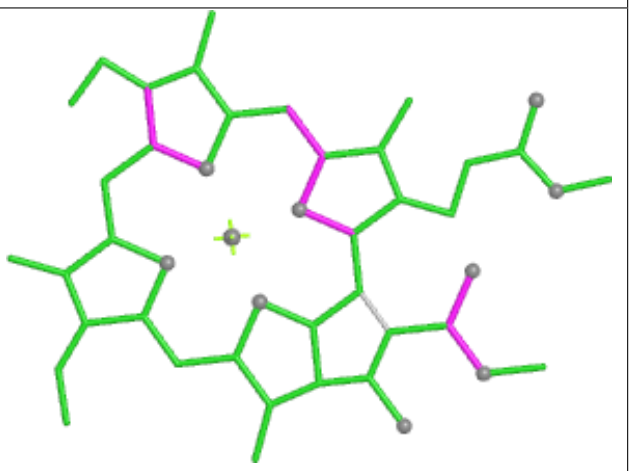


Rings

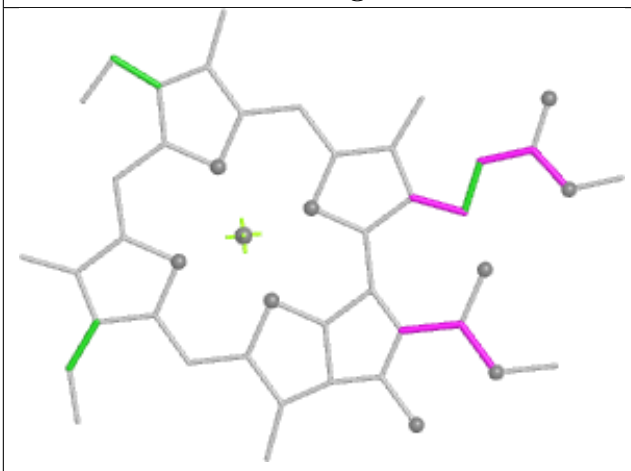
Ligand CLA 0 313



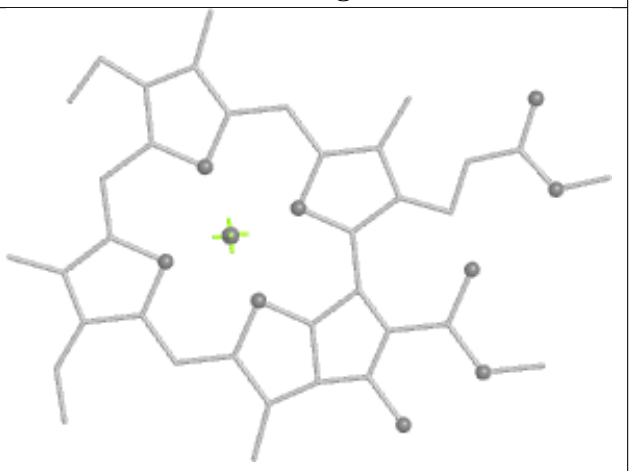
Bond lengths



Bond angles

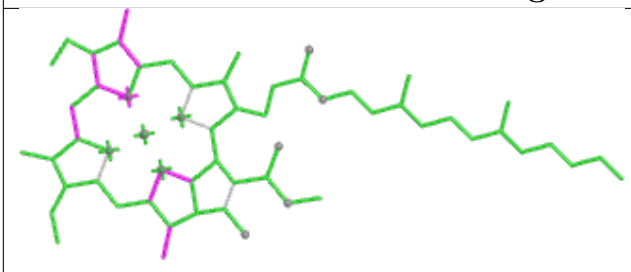


Torsions

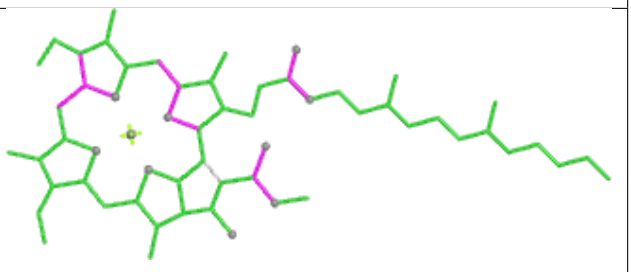


Rings

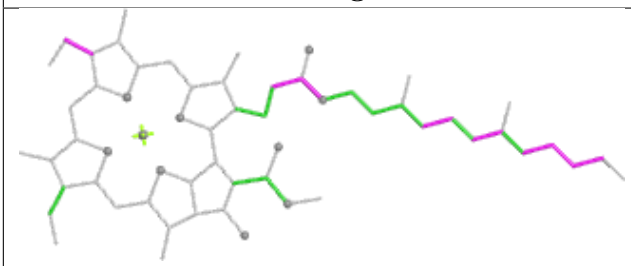
Ligand CLA 5 303



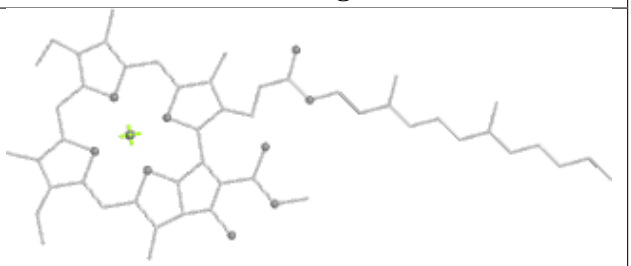
Bond lengths



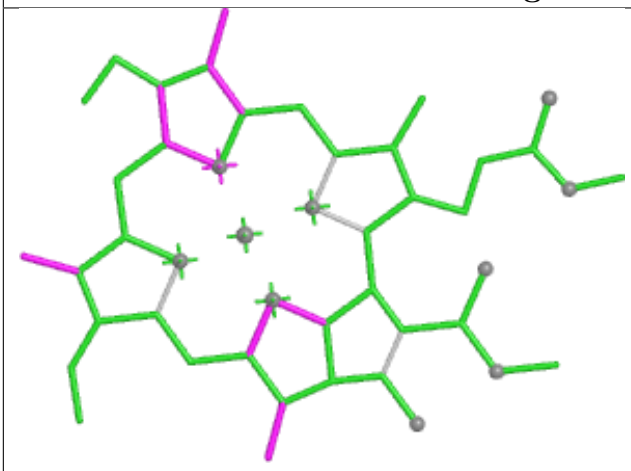
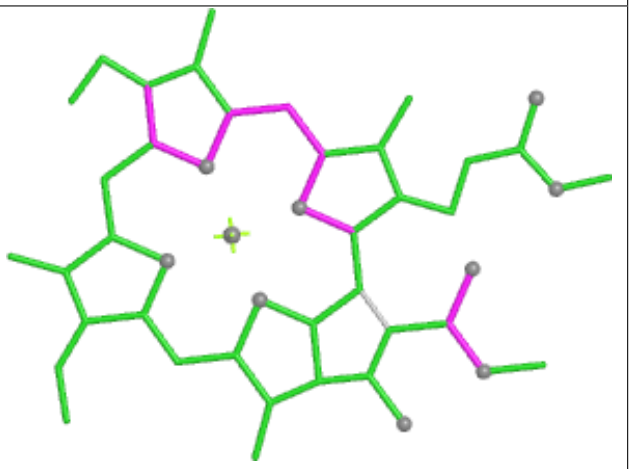
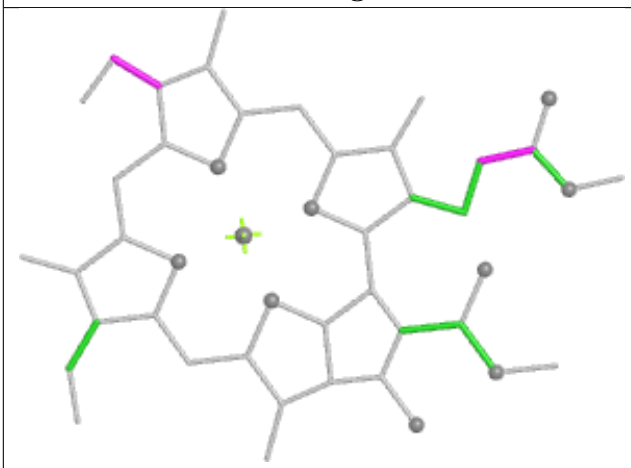
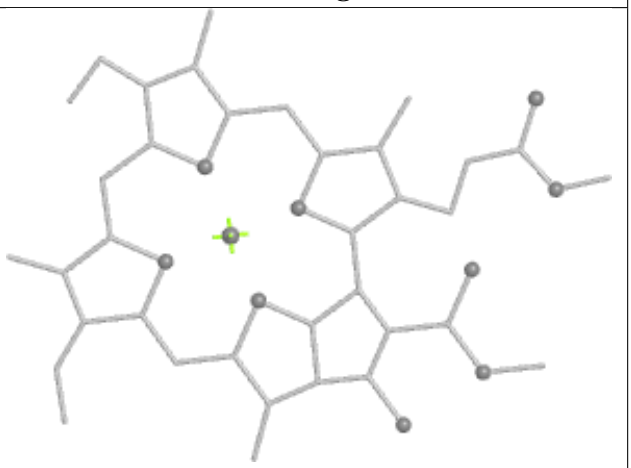
Bond angles



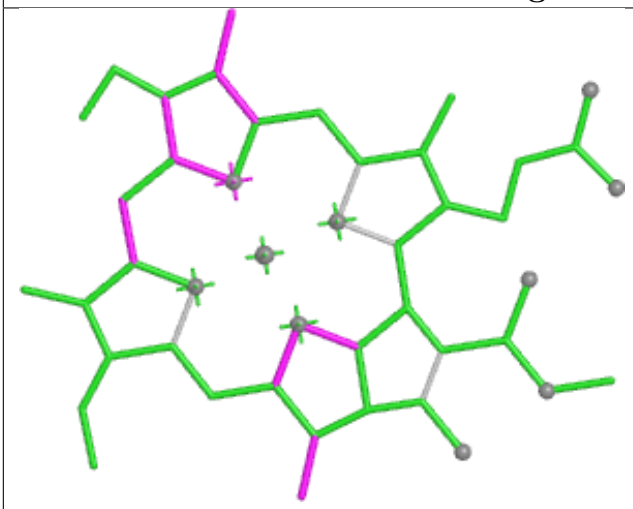
Torsions



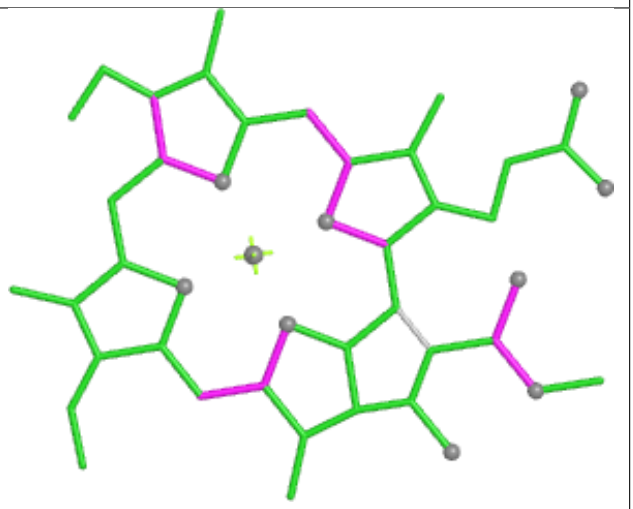
Rings

Ligand CLA A 834	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

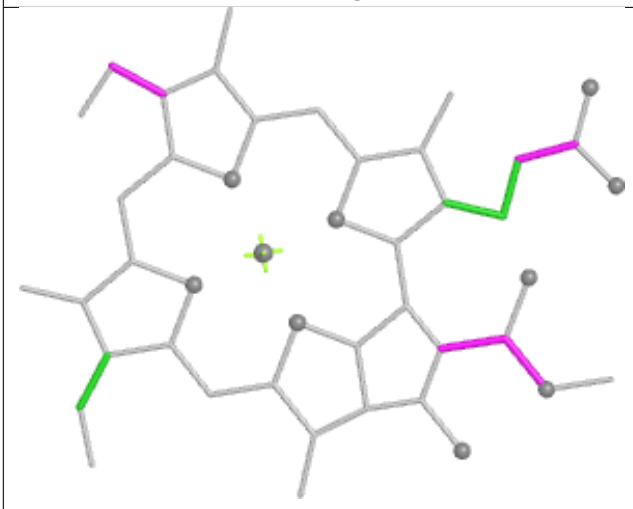
Ligand CLA 1 308



Bond lengths



Bond angles

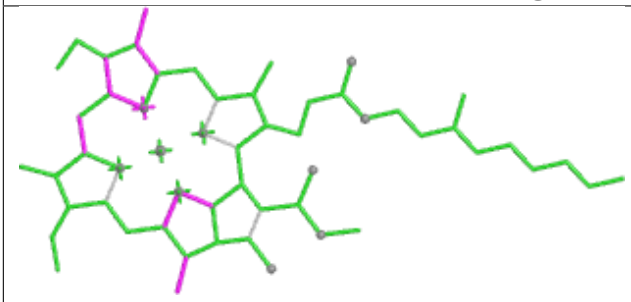


Torsions

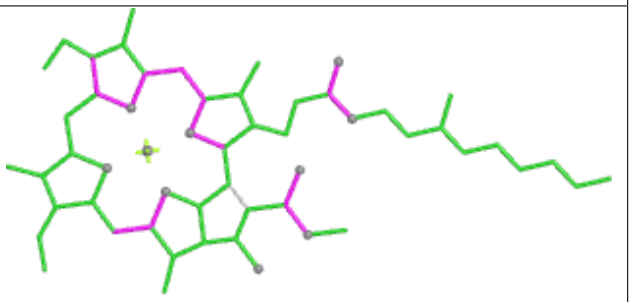


Rings

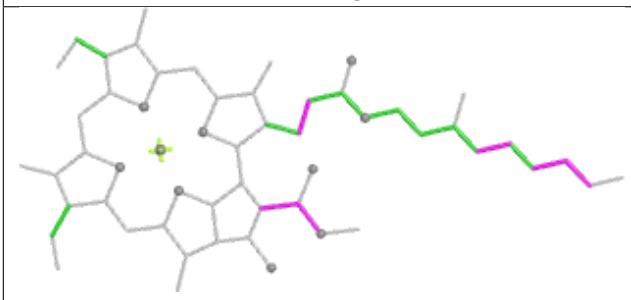
Ligand CLA c 613



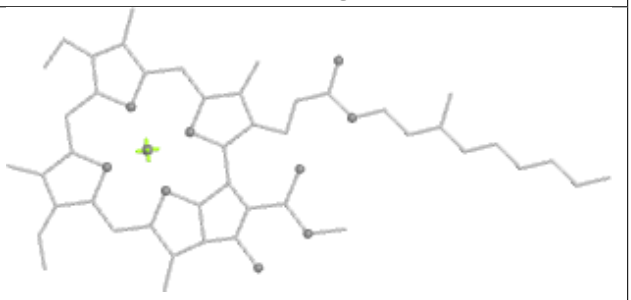
Bond lengths



Bond angles

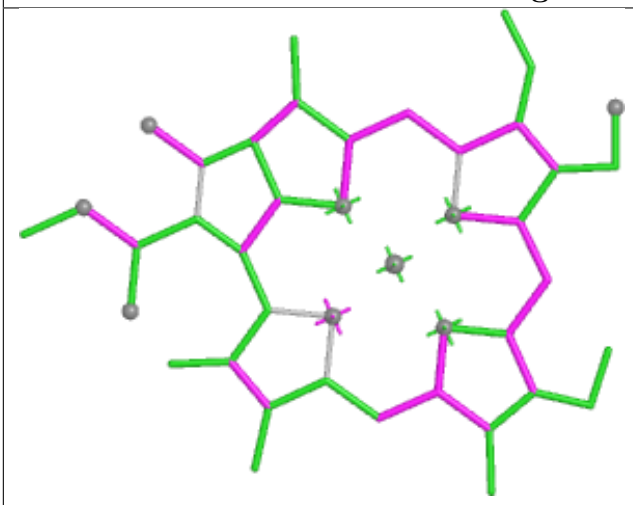


Torsions

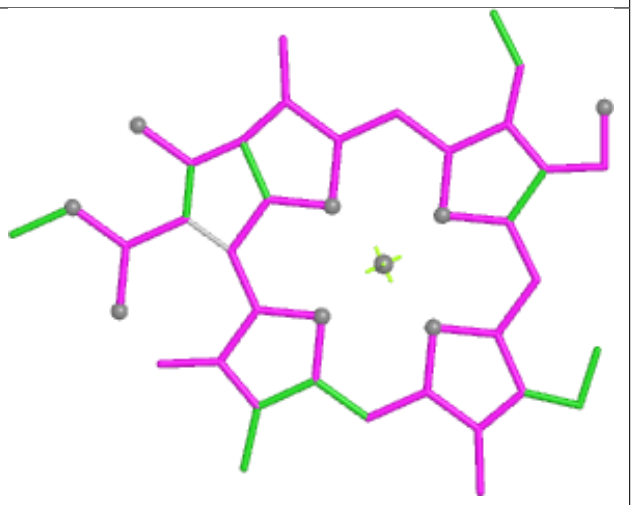


Rings

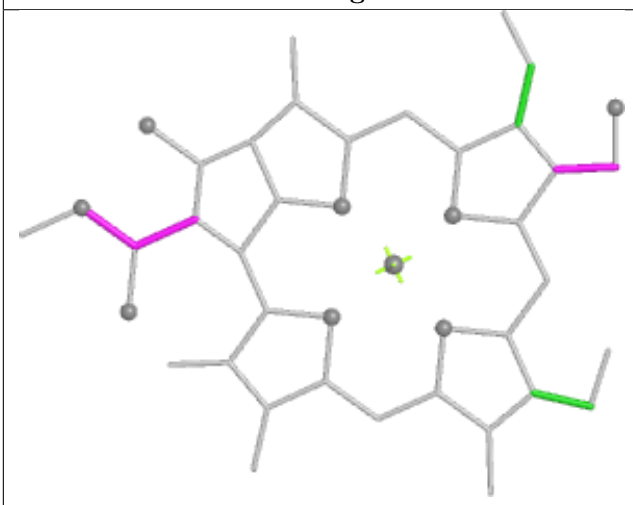
Ligand CHL f 614



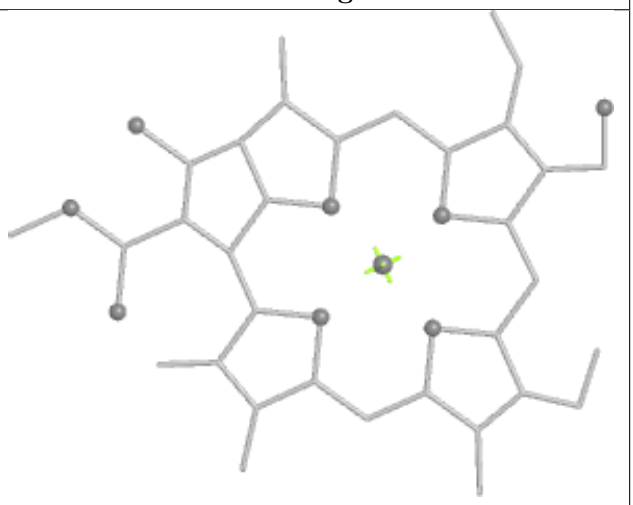
Bond lengths



Bond angles

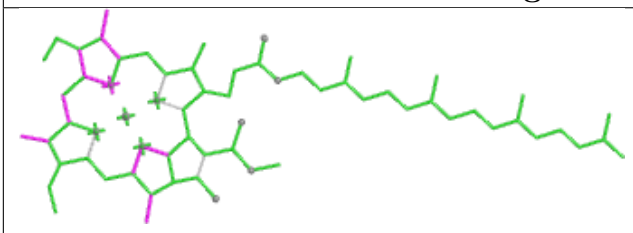


Torsions

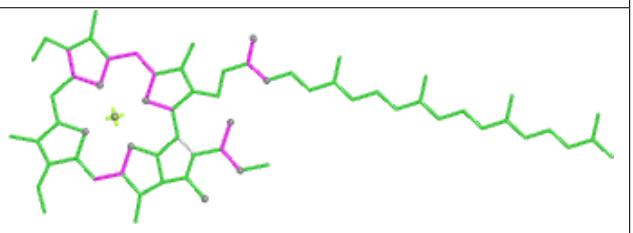


Rings

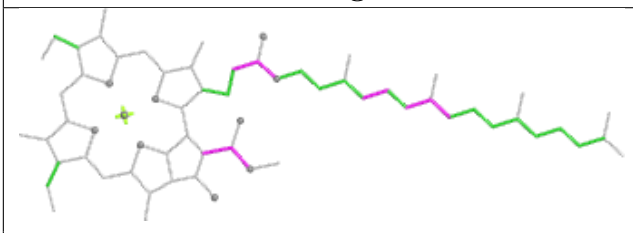
Ligand CLA A 833



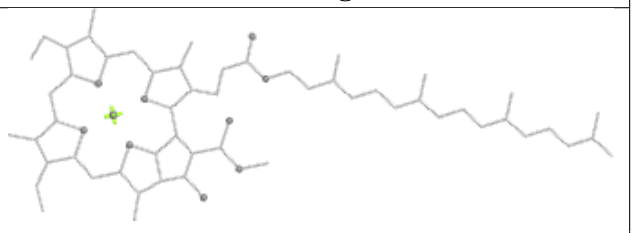
Bond lengths



Bond angles

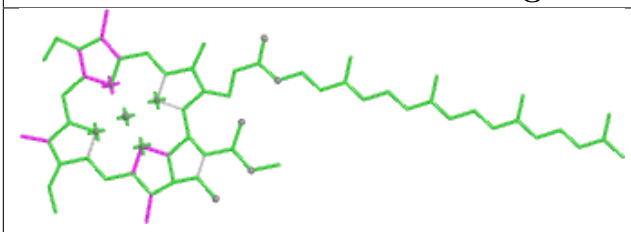


Torsions

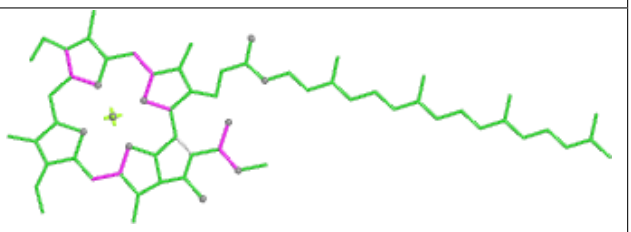


Rings

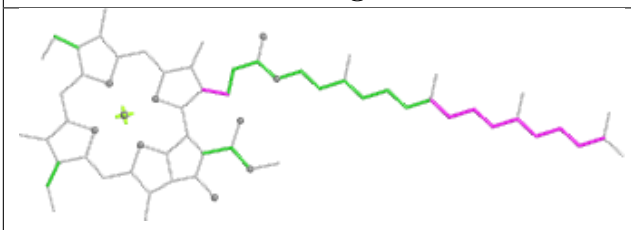
Ligand CLA A 811



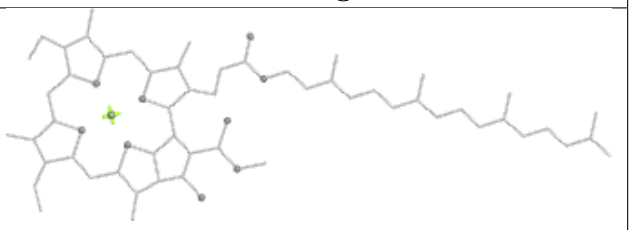
Bond lengths



Bond angles

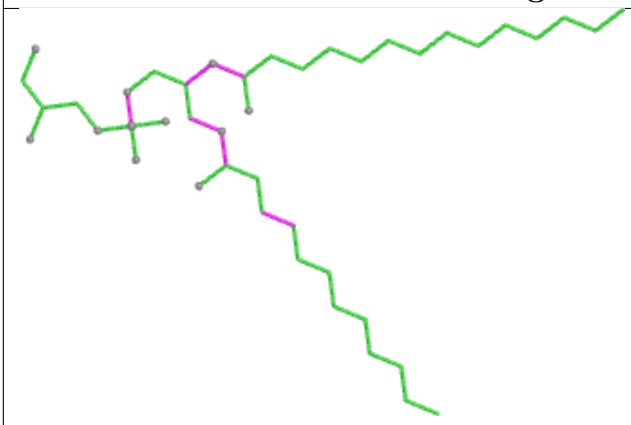


Torsions

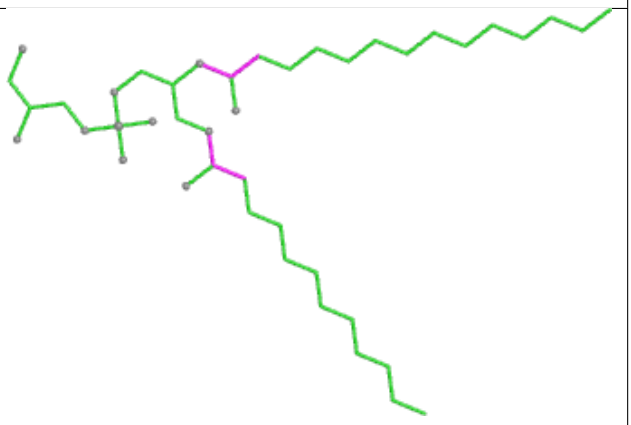


Rings

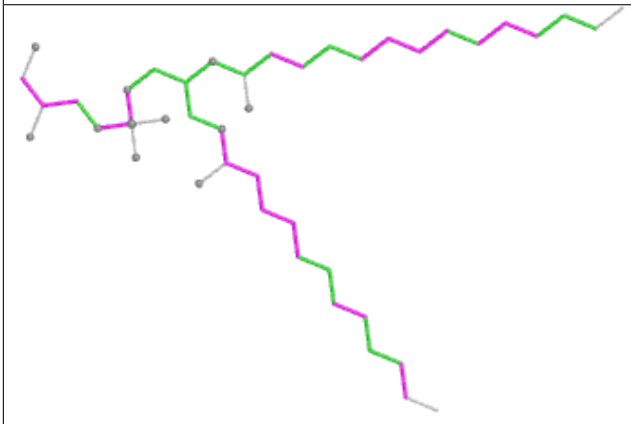
Ligand LHG e 630



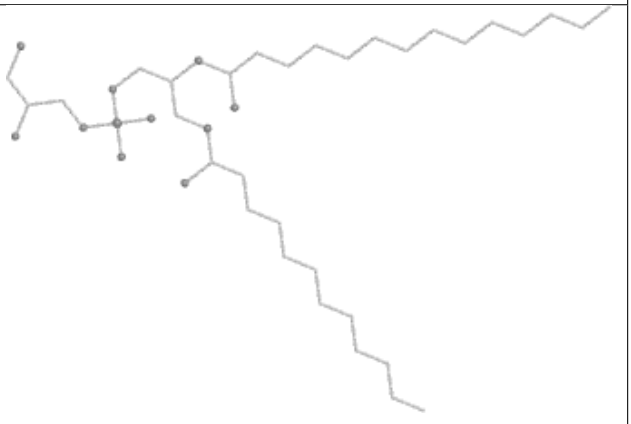
Bond lengths



Bond angles

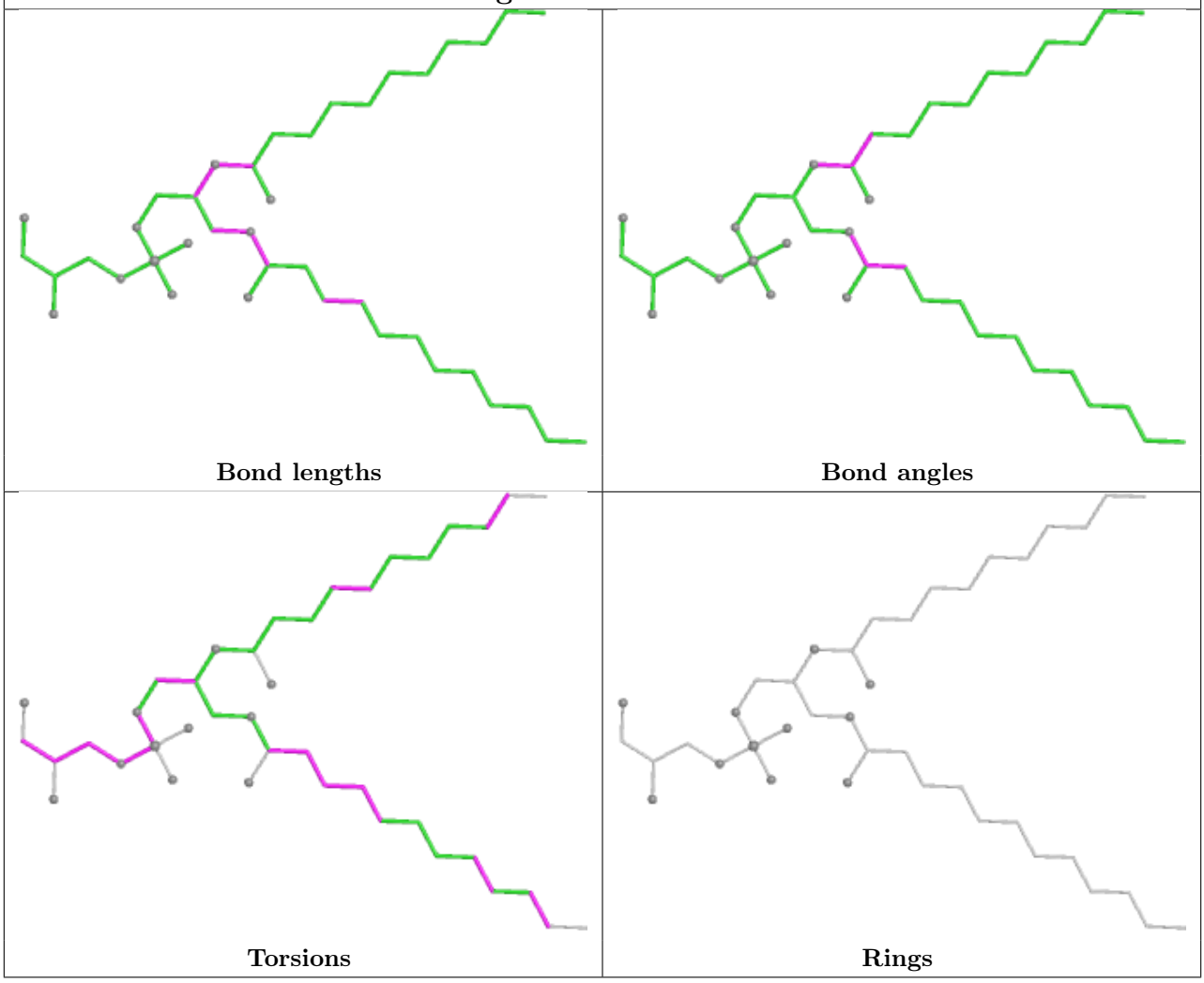


Torsions

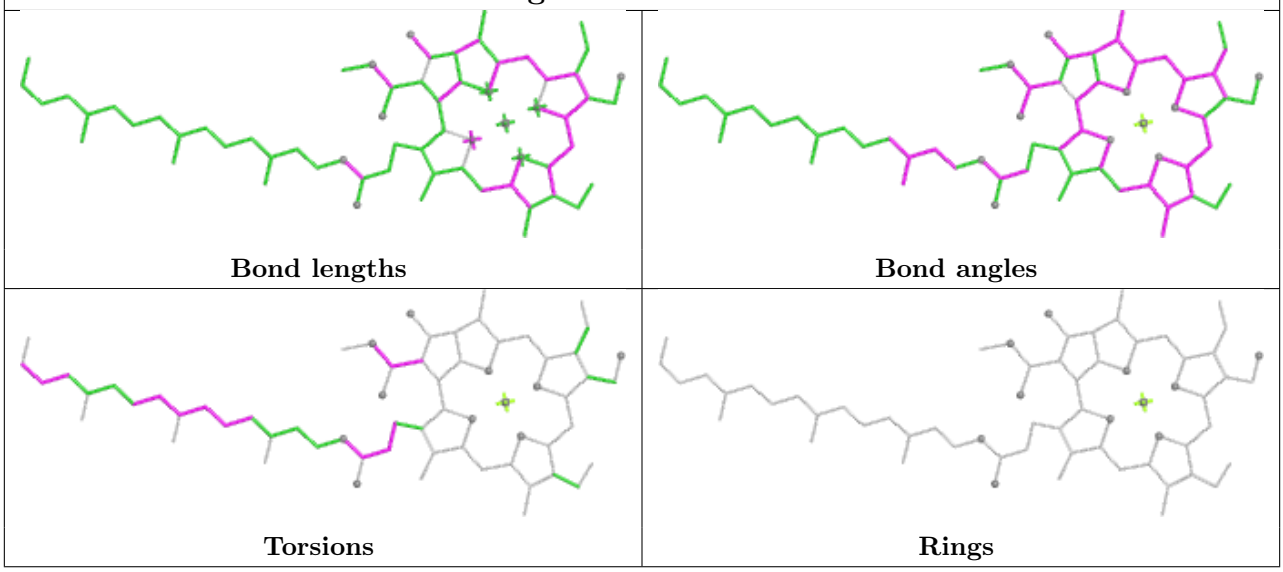


Rings

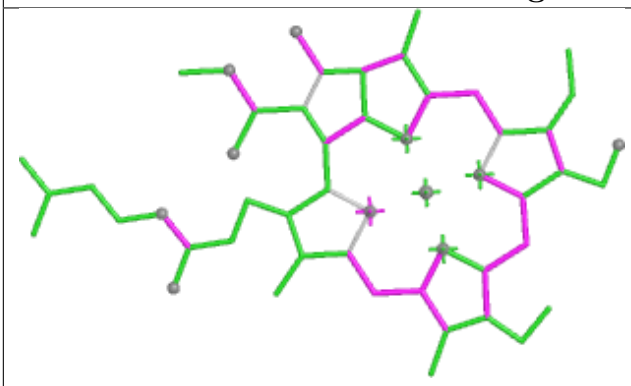
Ligand LHG c 630



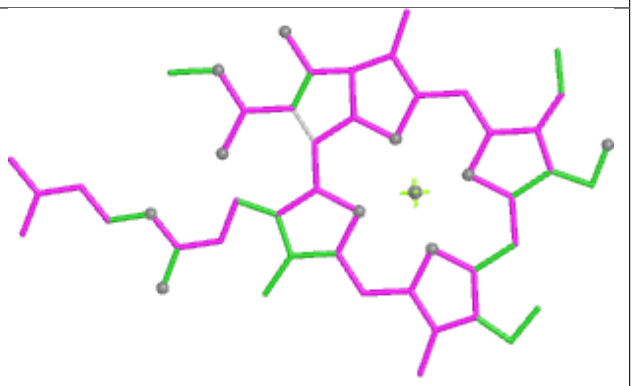
Ligand CHL h 602



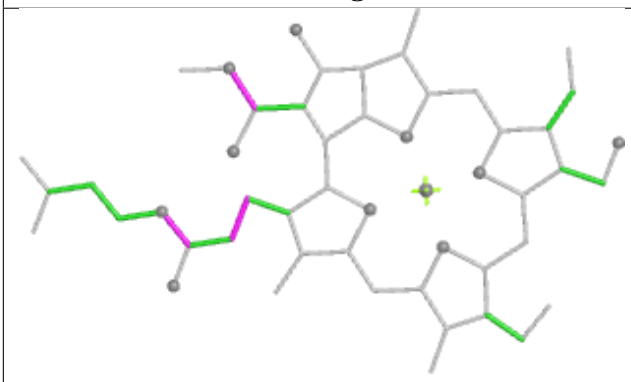
Ligand CHL 2 307



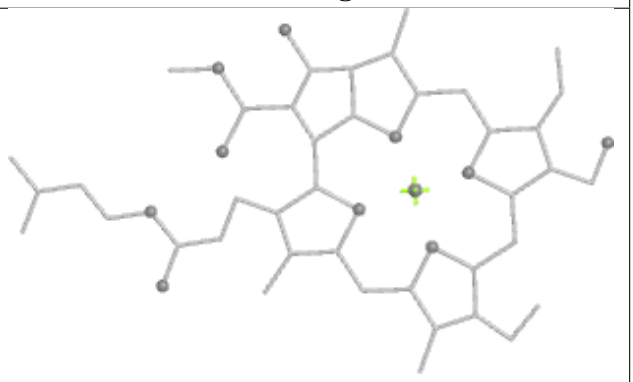
Bond lengths



Bond angles

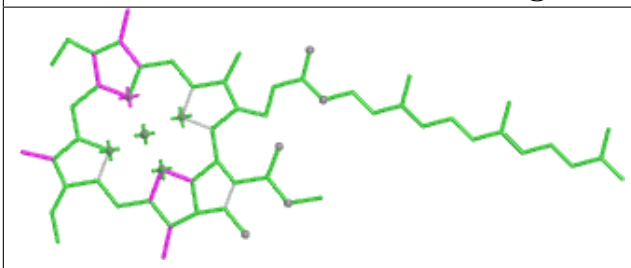


Torsions

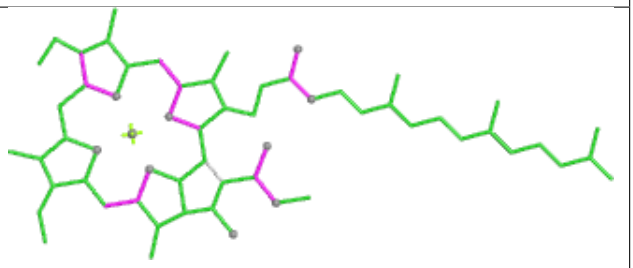


Rings

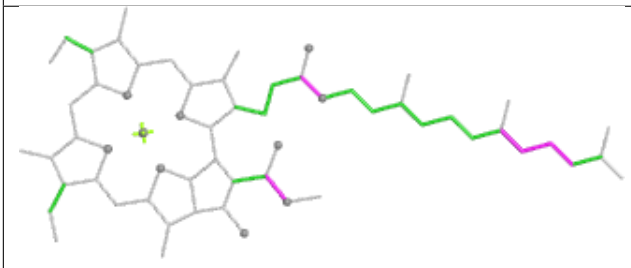
Ligand CLA 4 304



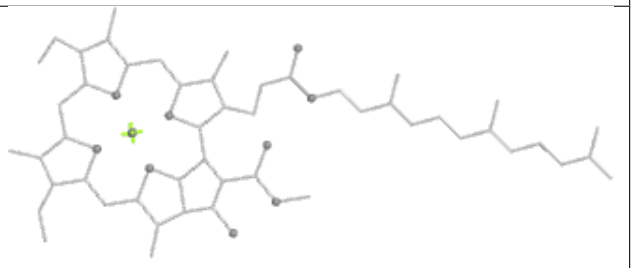
Bond lengths



Bond angles

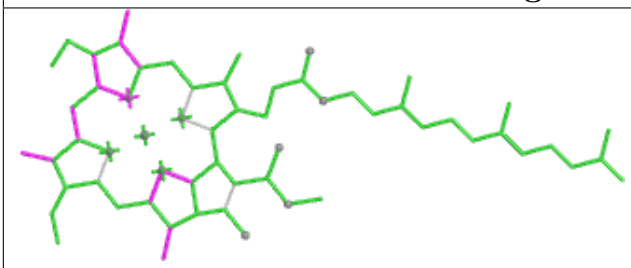


Torsions

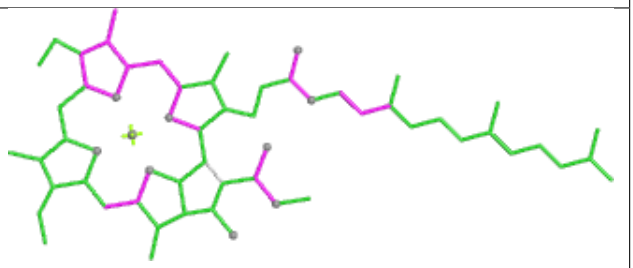


Rings

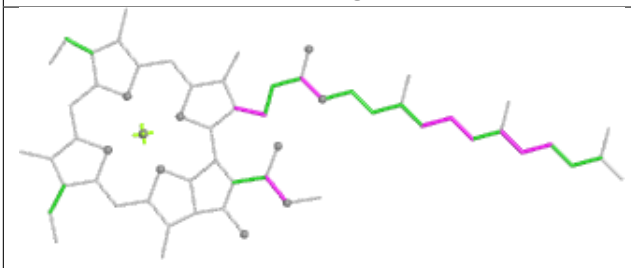
Ligand CLA B 836



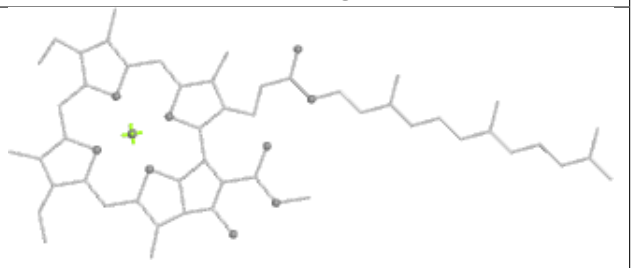
Bond lengths



Bond angles

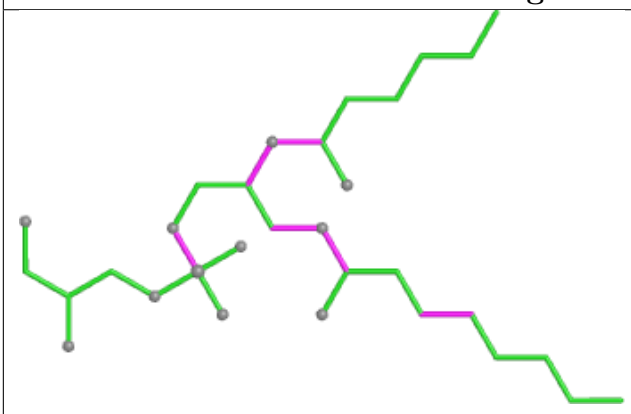


Torsions

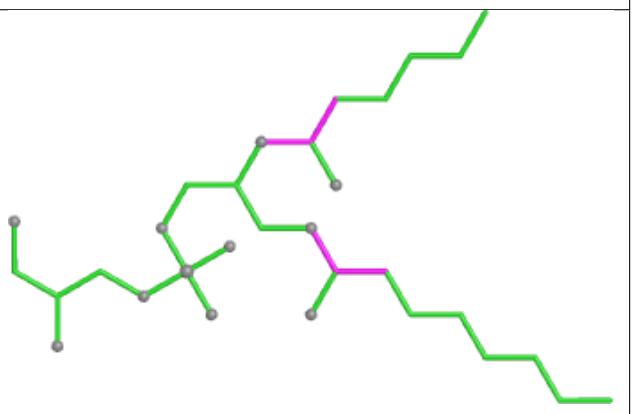


Rings

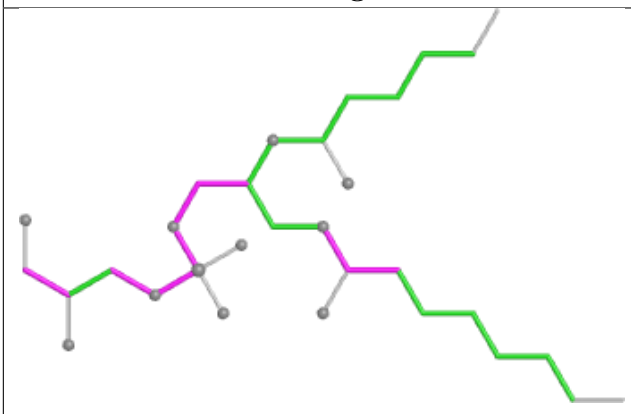
Ligand LHG 6 603



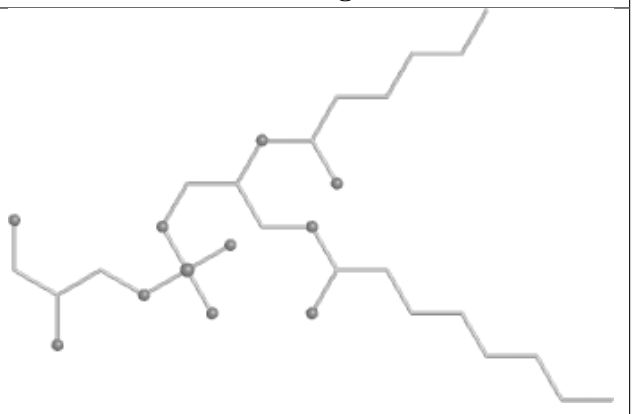
Bond lengths



Bond angles

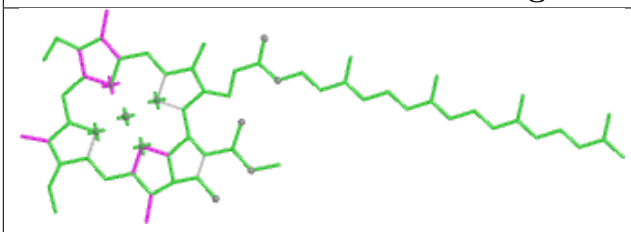


Torsions

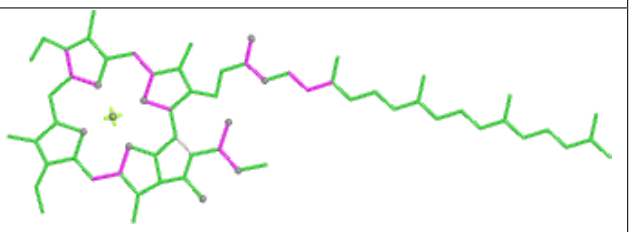


Rings

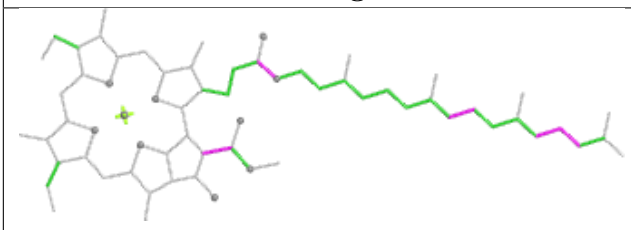
Ligand CLA 3 304



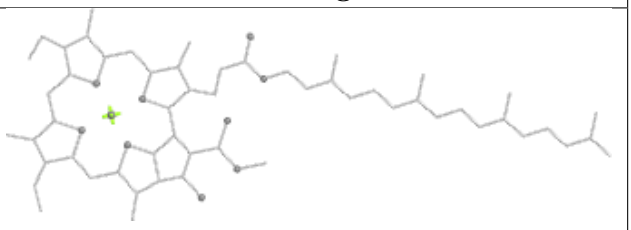
Bond lengths



Bond angles

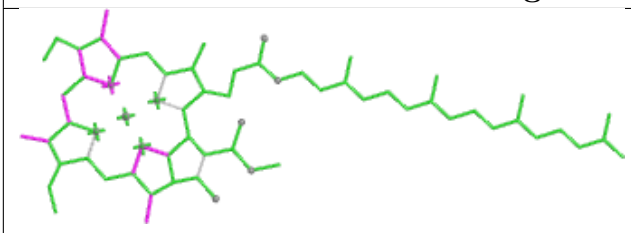


Torsions

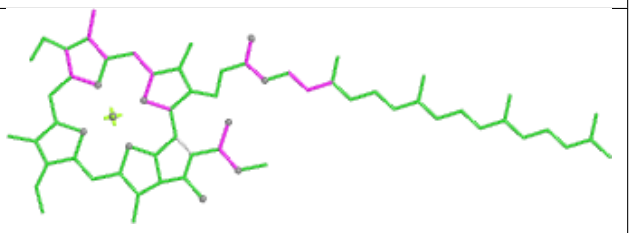


Rings

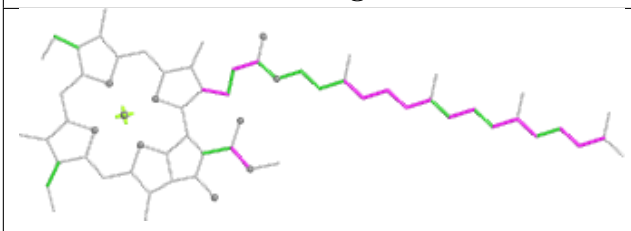
Ligand CLA A 828



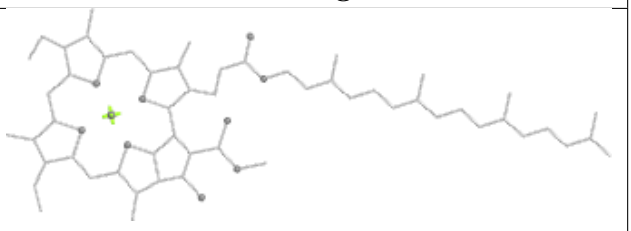
Bond lengths



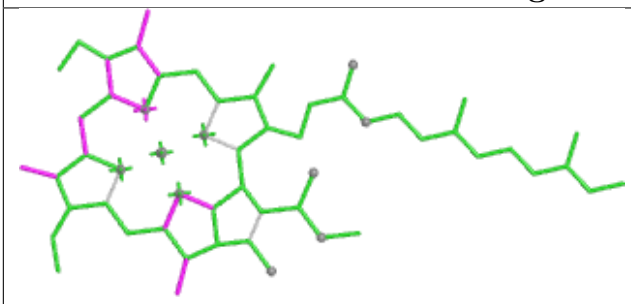
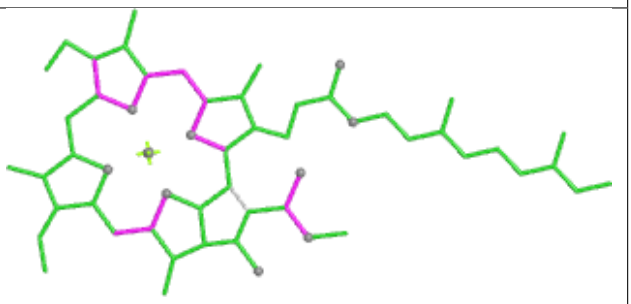
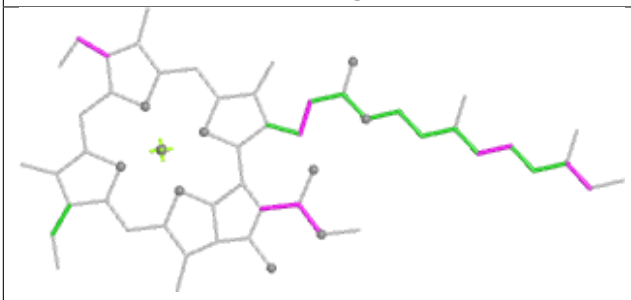
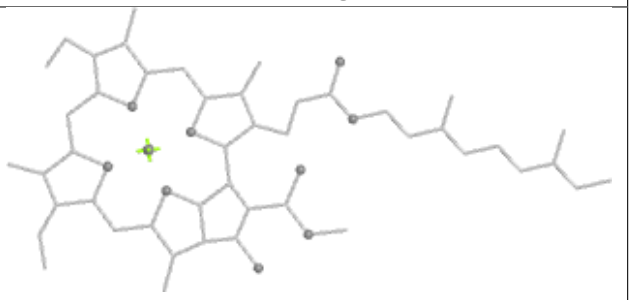
Bond angles

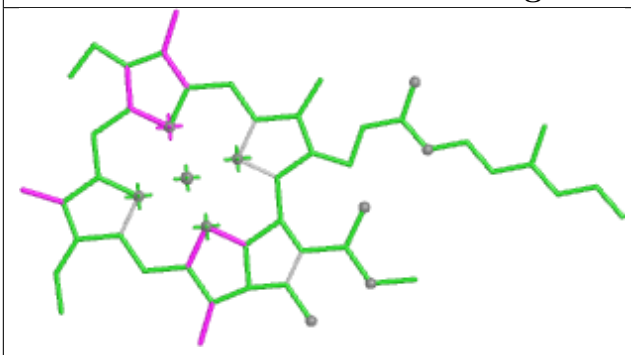
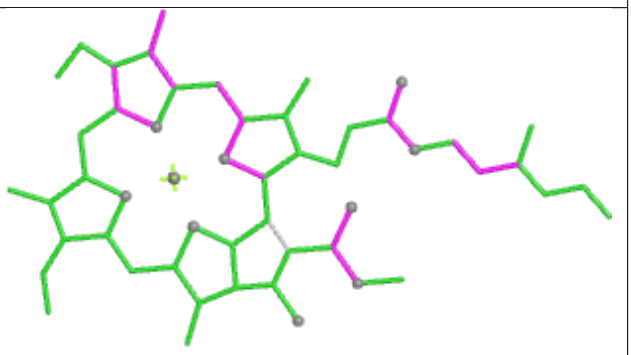
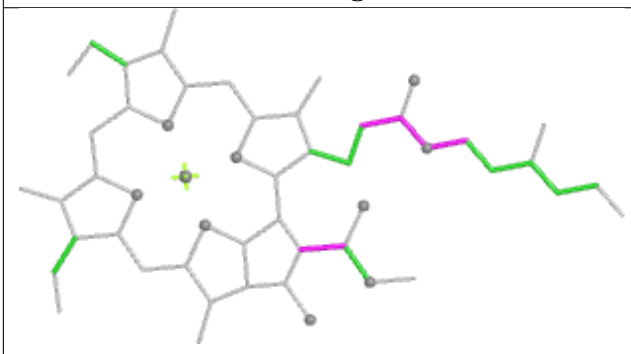
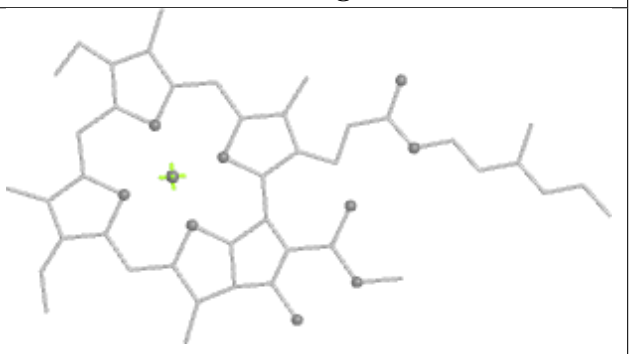


Torsions

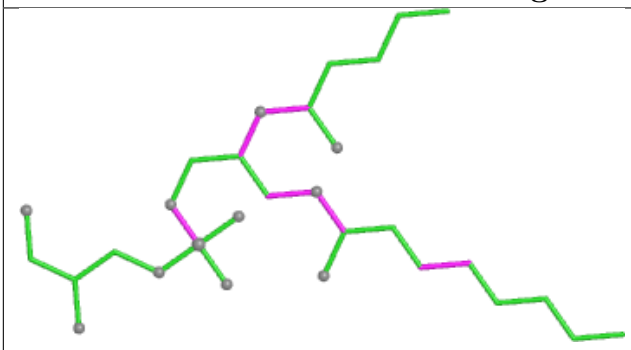


Rings

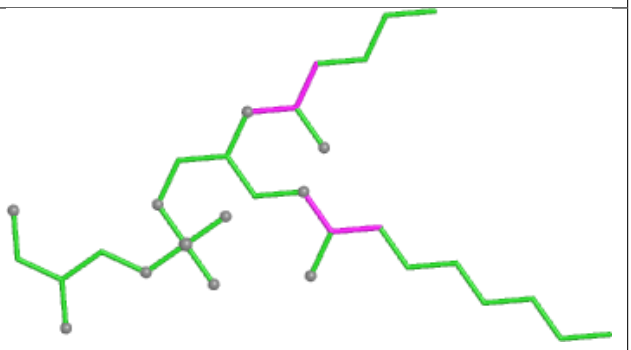
Ligand CLA 8 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

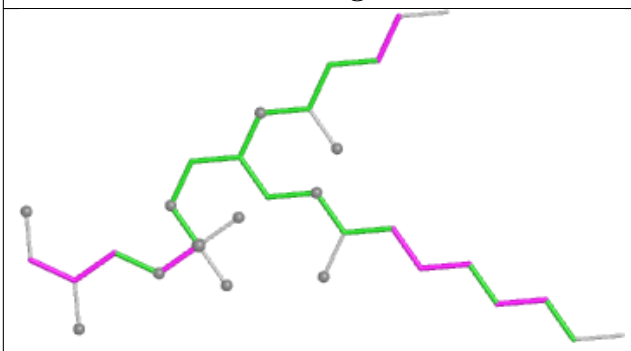
Ligand LHG i 630



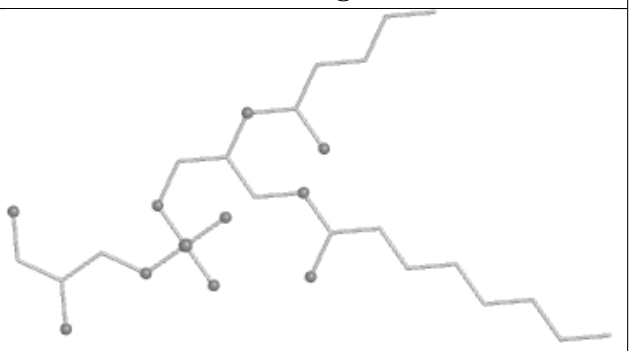
Bond lengths



Bond angles

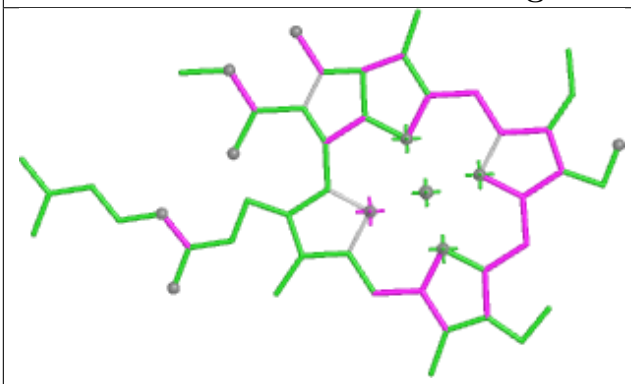


Torsions

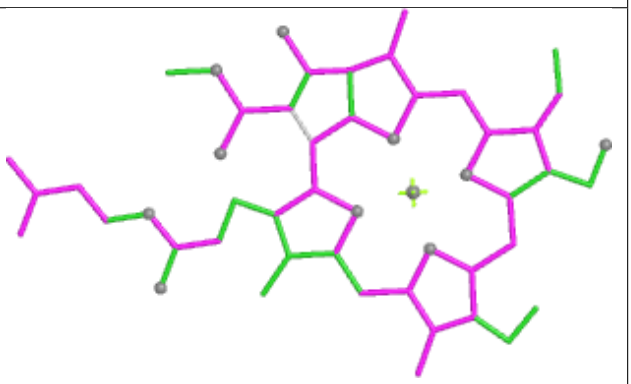


Rings

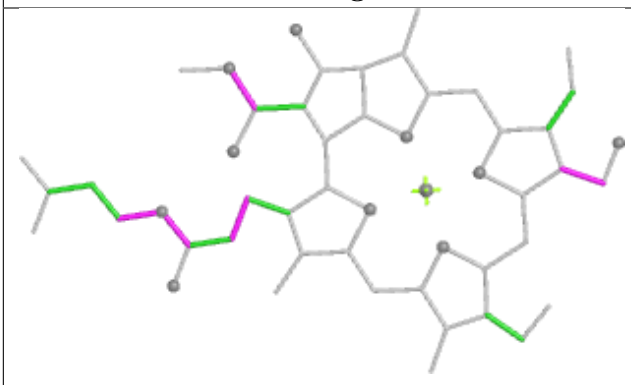
Ligand CHL d 606



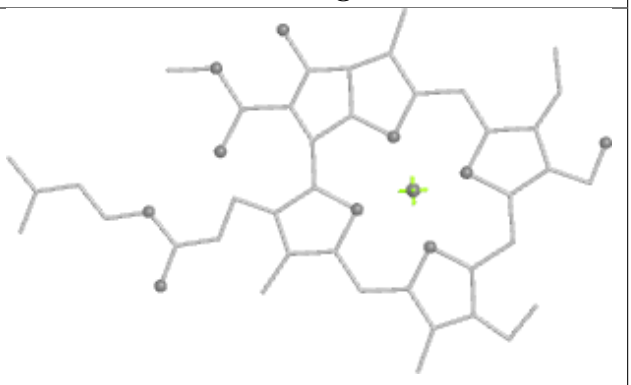
Bond lengths



Bond angles

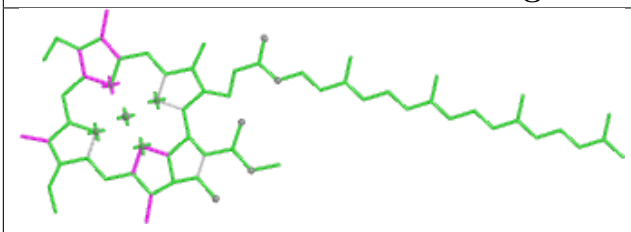


Torsions

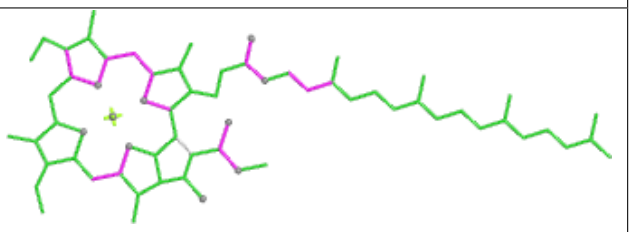


Rings

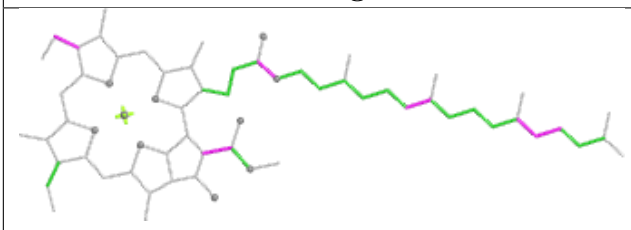
Ligand CLA A 815



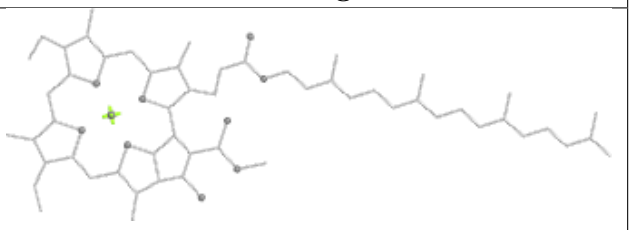
Bond lengths



Bond angles

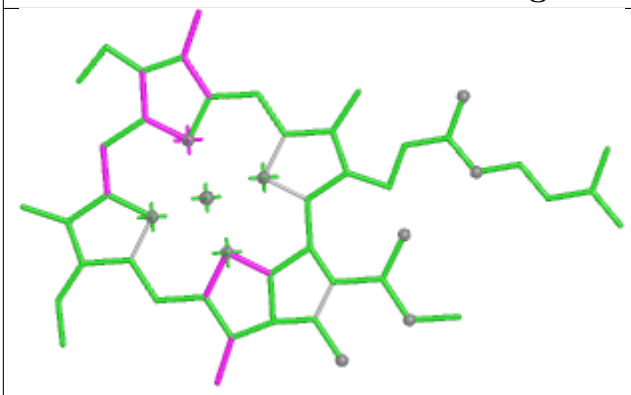


Torsions

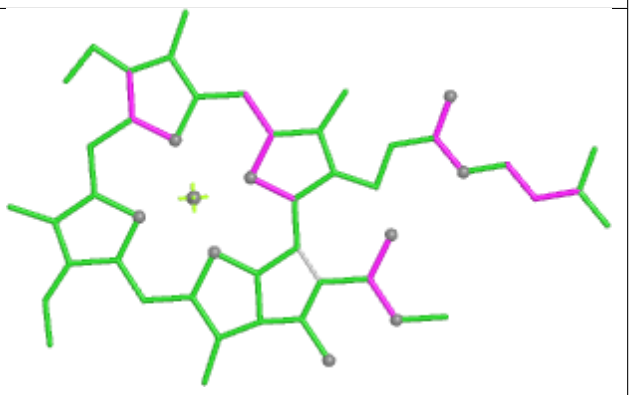


Rings

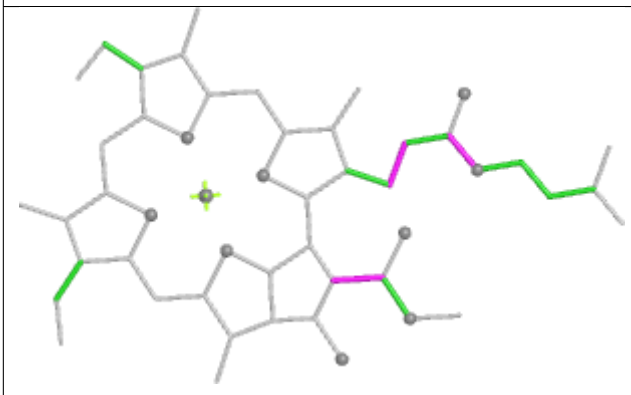
Ligand CLA c 604



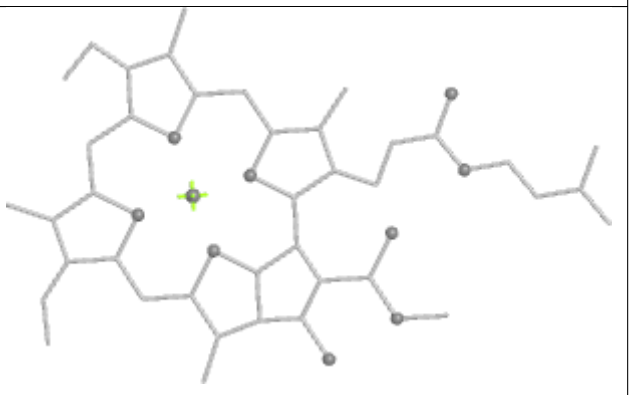
Bond lengths



Bond angles

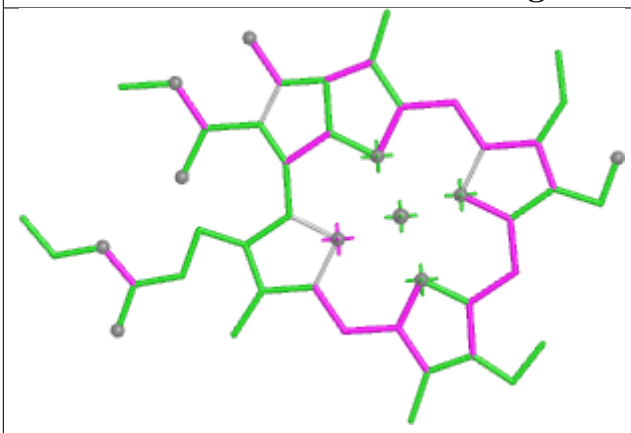


Torsions

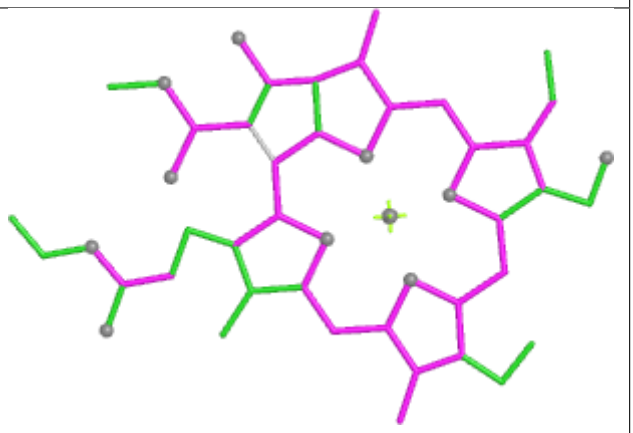


Rings

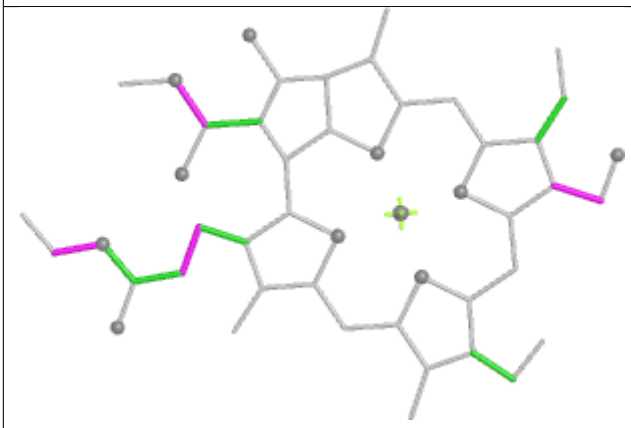
Ligand CHL 2 306



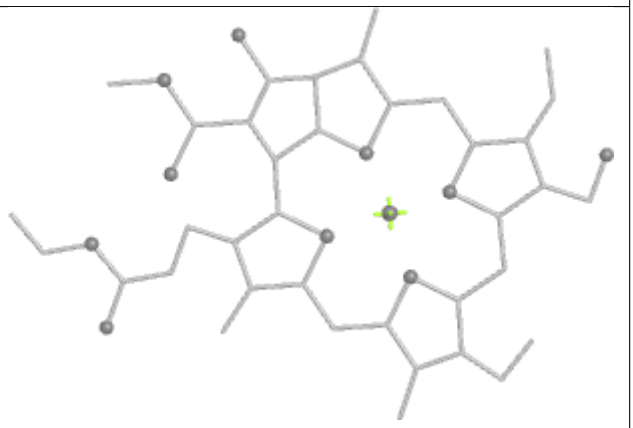
Bond lengths



Bond angles

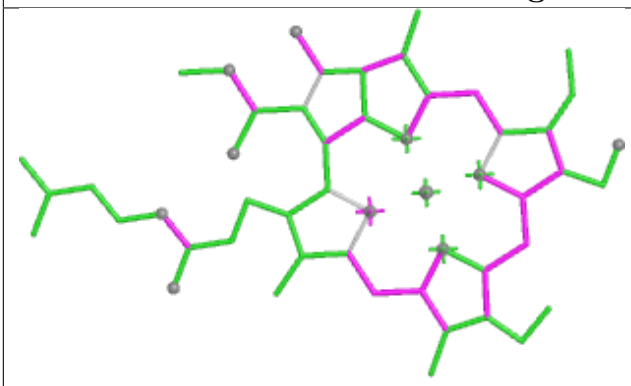


Torsions

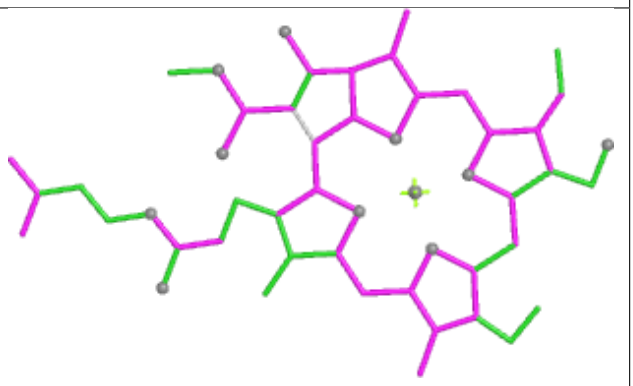


Rings

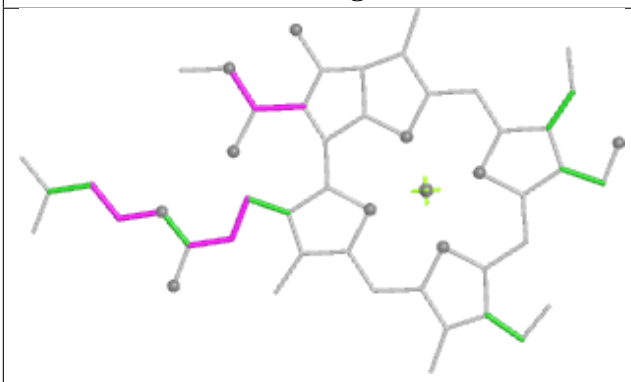
Ligand CHL 9 305



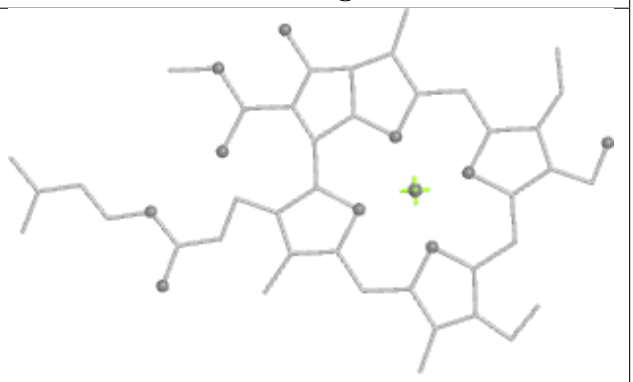
Bond lengths



Bond angles

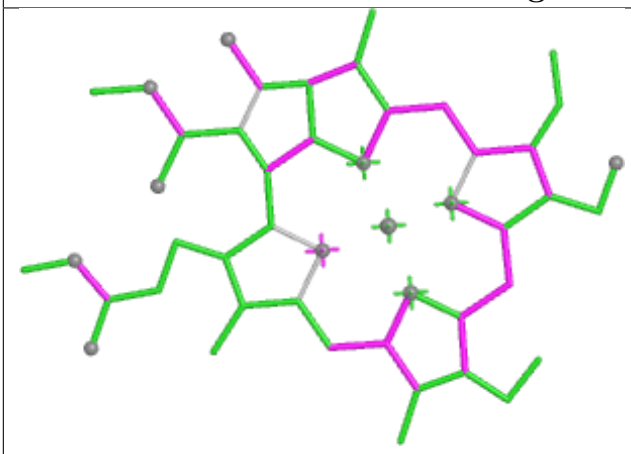


Torsions

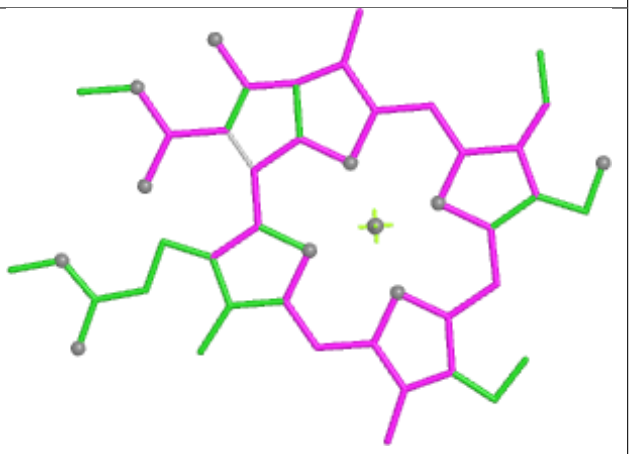


Rings

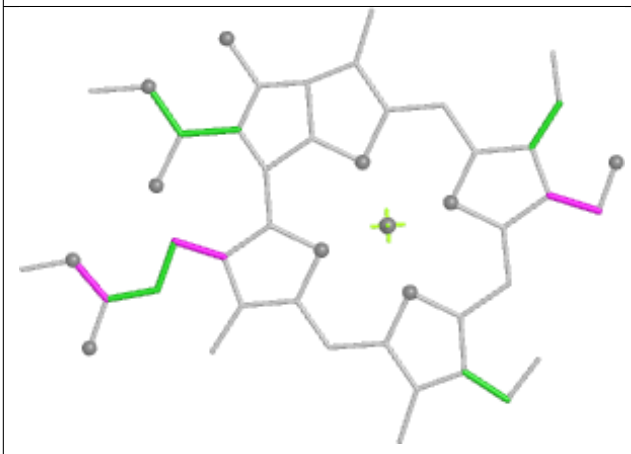
Ligand CHL 4 308



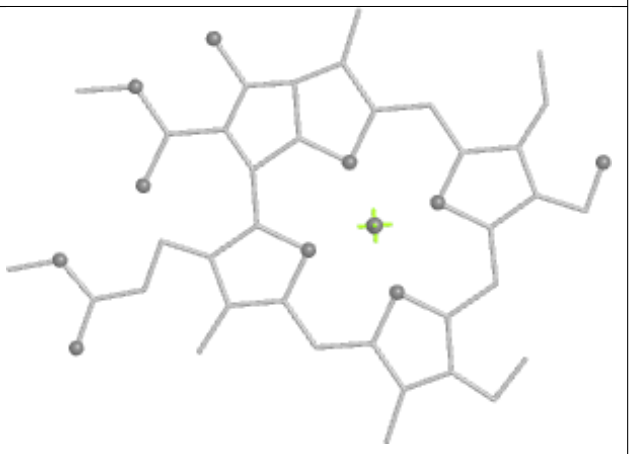
Bond lengths



Bond angles

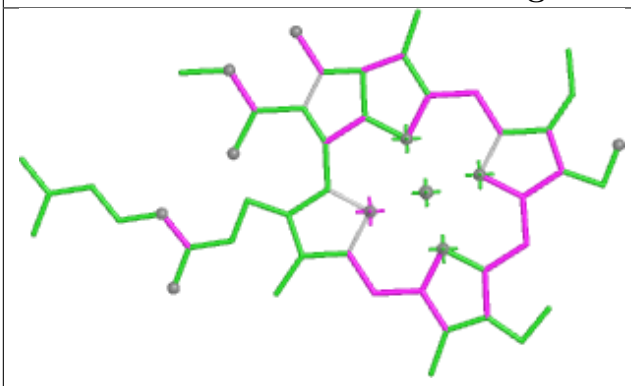


Torsions

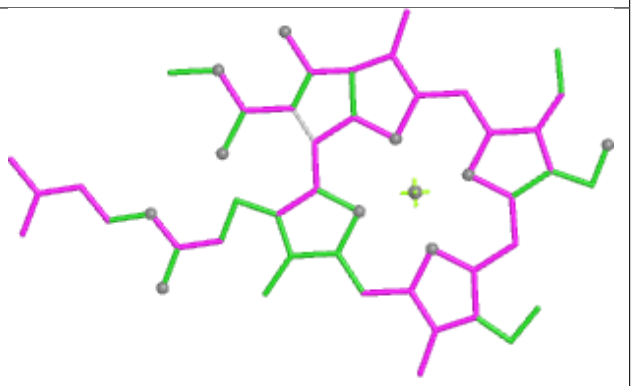


Rings

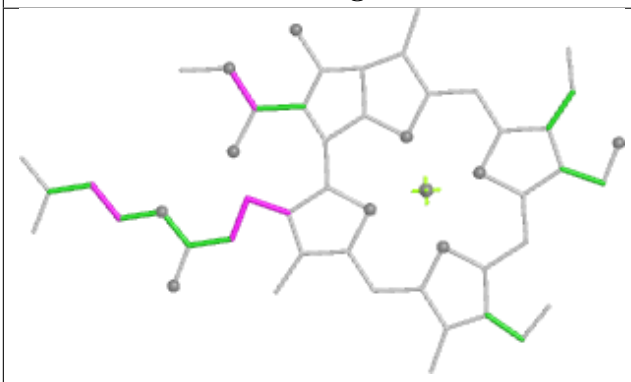
Ligand CHL 7 307



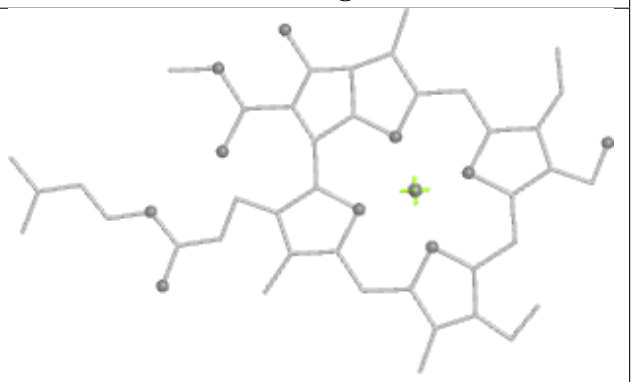
Bond lengths



Bond angles

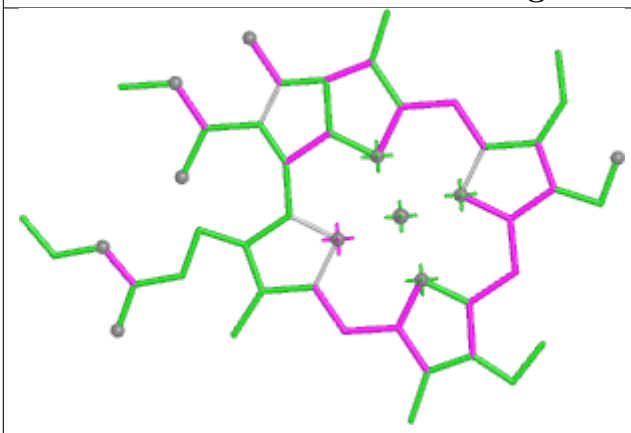


Torsions

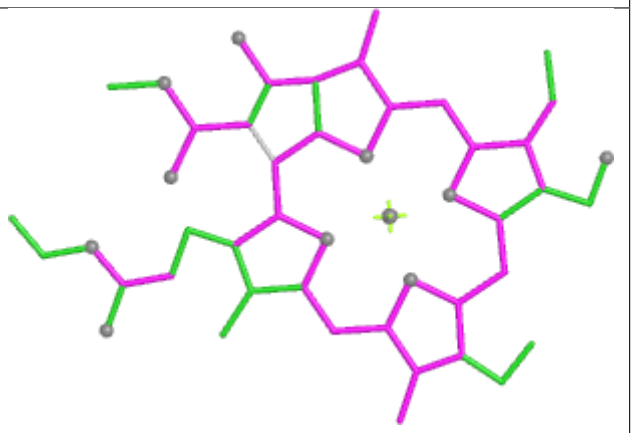


Rings

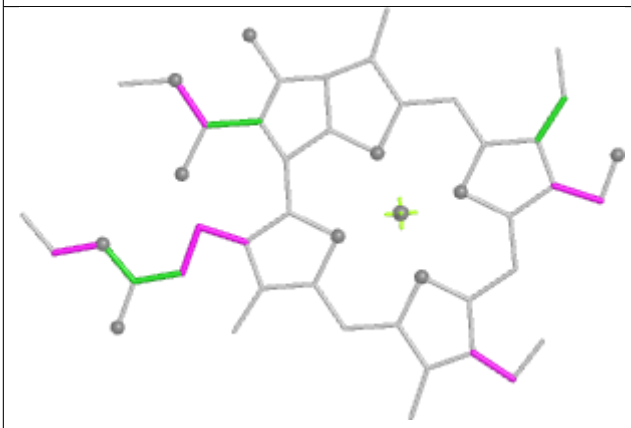
Ligand CHL 7 305



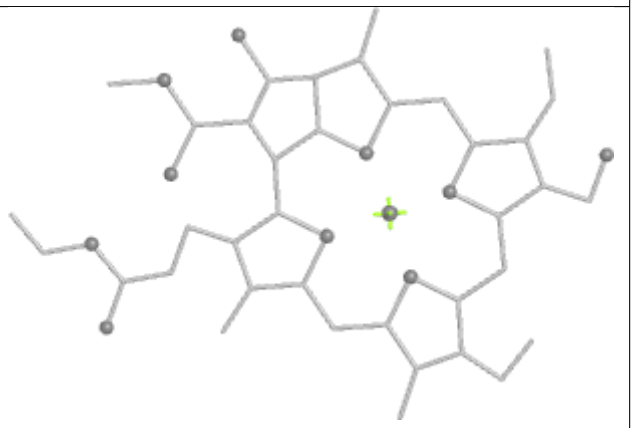
Bond lengths



Bond angles

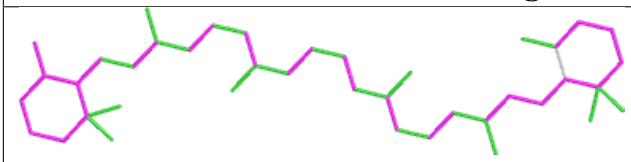


Torsions

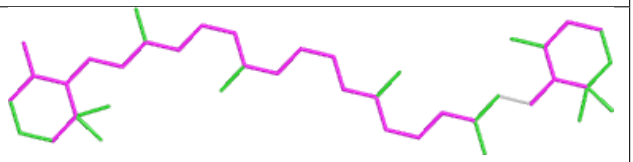


Rings

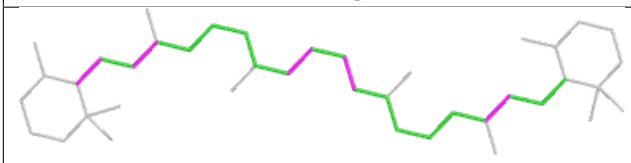
Ligand 8CT M 102



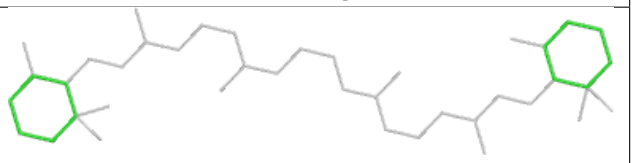
Bond lengths



Bond angles

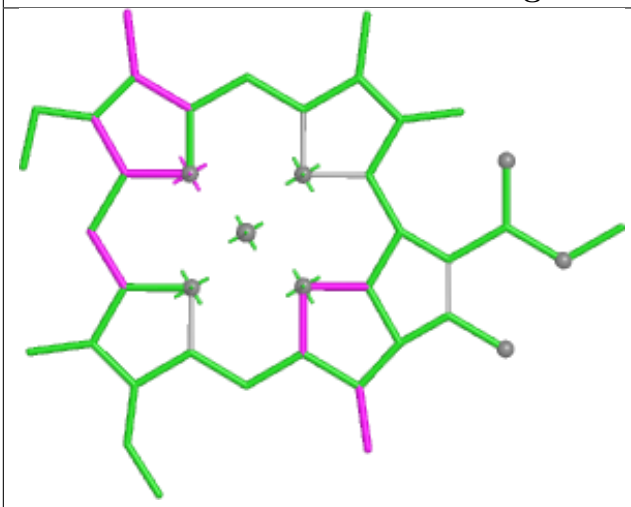


Torsions

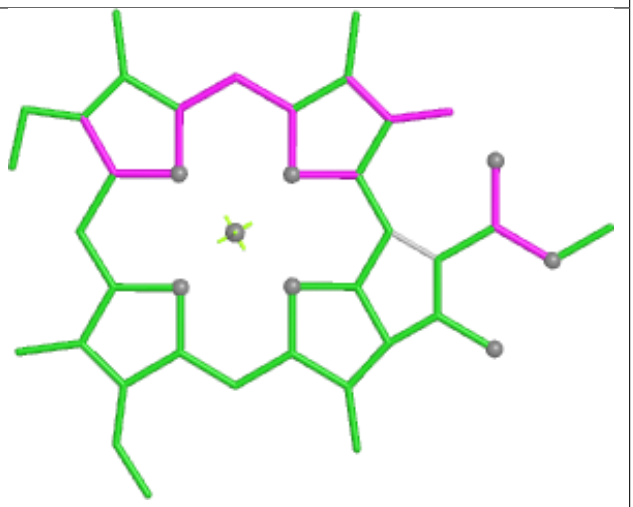


Rings

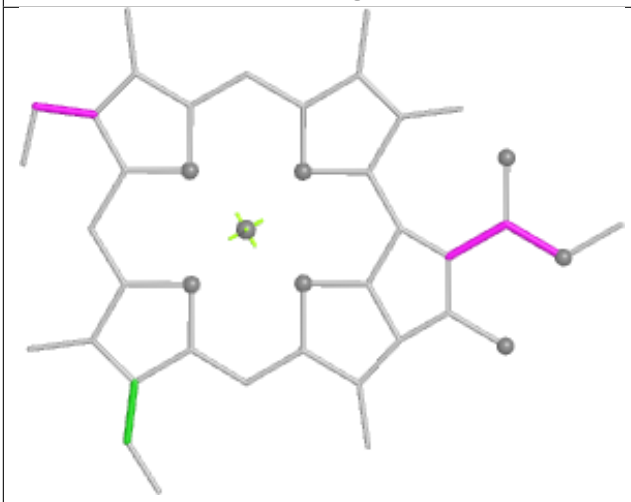
Ligand CLA O 201



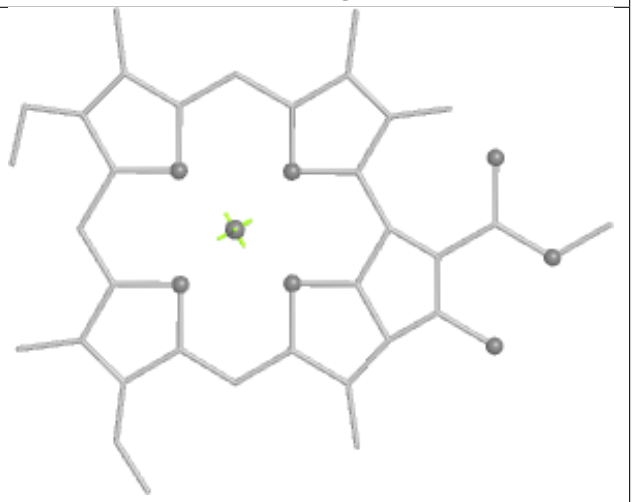
Bond lengths



Bond angles

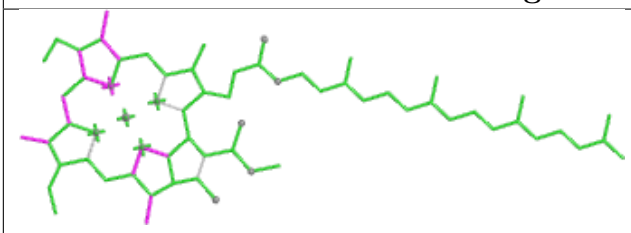


Torsions

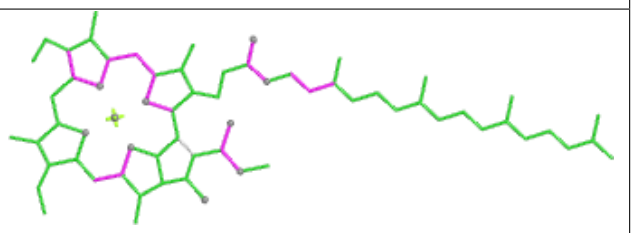


Rings

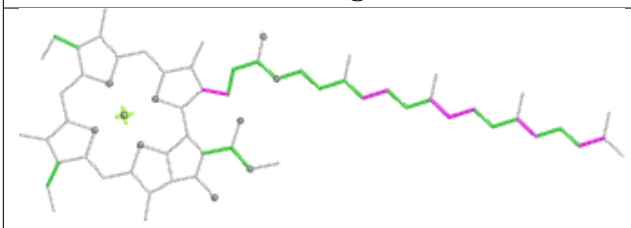
Ligand CLA A 803



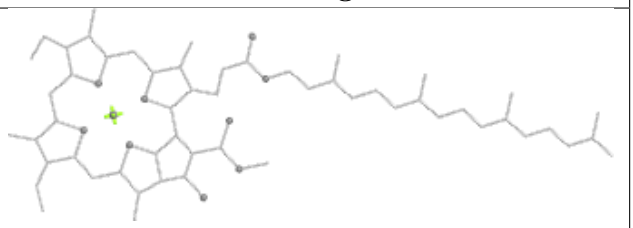
Bond lengths



Bond angles

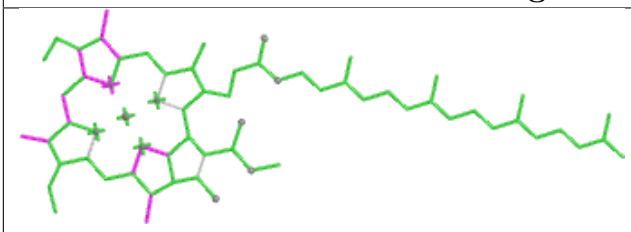


Torsions

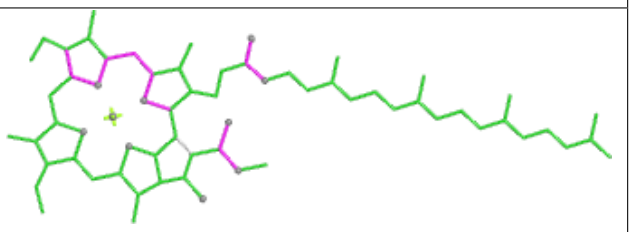


Rings

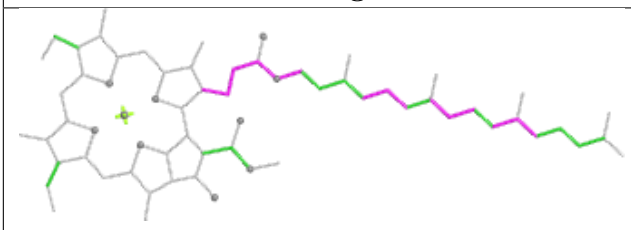
Ligand CLA 7 308



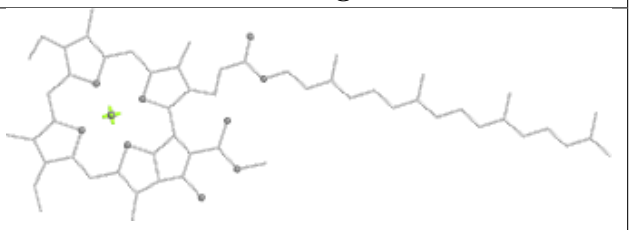
Bond lengths



Bond angles

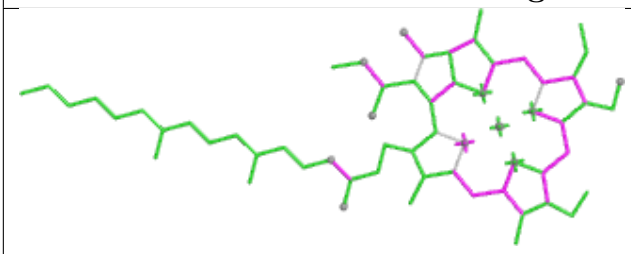


Torsions

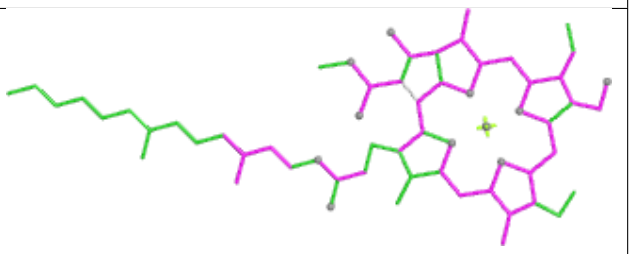


Rings

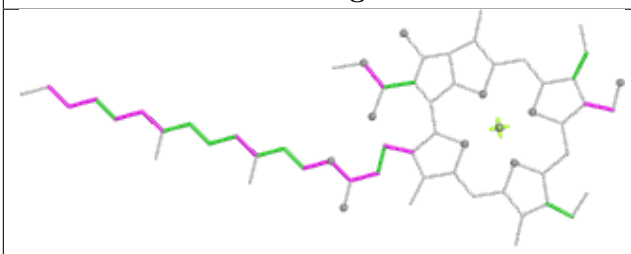
Ligand CHL 7 306



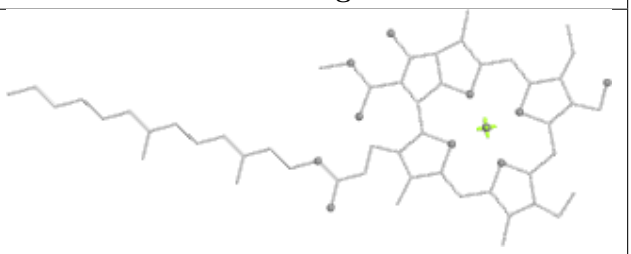
Bond lengths



Bond angles

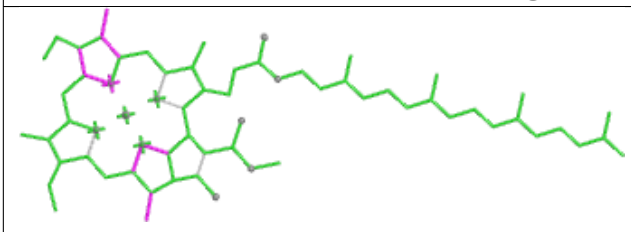


Torsions

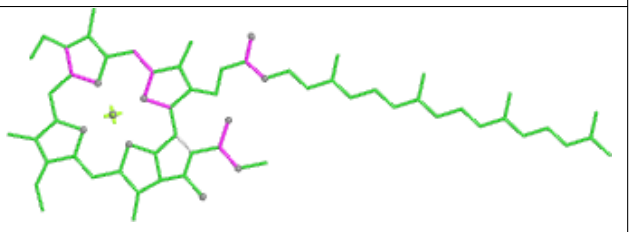


Rings

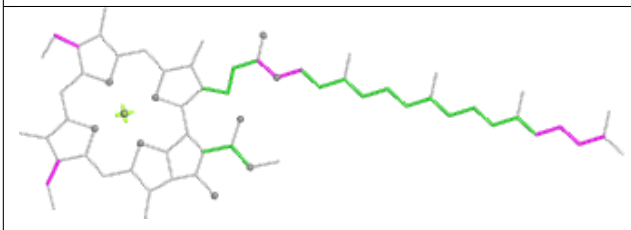
Ligand CLA B 840



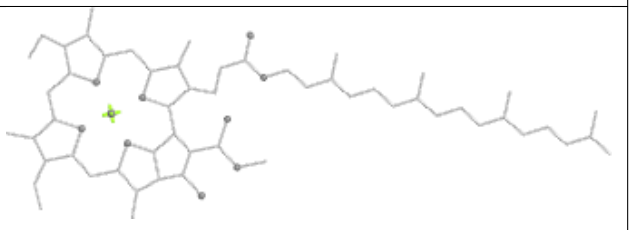
Bond lengths



Bond angles

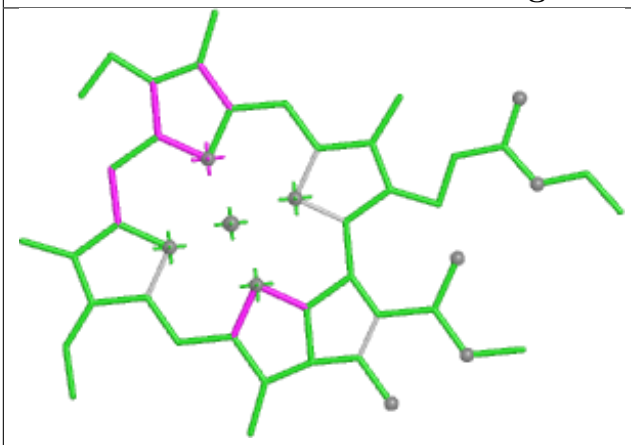


Torsions

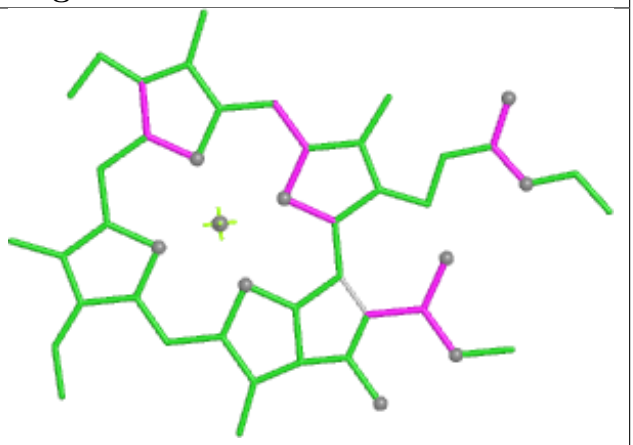


Rings

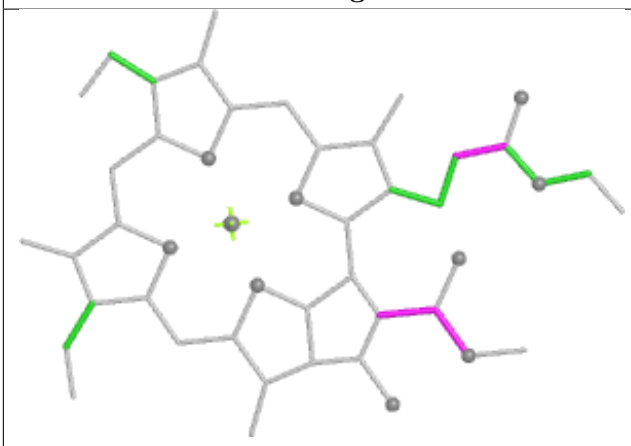
Ligand CLA g 613



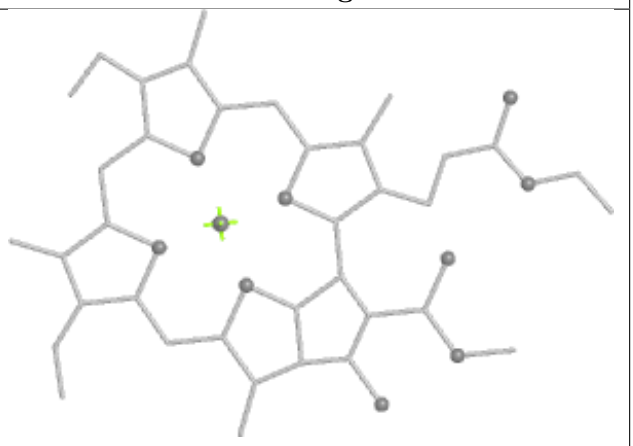
Bond lengths



Bond angles

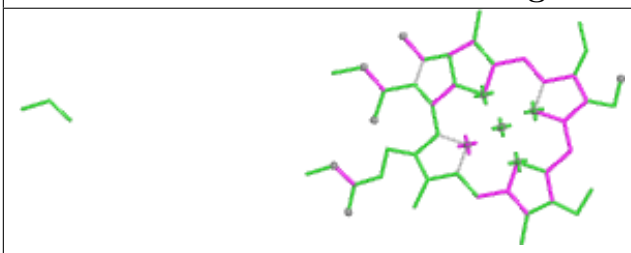


Torsions

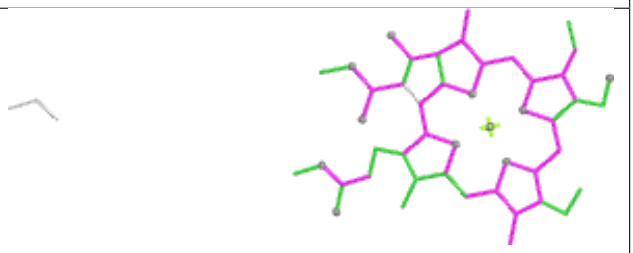


Rings

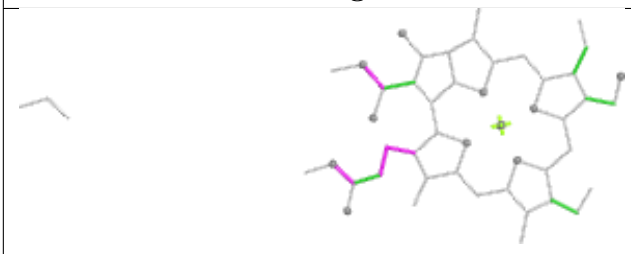
Ligand CHL a 607



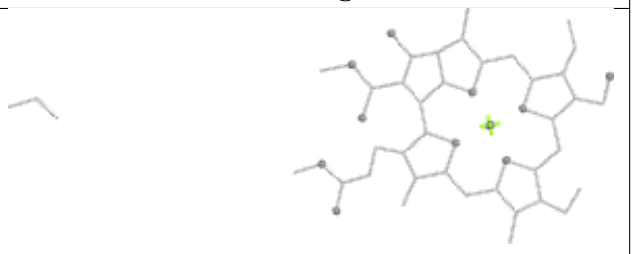
Bond lengths



Bond angles

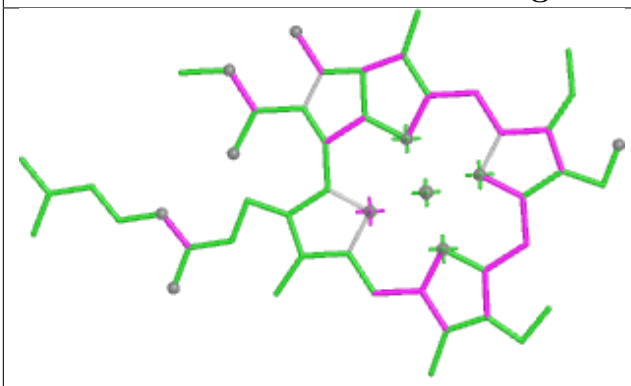


Torsions

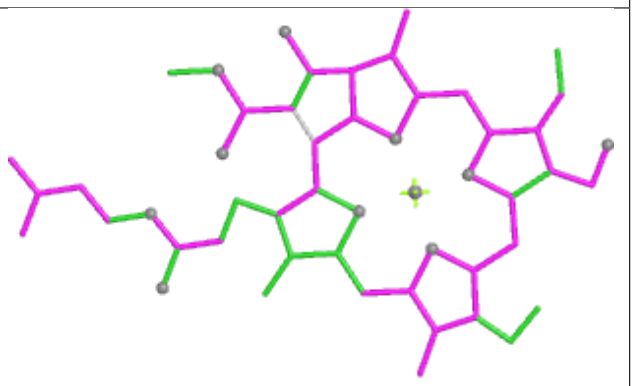


Rings

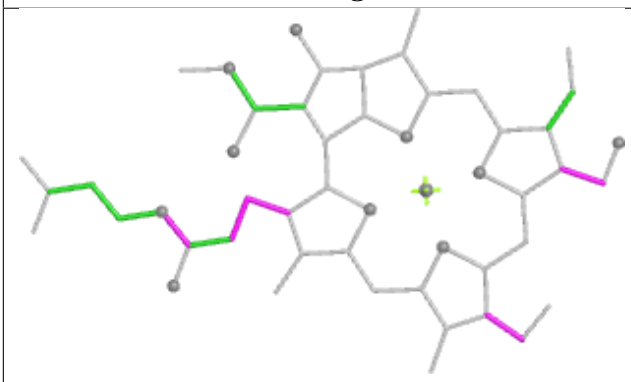
Ligand CHL f 606



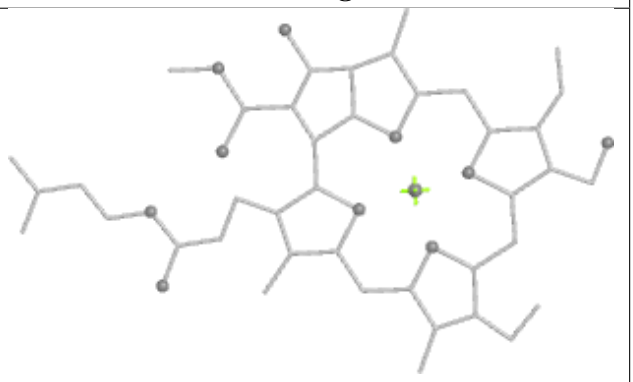
Bond lengths



Bond angles

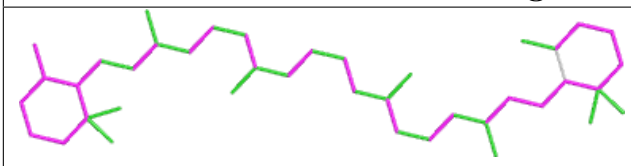


Torsions

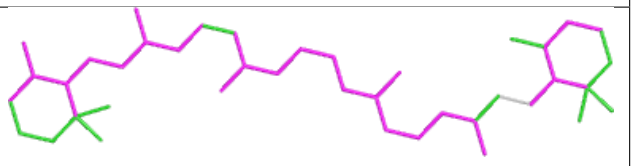


Rings

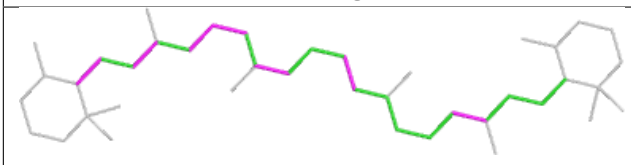
Ligand 8CT B 845



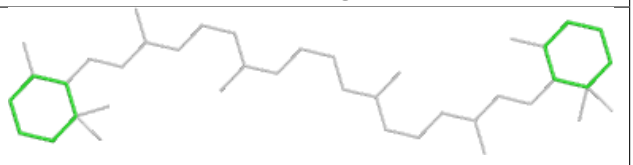
Bond lengths



Bond angles

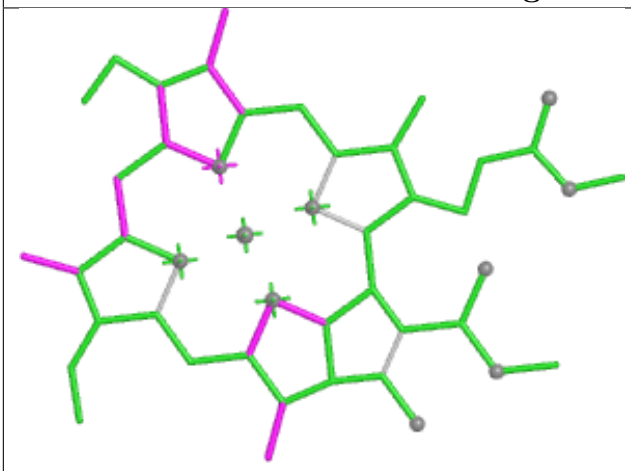


Torsions

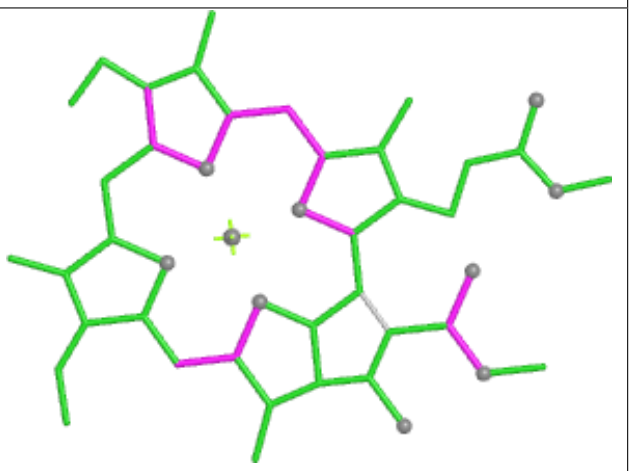


Rings

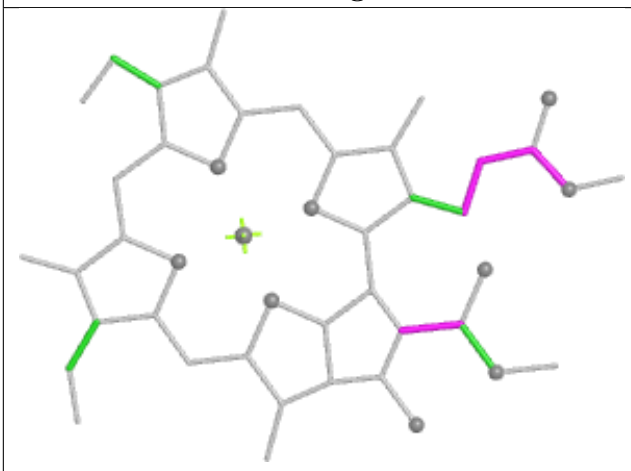
Ligand CLA K 104



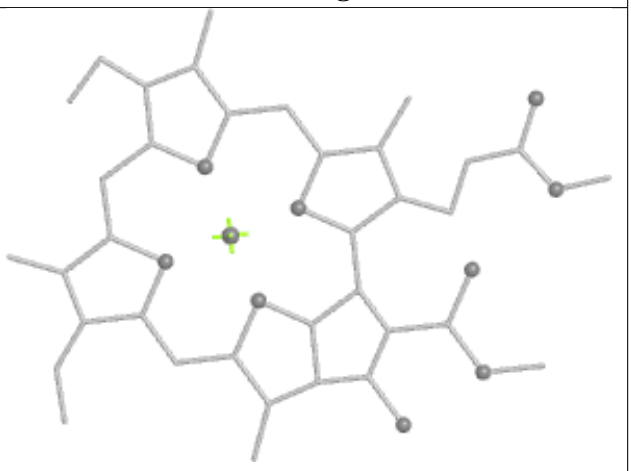
Bond lengths



Bond angles

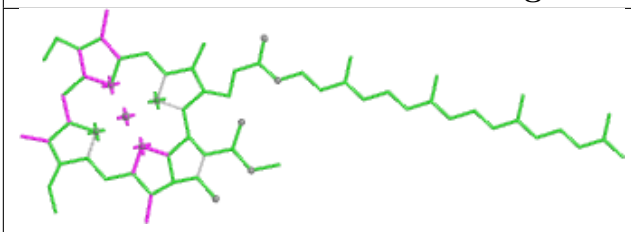


Torsions

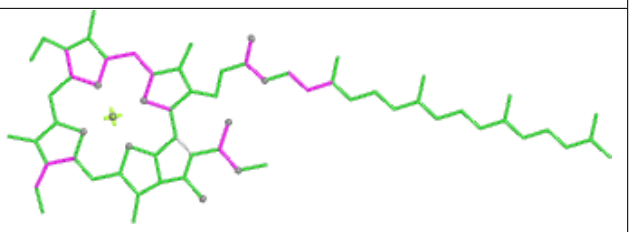


Rings

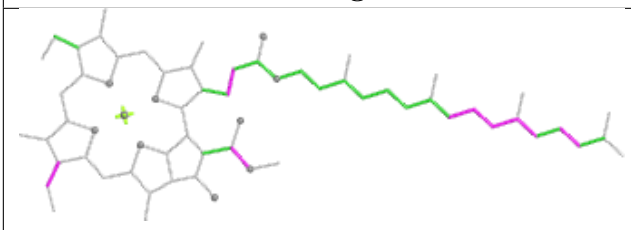
Ligand CLA B 806



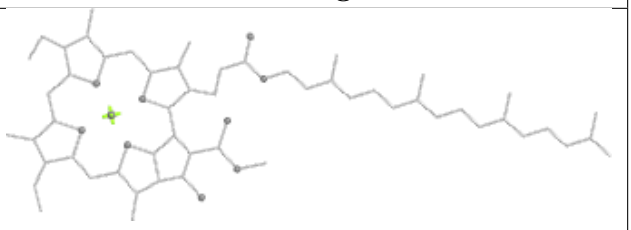
Bond lengths



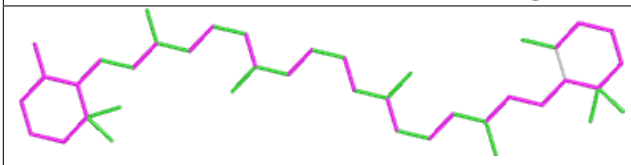
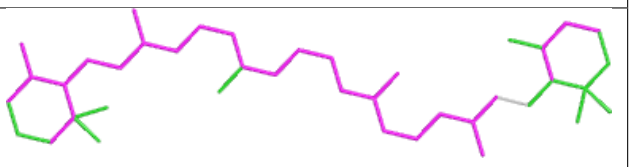
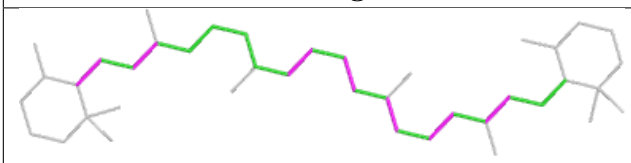
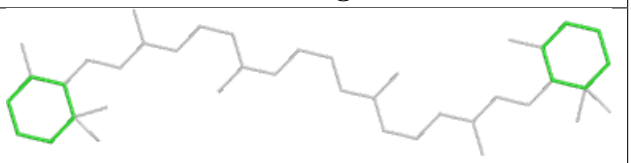
Bond angles

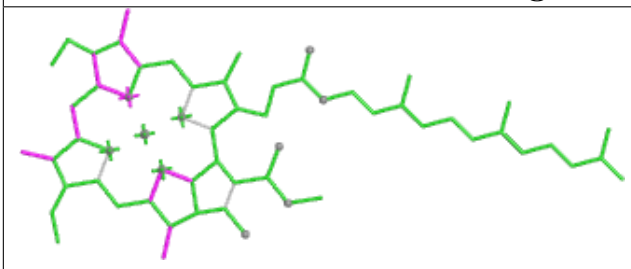
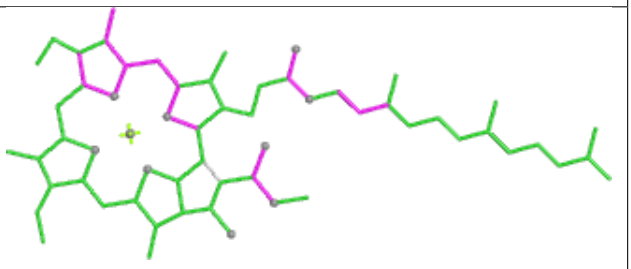
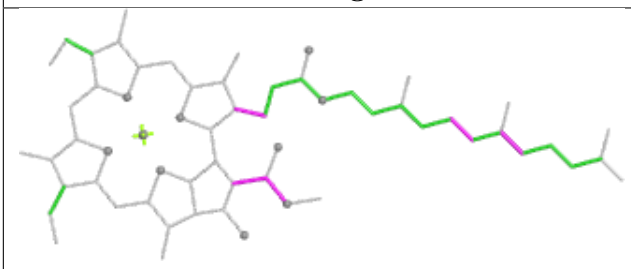
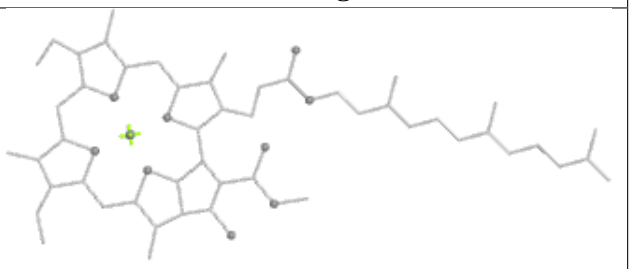


Torsions

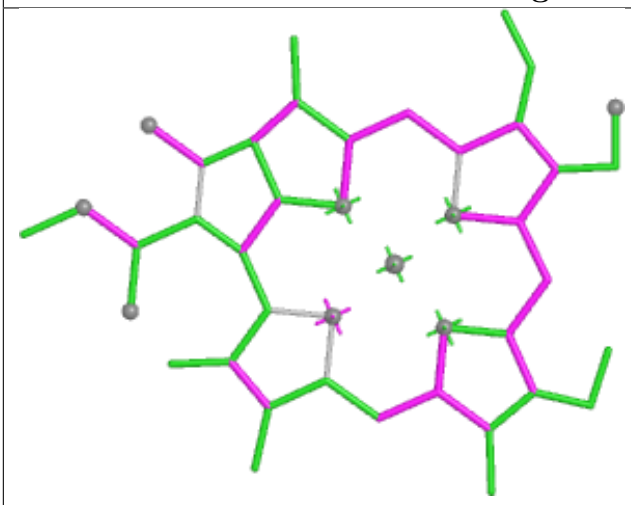


Rings

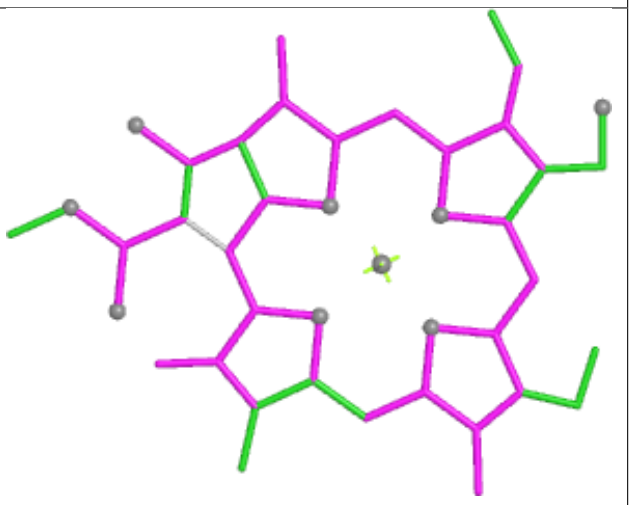
Ligand 8CT A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

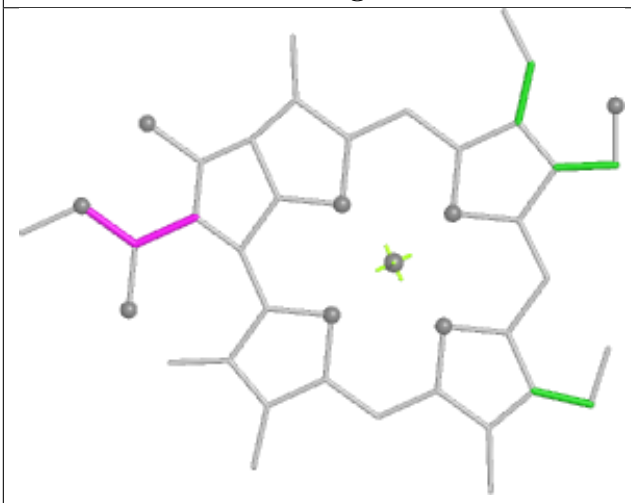
Ligand CHL i 614



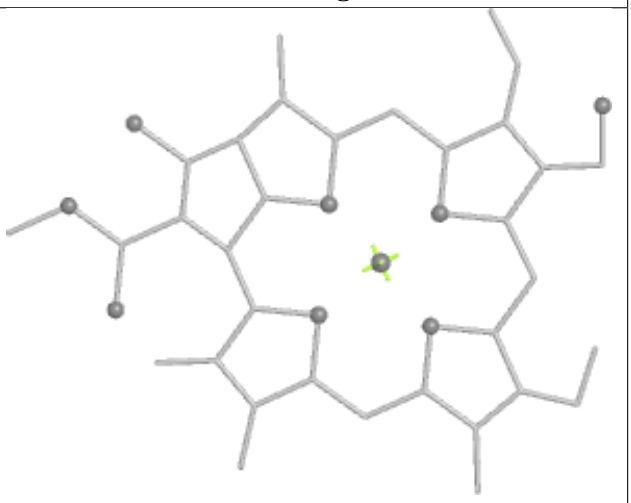
Bond lengths



Bond angles

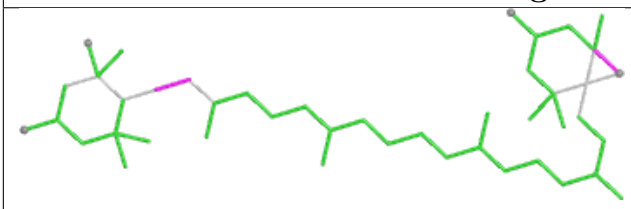


Torsions

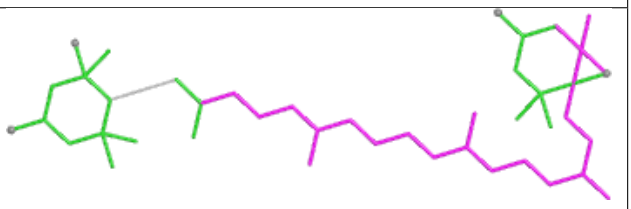


Rings

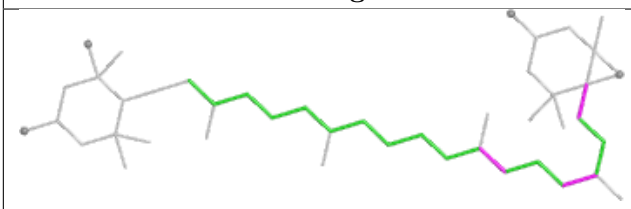
Ligand NEX i 523



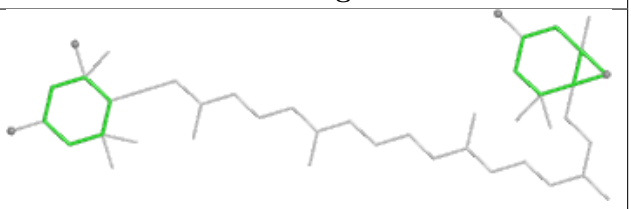
Bond lengths



Bond angles

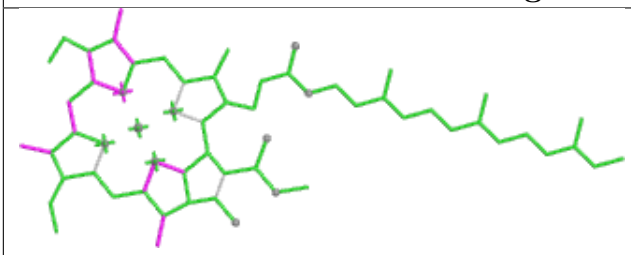


Torsions

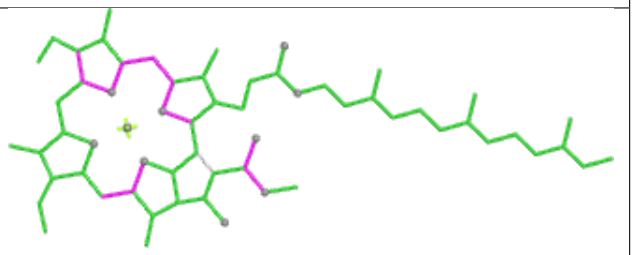


Rings

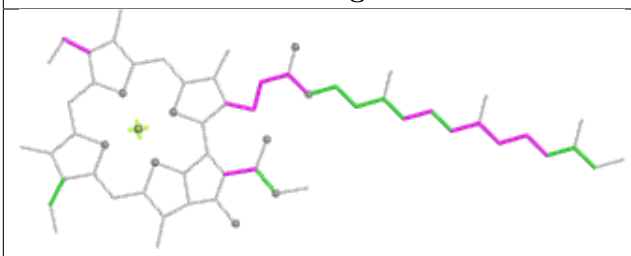
Ligand CLA B 834



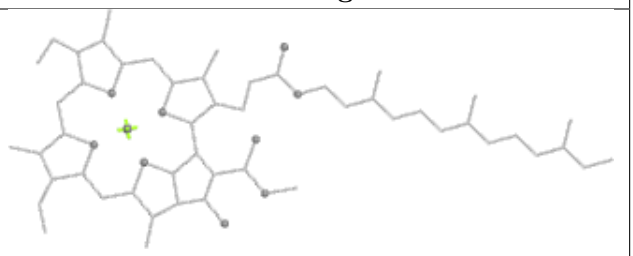
Bond lengths



Bond angles

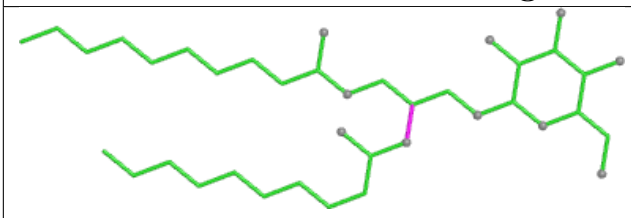


Torsions

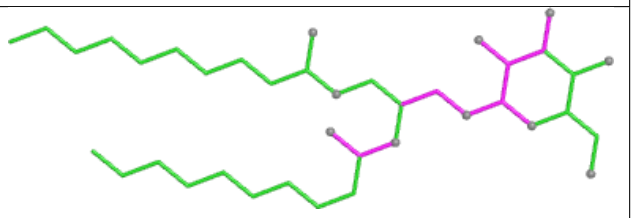


Rings

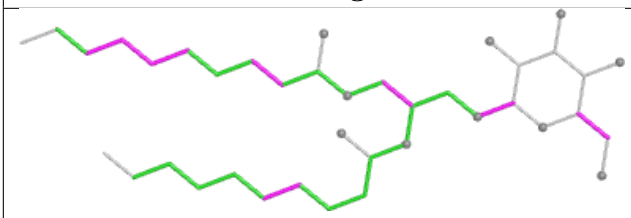
Ligand LMG O 207



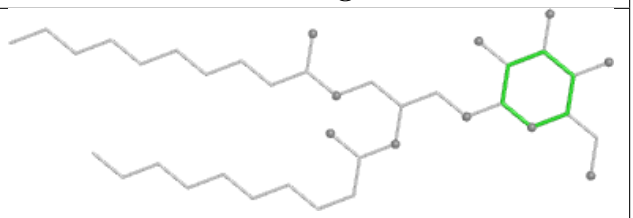
Bond lengths



Bond angles

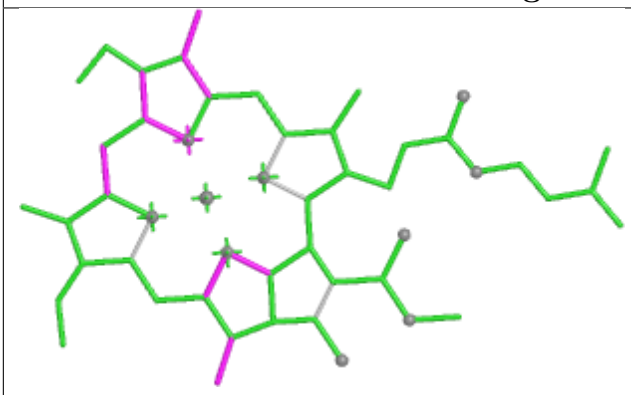


Torsions

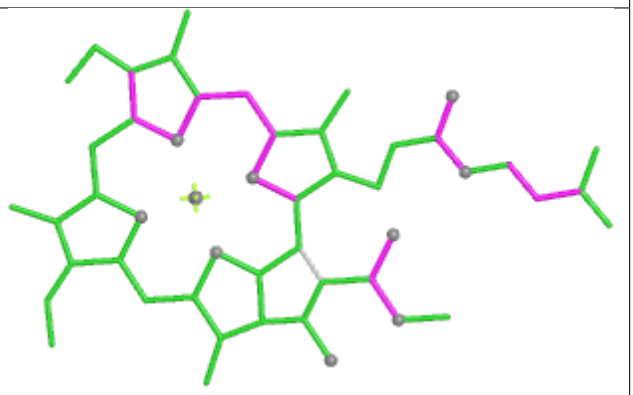


Rings

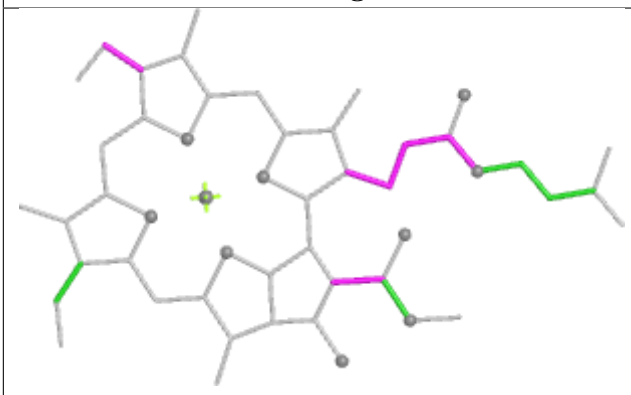
Ligand CLA K 105



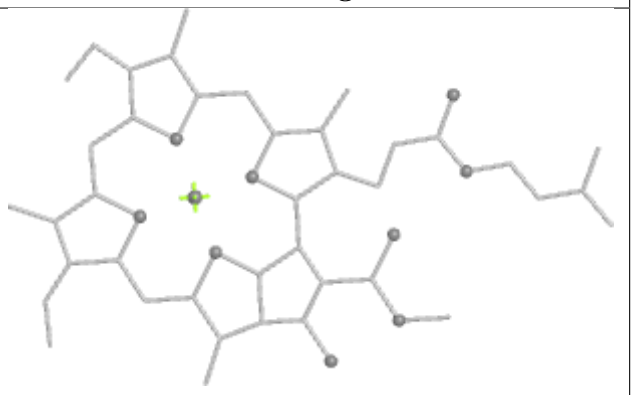
Bond lengths



Bond angles

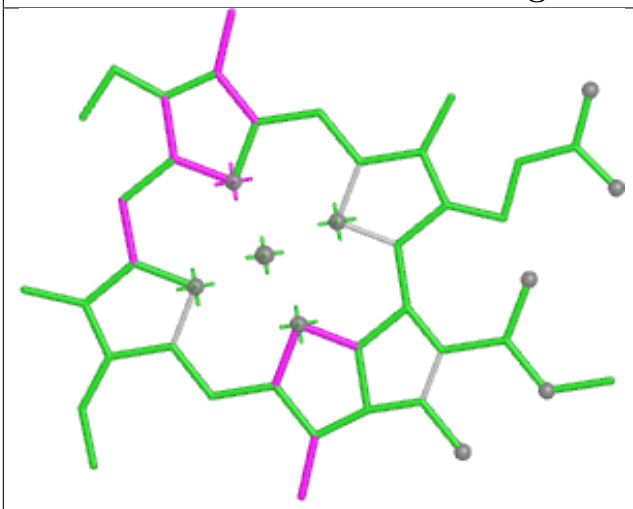


Torsions

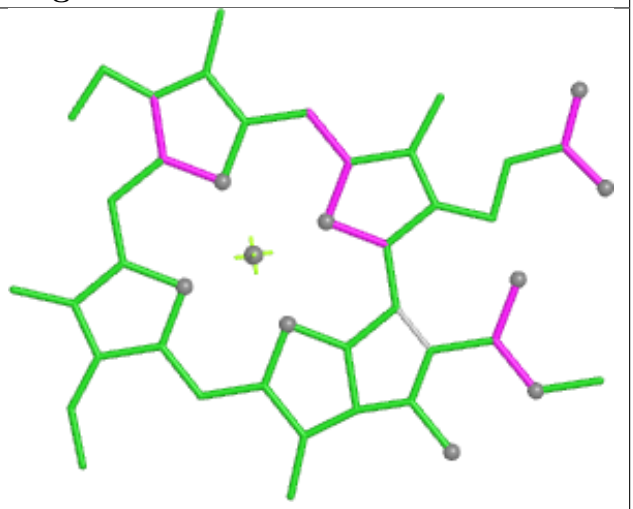


Rings

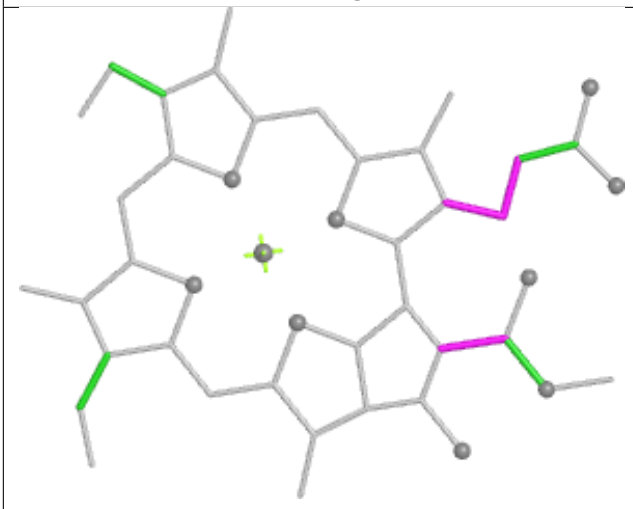
Ligand CLA g 604



Bond lengths



Bond angles

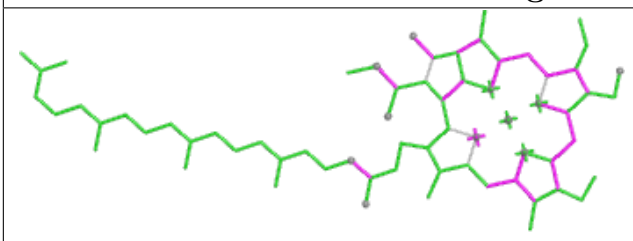


Torsions

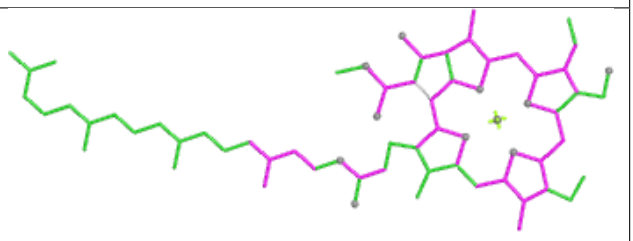


Rings

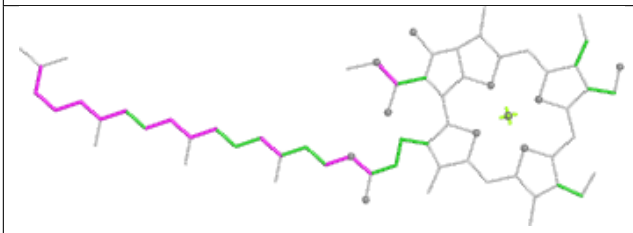
Ligand CHL d 609



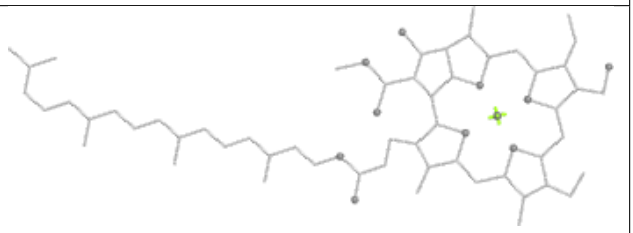
Bond lengths



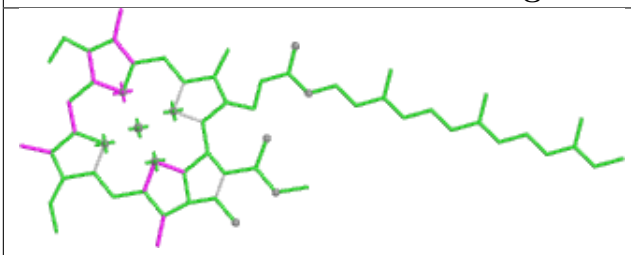
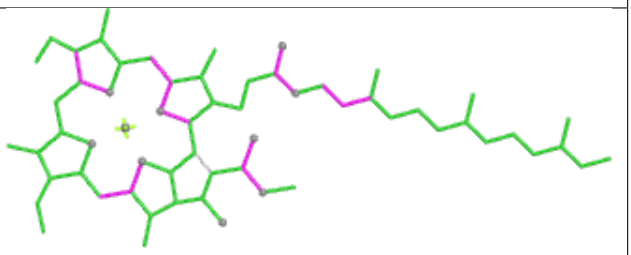
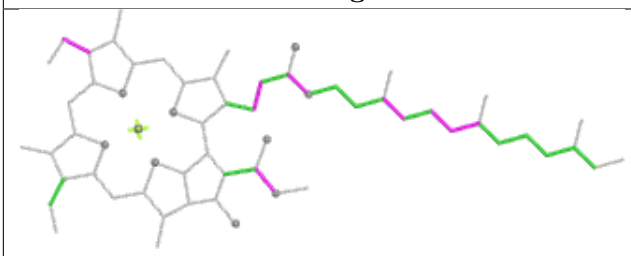
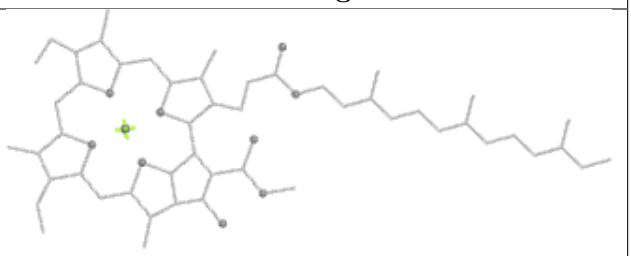
Bond angles

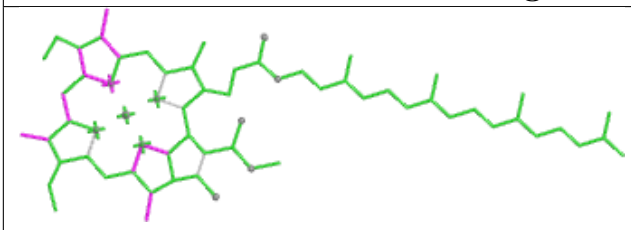
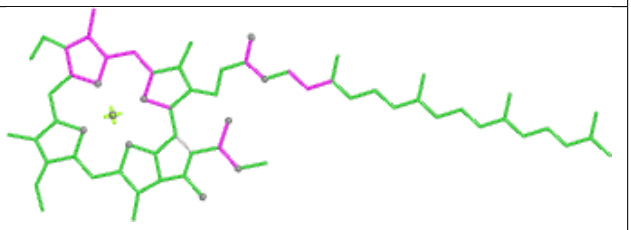
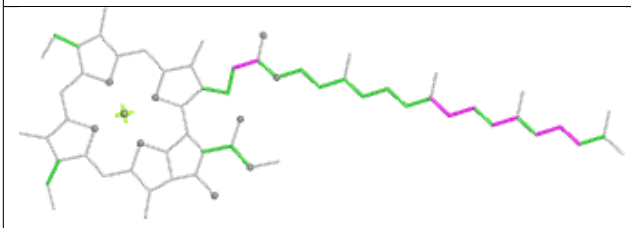
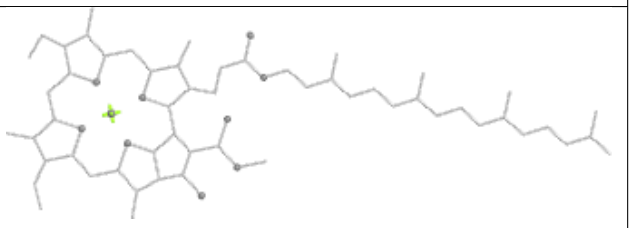


Torsions

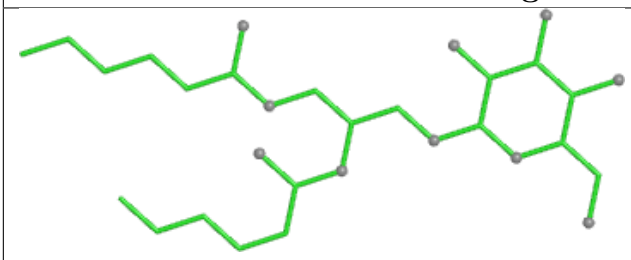


Rings

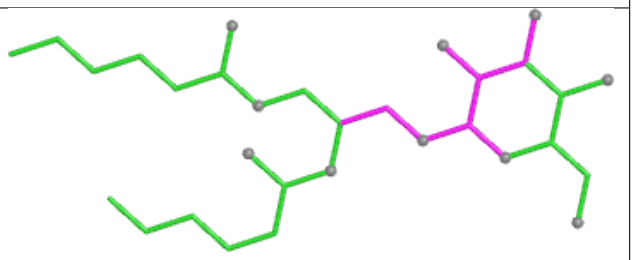
Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

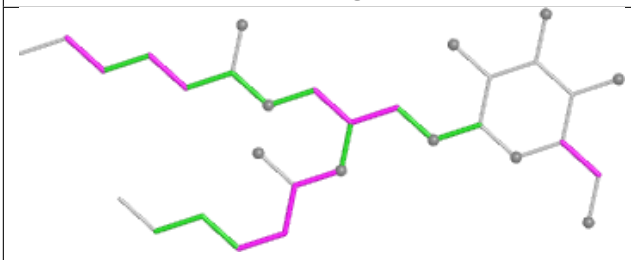
Ligand LMG L 210



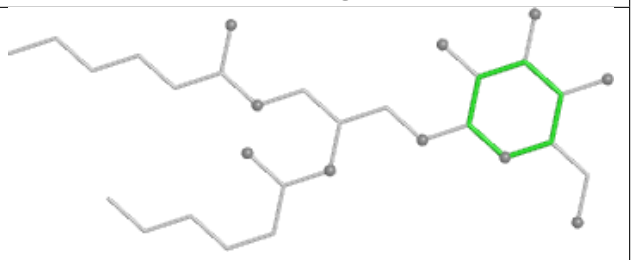
Bond lengths



Bond angles

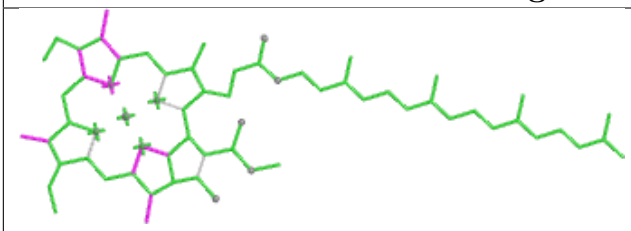


Torsions

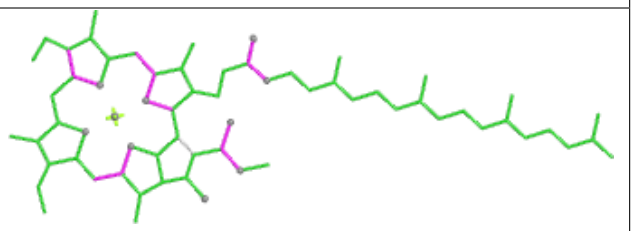


Rings

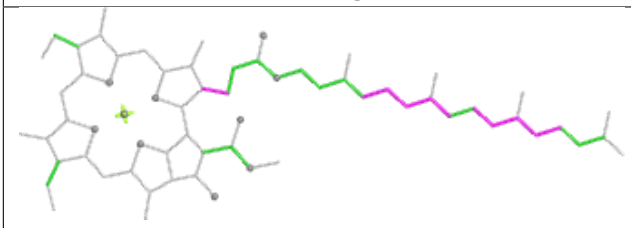
Ligand CLA 9 308



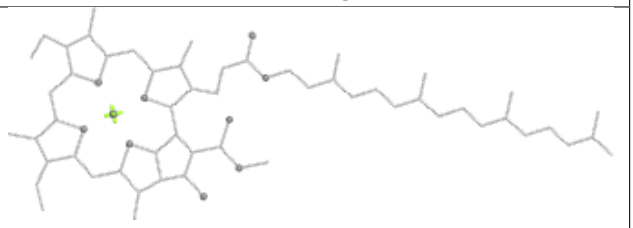
Bond lengths



Bond angles

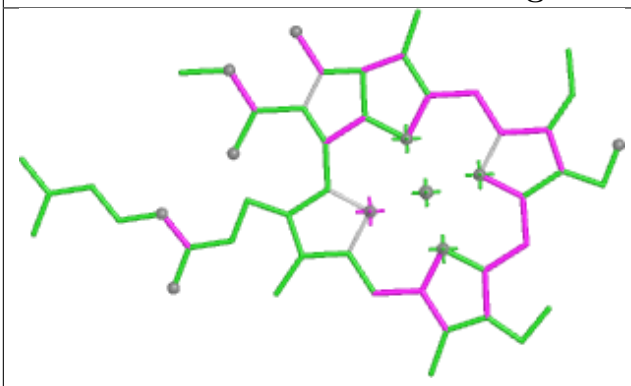


Torsions

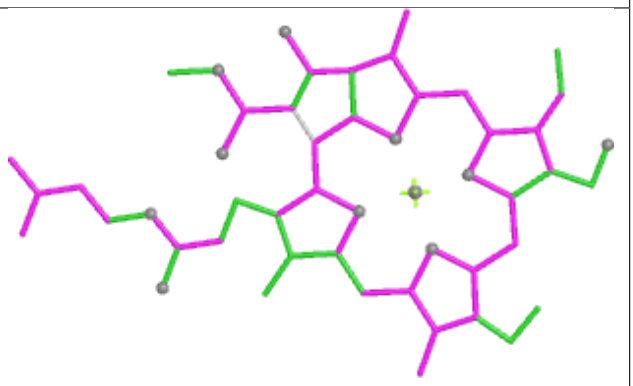


Rings

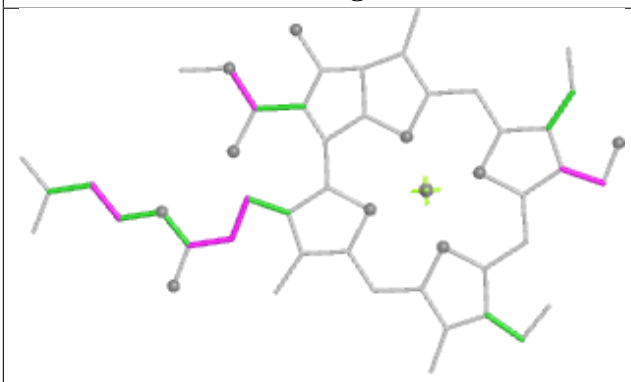
Ligand CHL h 606



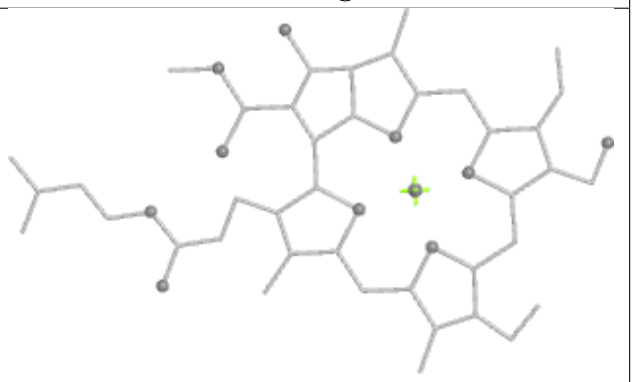
Bond lengths



Bond angles

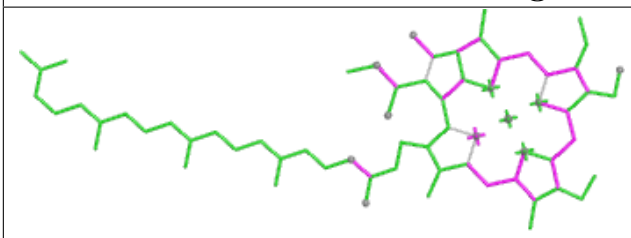


Torsions

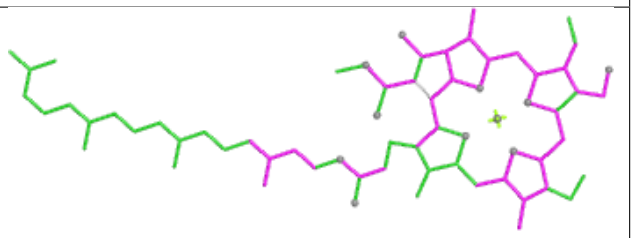


Rings

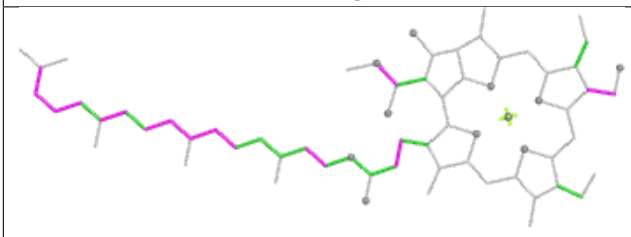
Ligand CHL e 608



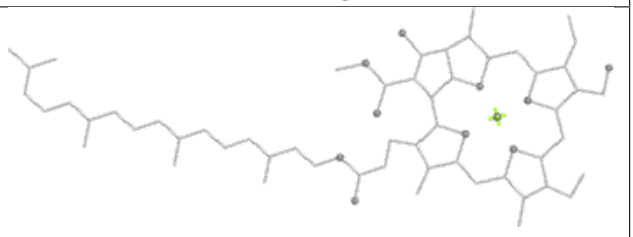
Bond lengths



Bond angles

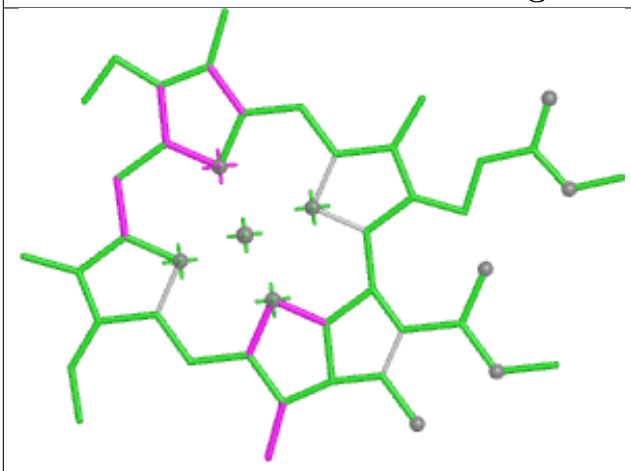


Torsions

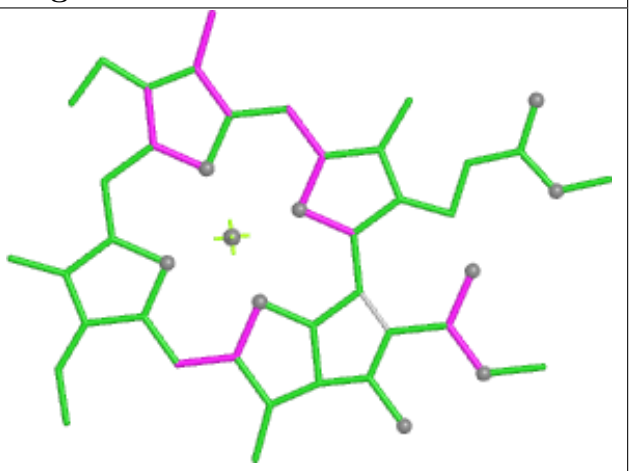


Rings

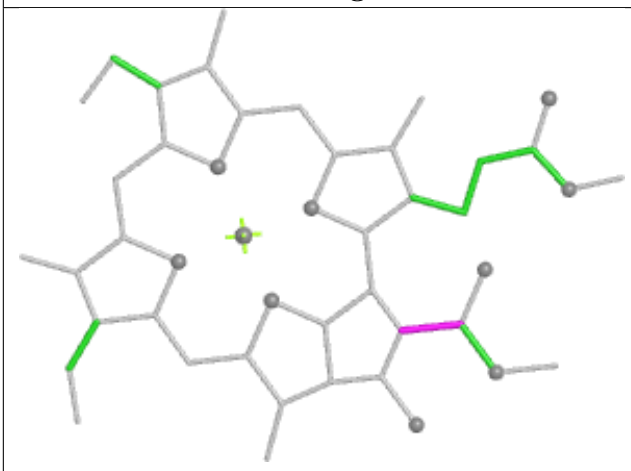
Ligand CLA g 611



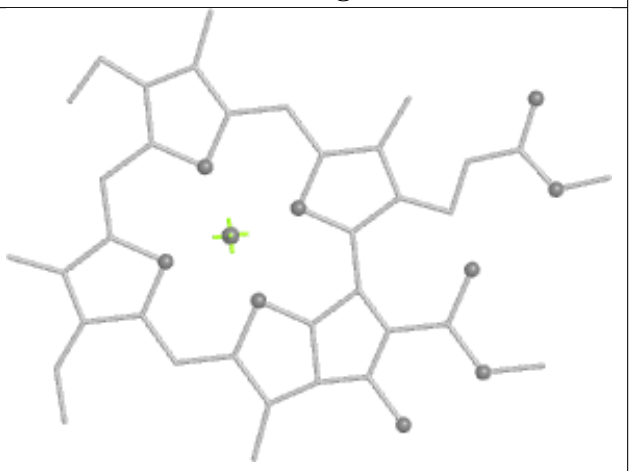
Bond lengths



Bond angles

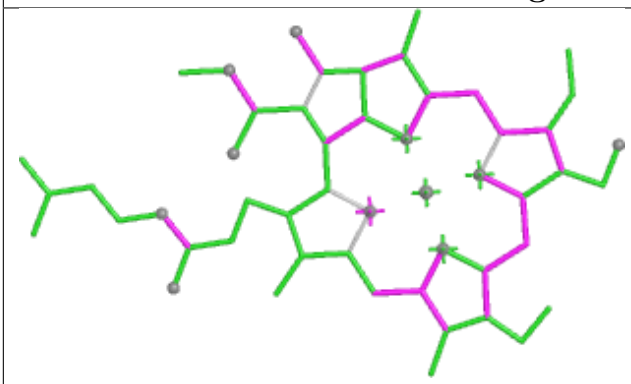


Torsions

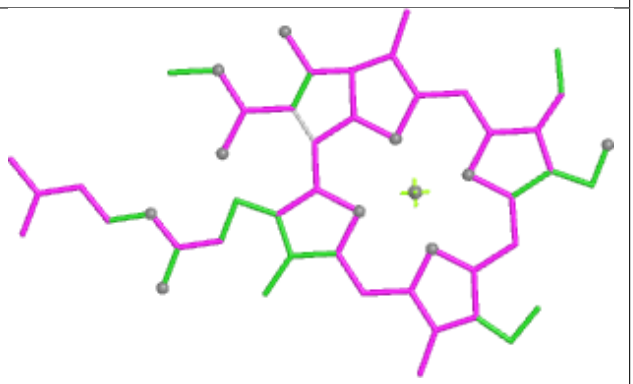


Rings

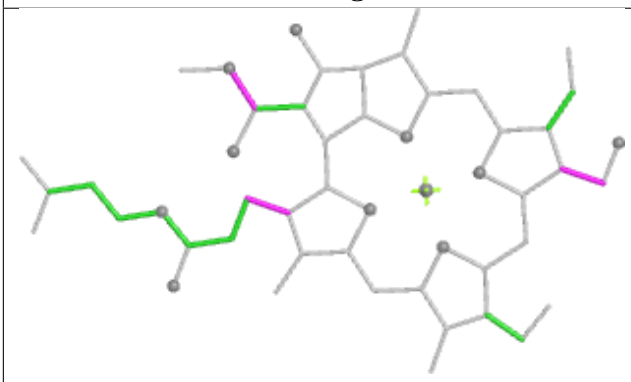
Ligand CHL e 601



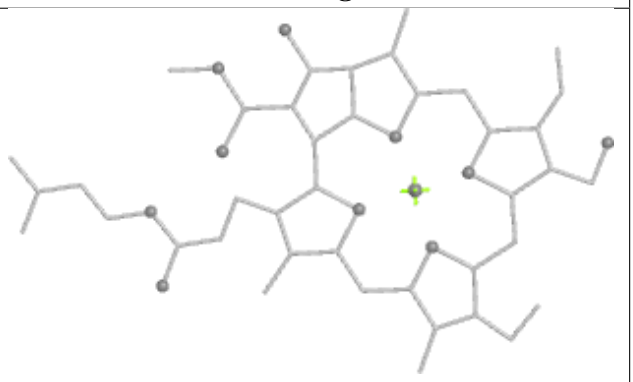
Bond lengths



Bond angles

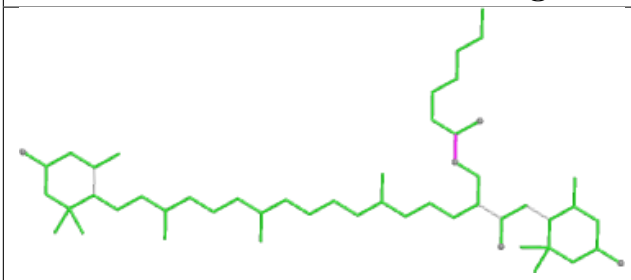


Torsions

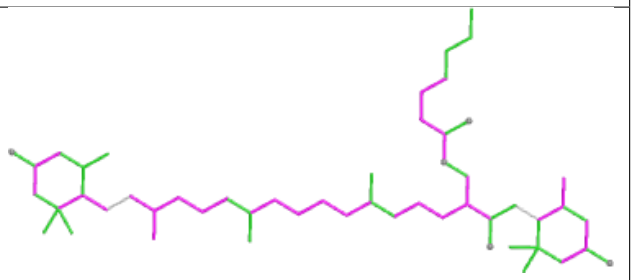


Rings

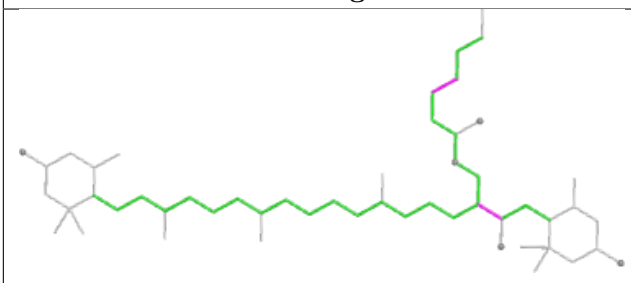
Ligand 0UR 1 501



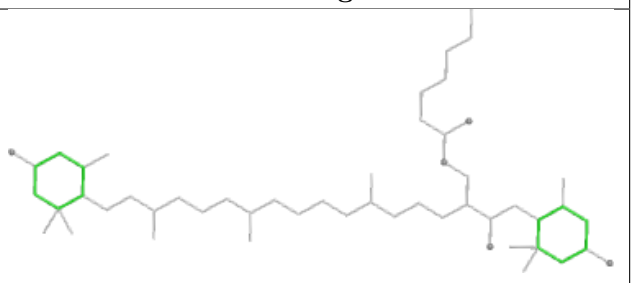
Bond lengths



Bond angles

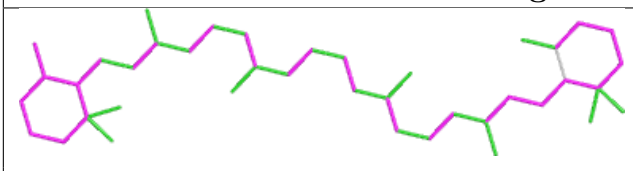


Torsions

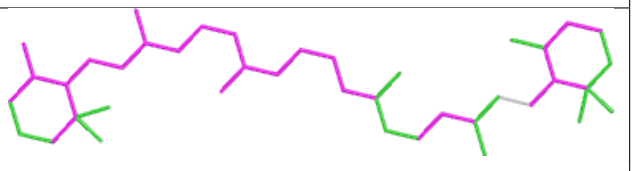


Rings

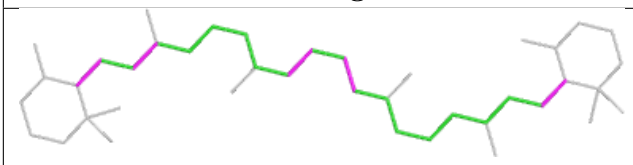
Ligand 8CT L 206



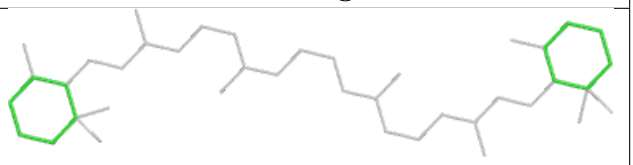
Bond lengths



Bond angles

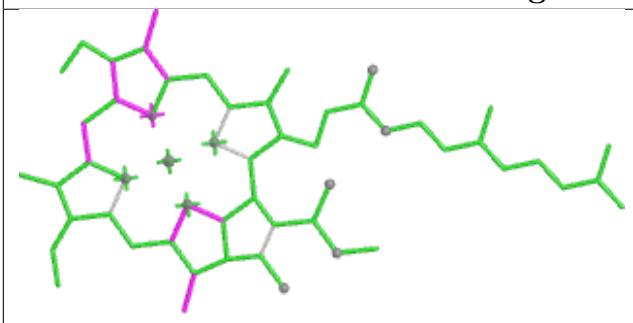


Torsions

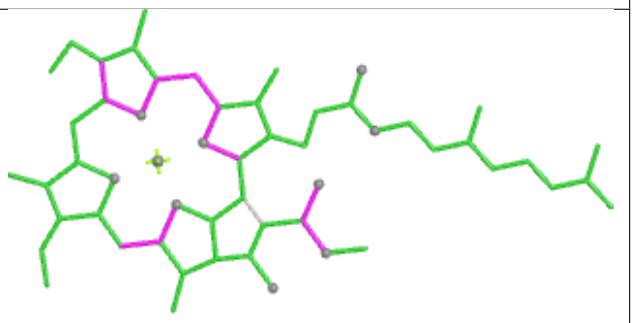


Rings

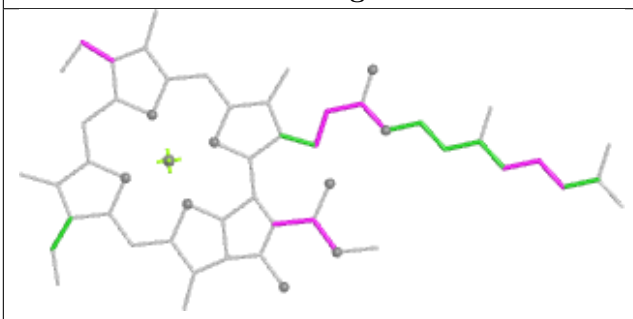
Ligand CLA 7 312



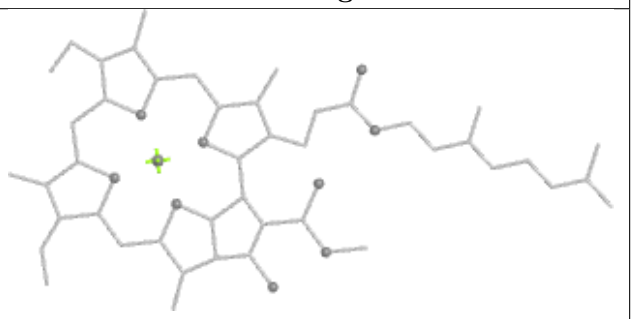
Bond lengths



Bond angles

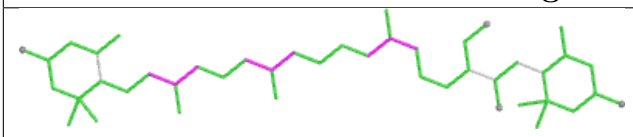


Torsions

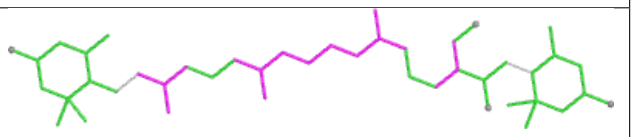


Rings

Ligand 0IE i 521



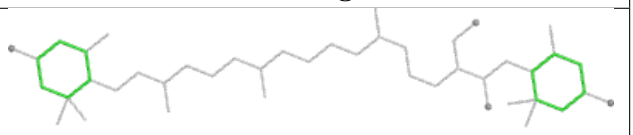
Bond lengths



Bond angles

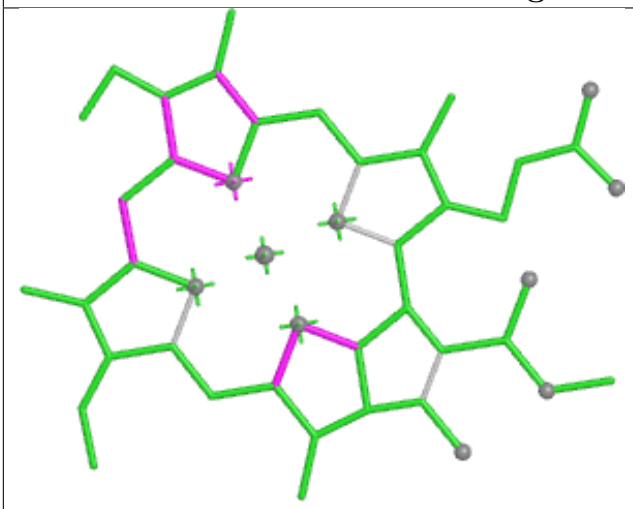


Torsions

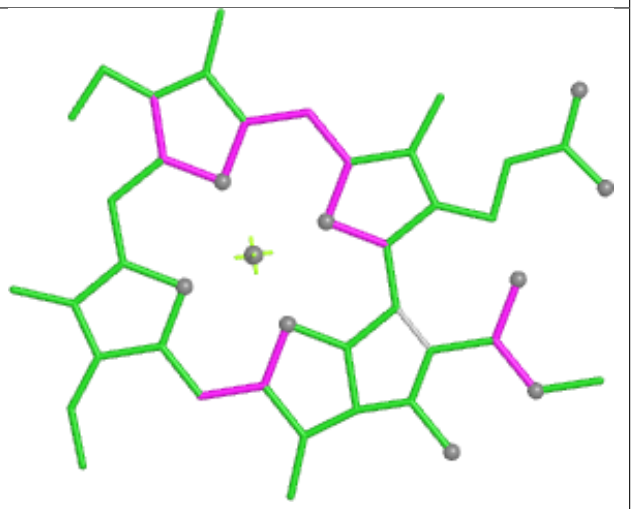


Rings

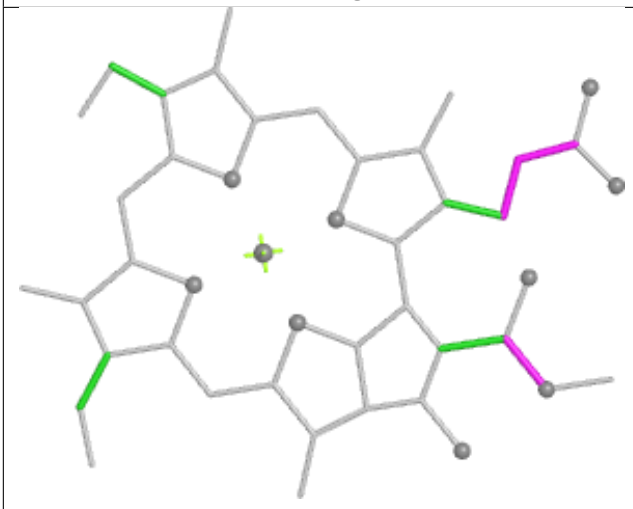
Ligand CLA h 613



Bond lengths



Bond angles

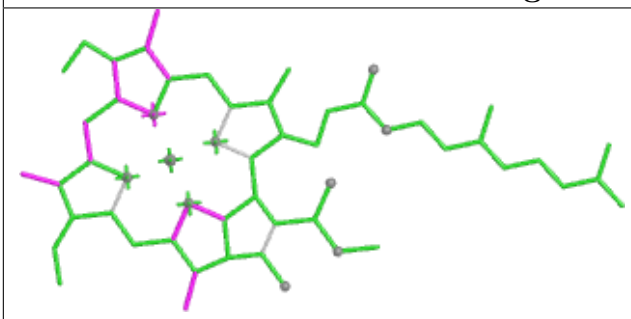


Torsions

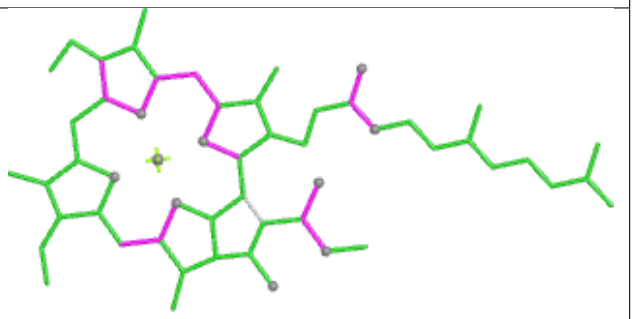


Rings

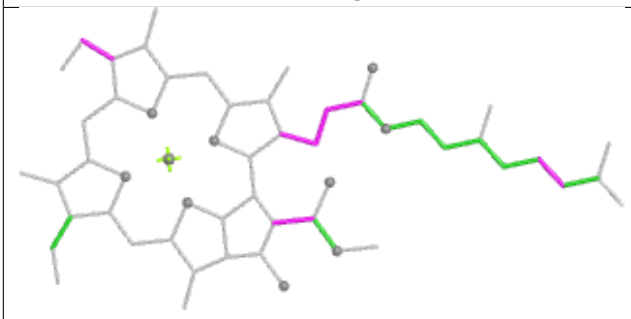
Ligand CLA A 820



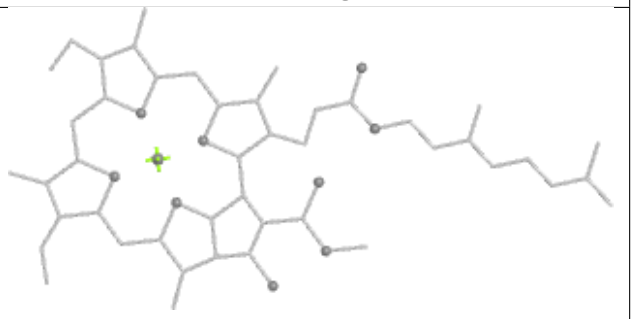
Bond lengths



Bond angles

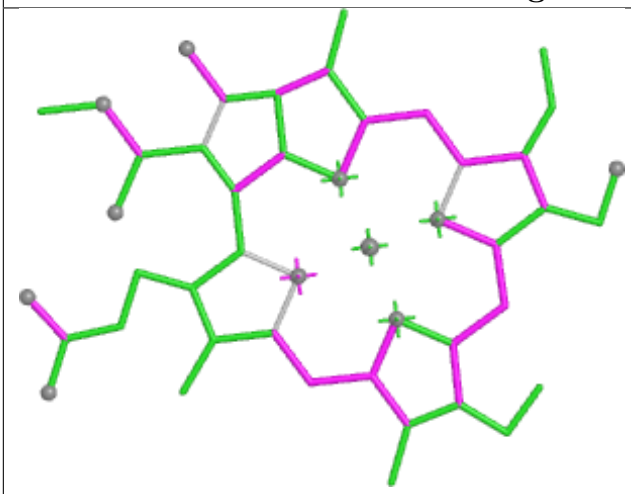


Torsions

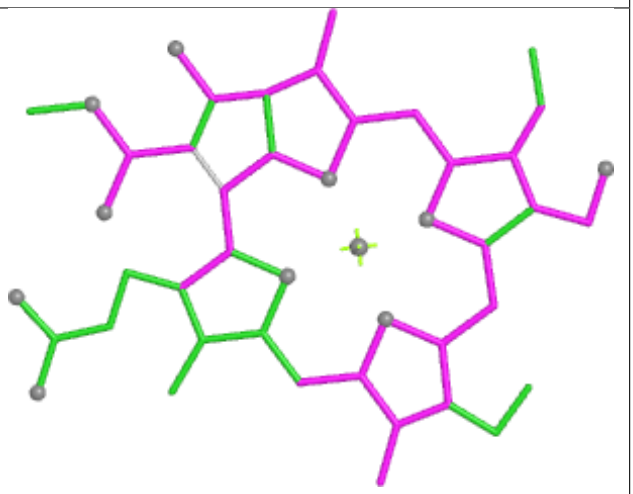


Rings

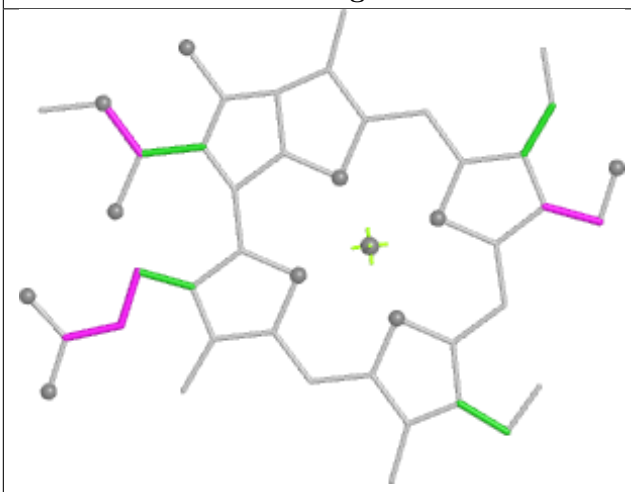
Ligand CHL 5 305



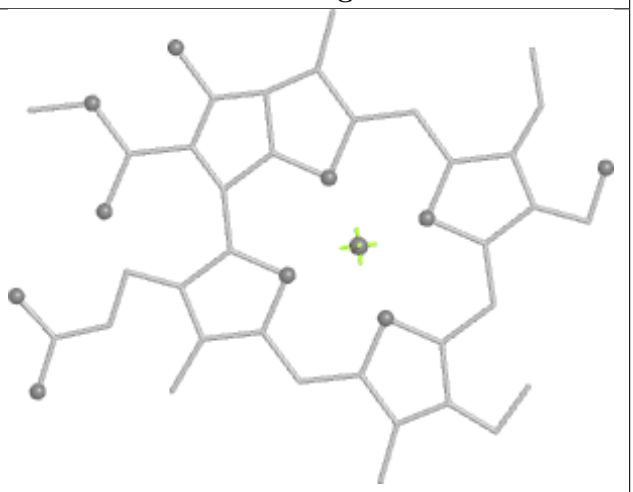
Bond lengths



Bond angles

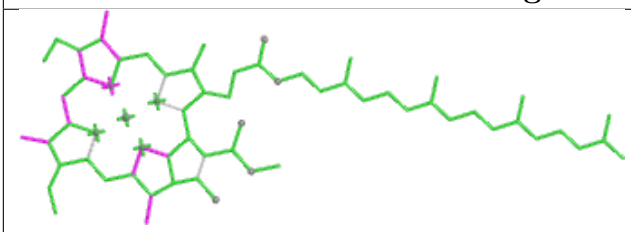


Torsions

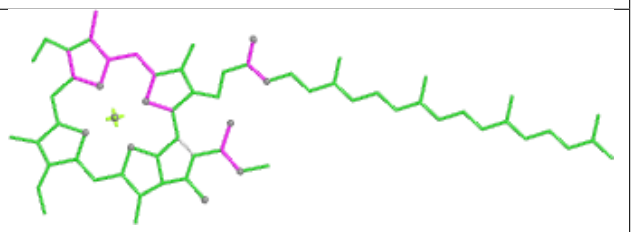


Rings

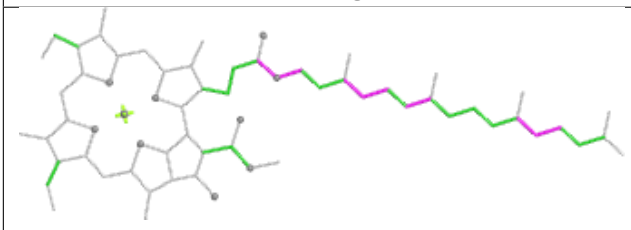
Ligand CLA A 821



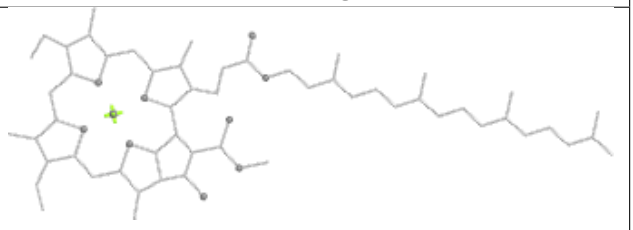
Bond lengths



Bond angles

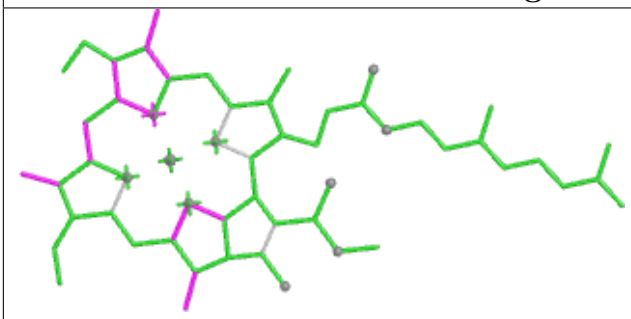


Torsions

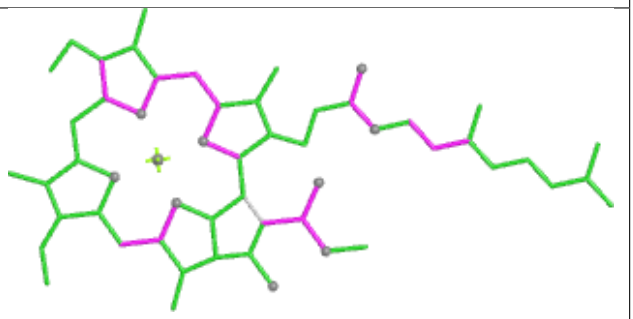


Rings

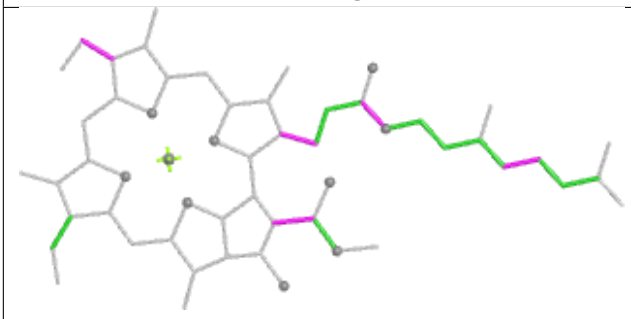
Ligand CLA B 833



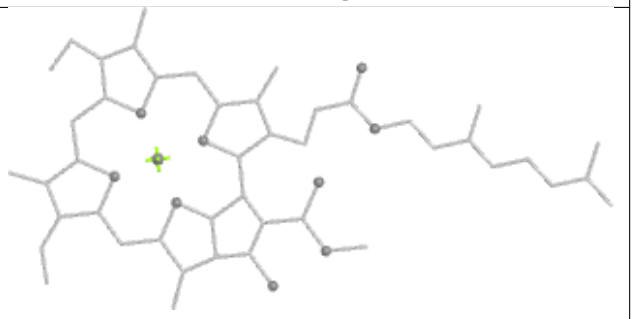
Bond lengths



Bond angles

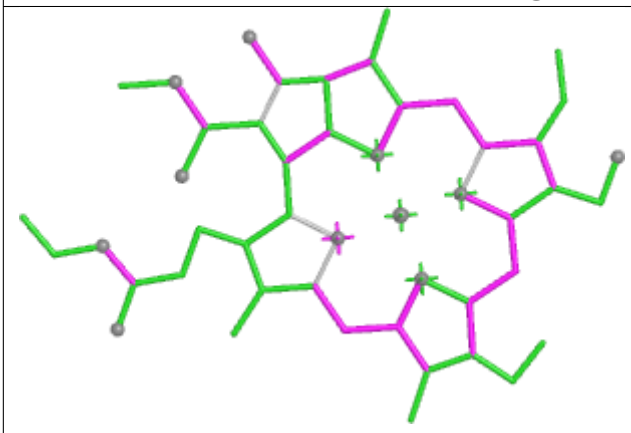


Torsions

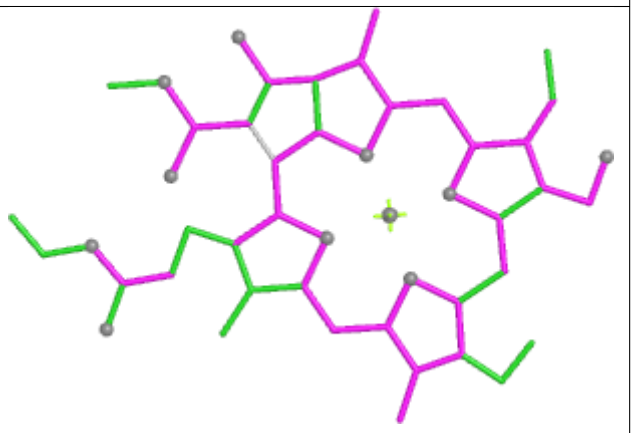


Rings

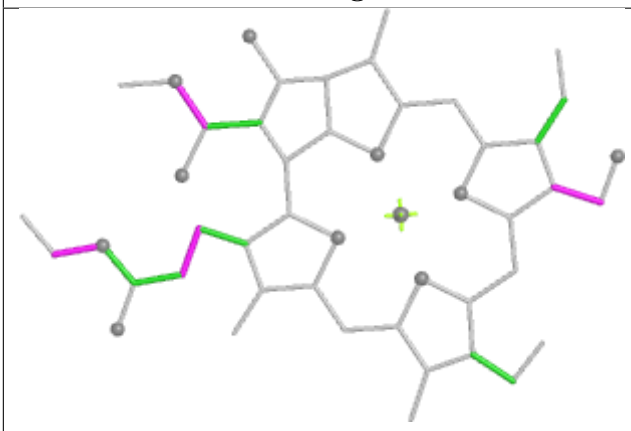
Ligand CHL 4 306



Bond lengths



Bond angles

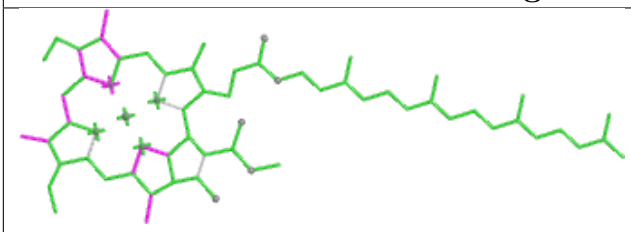


Torsions

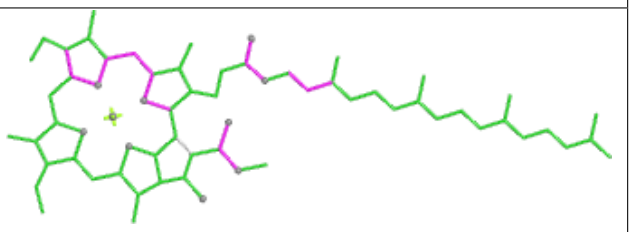


Rings

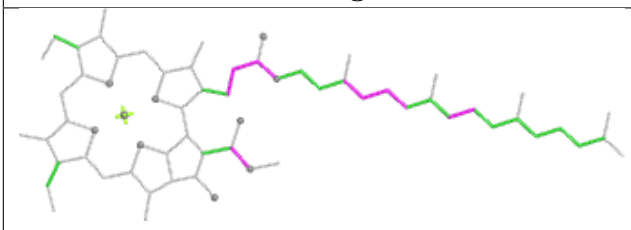
Ligand CLA A 841



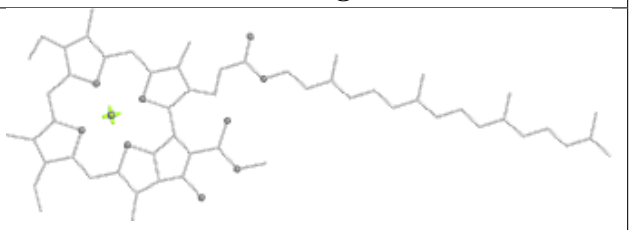
Bond lengths



Bond angles

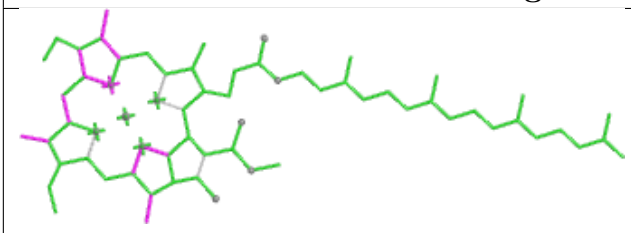


Torsions

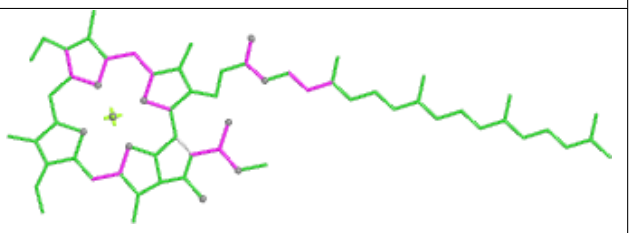


Rings

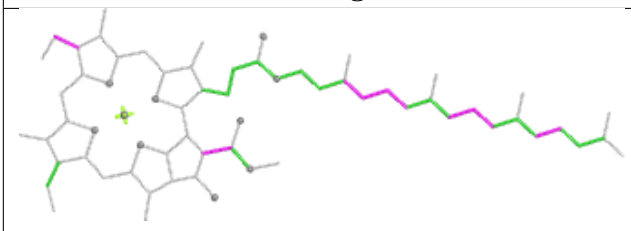
Ligand CLA B 811



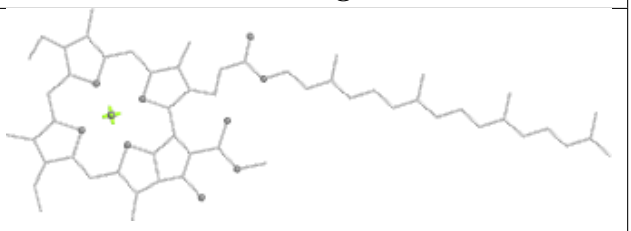
Bond lengths



Bond angles

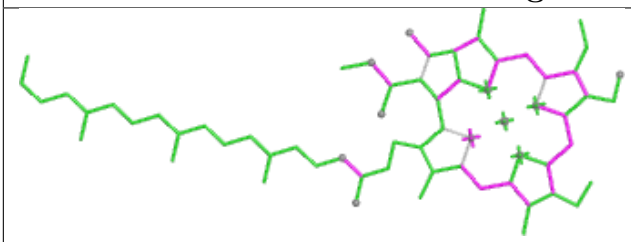


Torsions

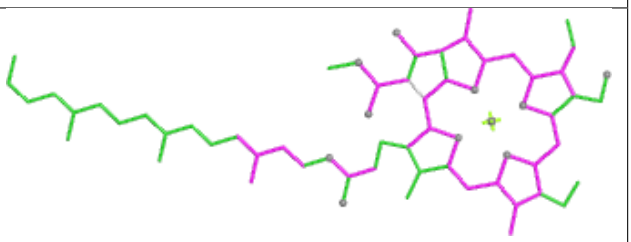


Rings

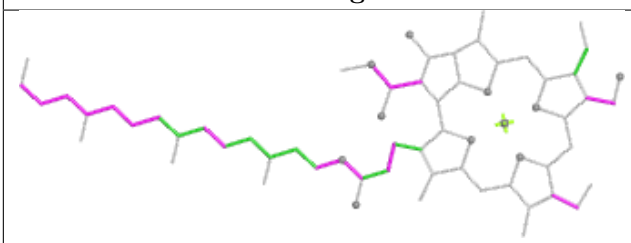
Ligand CHL b 602



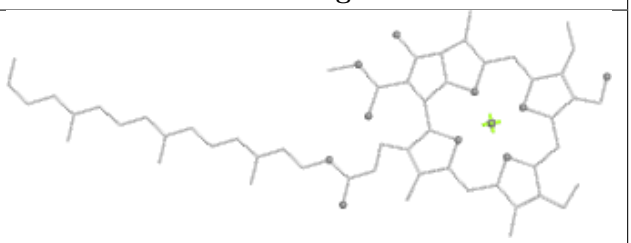
Bond lengths



Bond angles

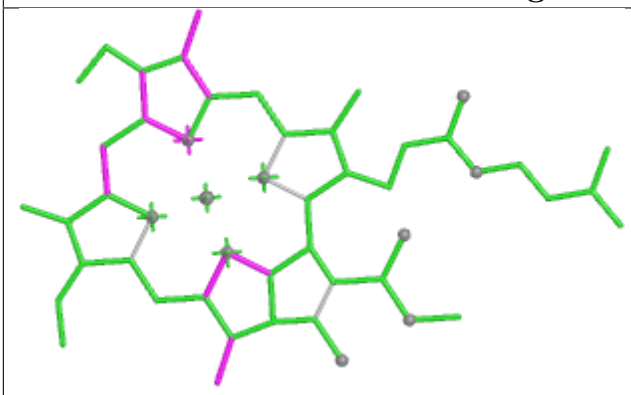


Torsions

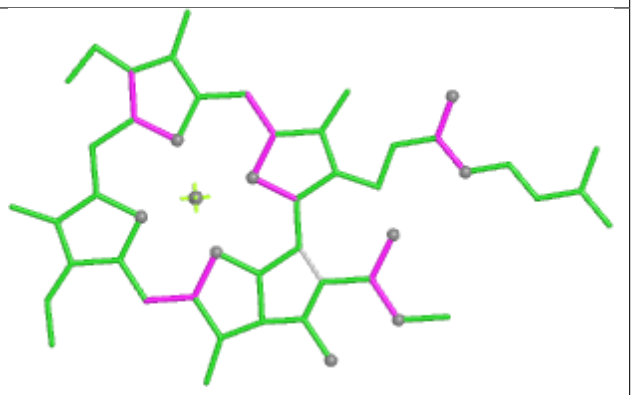


Rings

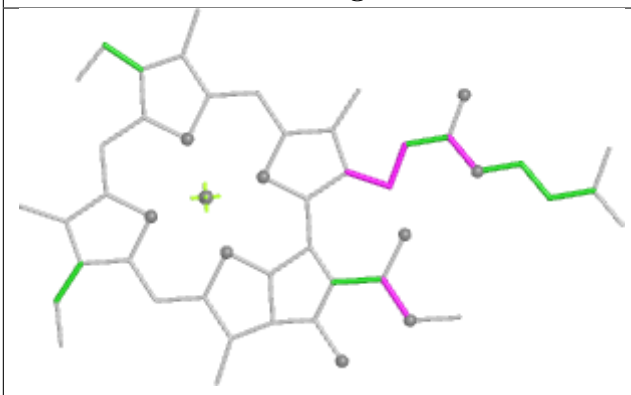
Ligand CLA b 604



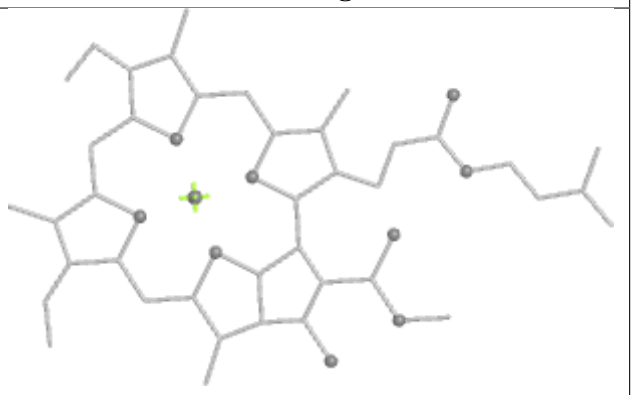
Bond lengths



Bond angles

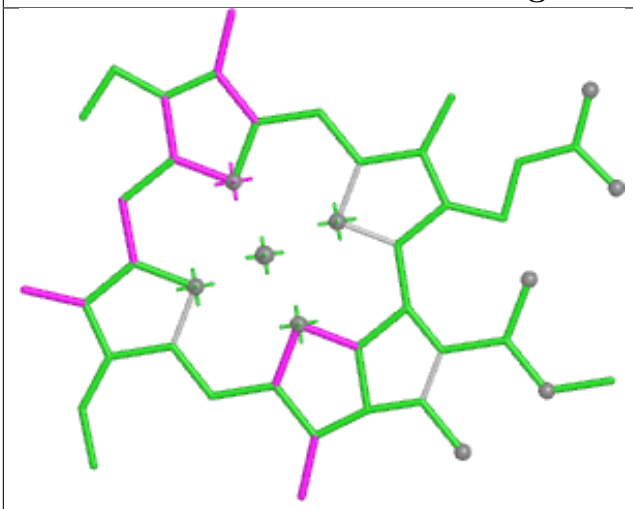


Torsions

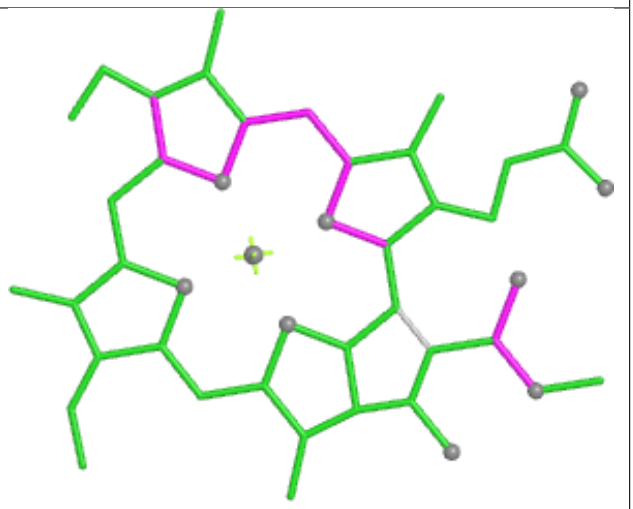


Rings

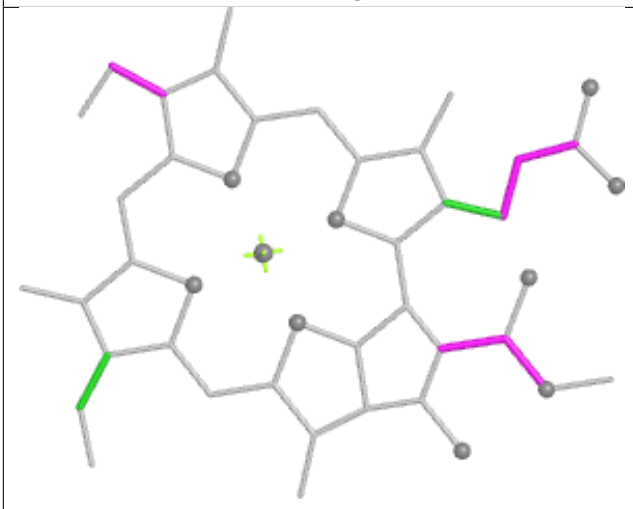
Ligand CLA 7 303



Bond lengths



Bond angles

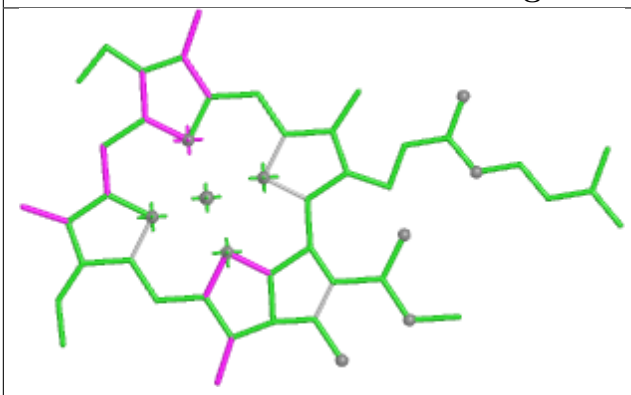


Torsions

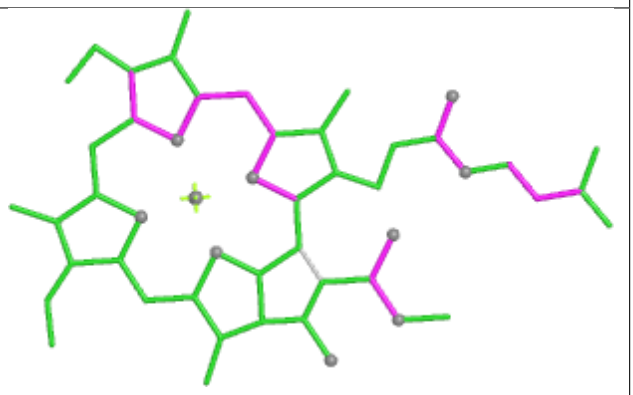


Rings

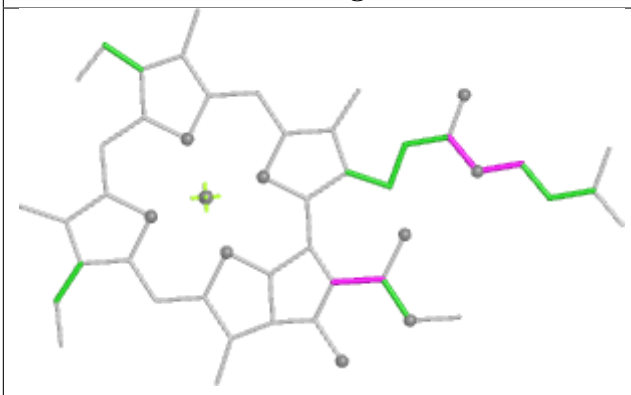
Ligand CLA A 831



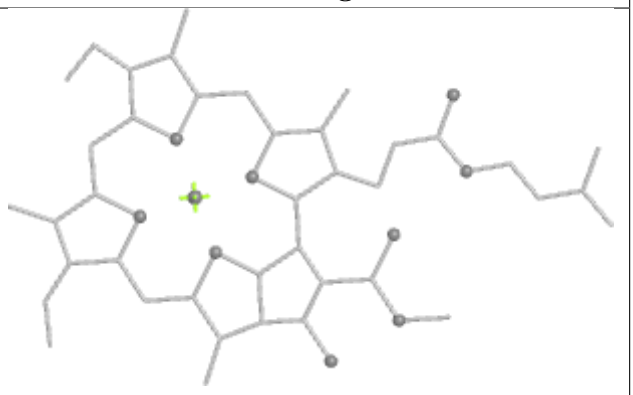
Bond lengths



Bond angles

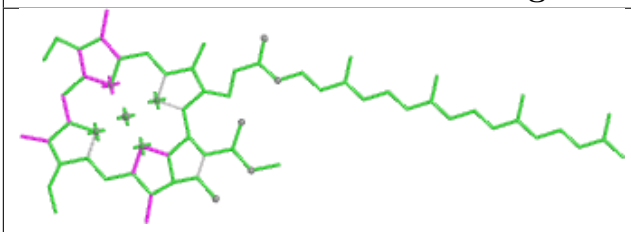


Torsions

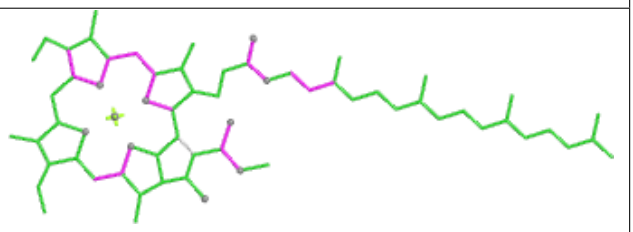


Rings

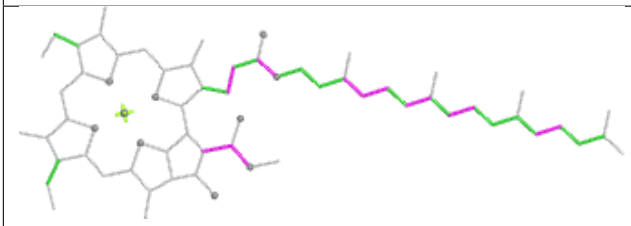
Ligand CLA 1 312



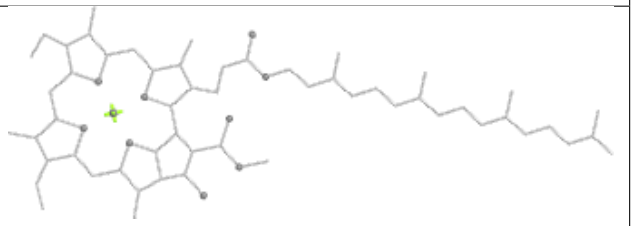
Bond lengths



Bond angles

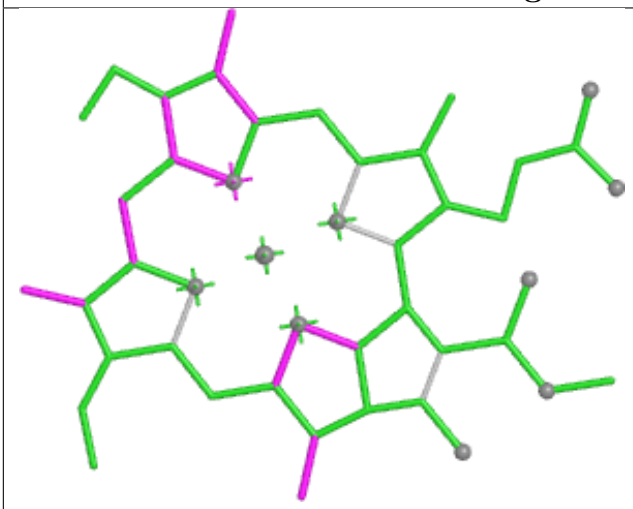


Torsions

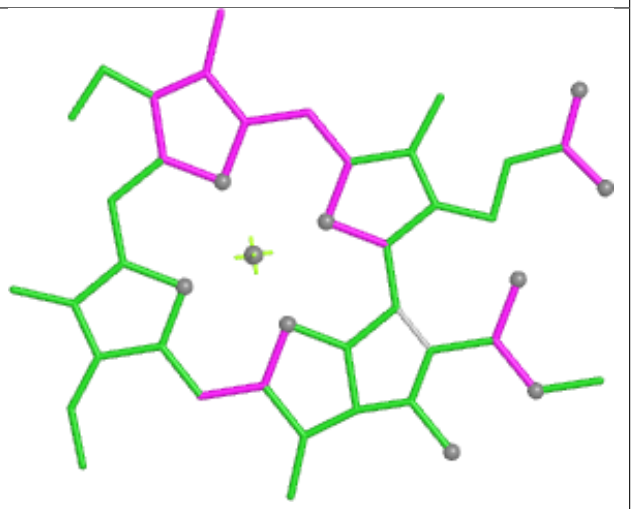


Rings

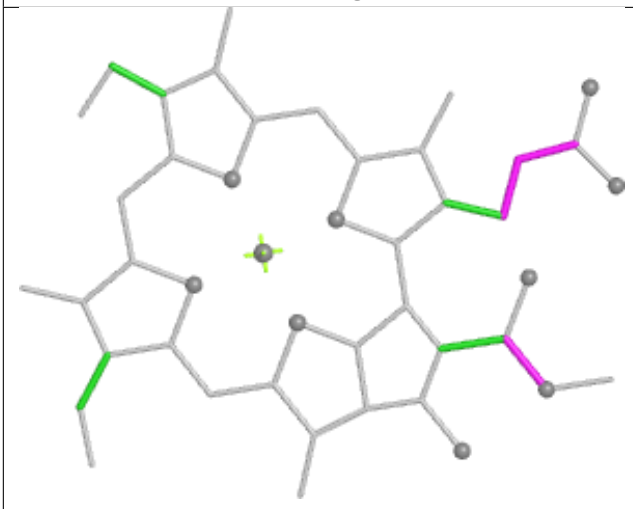
Ligand CLA B 807



Bond lengths



Bond angles

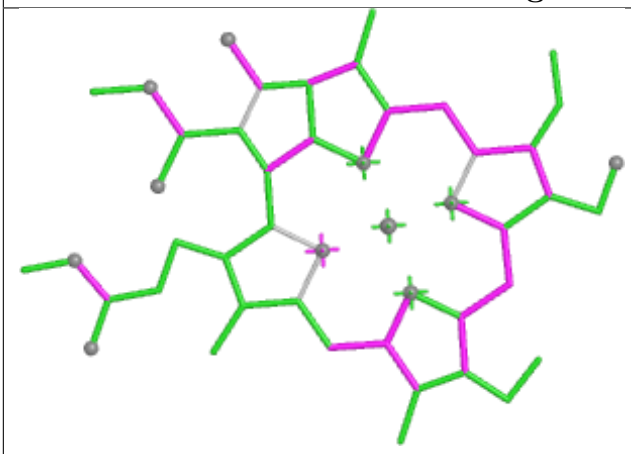


Torsions

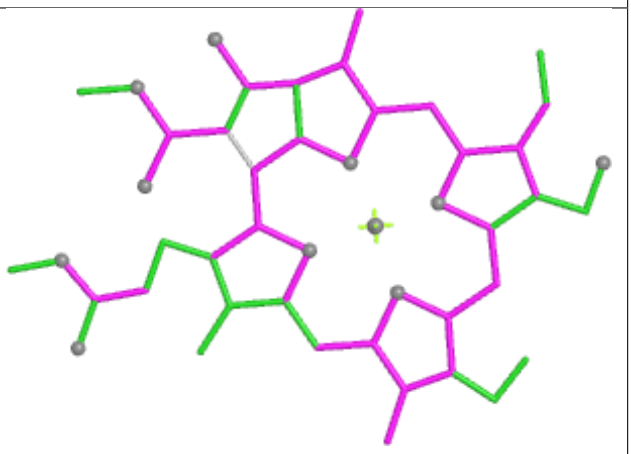


Rings

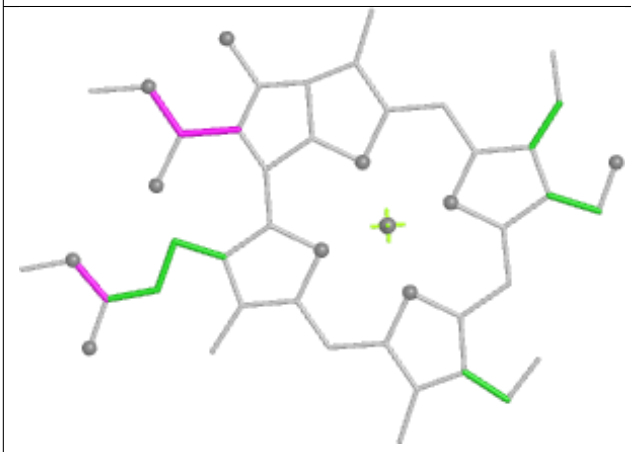
Ligand CHL b 607



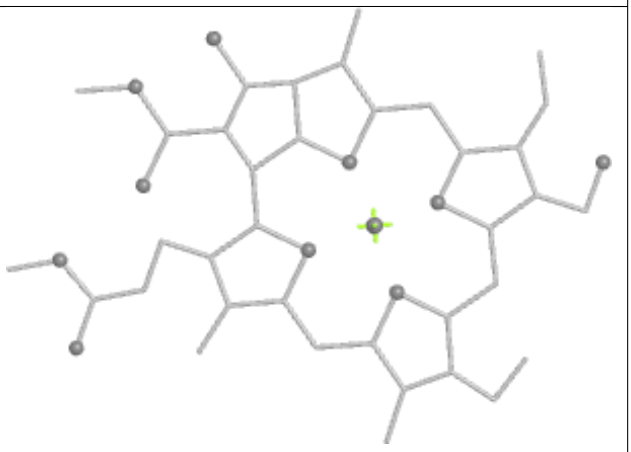
Bond lengths



Bond angles

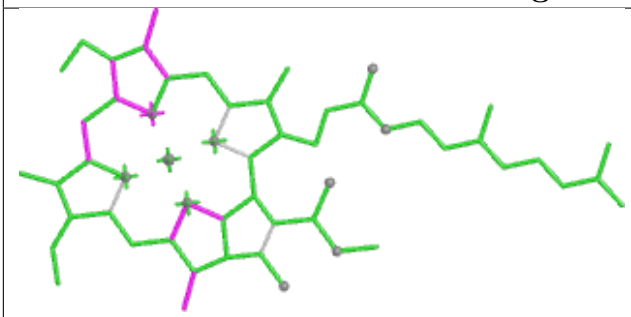


Torsions

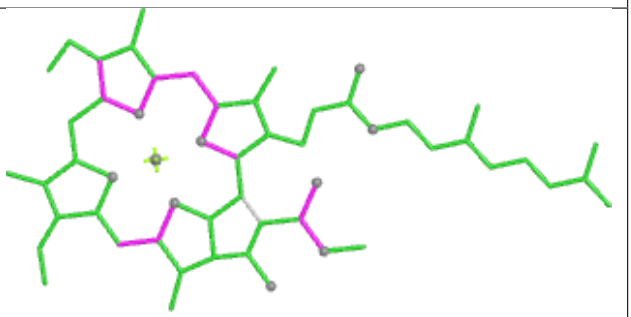


Rings

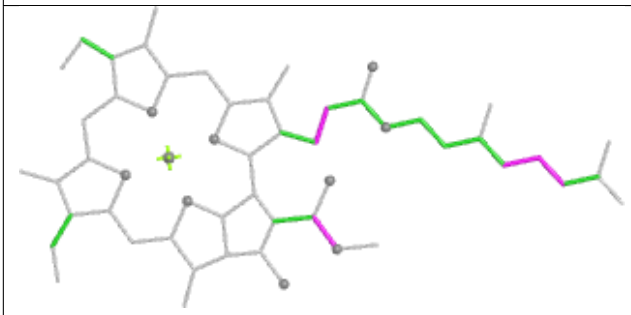
Ligand CLA f 611



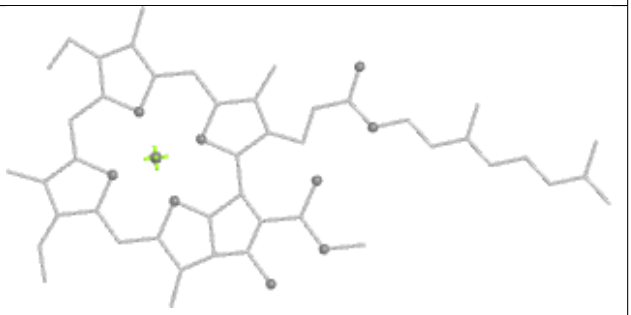
Bond lengths



Bond angles

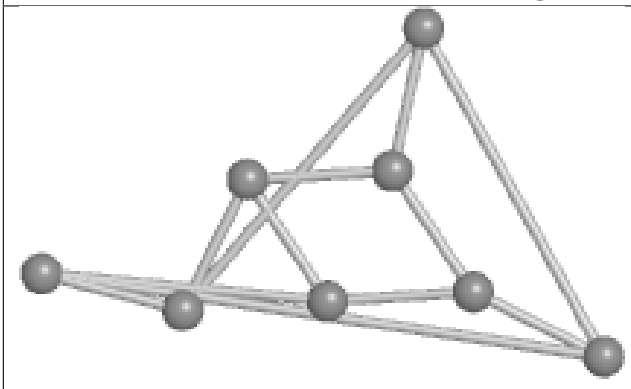


Torsions

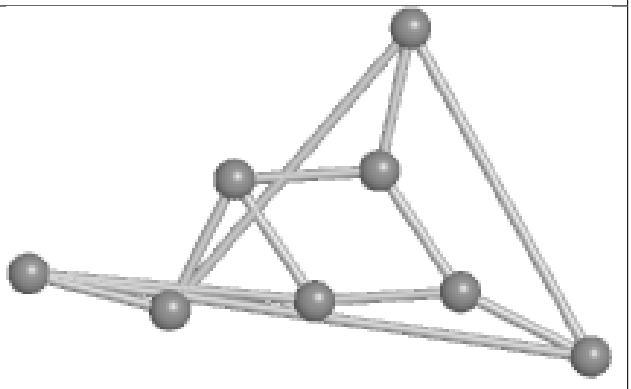


Rings

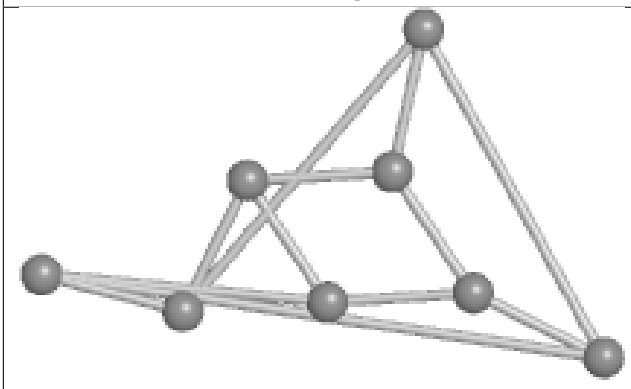
Ligand SF4 C 101



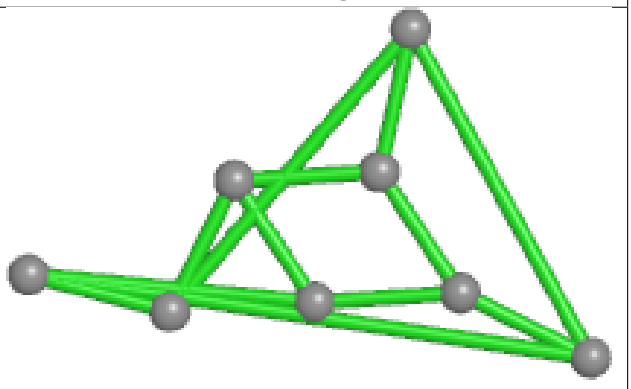
Bond lengths



Bond angles

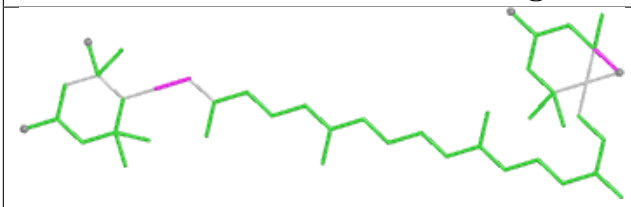


Torsions



Rings

Ligand NEX c 523



Bond lengths



Bond angles

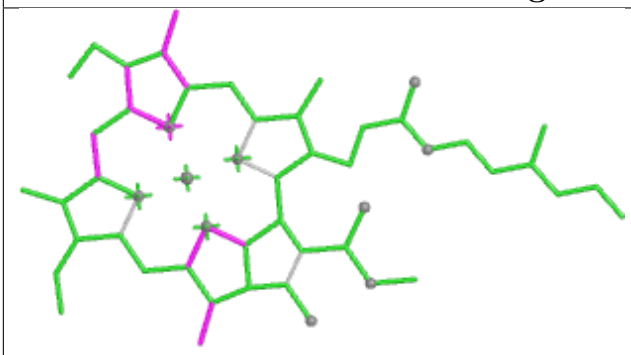


Torsions

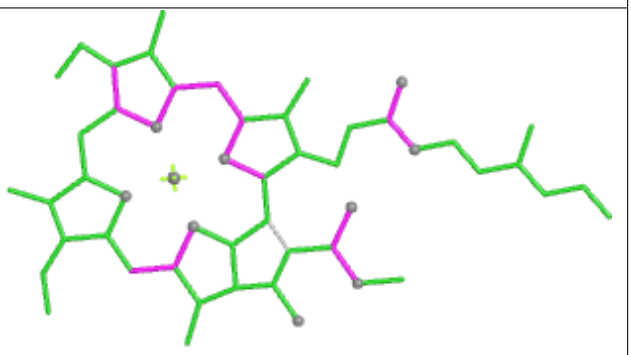


Rings

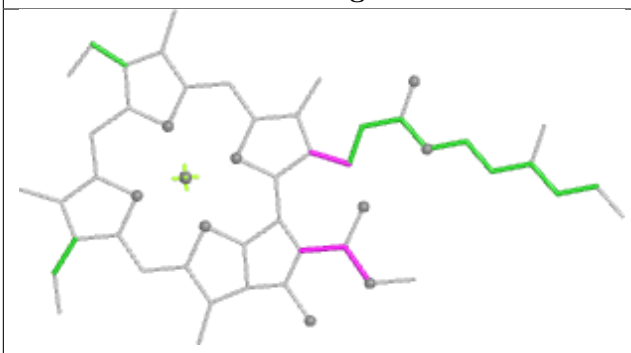
Ligand CLA 0 304



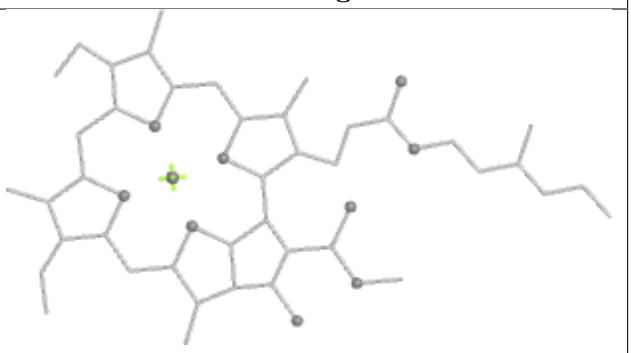
Bond lengths



Bond angles

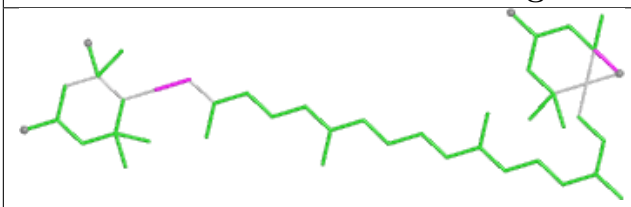


Torsions

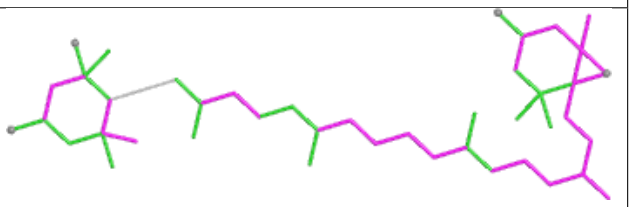


Rings

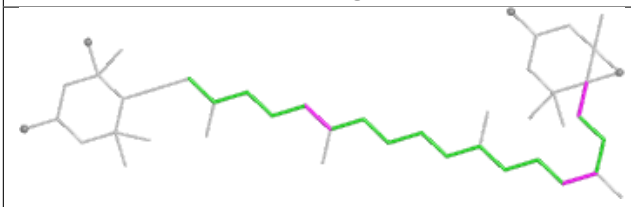
Ligand NEX e 523



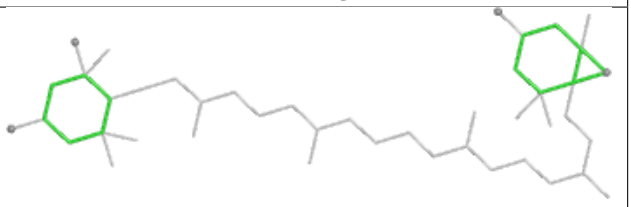
Bond lengths



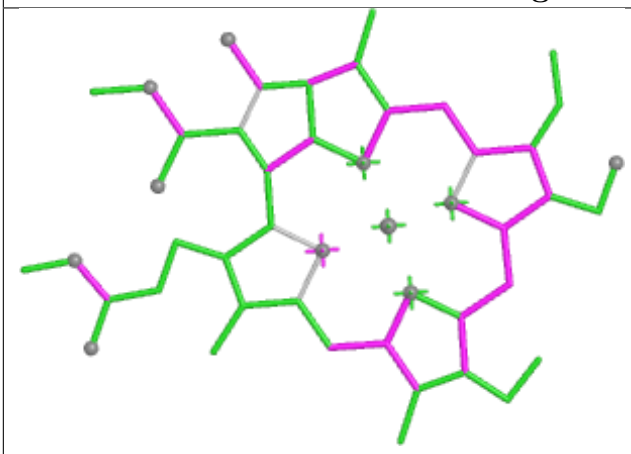
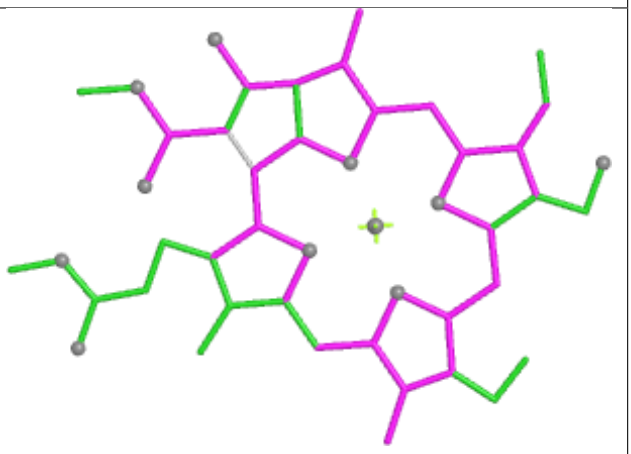
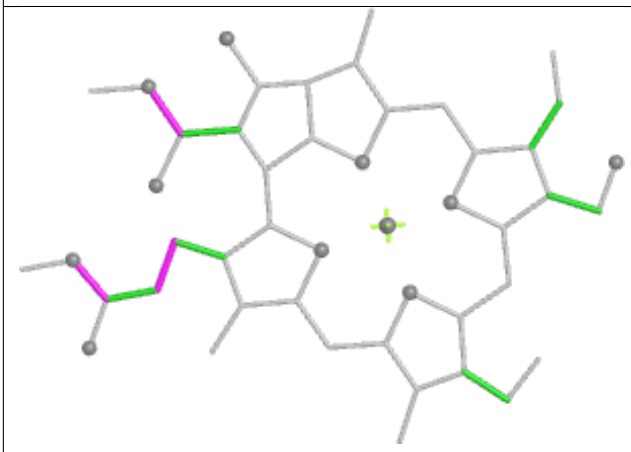
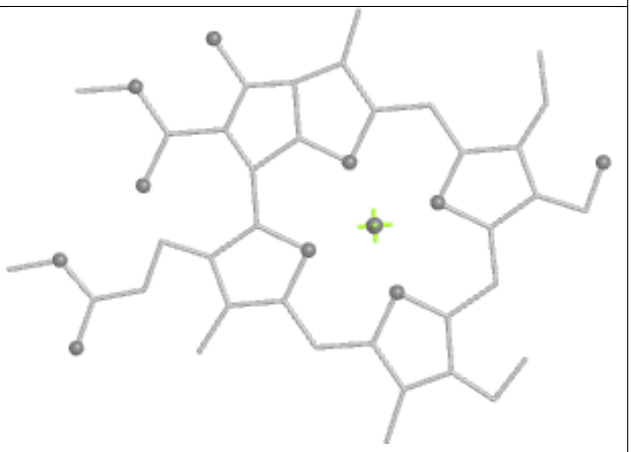
Bond angles

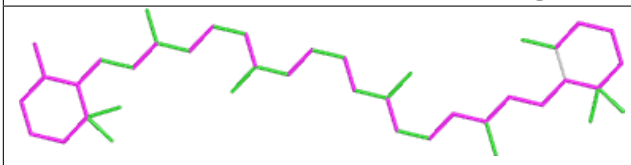
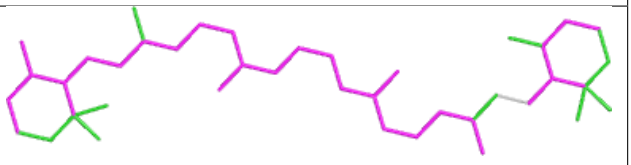
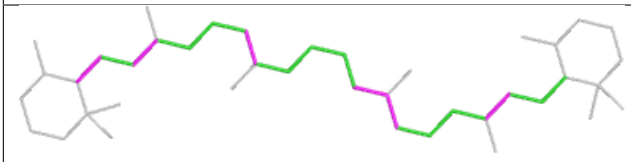
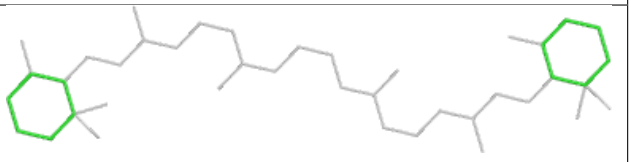


Torsions

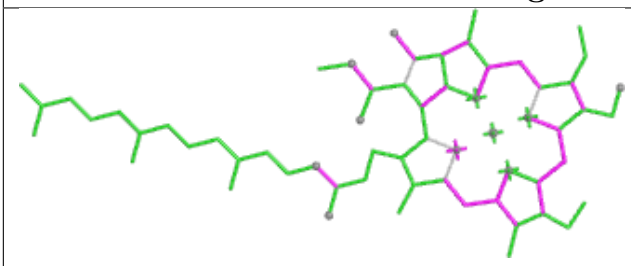


Rings

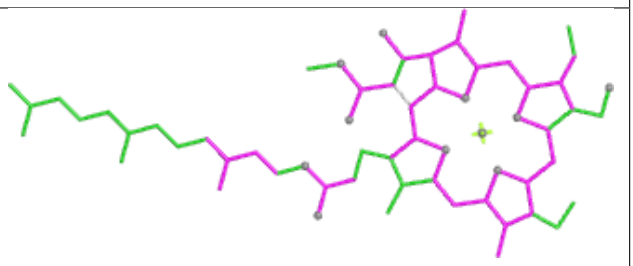
Ligand CHL i 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT 2 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

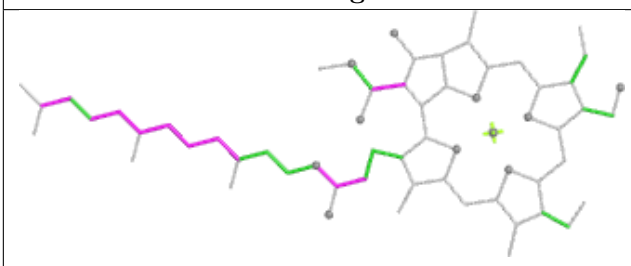
Ligand CHL 2 319



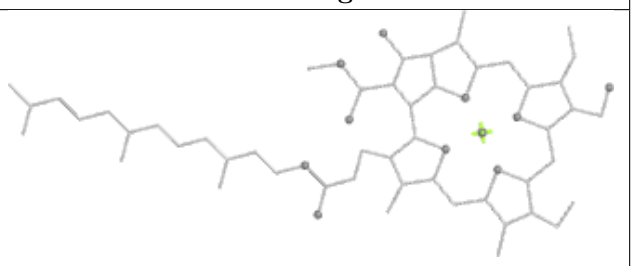
Bond lengths



Bond angles

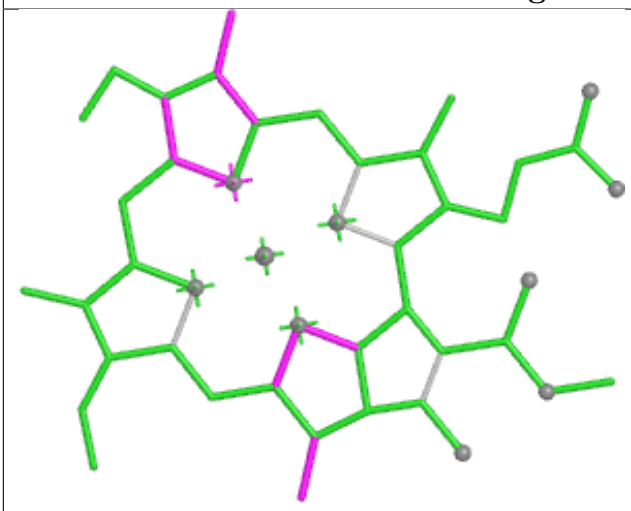


Torsions

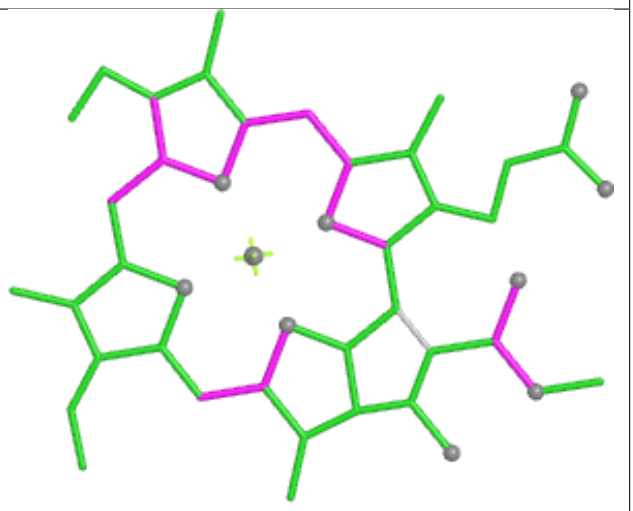


Rings

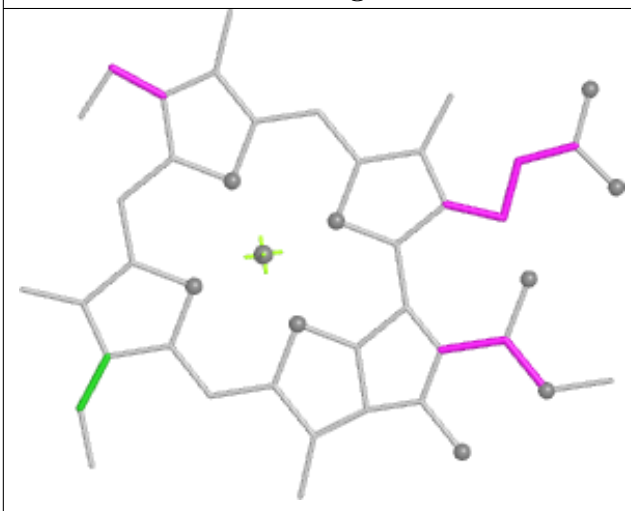
Ligand CLA 5 311



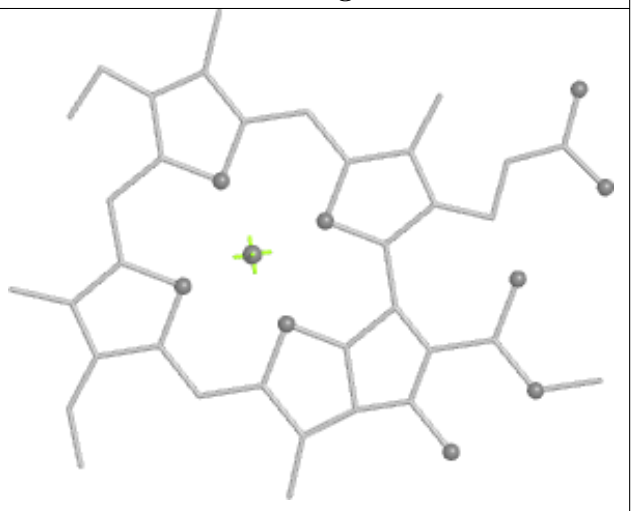
Bond lengths



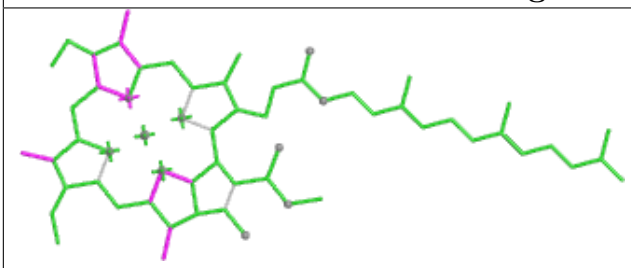
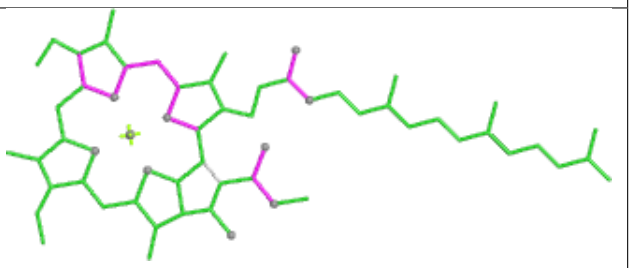
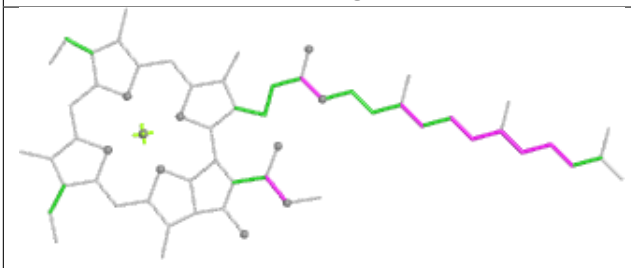
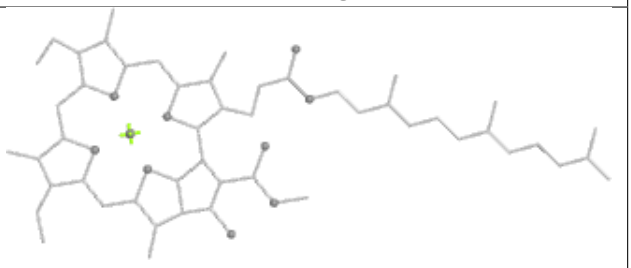
Bond angles

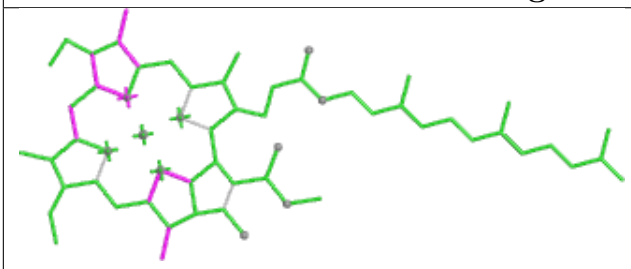
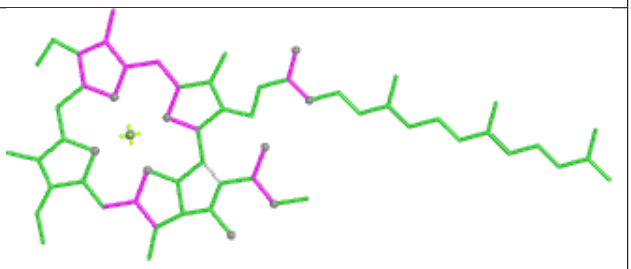
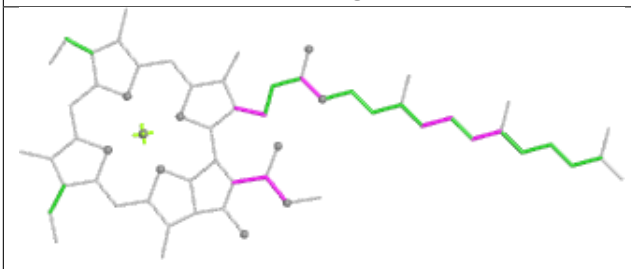
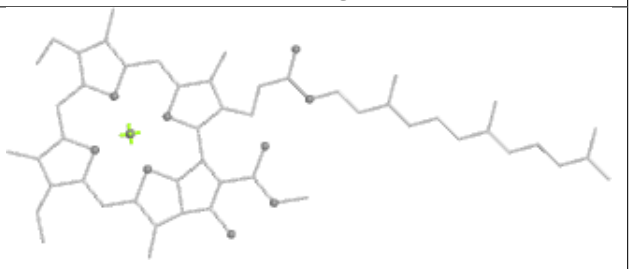


Torsions

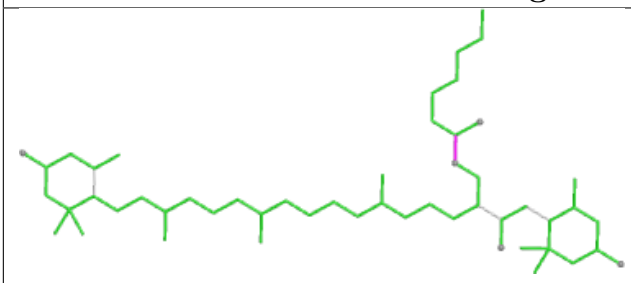


Rings

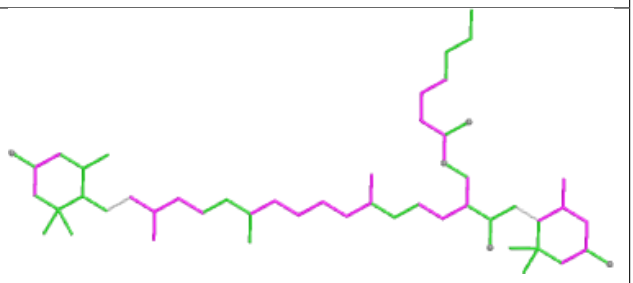
Ligand CLA 2 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

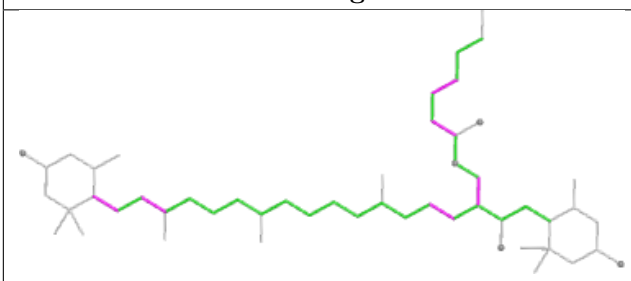
Ligand 0UR 5 502



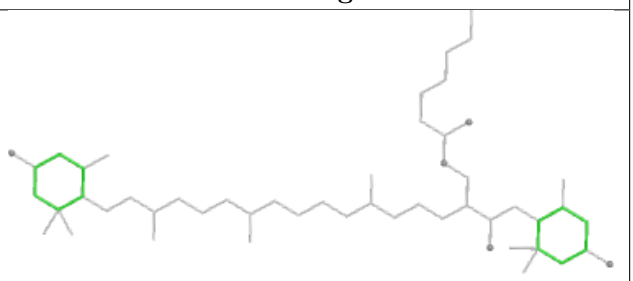
Bond lengths



Bond angles

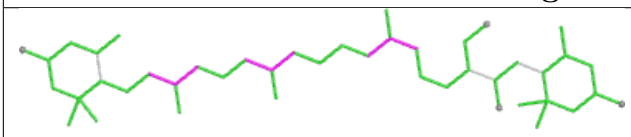


Torsions

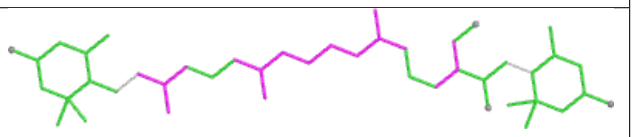


Rings

Ligand 0IE f 522



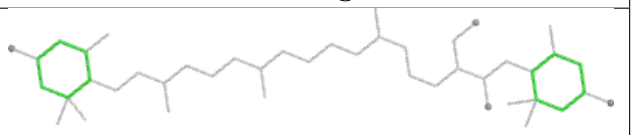
Bond lengths



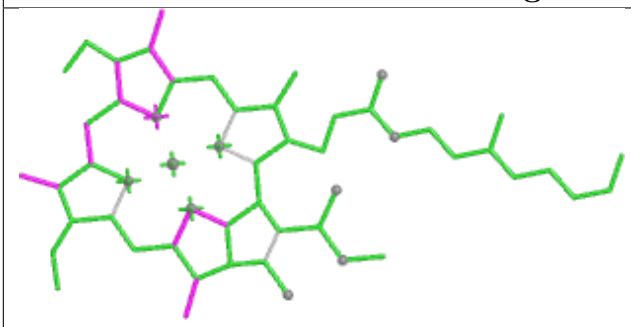
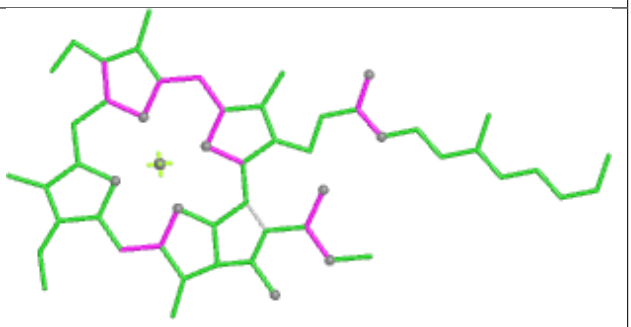
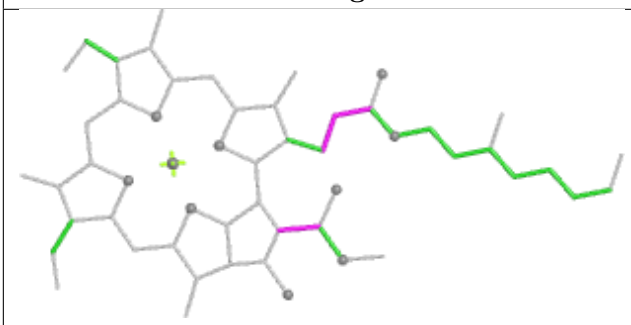
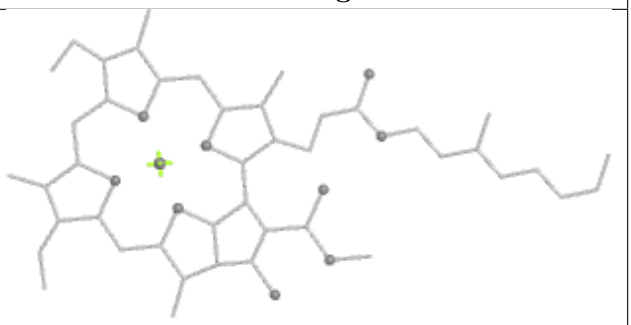
Bond angles

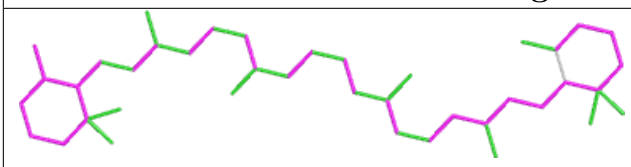
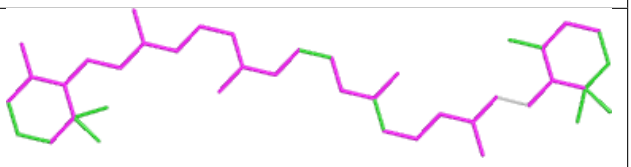
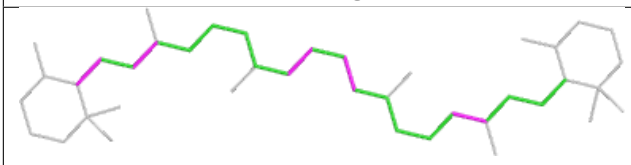
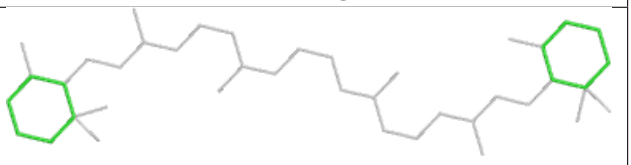


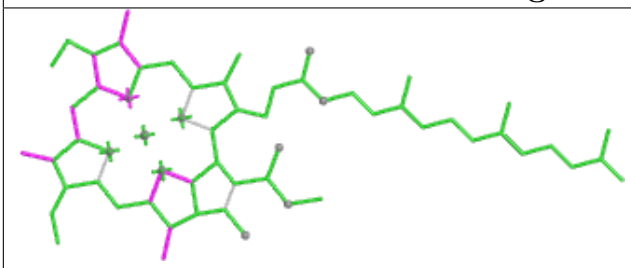
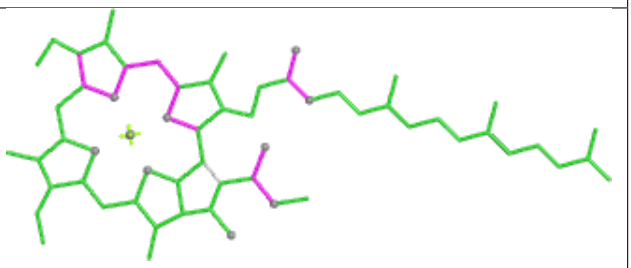
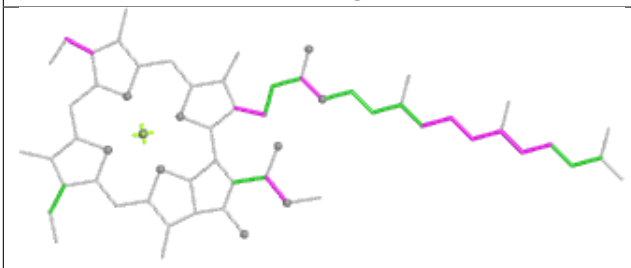
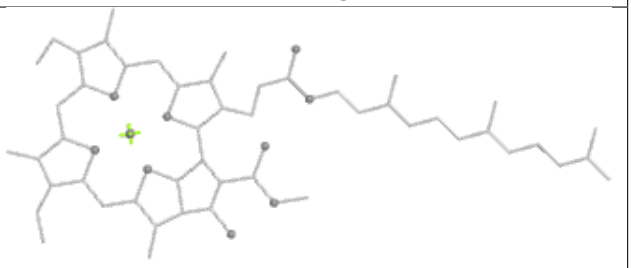
Torsions

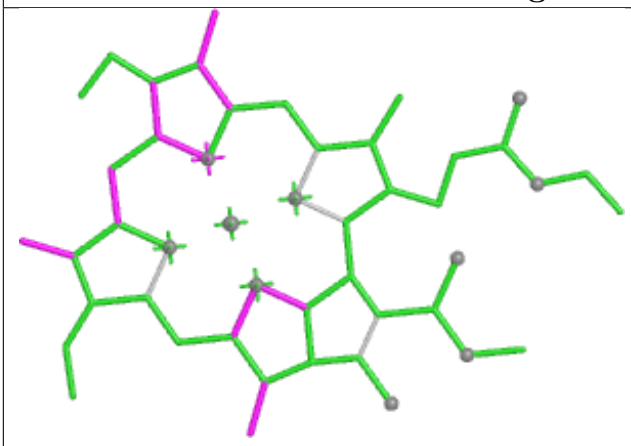
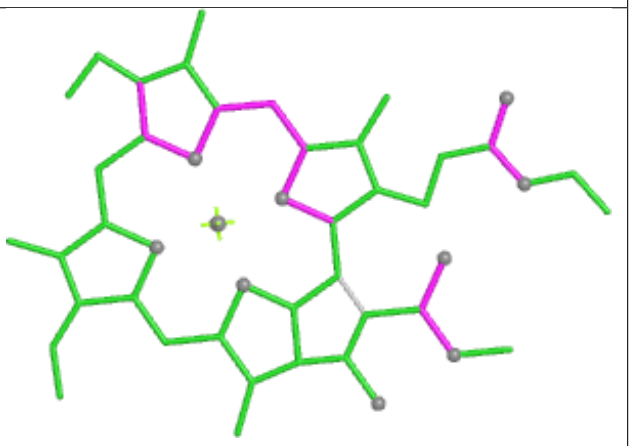
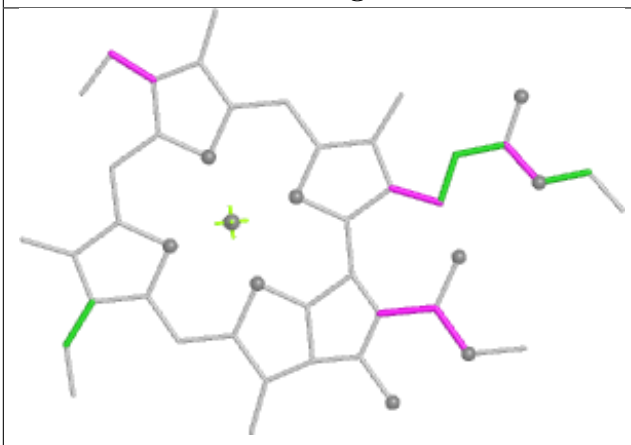
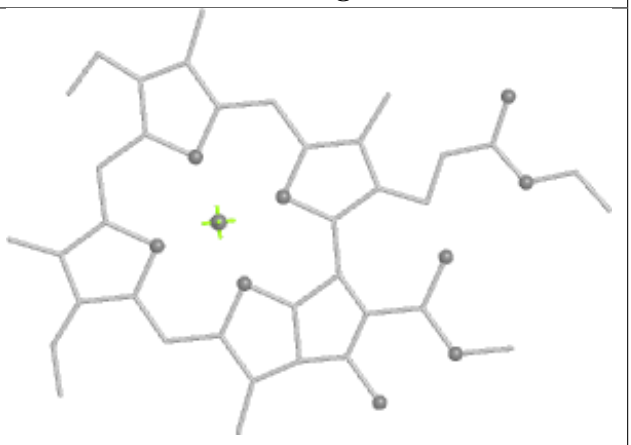


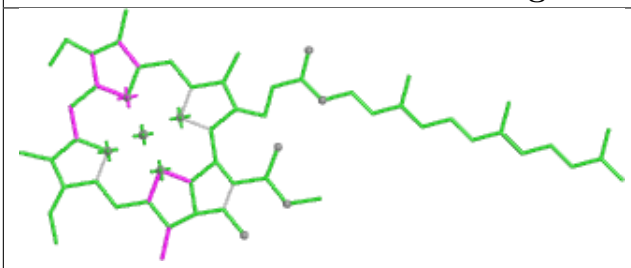
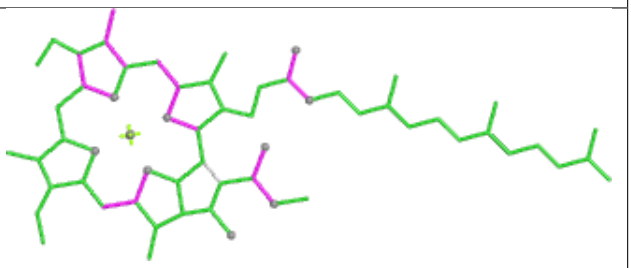
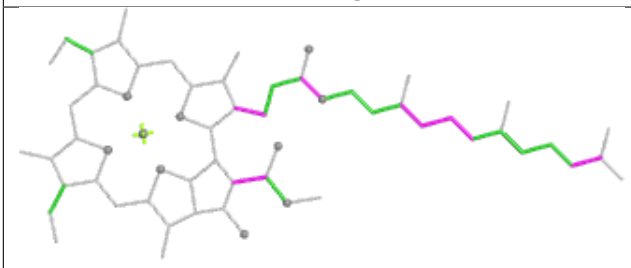
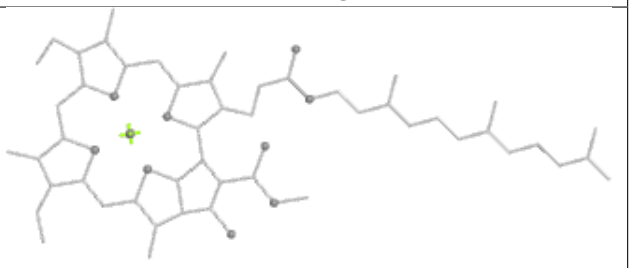
Rings

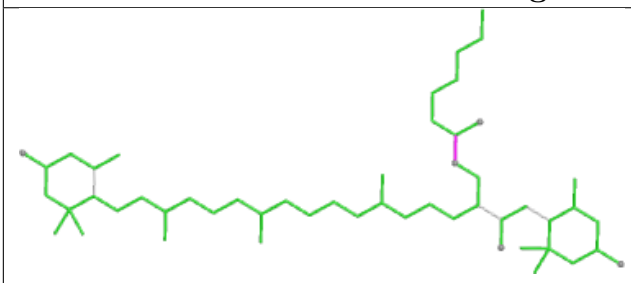
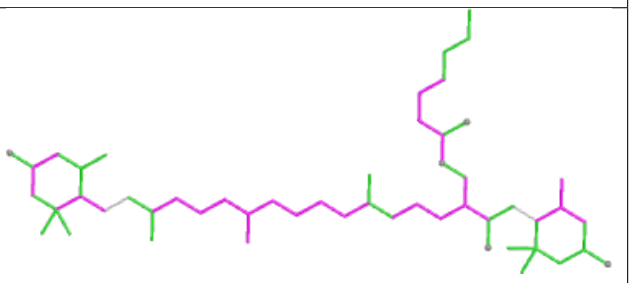
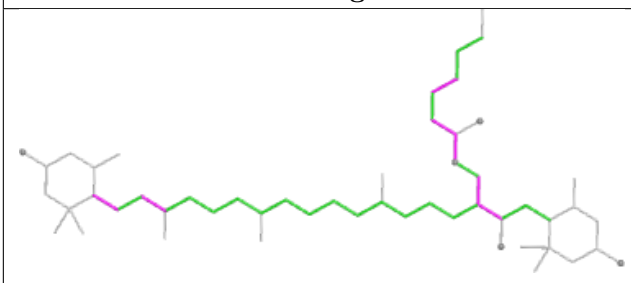
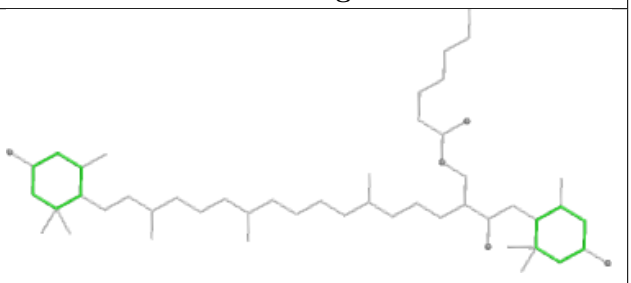
Ligand CLA A 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT 7 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

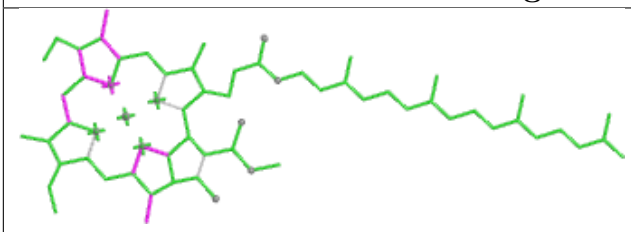
Ligand CLA 2 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

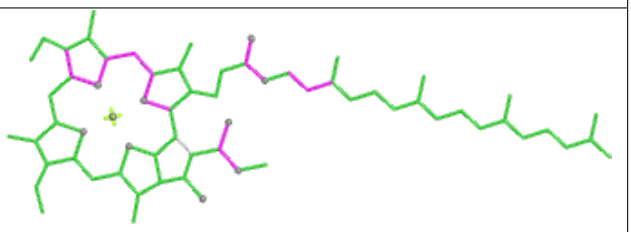
Ligand CLA 0 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 0UR 0 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

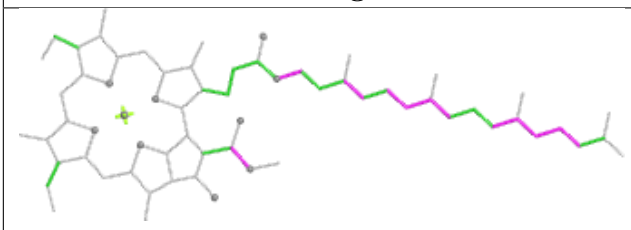
Ligand CLA A 853



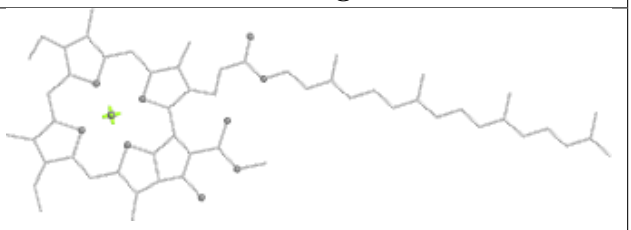
Bond lengths



Bond angles

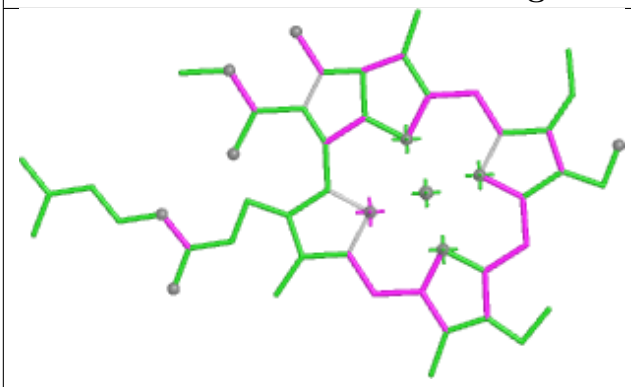


Torsions

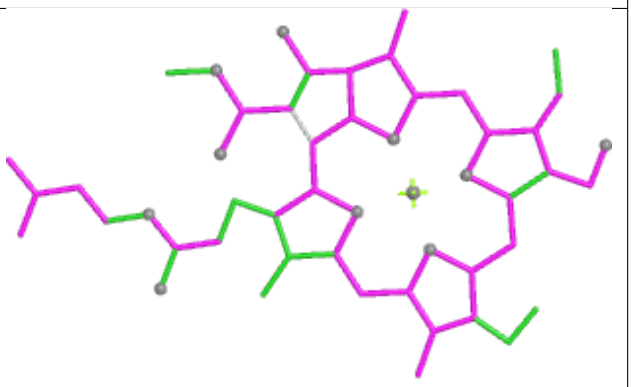


Rings

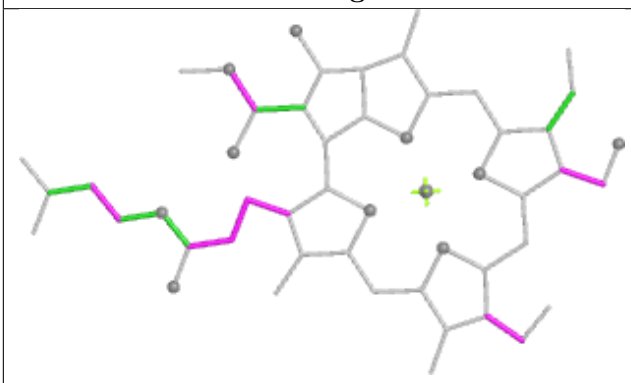
Ligand CHL 6 307



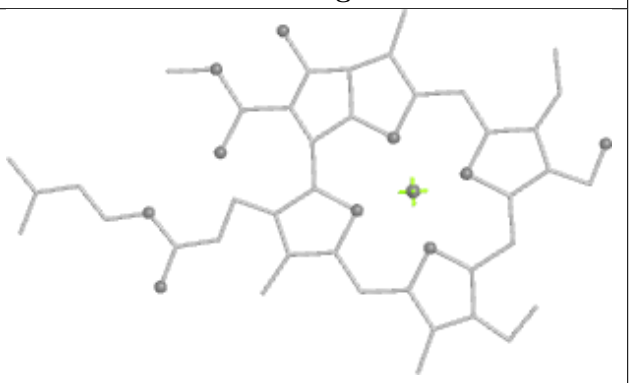
Bond lengths



Bond angles

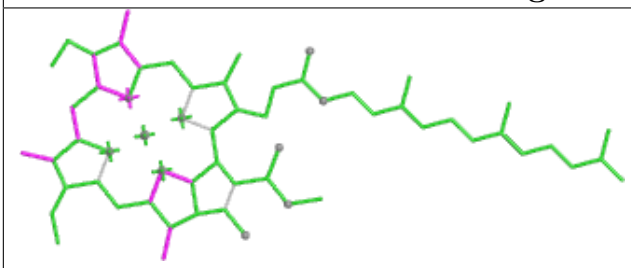


Torsions

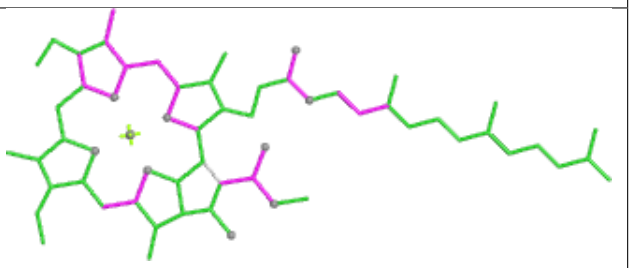


Rings

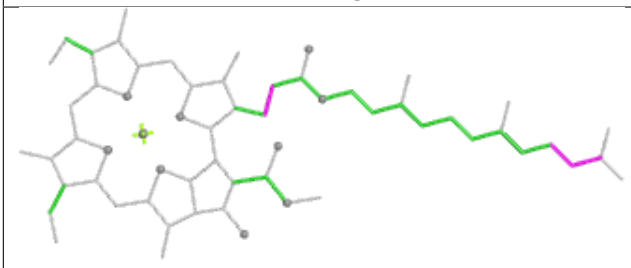
Ligand CLA 2 309



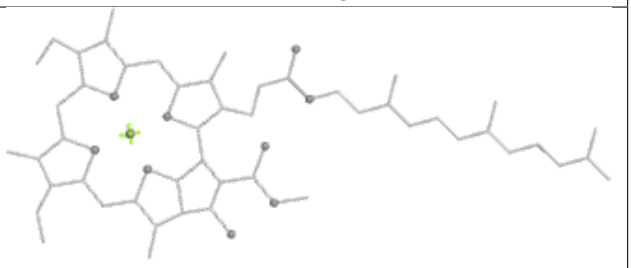
Bond lengths



Bond angles

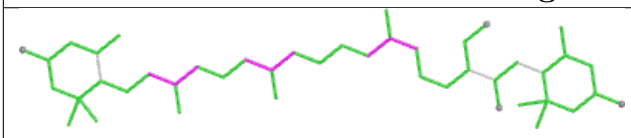


Torsions

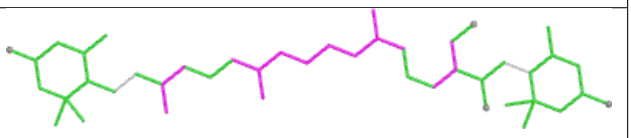


Rings

Ligand 0IE a 522



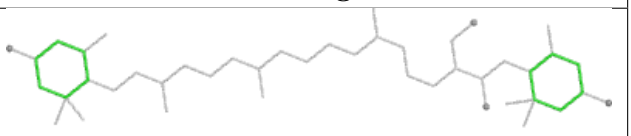
Bond lengths



Bond angles

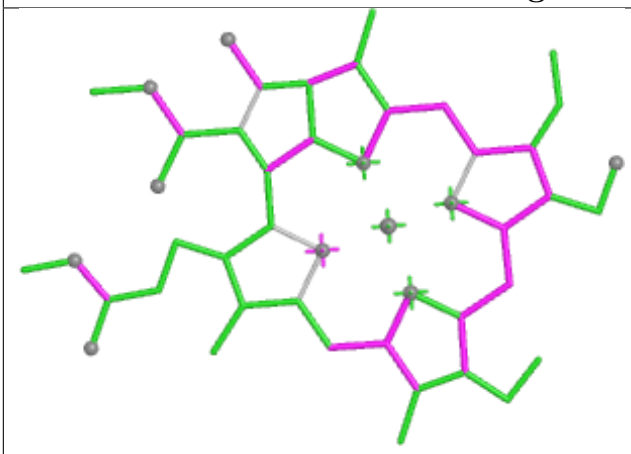


Torsions

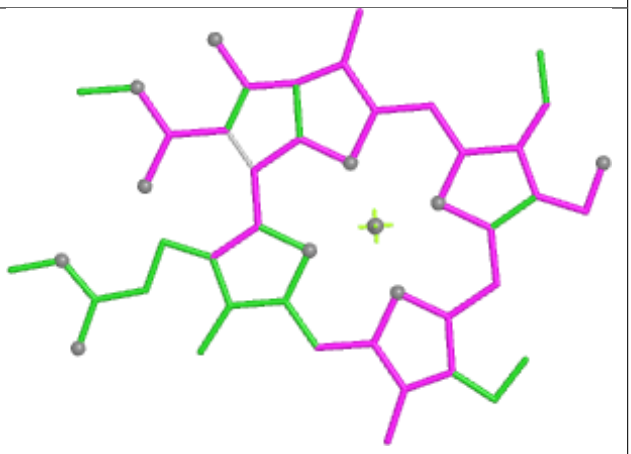


Rings

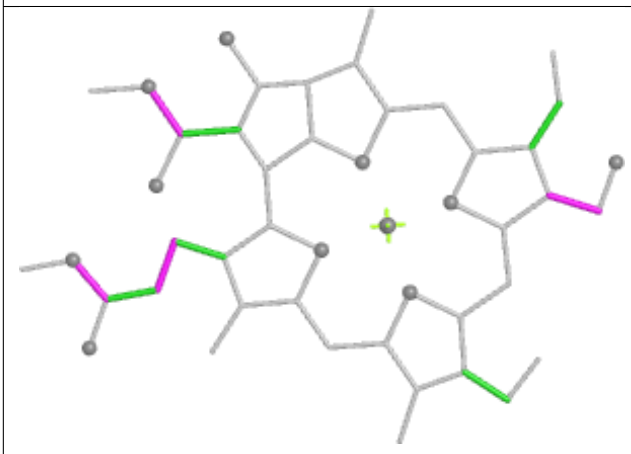
Ligand CHL 7 313



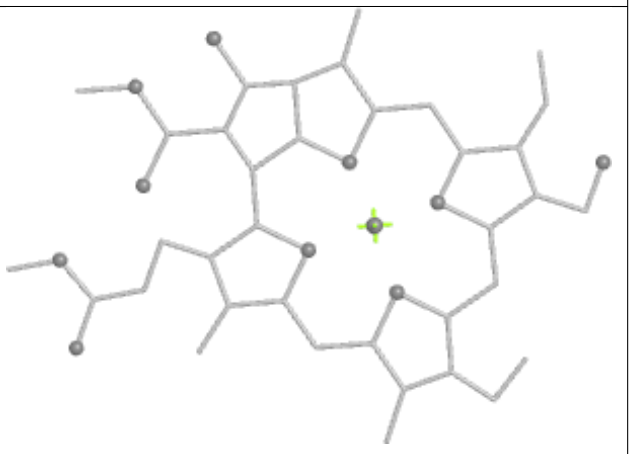
Bond lengths



Bond angles

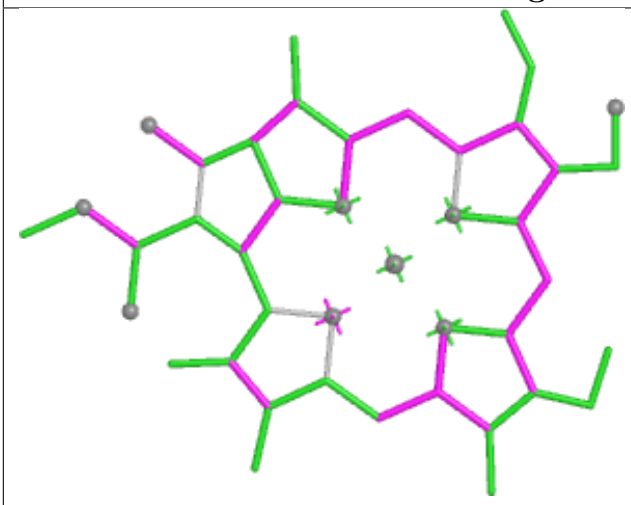


Torsions

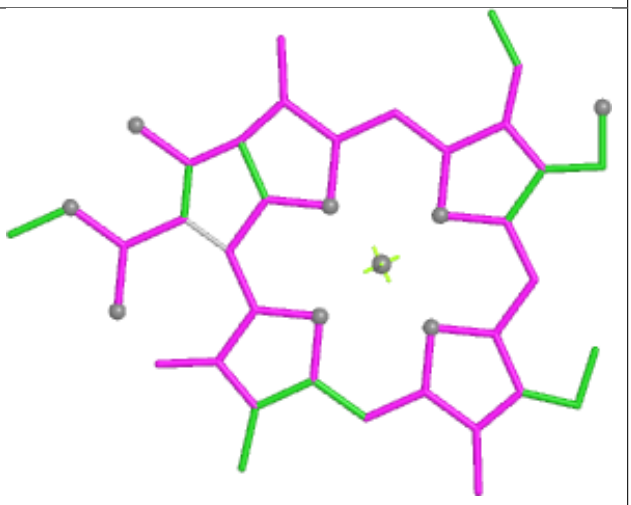


Rings

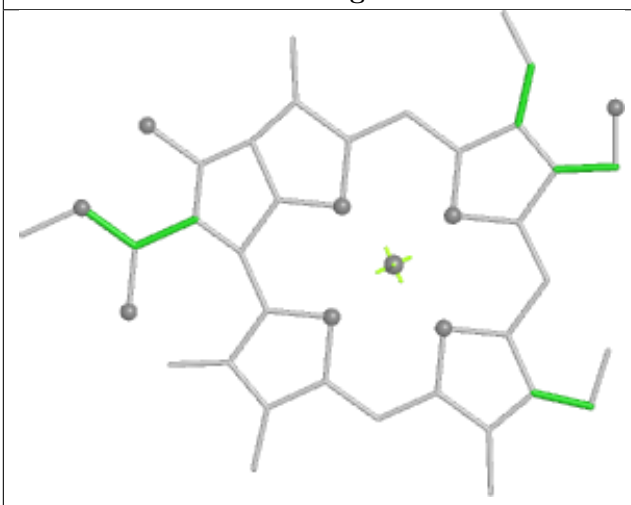
Ligand CHL a 614



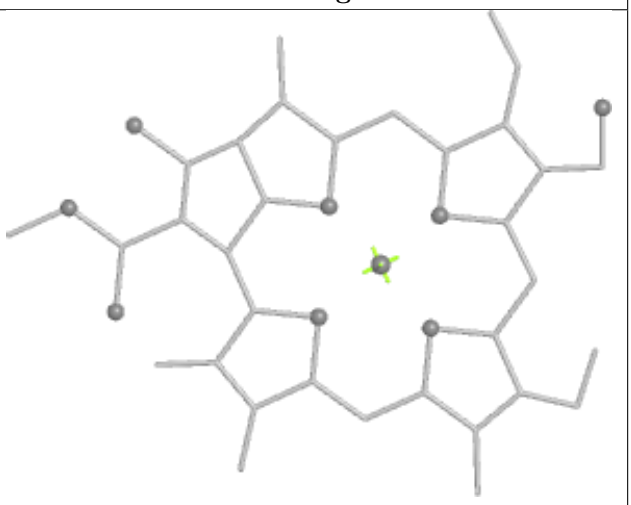
Bond lengths



Bond angles

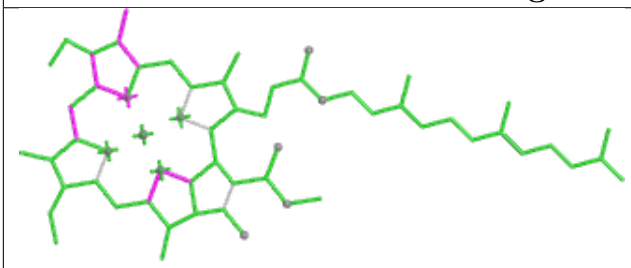


Torsions

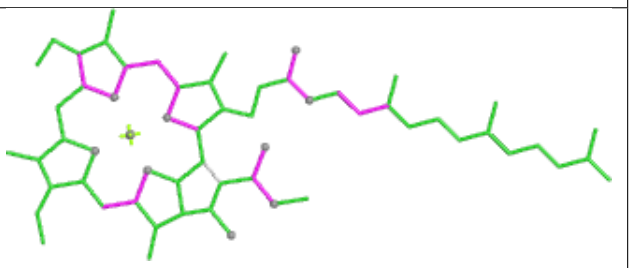


Rings

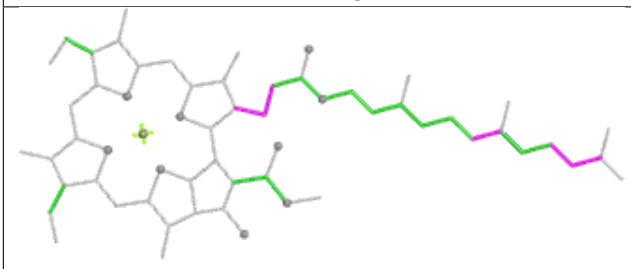
Ligand CLA 4 309



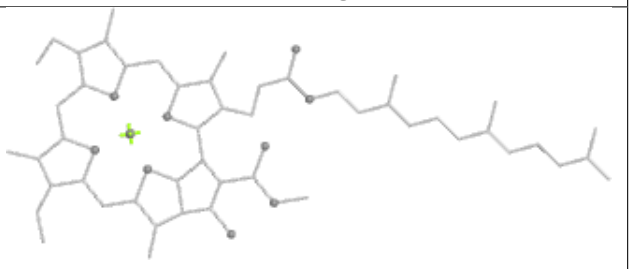
Bond lengths



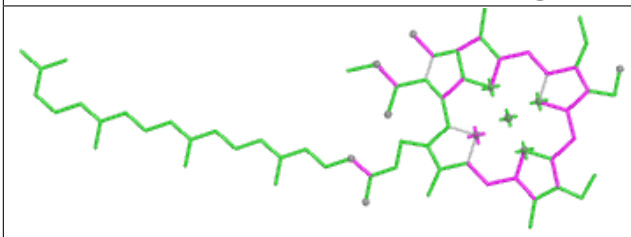
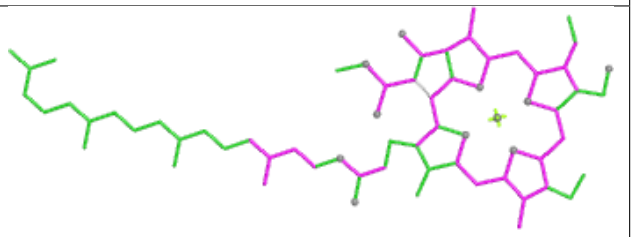
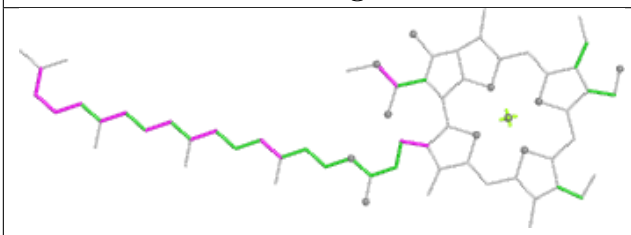
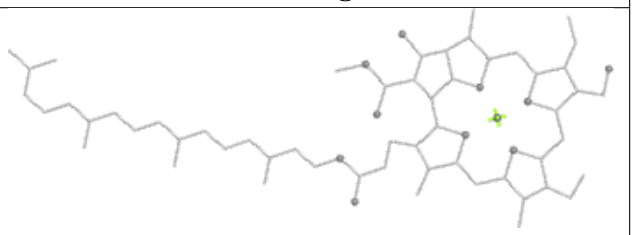
Bond angles

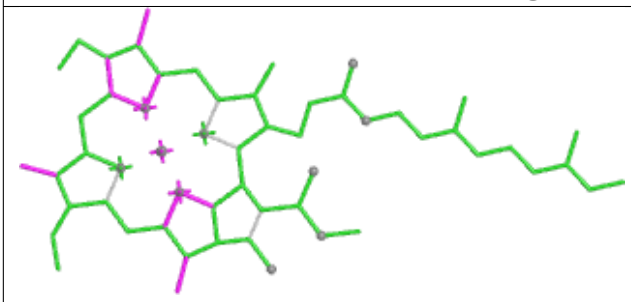
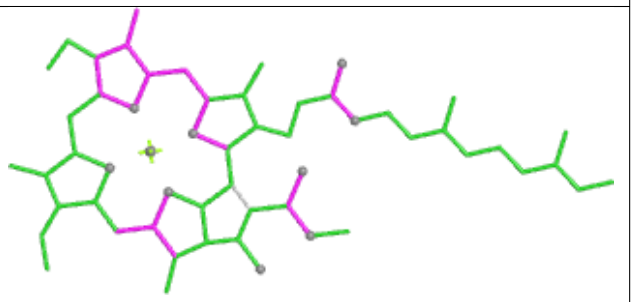
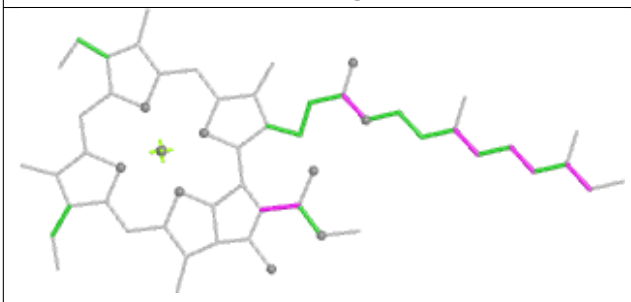
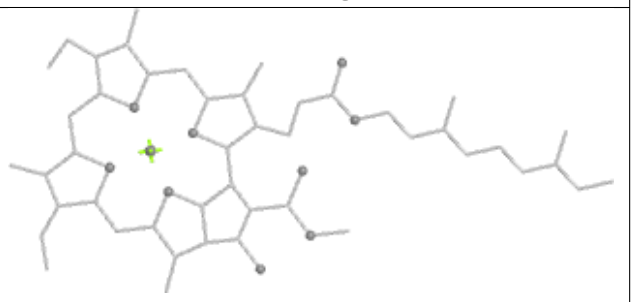


Torsions

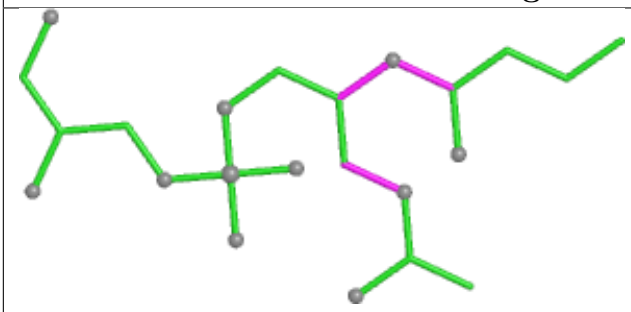


Rings

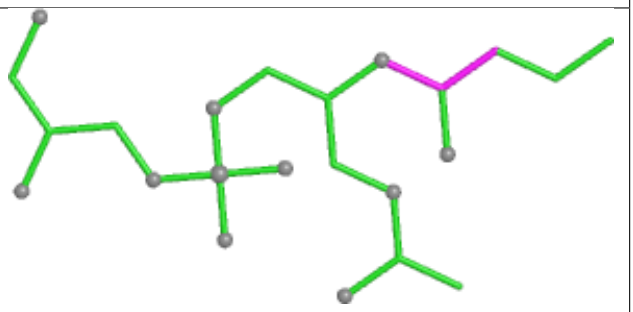
Ligand CHL f 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

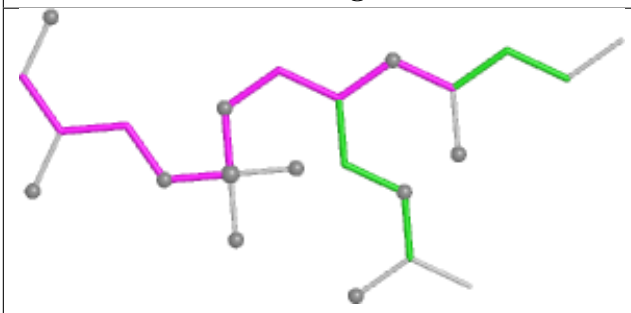
Ligand LHG B 852



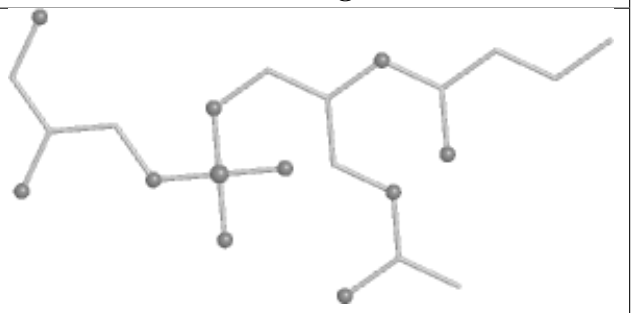
Bond lengths



Bond angles

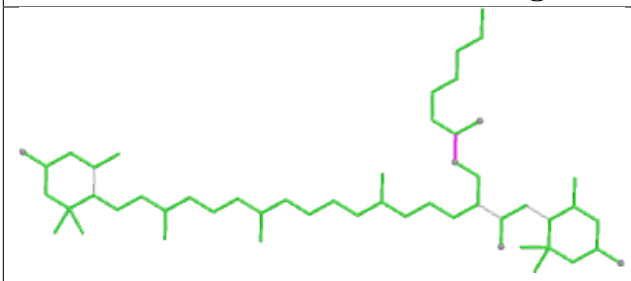


Torsions

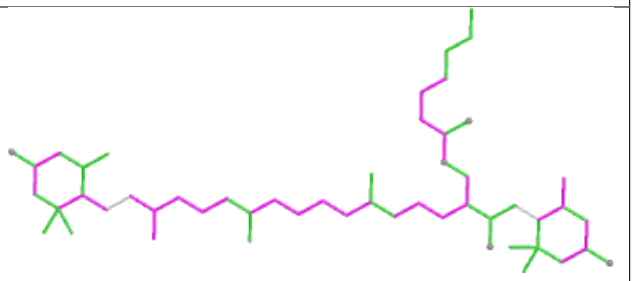


Rings

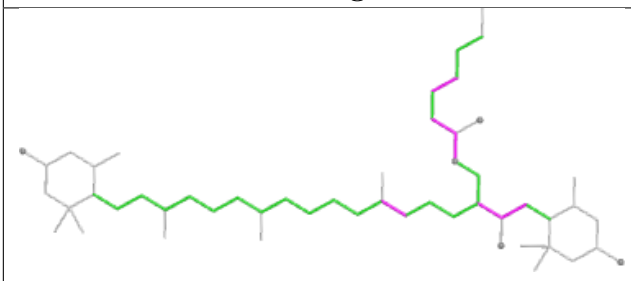
Ligand 0UR b 520



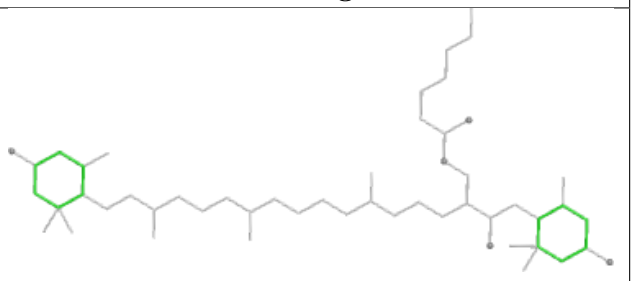
Bond lengths



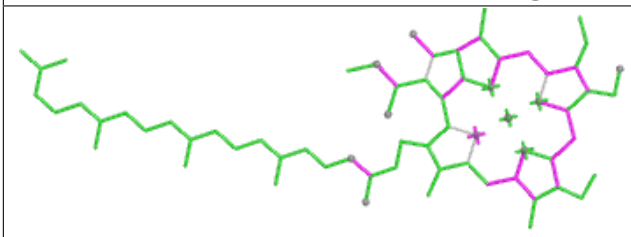
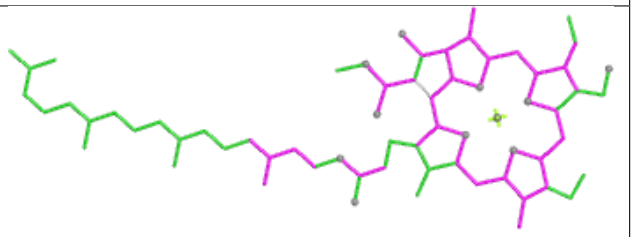
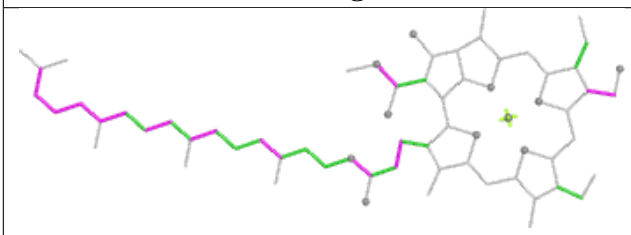
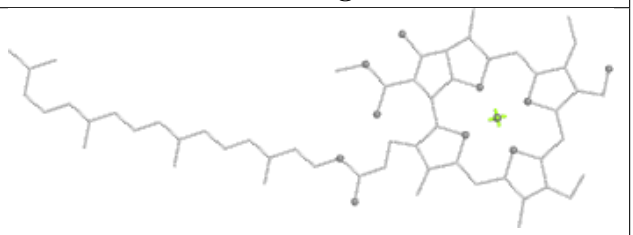
Bond angles

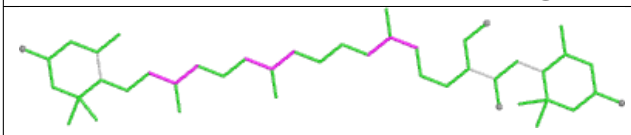
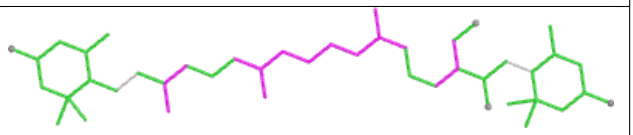
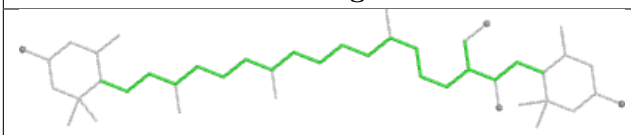
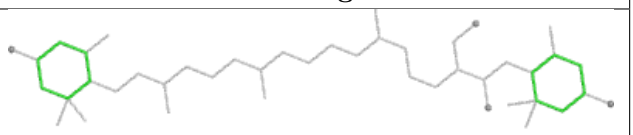


Torsions

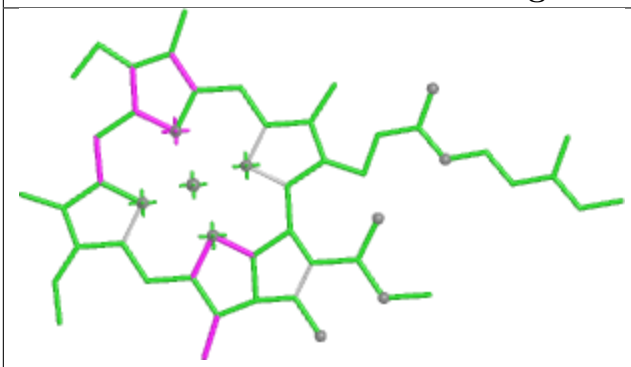


Rings

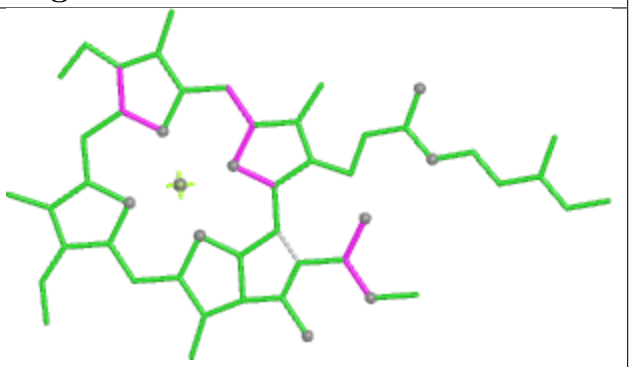
Ligand CHL b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 0IE h 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

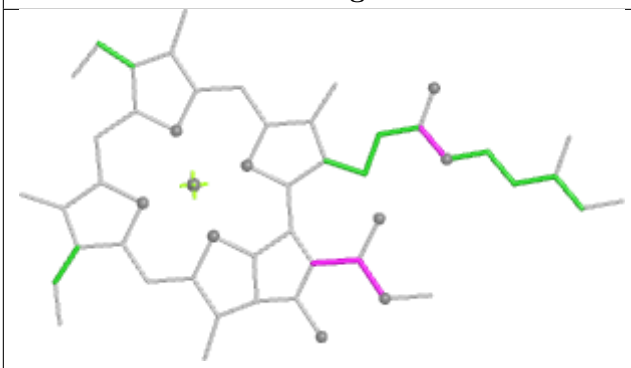
Ligand CLA g 603



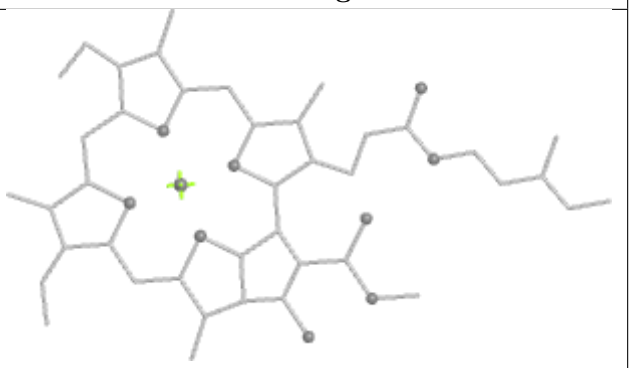
Bond lengths



Bond angles

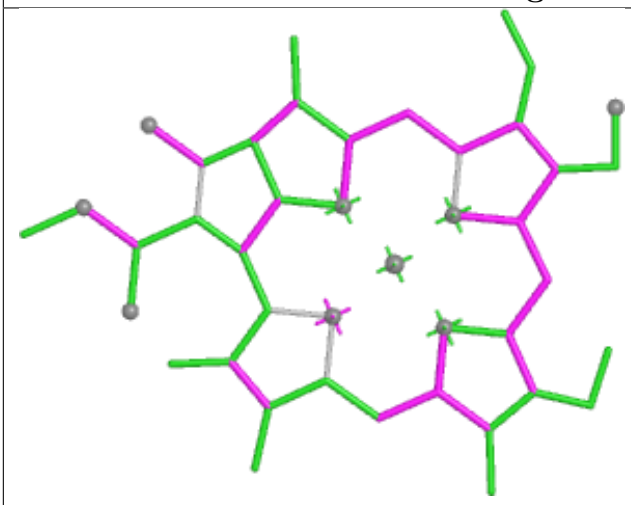


Torsions

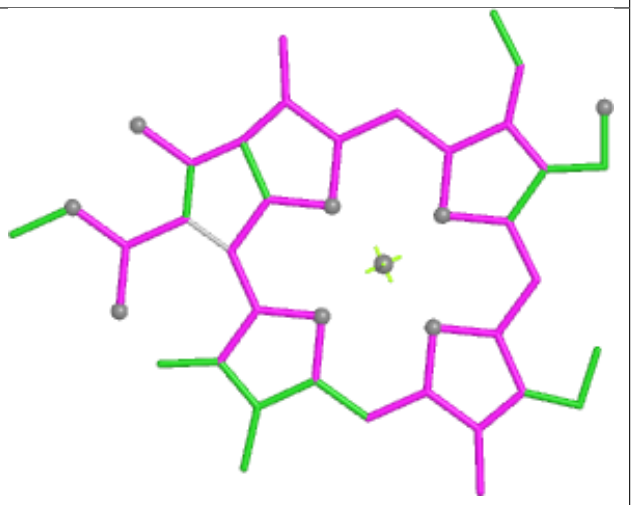


Rings

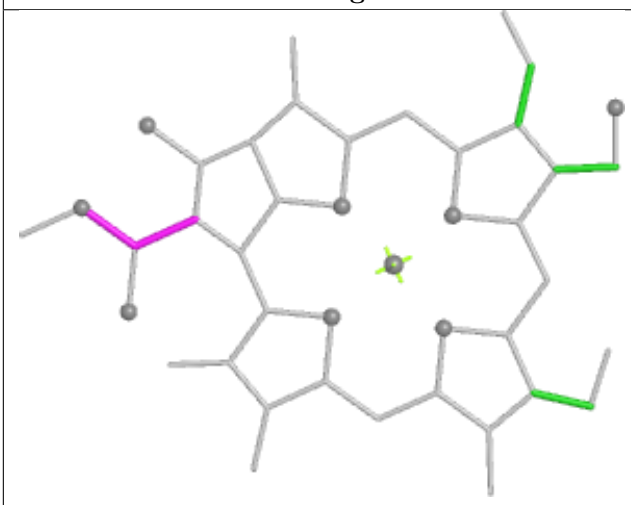
Ligand CHL h 614



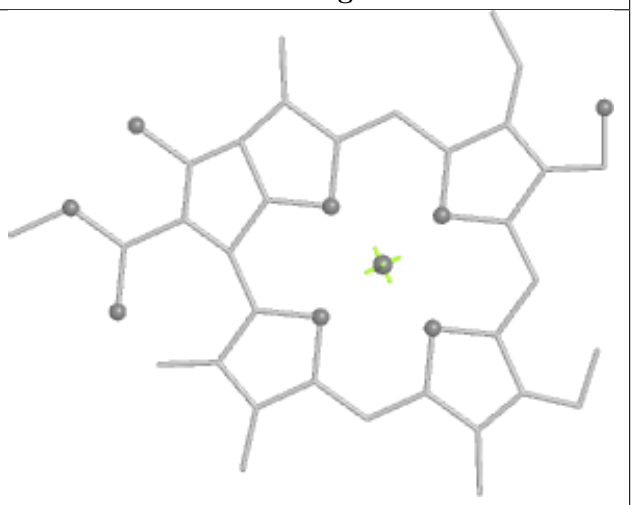
Bond lengths



Bond angles

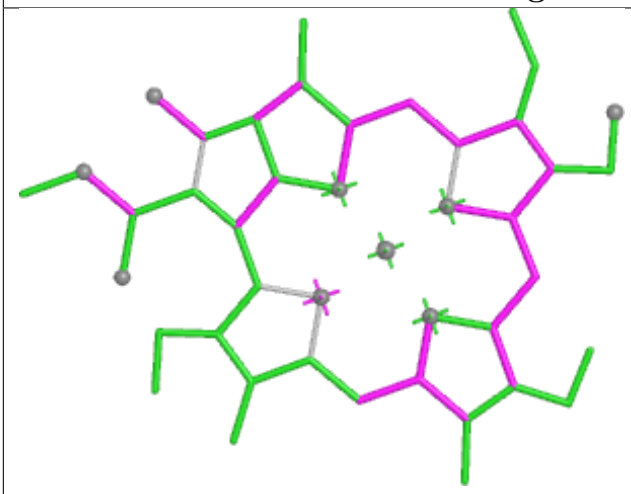


Torsions

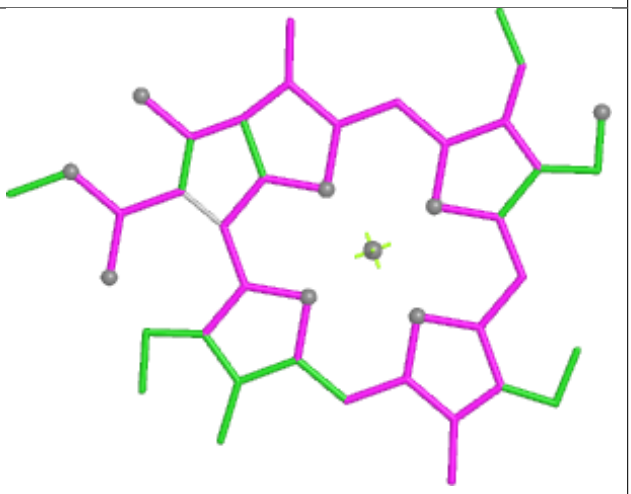


Rings

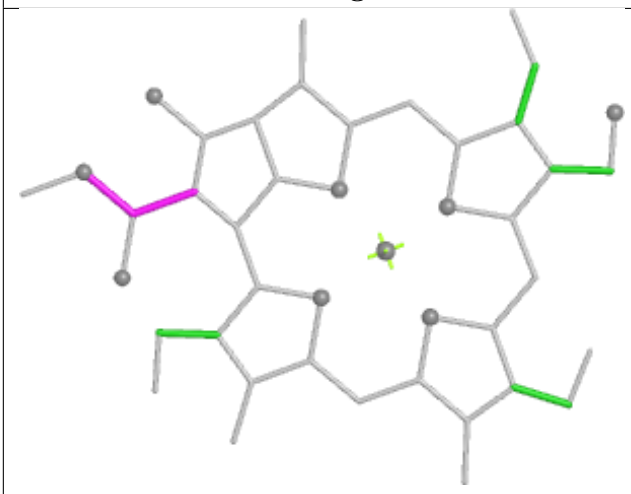
Ligand CHL 8 315



Bond lengths



Bond angles

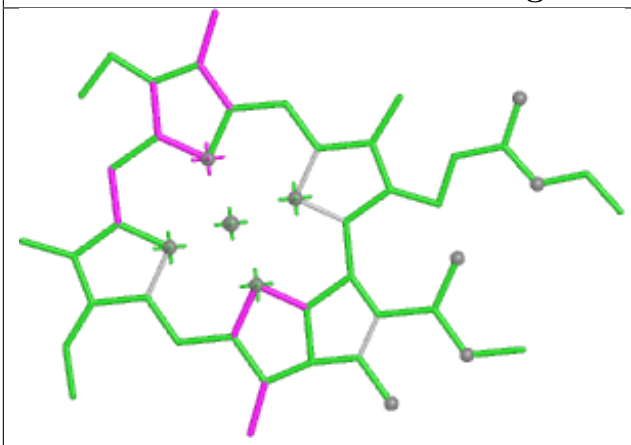


Torsions

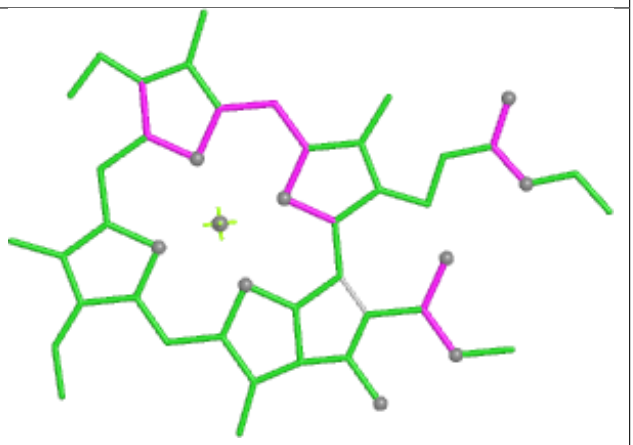


Rings

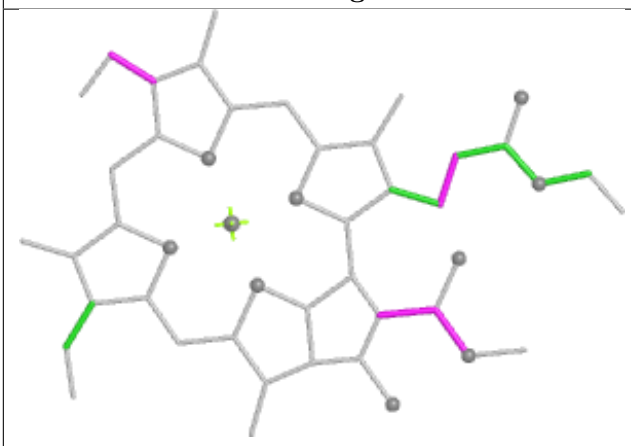
Ligand CLA L 207



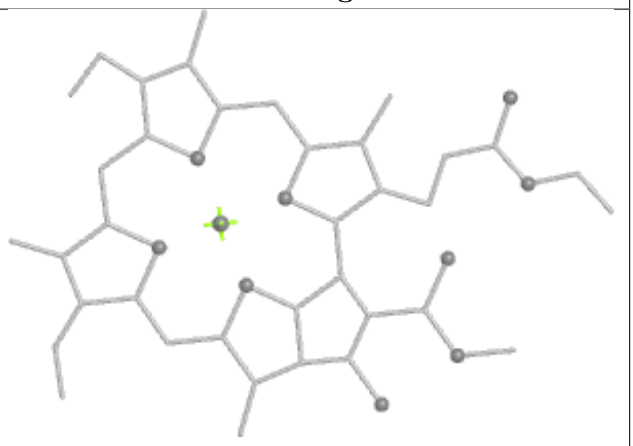
Bond lengths



Bond angles

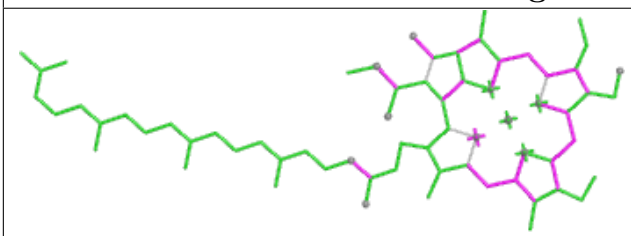


Torsions

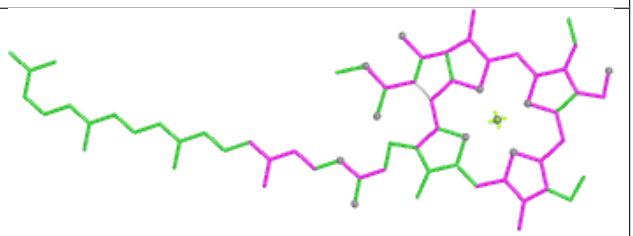


Rings

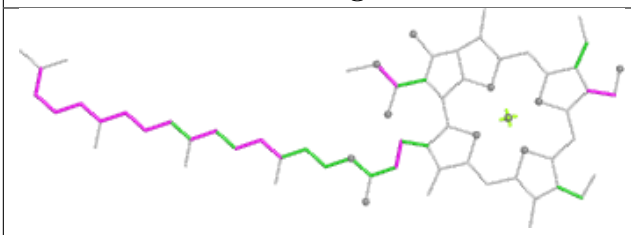
Ligand CHL c 608



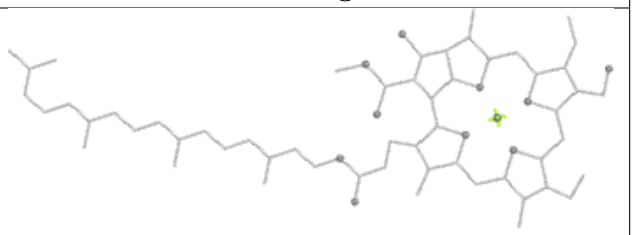
Bond lengths



Bond angles

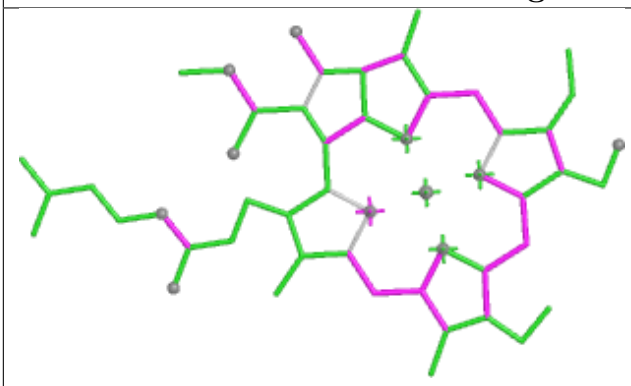


Torsions

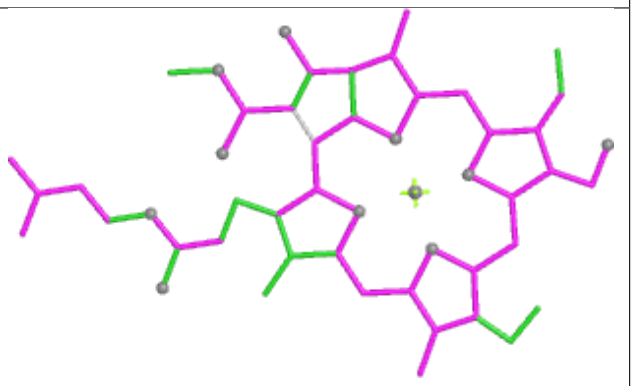


Rings

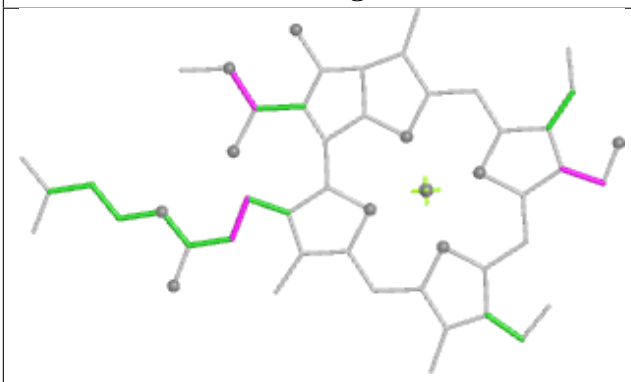
Ligand CHL 4 313



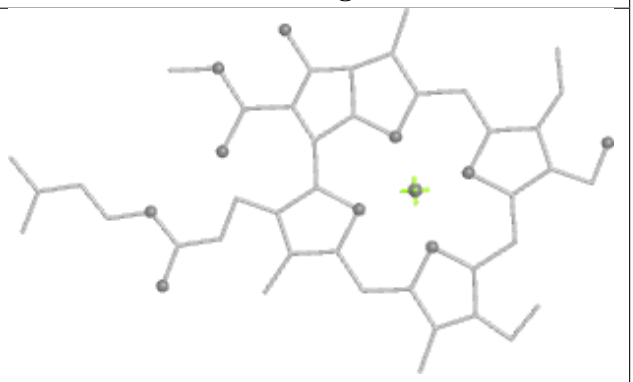
Bond lengths



Bond angles

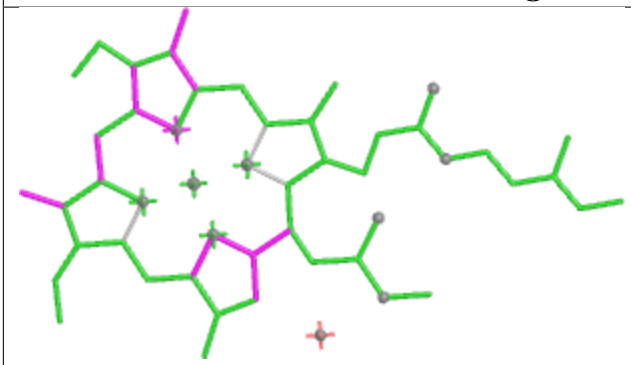


Torsions

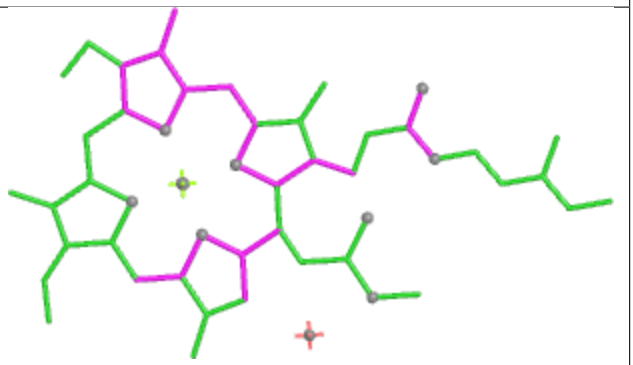


Rings

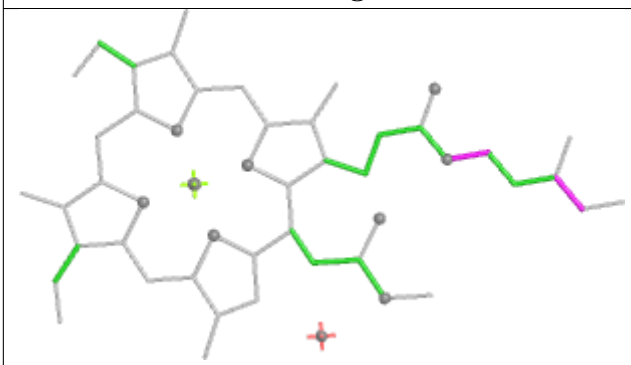
Ligand CLA B 826



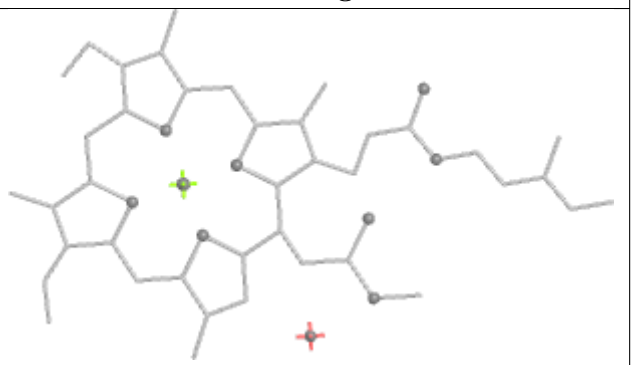
Bond lengths



Bond angles

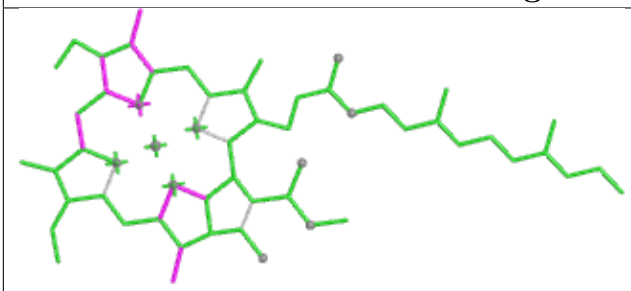


Torsions

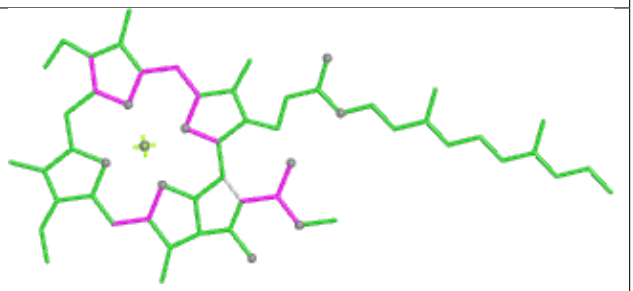


Rings

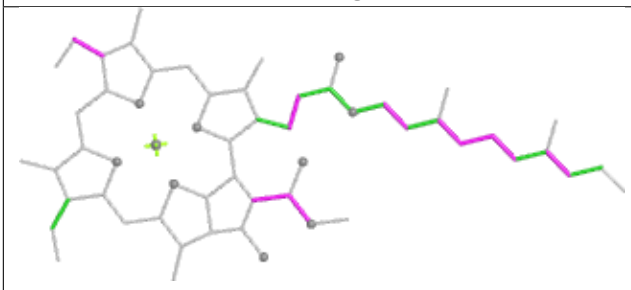
Ligand CLA A 835



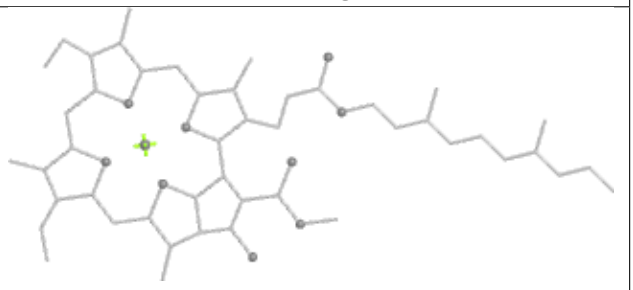
Bond lengths



Bond angles

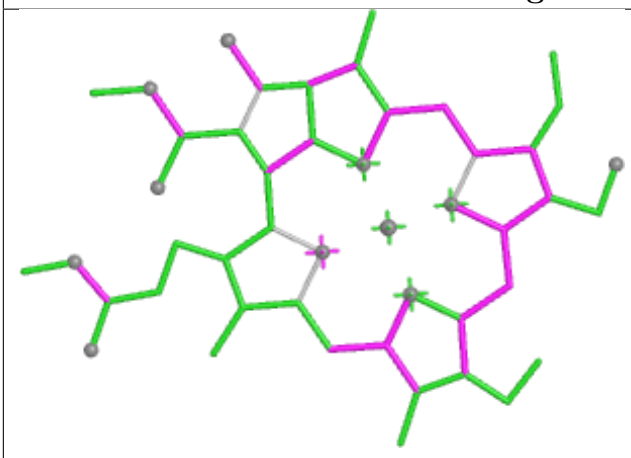


Torsions

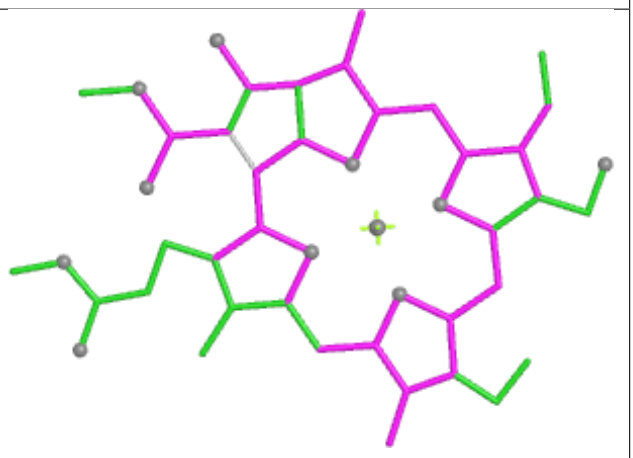


Rings

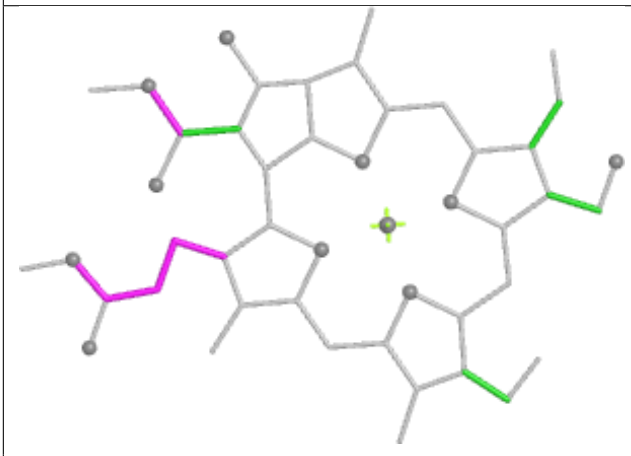
Ligand CHL d 607



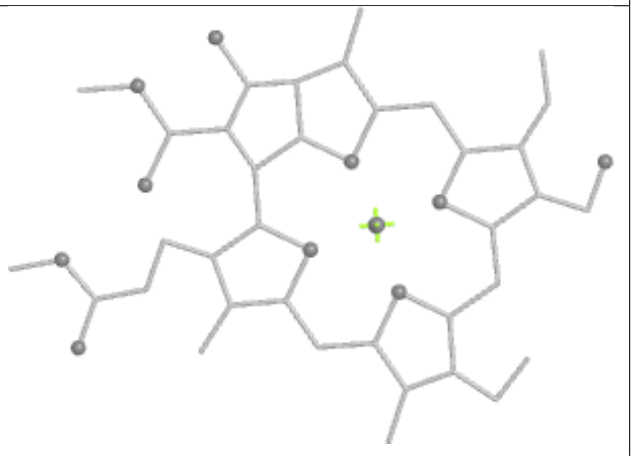
Bond lengths



Bond angles

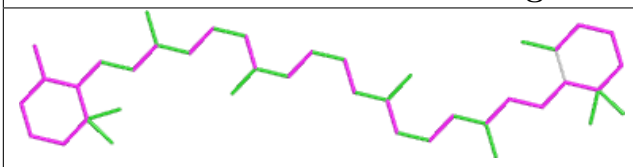


Torsions

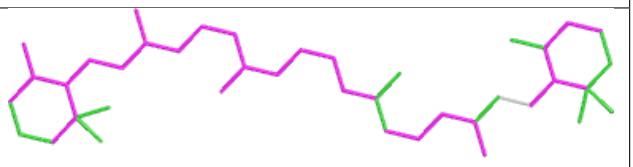


Rings

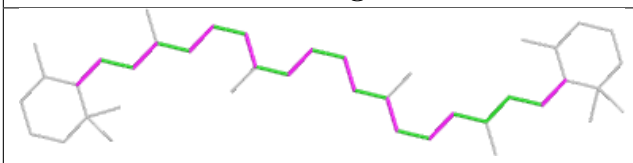
Ligand 8CT K 107



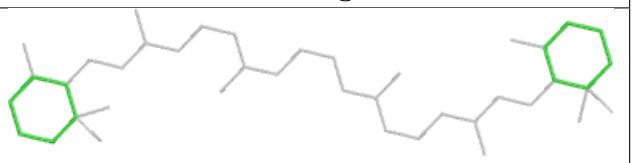
Bond lengths



Bond angles

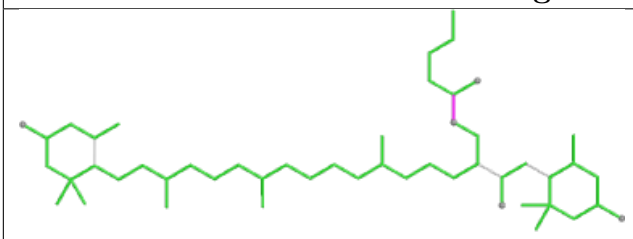


Torsions

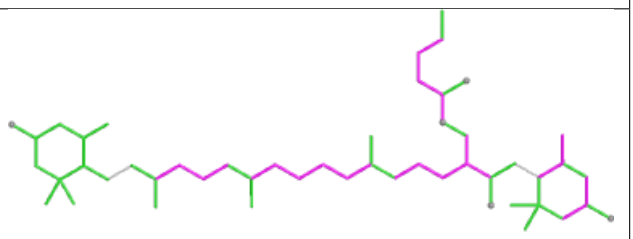


Rings

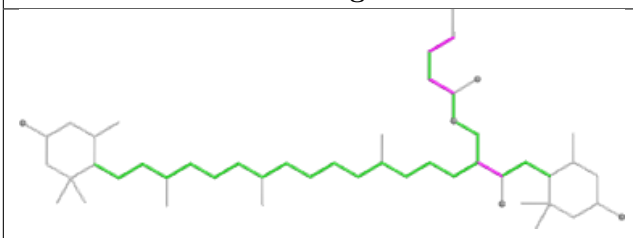
Ligand 0UR i 520



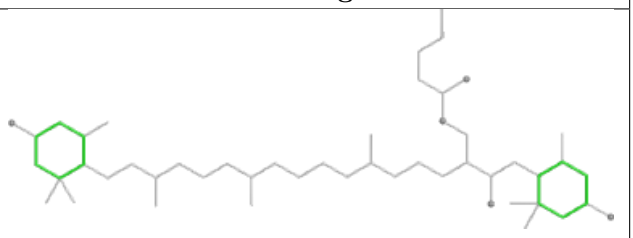
Bond lengths



Bond angles

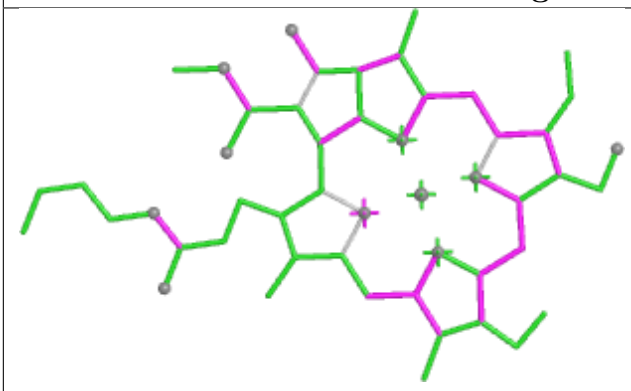


Torsions

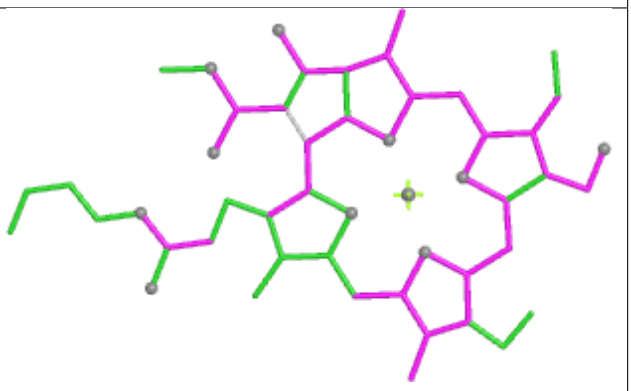


Rings

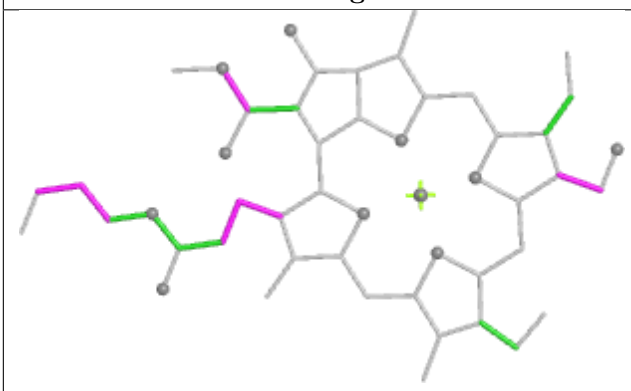
Ligand CHL i 608



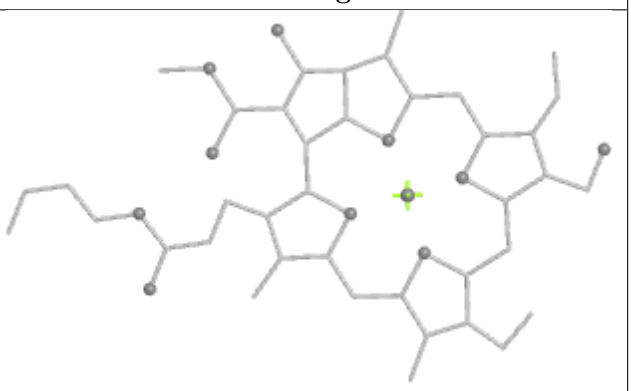
Bond lengths



Bond angles

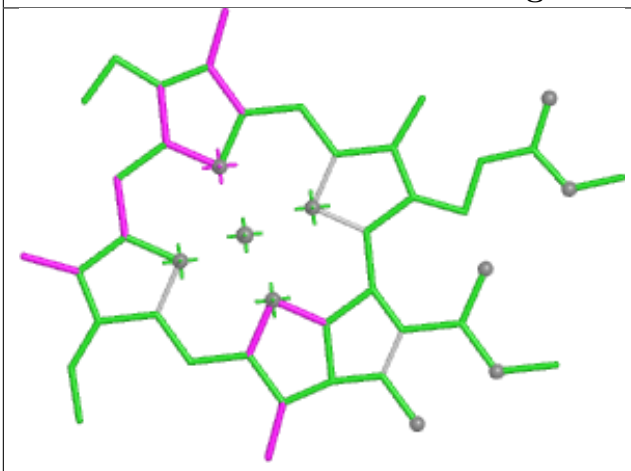


Torsions

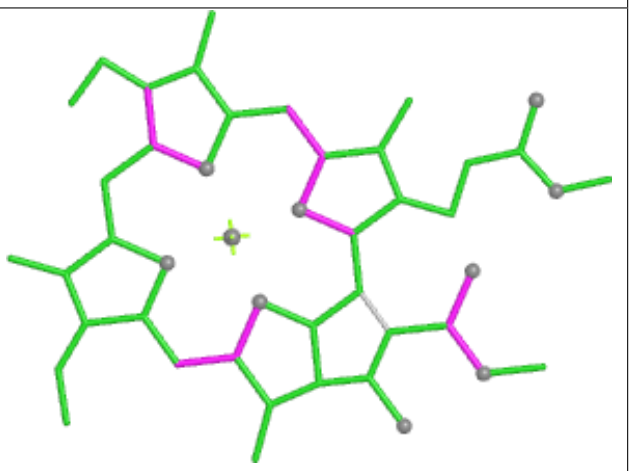


Rings

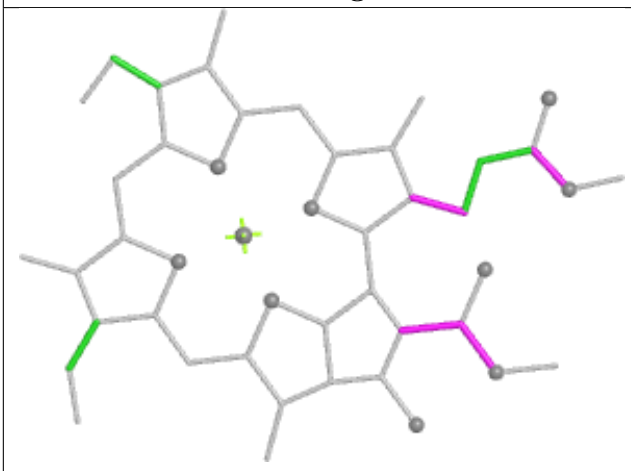
Ligand CLA L 204



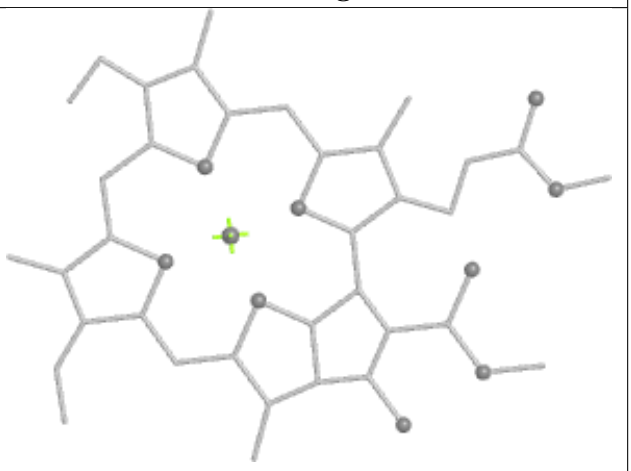
Bond lengths



Bond angles

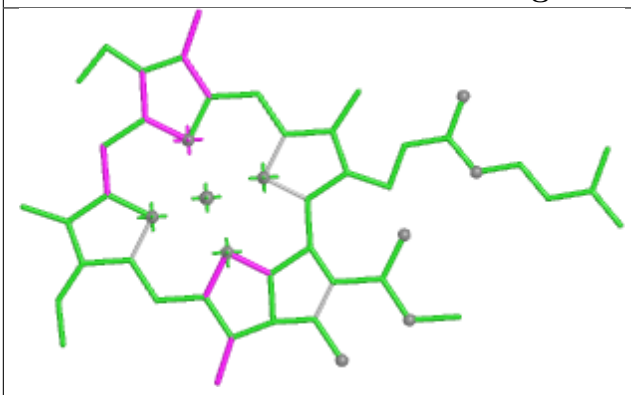


Torsions

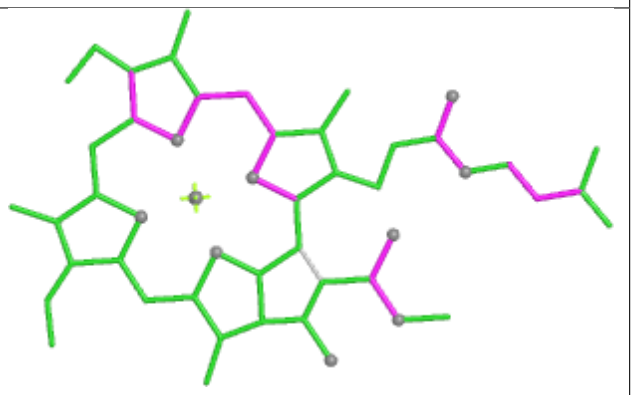


Rings

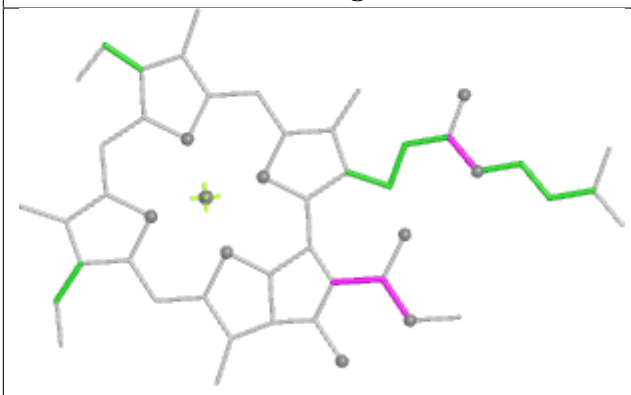
Ligand CLA f 604



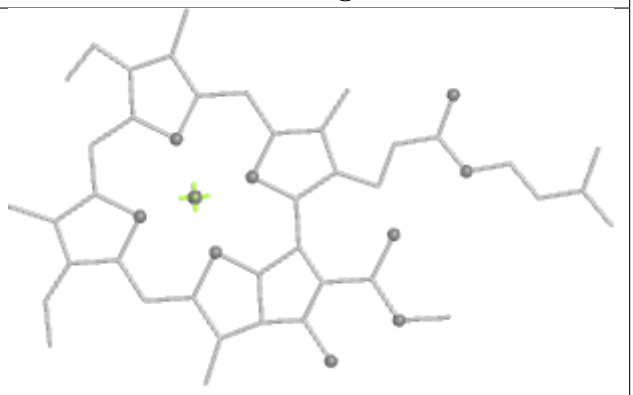
Bond lengths



Bond angles

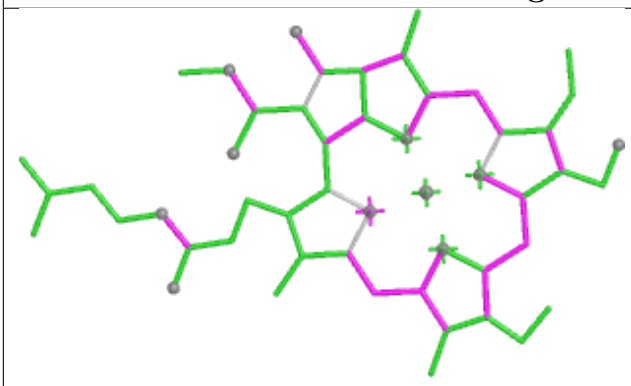


Torsions

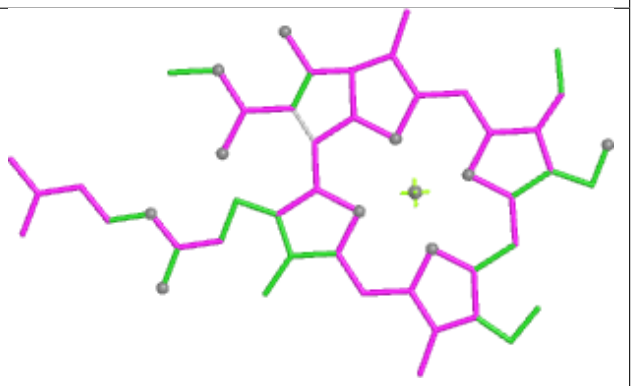


Rings

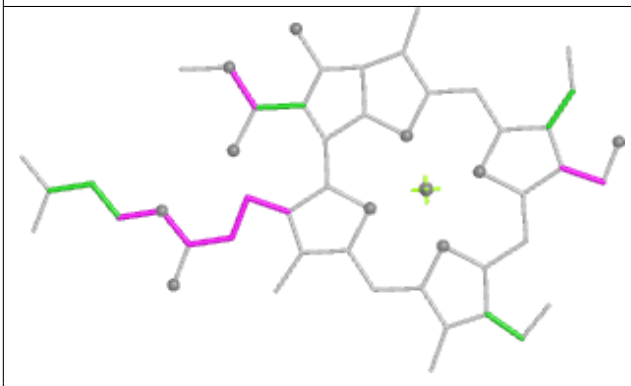
Ligand CHL 8 307



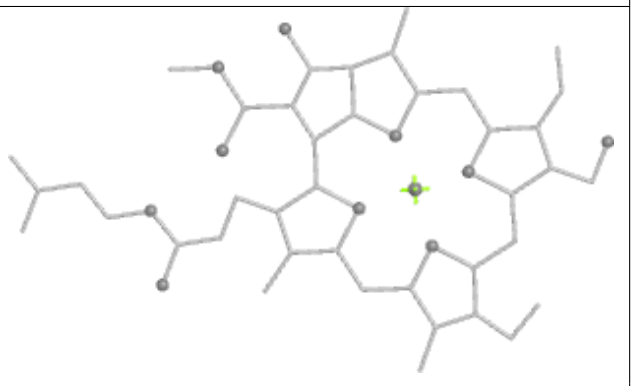
Bond lengths



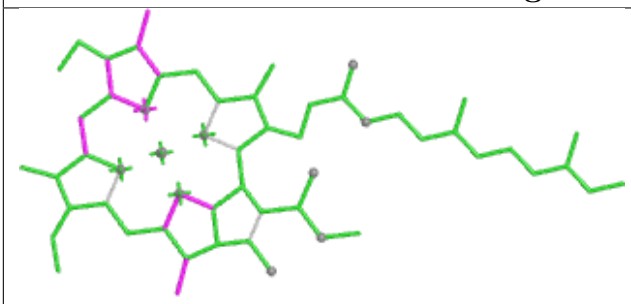
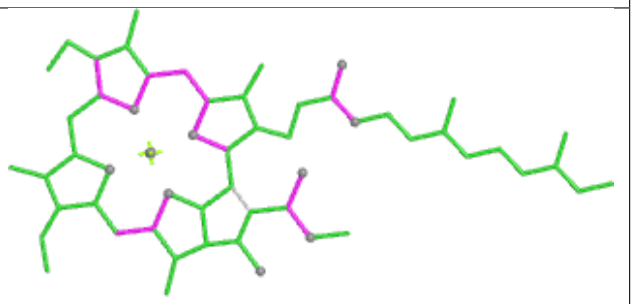
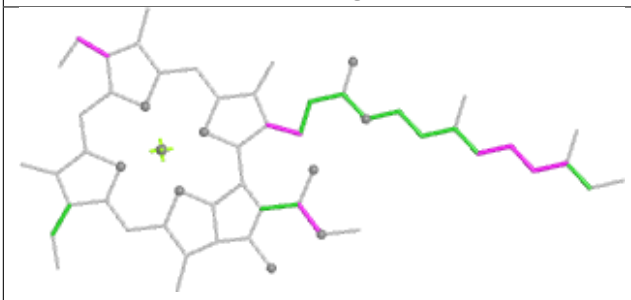
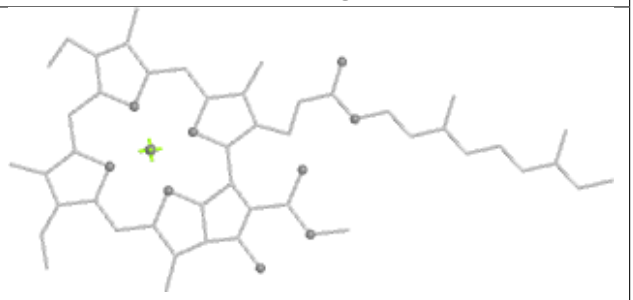
Bond angles

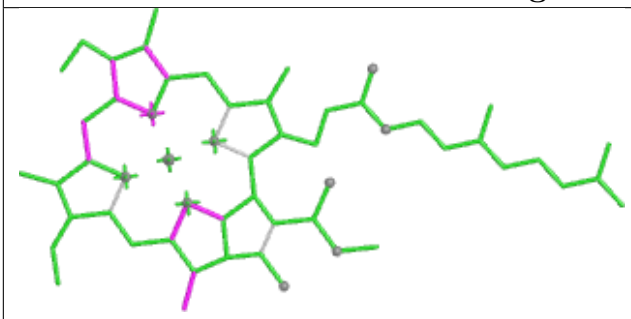
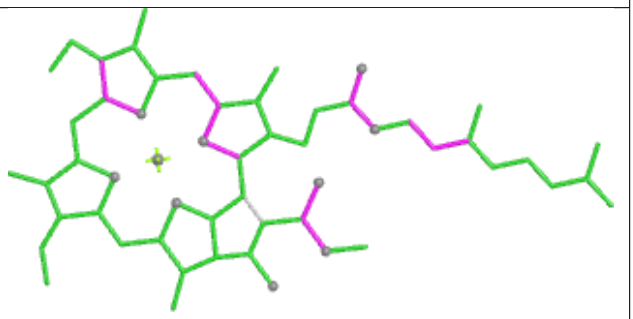
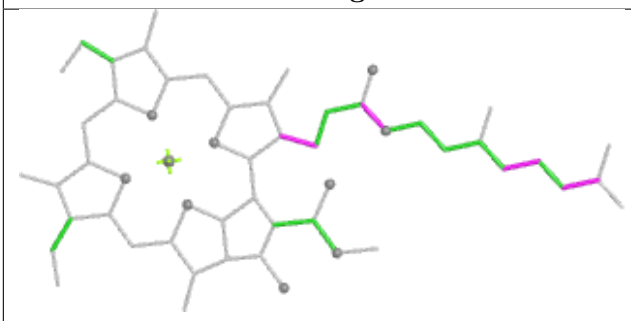
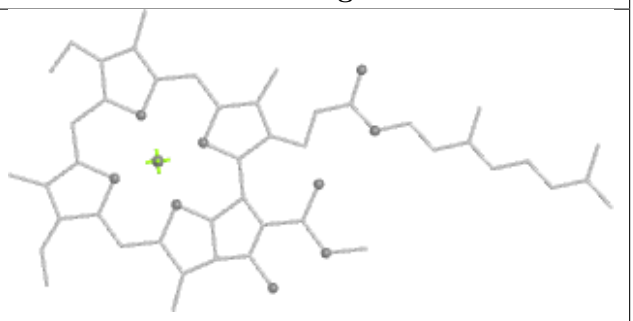


Torsions

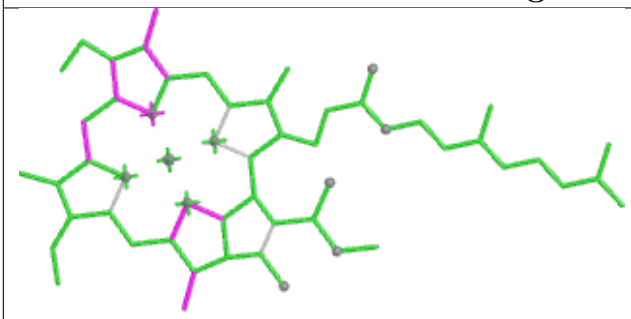


Rings

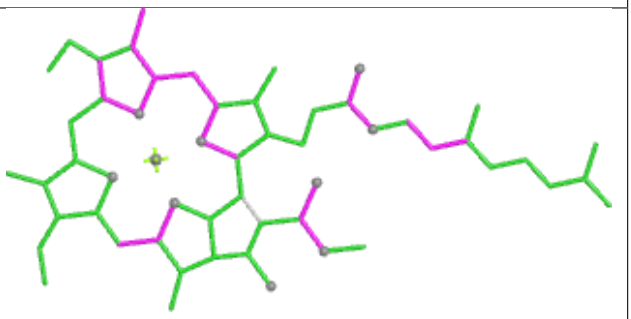
Ligand CLA B 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

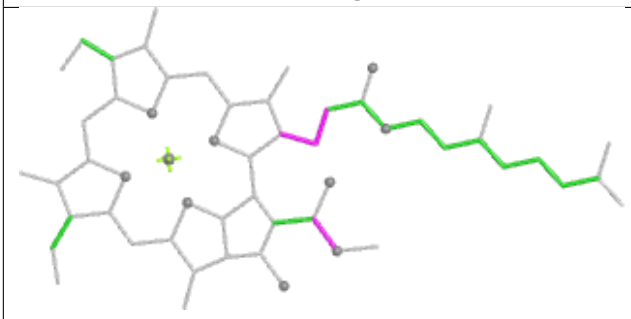
Ligand CLA b 610



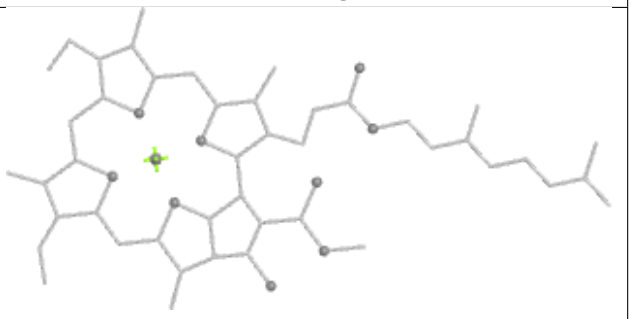
Bond lengths



Bond angles

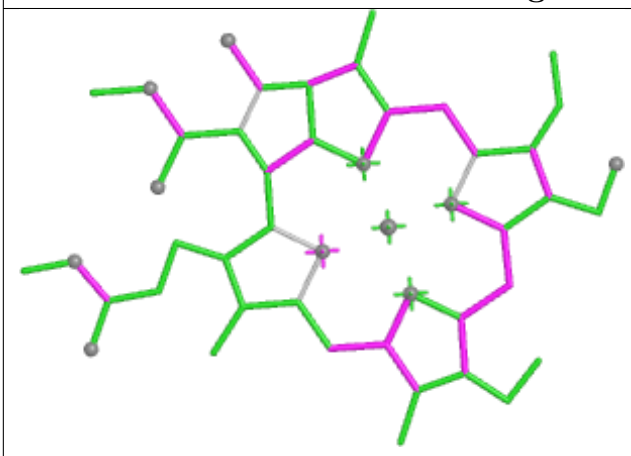


Torsions

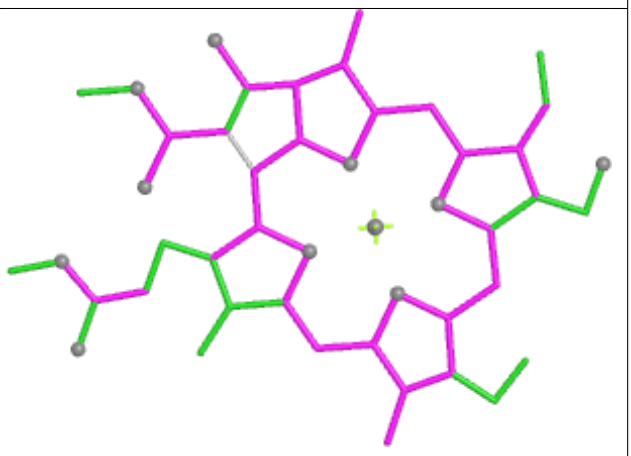


Rings

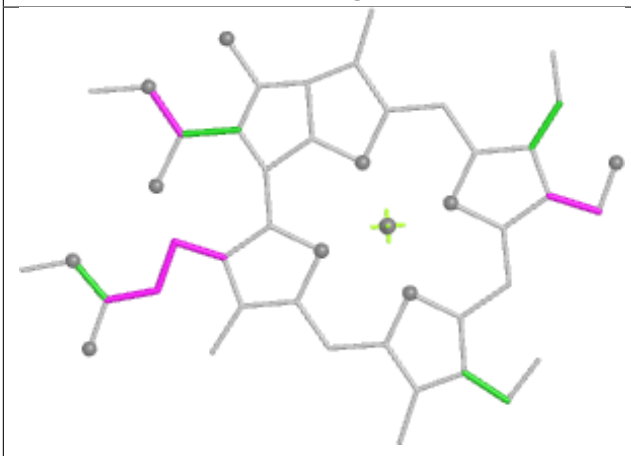
Ligand CHL 9 313



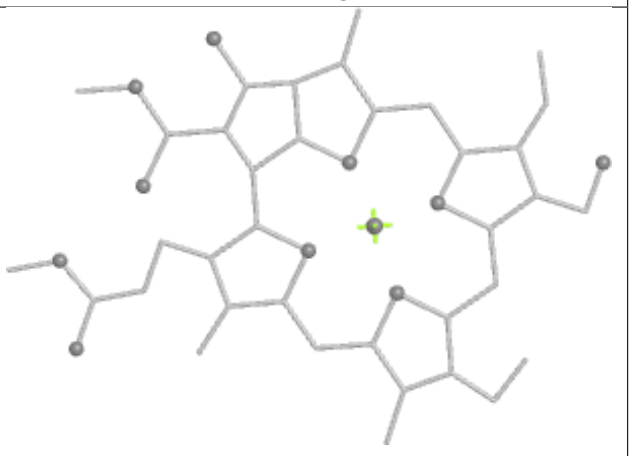
Bond lengths



Bond angles

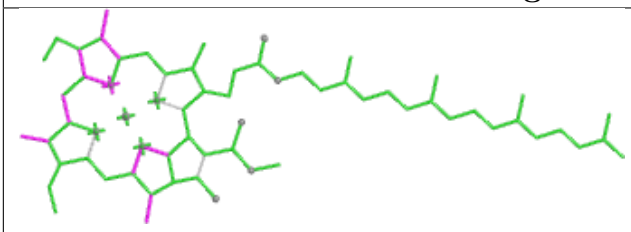


Torsions

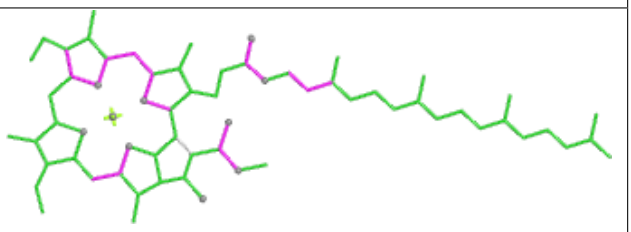


Rings

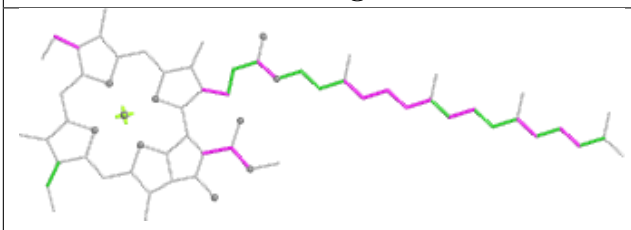
Ligand CLA A 806



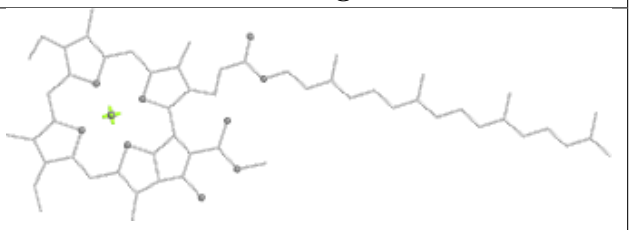
Bond lengths



Bond angles

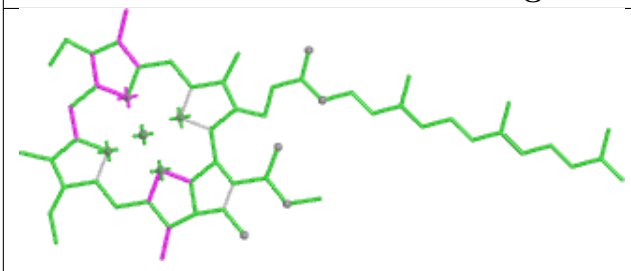


Torsions

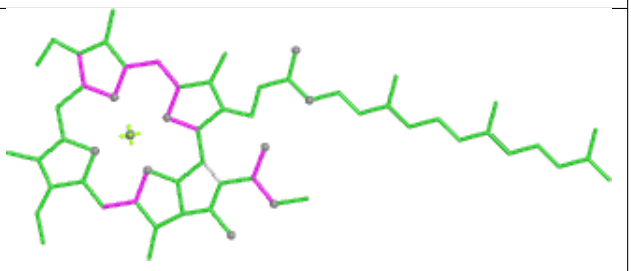


Rings

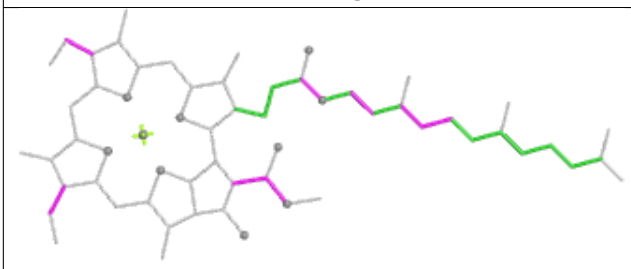
Ligand CLA B 822



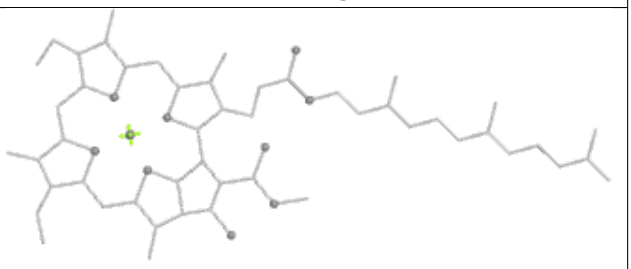
Bond lengths



Bond angles

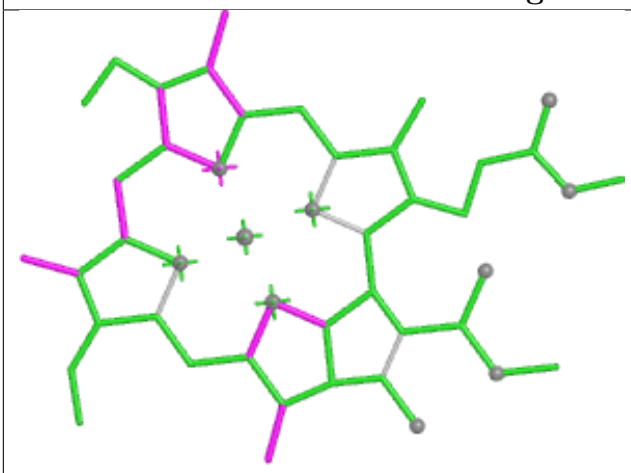


Torsions

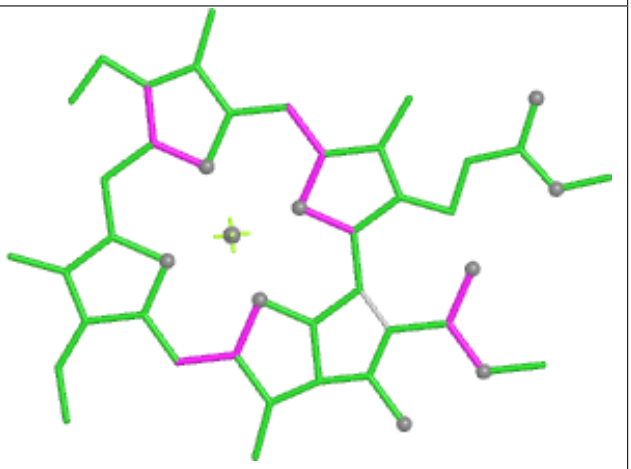


Rings

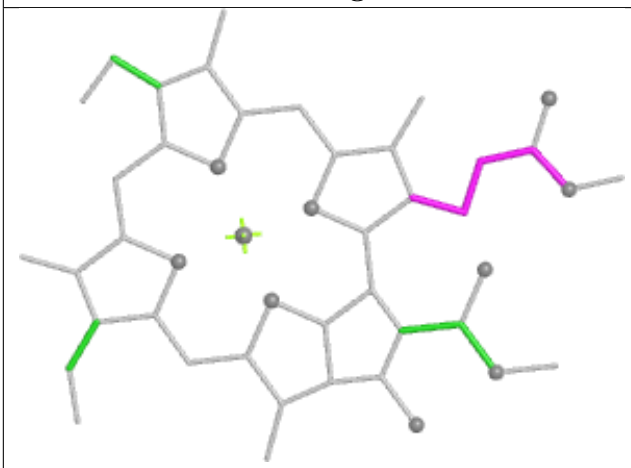
Ligand CLA L 202



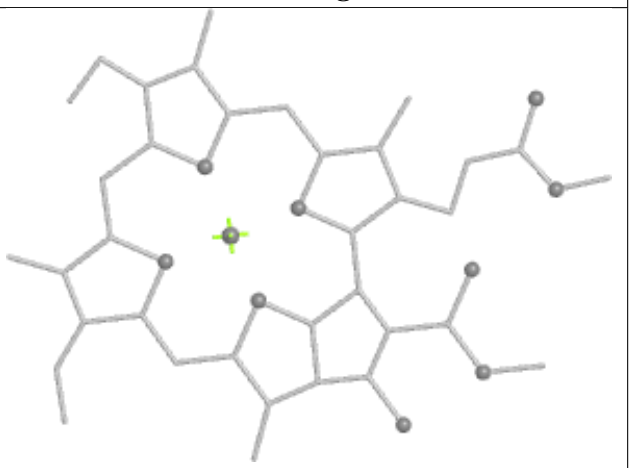
Bond lengths



Bond angles

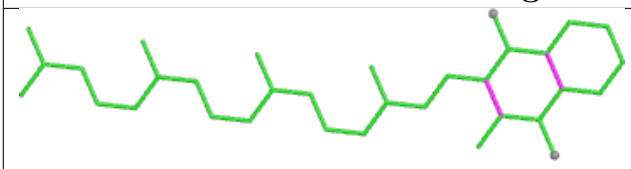


Torsions

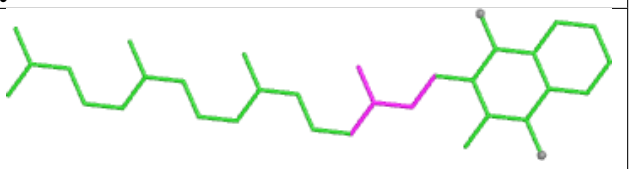


Rings

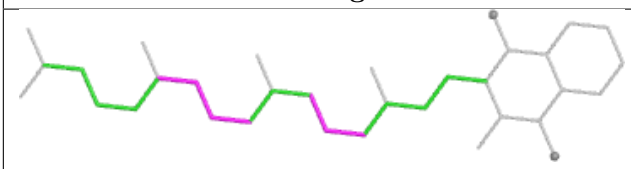
Ligand PQN B 842



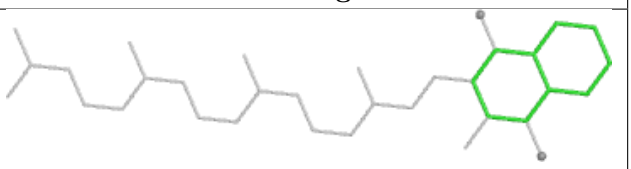
Bond lengths



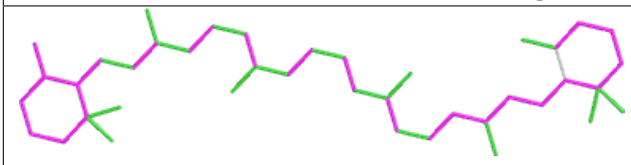
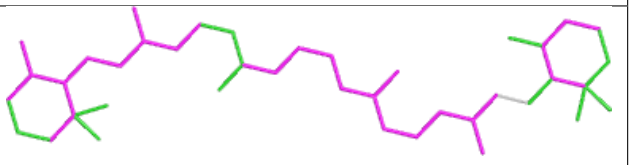
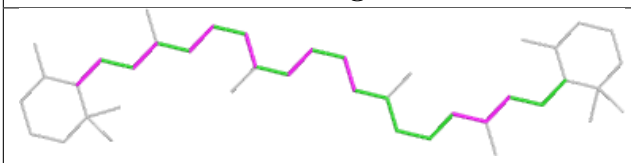
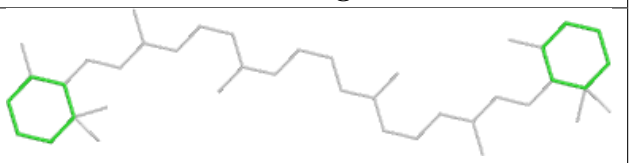
Bond angles

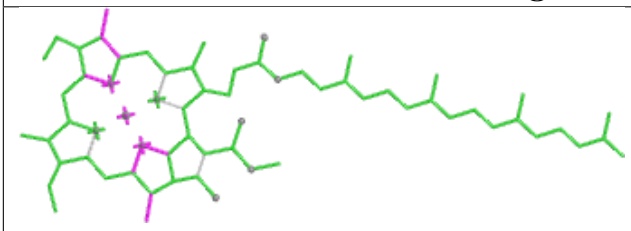
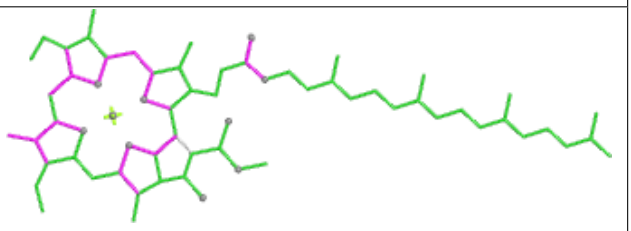
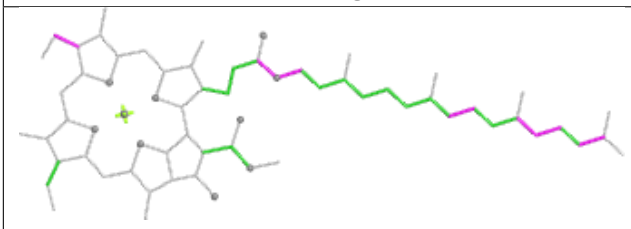
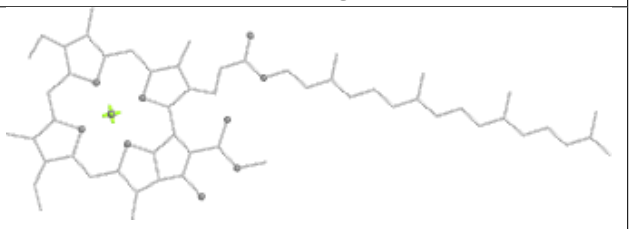


Torsions

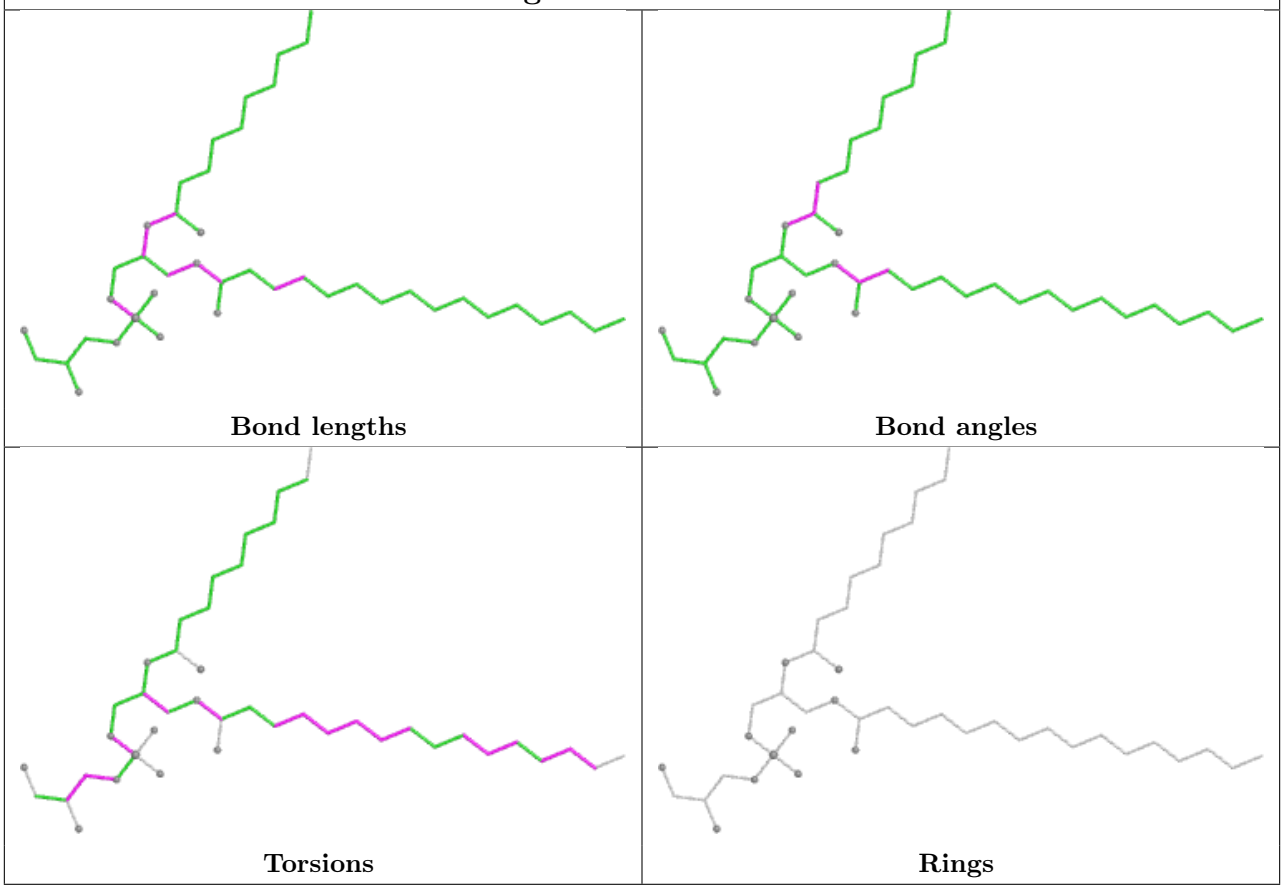


Rings

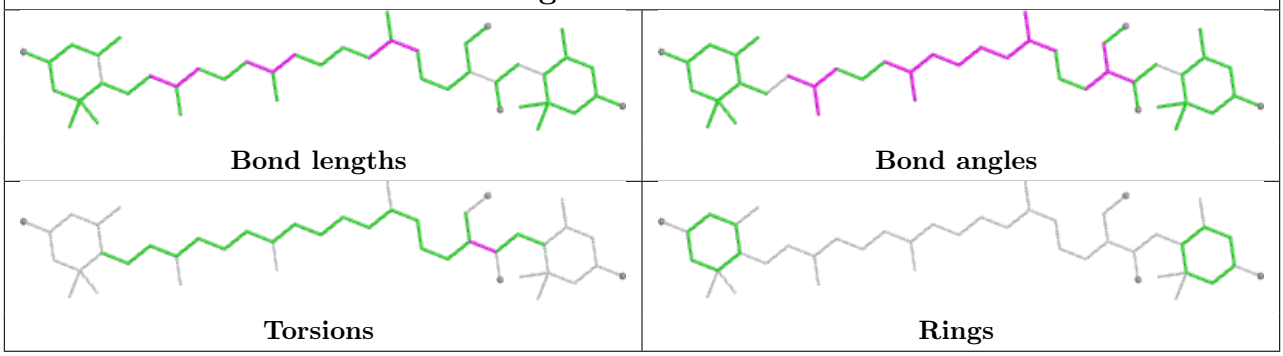
Ligand 8CT 8 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

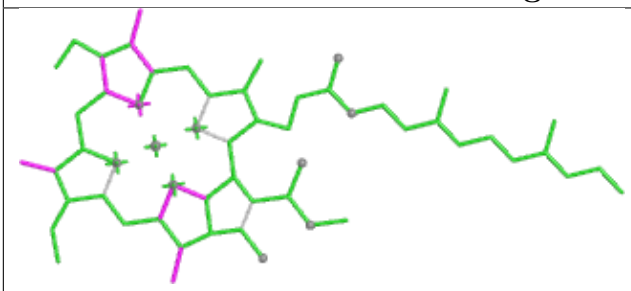
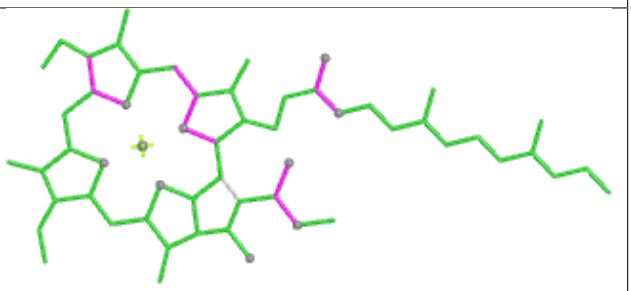
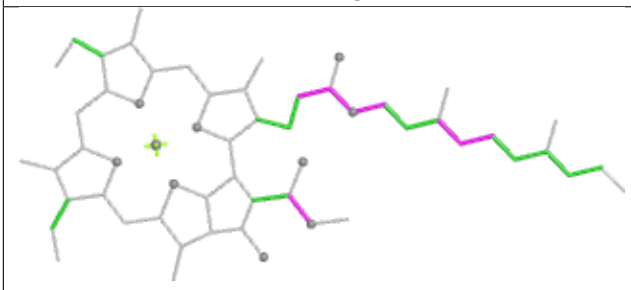
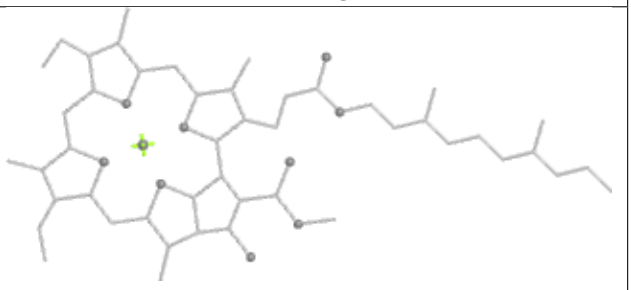
Ligand CL0 A 857	
 Bond lengths	 Bond angles
 Torsions	 Rings

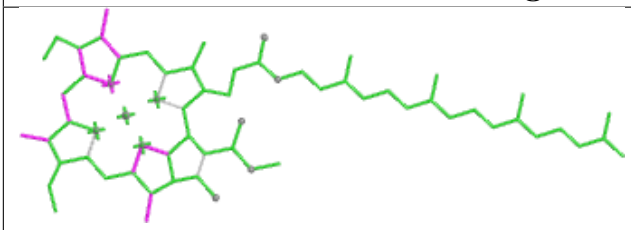
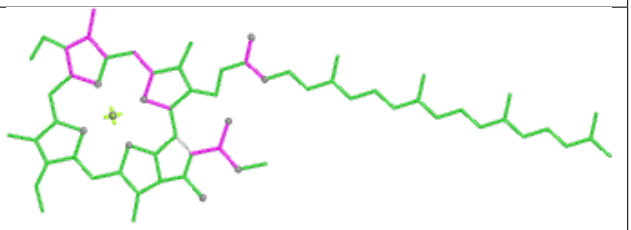
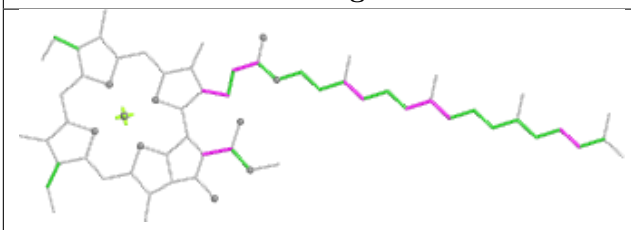
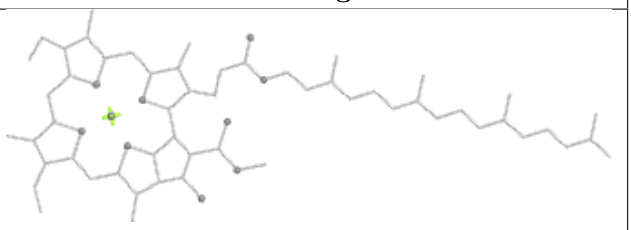
Ligand LHG B 854

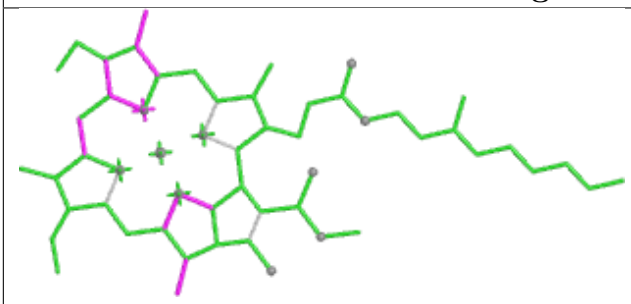
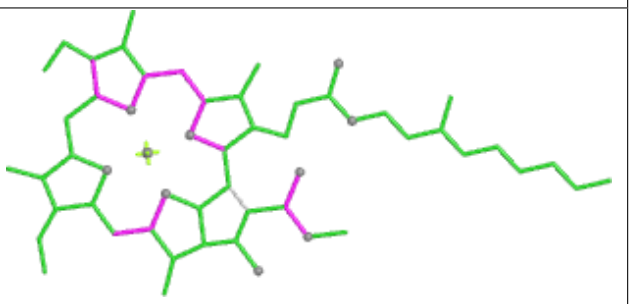
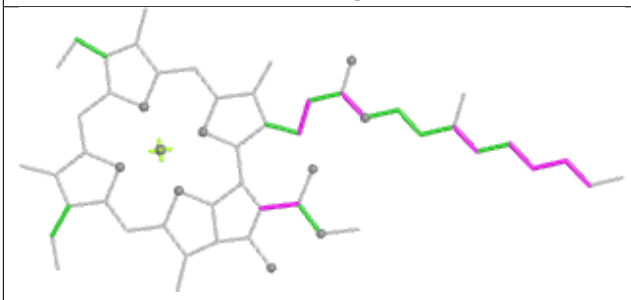
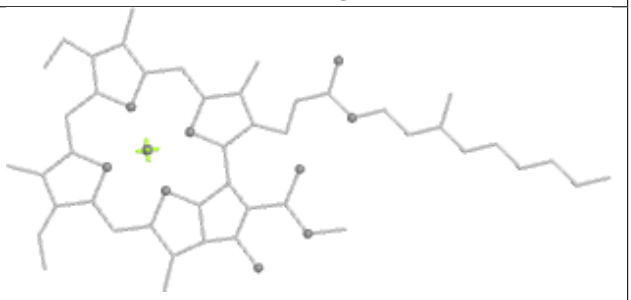


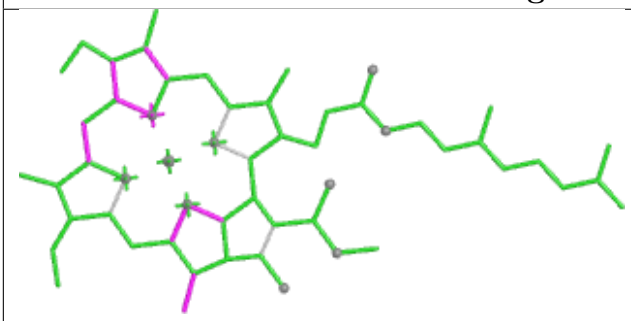
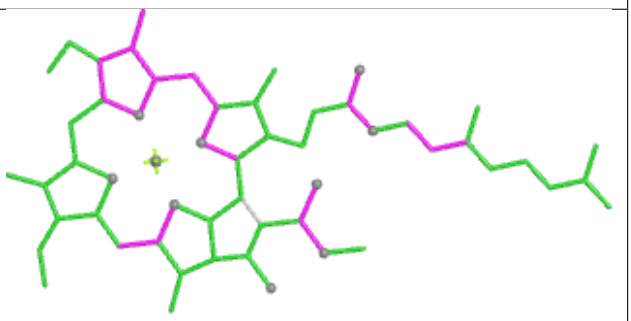
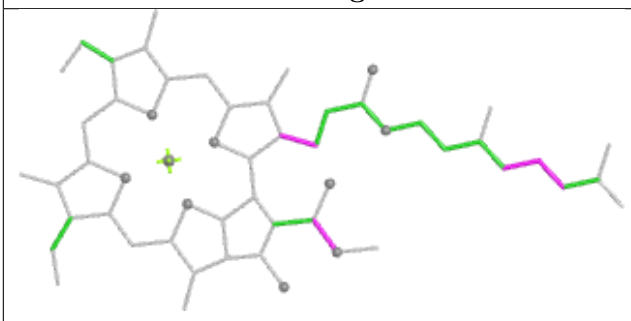
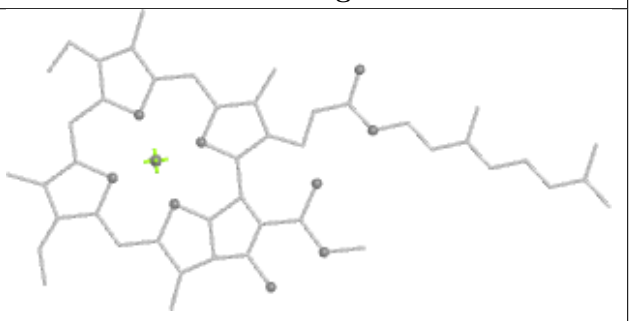
Ligand 0IE 3 502



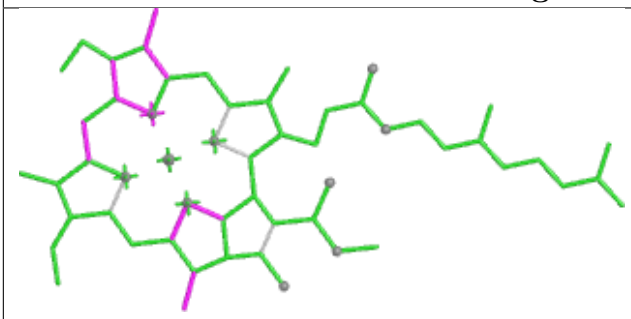
Ligand CLA A 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

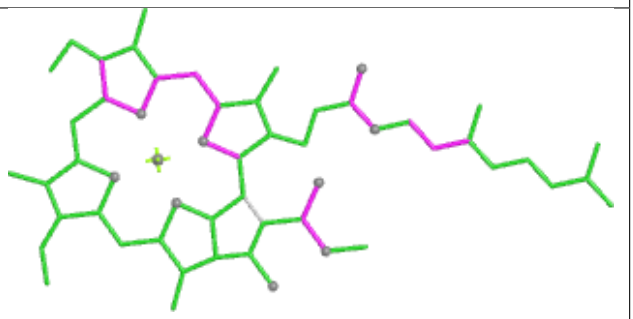
Ligand CLA f 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

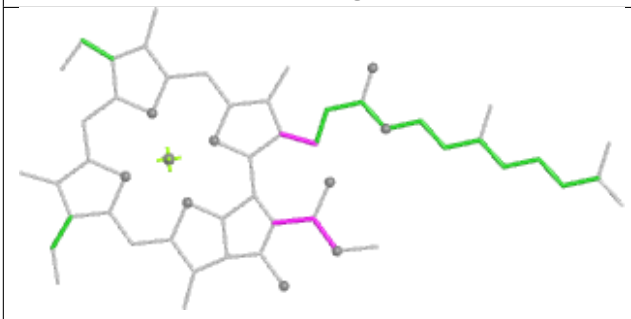
Ligand CLA f 610



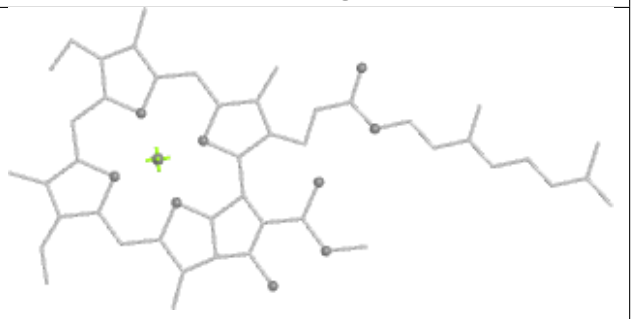
Bond lengths



Bond angles

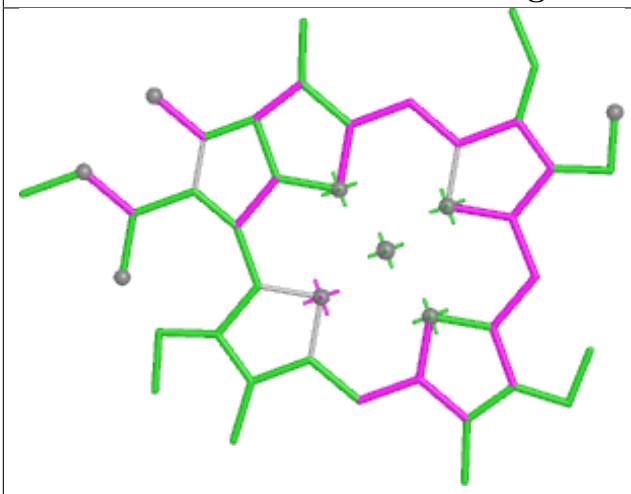


Torsions

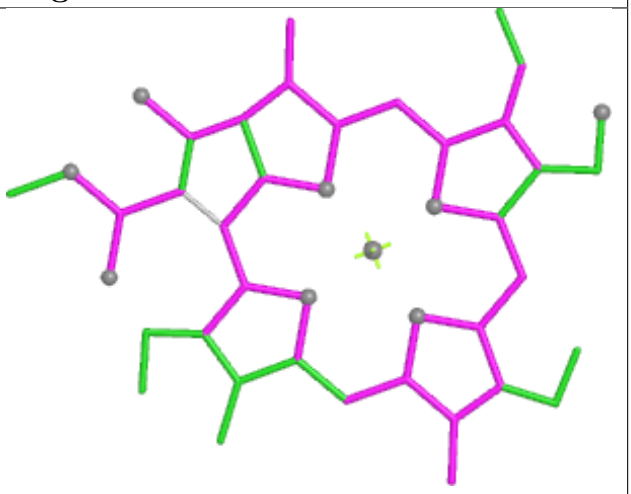


Rings

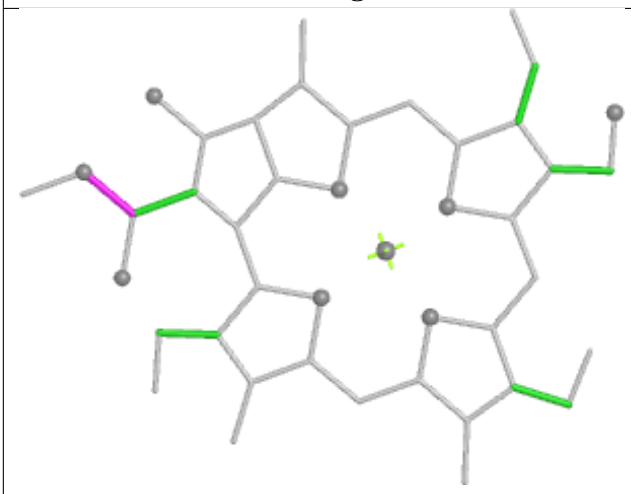
Ligand CHL g 605



Bond lengths



Bond angles

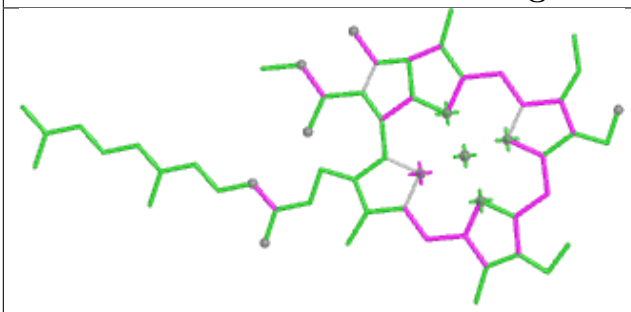


Torsions

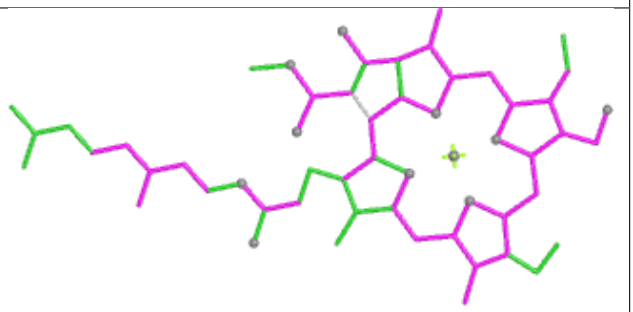


Rings

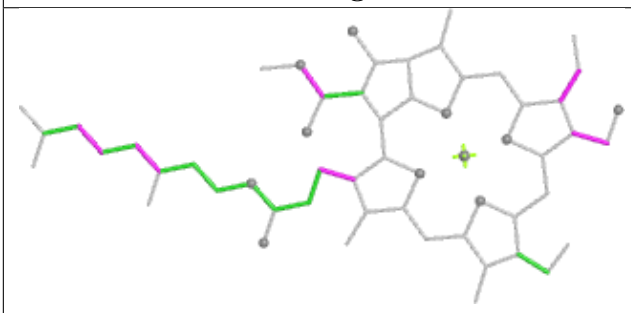
Ligand CHL c 601



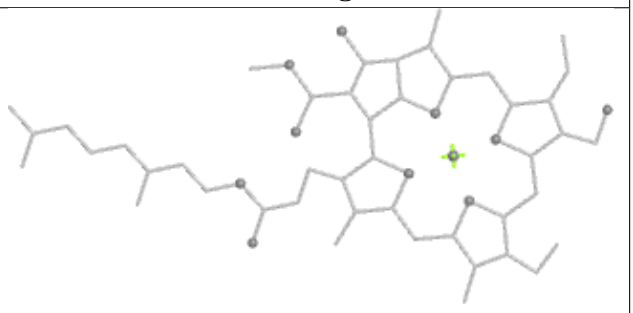
Bond lengths



Bond angles

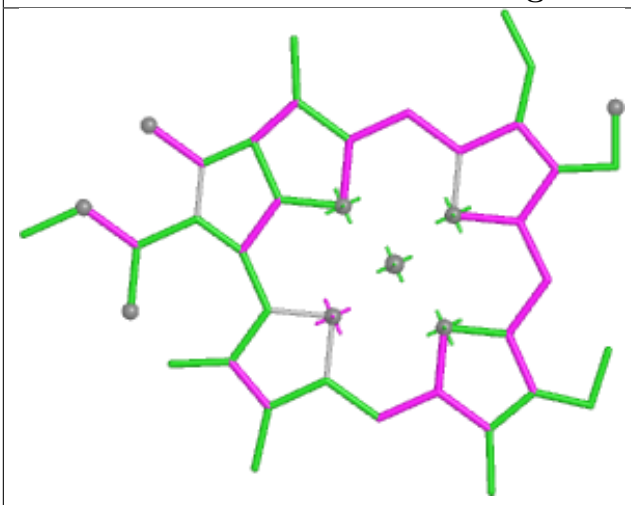


Torsions

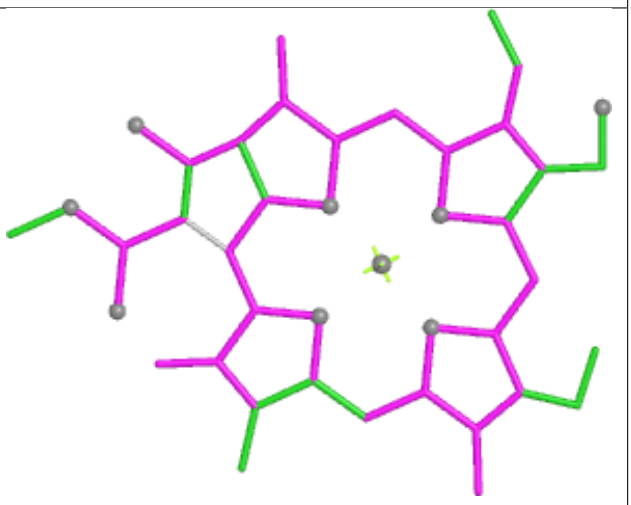


Rings

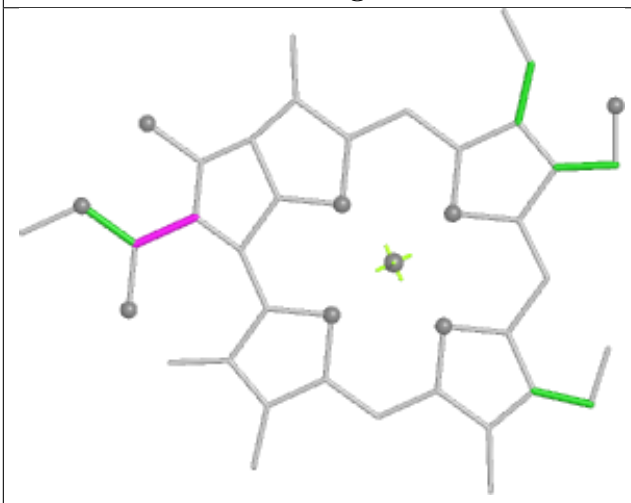
Ligand CHL d 614



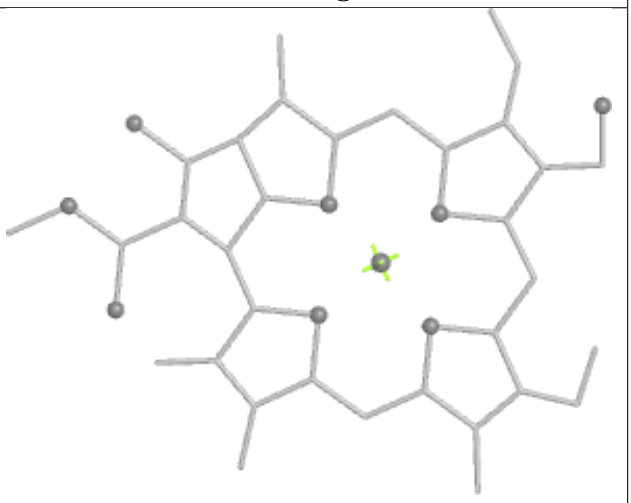
Bond lengths



Bond angles

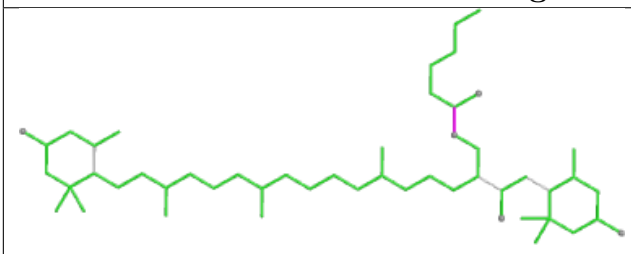


Torsions

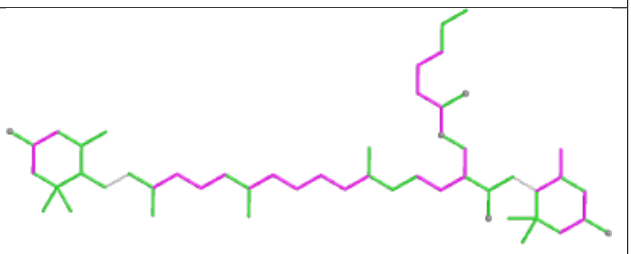


Rings

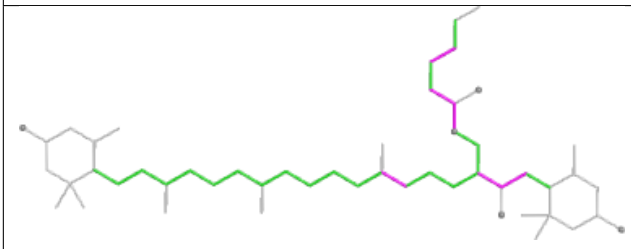
Ligand 0UR 5 501



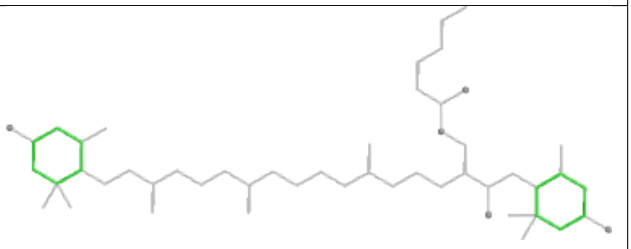
Bond lengths



Bond angles

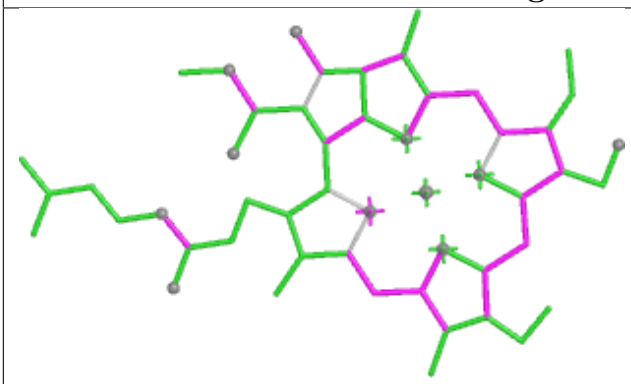


Torsions

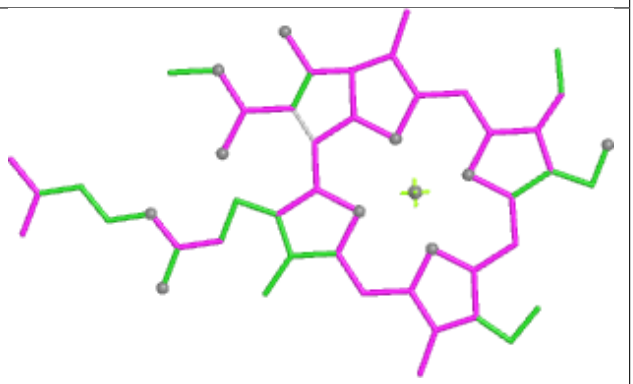


Rings

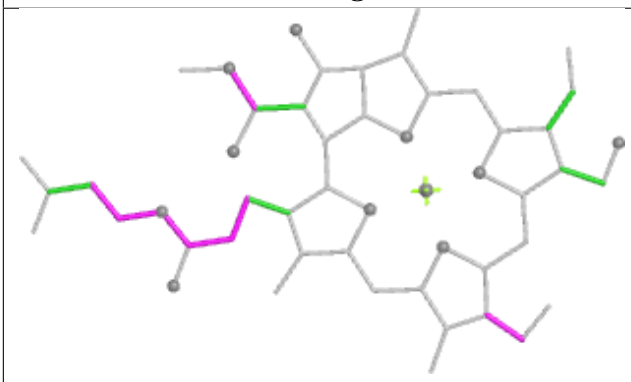
Ligand CHL 1 305



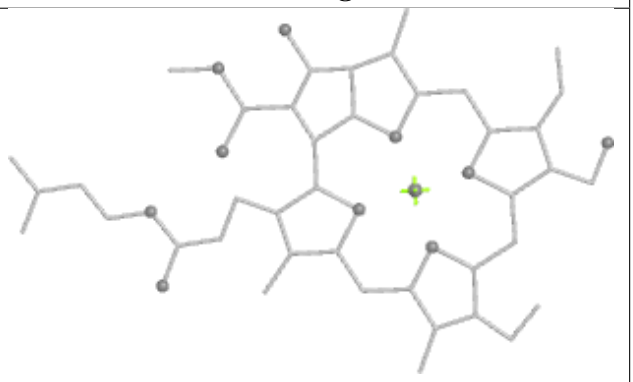
Bond lengths



Bond angles

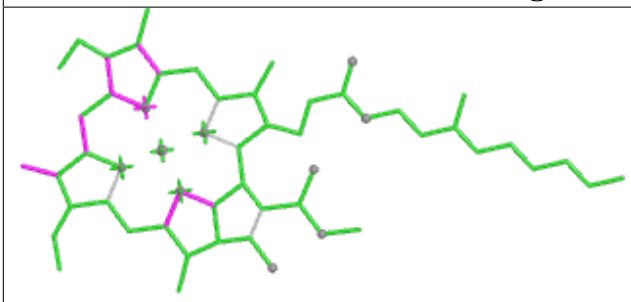


Torsions

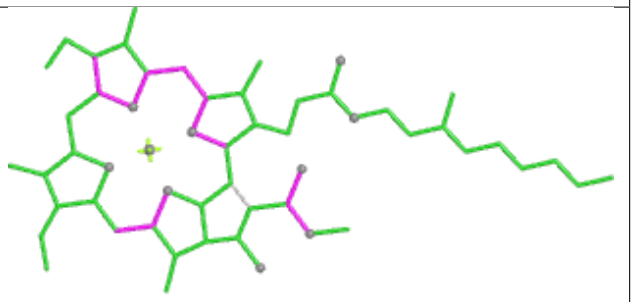


Rings

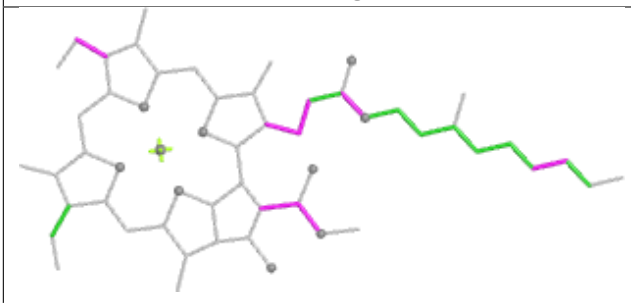
Ligand CLA a 613



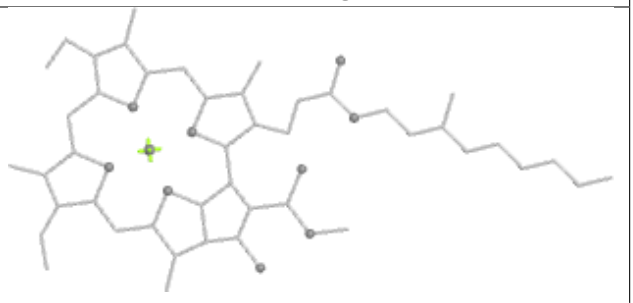
Bond lengths



Bond angles

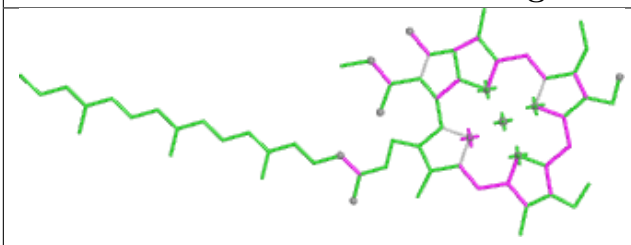


Torsions

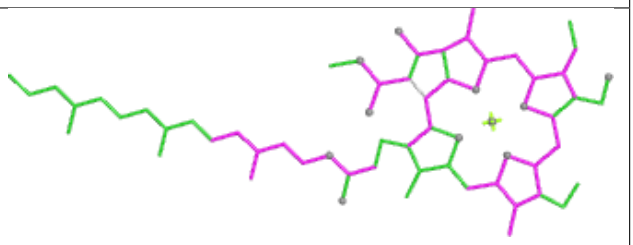


Rings

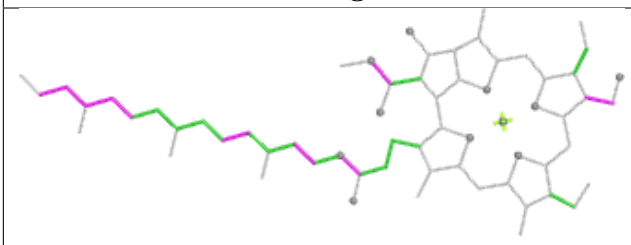
Ligand CHL 7 301



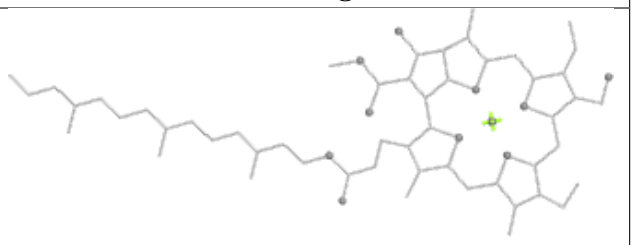
Bond lengths



Bond angles

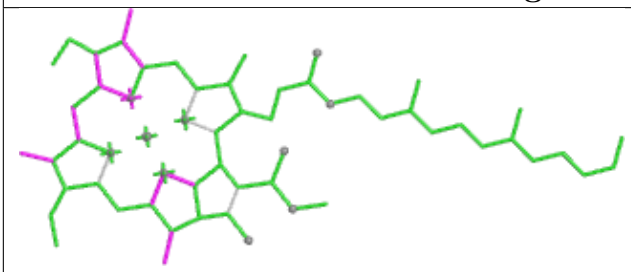


Torsions

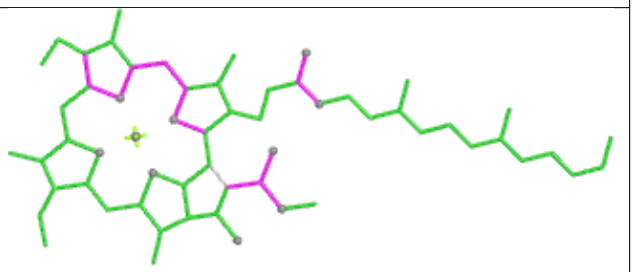


Rings

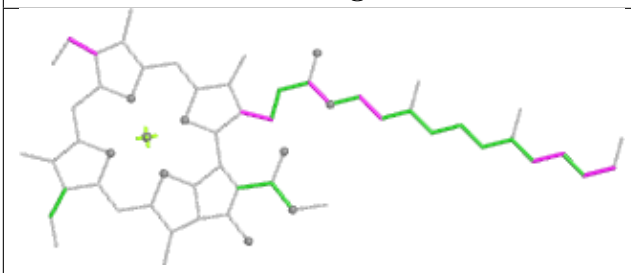
Ligand CLA B 818



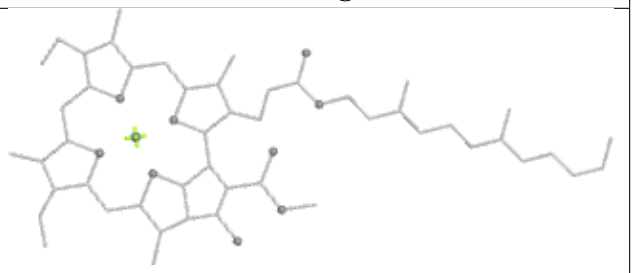
Bond lengths



Bond angles

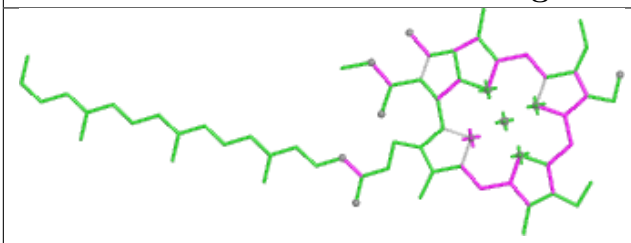


Torsions

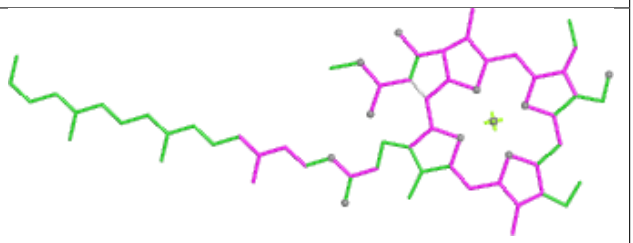


Rings

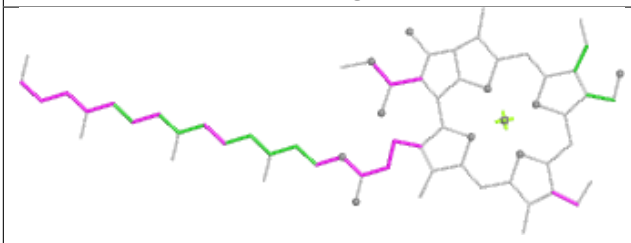
Ligand CHL f 602



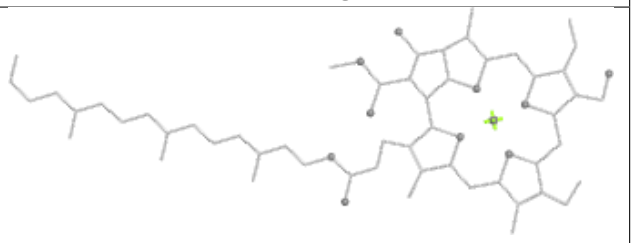
Bond lengths



Bond angles

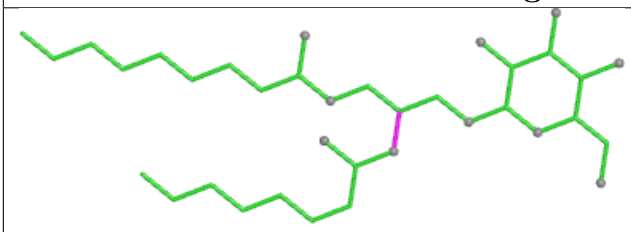


Torsions

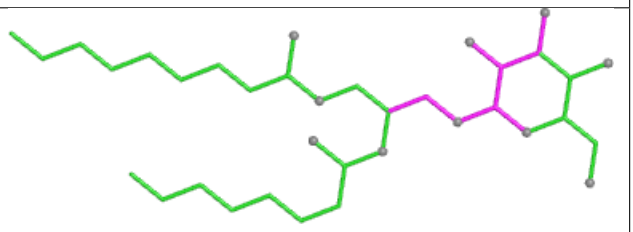


Rings

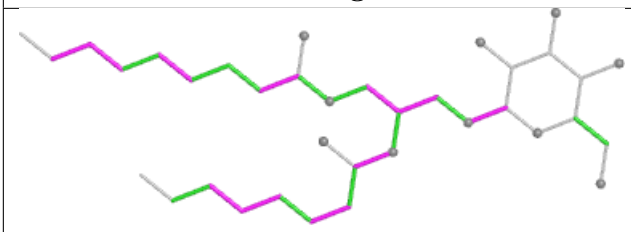
Ligand LMG 2 602



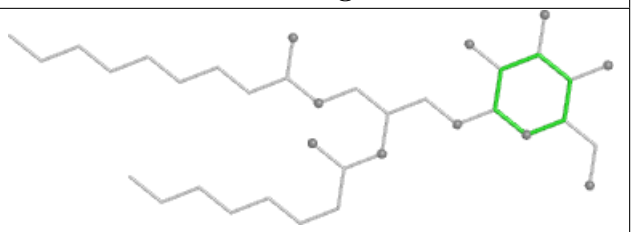
Bond lengths



Bond angles

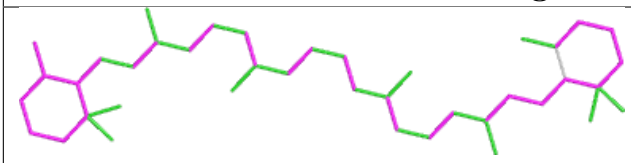


Torsions

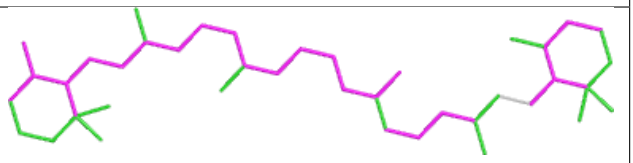


Rings

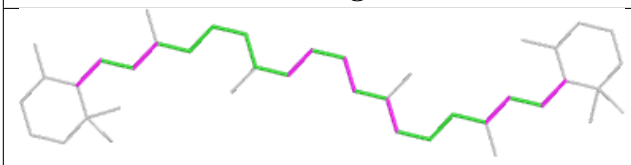
Ligand 8CT 9 401



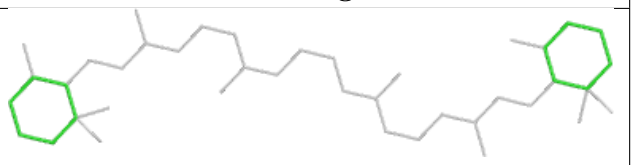
Bond lengths



Bond angles

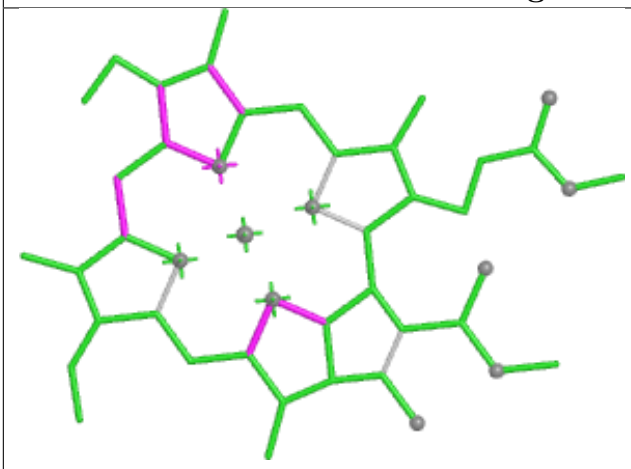


Torsions

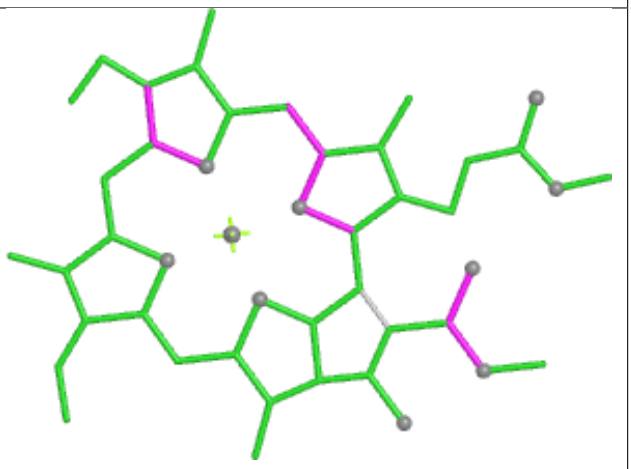


Rings

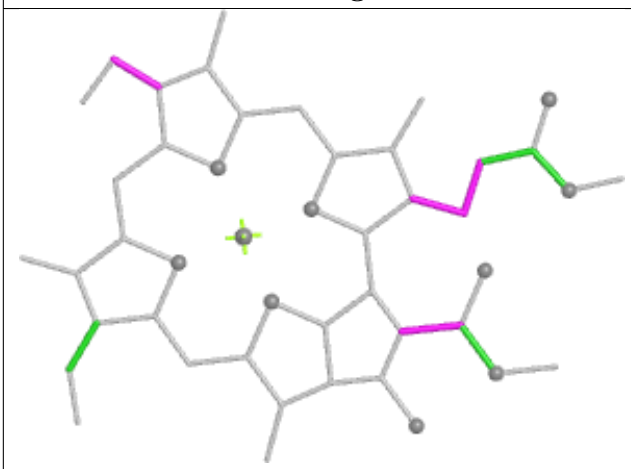
Ligand CLA d 611



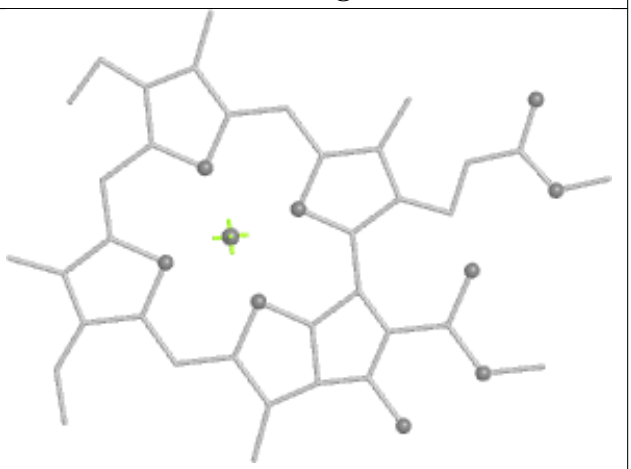
Bond lengths



Bond angles

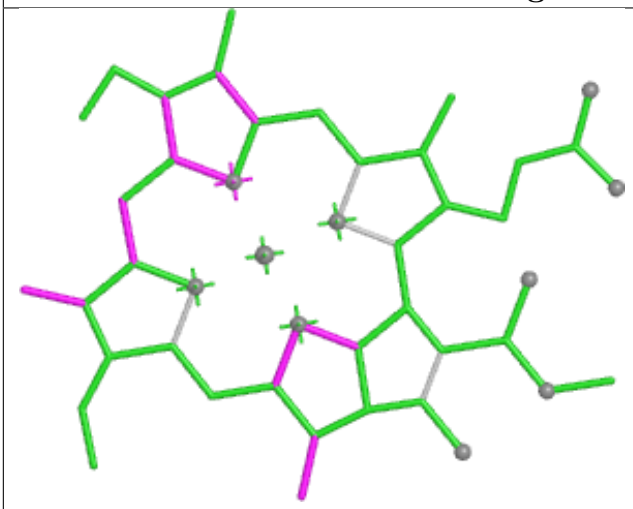


Torsions

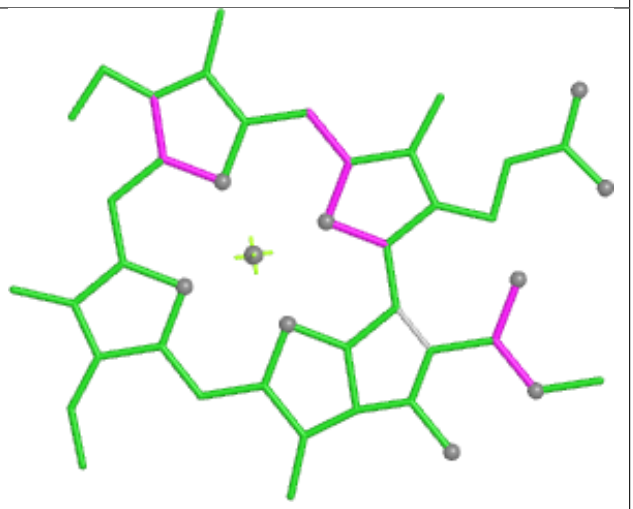


Rings

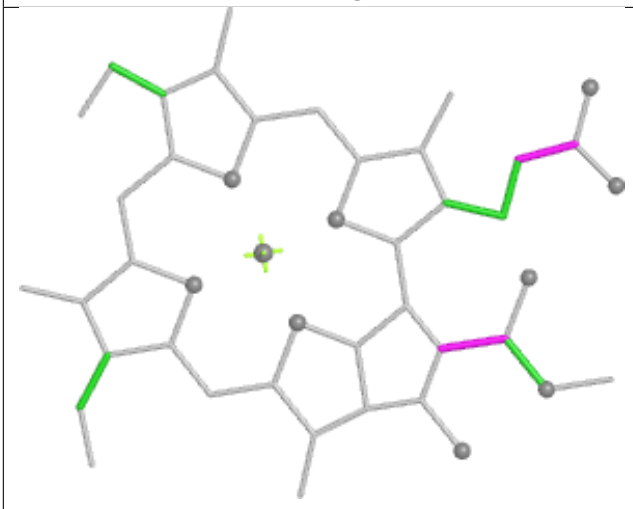
Ligand CLA b 612



Bond lengths



Bond angles

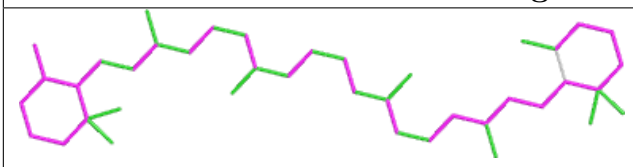


Torsions

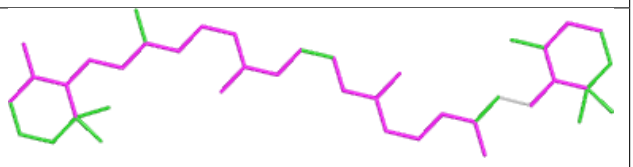


Rings

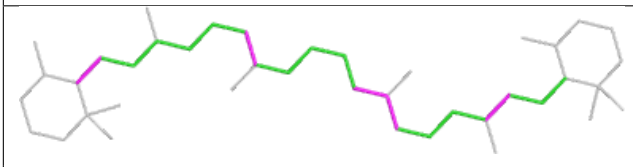
Ligand 8CT 4 402



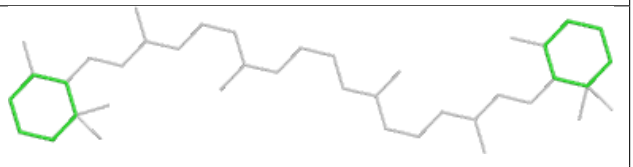
Bond lengths



Bond angles

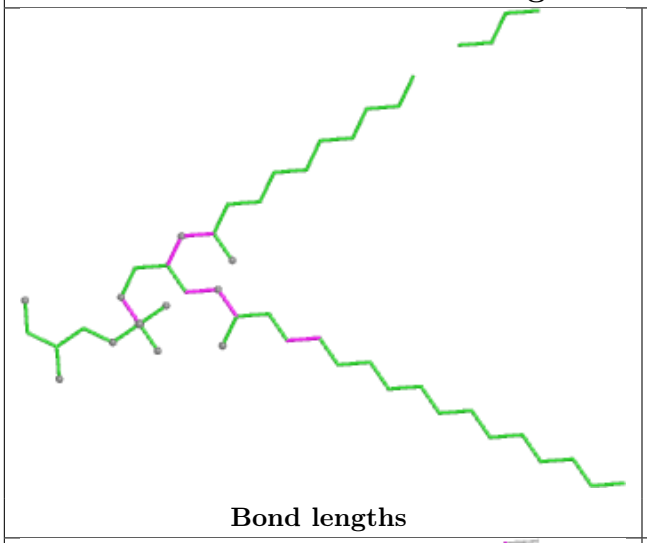


Torsions

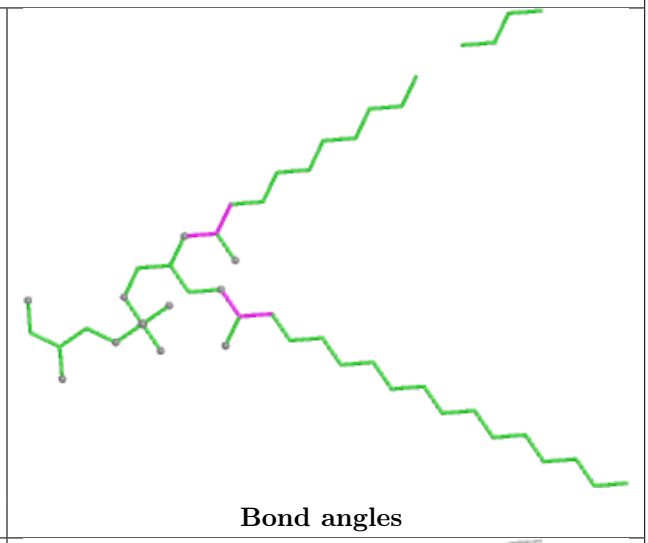


Rings

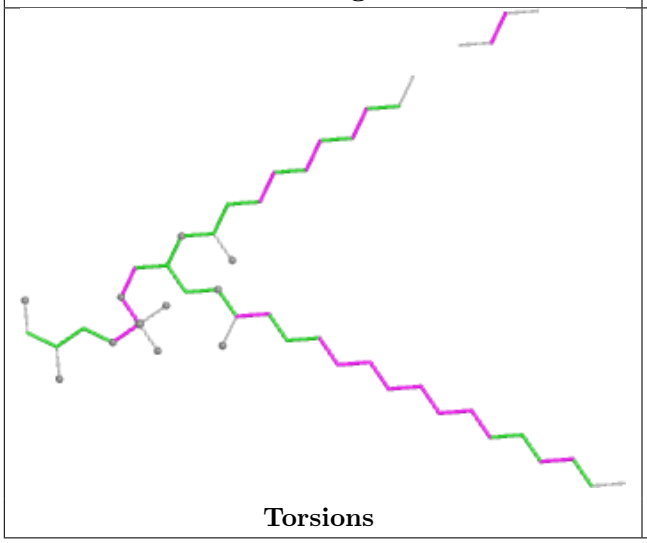
Ligand LHG 9 601



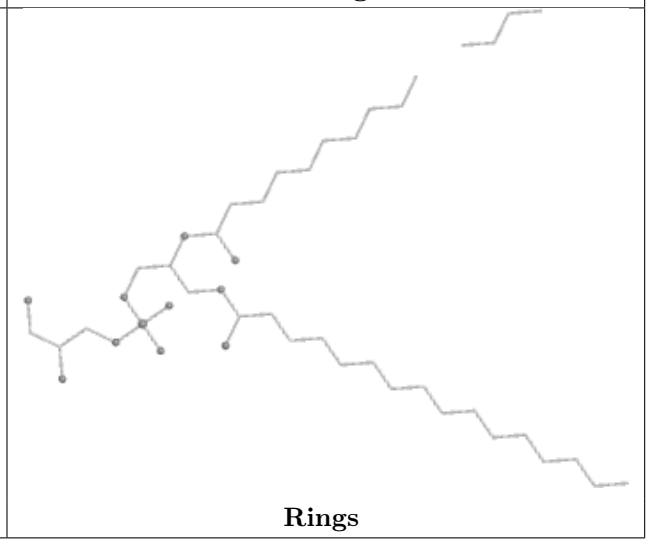
Bond lengths



Bond angles

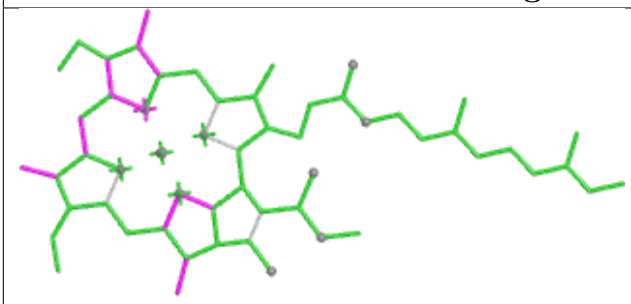


Torsions

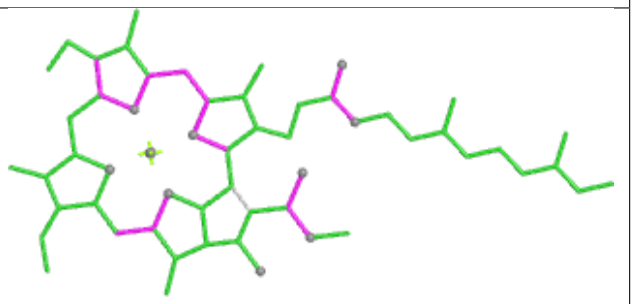


Rings

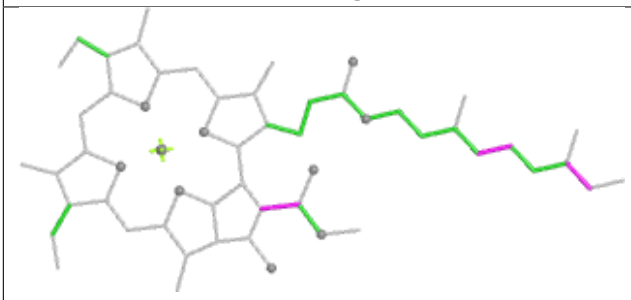
Ligand CLA A 838



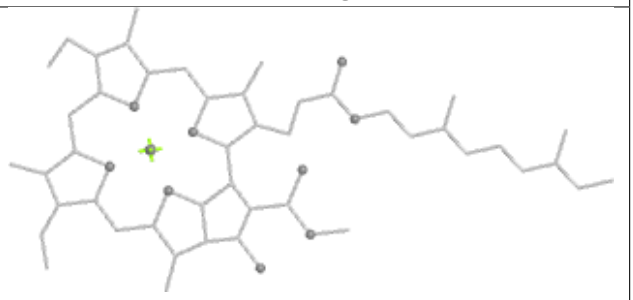
Bond lengths



Bond angles

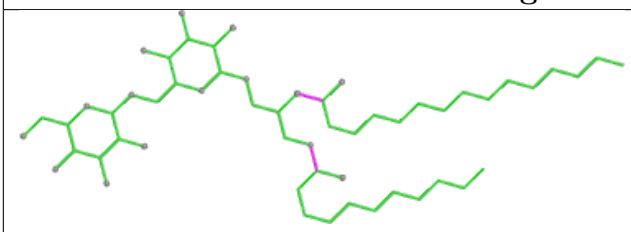


Torsions

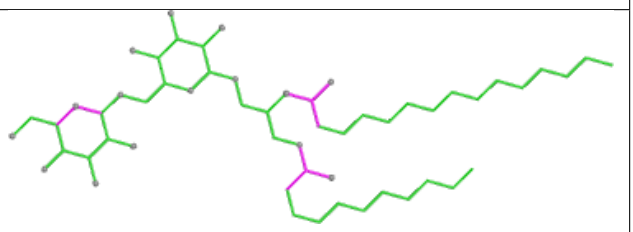


Rings

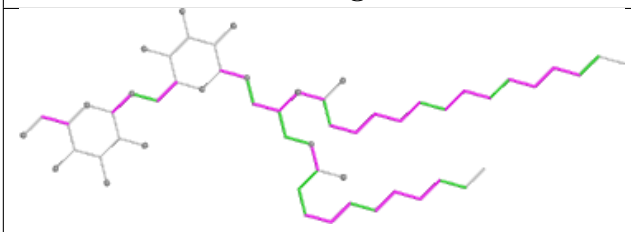
Ligand DGD B 849



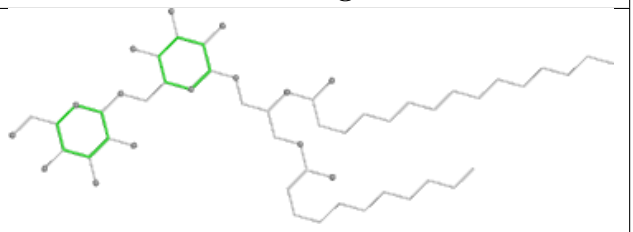
Bond lengths



Bond angles

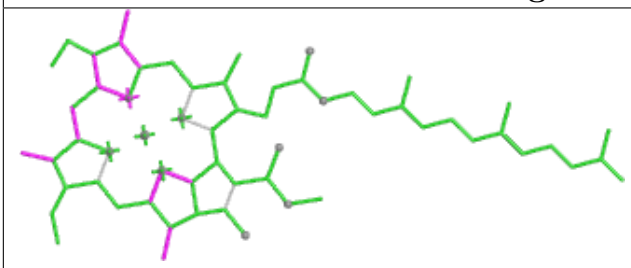


Torsions

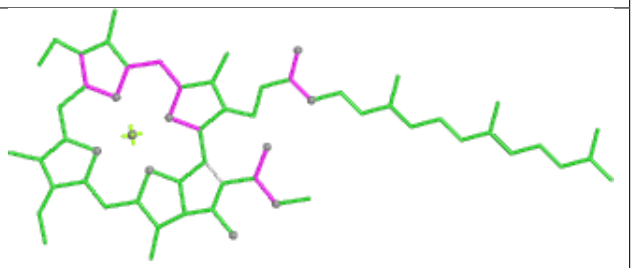


Rings

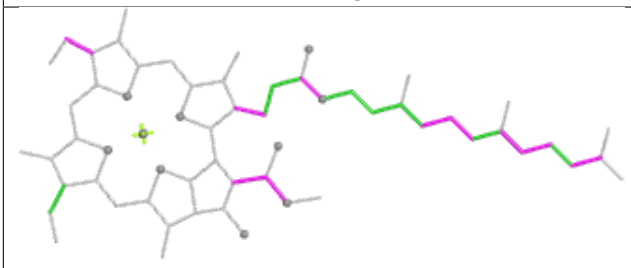
Ligand CLA 4 310



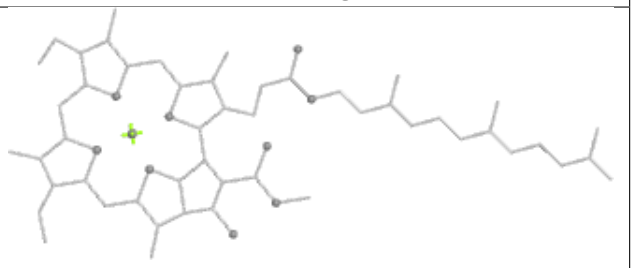
Bond lengths



Bond angles

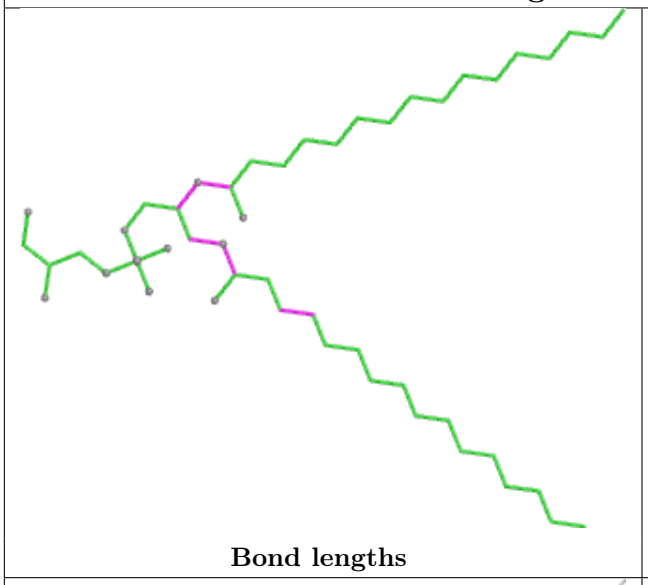


Torsions

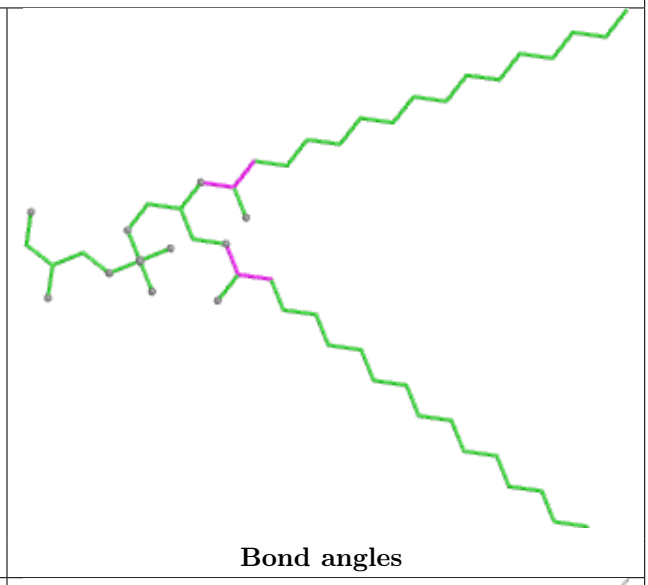


Rings

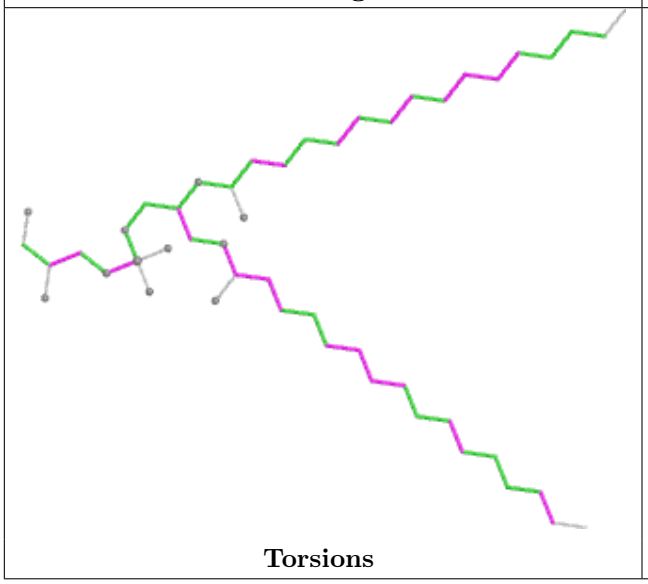
Ligand LHG 1 601



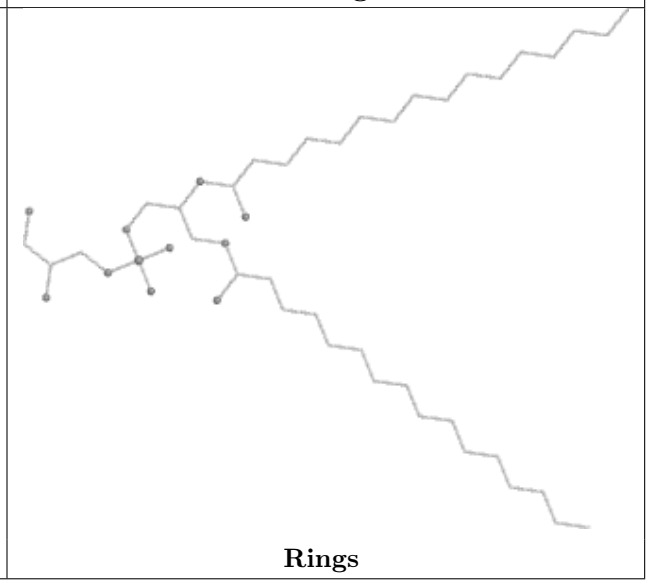
Bond lengths



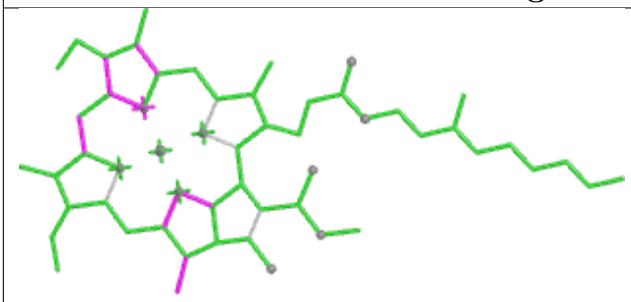
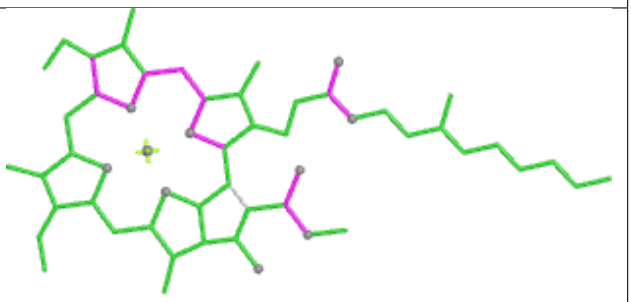
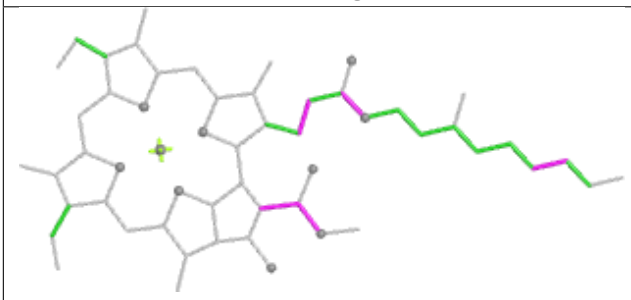
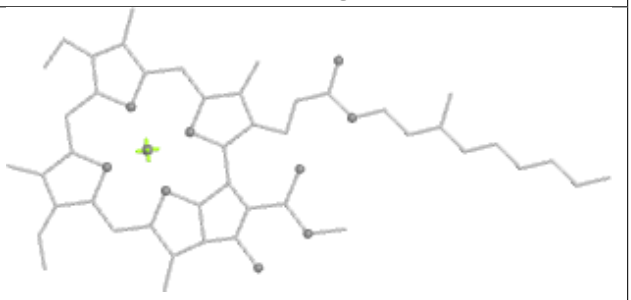
Bond angles

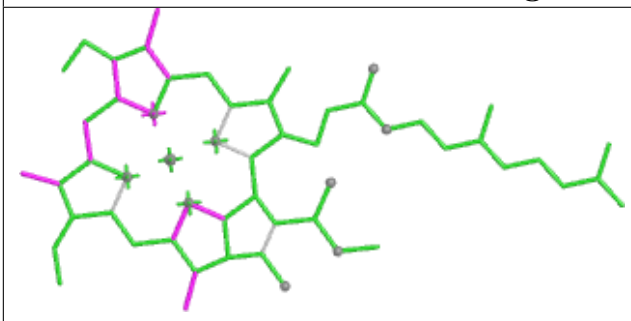
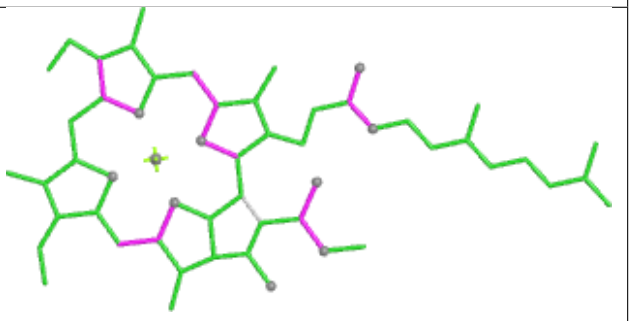
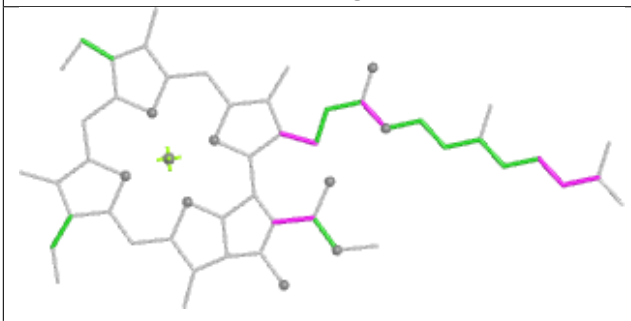
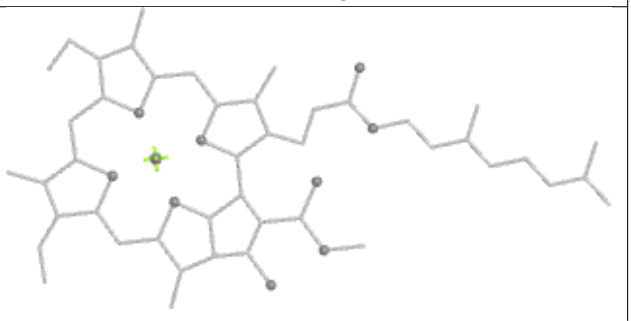


Torsions

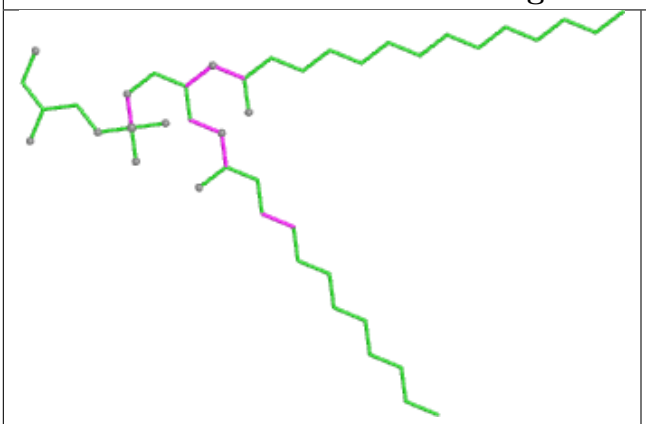


Rings

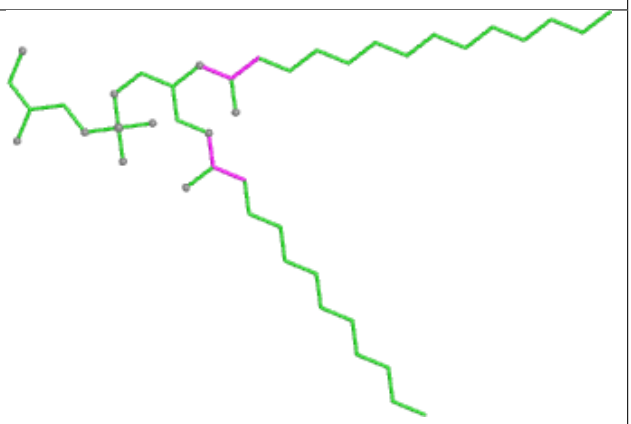
Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

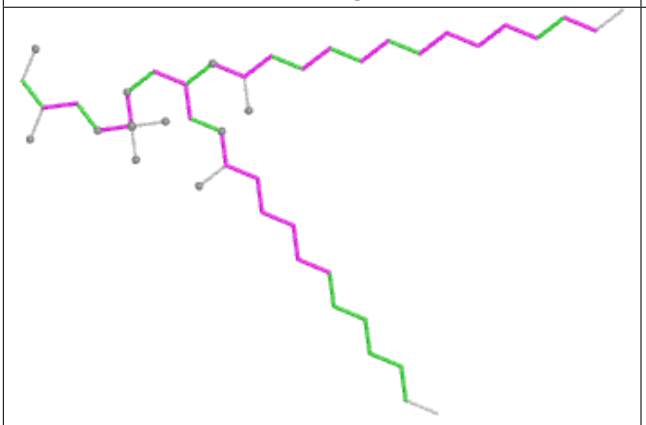
Ligand LHG a 630



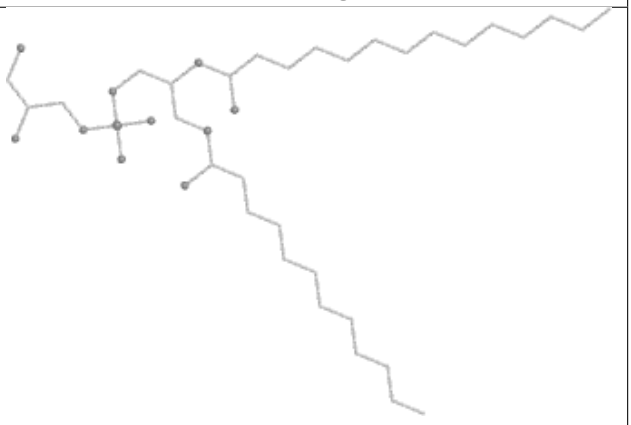
Bond lengths



Bond angles

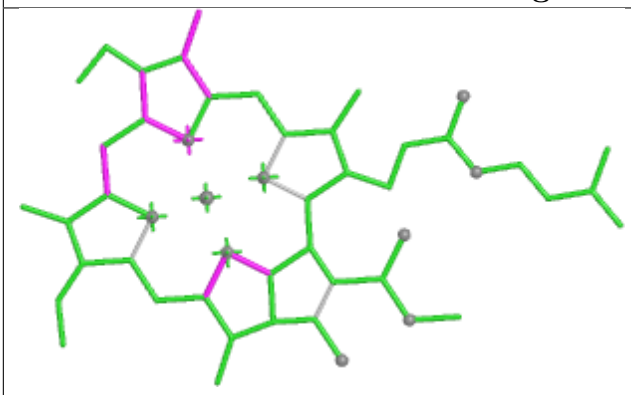


Torsions

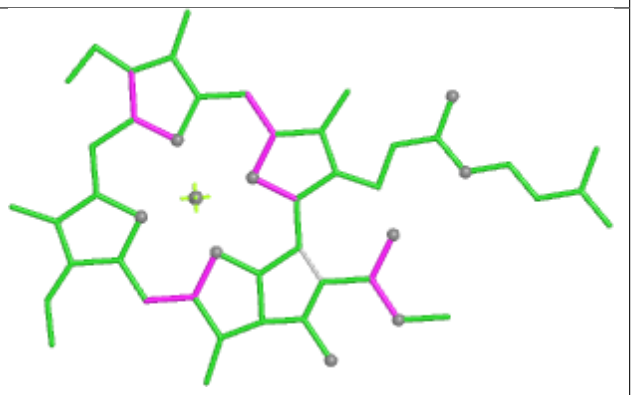


Rings

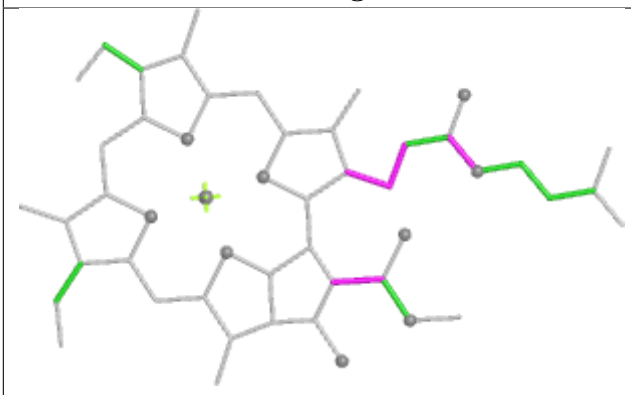
Ligand CLA i 604



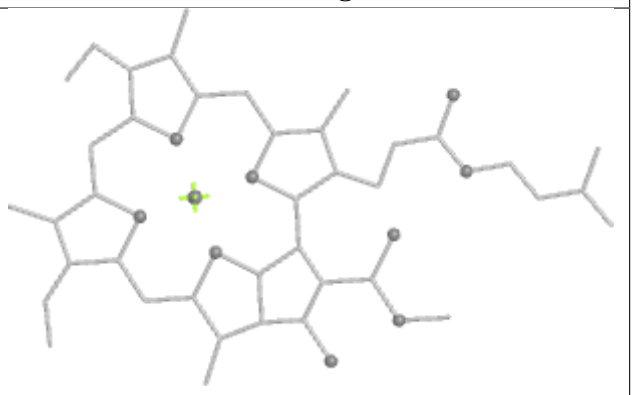
Bond lengths



Bond angles

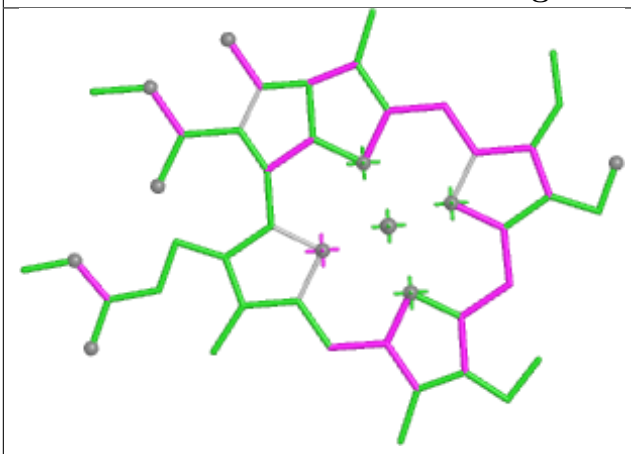


Torsions

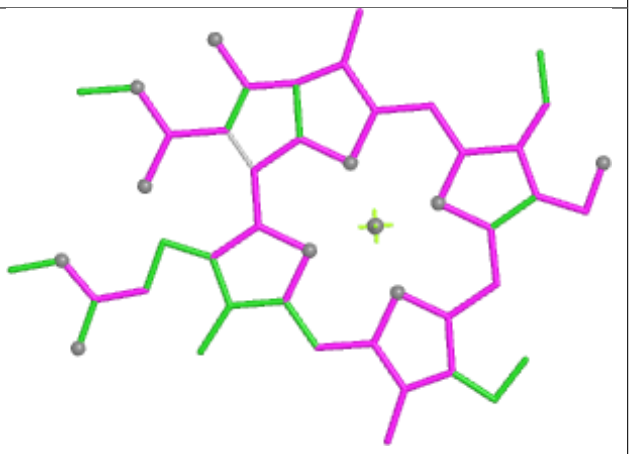


Rings

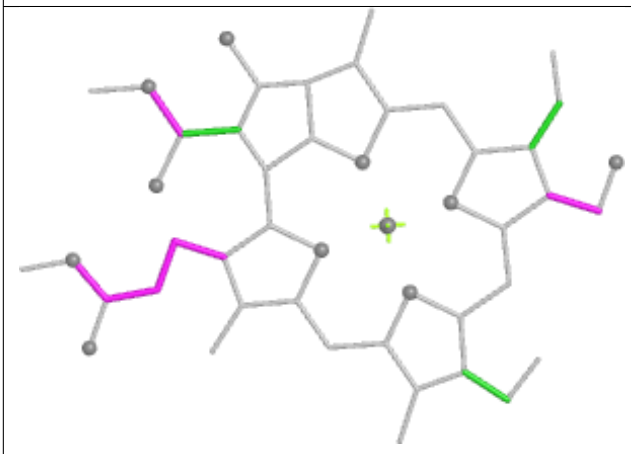
Ligand CHL i 607



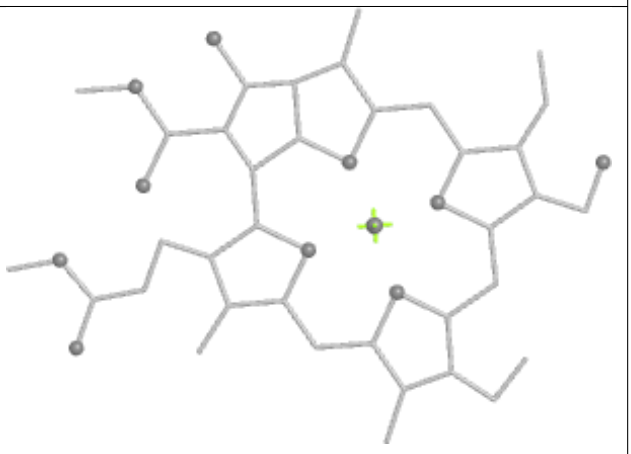
Bond lengths



Bond angles

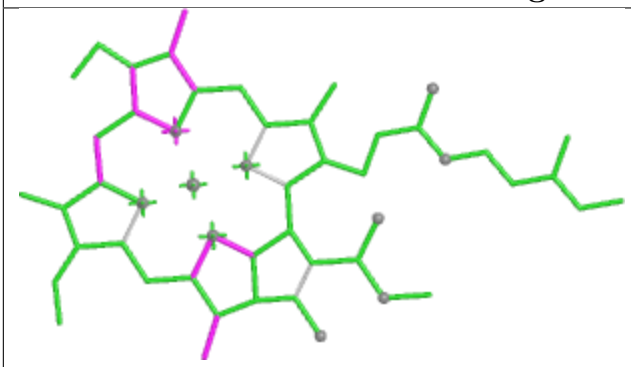


Torsions

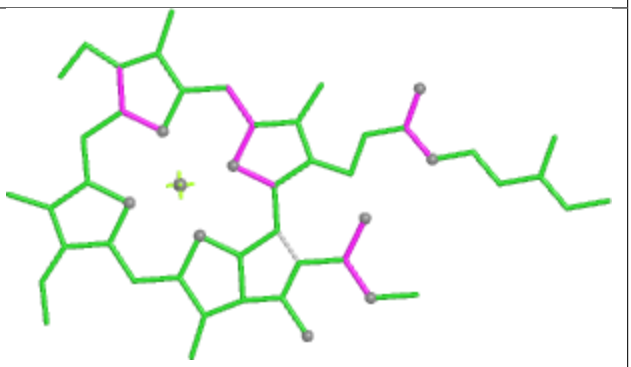


Rings

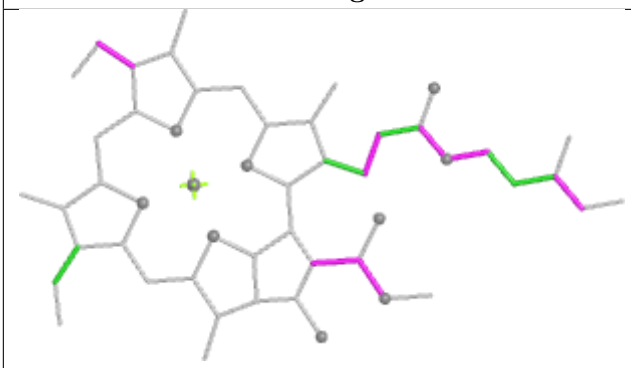
Ligand CLA 6 320



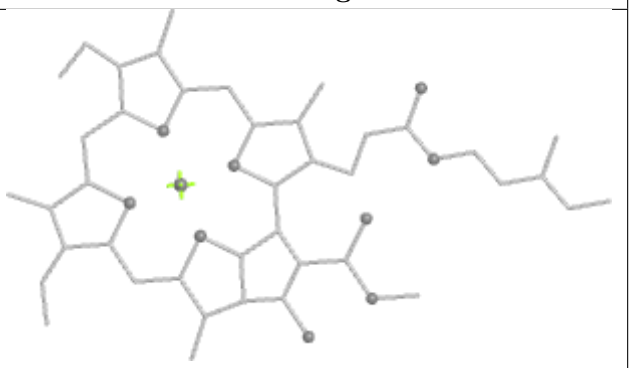
Bond lengths



Bond angles

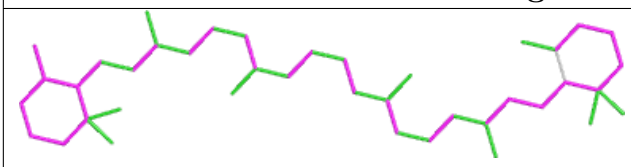


Torsions

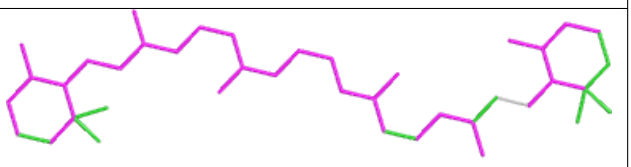


Rings

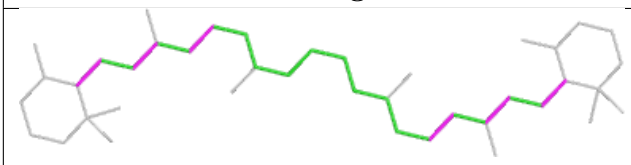
Ligand 8CT B 847



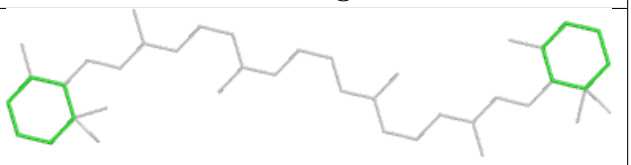
Bond lengths



Bond angles

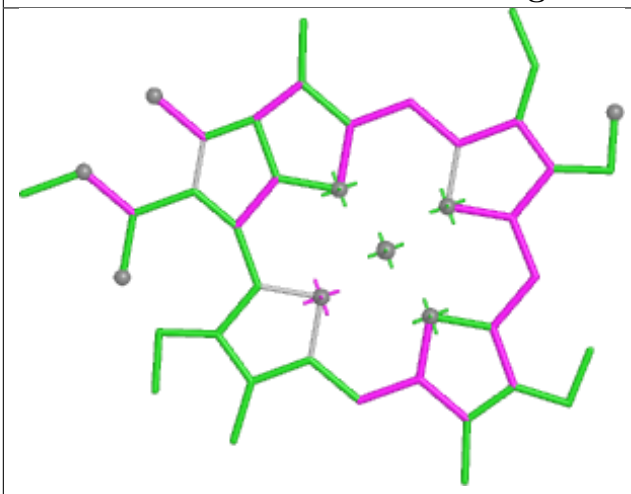


Torsions

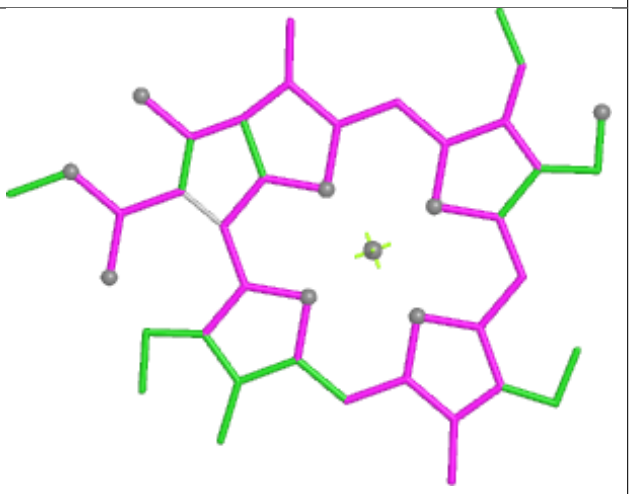


Rings

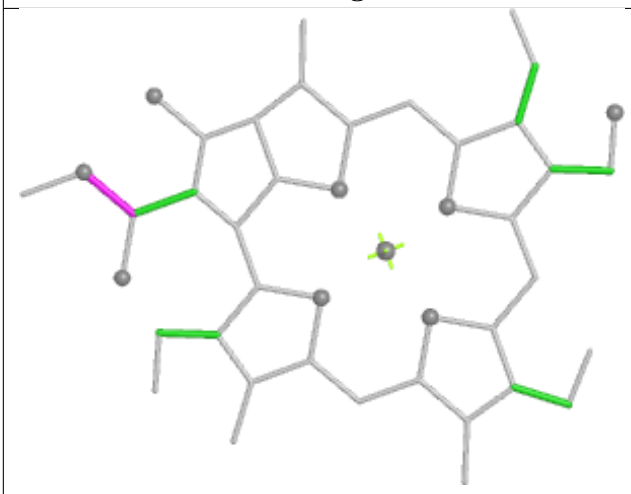
Ligand CHL a 605



Bond lengths



Bond angles

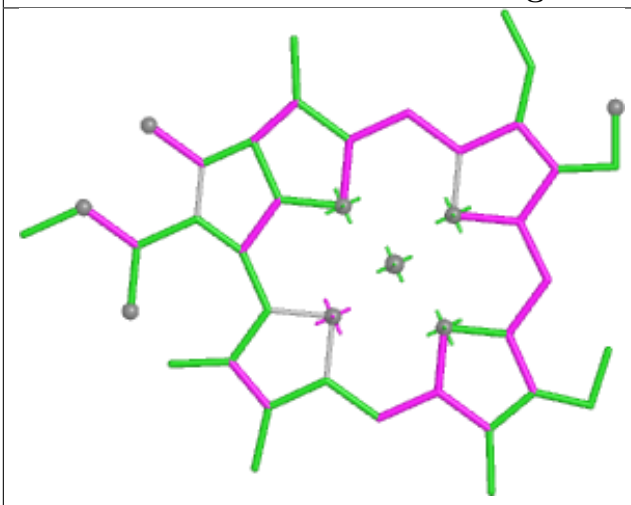


Torsions

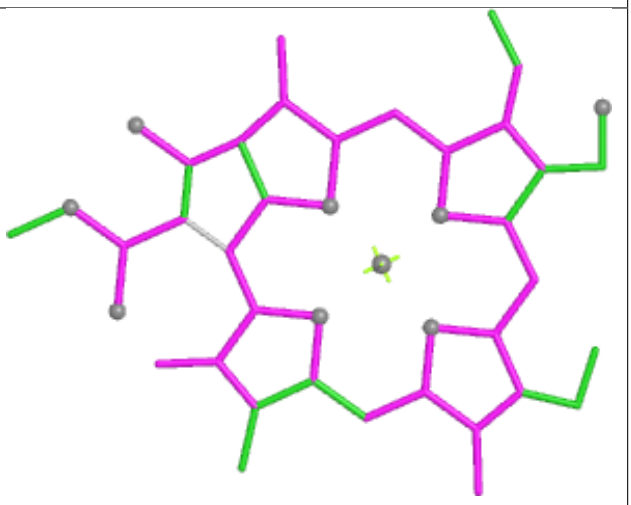


Rings

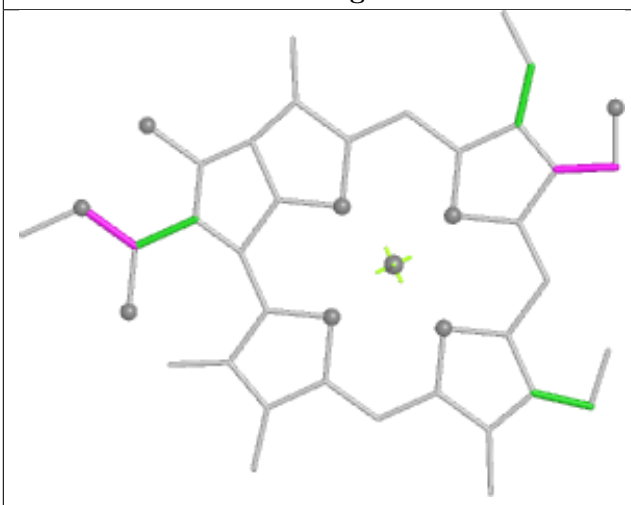
Ligand CHL b 614



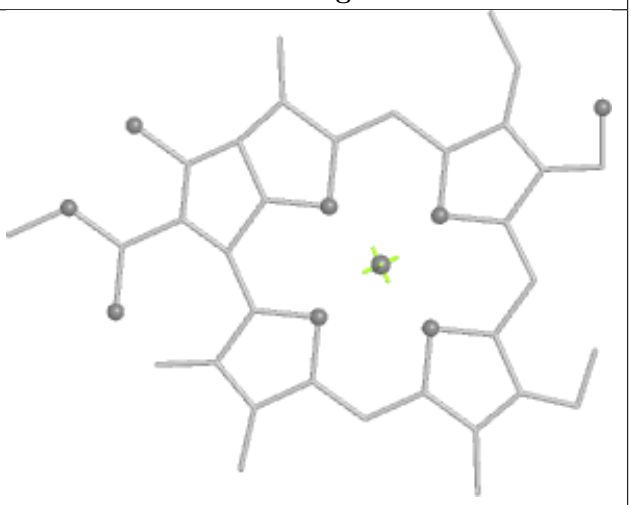
Bond lengths



Bond angles

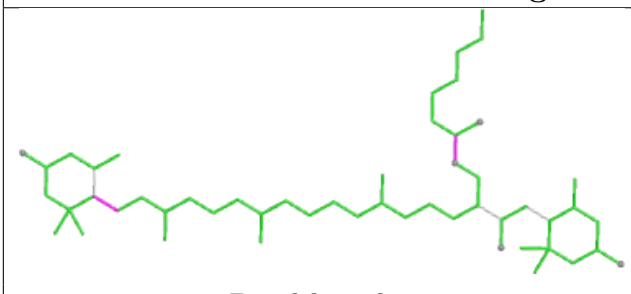


Torsions

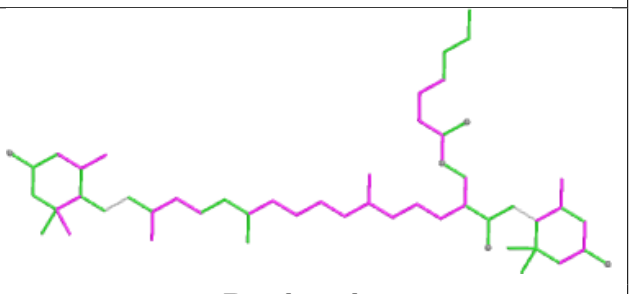


Rings

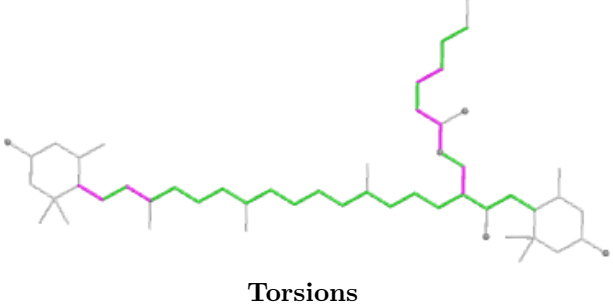
Ligand 0UR 1 502



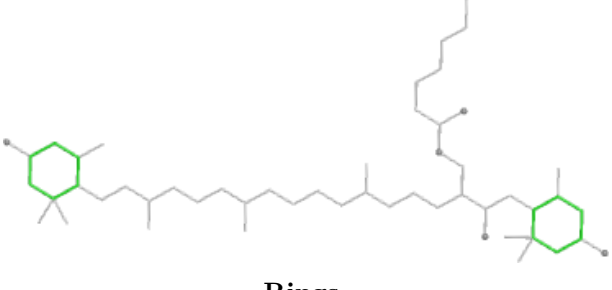
Bond lengths



Bond angles

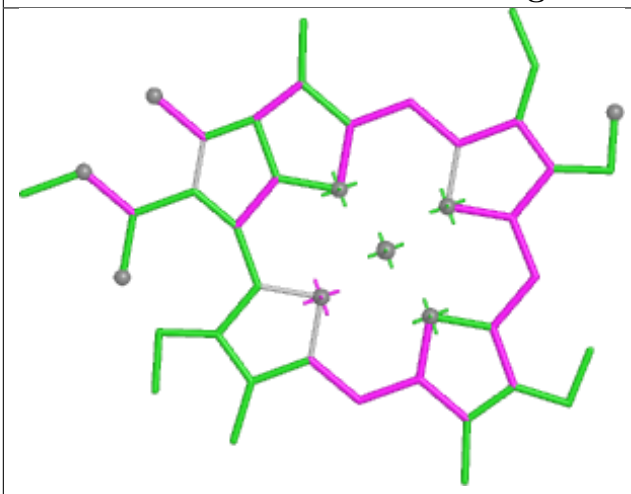


Torsions

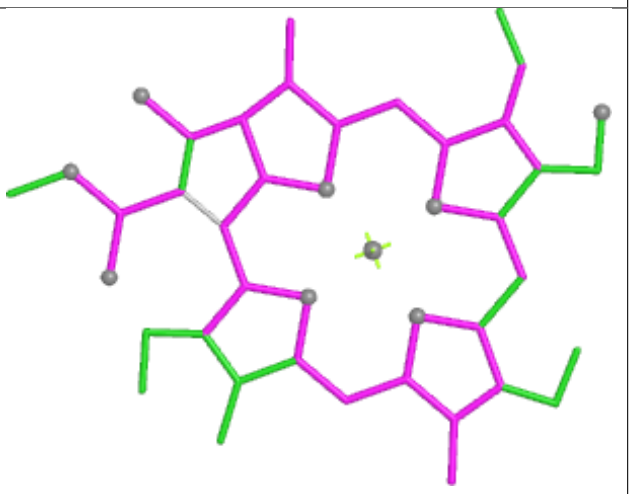


Rings

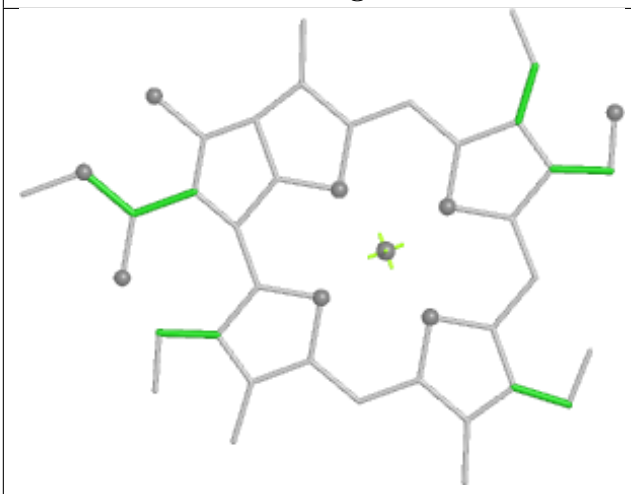
Ligand CHL 6 305



Bond lengths



Bond angles

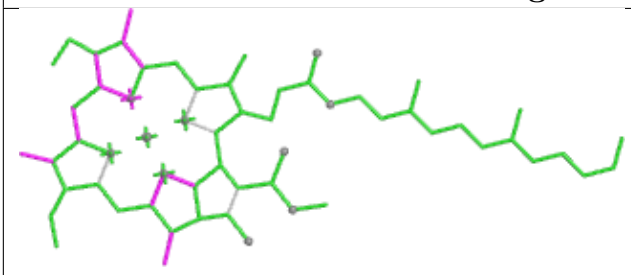


Torsions

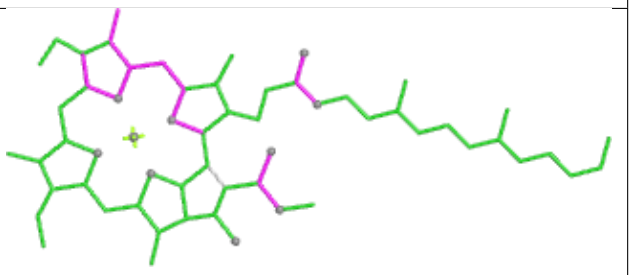


Rings

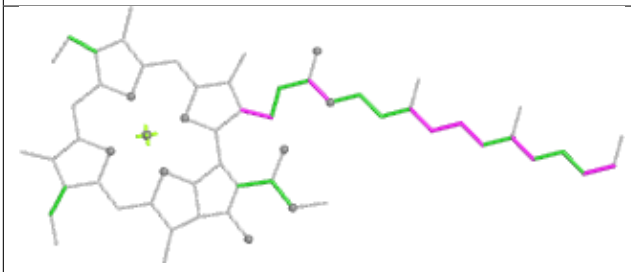
Ligand CLA 7 309



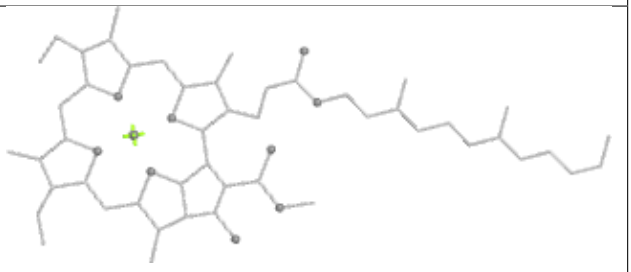
Bond lengths



Bond angles

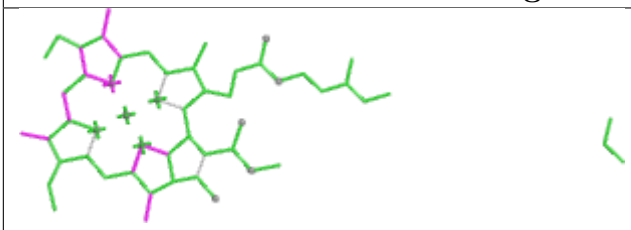


Torsions

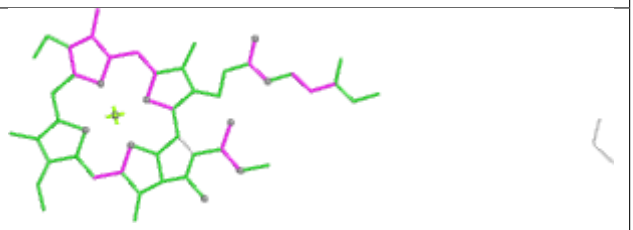


Rings

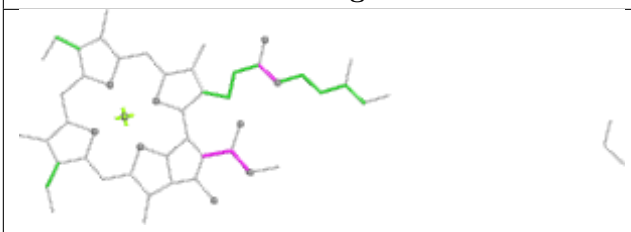
Ligand CLA A 807



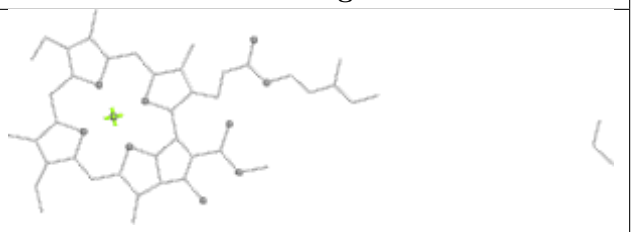
Bond lengths



Bond angles

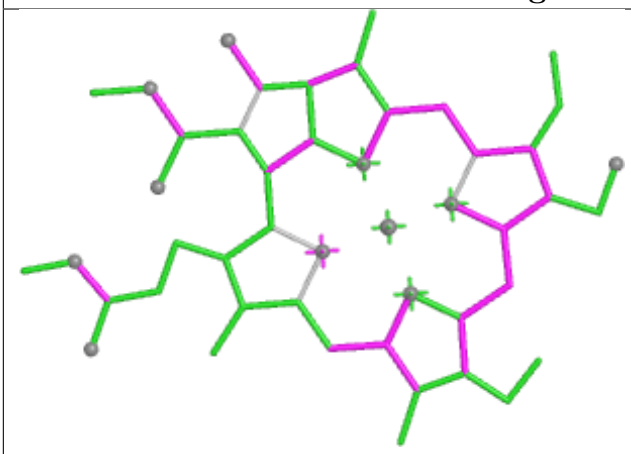


Torsions

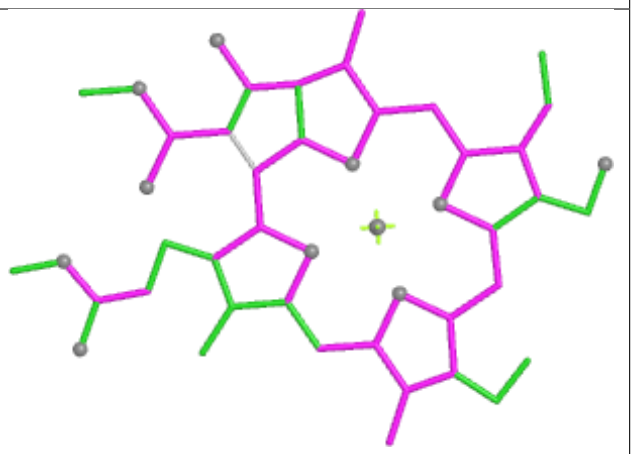


Rings

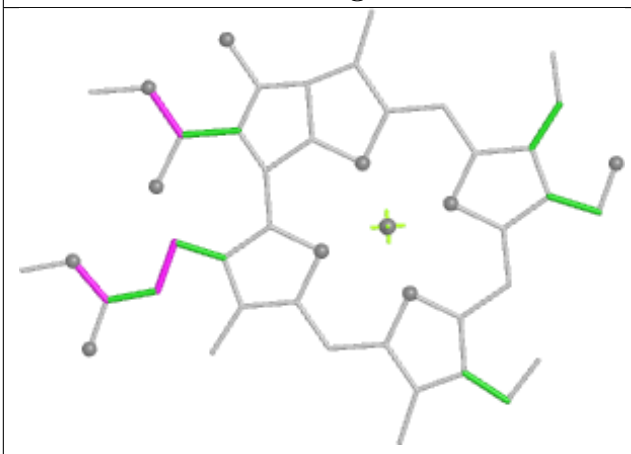
Ligand CHL e 607



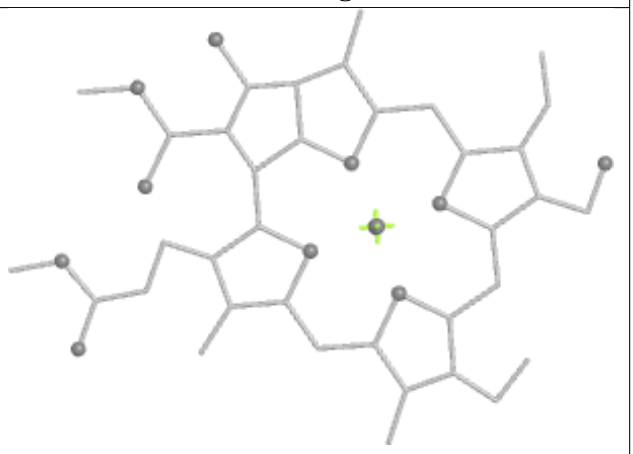
Bond lengths



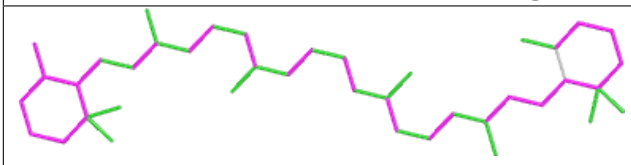
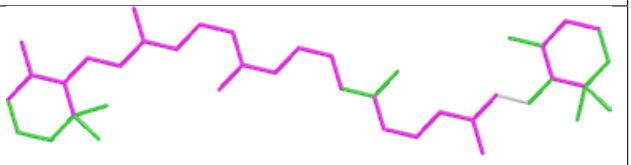
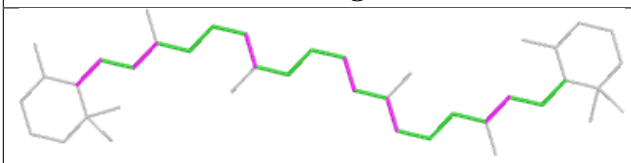
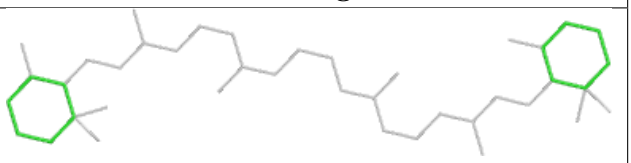
Bond angles

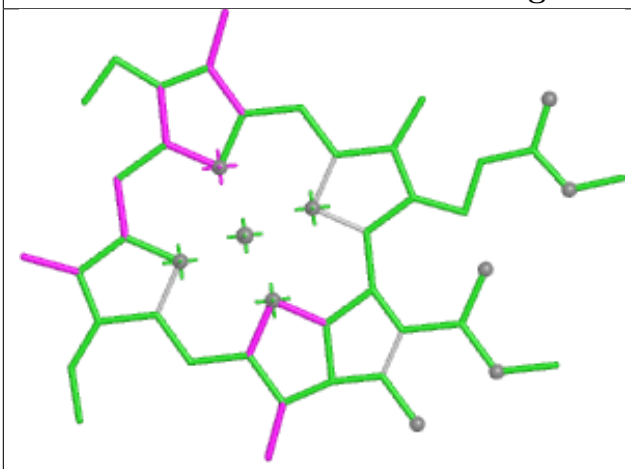
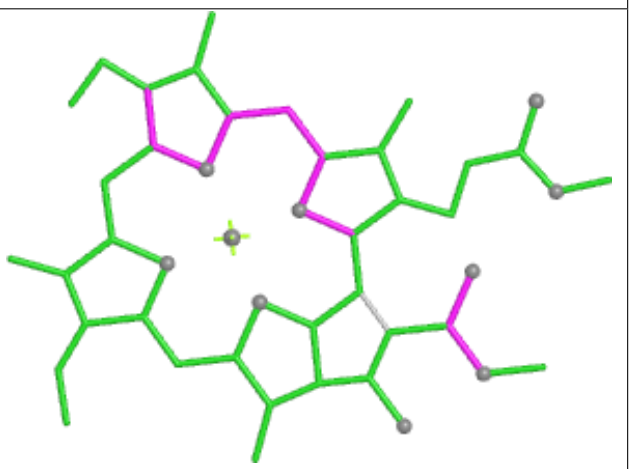
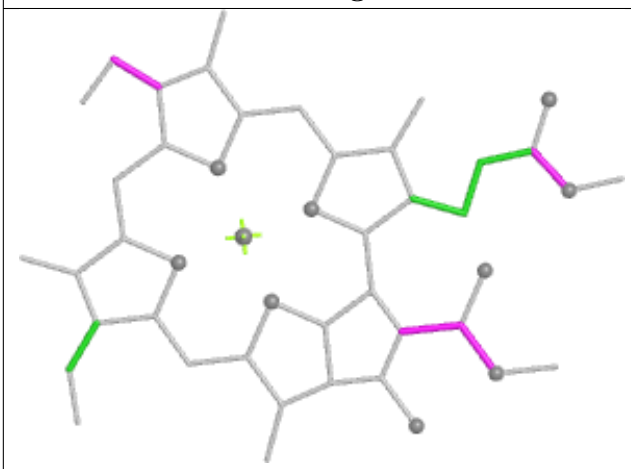
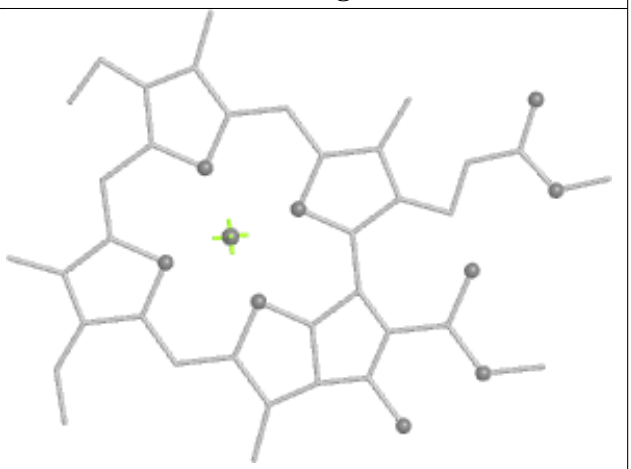


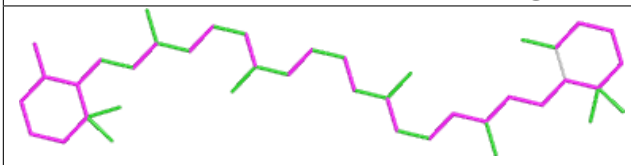
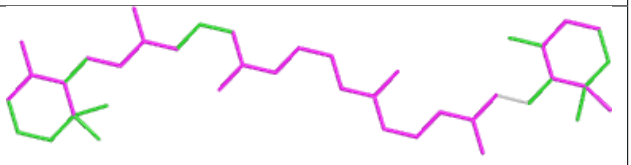
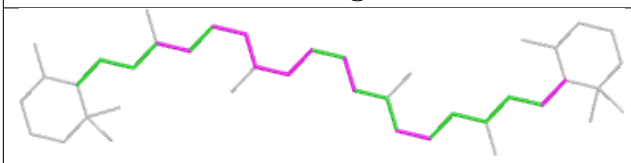
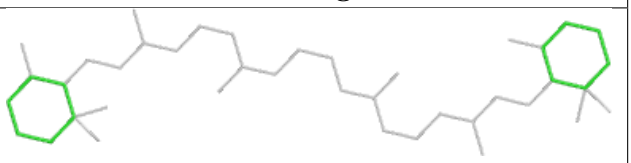
Torsions

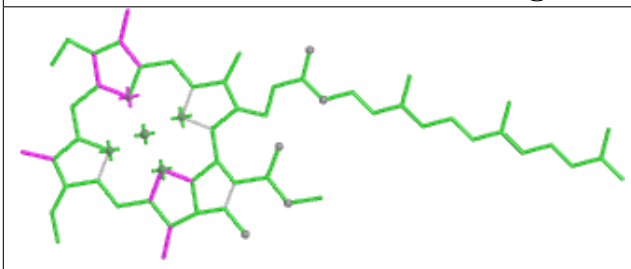
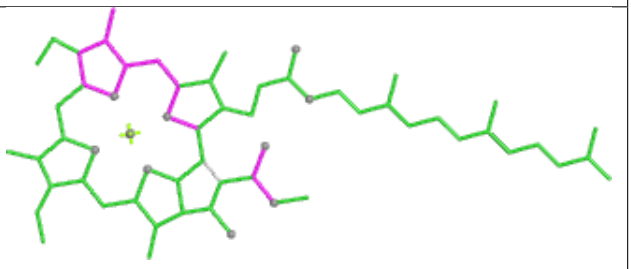
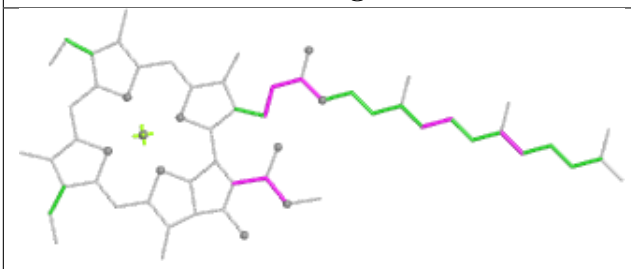
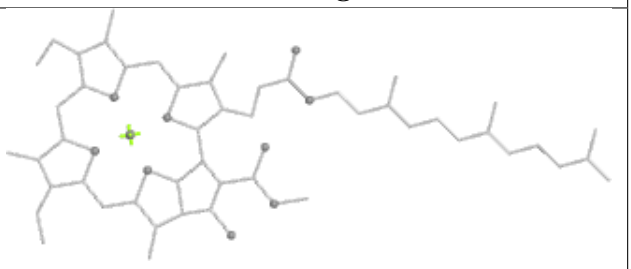


Rings

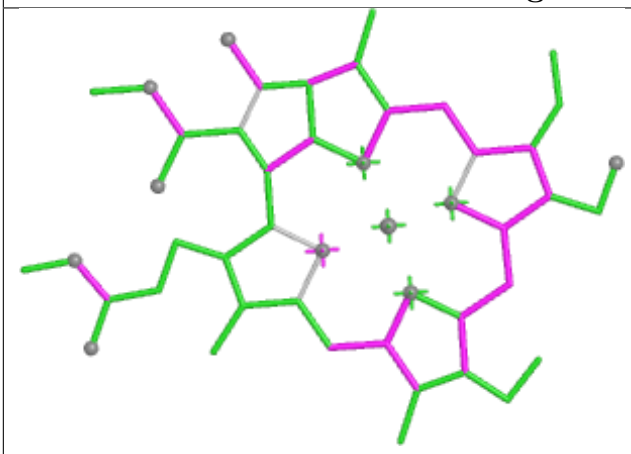
Ligand 8CT A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

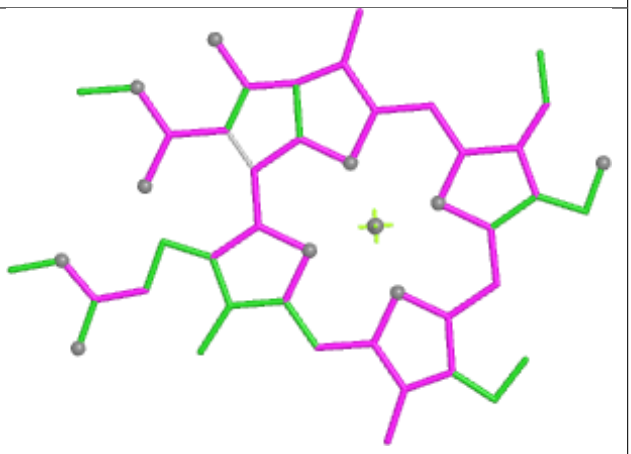
Ligand 8CT B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

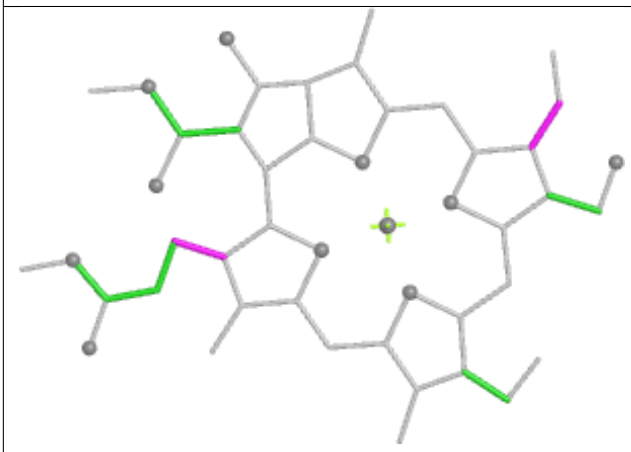
Ligand CHL h 609



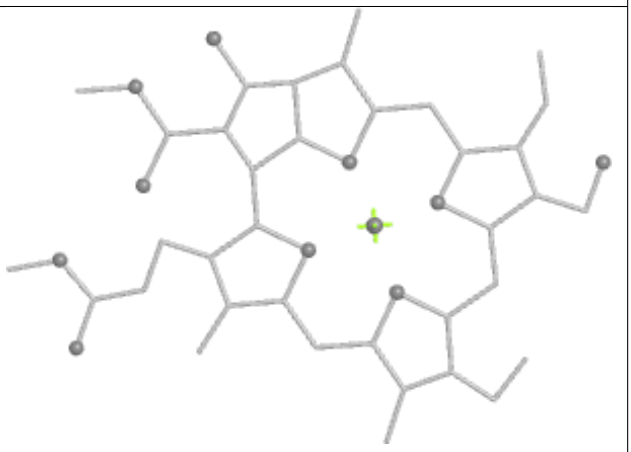
Bond lengths



Bond angles

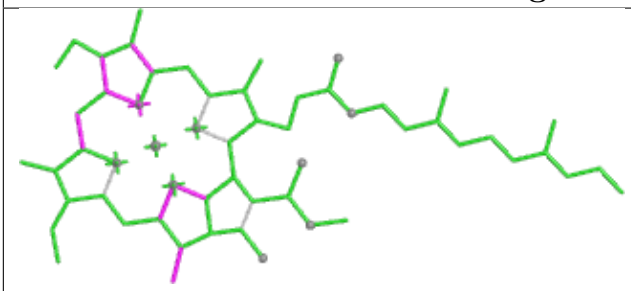


Torsions

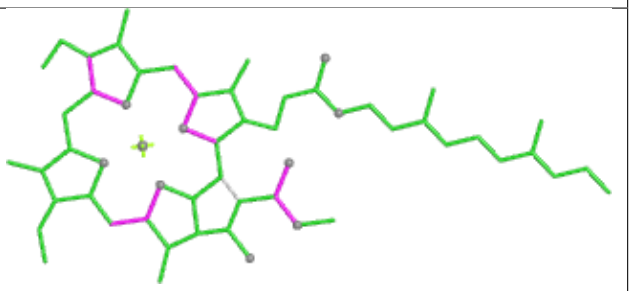


Rings

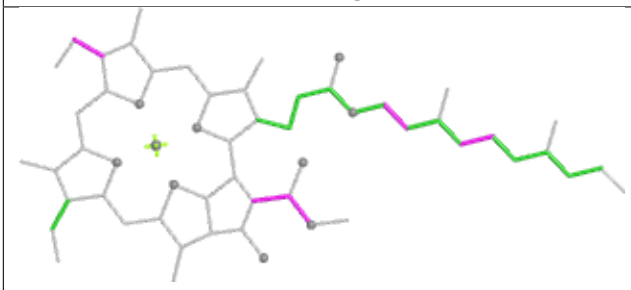
Ligand CLA e 603



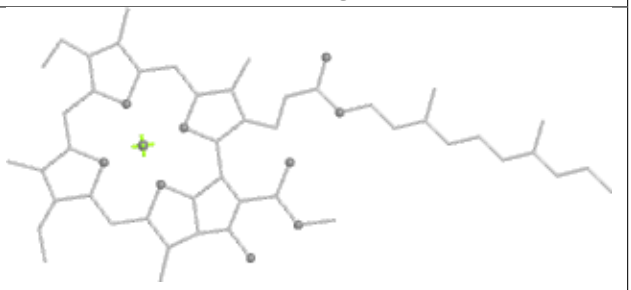
Bond lengths



Bond angles

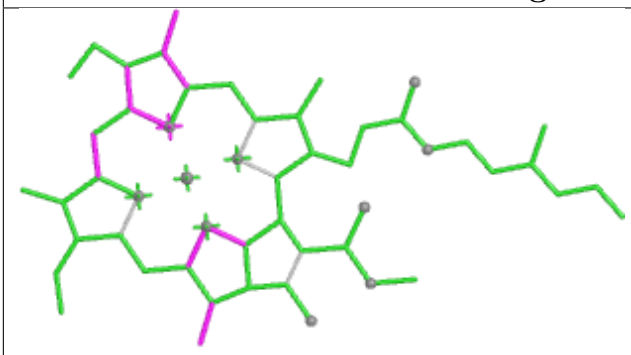


Torsions

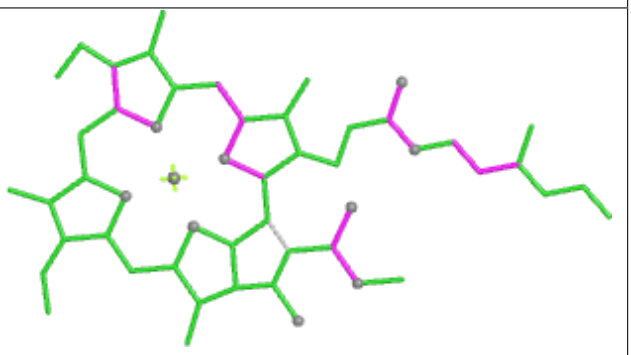


Rings

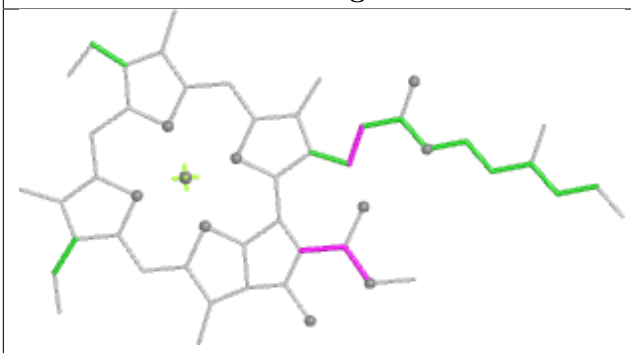
Ligand CLA c 603



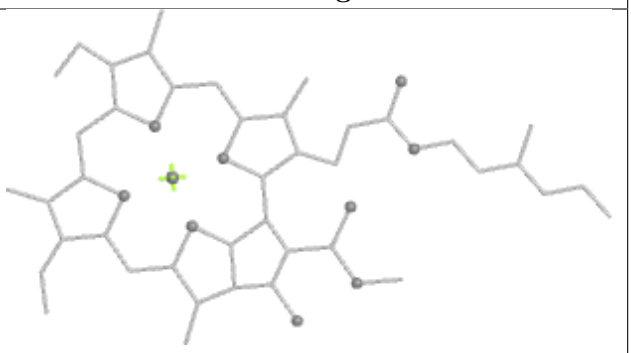
Bond lengths



Bond angles

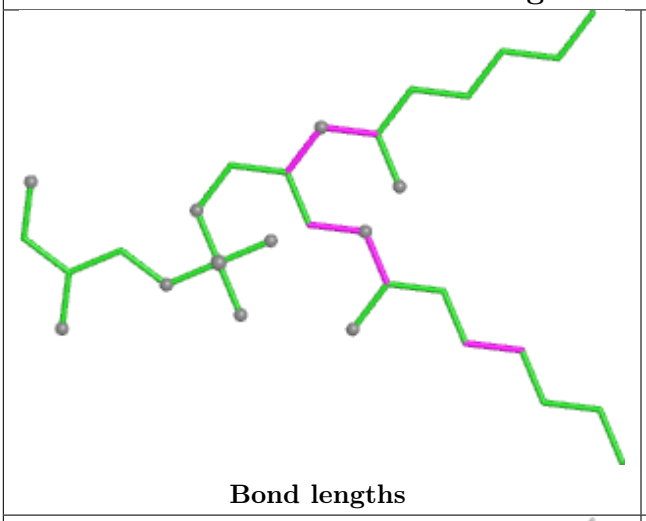


Torsions

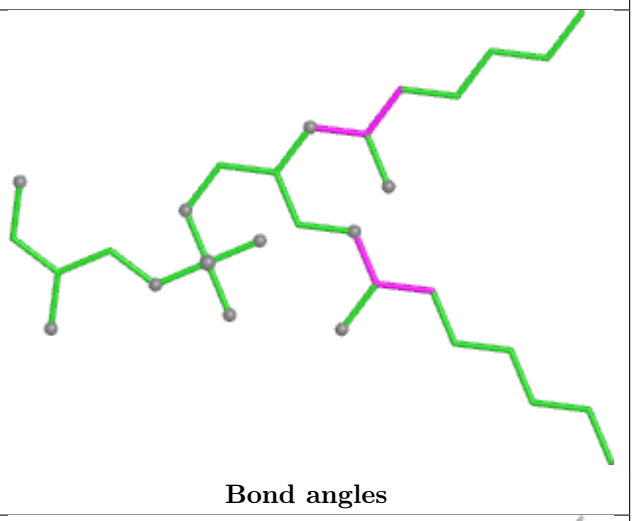


Rings

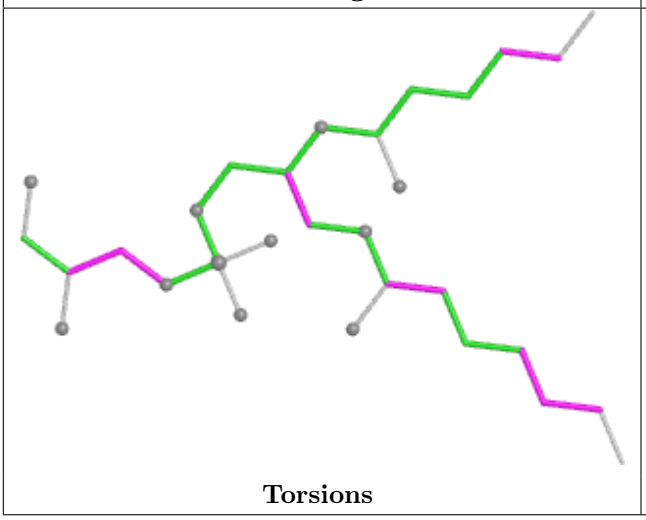
Ligand LHG 7 601



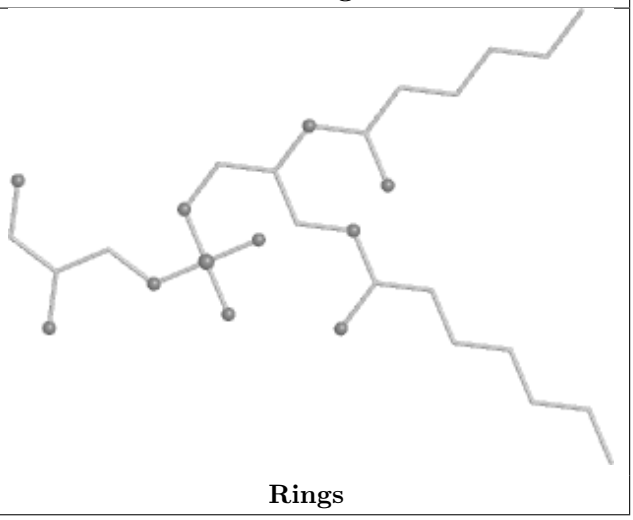
Bond lengths



Bond angles



Torsions

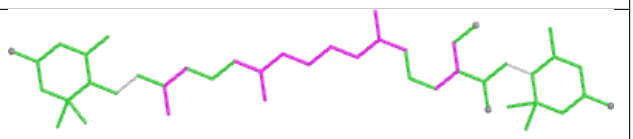


Rings

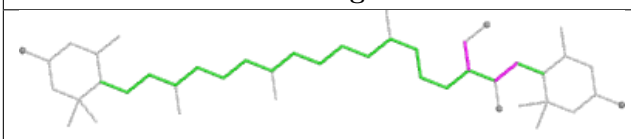
Ligand 0IE b 522



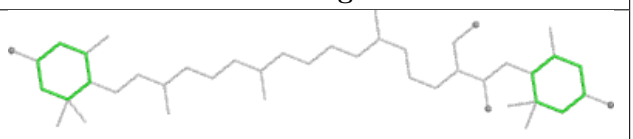
Bond lengths



Bond angles

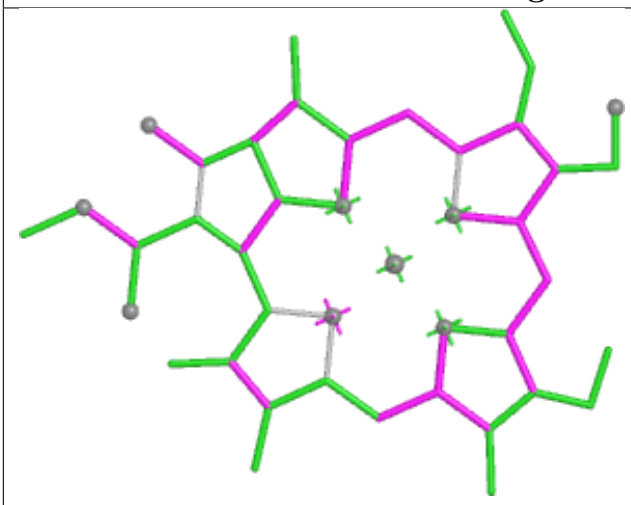


Torsions

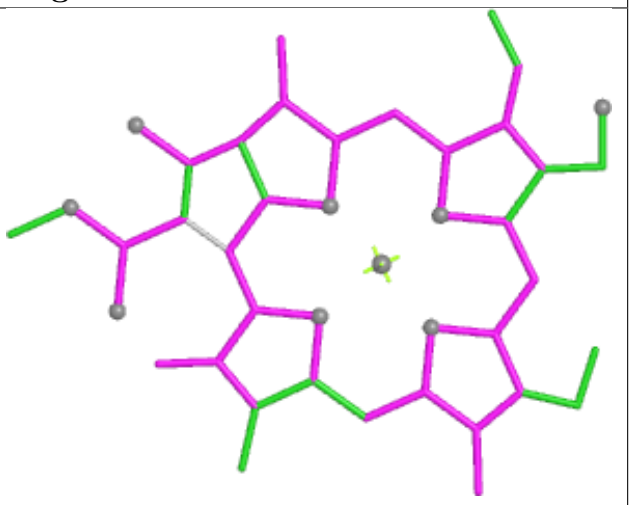


Rings

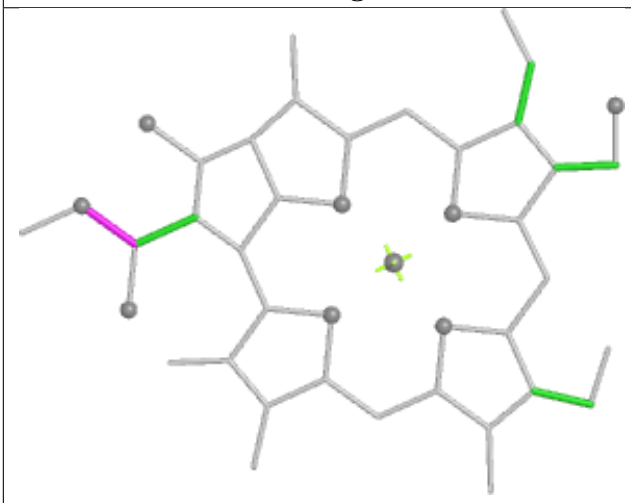
Ligand CHL g 614



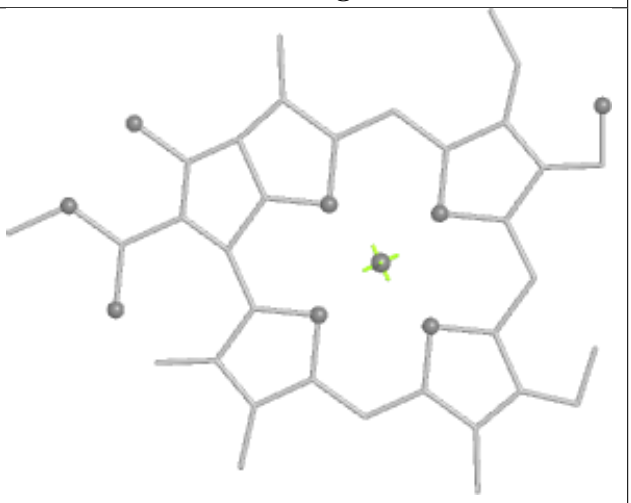
Bond lengths



Bond angles

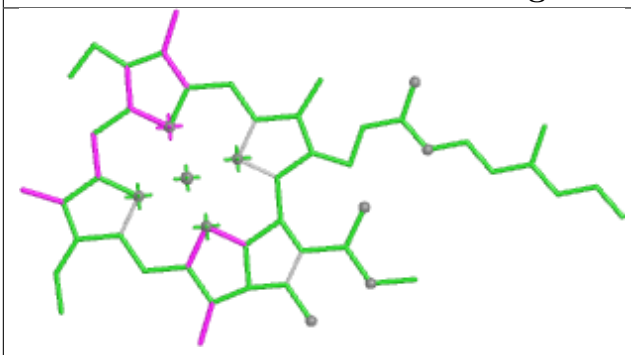


Torsions

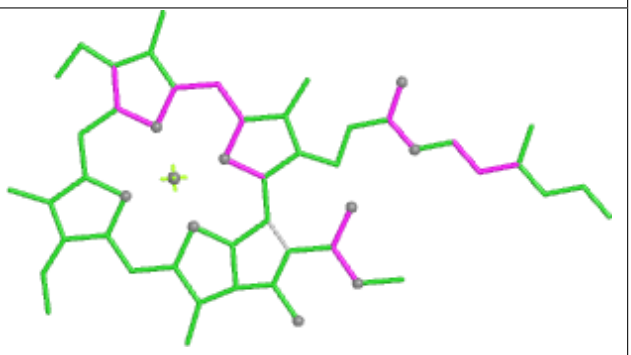


Rings

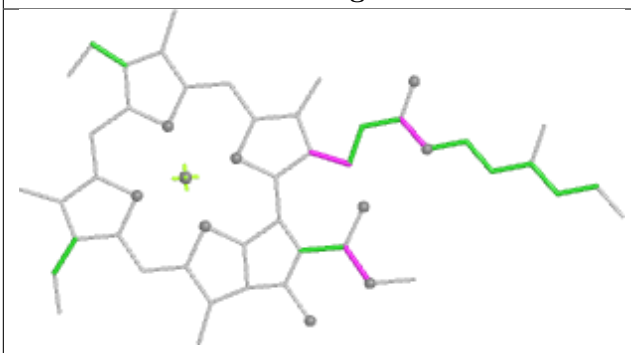
Ligand CLA 9 311



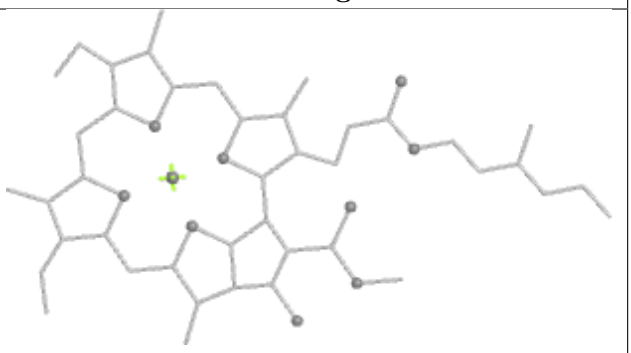
Bond lengths



Bond angles

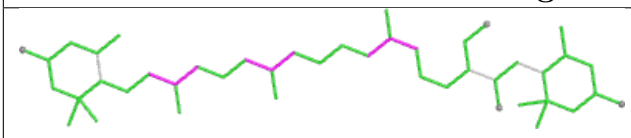


Torsions

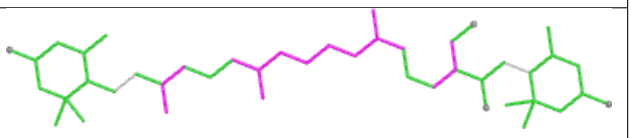


Rings

Ligand 0IE h 521



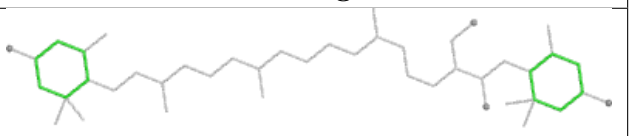
Bond lengths



Bond angles

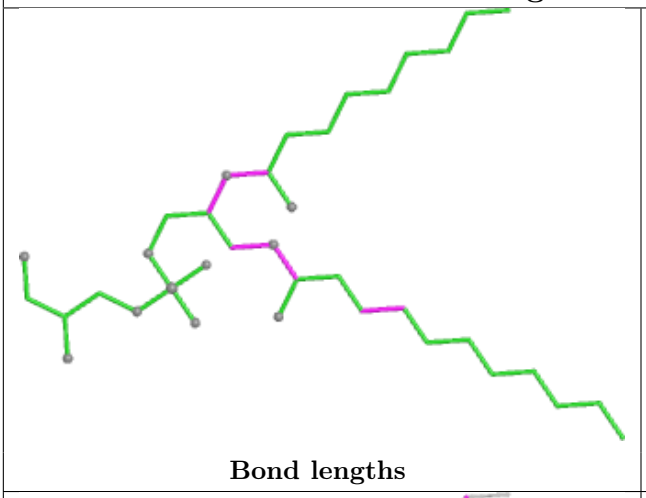


Torsions

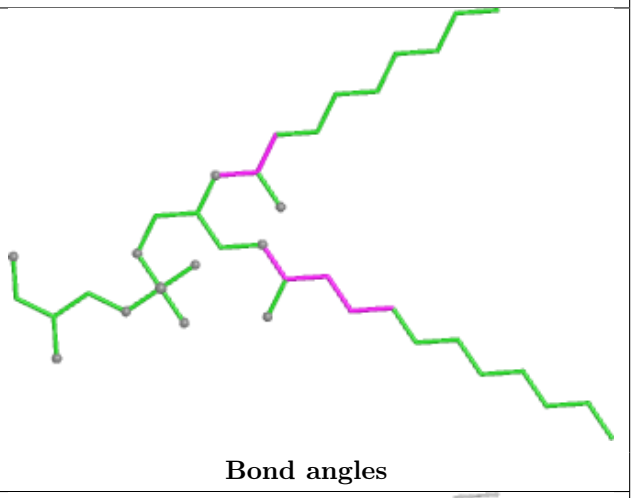


Rings

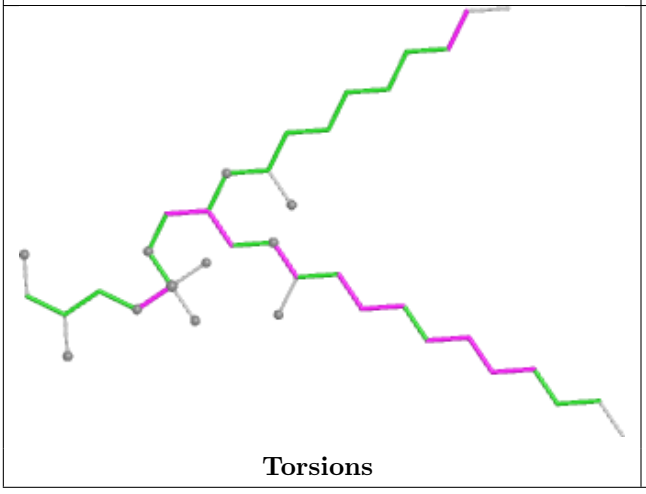
Ligand LHG 5 601



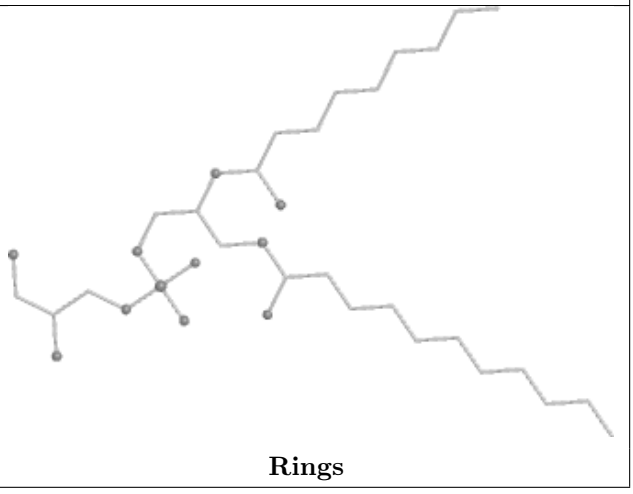
Bond lengths



Bond angles

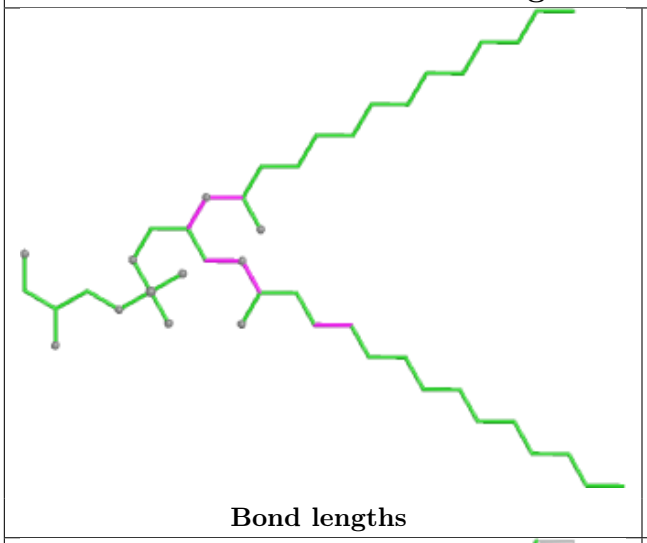


Torsions

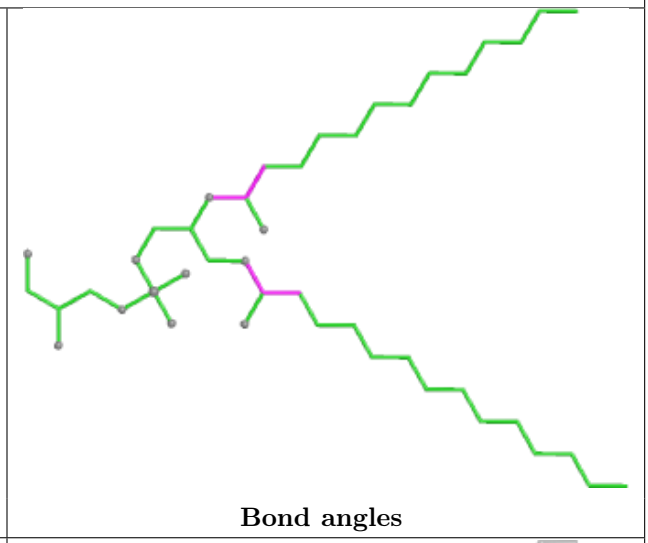


Rings

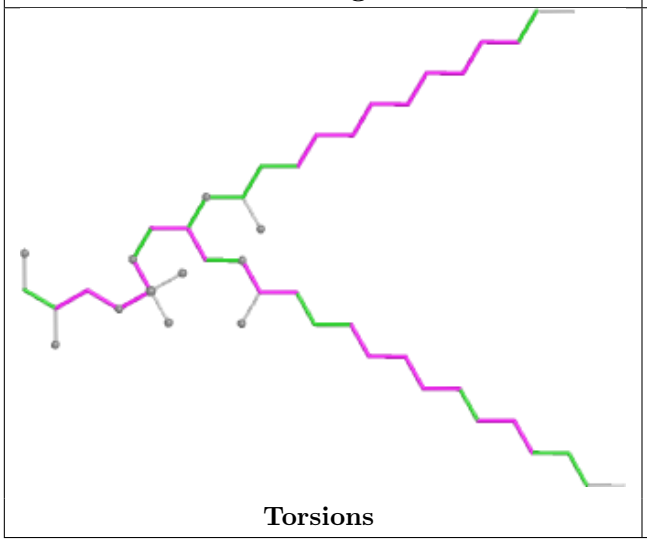
Ligand LHG 8 601



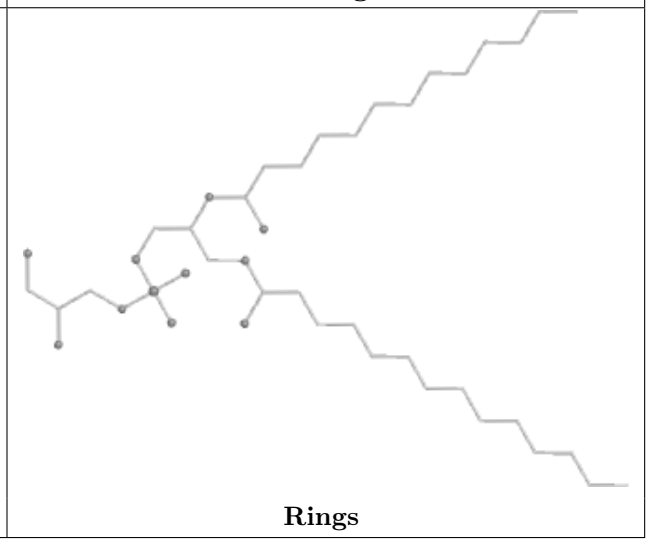
Bond lengths



Bond angles

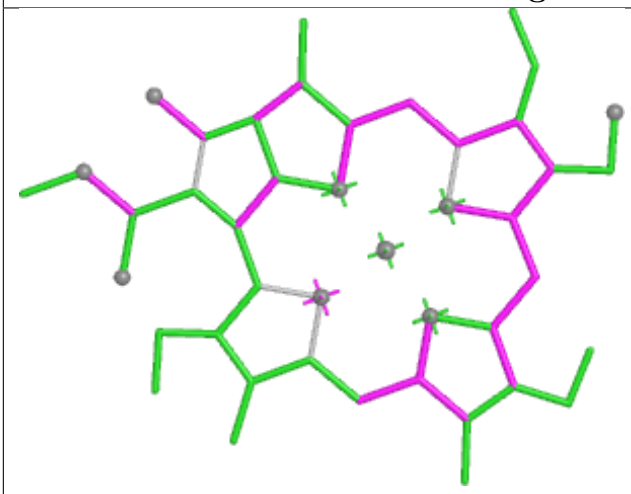


Torsions

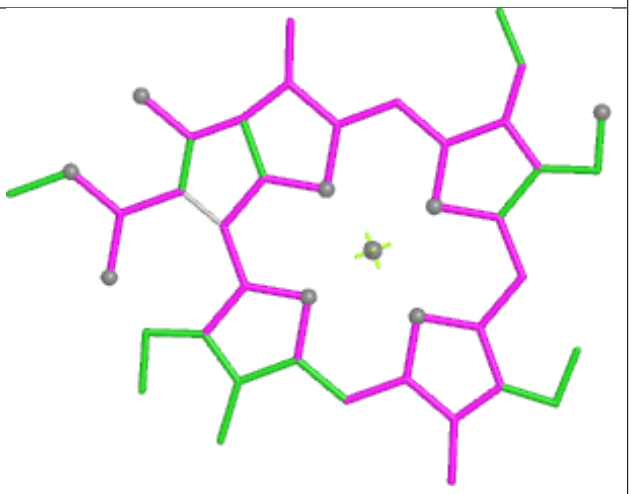


Rings

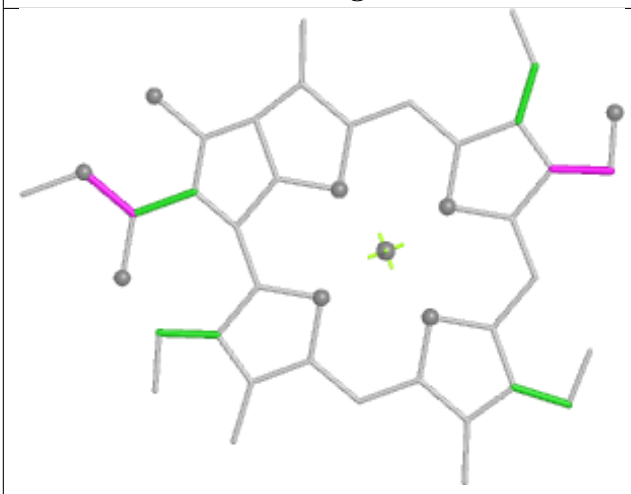
Ligand CHL e 605



Bond lengths



Bond angles

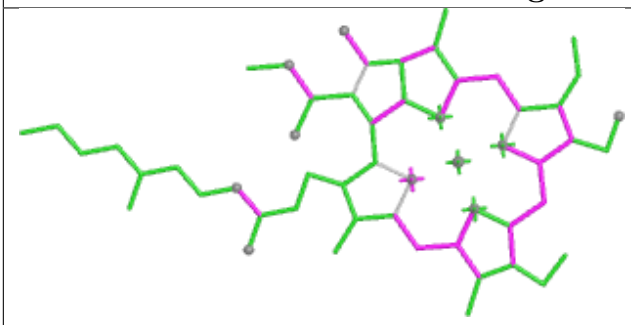


Torsions

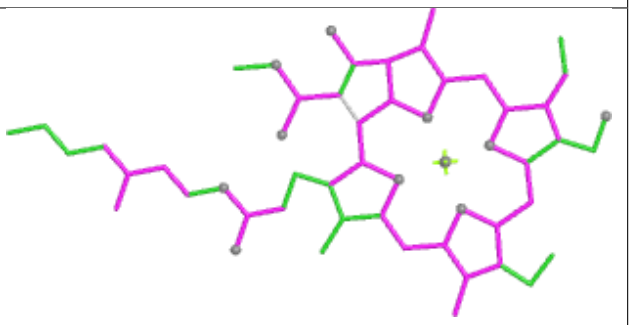


Rings

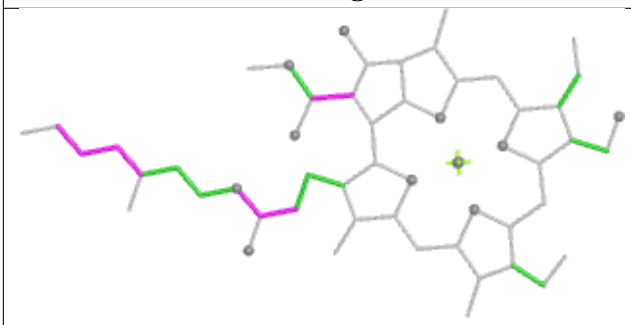
Ligand CHL 4 319



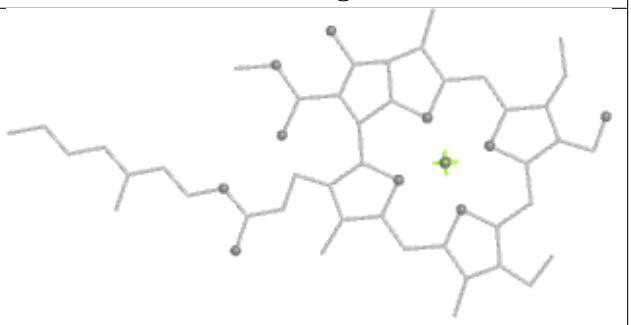
Bond lengths



Bond angles

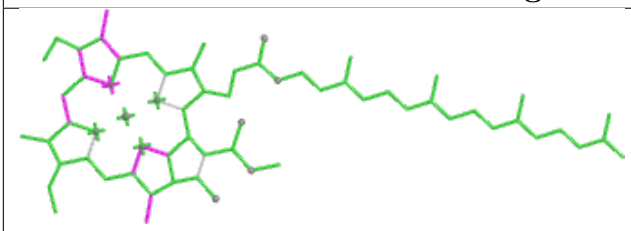


Torsions

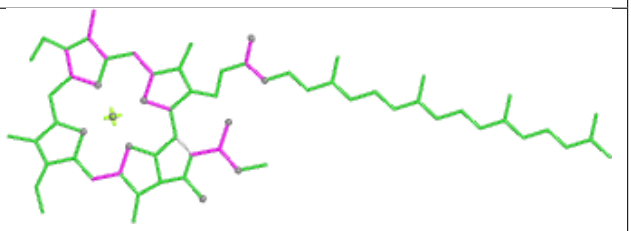


Rings

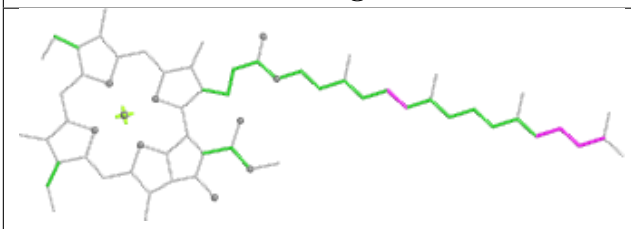
Ligand CLA B 837



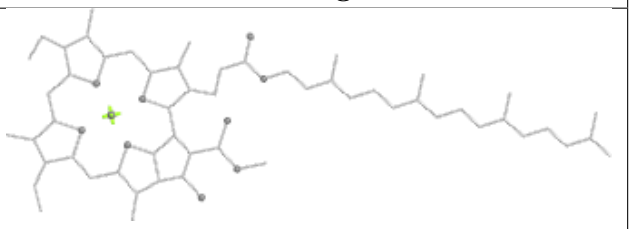
Bond lengths



Bond angles

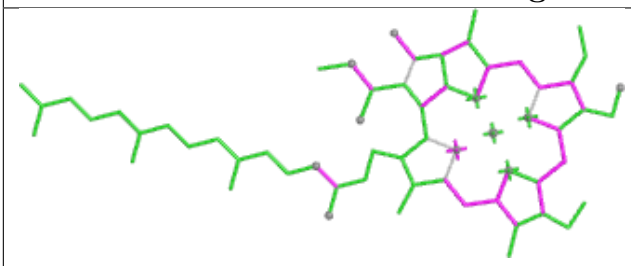


Torsions

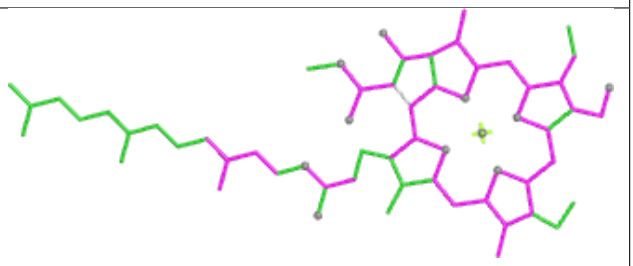


Rings

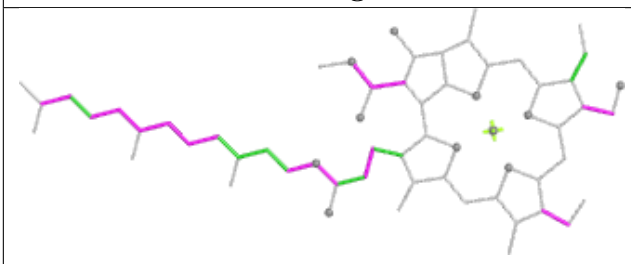
Ligand CHL c 602



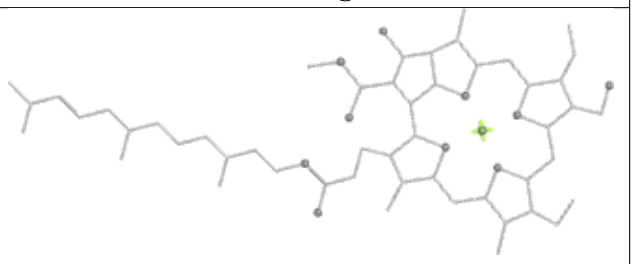
Bond lengths



Bond angles

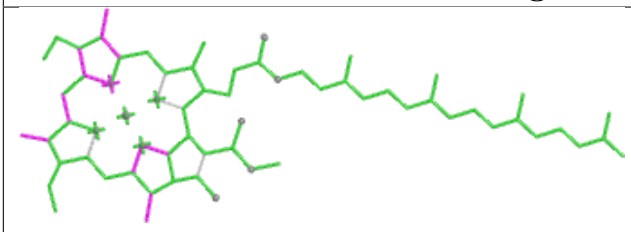


Torsions

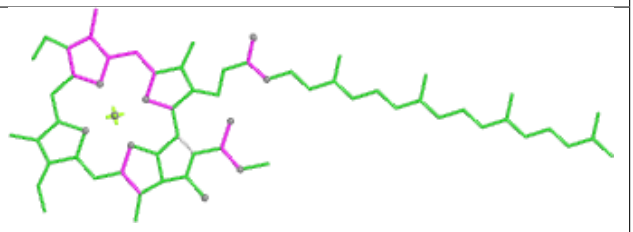


Rings

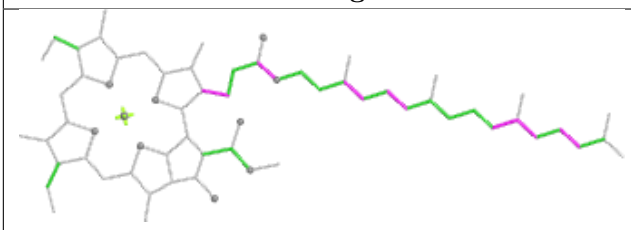
Ligand CLA 3 309



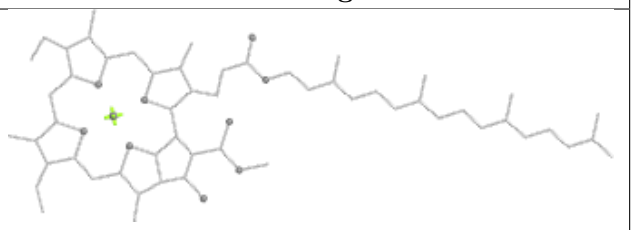
Bond lengths



Bond angles

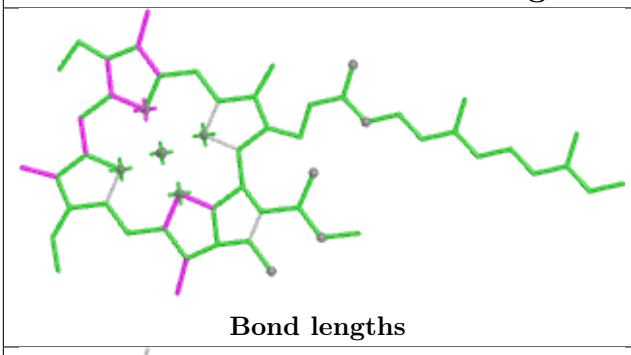


Torsions

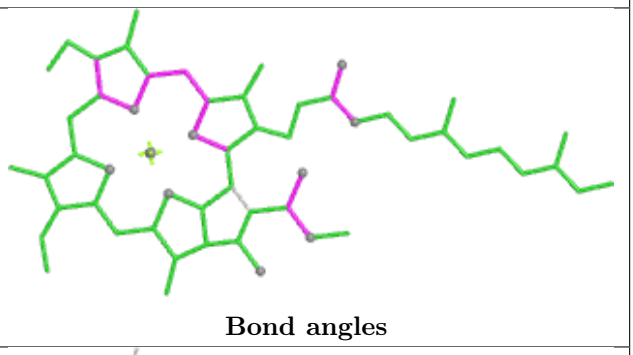


Rings

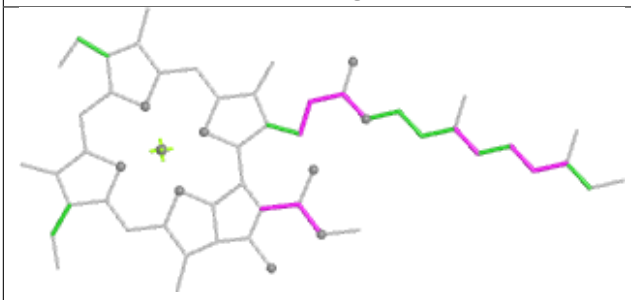
Ligand CLA 1 303



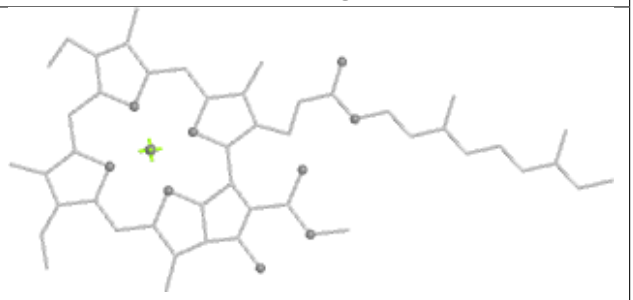
Bond lengths



Bond angles

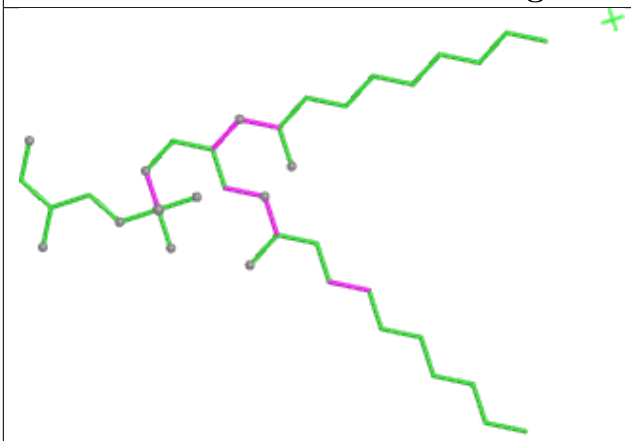


Torsions

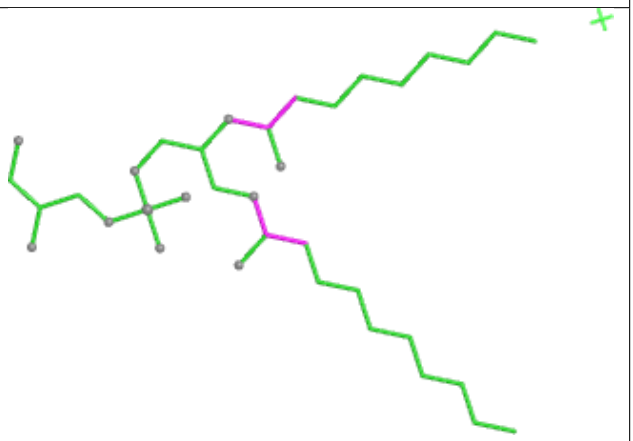


Rings

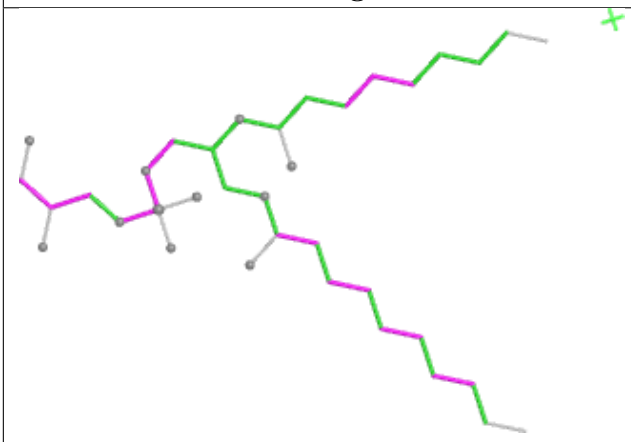
Ligand LHG 3 603



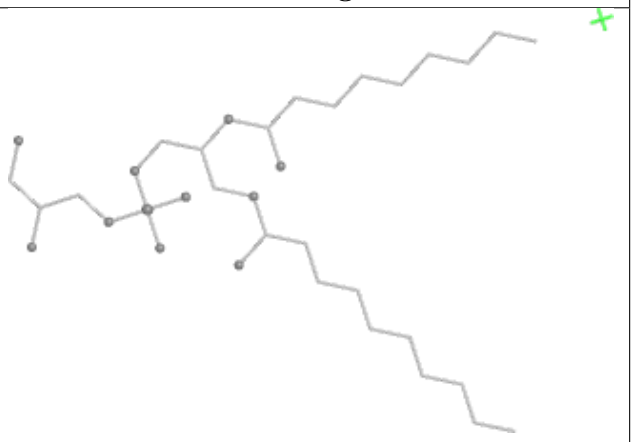
Bond lengths



Bond angles

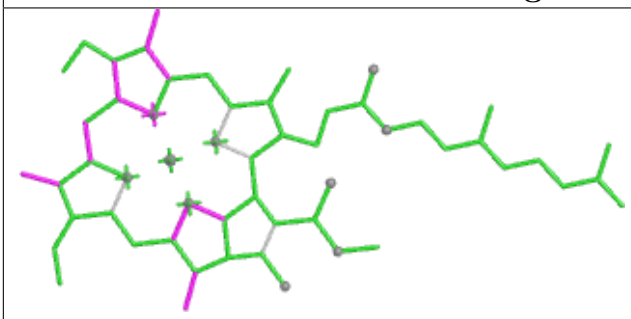


Torsions

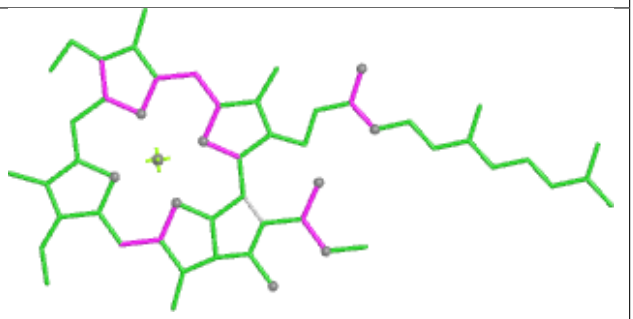


Rings

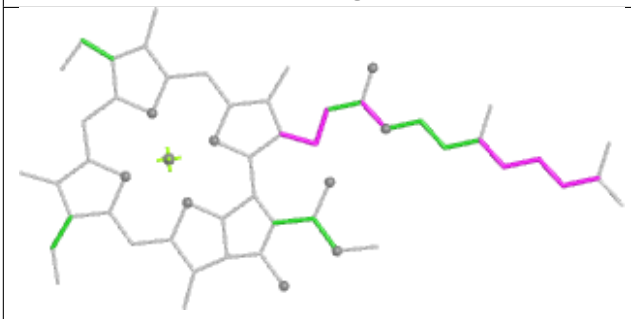
Ligand CLA B 813



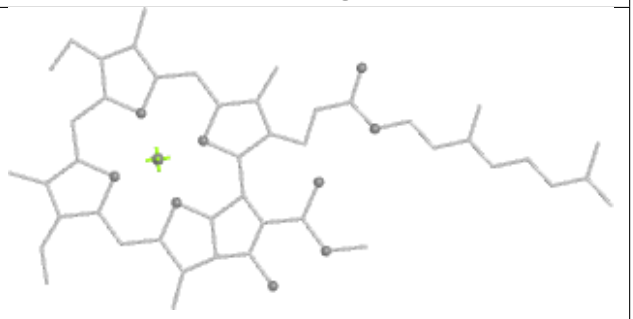
Bond lengths



Bond angles

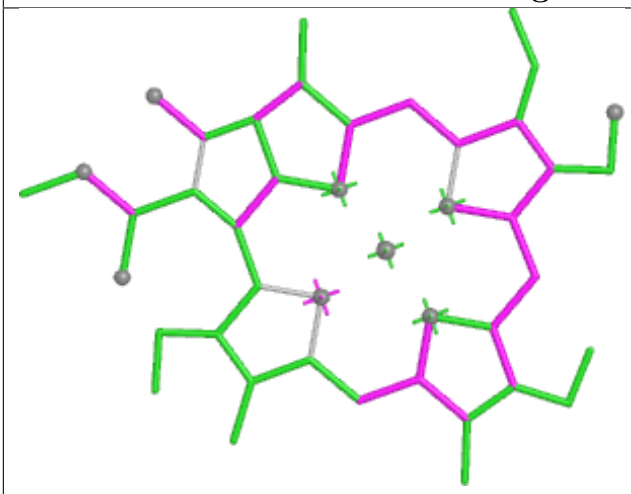


Torsions

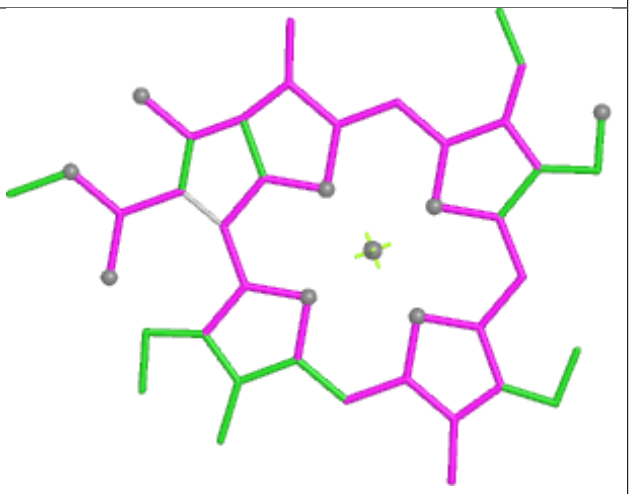


Rings

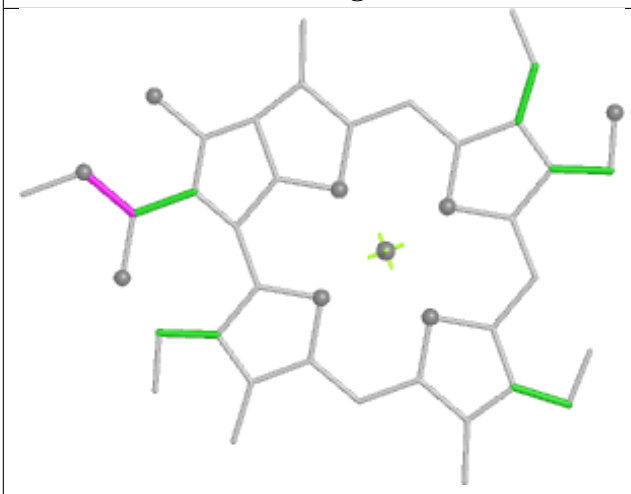
Ligand CHL i 605



Bond lengths



Bond angles

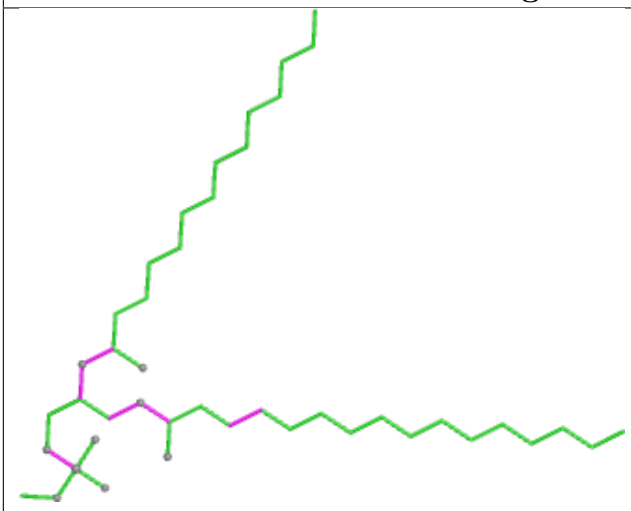


Torsions

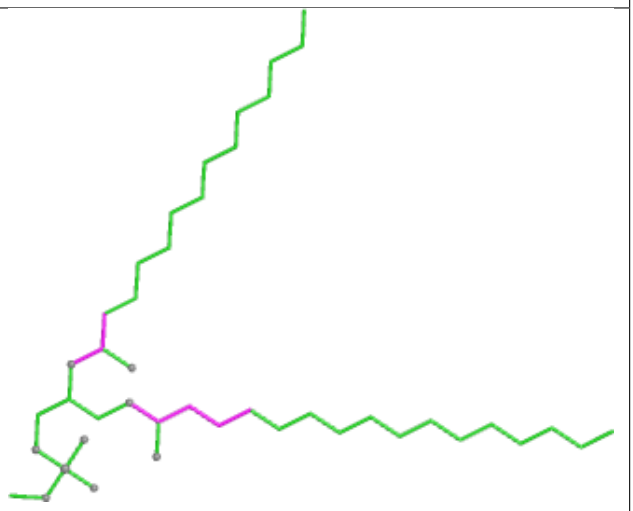


Rings

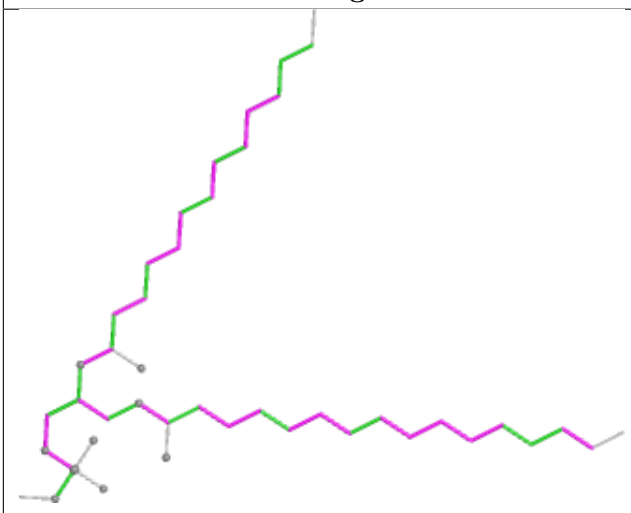
Ligand LHG K 106



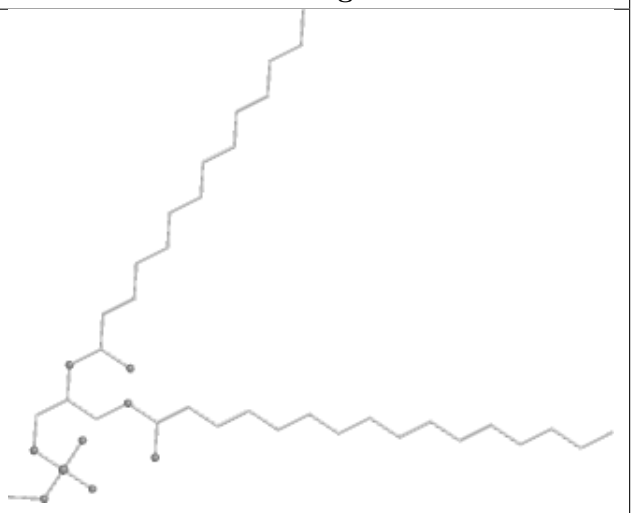
Bond lengths



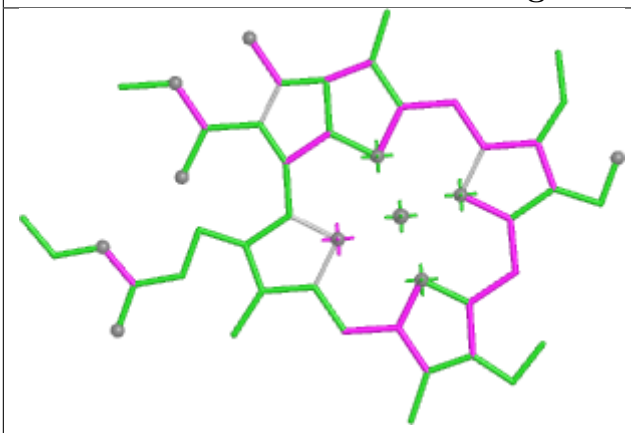
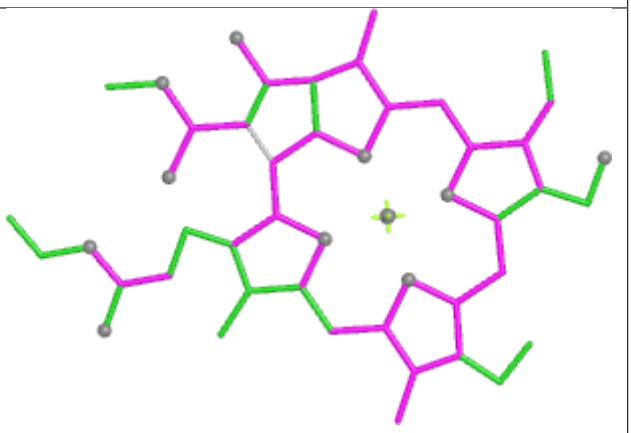
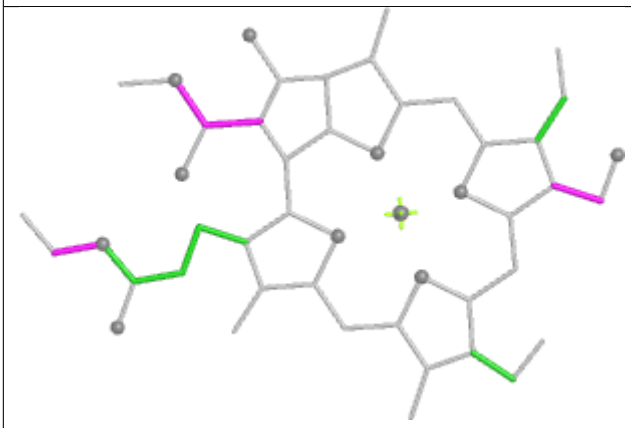
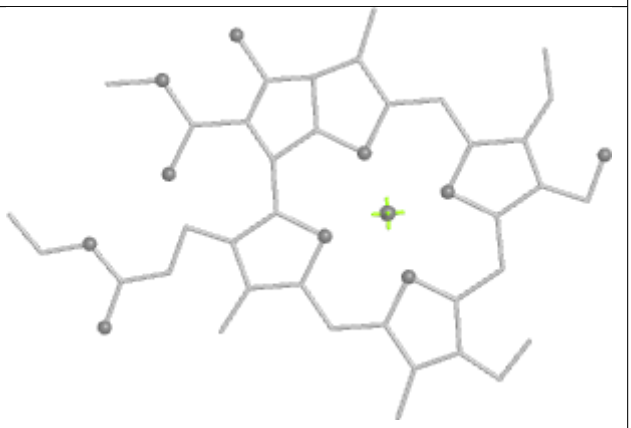
Bond angles

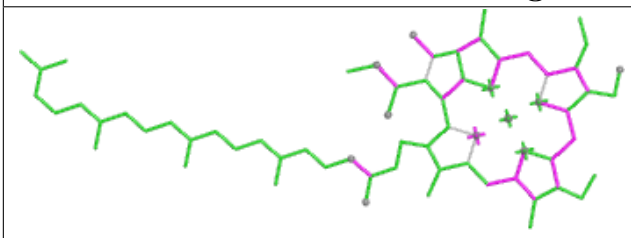
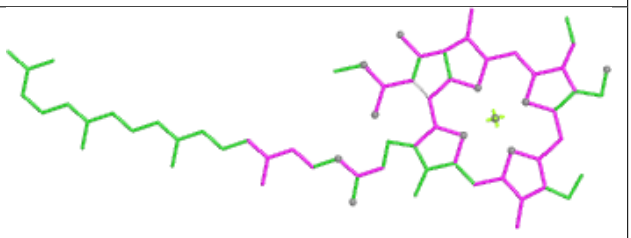
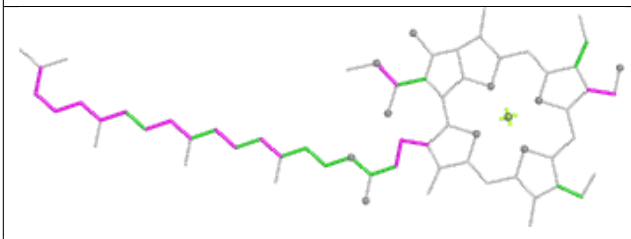
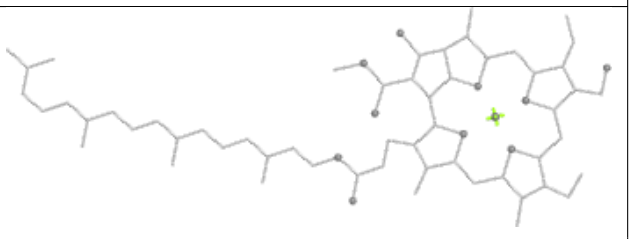


Torsions

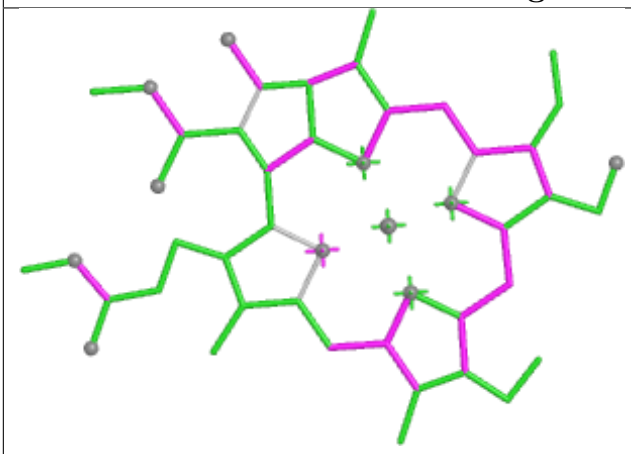


Rings

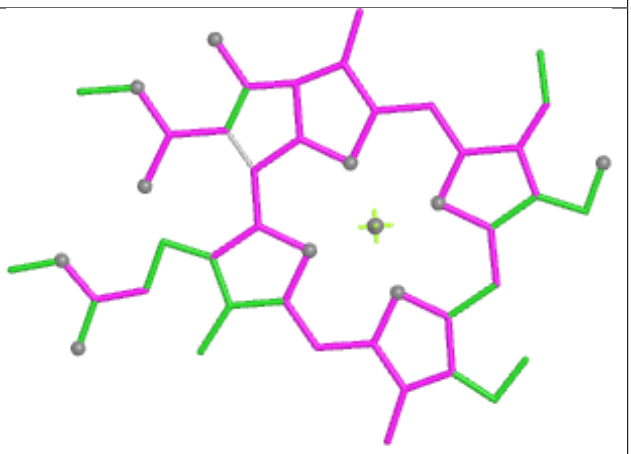
Ligand CHL 1 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

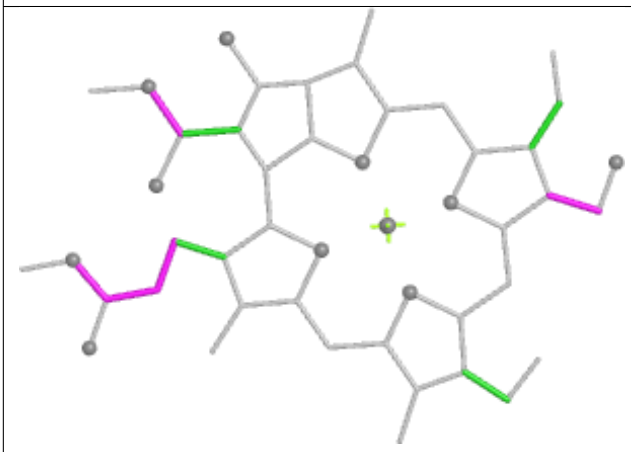
Ligand CHL 8 305



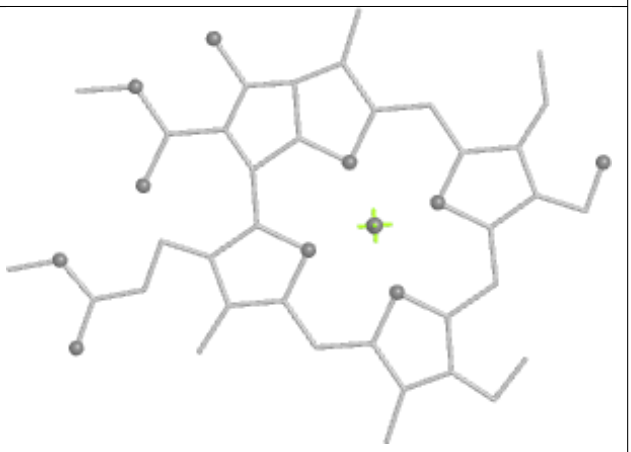
Bond lengths



Bond angles

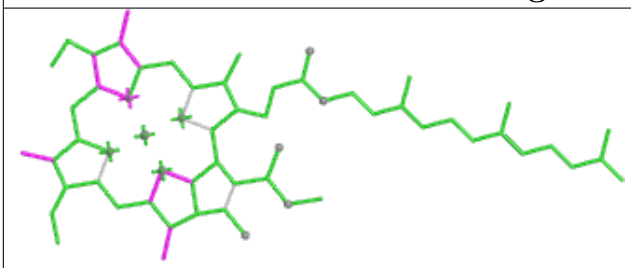


Torsions

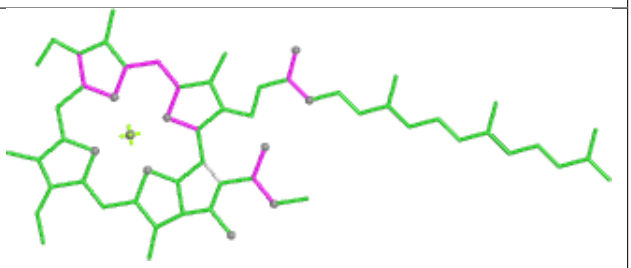


Rings

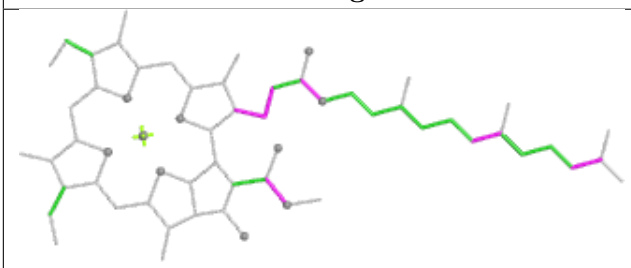
Ligand CLA 7 318



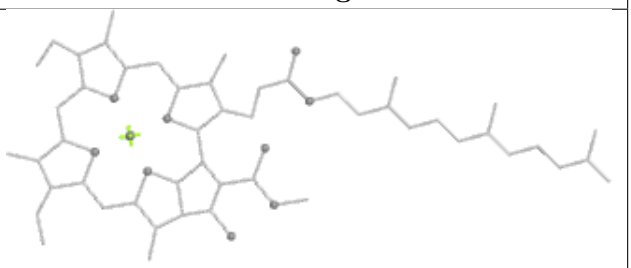
Bond lengths



Bond angles

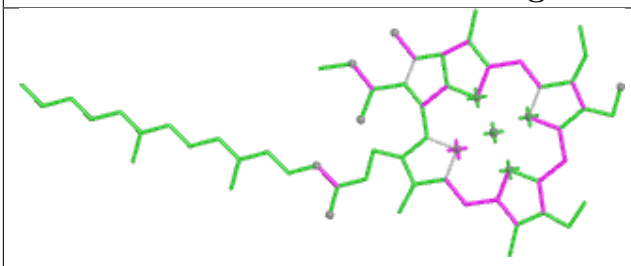


Torsions

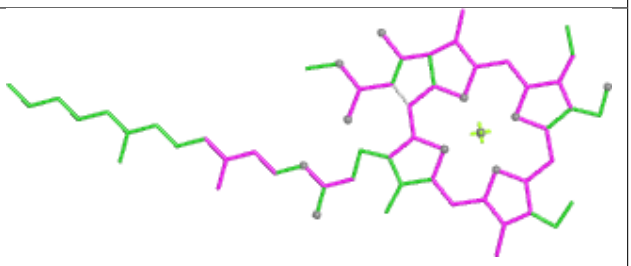


Rings

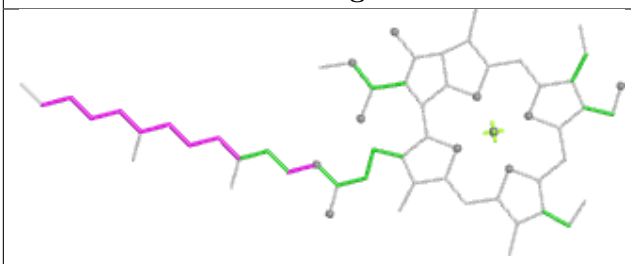
Ligand CHL 6 308



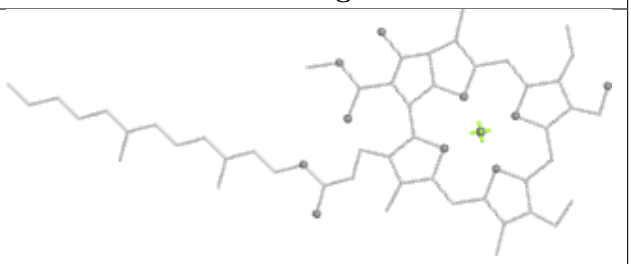
Bond lengths



Bond angles

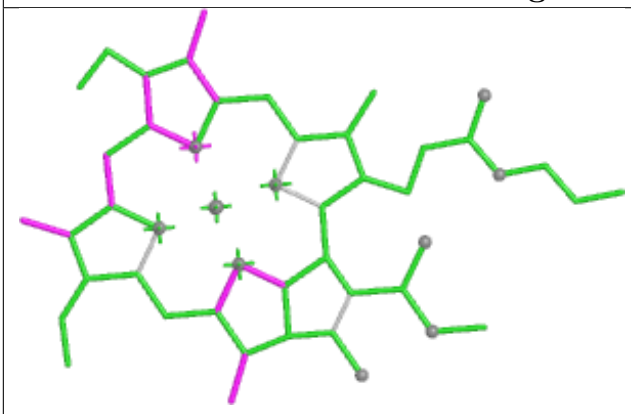


Torsions

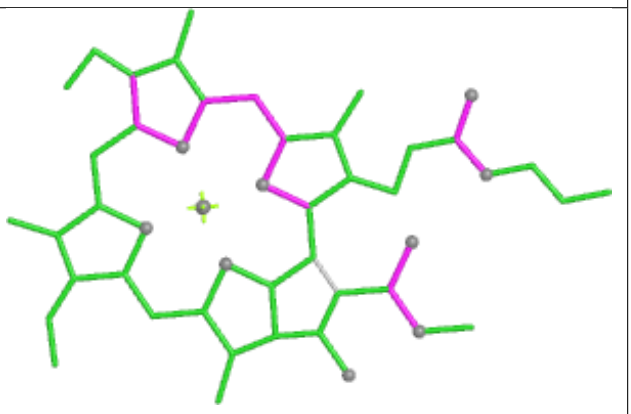


Rings

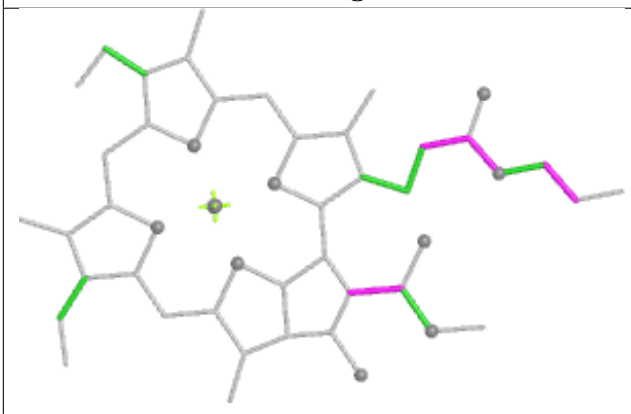
Ligand CLA 4 311



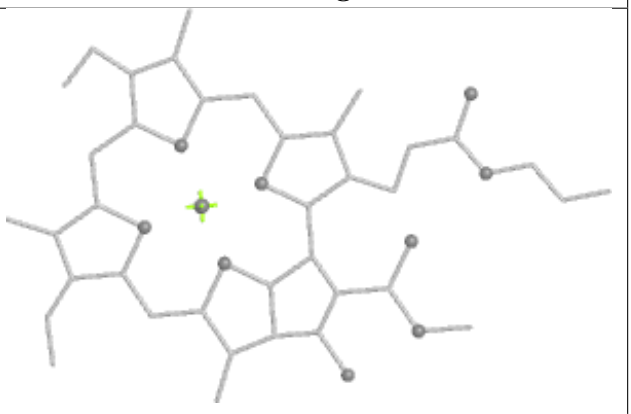
Bond lengths



Bond angles

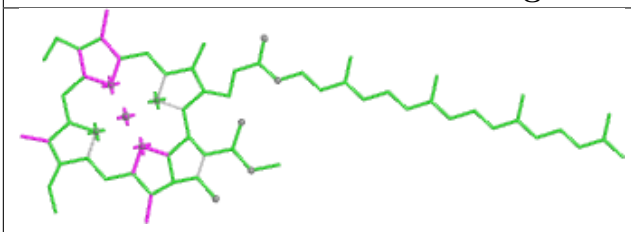


Torsions

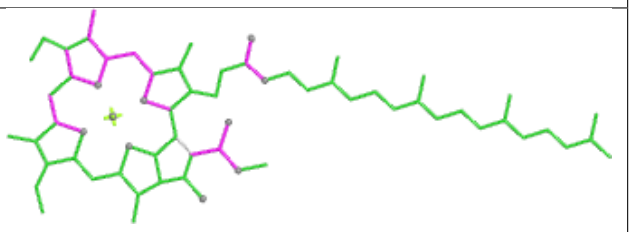


Rings

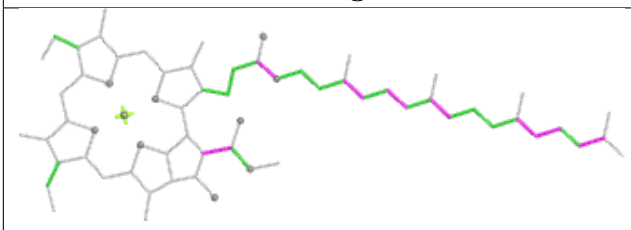
Ligand CLA A 830



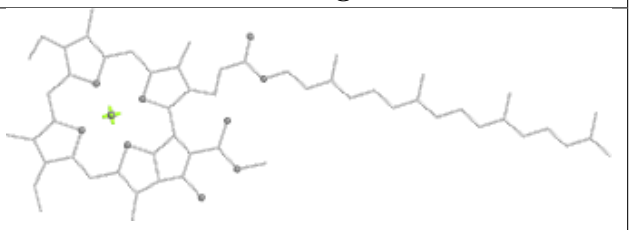
Bond lengths



Bond angles



Torsions



Rings

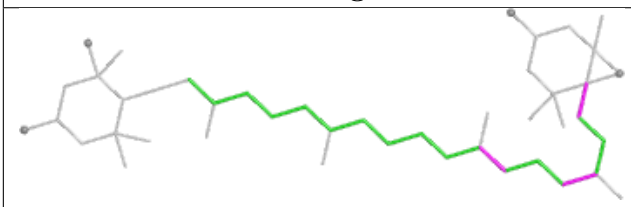
Ligand NEX f 523



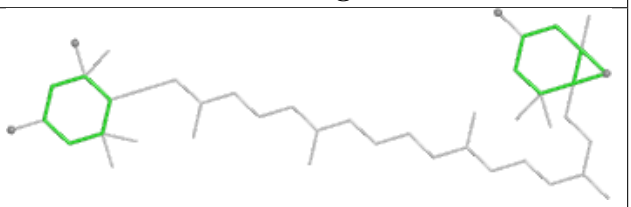
Bond lengths



Bond angles

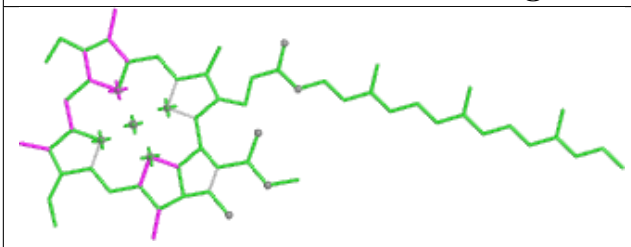


Torsions

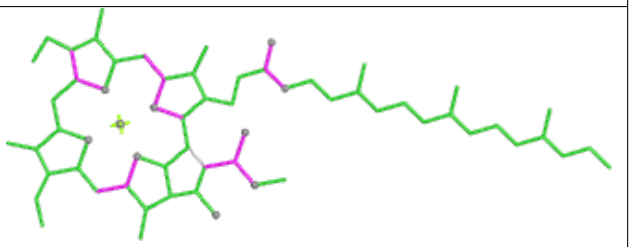


Rings

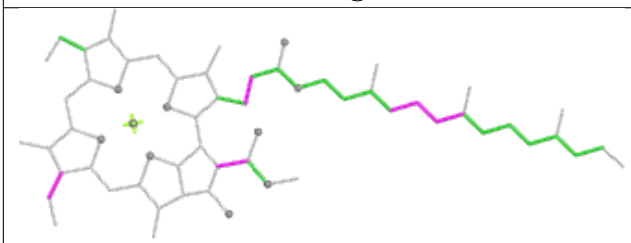
Ligand CLA B 810



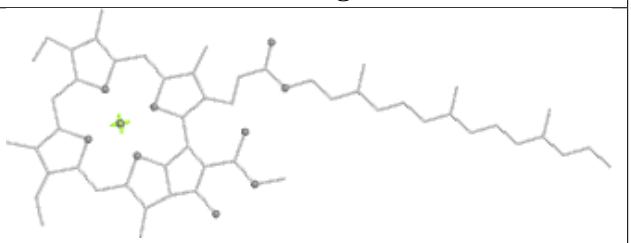
Bond lengths



Bond angles

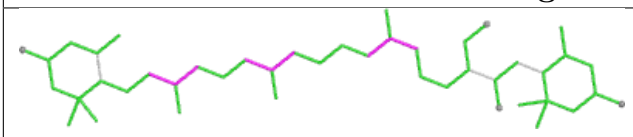


Torsions

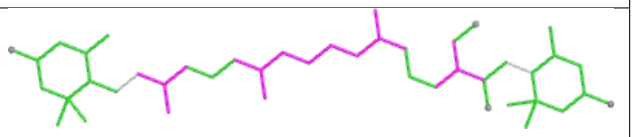


Rings

Ligand 0IE 7 502



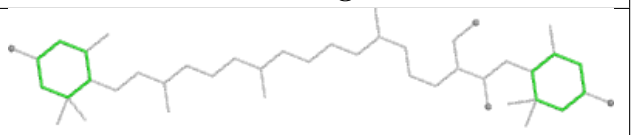
Bond lengths



Bond angles

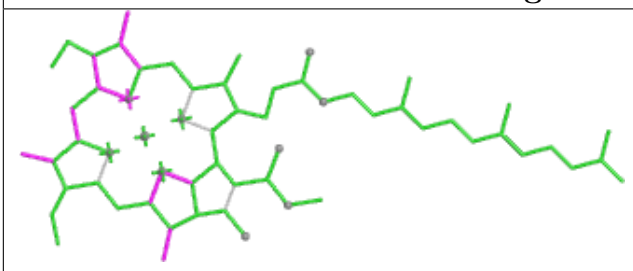


Torsions

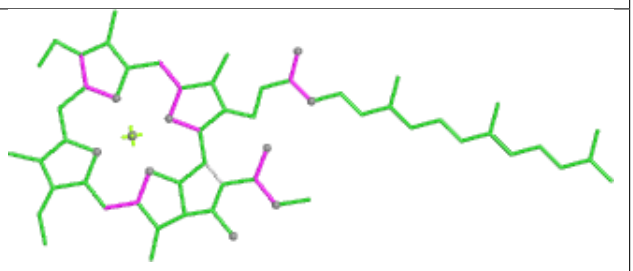


Rings

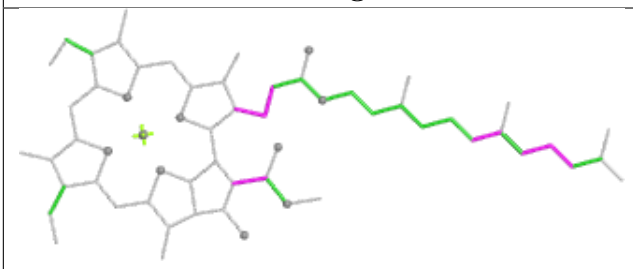
Ligand CLA B 828



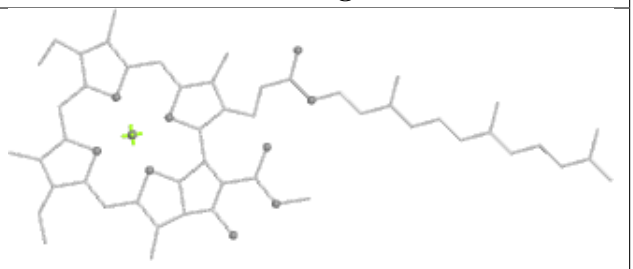
Bond lengths



Bond angles

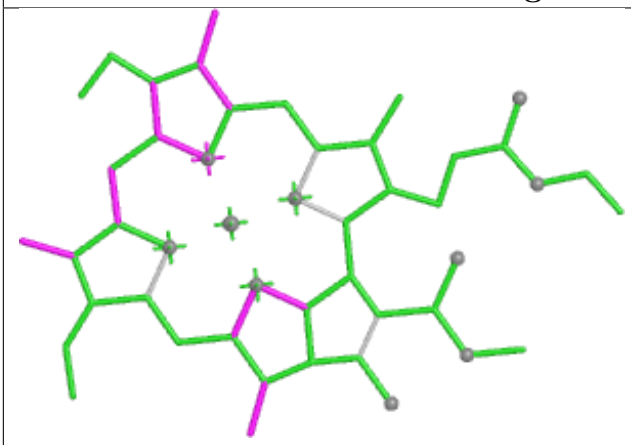


Torsions

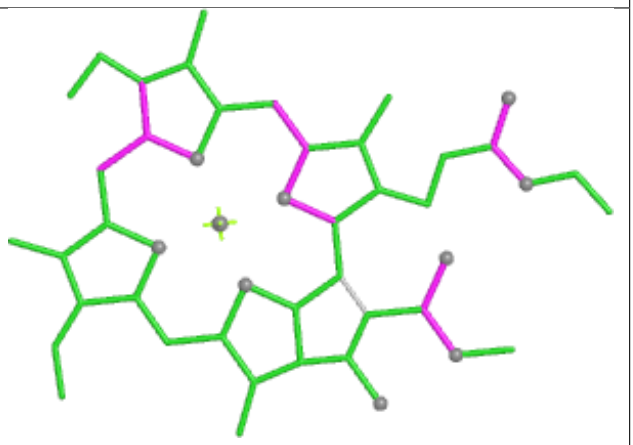


Rings

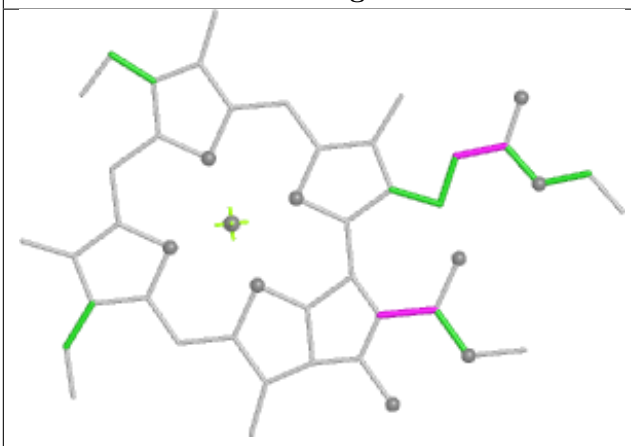
Ligand CLA B 838



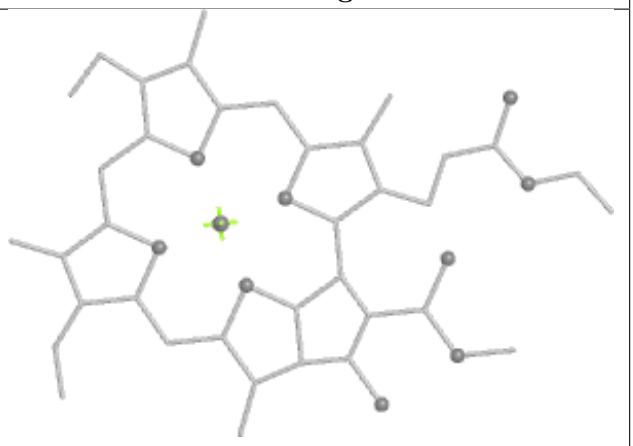
Bond lengths



Bond angles

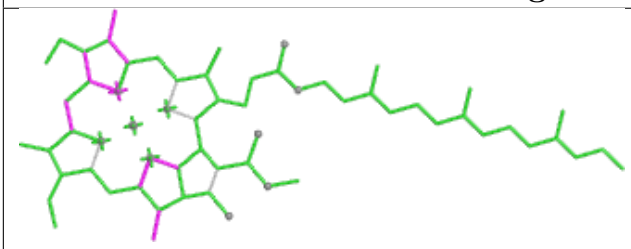


Torsions

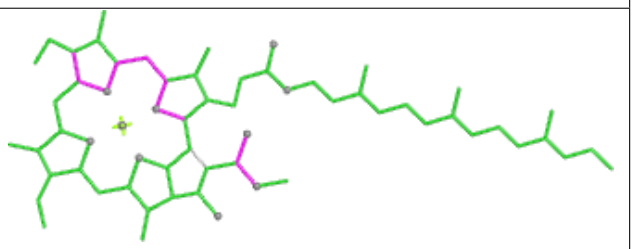


Rings

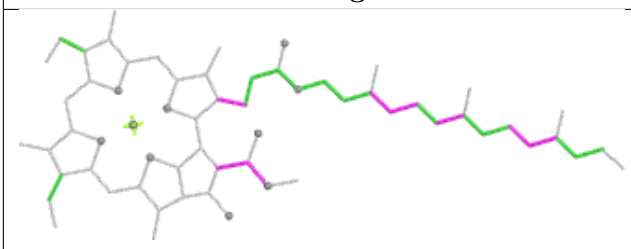
Ligand CLA 0 303



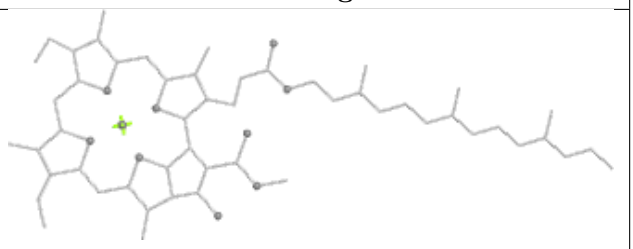
Bond lengths



Bond angles

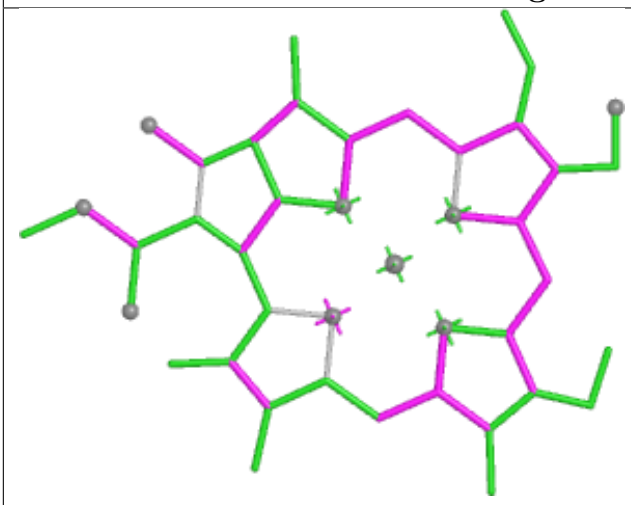


Torsions

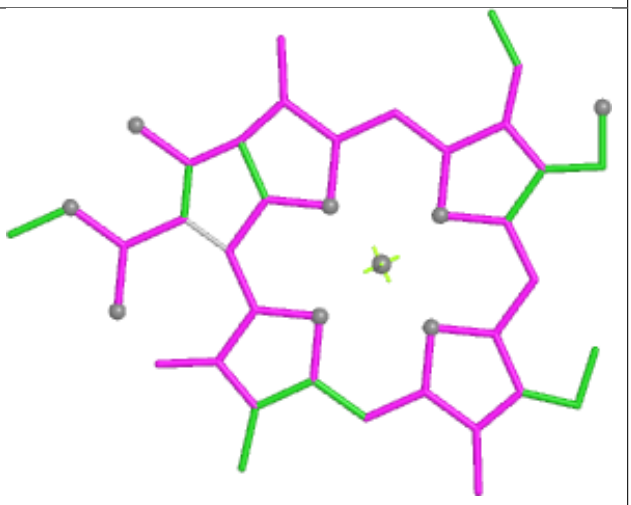


Rings

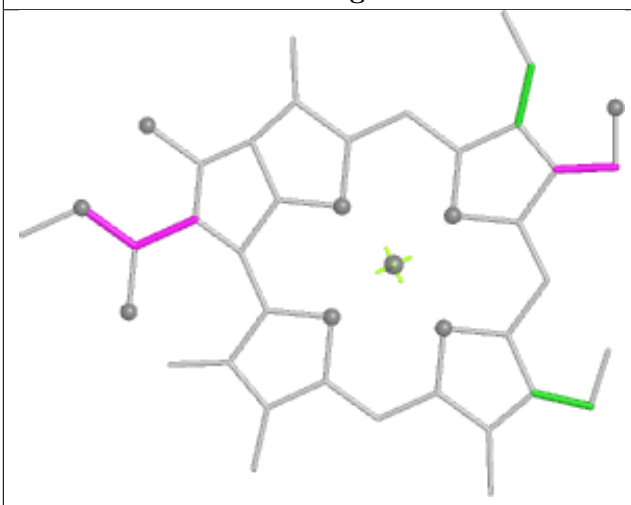
Ligand CHL c 614



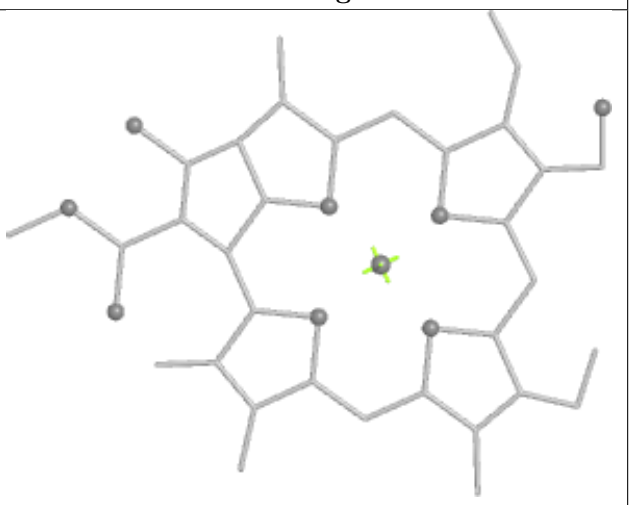
Bond lengths



Bond angles

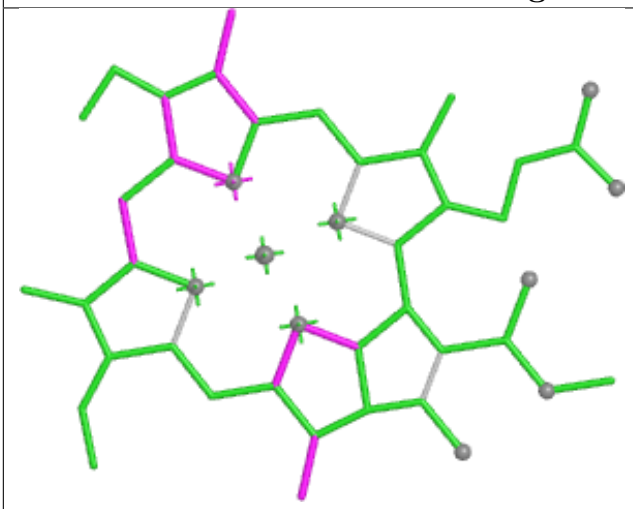


Torsions

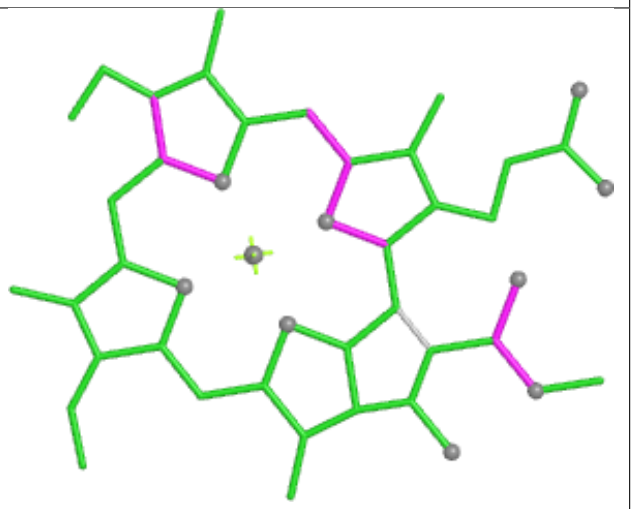


Rings

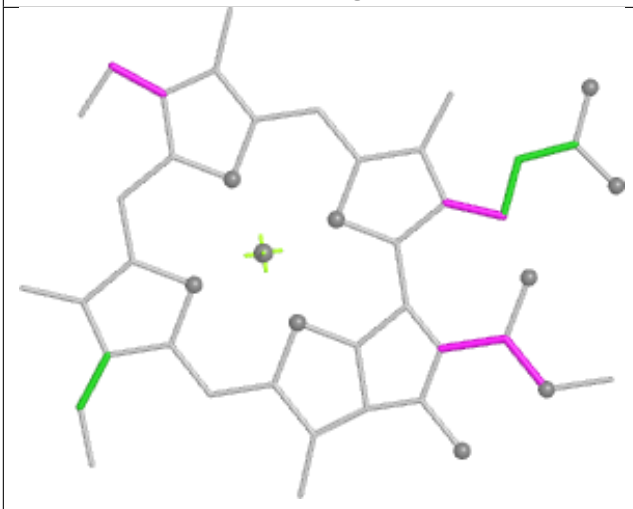
Ligand CLA 5 310



Bond lengths



Bond angles

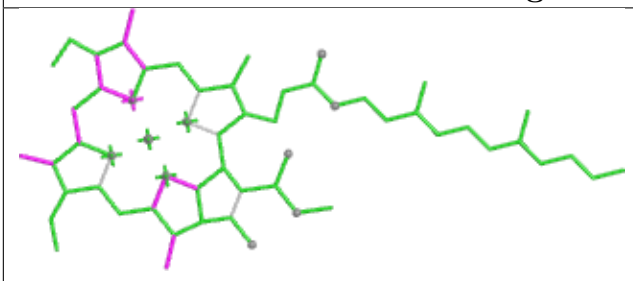


Torsions

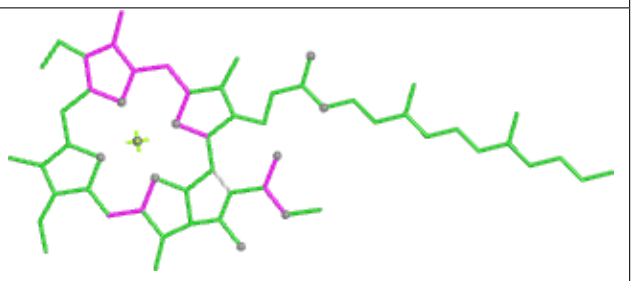


Rings

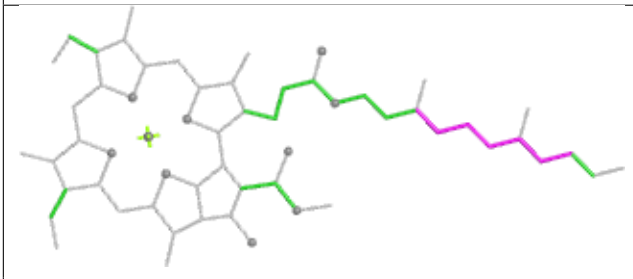
Ligand CLA L 201



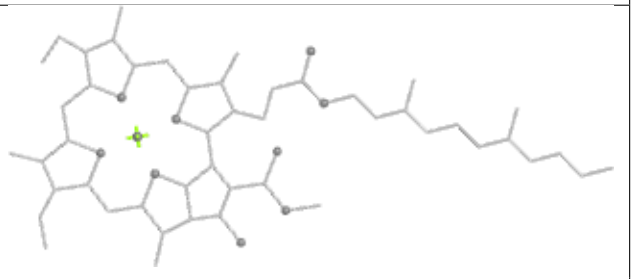
Bond lengths



Bond angles

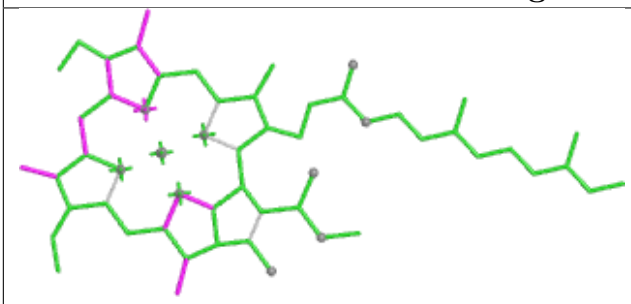


Torsions

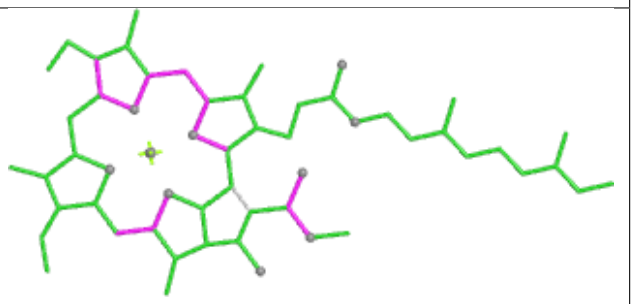


Rings

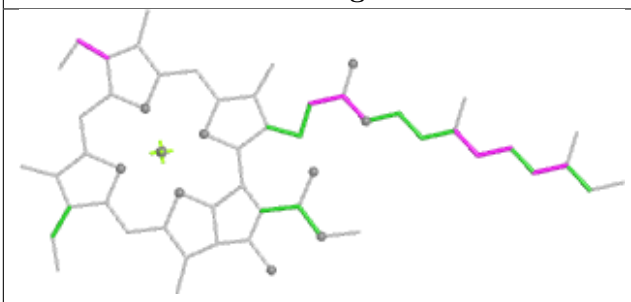
Ligand CLA 2 303



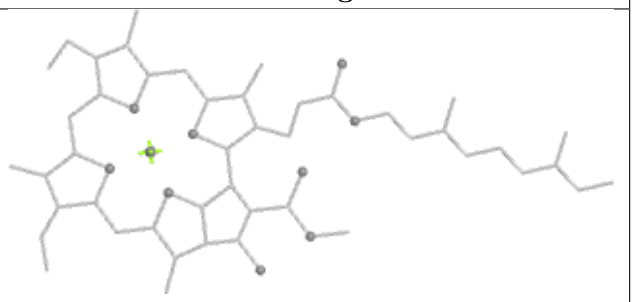
Bond lengths



Bond angles

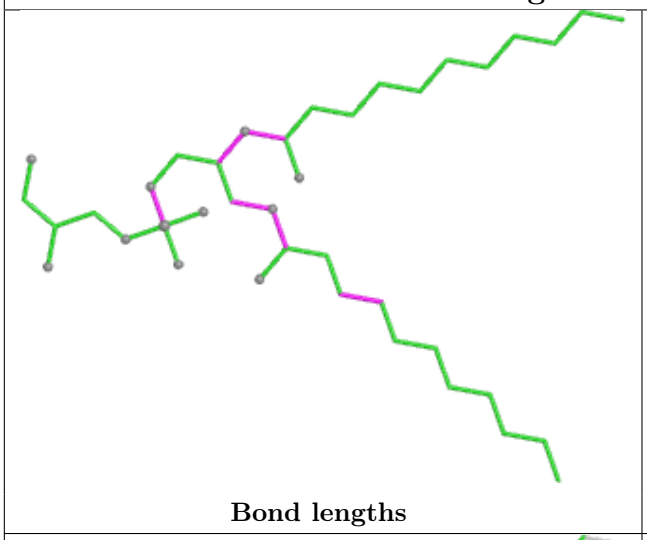


Torsions

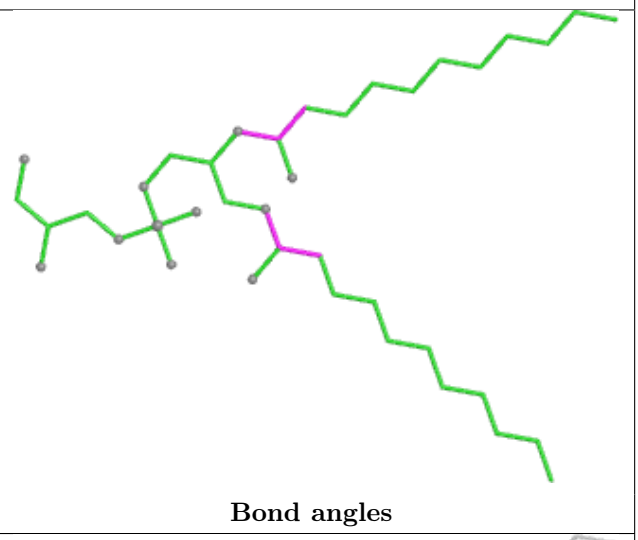


Rings

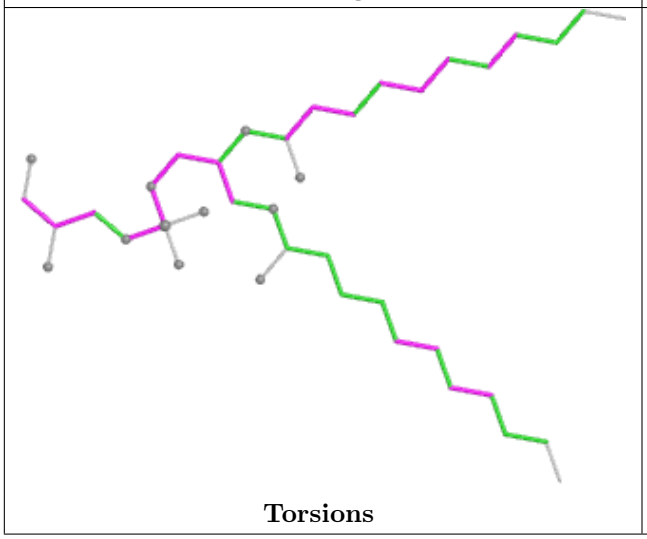
Ligand LHG 7 603



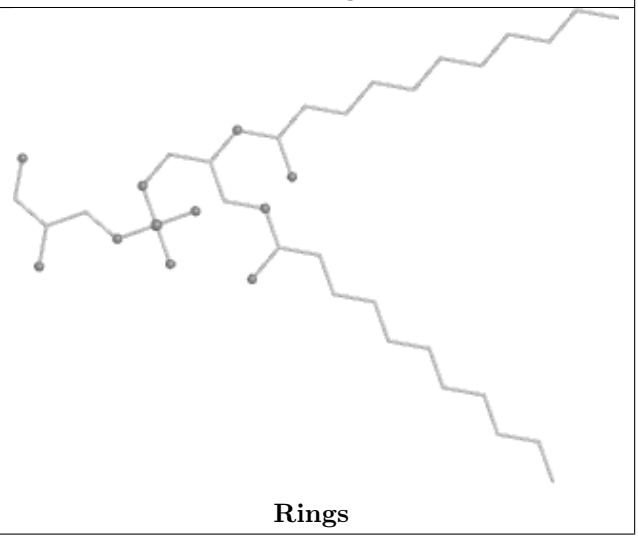
Bond lengths



Bond angles

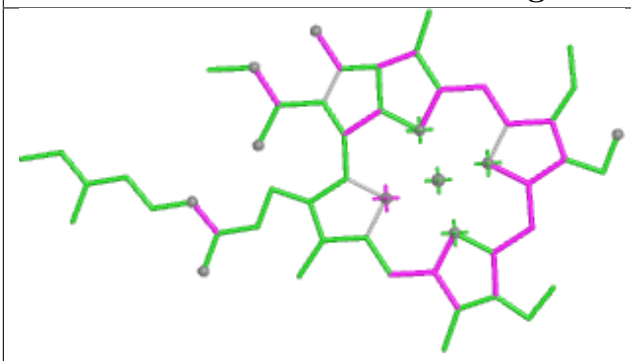


Torsions

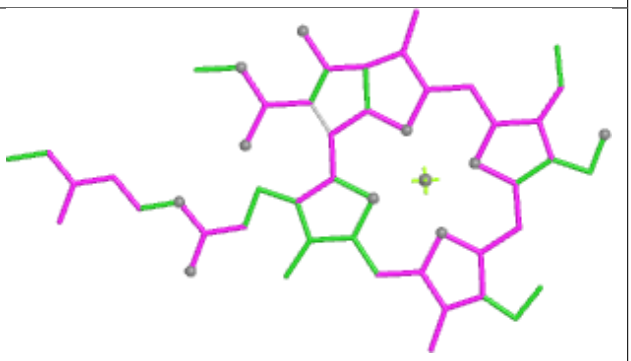


Rings

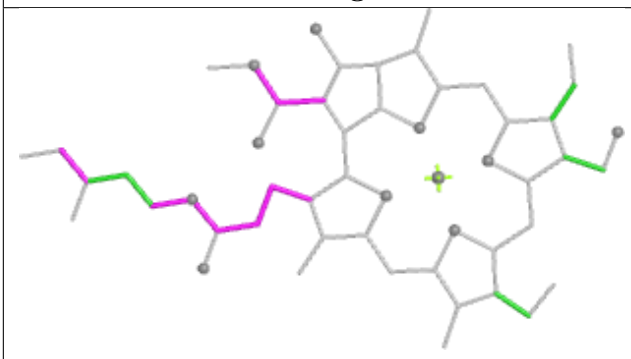
Ligand CHL 5 301



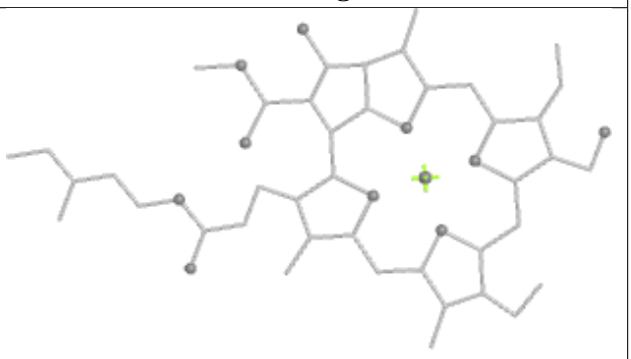
Bond lengths



Bond angles

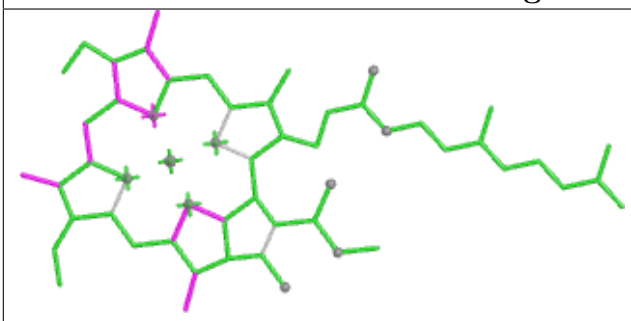


Torsions

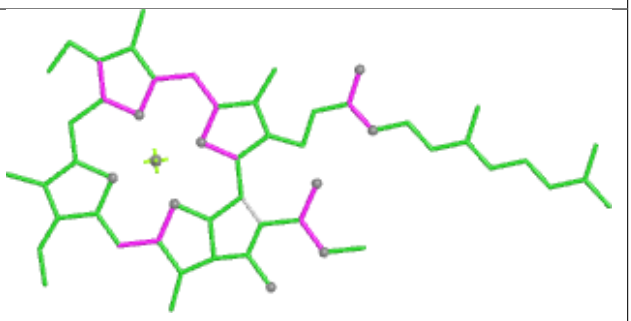


Rings

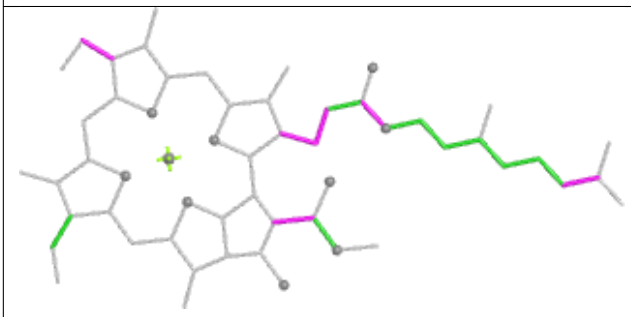
Ligand CLA A 824



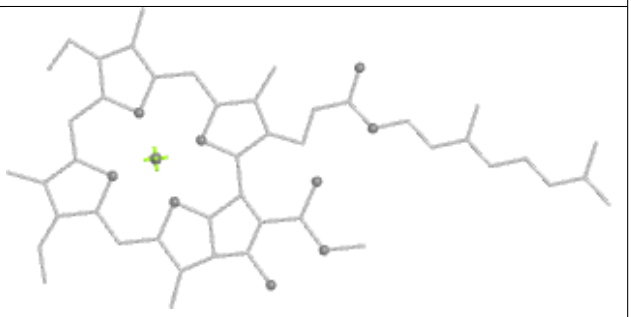
Bond lengths



Bond angles

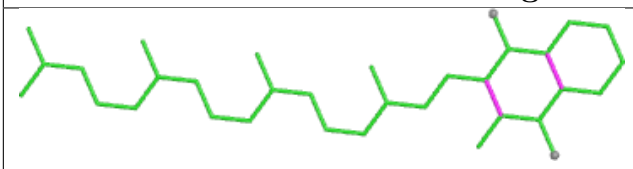


Torsions

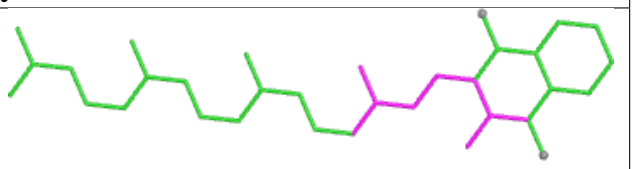


Rings

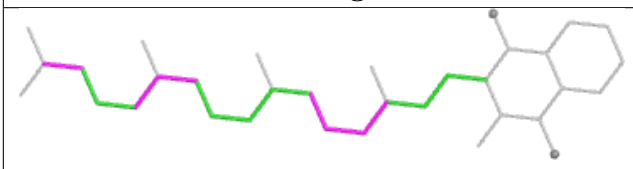
Ligand PQN A 842



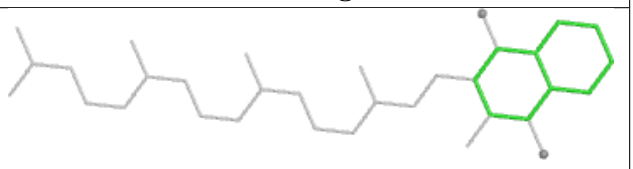
Bond lengths



Bond angles

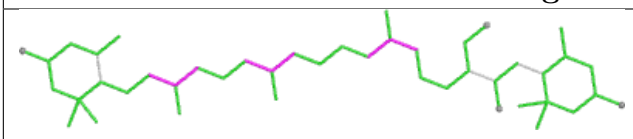


Torsions

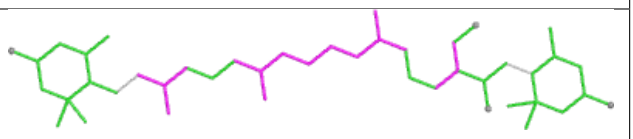


Rings

Ligand 0IE i 522



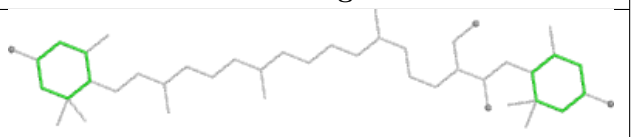
Bond lengths



Bond angles

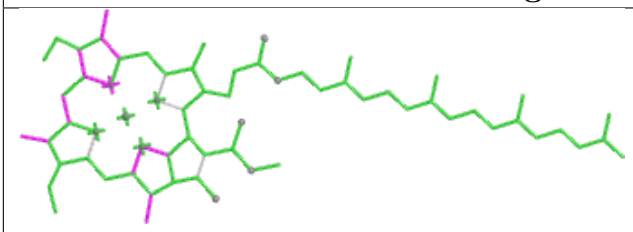


Torsions

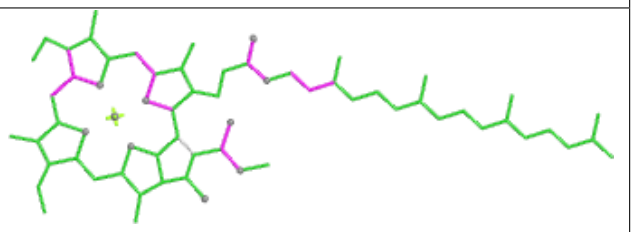


Rings

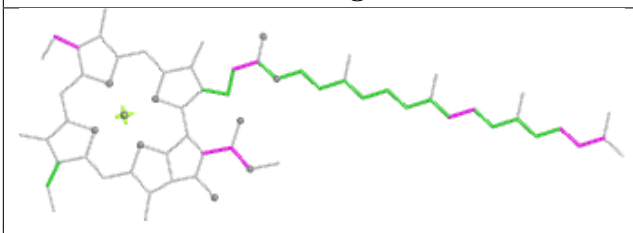
Ligand CLA B 805



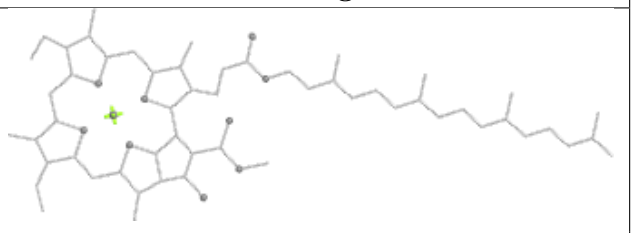
Bond lengths



Bond angles

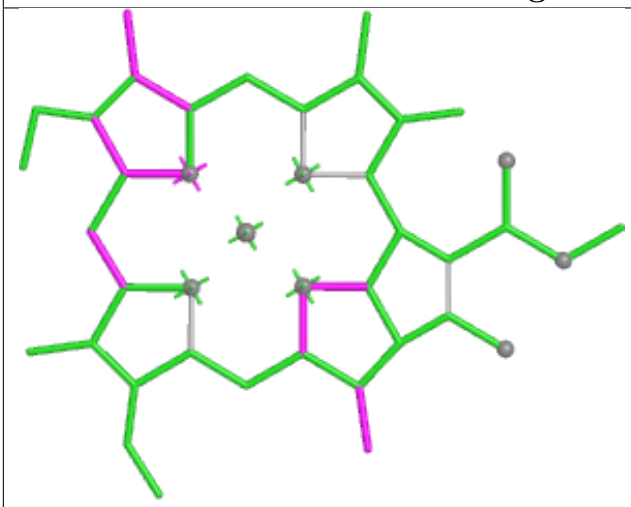


Torsions

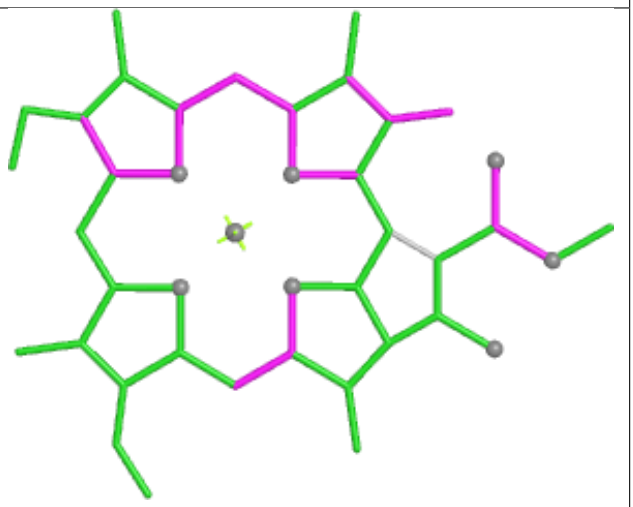


Rings

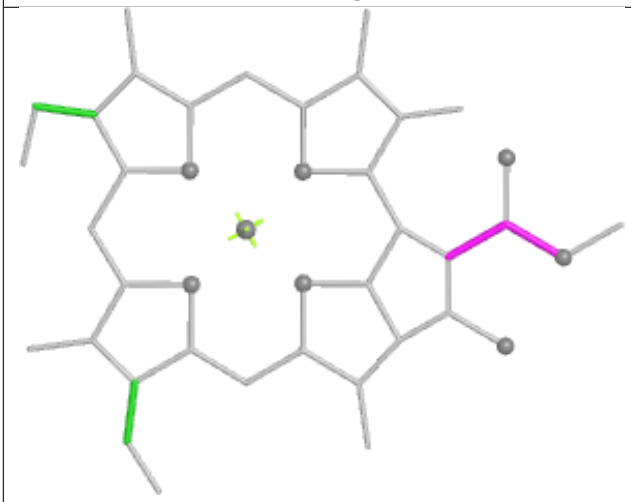
Ligand CLA 0 310



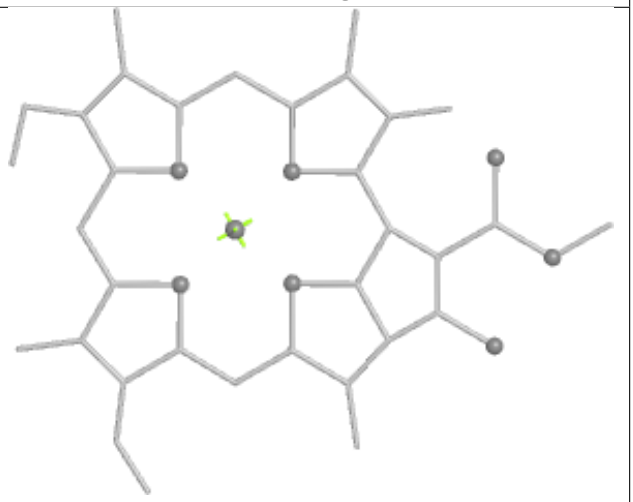
Bond lengths



Bond angles

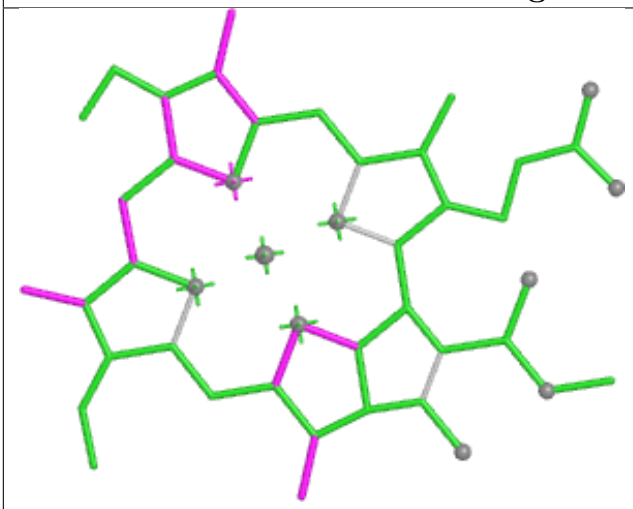


Torsions

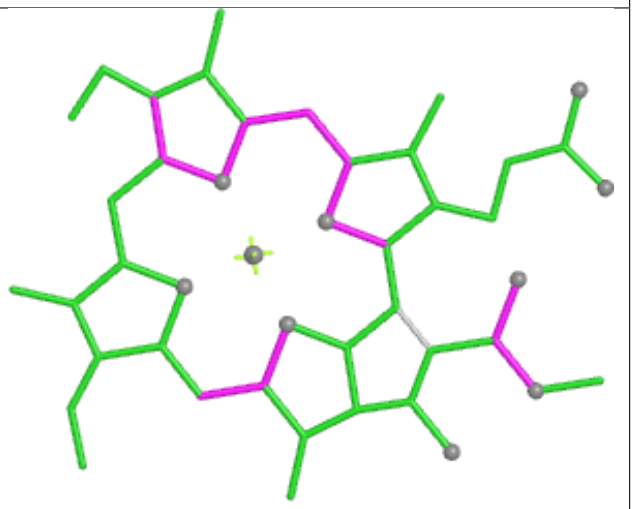


Rings

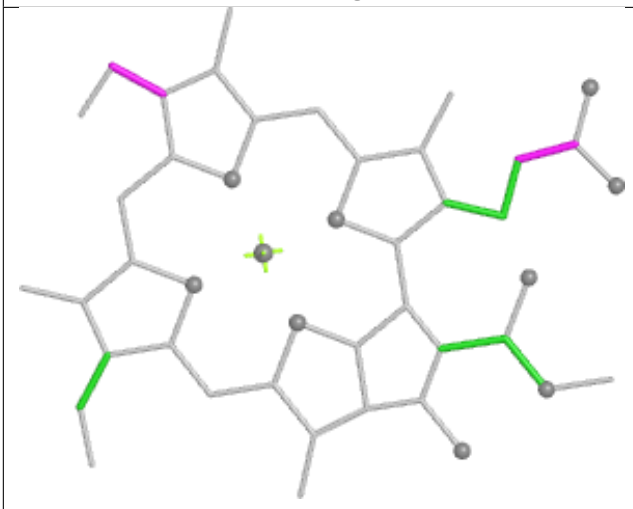
Ligand CLA 4 303



Bond lengths



Bond angles

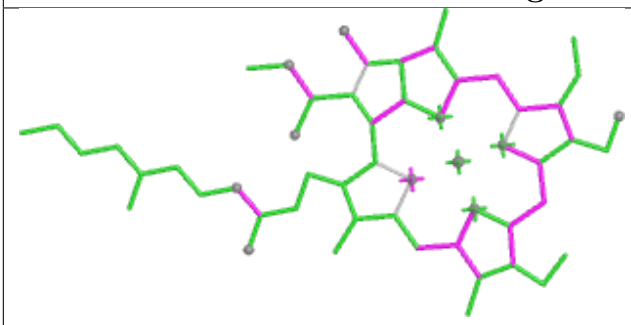


Torsions

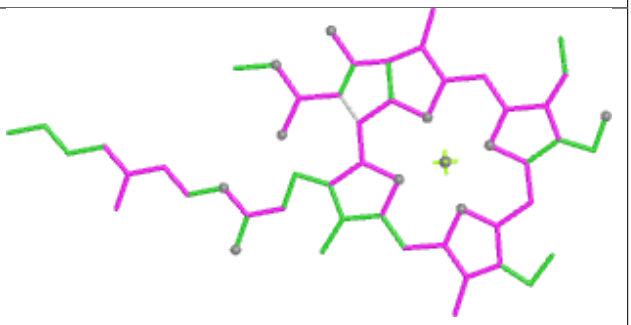


Rings

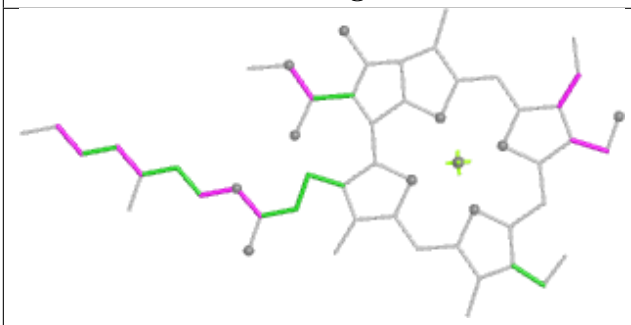
Ligand CHL b 609



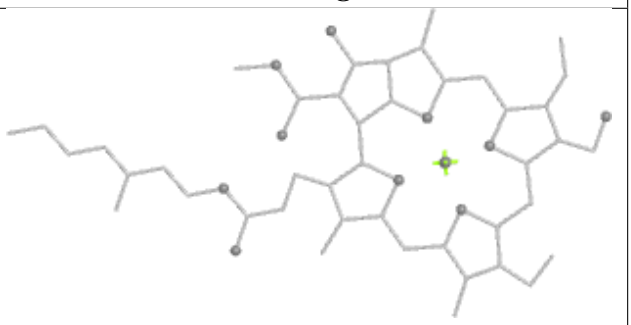
Bond lengths



Bond angles

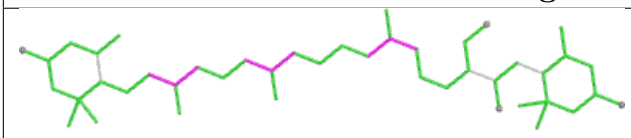


Torsions

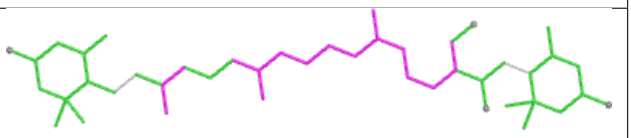


Rings

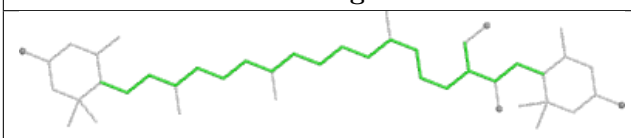
Ligand 0IE e 522



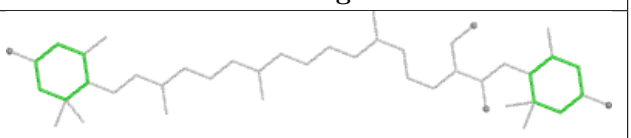
Bond lengths



Bond angles

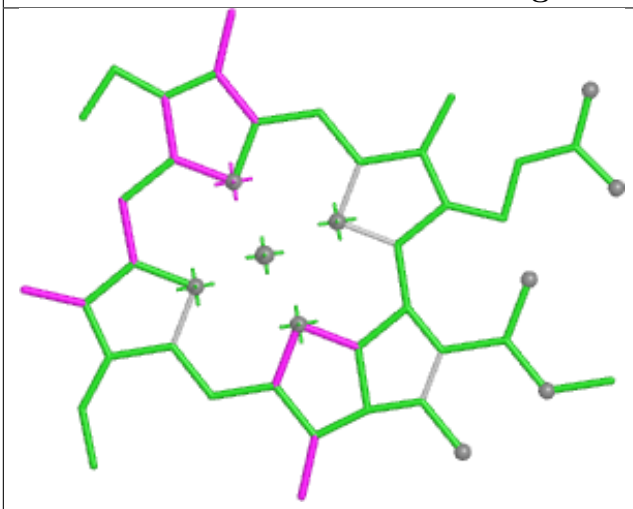


Torsions

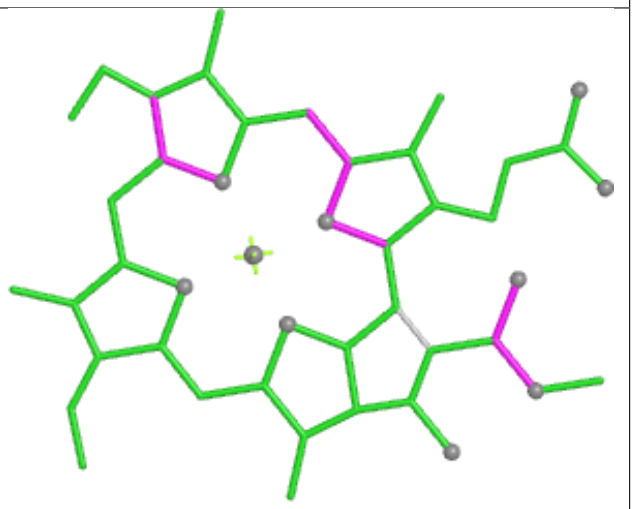


Rings

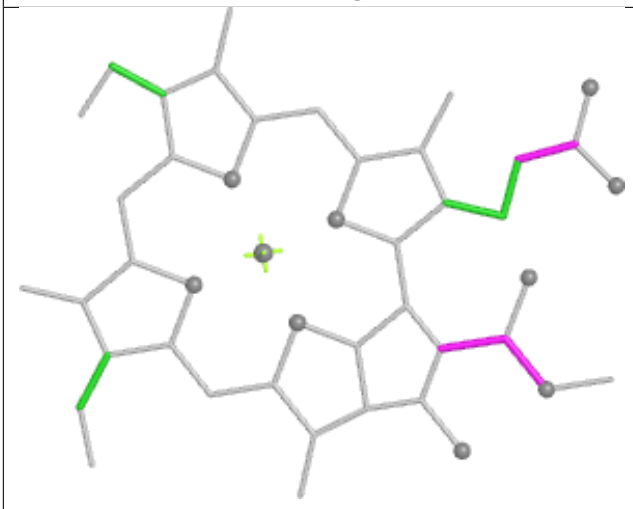
Ligand CLA f 612



Bond lengths



Bond angles

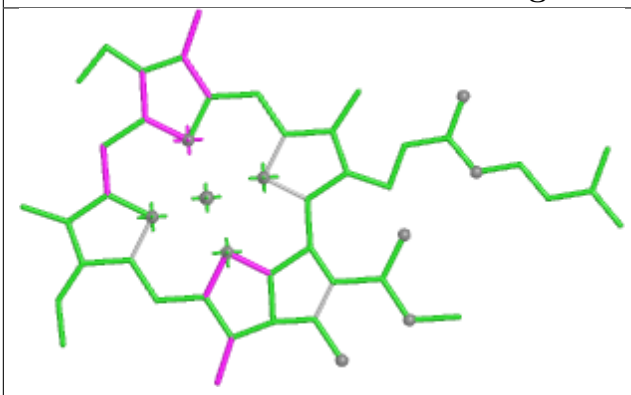


Torsions

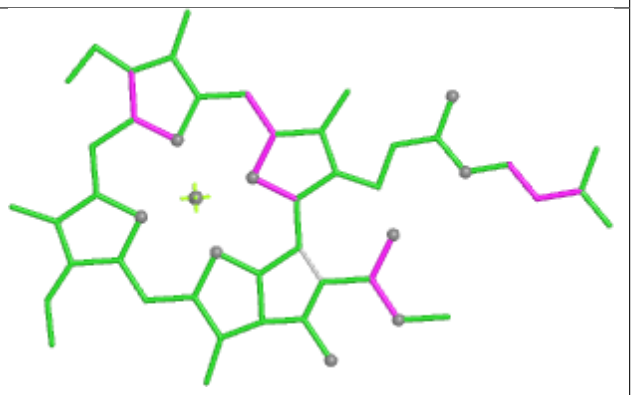


Rings

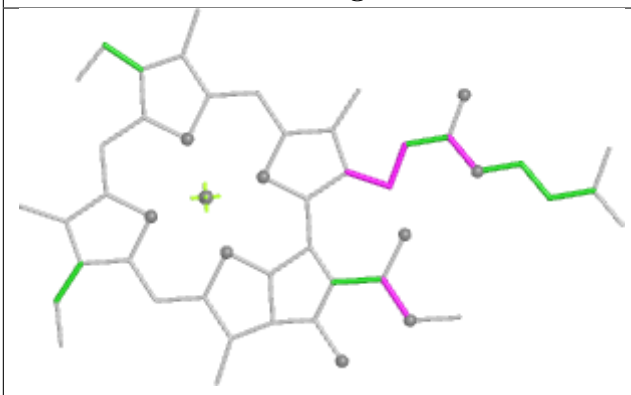
Ligand CLA e 604



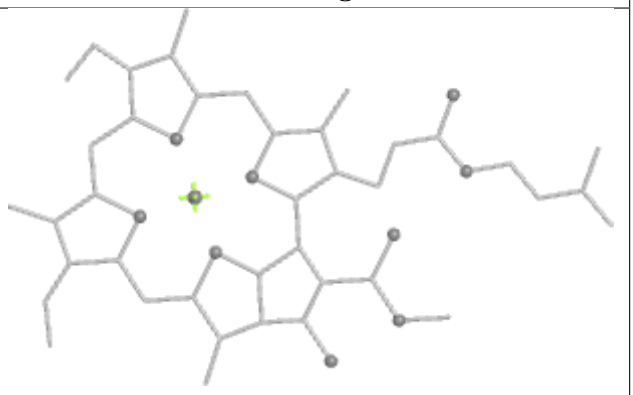
Bond lengths



Bond angles

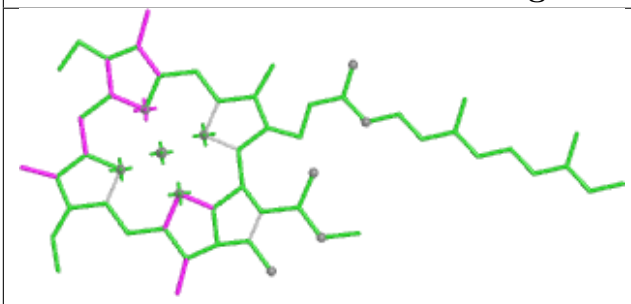


Torsions

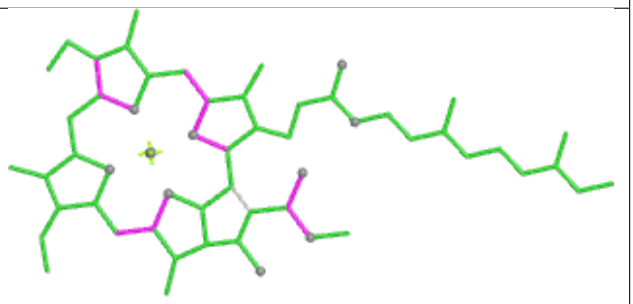


Rings

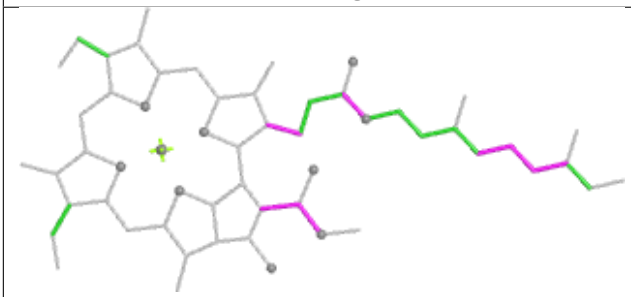
Ligand CLA 5 312



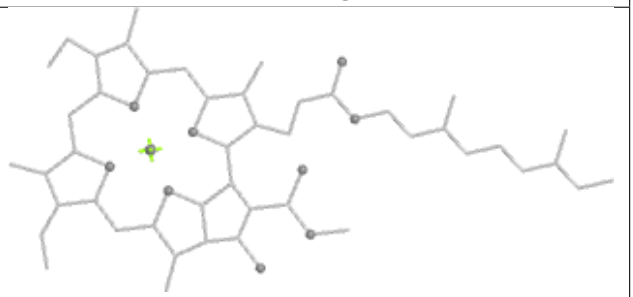
Bond lengths



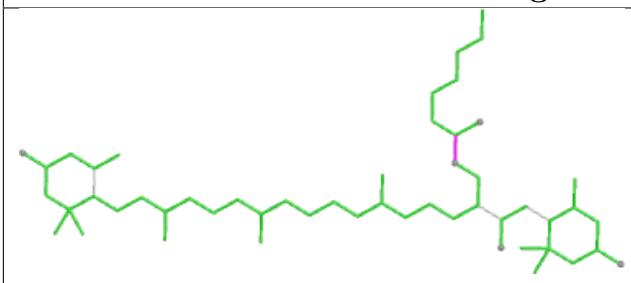
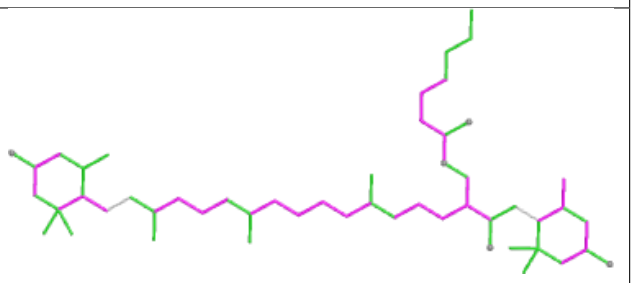
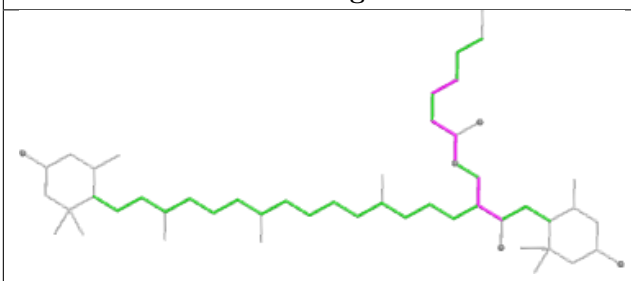
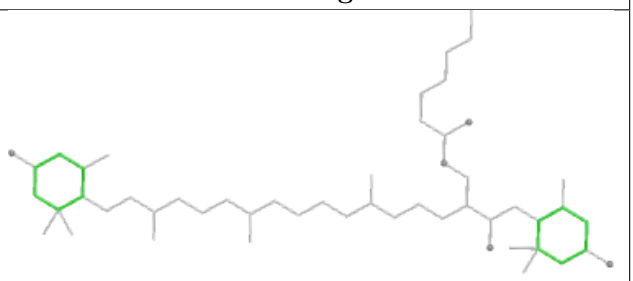
Bond angles

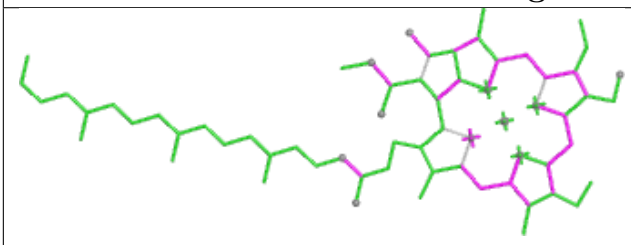
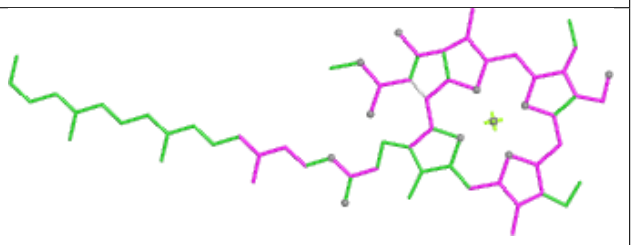
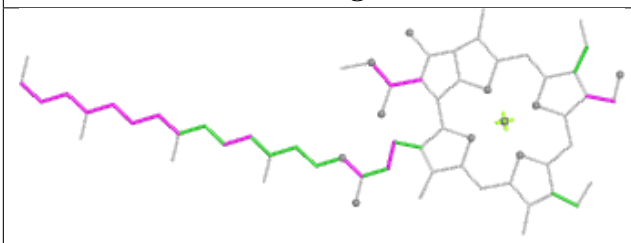
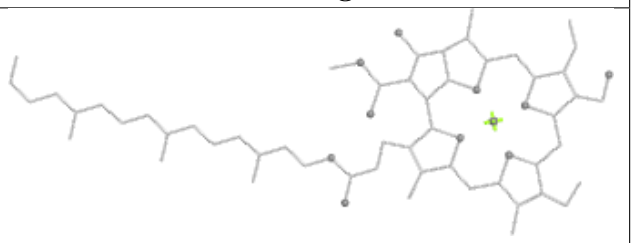


Torsions

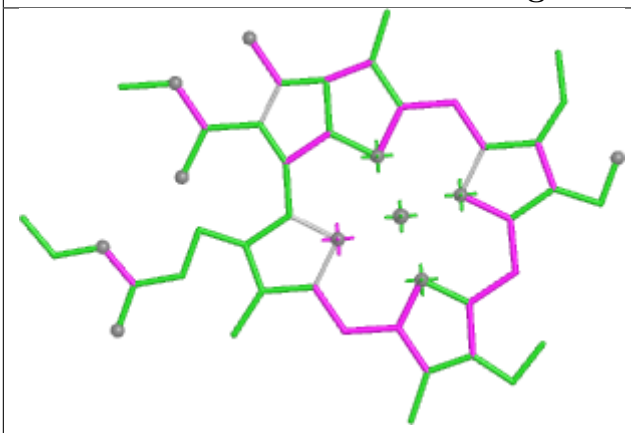


Rings

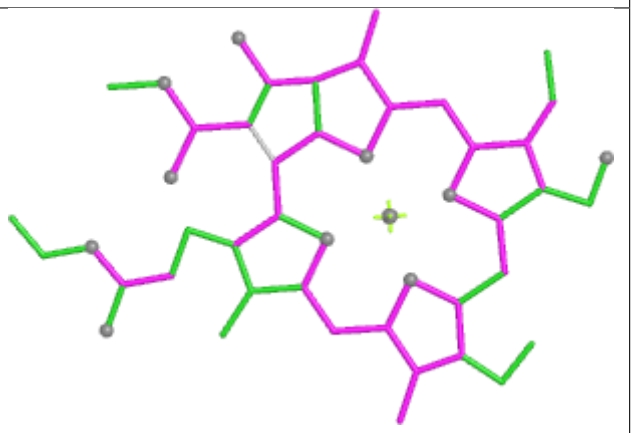
Ligand 0UR e 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL a 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

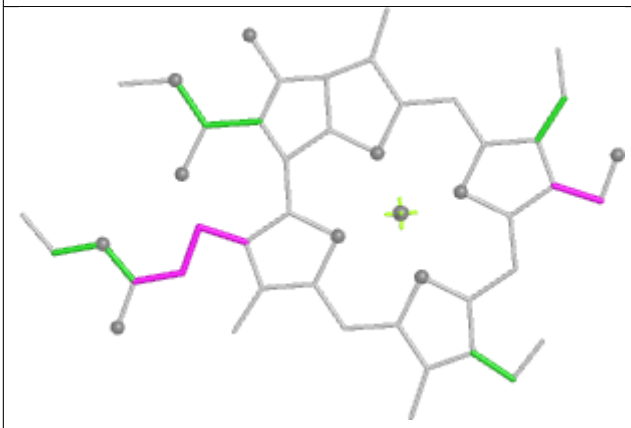
Ligand CHL 9 306



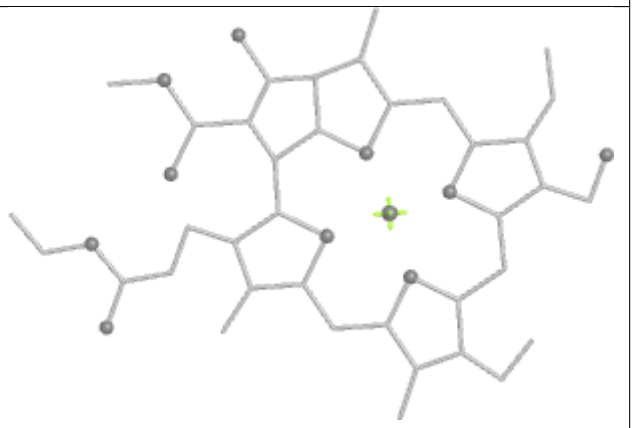
Bond lengths



Bond angles

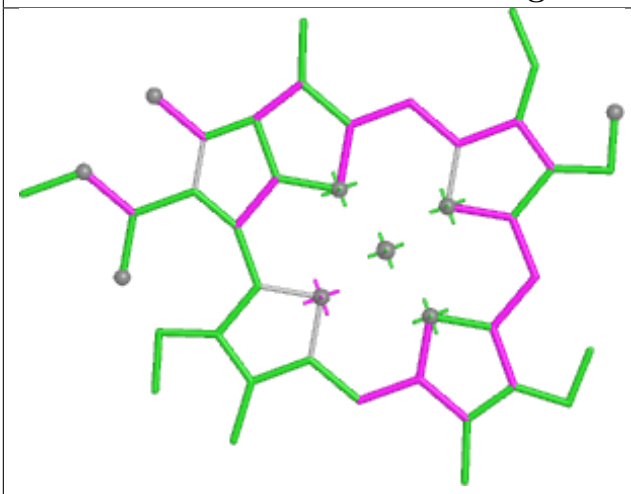


Torsions

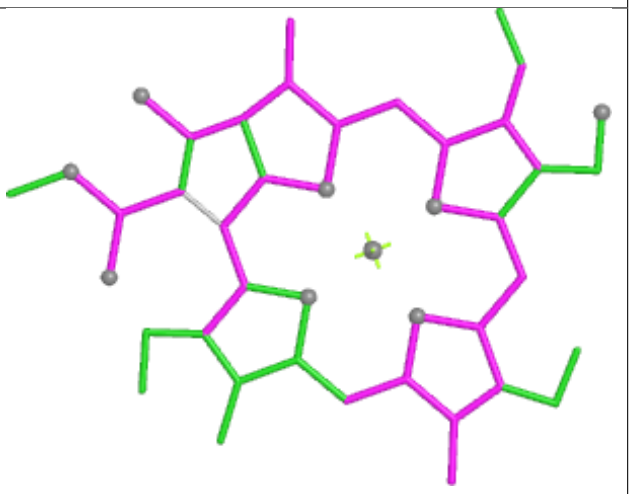


Rings

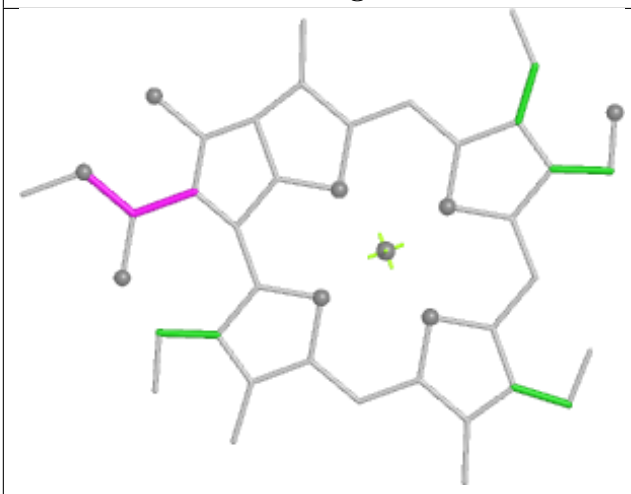
Ligand CHL 6 315



Bond lengths



Bond angles

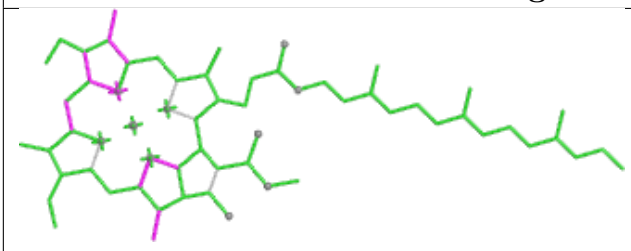


Torsions

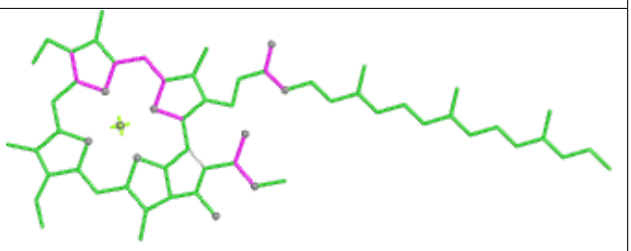


Rings

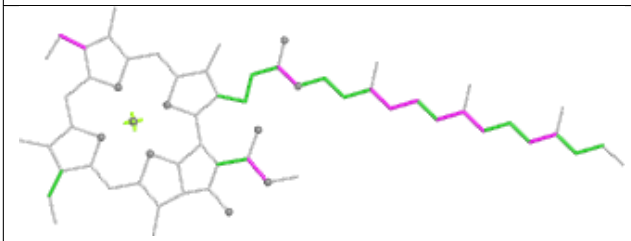
Ligand CLA 3 310



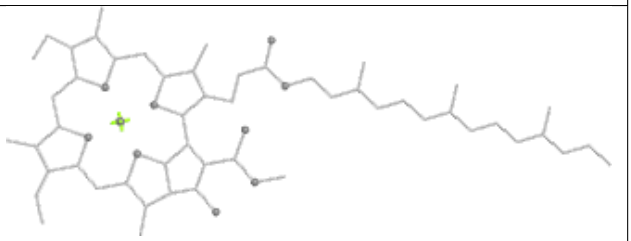
Bond lengths



Bond angles

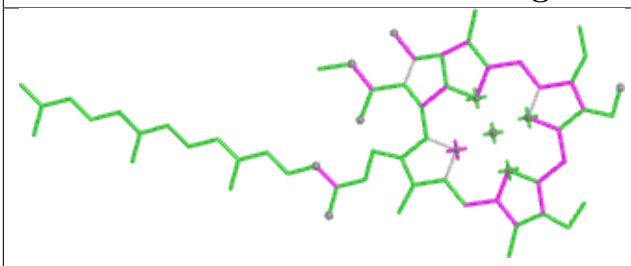


Torsions

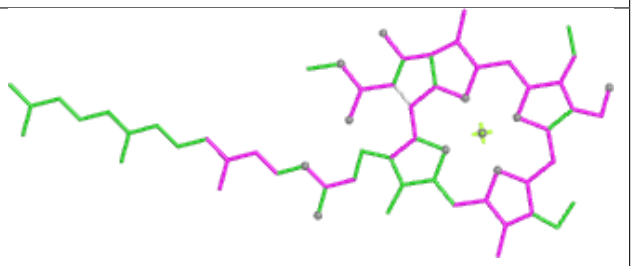


Rings

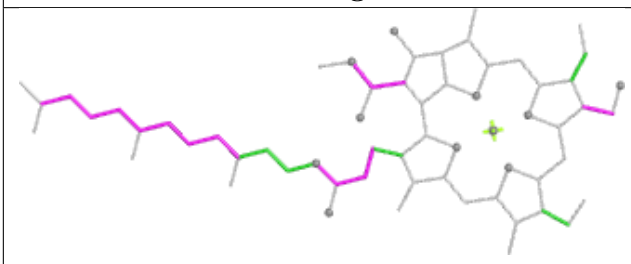
Ligand CHL i 602



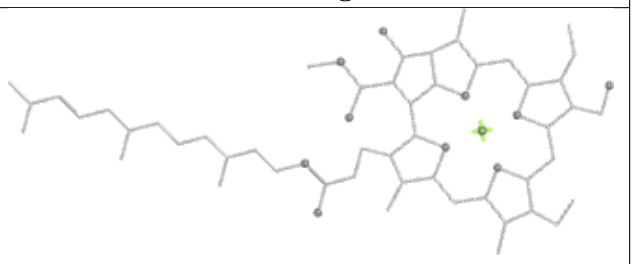
Bond lengths



Bond angles

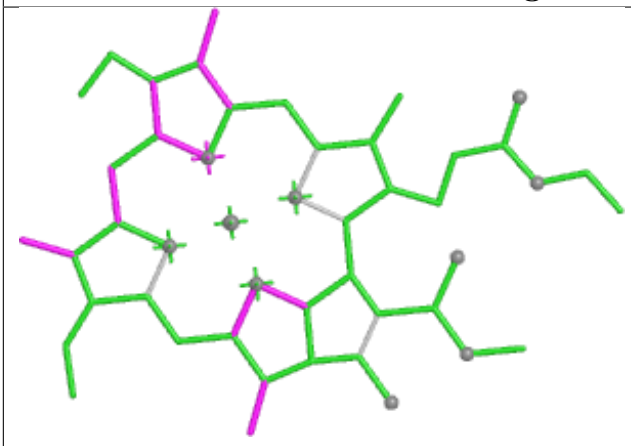


Torsions

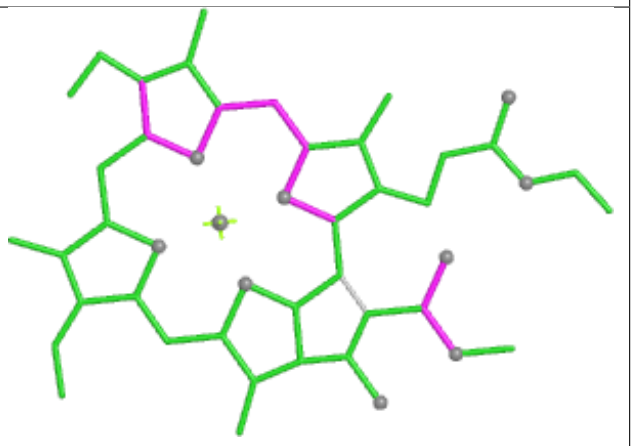


Rings

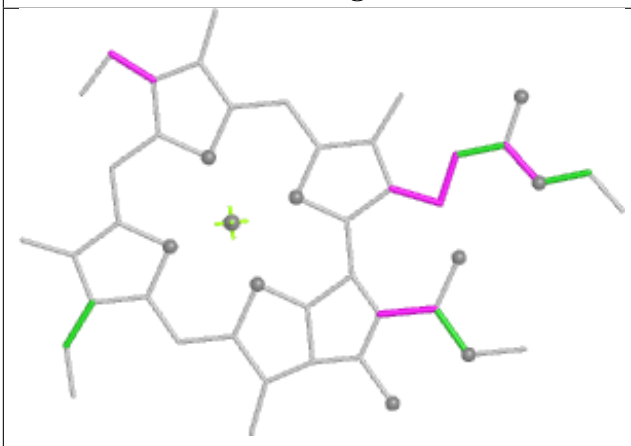
Ligand CLA H 202



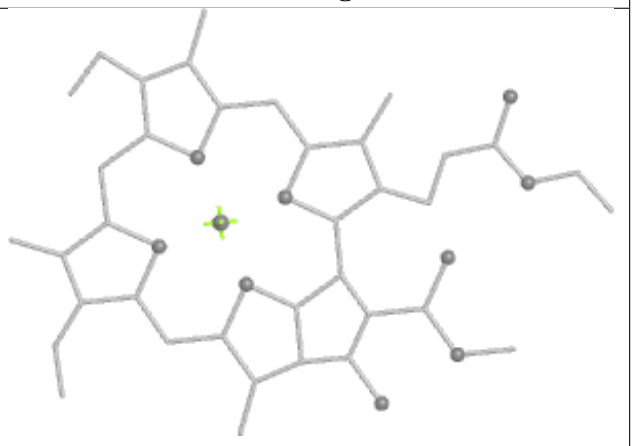
Bond lengths



Bond angles

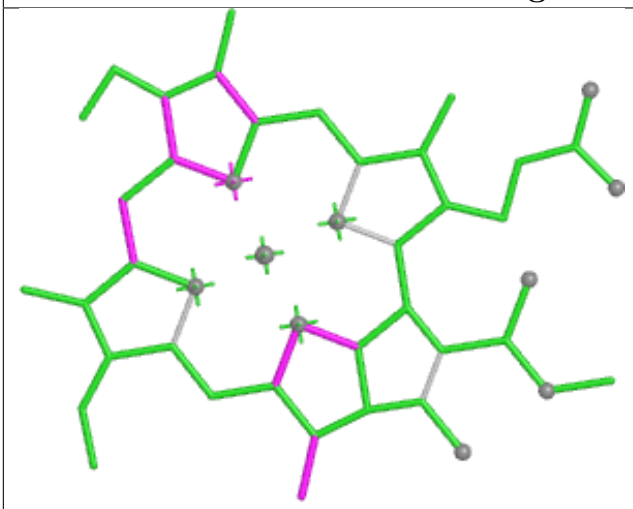


Torsions

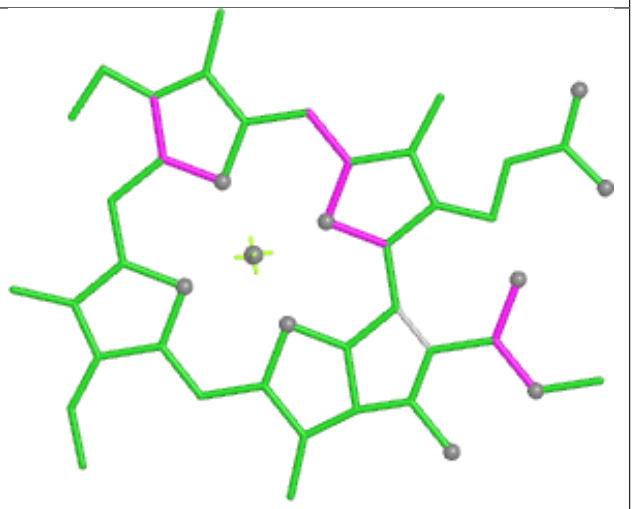


Rings

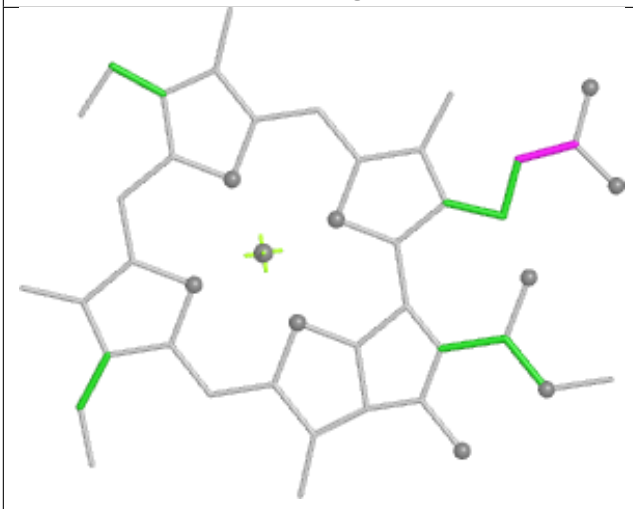
Ligand CLA a 612



Bond lengths



Bond angles

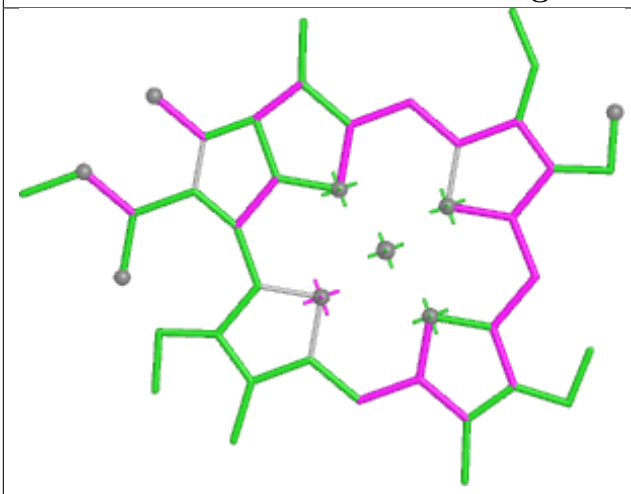


Torsions

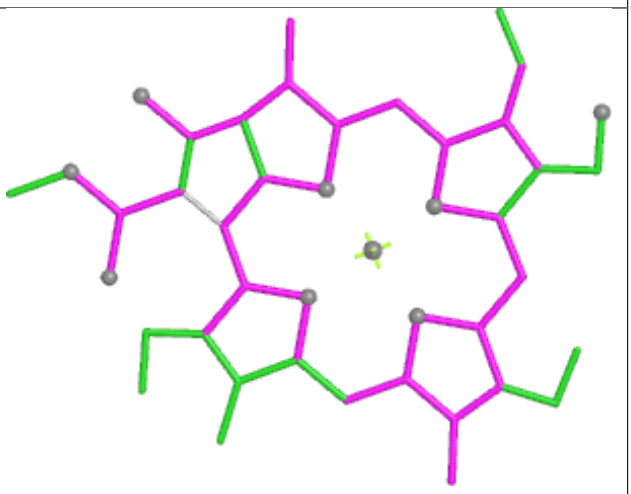


Rings

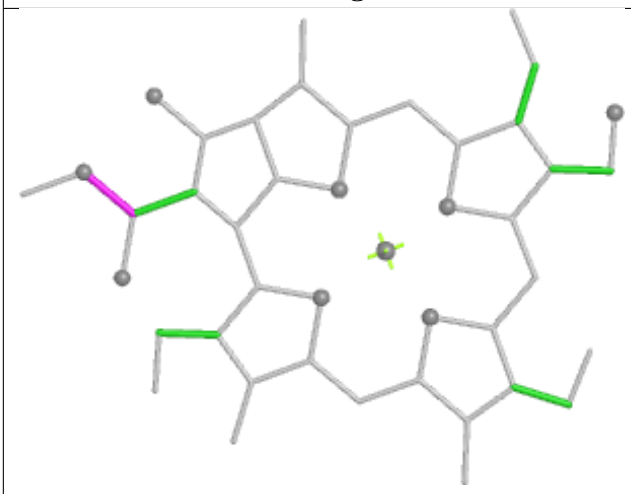
Ligand CHL f 605



Bond lengths



Bond angles

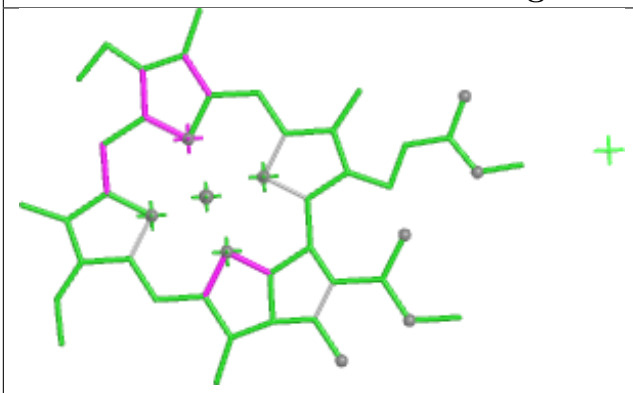


Torsions

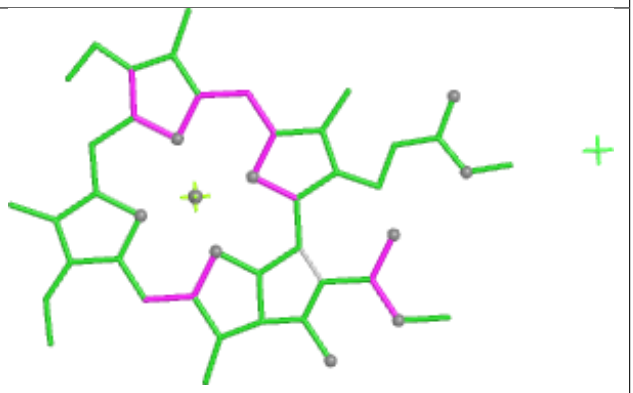


Rings

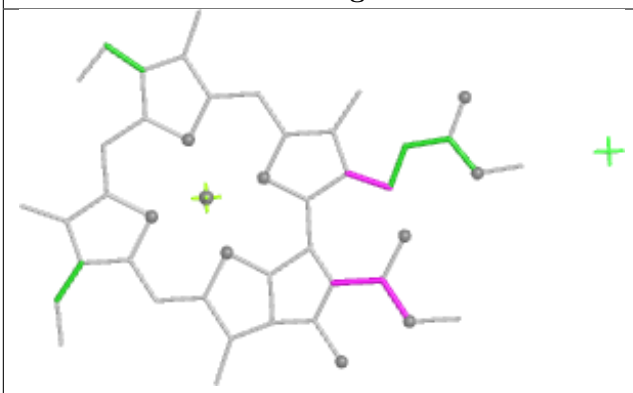
Ligand CLA h 610



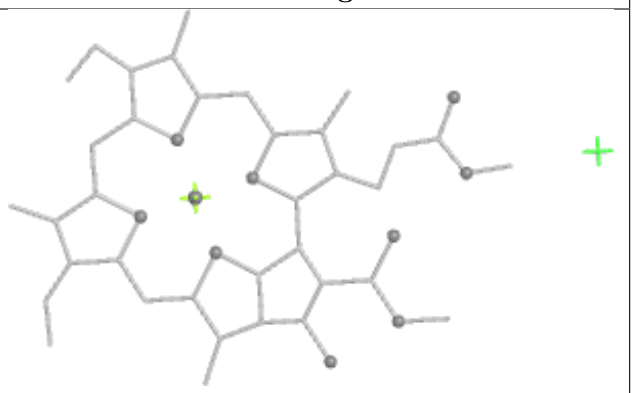
Bond lengths



Bond angles

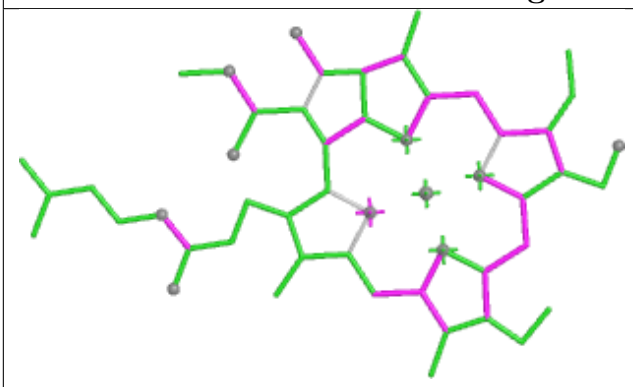


Torsions

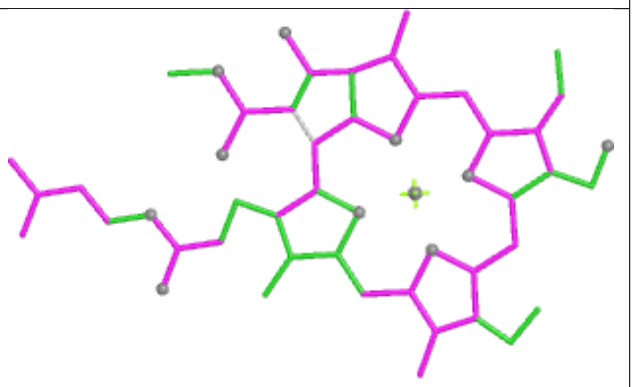


Rings

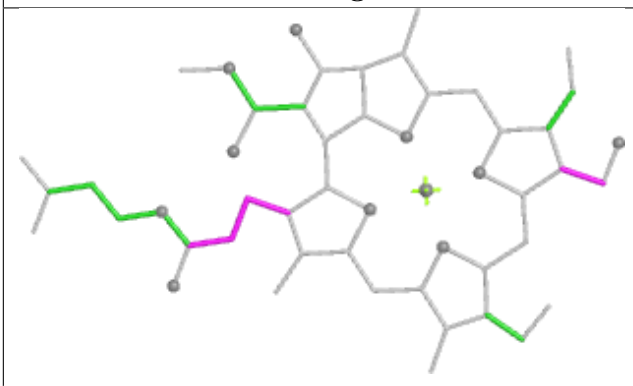
Ligand CHL 0 305



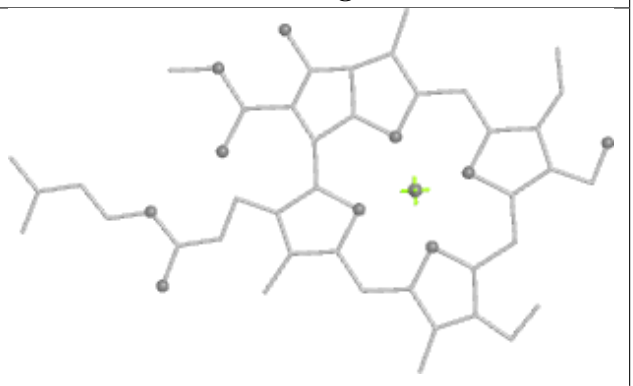
Bond lengths



Bond angles

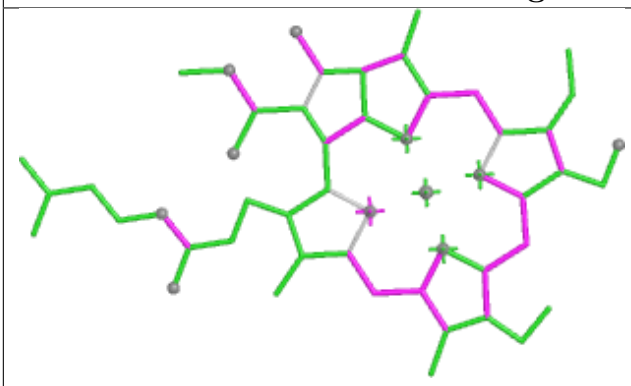


Torsions

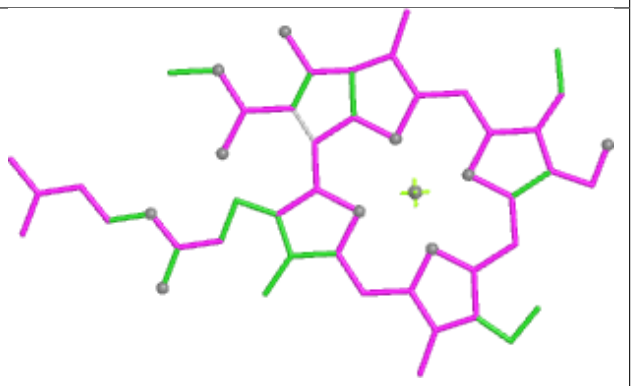


Rings

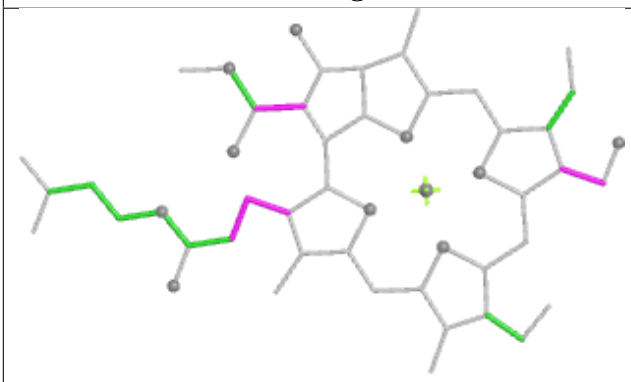
Ligand CHL 2 313



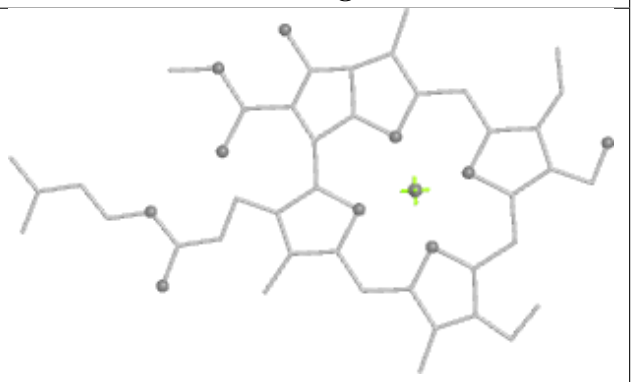
Bond lengths



Bond angles

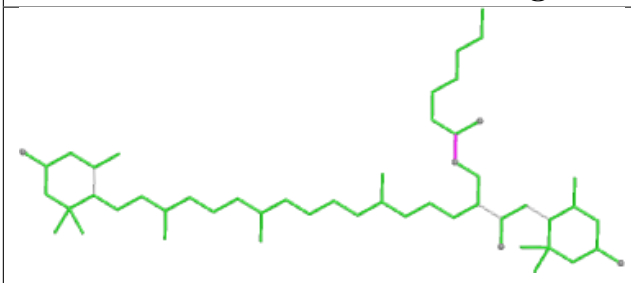


Torsions

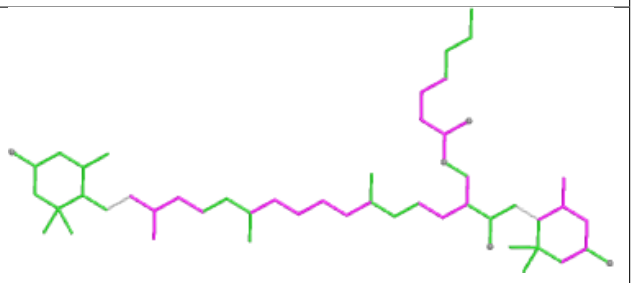


Rings

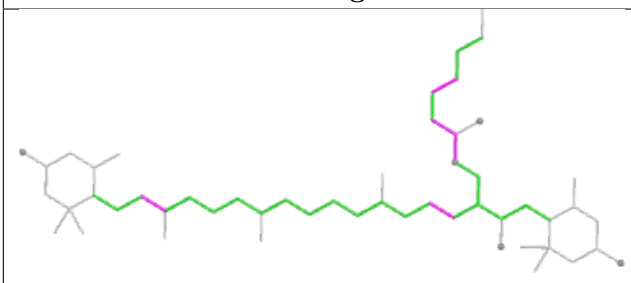
Ligand 0UR 8 502



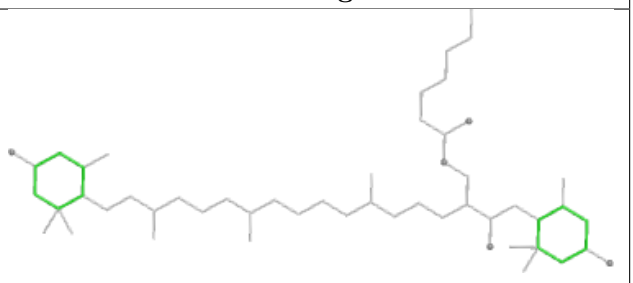
Bond lengths



Bond angles

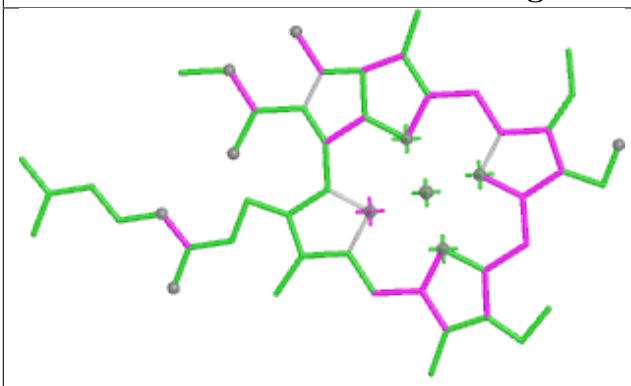


Torsions

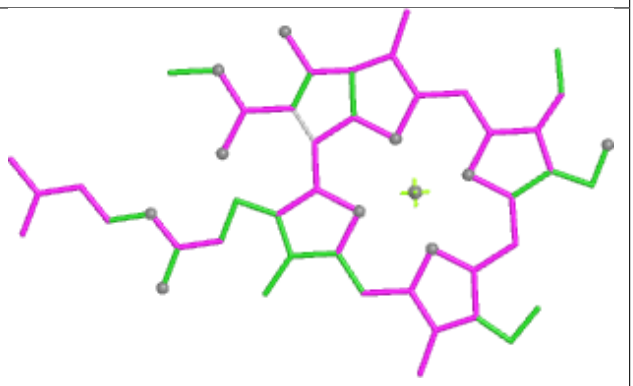


Rings

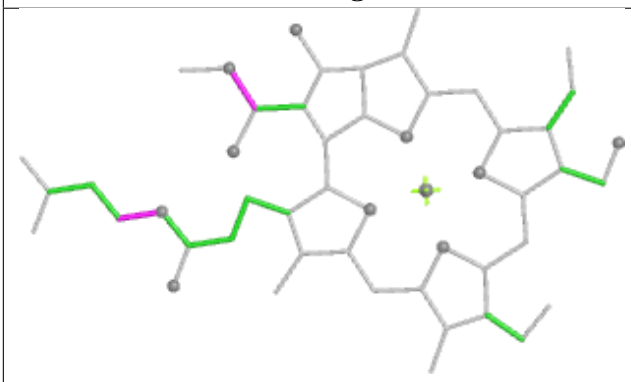
Ligand CHL d 601



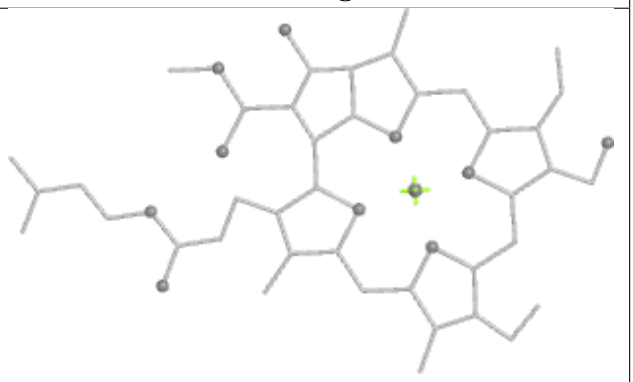
Bond lengths



Bond angles

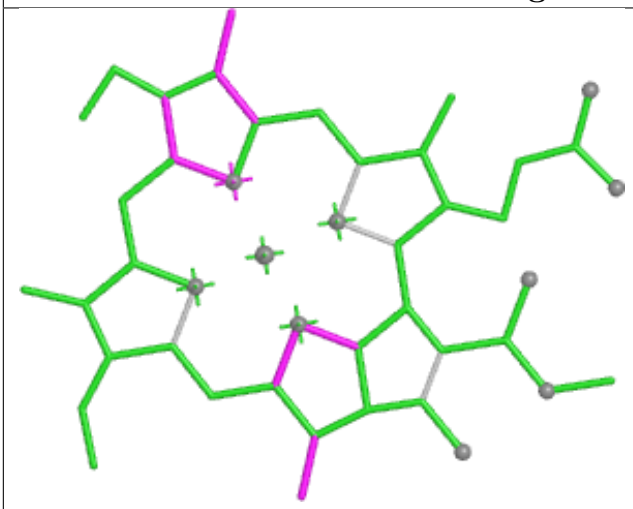


Torsions

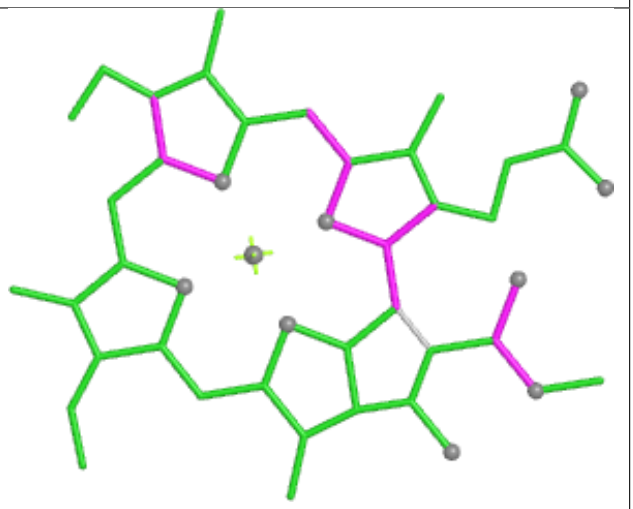


Rings

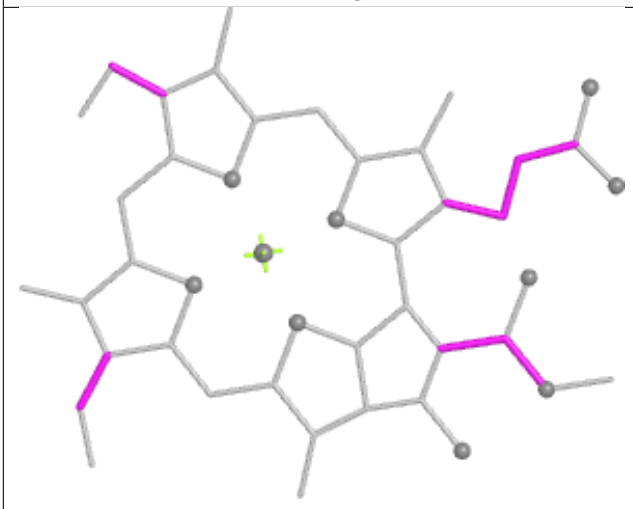
Ligand CLA 7 317



Bond lengths



Bond angles

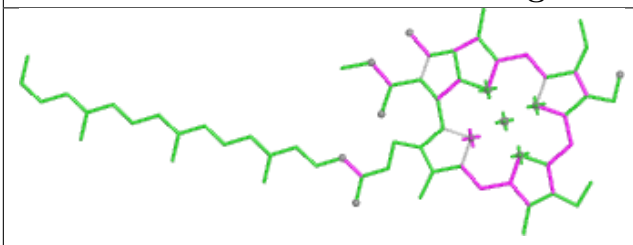


Torsions

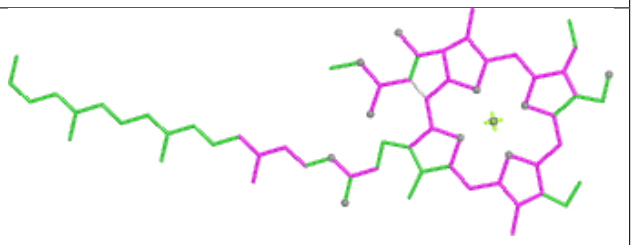


Rings

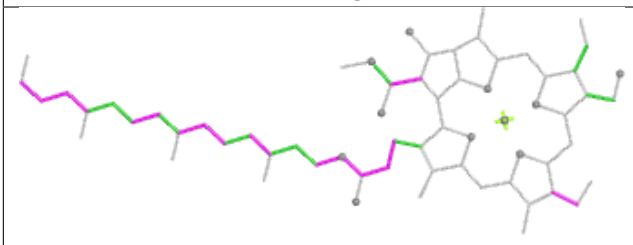
Ligand CHL 7 302



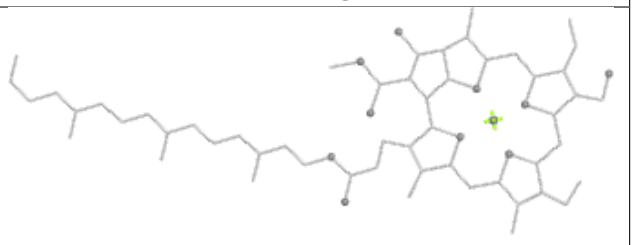
Bond lengths



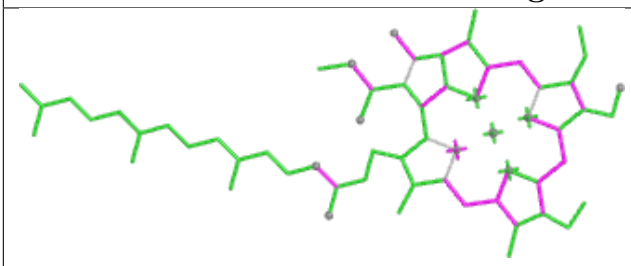
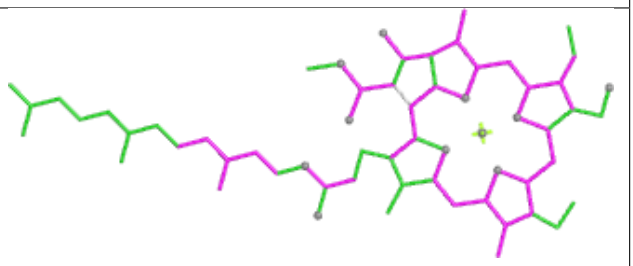
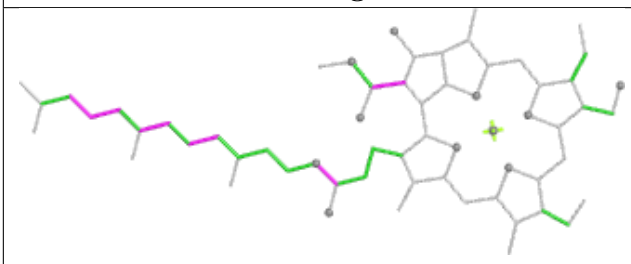
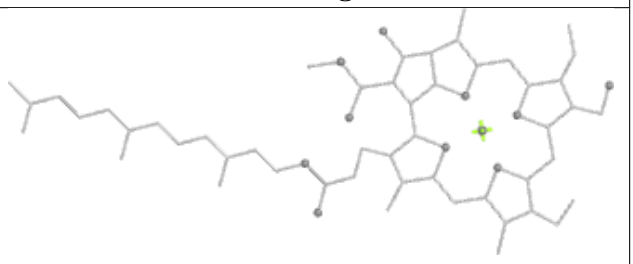
Bond angles

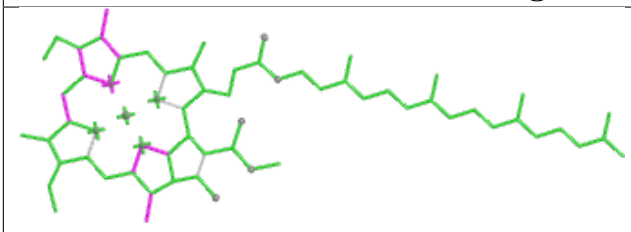
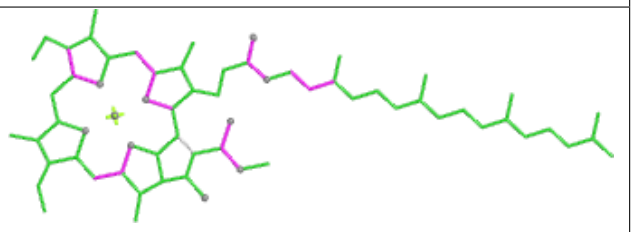
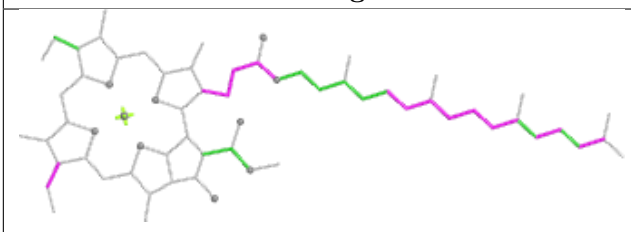
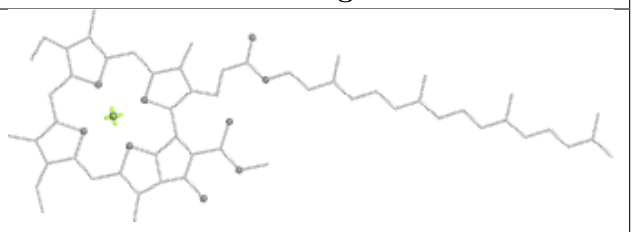


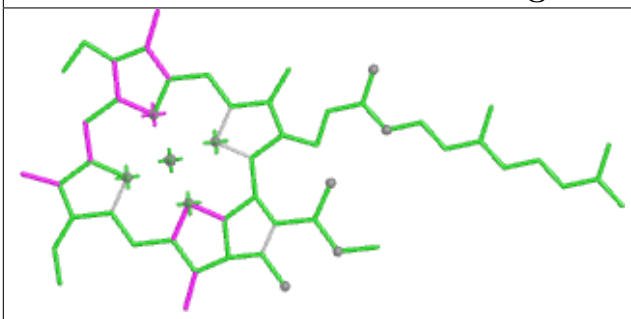
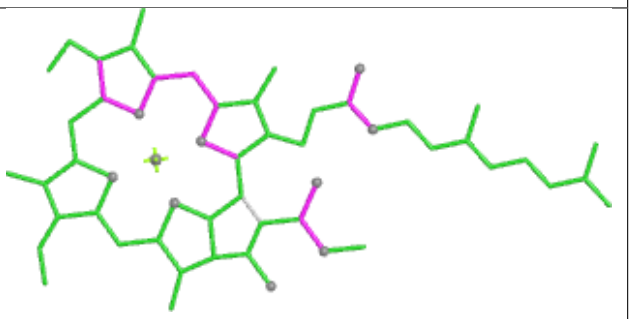
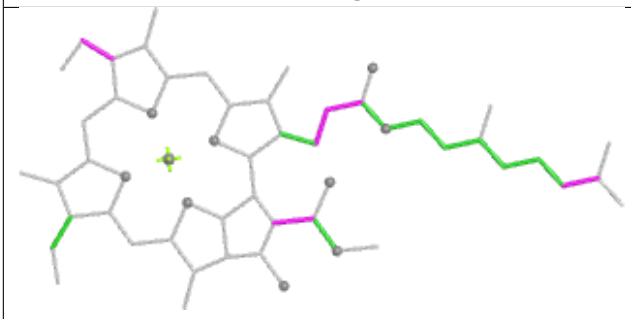
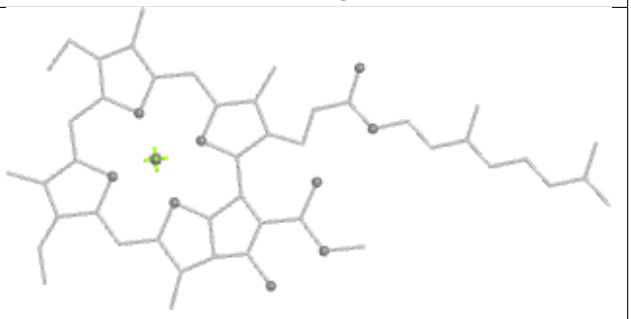
Torsions

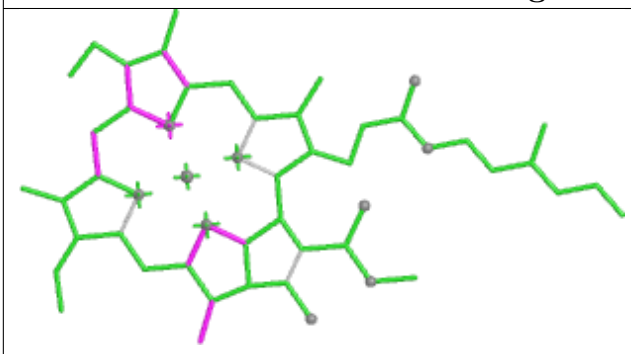
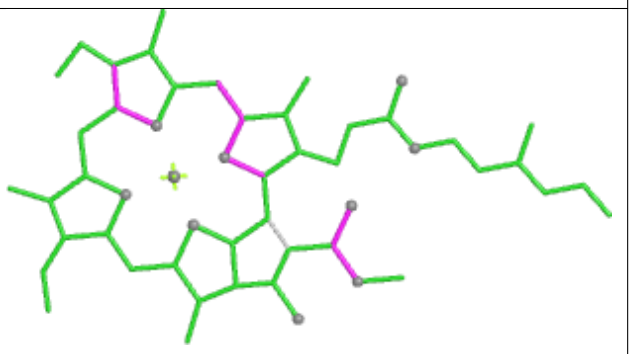
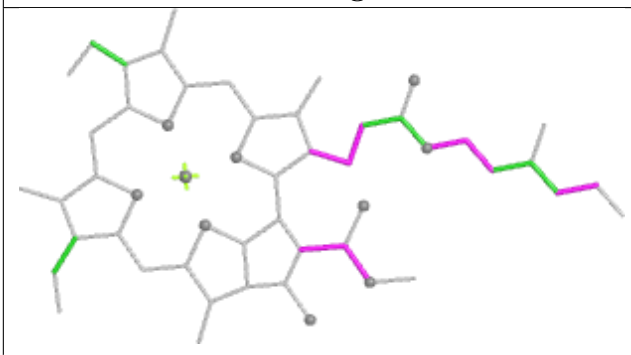
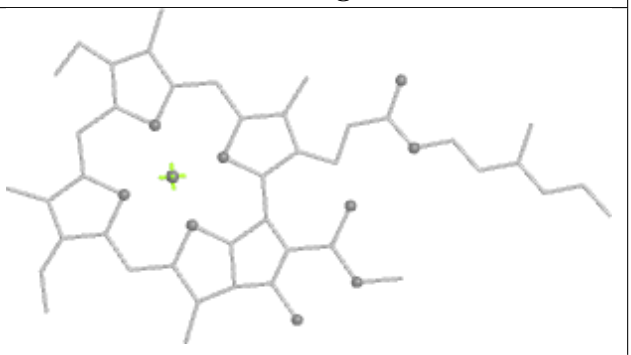


Rings

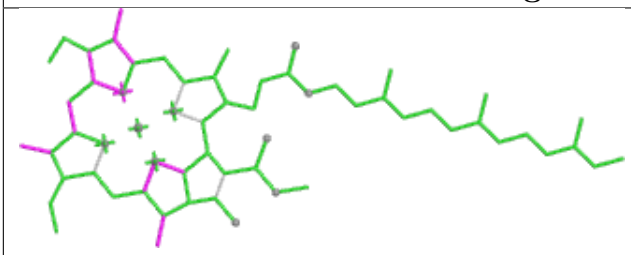
Ligand CHL 2 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

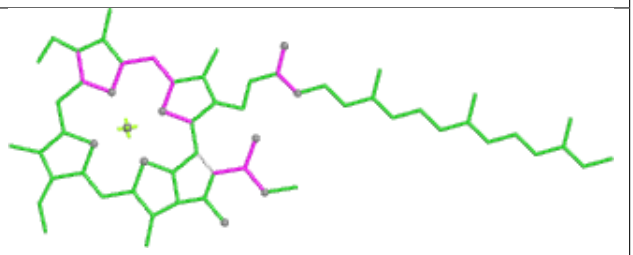
Ligand CLA 3 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

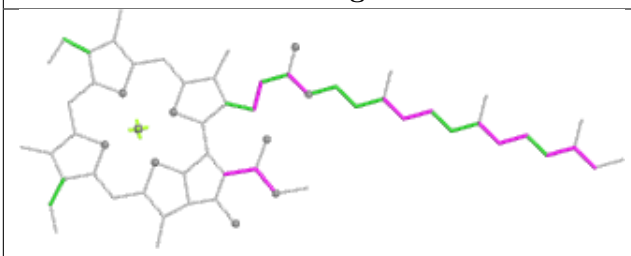
Ligand CLA A 817



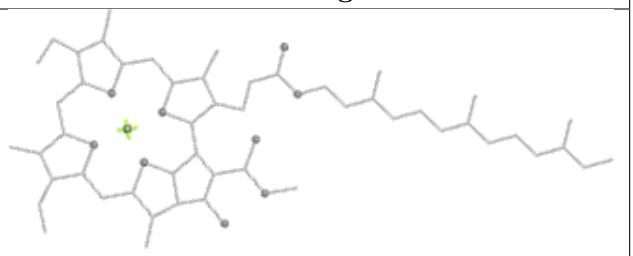
Bond lengths



Bond angles

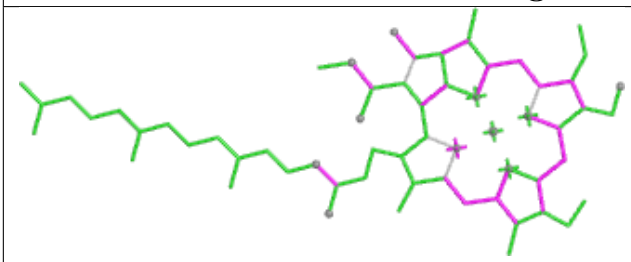


Torsions

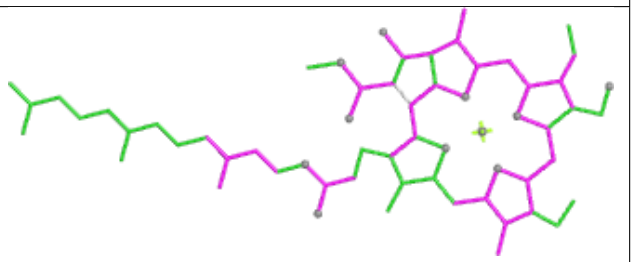


Rings

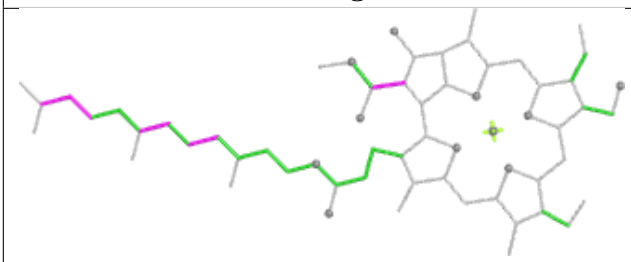
Ligand CHL 8 301



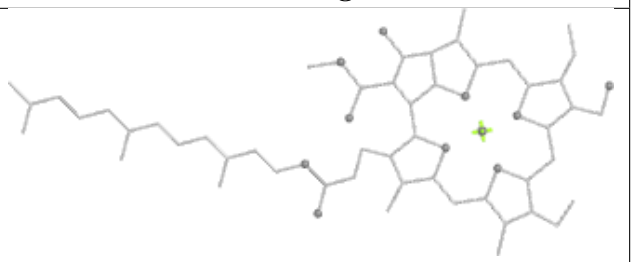
Bond lengths



Bond angles

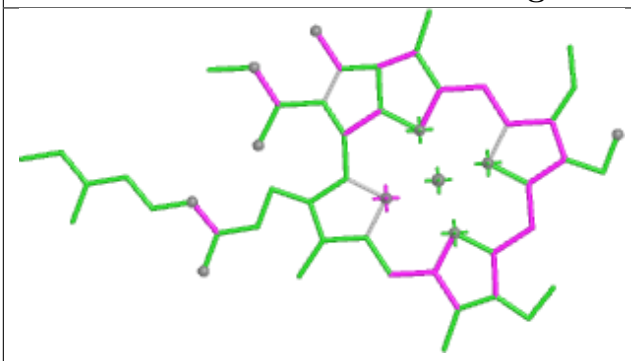


Torsions

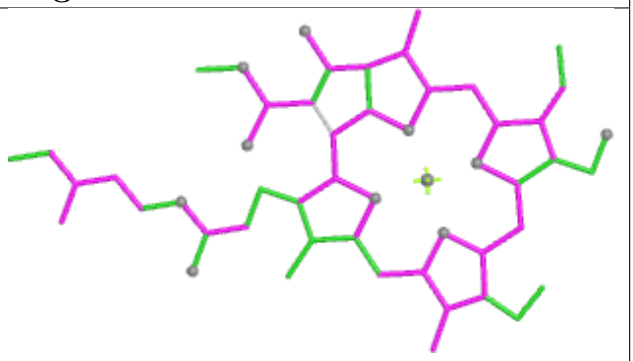


Rings

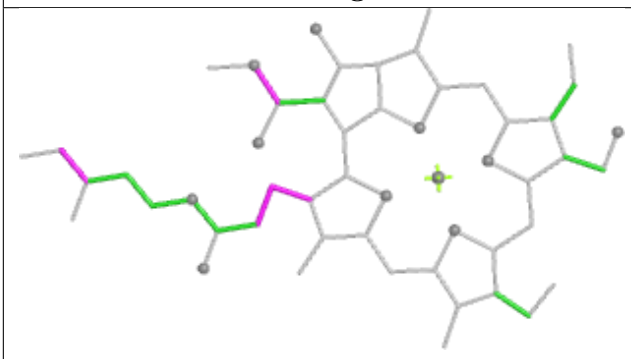
Ligand CHL g 601



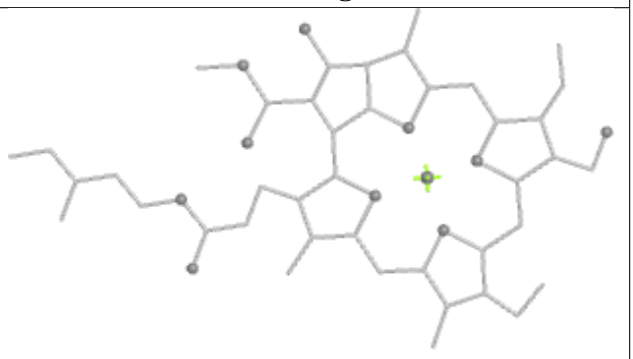
Bond lengths



Bond angles

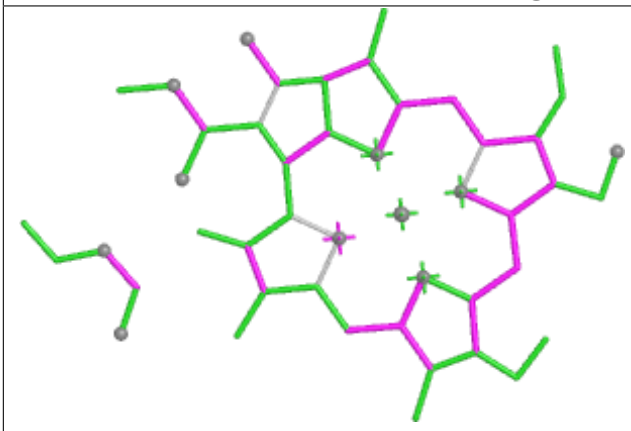


Torsions

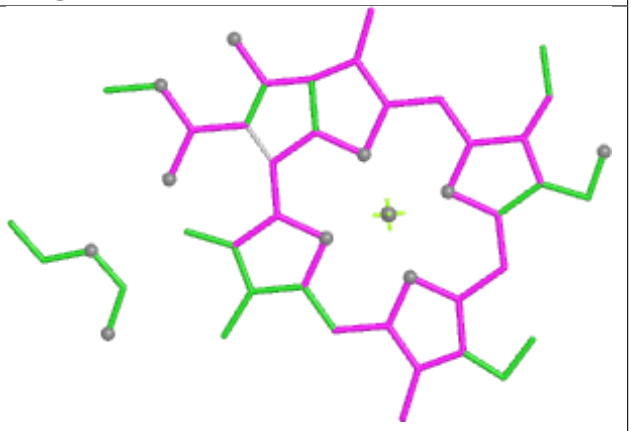


Rings

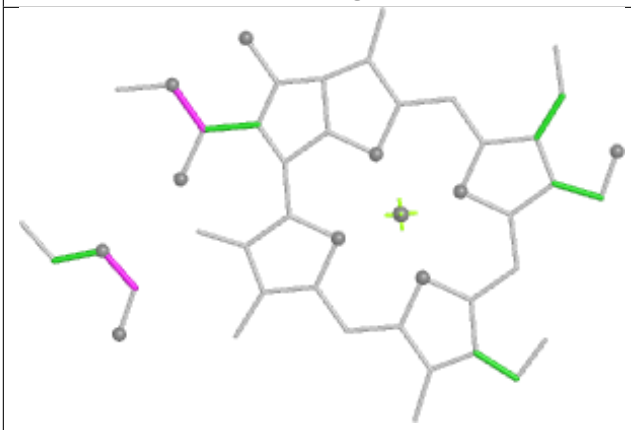
Ligand CHL g 609



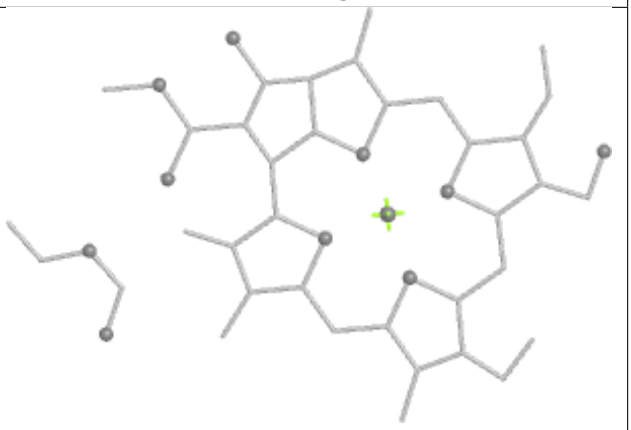
Bond lengths



Bond angles

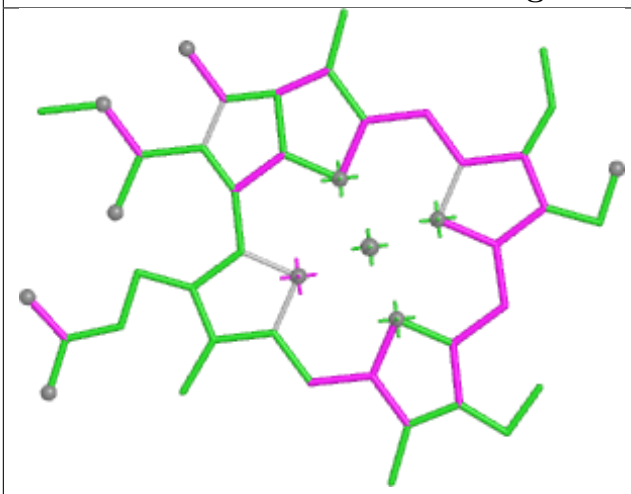


Torsions

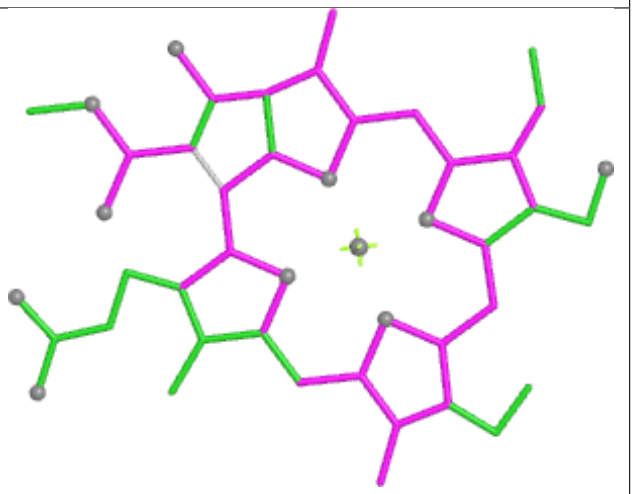


Rings

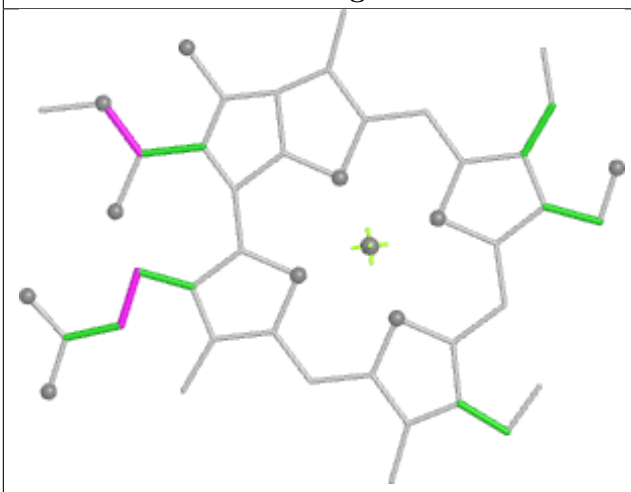
Ligand CHL h 607



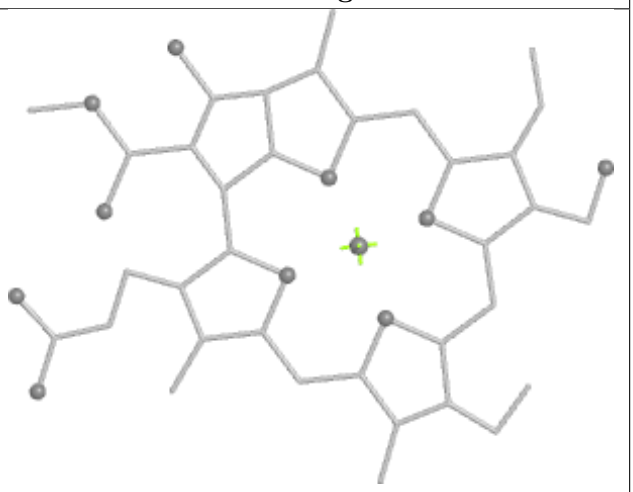
Bond lengths



Bond angles



Torsions

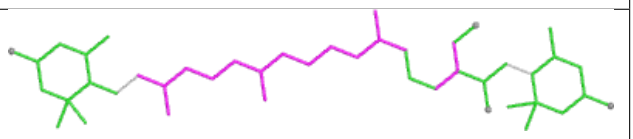


Rings

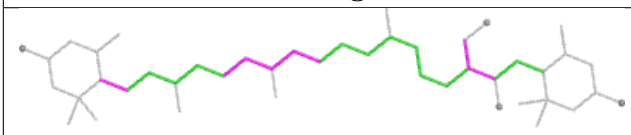
Ligand 0IE c 522



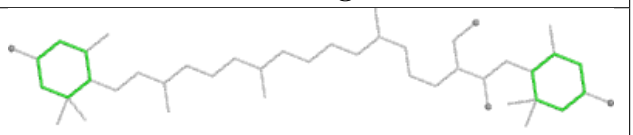
Bond lengths



Bond angles

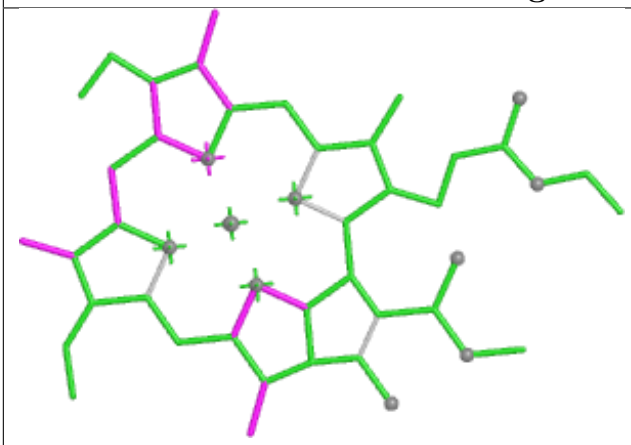


Torsions

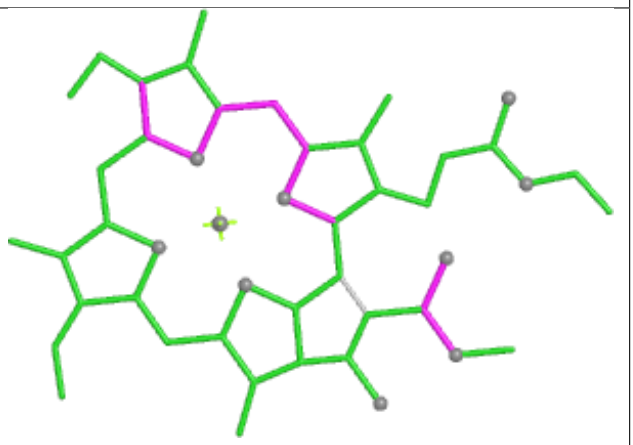


Rings

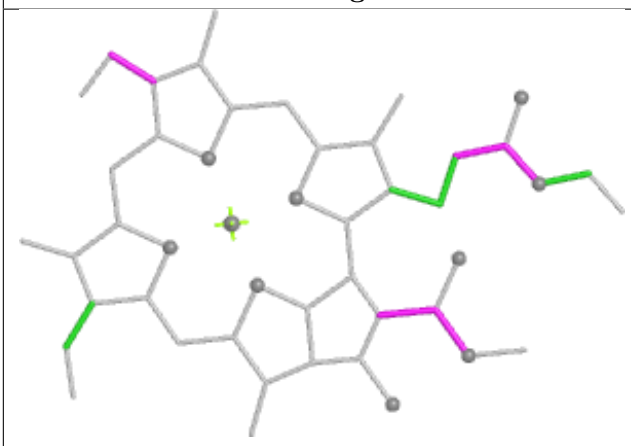
Ligand CLA 7 315



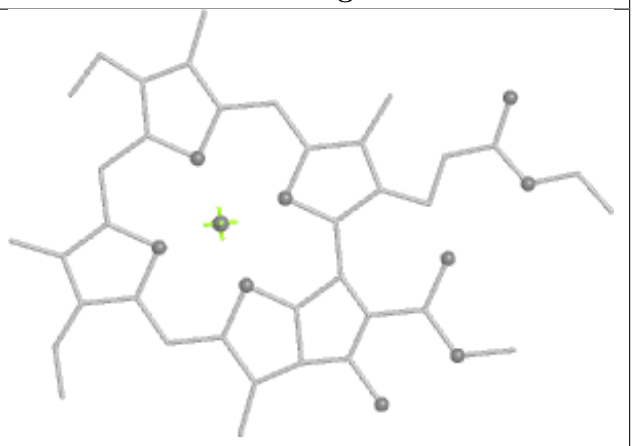
Bond lengths



Bond angles

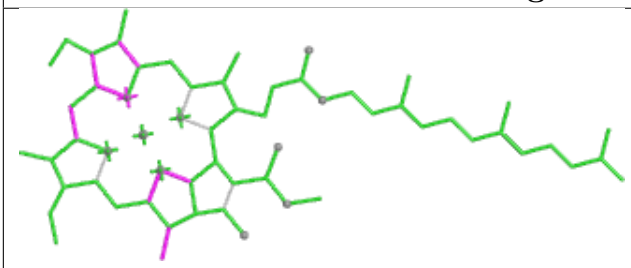


Torsions

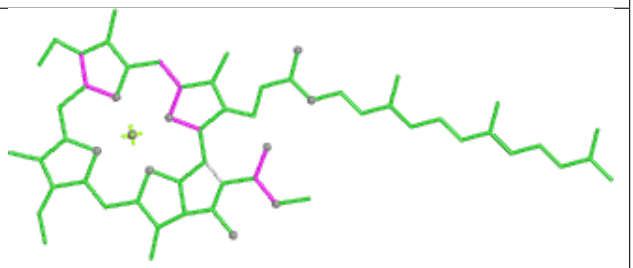


Rings

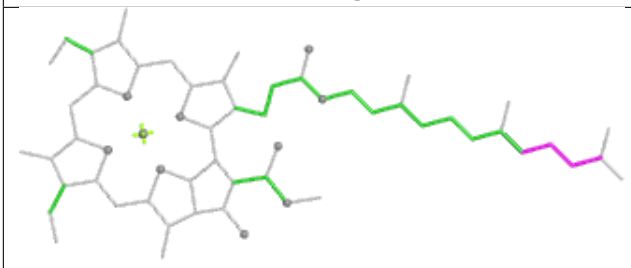
Ligand CLA b 611



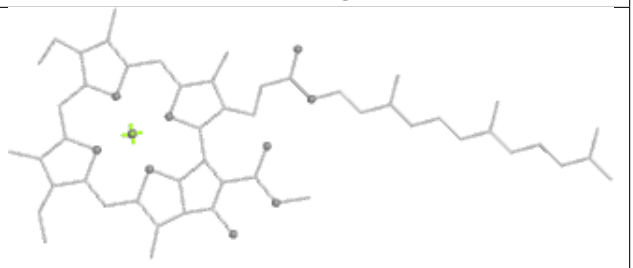
Bond lengths



Bond angles

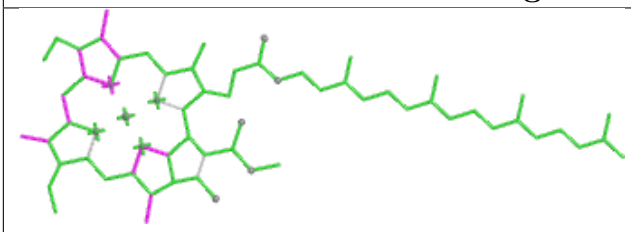


Torsions

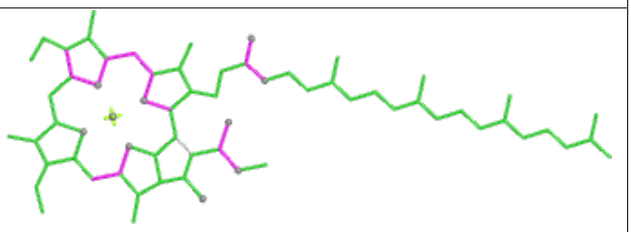


Rings

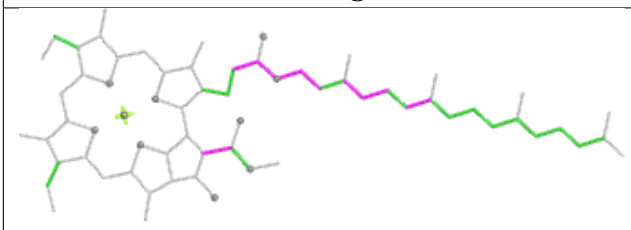
Ligand CLA A 805



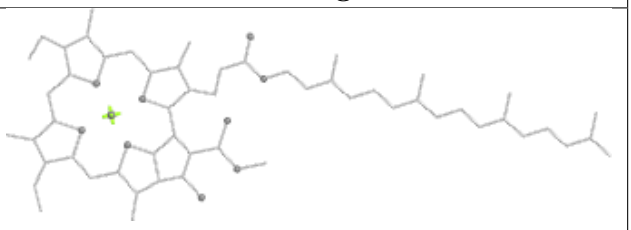
Bond lengths



Bond angles

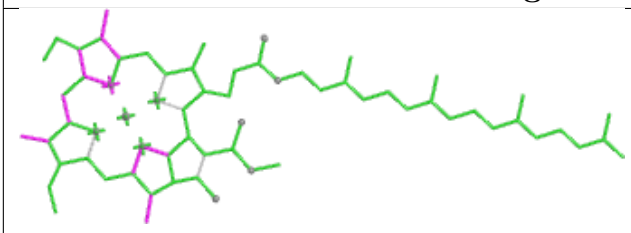


Torsions

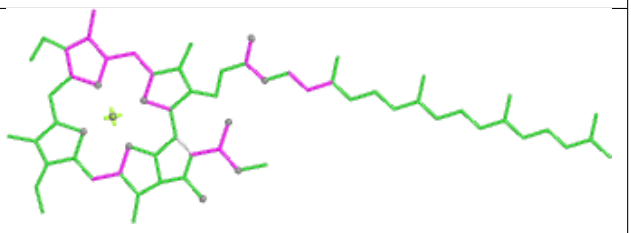


Rings

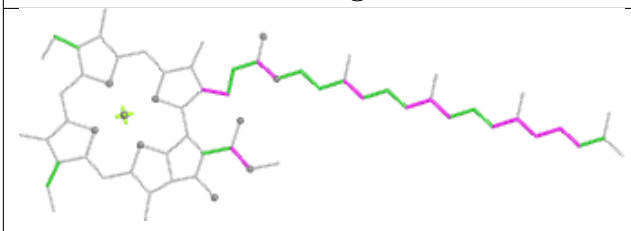
Ligand CLA A 819



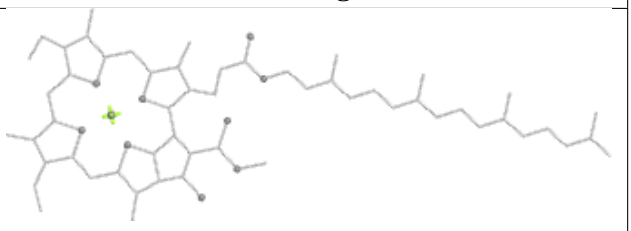
Bond lengths



Bond angles

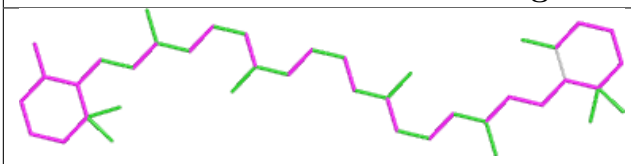


Torsions

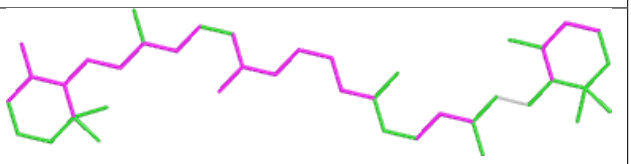


Rings

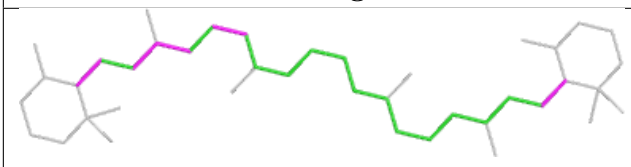
Ligand 8CT 3 402



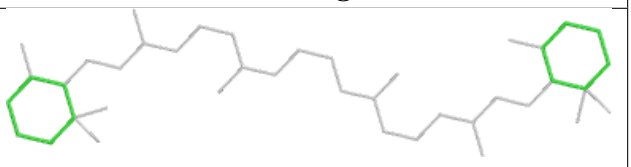
Bond lengths



Bond angles

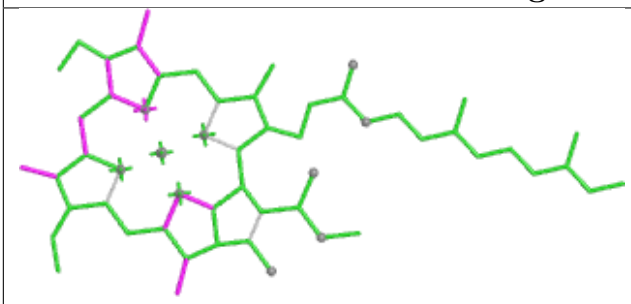


Torsions

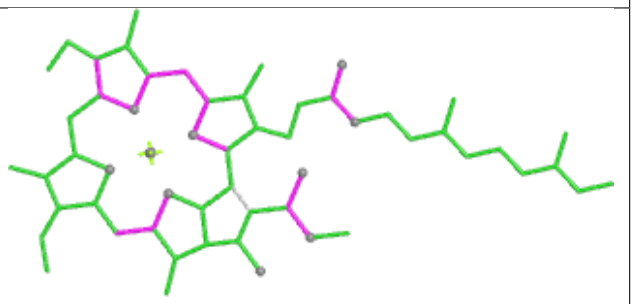


Rings

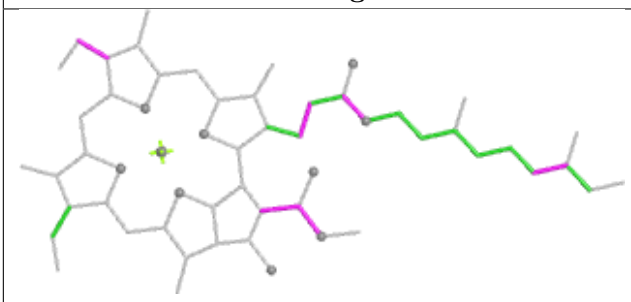
Ligand CLA 6 312



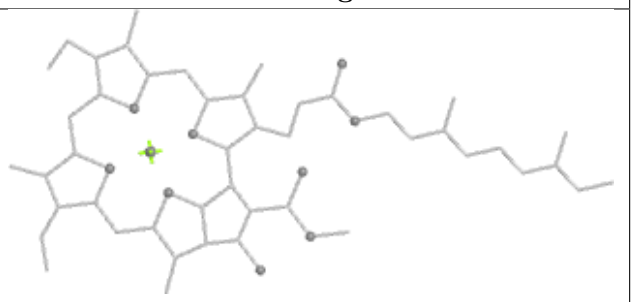
Bond lengths



Bond angles

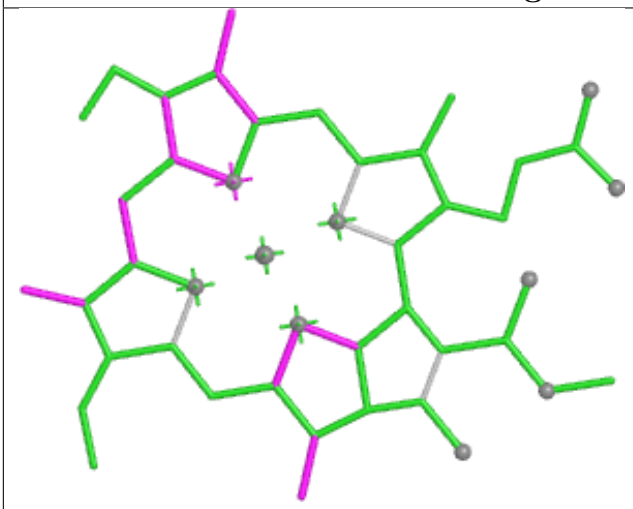


Torsions

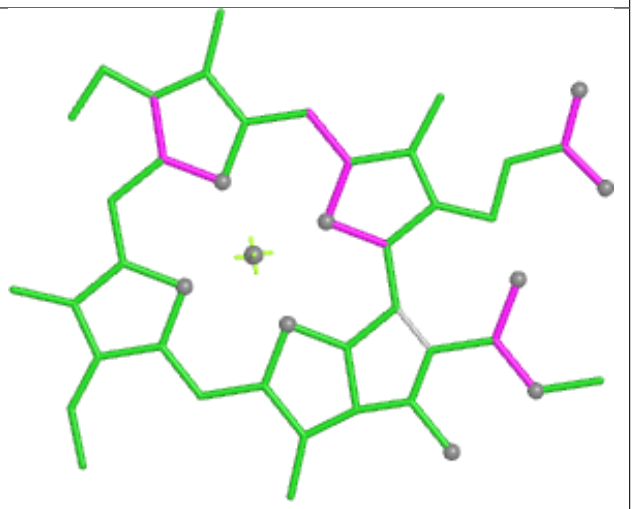


Rings

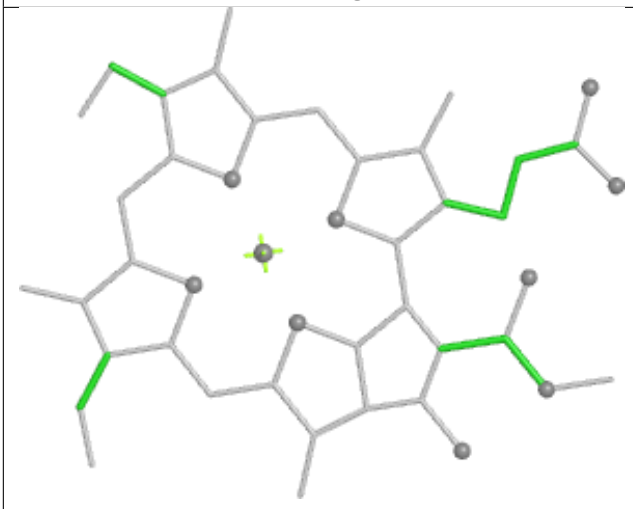
Ligand CLA B 835



Bond lengths



Bond angles

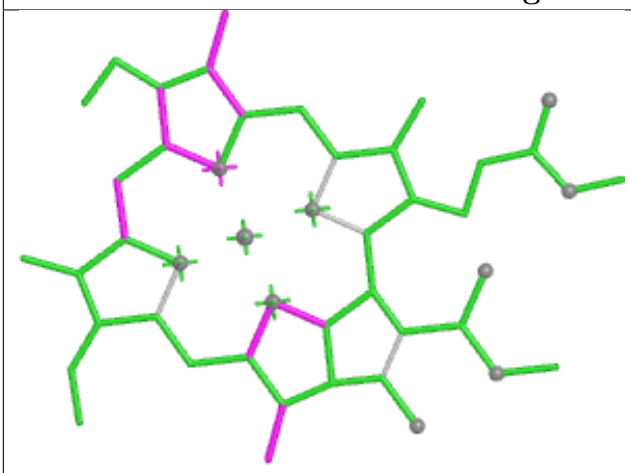


Torsions

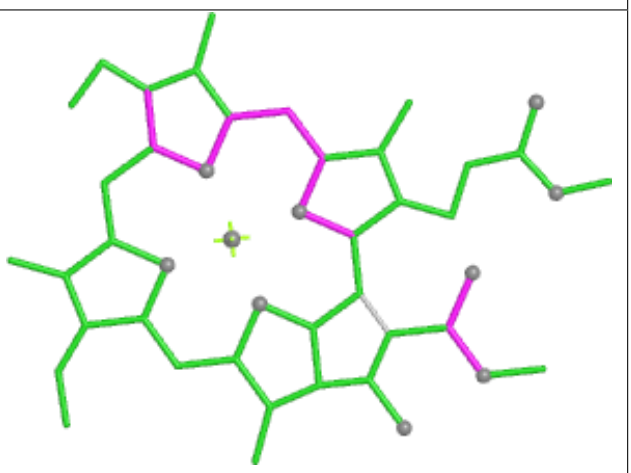


Rings

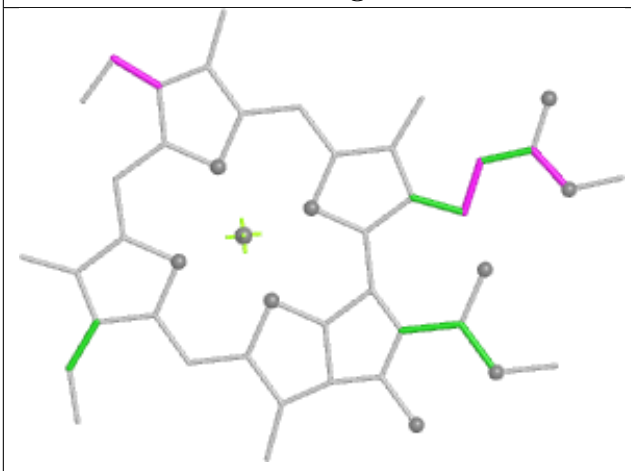
Ligand CLA G 103



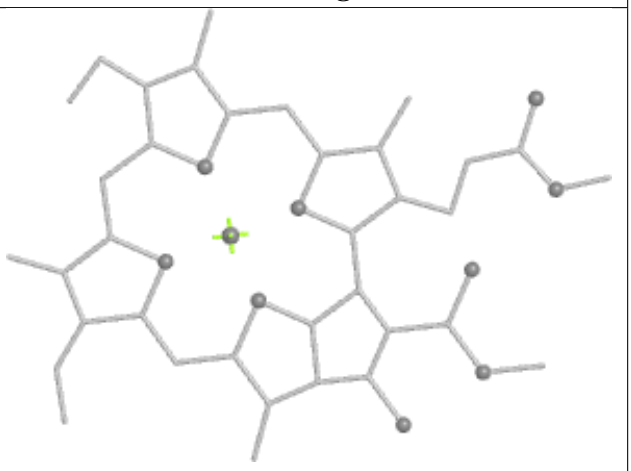
Bond lengths



Bond angles

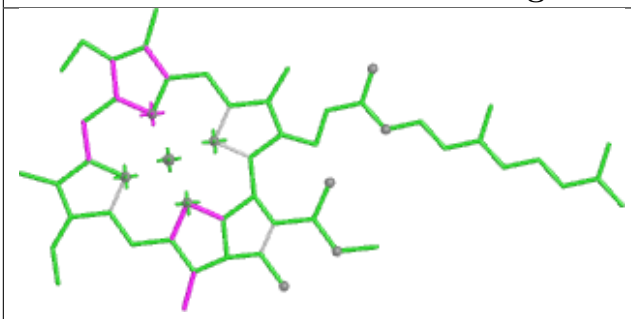


Torsions

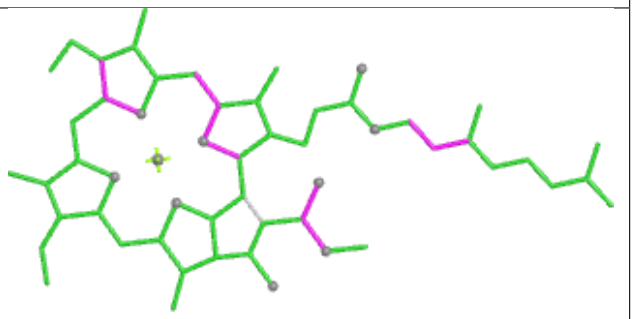


Rings

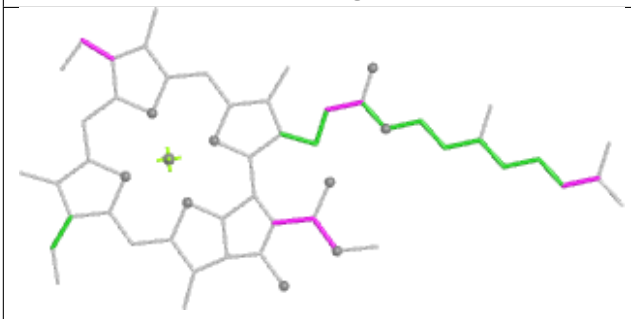
Ligand CLA d 603



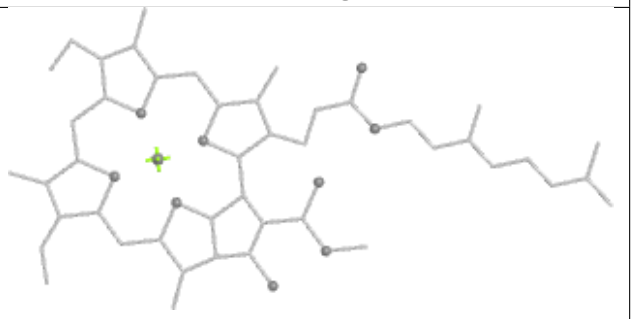
Bond lengths



Bond angles

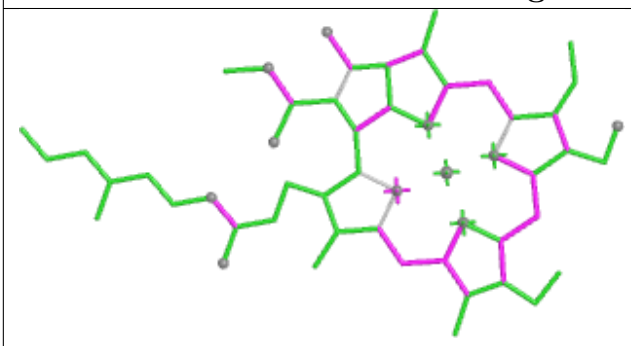


Torsions

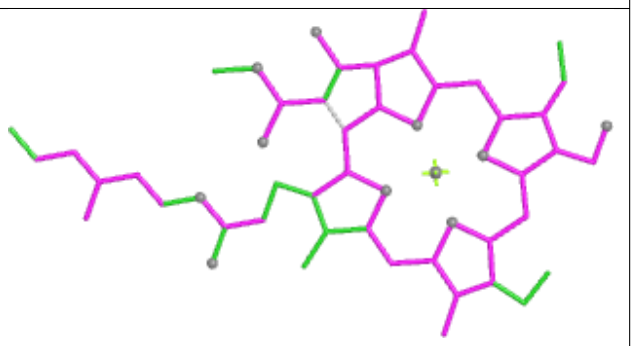


Rings

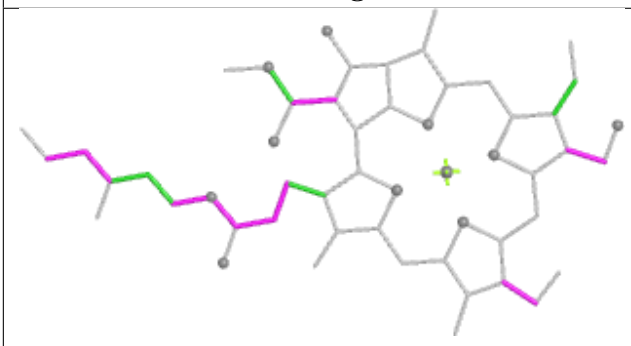
Ligand CHL 4 302



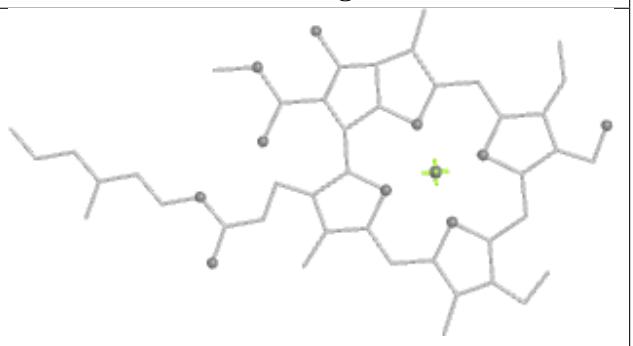
Bond lengths



Bond angles

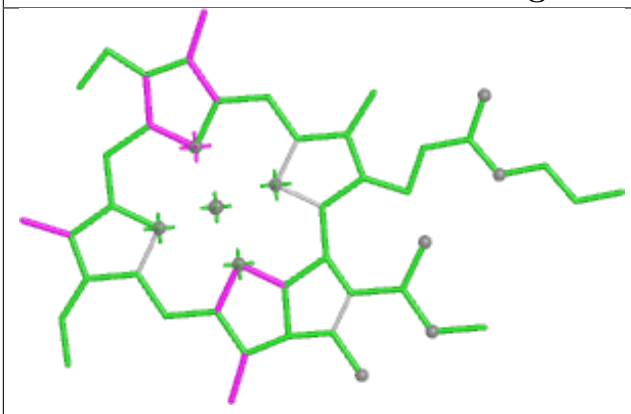


Torsions

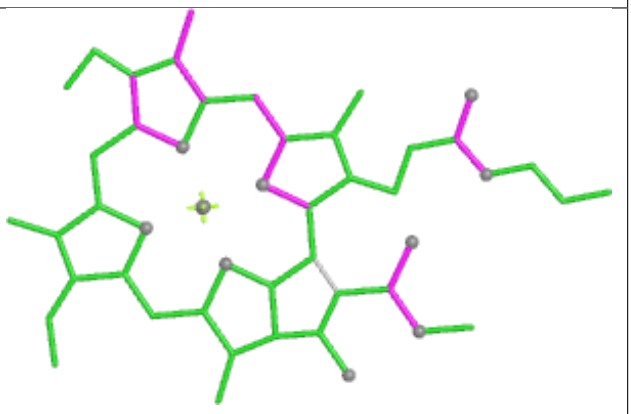


Rings

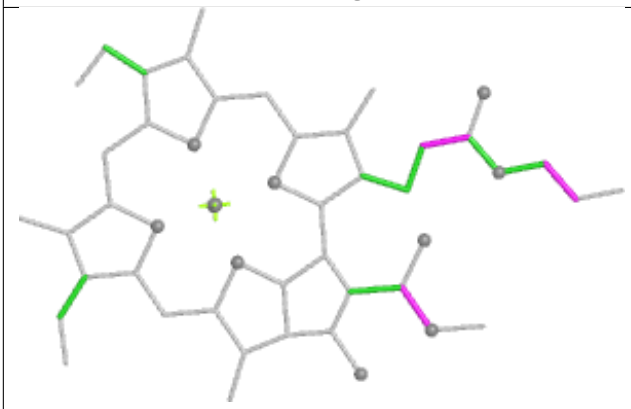
Ligand CLA 2 311



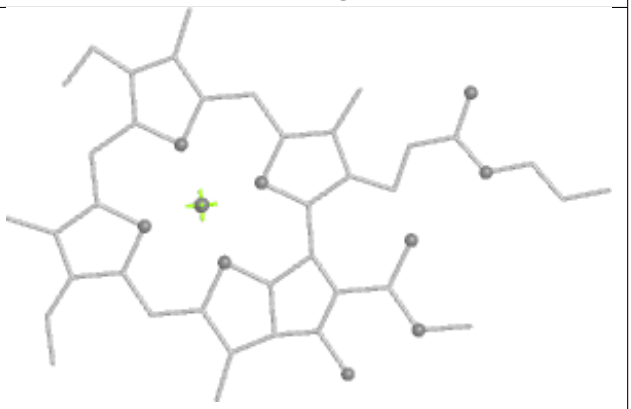
Bond lengths



Bond angles

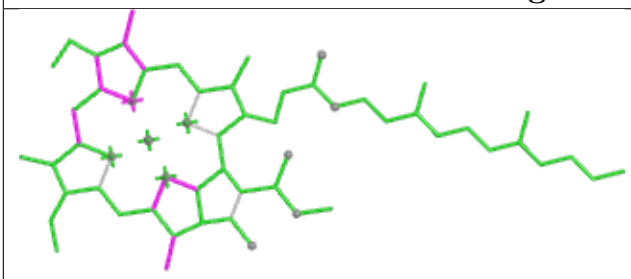


Torsions

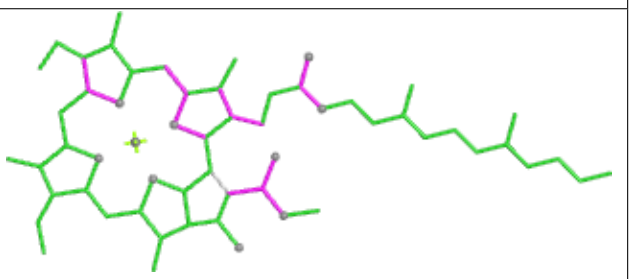


Rings

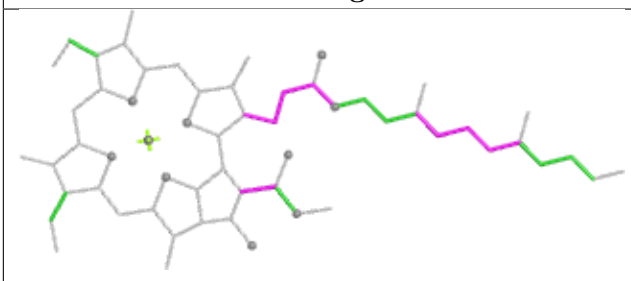
Ligand CLA 9 300



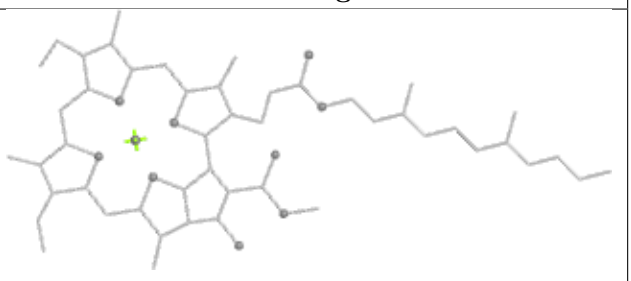
Bond lengths



Bond angles

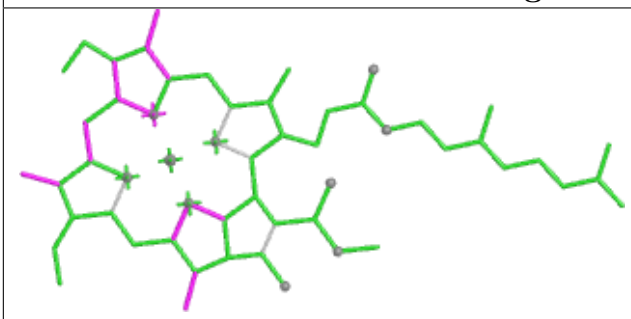


Torsions

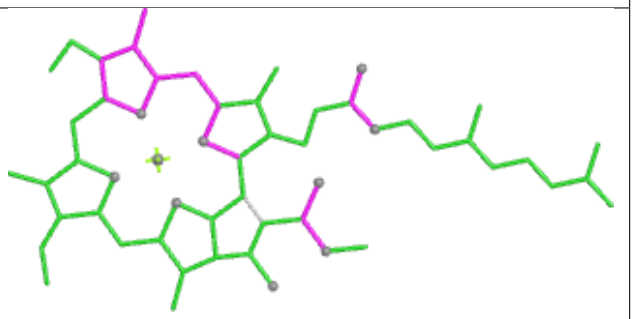


Rings

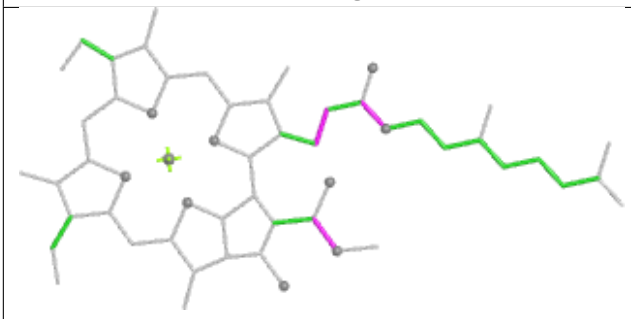
Ligand CLA B 815



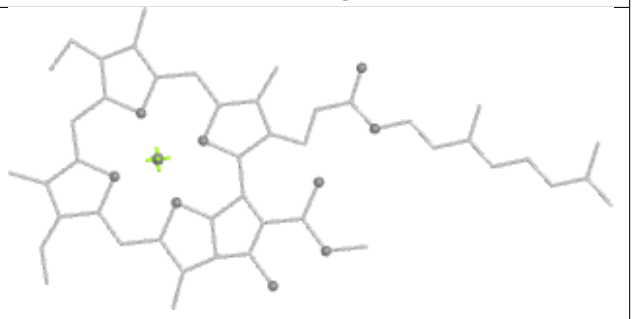
Bond lengths



Bond angles

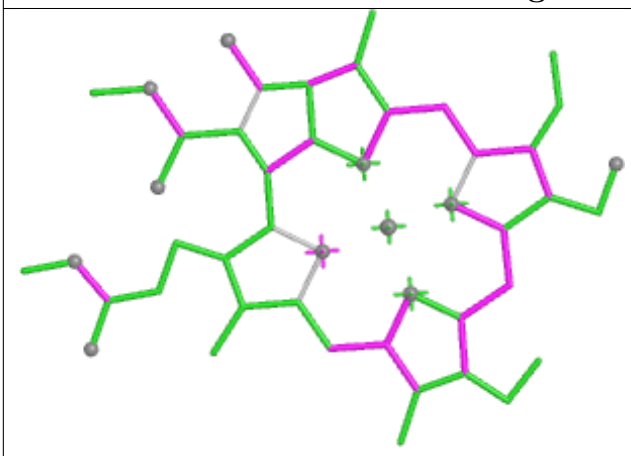


Torsions

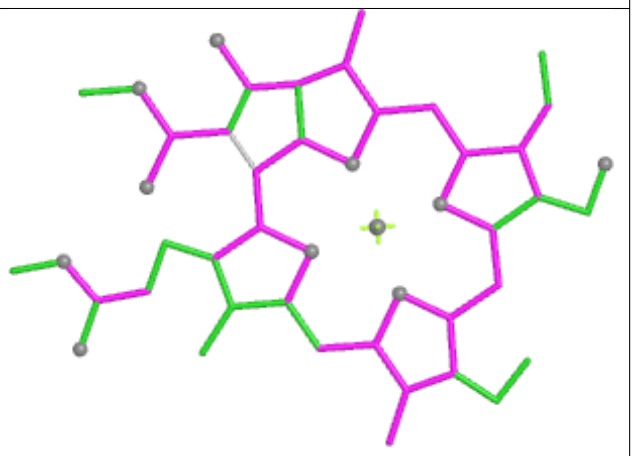


Rings

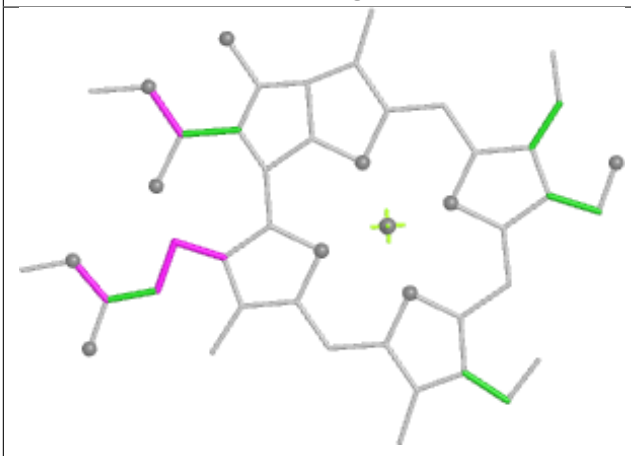
Ligand CHL a 601



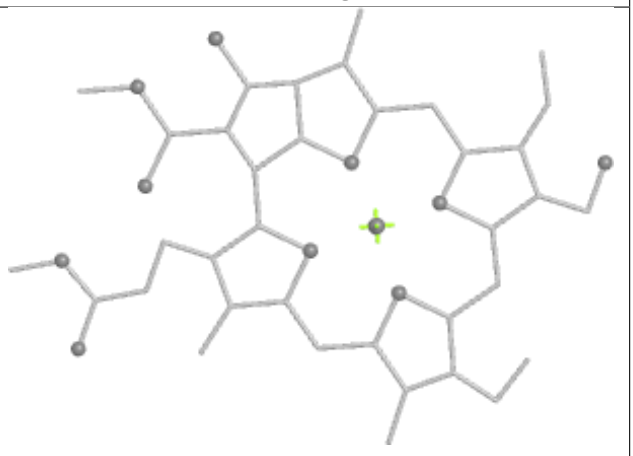
Bond lengths



Bond angles

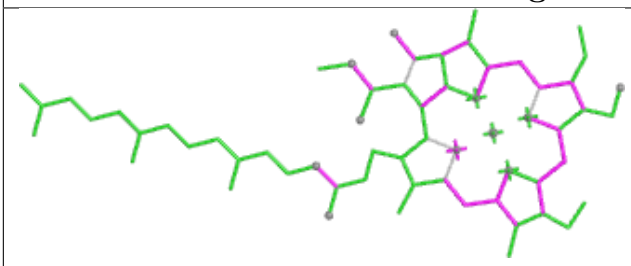


Torsions

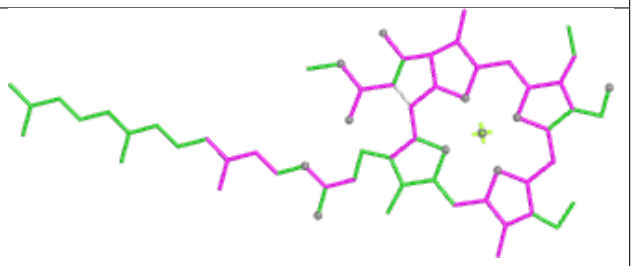


Rings

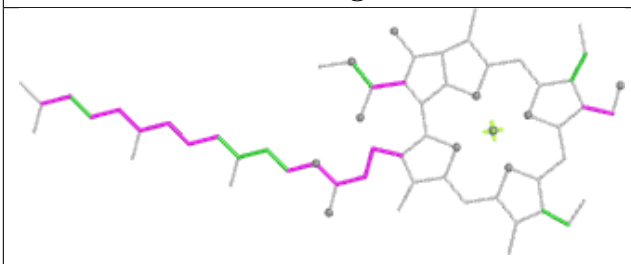
Ligand CHL e 602



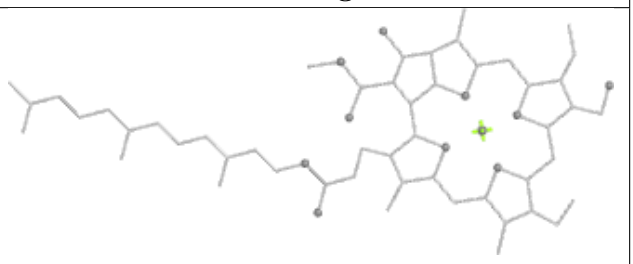
Bond lengths



Bond angles

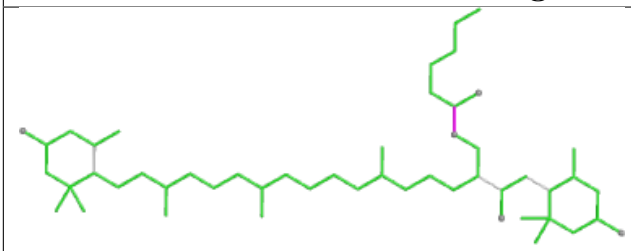


Torsions

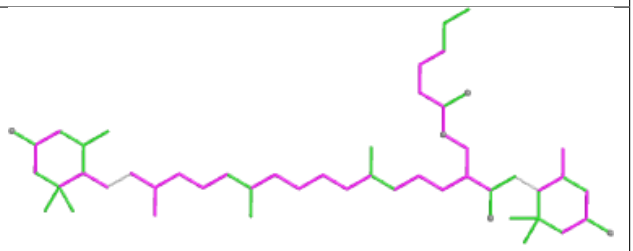


Rings

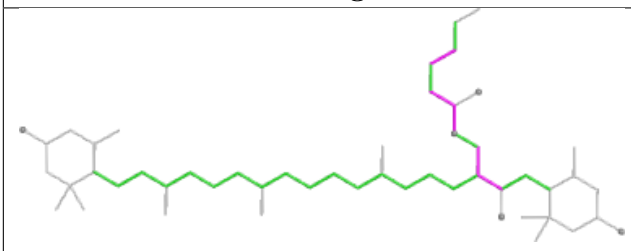
Ligand 0UR 4 501



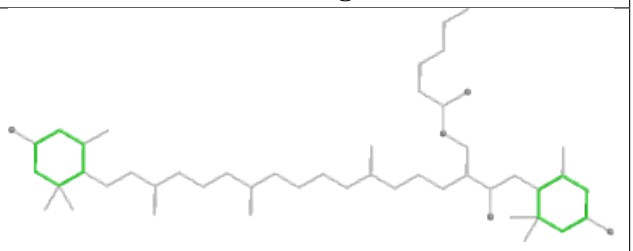
Bond lengths



Bond angles

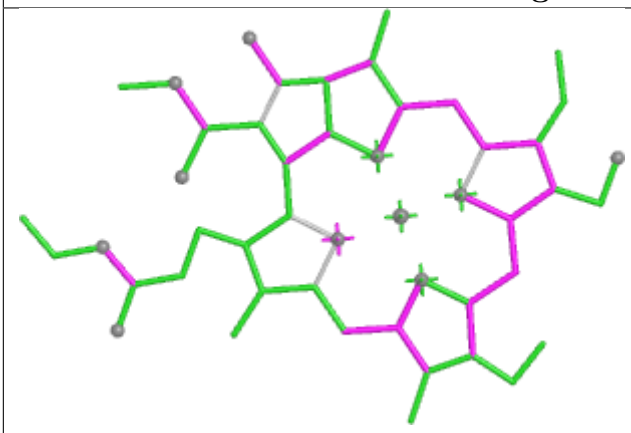


Torsions

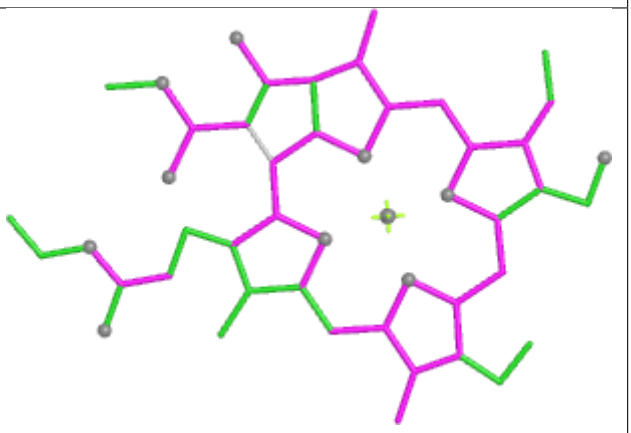


Rings

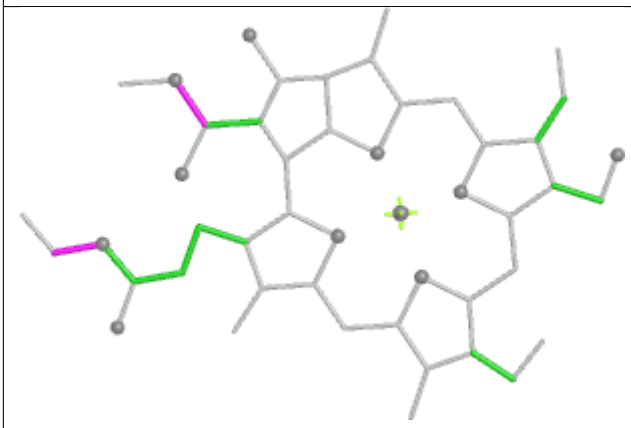
Ligand CHL i 609



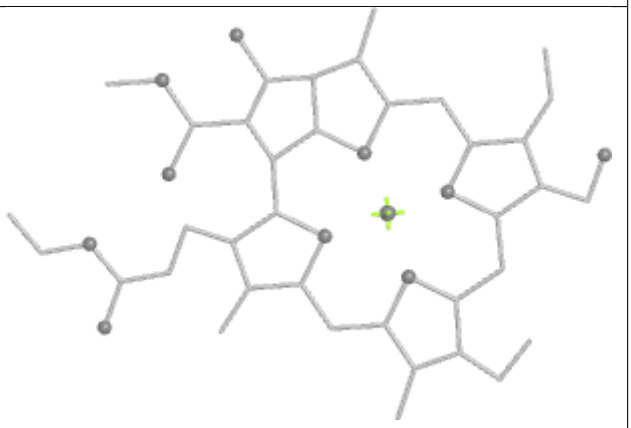
Bond lengths



Bond angles

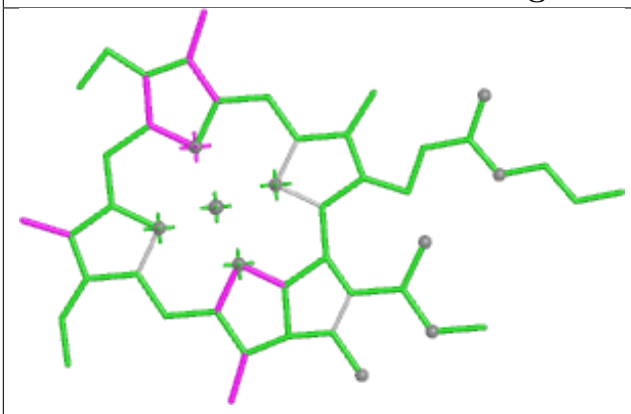


Torsions

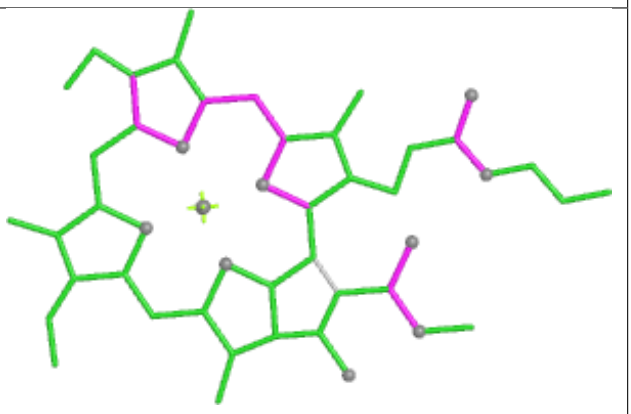


Rings

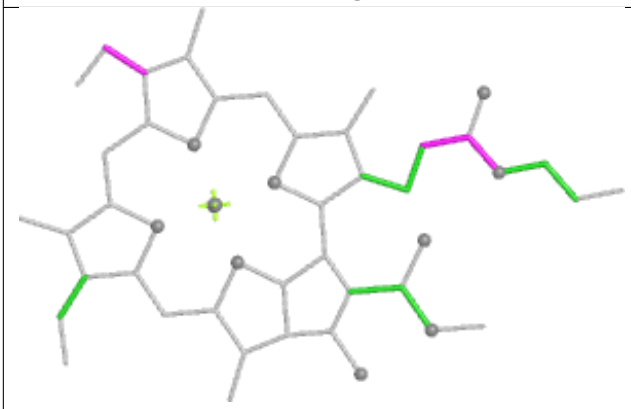
Ligand CLA 9 303



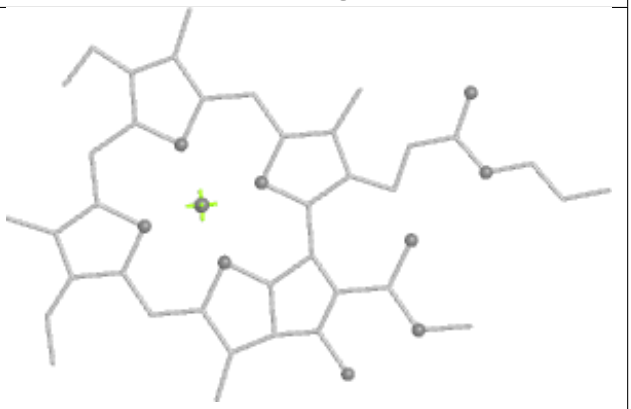
Bond lengths



Bond angles

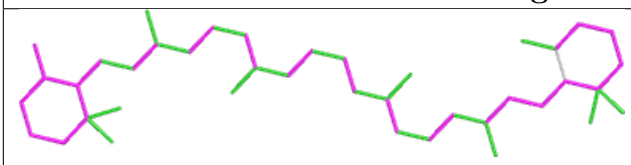


Torsions

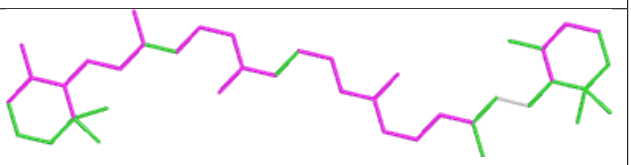


Rings

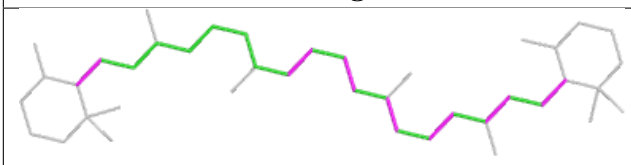
Ligand 8CT J 101



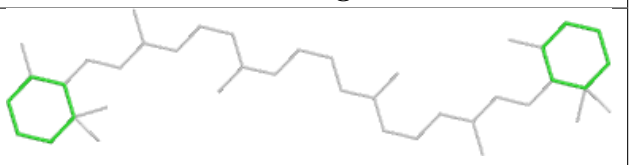
Bond lengths



Bond angles

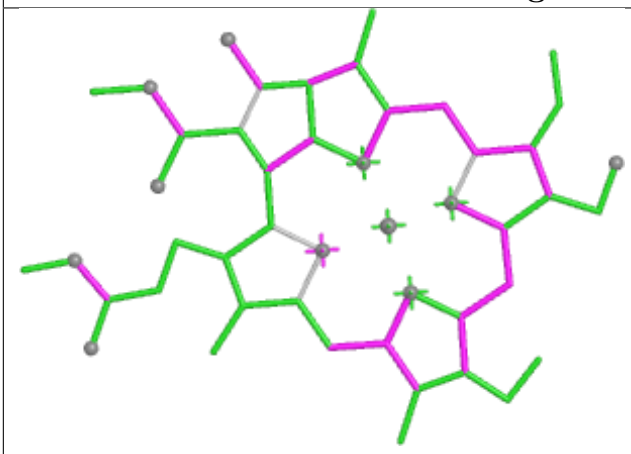


Torsions

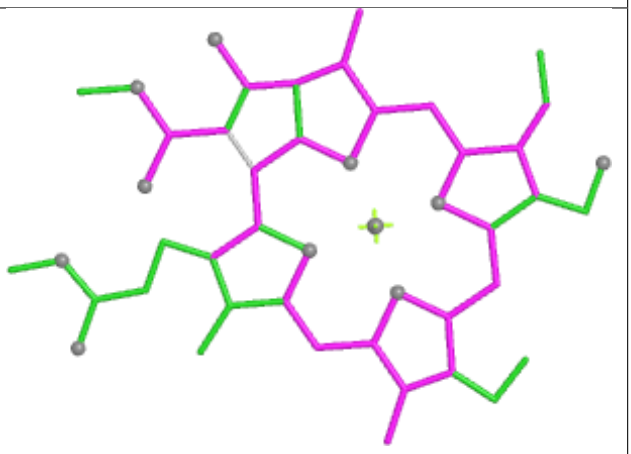


Rings

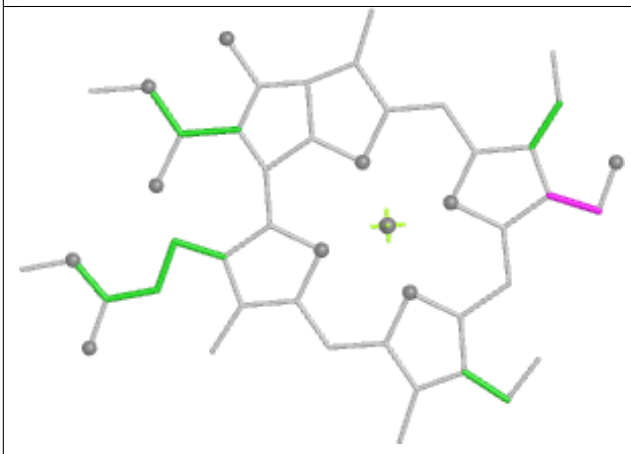
Ligand CHL 8 308



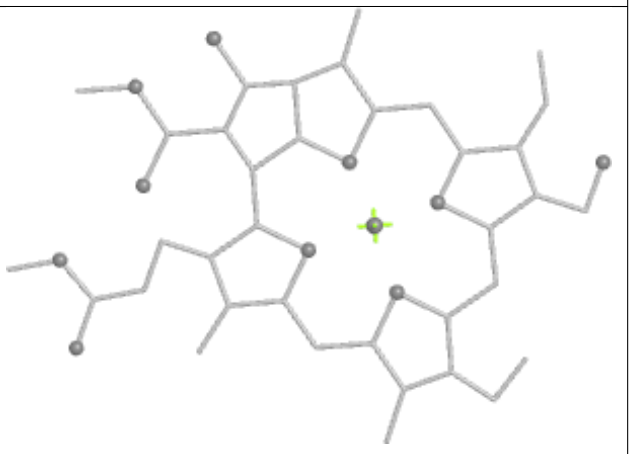
Bond lengths



Bond angles

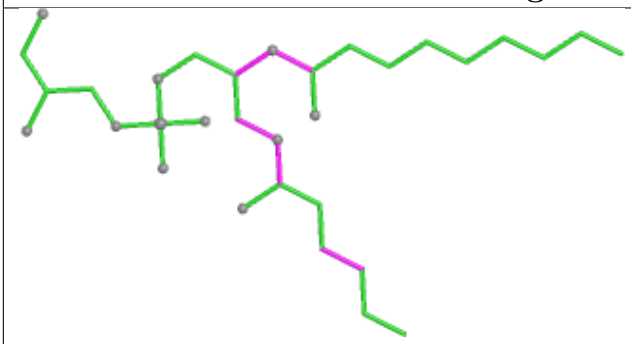


Torsions

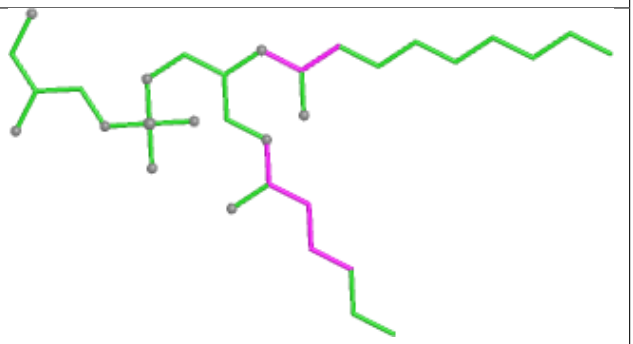


Rings

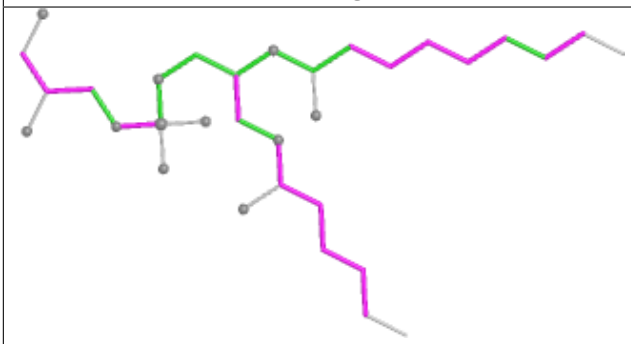
Ligand LHG 2 601



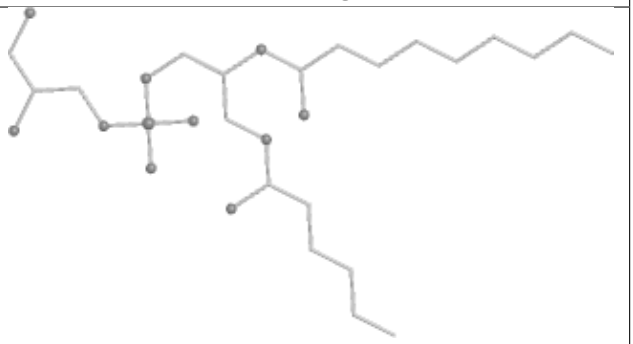
Bond lengths



Bond angles

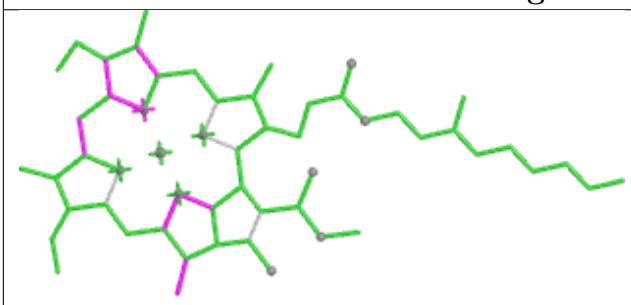


Torsions

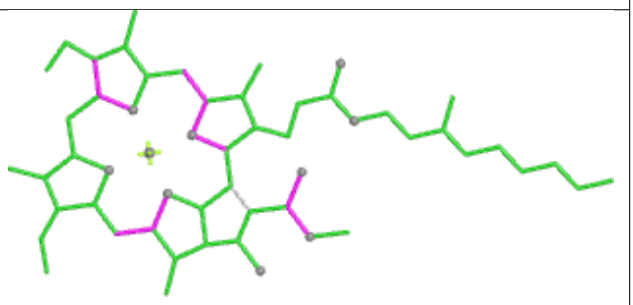


Rings

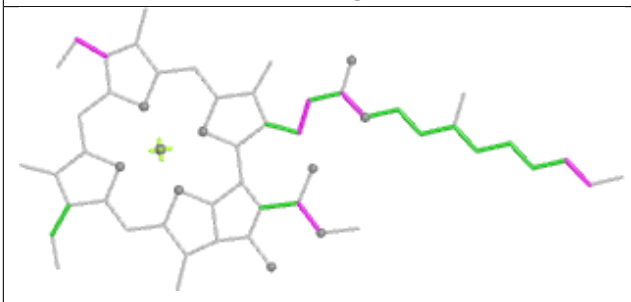
Ligand CLA d 613



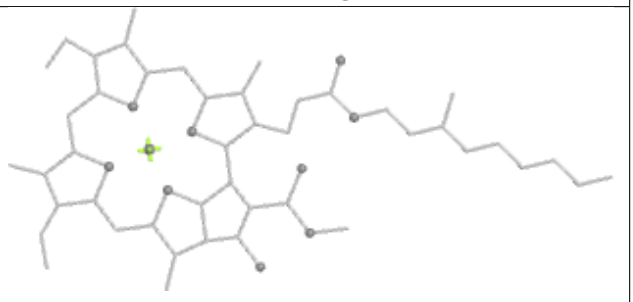
Bond lengths



Bond angles

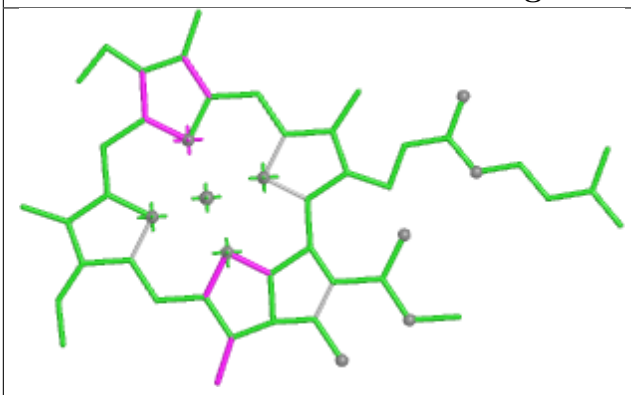


Torsions

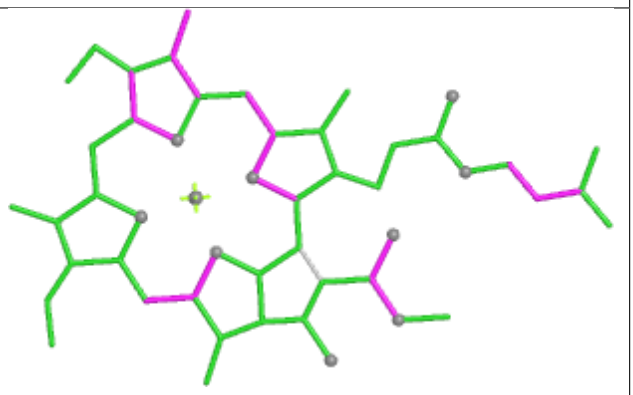


Rings

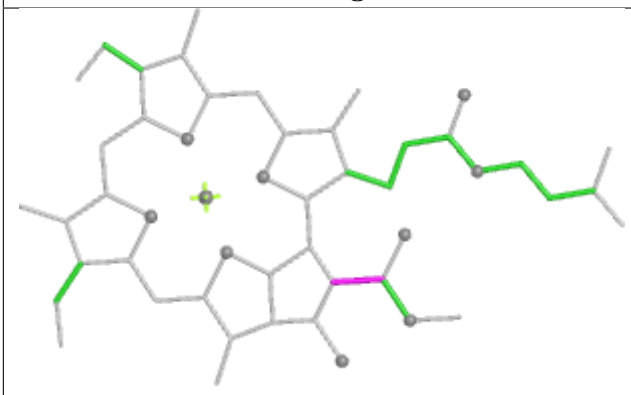
Ligand CLA B 821



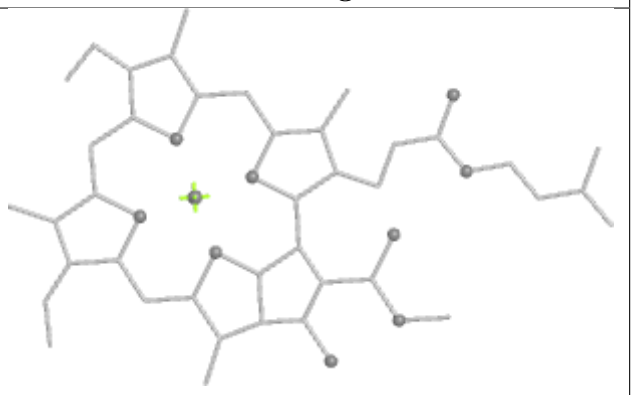
Bond lengths



Bond angles

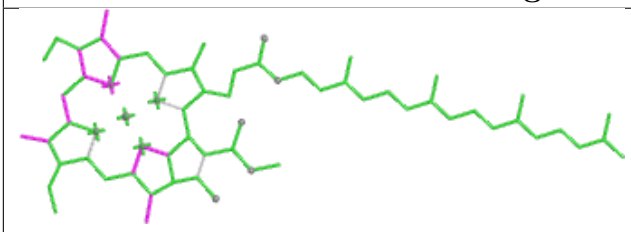


Torsions

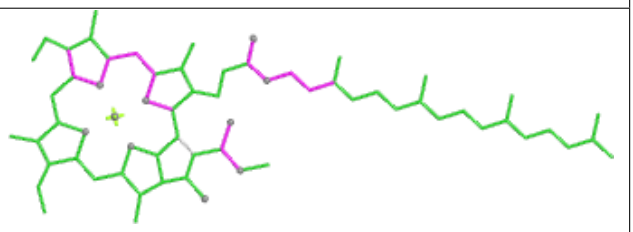


Rings

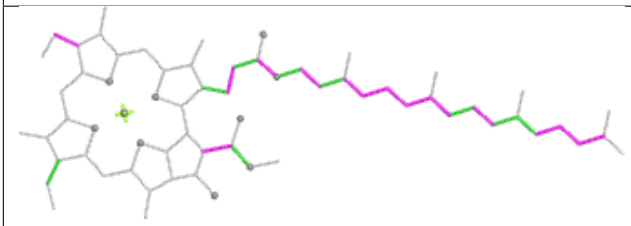
Ligand CLA A 840



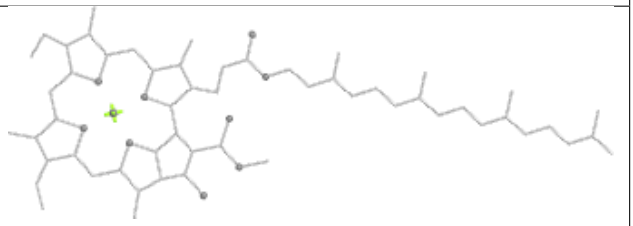
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

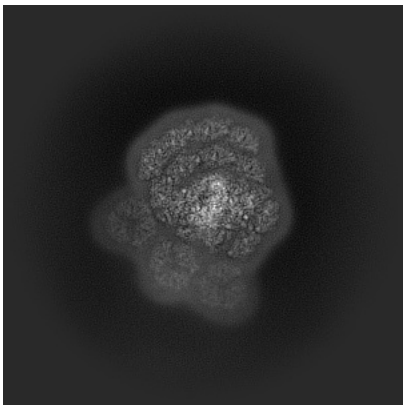
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61940. These allow visual inspection of the internal detail of the map and identification of artifacts.

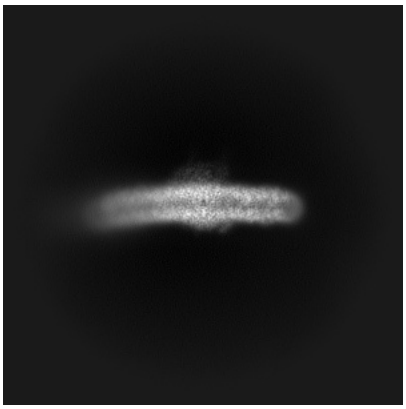
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

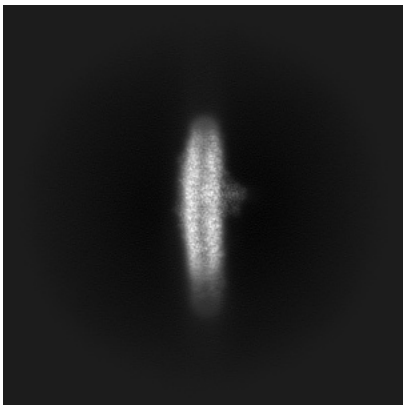
6.1.1 Primary map



X

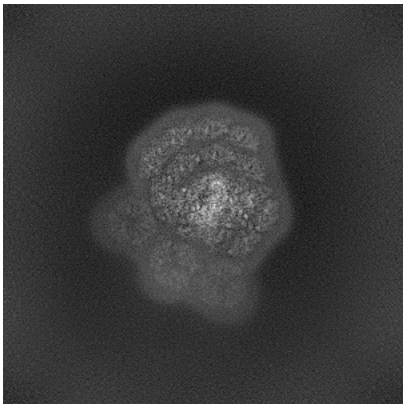


Y

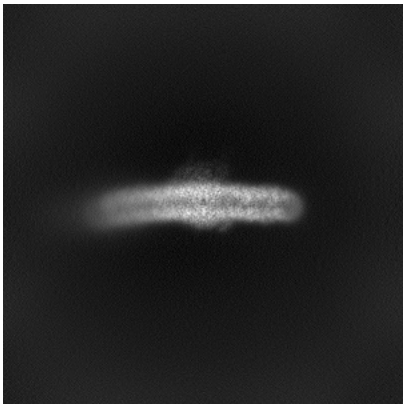


Z

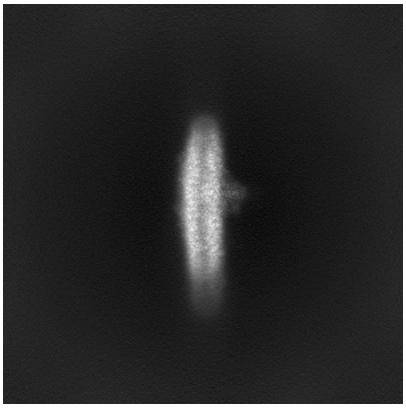
6.1.2 Raw map



X



Y

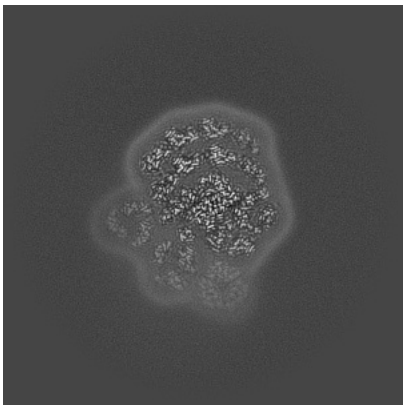


Z

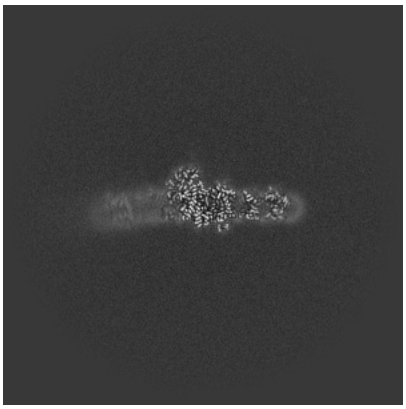
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

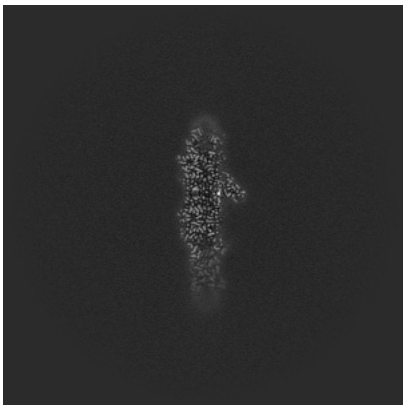
6.2.1 Primary map



X Index: 256

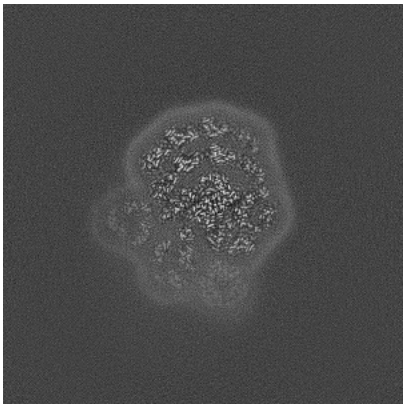


Y Index: 256

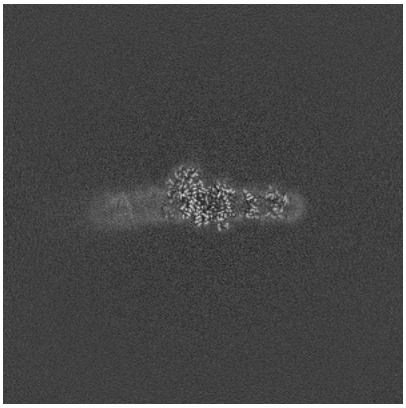


Z Index: 256

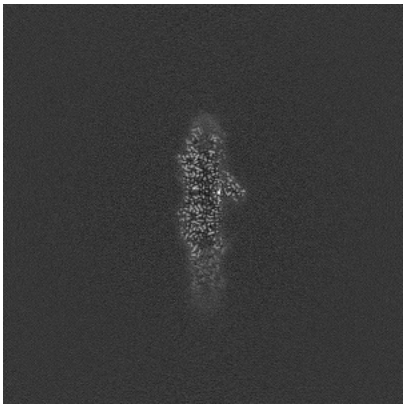
6.2.2 Raw map



X Index: 256



Y Index: 256

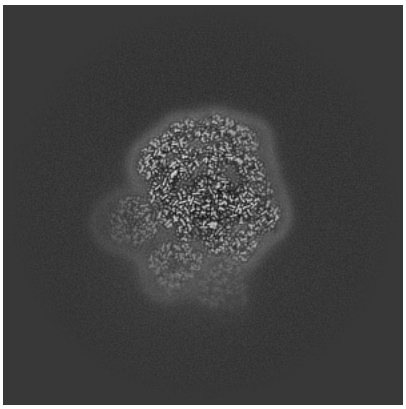


Z Index: 256

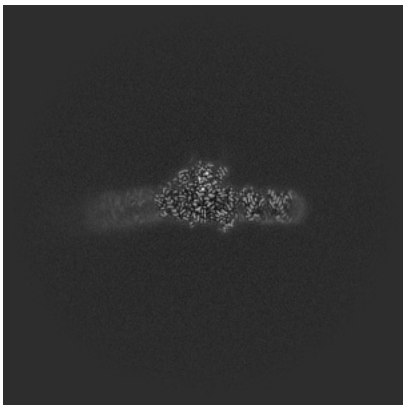
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 266

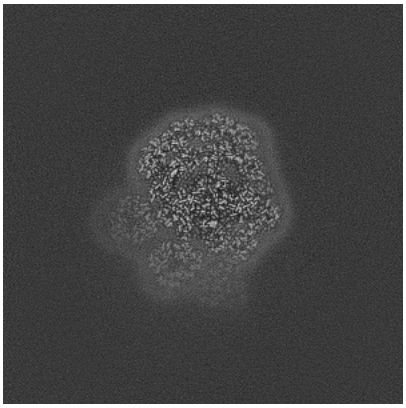


Y Index: 269

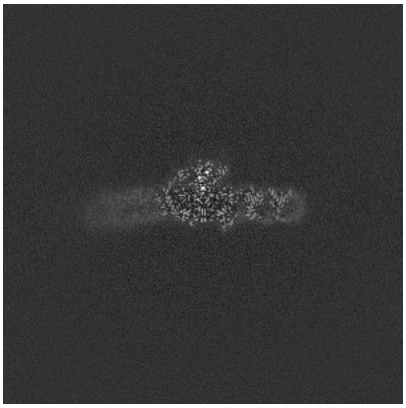


Z Index: 251

6.3.2 Raw map



X Index: 266



Y Index: 270

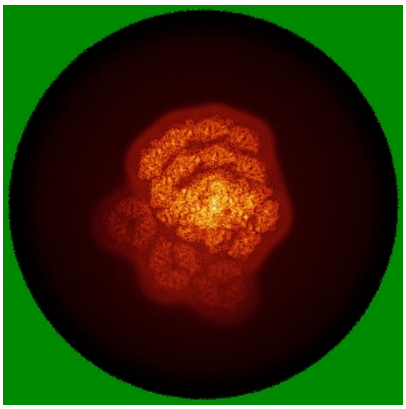


Z Index: 251

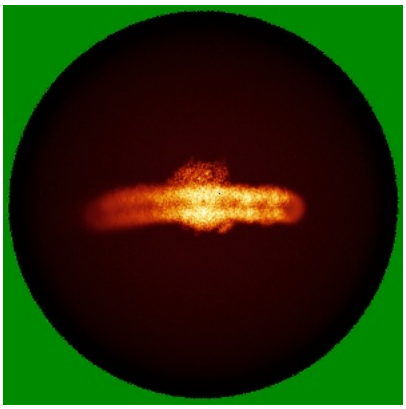
The images above show the largest variance slices of the map in three orthogonal directions.

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

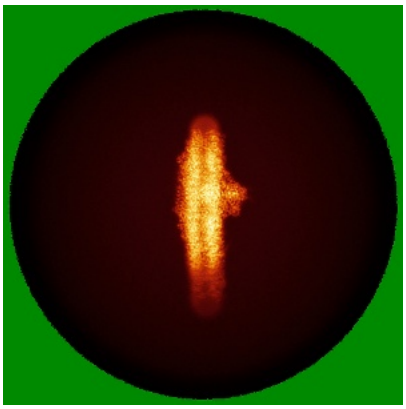
6.4.1 Primary map



X

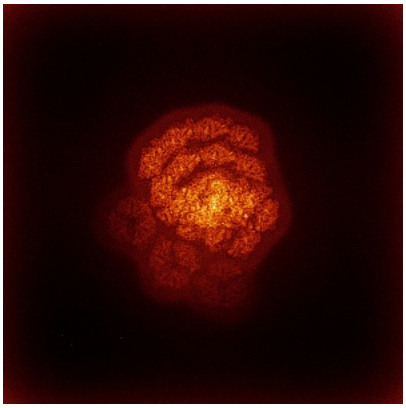


Y

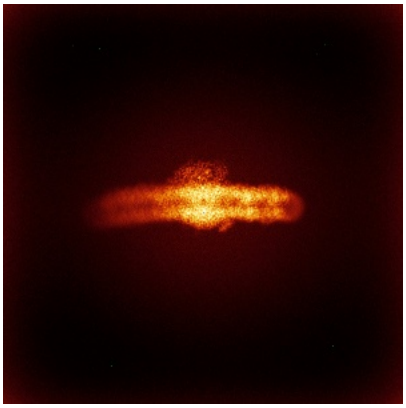


Z

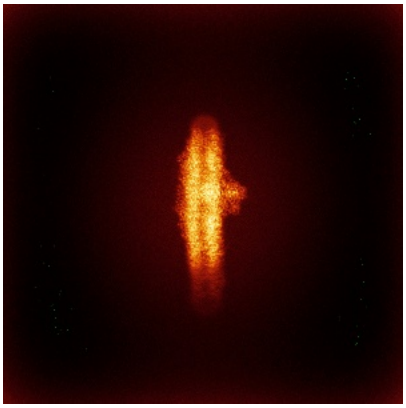
6.4.2 Raw map



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 0.217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

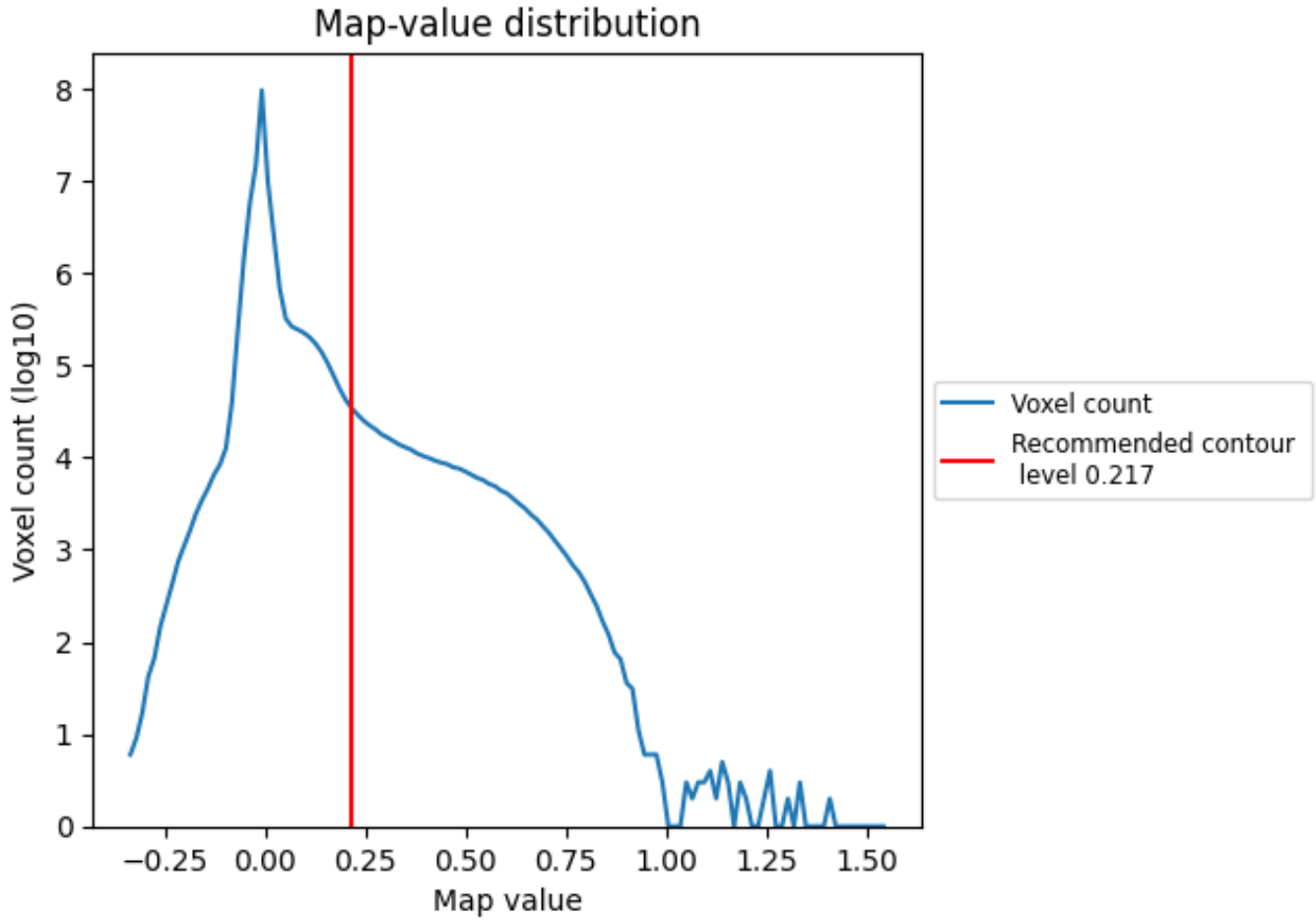
6.6 Mask visualisation (i)

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

7 Map analysis

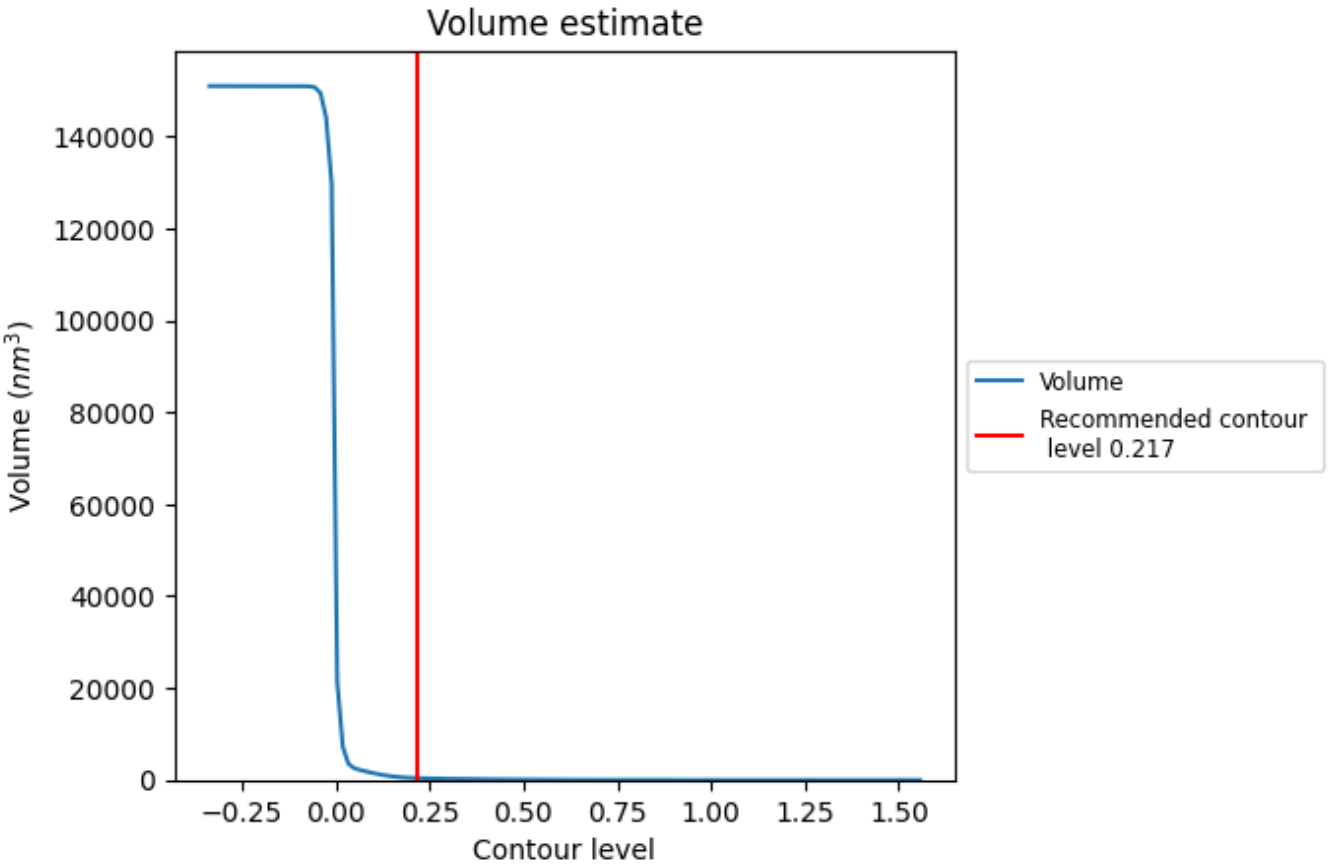
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

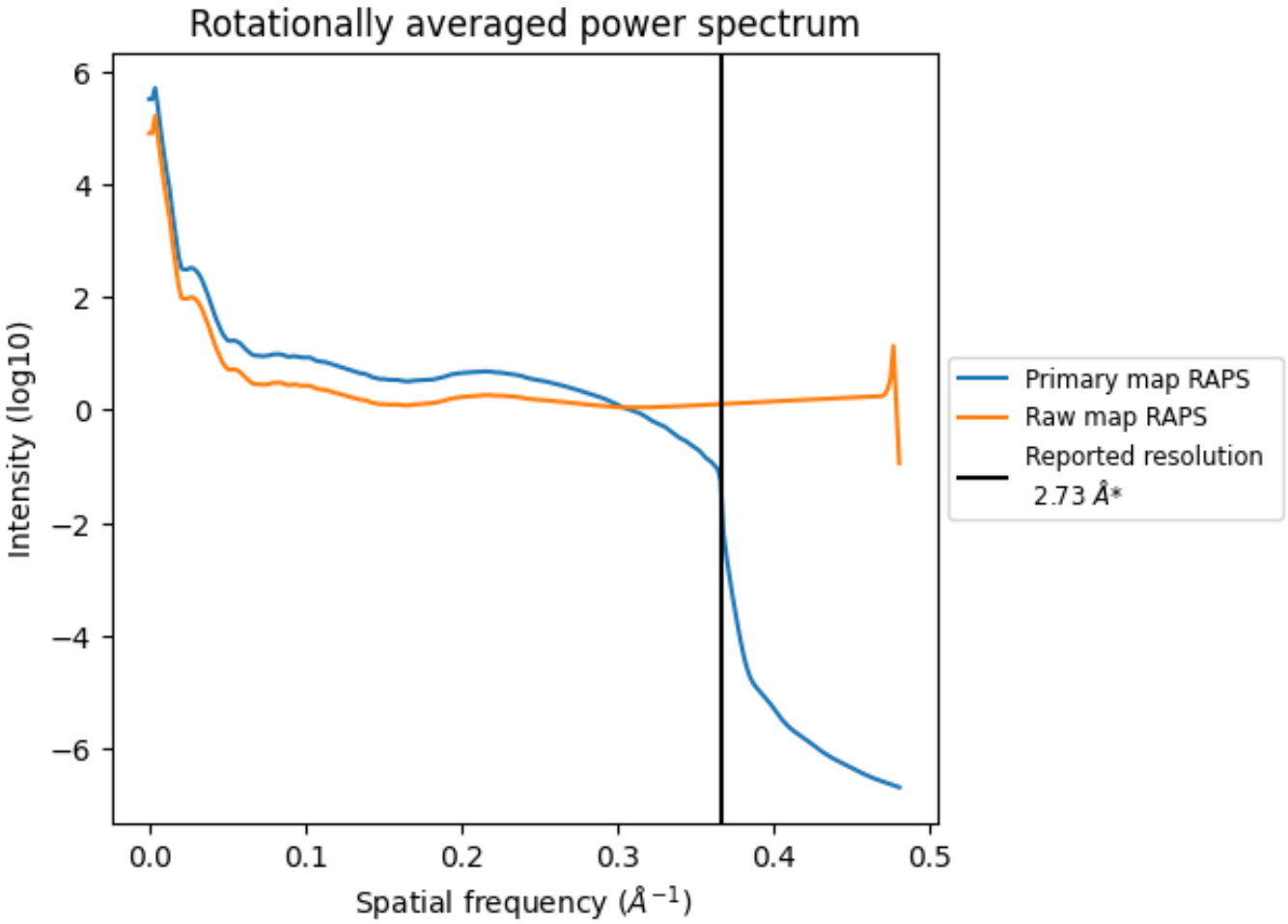
7.2 Volume estimate



The volume at the recommended contour level is 401 nm^3; this corresponds to an approximate mass of 362 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)

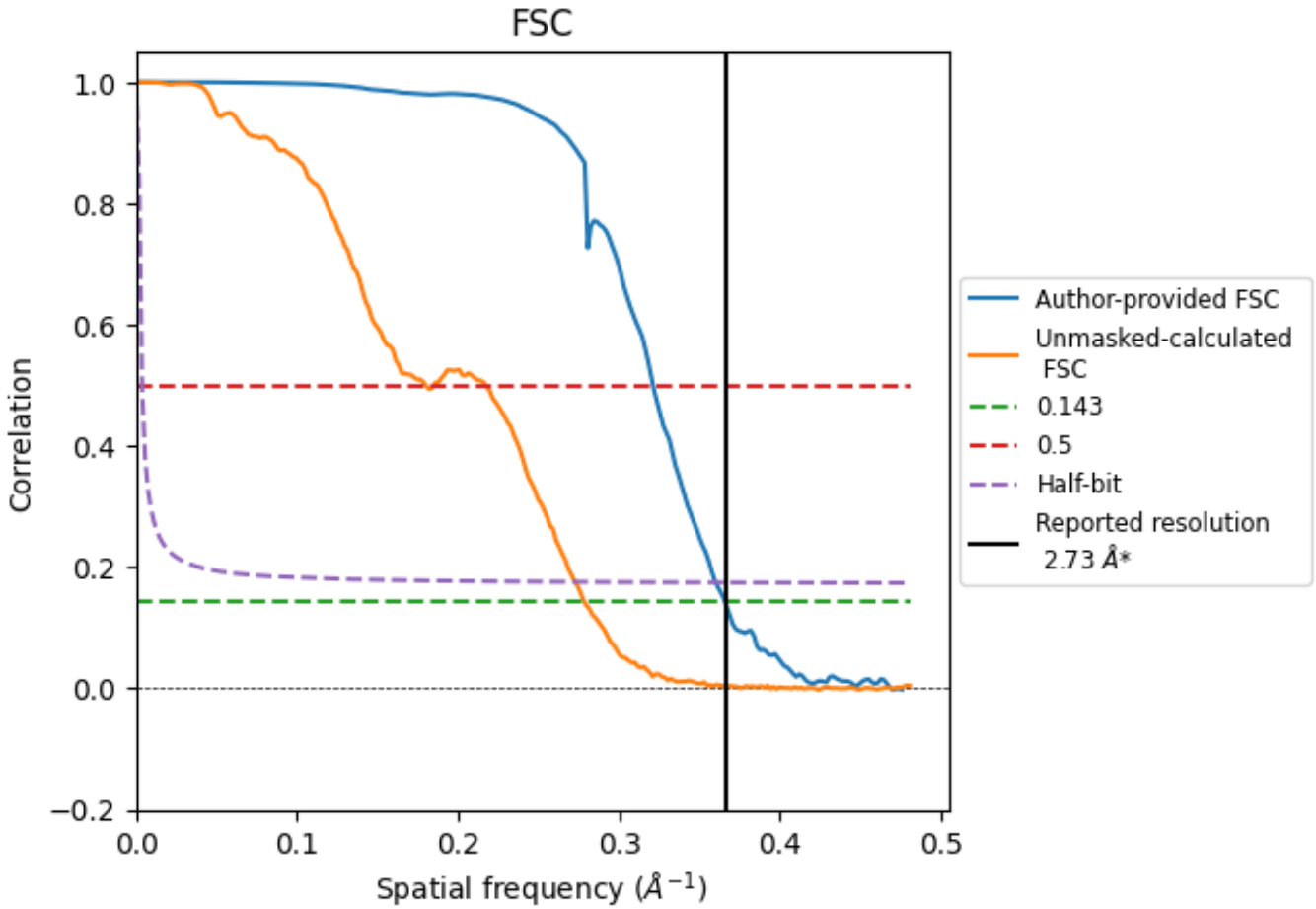


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

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 0.366 Å^{-1}

8.2 Resolution estimates (i)

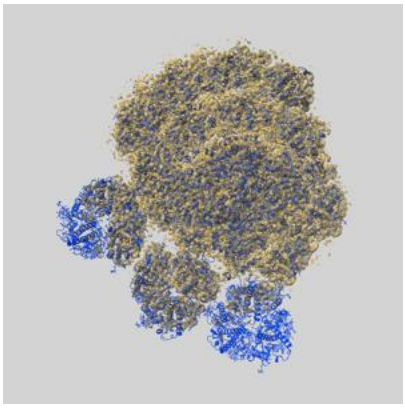
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.11	2.78
Unmasked-calculated*	3.59	5.56	3.66

*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 3.59 differs from the reported value 2.73 by more than 10 %

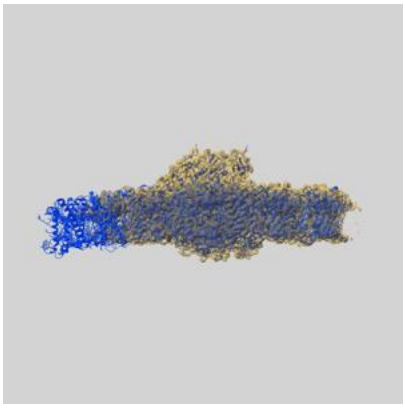
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61940 and PDB model 9JZR. Per-residue inclusion information can be found in section 3 on page 41.

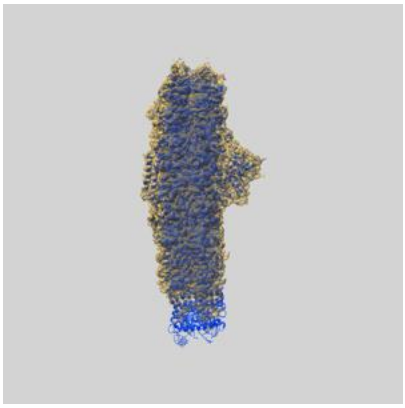
9.1 Map-model overlay



X



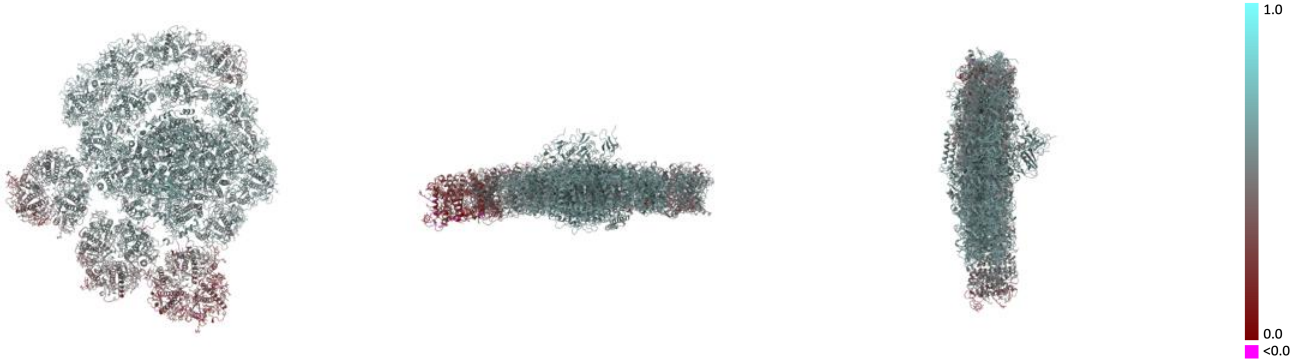
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.217 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.

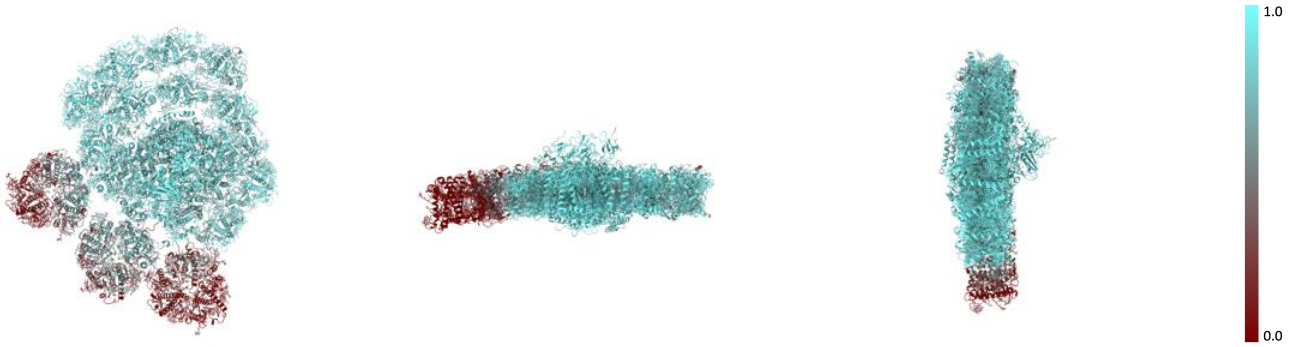
9.2 Q-score mapped to coordinate model (i)



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.

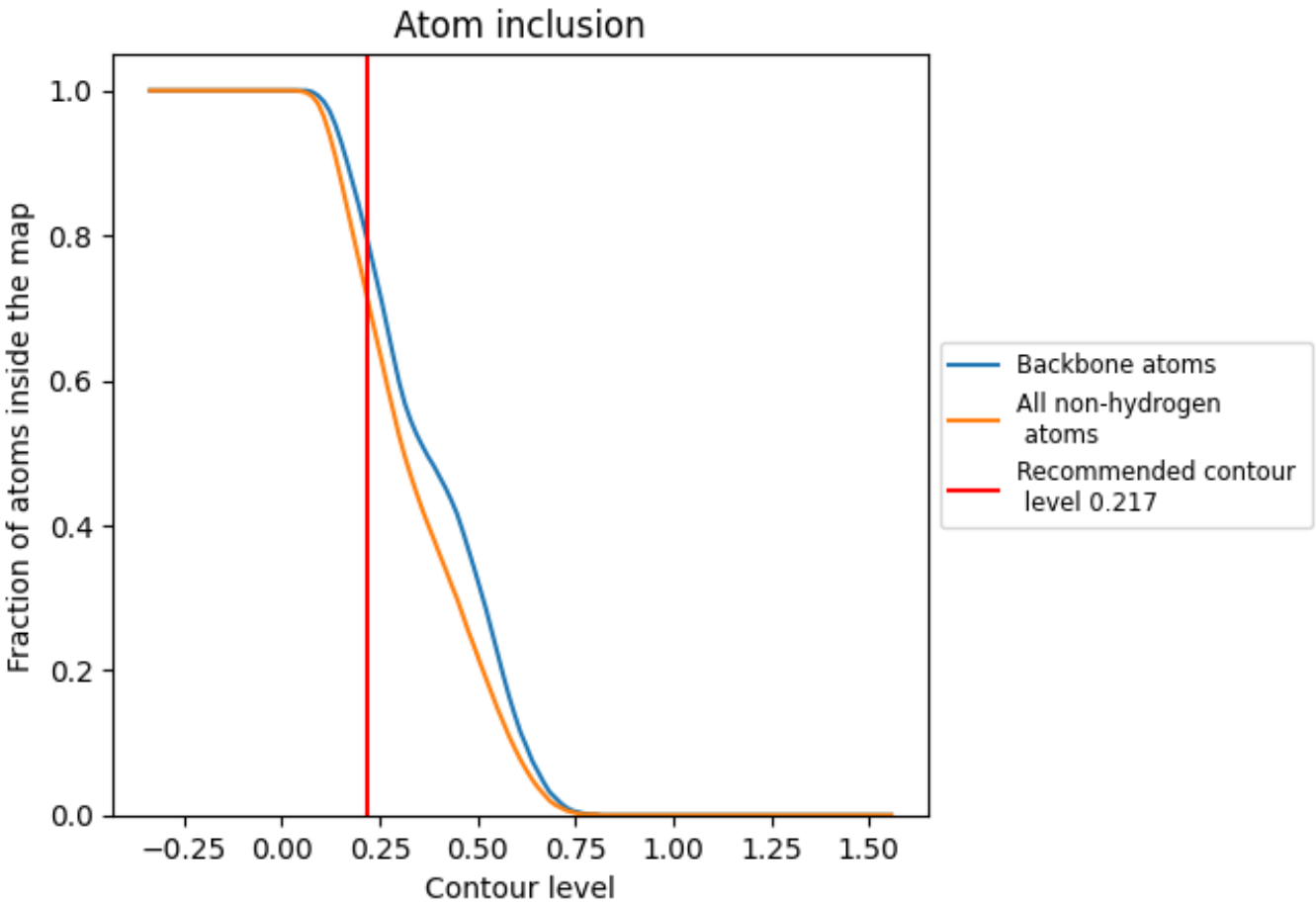
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.217).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7160	0.5260
0	0.8170	0.5440
1	0.8570	0.5600
2	0.9190	0.5900
3	0.9250	0.5940
4	0.8710	0.5490
5	0.7530	0.4730
6	0.9000	0.5700
7	0.8930	0.5770
8	0.8400	0.5370
9	0.8730	0.5690
A	0.9360	0.6060
B	0.9410	0.6020
C	0.9520	0.5880
D	0.9270	0.5990
E	0.8480	0.5730
F	0.8930	0.5690
G	0.7920	0.5390
H	0.8480	0.5790
I	0.9130	0.5760
J	0.9030	0.5870
K	0.8830	0.5830
L	0.8710	0.5780
M	0.8950	0.5860
O	0.8770	0.5710
a	0.0580	0.3680
b	0.4230	0.5140
c	0.5090	0.5130
d	0.2950	0.3960
e	0.4980	0.4730
f	0.6060	0.5100
g	0.0030	0.2200
h	0.0250	0.2680
i	0.2140	0.3760

