Full wwPDB EM Validation Report

Mar 5, 2026 – 04:22 AM UTC

PDB ID	:	6KIG / pdb_00006kig
EMDB ID	:	EMD-9995
Title	:	Structure of cyanobacterial photosystem I-IsiA supercomplex
Authors	:	Cao, P.; Cao, D.F.; Si, L.; Su, X.D.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2019-07-18
Resolution	:	2.90 Å(reported)

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

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

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

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

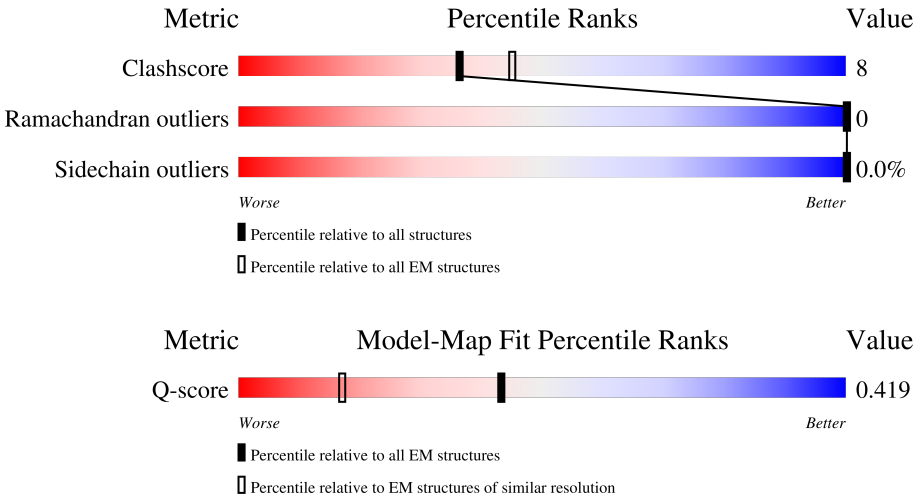
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



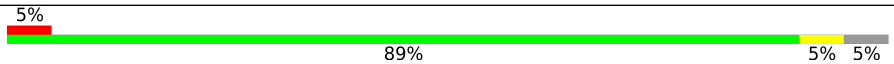
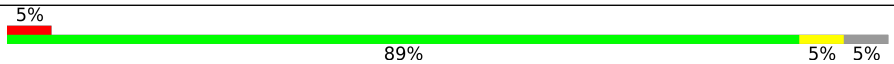
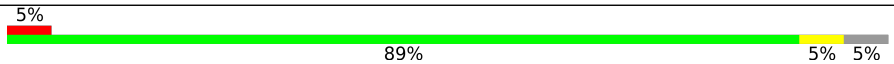
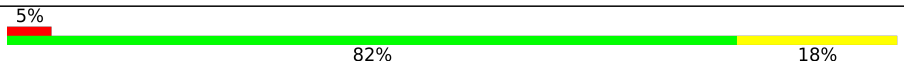
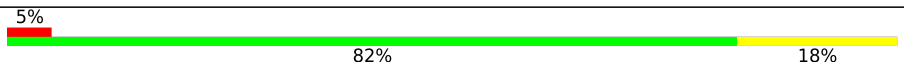
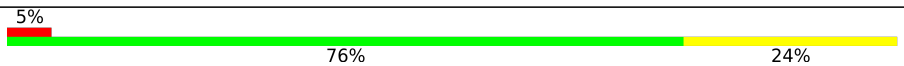
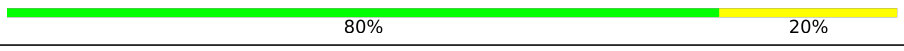
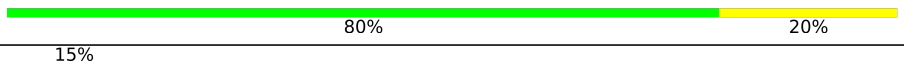
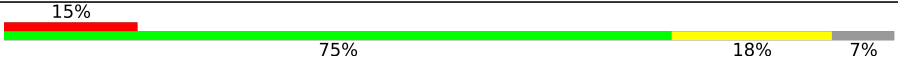
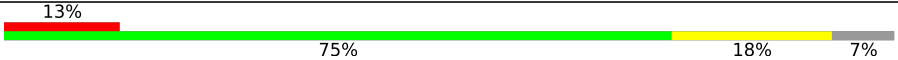
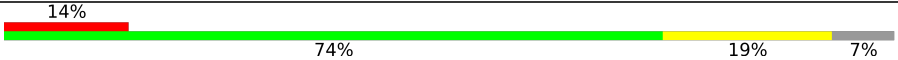
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	763	87% 12%
1	G	763	86% 12%
1	e	763	87% 12%
2	B	734	86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	734	
2	f	734	
3	C	81	
3	N	81	
3	g	81	
4	D	141	
4	O	141	
4	h	141	
5	E	75	
5	Q	75	
5	i	75	
6	F	159	
6	R	159	
6	j	159	
7	I	38	
7	S	38	
7	k	38	
8	J	41	
8	T	41	
8	l	41	
9	K	84	
9	U	84	
9	m	84	
10	L	166	
10	V	166	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	n	166	87% 12%
11	M	29	86% 14%
11	W	29	86% 14%
11	o	29	86% 14%
12	1	342	49% 88% 11%
12	2	342	40% 87% 12%
12	3	342	59% 89% 10%
12	4	342	94% 87% 13%
12	5	342	98% 90% 9%
12	6	342	91% 84% 15%
12	Y	342	49% 87% 12%
12	Z	342	38% 88% 11%
12	a	342	60% 90% 9%
12	b	342	95% 87% 13%
12	c	342	98% 91% 8%
12	d	342	90% 84% 15%
12	q	342	51% 87% 12%
12	r	342	41% 87% 12%
12	s	342	59% 88% 11%
12	t	342	93% 87% 12%
12	u	342	99% 90% 9%
12	v	342	90% 86% 13%

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
13	CLA	1	501	X	-	-	-
13	CLA	1	502	X	-	-	-
13	CLA	1	503	X	-	-	-
13	CLA	1	504	X	-	-	-
13	CLA	1	505	X	-	-	-
13	CLA	1	506	X	-	-	-
13	CLA	1	507	X	-	-	-
13	CLA	1	508	X	-	-	-
13	CLA	1	509	X	-	-	-
13	CLA	1	510	X	-	-	-
13	CLA	1	511	X	-	-	-
13	CLA	1	512	X	-	-	-
13	CLA	1	513	X	-	-	-
13	CLA	1	516	X	-	-	-
13	CLA	1	517	X	-	-	-
13	CLA	1	518	X	-	-	-
13	CLA	1	519	X	-	-	-
13	CLA	2	501	X	-	-	-
13	CLA	2	502	X	-	-	-
13	CLA	2	503	X	-	-	-
13	CLA	2	504	X	-	-	-
13	CLA	2	505	X	-	-	-
13	CLA	2	506	X	-	-	-
13	CLA	2	507	X	-	-	-
13	CLA	2	508	X	-	-	-
13	CLA	2	509	X	-	-	-
13	CLA	2	510	X	-	-	-
13	CLA	2	511	X	-	-	-
13	CLA	2	512	X	-	-	-
13	CLA	2	513	X	-	-	-
13	CLA	2	516	X	-	-	-
13	CLA	2	517	X	-	-	-
13	CLA	2	518	X	-	-	-
13	CLA	2	519	X	-	-	-
13	CLA	3	501	X	-	-	-
13	CLA	3	502	X	-	-	-
13	CLA	3	503	X	-	-	-
13	CLA	3	504	X	-	-	-
13	CLA	3	505	X	-	-	-
13	CLA	3	506	X	-	-	-
13	CLA	3	507	X	-	-	-
13	CLA	3	508	X	-	-	-
13	CLA	3	509	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	3	510	X	-	-	-
13	CLA	3	511	X	-	-	-
13	CLA	3	512	X	-	-	-
13	CLA	3	513	X	-	-	-
13	CLA	3	516	X	-	-	-
13	CLA	3	517	X	-	-	-
13	CLA	3	518	X	-	-	-
13	CLA	3	519	X	-	-	-
13	CLA	4	501	X	-	-	-
13	CLA	4	502	X	-	-	-
13	CLA	4	503	X	-	-	-
13	CLA	4	504	X	-	-	-
13	CLA	4	505	X	-	-	-
13	CLA	4	506	X	-	-	-
13	CLA	4	507	X	-	-	-
13	CLA	4	508	X	-	-	-
13	CLA	4	509	X	-	-	-
13	CLA	4	510	X	-	-	-
13	CLA	4	511	X	-	-	-
13	CLA	4	512	X	-	-	-
13	CLA	4	513	X	-	-	-
13	CLA	4	516	X	-	-	-
13	CLA	4	517	X	-	-	-
13	CLA	4	518	X	-	-	-
13	CLA	4	519	X	-	-	-
13	CLA	5	501	X	-	-	-
13	CLA	5	502	X	-	-	-
13	CLA	5	503	X	-	-	-
13	CLA	5	504	X	-	-	-
13	CLA	5	505	X	-	-	-
13	CLA	5	506	X	-	-	-
13	CLA	5	507	X	-	-	-
13	CLA	5	508	X	-	-	-
13	CLA	5	509	X	-	-	-
13	CLA	5	510	X	-	-	-
13	CLA	5	511	X	-	-	-
13	CLA	5	512	X	-	-	-
13	CLA	5	513	X	-	-	-
13	CLA	5	516	X	-	-	-
13	CLA	5	517	X	-	-	-
13	CLA	5	518	X	-	-	-
13	CLA	5	519	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	6	501	X	-	-	-
13	CLA	6	502	X	-	-	-
13	CLA	6	503	X	-	-	-
13	CLA	6	504	X	-	-	-
13	CLA	6	505	X	-	-	-
13	CLA	6	506	X	-	-	-
13	CLA	6	507	X	-	-	-
13	CLA	6	508	X	-	-	-
13	CLA	6	509	X	-	-	-
13	CLA	6	510	X	-	-	-
13	CLA	6	511	X	-	-	-
13	CLA	6	512	X	-	-	-
13	CLA	6	513	X	-	-	-
13	CLA	6	516	X	-	-	-
13	CLA	6	517	X	-	-	-
13	CLA	6	518	X	-	-	-
13	CLA	6	519	X	-	-	-
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1108	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1115	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1123	X	-	-	-
13	CLA	A	1124	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-
13	CLA	A	1130	X	-	-	-
13	CLA	A	1131	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1023	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1207	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1212	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1225	X	-	-	-
13	CLA	B	1226	X	-	-	-
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1235	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	B	1239	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	F	1302	X	-	-	-
13	CLA	G	1011	X	-	-	-
13	CLA	G	1013	X	-	-	-
13	CLA	G	1022	X	-	-	-
13	CLA	G	1101	X	-	-	-
13	CLA	G	1102	X	-	-	-
13	CLA	G	1103	X	-	-	-
13	CLA	G	1104	X	-	-	-
13	CLA	G	1105	X	-	-	-
13	CLA	G	1106	X	-	-	-
13	CLA	G	1107	X	-	-	-
13	CLA	G	1108	X	-	-	-
13	CLA	G	1109	X	-	-	-
13	CLA	G	1110	X	-	-	-
13	CLA	G	1111	X	-	-	-
13	CLA	G	1112	X	-	-	-
13	CLA	G	1113	X	-	-	-
13	CLA	G	1114	X	-	-	-
13	CLA	G	1115	X	-	-	-
13	CLA	G	1116	X	-	-	-
13	CLA	G	1117	X	-	-	-
13	CLA	G	1118	X	-	-	-
13	CLA	G	1119	X	-	-	-
13	CLA	G	1120	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	G	1121	X	-	-	-
13	CLA	G	1122	X	-	-	-
13	CLA	G	1123	X	-	-	-
13	CLA	G	1124	X	-	-	-
13	CLA	G	1125	X	-	-	-
13	CLA	G	1126	X	-	-	-
13	CLA	G	1127	X	-	-	-
13	CLA	G	1128	X	-	-	-
13	CLA	G	1129	X	-	-	-
13	CLA	G	1130	X	-	-	-
13	CLA	G	1131	X	-	-	-
13	CLA	G	1132	X	-	-	-
13	CLA	G	1133	X	-	-	-
13	CLA	G	1134	X	-	-	-
13	CLA	G	1135	X	-	-	-
13	CLA	G	1136	X	-	-	-
13	CLA	G	1137	X	-	-	-
13	CLA	G	1138	X	-	-	-
13	CLA	G	1139	X	-	-	-
13	CLA	G	1140	X	-	-	-
13	CLA	G	1237	X	-	-	-
13	CLA	G	1801	X	-	-	-
13	CLA	H	1012	X	-	-	-
13	CLA	H	1021	X	-	-	-
13	CLA	H	1023	X	-	-	-
13	CLA	H	1201	X	-	-	-
13	CLA	H	1202	X	-	-	-
13	CLA	H	1203	X	-	-	-
13	CLA	H	1204	X	-	-	-
13	CLA	H	1205	X	-	-	-
13	CLA	H	1206	X	-	-	-
13	CLA	H	1207	X	-	-	-
13	CLA	H	1208	X	-	-	-
13	CLA	H	1209	X	-	-	-
13	CLA	H	1210	X	-	-	-
13	CLA	H	1211	X	-	-	-
13	CLA	H	1212	X	-	-	-
13	CLA	H	1213	X	-	-	-
13	CLA	H	1214	X	-	-	-
13	CLA	H	1215	X	-	-	-
13	CLA	H	1216	X	-	-	-
13	CLA	H	1217	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	H	1218	X	-	-	-
13	CLA	H	1219	X	-	-	-
13	CLA	H	1220	X	-	-	-
13	CLA	H	1221	X	-	-	-
13	CLA	H	1222	X	-	-	-
13	CLA	H	1223	X	-	-	-
13	CLA	H	1224	X	-	-	-
13	CLA	H	1225	X	-	-	-
13	CLA	H	1226	X	-	-	-
13	CLA	H	1227	X	-	-	-
13	CLA	H	1228	X	-	-	-
13	CLA	H	1229	X	-	-	-
13	CLA	H	1230	X	-	-	-
13	CLA	H	1231	X	-	-	-
13	CLA	H	1232	X	-	-	-
13	CLA	H	1234	X	-	-	-
13	CLA	H	1235	X	-	-	-
13	CLA	H	1238	X	-	-	-
13	CLA	H	1239	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	J	1303	X	-	-	-
13	CLA	K	1103	X	-	-	-
13	CLA	K	1105	X	-	-	-
13	CLA	K	1401	X	-	-	-
13	CLA	L	1501	X	-	-	-
13	CLA	L	1502	X	-	-	-
13	CLA	L	1503	X	-	-	-
13	CLA	R	1301	X	-	-	-
13	CLA	R	1302	X	-	-	-
13	CLA	T	1302	X	-	-	-
13	CLA	T	1303	X	-	-	-
13	CLA	U	1103	X	-	-	-
13	CLA	U	1105	X	-	-	-
13	CLA	U	1401	X	-	-	-
13	CLA	V	1501	X	-	-	-
13	CLA	V	1502	X	-	-	-
13	CLA	V	1503	X	-	-	-
13	CLA	Y	501	X	-	-	-
13	CLA	Y	502	X	-	-	-
13	CLA	Y	503	X	-	-	-
13	CLA	Y	504	X	-	-	-
13	CLA	Y	505	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	Y	506	X	-	-	-
13	CLA	Y	507	X	-	-	-
13	CLA	Y	508	X	-	-	-
13	CLA	Y	509	X	-	-	-
13	CLA	Y	510	X	-	-	-
13	CLA	Y	511	X	-	-	-
13	CLA	Y	512	X	-	-	-
13	CLA	Y	513	X	-	-	-
13	CLA	Y	516	X	-	-	-
13	CLA	Y	517	X	-	-	-
13	CLA	Y	518	X	-	-	-
13	CLA	Y	519	X	-	-	-
13	CLA	Z	501	X	-	-	-
13	CLA	Z	502	X	-	-	-
13	CLA	Z	503	X	-	-	-
13	CLA	Z	504	X	-	-	-
13	CLA	Z	505	X	-	-	-
13	CLA	Z	506	X	-	-	-
13	CLA	Z	507	X	-	-	-
13	CLA	Z	508	X	-	-	-
13	CLA	Z	509	X	-	-	-
13	CLA	Z	510	X	-	-	-
13	CLA	Z	511	X	-	-	-
13	CLA	Z	512	X	-	-	-
13	CLA	Z	513	X	-	-	-
13	CLA	Z	516	X	-	-	-
13	CLA	Z	517	X	-	-	-
13	CLA	Z	518	X	-	-	-
13	CLA	Z	519	X	-	-	-
13	CLA	a	501	X	-	-	-
13	CLA	a	502	X	-	-	-
13	CLA	a	503	X	-	-	-
13	CLA	a	504	X	-	-	-
13	CLA	a	505	X	-	-	-
13	CLA	a	506	X	-	-	-
13	CLA	a	507	X	-	-	-
13	CLA	a	508	X	-	-	-
13	CLA	a	509	X	-	-	-
13	CLA	a	510	X	-	-	-
13	CLA	a	511	X	-	-	-
13	CLA	a	512	X	-	-	-
13	CLA	a	513	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	a	516	X	-	-	-
13	CLA	a	517	X	-	-	-
13	CLA	a	518	X	-	-	-
13	CLA	a	519	X	-	-	-
13	CLA	b	501	X	-	-	-
13	CLA	b	502	X	-	-	-
13	CLA	b	503	X	-	-	-
13	CLA	b	504	X	-	-	-
13	CLA	b	505	X	-	-	-
13	CLA	b	506	X	-	-	-
13	CLA	b	507	X	-	-	-
13	CLA	b	508	X	-	-	-
13	CLA	b	509	X	-	-	-
13	CLA	b	510	X	-	-	-
13	CLA	b	511	X	-	-	-
13	CLA	b	512	X	-	-	-
13	CLA	b	513	X	-	-	-
13	CLA	b	516	X	-	-	-
13	CLA	b	517	X	-	-	-
13	CLA	b	518	X	-	-	-
13	CLA	b	519	X	-	-	-
13	CLA	c	501	X	-	-	-
13	CLA	c	502	X	-	-	-
13	CLA	c	503	X	-	-	-
13	CLA	c	504	X	-	-	-
13	CLA	c	505	X	-	-	-
13	CLA	c	506	X	-	-	-
13	CLA	c	507	X	-	-	-
13	CLA	c	508	X	-	-	-
13	CLA	c	509	X	-	-	-
13	CLA	c	510	X	-	-	-
13	CLA	c	511	X	-	-	-
13	CLA	c	512	X	-	-	-
13	CLA	c	513	X	-	-	-
13	CLA	c	516	X	-	-	-
13	CLA	c	517	X	-	-	-
13	CLA	c	518	X	-	-	-
13	CLA	c	519	X	-	-	-
13	CLA	d	501	X	-	-	-
13	CLA	d	502	X	-	-	-
13	CLA	d	503	X	-	-	-
13	CLA	d	504	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	d	505	X	-	-	-
13	CLA	d	506	X	-	-	-
13	CLA	d	507	X	-	-	-
13	CLA	d	508	X	-	-	-
13	CLA	d	509	X	-	-	-
13	CLA	d	510	X	-	-	-
13	CLA	d	511	X	-	-	-
13	CLA	d	512	X	-	-	-
13	CLA	d	513	X	-	-	-
13	CLA	d	516	X	-	-	-
13	CLA	d	517	X	-	-	-
13	CLA	d	518	X	-	-	-
13	CLA	d	519	X	-	-	-
13	CLA	e	1011	X	-	-	-
13	CLA	e	1013	X	-	-	-
13	CLA	e	1022	X	-	-	-
13	CLA	e	1101	X	-	-	-
13	CLA	e	1102	X	-	-	-
13	CLA	e	1103	X	-	-	-
13	CLA	e	1104	X	-	-	-
13	CLA	e	1105	X	-	-	-
13	CLA	e	1106	X	-	-	-
13	CLA	e	1107	X	-	-	-
13	CLA	e	1108	X	-	-	-
13	CLA	e	1109	X	-	-	-
13	CLA	e	1110	X	-	-	-
13	CLA	e	1111	X	-	-	-
13	CLA	e	1112	X	-	-	-
13	CLA	e	1113	X	-	-	-
13	CLA	e	1114	X	-	-	-
13	CLA	e	1115	X	-	-	-
13	CLA	e	1116	X	-	-	-
13	CLA	e	1117	X	-	-	-
13	CLA	e	1118	X	-	-	-
13	CLA	e	1119	X	-	-	-
13	CLA	e	1120	X	-	-	-
13	CLA	e	1121	X	-	-	-
13	CLA	e	1122	X	-	-	-
13	CLA	e	1123	X	-	-	-
13	CLA	e	1124	X	-	-	-
13	CLA	e	1125	X	-	-	-
13	CLA	e	1126	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	e	1127	X	-	-	-
13	CLA	e	1128	X	-	-	-
13	CLA	e	1129	X	-	-	-
13	CLA	e	1130	X	-	-	-
13	CLA	e	1131	X	-	-	-
13	CLA	e	1132	X	-	-	-
13	CLA	e	1133	X	-	-	-
13	CLA	e	1134	X	-	-	-
13	CLA	e	1135	X	-	-	-
13	CLA	e	1136	X	-	-	-
13	CLA	e	1137	X	-	-	-
13	CLA	e	1138	X	-	-	-
13	CLA	e	1139	X	-	-	-
13	CLA	e	1140	X	-	-	-
13	CLA	e	1237	X	-	-	-
13	CLA	e	1801	X	-	-	-
13	CLA	f	1012	X	-	-	-
13	CLA	f	1021	X	-	-	-
13	CLA	f	1023	X	-	-	-
13	CLA	f	1201	X	-	-	-
13	CLA	f	1202	X	-	-	-
13	CLA	f	1203	X	-	-	-
13	CLA	f	1204	X	-	-	-
13	CLA	f	1205	X	-	-	-
13	CLA	f	1206	X	-	-	-
13	CLA	f	1207	X	-	-	-
13	CLA	f	1208	X	-	-	-
13	CLA	f	1209	X	-	-	-
13	CLA	f	1210	X	-	-	-
13	CLA	f	1211	X	-	-	-
13	CLA	f	1212	X	-	-	-
13	CLA	f	1213	X	-	-	-
13	CLA	f	1214	X	-	-	-
13	CLA	f	1215	X	-	-	-
13	CLA	f	1216	X	-	-	-
13	CLA	f	1217	X	-	-	-
13	CLA	f	1218	X	-	-	-
13	CLA	f	1219	X	-	-	-
13	CLA	f	1220	X	-	-	-
13	CLA	f	1221	X	-	-	-
13	CLA	f	1222	X	-	-	-
13	CLA	f	1223	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	f	1224	X	-	-	-
13	CLA	f	1225	X	-	-	-
13	CLA	f	1226	X	-	-	-
13	CLA	f	1227	X	-	-	-
13	CLA	f	1228	X	-	-	-
13	CLA	f	1229	X	-	-	-
13	CLA	f	1230	X	-	-	-
13	CLA	f	1231	X	-	-	-
13	CLA	f	1232	X	-	-	-
13	CLA	f	1234	X	-	-	-
13	CLA	f	1235	X	-	-	-
13	CLA	f	1238	X	-	-	-
13	CLA	f	1239	X	-	-	-
13	CLA	j	1301	X	-	-	-
13	CLA	j	1302	X	-	-	-
13	CLA	l	1302	X	-	-	-
13	CLA	l	1303	X	-	-	-
13	CLA	m	1103	X	-	-	-
13	CLA	m	1105	X	-	-	-
13	CLA	m	1401	X	-	-	-
13	CLA	n	1501	X	-	-	-
13	CLA	n	1502	X	-	-	-
13	CLA	n	1503	X	-	-	-
13	CLA	q	501	X	-	-	-
13	CLA	q	502	X	-	-	-
13	CLA	q	503	X	-	-	-
13	CLA	q	504	X	-	-	-
13	CLA	q	505	X	-	X	-
13	CLA	q	506	X	-	-	-
13	CLA	q	507	X	-	-	-
13	CLA	q	508	X	-	-	-
13	CLA	q	509	X	-	-	-
13	CLA	q	510	X	-	-	-
13	CLA	q	511	X	-	-	-
13	CLA	q	512	X	-	-	-
13	CLA	q	513	X	-	-	-
13	CLA	q	516	X	-	-	-
13	CLA	q	517	X	-	-	-
13	CLA	q	518	X	-	-	-
13	CLA	q	519	X	-	-	-
13	CLA	r	501	X	-	-	-
13	CLA	r	502	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	r	503	X	-	-	-
13	CLA	r	504	X	-	-	-
13	CLA	r	505	X	-	-	-
13	CLA	r	506	X	-	-	-
13	CLA	r	507	X	-	-	-
13	CLA	r	508	X	-	-	-
13	CLA	r	509	X	-	-	-
13	CLA	r	510	X	-	-	-
13	CLA	r	511	X	-	-	-
13	CLA	r	512	X	-	-	-
13	CLA	r	513	X	-	-	-
13	CLA	r	516	X	-	-	-
13	CLA	r	517	X	-	-	-
13	CLA	r	518	X	-	-	-
13	CLA	r	519	X	-	-	-
13	CLA	s	501	X	-	-	-
13	CLA	s	502	X	-	-	-
13	CLA	s	503	X	-	-	-
13	CLA	s	504	X	-	-	-
13	CLA	s	505	X	-	-	-
13	CLA	s	506	X	-	-	-
13	CLA	s	507	X	-	-	-
13	CLA	s	508	X	-	-	-
13	CLA	s	509	X	-	-	-
13	CLA	s	510	X	-	-	-
13	CLA	s	511	X	-	-	-
13	CLA	s	512	X	-	-	-
13	CLA	s	513	X	-	-	-
13	CLA	s	516	X	-	-	-
13	CLA	s	517	X	-	-	-
13	CLA	s	518	X	-	-	-
13	CLA	s	519	X	-	-	-
13	CLA	t	501	X	-	-	-
13	CLA	t	502	X	-	-	-
13	CLA	t	503	X	-	-	-
13	CLA	t	504	X	-	-	-
13	CLA	t	505	X	-	-	-
13	CLA	t	506	X	-	-	-
13	CLA	t	507	X	-	-	-
13	CLA	t	508	X	-	-	-
13	CLA	t	509	X	-	-	-
13	CLA	t	510	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	t	511	X	-	-	-
13	CLA	t	512	X	-	-	-
13	CLA	t	513	X	-	-	-
13	CLA	t	516	X	-	-	-
13	CLA	t	517	X	-	-	-
13	CLA	t	518	X	-	-	-
13	CLA	t	519	X	-	-	-
13	CLA	u	501	X	-	-	-
13	CLA	u	502	X	-	-	-
13	CLA	u	503	X	-	-	-
13	CLA	u	504	X	-	-	-
13	CLA	u	505	X	-	-	-
13	CLA	u	506	X	-	-	-
13	CLA	u	507	X	-	-	-
13	CLA	u	508	X	-	-	-
13	CLA	u	509	X	-	-	-
13	CLA	u	510	X	-	-	-
13	CLA	u	511	X	-	-	-
13	CLA	u	512	X	-	-	-
13	CLA	u	513	X	-	-	-
13	CLA	u	516	X	-	-	-
13	CLA	u	517	X	-	-	-
13	CLA	u	518	X	-	-	-
13	CLA	u	519	X	-	-	-
13	CLA	v	501	X	-	-	-
13	CLA	v	502	X	-	-	-
13	CLA	v	503	X	-	-	-
13	CLA	v	504	X	-	-	-
13	CLA	v	505	X	-	-	-
13	CLA	v	506	X	-	-	-
13	CLA	v	507	X	-	-	-
13	CLA	v	508	X	-	-	-
13	CLA	v	509	X	-	-	-
13	CLA	v	510	X	-	-	-
13	CLA	v	511	X	-	-	-
13	CLA	v	512	X	-	-	-
13	CLA	v	513	X	-	-	-
13	CLA	v	516	X	-	-	-
13	CLA	v	517	X	-	-	-
13	CLA	v	518	X	-	-	-
13	CLA	v	519	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 143022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	G	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	e	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	H	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	f	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	368	103	116	11		
3	N	80	Total	C	N	O	S	0	0
			598	368	103	116	11		
3	g	80	Total	C	N	O	S	0	0
			598	368	103	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		
4	h	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	71	Total	C	N	O	0	0
			543	343	95	105		
5	Q	71	Total	C	N	O	0	0
			543	343	95	105		
5	i	71	Total	C	N	O	0	0
			543	343	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	R	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	j	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		

- Molecule 7 is a protein called Photosystem I PsaI protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	S	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	k	38	Total	C	N	O	S	0	0
			282	191	38	51	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			335	228	52	54	1		
8	T	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	U	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	m	78	Total	C	N	O	S	0	0
			549	364	91	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	V	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	n	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		

- Molecule 11 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	W	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	o	29	Total	C	N	O	S	0	0
			228	151	36	40	1		

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

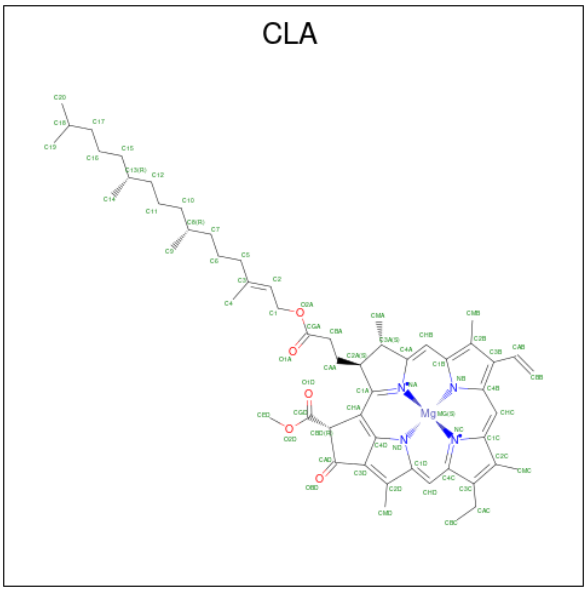
Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	5	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	6	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	Y	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	Z	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	a	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	b	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	c	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	d	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	q	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	r	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	s	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	t	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	u	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	v	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	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
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	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
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	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
13	1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	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
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	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
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	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
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	6	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
13	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	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
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	G	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
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	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
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	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
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	T	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Y	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
13	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	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
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	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
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	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
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	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
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	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
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	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
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	f	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
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	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
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	m	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	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
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	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
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	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
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

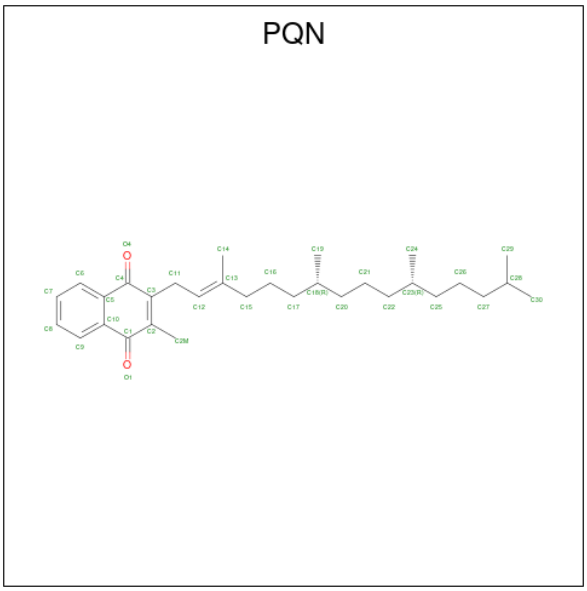
Mol	Chain	Residues	Atoms					AltConf
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

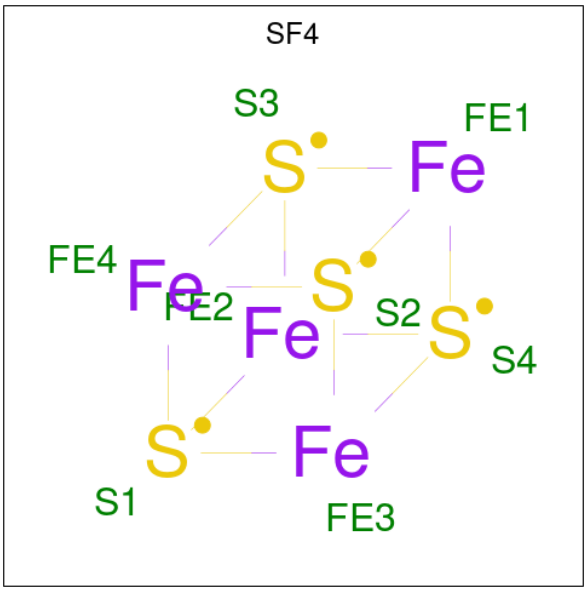
Mol	Chain	Residues	Atoms					AltConf
13	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	v	1	Total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

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



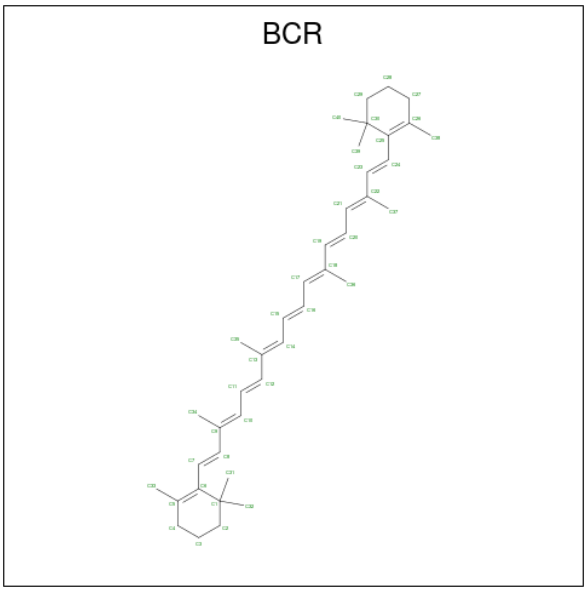
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C O 33 31 2	0
14	B	1	Total C O 33 31 2	0
14	G	1	Total C O 33 31 2	0
14	H	1	Total C O 33 31 2	0
14	e	1	Total C O 33 31 2	0
14	f	1	Total C O 33 31 2	0

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0
15	G	1	Total Fe S 8 4 4	0
15	N	1	Total Fe S 8 4 4	0
15	N	1	Total Fe S 8 4 4	0
15	e	1	Total Fe S 8 4 4	0
15	g	1	Total Fe S 8 4 4	0
15	g	1	Total Fe S 8 4 4	0

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	3	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	R	1	Total C 40 40	0
16	S	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	U	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	W	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Z	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

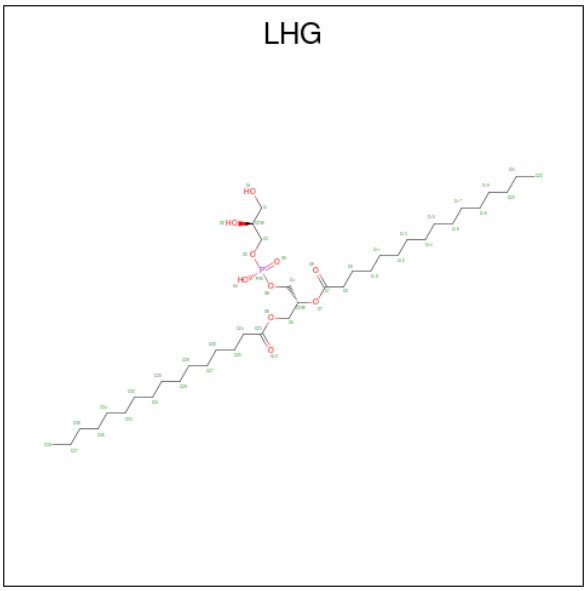
Mol	Chain	Residues	Atoms	AltConf
16	o	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
16	v	1	Total C 40 40	0
16	v	1	Total C 40 40	0
16	v	1	Total C 40 40	0
16	v	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C O P 39 28 10 1	0
17	A	1	Total C O P 36 25 10 1	0
17	A	1	Total C O P 45 34 10 1	0
17	A	1	Total C O P 45 34 10 1	0
17	A	1	Total C O P 47 36 10 1	0
17	A	1	Total C O P 35 24 10 1	0
17	A	1	Total C O P 49 38 10 1	0

Continued on next page...

Continued from previous page...

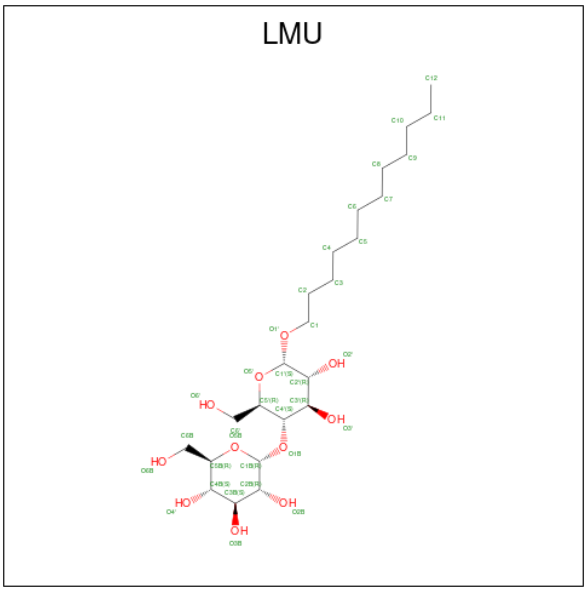
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			39	28	10	1	
17	B	1	Total	C	O	P	0
			44	33	10	1	
17	I	1	Total	C	O	P	0
			44	33	10	1	
17	L	1	Total	C	O	P	0
			38	27	10	1	
17	L	1	Total	C	O	P	0
			41	30	10	1	
17	L	1	Total	C	O	P	0
			49	38	10	1	
17	G	1	Total	C	O	P	0
			39	28	10	1	
17	G	1	Total	C	O	P	0
			36	25	10	1	
17	G	1	Total	C	O	P	0
			45	34	10	1	
17	G	1	Total	C	O	P	0
			45	34	10	1	
17	G	1	Total	C	O	P	0
			47	36	10	1	
17	G	1	Total	C	O	P	0
			35	24	10	1	
17	G	1	Total	C	O	P	0
			49	38	10	1	
17	G	1	Total	C	O	P	0
			49	38	10	1	
17	G	1	Total	C	O	P	0
			41	30	10	1	
17	H	1	Total	C	O	P	0
			39	28	10	1	
17	H	1	Total	C	O	P	0
			44	33	10	1	
17	S	1	Total	C	O	P	0
			44	33	10	1	
17	V	1	Total	C	O	P	0
			38	27	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
17	V	1	Total	C	O	P	0
			41	30	10	1	
17	V	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			39	28	10	1	
17	e	1	Total	C	O	P	0
			36	25	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			47	36	10	1	
17	e	1	Total	C	O	P	0
			35	24	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			41	30	10	1	
17	f	1	Total	C	O	P	0
			39	28	10	1	
17	f	1	Total	C	O	P	0
			44	33	10	1	
17	k	1	Total	C	O	P	0
			44	33	10	1	
17	n	1	Total	C	O	P	0
			38	27	10	1	
17	n	1	Total	C	O	P	0
			41	30	10	1	
17	n	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



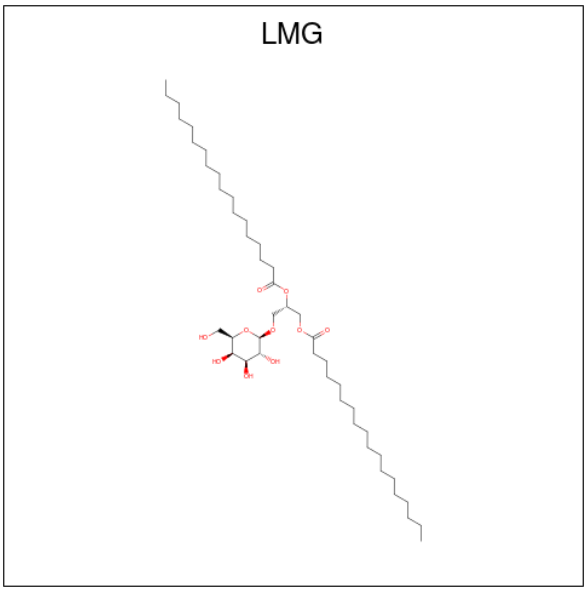
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			23	17	6	
18	B	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			22	16	6	
18	1	1	Total	C	O	0
			19	13	6	
18	2	1	Total	C	O	0
			23	17	6	
18	G	1	Total	C	O	0
			35	24	11	
18	G	1	Total	C	O	0
			23	17	6	
18	H	1	Total	C	O	0
			35	24	11	
18	T	1	Total	C	O	0
			22	16	6	
18	Y	1	Total	C	O	0
			19	13	6	
18	Z	1	Total	C	O	0
			23	17	6	
18	e	1	Total	C	O	0
			35	24	11	
18	e	1	Total	C	O	0
			23	17	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	f	1	Total C O 35 24 11	0
18	l	1	Total C O 22 16 6	0
18	q	1	Total C O 19 13 6	0
18	r	1	Total C O 23 17 6	0

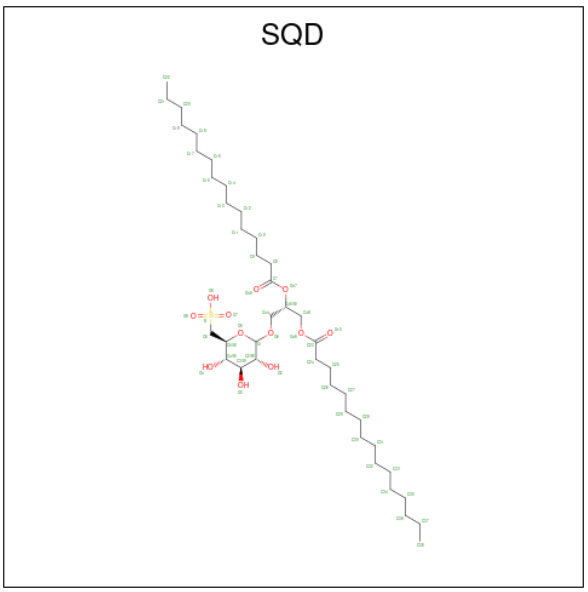
- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C O 54 44 10	0
19	J	1	Total C O 35 25 10	0
19	H	1	Total C O 54 44 10	0
19	T	1	Total C O 35 25 10	0
19	f	1	Total C O 54 44 10	0
19	l	1	Total C O 35 25 10	0

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	S	0
			45	32	12	1	
20	L	1	Total	C	O	S	0
			51	38	12	1	
20	1	1	Total	C	O	S	0
			48	35	12	1	
20	2	1	Total	C	O	S	0
			43	30	12	1	
20	3	1	Total	C	O	S	0
			43	30	12	1	
20	4	1	Total	C	O	S	0
			26	13	12	1	
20	5	1	Total	C	O	S	0
			29	16	12	1	
20	6	1	Total	C	O	S	0
			26	13	12	1	
20	H	1	Total	C	O	S	0
			45	32	12	1	
20	V	1	Total	C	O	S	0
			51	38	12	1	
20	Y	1	Total	C	O	S	0
			48	35	12	1	
20	Z	1	Total	C	O	S	0
			43	30	12	1	
20	a	1	Total	C	O	S	0
			43	30	12	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
20	b	1	Total	C	O	S	0
			26	13	12	1	
20	c	1	Total	C	O	S	0
			29	16	12	1	
20	d	1	Total	C	O	S	0
			26	13	12	1	
20	f	1	Total	C	O	S	0
			45	32	12	1	
20	n	1	Total	C	O	S	0
			51	38	12	1	
20	q	1	Total	C	O	S	0
			48	35	12	1	
20	r	1	Total	C	O	S	0
			43	30	12	1	
20	s	1	Total	C	O	S	0
			43	30	12	1	
20	t	1	Total	C	O	S	0
			26	13	12	1	
20	u	1	Total	C	O	S	0
			29	16	12	1	
20	v	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	9	Total	O	0
			9	9	
21	B	7	Total	O	0
			7	7	
21	F	1	Total	O	0
			1	1	
21	L	1	Total	O	0
			1	1	
21	G	9	Total	O	0
			9	9	
21	H	7	Total	O	0
			7	7	
21	R	1	Total	O	0
			1	1	
21	V	1	Total	O	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
21	e	9	Total O 9 9	0
21	f	7	Total O 7 7	0
21	j	1	Total O 1 1	0
21	n	1	Total O 1 1	0

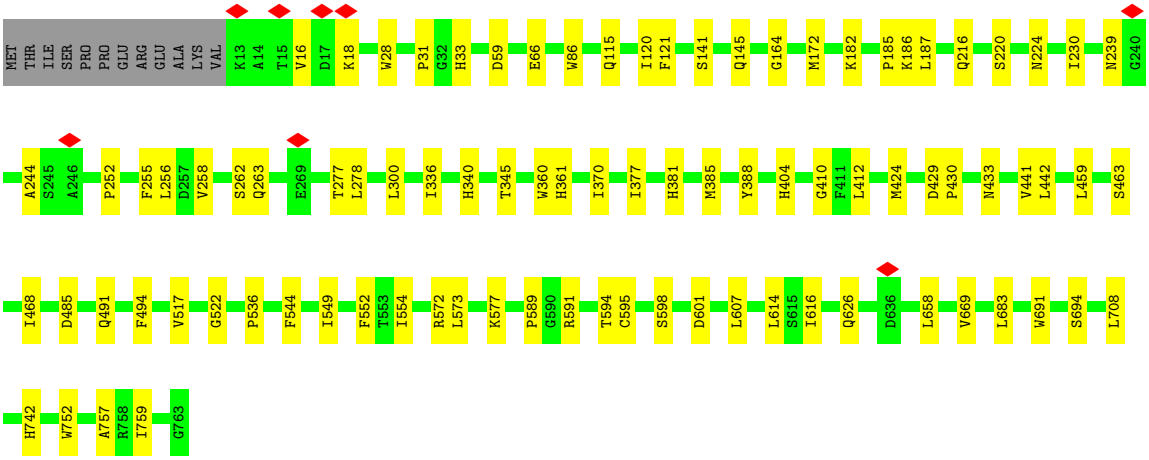
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

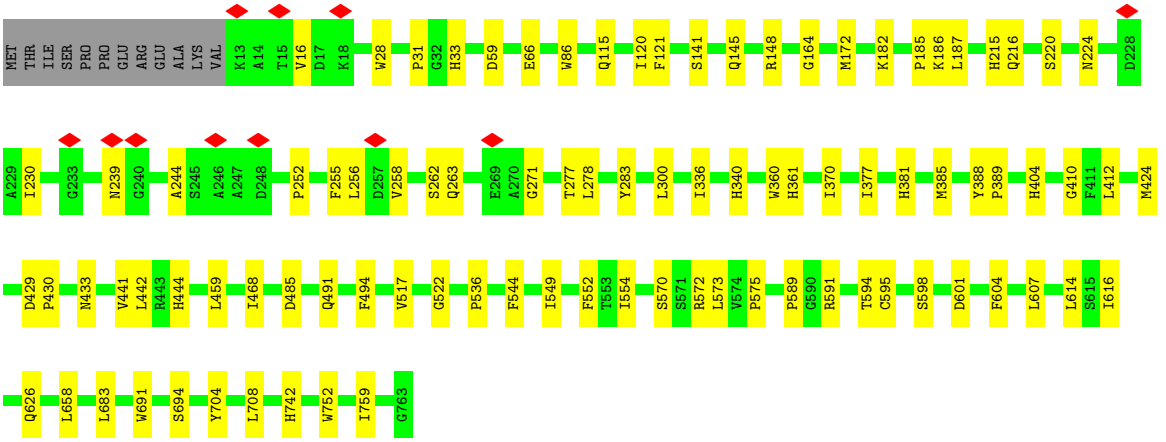




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

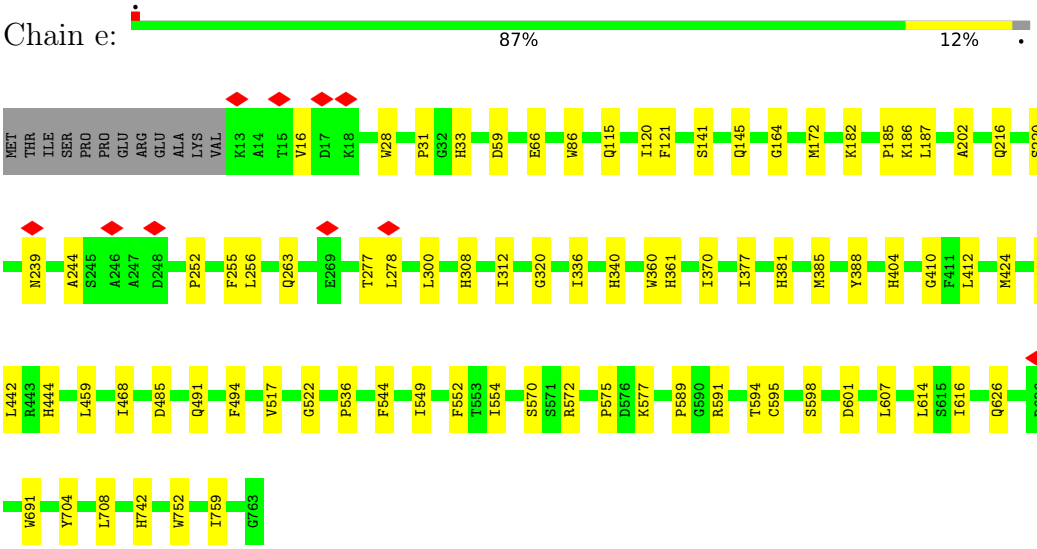
Chain G:





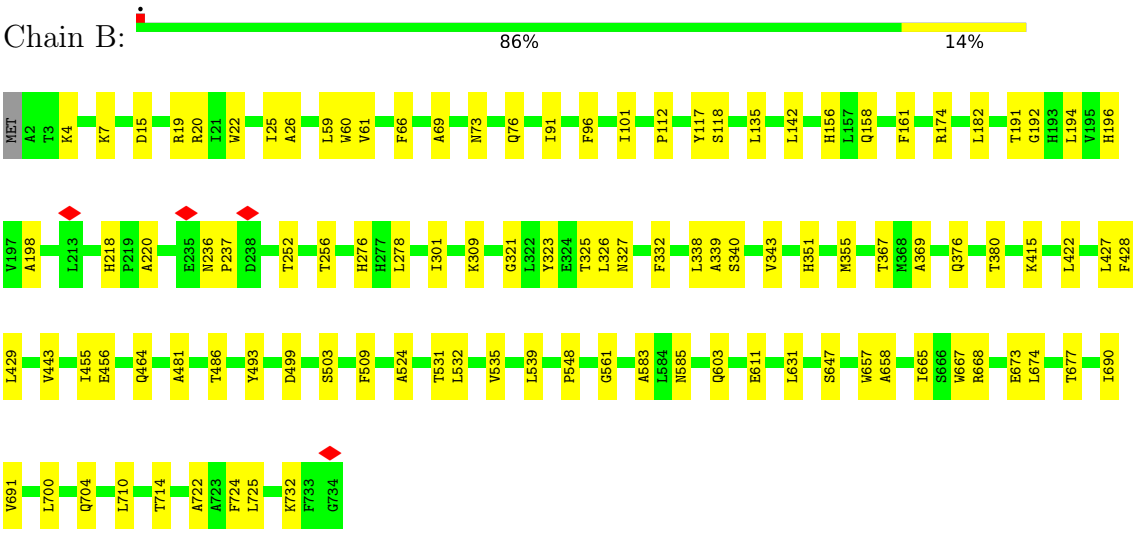
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e:



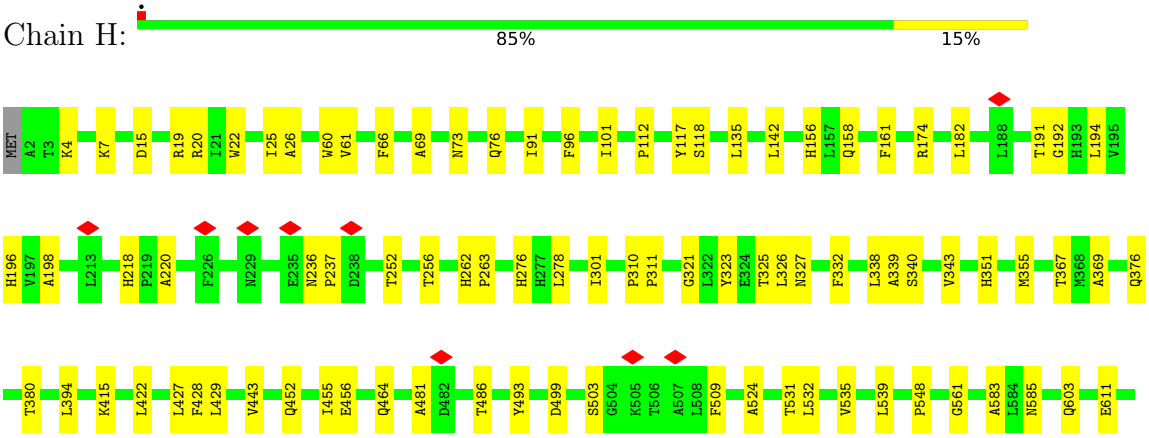
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

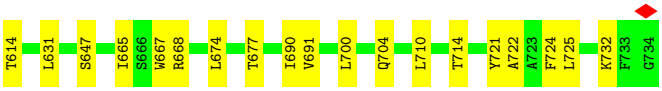
Chain B:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H:





• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f:

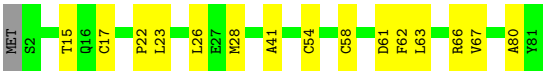




• Molecule 3: Photosystem I iron-sulfur center

Chain C:





• Molecule 3: Photosystem I iron-sulfur center

Chain N:

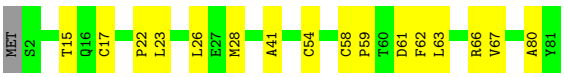




• Molecule 3: Photosystem I iron-sulfur center

Chain g:

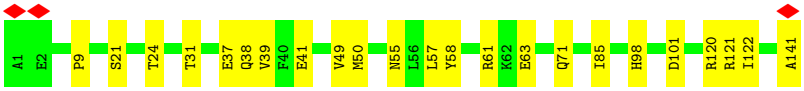




• Molecule 4: Photosystem I reaction center subunit II

Chain D:





• Molecule 4: Photosystem I reaction center subunit II

Chain O:

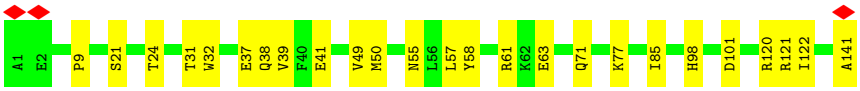




• Molecule 4: Photosystem I reaction center subunit II

Chain h:

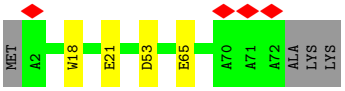




• Molecule 5: Photosystem I reaction center subunit IV

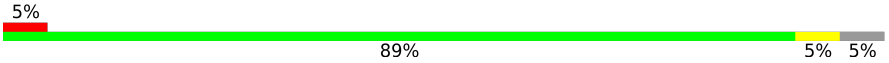
Chain E:

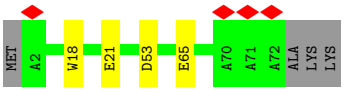




• Molecule 5: Photosystem I reaction center subunit IV

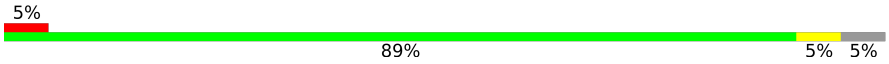
Chain Q:

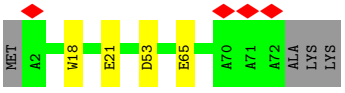




• Molecule 5: Photosystem I reaction center subunit IV

Chain i:

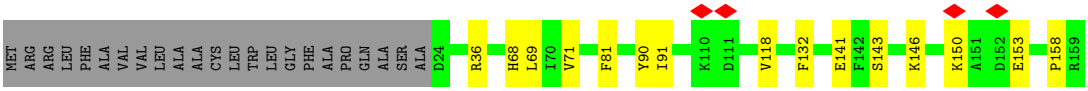




• Molecule 6: Photosystem I reaction center subunit III

Chain F:

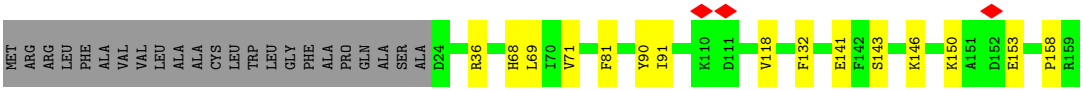




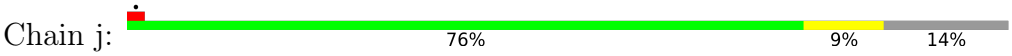
• Molecule 6: Photosystem I reaction center subunit III

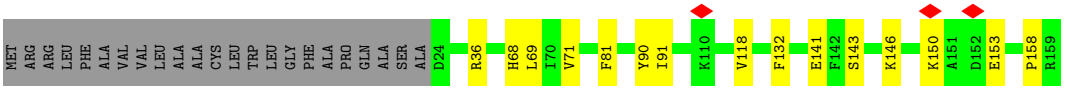
Chain R:



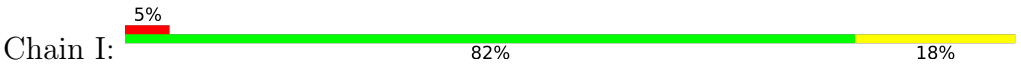


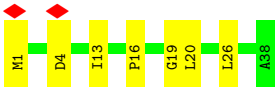
• Molecule 6: Photosystem I reaction center subunit III



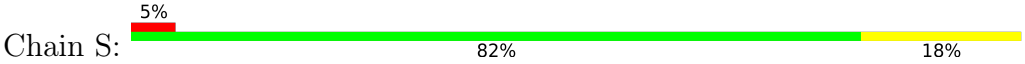


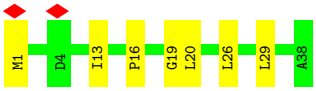
• Molecule 7: Photosystem I PsaI protein





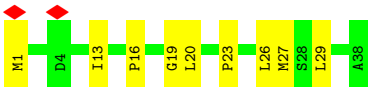
• Molecule 7: Photosystem I PsaI protein



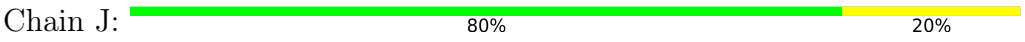


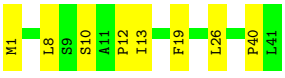
• Molecule 7: Photosystem I PsaI protein



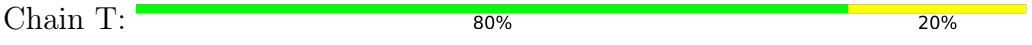


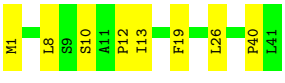
• Molecule 8: Photosystem I reaction center subunit IX





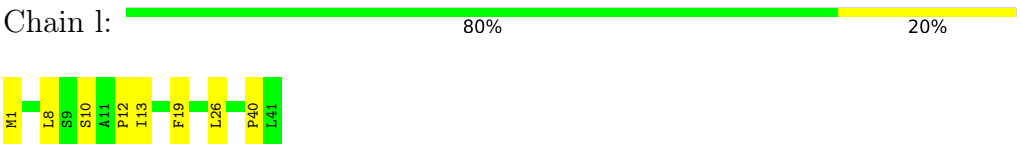
• Molecule 8: Photosystem I reaction center subunit IX





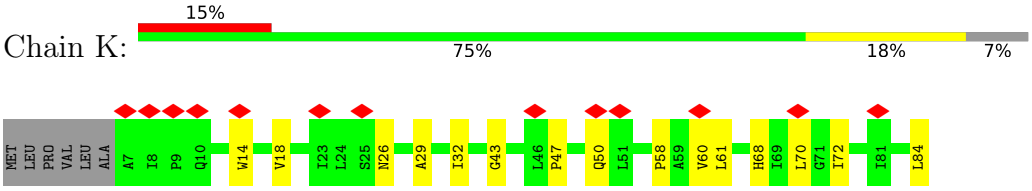
• Molecule 8: Photosystem I reaction center subunit IX

Chain l:



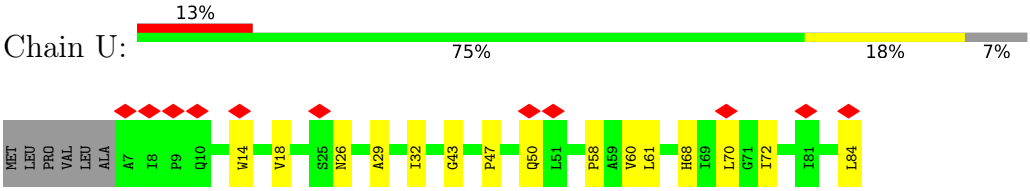
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



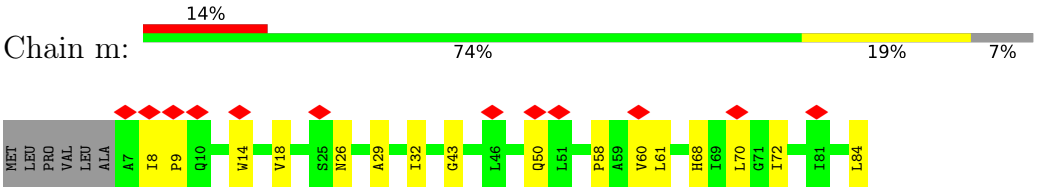
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain U:



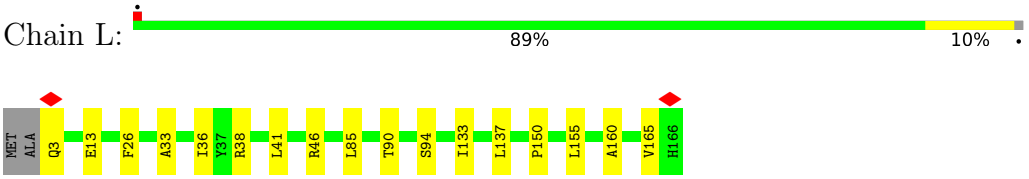
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain m:



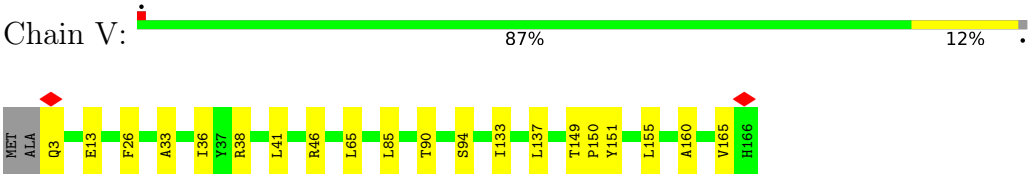
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



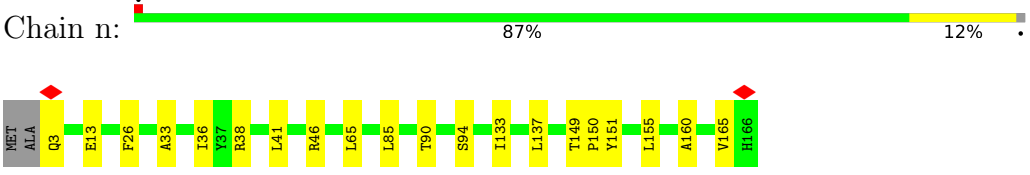
• Molecule 10: Photosystem I reaction center subunit XI

Chain V:



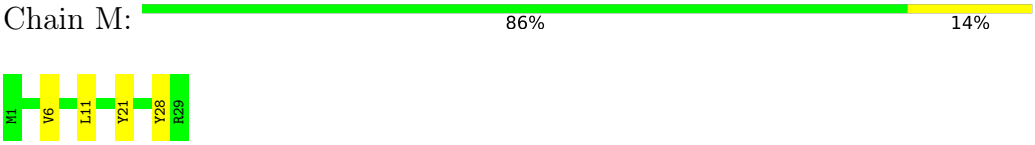
• Molecule 10: Photosystem I reaction center subunit XI

Chain n:



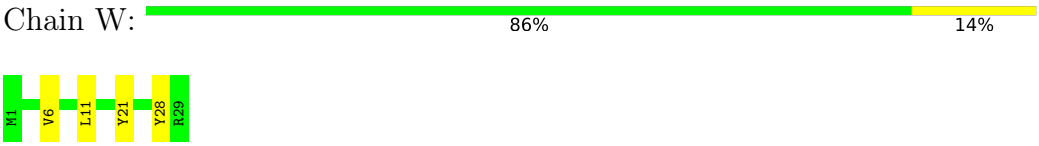
• Molecule 11: PsaM

Chain M:



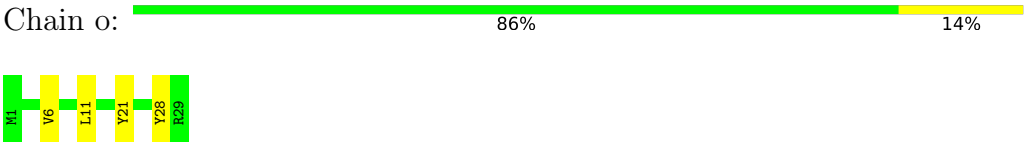
• Molecule 11: PsaM

Chain W:



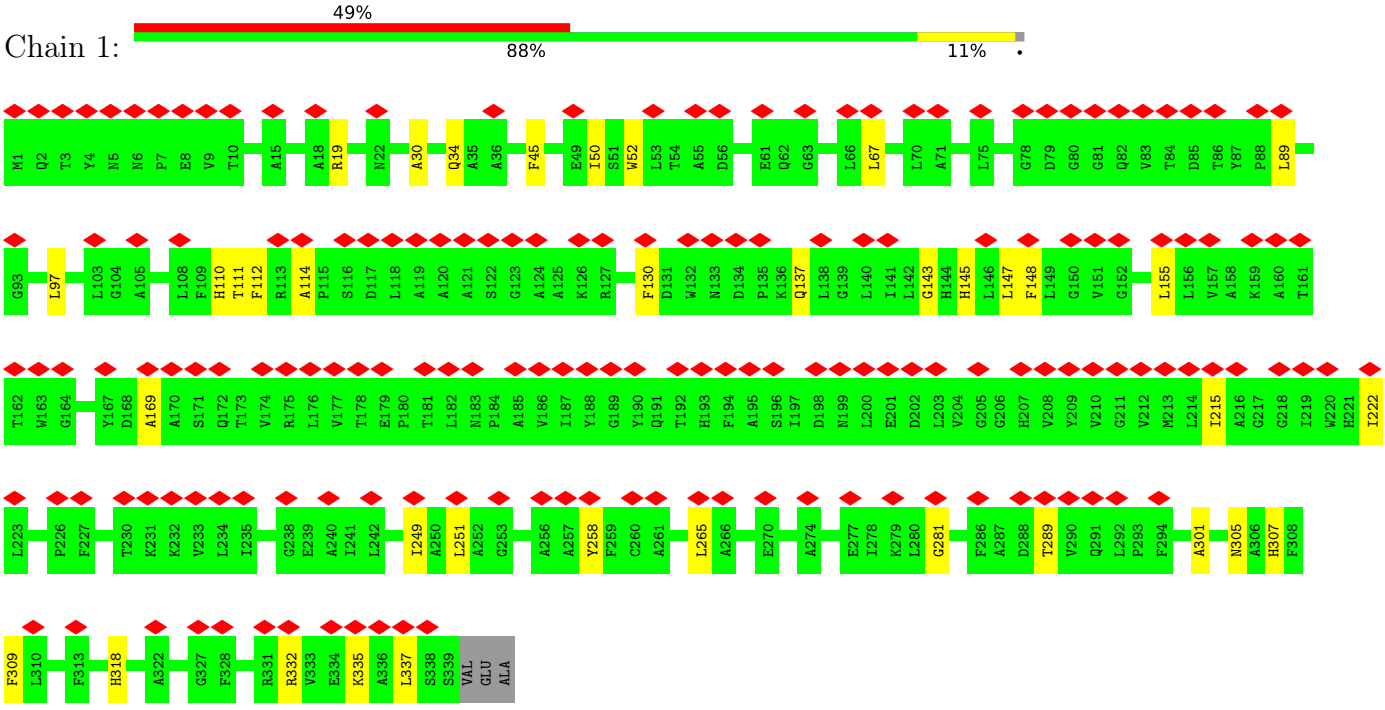
• Molecule 11: PsaM

Chain o:



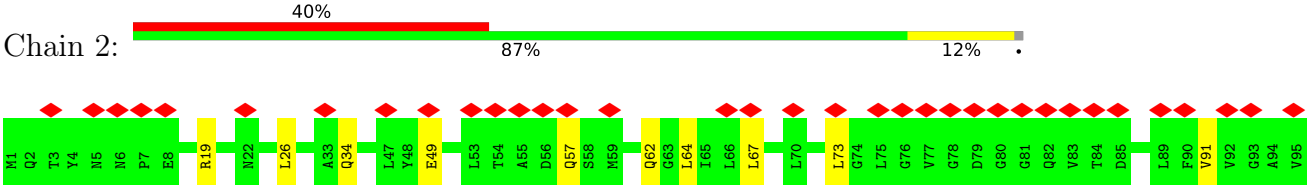
• Molecule 12: Iron stress-induced chlorophyll-binding protein

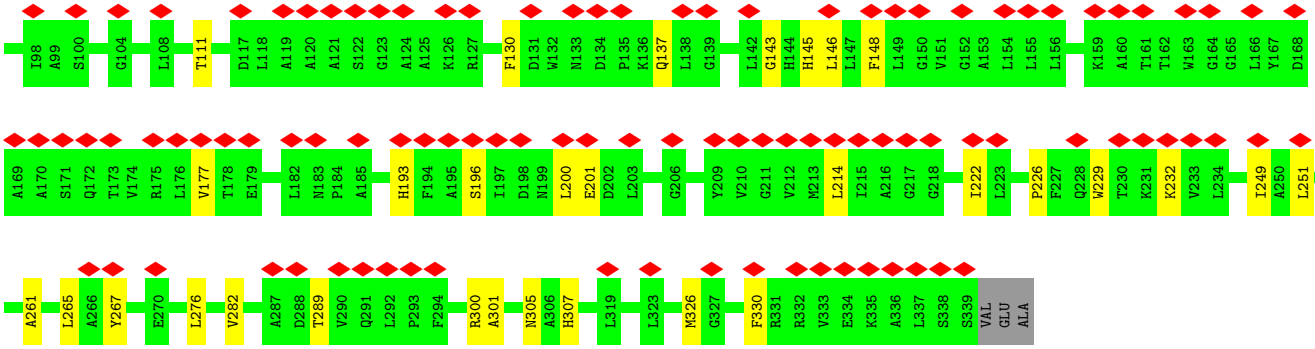
Chain 1:



• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 2:

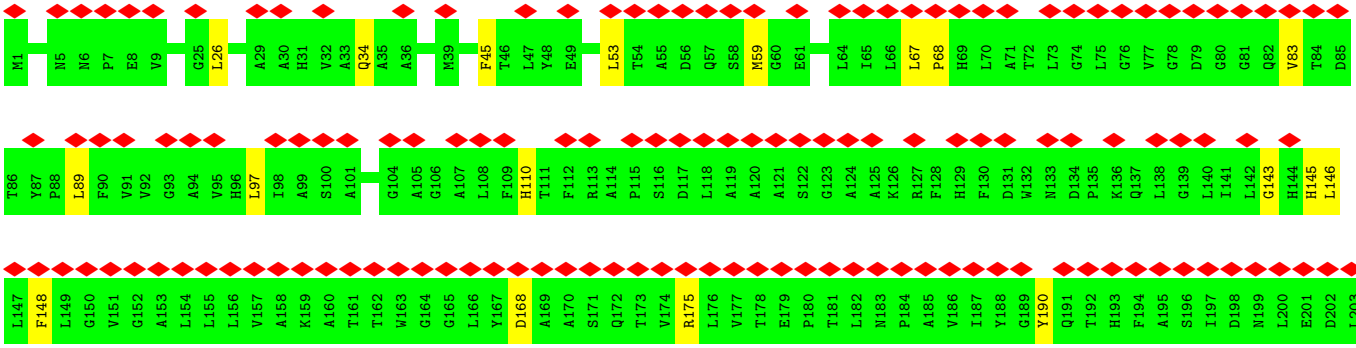




• Molecule 12: Iron stress-induced chlorophyll-binding protein

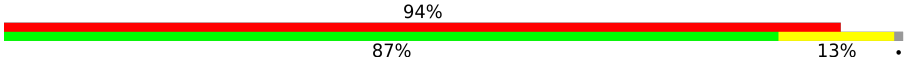
Chain 3:

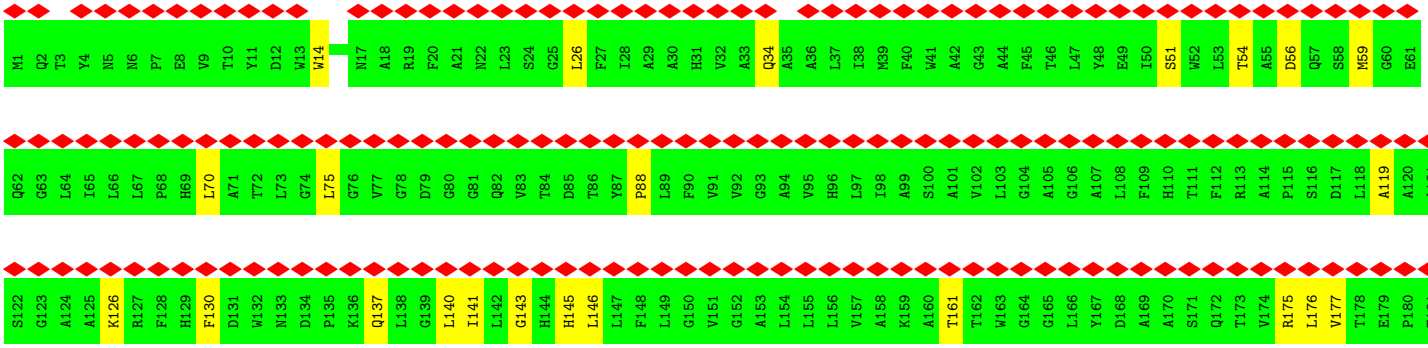


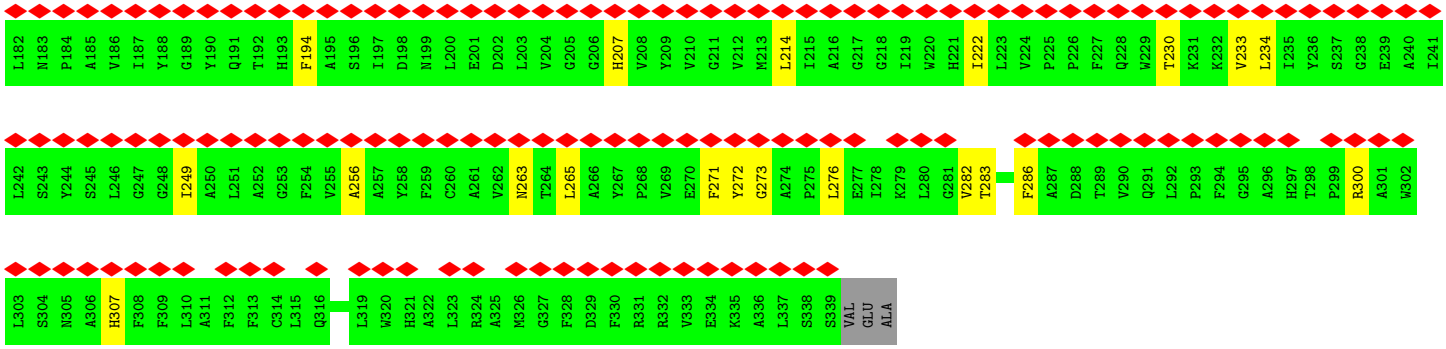


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 4:

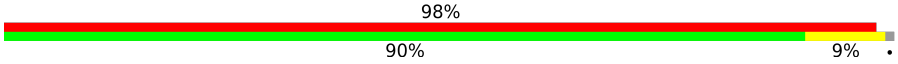


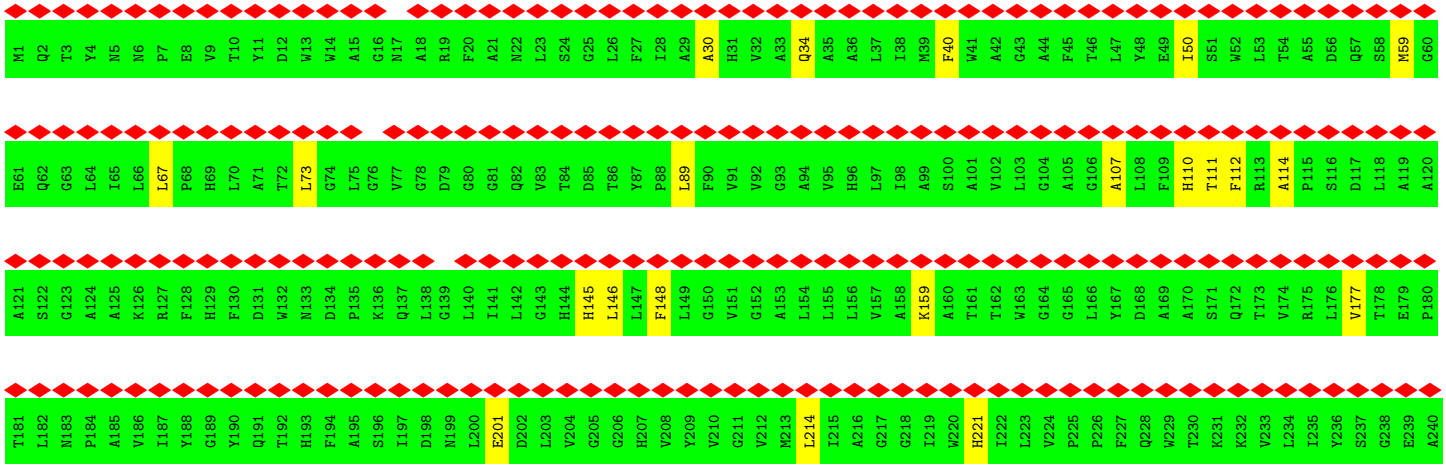


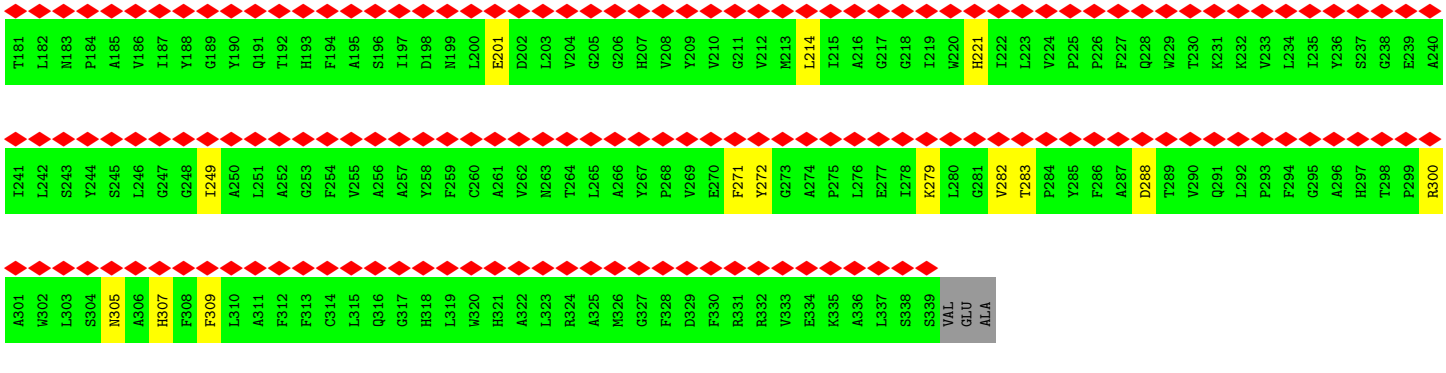


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 5:

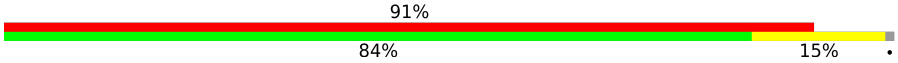


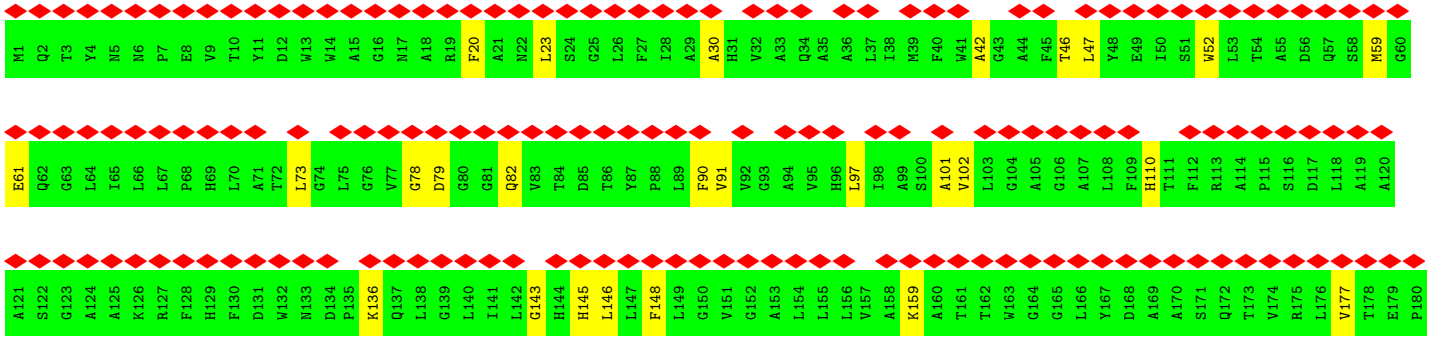


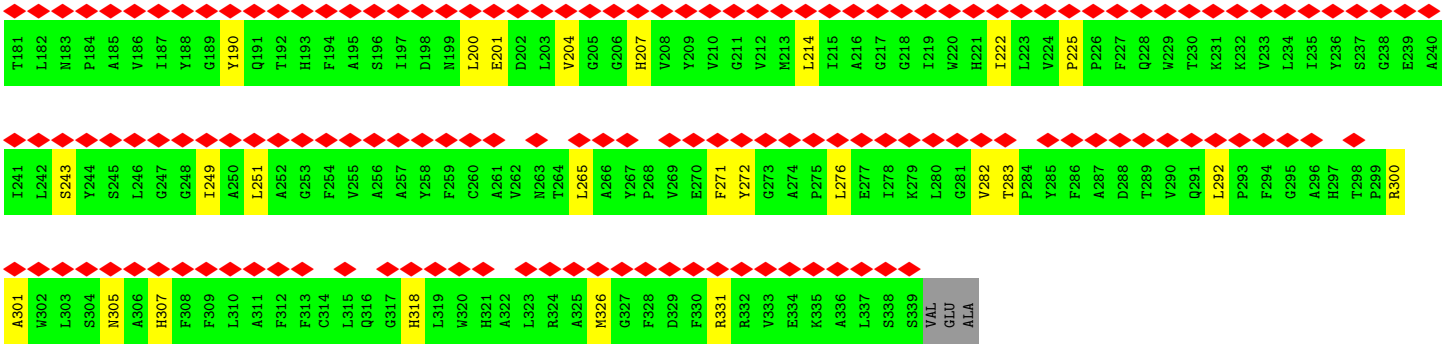


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 6:



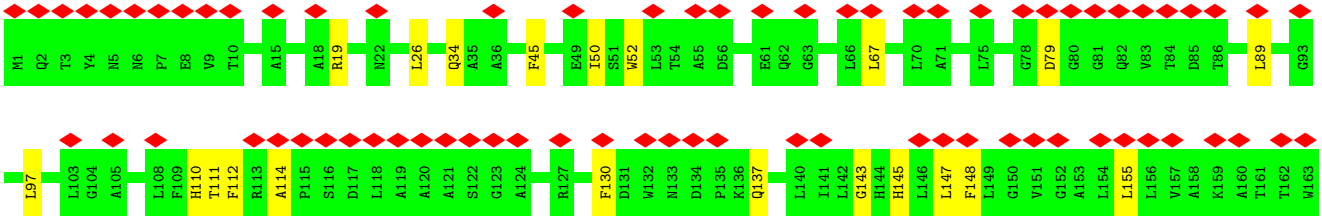




• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Y:

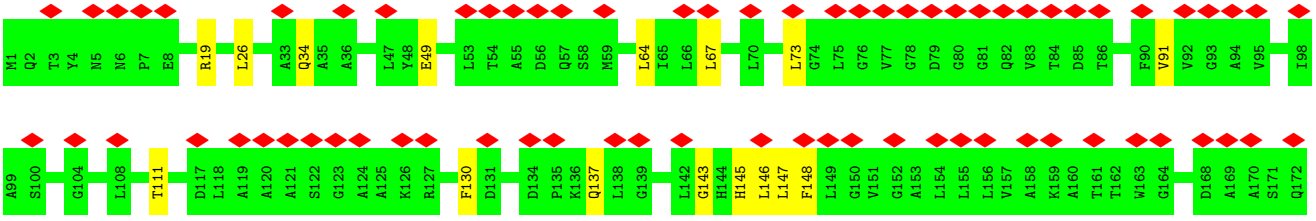


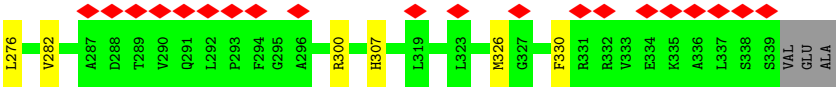


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Z:

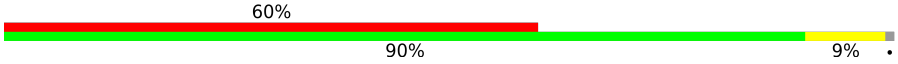


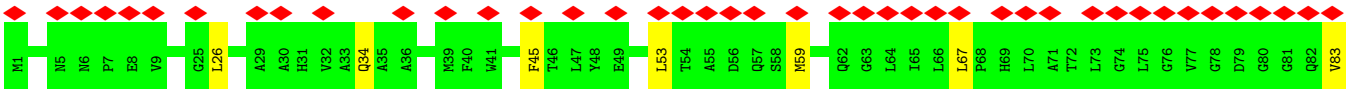


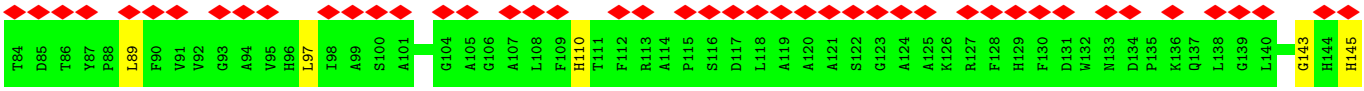


• Molecule 12: Iron stress-induced chlorophyll-binding protein

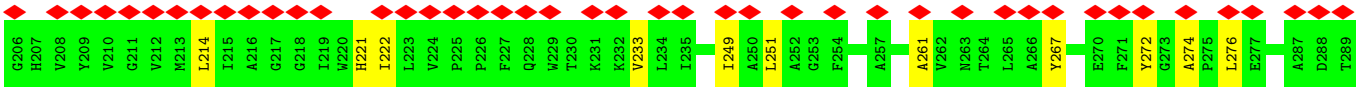
Chain a:

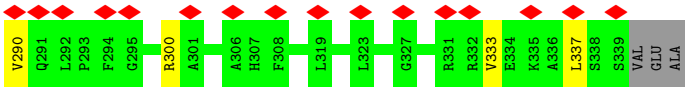






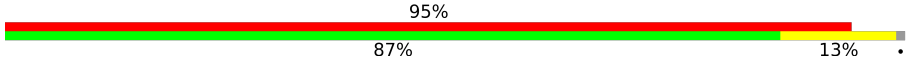


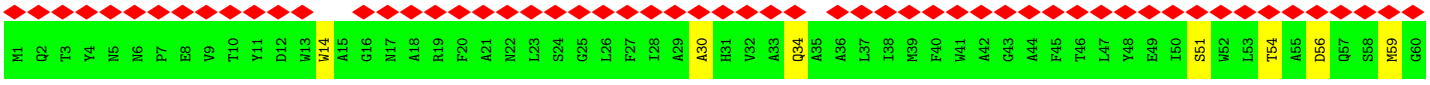


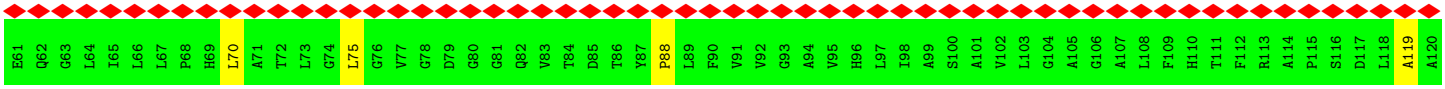


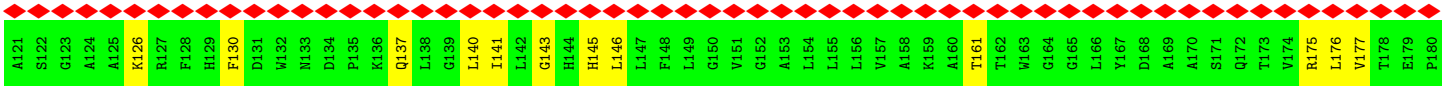
• Molecule 12: Iron stress-induced chlorophyll-binding protein

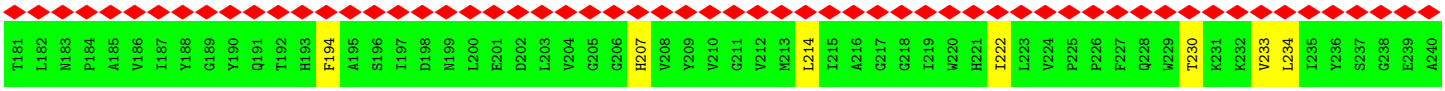
Chain b:

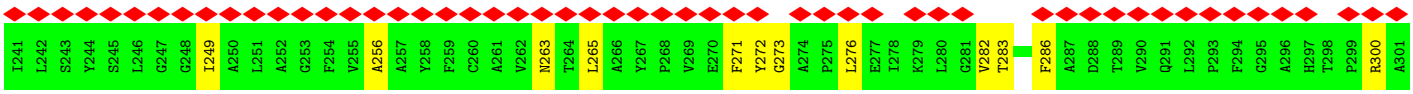


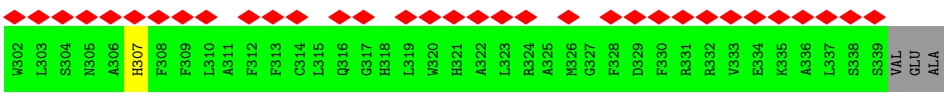






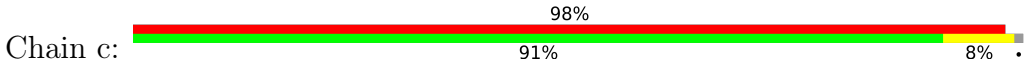


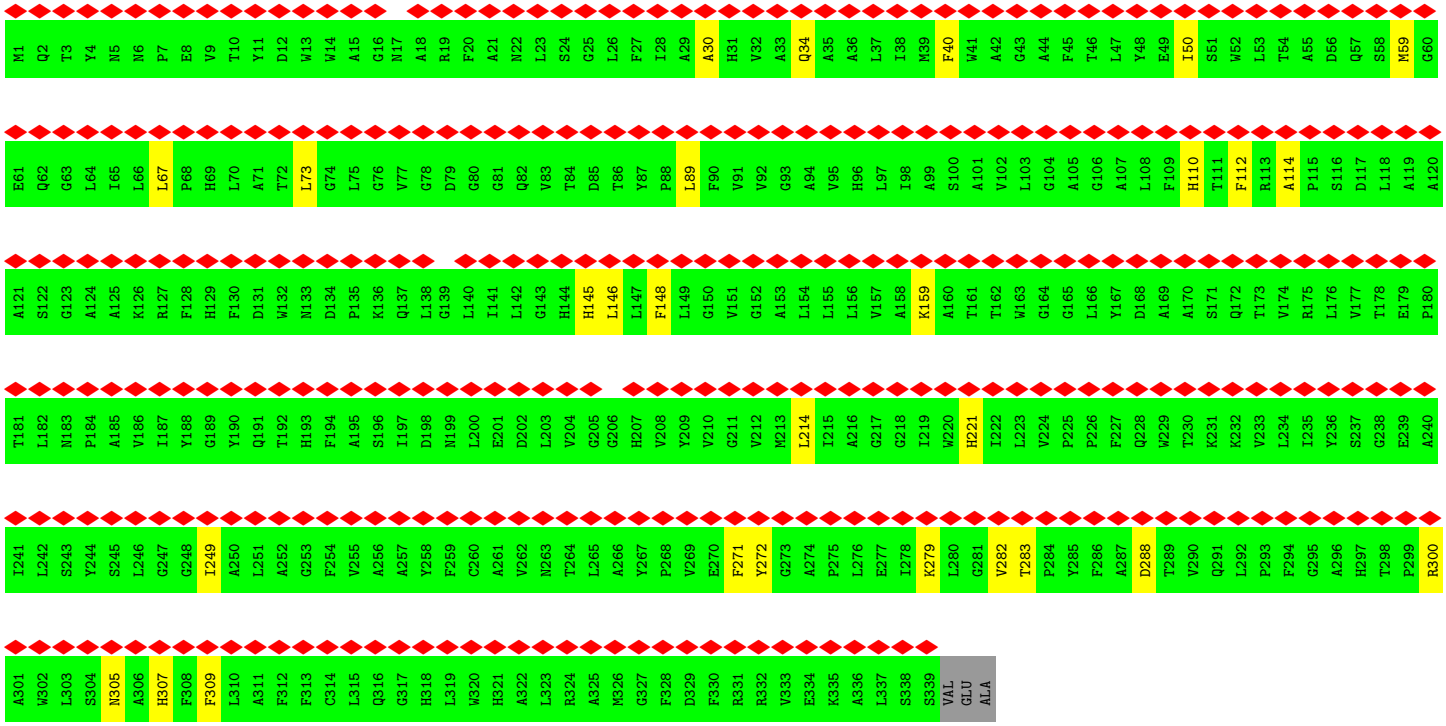




• Molecule 12: Iron stress-induced chlorophyll-binding protein

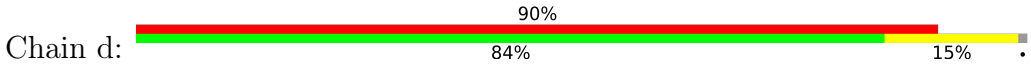
Chain c:

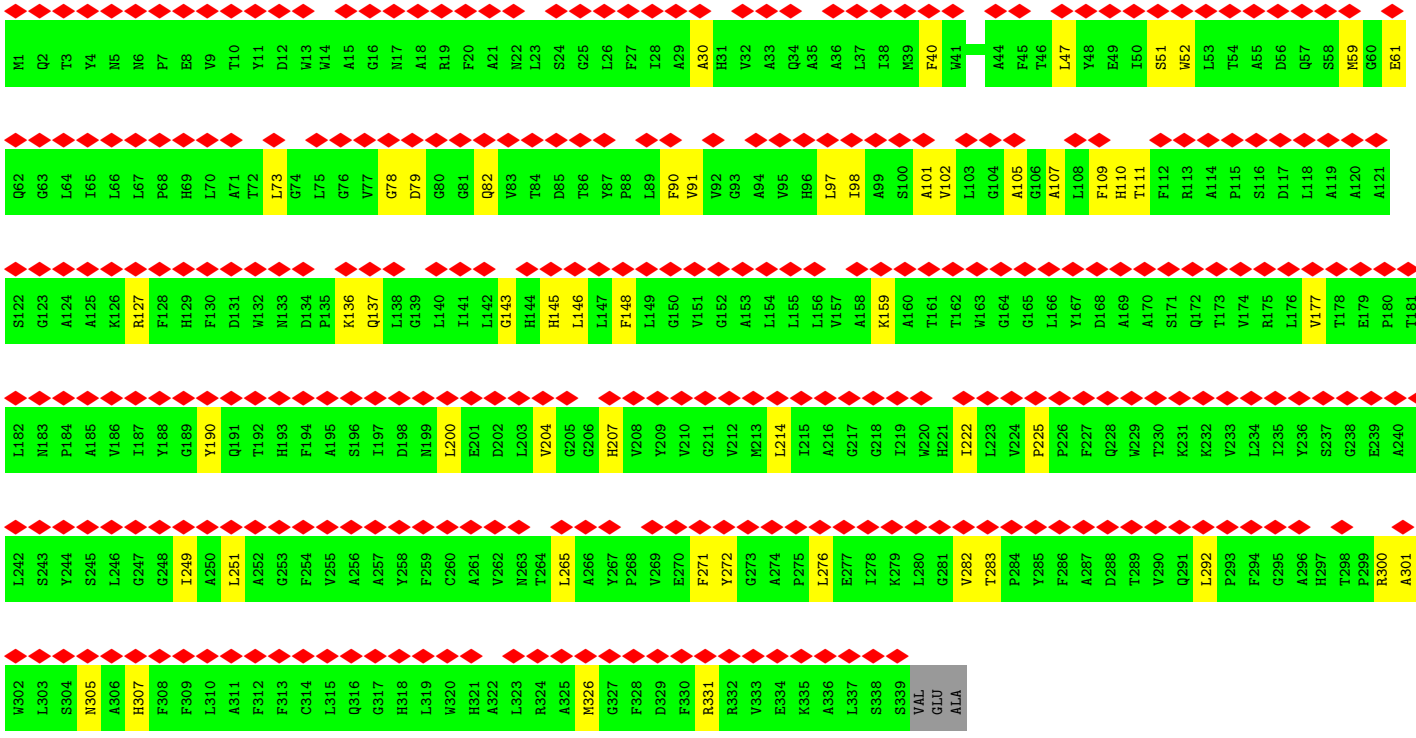




• Molecule 12: Iron stress-induced chlorophyll-binding protein

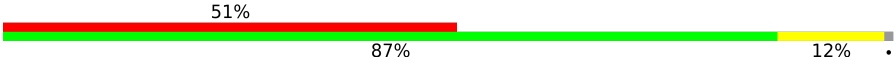
Chain d:

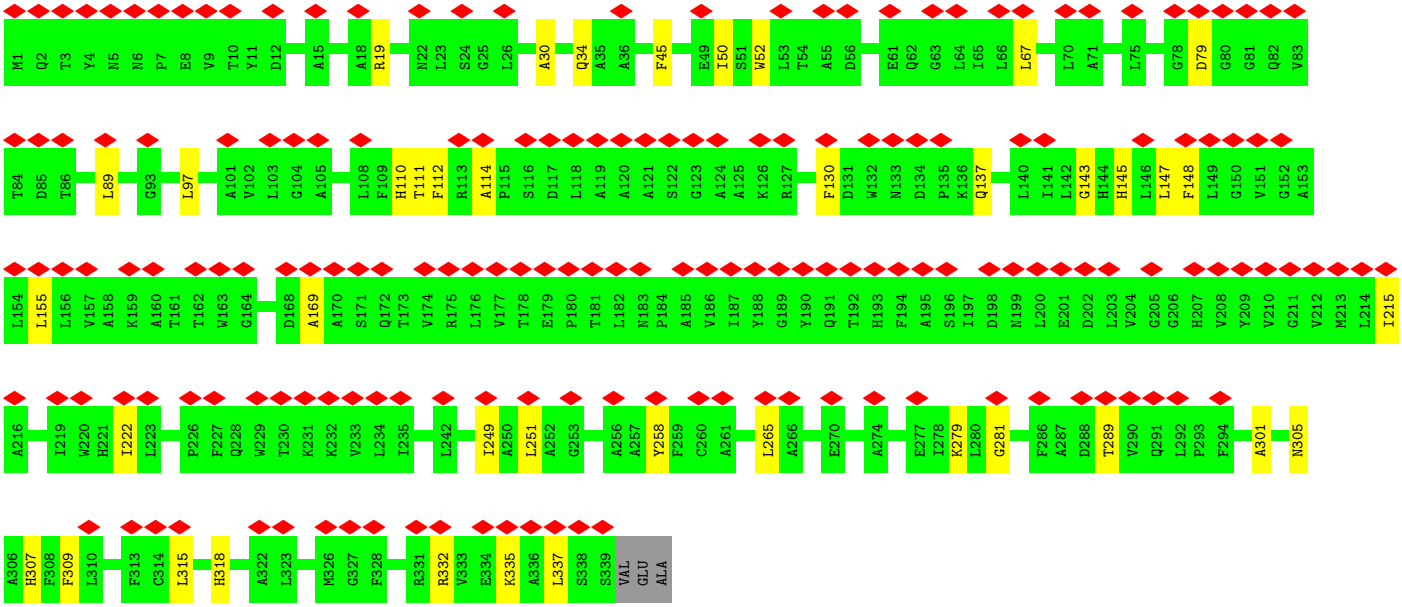




• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain q:

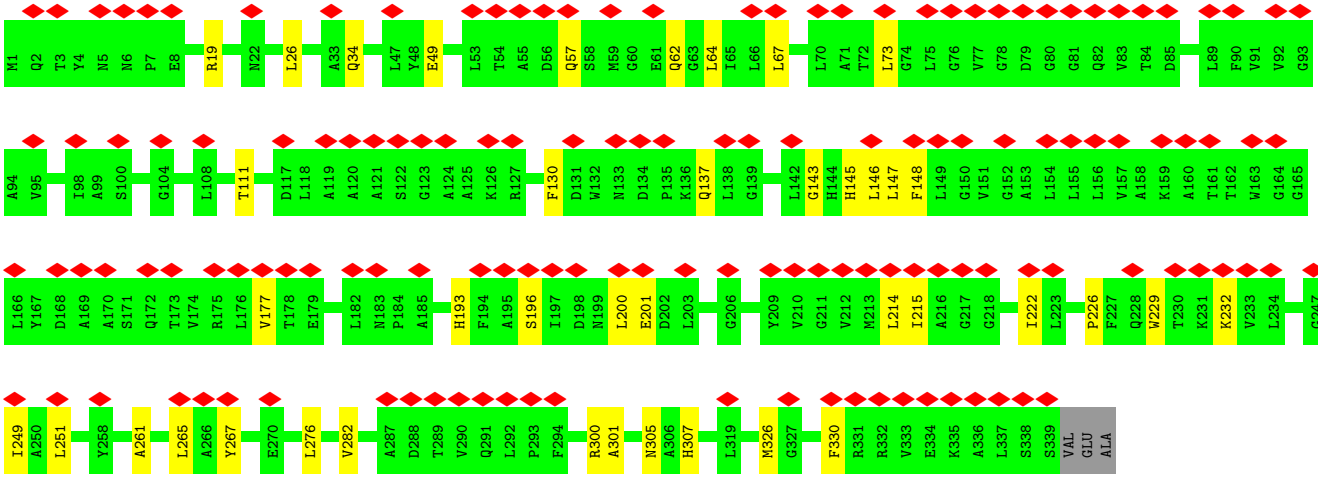




• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain r:

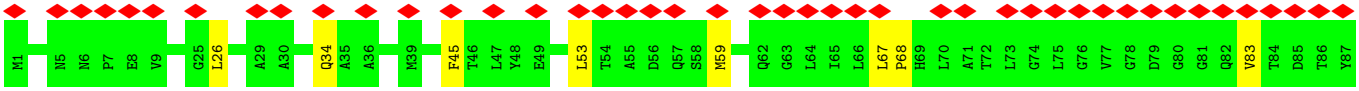


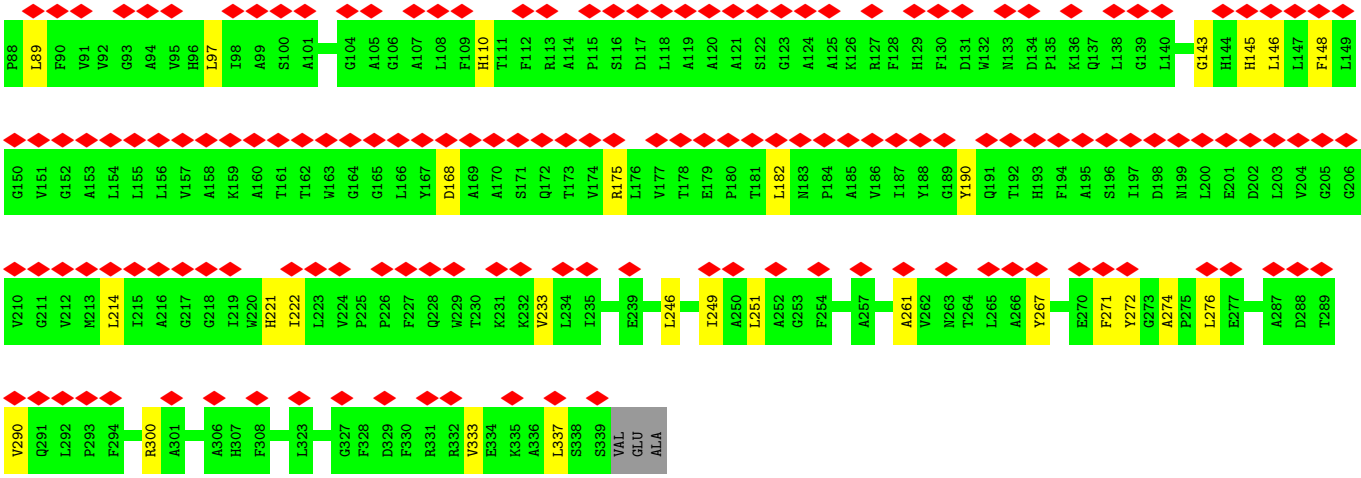


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain s:

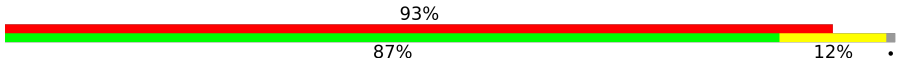


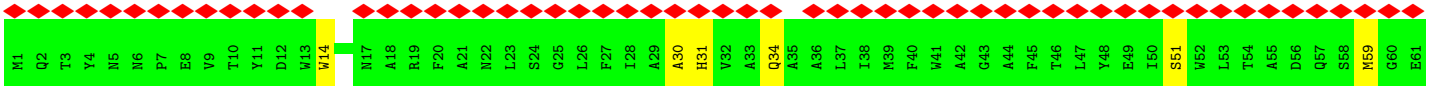


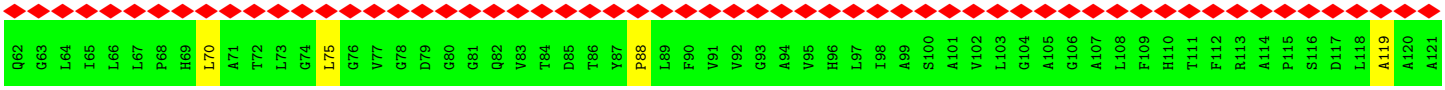


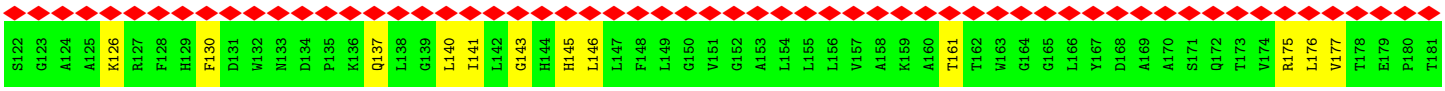
• Molecule 12: Iron stress-induced chlorophyll-binding protein

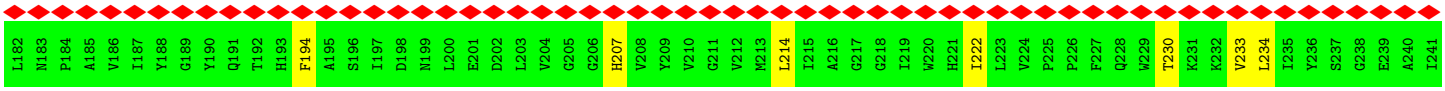
Chain t:

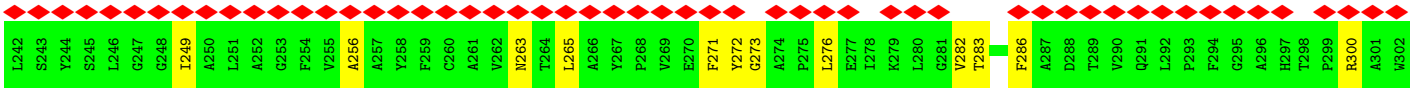


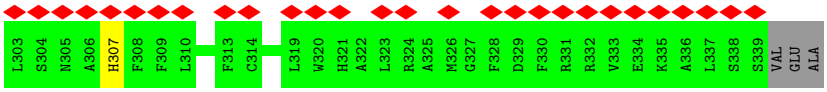






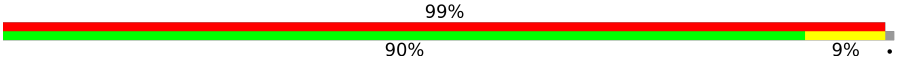


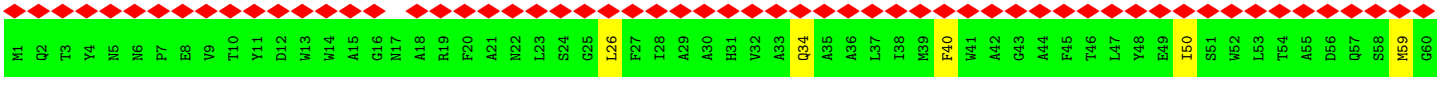


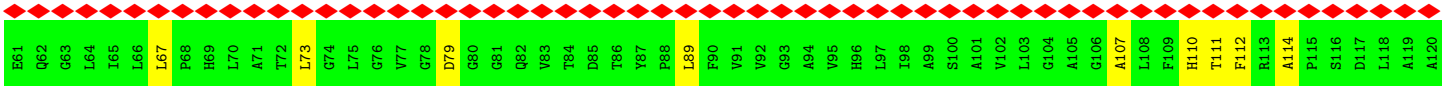


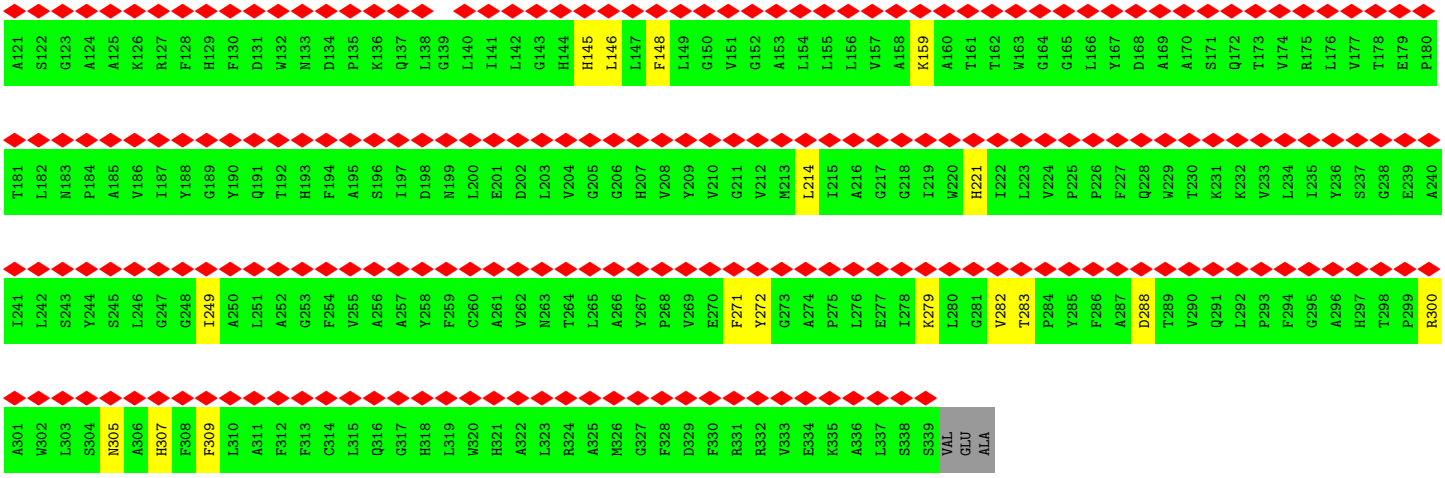
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain u:



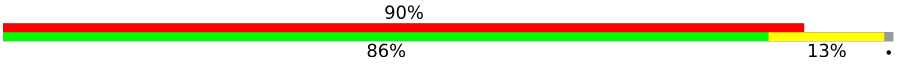


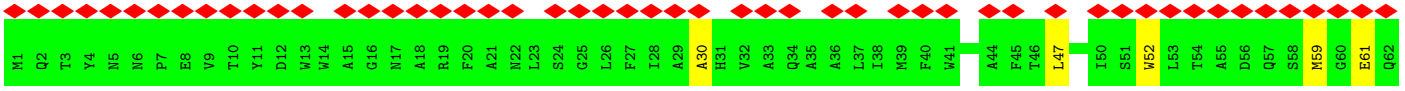


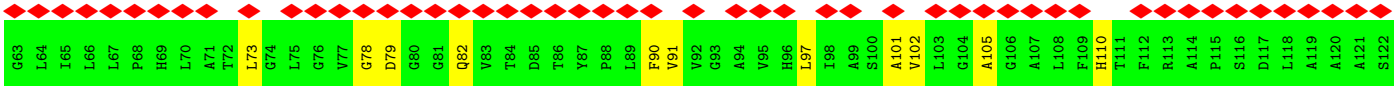


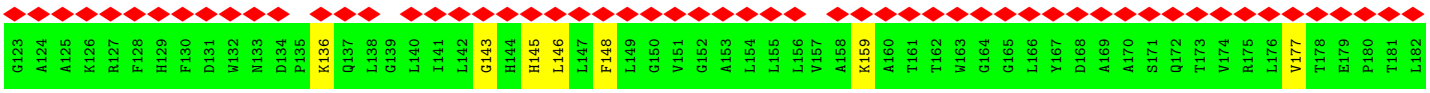
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain v:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	63332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMG, SF4, LMU, SQD, PQN, CLA, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.37	0/6064	0.51	0/8274
1	G	0.37	0/6064	0.51	0/8274
1	e	0.37	0/6064	0.51	0/8274
2	B	0.37	0/5999	0.53	2/8199 (0.0%)
2	H	0.37	0/5999	0.53	2/8199 (0.0%)
2	f	0.37	0/5999	0.53	2/8199 (0.0%)
3	C	0.38	0/608	0.57	0/823
3	N	0.39	0/608	0.56	0/823
3	g	0.39	0/608	0.56	0/823
4	D	0.29	0/1124	0.47	0/1516
4	O	0.30	0/1124	0.47	0/1516
4	h	0.30	0/1124	0.47	0/1516
5	E	0.27	0/553	0.41	0/750
5	Q	0.27	0/553	0.41	0/750
5	i	0.27	0/553	0.42	0/750
6	F	0.30	0/1062	0.50	0/1442
6	R	0.30	0/1062	0.50	0/1442
6	j	0.30	0/1062	0.50	0/1442
7	I	0.33	0/289	0.60	0/393
7	S	0.33	0/289	0.60	0/393
7	k	0.33	0/289	0.60	0/393
8	J	0.37	0/346	0.51	0/469
8	T	0.37	0/346	0.51	0/469
8	l	0.37	0/346	0.51	0/469
9	K	0.27	0/560	0.54	0/765
9	U	0.27	0/560	0.54	0/765
9	m	0.27	0/560	0.54	0/765
10	L	0.28	0/1242	0.49	0/1696
10	V	0.28	0/1242	0.49	0/1696
10	n	0.28	0/1242	0.49	0/1696
11	M	0.33	0/231	0.53	0/314
11	W	0.33	0/231	0.53	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	o	0.33	0/231	0.53	0/314
12	1	0.20	0/2689	0.42	0/3678
12	2	0.19	0/2689	0.41	0/3678
12	3	0.18	0/2689	0.39	0/3678
12	4	0.18	0/2689	0.41	0/3678
12	5	0.17	0/2689	0.40	2/3678 (0.1%)
12	6	0.16	0/2689	0.39	0/3678
12	Y	0.21	0/2689	0.42	0/3678
12	Z	0.20	0/2689	0.41	0/3678
12	a	0.18	0/2689	0.39	0/3678
12	b	0.18	0/2689	0.41	0/3678
12	c	0.17	0/2689	0.40	2/3678 (0.1%)
12	d	0.17	0/2689	0.39	0/3678
12	q	0.21	0/2689	0.42	0/3678
12	r	0.20	0/2689	0.41	0/3678
12	s	0.18	0/2689	0.39	0/3678
12	t	0.18	0/2689	0.40	0/3678
12	u	0.17	0/2689	0.40	2/3678 (0.1%)
12	v	0.17	0/2689	0.39	0/3678
All	All	0.28	0/102636	0.46	12/140127 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	665	ILE	N-CA-C	9.10	119.65	110.82
2	f	665	ILE	N-CA-C	9.10	119.65	110.82
2	H	665	ILE	N-CA-C	9.07	119.62	110.82
2	B	668	ARG	N-CA-C	8.15	120.16	111.28
2	f	668	ARG	N-CA-C	8.13	120.14	111.28
2	H	668	ARG	N-CA-C	8.12	120.13	111.28
12	c	288	ASP	CA-C-N	5.12	131.31	121.54
12	c	288	ASP	C-N-CA	5.12	131.31	121.54
12	u	288	ASP	CA-C-N	5.11	131.31	121.54
12	u	288	ASP	C-N-CA	5.11	131.31	121.54
12	5	288	ASP	CA-C-N	5.10	131.28	121.54
12	5	288	ASP	C-N-CA	5.10	131.28	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5865	0	5744	70	0
1	G	5865	0	5744	73	0
1	e	5865	0	5744	71	0
2	B	5789	0	5575	83	0
2	H	5789	0	5575	83	0
2	f	5789	0	5575	83	0
3	C	598	0	579	10	0
3	N	598	0	579	9	0
3	g	598	0	579	11	0
4	D	1098	0	1099	16	0
4	O	1098	0	1099	16	0
4	h	1098	0	1099	17	0
5	E	543	0	525	3	0
5	Q	543	0	525	3	0
5	i	543	0	525	3	0
6	F	1036	0	1031	12	0
6	R	1036	0	1031	12	0
6	j	1036	0	1031	12	0
7	I	282	0	291	10	0
7	S	282	0	291	11	0
7	k	282	0	291	11	0
8	J	335	0	344	8	0
8	T	335	0	344	8	0
8	l	335	0	344	8	0
9	K	549	0	597	13	0
9	U	549	0	597	13	0
9	m	549	0	597	13	0
10	L	1210	0	1206	15	0
10	V	1210	0	1206	17	0
10	n	1210	0	1206	16	0
11	M	228	0	246	4	0
11	W	228	0	246	4	0
11	o	228	0	246	4	0
12	1	2605	0	2564	34	0
12	2	2605	0	2564	34	0
12	3	2605	0	2564	26	0
12	4	2605	0	2564	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	5	2605	0	2564	28	0
12	6	2605	0	2564	38	0
12	Y	2605	0	2564	36	0
12	Z	2605	0	2564	32	0
12	a	2605	0	2564	25	0
12	b	2605	0	2564	35	0
12	c	2605	0	2564	26	0
12	d	2605	0	2564	54	0
12	q	2605	0	2564	36	0
12	r	2605	0	2564	33	0
12	s	2605	0	2564	28	0
12	t	2605	0	2564	35	0
12	u	2605	0	2564	27	0
12	v	2605	0	2564	38	0
13	1	951	0	894	39	0
13	2	993	0	981	34	0
13	3	950	0	900	24	0
13	4	860	0	725	20	0
13	5	857	0	721	20	0
13	6	823	0	658	21	0
13	A	2728	0	2800	99	0
13	B	2550	0	2680	93	0
13	F	110	0	105	4	0
13	G	2728	0	2800	102	0
13	H	2550	0	2680	97	0
13	J	123	0	127	5	0
13	K	150	0	121	4	0
13	L	190	0	203	10	0
13	R	110	0	105	3	0
13	T	123	0	127	3	0
13	U	150	0	121	4	0
13	V	190	0	203	11	0
13	Y	951	0	894	36	0
13	Z	993	0	981	35	0
13	a	950	0	900	23	0
13	b	860	0	725	18	0
13	c	857	0	721	21	0
13	d	823	0	658	20	0
13	e	2728	0	2800	110	0
13	f	2550	0	2680	95	0
13	j	110	0	105	4	0
13	l	123	0	127	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	150	0	121	4	0
13	n	190	0	203	11	0
13	q	951	0	894	57	0
13	r	993	0	981	37	0
13	s	950	0	900	22	0
13	t	860	0	725	20	0
13	u	857	0	721	23	0
13	v	823	0	658	18	0
14	A	33	0	46	3	0
14	B	33	0	46	2	0
14	G	33	0	46	3	0
14	H	33	0	46	4	0
14	e	33	0	46	2	0
14	f	33	0	46	3	0
15	A	8	0	0	0	0
15	C	16	0	0	1	0
15	G	8	0	0	0	0
15	N	16	0	0	1	0
15	e	8	0	0	0	0
15	g	16	0	0	1	0
16	1	160	0	224	11	0
16	2	160	0	224	13	0
16	3	160	0	224	14	0
16	4	160	0	224	6	0
16	5	160	0	224	9	0
16	6	160	0	224	16	0
16	A	240	0	336	18	0
16	B	280	0	392	29	0
16	F	40	0	56	5	0
16	G	240	0	336	17	0
16	H	280	0	392	23	0
16	I	40	0	56	3	0
16	J	120	0	168	12	0
16	K	40	0	56	7	0
16	L	160	0	224	12	0
16	M	40	0	56	2	0
16	R	40	0	56	4	0
16	S	40	0	56	5	0
16	T	120	0	168	16	0
16	U	40	0	56	6	0
16	V	160	0	224	15	0
16	W	40	0	56	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	160	0	224	13	0
16	Z	160	0	224	10	0
16	a	160	0	224	13	0
16	b	160	0	224	8	0
16	c	160	0	224	11	0
16	d	160	0	224	21	0
16	e	240	0	336	17	0
16	f	280	0	392	26	0
16	j	40	0	56	3	0
16	k	40	0	56	4	0
16	l	120	0	168	14	0
16	m	40	0	56	5	0
16	n	160	0	224	15	0
16	o	40	0	56	4	0
16	q	160	0	224	11	0
16	r	160	0	224	13	0
16	s	160	0	224	11	0
16	t	160	0	224	9	0
16	u	160	0	224	12	0
16	v	160	0	224	15	0
17	A	386	0	520	19	0
17	B	83	0	109	4	0
17	G	386	0	520	17	0
17	H	83	0	109	5	0
17	I	44	0	58	1	0
17	L	128	0	172	13	0
17	S	44	0	58	0	0
17	V	128	0	172	11	0
17	e	386	0	520	20	0
17	f	83	0	109	4	0
17	k	44	0	58	1	0
17	n	128	0	172	12	0
18	1	19	0	22	0	0
18	2	23	0	30	0	0
18	A	58	0	76	1	0
18	B	35	0	46	0	0
18	G	58	0	76	0	0
18	H	35	0	46	0	0
18	J	22	0	28	2	0
18	T	22	0	28	2	0
18	Y	19	0	22	0	0
18	Z	23	0	30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	e	58	0	76	1	0
18	f	35	0	46	0	0
18	l	22	0	28	2	0
18	q	19	0	22	0	0
18	r	23	0	30	0	0
19	B	54	0	81	7	0
19	H	54	0	81	7	0
19	J	35	0	40	0	0
19	T	35	0	40	0	0
19	f	54	0	81	7	0
19	l	35	0	40	0	0
20	1	48	0	63	4	0
20	2	43	0	49	1	0
20	3	43	0	50	1	0
20	4	26	0	16	0	0
20	5	29	0	22	0	0
20	6	26	0	16	1	0
20	B	45	0	53	7	0
20	H	45	0	53	10	0
20	L	51	0	69	4	0
20	V	51	0	69	3	0
20	Y	48	0	63	5	0
20	Z	43	0	49	1	0
20	a	43	0	50	1	0
20	b	26	0	16	0	0
20	c	29	0	22	0	0
20	d	26	0	16	1	0
20	f	45	0	53	8	0
20	n	51	0	69	4	0
20	q	48	0	63	4	0
20	r	43	0	49	1	0
20	s	43	0	50	1	0
20	t	26	0	16	0	0
20	u	29	0	22	0	0
20	v	26	0	16	1	0
21	A	9	0	0	0	0
21	B	7	0	0	0	0
21	F	1	0	0	0	0
21	G	9	0	0	0	0
21	H	7	0	0	0	0
21	L	1	0	0	0	0
21	R	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	1	0	0	0	0
21	e	9	0	0	0	0
21	f	7	0	0	0	0
21	j	1	0	0	0	0
21	n	1	0	0	0	0
All	All	143022	0	143508	2193	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 8.

All (2193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:1852:SQD:H91	17:e:5002:LHG:C23	2.07	0.84
17:L:5221:LHG:H252	13:f:1207:CLA:H42	1.60	0.83
13:B:1207:CLA:H42	17:V:5221:LHG:H252	1.58	0.83
13:H:1207:CLA:H42	17:n:5221:LHG:H252	1.59	0.83
20:H:1852:SQD:H91	17:e:5002:LHG:O10	1.81	0.81
13:B:1203:CLA:H152	13:B:1225:CLA:HBB2	1.65	0.79
13:H:1203:CLA:H152	13:H:1225:CLA:HBB2	1.65	0.77
13:a:518:CLA:HBC2	20:a:822:SQD:H282	1.67	0.77
13:f:1203:CLA:H152	13:f:1225:CLA:HBB2	1.65	0.77
13:s:518:CLA:HBC2	20:s:822:SQD:H282	1.67	0.75
12:t:75:LEU:HD12	12:t:75:LEU:O	1.87	0.75
12:4:75:LEU:HD12	12:4:75:LEU:O	1.87	0.75
13:e:1104:CLA:H42	13:e:1128:CLA:H2	1.69	0.74
17:A:5002:LHG:C23	20:f:1852:SQD:H91	2.16	0.74
12:b:75:LEU:HD12	12:b:75:LEU:O	1.87	0.74
13:3:518:CLA:HBC2	20:3:822:SQD:H282	1.67	0.74
4:O:41:GLU:H	4:O:71:GLN:HE22	1.36	0.73
13:G:1104:CLA:H42	13:G:1128:CLA:H2	1.69	0.73
13:e:1013:CLA:H111	16:e:4011:BCR:H23C	1.70	0.73
13:A:1013:CLA:H111	16:A:4011:BCR:H23C	1.70	0.73
17:L:5221:LHG:H342	13:f:1207:CLA:H142	1.68	0.73
4:D:41:GLU:H	4:D:71:GLN:HE22	1.36	0.72
13:G:1013:CLA:H111	16:G:4011:BCR:H23C	1.70	0.72
7:S:26:LEU:HD11	20:n:5216:SQD:H311	1.71	0.72
13:A:1104:CLA:H42	13:A:1128:CLA:H2	1.69	0.72
13:B:1207:CLA:H142	17:V:5221:LHG:H342	1.70	0.72
20:L:5216:SQD:H311	7:k:26:LEU:HD11	1.70	0.72
12:2:146:LEU:HD21	13:2:506:CLA:HAB	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:41:GLU:H	4:h:71:GLN:HE22	1.36	0.71
12:Z:146:LEU:HD21	13:Z:506:CLA:HAB	1.72	0.71
20:B:1852:SQD:H91	17:G:5002:LHG:C23	2.20	0.71
7:I:26:LEU:HD11	20:V:5216:SQD:H311	1.73	0.70
12:r:146:LEU:HD21	13:r:506:CLA:HAB	1.72	0.69
12:4:282:VAL:O	13:4:519:CLA:NB	2.25	0.69
12:4:145:HIS:NE2	13:4:512:CLA:NA	2.40	0.69
17:A:5002:LHG:O10	20:f:1852:SQD:H91	1.92	0.69
12:b:282:VAL:O	13:b:519:CLA:NB	2.26	0.69
16:U:4104:BCR:H24C	20:Y:822:SQD:H321	1.75	0.69
12:b:145:HIS:NE2	13:b:512:CLA:NA	2.40	0.69
16:d:522:BCR:HC41	12:q:258:TYR:HB2	1.75	0.69
16:K:4104:BCR:H24C	20:1:822:SQD:H321	1.75	0.68
12:t:282:VAL:O	13:t:519:CLA:NB	2.26	0.68
16:m:4104:BCR:H24C	20:q:822:SQD:H321	1.75	0.68
12:t:145:HIS:NE2	13:t:512:CLA:NA	2.40	0.68
20:B:1852:SQD:H91	17:G:5002:LHG:O10	1.93	0.68
1:e:410:GLY:HA3	1:e:614:LEU:HD11	1.76	0.67
1:G:410:GLY:HA3	1:G:614:LEU:HD11	1.76	0.67
13:A:1130:CLA:H101	16:L:4022:BCR:H322	1.77	0.67
13:6:505:CLA:H43	16:6:524:BCR:HC7	1.76	0.67
18:T:5105:LMU:H92	16:a:521:BCR:C40	2.25	0.67
13:G:1130:CLA:H101	16:V:4022:BCR:H322	1.77	0.67
18:l:5105:LMU:H92	16:s:521:BCR:C40	2.25	0.67
18:J:5105:LMU:H92	16:3:521:BCR:C40	2.25	0.66
13:H:1207:CLA:H142	17:n:5221:LHG:H342	1.75	0.66
13:d:505:CLA:H43	16:d:524:BCR:HC7	1.76	0.66
13:e:1130:CLA:H101	16:n:4022:BCR:H322	1.77	0.66
1:A:410:GLY:HA3	1:A:614:LEU:HD11	1.77	0.66
13:A:1130:CLA:H2	13:L:1502:CLA:H43	1.78	0.66
12:d:101:ALA:HB1	13:q:505:CLA:HAB	1.76	0.66
13:e:1130:CLA:H2	13:n:1502:CLA:H43	1.78	0.66
13:v:505:CLA:H43	16:v:524:BCR:HC7	1.77	0.66
13:G:1130:CLA:H2	13:V:1502:CLA:H43	1.78	0.66
12:4:75:LEU:HD13	12:4:88:PRO:HB2	1.78	0.66
2:B:112:PRO:HD2	7:I:1:MET:HB2	1.78	0.65
13:Y:501:CLA:HBB2	13:Y:507:CLA:H92	1.79	0.65
13:q:501:CLA:HBB2	13:q:507:CLA:H92	1.79	0.65
17:H:1855:LHG:HC82	17:H:1855:LHG:H252	1.79	0.65
2:f:112:PRO:HD2	7:k:1:MET:HB2	1.78	0.65
13:B:1231:CLA:H71	16:B:4010:BCR:H313	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:PRO:HD2	7:S:1:MET:HB2	1.78	0.65
18:T:5105:LMU:H92	16:a:521:BCR:H401	1.79	0.65
12:1:145:HIS:NE2	13:1:512:CLA:NA	2.45	0.65
17:B:1855:LHG:HC82	17:B:1855:LHG:H252	1.79	0.65
13:H:1231:CLA:H71	16:H:4010:BCR:H313	1.79	0.65
12:Y:145:HIS:NE2	13:Y:512:CLA:NA	2.45	0.65
13:e:1013:CLA:HBA2	2:f:427:LEU:HD12	1.79	0.65
18:l:5105:LMU:H92	16:s:521:BCR:H401	1.79	0.65
12:q:145:HIS:NE2	13:q:512:CLA:NA	2.45	0.65
12:b:75:LEU:HD13	12:b:88:PRO:HB2	1.78	0.64
12:t:75:LEU:HD13	12:t:88:PRO:HB2	1.78	0.64
13:A:1013:CLA:HBA2	2:B:427:LEU:HD12	1.79	0.64
18:J:5105:LMU:H92	16:3:521:BCR:H401	1.79	0.64
13:f:1231:CLA:H71	16:f:4010:BCR:H313	1.79	0.63
13:1:501:CLA:HBB2	13:1:507:CLA:H92	1.79	0.63
10:n:150:PRO:HG2	17:n:5221:LHG:HC62	1.80	0.63
13:G:1013:CLA:HBA2	2:H:427:LEU:HD12	1.79	0.63
10:V:160:ALA:HB1	10:V:165:VAL:HB	1.81	0.63
10:L:160:ALA:HB1	10:L:165:VAL:HB	1.81	0.63
2:B:326:LEU:HD13	2:B:332:PHE:CD2	2.34	0.63
13:2:502:CLA:H61	13:2:512:CLA:H42	1.81	0.63
2:H:158:GLN:HB3	20:H:1852:SQD:H5	1.81	0.63
17:f:1855:LHG:HC82	17:f:1855:LHG:H252	1.79	0.62
10:L:150:PRO:HG2	17:L:5221:LHG:HC62	1.80	0.62
16:A:4011:BCR:H362	13:B:1012:CLA:H2	1.81	0.62
12:b:30:ALA:HB2	13:b:511:CLA:HMA1	1.81	0.62
13:Z:502:CLA:H61	13:Z:512:CLA:H42	1.81	0.62
13:r:502:CLA:H61	13:r:512:CLA:H42	1.81	0.62
2:f:158:GLN:HB3	20:f:1852:SQD:H5	1.81	0.62
12:3:249:ILE:HG12	13:3:502:CLA:HAC1	1.81	0.62
2:f:326:LEU:HD13	2:f:332:PHE:CD2	2.34	0.62
2:B:158:GLN:HB3	20:B:1852:SQD:H5	1.81	0.62
16:G:4011:BCR:H362	13:H:1012:CLA:H2	1.81	0.62
10:n:160:ALA:HB1	10:n:165:VAL:HB	1.81	0.62
12:s:249:ILE:HG12	13:s:502:CLA:HAC1	1.81	0.62
12:3:272:TYR:HB3	12:3:300:ARG:HB2	1.82	0.62
1:G:494:PHE:HB3	13:G:1135:CLA:H11	1.82	0.62
13:e:1126:CLA:H201	16:l:4012:BCR:H12C	1.82	0.62
16:m:4104:BCR:H392	20:q:822:SQD:H301	1.82	0.62
2:B:323:TYR:O	2:B:327:ASN:HB2	2.00	0.61
13:H:1217:CLA:HAB	13:H:1217:CLA:H93	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:26:ASN:HB3	13:U:1103:CLA:H12	1.83	0.61
13:H:1225:CLA:H12	16:H:4005:BCR:H393	1.83	0.61
10:V:150:PRO:HG2	17:V:5221:LHG:HC62	1.80	0.61
1:A:494:PHE:HB3	13:A:1135:CLA:H11	1.82	0.61
16:K:4104:BCR:H392	20:1:822:SQD:H301	1.83	0.61
1:e:494:PHE:HB3	13:e:1135:CLA:H11	1.82	0.61
12:v:30:ALA:HB2	13:v:511:CLA:HMA1	1.82	0.61
12:1:289:THR:O	12:1:289:THR:HG22	2.01	0.61
13:G:1121:CLA:HAB	13:G:1801:CLA:HAB	1.83	0.61
1:e:33:HIS:NE2	13:e:1109:CLA:O1A	2.30	0.61
9:m:26:ASN:HB3	13:m:1103:CLA:H12	1.82	0.61
12:6:249:ILE:HG12	13:6:502:CLA:HAC1	1.83	0.61
13:H:1207:CLA:H42	17:n:5221:LHG:C25	2.31	0.61
12:d:52:TRP:CZ3	17:e:5009:LHG:HC11	2.35	0.61
13:e:1121:CLA:HAB	13:e:1801:CLA:HAB	1.83	0.61
16:e:4011:BCR:H362	13:f:1012:CLA:H2	1.81	0.61
12:q:289:THR:O	12:q:289:THR:HG22	2.01	0.61
13:A:1126:CLA:H201	16:J:4012:BCR:H12C	1.82	0.61
2:H:323:TYR:O	2:H:327:ASN:HB2	2.00	0.61
2:H:326:LEU:HD13	2:H:332:PHE:CD2	2.34	0.61
12:d:30:ALA:HB2	13:d:511:CLA:HMA1	1.82	0.61
12:t:30:ALA:HB2	13:t:511:CLA:HMA1	1.81	0.61
13:f:1217:CLA:HAB	13:f:1217:CLA:H93	1.82	0.61
16:L:4022:BCR:C24	10:n:137:LEU:HD13	2.31	0.61
17:L:5221:LHG:C25	13:f:1207:CLA:H42	2.30	0.61
17:H:1855:LHG:H192	13:R:1302:CLA:HBB1	1.83	0.61
2:f:323:TYR:O	2:f:327:ASN:HB2	2.00	0.61
12:6:136:LYS:HG3	12:6:225:PRO:HB3	1.83	0.60
12:d:249:ILE:HG12	13:d:502:CLA:HAC1	1.83	0.60
13:f:1225:CLA:H12	16:f:4005:BCR:H393	1.83	0.60
12:s:272:TYR:HB3	12:s:300:ARG:HB2	1.82	0.60
12:v:136:LYS:HG3	12:v:225:PRO:HB3	1.83	0.60
9:K:26:ASN:HB3	13:K:1103:CLA:H12	1.83	0.60
12:a:249:ILE:HG12	13:a:502:CLA:HAC1	1.82	0.60
12:a:272:TYR:HB3	12:a:300:ARG:HB2	1.82	0.60
12:c:146:LEU:HD21	13:c:506:CLA:HAB	1.83	0.60
10:L:137:LEU:HD13	16:V:4022:BCR:C24	2.30	0.60
16:U:4104:BCR:H392	20:Y:822:SQD:H301	1.82	0.60
17:B:1855:LHG:H192	13:F:1302:CLA:HBB1	1.83	0.60
12:v:249:ILE:HG12	13:v:502:CLA:HAC1	1.83	0.60
1:A:278:LEU:HD21	9:K:72:ILE:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1225:CLA:H12	16:B:4005:BCR:H393	1.83	0.60
13:A:1121:CLA:HAB	13:A:1801:CLA:HAB	1.83	0.60
13:B:1217:CLA:H93	13:B:1217:CLA:HAB	1.82	0.60
12:5:146:LEU:HD21	13:5:506:CLA:HAB	1.84	0.60
12:Y:289:THR:O	12:Y:289:THR:HG22	2.01	0.60
1:A:33:HIS:NE2	13:A:1109:CLA:O1A	2.30	0.60
12:6:30:ALA:HB2	13:6:511:CLA:HMA1	1.82	0.60
12:q:52:TRP:CE3	13:q:504:CLA:HED3	2.37	0.60
13:B:1207:CLA:H42	17:V:5221:LHG:C25	2.29	0.60
12:d:102:VAL:HA	13:q:505:CLA:H61	1.84	0.60
12:d:136:LYS:HG3	12:d:225:PRO:HB3	1.83	0.60
13:G:1126:CLA:H201	16:T:4012:BCR:H12C	1.82	0.59
13:q:502:CLA:H12	13:q:503:CLA:H42	1.84	0.59
17:e:5004:LHG:H102	12:r:282:VAL:HG13	1.82	0.59
13:l:1303:CLA:H62	12:t:282:VAL:HG22	1.84	0.59
17:A:5004:LHG:H102	12:2:282:VAL:HG13	1.82	0.59
13:G:1103:CLA:H121	16:G:4002:BCR:HC41	1.84	0.59
17:G:5004:LHG:H102	12:Z:282:VAL:HG13	1.82	0.59
12:u:146:LEU:HD21	13:u:506:CLA:HAB	1.83	0.59
12:1:52:TRP:CE3	13:1:504:CLA:HED3	2.37	0.59
13:1:502:CLA:H12	13:1:503:CLA:H42	1.84	0.59
6:R:141:GLU:HG3	6:R:146:LYS:HB3	1.84	0.59
11:W:21:TYR:OH	10:n:26:PHE:HB2	2.02	0.59
12:Y:52:TRP:CE3	13:Y:504:CLA:HED3	2.37	0.59
9:U:60:VAL:HG22	13:U:1105:CLA:HAC2	1.83	0.59
17:f:1855:LHG:H192	13:j:1302:CLA:HBB1	1.83	0.59
6:j:91:ILE:HG23	13:j:1301:CLA:HAA1	1.85	0.59
13:5:501:CLA:H72	13:5:501:CLA:HBB1	1.85	0.59
1:e:577:LYS:NZ	2:f:673:GLU:OE2	2.36	0.59
12:q:251:LEU:HD13	13:q:505:CLA:H122	1.85	0.59
12:1:30:ALA:HB2	13:1:511:CLA:HMA1	1.85	0.59
1:G:278:LEU:HD21	9:U:72:ILE:HD12	1.83	0.59
9:m:60:VAL:HG22	13:m:1105:CLA:HAC2	1.83	0.59
9:K:60:VAL:HG22	13:K:1105:CLA:HAC2	1.83	0.59
6:j:141:GLU:HG3	6:j:146:LYS:HB3	1.84	0.59
6:F:91:ILE:HG23	13:F:1301:CLA:HAA1	1.85	0.59
13:Y:502:CLA:H12	13:Y:503:CLA:H42	1.84	0.59
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.85	0.58
17:A:5009:LHG:HC11	12:v:52:TRP:CZ3	2.38	0.58
13:f:1222:CLA:HMA1	16:f:4010:BCR:H14C	1.85	0.58
12:1:251:LEU:HD13	13:1:505:CLA:H122	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1222:CLA:HMA1	16:B:4010:BCR:H14C	1.85	0.58
12:Z:267:TYR:O	12:Z:300:ARG:NH2	2.37	0.58
13:c:501:CLA:H72	13:c:501:CLA:HBB1	1.85	0.58
12:s:145:HIS:NE2	13:s:512:CLA:NA	2.52	0.58
6:F:141:GLU:HG3	6:F:146:LYS:HB3	1.84	0.58
12:a:145:HIS:NE2	13:a:512:CLA:NA	2.52	0.58
12:c:30:ALA:HB2	13:c:511:CLA:HMA1	1.85	0.58
12:6:146:LEU:HD21	13:6:506:CLA:HAB	1.86	0.58
1:e:278:LEU:HD21	9:m:72:ILE:HD12	1.83	0.58
2:f:15:ASP:HB3	2:f:20:ARG:HB2	1.85	0.58
13:u:501:CLA:H72	13:u:501:CLA:HBB1	1.85	0.58
1:A:59:ASP:OD2	1:A:361:HIS:NE2	2.37	0.58
12:1:258:TYR:HB2	16:v:522:BCR:HC41	1.84	0.58
13:H:1222:CLA:HMA1	16:H:4010:BCR:H14C	1.85	0.58
12:1:110:HIS:NE2	13:1:513:CLA:NB	2.52	0.58
1:G:59:ASP:OD2	1:G:361:HIS:NE2	2.37	0.58
1:e:59:ASP:OD2	1:e:361:HIS:NE2	2.37	0.58
13:e:1103:CLA:H121	16:e:4002:BCR:HC41	1.84	0.58
13:A:1103:CLA:H121	16:A:4002:BCR:HC41	1.84	0.57
12:3:168:ASP:OD2	12:3:175:ARG:NH2	2.37	0.57
12:d:146:LEU:HD21	13:d:506:CLA:HAB	1.86	0.57
12:2:267:TYR:O	12:2:300:ARG:NH2	2.37	0.57
12:3:145:HIS:NE2	13:3:512:CLA:NA	2.52	0.57
1:e:752:TRP:NE1	13:e:1126:CLA:O1A	2.32	0.57
13:f:1239:CLA:HBB1	16:f:4017:BCR:H363	1.86	0.57
12:q:30:ALA:HB2	13:q:511:CLA:HMA1	1.85	0.57
13:T:1303:CLA:H62	12:b:282:VAL:HG22	1.84	0.57
2:f:351:HIS:ND1	13:f:1214:CLA:OBD	2.38	0.57
13:J:1303:CLA:H62	12:4:282:VAL:HG22	1.84	0.57
12:5:30:ALA:HB2	13:5:511:CLA:HMA1	1.85	0.57
12:6:251:LEU:HD13	13:6:505:CLA:H122	1.87	0.57
17:G:5006:LHG:H241	12:Y:52:TRP:CH2	2.40	0.57
2:H:15:ASP:HB3	2:H:20:ARG:HB2	1.85	0.57
10:L:26:PHE:HB2	11:o:21:TYR:OH	2.04	0.57
1:G:752:TRP:NE1	13:G:1126:CLA:O1A	2.32	0.57
2:H:351:HIS:ND1	13:H:1214:CLA:OBD	2.38	0.57
12:Y:110:HIS:NE2	13:Y:513:CLA:NB	2.52	0.57
12:v:307:HIS:NE2	13:v:502:CLA:ND	2.53	0.57
12:Y:251:LEU:HD13	13:Y:505:CLA:H122	1.85	0.57
17:e:5006:LHG:H241	12:q:52:TRP:CH2	2.40	0.57
6:R:91:ILE:HG23	13:R:1301:CLA:HAA1	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:168:ASP:OD2	12:a:175:ARG:NH2	2.37	0.57
12:q:110:HIS:NE2	13:q:513:CLA:NB	2.52	0.57
12:s:168:ASP:OD2	12:s:175:ARG:NH2	2.37	0.57
12:v:146:LEU:HD21	13:v:506:CLA:HAB	1.86	0.57
17:A:5006:LHG:H241	12:1:52:TRP:CH2	2.40	0.57
12:Y:249:ILE:HG12	13:Y:502:CLA:HAC1	1.87	0.56
2:f:26:ALA:HA	13:f:1226:CLA:H43	1.87	0.56
12:r:267:TYR:O	12:r:300:ARG:NH2	2.37	0.56
9:U:18:VAL:HG22	9:U:84:LEU:HD21	1.87	0.56
9:U:50:GLN:HB2	12:Y:337:LEU:HD23	1.87	0.56
13:l:1303:CLA:H41	12:t:282:VAL:HG22	1.87	0.56
9:m:50:GLN:HB2	12:q:337:LEU:HD23	1.87	0.56
13:B:1239:CLA:HBB1	16:B:4017:BCR:H363	1.86	0.56
13:2:517:CLA:HBB1	16:2:524:BCR:H352	1.88	0.56
12:6:272:TYR:HB3	12:6:300:ARG:HB2	1.87	0.56
12:d:307:HIS:NE2	13:d:502:CLA:ND	2.53	0.56
12:v:272:TYR:HB3	12:v:300:ARG:HB2	1.87	0.56
2:B:351:HIS:ND1	13:B:1214:CLA:OBD	2.38	0.56
13:r:517:CLA:HBB1	16:r:524:BCR:H352	1.88	0.56
12:1:249:ILE:HG12	13:1:502:CLA:HAC1	1.87	0.56
12:d:102:VAL:HG22	13:q:505:CLA:H61	1.88	0.56
12:d:251:LEU:HD13	13:d:505:CLA:H122	1.87	0.56
9:K:50:GLN:HB2	12:1:337:LEU:HD23	1.87	0.56
12:d:110:HIS:NE2	13:d:513:CLA:NB	2.54	0.56
12:q:249:ILE:HG12	13:q:502:CLA:HAC1	1.87	0.56
12:v:251:LEU:HD13	13:v:505:CLA:H122	1.87	0.56
8:J:1:MET:HE3	12:3:337:LEU:HG	1.88	0.56
13:J:1303:CLA:H41	12:4:282:VAL:HG22	1.87	0.56
12:6:307:HIS:NE2	13:6:502:CLA:ND	2.53	0.56
13:Z:506:CLA:HBB2	13:Z:507:CLA:H51	1.88	0.56
13:Z:517:CLA:HBB1	16:Z:524:BCR:H352	1.88	0.56
13:A:1136:CLA:HBC1	17:L:5220:LHG:H282	1.88	0.56
11:M:21:TYR:OH	10:V:26:PHE:HB2	2.06	0.56
12:2:249:ILE:HG12	13:2:502:CLA:HAC1	1.88	0.56
13:G:1130:CLA:H121	13:V:1501:CLA:H201	1.88	0.56
13:H:1209:CLA:HBB2	13:H:1217:CLA:H102	1.88	0.56
12:d:272:TYR:HB3	12:d:300:ARG:HB2	1.87	0.56
13:e:1103:CLA:H142	16:e:4003:BCR:H372	1.88	0.56
4:h:61:ARG:NH1	4:h:63:GLU:OE1	2.39	0.56
4:D:61:ARG:NH1	4:D:63:GLU:OE1	2.39	0.55
12:6:110:HIS:NE2	13:6:513:CLA:NB	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:ARG:NH1	4:O:63:GLU:OE1	2.39	0.55
6:R:143:SER:HB2	12:b:14:TRP:CH2	2.41	0.55
8:T:1:MET:HE3	12:a:337:LEU:HG	1.88	0.55
8:l:1:MET:HE3	12:s:337:LEU:HG	1.88	0.55
12:r:249:ILE:HG12	13:r:502:CLA:HAC1	1.88	0.55
12:u:249:ILE:HG12	13:u:502:CLA:HAC1	1.88	0.55
13:A:1120:CLA:HMD2	16:A:4001:BCR:H24C	1.89	0.55
13:G:1120:CLA:HMD2	16:G:4001:BCR:H24C	1.88	0.55
12:c:249:ILE:HG12	13:c:502:CLA:HAC1	1.88	0.55
13:f:1209:CLA:HBB2	13:f:1217:CLA:H102	1.87	0.55
4:h:120:ARG:HH22	4:h:141:ALA:HB3	1.72	0.55
12:r:214:LEU:HD21	13:r:507:CLA:H71	1.88	0.55
13:A:1237:CLA:H152	16:L:4020:BCR:H16C	1.89	0.55
13:B:1202:CLA:H8	13:B:1221:CLA:HBA2	1.89	0.55
4:D:120:ARG:HH22	4:D:141:ALA:HB3	1.72	0.55
9:K:18:VAL:HG22	9:K:84:LEU:HD21	1.87	0.55
12:2:214:LEU:HD21	13:2:507:CLA:H71	1.89	0.55
2:H:603:GLN:HE21	2:H:732:LYS:HD3	1.72	0.55
13:A:1103:CLA:H142	16:A:4003:BCR:H372	1.88	0.55
10:L:41:LEU:O	10:L:46:ARG:NH1	2.40	0.55
12:2:34:GLN:OE1	13:2:510:CLA:NC	2.40	0.55
13:G:1103:CLA:H142	16:G:4003:BCR:H372	1.88	0.55
13:H:1239:CLA:HBB1	16:H:4017:BCR:H363	1.86	0.55
3:N:63:LEU:HD12	3:N:66:ARG:HH21	1.71	0.55
12:Z:214:LEU:HD21	13:Z:507:CLA:H71	1.89	0.55
13:f:1023:CLA:H142	16:k:4018:BCR:H271	1.88	0.55
13:f:1202:CLA:H8	13:f:1221:CLA:HBA2	1.89	0.55
4:D:85:ILE:HB	4:D:98:HIS:HB3	1.89	0.55
13:G:1136:CLA:HBC1	17:V:5220:LHG:H282	1.88	0.55
13:e:1237:CLA:H152	16:n:4020:BCR:H16C	1.89	0.55
2:B:26:ALA:HA	13:B:1226:CLA:H43	1.87	0.55
13:6:501:CLA:H72	13:6:501:CLA:HBB1	1.89	0.55
13:e:1120:CLA:HMD2	16:e:4001:BCR:H24C	1.89	0.55
12:r:34:GLN:OE1	13:r:510:CLA:NC	2.40	0.55
2:B:603:GLN:HE21	2:B:732:LYS:HD3	1.72	0.55
6:F:143:SER:HB2	12:4:14:TRP:CH2	2.41	0.55
13:2:506:CLA:HBB2	13:2:507:CLA:H51	1.88	0.55
6:j:143:SER:HB2	12:t:14:TRP:CH2	2.41	0.55
13:v:501:CLA:H72	13:v:501:CLA:HBB1	1.89	0.55
1:G:33:HIS:NE2	13:G:1109:CLA:O1A	2.30	0.55
2:H:26:ALA:HA	13:H:1226:CLA:H43	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:85:ILE:HB	4:h:98:HIS:HB3	1.89	0.55
10:n:41:LEU:O	10:n:46:ARG:NH1	2.40	0.55
12:s:251:LEU:HD13	13:s:505:CLA:H122	1.89	0.55
13:A:1130:CLA:H121	13:L:1501:CLA:H201	1.88	0.55
13:G:1237:CLA:H152	16:V:4020:BCR:H16C	1.89	0.55
13:H:1023:CLA:H142	16:S:4018:BCR:H271	1.88	0.55
4:O:85:ILE:HB	4:O:98:HIS:HB3	1.89	0.55
13:T:1303:CLA:H41	12:b:282:VAL:HG22	1.87	0.55
12:Y:45:PHE:HE2	13:Z:519:CLA:HBA2	1.72	0.55
13:d:501:CLA:H72	13:d:501:CLA:HBB1	1.89	0.55
12:5:249:ILE:HG12	13:5:502:CLA:HAC1	1.88	0.55
13:G:1121:CLA:HHB	13:G:1801:CLA:HBC3	1.90	0.55
12:Z:34:GLN:OE1	13:Z:510:CLA:NC	2.40	0.55
12:b:146:LEU:HD21	13:b:506:CLA:HAB	1.89	0.55
12:q:45:PHE:HE2	13:r:519:CLA:HBA2	1.72	0.55
12:v:110:HIS:NE2	13:v:513:CLA:NB	2.54	0.55
13:e:1136:CLA:HBC1	17:n:5220:LHG:H282	1.88	0.54
9:m:18:VAL:HG22	9:m:84:LEU:HD21	1.88	0.54
12:1:45:PHE:HE2	13:2:519:CLA:HBA2	1.72	0.54
13:6:505:CLA:H12	16:6:524:BCR:H312	1.89	0.54
13:B:1023:CLA:H142	16:I:4018:BCR:H271	1.88	0.54
4:O:120:ARG:HH22	4:O:141:ALA:HB3	1.72	0.54
13:Z:510:CLA:HED2	13:Z:510:CLA:H2	1.89	0.54
13:r:510:CLA:HED2	13:r:510:CLA:H2	1.89	0.54
12:t:146:LEU:HD21	13:t:506:CLA:HAB	1.89	0.54
13:v:505:CLA:H12	16:v:524:BCR:H312	1.89	0.54
13:2:510:CLA:H2	13:2:510:CLA:HED2	1.89	0.54
10:V:41:LEU:O	10:V:46:ARG:NH1	2.40	0.54
3:g:63:LEU:HD12	3:g:66:ARG:HH21	1.71	0.54
13:H:1234:CLA:HMB2	13:H:1236:CLA:HED1	1.89	0.54
8:T:12:PRO:HB2	16:T:4013:BCR:H381	1.90	0.54
13:d:505:CLA:H111	13:d:517:CLA:HBB2	1.90	0.54
1:e:412:LEU:HD21	13:e:1104:CLA:H142	1.89	0.54
1:e:459:LEU:HB3	1:e:552:PHE:HB2	1.90	0.54
13:e:1130:CLA:H121	13:n:1501:CLA:H201	1.88	0.54
13:r:506:CLA:HBB2	13:r:507:CLA:H51	1.88	0.54
1:A:459:LEU:HB3	1:A:552:PHE:HB2	1.90	0.54
13:B:1204:CLA:H111	16:I:4018:BCR:HC21	1.90	0.54
13:B:1234:CLA:HMB2	13:B:1236:CLA:HED1	1.89	0.54
3:C:63:LEU:HD12	3:C:66:ARG:HH21	1.71	0.54
1:G:683:LEU:HD21	13:G:1126:CLA:H142	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:1202:CLA:H8	13:H:1221:CLA:HBA2	1.89	0.54
2:f:66:PHE:HZ	11:o:6:VAL:HG13	1.73	0.54
13:f:1234:CLA:HMB2	13:f:1236:CLA:HED1	1.89	0.54
8:J:12:PRO:HB2	16:J:4013:BCR:H381	1.90	0.54
12:4:146:LEU:HD21	13:4:506:CLA:HAB	1.89	0.54
12:Z:249:ILE:HG12	13:Z:502:CLA:HAC1	1.88	0.54
10:n:38:ARG:O	10:n:46:ARG:NH2	2.41	0.54
1:G:485:ASP:OD1	1:G:491:GLN:NE2	2.40	0.54
13:s:505:CLA:H43	16:s:524:BCR:HC7	1.90	0.54
13:v:505:CLA:H111	13:v:517:CLA:HBB2	1.90	0.54
1:A:182:LYS:NZ	17:A:5008:LHG:O2	2.41	0.54
1:A:216:GLN:HA	1:A:220:SER:HB2	1.90	0.54
1:A:616:ILE:HD12	13:A:1011:CLA:H122	1.90	0.54
13:A:1121:CLA:HHB	13:A:1801:CLA:HBC3	1.89	0.54
13:B:1209:CLA:HBB2	13:B:1217:CLA:H102	1.88	0.54
13:6:505:CLA:H111	13:6:517:CLA:HBB2	1.90	0.54
1:G:182:LYS:NZ	17:G:5008:LHG:O2	2.41	0.53
13:H:1226:CLA:H112	19:H:5002:LMG:H212	1.90	0.53
12:d:98:ILE:HG23	13:q:505:CLA:C11	2.38	0.53
1:e:683:LEU:HD21	13:e:1126:CLA:H142	1.90	0.53
13:e:1121:CLA:HHB	13:e:1801:CLA:HBC3	1.89	0.53
13:3:505:CLA:H43	16:3:524:BCR:HC7	1.90	0.53
12:4:272:TYR:HB3	12:4:300:ARG:HB2	1.90	0.53
1:G:589:PRO:HD3	2:H:561:GLY:HA2	1.90	0.53
2:H:66:PHE:HZ	11:W:6:VAL:HG13	1.73	0.53
13:d:505:CLA:H12	16:d:524:BCR:H312	1.89	0.53
2:f:61:VAL:HG21	13:f:1225:CLA:H42	1.90	0.53
2:f:603:GLN:HE21	2:f:732:LYS:HD3	1.72	0.53
4:h:39:VAL:HG22	4:h:49:VAL:HG22	1.89	0.53
13:q:509:CLA:H101	13:q:512:CLA:HBD	1.91	0.53
1:G:216:GLN:HA	1:G:220:SER:HB2	1.90	0.53
1:G:412:LEU:HD21	13:G:1104:CLA:H142	1.89	0.53
1:G:459:LEU:HB3	1:G:552:PHE:HB2	1.90	0.53
4:O:39:VAL:HG22	4:O:49:VAL:HG22	1.89	0.53
12:b:272:TYR:HB3	12:b:300:ARG:HB2	1.90	0.53
12:d:98:ILE:HG12	13:q:505:CLA:H13	1.89	0.53
12:t:272:TYR:HB3	12:t:300:ARG:HB2	1.90	0.53
1:A:752:TRP:NE1	13:A:1126:CLA:O1A	2.32	0.53
2:B:524:ALA:HB2	13:B:1235:CLA:HMA1	1.91	0.53
12:a:251:LEU:HD13	13:a:505:CLA:H122	1.89	0.53
12:c:272:TYR:HB3	12:c:300:ARG:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:182:LYS:NZ	17:e:5008:LHG:O2	2.41	0.53
1:e:616:ILE:HD12	13:e:1011:CLA:H122	1.90	0.53
1:A:708:LEU:HD21	13:A:1013:CLA:HED2	1.91	0.53
10:V:38:ARG:O	10:V:46:ARG:NH2	2.41	0.53
12:Y:26:LEU:HB3	13:Y:511:CLA:HMA1	1.90	0.53
1:A:589:PRO:HD3	2:B:561:GLY:HA2	1.90	0.53
2:B:66:PHE:HZ	11:M:6:VAL:HG13	1.73	0.53
12:5:272:TYR:HB3	12:5:300:ARG:HB2	1.91	0.53
13:f:1204:CLA:H111	16:k:4018:BCR:HC21	1.90	0.53
4:h:121:ARG:NH1	5:i:65:GLU:OE2	2.42	0.53
1:A:683:LEU:HD21	13:A:1126:CLA:H142	1.90	0.53
2:B:61:VAL:HG21	13:B:1225:CLA:H42	1.90	0.53
4:D:39:VAL:HG22	4:D:49:VAL:HG22	1.89	0.53
4:D:121:ARG:NH1	5:E:65:GLU:OE2	2.42	0.53
13:1:509:CLA:H101	13:1:512:CLA:HBD	1.90	0.53
12:3:251:LEU:HD13	13:3:505:CLA:H122	1.89	0.53
13:5:507:CLA:HED2	13:5:507:CLA:H2A	1.91	0.53
1:G:708:LEU:HD21	13:G:1013:CLA:HED2	1.90	0.53
17:G:5009:LHG:H171	12:Y:309:PHE:CZ	2.44	0.53
1:e:216:GLN:HA	1:e:220:SER:HB2	1.90	0.53
1:e:589:PRO:HD3	2:f:561:GLY:HA2	1.90	0.53
13:f:1226:CLA:H112	19:f:5002:LMG:H212	1.89	0.53
13:A:1137:CLA:H13	16:A:4007:BCR:H271	1.91	0.53
10:L:38:ARG:O	10:L:46:ARG:NH2	2.41	0.53
12:1:301:ALA:O	12:1:305:ASN:ND2	2.41	0.53
1:e:517:VAL:HG23	13:e:1133:CLA:HED3	1.91	0.53
17:e:5009:LHG:H171	12:q:309:PHE:CZ	2.44	0.53
13:B:1226:CLA:H112	19:B:5002:LMG:H212	1.90	0.53
2:H:61:VAL:HG21	13:H:1225:CLA:H42	1.91	0.53
13:H:1204:CLA:H111	16:S:4018:BCR:HC21	1.90	0.53
12:a:45:PHE:HE2	13:b:519:CLA:HAA2	1.74	0.53
13:a:505:CLA:H43	16:a:524:BCR:HC7	1.90	0.53
1:e:277:THR:HB	9:m:14:TRP:HB2	1.91	0.53
13:f:1239:CLA:HBA2	14:f:2002:PQN:H251	1.91	0.53
12:r:111:THR:HG21	16:r:522:BCR:H271	1.91	0.53
13:B:1214:CLA:HBA2	13:B:1223:CLA:HBB2	1.91	0.53
13:L:1501:CLA:H141	13:L:1503:CLA:HBC2	1.91	0.53
12:6:73:LEU:O	12:6:159:LYS:NZ	2.42	0.53
13:H:1227:CLA:H191	13:H:1236:CLA:H51	1.91	0.53
12:s:45:PHE:HE2	13:t:519:CLA:HAA2	1.74	0.53
13:B:1227:CLA:H191	13:B:1236:CLA:H51	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:1117:CLA:H8	13:G:1117:CLA:HAB	1.92	0.52
13:G:1137:CLA:H13	16:G:4007:BCR:H271	1.91	0.52
8:l:12:PRO:HB2	16:l:4013:BCR:H381	1.90	0.52
12:u:272:TYR:HB3	12:u:300:ARG:HB2	1.91	0.52
12:v:73:LEU:O	12:v:159:LYS:NZ	2.42	0.52
12:4:175:ARG:NH2	12:4:176:LEU:O	2.43	0.52
8:T:40:PRO:HD2	16:T:4015:BCR:H382	1.91	0.52
1:e:31:PRO:HB3	13:e:1101:CLA:HAC1	1.92	0.52
13:f:1227:CLA:H191	13:f:1236:CLA:H51	1.91	0.52
1:A:412:LEU:HD21	13:A:1104:CLA:H142	1.89	0.52
17:A:5009:LHG:H171	12:1:309:PHE:CZ	2.44	0.52
12:4:26:LEU:HB3	13:4:511:CLA:HMA1	1.92	0.52
13:H:1214:CLA:HBA2	13:H:1223:CLA:HBB2	1.91	0.52
10:V:137:LEU:HD13	16:n:4022:BCR:C24	2.39	0.52
12:Y:318:HIS:NE2	13:Y:505:CLA:NB	2.57	0.52
12:d:73:LEU:O	12:d:159:LYS:NZ	2.42	0.52
16:d:522:BCR:H10C	13:q:505:CLA:H161	1.91	0.52
13:A:1117:CLA:H8	13:A:1117:CLA:HAB	1.92	0.52
12:1:318:HIS:NE2	13:1:505:CLA:NB	2.57	0.52
12:2:111:THR:HG21	16:2:522:BCR:H271	1.91	0.52
4:O:121:ARG:NH1	5:Q:65:GLU:OE2	2.42	0.52
13:Y:509:CLA:H101	13:Y:512:CLA:HBD	1.90	0.52
13:Z:502:CLA:H12	13:Z:503:CLA:H42	1.92	0.52
12:b:175:ARG:NH2	12:b:176:LEU:O	2.43	0.52
13:c:507:CLA:HED2	13:c:507:CLA:H2A	1.91	0.52
13:e:1137:CLA:H13	16:e:4007:BCR:H271	1.91	0.52
12:t:175:ARG:NH2	12:t:176:LEU:O	2.43	0.52
8:J:40:PRO:HD2	16:J:4015:BCR:H382	1.91	0.52
17:L:5221:LHG:C34	13:f:1207:CLA:H142	2.40	0.52
12:3:45:PHE:HE2	13:4:519:CLA:HAA2	1.74	0.52
1:G:517:VAL:HG23	13:G:1133:CLA:HED3	1.91	0.52
13:B:1239:CLA:HBA2	14:B:2002:PQN:H251	1.91	0.52
13:L:1501:CLA:H122	16:L:4219:BCR:H372	1.92	0.52
1:G:31:PRO:HB3	13:G:1101:CLA:HAC1	1.91	0.52
2:B:339:ALA:HB2	16:B:4010:BCR:H372	1.92	0.52
1:G:277:THR:HB	9:U:14:TRP:HB2	1.90	0.52
2:H:585:ASN:HB2	13:H:1012:CLA:HBC2	1.91	0.52
13:V:1501:CLA:H141	13:V:1503:CLA:HBC2	1.91	0.52
12:q:301:ALA:O	12:q:305:ASN:ND2	2.41	0.52
12:q:318:HIS:NE2	13:q:505:CLA:NB	2.57	0.52
12:t:207:HIS:NE2	13:t:501:CLA:NB	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:26:LEU:HB3	13:u:511:CLA:HMA1	1.91	0.52
1:A:517:VAL:HG23	13:A:1133:CLA:HED3	1.91	0.52
2:B:117:TYR:HA	2:B:367:THR:HG22	1.92	0.52
13:2:502:CLA:H12	13:2:503:CLA:H42	1.92	0.52
12:5:282:VAL:HG23	12:5:283:THR:HG23	1.92	0.52
8:l:40:PRO:HD2	16:l:4015:BCR:H382	1.91	0.52
13:n:1501:CLA:H122	16:n:4219:BCR:H372	1.92	0.52
12:5:67:LEU:HD22	12:5:89:LEU:HD13	1.92	0.52
2:H:524:ALA:HB2	13:H:1235:CLA:HMA1	1.91	0.52
12:b:207:HIS:NE2	13:b:501:CLA:NB	2.58	0.52
13:n:1501:CLA:H141	13:n:1503:CLA:HBC2	1.91	0.52
1:A:31:PRO:HB3	13:A:1101:CLA:HAC1	1.92	0.52
2:B:585:ASN:HB2	13:B:1012:CLA:HBC2	1.91	0.52
12:1:19:ARG:NH1	13:1:511:CLA:OBD	2.43	0.52
12:1:148:PHE:HZ	13:1:516:CLA:HBC2	1.74	0.52
1:G:616:ILE:HD12	13:G:1011:CLA:H122	1.90	0.52
1:A:277:THR:HB	9:K:14:TRP:HB2	1.90	0.51
2:B:340:SER:HB3	13:B:1221:CLA:H2	1.92	0.51
12:Y:148:PHE:HZ	13:Y:516:CLA:HBC2	1.74	0.51
13:e:1013:CLA:H142	16:e:4011:BCR:H21C	1.92	0.51
13:f:1214:CLA:HBA2	13:f:1223:CLA:HBB2	1.91	0.51
13:A:1122:CLA:HBB2	17:A:5003:LHG:HC82	1.92	0.51
2:H:422:LEU:HD13	2:H:532:LEU:HA	1.93	0.51
12:Z:64:LEU:HD13	12:Z:67:LEU:HD12	1.93	0.51
12:Z:148:PHE:HD2	13:Z:512:CLA:H3A	1.76	0.51
1:e:429:ASP:O	1:e:433:ASN:ND2	2.44	0.51
12:4:207:HIS:NE2	13:4:501:CLA:NB	2.58	0.51
17:G:5009:LHG:H241	9:U:14:TRP:HB3	1.93	0.51
12:d:145:HIS:NE2	13:d:512:CLA:NA	2.59	0.51
2:f:524:ALA:HB2	13:f:1235:CLA:HMA1	1.91	0.51
12:q:148:PHE:HZ	13:q:516:CLA:HBC2	1.74	0.51
12:Z:111:THR:HG21	16:Z:522:BCR:H271	1.91	0.51
2:f:340:SER:HB3	13:f:1221:CLA:H2	1.92	0.51
2:f:422:LEU:HD13	2:f:532:LEU:HA	1.93	0.51
2:f:585:ASN:HB2	13:f:1012:CLA:HBC2	1.91	0.51
12:v:145:HIS:NE2	13:v:512:CLA:NA	2.59	0.51
1:A:544:PHE:HZ	16:L:4219:BCR:H332	1.76	0.51
1:A:598:SER:OG	1:A:601:ASP:OD2	2.29	0.51
12:6:145:HIS:NE2	13:6:512:CLA:NA	2.59	0.51
17:G:5005:LHG:HC61	16:Z:521:BCR:HC22	1.92	0.51
13:H:1229:CLA:HBB2	16:H:4014:BCR:HC41	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:517:CLA:HED2	13:t:517:CLA:H2A	1.92	0.51
12:u:112:PHE:HB2	12:v:326:MET:HE3	1.93	0.51
12:u:282:VAL:HG23	12:u:283:THR:HG23	1.92	0.51
13:u:507:CLA:HED2	13:u:507:CLA:H2A	1.91	0.51
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.93	0.51
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.93	0.51
2:H:69:ALA:HB2	2:H:135:LEU:HB2	1.93	0.51
13:H:1239:CLA:HBA2	14:H:2002:PQN:H251	1.91	0.51
13:r:502:CLA:H12	13:r:503:CLA:H42	1.92	0.51
1:A:370:ILE:HD11	13:A:1119:CLA:H71	1.93	0.51
13:V:1501:CLA:H122	16:V:4219:BCR:H372	1.92	0.51
12:b:233:VAL:HG11	16:b:524:BCR:HC22	1.93	0.51
12:c:112:PHE:HB2	12:d:326:MET:HE3	1.93	0.51
13:e:1117:CLA:H8	13:e:1117:CLA:HAB	1.92	0.51
17:e:5008:LHG:H261	17:e:5008:LHG:HC92	1.93	0.51
13:r:505:CLA:H43	16:r:524:BCR:HC7	1.93	0.51
13:B:1229:CLA:HBB2	16:B:4014:BCR:HC41	1.92	0.51
12:6:52:TRP:CZ3	17:G:5009:LHG:HC11	2.46	0.51
16:6:522:BCR:HC41	12:Y:258:TYR:HB2	1.93	0.51
2:H:339:ALA:HB2	16:H:4010:BCR:H372	1.92	0.51
2:H:340:SER:HB3	13:H:1221:CLA:H2	1.92	0.51
12:a:53:LEU:HD21	12:a:83:VAL:HG11	1.93	0.51
1:e:370:ILE:HD11	13:e:1119:CLA:H71	1.93	0.51
1:e:708:LEU:HD21	13:e:1013:CLA:HED2	1.90	0.51
13:e:1122:CLA:HBB2	17:e:5003:LHG:HC82	1.92	0.51
13:e:1101:CLA:H91	16:l:4013:BCR:H21C	1.93	0.51
2:f:117:TYR:HA	2:f:367:THR:HG22	1.92	0.51
2:f:339:ALA:HB2	16:f:4010:BCR:H372	1.92	0.51
12:4:233:VAL:HG11	16:4:524:BCR:HC22	1.92	0.51
12:4:263:ASN:HD21	12:4:265:LEU:HB3	1.76	0.51
1:G:429:ASP:O	1:G:433:ASN:ND2	2.44	0.51
5:i:53:ASP:OD1	5:i:53:ASP:N	2.44	0.51
12:2:64:LEU:HD13	12:2:67:LEU:HD12	1.93	0.51
1:G:607:LEU:HD21	13:G:1128:CLA:HBC1	1.94	0.51
2:H:117:TYR:HA	2:H:367:THR:HG22	1.92	0.51
7:S:20:LEU:HD12	17:n:5221:LHG:H172	1.92	0.51
12:Y:148:PHE:HE2	13:Y:512:CLA:HHB	1.75	0.51
13:b:517:CLA:HED2	13:b:517:CLA:H2A	1.92	0.51
16:d:522:BCR:H323	13:q:505:CLA:H192	1.92	0.51
12:u:146:LEU:HD22	12:u:214:LEU:HD22	1.93	0.51
1:A:485:ASP:OD1	1:A:491:GLN:NE2	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1237:CLA:H141	10:L:85:LEU:HD11	1.93	0.50
12:1:148:PHE:HE2	13:1:512:CLA:HHB	1.76	0.50
13:G:1122:CLA:HBB2	17:G:5003:LHG:HC82	1.92	0.50
12:b:307:HIS:NE2	13:b:502:CLA:ND	2.60	0.50
12:c:282:VAL:HG23	12:c:283:THR:HG23	1.92	0.50
1:e:86:TRP:HA	13:e:1105:CLA:HBB2	1.93	0.50
17:e:5005:LHG:HC61	16:r:521:BCR:HC22	1.92	0.50
13:q:501:CLA:C4D	13:q:503:CLA:H2	2.41	0.50
17:L:5221:LHG:H121	13:f:1207:CLA:HMA2	1.93	0.50
13:4:517:CLA:H2A	13:4:517:CLA:HED2	1.92	0.50
12:5:112:PHE:HB2	12:6:326:MET:HE3	1.93	0.50
12:Y:301:ALA:O	12:Y:305:ASN:ND2	2.41	0.50
13:Y:501:CLA:C4D	13:Y:503:CLA:H2	2.41	0.50
12:a:146:LEU:HD22	12:a:214:LEU:HD22	1.94	0.50
12:b:263:ASN:HD21	12:b:265:LEU:HB3	1.76	0.50
1:e:549:ILE:HD12	13:e:1011:CLA:H172	1.94	0.50
2:f:69:ALA:HB2	2:f:135:LEU:HB2	1.93	0.50
12:t:263:ASN:HD21	12:t:265:LEU:HB3	1.76	0.50
13:A:1101:CLA:H91	16:J:4013:BCR:H21C	1.93	0.50
17:A:5005:LHG:HC61	16:2:521:BCR:HC22	1.92	0.50
12:4:307:HIS:NE2	13:4:502:CLA:ND	2.60	0.50
12:d:109:PHE:HB2	13:q:505:CLA:CAA	2.42	0.50
1:e:485:ASP:OD1	1:e:491:GLN:NE2	2.40	0.50
1:e:544:PHE:HZ	16:n:4219:BCR:H332	1.76	0.50
17:e:5009:LHG:H241	9:m:14:TRP:HB3	1.93	0.50
12:t:51:SER:HB2	12:u:279:LYS:HG2	1.94	0.50
12:u:110:HIS:NE2	13:u:513:CLA:NB	2.60	0.50
1:A:429:ASP:O	1:A:433:ASN:ND2	2.44	0.50
13:1:501:CLA:C4D	13:1:503:CLA:H2	2.41	0.50
13:Z:505:CLA:H43	16:Z:524:BCR:HC7	1.93	0.50
1:e:598:SER:OG	1:e:601:ASP:OD2	2.29	0.50
1:e:607:LEU:HD21	13:e:1128:CLA:HBC1	1.93	0.50
13:G:1013:CLA:H142	16:G:4011:BCR:H21C	1.92	0.50
20:H:1852:SQD:O3	10:n:3:GLN:NE2	2.40	0.50
13:Y:502:CLA:HBA2	13:Y:503:CLA:H171	1.93	0.50
13:f:1229:CLA:HBB2	16:f:4014:BCR:HC41	1.92	0.50
13:2:505:CLA:H43	16:2:524:BCR:HC7	1.93	0.50
12:5:110:HIS:NE2	13:5:513:CLA:NB	2.60	0.50
12:5:146:LEU:HD22	12:5:214:LEU:HD22	1.93	0.50
1:G:336:ILE:O	1:G:340:HIS:ND1	2.37	0.50
2:H:710:LEU:HD23	19:H:5002:LMG:H362	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:1237:CLA:H141	10:n:85:LEU:HD11	1.93	0.50
1:A:16:VAL:O	1:A:186:LYS:NZ	2.43	0.50
12:4:51:SER:HB2	12:5:279:LYS:HG2	1.94	0.50
12:4:256:ALA:HB2	13:4:501:CLA:H43	1.94	0.50
13:G:1101:CLA:H91	16:T:4013:BCR:H21C	1.93	0.50
17:G:5008:LHG:H261	17:G:5008:LHG:HC92	1.93	0.50
12:q:148:PHE:HE2	13:q:512:CLA:HHB	1.76	0.50
12:r:148:PHE:HD2	13:r:512:CLA:H3A	1.76	0.50
12:u:67:LEU:HD22	12:u:89:LEU:HD13	1.92	0.50
1:G:544:PHE:HZ	16:V:4219:BCR:H332	1.76	0.50
12:c:146:LEU:HD22	12:c:214:LEU:HD22	1.92	0.50
2:B:710:LEU:HD23	19:B:5002:LMG:H362	1.93	0.50
1:G:86:TRP:HA	13:G:1105:CLA:HBB2	1.93	0.50
2:H:611:GLU:OE2	6:R:36:ARG:NH1	2.44	0.50
4:O:9:PRO:HD2	4:O:57:LEU:HD13	1.94	0.50
12:b:140:LEU:HA	12:b:222:ILE:HG22	1.94	0.50
13:c:501:CLA:C4D	13:c:503:CLA:H2	2.42	0.50
12:d:105:ALA:O	13:q:505:CLA:HBA1	2.11	0.50
2:f:161:PHE:CE2	20:f:1852:SQD:H441	2.47	0.50
2:f:429:LEU:HD11	13:f:1235:CLA:HMB2	1.94	0.50
12:t:233:VAL:HG11	16:t:524:BCR:HC22	1.93	0.50
1:A:549:ILE:HD12	13:A:1011:CLA:H172	1.94	0.49
12:2:148:PHE:HD2	13:2:512:CLA:H3A	1.76	0.49
12:3:53:LEU:HD21	12:3:83:VAL:HG11	1.93	0.49
12:4:140:LEU:HA	12:4:222:ILE:HG22	1.94	0.49
1:G:598:SER:OG	1:G:601:ASP:OD2	2.29	0.49
12:c:67:LEU:HD22	12:c:89:LEU:HD13	1.92	0.49
12:d:276:LEU:HD11	12:d:300:ARG:HG2	1.94	0.49
13:u:501:CLA:C4D	13:u:503:CLA:H2	2.42	0.49
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.94	0.49
1:G:16:VAL:O	1:G:186:LYS:NZ	2.44	0.49
1:G:66:GLU:HG3	1:G:187:LEU:HB2	1.95	0.49
20:H:1852:SQD:H242	17:e:5002:LHG:H261	1.94	0.49
12:Y:19:ARG:NH1	13:Y:511:CLA:OBD	2.43	0.49
12:b:256:ALA:HB2	13:b:501:CLA:H43	1.94	0.49
4:h:9:PRO:HD2	4:h:57:LEU:HD13	1.94	0.49
1:A:86:TRP:HA	13:A:1105:CLA:HBB2	1.93	0.49
1:A:164:GLY:HA2	17:A:5007:LHG:H332	1.94	0.49
13:A:1013:CLA:H142	16:A:4011:BCR:H21C	1.92	0.49
17:A:5009:LHG:H241	9:K:14:TRP:HB3	1.93	0.49
13:3:510:CLA:H43	13:3:510:CLA:HED3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:549:ILE:HD12	13:G:1011:CLA:H172	1.94	0.49
12:b:51:SER:HB2	12:c:279:LYS:HG2	1.94	0.49
12:b:146:LEU:HD22	12:b:214:LEU:HD22	1.94	0.49
3:g:22:PRO:HG2	3:g:23:LEU:HD12	1.94	0.49
12:r:64:LEU:HD13	12:r:67:LEU:HD12	1.93	0.49
12:t:307:HIS:NE2	13:t:502:CLA:ND	2.60	0.49
2:B:73:ASN:HB2	2:B:76:GLN:HB2	1.94	0.49
13:B:1229:CLA:HAB	16:B:4014:BCR:H323	1.95	0.49
4:D:9:PRO:HD2	4:D:57:LEU:HD13	1.94	0.49
13:1:502:CLA:HBA2	13:1:503:CLA:H171	1.93	0.49
1:G:86:TRP:NE1	13:G:1126:CLA:OBD	2.46	0.49
1:G:370:ILE:HD11	13:G:1119:CLA:H71	1.93	0.49
13:G:1237:CLA:H141	10:V:85:LEU:HD11	1.93	0.49
2:H:161:PHE:CE2	20:H:1852:SQD:H441	2.47	0.49
16:d:522:BCR:H21C	13:q:518:CLA:O1D	2.13	0.49
12:s:53:LEU:HD21	12:s:83:VAL:HG11	1.93	0.49
12:s:146:LEU:HD22	12:s:214:LEU:HD22	1.93	0.49
12:t:256:ALA:HB2	13:t:501:CLA:H43	1.94	0.49
12:v:276:LEU:HD11	12:v:300:ARG:HG2	1.94	0.49
2:B:321:GLY:O	2:B:325:THR:OG1	2.28	0.49
3:N:15:THR:HG22	3:N:28:MET:HG3	1.94	0.49
12:d:102:VAL:HG22	13:q:505:CLA:C6	2.41	0.49
1:e:164:GLY:HA2	17:e:5007:LHG:H332	1.94	0.49
13:f:1229:CLA:HAB	16:f:4014:BCR:H323	1.95	0.49
12:q:307:HIS:NE2	13:q:502:CLA:ND	2.61	0.49
1:A:381:HIS:ND1	13:A:1116:CLA:OBD	2.46	0.49
1:A:607:LEU:HD21	13:A:1128:CLA:HBC1	1.94	0.49
12:1:307:HIS:NE2	13:1:502:CLA:ND	2.61	0.49
13:5:501:CLA:C4D	13:5:503:CLA:H2	2.42	0.49
12:Z:145:HIS:NE2	13:Z:512:CLA:NA	2.60	0.49
12:a:267:TYR:O	12:a:300:ARG:NH2	2.41	0.49
12:b:276:LEU:HB3	12:b:286:PHE:HB3	1.95	0.49
2:f:710:LEU:HD23	19:f:5002:LMG:H362	1.93	0.49
17:A:5008:LHG:HC92	17:A:5008:LHG:H261	1.93	0.49
2:B:161:PHE:CE2	20:B:1852:SQD:H441	2.47	0.49
12:Y:307:HIS:NE2	13:Y:502:CLA:ND	2.61	0.49
13:Y:501:CLA:H193	13:Y:507:CLA:HBB1	1.95	0.49
12:c:110:HIS:NE2	13:c:513:CLA:NB	2.60	0.49
1:e:381:HIS:ND1	13:e:1116:CLA:OBD	2.46	0.49
1:A:577:LYS:NZ	2:B:673:GLU:OE2	2.36	0.49
2:B:722:ALA:HB2	13:B:1224:CLA:HBB1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:251:LEU:HD13	13:2:505:CLA:H122	1.95	0.49
12:3:146:LEU:HD22	12:3:214:LEU:HD22	1.94	0.49
12:6:276:LEU:HD11	12:6:300:ARG:HG2	1.94	0.49
1:G:742:HIS:CE1	13:G:1140:CLA:NA	2.81	0.49
13:a:510:CLA:H43	13:a:510:CLA:HED3	1.94	0.49
17:A:5009:LHG:H291	13:K:1103:CLA:HED1	1.95	0.49
9:K:29:ALA:HA	9:K:32:ILE:HG12	1.95	0.49
2:H:722:ALA:HB2	13:H:1224:CLA:HBB1	1.95	0.49
13:H:1229:CLA:HAB	16:H:4014:BCR:H323	1.95	0.49
14:H:2002:PQN:H242	16:H:4017:BCR:H17C	1.95	0.49
13:e:1119:CLA:H61	16:e:4007:BCR:H352	1.95	0.49
10:n:33:ALA:HB1	13:n:1501:CLA:HAC1	1.94	0.49
12:r:145:HIS:NE2	13:r:512:CLA:NA	2.60	0.49
12:t:140:LEU:HA	12:t:222:ILE:HG22	1.94	0.49
1:A:66:GLU:HG3	1:A:187:LEU:HB2	1.95	0.48
3:C:15:THR:HG22	3:C:28:MET:HG3	1.94	0.48
20:L:5216:SQD:C3	2:f:4:LYS:HZ1	2.25	0.48
12:1:67:LEU:HD22	12:1:89:LEU:HD13	1.95	0.48
12:2:49:GLU:HB3	12:2:64:LEU:HD22	1.95	0.48
1:G:16:VAL:HA	1:G:185:PRO:HA	1.96	0.48
1:G:381:HIS:ND1	13:G:1116:CLA:OBD	2.46	0.48
13:G:1118:CLA:HBB1	16:U:4104:BCR:H342	1.95	0.48
12:Y:67:LEU:HD22	12:Y:89:LEU:HD13	1.95	0.48
12:d:101:ALA:HB1	13:q:505:CLA:CAB	2.42	0.48
1:e:16:VAL:O	1:e:186:LYS:NZ	2.43	0.48
1:e:16:VAL:HA	1:e:185:PRO:HA	1.95	0.48
2:f:73:ASN:HB2	2:f:76:GLN:HB2	1.94	0.48
13:f:1220:CLA:HAA1	16:f:4009:BCR:H16C	1.95	0.48
13:s:510:CLA:H43	13:s:510:CLA:HED3	1.94	0.48
12:v:331:ARG:NH2	20:v:822:SQD:O8	2.46	0.48
13:A:1103:CLA:H3A	13:A:1103:CLA:HBA1	1.54	0.48
2:B:429:LEU:HD11	13:B:1235:CLA:HMB2	1.94	0.48
13:1:501:CLA:H193	13:1:507:CLA:HBB1	1.95	0.48
12:4:276:LEU:HG	12:4:300:ARG:HD2	1.95	0.48
12:5:40:PHE:HE2	13:6:519:CLA:HBA1	1.77	0.48
17:G:5009:LHG:H291	13:U:1103:CLA:HED1	1.95	0.48
2:H:15:ASP:OD2	2:H:19:ARG:NH2	2.46	0.48
3:N:22:PRO:HG2	3:N:23:LEU:HD12	1.94	0.48
13:a:517:CLA:HBA1	13:a:517:CLA:H3A	1.50	0.48
1:e:377:ILE:HG21	13:e:1117:CLA:H201	1.95	0.48
13:e:1101:CLA:HHC	13:e:1101:CLA:HBB1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:67:VAL:HG21	15:g:3002:SF4:S2	2.53	0.48
9:m:29:ALA:HA	9:m:32:ILE:HG12	1.95	0.48
12:s:148:PHE:HZ	13:s:516:CLA:HBC2	1.78	0.48
13:s:507:CLA:H112	16:s:524:BCR:H362	1.95	0.48
1:A:742:HIS:CE1	13:A:1140:CLA:NA	2.81	0.48
2:B:96:PHE:HB2	7:I:1:MET:HE1	1.96	0.48
14:B:2002:PQN:H242	16:B:4017:BCR:H17C	1.95	0.48
1:G:377:ILE:HG21	13:G:1117:CLA:H201	1.95	0.48
2:H:429:LEU:HD11	13:H:1235:CLA:HMB2	1.94	0.48
13:H:1220:CLA:HAA1	16:H:4009:BCR:H16C	1.95	0.48
13:H:1227:CLA:HAB	13:H:1236:CLA:HBB2	1.96	0.48
10:V:33:ALA:HB1	13:V:1501:CLA:HAC1	1.94	0.48
12:r:49:GLU:HB3	12:r:64:LEU:HD22	1.96	0.48
13:A:1118:CLA:HBB1	16:K:4104:BCR:H342	1.96	0.48
13:B:1226:CLA:H42	19:B:5002:LMG:H302	1.95	0.48
10:L:33:ALA:HB1	13:L:1501:CLA:HAC1	1.94	0.48
13:1:505:CLA:HAB	12:v:101:ALA:HB1	1.95	0.48
2:H:73:ASN:HB2	2:H:76:GLN:HB2	1.94	0.48
3:N:67:VAL:HG21	15:N:3002:SF4:S2	2.53	0.48
12:a:148:PHE:HZ	13:a:516:CLA:HBC2	1.78	0.48
13:a:507:CLA:H112	16:a:524:BCR:H362	1.95	0.48
12:c:40:PHE:HE2	13:d:519:CLA:HBA1	1.77	0.48
1:e:86:TRP:NE1	13:e:1126:CLA:OBD	2.46	0.48
2:f:210:ASP:OD1	2:f:210:ASP:N	2.46	0.48
3:g:15:THR:HG22	3:g:28:MET:HG3	1.94	0.48
13:q:501:CLA:HMB2	16:q:524:BCR:H23C	1.96	0.48
2:B:15:ASP:OD2	2:B:19:ARG:NH2	2.46	0.48
2:B:326:LEU:HD13	2:B:332:PHE:HD2	1.77	0.48
12:4:282:VAL:HG23	12:4:283:THR:HG23	1.95	0.48
13:H:1207:CLA:HMA2	17:n:5221:LHG:H121	1.94	0.48
13:Y:501:CLA:HMB2	16:Y:524:BCR:H23C	1.96	0.48
12:Z:49:GLU:HB3	12:Z:64:LEU:HD22	1.96	0.48
12:d:102:VAL:CG2	13:q:505:CLA:H8	2.43	0.48
14:f:2002:PQN:H242	16:f:4017:BCR:H17C	1.95	0.48
13:q:502:CLA:HBA2	13:q:503:CLA:H171	1.93	0.48
12:s:267:TYR:O	12:s:300:ARG:NH2	2.41	0.48
12:1:130:PHE:HA	12:1:137:GLN:HG2	1.96	0.48
1:e:66:GLU:HG3	1:e:187:LEU:HB2	1.95	0.48
1:e:742:HIS:CE1	13:e:1140:CLA:NA	2.81	0.48
2:f:15:ASP:OD2	2:f:19:ARG:NH2	2.46	0.48
13:f:1226:CLA:H42	19:f:5002:LMG:H302	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:m:70:LEU:HD22	13:m:1401:CLA:HMC3	1.95	0.48
12:s:34:GLN:OE1	13:s:510:CLA:NC	2.47	0.48
13:B:1219:CLA:H142	17:B:1842:LHG:C36	2.44	0.48
13:1:501:CLA:HMB2	16:1:524:BCR:H23C	1.96	0.48
13:1:512:CLA:H3A	13:1:512:CLA:HBA1	1.62	0.48
12:3:34:GLN:OE1	13:3:510:CLA:NC	2.47	0.48
12:3:148:PHE:HZ	13:3:516:CLA:HBC2	1.78	0.48
12:4:146:LEU:HD22	12:4:214:LEU:HD22	1.94	0.48
2:H:631:LEU:O	2:H:647:SER:OG	2.29	0.48
13:H:1210:CLA:H2	13:H:1210:CLA:H62	1.64	0.48
12:Z:251:LEU:HD13	13:Z:505:CLA:H122	1.95	0.48
12:d:301:ALA:O	12:d:305:ASN:ND2	2.43	0.48
2:f:96:PHE:HB2	7:k:1:MET:HE1	1.96	0.48
2:f:456:GLU:OE1	6:j:68:HIS:ND1	2.47	0.48
13:f:1203:CLA:H191	19:f:5002:LMG:H252	1.96	0.48
12:q:67:LEU:HD22	12:q:89:LEU:HD13	1.95	0.48
13:q:516:CLA:HBA1	13:q:516:CLA:H3A	1.51	0.48
12:r:330:PHE:HB3	20:r:822:SQD:H82	1.96	0.48
1:A:220:SER:O	1:A:224:ASN:HB2	2.14	0.48
13:A:1140:CLA:HBA2	17:A:5001:LHG:H171	1.96	0.48
3:C:67:VAL:HG21	15:C:3002:SF4:S2	2.53	0.48
12:Z:200:LEU:HG	12:Z:265:LEU:HD11	1.96	0.48
12:b:59:MET:HB2	12:b:271:PHE:HA	1.96	0.48
12:d:61:GLU:HG3	12:d:292:LEU:HD13	1.96	0.48
13:e:1118:CLA:HBB1	16:m:4104:BCR:H342	1.95	0.48
17:e:5009:LHG:H291	13:m:1103:CLA:HED1	1.95	0.48
12:u:40:PHE:HE2	13:v:519:CLA:HBA1	1.77	0.48
12:2:145:HIS:NE2	13:2:512:CLA:NA	2.60	0.48
1:G:164:GLY:HA2	17:G:5007:LHG:H332	1.94	0.48
13:G:1140:CLA:HBA2	17:G:5001:LHG:H171	1.96	0.48
2:H:456:GLU:OE1	6:R:68:HIS:ND1	2.47	0.48
9:U:29:ALA:HA	9:U:32:ILE:HG12	1.95	0.48
12:Z:330:PHE:HB3	20:Z:822:SQD:H82	1.96	0.48
12:a:34:GLN:OE1	13:a:510:CLA:NC	2.47	0.48
12:b:276:LEU:HG	12:b:300:ARG:HD2	1.95	0.48
12:b:282:VAL:HG23	12:b:283:THR:HG23	1.95	0.48
13:q:501:CLA:H193	13:q:507:CLA:HBB1	1.95	0.48
13:r:511:CLA:H72	12:s:333:VAL:HG13	1.96	0.48
12:t:146:LEU:HD22	12:t:214:LEU:HD22	1.94	0.48
13:B:1227:CLA:HAB	13:B:1236:CLA:HBB2	1.96	0.48
13:3:509:CLA:HBD	13:3:509:CLA:H121	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:305:ASN:HB3	16:5:521:BCR:HC8	1.96	0.48
1:G:220:SER:O	1:G:224:ASN:HB2	2.14	0.48
13:H:1219:CLA:H142	17:H:1842:LHG:C36	2.44	0.48
2:f:722:ALA:HB2	13:f:1224:CLA:HBB1	1.95	0.48
12:r:251:LEU:HD23	13:r:501:CLA:H142	1.96	0.48
12:t:282:VAL:HG23	12:t:283:THR:HG23	1.95	0.48
12:2:301:ALA:O	12:2:305:ASN:ND2	2.41	0.47
12:4:59:MET:HB2	12:4:271:PHE:HA	1.96	0.47
12:4:276:LEU:HB3	12:4:286:PHE:HB3	1.95	0.47
13:a:509:CLA:HBD	13:a:509:CLA:H121	1.96	0.47
13:f:1235:CLA:H172	16:j:4016:BCR:H272	1.96	0.47
13:s:509:CLA:HBD	13:s:509:CLA:H121	1.96	0.47
12:t:59:MET:HB2	12:t:271:PHE:HA	1.96	0.47
12:t:276:LEU:HG	12:t:300:ARG:HD2	1.95	0.47
1:A:86:TRP:NE1	13:A:1126:CLA:OBD	2.46	0.47
12:2:330:PHE:HB3	20:2:822:SQD:H82	1.96	0.47
13:G:1119:CLA:H61	16:G:4007:BCR:H352	1.95	0.47
12:d:98:ILE:HG23	13:q:505:CLA:H112	1.96	0.47
13:e:1110:CLA:HBA2	13:e:1110:CLA:H3A	1.56	0.47
1:A:377:ILE:HG21	13:A:1117:CLA:H201	1.95	0.47
2:B:4:LYS:HZ1	20:V:5216:SQD:C3	2.26	0.47
13:B:1207:CLA:H142	17:V:5221:LHG:C34	2.41	0.47
13:3:502:CLA:HBD	13:3:503:CLA:H43	1.97	0.47
13:H:1222:CLA:H52	13:H:1234:CLA:H11	1.97	0.47
12:Z:148:PHE:CD2	13:Z:512:CLA:H3A	2.50	0.47
12:a:274:ALA:HB3	12:a:290:VAL:HG22	1.97	0.47
12:d:331:ARG:NH2	20:d:822:SQD:O8	2.46	0.47
13:e:1106:CLA:H3A	13:e:1106:CLA:HBA2	1.61	0.47
12:u:305:ASN:HB3	16:u:521:BCR:HC8	1.96	0.47
13:A:1119:CLA:H61	16:A:4007:BCR:H352	1.95	0.47
12:2:200:LEU:HG	12:2:265:LEU:HD11	1.96	0.47
12:6:331:ARG:NH2	20:6:822:SQD:O8	2.46	0.47
2:H:96:PHE:HB2	7:S:1:MET:HE1	1.96	0.47
9:U:70:LEU:HD22	13:U:1401:CLA:HMC3	1.95	0.47
13:r:506:CLA:H62	13:r:506:CLA:H41	1.71	0.47
7:I:20:LEU:HD12	17:V:5221:LHG:H172	1.95	0.47
13:G:1122:CLA:H91	13:G:1122:CLA:H111	1.77	0.47
2:H:481:ALA:HA	2:H:486:THR:HG21	1.97	0.47
13:H:1226:CLA:H42	19:H:5002:LMG:H302	1.95	0.47
13:Z:518:CLA:H61	13:Z:518:CLA:H41	1.62	0.47
1:e:220:SER:O	1:e:224:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:658:LEU:HD13	13:e:1022:CLA:HED1	1.96	0.47
13:e:1140:CLA:HBA2	17:e:5001:LHG:H171	1.96	0.47
13:f:1219:CLA:H142	17:f:1842:LHG:C36	2.44	0.47
12:t:276:LEU:HB3	12:t:286:PHE:HB3	1.95	0.47
13:B:1220:CLA:HAA1	16:B:4009:BCR:H16C	1.95	0.47
13:B:1235:CLA:H172	16:F:4016:BCR:H272	1.96	0.47
13:1:516:CLA:H3A	13:1:516:CLA:HBA1	1.51	0.47
13:3:507:CLA:H112	16:3:524:BCR:H362	1.95	0.47
13:4:509:CLA:HBD	13:4:509:CLA:H121	1.96	0.47
12:5:221:HIS:CE1	13:5:506:CLA:NA	2.83	0.47
12:6:200:LEU:HG	12:6:265:LEU:HD11	1.96	0.47
13:a:502:CLA:HBD	13:a:503:CLA:H43	1.97	0.47
16:d:522:BCR:H352	12:q:315:LEU:HD21	1.96	0.47
13:A:1108:CLA:HBA2	13:A:1108:CLA:H3A	1.71	0.47
2:B:301:ILE:HG21	13:B:1221:CLA:HAC1	1.97	0.47
13:B:1207:CLA:HMA2	17:V:5221:LHG:H121	1.95	0.47
10:L:155:LEU:HD22	7:k:13:ILE:HD11	1.96	0.47
12:6:61:GLU:HG3	12:6:292:LEU:HD13	1.96	0.47
1:G:658:LEU:HD13	13:G:1022:CLA:HED1	1.96	0.47
13:H:1203:CLA:H191	19:H:5002:LMG:H252	1.96	0.47
13:H:1215:CLA:H13	13:H:1221:CLA:H162	1.97	0.47
13:H:1235:CLA:H172	16:R:4016:BCR:H272	1.96	0.47
13:Z:501:CLA:C4D	13:Z:503:CLA:H2	2.45	0.47
13:Z:511:CLA:H72	12:a:333:VAL:HG13	1.96	0.47
16:a:524:BCR:H15C	16:a:524:BCR:H351	1.78	0.47
13:b:509:CLA:HBD	13:b:509:CLA:H121	1.96	0.47
12:c:221:HIS:CE1	13:c:506:CLA:NA	2.83	0.47
1:e:522:GLY:HA2	1:e:536:PRO:HB3	1.97	0.47
13:e:1116:CLA:HBA2	13:e:1116:CLA:H3A	1.46	0.47
13:f:1227:CLA:HAB	13:f:1236:CLA:HBB2	1.96	0.47
12:r:200:LEU:HG	12:r:265:LEU:HD11	1.96	0.47
12:r:251:LEU:HD13	13:r:505:CLA:H122	1.95	0.47
12:u:221:HIS:CE1	13:u:506:CLA:NA	2.83	0.47
13:A:1139:CLA:H41	13:A:1139:CLA:H61	1.62	0.47
13:B:1203:CLA:H191	19:B:5002:LMG:H252	1.96	0.47
7:I:1:MET:HB3	7:I:1:MET:HE2	1.81	0.47
9:K:70:LEU:HD22	13:K:1401:CLA:HMC3	1.95	0.47
13:6:517:CLA:HBA1	13:6:517:CLA:H3A	1.50	0.47
13:G:1101:CLA:HHC	13:G:1101:CLA:HBB1	1.96	0.47
12:c:305:ASN:HB3	16:c:521:BCR:HC8	1.96	0.47
16:c:522:BCR:H15C	16:c:522:BCR:H351	1.75	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:1215:CLA:H13	13:f:1221:CLA:H162	1.97	0.47
13:f:1222:CLA:H52	13:f:1234:CLA:H11	1.97	0.47
4:h:21:SER:HA	4:h:24:THR:HB	1.97	0.47
13:v:519:CLA:HED2	13:v:519:CLA:H2A	1.97	0.47
4:D:21:SER:HA	4:D:24:THR:HB	1.97	0.47
16:1:522:BCR:H351	16:1:522:BCR:H15C	1.80	0.47
12:4:230:THR:HG23	12:4:234:LEU:HD12	1.97	0.47
13:H:1207:CLA:H142	17:n:5221:LHG:C34	2.44	0.47
12:q:19:ARG:NH1	13:q:511:CLA:OBD	2.43	0.47
12:q:130:PHE:HA	12:q:137:GLN:HG2	1.96	0.47
12:s:143:GLY:HA3	12:s:222:ILE:HG13	1.97	0.47
13:s:502:CLA:HBD	13:s:503:CLA:H43	1.96	0.47
13:B:1220:CLA:HED3	13:B:1220:CLA:H2A	1.97	0.47
12:6:177:VAL:HG21	12:6:204:VAL:HG21	1.96	0.47
1:G:441:VAL:HG11	13:G:1119:CLA:H192	1.97	0.47
13:G:1130:CLA:HMC1	13:V:1502:CLA:H122	1.97	0.47
12:Y:281:GLY:O	13:Y:519:CLA:HED1	2.15	0.47
2:f:481:ALA:HA	2:f:486:THR:HG21	1.97	0.47
12:q:281:GLY:O	13:q:519:CLA:HED1	2.15	0.47
13:q:510:CLA:H61	13:q:510:CLA:H41	1.61	0.47
13:A:1101:CLA:HBB1	13:A:1101:CLA:HHC	1.96	0.46
12:2:148:PHE:CD2	13:2:512:CLA:H3A	2.50	0.46
7:S:29:LEU:HB3	20:n:5216:SQD:H241	1.97	0.46
12:b:230:THR:HG23	12:b:234:LEU:HD12	1.97	0.46
13:e:1013:CLA:H203	13:e:1140:CLA:H51	1.97	0.46
12:q:111:THR:HG21	16:q:522:BCR:H271	1.97	0.46
1:A:16:VAL:HA	1:A:185:PRO:HA	1.95	0.46
13:A:1126:CLA:H3A	13:A:1126:CLA:HBA2	1.60	0.46
12:1:111:THR:HG21	16:1:522:BCR:H271	1.97	0.46
13:1:505:CLA:H43	16:1:524:BCR:HC7	1.98	0.46
13:2:501:CLA:C4D	13:2:503:CLA:H2	2.45	0.46
2:H:326:LEU:HD13	2:H:332:PHE:HD2	1.77	0.46
12:d:251:LEU:HD23	13:d:501:CLA:H142	1.97	0.46
13:e:1140:CLA:HBA2	17:e:5001:LHG:H152	1.98	0.46
12:r:148:PHE:CD2	13:r:512:CLA:H3A	2.50	0.46
13:t:509:CLA:HBD	13:t:509:CLA:H121	1.96	0.46
2:B:481:ALA:HA	2:B:486:THR:HG21	1.97	0.46
12:2:251:LEU:HD23	13:2:501:CLA:H142	1.96	0.46
13:3:501:CLA:C4D	13:3:503:CLA:H2	2.46	0.46
12:4:70:LEU:HD21	13:4:503:CLA:HED2	1.97	0.46
13:G:1110:CLA:HBA2	13:G:1110:CLA:H3A	1.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:26:LEU:HA	3:N:41:ALA:O	2.16	0.46
12:Z:251:LEU:HD23	13:Z:501:CLA:H142	1.96	0.46
12:b:119:ALA:O	12:b:126:LYS:NZ	2.41	0.46
12:d:200:LEU:HG	12:d:265:LEU:HD11	1.96	0.46
12:v:61:GLU:HG3	12:v:292:LEU:HD13	1.96	0.46
2:B:118:SER:HA	13:B:1224:CLA:HMA2	1.98	0.46
2:B:355:MET:HE3	2:B:355:MET:HB2	1.79	0.46
13:B:1222:CLA:H52	13:B:1234:CLA:H11	1.97	0.46
10:L:3:GLN:NE2	20:f:1852:SQD:O3	2.47	0.46
13:G:1140:CLA:HBA2	17:G:5001:LHG:H152	1.98	0.46
2:H:118:SER:HA	13:H:1224:CLA:HMA2	1.97	0.46
12:Y:130:PHE:HA	12:Y:137:GLN:HG2	1.96	0.46
12:c:307:HIS:NE2	13:c:502:CLA:NA	2.64	0.46
12:d:79:ASP:OD1	12:d:79:ASP:N	2.48	0.46
13:d:519:CLA:HED2	13:d:519:CLA:H2A	1.97	0.46
16:d:522:BCR:C23	13:q:518:CLA:HED3	2.46	0.46
3:g:62:PHE:HD2	4:h:122:ILE:HD13	1.81	0.46
16:q:524:BCR:H15C	16:q:524:BCR:H351	1.79	0.46
12:s:274:ALA:HB3	12:s:290:VAL:HG22	1.96	0.46
12:v:251:LEU:HD23	13:v:501:CLA:H142	1.98	0.46
1:A:370:ILE:HG21	13:A:1123:CLA:HMA3	1.97	0.46
13:B:1215:CLA:H13	13:B:1221:CLA:H162	1.97	0.46
13:B:1215:CLA:HBA2	13:B:1215:CLA:H3A	1.58	0.46
13:B:1224:CLA:HBA2	13:B:1224:CLA:H3A	1.65	0.46
13:J:1302:CLA:H61	13:J:1302:CLA:H2	1.73	0.46
1:G:522:GLY:HA2	1:G:536:PRO:HB3	1.97	0.46
13:G:1134:CLA:H61	13:G:1134:CLA:H41	1.83	0.46
13:a:501:CLA:C4D	13:a:503:CLA:H2	2.46	0.46
13:q:505:CLA:H43	16:q:524:BCR:HC7	1.98	0.46
13:q:508:CLA:H43	13:q:511:CLA:HAC1	1.98	0.46
12:u:307:HIS:NE2	13:u:502:CLA:NA	2.64	0.46
12:v:200:LEU:HG	12:v:265:LEU:HD11	1.96	0.46
1:A:441:VAL:HG11	13:A:1119:CLA:H192	1.97	0.46
3:C:26:LEU:HA	3:C:41:ALA:O	2.16	0.46
12:6:190:TYR:HD2	16:6:524:BCR:H401	1.81	0.46
13:G:1013:CLA:H203	13:G:1140:CLA:H51	1.97	0.46
2:H:415:LYS:HD2	2:H:539:LEU:HB3	1.98	0.46
16:U:4104:BCR:H403	20:Y:822:SQD:H332	1.98	0.46
13:b:517:CLA:H3A	13:b:517:CLA:HBA1	1.68	0.46
12:c:309:PHE:CD2	16:c:521:BCR:H10C	2.51	0.46
13:e:1130:CLA:HMC1	13:n:1502:CLA:H122	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:415:LYS:HD2	2:f:539:LEU:HB3	1.98	0.46
13:f:1023:CLA:H122	16:k:4018:BCR:H281	1.98	0.46
13:l:1302:CLA:H2	13:l:1302:CLA:H61	1.73	0.46
13:r:501:CLA:C4D	13:r:503:CLA:H2	2.45	0.46
13:u:502:CLA:HBD	13:u:503:CLA:H43	1.98	0.46
12:v:59:MET:HB2	12:v:271:PHE:HA	1.98	0.46
16:B:4005:BCR:H15C	16:B:4005:BCR:H351	1.81	0.46
3:C:62:PHE:HD2	4:D:122:ILE:HD13	1.81	0.46
13:L:1501:CLA:HMD3	10:n:94:SER:HB2	1.97	0.46
17:L:5221:LHG:H172	7:k:20:LEU:HD12	1.96	0.46
16:2:524:BCR:H15C	16:2:524:BCR:H351	1.78	0.46
12:3:274:ALA:HB3	12:3:290:VAL:HG22	1.96	0.46
1:G:370:ILE:HG21	13:G:1123:CLA:HMA3	1.97	0.46
13:G:1013:CLA:H122	13:G:1140:CLA:H101	1.98	0.46
7:S:26:LEU:HD11	20:n:5216:SQD:H282	1.97	0.46
12:c:145:HIS:NE2	13:c:512:CLA:NA	2.64	0.46
12:d:177:VAL:HG21	12:d:204:VAL:HG21	1.97	0.46
13:e:1115:CLA:H62	13:e:1115:CLA:H41	1.65	0.46
2:f:118:SER:HA	13:f:1224:CLA:HMA2	1.97	0.46
2:f:156:HIS:CE1	13:f:1208:CLA:NA	2.84	0.46
2:f:343:VAL:HG13	13:f:1222:CLA:HED1	1.97	0.46
13:r:518:CLA:H61	13:r:518:CLA:H41	1.62	0.46
13:s:501:CLA:C4D	13:s:503:CLA:H2	2.46	0.46
13:s:517:CLA:H3A	13:s:517:CLA:HBA1	1.51	0.46
13:u:509:CLA:H92	13:u:509:CLA:H62	1.81	0.46
12:v:78:GLY:N	12:v:82:GLN:O	2.49	0.46
1:A:658:LEU:HD13	13:A:1022:CLA:HED1	1.97	0.46
16:A:4007:BCR:H15C	16:A:4007:BCR:H351	1.79	0.46
2:B:611:GLU:OE2	6:F:36:ARG:NH1	2.44	0.46
10:L:90:THR:HG21	10:L:133:ILE:HD12	1.98	0.46
12:6:251:LEU:HD23	13:6:501:CLA:H142	1.98	0.46
1:G:115:GLN:NE2	13:G:1107:CLA:OBD	2.43	0.46
14:G:2001:PQN:H301	8:T:19:PHE:HZ	1.81	0.46
2:H:156:HIS:CE1	13:H:1208:CLA:NA	2.84	0.46
2:H:301:ILE:HG21	13:H:1221:CLA:HAC1	1.97	0.46
13:H:1209:CLA:H3A	13:H:1209:CLA:HBA2	1.59	0.46
13:H:1221:CLA:H112	13:H:1221:CLA:H72	1.75	0.46
16:H:4009:BCR:H351	16:H:4009:BCR:H15C	1.82	0.46
12:Y:111:THR:HG21	16:Y:522:BCR:H271	1.97	0.46
16:c:521:BCR:H24C	16:c:521:BCR:H371	1.82	0.46
2:f:326:LEU:HD13	2:f:332:PHE:HD2	1.77	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:1201:CLA:H2	16:o:4021:BCR:H323	1.98	0.46
4:h:101:ASP:OD1	4:h:101:ASP:N	2.48	0.46
13:s:501:CLA:HBB2	13:s:507:CLA:H92	1.98	0.46
16:u:521:BCR:H15C	16:u:521:BCR:H351	1.85	0.46
13:B:1221:CLA:H141	13:B:1221:CLA:H161	1.78	0.46
12:1:281:GLY:O	13:1:519:CLA:HED1	2.15	0.46
12:3:26:LEU:HB3	13:3:511:CLA:HMA1	1.98	0.46
13:Y:512:CLA:H3A	13:Y:512:CLA:HBA1	1.62	0.46
12:c:73:LEU:O	12:c:159:LYS:NZ	2.49	0.46
16:m:4104:BCR:H403	20:q:822:SQD:H332	1.98	0.46
10:n:90:THR:HG21	10:n:133:ILE:HD12	1.98	0.46
12:q:97:LEU:HG	16:q:522:BCR:H12C	1.98	0.46
13:r:501:CLA:H41	13:r:501:CLA:H62	1.61	0.46
1:A:522:GLY:HA2	1:A:536:PRO:HB3	1.97	0.46
13:A:1105:CLA:HMB3	13:A:1106:CLA:HHB	1.98	0.46
13:A:1130:CLA:HMC1	13:L:1502:CLA:H122	1.97	0.46
16:A:4003:BCR:H15C	16:A:4003:BCR:H351	1.81	0.46
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.98	0.46
7:I:13:ILE:HD11	10:V:155:LEU:HD22	1.96	0.46
13:1:508:CLA:H62	13:1:508:CLA:H41	1.62	0.46
13:3:501:CLA:HBB2	13:3:507:CLA:H92	1.98	0.46
12:5:148:PHE:HD2	13:5:512:CLA:H3A	1.81	0.46
12:5:309:PHE:HD2	16:5:521:BCR:H10C	1.81	0.46
12:6:146:LEU:HD22	12:6:214:LEU:HD22	1.98	0.46
13:G:1102:CLA:H202	13:G:1102:CLA:H161	1.82	0.46
13:H:1215:CLA:HBA2	13:H:1215:CLA:H3A	1.58	0.46
13:H:1217:CLA:HBA2	13:H:1217:CLA:H3A	1.41	0.46
12:b:70:LEU:HD21	13:b:503:CLA:HED2	1.97	0.46
12:d:146:LEU:HD22	12:d:214:LEU:HD22	1.98	0.46
1:e:360:TRP:HB3	13:e:1103:CLA:HAC1	1.98	0.46
13:e:1022:CLA:H192	13:f:1206:CLA:H51	1.98	0.46
16:l:4015:BCR:H15C	16:l:4015:BCR:H351	1.79	0.46
12:t:70:LEU:HD21	13:t:503:CLA:HED2	1.97	0.46
12:u:73:LEU:O	12:u:159:LYS:NZ	2.49	0.46
1:A:115:GLN:NE2	13:A:1107:CLA:OBD	2.43	0.45
13:A:1140:CLA:HBA2	17:A:5001:LHG:H152	1.98	0.45
2:B:343:VAL:HG13	13:B:1222:CLA:HED1	1.97	0.45
13:B:1201:CLA:H2	16:M:4021:BCR:H323	1.98	0.45
16:F:4016:BCR:H11C	16:F:4016:BCR:H341	1.77	0.45
16:1:521:BCR:H15C	16:1:521:BCR:H351	1.82	0.45
12:3:59:MET:HE2	12:3:67:LEU:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:519:CLA:HED2	13:6:519:CLA:H2A	1.97	0.45
13:H:1224:CLA:H72	13:H:1224:CLA:H111	1.68	0.45
16:H:4014:BCR:H332	16:T:4012:BCR:HC32	1.99	0.45
12:Z:226:PRO:HA	13:Z:506:CLA:HED3	1.98	0.45
12:d:102:VAL:HG22	13:q:505:CLA:C7	2.46	0.45
12:d:102:VAL:HG13	13:q:505:CLA:H52	1.98	0.45
13:f:1228:CLA:HAB	13:f:1229:CLA:H202	1.98	0.45
12:v:143:GLY:HA3	12:v:222:ILE:HG13	1.98	0.45
12:v:190:TYR:HD2	16:v:524:BCR:H401	1.81	0.45
13:A:1013:CLA:H203	13:A:1140:CLA:H51	1.97	0.45
13:A:1122:CLA:H41	13:A:1122:CLA:H62	1.68	0.45
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.99	0.45
2:B:415:LYS:HD2	2:B:539:LEU:HB3	1.98	0.45
13:B:1212:CLA:H61	13:B:1212:CLA:H41	1.70	0.45
4:D:37:GLU:HA	4:D:50:MET:O	2.16	0.45
16:1:524:BCR:H15C	16:1:524:BCR:H351	1.79	0.45
13:2:511:CLA:H72	12:3:333:VAL:HG13	1.96	0.45
13:5:512:CLA:H3A	13:5:512:CLA:HBA1	1.68	0.45
13:6:501:CLA:HMB2	16:6:524:BCR:H23C	1.98	0.45
12:b:143:GLY:HA3	12:b:222:ILE:HG23	1.98	0.45
16:c:521:BCR:H15C	16:c:521:BCR:H351	1.84	0.45
1:e:441:VAL:HG11	13:e:1119:CLA:H192	1.97	0.45
13:f:1220:CLA:H2A	13:f:1220:CLA:HED3	1.97	0.45
12:t:230:THR:HG23	12:t:234:LEU:HD12	1.97	0.45
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.99	0.45
2:B:156:HIS:CE1	13:B:1208:CLA:NA	2.84	0.45
2:B:376:GLN:O	2:B:380:THR:OG1	2.33	0.45
13:B:1219:CLA:H2	13:B:1219:CLA:H61	1.65	0.45
13:B:1222:CLA:H2	13:B:1231:CLA:HBB2	1.99	0.45
16:L:4219:BCR:H15C	16:L:4219:BCR:H351	1.78	0.45
12:2:19:ARG:NH1	13:2:511:CLA:OBD	2.50	0.45
12:2:226:PRO:HA	13:2:506:CLA:HED3	1.98	0.45
12:6:59:MET:HB2	12:6:271:PHE:HA	1.98	0.45
13:G:1139:CLA:H61	13:G:1139:CLA:H41	1.62	0.45
2:H:343:VAL:HG13	13:H:1222:CLA:HED1	1.97	0.45
13:H:1220:CLA:HED3	13:H:1220:CLA:H2A	1.97	0.45
16:T:4015:BCR:H11C	16:T:4015:BCR:H341	1.84	0.45
12:a:143:GLY:HA3	12:a:222:ILE:HG13	1.97	0.45
13:j:1301:CLA:H102	13:j:1301:CLA:H13	1.80	0.45
12:r:19:ARG:NH1	13:r:511:CLA:OBD	2.50	0.45
13:A:1013:CLA:H122	13:A:1140:CLA:H101	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:507:CLA:H62	13:2:507:CLA:H41	1.71	0.45
12:4:143:GLY:HA3	12:4:222:ILE:HG23	1.99	0.45
2:H:321:GLY:O	2:H:325:THR:OG1	2.28	0.45
13:d:501:CLA:HMB2	16:d:524:BCR:H23C	1.98	0.45
13:e:1105:CLA:HMB3	13:e:1106:CLA:HHB	1.98	0.45
13:f:1210:CLA:H112	13:f:1210:CLA:H51	1.98	0.45
16:f:4010:BCR:H351	16:f:4010:BCR:H15C	1.74	0.45
12:t:143:GLY:HA3	12:t:222:ILE:HG23	1.98	0.45
13:t:512:CLA:HAB	13:t:516:CLA:HMD2	1.99	0.45
12:u:145:HIS:NE2	13:u:512:CLA:NA	2.64	0.45
1:A:252:PRO:HA	1:A:255:PHE:HD2	1.82	0.45
16:B:4017:BCR:H15C	16:B:4017:BCR:H351	1.85	0.45
16:B:4014:BCR:H332	16:J:4012:BCR:HC32	1.99	0.45
12:2:177:VAL:HG13	12:2:201:GLU:HG3	1.98	0.45
12:5:309:PHE:CD2	16:5:521:BCR:H10C	2.51	0.45
2:H:158:GLN:HG3	20:H:1852:SQD:H1	1.98	0.45
13:H:1210:CLA:H112	13:H:1210:CLA:H51	1.99	0.45
16:H:4017:BCR:H371	16:H:4017:BCR:H24C	1.80	0.45
9:U:43:GLY:HA3	9:U:58:PRO:HG2	1.98	0.45
16:V:4219:BCR:H15C	16:V:4219:BCR:H351	1.78	0.45
16:Y:521:BCR:H15C	16:Y:521:BCR:H351	1.82	0.45
12:a:26:LEU:HB3	13:a:511:CLA:HMA1	1.98	0.45
12:d:190:TYR:HD2	16:d:524:BCR:H401	1.81	0.45
13:e:1013:CLA:H93	13:e:1013:CLA:H61	1.79	0.45
14:e:2001:PQN:H301	8:l:19:PHE:HZ	1.81	0.45
2:f:301:ILE:HG21	13:f:1221:CLA:HAC1	1.97	0.45
2:f:301:ILE:HG23	13:f:1216:CLA:HED3	1.98	0.45
4:h:37:GLU:HA	4:h:50:MET:O	2.16	0.45
12:u:309:PHE:HD2	16:u:521:BCR:H10C	1.81	0.45
13:u:509:CLA:HBA1	13:u:509:CLA:H3A	1.78	0.45
12:v:146:LEU:HD22	12:v:214:LEU:HD22	1.98	0.45
2:B:301:ILE:HG23	13:B:1216:CLA:HED3	1.98	0.45
13:1:509:CLA:H92	13:1:509:CLA:H62	1.82	0.45
13:1:518:CLA:H61	13:1:518:CLA:H41	1.73	0.45
12:3:143:GLY:HA3	12:3:222:ILE:HG13	1.97	0.45
16:6:524:BCR:H15C	16:6:524:BCR:H351	1.81	0.45
2:H:191:THR:HG21	2:H:278:LEU:HB2	1.99	0.45
2:H:301:ILE:HG23	13:H:1216:CLA:HED3	1.98	0.45
10:V:90:THR:HG21	10:V:133:ILE:HD12	1.98	0.45
13:Y:509:CLA:H92	13:Y:509:CLA:H62	1.82	0.45
13:b:512:CLA:HAB	13:b:516:CLA:HMD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:78:GLY:N	12:d:82:GLN:O	2.49	0.45
12:d:102:VAL:HG22	13:q:505:CLA:H8	1.99	0.45
12:d:105:ALA:N	13:q:505:CLA:HMB2	2.32	0.45
12:d:282:VAL:HG23	12:d:283:THR:HG23	1.98	0.45
1:e:252:PRO:HA	1:e:255:PHE:HD2	1.82	0.45
4:h:38:GLN:HG3	4:h:50:MET:HE3	1.97	0.45
12:v:282:VAL:HG23	12:v:283:THR:HG23	1.98	0.45
16:v:522:BCR:H371	16:v:522:BCR:H24C	1.82	0.45
16:A:4002:BCR:H24C	16:A:4002:BCR:H371	1.81	0.45
16:A:4011:BCR:H15C	16:A:4011:BCR:H351	1.86	0.45
3:C:17:CYS:HB2	3:C:54:CYS:HB2	1.99	0.45
4:D:38:GLN:HG3	4:D:50:MET:HE3	1.97	0.45
12:6:79:ASP:OD1	12:6:79:ASP:N	2.48	0.45
13:H:1023:CLA:H122	16:S:4018:BCR:H281	1.98	0.45
4:O:38:GLN:HG3	4:O:50:MET:HE3	1.97	0.45
12:Z:143:GLY:HA3	12:Z:222:ILE:HG13	1.99	0.45
12:d:59:MET:HB2	12:d:271:PHE:HA	1.98	0.45
2:f:191:THR:HG21	2:f:278:LEU:HB2	1.99	0.45
2:f:236:ASN:OD1	2:f:236:ASN:N	2.49	0.45
2:f:548:PRO:HB3	6:j:158:PRO:HG2	1.98	0.45
13:f:1224:CLA:H111	13:f:1224:CLA:H72	1.68	0.45
12:r:177:VAL:HG13	12:r:201:GLU:HG3	1.98	0.45
12:4:119:ALA:O	12:4:126:LYS:NZ	2.41	0.45
12:5:307:HIS:NE2	13:5:502:CLA:NA	2.64	0.45
13:5:502:CLA:HBD	13:5:503:CLA:H43	1.98	0.45
12:6:143:GLY:HA3	12:6:222:ILE:HG13	1.98	0.45
13:G:1022:CLA:H192	13:H:1206:CLA:H51	1.98	0.45
13:H:1201:CLA:H2	16:W:4021:BCR:H323	1.98	0.45
13:H:1219:CLA:HBA2	13:H:1219:CLA:H43	1.99	0.45
3:N:58:CYS:HB3	3:N:63:LEU:HD22	1.98	0.45
16:T:4015:BCR:H20C	16:T:4015:BCR:H361	1.81	0.45
16:Y:524:BCR:H15C	16:Y:524:BCR:H351	1.79	0.45
13:Z:506:CLA:H62	13:Z:506:CLA:H41	1.71	0.45
12:a:110:HIS:NE2	13:a:513:CLA:NB	2.65	0.45
12:c:309:PHE:HD2	16:c:521:BCR:H10C	1.81	0.45
12:d:98:ILE:HG23	13:q:505:CLA:H111	1.98	0.45
13:d:517:CLA:H3A	13:d:517:CLA:HBA1	1.50	0.45
1:e:554:ILE:HD11	13:e:1135:CLA:HBB1	1.99	0.45
16:e:4008:BCR:H15C	16:e:4008:BCR:H351	1.82	0.45
2:f:355:MET:HE3	2:f:355:MET:HB2	1.79	0.45
3:g:17:CYS:HB2	3:g:54:CYS:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:32:TRP:NE1	4:h:50:MET:SD	2.76	0.45
13:u:512:CLA:HBA1	13:u:512:CLA:H3A	1.68	0.45
12:v:177:VAL:HG21	12:v:204:VAL:HG21	1.96	0.45
1:A:336:ILE:O	1:A:340:HIS:ND1	2.37	0.45
1:A:360:TRP:HB3	13:A:1103:CLA:HAC1	1.98	0.45
13:B:1023:CLA:H122	16:I:4018:BCR:H281	1.98	0.45
13:B:1210:CLA:H112	13:B:1210:CLA:H51	1.98	0.45
13:1:508:CLA:H43	13:1:511:CLA:HAC1	1.98	0.45
13:1:510:CLA:H41	13:1:510:CLA:H61	1.60	0.45
12:6:301:ALA:O	12:6:305:ASN:ND2	2.43	0.45
13:G:1102:CLA:H112	13:G:1102:CLA:H151	1.73	0.45
13:G:1105:CLA:HMB3	13:G:1106:CLA:HHB	1.98	0.45
13:G:1122:CLA:H62	13:G:1122:CLA:H41	1.68	0.45
13:H:1207:CLA:HAB	7:S:19:GLY:HA3	1.99	0.45
4:O:37:GLU:HA	4:O:50:MET:O	2.16	0.45
13:Y:508:CLA:H43	13:Y:511:CLA:HAC1	1.98	0.45
12:Z:19:ARG:NH1	13:Z:511:CLA:OBD	2.50	0.45
12:a:59:MET:HE2	12:a:67:LEU:HB3	1.98	0.45
2:f:25:ILE:HA	13:f:1201:CLA:HMD2	1.99	0.45
6:j:90:TYR:OH	6:j:132:PHE:O	2.33	0.45
11:o:11:LEU:HD21	16:o:4021:BCR:H272	1.99	0.45
13:v:501:CLA:HMB2	16:v:524:BCR:H23C	1.98	0.45
13:v:517:CLA:H3A	13:v:517:CLA:HBA1	1.50	0.45
13:A:1124:CLA:H2	13:A:1124:CLA:H61	1.79	0.45
14:A:2001:PQN:H301	8:J:19:PHE:HZ	1.81	0.45
2:B:236:ASN:OD1	2:B:236:ASN:N	2.49	0.45
2:B:456:GLU:OE1	6:F:68:HIS:ND1	2.47	0.45
13:B:1224:CLA:H111	13:B:1224:CLA:H72	1.68	0.45
3:C:61:ASP:HA	3:C:62:PHE:HA	1.83	0.45
12:3:110:HIS:NE2	13:3:513:CLA:NB	2.65	0.45
12:5:73:LEU:O	12:5:159:LYS:NZ	2.49	0.45
12:5:145:HIS:NE2	13:5:512:CLA:NA	2.64	0.45
12:6:101:ALA:HB1	13:Y:505:CLA:HAB	1.99	0.45
13:6:501:CLA:H41	13:6:501:CLA:H62	1.76	0.45
1:G:252:PRO:HA	1:G:255:PHE:HD2	1.82	0.45
1:G:360:TRP:HB3	13:G:1103:CLA:HAC1	1.98	0.45
13:H:1219:CLA:H61	13:H:1219:CLA:H2	1.65	0.45
20:H:1852:SQD:O10	13:e:1801:CLA:HBD	2.17	0.45
3:N:62:PHE:HD2	4:O:122:ILE:HD13	1.81	0.45
16:Z:521:BCR:H15C	16:Z:521:BCR:H351	1.83	0.45
1:e:370:ILE:HG21	13:e:1123:CLA:HMA3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:1013:CLA:H122	13:e:1140:CLA:H101	1.98	0.45
2:f:674:LEU:O	2:f:677:THR:OG1	2.34	0.45
3:g:26:LEU:HA	3:g:41:ALA:O	2.16	0.45
16:k:4018:BCR:H11C	16:k:4018:BCR:H341	1.86	0.45
13:n:1501:CLA:H41	13:n:1501:CLA:H61	1.75	0.45
16:n:4022:BCR:H11C	16:n:4022:BCR:H341	1.84	0.45
12:t:273:GLY:O	12:t:300:ARG:NH2	2.45	0.45
2:B:25:ILE:HA	13:B:1201:CLA:HMD2	1.99	0.44
20:B:1852:SQD:H252	20:B:1852:SQD:H102	1.99	0.44
5:E:53:ASP:OD1	5:E:53:ASP:N	2.44	0.44
1:G:300:LEU:HD21	1:G:385:MET:HB3	1.99	0.44
4:O:21:SER:HA	4:O:24:THR:HB	1.97	0.44
13:V:1501:CLA:HAA2	16:V:4022:BCR:H363	1.99	0.44
12:d:143:GLY:HA3	12:d:222:ILE:HG13	1.98	0.44
13:f:1212:CLA:H61	13:f:1212:CLA:H41	1.70	0.44
16:l:4015:BCR:H20C	16:l:4015:BCR:H361	1.82	0.44
12:s:26:LEU:HB3	13:s:511:CLA:HMA1	1.98	0.44
16:t:524:BCR:H351	16:t:524:BCR:H15C	1.79	0.44
12:u:309:PHE:CD2	16:u:521:BCR:H10C	2.51	0.44
13:u:505:CLA:H91	13:u:505:CLA:H112	1.81	0.44
13:A:1022:CLA:H192	13:B:1206:CLA:H51	1.98	0.44
2:B:158:GLN:HG3	20:B:1852:SQD:H1	1.98	0.44
16:K:4104:BCR:H403	20:1:822:SQD:H332	1.98	0.44
11:M:11:LEU:HD21	16:M:4021:BCR:H272	1.99	0.44
2:H:4:LYS:HZ1	20:n:5216:SQD:C3	2.29	0.44
11:W:11:LEU:HD21	16:W:4021:BCR:H272	1.99	0.44
13:c:501:CLA:HMB2	16:c:524:BCR:H23C	2.00	0.44
16:e:4002:BCR:H361	16:e:4002:BCR:H20C	1.77	0.44
13:f:1210:CLA:H2	13:f:1210:CLA:H62	1.64	0.44
13:f:1219:CLA:HBA2	13:f:1219:CLA:H43	1.99	0.44
13:B:1228:CLA:HAB	13:B:1229:CLA:H202	1.98	0.44
12:4:273:GLY:O	12:4:300:ARG:NH2	2.45	0.44
2:H:548:PRO:HB3	6:R:158:PRO:HG2	1.98	0.44
13:Y:505:CLA:H43	16:Y:524:BCR:HC7	1.98	0.44
13:c:503:CLA:H62	13:c:503:CLA:H41	1.83	0.44
16:d:524:BCR:H15C	16:d:524:BCR:H351	1.81	0.44
13:f:1221:CLA:H141	13:f:1221:CLA:H161	1.78	0.44
13:f:1207:CLA:HAB	7:k:19:GLY:HA3	1.99	0.44
12:u:148:PHE:HD2	13:u:512:CLA:H3A	1.81	0.44
1:A:595:CYS:HB2	2:B:667:TRP:HB3	2.00	0.44
2:B:674:LEU:O	2:B:677:THR:OG1	2.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1202:CLA:HBD	13:B:1202:CLA:H122	2.00	0.44
16:6:522:BCR:H15C	16:6:522:BCR:H351	1.81	0.44
1:G:752:TRP:HD1	13:G:1126:CLA:HMB2	1.83	0.44
16:G:4003:BCR:H20C	16:G:4003:BCR:H361	1.88	0.44
2:H:25:ILE:HA	13:H:1201:CLA:HMD2	1.99	0.44
2:H:91:ILE:HB	2:H:112:PRO:HB2	1.99	0.44
13:H:1212:CLA:H61	13:H:1212:CLA:H41	1.70	0.44
6:R:150:LYS:HA	6:R:150:LYS:HD3	1.72	0.44
16:T:4013:BCR:H351	16:T:4013:BCR:H15C	1.82	0.44
12:Z:73:LEU:HD11	13:Z:503:CLA:HAA2	1.99	0.44
1:e:430:PRO:HG2	4:h:41:GLU:HB2	2.00	0.44
12:r:226:PRO:HA	13:r:506:CLA:HED3	1.98	0.44
13:r:507:CLA:H62	13:r:507:CLA:H41	1.71	0.44
12:s:59:MET:HE2	12:s:67:LEU:HB3	1.98	0.44
16:t:523:BCR:H11C	16:t:523:BCR:H341	1.90	0.44
13:u:501:CLA:HMB2	16:u:524:BCR:H23C	1.99	0.44
16:v:521:BCR:H15C	16:v:521:BCR:H351	1.83	0.44
13:A:1102:CLA:H141	13:A:1102:CLA:H162	1.79	0.44
12:1:97:LEU:HG	16:1:522:BCR:H12C	1.98	0.44
12:1:112:PHE:HB2	12:2:326:MET:HE3	2.00	0.44
13:5:501:CLA:HMB2	16:5:524:BCR:H23C	1.99	0.44
2:H:182:LEU:HD13	13:H:1210:CLA:HHB	1.99	0.44
2:H:674:LEU:O	2:H:677:THR:OG1	2.34	0.44
2:H:700:LEU:HD22	2:H:704:GLN:NE2	2.33	0.44
13:H:1208:CLA:H202	13:H:1208:CLA:H161	1.80	0.44
7:S:1:MET:HE2	7:S:1:MET:HB3	1.81	0.44
12:Y:112:PHE:HB2	12:Z:326:MET:HE3	2.00	0.44
12:c:148:PHE:HD2	13:c:512:CLA:H3A	1.81	0.44
13:c:502:CLA:HBD	13:c:503:CLA:H43	1.98	0.44
13:c:509:CLA:H92	13:c:509:CLA:H62	1.81	0.44
16:d:523:BCR:H15C	16:d:523:BCR:H351	1.81	0.44
16:f:4017:BCR:H24C	16:f:4017:BCR:H371	1.80	0.44
16:f:4014:BCR:H332	16:l:4012:BCR:HC32	1.98	0.44
6:j:150:LYS:HD3	6:j:150:LYS:HA	1.72	0.44
9:m:43:GLY:HA3	9:m:58:PRO:HG2	1.98	0.44
12:q:143:GLY:HA3	12:q:222:ILE:HG13	2.00	0.44
12:u:110:HIS:HA	12:u:114:ALA:HB3	2.00	0.44
13:u:501:CLA:H41	13:u:501:CLA:H62	1.70	0.44
2:B:548:PRO:HB3	6:F:158:PRO:HG2	1.98	0.44
13:B:1207:CLA:HAB	7:I:19:GLY:HA3	1.99	0.44
7:I:16:PRO:HB3	17:V:5221:LHG:H151	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:5001:LHG:H131	20:V:5216:SQD:H291	2.00	0.44
13:J:1303:CLA:HAB	13:J:1303:CLA:H161	2.00	0.44
12:2:130:PHE:HA	12:2:137:GLN:HG2	2.00	0.44
13:G:1102:CLA:H141	13:G:1102:CLA:H162	1.79	0.44
14:G:2001:PQN:H142	14:G:2001:PQN:H112	1.89	0.44
20:H:1852:SQD:H102	20:H:1852:SQD:H252	1.99	0.44
3:N:17:CYS:HB2	3:N:54:CYS:HB2	1.99	0.44
12:Y:97:LEU:HG	16:Y:522:BCR:H12C	1.98	0.44
12:Z:130:PHE:HA	12:Z:137:GLN:HG2	2.00	0.44
12:Z:177:VAL:HG13	12:Z:201:GLU:HG3	1.98	0.44
12:b:161:THR:HA	12:b:177:VAL:HB	1.99	0.44
12:c:148:PHE:CE2	13:c:512:CLA:HHB	2.53	0.44
12:d:107:ALA:O	12:d:111:THR:OG1	2.31	0.44
1:e:336:ILE:O	1:e:340:HIS:ND1	2.37	0.44
1:e:752:TRP:HD1	13:e:1126:CLA:HMB2	1.83	0.44
16:e:4003:BCR:H20C	16:e:4003:BCR:H361	1.88	0.44
2:f:158:GLN:HG3	20:f:1852:SQD:H1	1.98	0.44
13:f:1217:CLA:H3A	13:f:1217:CLA:HBA2	1.41	0.44
3:g:58:CYS:HB3	3:g:63:LEU:HD22	1.98	0.44
13:l:1303:CLA:HAB	13:l:1303:CLA:H161	2.00	0.44
12:r:130:PHE:HA	12:r:137:GLN:HG2	2.00	0.44
12:r:143:GLY:HA3	12:r:222:ILE:HG13	1.99	0.44
1:A:430:PRO:HG2	4:D:41:GLU:HB2	2.00	0.44
13:B:1219:CLA:HBA2	13:B:1219:CLA:H43	1.99	0.44
13:1:505:CLA:H61	12:v:102:VAL:HA	1.99	0.44
12:6:78:GLY:N	12:6:82:GLN:O	2.49	0.44
1:G:230:ILE:HG12	1:G:244:ALA:HA	2.00	0.44
13:H:1222:CLA:H2	13:H:1231:CLA:HBB2	1.99	0.44
4:O:31:THR:HA	4:O:55:ASN:O	2.18	0.44
13:Y:502:CLA:H61	13:Y:512:CLA:H42	1.99	0.44
16:Y:523:BCR:H15C	16:Y:523:BCR:H351	1.88	0.44
12:c:110:HIS:HA	12:c:114:ALA:HB3	1.99	0.44
2:f:91:ILE:HB	2:f:112:PRO:HB2	1.99	0.44
13:f:1209:CLA:H3A	13:f:1209:CLA:HBA2	1.59	0.44
13:f:1218:CLA:H61	13:f:1218:CLA:H2	1.72	0.44
7:k:1:MET:HE2	7:k:1:MET:HB3	1.81	0.44
12:r:301:ALA:O	12:r:305:ASN:ND2	2.41	0.44
12:t:249:ILE:HG12	13:t:502:CLA:HAC1	2.00	0.44
13:F:1302:CLA:H3A	13:F:1302:CLA:HBA1	1.70	0.44
12:6:282:VAL:HG23	12:6:283:THR:HG23	1.98	0.44
1:G:172:MET:HE1	13:G:1111:CLA:H92	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:554:ILE:HD11	13:G:1135:CLA:HBB1	1.99	0.44
7:S:16:PRO:HB3	17:n:5221:LHG:H151	2.00	0.44
2:f:700:LEU:HD22	2:f:704:GLN:NE2	2.33	0.44
16:f:4004:BCR:H11C	16:f:4004:BCR:H341	1.88	0.44
16:f:4006:BCR:H24C	16:f:4006:BCR:H371	1.75	0.44
12:q:155:LEU:HB3	13:q:502:CLA:H121	2.00	0.44
1:A:752:TRP:HD1	13:A:1126:CLA:HMB2	1.83	0.44
6:F:90:TYR:OH	6:F:132:PHE:O	2.33	0.44
16:2:521:BCR:H15C	16:2:521:BCR:H351	1.83	0.44
12:3:190:TYR:HD2	16:3:524:BCR:H401	1.83	0.44
13:3:517:CLA:H3A	13:3:517:CLA:HBA1	1.50	0.44
12:5:148:PHE:CE2	13:5:512:CLA:HHB	2.53	0.44
13:G:1013:CLA:H141	13:G:1013:CLA:H161	1.84	0.44
13:H:1205:CLA:H143	13:H:1205:CLA:H161	1.90	0.44
16:H:4004:BCR:H351	16:H:4004:BCR:H15C	1.77	0.44
16:R:4016:BCR:H24C	16:R:4016:BCR:H371	1.80	0.44
7:S:13:ILE:HD11	10:n:155:LEU:HD22	1.99	0.44
13:T:1303:CLA:HAB	13:T:1303:CLA:H161	2.00	0.44
16:e:4003:BCR:H15C	16:e:4003:BCR:H351	1.81	0.44
2:f:611:GLU:OE2	6:j:36:ARG:NH1	2.44	0.44
16:f:4004:BCR:H15C	16:f:4004:BCR:H351	1.77	0.44
3:g:58:CYS:HA	3:g:59:PRO:HD3	1.87	0.44
13:q:502:CLA:H61	13:q:512:CLA:H42	1.99	0.44
12:u:34:GLN:OE1	13:u:510:CLA:NC	2.51	0.44
12:u:148:PHE:CE2	13:u:512:CLA:HHB	2.53	0.44
1:A:172:MET:HE1	13:A:1111:CLA:H92	2.00	0.43
17:A:5002:LHG:H261	20:f:1852:SQD:H242	1.99	0.43
13:B:1213:CLA:H162	13:B:1213:CLA:H141	1.80	0.43
9:K:43:GLY:HA3	9:K:58:PRO:HG2	1.98	0.43
16:3:524:BCR:H351	16:3:524:BCR:H15C	1.78	0.43
16:5:522:BCR:H24C	16:5:522:BCR:H371	1.84	0.43
1:G:424:MET:HE1	1:G:442:LEU:HD11	2.00	0.43
1:G:595:CYS:HB2	2:H:667:TRP:HB3	2.00	0.43
2:H:332:PHE:CD1	16:H:4010:BCR:H391	2.53	0.43
13:H:1215:CLA:H142	13:H:1215:CLA:H112	1.88	0.43
13:H:1228:CLA:HAB	13:H:1229:CLA:H202	1.98	0.43
13:H:1228:CLA:HBC2	13:H:1236:CLA:HMC2	2.00	0.43
13:Y:516:CLA:H3A	13:Y:516:CLA:HBA1	1.51	0.43
13:Z:517:CLA:H3A	13:Z:517:CLA:HBA1	1.79	0.43
13:a:501:CLA:HBB2	13:a:507:CLA:H92	1.98	0.43
1:e:591:ARG:HH21	1:e:594:THR:HG21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:1222:CLA:H2	13:f:1231:CLA:HBB2	1.99	0.43
13:f:1228:CLA:HBC2	13:f:1236:CLA:HMC2	2.00	0.43
12:r:307:HIS:NE2	13:r:502:CLA:NA	2.66	0.43
12:s:110:HIS:NE2	13:s:513:CLA:NB	2.65	0.43
1:A:554:ILE:HD11	13:A:1135:CLA:HBB1	1.99	0.43
1:A:691:TRP:O	1:A:694:SER:OG	2.30	0.43
13:A:1104:CLA:H201	17:A:5001:LHG:H221	2.00	0.43
2:B:22:TRP:HE1	13:B:1238:CLA:HBB1	1.84	0.43
4:D:31:THR:HA	4:D:55:ASN:O	2.18	0.43
6:F:71:VAL:HG12	6:F:81:PHE:HB2	2.00	0.43
16:2:521:BCR:H371	16:2:521:BCR:H24C	1.78	0.43
12:3:267:TYR:O	12:3:300:ARG:NH2	2.41	0.43
13:G:1104:CLA:H201	17:G:5001:LHG:H221	2.00	0.43
13:G:1116:CLA:H93	13:G:1116:CLA:H61	1.90	0.43
13:H:1021:CLA:H62	13:H:1021:CLA:H102	1.85	0.43
13:H:1218:CLA:H61	13:H:1218:CLA:H2	1.72	0.43
13:R:1302:CLA:HBA1	13:R:1302:CLA:H3A	1.70	0.43
12:Y:155:LEU:HB3	13:Y:502:CLA:H121	2.00	0.43
1:e:404:HIS:CE1	13:e:1126:CLA:ND	2.86	0.43
13:f:1224:CLA:H3A	13:f:1224:CLA:HBA2	1.65	0.43
13:f:1239:CLA:H91	13:f:1239:CLA:H112	1.88	0.43
16:n:4020:BCR:H371	16:n:4020:BCR:H24C	1.71	0.43
1:A:300:LEU:HD21	1:A:385:MET:HB3	1.99	0.43
1:A:404:HIS:CE1	13:A:1126:CLA:ND	2.86	0.43
13:B:1221:CLA:H72	13:B:1221:CLA:H112	1.75	0.43
10:L:85:LEU:HD12	10:L:85:LEU:HA	1.86	0.43
12:1:169:ALA:HB3	12:1:265:LEU:HD12	2.00	0.43
12:2:143:GLY:HA3	12:2:222:ILE:HG13	1.99	0.43
16:5:524:BCR:H15C	16:5:524:BCR:H351	1.80	0.43
1:G:404:HIS:CE1	13:G:1126:CLA:ND	2.86	0.43
13:Z:506:CLA:H72	16:Z:524:BCR:H10C	2.00	0.43
12:b:249:ILE:HG12	13:b:502:CLA:HAC1	2.00	0.43
13:e:1103:CLA:H3A	13:e:1103:CLA:HBA1	1.54	0.43
13:e:1122:CLA:H41	13:e:1122:CLA:H62	1.68	0.43
2:f:369:ALA:HB1	2:f:725:LEU:HD11	2.00	0.43
13:f:1234:CLA:H193	13:f:1234:CLA:H161	1.87	0.43
13:n:1501:CLA:HAA2	16:n:4022:BCR:H363	1.99	0.43
16:q:521:BCR:H11C	16:q:521:BCR:H341	1.88	0.43
12:t:161:THR:HA	12:t:177:VAL:HB	1.99	0.43
13:4:512:CLA:HAB	13:4:516:CLA:HMD2	1.99	0.43
16:4:524:BCR:H351	16:4:524:BCR:H15C	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:34:GLN:OE1	13:5:510:CLA:NC	2.51	0.43
2:H:218:HIS:HD2	2:H:220:ALA:H	1.66	0.43
13:H:1221:CLA:H141	13:H:1221:CLA:H161	1.78	0.43
13:H:1224:CLA:H141	19:H:5002:LMG:H261	2.00	0.43
16:Z:524:BCR:H15C	16:Z:524:BCR:H351	1.78	0.43
12:c:34:GLN:OE1	13:c:510:CLA:NC	2.51	0.43
16:d:522:BCR:H24C	16:d:522:BCR:H371	1.82	0.43
13:e:1104:CLA:H41	13:e:1104:CLA:H62	1.64	0.43
18:e:1849:LMU:H62	18:e:1849:LMU:H91	1.85	0.43
2:f:182:LEU:HD13	13:f:1210:CLA:HHB	2.00	0.43
13:r:501:CLA:HMB2	16:r:524:BCR:H23C	2.01	0.43
12:s:190:TYR:HD2	16:s:524:BCR:H401	1.83	0.43
13:B:1228:CLA:HBC2	13:B:1236:CLA:HMC2	2.00	0.43
16:L:4020:BCR:H24C	16:L:4020:BCR:H371	1.71	0.43
12:2:73:LEU:HD11	13:2:503:CLA:HAA2	1.99	0.43
12:2:307:HIS:NE2	13:2:502:CLA:NA	2.66	0.43
12:4:161:THR:HA	12:4:177:VAL:HB	1.99	0.43
1:G:626:GLN:HE21	1:G:759:ILE:HD13	1.83	0.43
6:R:150:LYS:HB3	6:R:153:GLU:HG3	2.01	0.43
13:Y:507:CLA:H112	16:Y:524:BCR:H362	2.00	0.43
13:Z:502:CLA:H11	13:Z:503:CLA:H161	2.01	0.43
12:a:190:TYR:HD2	16:a:524:BCR:H401	1.83	0.43
16:r:522:BCR:H24C	16:r:522:BCR:H371	1.86	0.43
2:B:182:LEU:HD13	13:B:1210:CLA:HHB	2.00	0.43
2:B:332:PHE:CD1	16:B:4010:BCR:H391	2.53	0.43
13:L:1501:CLA:HAA2	16:L:4022:BCR:H363	1.99	0.43
12:4:249:ILE:HG12	13:4:502:CLA:HAC1	2.00	0.43
2:H:22:TRP:HE1	13:H:1238:CLA:HBB1	1.84	0.43
2:H:310:PRO:HA	2:H:311:PRO:HD3	1.88	0.43
2:H:369:ALA:HB1	2:H:725:LEU:HD11	2.01	0.43
6:R:118:VAL:HA	8:T:10:SER:HA	2.01	0.43
12:d:105:ALA:HA	13:q:505:CLA:CHB	2.49	0.43
2:f:332:PHE:CD1	16:f:4010:BCR:H391	2.53	0.43
13:f:1202:CLA:H122	13:f:1202:CLA:HBD	2.00	0.43
13:f:1227:CLA:H142	16:f:4009:BCR:H17C	2.01	0.43
12:q:112:PHE:HB2	12:r:326:MET:HE3	2.00	0.43
12:r:34:GLN:HG2	13:r:509:CLA:HHB	2.00	0.43
13:r:506:CLA:H72	16:r:524:BCR:H10C	1.99	0.43
16:A:4002:BCR:H11C	16:A:4002:BCR:H341	1.82	0.43
2:B:7:LYS:HD2	11:M:28:TYR:CZ	2.54	0.43
2:B:309:LYS:HE2	2:B:309:LYS:HB2	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ALA:HB1	2:B:725:LEU:HD11	2.01	0.43
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.33	0.43
13:B:1227:CLA:H142	16:B:4009:BCR:H17C	2.01	0.43
6:F:118:VAL:HA	8:J:10:SER:HA	2.01	0.43
13:1:502:CLA:H61	13:1:512:CLA:H42	1.99	0.43
13:1:509:CLA:H91	13:1:512:CLA:HAA2	2.01	0.43
13:2:506:CLA:H72	16:2:524:BCR:H10C	2.00	0.43
16:2:521:BCR:H20C	16:2:521:BCR:H361	1.87	0.43
12:3:67:LEU:HD22	12:3:89:LEU:HD13	2.01	0.43
16:4:524:BCR:H11C	16:4:524:BCR:H341	1.83	0.43
13:H:1202:CLA:HBD	13:H:1202:CLA:H122	2.00	0.43
13:H:1224:CLA:HBA2	13:H:1224:CLA:H3A	1.65	0.43
6:R:71:VAL:HG12	6:R:81:PHE:HB2	2.00	0.43
16:Y:522:BCR:H24C	16:Y:522:BCR:H371	1.84	0.43
12:Z:307:HIS:NE2	13:Z:502:CLA:NA	2.66	0.43
12:c:221:HIS:HE1	13:c:506:CLA:NA	2.17	0.43
2:f:7:LYS:HD2	11:o:28:TYR:CZ	2.54	0.43
4:h:31:THR:HA	4:h:55:ASN:O	2.17	0.43
16:l:4013:BCR:H11C	16:l:4013:BCR:H341	1.88	0.43
16:n:4022:BCR:H15C	16:n:4022:BCR:H351	1.85	0.43
16:t:524:BCR:H11C	16:t:524:BCR:H341	1.84	0.43
1:A:424:MET:HE1	1:A:442:LEU:HD11	2.00	0.43
13:A:1108:CLA:H41	13:A:1108:CLA:H61	1.78	0.43
16:A:4008:BCR:H11C	16:A:4008:BCR:H341	1.89	0.43
2:B:174:ARG:HB2	13:B:1210:CLA:HBC2	2.01	0.43
13:B:1219:CLA:HBC2	13:B:1220:CLA:HBA1	2.00	0.43
4:D:101:ASP:OD1	4:D:101:ASP:N	2.48	0.43
16:J:4015:BCR:H20C	16:J:4015:BCR:H361	1.81	0.43
10:L:94:SER:HB2	13:V:1501:CLA:HMD3	2.00	0.43
12:1:110:HIS:HA	12:1:114:ALA:HB3	2.01	0.43
12:2:261:ALA:HA	12:2:276:LEU:HD12	2.01	0.43
13:2:501:CLA:H62	13:2:501:CLA:H41	1.62	0.43
13:G:1109:CLA:H141	13:G:1109:CLA:H161	1.82	0.43
13:Y:509:CLA:H91	13:Y:512:CLA:HAA2	2.01	0.43
13:Y:518:CLA:H41	13:Y:518:CLA:H61	1.73	0.43
12:a:67:LEU:HD22	12:a:89:LEU:HD13	2.01	0.43
16:d:522:BCR:H321	13:q:505:CLA:H172	1.99	0.43
1:e:230:ILE:HG12	1:e:244:ALA:HA	2.00	0.43
1:e:595:CYS:HB2	2:f:667:TRP:HB3	2.00	0.43
12:r:193:HIS:HB2	12:r:196:SER:HB3	2.00	0.43
13:s:503:CLA:H18	13:s:510:CLA:HBB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:s:523:BCR:H11C	16:s:523:BCR:H341	1.90	0.43
16:s:523:BCR:H15C	16:s:523:BCR:H351	1.79	0.43
16:u:522:BCR:H24C	16:u:522:BCR:H371	1.84	0.43
1:A:28:TRP:CD1	13:A:1109:CLA:HBA1	2.54	0.43
2:B:531:THR:O	2:B:535:VAL:HB	2.19	0.43
13:B:1208:CLA:H202	13:B:1208:CLA:H161	1.80	0.43
13:B:1228:CLA:H12	13:B:1228:CLA:H52	1.80	0.43
16:J:4013:BCR:H11C	16:J:4013:BCR:H341	1.88	0.43
17:L:5221:LHG:H252	13:f:1207:CLA:C4	2.40	0.43
12:1:155:LEU:HB3	13:1:502:CLA:H121	2.00	0.43
13:1:505:CLA:H161	16:v:522:BCR:H10C	2.01	0.43
12:2:26:LEU:HB3	13:2:511:CLA:HMA1	2.01	0.43
13:2:501:CLA:HMB2	16:2:524:BCR:H23C	2.01	0.43
12:4:141:ILE:HD13	13:4:509:CLA:H191	2.01	0.43
1:G:430:PRO:HG2	4:O:41:GLU:HB2	2.00	0.43
13:G:1118:CLA:H3A	9:U:61:LEU:HD23	2.01	0.43
13:H:1219:CLA:HBC2	13:H:1220:CLA:HBA1	2.00	0.43
12:Y:169:ALA:HB3	12:Y:265:LEU:HD12	2.00	0.43
13:Z:501:CLA:HMB2	16:Z:524:BCR:H23C	2.01	0.43
16:Z:522:BCR:H24C	16:Z:522:BCR:H371	1.86	0.43
12:b:141:ILE:HD13	13:b:509:CLA:H191	2.01	0.43
12:d:97:LEU:HG	16:d:522:BCR:H12C	2.00	0.43
13:q:507:CLA:H112	16:q:524:BCR:H362	2.00	0.43
13:q:509:CLA:H91	13:q:512:CLA:HAA2	2.01	0.43
12:u:221:HIS:HE1	13:u:506:CLA:NA	2.17	0.43
13:A:1102:CLA:H151	13:A:1102:CLA:H112	1.73	0.43
16:B:4010:BCR:H351	16:B:4010:BCR:H15C	1.74	0.43
12:5:110:HIS:HA	12:5:114:ALA:HB3	1.99	0.43
13:G:1104:CLA:H41	13:G:1104:CLA:H62	1.64	0.43
16:G:4003:BCR:H11C	16:G:4003:BCR:H341	1.90	0.43
1:e:300:LEU:HD21	1:e:385:MET:HB3	1.99	0.43
16:n:4020:BCR:H15C	16:n:4020:BCR:H351	1.87	0.43
13:q:508:CLA:H62	13:q:508:CLA:H41	1.62	0.43
12:r:73:LEU:HD11	13:r:503:CLA:HAA2	1.99	0.43
13:r:518:CLA:H142	13:r:518:CLA:H111	1.85	0.43
12:v:148:PHE:HE2	13:v:512:CLA:HHB	1.84	0.43
1:A:239:ASN:HD22	1:A:263:GLN:HE22	1.66	0.42
1:A:691:TRP:CE2	13:A:1011:CLA:HBA2	2.54	0.42
13:A:1109:CLA:H141	13:A:1109:CLA:H161	1.82	0.42
13:A:1128:CLA:H142	13:A:1128:CLA:H111	1.87	0.42
13:A:1139:CLA:H121	13:A:1139:CLA:H161	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:HIS:HD2	2:B:220:ALA:H	1.66	0.42
2:B:493:TYR:HE2	13:B:1231:CLA:HED1	1.84	0.42
16:B:4009:BCR:H11C	16:B:4009:BCR:H341	1.86	0.42
12:1:143:GLY:HA3	12:1:222:ILE:HG13	2.00	0.42
13:1:507:CLA:H112	16:1:524:BCR:H362	2.00	0.42
13:2:502:CLA:H11	13:2:503:CLA:H161	2.00	0.42
13:G:1119:CLA:H171	13:G:1129:CLA:HBC1	2.01	0.42
12:Z:193:HIS:HB2	12:Z:196:SER:HB3	2.00	0.42
13:a:513:CLA:HBB1	16:a:523:BCR:H402	2.01	0.42
1:e:626:GLN:HE21	1:e:759:ILE:HD13	1.83	0.42
13:e:1108:CLA:H3A	13:e:1108:CLA:HBA2	1.71	0.42
2:f:22:TRP:HE1	13:f:1238:CLA:HBB1	1.84	0.42
2:f:531:THR:O	2:f:535:VAL:HB	2.19	0.42
2:f:631:LEU:O	2:f:647:SER:OG	2.29	0.42
20:f:1852:SQD:H102	20:f:1852:SQD:H252	1.99	0.42
6:j:118:VAL:HA	8:l:10:SER:HA	2.01	0.42
16:n:4019:BCR:H351	16:n:4019:BCR:H15C	1.80	0.42
12:u:107:ALA:O	12:u:111:THR:OG1	2.30	0.42
13:A:1102:CLA:H202	13:A:1102:CLA:H161	1.82	0.42
13:A:1102:CLA:HBA2	13:A:1102:CLA:H3A	1.81	0.42
13:A:1119:CLA:H171	13:A:1129:CLA:HBC1	2.01	0.42
13:A:1123:CLA:H141	13:A:1123:CLA:H161	1.80	0.42
2:B:59:LEU:HD23	2:B:59:LEU:HA	1.89	0.42
13:B:1012:CLA:H122	13:B:1012:CLA:H8	1.88	0.42
16:B:4005:BCR:H11C	16:B:4005:BCR:H341	1.86	0.42
12:1:34:GLN:OE1	13:1:510:CLA:NC	2.52	0.42
13:4:505:CLA:H112	13:4:505:CLA:H91	1.86	0.42
1:G:691:TRP:CE2	13:G:1011:CLA:HBA2	2.54	0.42
13:H:1227:CLA:H142	16:H:4009:BCR:H17C	2.01	0.42
16:T:4013:BCR:H11C	16:T:4013:BCR:H341	1.88	0.42
13:Y:502:CLA:HBD	13:Y:503:CLA:H43	2.01	0.42
13:e:1118:CLA:H3A	9:m:61:LEU:HD23	2.01	0.42
6:j:150:LYS:HB3	6:j:153:GLU:HG3	2.01	0.42
13:q:512:CLA:H3A	13:q:512:CLA:HBA1	1.62	0.42
13:s:513:CLA:HBB1	16:s:523:BCR:H402	2.01	0.42
1:A:591:ARG:HH21	1:A:594:THR:HG21	1.83	0.42
1:A:626:GLN:HE21	1:A:759:ILE:HD13	1.83	0.42
13:A:1011:CLA:H62	13:A:1011:CLA:H102	1.87	0.42
13:A:1013:CLA:H93	13:A:1013:CLA:H61	1.79	0.42
13:B:1210:CLA:H62	13:B:1210:CLA:H2	1.64	0.42
16:B:4004:BCR:H15C	16:B:4004:BCR:H351	1.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:4017:BCR:H371	16:B:4017:BCR:H24C	1.80	0.42
16:B:4009:BCR:H15C	16:B:4009:BCR:H351	1.82	0.42
1:G:28:TRP:CD1	13:G:1109:CLA:HBA1	2.54	0.42
2:H:101:ILE:HG12	7:S:1:MET:HE2	2.02	0.42
2:H:380:THR:HG22	2:H:583:ALA:HB1	2.02	0.42
12:Y:143:GLY:HA3	12:Y:222:ILE:HG13	2.00	0.42
1:e:28:TRP:CD1	13:e:1109:CLA:HBA1	2.54	0.42
13:e:1102:CLA:H162	13:e:1102:CLA:H141	1.79	0.42
13:e:1129:CLA:H11	13:e:1129:CLA:H51	1.80	0.42
12:q:34:GLN:OE1	13:q:510:CLA:NC	2.52	0.42
12:q:169:ALA:HB3	12:q:265:LEU:HD12	2.00	0.42
12:r:26:LEU:HB3	13:r:511:CLA:HMA1	2.01	0.42
13:t:517:CLA:H3A	13:t:517:CLA:HBA1	1.68	0.42
13:u:505:CLA:H42	16:u:524:BCR:HC7	2.02	0.42
13:B:1220:CLA:H61	13:B:1220:CLA:H2	1.85	0.42
13:3:503:CLA:H18	13:3:510:CLA:HBB2	2.00	0.42
16:3:522:BCR:H15C	16:3:522:BCR:H351	1.80	0.42
13:G:1104:CLA:H191	17:G:5001:LHG:H211	2.02	0.42
13:G:1138:CLA:HAA2	13:H:1228:CLA:HMB1	2.01	0.42
13:H:1216:CLA:H93	13:H:1216:CLA:H111	1.89	0.42
13:H:1228:CLA:H12	13:H:1228:CLA:H52	1.80	0.42
4:O:32:TRP:NE1	4:O:50:MET:SD	2.76	0.42
8:T:26:LEU:HD13	16:T:4012:BCR:HC7	2.02	0.42
9:U:68:HIS:O	9:U:72:ILE:HG12	2.20	0.42
12:Y:34:GLN:OE1	13:Y:510:CLA:NC	2.52	0.42
12:Y:147:LEU:HD12	12:Y:215:ILE:HG12	2.01	0.42
1:e:424:MET:HE1	1:e:442:LEU:HD11	2.00	0.42
13:e:1122:CLA:H91	13:e:1122:CLA:H111	1.77	0.42
13:e:1140:CLA:H11	13:e:1140:CLA:CHA	2.50	0.42
17:n:5220:LHG:H311	17:n:5220:LHG:H171	2.01	0.42
12:q:34:GLN:HG2	13:q:509:CLA:HHB	2.02	0.42
12:r:261:ALA:HA	12:r:276:LEU:HD12	2.01	0.42
13:u:503:CLA:H62	13:u:503:CLA:H41	1.83	0.42
16:B:4004:BCR:H11C	16:B:4004:BCR:H341	1.88	0.42
8:J:26:LEU:HD13	16:J:4012:BCR:HC7	2.02	0.42
16:J:4013:BCR:H15C	16:J:4013:BCR:H351	1.82	0.42
9:K:68:HIS:O	9:K:72:ILE:HG12	2.20	0.42
12:6:97:LEU:HG	16:6:522:BCR:H12C	2.00	0.42
16:Y:522:BCR:H20C	16:Y:522:BCR:H361	1.94	0.42
13:Z:501:CLA:H41	13:Z:501:CLA:H62	1.61	0.42
16:b:521:BCR:H15C	16:b:521:BCR:H351	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:50:ILE:HD11	12:c:89:LEU:HB2	2.01	0.42
12:d:40:PHE:CZ	13:q:518:CLA:C2	3.02	0.42
13:e:1116:CLA:H91	13:e:1116:CLA:H111	1.83	0.42
13:f:1219:CLA:HBC2	13:f:1220:CLA:HBA1	2.01	0.42
13:f:1224:CLA:H141	19:f:5002:LMG:H261	2.00	0.42
12:s:67:LEU:HD22	12:s:89:LEU:HD13	2.01	0.42
1:A:230:ILE:HG12	1:A:244:ALA:HA	2.00	0.42
13:B:1217:CLA:H41	13:B:1217:CLA:H61	1.73	0.42
13:L:1501:CLA:H202	13:L:1501:CLA:H161	1.88	0.42
12:2:148:PHE:CE2	13:2:512:CLA:HHB	2.55	0.42
16:3:522:BCR:H11C	16:3:522:BCR:H341	1.92	0.42
12:5:50:ILE:HD11	12:5:89:LEU:HB2	2.01	0.42
13:G:1106:CLA:H3A	13:G:1106:CLA:HBA2	1.61	0.42
2:H:7:LYS:HD2	11:W:28:TYR:CZ	2.54	0.42
2:H:236:ASN:OD1	2:H:236:ASN:N	2.49	0.42
8:T:13:ILE:HD11	16:T:4013:BCR:H281	2.02	0.42
16:T:4013:BCR:H362	16:T:4012:BCR:H17C	2.01	0.42
12:Z:26:LEU:HB3	13:Z:511:CLA:HMA1	2.01	0.42
13:a:519:CLA:HED2	13:a:519:CLA:H2A	2.02	0.42
16:a:523:BCR:H15C	16:a:523:BCR:H351	1.79	0.42
13:e:1119:CLA:H171	13:e:1129:CLA:HBC1	2.01	0.42
13:e:1138:CLA:HAA2	13:f:1228:CLA:HMB1	2.01	0.42
2:f:60:TRP:NE1	13:f:1224:CLA:OBD	2.53	0.42
2:f:174:ARG:HB2	13:f:1210:CLA:HBC2	2.01	0.42
2:f:326:LEU:HD12	2:f:326:LEU:O	2.20	0.42
2:f:338:LEU:HD21	13:f:1226:CLA:HAB	2.02	0.42
13:f:1226:CLA:H91	19:f:5002:LMG:H372	2.01	0.42
6:j:71:VAL:HG12	6:j:81:PHE:HB2	2.00	0.42
16:l:4013:BCR:H362	16:l:4012:BCR:H17C	2.01	0.42
12:q:110:HIS:HA	12:q:114:ALA:HB3	2.01	0.42
13:A:1104:CLA:H191	17:A:5001:LHG:H211	2.02	0.42
13:A:1118:CLA:H3A	9:K:61:LEU:HD23	2.01	0.42
13:A:1138:CLA:HAA2	13:B:1228:CLA:HMB1	2.01	0.42
2:B:192:GLY:O	2:B:196:HIS:HB2	2.20	0.42
13:B:1224:CLA:H141	19:B:5002:LMG:H261	2.00	0.42
17:L:5221:LHG:H151	7:k:16:PRO:HB3	2.02	0.42
12:1:34:GLN:HG2	13:1:509:CLA:HHB	2.02	0.42
12:1:289:THR:O	12:1:289:THR:CG2	2.67	0.42
16:1:523:BCR:H15C	16:1:523:BCR:H351	1.88	0.42
12:4:194:PHE:HB2	16:4:524:BCR:H391	2.01	0.42
1:G:591:ARG:HH21	1:G:594:THR:HG21	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:94:SER:HB2	13:n:1501:CLA:HMD3	2.01	0.42
16:V:4020:BCR:H15C	16:V:4020:BCR:H351	1.87	0.42
16:Y:522:BCR:H15C	16:Y:522:BCR:H351	1.80	0.42
12:c:73:LEU:HD23	12:c:73:LEU:HA	1.91	0.42
13:c:512:CLA:H3A	13:c:512:CLA:HBA1	1.68	0.42
12:d:51:SER:HB2	12:q:279:LYS:HA	2.02	0.42
1:e:115:GLN:NE2	13:e:1107:CLA:OBD	2.43	0.42
13:e:1104:CLA:H193	13:e:1104:CLA:H161	1.85	0.42
13:e:1139:CLA:H41	13:e:1139:CLA:H61	1.62	0.42
2:f:101:ILE:HG12	7:k:1:MET:HE2	2.01	0.42
2:f:380:THR:HG22	2:f:583:ALA:HB1	2.01	0.42
2:f:690:ILE:HG13	10:n:36:ILE:HG12	2.02	0.42
13:f:1229:CLA:H61	16:j:4016:BCR:HC32	2.02	0.42
16:r:523:BCR:H15C	16:r:523:BCR:H351	1.85	0.42
16:v:521:BCR:H20C	16:v:521:BCR:H361	1.80	0.42
16:A:4007:BCR:H11C	16:A:4007:BCR:H341	1.88	0.42
2:B:690:ILE:HG13	10:L:36:ILE:HG12	2.02	0.42
8:J:13:ILE:HD11	16:J:4013:BCR:H281	2.02	0.42
20:L:5216:SQD:H291	17:k:5001:LHG:H131	2.02	0.42
13:3:513:CLA:HBB1	16:3:523:BCR:H402	2.01	0.42
13:5:503:CLA:H62	13:5:503:CLA:H41	1.83	0.42
12:6:102:VAL:HG22	13:Y:505:CLA:H61	2.01	0.42
14:H:2002:PQN:H261	14:H:2002:PQN:H222	1.83	0.42
16:Y:521:BCR:H11C	16:Y:521:BCR:H341	1.88	0.42
13:b:513:CLA:HBB1	16:b:523:BCR:H402	2.02	0.42
16:b:523:BCR:H15C	16:b:523:BCR:H351	1.84	0.42
13:e:1104:CLA:H201	17:e:5001:LHG:H221	2.00	0.42
13:e:1124:CLA:H2	13:e:1124:CLA:H61	1.79	0.42
13:e:1139:CLA:H101	13:e:1139:CLA:H203	2.02	0.42
2:f:218:HIS:HD2	2:f:220:ALA:H	1.66	0.42
16:n:4019:BCR:H11C	16:n:4019:BCR:H341	1.90	0.42
12:t:141:ILE:HD13	13:t:509:CLA:H191	2.01	0.42
13:t:518:CLA:C2	13:t:518:CLA:H3A	2.50	0.42
16:t:523:BCR:H15C	16:t:523:BCR:H351	1.84	0.42
16:u:522:BCR:H20C	16:u:522:BCR:H361	1.94	0.42
12:v:79:ASP:OD1	12:v:79:ASP:N	2.48	0.42
12:v:148:PHE:CE2	13:v:512:CLA:HHB	2.55	0.42
13:A:1139:CLA:H203	13:A:1139:CLA:H101	2.02	0.42
16:A:4002:BCR:H361	16:A:4002:BCR:H20C	1.77	0.42
18:A:1849:LMU:H91	18:A:1849:LMU:H62	1.85	0.42
2:B:326:LEU:O	2:B:326:LEU:HD12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1218:CLA:HMD2	16:B:4004:BCR:H23C	2.02	0.42
13:B:1226:CLA:H91	19:B:5002:LMG:H372	2.02	0.42
16:F:4016:BCR:H371	16:F:4016:BCR:H24C	1.80	0.42
12:3:97:LEU:HG	16:3:522:BCR:H12C	2.02	0.42
12:5:221:HIS:HE1	13:5:506:CLA:NA	2.17	0.42
16:5:521:BCR:H15C	16:5:521:BCR:H351	1.85	0.42
16:6:523:BCR:H15C	16:6:523:BCR:H351	1.81	0.42
13:G:1108:CLA:HBA2	13:G:1108:CLA:H3A	1.71	0.42
12:Z:34:GLN:HG2	13:Z:509:CLA:HHB	2.00	0.42
12:a:221:HIS:CE1	13:a:506:CLA:NA	2.88	0.42
16:a:521:BCR:H24C	16:a:521:BCR:H371	1.89	0.42
16:a:524:BCR:H20C	16:a:524:BCR:H361	1.92	0.42
12:b:194:PHE:HB2	16:b:524:BCR:H391	2.01	0.42
16:b:521:BCR:H11C	16:b:521:BCR:H341	1.91	0.42
12:c:59:MET:HB2	12:c:271:PHE:HA	2.02	0.42
12:d:148:PHE:CE2	13:d:512:CLA:HHB	2.55	0.42
1:e:172:MET:HE1	13:e:1111:CLA:H92	2.00	0.42
1:e:239:ASN:HD22	1:e:263:GLN:HE22	1.67	0.42
13:e:1102:CLA:H112	13:e:1102:CLA:H151	1.73	0.42
16:e:4002:BCR:H11C	16:e:4002:BCR:H341	1.82	0.42
2:f:428:PHE:CZ	16:l:4015:BCR:HC41	2.55	0.42
13:r:502:CLA:H11	13:r:503:CLA:H161	2.00	0.42
16:r:523:BCR:H11C	16:r:523:BCR:H341	1.88	0.42
13:s:519:CLA:HED2	13:s:519:CLA:H2A	2.02	0.42
12:t:130:PHE:HA	12:t:137:GLN:HG2	2.02	0.42
13:t:505:CLA:H91	13:t:505:CLA:H112	1.86	0.42
2:B:101:ILE:HG12	7:I:1:MET:HE2	2.02	0.42
16:L:4022:BCR:H24C	16:L:4022:BCR:H371	1.85	0.42
13:4:513:CLA:HBB1	16:4:523:BCR:H402	2.02	0.42
16:6:521:BCR:H361	16:6:521:BCR:H20C	1.80	0.42
1:G:239:ASN:HD22	1:G:263:GLN:HE22	1.67	0.42
13:G:1140:CLA:H11	13:G:1140:CLA:CHA	2.50	0.42
2:H:464:GLN:HG2	2:H:509:PHE:CD1	2.55	0.42
13:Y:517:CLA:HBA1	13:Y:517:CLA:H3A	1.76	0.42
3:g:61:ASP:HA	3:g:62:PHE:HA	1.83	0.42
12:u:79:ASP:OD1	12:u:79:ASP:N	2.45	0.42
16:u:522:BCR:H351	16:u:522:BCR:H15C	1.75	0.42
12:v:97:LEU:HG	16:v:522:BCR:H12C	2.00	0.42
2:B:464:GLN:HG2	2:B:509:PHE:CD1	2.55	0.41
6:F:150:LYS:HB3	6:F:153:GLU:HG3	2.01	0.41
13:2:518:CLA:H41	13:2:518:CLA:H61	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:148:PHE:CE2	13:6:512:CLA:HHB	2.55	0.41
1:G:544:PHE:CZ	16:V:4219:BCR:H332	2.54	0.41
13:G:1116:CLA:HBA2	13:G:1116:CLA:H3A	1.46	0.41
13:G:1138:CLA:H202	13:G:1138:CLA:H162	1.88	0.41
2:H:326:LEU:HD12	2:H:326:LEU:O	2.20	0.41
2:H:376:GLN:O	2:H:380:THR:OG1	2.33	0.41
2:H:531:THR:O	2:H:535:VAL:HB	2.19	0.41
13:H:1219:CLA:H192	13:H:1219:CLA:H162	1.84	0.41
17:H:1855:LHG:HC82	17:H:1855:LHG:H112	1.93	0.41
16:V:4022:BCR:H371	16:V:4022:BCR:H24C	1.85	0.41
12:Y:34:GLN:HG2	13:Y:509:CLA:HHB	2.02	0.41
12:Y:50:ILE:HD11	12:Y:89:LEU:HB2	2.02	0.41
13:a:503:CLA:H18	13:a:510:CLA:HBB2	2.00	0.41
16:c:523:BCR:H15C	16:c:523:BCR:H351	1.79	0.41
16:c:524:BCR:H20C	16:c:524:BCR:H361	1.94	0.41
1:e:312:ILE:HD13	1:e:312:ILE:HA	1.87	0.41
1:e:704:TYR:OH	13:e:1013:CLA:OBD	2.28	0.41
13:e:1136:CLA:H92	13:e:1136:CLA:H62	1.82	0.41
2:f:493:TYR:HE2	13:f:1231:CLA:HED1	1.84	0.41
16:f:4006:BCR:H351	16:f:4006:BCR:H15C	1.83	0.41
13:q:502:CLA:HBD	13:q:503:CLA:H43	2.01	0.41
12:r:148:PHE:CE2	13:r:512:CLA:HHB	2.55	0.41
12:s:221:HIS:CE1	13:s:506:CLA:NA	2.88	0.41
16:s:521:BCR:H15C	16:s:521:BCR:H351	1.82	0.41
12:u:50:ILE:HD11	12:u:89:LEU:HB2	2.01	0.41
12:v:246:LEU:HD23	12:v:246:LEU:HA	1.92	0.41
1:A:141:SER:HB3	13:A:1126:CLA:HAA2	2.02	0.41
13:A:1104:CLA:H3A	13:A:1128:CLA:CAB	2.51	0.41
2:B:60:TRP:NE1	13:B:1224:CLA:OBD	2.53	0.41
2:B:338:LEU:HD21	13:B:1226:CLA:HAB	2.02	0.41
2:B:428:PHE:CZ	16:J:4015:BCR:HC41	2.55	0.41
2:B:631:LEU:O	2:B:647:SER:OG	2.29	0.41
16:K:4104:BCR:H11C	16:K:4104:BCR:H341	1.91	0.41
12:1:147:LEU:HD12	12:1:215:ILE:HG12	2.01	0.41
12:3:221:HIS:CE1	13:3:506:CLA:NA	2.88	0.41
12:6:42:ALA:O	12:6:46:THR:OG1	2.33	0.41
16:G:4008:BCR:H11C	16:G:4008:BCR:H341	1.89	0.41
2:H:174:ARG:HB2	13:H:1210:CLA:HBC2	2.01	0.41
2:H:338:LEU:HD21	13:H:1226:CLA:HAB	2.02	0.41
13:H:1234:CLA:H193	13:H:1234:CLA:H161	1.87	0.41
12:Y:110:HIS:HA	12:Y:114:ALA:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:518:CLA:H102	13:Y:518:CLA:H62	1.85	0.41
13:a:505:CLA:H92	13:a:505:CLA:H61	1.89	0.41
13:b:518:CLA:C2	13:b:518:CLA:H3A	2.50	0.41
1:e:570:SER:HB2	1:e:575:PRO:HA	2.03	0.41
1:e:691:TRP:CE2	13:e:1011:CLA:HBA2	2.54	0.41
13:e:1116:CLA:H93	13:e:1116:CLA:H61	1.90	0.41
17:e:5001:LHG:H372	17:e:5001:LHG:H341	1.82	0.41
2:f:464:GLN:HG2	2:f:509:PHE:CD1	2.55	0.41
14:f:2002:PQN:H211	14:f:2002:PQN:H172	1.88	0.41
16:u:524:BCR:H11C	16:u:524:BCR:H341	1.92	0.41
13:A:1106:CLA:H3A	13:A:1106:CLA:HBA2	1.61	0.41
13:A:1116:CLA:H91	13:A:1116:CLA:H111	1.83	0.41
13:A:1140:CLA:H11	13:A:1140:CLA:CHA	2.50	0.41
2:B:194:LEU:HA	2:B:198:ALA:HB3	2.02	0.41
2:B:276:HIS:HE2	13:B:1215:CLA:C2B	2.33	0.41
7:I:4:ASP:OD1	7:I:4:ASP:N	2.42	0.41
16:J:4013:BCR:H362	16:J:4012:BCR:H17C	2.01	0.41
13:3:519:CLA:HED2	13:3:519:CLA:H2A	2.02	0.41
12:6:148:PHE:HE2	13:6:512:CLA:HHB	1.84	0.41
13:G:1104:CLA:H161	13:G:1104:CLA:H193	1.85	0.41
13:G:1126:CLA:H192	13:G:1126:CLA:H161	1.96	0.41
2:H:493:TYR:HE2	13:H:1231:CLA:HED1	1.84	0.41
13:H:1226:CLA:H112	13:H:1226:CLA:H71	1.92	0.41
5:Q:53:ASP:OD1	5:Q:53:ASP:N	2.44	0.41
9:U:47:PRO:HG2	20:Y:822:SQD:H241	2.03	0.41
13:V:1503:CLA:H93	13:V:1503:CLA:H61	1.90	0.41
12:a:261:ALA:HA	12:a:276:LEU:HD12	2.02	0.41
1:e:468:ILE:HG23	13:e:1022:CLA:H61	2.02	0.41
2:f:192:GLY:O	2:f:196:HIS:HB2	2.20	0.41
2:f:237:PRO:HB3	2:f:256:THR:HG21	2.02	0.41
2:f:499:ASP:O	2:f:503:SER:HB3	2.20	0.41
13:f:1023:CLA:H202	13:f:1023:CLA:H162	1.94	0.41
13:f:1218:CLA:HMD2	16:f:4004:BCR:H23C	2.02	0.41
13:j:1301:CLA:H72	13:j:1301:CLA:H111	1.78	0.41
12:q:79:ASP:OD1	12:q:79:ASP:N	2.53	0.41
2:B:631:LEU:HD22	2:B:724:PHE:HA	2.02	0.41
16:B:4004:BCR:H361	16:B:4004:BCR:H20C	1.75	0.41
16:B:4010:BCR:H20C	16:B:4010:BCR:H361	1.92	0.41
16:K:4104:BCR:H20C	16:K:4104:BCR:H361	1.87	0.41
13:1:502:CLA:HBD	13:1:503:CLA:H43	2.01	0.41
12:2:34:GLN:HG2	13:2:509:CLA:HHB	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:193:HIS:HB2	12:2:196:SER:HB3	2.00	0.41
12:4:130:PHE:HA	12:4:137:GLN:HG2	2.02	0.41
1:G:258:VAL:O	1:G:262:SER:HB2	2.21	0.41
1:G:573:LEU:O	4:O:61:ARG:NH2	2.49	0.41
1:G:691:TRP:O	1:G:694:SER:OG	2.30	0.41
13:G:1103:CLA:H3A	13:G:1103:CLA:HBA1	1.54	0.41
14:G:2001:PQN:H162	16:H:4014:BCR:H382	2.03	0.41
16:G:4002:BCR:H24C	16:G:4002:BCR:H371	1.82	0.41
2:H:276:HIS:HE2	13:H:1215:CLA:C2B	2.34	0.41
2:H:428:PHE:CZ	16:T:4015:BCR:HC41	2.55	0.41
2:H:690:ILE:HG13	10:V:36:ILE:HG12	2.02	0.41
13:H:1203:CLA:H12	13:H:1226:CLA:HBA1	2.02	0.41
13:H:1226:CLA:H91	19:H:5002:LMG:H372	2.01	0.41
14:H:2002:PQN:H211	14:H:2002:PQN:H172	1.88	0.41
13:e:1120:CLA:C1B	13:e:1120:CLA:H2	2.50	0.41
13:e:1123:CLA:H162	13:e:1123:CLA:H193	1.83	0.41
13:e:1138:CLA:H202	13:e:1138:CLA:H162	1.88	0.41
16:e:4007:BCR:H15C	16:e:4007:BCR:H351	1.79	0.41
13:f:1204:CLA:H93	13:f:1204:CLA:H61	1.92	0.41
16:f:4009:BCR:H11C	16:f:4009:BCR:H341	1.86	0.41
12:q:147:LEU:HD12	12:q:215:ILE:HG12	2.01	0.41
16:r:521:BCR:H371	16:r:521:BCR:H24C	1.78	0.41
12:s:148:PHE:HD2	13:s:512:CLA:H3A	1.85	0.41
1:A:468:ILE:HG23	13:A:1022:CLA:H61	2.02	0.41
13:A:1129:CLA:H11	13:A:1129:CLA:H51	1.80	0.41
13:B:1229:CLA:H61	16:F:4016:BCR:HC32	2.02	0.41
12:3:261:ALA:HA	12:3:276:LEU:HD12	2.02	0.41
13:4:518:CLA:C2	13:4:518:CLA:H3A	2.50	0.41
13:G:1124:CLA:H61	13:G:1124:CLA:H2	1.79	0.41
13:H:1229:CLA:H61	16:R:4016:BCR:HC32	2.02	0.41
6:R:90:TYR:OH	6:R:132:PHE:O	2.33	0.41
12:Y:289:THR:O	12:Y:289:THR:CG2	2.67	0.41
16:Y:524:BCR:H20C	16:Y:524:BCR:H361	1.91	0.41
12:Z:148:PHE:CE2	13:Z:512:CLA:HHB	2.55	0.41
12:Z:261:ALA:HA	12:Z:276:LEU:HD12	2.01	0.41
13:a:513:CLA:H143	13:a:513:CLA:H111	1.92	0.41
13:e:1108:CLA:H41	13:e:1108:CLA:H61	1.78	0.41
13:e:1109:CLA:H141	13:e:1109:CLA:H161	1.82	0.41
13:e:1126:CLA:H3A	13:e:1126:CLA:HBA2	1.60	0.41
2:f:631:LEU:HD22	2:f:724:PHE:HA	2.02	0.41
2:f:658:ALA:HB3	13:f:1023:CLA:HBB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:696:LYS:HA	2:f:697:PRO:HD3	1.96	0.41
16:f:4017:BCR:H20C	16:f:4017:BCR:H361	1.89	0.41
16:f:4009:BCR:H15C	16:f:4009:BCR:H351	1.82	0.41
4:h:77:LYS:HD3	4:h:77:LYS:HA	1.92	0.41
9:m:68:HIS:O	9:m:72:ILE:HG12	2.20	0.41
12:q:50:ILE:HD11	12:q:89:LEU:HB2	2.02	0.41
13:r:513:CLA:H143	13:r:513:CLA:H111	1.91	0.41
12:v:91:VAL:HG22	16:v:523:BCR:HC22	2.02	0.41
1:A:258:VAL:O	1:A:262:SER:HB2	2.21	0.41
13:A:1237:CLA:HAB	2:B:691:VAL:HG11	2.03	0.41
13:B:1219:CLA:H61	13:B:1219:CLA:H92	1.91	0.41
16:B:4017:BCR:H20C	16:B:4017:BCR:H361	1.89	0.41
13:L:1501:CLA:H112	16:L:4022:BCR:H10C	2.03	0.41
16:1:522:BCR:H24C	16:1:522:BCR:H371	1.84	0.41
12:2:91:VAL:HG22	16:2:523:BCR:HC22	2.03	0.41
12:5:107:ALA:O	12:5:111:THR:OG1	2.30	0.41
1:G:271:GLY:O	1:G:283:TYR:OH	2.29	0.41
1:G:441:VAL:HA	1:G:444:HIS:CE1	2.56	0.41
2:H:192:GLY:O	2:H:196:HIS:HB2	2.20	0.41
2:H:236:ASN:OD1	2:H:252:THR:OG1	2.39	0.41
2:H:355:MET:HE3	2:H:355:MET:HB2	1.79	0.41
2:H:499:ASP:O	2:H:503:SER:HB3	2.20	0.41
2:H:714:THR:HG21	19:H:5002:LMG:H402	2.03	0.41
16:R:4016:BCR:H11C	16:R:4016:BCR:H341	1.77	0.41
13:Z:518:CLA:H111	13:Z:518:CLA:H142	1.85	0.41
12:a:97:LEU:HG	16:a:522:BCR:H12C	2.02	0.41
12:b:34:GLN:OE1	13:b:510:CLA:NC	2.54	0.41
12:d:148:PHE:HE2	13:d:512:CLA:HHB	1.84	0.41
12:d:207:HIS:CE1	16:d:524:BCR:H381	2.56	0.41
16:d:521:BCR:H20C	16:d:521:BCR:H361	1.80	0.41
13:e:1104:CLA:H3A	13:e:1128:CLA:CAB	2.51	0.41
13:e:1022:CLA:H122	16:f:4017:BCR:H12C	2.03	0.41
13:f:1219:CLA:H192	13:f:1219:CLA:H162	1.84	0.41
13:r:505:CLA:HBA2	13:r:505:CLA:H11	1.88	0.41
12:s:261:ALA:HA	12:s:276:LEU:HD12	2.02	0.41
12:t:34:GLN:OE1	13:t:510:CLA:NC	2.54	0.41
1:A:120:ILE:HG13	1:A:121:PHE:CD2	2.56	0.41
13:A:1137:CLA:H93	13:A:1137:CLA:H111	1.91	0.41
13:A:1138:CLA:H91	13:F:1301:CLA:HAC2	2.03	0.41
14:A:2001:PQN:H2M1	14:A:2001:PQN:H111	1.91	0.41
20:B:1852:SQD:O3	10:V:3:GLN:NE2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:8:LEU:HA	8:J:13:ILE:HG21	2.02	0.41
16:L:4219:BCR:H393	17:L:5221:LHG:H322	2.03	0.41
17:L:5220:LHG:H311	17:L:5220:LHG:H171	2.02	0.41
13:2:505:CLA:HBC2	16:2:524:BCR:H341	2.03	0.41
13:2:506:CLA:H41	13:2:506:CLA:H62	1.71	0.41
12:3:233:VAL:HG13	16:3:524:BCR:HC21	2.03	0.41
16:5:522:BCR:H351	16:5:522:BCR:H15C	1.75	0.41
16:6:521:BCR:H15C	16:6:521:BCR:H351	1.83	0.41
16:6:522:BCR:H371	16:6:522:BCR:H24C	1.82	0.41
1:G:572:ARG:HD3	3:N:80:ALA:HB3	2.03	0.41
1:G:704:TYR:OH	13:G:1013:CLA:OBD	2.28	0.41
13:G:1131:CLA:HBB2	10:V:65:LEU:HD13	2.02	0.41
13:G:1135:CLA:H62	13:G:1135:CLA:H41	1.79	0.41
2:H:394:LEU:HD23	2:H:394:LEU:HA	1.92	0.41
17:V:5220:LHG:H311	17:V:5220:LHG:H171	2.01	0.41
16:a:522:BCR:H24C	16:a:522:BCR:H371	1.87	0.41
13:c:501:CLA:H62	13:c:501:CLA:H41	1.70	0.41
1:e:120:ILE:HG13	1:e:121:PHE:CD2	2.56	0.41
1:e:141:SER:HB3	13:e:1126:CLA:HAA2	2.02	0.41
1:e:572:ARG:HD3	3:g:80:ALA:HB3	2.03	0.41
13:e:1121:CLA:HAB	13:e:1801:CLA:CAB	2.50	0.41
2:f:714:THR:HG21	19:f:5002:LMG:H402	2.03	0.41
8:l:8:LEU:HA	8:l:13:ILE:HG21	2.02	0.41
16:q:524:BCR:H24C	16:q:524:BCR:H371	1.90	0.41
12:v:47:LEU:HD21	12:v:90:PHE:HD1	1.86	0.41
13:A:1104:CLA:H41	13:A:1104:CLA:H62	1.64	0.41
16:A:4008:BCR:H20C	16:A:4008:BCR:H361	1.84	0.41
2:B:380:THR:HG22	2:B:583:ALA:HB1	2.02	0.41
13:B:1205:CLA:H193	13:B:1205:CLA:H161	1.91	0.41
5:E:18:TRP:HB3	5:E:21:GLU:HB2	2.03	0.41
6:F:150:LYS:HD3	6:F:150:LYS:HA	1.72	0.41
17:L:5221:LHG:H121	13:f:1207:CLA:CMA	2.51	0.41
16:1:524:BCR:H20C	16:1:524:BCR:H361	1.91	0.41
12:6:47:LEU:HD21	12:6:90:PHE:HD1	1.86	0.41
16:6:524:BCR:H11C	16:6:524:BCR:H341	1.88	0.41
1:G:256:LEU:HD12	13:G:1114:CLA:HBC2	2.03	0.41
13:G:1136:CLA:H62	13:G:1136:CLA:H92	1.82	0.41
13:G:1237:CLA:HAB	2:H:691:VAL:HG11	2.03	0.41
10:V:149:THR:HG22	10:V:151:TYR:H	1.86	0.41
16:b:524:BCR:H11C	16:b:524:BCR:H341	1.83	0.41
13:c:505:CLA:H42	16:c:524:BCR:HC7	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:512:CLA:HED2	13:d:512:CLA:H2A	2.03	0.41
16:d:521:BCR:H371	16:d:521:BCR:H24C	1.82	0.41
13:e:1131:CLA:HBB2	10:n:65:LEU:HD13	2.02	0.41
13:e:1135:CLA:HAB	13:e:1135:CLA:HHC	1.87	0.41
2:f:34:HIS:HE1	13:f:1201:CLA:HED1	1.86	0.41
8:l:13:ILE:HD11	16:l:4013:BCR:H281	2.02	0.41
10:n:149:THR:HG22	10:n:151:TYR:H	1.86	0.41
16:n:4219:BCR:H393	17:n:5221:LHG:H322	2.03	0.41
16:o:4021:BCR:H15C	16:o:4021:BCR:H351	1.84	0.41
16:o:4021:BCR:H24C	16:o:4021:BCR:H371	1.85	0.41
12:r:147:LEU:HD12	12:r:215:ILE:HG12	2.03	0.41
16:r:524:BCR:H351	16:r:524:BCR:H15C	1.78	0.41
13:s:510:CLA:H143	13:s:510:CLA:H111	1.91	0.41
13:t:513:CLA:HBB1	16:t:523:BCR:H402	2.02	0.41
16:t:524:BCR:H24C	16:t:524:BCR:H371	1.92	0.41
1:A:145:GLN:HB3	1:A:388:TYR:HB3	2.02	0.41
13:A:1120:CLA:H2	13:A:1120:CLA:C1B	2.50	0.41
2:B:714:THR:HG21	19:B:5002:LMG:H402	2.03	0.41
4:D:58:TYR:H	10:L:13:GLU:HG2	1.86	0.41
9:K:47:PRO:HG2	20:1:822:SQD:H241	2.02	0.41
20:L:5216:SQD:H241	7:k:29:LEU:HB3	2.02	0.41
13:1:505:CLA:H61	12:v:102:VAL:HG22	2.02	0.41
12:2:289:THR:HG22	12:2:289:THR:O	2.21	0.41
12:3:68:PRO:HB3	12:3:271:PHE:HB3	2.03	0.41
12:3:148:PHE:HD2	13:3:512:CLA:H3A	1.85	0.41
13:3:511:CLA:H2	16:3:522:BCR:H282	2.03	0.41
16:3:522:BCR:H24C	16:3:522:BCR:H371	1.87	0.41
16:3:524:BCR:H20C	16:3:524:BCR:H361	1.91	0.41
13:5:501:CLA:H62	13:5:501:CLA:H41	1.70	0.41
12:6:177:VAL:HG13	12:6:201:GLU:HG2	2.02	0.41
13:6:512:CLA:HED2	13:6:512:CLA:H2A	2.03	0.41
1:G:145:GLN:HB3	1:G:388:TYR:HB3	2.02	0.41
1:G:601:ASP:HA	1:G:604:PHE:HB3	2.03	0.41
13:G:1120:CLA:C1B	13:G:1120:CLA:H2	2.50	0.41
13:G:1123:CLA:H141	13:G:1123:CLA:H161	1.80	0.41
2:H:262:HIS:HA	2:H:263:PRO:HD3	1.98	0.41
2:H:631:LEU:HD22	2:H:724:PHE:HA	2.02	0.41
16:H:4004:BCR:H361	16:H:4004:BCR:H20C	1.75	0.41
16:H:4005:BCR:H15C	16:H:4005:BCR:H351	1.81	0.41
4:O:58:TYR:H	10:V:13:GLU:HG2	1.86	0.41
16:S:4018:BCR:H11C	16:S:4018:BCR:H341	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:4018:BCR:H24C	16:S:4018:BCR:H371	1.90	0.41
16:U:4104:BCR:H24C	20:Y:822:SQD:H341	2.03	0.41
10:V:85:LEU:HA	10:V:85:LEU:HD12	1.86	0.41
16:W:4021:BCR:H15C	16:W:4021:BCR:H351	1.84	0.41
12:Z:229:TRP:HA	12:Z:232:LYS:HB2	2.03	0.41
12:a:233:VAL:HG13	16:a:524:BCR:HC21	2.03	0.41
12:d:47:LEU:HD21	12:d:90:PHE:HD1	1.86	0.41
1:e:145:GLN:HB3	1:e:388:TYR:HB3	2.02	0.41
13:e:1137:CLA:H93	13:e:1137:CLA:H111	1.91	0.41
2:f:142:LEU:HG	16:f:4006:BCR:H382	2.02	0.41
13:f:1203:CLA:H12	13:f:1226:CLA:HBA1	2.02	0.41
13:f:1217:CLA:H41	13:f:1217:CLA:H61	1.73	0.41
9:m:8:ILE:HA	9:m:9:PRO:HD3	1.93	0.41
16:q:522:BCR:H24C	16:q:522:BCR:H371	1.84	0.41
13:r:510:CLA:H41	13:r:510:CLA:H62	1.81	0.41
12:s:68:PRO:HB3	12:s:271:PHE:HB3	2.02	0.41
12:s:233:VAL:HG13	16:s:524:BCR:HC21	2.03	0.41
12:t:194:PHE:HB2	16:t:524:BCR:H391	2.01	0.41
12:u:59:MET:HB2	12:u:271:PHE:HA	2.02	0.41
12:v:177:VAL:HG13	12:v:201:GLU:HG2	2.02	0.41
1:A:573:LEU:O	4:D:61:ARG:NH2	2.49	0.41
13:A:1121:CLA:HAB	13:A:1801:CLA:CAB	2.50	0.41
14:A:2001:PQN:H162	16:B:4014:BCR:H382	2.03	0.41
2:B:236:ASN:OD1	2:B:252:THR:OG1	2.39	0.41
2:B:499:ASP:O	2:B:503:SER:HB3	2.20	0.41
13:B:1240:CLA:H62	13:B:1240:CLA:H41	1.88	0.41
13:J:1303:CLA:H62	13:J:1303:CLA:H41	1.83	0.41
12:5:59:MET:HB2	12:5:271:PHE:HA	2.02	0.41
13:5:505:CLA:H42	16:5:524:BCR:HC7	2.02	0.41
12:6:243:SER:O	12:6:318:HIS:ND1	2.54	0.41
1:G:148:ARG:HD3	1:G:389:PRO:HB2	2.03	0.41
13:G:1137:CLA:H93	13:G:1137:CLA:H61	1.94	0.41
13:G:1237:CLA:H202	16:V:4019:BCR:H391	2.03	0.41
13:G:1101:CLA:H102	13:G:1101:CLA:H62	1.84	0.41
2:H:142:LEU:HG	16:H:4006:BCR:H382	2.02	0.41
2:H:194:LEU:HA	2:H:198:ALA:HB3	2.02	0.41
13:H:1217:CLA:H61	13:H:1217:CLA:H41	1.73	0.41
16:T:4012:BCR:H20C	16:T:4012:BCR:H361	1.94	0.41
16:V:4022:BCR:H11C	16:V:4022:BCR:H341	1.84	0.41
12:Y:79:ASP:OD1	12:Y:79:ASP:N	2.54	0.41
12:Z:91:VAL:HG22	16:Z:523:BCR:HC22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:148:PHE:HD2	13:a:512:CLA:H3A	1.85	0.41
13:d:517:CLA:HBB1	16:d:524:BCR:H352	2.04	0.41
16:d:524:BCR:H24C	16:d:524:BCR:H371	1.87	0.41
1:e:256:LEU:HD12	13:e:1114:CLA:HBC2	2.03	0.41
1:e:308:HIS:HE2	13:e:1117:CLA:C2B	2.34	0.41
13:e:1104:CLA:H191	17:e:5001:LHG:H211	2.02	0.41
16:e:4003:BCR:H11C	16:e:4003:BCR:H341	1.90	0.41
2:f:194:LEU:HA	2:f:198:ALA:HB3	2.02	0.41
2:f:276:HIS:HE2	13:f:1215:CLA:C2B	2.33	0.41
2:f:321:GLY:O	2:f:325:THR:OG1	2.28	0.41
2:f:455:ILE:HD13	6:j:69:LEU:HB2	2.03	0.41
13:f:1223:CLA:H102	13:f:1223:CLA:H61	1.97	0.41
16:j:4016:BCR:H11C	16:j:4016:BCR:H341	1.77	0.41
8:l:26:LEU:HD13	16:l:4012:BCR:HC7	2.02	0.41
16:m:4104:BCR:H24C	20:q:822:SQD:H341	2.03	0.41
1:A:18:LYS:HA	1:A:18:LYS:HD2	1.94	0.40
1:A:459:LEU:O	1:A:463:SER:OG	2.37	0.40
2:B:142:LEU:HG	16:B:4006:BCR:H382	2.02	0.40
2:B:658:ALA:HB3	13:B:1023:CLA:HBB2	2.02	0.40
13:B:1206:CLA:H3A	13:B:1206:CLA:HBA1	1.58	0.40
16:L:4020:BCR:H20C	16:L:4020:BCR:H361	1.89	0.40
12:1:50:ILE:HD11	12:1:89:LEU:HB2	2.02	0.40
12:1:332:ARG:HA	12:1:335:LYS:HB3	2.03	0.40
13:2:518:CLA:H142	13:2:518:CLA:H111	1.85	0.40
12:5:177:VAL:HG13	12:5:201:GLU:HG2	2.04	0.40
1:G:468:ILE:HG23	13:G:1022:CLA:H61	2.02	0.40
13:G:1104:CLA:H3A	13:G:1128:CLA:CAB	2.51	0.40
16:G:4007:BCR:H371	16:G:4007:BCR:H24C	1.89	0.40
2:H:237:PRO:HB3	2:H:256:THR:HG21	2.02	0.40
13:H:1218:CLA:HMD2	16:H:4004:BCR:H23C	2.02	0.40
16:U:4104:BCR:H15C	16:U:4104:BCR:H351	1.84	0.40
16:V:4219:BCR:H393	17:V:5221:LHG:H322	2.03	0.40
12:b:130:PHE:HA	12:b:137:GLN:HG2	2.02	0.40
13:e:1126:CLA:H143	13:e:1126:CLA:H112	1.87	0.40
13:e:1128:CLA:H91	13:e:1128:CLA:H112	1.89	0.40
13:e:1137:CLA:H62	13:e:1137:CLA:H41	1.80	0.40
16:f:4009:BCR:H321	17:f:1842:LHG:H322	2.03	0.40
4:h:58:TYR:H	10:n:13:GLU:HG2	1.86	0.40
16:q:523:BCR:H15C	16:q:523:BCR:H351	1.88	0.40
12:r:229:TRP:HA	12:r:232:LYS:HB2	2.03	0.40
12:s:246:LEU:HD23	12:s:246:LEU:HA	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:523:BCR:H351	16:u:523:BCR:H15C	1.80	0.40
16:v:523:BCR:H15C	16:v:523:BCR:H351	1.81	0.40
1:A:256:LEU:HD12	13:A:1114:CLA:HBC2	2.03	0.40
1:A:669:VAL:HG22	1:A:757:ALA:HB3	2.04	0.40
13:A:1115:CLA:H142	13:A:1115:CLA:H112	1.92	0.40
12:2:57:GLN:HB2	12:2:62:GLN:HE21	1.86	0.40
12:2:229:TRP:HA	12:2:232:LYS:HB2	2.03	0.40
12:4:34:GLN:OE1	13:4:510:CLA:NC	2.54	0.40
13:4:509:CLA:H3A	13:4:509:CLA:HBA1	1.87	0.40
1:G:141:SER:HB3	13:G:1126:CLA:HAA2	2.02	0.40
13:G:1107:CLA:H152	16:T:4012:BCR:H272	2.03	0.40
13:H:1201:CLA:H2	16:W:4021:BCR:HC31	2.03	0.40
16:H:4010:BCR:H20C	16:H:4010:BCR:H361	1.92	0.40
12:Y:332:ARG:HA	12:Y:335:LYS:HB3	2.03	0.40
16:b:524:BCR:H15C	16:b:524:BCR:H351	1.80	0.40
13:e:1107:CLA:H152	16:l:4012:BCR:H272	2.03	0.40
13:e:1128:CLA:H142	13:e:1128:CLA:H111	1.87	0.40
13:e:1237:CLA:HAB	2:f:691:VAL:HG11	2.03	0.40
7:k:23:PRO:O	7:k:27:MET:HB2	2.21	0.40
12:s:97:LEU:HG	16:s:522:BCR:H12C	2.02	0.40
13:A:1137:CLA:H122	16:A:4007:BCR:H393	2.04	0.40
13:B:1221:CLA:H112	13:B:1221:CLA:H151	1.82	0.40
13:B:1229:CLA:H192	16:F:4016:BCR:H17C	2.04	0.40
16:B:4009:BCR:H321	17:B:1842:LHG:H322	2.03	0.40
13:3:513:CLA:H143	13:3:513:CLA:H111	1.91	0.40
16:4:521:BCR:H24C	16:4:521:BCR:H371	1.91	0.40
12:6:20:PHE:HA	12:6:23:LEU:HD12	2.03	0.40
12:6:207:HIS:CE1	16:6:524:BCR:H381	2.56	0.40
1:G:120:ILE:HG13	1:G:121:PHE:CD2	2.56	0.40
1:G:570:SER:HB2	1:G:575:PRO:HA	2.03	0.40
13:G:1117:CLA:H203	13:G:1125:CLA:HAA1	2.03	0.40
13:G:1139:CLA:H101	13:G:1139:CLA:H203	2.02	0.40
16:G:4007:BCR:H11C	16:G:4007:BCR:H341	1.88	0.40
16:G:4007:BCR:H15C	16:G:4007:BCR:H351	1.79	0.40
2:H:60:TRP:NE1	13:H:1224:CLA:OBD	2.53	0.40
13:H:1213:CLA:H3A	13:H:1213:CLA:HBA2	1.84	0.40
16:H:4009:BCR:H321	17:H:1842:LHG:H322	2.03	0.40
16:T:4015:BCR:H15C	16:T:4015:BCR:H351	1.79	0.40
13:V:1501:CLA:H112	16:V:4022:BCR:H10C	2.03	0.40
16:V:4020:BCR:H24C	16:V:4020:BCR:H371	1.71	0.40
12:Y:261:ALA:HA	12:Y:276:LEU:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:147:LEU:HD12	12:Z:215:ILE:HG12	2.03	0.40
13:Z:513:CLA:H143	13:Z:513:CLA:H111	1.91	0.40
12:d:91:VAL:HG22	16:d:523:BCR:HC22	2.02	0.40
12:d:127:ARG:O	12:d:137:GLN:NE2	2.50	0.40
1:e:221:LEU:HD23	1:e:221:LEU:HA	1.89	0.40
13:e:1119:CLA:H111	13:e:1119:CLA:H152	1.87	0.40
16:e:4001:BCR:H11C	16:e:4001:BCR:H341	1.87	0.40
13:f:1234:CLA:H71	13:f:1235:CLA:H12	2.03	0.40
5:i:18:TRP:HB3	5:i:21:GLU:HB2	2.03	0.40
16:l:4013:BCR:H351	16:l:4013:BCR:H15C	1.82	0.40
13:n:1501:CLA:H102	13:n:1503:CLA:H122	2.03	0.40
17:n:5221:LHG:H241	17:n:5221:LHG:HC92	2.03	0.40
12:q:332:ARG:HA	12:q:335:LYS:HB3	2.03	0.40
13:q:518:CLA:H41	13:q:518:CLA:H61	1.73	0.40
16:q:522:BCR:H15C	16:q:522:BCR:H351	1.80	0.40
16:r:524:BCR:H11C	16:r:524:BCR:H341	1.97	0.40
12:s:182:LEU:O	12:s:209:TYR:OH	2.37	0.40
12:t:119:ALA:O	12:t:126:LYS:NZ	2.41	0.40
12:v:47:LEU:HD23	12:v:47:LEU:HA	1.94	0.40
12:v:207:HIS:CE1	16:v:524:BCR:H381	2.56	0.40
16:v:523:BCR:H20C	16:v:523:BCR:H361	1.93	0.40
16:v:524:BCR:H371	16:v:524:BCR:H24C	1.87	0.40
1:A:345:THR:HG21	17:A:5003:LHG:HC11	2.04	0.40
13:A:1022:CLA:H122	16:B:4017:BCR:H12C	2.02	0.40
2:B:455:ILE:HD13	6:F:69:LEU:HB2	2.03	0.40
13:1:505:CLA:HBA1	12:v:105:ALA:O	2.21	0.40
16:2:522:BCR:H24C	16:2:522:BCR:H371	1.86	0.40
12:6:91:VAL:HG22	16:6:523:BCR:HC22	2.02	0.40
16:G:4001:BCR:H11C	16:G:4001:BCR:H341	1.87	0.40
2:H:721:TYR:HB2	13:H:1021:CLA:HED3	2.03	0.40
20:H:1852:SQD:C9	17:e:5002:LHG:C23	2.90	0.40
8:T:8:LEU:HA	8:T:13:ILE:HG21	2.02	0.40
13:V:1501:CLA:H102	13:V:1503:CLA:H122	2.04	0.40
1:e:441:VAL:HA	1:e:444:HIS:CE1	2.56	0.40
2:f:236:ASN:OD1	2:f:252:THR:OG1	2.39	0.40
2:f:657:TRP:CZ3	13:f:1021:CLA:HHB	2.57	0.40
13:f:1213:CLA:H141	13:f:1213:CLA:H162	1.80	0.40
13:n:1501:CLA:H112	16:n:4022:BCR:H10C	2.03	0.40
16:t:521:BCR:H15C	16:t:521:BCR:H351	1.93	0.40
1:A:572:ARG:HD3	3:C:80:ALA:HB3	2.03	0.40
13:A:1128:CLA:H91	13:A:1128:CLA:H112	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:PRO:HB3	2:B:256:THR:HG21	2.02	0.40
2:B:657:TRP:CZ3	13:B:1021:CLA:HHB	2.57	0.40
13:B:1227:CLA:HMC1	13:B:1236:CLA:HAB	2.03	0.40
16:K:4104:BCR:H15C	16:K:4104:BCR:H351	1.84	0.40
13:3:503:CLA:H62	13:3:503:CLA:H101	1.89	0.40
12:4:54:THR:HG22	12:4:56:ASP:H	1.87	0.40
13:4:517:CLA:HBA1	13:4:517:CLA:H3A	1.68	0.40
12:5:73:LEU:HD23	12:5:73:LEU:HA	1.91	0.40
13:6:517:CLA:HBB1	16:6:524:BCR:H352	2.03	0.40
1:G:215:HIS:CE1	13:G:1112:CLA:NA	2.90	0.40
16:G:4002:BCR:H361	16:G:4002:BCR:H20C	1.77	0.40
2:H:452:GLN:NE2	2:H:614:THR:OG1	2.55	0.40
2:H:455:ILE:HD13	6:R:69:LEU:HB2	2.03	0.40
13:H:1206:CLA:H3A	13:H:1206:CLA:HBA1	1.58	0.40
13:H:1234:CLA:H71	13:H:1235:CLA:H12	2.03	0.40
16:H:4010:BCR:H15C	16:H:4010:BCR:H351	1.74	0.40
5:Q:18:TRP:HB3	5:Q:21:GLU:HB2	2.03	0.40
13:Z:511:CLA:H93	13:Z:511:CLA:H61	1.91	0.40
12:b:54:THR:HG22	12:b:56:ASP:H	1.87	0.40
12:b:273:GLY:O	12:b:300:ARG:NH2	2.45	0.40
16:c:522:BCR:H24C	16:c:522:BCR:H371	1.84	0.40
12:d:109:PHE:HB2	13:q:505:CLA:HAA2	2.02	0.40
1:e:202:ALA:HB2	1:e:320:GLY:HA3	2.04	0.40
1:e:278:LEU:HD23	1:e:278:LEU:HA	1.92	0.40
13:e:1137:CLA:H122	16:e:4007:BCR:H393	2.04	0.40
14:e:2001:PQN:H162	16:f:4014:BCR:H382	2.03	0.40
13:f:1202:CLA:H202	13:f:1202:CLA:H161	1.88	0.40
13:f:1220:CLA:H51	13:f:1221:CLA:H142	2.04	0.40
16:n:4219:BCR:H351	16:n:4219:BCR:H15C	1.78	0.40
12:r:57:GLN:HB2	12:r:62:GLN:HE21	1.86	0.40
13:r:505:CLA:HBC2	16:r:524:BCR:H341	2.03	0.40
12:t:31:HIS:NE2	13:t:509:CLA:NB	2.70	0.40
16:u:523:BCR:H11C	16:u:523:BCR:H341	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	G	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	e	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
2	B	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	H	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	f	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	g	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	O	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	h	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	Q	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	i	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
6	F	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	R	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	j	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
7	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	S	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	k	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	39/41 (95%)	39 (100%)	0	0	100	100
8	l	39/41 (95%)	39 (100%)	0	0	100	100
9	K	76/84 (90%)	75 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	U	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	m	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
10	L	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	V	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	n	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
11	M	27/29 (93%)	27 (100%)	0	0	100	100
11	W	27/29 (93%)	27 (100%)	0	0	100	100
11	o	27/29 (93%)	27 (100%)	0	0	100	100
12	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	2	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	4	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Z	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	b	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	r	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	t	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	12786/13089 (98%)	12420 (97%)	366 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/611 (98%)	600 (100%)	0	100	100
1	G	600/611 (98%)	600 (100%)	0	100	100
1	e	600/611 (98%)	600 (100%)	0	100	100
2	B	583/584 (100%)	582 (100%)	1 (0%)	87	96
2	H	583/584 (100%)	582 (100%)	1 (0%)	87	96
2	f	583/584 (100%)	582 (100%)	1 (0%)	87	96
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	g	67/68 (98%)	67 (100%)	0	100	100
4	D	114/114 (100%)	114 (100%)	0	100	100
4	O	114/114 (100%)	114 (100%)	0	100	100
4	h	114/114 (100%)	114 (100%)	0	100	100
5	E	56/59 (95%)	56 (100%)	0	100	100
5	Q	56/59 (95%)	56 (100%)	0	100	100
5	i	56/59 (95%)	56 (100%)	0	100	100
6	F	105/121 (87%)	105 (100%)	0	100	100
6	R	105/121 (87%)	105 (100%)	0	100	100
6	j	105/121 (87%)	105 (100%)	0	100	100
7	I	30/30 (100%)	30 (100%)	0	100	100
7	S	30/30 (100%)	30 (100%)	0	100	100
7	k	30/30 (100%)	30 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
8	T	35/35 (100%)	35 (100%)	0	100	100
8	l	35/35 (100%)	35 (100%)	0	100	100
9	K	56/61 (92%)	56 (100%)	0	100	100
9	U	56/61 (92%)	56 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	m	56/61 (92%)	56 (100%)	0	100	100
10	L	127/128 (99%)	127 (100%)	0	100	100
10	V	127/128 (99%)	127 (100%)	0	100	100
10	n	127/128 (99%)	127 (100%)	0	100	100
11	M	24/24 (100%)	24 (100%)	0	100	100
11	W	24/24 (100%)	24 (100%)	0	100	100
11	o	24/24 (100%)	24 (100%)	0	100	100
12	1	257/259 (99%)	257 (100%)	0	100	100
12	2	257/259 (99%)	257 (100%)	0	100	100
12	3	257/259 (99%)	257 (100%)	0	100	100
12	4	257/259 (99%)	257 (100%)	0	100	100
12	5	257/259 (99%)	257 (100%)	0	100	100
12	6	257/259 (99%)	257 (100%)	0	100	100
12	Y	257/259 (99%)	257 (100%)	0	100	100
12	Z	257/259 (99%)	257 (100%)	0	100	100
12	a	257/259 (99%)	257 (100%)	0	100	100
12	b	257/259 (99%)	257 (100%)	0	100	100
12	c	257/259 (99%)	257 (100%)	0	100	100
12	d	257/259 (99%)	257 (100%)	0	100	100
12	q	257/259 (99%)	257 (100%)	0	100	100
12	r	257/259 (99%)	257 (100%)	0	100	100
12	s	257/259 (99%)	257 (100%)	0	100	100
12	t	257/259 (99%)	257 (100%)	0	100	100
12	u	257/259 (99%)	257 (100%)	0	100	100
12	v	257/259 (99%)	257 (100%)	0	100	100
All	All	10017/10167 (98%)	10014 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	443	VAL
2	H	443	VAL
2	f	443	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	135	HIS
1	A	179	HIS
1	A	192	ASN
1	A	216	GLN
1	A	253	HIS
1	A	263	GLN
1	A	742	HIS
2	B	34	HIS
2	B	98	GLN
2	B	114	ASN
2	B	218	HIS
2	B	452	GLN
2	B	603	GLN
2	B	704	GLN
4	D	71	GLN
4	D	137	GLN
6	F	77	HIS
8	J	39	HIS
9	K	26	ASN
10	L	3	GLN
12	1	144	HIS
12	1	207	HIS
12	2	207	HIS
12	2	221	HIS
12	2	263	ASN
12	2	316	GLN
12	3	129	HIS
12	3	263	ASN
12	4	62	GLN
12	4	263	ASN
12	5	129	HIS
12	5	133	ASN
12	5	207	HIS
12	5	221	HIS
12	5	291	GLN
12	6	133	ASN
12	6	144	HIS
12	6	263	ASN
1	G	19	ASN
1	G	56	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	135	HIS
1	G	179	HIS
1	G	192	ASN
1	G	216	GLN
1	G	253	HIS
1	G	263	GLN
1	G	742	HIS
2	H	34	HIS
2	H	98	GLN
2	H	114	ASN
2	H	218	HIS
2	H	452	GLN
2	H	603	GLN
2	H	704	GLN
4	O	71	GLN
6	R	77	HIS
8	T	39	HIS
9	U	26	ASN
12	Y	144	HIS
12	Y	207	HIS
12	Z	129	HIS
12	Z	221	HIS
12	Z	263	ASN
12	Z	316	GLN
12	a	129	HIS
12	a	263	ASN
12	b	62	GLN
12	b	263	ASN
12	c	133	ASN
12	c	207	HIS
12	c	291	GLN
12	d	133	ASN
12	d	263	ASN
1	e	19	ASN
1	e	115	GLN
1	e	135	HIS
1	e	179	HIS
1	e	192	ASN
1	e	216	GLN
1	e	253	HIS
1	e	263	GLN
1	e	294	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	742	HIS
2	f	34	HIS
2	f	98	GLN
2	f	114	ASN
2	f	218	HIS
2	f	452	GLN
2	f	603	GLN
2	f	704	GLN
4	h	71	GLN
4	h	137	GLN
6	j	77	HIS
8	l	39	HIS
9	m	26	ASN
9	m	80	ASN
10	n	3	GLN
12	q	144	HIS
12	q	207	HIS
12	r	221	HIS
12	r	263	ASN
12	r	316	GLN
12	s	129	HIS
12	s	221	HIS
12	s	263	ASN
12	t	62	GLN
12	t	263	ASN
12	u	129	HIS
12	u	133	ASN
12	u	207	HIS
12	u	221	HIS
12	u	291	GLN
12	v	133	ASN
12	v	144	HIS
12	v	263	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

846 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	$\#\|Z\| > 2$
13	CLA	6	519	12	50,54,73	1.36	8 (16%)	59,90,113	1.44	4 (6%)
13	CLA	H	1226	2	69,73,73	1.27	9 (13%)	82,113,113	1.64	15 (18%)
13	CLA	A	1114	21	54,58,73	1.31	9 (16%)	64,95,113	1.49	7 (10%)
13	CLA	Y	508	12	59,63,73	1.26	9 (15%)	70,101,113	1.53	10 (14%)
13	CLA	d	513	12	49,53,73	1.41	7 (14%)	58,89,113	1.40	4 (6%)
13	CLA	e	1128	1	69,73,73	1.24	8 (11%)	82,113,113	1.50	8 (9%)
18	LMU	2	901	-	23,23,36	1.11	1 (4%)	28,28,47	0.93	0
13	CLA	B	1228	2	59,63,73	1.20	9 (15%)	70,101,113	1.49	9 (12%)
13	CLA	4	516	12	49,53,73	1.39	7 (14%)	58,89,113	1.42	5 (8%)
13	CLA	A	1111	1	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
13	CLA	B	1235	2	69,73,73	1.14	9 (13%)	82,113,113	1.42	7 (8%)
13	CLA	f	1226	2	69,73,73	1.27	9 (13%)	82,113,113	1.64	16 (19%)
16	BCR	r	524	-	41,41,41	0.69	0	56,56,56	1.68	13 (23%)
13	CLA	H	1220	2	59,63,73	1.22	8 (13%)	70,101,113	1.53	7 (10%)
13	CLA	c	510	12	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
13	CLA	m	1103	9	54,58,73	1.31	7 (12%)	64,95,113	1.53	8 (12%)
13	CLA	U	1401	-	59,63,73	1.24	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	u	502	12	54,58,73	1.33	9 (16%)	64,95,113	1.45	5 (7%)
13	CLA	v	502	12	54,58,73	1.32	7 (12%)	64,95,113	1.46	5 (7%)
17	LHG	H	1842	13	38,38,48	0.67	1 (2%)	41,44,54	1.26	4 (9%)
13	CLA	b	507	-	49,53,73	1.38	8 (16%)	58,89,113	1.52	6 (10%)
13	CLA	e	1136	1	64,68,73	1.19	7 (10%)	76,107,113	1.46	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	Y	518	12	64,68,73	1.19	7 (10%)	76,107,113	1.41	6 (7%)
13	CLA	B	1210	2	69,73,73	1.15	8 (11%)	82,113,113	1.41	13 (15%)
16	BCR	q	524	-	41,41,41	0.68	0	56,56,56	1.84	16 (28%)
13	CLA	3	501	12	69,73,73	1.16	8 (11%)	82,113,113	1.37	8 (9%)
13	CLA	e	1114	21	54,58,73	1.31	9 (16%)	64,95,113	1.49	6 (9%)
16	BCR	u	521	-	41,41,41	0.67	0	56,56,56	1.95	16 (28%)
13	CLA	f	1221	21	69,73,73	1.19	12 (17%)	82,113,113	1.49	13 (15%)
13	CLA	U	1105	9	49,53,73	1.40	8 (16%)	58,89,113	1.67	7 (12%)
13	CLA	s	508	12	59,63,73	1.28	9 (15%)	70,101,113	1.42	8 (11%)
13	CLA	G	1130	1	69,73,73	1.15	9 (13%)	82,113,113	1.39	12 (14%)
18	LMU	r	901	-	23,23,36	1.11	1 (4%)	28,28,47	0.94	0
13	CLA	Y	502	12	64,68,73	1.22	7 (10%)	76,107,113	1.36	7 (9%)
13	CLA	2	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	4 (6%)
13	CLA	A	1119	21	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
13	CLA	A	1011	1	69,73,73	1.17	8 (11%)	82,113,113	1.54	10 (12%)
13	CLA	6	516	12	49,53,73	1.39	8 (16%)	58,89,113	1.44	5 (8%)
13	CLA	G	1102	1	69,73,73	1.12	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	G	1103	1	69,73,73	1.14	7 (10%)	82,113,113	1.49	9 (10%)
13	CLA	3	506	12	54,58,73	1.33	9 (16%)	64,95,113	1.46	5 (7%)
16	BCR	H	4009	-	41,41,41	0.71	0	56,56,56	1.94	21 (37%)
13	CLA	H	1218	2	64,68,73	1.17	8 (12%)	76,107,113	1.37	6 (7%)
13	CLA	t	513	12	49,53,73	1.40	9 (18%)	58,89,113	1.46	4 (6%)
16	BCR	v	521	-	41,41,41	0.64	0	56,56,56	1.92	12 (21%)
13	CLA	H	1204	2	69,73,73	1.11	9 (13%)	82,113,113	1.29	6 (7%)
13	CLA	a	513	12	69,73,73	1.16	8 (11%)	82,113,113	1.32	5 (6%)
13	CLA	2	512	12	57,61,73	1.27	7 (12%)	67,98,113	1.37	5 (7%)
13	CLA	5	519	12	50,54,73	1.35	9 (18%)	59,90,113	1.44	4 (6%)
16	BCR	e	4002	-	41,41,41	0.74	1 (2%)	56,56,56	1.87	16 (28%)
17	LHG	n	5218	-	37,37,48	0.76	2 (5%)	40,43,54	1.26	4 (10%)
16	BCR	u	524	-	41,41,41	0.66	0	56,56,56	1.69	15 (26%)
13	CLA	A	1120	1	57,61,73	1.22	9 (15%)	67,98,113	1.50	7 (10%)
13	CLA	B	1223	2	69,73,73	1.15	9 (13%)	82,113,113	1.40	7 (8%)
13	CLA	H	1213	2	69,73,73	1.13	10 (14%)	82,113,113	1.42	10 (12%)
13	CLA	c	518	12	59,63,73	1.26	8 (13%)	70,101,113	1.32	5 (7%)
13	CLA	B	1214	2	69,73,73	1.16	9 (13%)	82,113,113	1.40	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	f	4009	-	41,41,41	0.71	0	56,56,56	1.94	21 (37%)
13	CLA	1	508	12	59,63,73	1.26	9 (15%)	70,101,113	1.52	10 (14%)
13	CLA	3	519	12	59,63,73	1.26	9 (15%)	70,101,113	1.39	5 (7%)
13	CLA	t	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.38	5 (7%)
16	BCR	T	4012	-	41,41,41	0.69	0	56,56,56	1.67	13 (23%)
13	CLA	n	1503	21	64,68,73	1.18	9 (14%)	76,107,113	1.37	6 (7%)
13	CLA	q	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
13	CLA	b	519	12	59,63,73	1.25	9 (15%)	70,101,113	1.39	4 (5%)
13	CLA	A	1135	1	56,60,73	1.26	8 (14%)	65,97,113	1.55	10 (15%)
17	LHG	G	5005	-	44,44,48	0.69	1 (2%)	47,50,54	1.30	6 (12%)
16	BCR	A	4011	-	41,41,41	0.66	0	56,56,56	1.83	12 (21%)
13	CLA	b	517	-	49,53,73	1.39	9 (18%)	58,89,113	1.49	5 (8%)
13	CLA	5	513	12	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
13	CLA	H	1225	2	69,73,73	1.13	10 (14%)	82,113,113	1.28	7 (8%)
13	CLA	u	506	12	49,53,73	1.39	9 (18%)	58,89,113	1.49	5 (8%)
14	PQN	e	2001	-	34,34,34	2.90	11 (32%)	43,45,45	2.04	6 (13%)
13	CLA	B	1230	2	64,68,73	1.20	8 (12%)	76,107,113	1.43	8 (10%)
13	CLA	r	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	4 (6%)
13	CLA	G	1137	1	69,73,73	1.13	8 (11%)	82,113,113	1.42	6 (7%)
13	CLA	v	505	12	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
13	CLA	G	1135	1	56,60,73	1.26	8 (14%)	65,97,113	1.55	10 (15%)
13	CLA	Y	510	12	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
13	CLA	a	511	12	54,58,73	1.33	9 (16%)	64,95,113	1.47	6 (9%)
13	CLA	a	519	12	59,63,73	1.26	9 (15%)	70,101,113	1.39	5 (7%)
13	CLA	u	519	12	50,54,73	1.35	9 (18%)	59,90,113	1.45	4 (6%)
17	LHG	I	5001	-	43,43,48	0.65	0	46,49,54	1.25	4 (8%)
13	CLA	1	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.38	9 (11%)
16	BCR	H	4006	-	41,41,41	0.69	0	56,56,56	1.99	19 (33%)
13	CLA	G	1136	1	64,68,73	1.18	7 (10%)	76,107,113	1.46	9 (11%)
16	BCR	l	4012	-	41,41,41	0.70	0	56,56,56	1.67	13 (23%)
13	CLA	s	509	12	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
13	CLA	e	1119	21	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
13	CLA	6	510	12	49,53,73	1.38	8 (16%)	58,89,113	1.40	4 (6%)
16	BCR	t	523	-	41,41,41	0.66	0	56,56,56	1.67	13 (23%)
13	CLA	A	1139	21	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LMU	q	902	-	19,19,36	1.23	1 (5%)	24,24,47	1.09	3 (12%)
13	CLA	H	1230	2	64,68,73	1.20	8 (12%)	76,107,113	1.43	8 (10%)
13	CLA	A	1013	-	69,73,73	1.18	10 (14%)	82,113,113	1.55	9 (10%)
13	CLA	1	503	12	68,72,73	1.19	8 (11%)	80,111,113	1.33	7 (8%)
16	BCR	Z	523	-	41,41,41	0.66	0	56,56,56	1.77	15 (26%)
13	CLA	Z	507	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
13	CLA	G	1013	-	69,73,73	1.19	10 (14%)	82,113,113	1.55	9 (10%)
13	CLA	2	509	12	69,73,73	1.18	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	2	519	12	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
13	CLA	H	1236	2	59,63,73	1.23	8 (13%)	70,101,113	1.29	6 (8%)
13	CLA	r	503	12	69,73,73	1.18	8 (11%)	82,113,113	1.31	7 (8%)
16	BCR	s	524	-	41,41,41	0.70	0	56,56,56	1.83	18 (32%)
13	CLA	B	1232	21	54,58,73	1.29	10 (18%)	64,95,113	1.58	7 (10%)
13	CLA	f	1228	2	59,63,73	1.20	9 (15%)	70,101,113	1.48	9 (12%)
13	CLA	s	506	12	54,58,73	1.32	8 (14%)	64,95,113	1.46	5 (7%)
16	BCR	5	522	-	41,41,41	0.70	0	56,56,56	1.94	21 (37%)
20	SQD	f	1852	-	43,45,54	1.02	4 (9%)	53,56,65	1.77	14 (26%)
13	CLA	1	502	12	64,68,73	1.22	8 (12%)	76,107,113	1.36	6 (7%)
13	CLA	Z	509	12	69,73,73	1.17	9 (13%)	82,113,113	1.34	7 (8%)
20	SQD	H	1852	-	43,45,54	1.03	3 (6%)	53,56,65	1.77	14 (26%)
13	CLA	B	1222	21	64,68,73	1.18	9 (14%)	76,107,113	1.38	9 (11%)
13	CLA	t	517	-	49,53,73	1.39	9 (18%)	58,89,113	1.50	5 (8%)
13	CLA	G	1138	1	69,73,73	1.12	9 (13%)	82,113,113	1.35	6 (7%)
13	CLA	B	1219	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	f	1240	17	69,73,73	1.17	9 (13%)	82,113,113	1.33	8 (9%)
13	CLA	G	1022	21	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
16	BCR	1	524	-	41,41,41	0.68	0	56,56,56	1.84	16 (28%)
15	SF4	N	3003	3	0,12,12	-	-	-		
13	CLA	c	519	12	50,54,73	1.35	9 (18%)	59,90,113	1.45	4 (6%)
16	BCR	H	4014	-	41,41,41	0.68	0	56,56,56	1.87	13 (23%)
13	CLA	G	1104	1	69,73,73	1.13	8 (11%)	82,113,113	1.38	9 (10%)
13	CLA	H	1238	21	69,73,73	1.12	9 (13%)	82,113,113	1.39	9 (10%)
17	LHG	G	5002	-	38,38,48	0.71	1 (2%)	41,44,54	1.25	5 (12%)
16	BCR	a	524	-	41,41,41	0.70	0	56,56,56	1.83	18 (32%)
13	CLA	d	519	12	50,54,73	1.37	7 (14%)	59,90,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	SQD	r	822	-	41,43,54	1.07	3 (7%)	51,54,65	1.55	10 (19%)
16	BCR	c	523	-	41,41,41	0.68	1 (2%)	56,56,56	1.81	17 (30%)
16	BCR	B	4009	-	41,41,41	0.71	0	56,56,56	1.94	21 (37%)
13	CLA	q	512	12	56,60,73	1.29	8 (14%)	65,97,113	1.38	4 (6%)
16	BCR	u	523	-	41,41,41	0.68	0	56,56,56	1.80	17 (30%)
13	CLA	r	510	12	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
13	CLA	v	516	12	49,53,73	1.39	7 (14%)	58,89,113	1.44	5 (8%)
16	BCR	5	521	-	41,41,41	0.67	0	56,56,56	1.95	16 (28%)
13	CLA	e	1107	1	69,73,73	1.15	10 (14%)	82,113,113	1.34	8 (9%)
13	CLA	q	502	12	64,68,73	1.22	8 (12%)	76,107,113	1.35	6 (7%)
13	CLA	s	513	12	69,73,73	1.16	8 (11%)	82,113,113	1.32	5 (6%)
13	CLA	B	1240	17	69,73,73	1.17	9 (13%)	82,113,113	1.33	8 (9%)
16	BCR	3	522	-	41,41,41	0.65	0	56,56,56	1.92	18 (32%)
17	LHG	e	5005	-	44,44,48	0.69	1 (2%)	47,50,54	1.30	6 (12%)
17	LHG	n	5221	-	48,48,48	0.67	2 (4%)	51,54,54	1.32	6 (11%)
16	BCR	V	4022	-	41,41,41	0.72	0	56,56,56	1.93	15 (26%)
16	BCR	2	522	-	41,41,41	0.67	0	56,56,56	1.76	19 (33%)
17	LHG	L	5221	-	48,48,48	0.67	2 (4%)	51,54,54	1.32	6 (11%)
13	CLA	B	1012	21	69,73,73	1.18	9 (13%)	82,113,113	1.37	8 (9%)
20	SQD	d	822	-	24,26,54	1.32	4 (16%)	34,37,65	1.85	10 (29%)
13	CLA	H	1201	2	64,68,73	1.17	9 (14%)	76,107,113	1.49	8 (10%)
13	CLA	A	1130	1	69,73,73	1.15	9 (13%)	82,113,113	1.39	12 (14%)
13	CLA	r	508	12	59,63,73	1.27	9 (15%)	70,101,113	1.42	8 (11%)
13	CLA	v	508	12	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
17	LHG	B	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.24	5 (10%)
13	CLA	A	1129	1	55,59,73	1.28	7 (12%)	64,96,113	1.51	9 (14%)
16	BCR	M	4021	-	41,41,41	0.64	0	56,56,56	1.84	16 (28%)
16	BCR	3	521	-	41,41,41	0.64	0	56,56,56	1.77	10 (17%)
18	LMU	l	5105	-	22,22,36	1.15	1 (4%)	27,27,47	0.81	0
13	CLA	1	513	12	59,63,73	1.26	9 (15%)	70,101,113	1.35	5 (7%)
13	CLA	u	517	-	49,53,73	1.39	9 (18%)	58,89,113	1.38	4 (6%)
13	CLA	H	1211	2	60,64,73	1.22	7 (11%)	71,102,113	1.58	5 (7%)
13	CLA	a	504	-	49,53,73	1.37	8 (16%)	58,89,113	1.50	7 (12%)
13	CLA	t	512	12	49,53,73	1.39	7 (14%)	58,89,113	1.48	4 (6%)
13	CLA	c	508	12	49,53,73	1.39	9 (18%)	58,89,113	1.53	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1115	1	64,68,73	1.16	8 (12%)	76,107,113	1.45	8 (10%)
13	CLA	e	1123	21	69,73,73	1.15	9 (13%)	82,113,113	1.35	9 (10%)
13	CLA	s	519	12	59,63,73	1.25	9 (15%)	70,101,113	1.39	5 (7%)
13	CLA	H	1219	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	d	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
13	CLA	j	1301	21	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
13	CLA	A	1126	1	69,73,73	1.12	9 (13%)	82,113,113	1.39	7 (8%)
13	CLA	f	1213	2	69,73,73	1.13	10 (14%)	82,113,113	1.42	10 (12%)
13	CLA	e	1127	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	9 (10%)
16	BCR	e	4003	-	41,41,41	0.71	0	56,56,56	1.75	12 (21%)
17	LHG	f	1842	13	38,38,48	0.66	1 (2%)	41,44,54	1.26	4 (9%)
13	CLA	G	1125	1	69,73,73	1.14	9 (13%)	82,113,113	1.42	9 (10%)
13	CLA	q	510	12	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
16	BCR	l	4015	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
13	CLA	B	1229	2	69,73,73	1.13	9 (13%)	82,113,113	1.39	10 (12%)
13	CLA	b	512	12	49,53,73	1.39	8 (16%)	58,89,113	1.49	4 (6%)
13	CLA	A	1106	1	69,73,73	1.12	9 (13%)	82,113,113	1.43	9 (10%)
13	CLA	6	505	12	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
13	CLA	B	1023	-	69,73,73	1.14	10 (14%)	82,113,113	1.69	14 (17%)
17	LHG	e	5006	-	44,44,48	0.63	1 (2%)	47,50,54	1.28	5 (10%)
13	CLA	1	510	12	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
13	CLA	5	504	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
16	BCR	o	4021	-	41,41,41	0.64	0	56,56,56	1.84	15 (26%)
16	BCR	S	4018	-	41,41,41	0.76	2 (4%)	56,56,56	1.87	16 (28%)
16	BCR	Y	521	-	41,41,41	0.63	0	56,56,56	1.81	11 (19%)
13	CLA	H	1203	2	69,73,73	1.16	11 (15%)	82,113,113	1.32	7 (8%)
20	SQD	Z	822	-	41,43,54	1.07	3 (7%)	51,54,65	1.55	10 (19%)
13	CLA	Z	506	12	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
16	BCR	v	522	-	41,41,41	0.67	0	56,56,56	1.85	16 (28%)
13	CLA	e	1131	1	69,73,73	1.14	8 (11%)	82,113,113	1.33	7 (8%)
13	CLA	e	1126	1	69,73,73	1.12	9 (13%)	82,113,113	1.40	8 (9%)
13	CLA	5	508	12	49,53,73	1.39	9 (18%)	58,89,113	1.53	5 (8%)
13	CLA	d	511	12	49,53,73	1.39	9 (18%)	58,89,113	1.48	4 (6%)
17	LHG	G	5004	-	35,35,48	0.76	1 (2%)	38,41,54	1.29	4 (10%)
13	CLA	q	503	12	68,72,73	1.19	8 (11%)	80,111,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	B	4010	-	41,41,41	0.81	0	56,56,56	2.31	24 (42%)
16	BCR	n	4020	-	41,41,41	0.73	0	56,56,56	1.96	15 (26%)
18	LMU	Z	901	-	23,23,36	1.11	1 (4%)	28,28,47	0.94	0
13	CLA	r	502	12	64,68,73	1.23	8 (12%)	76,107,113	1.37	6 (7%)
13	CLA	e	1137	1	69,73,73	1.14	8 (11%)	82,113,113	1.41	6 (7%)
13	CLA	r	504	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	6 (9%)
13	CLA	5	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.38	6 (8%)
13	CLA	V	1502	10	69,73,73	1.12	9 (13%)	82,113,113	1.37	5 (6%)
13	CLA	H	1207	2	69,73,73	1.16	9 (13%)	82,113,113	1.30	4 (4%)
13	CLA	H	1012	21	69,73,73	1.18	9 (13%)	82,113,113	1.37	8 (9%)
13	CLA	A	1128	1	69,73,73	1.23	8 (11%)	82,113,113	1.50	8 (9%)
13	CLA	r	505	12	69,73,73	1.15	7 (10%)	82,113,113	1.26	5 (6%)
13	CLA	c	504	-	49,53,73	1.39	8 (16%)	58,89,113	1.46	4 (6%)
16	BCR	a	523	-	41,41,41	0.64	0	56,56,56	1.78	17 (30%)
13	CLA	H	1224	2	64,68,73	1.17	8 (12%)	76,107,113	1.42	9 (11%)
13	CLA	q	516	12	49,53,73	1.38	8 (16%)	58,89,113	1.63	7 (12%)
17	LHG	A	5007	-	46,46,48	0.69	1 (2%)	49,52,54	1.27	5 (10%)
13	CLA	e	1118	1	64,68,73	1.19	8 (12%)	76,107,113	1.39	7 (9%)
16	BCR	J	4015	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
13	CLA	v	519	12	50,54,73	1.36	8 (16%)	59,90,113	1.44	4 (6%)
16	BCR	c	521	-	41,41,41	0.68	0	56,56,56	1.95	16 (28%)
13	CLA	B	1231	21	69,73,73	1.12	7 (10%)	82,113,113	1.40	8 (9%)
13	CLA	q	508	12	59,63,73	1.26	9 (15%)	70,101,113	1.52	10 (14%)
16	BCR	J	4013	-	41,41,41	0.70	0	56,56,56	1.98	15 (26%)
13	CLA	G	1109	1	69,73,73	1.12	9 (13%)	82,113,113	1.40	6 (7%)
13	CLA	v	506	12	49,53,73	1.40	9 (18%)	58,89,113	1.46	5 (8%)
13	CLA	r	511	12	59,63,73	1.28	9 (15%)	70,101,113	1.41	6 (8%)
13	CLA	2	504	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	6 (9%)
13	CLA	G	1107	1	69,73,73	1.15	11 (15%)	82,113,113	1.34	8 (9%)
14	PQN	A	2001	-	34,34,34	2.90	11 (32%)	43,45,45	2.04	6 (13%)
16	BCR	k	4018	-	41,41,41	0.76	2 (4%)	56,56,56	1.86	15 (26%)
17	LHG	e	5007	-	46,46,48	0.69	1 (2%)	49,52,54	1.27	5 (10%)
17	LHG	V	5220	-	40,40,48	0.65	0	43,46,54	1.26	4 (9%)
13	CLA	b	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.38	5 (7%)
13	CLA	a	509	12	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	H	1221	21	69,73,73	1.18	12 (17%)	82,113,113	1.50	12 (14%)
13	CLA	f	1012	21	69,73,73	1.18	9 (13%)	82,113,113	1.37	8 (9%)
13	CLA	a	517	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
20	SQD	c	822	-	27,29,54	1.26	3 (11%)	37,40,65	1.83	13 (35%)
13	CLA	c	506	12	49,53,73	1.39	9 (18%)	58,89,113	1.49	5 (8%)
13	CLA	B	1209	2	56,60,73	1.27	8 (14%)	65,97,113	1.56	7 (10%)
16	BCR	c	522	-	41,41,41	0.70	0	56,56,56	1.94	21 (37%)
16	BCR	G	4007	-	41,41,41	0.69	0	56,56,56	2.13	18 (32%)
13	CLA	f	1217	2	61,65,73	1.22	9 (14%)	72,103,113	1.41	7 (9%)
13	CLA	U	1103	9	54,58,73	1.30	7 (12%)	64,95,113	1.54	8 (12%)
16	BCR	f	4004	-	41,41,41	0.68	0	56,56,56	1.87	13 (23%)
13	CLA	B	1239	2	69,73,73	1.17	6 (8%)	82,113,113	1.51	12 (14%)
20	SQD	n	5216	-	49,51,54	0.98	3 (6%)	59,62,65	1.57	12 (20%)
20	SQD	t	822	-	24,26,54	1.33	3 (12%)	34,37,65	1.77	11 (32%)
13	CLA	r	512	12	57,61,73	1.27	7 (12%)	67,98,113	1.37	5 (7%)
14	PQN	H	2002	-	34,34,34	2.89	11 (32%)	43,45,45	2.10	5 (11%)
13	CLA	B	1216	21	64,68,73	1.22	9 (14%)	76,107,113	1.35	6 (7%)
13	CLA	t	505	12	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
16	BCR	T	4013	-	41,41,41	0.70	0	56,56,56	1.98	15 (26%)
13	CLA	t	503	12	59,63,73	1.29	6 (10%)	70,101,113	1.39	8 (11%)
13	CLA	A	1801	17	49,53,73	1.39	10 (20%)	58,89,113	1.59	7 (12%)
13	CLA	f	1230	2	64,68,73	1.20	8 (12%)	76,107,113	1.43	8 (10%)
13	CLA	A	1118	1	64,68,73	1.19	8 (12%)	76,107,113	1.40	7 (9%)
13	CLA	G	1115	1	64,68,73	1.17	9 (14%)	76,107,113	1.45	8 (10%)
13	CLA	m	1401	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	A	1112	1	54,58,73	1.27	9 (16%)	64,95,113	1.56	8 (12%)
13	CLA	K	1105	9	49,53,73	1.40	8 (16%)	58,89,113	1.67	7 (12%)
16	BCR	5	524	-	41,41,41	0.66	0	56,56,56	1.69	15 (26%)
16	BCR	A	4001	-	41,41,41	0.70	0	56,56,56	1.74	12 (21%)
17	LHG	n	5220	-	40,40,48	0.65	0	43,46,54	1.26	4 (9%)
17	LHG	G	5009	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	7 (13%)
16	BCR	G	4003	-	41,41,41	0.72	0	56,56,56	1.75	12 (21%)
17	LHG	L	5220	-	40,40,48	0.66	0	43,46,54	1.26	4 (9%)
13	CLA	6	513	12	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
13	CLA	G	1121	1	59,63,73	1.25	8 (13%)	70,101,113	1.47	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	G	1132	1	69,73,73	1.13	9 (13%)	82,113,113	1.36	7 (8%)
13	CLA	3	511	12	54,58,73	1.34	9 (16%)	64,95,113	1.47	5 (7%)
13	CLA	c	503	12	59,63,73	1.28	7 (11%)	70,101,113	1.38	6 (8%)
13	CLA	f	1204	2	69,73,73	1.11	8 (11%)	82,113,113	1.29	6 (7%)
13	CLA	u	504	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
17	LHG	G	5007	-	46,46,48	0.70	1 (2%)	49,52,54	1.27	5 (10%)
13	CLA	G	1131	1	69,73,73	1.14	8 (11%)	82,113,113	1.33	7 (8%)
13	CLA	c	509	12	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
17	LHG	k	5001	-	43,43,48	0.66	0	46,49,54	1.25	4 (8%)
17	LHG	A	5008	-	34,34,48	0.78	1 (2%)	37,40,54	1.31	4 (10%)
13	CLA	G	1108	1	58,62,73	1.26	9 (15%)	68,99,113	1.34	5 (7%)
13	CLA	b	509	12	69,73,73	1.17	7 (10%)	82,113,113	1.37	8 (9%)
16	BCR	e	4001	-	41,41,41	0.70	0	56,56,56	1.74	12 (21%)
13	CLA	u	510	12	49,53,73	1.39	8 (16%)	58,89,113	1.45	4 (6%)
16	BCR	Y	524	-	41,41,41	0.69	0	56,56,56	1.84	16 (28%)
13	CLA	1	519	12	54,58,73	1.30	8 (14%)	64,95,113	1.42	6 (9%)
13	CLA	e	1113	1	49,53,73	1.32	9 (18%)	58,89,113	1.56	6 (10%)
13	CLA	B	1225	2	69,73,73	1.13	10 (14%)	82,113,113	1.29	7 (8%)
13	CLA	t	510	12	54,58,73	1.32	8 (14%)	64,95,113	1.47	5 (7%)
13	CLA	H	1239	2	69,73,73	1.17	6 (8%)	82,113,113	1.51	12 (14%)
20	SQD	5	822	-	27,29,54	1.26	3 (11%)	37,40,65	1.83	13 (35%)
16	BCR	A	4002	-	41,41,41	0.75	1 (2%)	56,56,56	1.87	16 (28%)
15	SF4	G	3001	1,2	0,12,12	-	-	-		
13	CLA	q	506	12	49,53,73	1.38	7 (14%)	58,89,113	1.46	6 (10%)
20	SQD	L	5216	-	49,51,54	0.98	3 (6%)	59,62,65	1.57	11 (18%)
13	CLA	F	1301	21	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
13	CLA	v	513	12	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
13	CLA	u	507	-	49,53,73	1.37	7 (14%)	58,89,113	1.51	7 (12%)
13	CLA	v	507	-	49,53,73	1.38	8 (16%)	58,89,113	1.49	6 (10%)
16	BCR	q	522	-	41,41,41	0.69	0	56,56,56	1.91	20 (35%)
13	CLA	f	1219	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	2	516	12	49,53,73	1.38	9 (18%)	58,89,113	1.50	5 (8%)
13	CLA	d	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.36	5 (7%)
13	CLA	G	1118	1	64,68,73	1.19	8 (12%)	76,107,113	1.39	7 (9%)
13	CLA	4	513	12	49,53,73	1.40	9 (18%)	58,89,113	1.46	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	6	522	-	41,41,41	0.67	0	56,56,56	1.84	17 (30%)
13	CLA	B	1204	2	69,73,73	1.11	9 (13%)	82,113,113	1.30	6 (7%)
13	CLA	d	502	12	54,58,73	1.32	7 (12%)	64,95,113	1.46	5 (7%)
13	CLA	6	503	12	56,60,73	1.30	8 (14%)	65,97,113	1.44	7 (10%)
13	CLA	2	518	12	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	H	1217	2	61,65,73	1.22	8 (13%)	72,103,113	1.41	7 (9%)
13	CLA	Y	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.38	9 (11%)
18	LMU	e	1848	-	36,36,36	1.14	2 (5%)	47,47,47	1.09	2 (4%)
13	CLA	d	505	12	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
13	CLA	s	511	12	54,58,73	1.34	9 (16%)	64,95,113	1.47	5 (7%)
13	CLA	b	502	12	54,58,73	1.32	9 (16%)	64,95,113	1.47	5 (7%)
13	CLA	G	1133	1	69,73,73	1.11	7 (10%)	82,113,113	1.37	6 (7%)
20	SQD	a	822	-	41,43,54	1.07	4 (9%)	51,54,65	1.53	12 (23%)
16	BCR	e	4011	-	41,41,41	0.66	0	56,56,56	1.84	12 (21%)
13	CLA	a	506	12	54,58,73	1.33	9 (16%)	64,95,113	1.46	5 (7%)
16	BCR	4	521	-	41,41,41	0.62	0	56,56,56	1.80	12 (21%)
16	BCR	Y	522	-	41,41,41	0.68	0	56,56,56	1.92	20 (35%)
13	CLA	a	503	12	69,73,73	1.19	8 (11%)	82,113,113	1.30	5 (6%)
13	CLA	t	502	12	54,58,73	1.32	8 (14%)	64,95,113	1.46	5 (7%)
20	SQD	4	822	-	24,26,54	1.33	4 (16%)	34,37,65	1.77	11 (32%)
13	CLA	u	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.38	6 (8%)
13	CLA	H	1228	2	59,63,73	1.20	9 (15%)	70,101,113	1.49	9 (12%)
17	LHG	A	5001	-	48,48,48	0.81	1 (2%)	51,54,54	1.28	6 (11%)
13	CLA	3	509	12	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
13	CLA	e	1111	1	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
13	CLA	3	512	12	49,53,73	1.37	9 (18%)	58,89,113	1.48	4 (6%)
13	CLA	V	1501	10	69,73,73	1.15	9 (13%)	82,113,113	1.39	8 (9%)
13	CLA	j	1302	6	49,53,73	1.36	8 (16%)	58,89,113	1.45	4 (6%)
13	CLA	A	1123	21	69,73,73	1.15	9 (13%)	82,113,113	1.36	9 (10%)
17	LHG	G	5006	-	44,44,48	0.63	1 (2%)	47,50,54	1.28	5 (10%)
15	SF4	g	3003	3	0,12,12	-	-	-		
17	LHG	A	5005	-	44,44,48	0.69	1 (2%)	47,50,54	1.30	6 (12%)
17	LHG	e	5003	13	40,40,48	0.76	1 (2%)	43,46,54	1.36	6 (13%)
20	SQD	2	822	-	41,43,54	1.07	3 (7%)	51,54,65	1.55	10 (19%)
13	CLA	J	1302	8	62,66,73	1.20	8 (12%)	73,104,113	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	6	521	-	41,41,41	0.64	0	56,56,56	1.92	12 (21%)
13	CLA	Z	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.41	6 (8%)
13	CLA	5	503	12	59,63,73	1.28	7 (11%)	70,101,113	1.38	5 (7%)
13	CLA	A	1117	1	69,73,73	1.14	10 (14%)	82,113,113	1.55	10 (12%)
13	CLA	A	1124	21	60,64,73	1.26	8 (13%)	71,102,113	1.45	10 (14%)
16	BCR	5	523	-	41,41,41	0.68	0	56,56,56	1.81	17 (30%)
13	CLA	f	1208	2	69,73,73	1.12	7 (10%)	82,113,113	1.30	5 (6%)
16	BCR	3	524	-	41,41,41	0.70	0	56,56,56	1.83	18 (32%)
13	CLA	1	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.43	8 (11%)
13	CLA	b	508	12	49,53,73	1.41	8 (16%)	58,89,113	1.54	6 (10%)
13	CLA	d	509	12	49,53,73	1.40	8 (16%)	58,89,113	1.44	5 (8%)
19	LMG	f	5002	-	54,54,55	0.81	3 (5%)	62,62,63	1.43	10 (16%)
13	CLA	R	1302	6	49,53,73	1.36	8 (16%)	58,89,113	1.46	4 (6%)
13	CLA	L	1503	21	64,68,73	1.18	9 (14%)	76,107,113	1.37	5 (6%)
16	BCR	n	4022	-	41,41,41	0.72	0	56,56,56	1.93	16 (28%)
13	CLA	v	504	-	49,53,73	1.38	7 (14%)	58,89,113	1.50	7 (12%)
13	CLA	a	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.36	6 (8%)
16	BCR	1	523	-	41,41,41	0.64	0	56,56,56	1.66	18 (32%)
13	CLA	Z	505	12	69,73,73	1.16	7 (10%)	82,113,113	1.27	5 (6%)
16	BCR	b	523	-	41,41,41	0.66	0	56,56,56	1.67	13 (23%)
13	CLA	a	510	12	69,73,73	1.17	7 (10%)	82,113,113	1.34	9 (10%)
13	CLA	6	504	-	49,53,73	1.39	8 (16%)	58,89,113	1.50	7 (12%)
16	BCR	c	524	-	41,41,41	0.66	0	56,56,56	1.69	15 (26%)
13	CLA	B	1236	2	59,63,73	1.24	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	e	1109	1	69,73,73	1.12	8 (11%)	82,113,113	1.40	6 (7%)
20	SQD	3	822	-	41,43,54	1.06	4 (9%)	51,54,65	1.53	12 (23%)
13	CLA	B	1224	2	64,68,73	1.18	8 (12%)	76,107,113	1.42	9 (11%)
13	CLA	e	1117	1	69,73,73	1.14	10 (14%)	82,113,113	1.55	10 (12%)
13	CLA	e	1105	1	59,63,73	1.20	9 (15%)	70,101,113	1.50	8 (11%)
16	BCR	A	4003	-	41,41,41	0.71	0	56,56,56	1.75	12 (21%)
13	CLA	1	505	12	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
13	CLA	G	1122	1	64,68,73	1.18	7 (10%)	76,107,113	1.39	5 (6%)
16	BCR	Y	523	-	41,41,41	0.64	0	56,56,56	1.66	17 (30%)
13	CLA	Y	512	12	56,60,73	1.29	8 (14%)	65,97,113	1.39	4 (6%)
13	CLA	e	1101	1	69,73,73	1.17	9 (13%)	82,113,113	1.39	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	3	513	12	69,73,73	1.16	8 (11%)	82,113,113	1.32	5 (6%)
16	BCR	d	524	-	41,41,41	0.69	0	56,56,56	1.89	13 (23%)
13	CLA	r	516	12	49,53,73	1.38	9 (18%)	58,89,113	1.51	5 (8%)
13	CLA	a	507	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	6 (7%)
13	CLA	Z	518	12	69,73,73	1.15	9 (13%)	82,113,113	1.35	7 (8%)
13	CLA	l	1303	8	69,73,73	1.15	8 (11%)	82,113,113	1.38	9 (10%)
16	BCR	R	4016	-	41,41,41	0.68	0	56,56,56	1.80	13 (23%)
16	BCR	j	4016	-	41,41,41	0.68	0	56,56,56	1.81	13 (23%)
13	CLA	B	1021	2	69,73,73	1.16	8 (11%)	82,113,113	1.35	7 (8%)
13	CLA	A	1116	1	64,68,73	1.20	9 (14%)	76,107,113	1.34	7 (9%)
16	BCR	H	4010	-	41,41,41	0.81	0	56,56,56	2.31	24 (42%)
17	LHG	G	5003	13	40,40,48	0.76	1 (2%)	43,46,54	1.36	6 (13%)
13	CLA	e	1125	1	69,73,73	1.14	9 (13%)	82,113,113	1.43	9 (10%)
17	LHG	A	5004	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	H	1227	2	69,73,73	1.13	9 (13%)	82,113,113	1.38	6 (7%)
13	CLA	a	505	12	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
13	CLA	V	1503	21	64,68,73	1.18	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	5	510	12	49,53,73	1.38	8 (16%)	58,89,113	1.45	4 (6%)
13	CLA	1	509	12	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
16	BCR	2	523	-	41,41,41	0.66	0	56,56,56	1.77	15 (26%)
13	CLA	G	1113	1	49,53,73	1.32	8 (16%)	58,89,113	1.55	6 (10%)
16	BCR	f	4010	-	41,41,41	0.81	0	56,56,56	2.31	24 (42%)
13	CLA	s	507	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
16	BCR	v	524	-	41,41,41	0.69	0	56,56,56	1.89	13 (23%)
13	CLA	A	1134	1	60,64,73	1.21	8 (13%)	71,102,113	1.43	5 (7%)
13	CLA	T	1303	8	69,73,73	1.15	8 (11%)	82,113,113	1.38	10 (12%)
13	CLA	4	504	-	49,53,73	1.38	7 (14%)	58,89,113	1.46	4 (6%)
13	CLA	a	501	12	69,73,73	1.16	8 (11%)	82,113,113	1.37	8 (9%)
13	CLA	2	513	12	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
13	CLA	H	1214	2	69,73,73	1.16	9 (13%)	82,113,113	1.41	6 (7%)
16	BCR	b	521	-	41,41,41	0.61	0	56,56,56	1.80	12 (21%)
13	CLA	H	1205	2	69,73,73	1.15	9 (13%)	82,113,113	1.44	8 (9%)
16	BCR	G	4002	-	41,41,41	0.75	1 (2%)	56,56,56	1.87	16 (28%)
13	CLA	H	1223	2	69,73,73	1.15	9 (13%)	82,113,113	1.40	6 (7%)
13	CLA	G	1114	21	54,58,73	1.31	9 (16%)	64,95,113	1.49	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	V	4219	-	41,41,41	0.68	0	56,56,56	1.84	13 (23%)
13	CLA	e	1139	21	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
13	CLA	3	505	12	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
13	CLA	e	1237	21	69,73,73	1.16	8 (11%)	82,113,113	1.41	8 (9%)
13	CLA	Y	519	12	54,58,73	1.29	8 (14%)	64,95,113	1.43	6 (9%)
13	CLA	d	508	12	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
16	BCR	t	522	-	41,41,41	0.69	0	56,56,56	1.86	18 (32%)
13	CLA	f	1021	2	69,73,73	1.16	8 (11%)	82,113,113	1.35	7 (8%)
13	CLA	s	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
13	CLA	1	506	12	49,53,73	1.37	7 (14%)	58,89,113	1.45	6 (10%)
13	CLA	5	517	-	49,53,73	1.40	9 (18%)	58,89,113	1.38	4 (6%)
13	CLA	e	1108	1	58,62,73	1.25	9 (15%)	68,99,113	1.34	5 (7%)
17	LHG	H	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.24	5 (10%)
13	CLA	B	1215	2	69,73,73	1.15	9 (13%)	82,113,113	1.42	8 (9%)
13	CLA	2	510	12	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
13	CLA	4	507	-	49,53,73	1.38	7 (14%)	58,89,113	1.52	6 (10%)
16	BCR	T	4015	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
13	CLA	t	504	-	49,53,73	1.38	7 (14%)	58,89,113	1.46	4 (6%)
13	CLA	e	1110	1	55,59,73	1.30	9 (16%)	64,96,113	1.48	5 (7%)
13	CLA	B	1205	2	69,73,73	1.15	9 (13%)	82,113,113	1.43	8 (9%)
13	CLA	4	505	12	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
16	BCR	F	4016	-	41,41,41	0.68	0	56,56,56	1.80	13 (23%)
13	CLA	G	1119	21	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
13	CLA	H	1212	2	59,63,73	1.23	9 (15%)	70,101,113	1.46	8 (11%)
13	CLA	B	1238	21	69,73,73	1.13	9 (13%)	82,113,113	1.38	9 (10%)
13	CLA	2	507	-	69,73,73	1.14	7 (10%)	82,113,113	1.37	5 (6%)
13	CLA	3	502	12	54,58,73	1.31	9 (16%)	64,95,113	1.49	6 (9%)
16	BCR	4	523	-	41,41,41	0.66	0	56,56,56	1.67	13 (23%)
13	CLA	t	508	12	49,53,73	1.41	8 (16%)	58,89,113	1.54	6 (10%)
13	CLA	u	509	12	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
13	CLA	q	513	12	59,63,73	1.25	9 (15%)	70,101,113	1.35	5 (7%)
13	CLA	A	1110	1	55,59,73	1.30	9 (16%)	64,96,113	1.47	5 (7%)
13	CLA	q	519	12	54,58,73	1.30	8 (14%)	64,95,113	1.43	6 (9%)
13	CLA	6	507	-	49,53,73	1.38	8 (16%)	58,89,113	1.50	6 (10%)
13	CLA	B	1226	2	69,73,73	1.27	9 (13%)	82,113,113	1.64	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LHG	B	1842	13	38,38,48	0.67	1 (2%)	41,44,54	1.26	4 (9%)
13	CLA	f	1212	2	59,63,73	1.23	8 (13%)	70,101,113	1.47	8 (11%)
16	BCR	s	523	-	41,41,41	0.65	0	56,56,56	1.78	17 (30%)
13	CLA	6	508	12	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
13	CLA	4	501	12	64,68,73	1.22	8 (12%)	76,107,113	1.33	4 (5%)
13	CLA	f	1236	2	59,63,73	1.23	7 (11%)	70,101,113	1.30	6 (8%)
13	CLA	f	1227	2	69,73,73	1.13	9 (13%)	82,113,113	1.39	6 (7%)
13	CLA	Y	509	12	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
16	BCR	l	4013	-	41,41,41	0.70	0	56,56,56	1.98	15 (26%)
13	CLA	Y	513	12	59,63,73	1.26	9 (15%)	70,101,113	1.34	4 (5%)
13	CLA	s	516	12	49,53,73	1.39	7 (14%)	58,89,113	1.68	9 (15%)
13	CLA	u	512	12	49,53,73	1.38	8 (16%)	58,89,113	1.46	4 (6%)
13	CLA	1	518	12	64,68,73	1.19	8 (12%)	76,107,113	1.42	6 (7%)
13	CLA	n	1502	10	69,73,73	1.12	9 (13%)	82,113,113	1.37	5 (6%)
17	LHG	f	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.24	5 (10%)
13	CLA	L	1502	10	69,73,73	1.12	9 (13%)	82,113,113	1.37	5 (6%)
16	BCR	G	4011	-	41,41,41	0.66	0	56,56,56	1.84	12 (21%)
16	BCR	H	4004	-	41,41,41	0.68	0	56,56,56	1.87	13 (23%)
20	SQD	6	822	-	24,26,54	1.32	3 (12%)	34,37,65	1.84	10 (29%)
13	CLA	v	501	12	64,68,73	1.20	8 (12%)	76,107,113	1.39	6 (7%)
16	BCR	d	521	-	41,41,41	0.64	0	56,56,56	1.92	13 (23%)
13	CLA	e	1129	1	55,59,73	1.28	8 (14%)	64,96,113	1.51	10 (15%)
16	BCR	H	4005	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
13	CLA	A	1101	1	69,73,73	1.17	9 (13%)	82,113,113	1.39	7 (8%)
18	LMU	Y	902	-	19,19,36	1.23	1 (5%)	24,24,47	1.09	3 (12%)
13	CLA	6	501	12	64,68,73	1.20	8 (12%)	76,107,113	1.39	6 (7%)
13	CLA	4	511	12	49,53,73	1.41	8 (16%)	58,89,113	1.51	5 (8%)
13	CLA	G	1111	1	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
13	CLA	5	518	12	59,63,73	1.26	8 (13%)	70,101,113	1.32	5 (7%)
13	CLA	6	502	12	54,58,73	1.32	7 (12%)	64,95,113	1.46	5 (7%)
13	CLA	Y	506	12	49,53,73	1.37	7 (14%)	58,89,113	1.45	6 (10%)
13	CLA	e	1135	1	56,60,73	1.26	7 (12%)	65,97,113	1.55	10 (15%)
13	CLA	A	1102	1	69,73,73	1.12	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	A	1103	1	69,73,73	1.14	8 (11%)	82,113,113	1.48	9 (10%)
13	CLA	G	1112	1	54,58,73	1.27	9 (16%)	64,95,113	1.56	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1120	1	57,61,73	1.23	10 (17%)	67,98,113	1.51	7 (10%)
13	CLA	f	1225	2	69,73,73	1.12	10 (14%)	82,113,113	1.29	8 (9%)
13	CLA	n	1501	10	69,73,73	1.15	8 (11%)	82,113,113	1.39	8 (9%)
13	CLA	q	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.39	9 (11%)
13	CLA	e	1130	1	69,73,73	1.15	9 (13%)	82,113,113	1.39	12 (14%)
13	CLA	d	512	12	49,53,73	1.38	9 (18%)	58,89,113	1.47	4 (6%)
13	CLA	b	504	-	49,53,73	1.38	6 (12%)	58,89,113	1.46	4 (6%)
13	CLA	Z	501	12	69,73,73	1.16	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	b	506	12	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
16	BCR	G	4008	-	41,41,41	0.74	0	56,56,56	2.05	17 (30%)
18	LMU	T	5105	-	22,22,36	1.15	1 (4%)	27,27,47	0.81	0
13	CLA	G	1237	21	69,73,73	1.16	8 (11%)	82,113,113	1.42	8 (9%)
13	CLA	G	1128	1	69,73,73	1.23	8 (11%)	82,113,113	1.49	8 (9%)
13	CLA	Z	516	12	49,53,73	1.38	9 (18%)	58,89,113	1.50	5 (8%)
13	CLA	f	1220	2	59,63,73	1.22	8 (13%)	70,101,113	1.52	7 (10%)
13	CLA	e	1011	1	69,73,73	1.17	7 (10%)	82,113,113	1.54	10 (12%)
13	CLA	f	1224	2	64,68,73	1.18	8 (12%)	76,107,113	1.42	9 (11%)
13	CLA	b	513	12	49,53,73	1.40	9 (18%)	58,89,113	1.46	4 (6%)
16	BCR	Z	521	-	41,41,41	0.65	0	56,56,56	1.88	11 (19%)
13	CLA	e	1106	1	69,73,73	1.12	9 (13%)	82,113,113	1.43	9 (10%)
18	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.09	2 (4%)
16	BCR	L	4020	-	41,41,41	0.74	0	56,56,56	1.96	16 (28%)
13	CLA	G	1139	21	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)
13	CLA	H	1023	-	69,73,73	1.14	10 (14%)	82,113,113	1.69	14 (17%)
13	CLA	c	517	-	49,53,73	1.40	9 (18%)	58,89,113	1.38	4 (6%)
13	CLA	q	509	12	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
13	CLA	e	1122	1	64,68,73	1.18	7 (10%)	76,107,113	1.40	5 (6%)
13	CLA	e	1801	17	49,53,73	1.39	10 (20%)	58,89,113	1.60	7 (12%)
13	CLA	Y	504	-	49,53,73	1.39	9 (18%)	58,89,113	1.47	6 (10%)
13	CLA	Z	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.46	4 (6%)
13	CLA	5	502	12	54,58,73	1.32	9 (16%)	64,95,113	1.44	5 (7%)
13	CLA	G	1127	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	9 (10%)
13	CLA	A	1137	1	69,73,73	1.14	8 (11%)	82,113,113	1.41	6 (7%)
13	CLA	e	1112	1	54,58,73	1.27	9 (16%)	64,95,113	1.56	8 (12%)
13	CLA	G	1105	1	59,63,73	1.20	9 (15%)	70,101,113	1.51	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	t	506	12	49,53,73	1.40	8 (16%)	58,89,113	1.48	4 (6%)
16	BCR	L	4019	-	41,41,41	0.68	0	56,56,56	1.94	13 (23%)
18	LMU	G	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
13	CLA	F	1302	6	49,53,73	1.36	8 (16%)	58,89,113	1.46	4 (6%)
19	LMG	B	5002	-	54,54,55	0.80	3 (5%)	62,62,63	1.43	10 (16%)
14	PQN	B	2002	-	34,34,34	2.89	11 (32%)	43,45,45	2.11	5 (11%)
13	CLA	r	507	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	5 (6%)
13	CLA	1	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
16	BCR	q	521	-	41,41,41	0.64	0	56,56,56	1.81	11 (19%)
19	LMG	J	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
13	CLA	B	1221	21	69,73,73	1.18	12 (17%)	82,113,113	1.49	12 (14%)
18	LMU	1	902	-	19,19,36	1.23	1 (5%)	24,24,47	1.09	3 (12%)
13	CLA	f	1205	2	69,73,73	1.15	9 (13%)	82,113,113	1.42	8 (9%)
20	SQD	u	822	-	27,29,54	1.27	3 (11%)	37,40,65	1.83	13 (35%)
20	SQD	v	822	-	24,26,54	1.31	3 (12%)	34,37,65	1.84	10 (29%)
13	CLA	6	506	12	49,53,73	1.39	9 (18%)	58,89,113	1.47	5 (8%)
13	CLA	4	509	12	69,73,73	1.17	8 (11%)	82,113,113	1.37	8 (9%)
13	CLA	u	503	12	59,63,73	1.28	7 (11%)	70,101,113	1.38	5 (7%)
13	CLA	B	1212	2	59,63,73	1.23	8 (13%)	70,101,113	1.46	8 (11%)
13	CLA	s	504	-	49,53,73	1.37	9 (18%)	58,89,113	1.51	7 (12%)
16	BCR	H	4017	-	41,41,41	0.72	0	56,56,56	1.61	12 (21%)
13	CLA	a	512	12	49,53,73	1.38	9 (18%)	58,89,113	1.49	4 (6%)
13	CLA	b	501	12	64,68,73	1.22	8 (12%)	76,107,113	1.34	4 (5%)
16	BCR	f	4017	-	41,41,41	0.72	0	56,56,56	1.60	11 (19%)
13	CLA	H	1229	2	69,73,73	1.13	9 (13%)	82,113,113	1.38	10 (12%)
13	CLA	3	516	12	49,53,73	1.39	8 (16%)	58,89,113	1.68	9 (15%)
20	SQD	Y	822	-	46,48,54	0.99	3 (6%)	56,59,65	1.69	13 (23%)
15	SF4	e	3001	1,2	0,12,12	-	-	-		
13	CLA	q	504	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
16	BCR	d	522	-	41,41,41	0.67	0	56,56,56	1.84	17 (30%)
13	CLA	t	501	12	64,68,73	1.22	8 (12%)	76,107,113	1.32	4 (5%)
13	CLA	B	1208	2	69,73,73	1.12	8 (11%)	82,113,113	1.29	5 (6%)
13	CLA	A	1125	1	69,73,73	1.14	9 (13%)	82,113,113	1.42	9 (10%)
16	BCR	4	524	-	41,41,41	0.66	0	56,56,56	1.86	16 (28%)
13	CLA	H	1235	2	69,73,73	1.15	9 (13%)	82,113,113	1.42	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	f	4006	-	41,41,41	0.68	0	56,56,56	1.99	19 (33%)
13	CLA	G	1123	21	69,73,73	1.15	9 (13%)	82,113,113	1.35	9 (10%)
13	CLA	A	1127	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	10 (12%)
13	CLA	d	503	12	56,60,73	1.30	8 (14%)	65,97,113	1.43	7 (10%)
13	CLA	e	1116	1	64,68,73	1.21	10 (15%)	76,107,113	1.33	7 (9%)
16	BCR	t	521	-	41,41,41	0.63	0	56,56,56	1.79	12 (21%)
13	CLA	e	1104	1	69,73,73	1.13	8 (11%)	82,113,113	1.37	9 (10%)
13	CLA	c	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.38	6 (8%)
13	CLA	t	509	12	69,73,73	1.17	7 (10%)	82,113,113	1.37	7 (8%)
13	CLA	5	509	12	69,73,73	1.16	9 (13%)	82,113,113	1.32	8 (9%)
13	CLA	e	1013	-	69,73,73	1.18	10 (14%)	82,113,113	1.55	9 (10%)
13	CLA	3	508	12	59,63,73	1.29	9 (15%)	70,101,113	1.42	8 (11%)
13	CLA	5	512	12	49,53,73	1.37	8 (16%)	58,89,113	1.45	4 (6%)
13	CLA	A	1022	21	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
13	CLA	5	506	12	49,53,73	1.39	9 (18%)	58,89,113	1.49	5 (8%)
13	CLA	Y	501	12	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	t	507	-	49,53,73	1.39	7 (14%)	58,89,113	1.53	6 (10%)
20	SQD	s	822	-	41,43,54	1.07	4 (9%)	51,54,65	1.53	12 (23%)
13	CLA	b	503	12	59,63,73	1.30	7 (11%)	70,101,113	1.40	8 (11%)
13	CLA	d	516	12	49,53,73	1.39	7 (14%)	58,89,113	1.45	5 (8%)
13	CLA	5	505	12	65,69,73	1.20	7 (10%)	77,108,113	1.26	4 (5%)
13	CLA	3	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
13	CLA	6	518	12	59,63,73	1.26	9 (15%)	70,101,113	1.35	5 (7%)
13	CLA	s	503	12	69,73,73	1.19	8 (11%)	82,113,113	1.30	5 (6%)
13	CLA	u	518	12	59,63,73	1.26	8 (13%)	70,101,113	1.32	5 (7%)
13	CLA	G	1120	1	57,61,73	1.22	9 (15%)	67,98,113	1.51	7 (10%)
13	CLA	A	1104	1	69,73,73	1.13	9 (13%)	82,113,113	1.38	9 (10%)
13	CLA	B	1202	2	69,73,73	1.14	10 (14%)	82,113,113	1.48	9 (10%)
13	CLA	B	1220	2	59,63,73	1.22	8 (13%)	70,101,113	1.53	7 (10%)
13	CLA	c	505	12	65,69,73	1.20	8 (12%)	77,108,113	1.26	4 (5%)
13	CLA	e	1103	1	69,73,73	1.14	8 (11%)	82,113,113	1.48	9 (10%)
13	CLA	A	1121	1	59,63,73	1.25	7 (11%)	70,101,113	1.47	9 (12%)
13	CLA	B	1234	2	69,73,73	1.17	10 (14%)	82,113,113	1.52	14 (17%)
13	CLA	3	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.37	6 (8%)
13	CLA	H	1208	2	69,73,73	1.12	8 (11%)	82,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	u	505	12	65,69,73	1.20	6 (9%)	77,108,113	1.26	4 (5%)
13	CLA	v	503	12	56,60,73	1.30	8 (14%)	65,97,113	1.44	7 (10%)
16	BCR	t	524	-	41,41,41	0.67	0	56,56,56	1.86	17 (30%)
13	CLA	e	1022	21	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
18	LMU	f	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.12	3 (6%)
13	CLA	G	1011	1	69,73,73	1.18	7 (10%)	82,113,113	1.53	10 (12%)
13	CLA	r	506	12	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
13	CLA	c	502	12	54,58,73	1.32	9 (16%)	64,95,113	1.44	5 (7%)
13	CLA	3	510	12	69,73,73	1.17	7 (10%)	82,113,113	1.34	9 (10%)
13	CLA	4	517	-	49,53,73	1.39	9 (18%)	58,89,113	1.50	5 (8%)
13	CLA	A	1108	1	58,62,73	1.26	9 (15%)	68,99,113	1.34	5 (7%)
13	CLA	Y	505	12	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
13	CLA	r	519	12	59,63,73	1.26	9 (15%)	70,101,113	1.37	6 (8%)
13	CLA	A	1115	1	64,68,73	1.16	8 (12%)	76,107,113	1.45	8 (10%)
13	CLA	2	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.41	6 (8%)
13	CLA	c	501	12	69,73,73	1.16	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	f	1235	2	69,73,73	1.14	8 (11%)	82,113,113	1.41	7 (8%)
16	BCR	A	4007	-	41,41,41	0.68	0	56,56,56	2.13	18 (32%)
16	BCR	6	523	-	41,41,41	0.67	0	56,56,56	1.75	15 (26%)
13	CLA	u	501	12	69,73,73	1.16	9 (13%)	82,113,113	1.35	5 (6%)
16	BCR	b	524	-	41,41,41	0.66	0	56,56,56	1.86	17 (30%)
13	CLA	Z	503	12	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
13	CLA	G	1140	1	69,73,73	1.17	9 (13%)	82,113,113	1.39	13 (15%)
13	CLA	G	1116	1	64,68,73	1.20	10 (15%)	76,107,113	1.34	7 (9%)
13	CLA	3	507	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	6 (7%)
13	CLA	c	516	12	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
13	CLA	K	1103	9	54,58,73	1.30	7 (12%)	64,95,113	1.53	8 (12%)
13	CLA	H	1202	2	69,73,73	1.14	10 (14%)	82,113,113	1.48	9 (10%)
13	CLA	s	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.37	6 (8%)
16	BCR	m	4104	-	41,41,41	0.71	0	56,56,56	1.88	15 (26%)
13	CLA	J	1303	8	69,73,73	1.15	8 (11%)	82,113,113	1.38	10 (12%)
13	CLA	H	1234	2	69,73,73	1.17	10 (14%)	82,113,113	1.51	14 (17%)
13	CLA	d	501	12	64,68,73	1.20	8 (12%)	76,107,113	1.39	6 (7%)
13	CLA	s	510	12	69,73,73	1.17	7 (10%)	82,113,113	1.33	9 (10%)
16	BCR	a	522	-	41,41,41	0.65	0	56,56,56	1.92	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	2	501	12	69,73,73	1.16	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	A	1109	1	69,73,73	1.12	8 (11%)	82,113,113	1.40	6 (7%)
13	CLA	T	1302	8	62,66,73	1.21	8 (12%)	73,104,113	1.39	6 (8%)
13	CLA	f	1215	2	69,73,73	1.15	9 (13%)	82,113,113	1.42	8 (9%)
16	BCR	4	522	-	41,41,41	0.69	0	56,56,56	1.86	18 (32%)
13	CLA	Z	508	12	59,63,73	1.27	9 (15%)	70,101,113	1.41	8 (11%)
13	CLA	v	510	12	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
13	CLA	q	511	12	59,63,73	1.27	8 (13%)	70,101,113	1.42	8 (11%)
13	CLA	a	516	12	49,53,73	1.39	7 (14%)	58,89,113	1.68	9 (15%)
20	SQD	V	5216	-	49,51,54	0.97	3 (6%)	59,62,65	1.57	10 (16%)
13	CLA	r	518	12	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
16	BCR	2	521	-	41,41,41	0.65	0	56,56,56	1.88	11 (19%)
13	CLA	G	1129	1	55,59,73	1.28	7 (12%)	64,96,113	1.51	9 (14%)
16	BCR	e	4008	-	41,41,41	0.74	0	56,56,56	2.04	17 (30%)
13	CLA	2	506	12	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
13	CLA	d	504	-	49,53,73	1.39	8 (16%)	58,89,113	1.50	7 (12%)
16	BCR	a	521	-	41,41,41	0.65	0	56,56,56	1.76	10 (17%)
13	CLA	f	1239	2	69,73,73	1.17	6 (8%)	82,113,113	1.50	11 (13%)
13	CLA	s	505	12	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
13	CLA	H	1232	21	54,58,73	1.29	10 (18%)	64,95,113	1.58	7 (10%)
16	BCR	B	4006	-	41,41,41	0.68	0	56,56,56	1.99	19 (33%)
13	CLA	Y	511	12	59,63,73	1.28	9 (15%)	70,101,113	1.43	8 (11%)
13	CLA	4	518	12	59,63,73	1.27	9 (15%)	70,101,113	1.38	5 (7%)
13	CLA	Z	510	12	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
13	CLA	l	1302	8	62,66,73	1.20	8 (12%)	73,104,113	1.41	6 (8%)
18	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
13	CLA	s	502	12	54,58,73	1.31	8 (14%)	64,95,113	1.48	6 (9%)
13	CLA	G	1126	1	69,73,73	1.12	9 (13%)	82,113,113	1.39	7 (8%)
13	CLA	a	508	12	59,63,73	1.29	9 (15%)	70,101,113	1.42	8 (11%)
20	SQD	b	822	-	24,26,54	1.33	4 (16%)	34,37,65	1.78	11 (32%)
16	BCR	q	523	-	41,41,41	0.64	0	56,56,56	1.66	18 (32%)
17	LHG	e	5001	-	48,48,48	0.81	1 (2%)	51,54,54	1.28	6 (11%)
20	SQD	B	1852	-	43,45,54	1.02	4 (9%)	53,56,65	1.77	14 (26%)
13	CLA	s	501	12	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)
13	CLA	B	1207	2	69,73,73	1.15	9 (13%)	82,113,113	1.29	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	H	1021	2	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
13	CLA	G	1106	1	69,73,73	1.12	10 (14%)	82,113,113	1.44	9 (10%)
16	BCR	f	4005	-	41,41,41	0.67	0	56,56,56	1.80	12 (21%)
20	SQD	q	822	-	46,48,54	0.99	3 (6%)	56,59,65	1.69	13 (23%)
13	CLA	m	1105	9	49,53,73	1.40	8 (16%)	58,89,113	1.67	8 (13%)
13	CLA	q	501	12	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
18	LMU	e	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
16	BCR	s	521	-	41,41,41	0.64	0	56,56,56	1.77	10 (17%)
17	LHG	e	5002	-	38,38,48	0.71	1 (2%)	41,44,54	1.25	5 (12%)
13	CLA	G	1801	17	49,53,73	1.39	10 (20%)	58,89,113	1.59	7 (12%)
16	BCR	b	522	-	41,41,41	0.70	0	56,56,56	1.86	18 (32%)
16	BCR	n	4219	-	41,41,41	0.68	0	56,56,56	1.84	13 (23%)
13	CLA	f	1229	2	69,73,73	1.13	9 (13%)	82,113,113	1.39	10 (12%)
13	CLA	e	1124	21	60,64,73	1.26	8 (13%)	71,102,113	1.44	10 (14%)
16	BCR	K	4104	-	41,41,41	0.71	0	56,56,56	1.87	15 (26%)
18	LMU	B	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.12	3 (6%)
13	CLA	a	502	12	54,58,73	1.31	8 (14%)	64,95,113	1.49	6 (9%)
16	BCR	A	4008	-	41,41,41	0.74	0	56,56,56	2.05	17 (30%)
13	CLA	f	1201	2	64,68,73	1.17	9 (14%)	76,107,113	1.49	8 (10%)
13	CLA	f	1234	2	69,73,73	1.16	10 (14%)	82,113,113	1.52	14 (17%)
13	CLA	A	1105	1	59,63,73	1.20	9 (15%)	70,101,113	1.50	8 (11%)
13	CLA	Z	502	12	64,68,73	1.22	8 (12%)	76,107,113	1.37	6 (7%)
16	BCR	G	4001	-	41,41,41	0.70	0	56,56,56	1.74	12 (21%)
13	CLA	B	1227	2	69,73,73	1.13	9 (13%)	82,113,113	1.39	6 (7%)
13	CLA	f	1206	2	69,73,73	1.17	9 (13%)	82,113,113	1.43	5 (6%)
13	CLA	B	1213	2	69,73,73	1.14	10 (14%)	82,113,113	1.42	10 (12%)
13	CLA	f	1218	2	64,68,73	1.18	8 (12%)	76,107,113	1.38	7 (9%)
13	CLA	r	513	12	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
13	CLA	t	511	12	49,53,73	1.41	8 (16%)	58,89,113	1.52	5 (8%)
13	CLA	4	510	12	54,58,73	1.32	8 (14%)	64,95,113	1.46	5 (7%)
13	CLA	A	1122	1	64,68,73	1.18	7 (10%)	76,107,113	1.40	5 (6%)
13	CLA	H	1216	21	64,68,73	1.22	9 (14%)	76,107,113	1.35	6 (7%)
16	BCR	V	4020	-	41,41,41	0.74	0	56,56,56	1.96	16 (28%)
18	LMU	J	5105	-	22,22,36	1.15	1 (4%)	27,27,47	0.81	0
13	CLA	6	509	12	49,53,73	1.39	8 (16%)	58,89,113	1.44	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	K	1401	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	A	1107	1	69,73,73	1.16	11 (15%)	82,113,113	1.34	8 (9%)
13	CLA	G	1134	1	60,64,73	1.21	8 (13%)	71,102,113	1.42	5 (7%)
13	CLA	2	502	12	64,68,73	1.22	8 (12%)	76,107,113	1.38	6 (7%)
13	CLA	s	512	12	49,53,73	1.37	9 (18%)	58,89,113	1.49	4 (6%)
16	BCR	r	521	-	41,41,41	0.65	0	56,56,56	1.88	11 (19%)
13	CLA	f	1216	21	64,68,73	1.22	9 (14%)	76,107,113	1.36	6 (7%)
17	LHG	G	5008	-	34,34,48	0.78	1 (2%)	37,40,54	1.31	4 (10%)
15	SF4	C	3002	3	0,12,12	-	-	-		
16	BCR	Z	524	-	41,41,41	0.70	0	56,56,56	1.68	12 (21%)
17	LHG	V	5218	-	37,37,48	0.77	2 (5%)	40,43,54	1.26	4 (10%)
13	CLA	H	1222	21	64,68,73	1.17	9 (14%)	76,107,113	1.38	9 (11%)
17	LHG	L	5218	-	37,37,48	0.76	2 (5%)	40,43,54	1.26	4 (10%)
20	SQD	1	822	-	46,48,54	0.99	3 (6%)	56,59,65	1.69	13 (23%)
13	CLA	f	1214	2	69,73,73	1.16	9 (13%)	82,113,113	1.41	6 (7%)
13	CLA	Z	512	12	57,61,73	1.27	7 (12%)	67,98,113	1.37	5 (7%)
16	BCR	6	524	-	41,41,41	0.69	0	56,56,56	1.88	13 (23%)
17	LHG	A	5002	-	38,38,48	0.71	1 (2%)	41,44,54	1.25	5 (12%)
13	CLA	c	507	-	49,53,73	1.36	7 (14%)	58,89,113	1.52	7 (12%)
16	BCR	J	4012	-	41,41,41	0.70	0	56,56,56	1.67	13 (23%)
16	BCR	I	4018	-	41,41,41	0.76	1 (2%)	56,56,56	1.86	16 (28%)
16	BCR	u	522	-	41,41,41	0.70	0	56,56,56	1.94	21 (37%)
17	LHG	e	5009	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	7 (13%)
16	BCR	n	4019	-	41,41,41	0.68	0	56,56,56	1.94	13 (23%)
13	CLA	B	1211	2	60,64,73	1.23	6 (10%)	71,102,113	1.57	5 (7%)
13	CLA	B	1206	2	69,73,73	1.17	9 (13%)	82,113,113	1.43	5 (6%)
13	CLA	B	1218	2	64,68,73	1.17	9 (14%)	76,107,113	1.37	7 (9%)
13	CLA	1	512	12	56,60,73	1.29	8 (14%)	65,97,113	1.39	4 (6%)
13	CLA	f	1232	21	54,58,73	1.29	10 (18%)	64,95,113	1.58	7 (10%)
16	BCR	v	523	-	41,41,41	0.67	0	56,56,56	1.75	15 (26%)
19	LMG	l	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
16	BCR	r	522	-	41,41,41	0.67	0	56,56,56	1.76	19 (33%)
16	BCR	W	4021	-	41,41,41	0.64	0	56,56,56	1.84	16 (28%)
13	CLA	3	503	12	69,73,73	1.19	8 (11%)	82,113,113	1.30	5 (6%)
19	LMG	H	5002	-	54,54,55	0.80	3 (5%)	62,62,63	1.43	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LHG	A	5009	-	48,48,48	0.64	1 (2%)	51,54,54	1.29	7 (13%)
17	LHG	A	5006	-	44,44,48	0.63	1 (2%)	47,50,54	1.28	5 (10%)
16	BCR	d	523	-	41,41,41	0.67	0	56,56,56	1.75	15 (26%)
16	BCR	e	4007	-	41,41,41	0.68	0	56,56,56	2.13	18 (32%)
13	CLA	6	511	12	49,53,73	1.39	9 (18%)	58,89,113	1.49	5 (8%)
13	CLA	B	1203	2	69,73,73	1.16	11 (15%)	82,113,113	1.32	7 (8%)
13	CLA	v	518	12	59,63,73	1.26	8 (13%)	70,101,113	1.35	5 (7%)
13	CLA	4	502	12	54,58,73	1.32	8 (14%)	64,95,113	1.47	5 (7%)
13	CLA	A	1131	1	69,73,73	1.14	8 (11%)	82,113,113	1.33	7 (8%)
13	CLA	4	503	12	59,63,73	1.29	6 (10%)	70,101,113	1.39	7 (10%)
13	CLA	v	509	12	49,53,73	1.40	9 (18%)	58,89,113	1.45	5 (8%)
13	CLA	v	512	12	49,53,73	1.38	8 (16%)	58,89,113	1.46	4 (6%)
19	LMG	T	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
13	CLA	2	505	12	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
13	CLA	f	1210	2	69,73,73	1.15	8 (11%)	82,113,113	1.41	13 (15%)
16	BCR	L	4219	-	41,41,41	0.68	0	56,56,56	1.84	13 (23%)
13	CLA	v	511	12	49,53,73	1.39	8 (16%)	58,89,113	1.49	4 (6%)
13	CLA	f	1222	21	64,68,73	1.18	9 (14%)	76,107,113	1.38	9 (11%)
16	BCR	B	4004	-	41,41,41	0.68	0	56,56,56	1.87	13 (23%)
17	LHG	V	5221	-	48,48,48	0.68	2 (4%)	51,54,54	1.32	6 (11%)
13	CLA	e	1132	1	69,73,73	1.13	10 (14%)	82,113,113	1.35	7 (8%)
13	CLA	B	1217	2	61,65,73	1.22	9 (14%)	72,103,113	1.41	7 (9%)
13	CLA	Y	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
13	CLA	2	503	12	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
15	SF4	A	3001	1,2	0,12,12	-	-	-		
16	BCR	B	4005	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
13	CLA	B	1201	2	64,68,73	1.17	9 (14%)	76,107,113	1.49	8 (10%)
13	CLA	A	1140	1	69,73,73	1.17	9 (13%)	82,113,113	1.38	11 (13%)
17	LHG	e	5004	-	35,35,48	0.76	1 (2%)	38,41,54	1.29	4 (10%)
16	BCR	f	4014	-	41,41,41	0.69	0	56,56,56	1.87	13 (23%)
13	CLA	6	517	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
13	CLA	H	1206	2	69,73,73	1.17	9 (13%)	82,113,113	1.43	5 (6%)
13	CLA	4	508	12	49,53,73	1.41	8 (16%)	58,89,113	1.54	7 (12%)
13	CLA	5	501	12	69,73,73	1.16	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	G	1117	1	69,73,73	1.14	10 (14%)	82,113,113	1.55	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	G	1124	21	60,64,73	1.26	8 (13%)	71,102,113	1.46	10 (14%)
13	CLA	e	1133	1	69,73,73	1.11	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	f	1238	21	69,73,73	1.13	9 (13%)	82,113,113	1.38	9 (10%)
16	BCR	Z	522	-	41,41,41	0.67	0	56,56,56	1.76	19 (33%)
13	CLA	G	1101	1	69,73,73	1.17	9 (13%)	82,113,113	1.40	7 (8%)
16	BCR	r	523	-	41,41,41	0.66	0	56,56,56	1.77	15 (26%)
13	CLA	q	505	12	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
13	CLA	f	1202	2	69,73,73	1.14	10 (14%)	82,113,113	1.47	9 (10%)
16	BCR	1	522	-	41,41,41	0.68	0	56,56,56	1.92	20 (35%)
13	CLA	c	512	12	49,53,73	1.37	8 (16%)	58,89,113	1.46	4 (6%)
16	BCR	L	4022	-	41,41,41	0.72	0	56,56,56	1.93	16 (28%)
13	CLA	1	501	12	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	2	508	12	59,63,73	1.27	9 (15%)	70,101,113	1.42	8 (11%)
13	CLA	3	504	-	49,53,73	1.37	9 (18%)	58,89,113	1.51	7 (12%)
15	SF4	C	3003	3	0,12,12	-	-	-		
13	CLA	A	1133	1	69,73,73	1.11	9 (13%)	82,113,113	1.36	6 (7%)
13	CLA	t	516	12	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
16	BCR	V	4019	-	41,41,41	0.68	0	56,56,56	1.94	13 (23%)
13	CLA	5	507	-	49,53,73	1.37	7 (14%)	58,89,113	1.52	7 (12%)
13	CLA	r	501	12	69,73,73	1.16	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	H	1209	2	56,60,73	1.27	8 (14%)	65,97,113	1.56	7 (10%)
13	CLA	u	513	12	49,53,73	1.39	9 (18%)	58,89,113	1.41	4 (6%)
13	CLA	q	518	12	64,68,73	1.19	7 (10%)	76,107,113	1.41	6 (7%)
16	BCR	1	521	-	41,41,41	0.64	0	56,56,56	1.82	11 (19%)
14	PQN	G	2001	-	34,34,34	2.90	11 (32%)	43,45,45	2.05	6 (13%)
13	CLA	v	517	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
13	CLA	e	1140	1	69,73,73	1.17	9 (13%)	82,113,113	1.38	11 (13%)
13	CLA	1	516	12	49,53,73	1.39	8 (16%)	58,89,113	1.64	7 (12%)
16	BCR	B	4014	-	41,41,41	0.68	0	56,56,56	1.87	13 (23%)
13	CLA	b	516	12	49,53,73	1.39	7 (14%)	58,89,113	1.41	5 (8%)
13	CLA	Z	513	12	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
13	CLA	r	509	12	69,73,73	1.18	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	d	506	12	49,53,73	1.39	9 (18%)	58,89,113	1.47	5 (8%)
16	BCR	B	4017	-	41,41,41	0.72	0	56,56,56	1.60	11 (19%)
13	CLA	A	1237	21	69,73,73	1.17	8 (11%)	82,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	f	1211	2	60,64,73	1.22	7 (11%)	71,102,113	1.57	5 (7%)
13	CLA	t	519	12	59,63,73	1.25	9 (15%)	70,101,113	1.40	4 (5%)
17	LHG	G	5001	-	48,48,48	0.81	1 (2%)	51,54,54	1.28	6 (11%)
16	BCR	s	522	-	41,41,41	0.65	0	56,56,56	1.92	18 (32%)
13	CLA	Z	519	12	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
13	CLA	e	1102	1	69,73,73	1.12	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	f	1231	21	69,73,73	1.12	7 (10%)	82,113,113	1.41	8 (9%)
13	CLA	b	505	12	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
15	SF4	N	3002	3	0,12,12	-	-	-		
13	CLA	H	1231	21	69,73,73	1.12	7 (10%)	82,113,113	1.40	8 (9%)
13	CLA	R	1301	21	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
17	LHG	S	5001	-	43,43,48	0.65	0	46,49,54	1.25	4 (8%)
13	CLA	6	512	12	49,53,73	1.38	9 (18%)	58,89,113	1.46	4 (6%)
18	LMU	H	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.12	3 (6%)
13	CLA	e	1121	1	59,63,73	1.25	8 (13%)	70,101,113	1.46	10 (14%)
13	CLA	b	510	12	54,58,73	1.32	8 (14%)	64,95,113	1.47	5 (7%)
13	CLA	A	1138	1	69,73,73	1.11	9 (13%)	82,113,113	1.35	6 (7%)
13	CLA	5	516	12	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
13	CLA	f	1203	2	69,73,73	1.16	11 (15%)	82,113,113	1.32	7 (8%)
13	CLA	e	1134	1	60,64,73	1.21	8 (13%)	71,102,113	1.42	5 (7%)
13	CLA	d	510	12	49,53,73	1.38	8 (16%)	58,89,113	1.39	4 (6%)
13	CLA	4	506	12	49,53,73	1.40	8 (16%)	58,89,113	1.48	4 (6%)
13	CLA	L	1501	10	69,73,73	1.15	8 (11%)	82,113,113	1.39	8 (9%)
13	CLA	f	1223	2	69,73,73	1.15	8 (11%)	82,113,113	1.41	7 (8%)
16	BCR	3	523	-	41,41,41	0.65	0	56,56,56	1.78	17 (30%)
13	CLA	u	516	12	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
17	LHG	e	5008	-	34,34,48	0.78	1 (2%)	37,40,54	1.30	4 (10%)
13	CLA	A	1136	1	64,68,73	1.18	7 (10%)	76,107,113	1.46	8 (10%)
17	LHG	A	5003	13	40,40,48	0.76	1 (2%)	43,46,54	1.36	6 (13%)
16	BCR	U	4104	-	41,41,41	0.71	0	56,56,56	1.87	15 (26%)
13	CLA	4	519	12	59,63,73	1.25	9 (15%)	70,101,113	1.40	4 (5%)
14	PQN	f	2002	-	34,34,34	2.89	11 (32%)	43,45,45	2.10	5 (11%)
16	BCR	2	524	-	41,41,41	0.69	0	56,56,56	1.69	12 (21%)
13	CLA	f	1023	-	69,73,73	1.14	10 (14%)	82,113,113	1.69	13 (15%)
18	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.09	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	d	507	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	6 (10%)
13	CLA	Z	504	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	6 (9%)
13	CLA	f	1207	2	69,73,73	1.15	9 (13%)	82,113,113	1.29	4 (4%)
13	CLA	e	1138	1	69,73,73	1.11	9 (13%)	82,113,113	1.35	6 (7%)
13	CLA	Y	503	12	68,72,73	1.19	8 (11%)	80,111,113	1.32	7 (8%)
13	CLA	Y	516	12	49,53,73	1.39	8 (16%)	58,89,113	1.63	7 (12%)
13	CLA	A	1113	1	49,53,73	1.32	9 (18%)	58,89,113	1.55	6 (10%)
13	CLA	H	1215	2	69,73,73	1.15	9 (13%)	82,113,113	1.42	9 (10%)
15	SF4	g	3002	3	0,12,12	-	-	-		
13	CLA	1	504	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	6 (10%)
13	CLA	H	1240	17	69,73,73	1.17	9 (13%)	82,113,113	1.33	8 (9%)
13	CLA	A	1132	1	69,73,73	1.13	10 (14%)	82,113,113	1.36	7 (8%)
13	CLA	H	1210	2	69,73,73	1.15	8 (11%)	82,113,113	1.41	12 (14%)
13	CLA	u	508	12	49,53,73	1.39	9 (18%)	58,89,113	1.53	5 (8%)
13	CLA	4	512	12	49,53,73	1.39	7 (14%)	58,89,113	1.48	4 (6%)
13	CLA	c	513	12	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
13	CLA	f	1209	2	56,60,73	1.27	8 (14%)	65,97,113	1.56	7 (10%)
13	CLA	b	511	12	49,53,73	1.41	8 (16%)	58,89,113	1.51	5 (8%)
13	CLA	G	1110	1	55,59,73	1.29	9 (16%)	64,96,113	1.47	5 (7%)

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
13	CLA	6	519	12	1/1/11/20	9/17/93/115	-
13	CLA	H	1226	2	1/1/15/20	11/39/115/115	-
13	CLA	A	1114	21	1/1/12/20	2/21/97/115	-
13	CLA	Y	508	12	1/1/13/20	11/27/103/115	-
13	CLA	d	513	12	1/1/11/20	5/15/91/115	-
13	CLA	e	1128	1	1/1/15/20	12/39/115/115	-
18	LMU	2	901	-	-	8/14/34/61	0/1/1/2
13	CLA	B	1228	2	1/1/13/20	8/27/103/115	-
13	CLA	4	516	12	1/1/11/20	6/15/91/115	-
13	CLA	A	1111	1	1/1/15/20	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1235	2	1/1/15/20	8/39/115/115	-
13	CLA	f	1226	2	1/1/15/20	11/39/115/115	-
16	BCR	r	524	-	-	2/29/63/63	0/2/2/2
13	CLA	H	1220	2	1/1/13/20	9/27/103/115	-
13	CLA	c	510	12	1/1/11/20	8/15/91/115	-
13	CLA	m	1103	9	1/1/12/20	8/21/97/115	-
13	CLA	U	1401	-	1/1/13/20	8/27/103/115	-
13	CLA	u	502	12	1/1/12/20	6/21/97/115	-
13	CLA	v	502	12	1/1/12/20	6/21/97/115	-
17	LHG	H	1842	13	-	21/43/43/53	-
13	CLA	b	507	-	1/1/11/20	8/15/91/115	-
13	CLA	e	1136	1	1/1/14/20	5/33/109/115	-
13	CLA	Y	518	12	1/1/14/20	17/33/109/115	-
13	CLA	B	1210	2	1/1/15/20	20/39/115/115	-
16	BCR	q	524	-	-	2/29/63/63	0/2/2/2
13	CLA	3	501	12	1/1/15/20	6/39/115/115	-
13	CLA	e	1114	21	1/1/12/20	2/21/97/115	-
16	BCR	u	521	-	-	6/29/63/63	0/2/2/2
13	CLA	f	1221	21	1/1/15/20	14/39/115/115	-
13	CLA	U	1105	9	1/1/11/20	11/15/91/115	-
13	CLA	s	508	12	1/1/13/20	6/27/103/115	-
13	CLA	G	1130	1	1/1/15/20	9/39/115/115	-
18	LMU	r	901	-	-	8/14/34/61	0/1/1/2
13	CLA	Y	502	12	1/1/14/20	15/33/109/115	-
13	CLA	2	517	-	1/1/11/20	3/15/91/115	-
13	CLA	A	1119	21	1/1/15/20	12/39/115/115	-
13	CLA	A	1011	1	1/1/15/20	11/39/115/115	-
13	CLA	6	516	12	1/1/11/20	9/15/91/115	-
13	CLA	G	1102	1	1/1/15/20	11/39/115/115	-
13	CLA	G	1103	1	1/1/15/20	19/39/115/115	-
13	CLA	3	506	12	1/1/12/20	4/21/97/115	-
16	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	H	1218	2	1/1/14/20	7/33/109/115	-
13	CLA	t	513	12	1/1/11/20	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	v	521	-	-	5/29/63/63	0/2/2/2
13	CLA	H	1204	2	1/1/15/20	8/39/115/115	-
13	CLA	a	513	12	1/1/15/20	15/39/115/115	-
13	CLA	2	512	12	1/1/12/20	6/25/101/115	-
13	CLA	5	519	12	1/1/11/20	6/17/93/115	-
16	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
17	LHG	n	5218	-	-	23/42/42/53	-
16	BCR	u	524	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1120	1	1/1/12/20	4/25/101/115	-
13	CLA	B	1223	2	1/1/15/20	12/39/115/115	-
13	CLA	H	1213	2	1/1/15/20	11/39/115/115	-
13	CLA	c	518	12	1/1/13/20	14/27/103/115	-
13	CLA	B	1214	2	1/1/15/20	14/39/115/115	-
16	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	1	508	12	1/1/13/20	11/27/103/115	-
13	CLA	3	519	12	1/1/13/20	11/27/103/115	-
13	CLA	t	518	12	1/1/13/20	11/27/103/115	-
16	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	n	1503	21	1/1/14/20	9/33/109/115	-
13	CLA	q	517	-	1/1/11/20	5/15/91/115	-
13	CLA	b	519	12	1/1/13/20	11/27/103/115	-
13	CLA	A	1135	1	1/1/12/20	10/24/100/115	-
17	LHG	G	5005	-	-	29/49/49/53	-
16	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
13	CLA	b	517	-	1/1/11/20	8/15/91/115	-
13	CLA	5	513	12	1/1/11/20	6/15/91/115	-
13	CLA	H	1225	2	1/1/15/20	7/39/115/115	-
13	CLA	u	506	12	1/1/11/20	6/15/91/115	-
14	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	B	1230	2	1/1/14/20	11/33/109/115	-
13	CLA	r	517	-	1/1/11/20	3/15/91/115	-
13	CLA	G	1137	1	1/1/15/20	19/39/115/115	-
13	CLA	v	505	12	1/1/15/20	15/39/115/115	-
13	CLA	G	1135	1	1/1/12/20	10/24/100/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	Y	510	12	1/1/15/20	12/39/115/115	-
13	CLA	a	511	12	1/1/12/20	7/21/97/115	-
13	CLA	a	519	12	1/1/13/20	11/27/103/115	-
13	CLA	u	519	12	1/1/11/20	6/17/93/115	-
17	LHG	I	5001	-	-	22/48/48/53	-
13	CLA	1	507	-	1/1/14/20	15/33/109/115	-
16	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1136	1	1/1/14/20	5/33/109/115	-
16	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	s	509	12	1/1/15/20	3/39/115/115	-
13	CLA	e	1119	21	1/1/15/20	12/39/115/115	-
13	CLA	6	510	12	1/1/11/20	8/15/91/115	-
16	BCR	t	523	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1139	21	1/1/15/20	12/39/115/115	-
18	LMU	q	902	-	-	6/10/30/61	0/1/1/2
13	CLA	H	1230	2	1/1/14/20	11/33/109/115	-
13	CLA	A	1013	-	1/1/15/20	10/39/115/115	-
13	CLA	1	503	12	1/1/14/20	10/38/114/115	-
16	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
13	CLA	Z	507	-	1/1/15/20	16/39/115/115	-
13	CLA	G	1013	-	1/1/15/20	10/39/115/115	-
13	CLA	2	509	12	1/1/15/20	5/39/115/115	-
13	CLA	2	519	12	1/1/13/20	8/27/103/115	-
13	CLA	H	1236	2	-	5/27/103/115	-
13	CLA	r	503	12	1/1/15/20	8/39/115/115	-
16	BCR	s	524	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1232	21	1/1/12/20	5/21/97/115	-
13	CLA	f	1228	2	1/1/13/20	8/27/103/115	-
13	CLA	s	506	12	1/1/12/20	4/21/97/115	-
16	BCR	5	522	-	-	5/29/63/63	0/2/2/2
20	SQD	f	1852	-	-	20/40/60/69	0/1/1/1
13	CLA	1	502	12	1/1/14/20	15/33/109/115	-
13	CLA	Z	509	12	1/1/15/20	5/39/115/115	-
20	SQD	H	1852	-	-	20/40/60/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1222	21	1/1/14/20	7/33/109/115	-
13	CLA	t	517	-	1/1/11/20	8/15/91/115	-
13	CLA	G	1138	1	1/1/15/20	12/39/115/115	-
13	CLA	B	1219	2	1/1/15/20	17/39/115/115	-
13	CLA	f	1240	17	-	13/39/115/115	-
13	CLA	G	1022	21	1/1/15/20	8/39/115/115	-
16	BCR	1	524	-	-	2/29/63/63	0/2/2/2
15	SF4	N	3003	3	-	-	0/6/5/5
13	CLA	c	519	12	1/1/11/20	6/17/93/115	-
16	BCR	H	4014	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1104	1	1/1/15/20	12/39/115/115	-
13	CLA	H	1238	21	1/1/15/20	3/39/115/115	-
17	LHG	G	5002	-	-	26/43/43/53	-
16	BCR	a	524	-	-	5/29/63/63	0/2/2/2
13	CLA	d	519	12	1/1/11/20	9/17/93/115	-
20	SQD	r	822	-	-	13/38/58/69	0/1/1/1
16	BCR	c	523	-	-	4/29/63/63	0/2/2/2
16	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	q	512	12	1/1/12/20	10/24/100/115	-
16	BCR	u	523	-	-	4/29/63/63	0/2/2/2
13	CLA	r	510	12	1/1/15/20	7/39/115/115	-
13	CLA	v	516	12	1/1/11/20	9/15/91/115	-
16	BCR	5	521	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1107	1	1/1/15/20	15/39/115/115	-
13	CLA	q	502	12	1/1/14/20	15/33/109/115	-
13	CLA	s	513	12	1/1/15/20	15/39/115/115	-
13	CLA	B	1240	17	-	13/39/115/115	-
16	BCR	3	522	-	-	5/29/63/63	0/2/2/2
17	LHG	e	5005	-	-	29/49/49/53	-
17	LHG	n	5221	-	-	30/53/53/53	-
16	BCR	V	4022	-	-	2/29/63/63	0/2/2/2
16	BCR	2	522	-	-	6/29/63/63	0/2/2/2
17	LHG	L	5221	-	-	30/53/53/53	-
13	CLA	B	1012	21	1/1/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	SQD	d	822	-	-	9/19/39/69	0/1/1/1
13	CLA	H	1201	2	1/1/14/20	10/33/109/115	-
13	CLA	A	1130	1	1/1/15/20	9/39/115/115	-
13	CLA	r	508	12	1/1/13/20	8/27/103/115	-
13	CLA	v	508	12	1/1/11/20	3/15/91/115	-
17	LHG	B	1855	-	-	28/48/48/53	-
13	CLA	A	1129	1	1/1/12/20	6/23/99/115	-
16	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
16	BCR	3	521	-	-	7/29/63/63	0/2/2/2
18	LMU	l	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	1	513	12	1/1/13/20	3/27/103/115	-
13	CLA	u	517	-	1/1/11/20	9/15/91/115	-
13	CLA	H	1211	2	1/1/13/20	6/29/105/115	-
13	CLA	a	504	-	1/1/11/20	5/15/91/115	-
13	CLA	t	512	12	1/1/11/20	6/15/91/115	-
13	CLA	c	508	12	1/1/11/20	6/15/91/115	-
13	CLA	e	1115	1	1/1/14/20	10/33/109/115	-
13	CLA	e	1123	21	1/1/15/20	11/39/115/115	-
13	CLA	s	519	12	1/1/13/20	11/27/103/115	-
13	CLA	H	1219	2	1/1/15/20	17/39/115/115	-
13	CLA	d	517	-	1/1/11/20	10/15/91/115	-
13	CLA	j	1301	21	1/1/15/20	12/39/115/115	-
13	CLA	A	1126	1	1/1/15/20	17/39/115/115	-
13	CLA	f	1213	2	1/1/15/20	11/39/115/115	-
13	CLA	e	1127	1	1/1/15/20	12/39/115/115	-
16	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
17	LHG	f	1842	13	-	21/43/43/53	-
13	CLA	G	1125	1	1/1/15/20	12/39/115/115	-
13	CLA	q	510	12	1/1/15/20	12/39/115/115	-
16	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1229	2	1/1/15/20	13/39/115/115	-
13	CLA	b	512	12	1/1/11/20	6/15/91/115	-
13	CLA	A	1106	1	1/1/15/20	23/39/115/115	-
13	CLA	6	505	12	1/1/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1023	-	1/1/15/20	8/39/115/115	-
17	LHG	e	5006	-	-	21/49/49/53	-
13	CLA	1	510	12	1/1/15/20	12/39/115/115	-
13	CLA	5	504	-	1/1/11/20	4/15/91/115	-
16	BCR	o	4021	-	-	7/29/63/63	0/2/2/2
16	BCR	S	4018	-	-	1/29/63/63	0/2/2/2
16	BCR	Y	521	-	-	6/29/63/63	0/2/2/2
13	CLA	H	1203	2	1/1/15/20	17/39/115/115	-
20	SQD	Z	822	-	-	13/38/58/69	0/1/1/1
13	CLA	Z	506	12	1/1/13/20	7/27/103/115	-
16	BCR	v	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1131	1	1/1/15/20	9/39/115/115	-
13	CLA	e	1126	1	1/1/15/20	17/39/115/115	-
13	CLA	5	508	12	1/1/11/20	6/15/91/115	-
13	CLA	d	511	12	1/1/11/20	6/15/91/115	-
17	LHG	G	5004	-	-	21/40/40/53	-
13	CLA	q	503	12	1/1/14/20	10/38/114/115	-
16	BCR	B	4010	-	-	5/29/63/63	0/2/2/2
16	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
18	LMU	Z	901	-	-	7/14/34/61	0/1/1/2
13	CLA	r	502	12	1/1/14/20	12/33/109/115	-
13	CLA	e	1137	1	1/1/15/20	19/39/115/115	-
13	CLA	r	504	-	1/1/12/20	6/21/97/115	-
13	CLA	5	511	12	1/1/13/20	7/27/103/115	-
13	CLA	V	1502	10	1/1/15/20	10/39/115/115	-
13	CLA	H	1207	2	1/1/15/20	15/39/115/115	-
13	CLA	H	1012	21	1/1/15/20	15/39/115/115	-
13	CLA	A	1128	1	1/1/15/20	12/39/115/115	-
13	CLA	r	505	12	1/1/15/20	14/39/115/115	-
13	CLA	c	504	-	1/1/11/20	4/15/91/115	-
16	BCR	a	523	-	-	4/29/63/63	0/2/2/2
13	CLA	H	1224	2	1/1/14/20	13/33/109/115	-
13	CLA	q	516	12	1/1/11/20	13/15/91/115	-
17	LHG	A	5007	-	-	23/51/51/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1118	1	1/1/14/20	11/33/109/115	-
16	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	v	519	12	1/1/11/20	9/17/93/115	-
16	BCR	c	521	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1231	21	1/1/15/20	8/39/115/115	-
13	CLA	q	508	12	1/1/13/20	11/27/103/115	-
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1109	1	1/1/15/20	10/39/115/115	-
13	CLA	v	506	12	1/1/11/20	5/15/91/115	-
13	CLA	r	511	12	1/1/13/20	6/27/103/115	-
13	CLA	2	504	-	1/1/12/20	6/21/97/115	-
13	CLA	G	1107	1	1/1/15/20	16/39/115/115	-
14	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
16	BCR	k	4018	-	-	1/29/63/63	0/2/2/2
17	LHG	e	5007	-	-	22/51/51/53	-
17	LHG	V	5220	-	-	24/45/45/53	-
13	CLA	b	518	12	1/1/13/20	11/27/103/115	-
13	CLA	a	509	12	1/1/15/20	3/39/115/115	-
13	CLA	H	1221	21	1/1/15/20	14/39/115/115	-
13	CLA	f	1012	21	1/1/15/20	15/39/115/115	-
13	CLA	a	517	-	1/1/11/20	8/15/91/115	-
20	SQD	c	822	-	-	7/24/44/69	0/1/1/1
13	CLA	c	506	12	1/1/11/20	6/15/91/115	-
13	CLA	B	1209	2	1/1/12/20	8/24/100/115	-
16	BCR	c	522	-	-	5/29/63/63	0/2/2/2
16	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	f	1217	2	1/1/13/20	13/30/106/115	-
13	CLA	U	1103	9	1/1/12/20	8/21/97/115	-
16	BCR	f	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	B	1239	2	1/1/15/20	17/39/115/115	-
20	SQD	n	5216	-	-	17/46/66/69	0/1/1/1
20	SQD	t	822	-	-	9/19/39/69	0/1/1/1
13	CLA	r	512	12	1/1/12/20	6/25/101/115	-
14	PQN	H	2002	-	-	9/23/43/43	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1216	21	1/1/14/20	6/33/109/115	-
13	CLA	t	505	12	1/1/15/20	12/39/115/115	-
16	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	t	503	12	1/1/13/20	5/27/103/115	-
13	CLA	A	1801	17	1/1/11/20	4/15/91/115	-
13	CLA	f	1230	2	1/1/14/20	11/33/109/115	-
13	CLA	A	1118	1	1/1/14/20	11/33/109/115	-
13	CLA	G	1115	1	1/1/14/20	10/33/109/115	-
13	CLA	m	1401	-	1/1/13/20	8/27/103/115	-
13	CLA	A	1112	1	1/1/12/20	4/21/97/115	-
13	CLA	K	1105	9	1/1/11/20	11/15/91/115	-
16	BCR	5	524	-	-	2/29/63/63	0/2/2/2
16	BCR	A	4001	-	-	7/29/63/63	0/2/2/2
17	LHG	n	5220	-	-	24/45/45/53	-
17	LHG	G	5009	-	-	27/53/53/53	-
16	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
17	LHG	L	5220	-	-	24/45/45/53	-
13	CLA	6	513	12	1/1/11/20	5/15/91/115	-
13	CLA	G	1121	1	1/1/13/20	8/27/103/115	-
13	CLA	G	1132	1	1/1/15/20	17/39/115/115	-
13	CLA	3	511	12	1/1/12/20	7/21/97/115	-
13	CLA	c	503	12	1/1/13/20	11/27/103/115	-
13	CLA	f	1204	2	1/1/15/20	8/39/115/115	-
13	CLA	u	504	-	1/1/11/20	4/15/91/115	-
17	LHG	G	5007	-	-	23/51/51/53	-
13	CLA	G	1131	1	1/1/15/20	9/39/115/115	-
13	CLA	c	509	12	1/1/15/20	12/39/115/115	-
17	LHG	k	5001	-	-	22/48/48/53	-
17	LHG	A	5008	-	-	19/39/39/53	-
13	CLA	G	1108	1	1/1/12/20	16/26/102/115	-
13	CLA	b	509	12	1/1/15/20	7/39/115/115	-
16	BCR	e	4001	-	-	7/29/63/63	0/2/2/2
13	CLA	u	510	12	1/1/11/20	8/15/91/115	-
16	BCR	Y	524	-	-	2/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	519	12	1/1/12/20	6/21/97/115	-
13	CLA	e	1113	1	1/1/11/20	3/15/91/115	-
13	CLA	B	1225	2	1/1/15/20	7/39/115/115	-
13	CLA	t	510	12	1/1/12/20	8/21/97/115	-
13	CLA	H	1239	2	1/1/15/20	17/39/115/115	-
20	SQD	5	822	-	-	7/24/44/69	0/1/1/1
16	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
15	SF4	G	3001	1,2	-	-	0/6/5/5
13	CLA	q	506	12	1/1/11/20	5/15/91/115	-
20	SQD	L	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	F	1301	21	1/1/15/20	12/39/115/115	-
13	CLA	v	513	12	1/1/11/20	5/15/91/115	-
13	CLA	u	507	-	1/1/11/20	9/15/91/115	-
13	CLA	v	507	-	1/1/11/20	6/15/91/115	-
16	BCR	q	522	-	-	6/29/63/63	0/2/2/2
13	CLA	f	1219	2	1/1/15/20	17/39/115/115	-
13	CLA	2	516	12	1/1/11/20	10/15/91/115	-
13	CLA	d	518	12	1/1/13/20	11/27/103/115	-
13	CLA	G	1118	1	1/1/14/20	11/33/109/115	-
13	CLA	4	513	12	1/1/11/20	7/15/91/115	-
16	BCR	6	522	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1204	2	1/1/15/20	8/39/115/115	-
13	CLA	d	502	12	1/1/12/20	6/21/97/115	-
13	CLA	6	503	12	1/1/12/20	9/24/100/115	-
13	CLA	2	518	12	1/1/15/20	15/39/115/115	-
13	CLA	H	1217	2	1/1/13/20	13/30/106/115	-
13	CLA	Y	507	-	1/1/14/20	15/33/109/115	-
18	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	d	505	12	1/1/15/20	15/39/115/115	-
13	CLA	s	511	12	1/1/12/20	7/21/97/115	-
13	CLA	b	502	12	1/1/12/20	7/21/97/115	-
13	CLA	G	1133	1	1/1/15/20	16/39/115/115	-
20	SQD	a	822	-	-	22/38/58/69	0/1/1/1
16	BCR	e	4011	-	-	12/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	506	12	1/1/12/20	4/21/97/115	-
16	BCR	4	521	-	-	10/29/63/63	0/2/2/2
16	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
13	CLA	a	503	12	1/1/15/20	8/39/115/115	-
13	CLA	t	502	12	1/1/12/20	7/21/97/115	-
20	SQD	4	822	-	-	9/19/39/69	0/1/1/1
13	CLA	u	511	12	1/1/13/20	7/27/103/115	-
13	CLA	H	1228	2	1/1/13/20	8/27/103/115	-
17	LHG	A	5001	-	-	24/53/53/53	-
13	CLA	3	509	12	1/1/15/20	3/39/115/115	-
13	CLA	e	1111	1	1/1/15/20	10/39/115/115	-
13	CLA	3	512	12	1/1/11/20	7/15/91/115	-
13	CLA	V	1501	10	1/1/15/20	19/39/115/115	-
13	CLA	j	1302	6	1/1/11/20	9/15/91/115	-
13	CLA	A	1123	21	1/1/15/20	11/39/115/115	-
17	LHG	G	5006	-	-	21/49/49/53	-
17	LHG	A	5005	-	-	29/49/49/53	-
15	SF4	g	3003	3	-	-	0/6/5/5
17	LHG	e	5003	13	-	15/45/45/53	-
20	SQD	2	822	-	-	13/38/58/69	0/1/1/1
13	CLA	J	1302	8	1/1/13/20	13/31/107/115	-
16	BCR	6	521	-	-	5/29/63/63	0/2/2/2
13	CLA	Z	511	12	1/1/13/20	6/27/103/115	-
13	CLA	5	503	12	1/1/13/20	11/27/103/115	-
13	CLA	A	1117	1	1/1/15/20	13/39/115/115	-
13	CLA	A	1124	21	1/1/13/20	12/29/105/115	-
16	BCR	5	523	-	-	4/29/63/63	0/2/2/2
13	CLA	f	1208	2	1/1/15/20	16/39/115/115	-
16	BCR	3	524	-	-	5/29/63/63	0/2/2/2
13	CLA	1	511	12	1/1/13/20	4/27/103/115	-
13	CLA	b	508	12	1/1/11/20	6/15/91/115	-
13	CLA	d	509	12	1/1/11/20	4/15/91/115	-
19	LMG	f	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	R	1302	6	1/1/11/20	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	L	1503	21	1/1/14/20	9/33/109/115	-
16	BCR	n	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	v	504	-	1/1/11/20	6/15/91/115	-
13	CLA	a	518	12	1/1/13/20	11/27/103/115	-
16	BCR	1	523	-	-	6/29/63/63	0/2/2/2
13	CLA	Z	505	12	1/1/15/20	14/39/115/115	-
16	BCR	b	523	-	-	4/29/63/63	0/2/2/2
13	CLA	a	510	12	1/1/15/20	16/39/115/115	-
13	CLA	6	504	-	1/1/11/20	6/15/91/115	-
16	BCR	c	524	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1236	2	-	5/27/103/115	-
13	CLA	e	1109	1	1/1/15/20	10/39/115/115	-
20	SQD	3	822	-	-	22/38/58/69	0/1/1/1
13	CLA	B	1224	2	1/1/14/20	13/33/109/115	-
13	CLA	e	1117	1	1/1/15/20	13/39/115/115	-
13	CLA	e	1105	1	1/1/13/20	5/27/103/115	-
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	1	505	12	1/1/15/20	11/39/115/115	-
13	CLA	G	1122	1	1/1/14/20	13/33/109/115	-
16	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
13	CLA	Y	512	12	1/1/12/20	9/24/100/115	-
13	CLA	e	1101	1	1/1/15/20	13/39/115/115	-
13	CLA	3	513	12	1/1/15/20	15/39/115/115	-
16	BCR	d	524	-	-	3/29/63/63	0/2/2/2
13	CLA	r	516	12	1/1/11/20	10/15/91/115	-
13	CLA	a	507	-	1/1/15/20	14/39/115/115	-
13	CLA	Z	518	12	1/1/15/20	15/39/115/115	-
13	CLA	l	1303	8	1/1/15/20	16/39/115/115	-
16	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
16	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1021	2	1/1/15/20	10/39/115/115	-
13	CLA	A	1116	1	1/1/14/20	15/33/109/115	-
16	BCR	H	4010	-	-	5/29/63/63	0/2/2/2
17	LHG	G	5003	13	-	15/45/45/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1125	1	1/1/15/20	12/39/115/115	-
17	LHG	A	5004	-	-	21/40/40/53	-
13	CLA	H	1227	2	1/1/15/20	14/39/115/115	-
13	CLA	a	505	12	1/1/15/20	18/39/115/115	-
13	CLA	V	1503	21	1/1/14/20	9/33/109/115	-
13	CLA	5	510	12	1/1/11/20	8/15/91/115	-
13	CLA	1	509	12	1/1/15/20	6/39/115/115	-
16	BCR	2	523	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1113	1	1/1/11/20	3/15/91/115	-
16	BCR	f	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	s	507	-	1/1/15/20	14/39/115/115	-
16	BCR	v	524	-	-	3/29/63/63	0/2/2/2
13	CLA	A	1134	1	1/1/13/20	11/29/105/115	-
13	CLA	T	1303	8	1/1/15/20	16/39/115/115	-
13	CLA	4	504	-	1/1/11/20	6/15/91/115	-
13	CLA	a	501	12	1/1/15/20	6/39/115/115	-
13	CLA	2	513	12	1/1/15/20	15/39/115/115	-
13	CLA	H	1214	2	1/1/15/20	14/39/115/115	-
16	BCR	b	521	-	-	10/29/63/63	0/2/2/2
13	CLA	H	1205	2	1/1/15/20	11/39/115/115	-
16	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	H	1223	2	1/1/15/20	12/39/115/115	-
13	CLA	G	1114	21	1/1/12/20	2/21/97/115	-
16	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	e	1139	21	1/1/15/20	12/39/115/115	-
13	CLA	3	505	12	1/1/15/20	18/39/115/115	-
13	CLA	e	1237	21	1/1/15/20	20/39/115/115	-
13	CLA	Y	519	12	1/1/12/20	6/21/97/115	-
13	CLA	d	508	12	1/1/11/20	3/15/91/115	-
16	BCR	t	522	-	-	4/29/63/63	0/2/2/2
13	CLA	f	1021	2	1/1/15/20	10/39/115/115	-
13	CLA	s	517	-	1/1/11/20	8/15/91/115	-
13	CLA	1	506	12	1/1/11/20	5/15/91/115	-
13	CLA	5	517	-	1/1/11/20	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1108	1	1/1/12/20	16/26/102/115	-
17	LHG	H	1855	-	-	28/48/48/53	-
13	CLA	B	1215	2	1/1/15/20	17/39/115/115	-
13	CLA	2	510	12	1/1/15/20	7/39/115/115	-
13	CLA	4	507	-	1/1/11/20	8/15/91/115	-
16	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	t	504	-	1/1/11/20	6/15/91/115	-
13	CLA	e	1110	1	1/1/12/20	10/23/99/115	-
13	CLA	B	1205	2	1/1/15/20	11/39/115/115	-
13	CLA	4	505	12	1/1/15/20	12/39/115/115	-
16	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	G	1119	21	1/1/15/20	12/39/115/115	-
13	CLA	H	1212	2	1/1/13/20	11/27/103/115	-
13	CLA	B	1238	21	1/1/15/20	3/39/115/115	-
13	CLA	2	507	-	1/1/15/20	16/39/115/115	-
13	CLA	3	502	12	1/1/12/20	6/21/97/115	-
16	BCR	4	523	-	-	4/29/63/63	0/2/2/2
13	CLA	t	508	12	1/1/11/20	6/15/91/115	-
13	CLA	u	509	12	1/1/15/20	12/39/115/115	-
13	CLA	q	513	12	1/1/13/20	3/27/103/115	-
13	CLA	A	1110	1	1/1/12/20	10/23/99/115	-
13	CLA	q	519	12	1/1/12/20	6/21/97/115	-
13	CLA	6	507	-	1/1/11/20	6/15/91/115	-
13	CLA	B	1226	2	1/1/15/20	11/39/115/115	-
17	LHG	B	1842	13	-	21/43/43/53	-
13	CLA	f	1212	2	1/1/13/20	11/27/103/115	-
16	BCR	s	523	-	-	4/29/63/63	0/2/2/2
13	CLA	6	508	12	1/1/11/20	3/15/91/115	-
13	CLA	4	501	12	1/1/14/20	11/33/109/115	-
13	CLA	f	1236	2	-	5/27/103/115	-
13	CLA	f	1227	2	1/1/15/20	14/39/115/115	-
13	CLA	Y	509	12	1/1/15/20	6/39/115/115	-
16	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	Y	513	12	1/1/13/20	3/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	s	516	12	1/1/11/20	10/15/91/115	-
13	CLA	u	512	12	1/1/11/20	8/15/91/115	-
13	CLA	1	518	12	1/1/14/20	17/33/109/115	-
13	CLA	n	1502	10	1/1/15/20	10/39/115/115	-
17	LHG	f	1855	-	-	28/48/48/53	-
13	CLA	L	1502	10	1/1/15/20	10/39/115/115	-
16	BCR	G	4011	-	-	11/29/63/63	0/2/2/2
16	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
20	SQD	6	822	-	-	9/19/39/69	0/1/1/1
13	CLA	v	501	12	1/1/14/20	18/33/109/115	-
16	BCR	d	521	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1129	1	1/1/12/20	6/23/99/115	-
16	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1101	1	1/1/15/20	13/39/115/115	-
18	LMU	Y	902	-	-	6/10/30/61	0/1/1/2
13	CLA	6	501	12	1/1/14/20	18/33/109/115	-
13	CLA	4	511	12	1/1/11/20	5/15/91/115	-
13	CLA	G	1111	1	1/1/15/20	10/39/115/115	-
13	CLA	5	518	12	1/1/13/20	14/27/103/115	-
13	CLA	6	502	12	1/1/12/20	6/21/97/115	-
13	CLA	Y	506	12	1/1/11/20	5/15/91/115	-
13	CLA	e	1135	1	1/1/12/20	10/24/100/115	-
13	CLA	A	1102	1	1/1/15/20	11/39/115/115	-
13	CLA	A	1103	1	1/1/15/20	19/39/115/115	-
13	CLA	G	1112	1	1/1/12/20	4/21/97/115	-
13	CLA	e	1120	1	1/1/12/20	4/25/101/115	-
13	CLA	f	1225	2	1/1/15/20	7/39/115/115	-
13	CLA	n	1501	10	1/1/15/20	19/39/115/115	-
13	CLA	q	507	-	1/1/14/20	15/33/109/115	-
13	CLA	e	1130	1	1/1/15/20	9/39/115/115	-
13	CLA	d	512	12	1/1/11/20	10/15/91/115	-
13	CLA	b	504	-	1/1/11/20	6/15/91/115	-
13	CLA	Z	501	12	1/1/15/20	13/39/115/115	-
13	CLA	b	506	12	1/1/11/20	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	G	4008	-	-	5/29/63/63	0/2/2/2
18	LMU	T	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	G	1237	21	1/1/15/20	20/39/115/115	-
13	CLA	G	1128	1	1/1/15/20	12/39/115/115	-
13	CLA	Z	516	12	1/1/11/20	10/15/91/115	-
13	CLA	f	1220	2	1/1/13/20	9/27/103/115	-
13	CLA	e	1011	1	1/1/15/20	11/39/115/115	-
13	CLA	f	1224	2	1/1/14/20	13/33/109/115	-
13	CLA	b	513	12	1/1/11/20	7/15/91/115	-
16	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1106	1	1/1/15/20	23/39/115/115	-
18	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
16	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1139	21	1/1/15/20	12/39/115/115	-
13	CLA	H	1023	-	1/1/15/20	8/39/115/115	-
13	CLA	c	517	-	1/1/11/20	9/15/91/115	-
13	CLA	q	509	12	1/1/15/20	6/39/115/115	-
13	CLA	e	1122	1	1/1/14/20	13/33/109/115	-
13	CLA	e	1801	17	1/1/11/20	4/15/91/115	-
13	CLA	Y	504	-	1/1/11/20	6/15/91/115	-
13	CLA	Z	517	-	1/1/11/20	3/15/91/115	-
13	CLA	5	502	12	1/1/12/20	6/21/97/115	-
13	CLA	G	1127	1	1/1/15/20	12/39/115/115	-
13	CLA	A	1137	1	1/1/15/20	19/39/115/115	-
13	CLA	e	1112	1	1/1/12/20	4/21/97/115	-
13	CLA	G	1105	1	1/1/13/20	5/27/103/115	-
13	CLA	t	506	12	1/1/11/20	6/15/91/115	-
16	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
18	LMU	G	1849	-	-	5/14/34/61	0/1/1/2
13	CLA	F	1302	6	1/1/11/20	9/15/91/115	-
19	LMG	B	5002	-	-	24/49/69/70	0/1/1/1
14	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	r	507	-	1/1/15/20	16/39/115/115	-
13	CLA	1	517	-	1/1/11/20	5/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	q	521	-	-	7/29/63/63	0/2/2/2
19	LMG	J	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	B	1221	21	1/1/15/20	14/39/115/115	-
18	LMU	1	902	-	-	6/10/30/61	0/1/1/2
13	CLA	f	1205	2	1/1/15/20	11/39/115/115	-
20	SQD	u	822	-	-	7/24/44/69	0/1/1/1
20	SQD	v	822	-	-	9/19/39/69	0/1/1/1
13	CLA	6	506	12	1/1/11/20	5/15/91/115	-
13	CLA	4	509	12	1/1/15/20	7/39/115/115	-
13	CLA	u	503	12	1/1/13/20	11/27/103/115	-
13	CLA	B	1212	2	1/1/13/20	11/27/103/115	-
13	CLA	s	504	-	1/1/11/20	5/15/91/115	-
16	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	a	512	12	1/1/11/20	7/15/91/115	-
13	CLA	b	501	12	1/1/14/20	11/33/109/115	-
16	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	H	1229	2	1/1/15/20	13/39/115/115	-
13	CLA	3	516	12	1/1/11/20	10/15/91/115	-
20	SQD	Y	822	-	-	20/43/63/69	0/1/1/1
15	SF4	e	3001	1,2	-	-	0/6/5/5
13	CLA	q	504	-	1/1/11/20	6/15/91/115	-
16	BCR	d	522	-	-	5/29/63/63	0/2/2/2
13	CLA	t	501	12	1/1/14/20	11/33/109/115	-
13	CLA	B	1208	2	1/1/15/20	16/39/115/115	-
13	CLA	A	1125	1	1/1/15/20	12/39/115/115	-
16	BCR	4	524	-	-	4/29/63/63	0/2/2/2
13	CLA	H	1235	2	1/1/15/20	8/39/115/115	-
16	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1123	21	1/1/15/20	11/39/115/115	-
13	CLA	A	1127	1	1/1/15/20	12/39/115/115	-
13	CLA	d	503	12	1/1/12/20	9/24/100/115	-
13	CLA	e	1116	1	1/1/14/20	15/33/109/115	-
16	BCR	t	521	-	-	10/29/63/63	0/2/2/2
13	CLA	e	1104	1	1/1/15/20	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	c	511	12	1/1/13/20	7/27/103/115	-
13	CLA	t	509	12	1/1/15/20	7/39/115/115	-
13	CLA	5	509	12	1/1/15/20	12/39/115/115	-
13	CLA	e	1013	-	1/1/15/20	10/39/115/115	-
13	CLA	3	508	12	1/1/13/20	6/27/103/115	-
13	CLA	5	512	12	1/1/11/20	8/15/91/115	-
13	CLA	A	1022	21	1/1/15/20	8/39/115/115	-
13	CLA	5	506	12	1/1/11/20	6/15/91/115	-
13	CLA	Y	501	12	1/1/15/20	16/39/115/115	-
13	CLA	t	507	-	1/1/11/20	8/15/91/115	-
20	SQD	s	822	-	-	22/38/58/69	0/1/1/1
13	CLA	b	503	12	1/1/13/20	5/27/103/115	-
13	CLA	d	516	12	1/1/11/20	9/15/91/115	-
13	CLA	5	505	12	1/1/14/20	18/35/111/115	-
13	CLA	3	517	-	1/1/11/20	8/15/91/115	-
13	CLA	6	518	12	1/1/13/20	11/27/103/115	-
13	CLA	s	503	12	1/1/15/20	8/39/115/115	-
13	CLA	u	518	12	1/1/13/20	14/27/103/115	-
13	CLA	G	1120	1	1/1/12/20	4/25/101/115	-
13	CLA	A	1104	1	1/1/15/20	12/39/115/115	-
13	CLA	B	1202	2	1/1/15/20	11/39/115/115	-
13	CLA	B	1220	2	1/1/13/20	9/27/103/115	-
13	CLA	c	505	12	1/1/14/20	18/35/111/115	-
13	CLA	e	1103	1	1/1/15/20	19/39/115/115	-
13	CLA	A	1121	1	1/1/13/20	8/27/103/115	-
13	CLA	B	1234	2	1/1/15/20	12/39/115/115	-
13	CLA	3	518	12	1/1/13/20	11/27/103/115	-
13	CLA	H	1208	2	1/1/15/20	16/39/115/115	-
13	CLA	u	505	12	1/1/14/20	18/35/111/115	-
13	CLA	v	503	12	1/1/12/20	9/24/100/115	-
16	BCR	t	524	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1022	21	1/1/15/20	8/39/115/115	-
18	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	G	1011	1	1/1/15/20	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	r	506	12	1/1/13/20	7/27/103/115	-
13	CLA	c	502	12	1/1/12/20	6/21/97/115	-
13	CLA	3	510	12	1/1/15/20	16/39/115/115	-
13	CLA	4	517	-	1/1/11/20	8/15/91/115	-
13	CLA	A	1108	1	1/1/12/20	16/26/102/115	-
13	CLA	Y	505	12	1/1/15/20	11/39/115/115	-
13	CLA	r	519	12	1/1/13/20	8/27/103/115	-
13	CLA	A	1115	1	1/1/14/20	10/33/109/115	-
13	CLA	2	511	12	1/1/13/20	6/27/103/115	-
13	CLA	c	501	12	1/1/15/20	20/39/115/115	-
13	CLA	f	1235	2	1/1/15/20	8/39/115/115	-
16	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
16	BCR	6	523	-	-	4/29/63/63	0/2/2/2
13	CLA	u	501	12	1/1/15/20	20/39/115/115	-
16	BCR	b	524	-	-	4/29/63/63	0/2/2/2
13	CLA	Z	503	12	1/1/15/20	8/39/115/115	-
13	CLA	G	1140	1	1/1/15/20	13/39/115/115	-
13	CLA	G	1116	1	1/1/14/20	15/33/109/115	-
13	CLA	3	507	-	1/1/15/20	14/39/115/115	-
13	CLA	c	516	12	1/1/11/20	4/15/91/115	-
13	CLA	K	1103	9	1/1/12/20	8/21/97/115	-
13	CLA	H	1202	2	1/1/15/20	11/39/115/115	-
13	CLA	s	518	12	1/1/13/20	11/27/103/115	-
16	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	J	1303	8	1/1/15/20	16/39/115/115	-
13	CLA	H	1234	2	1/1/15/20	12/39/115/115	-
13	CLA	d	501	12	1/1/14/20	18/33/109/115	-
13	CLA	s	510	12	1/1/15/20	16/39/115/115	-
16	BCR	a	522	-	-	5/29/63/63	0/2/2/2
13	CLA	2	501	12	1/1/15/20	13/39/115/115	-
13	CLA	A	1109	1	1/1/15/20	10/39/115/115	-
13	CLA	T	1302	8	1/1/13/20	13/31/107/115	-
13	CLA	f	1215	2	1/1/15/20	17/39/115/115	-
16	BCR	4	522	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	Z	508	12	1/1/13/20	8/27/103/115	-
13	CLA	v	510	12	1/1/11/20	8/15/91/115	-
13	CLA	q	511	12	1/1/13/20	4/27/103/115	-
13	CLA	a	516	12	1/1/11/20	10/15/91/115	-
20	SQD	V	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	r	518	12	1/1/15/20	15/39/115/115	-
16	BCR	2	521	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1129	1	1/1/12/20	6/23/99/115	-
16	BCR	e	4008	-	-	5/29/63/63	0/2/2/2
13	CLA	2	506	12	1/1/13/20	7/27/103/115	-
13	CLA	d	504	-	1/1/11/20	6/15/91/115	-
16	BCR	a	521	-	-	7/29/63/63	0/2/2/2
13	CLA	f	1239	2	1/1/15/20	17/39/115/115	-
13	CLA	s	505	12	1/1/15/20	18/39/115/115	-
13	CLA	H	1232	21	1/1/12/20	5/21/97/115	-
16	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	Y	511	12	1/1/13/20	4/27/103/115	-
13	CLA	4	518	12	1/1/13/20	11/27/103/115	-
13	CLA	Z	510	12	1/1/15/20	7/39/115/115	-
13	CLA	l	1302	8	1/1/13/20	13/31/107/115	-
18	LMU	A	1849	-	-	5/14/34/61	0/1/1/2
13	CLA	s	502	12	1/1/12/20	6/21/97/115	-
13	CLA	G	1126	1	1/1/15/20	17/39/115/115	-
13	CLA	a	508	12	1/1/13/20	6/27/103/115	-
20	SQD	b	822	-	-	9/19/39/69	0/1/1/1
16	BCR	q	523	-	-	6/29/63/63	0/2/2/2
17	LHG	e	5001	-	-	24/53/53/53	-
20	SQD	B	1852	-	-	20/40/60/69	0/1/1/1
13	CLA	s	501	12	1/1/15/20	6/39/115/115	-
13	CLA	B	1207	2	1/1/15/20	15/39/115/115	-
13	CLA	H	1021	2	1/1/15/20	10/39/115/115	-
13	CLA	G	1106	1	1/1/15/20	23/39/115/115	-
16	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
20	SQD	q	822	-	-	20/43/63/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	m	1105	9	1/1/11/20	11/15/91/115	-
13	CLA	q	501	12	1/1/15/20	16/39/115/115	-
18	LMU	e	1849	-	-	5/14/34/61	0/1/1/2
16	BCR	s	521	-	-	7/29/63/63	0/2/2/2
17	LHG	e	5002	-	-	26/43/43/53	-
13	CLA	G	1801	17	1/1/11/20	4/15/91/115	-
16	BCR	b	522	-	-	4/29/63/63	0/2/2/2
16	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1229	2	1/1/15/20	13/39/115/115	-
13	CLA	e	1124	21	1/1/13/20	12/29/105/115	-
16	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
18	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	a	502	12	1/1/12/20	6/21/97/115	-
16	BCR	A	4008	-	-	5/29/63/63	0/2/2/2
13	CLA	f	1201	2	1/1/14/20	10/33/109/115	-
13	CLA	f	1234	2	1/1/15/20	12/39/115/115	-
13	CLA	A	1105	1	1/1/13/20	5/27/103/115	-
13	CLA	Z	502	12	1/1/14/20	12/33/109/115	-
16	BCR	G	4001	-	-	7/29/63/63	0/2/2/2
13	CLA	B	1227	2	1/1/15/20	14/39/115/115	-
13	CLA	f	1206	2	1/1/15/20	15/39/115/115	-
13	CLA	B	1213	2	1/1/15/20	11/39/115/115	-
13	CLA	f	1218	2	1/1/14/20	7/33/109/115	-
13	CLA	r	513	12	1/1/15/20	15/39/115/115	-
13	CLA	t	511	12	1/1/11/20	5/15/91/115	-
13	CLA	4	510	12	1/1/12/20	8/21/97/115	-
13	CLA	A	1122	1	1/1/14/20	13/33/109/115	-
13	CLA	H	1216	21	1/1/14/20	6/33/109/115	-
16	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
18	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	6	509	12	1/1/11/20	4/15/91/115	-
13	CLA	K	1401	-	1/1/13/20	8/27/103/115	-
13	CLA	A	1107	1	1/1/15/20	16/39/115/115	-
13	CLA	G	1134	1	1/1/13/20	11/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	502	12	1/1/14/20	12/33/109/115	-
13	CLA	s	512	12	1/1/11/20	7/15/91/115	-
16	BCR	r	521	-	-	4/29/63/63	0/2/2/2
13	CLA	f	1216	21	1/1/14/20	6/33/109/115	-
17	LHG	G	5008	-	-	19/39/39/53	-
16	BCR	Z	524	-	-	3/29/63/63	0/2/2/2
15	SF4	C	3002	3	-	-	0/6/5/5
17	LHG	V	5218	-	-	23/42/42/53	-
13	CLA	H	1222	21	1/1/14/20	7/33/109/115	-
17	LHG	L	5218	-	-	23/42/42/53	-
20	SQD	1	822	-	-	20/43/63/69	0/1/1/1
13	CLA	f	1214	2	1/1/15/20	14/39/115/115	-
13	CLA	Z	512	12	1/1/12/20	6/25/101/115	-
16	BCR	6	524	-	-	3/29/63/63	0/2/2/2
17	LHG	A	5002	-	-	26/43/43/53	-
13	CLA	c	507	-	1/1/11/20	9/15/91/115	-
16	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
16	BCR	I	4018	-	-	1/29/63/63	0/2/2/2
16	BCR	u	522	-	-	5/29/63/63	0/2/2/2
17	LHG	e	5009	-	-	27/53/53/53	-
16	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1211	2	1/1/13/20	6/29/105/115	-
13	CLA	B	1206	2	1/1/15/20	15/39/115/115	-
13	CLA	B	1218	2	1/1/14/20	7/33/109/115	-
13	CLA	1	512	12	1/1/12/20	10/24/100/115	-
13	CLA	f	1232	21	1/1/12/20	5/21/97/115	-
16	BCR	v	523	-	-	4/29/63/63	0/2/2/2
19	LMG	l	5104	-	-	17/30/50/70	0/1/1/1
16	BCR	r	522	-	-	6/29/63/63	0/2/2/2
16	BCR	W	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	3	503	12	1/1/15/20	8/39/115/115	-
19	LMG	H	5002	-	-	24/49/69/70	0/1/1/1
17	LHG	A	5009	-	-	27/53/53/53	-
17	LHG	A	5006	-	-	21/49/49/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	d	523	-	-	4/29/63/63	0/2/2/2
16	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	6	511	12	1/1/11/20	6/15/91/115	-
13	CLA	B	1203	2	1/1/15/20	17/39/115/115	-
13	CLA	v	518	12	1/1/13/20	11/27/103/115	-
13	CLA	4	502	12	1/1/12/20	7/21/97/115	-
13	CLA	A	1131	1	1/1/15/20	9/39/115/115	-
13	CLA	4	503	12	1/1/13/20	5/27/103/115	-
13	CLA	v	509	12	1/1/11/20	4/15/91/115	-
13	CLA	v	512	12	1/1/11/20	10/15/91/115	-
19	LMG	T	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	2	505	12	1/1/15/20	14/39/115/115	-
13	CLA	f	1210	2	1/1/15/20	20/39/115/115	-
16	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	v	511	12	1/1/11/20	6/15/91/115	-
13	CLA	f	1222	21	1/1/14/20	6/33/109/115	-
16	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
17	LHG	V	5221	-	-	30/53/53/53	-
13	CLA	e	1132	1	1/1/15/20	17/39/115/115	-
13	CLA	B	1217	2	1/1/13/20	13/30/106/115	-
13	CLA	Y	517	-	1/1/11/20	5/15/91/115	-
13	CLA	2	503	12	1/1/15/20	8/39/115/115	-
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
17	LHG	e	5004	-	-	21/40/40/53	-
13	CLA	B	1201	2	1/1/14/20	10/33/109/115	-
13	CLA	A	1140	1	1/1/15/20	13/39/115/115	-
15	SF4	A	3001	1,2	-	-	0/6/5/5
16	BCR	f	4014	-	-	6/29/63/63	0/2/2/2
13	CLA	6	517	-	1/1/11/20	10/15/91/115	-
13	CLA	H	1206	2	1/1/15/20	15/39/115/115	-
13	CLA	4	508	12	1/1/11/20	6/15/91/115	-
13	CLA	5	501	12	1/1/15/20	20/39/115/115	-
13	CLA	G	1117	1	1/1/15/20	13/39/115/115	-
13	CLA	G	1124	21	1/1/13/20	12/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1133	1	1/1/15/20	16/39/115/115	-
13	CLA	f	1238	21	1/1/15/20	3/39/115/115	-
16	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1101	1	1/1/15/20	13/39/115/115	-
16	BCR	r	523	-	-	6/29/63/63	0/2/2/2
13	CLA	q	505	12	1/1/15/20	11/39/115/115	-
13	CLA	f	1202	2	1/1/15/20	11/39/115/115	-
16	BCR	1	522	-	-	6/29/63/63	0/2/2/2
13	CLA	c	512	12	1/1/11/20	8/15/91/115	-
16	BCR	L	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	1	501	12	1/1/15/20	16/39/115/115	-
13	CLA	2	508	12	1/1/13/20	8/27/103/115	-
13	CLA	3	504	-	1/1/11/20	5/15/91/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	A	1133	1	1/1/15/20	16/39/115/115	-
13	CLA	t	516	12	1/1/11/20	6/15/91/115	-
16	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	5	507	-	1/1/11/20	9/15/91/115	-
13	CLA	r	501	12	1/1/15/20	13/39/115/115	-
13	CLA	H	1209	2	1/1/12/20	8/24/100/115	-
13	CLA	u	513	12	1/1/11/20	6/15/91/115	-
13	CLA	q	518	12	1/1/14/20	17/33/109/115	-
16	BCR	1	521	-	-	7/29/63/63	0/2/2/2
14	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	v	517	-	1/1/11/20	10/15/91/115	-
13	CLA	e	1140	1	1/1/15/20	13/39/115/115	-
13	CLA	1	516	12	1/1/11/20	13/15/91/115	-
16	BCR	B	4014	-	-	6/29/63/63	0/2/2/2
13	CLA	b	516	12	1/1/11/20	6/15/91/115	-
13	CLA	Z	513	12	1/1/15/20	15/39/115/115	-
13	CLA	r	509	12	1/1/15/20	5/39/115/115	-
13	CLA	d	506	12	1/1/11/20	5/15/91/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1237	21	1/1/15/20	20/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1211	2	1/1/13/20	6/29/105/115	-
13	CLA	t	519	12	1/1/13/20	11/27/103/115	-
17	LHG	G	5001	-	-	24/53/53/53	-
16	BCR	s	522	-	-	5/29/63/63	0/2/2/2
13	CLA	Z	519	12	1/1/13/20	8/27/103/115	-
13	CLA	e	1102	1	1/1/15/20	11/39/115/115	-
13	CLA	f	1231	21	1/1/15/20	8/39/115/115	-
13	CLA	b	505	12	1/1/15/20	12/39/115/115	-
17	LHG	S	5001	-	-	22/48/48/53	-
13	CLA	H	1231	21	1/1/15/20	8/39/115/115	-
13	CLA	R	1301	21	1/1/15/20	12/39/115/115	-
15	SF4	N	3002	3	-	-	0/6/5/5
13	CLA	6	512	12	1/1/11/20	10/15/91/115	-
18	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	e	1121	1	1/1/13/20	8/27/103/115	-
13	CLA	b	510	12	1/1/12/20	8/21/97/115	-
13	CLA	A	1138	1	1/1/15/20	12/39/115/115	-
13	CLA	5	516	12	1/1/11/20	4/15/91/115	-
13	CLA	f	1203	2	1/1/15/20	17/39/115/115	-
13	CLA	e	1134	1	1/1/13/20	11/29/105/115	-
13	CLA	d	510	12	1/1/11/20	8/15/91/115	-
13	CLA	4	506	12	1/1/11/20	6/15/91/115	-
13	CLA	L	1501	10	1/1/15/20	19/39/115/115	-
13	CLA	f	1223	2	1/1/15/20	12/39/115/115	-
16	BCR	3	523	-	-	4/29/63/63	0/2/2/2
13	CLA	u	516	12	1/1/11/20	4/15/91/115	-
17	LHG	e	5008	-	-	19/39/39/53	-
13	CLA	A	1136	1	1/1/14/20	5/33/109/115	-
17	LHG	A	5003	13	-	15/45/45/53	-
16	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	4	519	12	1/1/13/20	11/27/103/115	-
14	PQN	f	2002	-	-	9/23/43/43	0/2/2/2
16	BCR	2	524	-	-	3/29/63/63	0/2/2/2
13	CLA	f	1023	-	1/1/15/20	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	d	507	-	1/1/11/20	6/15/91/115	-
13	CLA	Z	504	-	1/1/12/20	6/21/97/115	-
13	CLA	f	1207	2	1/1/15/20	15/39/115/115	-
13	CLA	e	1138	1	1/1/15/20	12/39/115/115	-
13	CLA	Y	503	12	1/1/14/20	10/38/114/115	-
13	CLA	Y	516	12	1/1/11/20	13/15/91/115	-
13	CLA	A	1113	1	1/1/11/20	3/15/91/115	-
13	CLA	H	1215	2	1/1/15/20	17/39/115/115	-
15	SF4	g	3002	3	-	-	0/6/5/5
13	CLA	1	504	-	1/1/11/20	6/15/91/115	-
13	CLA	H	1240	17	-	13/39/115/115	-
13	CLA	A	1132	1	1/1/15/20	17/39/115/115	-
13	CLA	H	1210	2	1/1/15/20	20/39/115/115	-
13	CLA	u	508	12	1/1/11/20	6/15/91/115	-
13	CLA	4	512	12	1/1/11/20	6/15/91/115	-
13	CLA	c	513	12	1/1/11/20	6/15/91/115	-
13	CLA	f	1209	2	1/1/12/20	8/24/100/115	-
13	CLA	b	511	12	1/1/11/20	5/15/91/115	-
13	CLA	G	1110	1	1/1/12/20	9/23/99/115	-

All (5253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C12-C13	9.04	1.53	1.33
14	f	2002	PQN	C12-C13	9.03	1.53	1.33
14	H	2002	PQN	C12-C13	9.03	1.53	1.33
14	G	2001	PQN	C12-C13	8.99	1.53	1.33
14	e	2001	PQN	C12-C13	8.99	1.53	1.33
14	A	2001	PQN	C12-C13	8.98	1.53	1.33
14	f	2002	PQN	O1-C1	7.93	1.39	1.23
14	B	2002	PQN	O1-C1	7.92	1.39	1.23
14	G	2001	PQN	O1-C1	7.88	1.39	1.23
14	H	2002	PQN	O1-C1	7.88	1.39	1.23
14	e	2001	PQN	O1-C1	7.88	1.39	1.23
14	A	2001	PQN	O1-C1	7.86	1.39	1.23
14	e	2001	PQN	O4-C4	7.66	1.39	1.23
14	A	2001	PQN	O4-C4	7.66	1.39	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	2001	PQN	O4-C4	7.63	1.39	1.23
14	H	2002	PQN	O4-C4	7.53	1.38	1.23
14	f	2002	PQN	O4-C4	7.51	1.38	1.23
14	B	2002	PQN	O4-C4	7.51	1.38	1.23
14	B	2002	PQN	C2-C1	-4.41	1.37	1.47
14	f	2002	PQN	C2-C1	-4.41	1.37	1.47
14	H	2002	PQN	C2-C1	-4.38	1.37	1.47
13	e	1128	CLA	CMB-C2B	-4.21	1.42	1.50
13	G	1128	CLA	CMB-C2B	-4.19	1.42	1.50
13	A	1128	CLA	CMB-C2B	-4.18	1.42	1.50
13	H	1226	CLA	CMB-C2B	-4.18	1.42	1.50
13	B	1226	CLA	CMB-C2B	-4.17	1.42	1.50
13	f	1226	CLA	CMB-C2B	-4.16	1.42	1.50
13	e	1011	CLA	C1D-ND	4.03	1.43	1.37
13	A	1011	CLA	C1D-ND	4.03	1.43	1.37
13	G	1011	CLA	C1D-ND	4.02	1.43	1.37
14	e	2001	PQN	C2-C1	-3.99	1.38	1.47
14	A	2001	PQN	C2-C1	-3.97	1.38	1.47
14	G	2001	PQN	C2-C1	-3.96	1.38	1.47
13	b	503	CLA	C1D-ND	3.81	1.42	1.37
18	G	1849	LMU	O5'-C1'	3.80	1.51	1.41
13	t	503	CLA	C1D-ND	3.80	1.42	1.37
18	A	1849	LMU	O5'-C1'	3.80	1.51	1.41
18	e	1849	LMU	O5'-C1'	3.79	1.51	1.41
13	4	503	CLA	C1D-ND	3.79	1.42	1.37
13	c	503	CLA	C1D-ND	3.72	1.42	1.37
13	s	503	CLA	C1D-ND	3.69	1.42	1.37
13	u	503	CLA	C1D-ND	3.69	1.42	1.37
13	a	503	CLA	C1D-ND	3.68	1.42	1.37
13	5	503	CLA	C1D-ND	3.67	1.42	1.37
13	t	516	CLA	C1D-ND	3.67	1.42	1.37
13	3	503	CLA	C1D-ND	3.65	1.42	1.37
13	q	503	CLA	C1D-ND	3.63	1.42	1.37
13	b	516	CLA	C1D-ND	3.61	1.42	1.37
13	1	503	CLA	C1D-ND	3.61	1.42	1.37
13	c	517	CLA	C1D-ND	3.61	1.42	1.37
13	t	510	CLA	C1D-ND	3.61	1.42	1.37
18	f	1843	LMU	O5'-C1'	3.60	1.51	1.41
18	H	1843	LMU	O5'-C1'	3.60	1.51	1.41
13	d	506	CLA	C1D-ND	3.60	1.42	1.37
13	Y	506	CLA	C1D-ND	3.60	1.42	1.37
13	H	1226	CLA	CMD-C2D	-3.60	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	516	CLA	C1D-ND	3.59	1.42	1.37
18	B	1843	LMU	O5'-C1'	3.59	1.51	1.41
13	b	510	CLA	C1D-ND	3.59	1.42	1.37
13	6	506	CLA	C1D-ND	3.59	1.42	1.37
13	B	1226	CLA	CMD-C2D	-3.58	1.43	1.50
13	4	517	CLA	C1D-ND	3.58	1.42	1.37
13	1	506	CLA	C1D-ND	3.58	1.42	1.37
13	3	506	CLA	C1D-ND	3.58	1.42	1.37
13	a	506	CLA	C1D-ND	3.58	1.42	1.37
13	2	503	CLA	C1D-ND	3.57	1.42	1.37
13	4	510	CLA	C1D-ND	3.57	1.42	1.37
13	5	517	CLA	C1D-ND	3.57	1.42	1.37
13	r	503	CLA	C1D-ND	3.57	1.42	1.37
13	v	506	CLA	C1D-ND	3.57	1.42	1.37
13	f	1226	CLA	CMD-C2D	-3.57	1.43	1.50
13	c	516	CLA	C1D-ND	3.57	1.42	1.37
13	r	511	CLA	C1D-ND	3.57	1.42	1.37
13	Y	503	CLA	C1D-ND	3.57	1.42	1.37
13	q	506	CLA	C1D-ND	3.56	1.42	1.37
13	Z	503	CLA	C1D-ND	3.56	1.42	1.37
13	b	517	CLA	C1D-ND	3.56	1.42	1.37
13	4	507	CLA	C1D-ND	3.55	1.42	1.37
13	a	513	CLA	C1D-ND	3.54	1.42	1.37
13	d	501	CLA	C1D-ND	3.54	1.42	1.37
18	q	902	LMU	O5'-C1'	3.54	1.51	1.41
13	4	513	CLA	C1D-ND	3.54	1.42	1.37
18	1	902	LMU	O5'-C1'	3.54	1.50	1.41
13	t	502	CLA	C1D-ND	3.54	1.42	1.37
13	t	513	CLA	C1D-ND	3.54	1.42	1.37
18	J	5105	LMU	O5'-C1'	3.54	1.50	1.41
18	l	5105	LMU	O5'-C1'	3.54	1.50	1.41
13	s	507	CLA	C1D-ND	3.54	1.42	1.37
13	b	513	CLA	C1D-ND	3.54	1.42	1.37
13	u	517	CLA	C1D-ND	3.54	1.42	1.37
18	Y	902	LMU	O5'-C1'	3.53	1.50	1.41
13	6	503	CLA	C1D-ND	3.53	1.42	1.37
13	a	507	CLA	C1D-ND	3.53	1.42	1.37
13	t	517	CLA	C1D-ND	3.53	1.42	1.37
13	s	506	CLA	C1D-ND	3.53	1.42	1.37
13	b	502	CLA	C1D-ND	3.53	1.42	1.37
13	4	501	CLA	C1D-ND	3.53	1.42	1.37
13	d	513	CLA	C1D-ND	3.53	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	507	CLA	C1D-ND	3.52	1.42	1.37
13	Y	507	CLA	C1D-ND	3.52	1.42	1.37
13	v	501	CLA	C1D-ND	3.52	1.42	1.37
18	G	1848	LMU	O5B-C1B	3.52	1.50	1.41
13	t	501	CLA	C1D-ND	3.52	1.42	1.37
18	T	5105	LMU	O5'-C1'	3.51	1.50	1.41
13	b	507	CLA	C1D-ND	3.51	1.42	1.37
13	Y	513	CLA	C1D-ND	3.51	1.42	1.37
13	5	516	CLA	C1D-ND	3.51	1.42	1.37
13	v	503	CLA	C1D-ND	3.51	1.42	1.37
13	6	501	CLA	C1D-ND	3.51	1.42	1.37
13	d	519	CLA	C1D-ND	3.51	1.42	1.37
13	4	502	CLA	C1D-ND	3.50	1.42	1.37
13	v	519	CLA	C1D-ND	3.50	1.42	1.37
13	u	510	CLA	C1D-ND	3.50	1.42	1.37
18	A	1848	LMU	O5B-C1B	3.50	1.50	1.41
13	b	509	CLA	C1D-ND	3.50	1.42	1.37
13	3	513	CLA	C1D-ND	3.50	1.42	1.37
13	b	501	CLA	C1D-ND	3.50	1.42	1.37
13	q	513	CLA	C1D-ND	3.49	1.42	1.37
13	1	513	CLA	C1D-ND	3.49	1.42	1.37
13	v	502	CLA	C1D-ND	3.49	1.42	1.37
18	e	1848	LMU	O5B-C1B	3.49	1.50	1.41
13	d	503	CLA	C1D-ND	3.49	1.42	1.37
13	r	516	CLA	C1D-ND	3.49	1.42	1.37
13	2	511	CLA	C1D-ND	3.49	1.42	1.37
13	u	508	CLA	C1D-ND	3.49	1.42	1.37
13	c	509	CLA	C1D-ND	3.49	1.42	1.37
13	5	508	CLA	C1D-ND	3.49	1.42	1.37
13	6	519	CLA	C1D-ND	3.49	1.42	1.37
13	Z	501	CLA	C1D-ND	3.49	1.42	1.37
13	q	507	CLA	C1D-ND	3.49	1.42	1.37
13	s	501	CLA	C1D-ND	3.49	1.42	1.37
13	u	516	CLA	C1D-ND	3.49	1.42	1.37
13	t	509	CLA	C1D-ND	3.48	1.42	1.37
13	Z	511	CLA	C1D-ND	3.48	1.42	1.37
13	3	519	CLA	C1D-ND	3.48	1.42	1.37
13	6	513	CLA	C1D-ND	3.48	1.42	1.37
13	a	519	CLA	C1D-ND	3.48	1.42	1.37
13	v	509	CLA	C1D-ND	3.48	1.42	1.37
13	3	518	CLA	C1D-ND	3.48	1.42	1.37
13	Z	516	CLA	C1D-ND	3.48	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	518	CLA	C1D-ND	3.47	1.42	1.37
13	2	516	CLA	C1D-ND	3.47	1.42	1.37
13	a	501	CLA	C1D-ND	3.47	1.42	1.37
13	6	518	CLA	C1D-ND	3.47	1.42	1.37
13	s	518	CLA	C1D-ND	3.47	1.42	1.37
13	Z	513	CLA	C1D-ND	3.47	1.42	1.37
13	3	507	CLA	C1D-ND	3.47	1.42	1.37
13	6	502	CLA	C1D-ND	3.47	1.42	1.37
13	1	507	CLA	C1D-ND	3.46	1.42	1.37
13	r	501	CLA	C1D-ND	3.46	1.42	1.37
13	t	518	CLA	C1D-ND	3.46	1.42	1.37
13	d	510	CLA	C1D-ND	3.46	1.42	1.37
13	s	513	CLA	C1D-ND	3.46	1.42	1.37
13	4	509	CLA	C1D-ND	3.46	1.42	1.37
13	c	519	CLA	C1D-ND	3.46	1.42	1.37
13	2	506	CLA	C1D-ND	3.46	1.42	1.37
13	d	509	CLA	C1D-ND	3.46	1.42	1.37
13	G	1124	CLA	C1D-ND	3.46	1.42	1.37
13	b	518	CLA	C1D-ND	3.46	1.42	1.37
13	c	508	CLA	C1D-ND	3.45	1.42	1.37
13	d	511	CLA	C1D-ND	3.45	1.42	1.37
13	v	513	CLA	C1D-ND	3.45	1.42	1.37
13	s	511	CLA	C1D-ND	3.45	1.42	1.37
13	3	501	CLA	C1D-ND	3.45	1.42	1.37
13	6	511	CLA	C1D-ND	3.45	1.42	1.37
13	c	506	CLA	C1D-ND	3.45	1.42	1.37
13	6	507	CLA	C1D-ND	3.45	1.42	1.37
13	t	506	CLA	C1D-ND	3.45	1.42	1.37
13	u	504	CLA	C1D-ND	3.45	1.42	1.37
13	6	510	CLA	C1D-ND	3.45	1.42	1.37
13	5	509	CLA	C1D-ND	3.45	1.42	1.37
13	c	511	CLA	C1D-ND	3.44	1.42	1.37
13	v	517	CLA	C1D-ND	3.44	1.42	1.37
13	A	1124	CLA	C1D-ND	3.44	1.42	1.37
13	5	513	CLA	C1D-ND	3.44	1.42	1.37
13	v	511	CLA	C1D-ND	3.44	1.42	1.37
13	1	510	CLA	C1D-ND	3.44	1.42	1.37
13	Y	511	CLA	C1D-ND	3.44	1.42	1.37
13	d	518	CLA	C1D-ND	3.44	1.42	1.37
13	Z	506	CLA	C1D-ND	3.44	1.42	1.37
13	5	506	CLA	C1D-ND	3.44	1.42	1.37
13	2	501	CLA	C1D-ND	3.44	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	508	CLA	C1D-ND	3.44	1.42	1.37
13	s	519	CLA	C1D-ND	3.44	1.42	1.37
13	6	509	CLA	C1D-ND	3.44	1.42	1.37
13	u	509	CLA	C1D-ND	3.43	1.42	1.37
13	d	502	CLA	C1D-ND	3.43	1.42	1.37
13	5	510	CLA	C1D-ND	3.43	1.42	1.37
13	4	504	CLA	C1D-ND	3.43	1.42	1.37
13	e	1124	CLA	C1D-ND	3.43	1.42	1.37
13	d	508	CLA	C1D-ND	3.43	1.42	1.37
13	4	506	CLA	C1D-ND	3.43	1.42	1.37
13	6	508	CLA	C1D-ND	3.43	1.42	1.37
13	v	518	CLA	C1D-ND	3.43	1.42	1.37
13	G	1116	CLA	C1D-ND	3.43	1.42	1.37
13	c	513	CLA	C1D-ND	3.43	1.42	1.37
13	r	506	CLA	C1D-ND	3.43	1.42	1.37
14	A	2001	PQN	C3-C2	3.42	1.41	1.35
13	t	504	CLA	C1D-ND	3.42	1.42	1.37
14	G	2001	PQN	C3-C2	3.42	1.41	1.35
13	t	511	CLA	C1D-ND	3.42	1.42	1.37
13	5	519	CLA	C1D-ND	3.42	1.42	1.37
13	Y	510	CLA	C1D-ND	3.42	1.42	1.37
13	b	506	CLA	C1D-ND	3.42	1.42	1.37
13	4	518	CLA	C1D-ND	3.42	1.42	1.37
13	q	501	CLA	C1D-ND	3.42	1.42	1.37
14	B	2002	PQN	C3-C4	-3.42	1.38	1.47
13	d	516	CLA	C1D-ND	3.42	1.42	1.37
13	u	511	CLA	C1D-ND	3.42	1.42	1.37
13	3	511	CLA	C1D-ND	3.42	1.42	1.37
14	H	2002	PQN	C3-C4	-3.42	1.38	1.47
13	Y	502	CLA	C1D-ND	3.42	1.42	1.37
13	v	507	CLA	C1D-ND	3.42	1.42	1.37
13	5	504	CLA	C1D-ND	3.41	1.42	1.37
13	d	507	CLA	C1D-ND	3.41	1.42	1.37
13	6	516	CLA	C1D-ND	3.41	1.42	1.37
13	c	504	CLA	C1D-ND	3.41	1.42	1.37
13	u	519	CLA	C1D-ND	3.41	1.42	1.37
13	v	510	CLA	C1D-ND	3.41	1.42	1.37
13	u	513	CLA	C1D-ND	3.41	1.42	1.37
13	u	506	CLA	C1D-ND	3.41	1.42	1.37
13	4	508	CLA	C1D-ND	3.41	1.42	1.37
13	6	517	CLA	C1D-ND	3.41	1.42	1.37
13	a	508	CLA	C1D-ND	3.41	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	1105	CLA	C1D-ND	3.41	1.42	1.37
13	u	502	CLA	C1D-ND	3.41	1.42	1.37
13	Y	501	CLA	C1D-ND	3.41	1.42	1.37
13	e	1116	CLA	C1D-ND	3.40	1.42	1.37
13	1	511	CLA	C1D-ND	3.40	1.42	1.37
13	Y	517	CLA	C1D-ND	3.40	1.42	1.37
13	c	510	CLA	C1D-ND	3.40	1.42	1.37
13	v	516	CLA	C1D-ND	3.40	1.42	1.37
13	K	1105	CLA	C1D-ND	3.40	1.42	1.37
13	5	511	CLA	C1D-ND	3.40	1.42	1.37
13	a	511	CLA	C1D-ND	3.40	1.42	1.37
13	U	1105	CLA	C1D-ND	3.40	1.42	1.37
13	a	517	CLA	C1D-ND	3.40	1.42	1.37
18	Z	901	LMU	O5'-C1'	3.40	1.50	1.41
13	4	511	CLA	C1D-ND	3.39	1.42	1.37
13	6	504	CLA	C1D-ND	3.39	1.42	1.37
13	a	510	CLA	C1D-ND	3.39	1.42	1.37
14	e	2001	PQN	C3-C2	3.39	1.41	1.35
18	H	1843	LMU	O5B-C1B	3.39	1.50	1.41
13	1	517	CLA	C1D-ND	3.39	1.42	1.37
18	2	901	LMU	O5'-C1'	3.39	1.50	1.41
13	v	508	CLA	C1D-ND	3.39	1.42	1.37
13	5	507	CLA	C1D-ND	3.39	1.42	1.37
13	1	501	CLA	C1D-ND	3.39	1.42	1.37
13	3	517	CLA	C1D-ND	3.39	1.42	1.37
13	5	502	CLA	C1D-ND	3.39	1.42	1.37
13	t	508	CLA	C1D-ND	3.39	1.42	1.37
18	f	1843	LMU	O5B-C1B	3.39	1.50	1.41
13	2	513	CLA	C1D-ND	3.39	1.42	1.37
14	f	2002	PQN	C3-C4	-3.39	1.38	1.47
18	B	1843	LMU	O5B-C1B	3.38	1.50	1.41
13	2	519	CLA	C1D-ND	3.38	1.42	1.37
18	r	901	LMU	O5'-C1'	3.38	1.50	1.41
13	q	510	CLA	C1D-ND	3.38	1.42	1.37
13	q	517	CLA	C1D-ND	3.38	1.42	1.37
13	d	504	CLA	C1D-ND	3.38	1.42	1.37
13	Z	508	CLA	C1D-ND	3.38	1.42	1.37
13	b	511	CLA	C1D-ND	3.38	1.42	1.37
13	u	518	CLA	C1D-ND	3.38	1.42	1.37
13	c	502	CLA	C1D-ND	3.37	1.42	1.37
13	s	517	CLA	C1D-ND	3.37	1.42	1.37
13	3	508	CLA	C1D-ND	3.37	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	519	CLA	C1D-ND	3.37	1.42	1.37
13	b	504	CLA	C1D-ND	3.37	1.42	1.37
13	A	1116	CLA	C1D-ND	3.37	1.42	1.37
13	1	502	CLA	C1D-ND	3.36	1.42	1.37
13	5	518	CLA	C1D-ND	3.36	1.42	1.37
13	n	1503	CLA	C1D-ND	3.36	1.42	1.37
13	u	507	CLA	C1D-ND	3.36	1.42	1.37
13	1	509	CLA	C1D-ND	3.36	1.42	1.37
13	c	505	CLA	C1D-ND	3.36	1.42	1.37
13	r	508	CLA	C1D-ND	3.36	1.42	1.37
13	2	508	CLA	C1D-ND	3.36	1.42	1.37
13	V	1503	CLA	C1D-ND	3.36	1.42	1.37
13	d	517	CLA	C1D-ND	3.36	1.42	1.37
13	r	519	CLA	C1D-ND	3.35	1.42	1.37
13	s	509	CLA	C1D-ND	3.35	1.42	1.37
13	d	505	CLA	C1D-ND	3.35	1.42	1.37
13	3	509	CLA	C1D-ND	3.35	1.42	1.37
13	5	501	CLA	C1D-ND	3.35	1.42	1.37
13	c	501	CLA	C1D-ND	3.35	1.42	1.37
13	r	513	CLA	C1D-ND	3.35	1.42	1.37
13	L	1503	CLA	C1D-ND	3.35	1.42	1.37
13	Z	510	CLA	C1D-ND	3.35	1.42	1.37
13	c	507	CLA	C1D-ND	3.35	1.42	1.37
13	Y	509	CLA	C1D-ND	3.35	1.42	1.37
13	a	509	CLA	C1D-ND	3.35	1.42	1.37
13	s	508	CLA	C1D-ND	3.34	1.42	1.37
14	G	2001	PQN	C3-C4	-3.34	1.38	1.47
13	4	505	CLA	C1D-ND	3.34	1.42	1.37
13	2	517	CLA	C1D-ND	3.34	1.42	1.37
13	q	509	CLA	C1D-ND	3.34	1.42	1.37
13	v	505	CLA	C1D-ND	3.34	1.42	1.37
14	e	2001	PQN	C3-C4	-3.33	1.38	1.47
13	d	513	CLA	C4B-NB	3.33	1.42	1.37
13	6	505	CLA	C1D-ND	3.33	1.42	1.37
13	2	510	CLA	C1D-ND	3.33	1.42	1.37
13	b	505	CLA	C1D-ND	3.33	1.42	1.37
13	v	504	CLA	C1D-ND	3.33	1.42	1.37
13	r	510	CLA	C1D-ND	3.33	1.42	1.37
13	e	1110	CLA	C1D-ND	3.33	1.42	1.37
13	5	505	CLA	C1D-ND	3.33	1.42	1.37
13	s	510	CLA	C1D-ND	3.33	1.42	1.37
14	A	2001	PQN	C3-C4	-3.33	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	518	CLA	C1D-ND	3.33	1.42	1.37
13	3	510	CLA	C1D-ND	3.33	1.42	1.37
13	r	507	CLA	C1D-ND	3.33	1.42	1.37
13	u	505	CLA	C1D-ND	3.32	1.42	1.37
13	G	1110	CLA	C1D-ND	3.32	1.42	1.37
13	f	1218	CLA	C1D-ND	3.32	1.42	1.37
13	q	502	CLA	C1D-ND	3.32	1.42	1.37
13	t	505	CLA	C1D-ND	3.32	1.42	1.37
13	Z	517	CLA	C1D-ND	3.32	1.42	1.37
13	1	505	CLA	C1D-ND	3.32	1.42	1.37
13	q	511	CLA	C1D-ND	3.32	1.42	1.37
13	A	1140	CLA	C1D-ND	3.32	1.42	1.37
13	Y	508	CLA	C1D-ND	3.32	1.42	1.37
13	6	513	CLA	C4B-NB	3.31	1.42	1.37
13	u	501	CLA	C1D-ND	3.31	1.42	1.37
13	Z	509	CLA	C1D-ND	3.31	1.42	1.37
13	e	1136	CLA	C1D-ND	3.31	1.42	1.37
13	L	1501	CLA	C1D-ND	3.31	1.42	1.37
13	e	1801	CLA	C1D-ND	3.31	1.42	1.37
13	q	508	CLA	C1D-ND	3.31	1.42	1.37
13	1	508	CLA	C1D-ND	3.31	1.42	1.37
13	Z	518	CLA	C1D-ND	3.31	1.42	1.37
13	A	1110	CLA	C1D-ND	3.30	1.42	1.37
13	A	1131	CLA	C1D-ND	3.30	1.42	1.37
13	2	507	CLA	C1D-ND	3.30	1.42	1.37
13	r	517	CLA	C1D-ND	3.30	1.42	1.37
13	H	1222	CLA	C1D-ND	3.30	1.42	1.37
13	H	1211	CLA	C1D-ND	3.30	1.42	1.37
13	V	1501	CLA	C1D-ND	3.30	1.42	1.37
13	f	1222	CLA	C1D-ND	3.30	1.42	1.37
13	H	1209	CLA	C1D-ND	3.30	1.42	1.37
13	B	1222	CLA	C1D-ND	3.30	1.42	1.37
13	e	1131	CLA	C1D-ND	3.30	1.42	1.37
13	2	509	CLA	C1D-ND	3.30	1.42	1.37
13	f	1209	CLA	C1D-ND	3.30	1.42	1.37
13	c	518	CLA	C1D-ND	3.30	1.42	1.37
13	e	1140	CLA	C1D-ND	3.30	1.42	1.37
13	B	1211	CLA	C1D-ND	3.30	1.42	1.37
13	m	1103	CLA	C1D-ND	3.29	1.42	1.37
13	G	1140	CLA	C1D-ND	3.29	1.42	1.37
13	q	505	CLA	C1D-ND	3.29	1.42	1.37
13	G	1131	CLA	C1D-ND	3.29	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	505	CLA	C1D-ND	3.29	1.42	1.37
13	r	509	CLA	C1D-ND	3.29	1.42	1.37
13	s	502	CLA	C1D-ND	3.29	1.42	1.37
13	A	1122	CLA	C1D-ND	3.29	1.42	1.37
13	H	1218	CLA	C1D-ND	3.29	1.42	1.37
13	u	512	CLA	C1D-ND	3.29	1.42	1.37
13	B	1236	CLA	C1D-ND	3.28	1.42	1.37
13	Z	507	CLA	C1D-ND	3.28	1.42	1.37
13	H	1240	CLA	C1D-ND	3.28	1.42	1.37
13	5	512	CLA	C1D-ND	3.28	1.42	1.37
13	G	1136	CLA	C1D-ND	3.28	1.42	1.37
13	B	1218	CLA	C1D-ND	3.28	1.42	1.37
13	e	1137	CLA	C1D-ND	3.28	1.42	1.37
13	r	518	CLA	C1D-ND	3.28	1.42	1.37
20	b	822	SQD	O47-C7	3.27	1.42	1.35
20	v	822	SQD	O47-C7	3.27	1.42	1.35
13	G	1122	CLA	C1D-ND	3.27	1.42	1.37
13	A	1801	CLA	C1D-ND	3.27	1.42	1.37
13	f	1211	CLA	C1D-ND	3.27	1.42	1.37
13	B	1209	CLA	C1D-ND	3.27	1.42	1.37
13	r	502	CLA	C1D-ND	3.27	1.42	1.37
13	2	504	CLA	C1D-ND	3.27	1.42	1.37
20	4	822	SQD	O47-C7	3.27	1.42	1.35
20	6	822	SQD	O47-C7	3.27	1.42	1.35
13	s	505	CLA	C1D-ND	3.27	1.42	1.37
13	3	502	CLA	C1D-ND	3.26	1.42	1.37
13	Y	516	CLA	C1D-ND	3.26	1.42	1.37
13	f	1236	CLA	C1D-ND	3.26	1.42	1.37
20	d	822	SQD	O47-C7	3.26	1.42	1.35
13	K	1401	CLA	C1D-ND	3.26	1.42	1.37
13	f	1232	CLA	C1D-ND	3.26	1.42	1.37
13	l	1302	CLA	C1D-ND	3.26	1.42	1.37
13	A	1136	CLA	C1D-ND	3.25	1.42	1.37
13	U	1103	CLA	C1D-ND	3.25	1.42	1.37
13	J	1302	CLA	C1D-ND	3.25	1.42	1.37
13	U	1401	CLA	C1D-ND	3.25	1.42	1.37
13	3	505	CLA	C1D-ND	3.25	1.42	1.37
13	T	1302	CLA	C1D-ND	3.25	1.42	1.37
13	H	1236	CLA	C1D-ND	3.25	1.42	1.37
13	m	1401	CLA	C1D-ND	3.25	1.42	1.37
13	G	1111	CLA	C1D-ND	3.24	1.42	1.37
13	n	1501	CLA	C1D-ND	3.24	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	512	CLA	C1D-ND	3.24	1.42	1.37
13	e	1122	CLA	C1D-ND	3.24	1.42	1.37
13	H	1210	CLA	C1D-ND	3.24	1.42	1.37
13	Y	504	CLA	C1D-ND	3.24	1.42	1.37
13	B	1210	CLA	C1D-ND	3.24	1.42	1.37
13	d	512	CLA	C1D-ND	3.24	1.42	1.37
13	a	502	CLA	C1D-ND	3.24	1.42	1.37
13	A	1137	CLA	C1D-ND	3.24	1.42	1.37
13	K	1103	CLA	C1D-ND	3.24	1.42	1.37
13	1	516	CLA	C1D-ND	3.24	1.42	1.37
13	J	1303	CLA	C1D-ND	3.24	1.42	1.37
13	l	1303	CLA	C1D-ND	3.24	1.42	1.37
13	v	513	CLA	C4B-NB	3.23	1.42	1.37
20	t	822	SQD	O47-C7	3.23	1.42	1.35
13	Z	504	CLA	C1D-ND	3.23	1.42	1.37
13	f	1210	CLA	C1D-ND	3.23	1.42	1.37
13	v	512	CLA	C1D-ND	3.23	1.42	1.37
13	6	512	CLA	C1D-ND	3.23	1.42	1.37
13	H	1212	CLA	C1D-ND	3.23	1.42	1.37
13	B	1240	CLA	C1D-ND	3.22	1.42	1.37
13	2	502	CLA	C1D-ND	3.22	1.42	1.37
13	H	1232	CLA	C1D-ND	3.22	1.42	1.37
13	B	1232	CLA	C1D-ND	3.22	1.42	1.37
13	q	516	CLA	C1D-ND	3.21	1.42	1.37
13	a	505	CLA	C1D-ND	3.21	1.42	1.37
13	r	504	CLA	C1D-ND	3.21	1.42	1.37
13	e	1117	CLA	C1D-ND	3.21	1.42	1.37
13	u	513	CLA	C4B-NB	3.20	1.42	1.37
13	B	1239	CLA	C1D-ND	3.20	1.42	1.37
20	n	5216	SQD	O48-C23	3.20	1.42	1.33
13	T	1303	CLA	C1D-ND	3.19	1.42	1.37
20	L	5216	SQD	O48-C23	3.19	1.42	1.33
13	G	1801	CLA	C1D-ND	3.19	1.42	1.37
13	f	1239	CLA	C1D-ND	3.19	1.42	1.37
13	B	1212	CLA	C1D-ND	3.19	1.42	1.37
13	A	1117	CLA	C1D-ND	3.19	1.42	1.37
13	H	1239	CLA	C1D-ND	3.19	1.42	1.37
13	G	1137	CLA	C1D-ND	3.18	1.42	1.37
14	B	2002	PQN	C3-C2	3.18	1.40	1.35
13	j	1301	CLA	C1D-ND	3.18	1.42	1.37
13	t	512	CLA	C1D-ND	3.18	1.42	1.37
20	V	5216	SQD	O48-C23	3.18	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1111	CLA	C1D-ND	3.18	1.42	1.37
13	f	1240	CLA	C1D-ND	3.18	1.42	1.37
13	e	1114	CLA	C1D-ND	3.18	1.42	1.37
13	a	508	CLA	C4B-NB	3.17	1.42	1.37
13	a	504	CLA	C1D-ND	3.17	1.42	1.37
13	1	504	CLA	C1D-ND	3.17	1.42	1.37
13	G	1114	CLA	C1D-ND	3.17	1.42	1.37
13	R	1301	CLA	C1D-ND	3.17	1.42	1.37
13	b	512	CLA	C1D-ND	3.17	1.42	1.37
13	G	1117	CLA	C1D-ND	3.17	1.42	1.37
13	Z	502	CLA	C1D-ND	3.17	1.42	1.37
13	B	1208	CLA	C1D-ND	3.17	1.42	1.37
13	F	1301	CLA	C1D-ND	3.17	1.42	1.37
13	f	1212	CLA	C1D-ND	3.17	1.42	1.37
13	H	1209	CLA	C4B-NB	3.17	1.42	1.37
13	s	504	CLA	C1D-ND	3.17	1.42	1.37
13	e	1105	CLA	C1D-ND	3.17	1.42	1.37
13	A	1114	CLA	C1D-ND	3.16	1.42	1.37
13	5	513	CLA	C4B-NB	3.16	1.42	1.37
13	G	1134	CLA	C1D-ND	3.16	1.42	1.37
17	e	5001	LHG	O7-C5	-3.16	1.39	1.46
13	f	1208	CLA	C1D-ND	3.16	1.42	1.37
13	f	1213	CLA	C1D-ND	3.16	1.42	1.37
13	A	1134	CLA	C1D-ND	3.15	1.42	1.37
13	G	1105	CLA	C1D-ND	3.15	1.42	1.37
13	t	512	CLA	C4B-NB	3.15	1.42	1.37
13	4	512	CLA	C1D-ND	3.15	1.42	1.37
13	e	1109	CLA	C1D-ND	3.15	1.42	1.37
13	B	1220	CLA	C1D-ND	3.15	1.42	1.37
13	f	1209	CLA	C4B-NB	3.15	1.42	1.37
13	f	1201	CLA	C1D-ND	3.15	1.42	1.37
17	G	5001	LHG	O7-C5	-3.15	1.39	1.46
13	B	1207	CLA	C1D-ND	3.15	1.42	1.37
13	B	1209	CLA	C4B-NB	3.15	1.42	1.37
13	f	1207	CLA	C1D-ND	3.15	1.42	1.37
13	A	1108	CLA	C1D-ND	3.15	1.42	1.37
13	H	1207	CLA	C1D-ND	3.15	1.42	1.37
13	c	513	CLA	C4B-NB	3.14	1.42	1.37
13	H	1220	CLA	C1D-ND	3.14	1.42	1.37
13	e	1134	CLA	C1D-ND	3.14	1.42	1.37
13	q	504	CLA	C1D-ND	3.14	1.42	1.37
17	A	5001	LHG	O7-C5	-3.14	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1208	CLA	C1D-ND	3.14	1.42	1.37
13	B	1023	CLA	CMC-C2C	-3.14	1.44	1.50
13	f	1223	CLA	C1D-ND	3.14	1.42	1.37
13	2	505	CLA	C1D-ND	3.14	1.42	1.37
13	3	504	CLA	C1D-ND	3.14	1.42	1.37
13	4	512	CLA	C4B-NB	3.14	1.42	1.37
14	H	2002	PQN	C3-C2	3.14	1.40	1.35
14	f	2002	PQN	C3-C2	3.14	1.40	1.35
13	B	1201	CLA	C1D-ND	3.13	1.42	1.37
13	B	1213	CLA	C1D-ND	3.13	1.42	1.37
13	f	1235	CLA	C1D-ND	3.13	1.42	1.37
13	Z	505	CLA	C1D-ND	3.13	1.42	1.37
13	c	517	CLA	C4B-NB	3.13	1.42	1.37
13	e	1123	CLA	C1D-ND	3.13	1.42	1.37
13	v	517	CLA	C4B-NB	3.13	1.42	1.37
13	d	510	CLA	C4B-NB	3.13	1.42	1.37
13	v	510	CLA	C4B-NB	3.13	1.42	1.37
13	A	1105	CLA	C1D-ND	3.13	1.42	1.37
13	f	1220	CLA	C1D-ND	3.13	1.42	1.37
13	s	516	CLA	C1D-ND	3.13	1.42	1.37
13	3	508	CLA	C4B-NB	3.13	1.42	1.37
13	f	1023	CLA	CMC-C2C	-3.12	1.44	1.50
20	q	822	SQD	O48-C23	3.12	1.42	1.33
13	e	1108	CLA	C1D-ND	3.12	1.42	1.37
13	t	506	CLA	C4B-NB	3.12	1.42	1.37
13	A	1123	CLA	C1D-ND	3.12	1.42	1.37
13	e	1132	CLA	C1D-ND	3.12	1.42	1.37
13	5	517	CLA	C4B-NB	3.12	1.42	1.37
13	e	1111	CLA	C1D-ND	3.12	1.42	1.37
20	1	822	SQD	O48-C23	3.12	1.42	1.33
13	b	512	CLA	C4B-NB	3.12	1.42	1.37
13	B	1223	CLA	C1D-ND	3.12	1.42	1.37
13	b	513	CLA	C4B-NB	3.12	1.42	1.37
13	6	510	CLA	C4B-NB	3.12	1.42	1.37
13	H	1235	CLA	C1D-ND	3.12	1.42	1.37
13	q	501	CLA	C4B-NB	3.12	1.42	1.37
13	H	1213	CLA	C1D-ND	3.12	1.42	1.37
20	Y	822	SQD	O48-C23	3.11	1.42	1.33
13	5	502	CLA	C4B-NB	3.11	1.42	1.37
13	3	516	CLA	C1D-ND	3.11	1.41	1.37
13	6	516	CLA	C4B-NB	3.11	1.41	1.37
13	G	1115	CLA	C1D-ND	3.11	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	516	CLA	C1D-ND	3.11	1.41	1.37
13	d	516	CLA	C4B-NB	3.11	1.41	1.37
13	H	1023	CLA	CMC-C2C	-3.11	1.44	1.50
13	A	1132	CLA	C1D-ND	3.11	1.41	1.37
13	4	506	CLA	C4B-NB	3.11	1.41	1.37
13	G	1121	CLA	C1D-ND	3.11	1.41	1.37
20	a	822	SQD	O48-C23	3.11	1.42	1.33
20	s	822	SQD	O48-C23	3.11	1.42	1.33
13	B	1235	CLA	C1D-ND	3.10	1.41	1.37
20	r	822	SQD	O48-C23	3.10	1.42	1.33
13	A	1109	CLA	C1D-ND	3.10	1.41	1.37
13	G	1108	CLA	C1D-ND	3.10	1.41	1.37
13	Y	504	CLA	C4B-NB	3.10	1.41	1.37
13	4	513	CLA	C4B-NB	3.10	1.41	1.37
13	c	503	CLA	C4B-NB	3.10	1.41	1.37
13	A	1130	CLA	C1D-ND	3.09	1.41	1.37
13	c	502	CLA	C4B-NB	3.09	1.41	1.37
20	2	822	SQD	O48-C23	3.09	1.42	1.33
13	u	517	CLA	C4B-NB	3.09	1.41	1.37
13	H	1236	CLA	C4B-NB	3.09	1.41	1.37
20	Z	822	SQD	O48-C23	3.09	1.42	1.33
13	r	513	CLA	C4B-NB	3.09	1.41	1.37
13	e	1121	CLA	C1D-ND	3.09	1.41	1.37
20	3	822	SQD	O48-C23	3.09	1.42	1.33
13	G	1123	CLA	C1D-ND	3.09	1.41	1.37
13	H	1223	CLA	C1D-ND	3.08	1.41	1.37
13	r	505	CLA	C1D-ND	3.08	1.41	1.37
13	H	1201	CLA	C1D-ND	3.08	1.41	1.37
13	G	1109	CLA	C1D-ND	3.08	1.41	1.37
13	s	508	CLA	C4B-NB	3.07	1.41	1.37
13	4	519	CLA	C1D-ND	3.07	1.41	1.37
13	e	1101	CLA	C4B-NB	3.07	1.41	1.37
13	H	1203	CLA	C1D-ND	3.07	1.41	1.37
20	c	822	SQD	O48-C23	3.07	1.42	1.33
13	Z	504	CLA	C4B-NB	3.07	1.41	1.37
13	q	504	CLA	C4B-NB	3.07	1.41	1.37
13	H	1214	CLA	C1D-ND	3.07	1.41	1.37
13	G	1138	CLA	C1D-ND	3.07	1.41	1.37
13	t	519	CLA	C1D-ND	3.07	1.41	1.37
13	b	506	CLA	C4B-NB	3.06	1.41	1.37
13	v	506	CLA	C4B-NB	3.06	1.41	1.37
13	t	513	CLA	C4B-NB	3.06	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1237	CLA	C1D-ND	3.06	1.41	1.37
13	6	517	CLA	C4B-NB	3.06	1.41	1.37
13	e	1127	CLA	C1D-ND	3.06	1.41	1.37
13	e	1237	CLA	C1D-ND	3.06	1.41	1.37
13	f	1231	CLA	C1D-ND	3.06	1.41	1.37
13	A	1121	CLA	C1D-ND	3.06	1.41	1.37
13	e	1138	CLA	C1D-ND	3.06	1.41	1.37
13	B	1203	CLA	C1D-ND	3.06	1.41	1.37
13	2	513	CLA	C4B-NB	3.06	1.41	1.37
13	d	517	CLA	C4B-NB	3.06	1.41	1.37
13	1	501	CLA	C4B-NB	3.06	1.41	1.37
13	G	1113	CLA	C1D-ND	3.06	1.41	1.37
13	Z	513	CLA	C4B-NB	3.06	1.41	1.37
13	v	503	CLA	C4B-NB	3.06	1.41	1.37
13	e	1130	CLA	C1D-ND	3.06	1.41	1.37
13	G	1132	CLA	C1D-ND	3.05	1.41	1.37
13	b	519	CLA	C1D-ND	3.05	1.41	1.37
13	B	1236	CLA	C4B-NB	3.05	1.41	1.37
20	5	822	SQD	O48-C23	3.05	1.42	1.33
13	A	1115	CLA	C1D-ND	3.05	1.41	1.37
13	Y	501	CLA	C4B-NB	3.05	1.41	1.37
13	A	1237	CLA	C1D-ND	3.05	1.41	1.37
13	t	501	CLA	C4B-NB	3.05	1.41	1.37
18	A	1848	LMU	O5'-C1'	3.05	1.49	1.41
13	1	504	CLA	C4B-NB	3.05	1.41	1.37
13	A	1101	CLA	C4B-NB	3.05	1.41	1.37
13	f	1236	CLA	C4B-NB	3.05	1.41	1.37
13	u	502	CLA	C4B-NB	3.05	1.41	1.37
13	u	506	CLA	C4B-NB	3.05	1.41	1.37
18	G	1848	LMU	O5'-C1'	3.05	1.49	1.41
13	G	1130	CLA	C1D-ND	3.05	1.41	1.37
13	v	512	CLA	C4B-NB	3.04	1.41	1.37
13	H	1206	CLA	CMB-C2B	-3.04	1.44	1.50
20	u	822	SQD	O48-C23	3.04	1.42	1.33
13	a	506	CLA	C4B-NB	3.04	1.41	1.37
13	j	1302	CLA	C1D-ND	3.04	1.41	1.37
18	e	1848	LMU	O5'-C1'	3.04	1.49	1.41
13	4	517	CLA	C4B-NB	3.04	1.41	1.37
13	H	1216	CLA	CMB-C2B	-3.04	1.44	1.50
13	a	511	CLA	C4B-NB	3.04	1.41	1.37
13	b	503	CLA	C4B-NB	3.04	1.41	1.37
13	s	512	CLA	C1D-ND	3.04	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	511	CLA	C4B-NB	3.04	1.41	1.37
13	2	504	CLA	C4B-NB	3.04	1.41	1.37
13	3	511	CLA	C4B-NB	3.04	1.41	1.37
13	Y	513	CLA	C4B-NB	3.04	1.41	1.37
13	v	516	CLA	C4B-NB	3.04	1.41	1.37
13	B	1214	CLA	C1D-ND	3.04	1.41	1.37
13	u	503	CLA	C4B-NB	3.04	1.41	1.37
13	B	1206	CLA	CMB-C2B	-3.03	1.44	1.50
14	H	2002	PQN	C10-C1	-3.03	1.42	1.48
13	A	1138	CLA	C1D-ND	3.03	1.41	1.37
13	5	503	CLA	C4B-NB	3.03	1.41	1.37
13	6	503	CLA	C4B-NB	3.03	1.41	1.37
13	6	512	CLA	C4B-NB	3.03	1.41	1.37
13	B	1231	CLA	C1D-ND	3.03	1.41	1.37
13	G	1127	CLA	C1D-ND	3.03	1.41	1.37
13	q	517	CLA	C4B-NB	3.03	1.41	1.37
13	r	504	CLA	C4B-NB	3.03	1.41	1.37
13	b	501	CLA	C4B-NB	3.03	1.41	1.37
13	s	511	CLA	C4B-NB	3.03	1.41	1.37
13	u	516	CLA	C4B-NB	3.03	1.41	1.37
13	d	506	CLA	C4B-NB	3.03	1.41	1.37
14	f	2002	PQN	C10-C1	-3.03	1.42	1.48
13	b	517	CLA	C4B-NB	3.03	1.41	1.37
13	A	1127	CLA	C1D-ND	3.03	1.41	1.37
13	H	1231	CLA	C1D-ND	3.03	1.41	1.37
13	b	511	CLA	C4B-NB	3.02	1.41	1.37
13	4	511	CLA	C4B-NB	3.02	1.41	1.37
13	1	512	CLA	C1D-ND	3.02	1.41	1.37
13	G	1125	CLA	C1D-ND	3.02	1.41	1.37
13	a	512	CLA	C1D-ND	3.02	1.41	1.37
13	e	1115	CLA	C1D-ND	3.02	1.41	1.37
13	f	1216	CLA	CMB-C2B	-3.02	1.44	1.50
13	G	1126	CLA	C1D-ND	3.02	1.41	1.37
13	b	502	CLA	C4B-NB	3.02	1.41	1.37
13	B	1215	CLA	C1D-ND	3.02	1.41	1.37
13	Y	519	CLA	C1D-ND	3.02	1.41	1.37
13	A	1126	CLA	C1D-ND	3.02	1.41	1.37
13	6	506	CLA	C4B-NB	3.02	1.41	1.37
13	G	1101	CLA	C4B-NB	3.02	1.41	1.37
14	B	2002	PQN	C10-C1	-3.02	1.42	1.48
13	d	519	CLA	C4B-NB	3.01	1.41	1.37
13	t	504	CLA	C4B-NB	3.01	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1113	CLA	C1D-ND	3.01	1.41	1.37
13	d	512	CLA	C4B-NB	3.01	1.41	1.37
13	Y	517	CLA	C4B-NB	3.01	1.41	1.37
13	u	511	CLA	C4B-NB	3.01	1.41	1.37
13	3	506	CLA	C4B-NB	3.01	1.41	1.37
13	5	506	CLA	C4B-NB	3.01	1.41	1.37
13	H	1215	CLA	C1D-ND	3.01	1.41	1.37
13	1	513	CLA	C4B-NB	3.01	1.41	1.37
13	4	501	CLA	C4B-NB	3.00	1.41	1.37
13	R	1302	CLA	C4B-NB	3.00	1.41	1.37
13	q	512	CLA	C1D-ND	3.00	1.41	1.37
13	G	1130	CLA	C4B-NB	3.00	1.41	1.37
13	f	1219	CLA	C1D-ND	3.00	1.41	1.37
13	2	511	CLA	C4B-NB	3.00	1.41	1.37
13	1	517	CLA	C4B-NB	3.00	1.41	1.37
13	f	1203	CLA	C1D-ND	3.00	1.41	1.37
13	5	511	CLA	C4B-NB	3.00	1.41	1.37
13	Y	512	CLA	C1D-ND	3.00	1.41	1.37
13	d	511	CLA	C4B-NB	3.00	1.41	1.37
13	e	1113	CLA	C1D-ND	3.00	1.41	1.37
13	1	519	CLA	C1D-ND	3.00	1.41	1.37
13	5	516	CLA	C4B-NB	3.00	1.41	1.37
13	v	509	CLA	C4B-NB	3.00	1.41	1.37
13	6	504	CLA	C4B-NB	3.00	1.41	1.37
13	Y	506	CLA	C4B-NB	3.00	1.41	1.37
13	c	516	CLA	C4B-NB	3.00	1.41	1.37
13	d	503	CLA	C4B-NB	3.00	1.41	1.37
13	u	504	CLA	C4B-NB	3.00	1.41	1.37
13	e	1130	CLA	C4B-NB	3.00	1.41	1.37
13	u	501	CLA	C4B-NB	3.00	1.41	1.37
13	v	519	CLA	C4B-NB	3.00	1.41	1.37
13	4	502	CLA	C4B-NB	2.99	1.41	1.37
13	r	501	CLA	C4B-NB	2.99	1.41	1.37
13	s	506	CLA	C4B-NB	2.99	1.41	1.37
13	f	1214	CLA	C1D-ND	2.99	1.41	1.37
13	v	518	CLA	C4B-NB	2.99	1.41	1.37
13	t	518	CLA	C4B-NB	2.99	1.41	1.37
13	Z	511	CLA	C4B-NB	2.99	1.41	1.37
13	e	1126	CLA	C1D-ND	2.99	1.41	1.37
13	r	511	CLA	C4B-NB	2.99	1.41	1.37
13	b	510	CLA	C4B-NB	2.99	1.41	1.37
13	u	518	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)
13	4	503	CLA	C4B-NB	2.99	1.41	1.37
13	t	508	CLA	C4B-NB	2.99	1.41	1.37
13	B	1219	CLA	C1D-ND	2.99	1.41	1.37
13	F	1302	CLA	C1D-ND	2.99	1.41	1.37
13	A	1130	CLA	C4B-NB	2.99	1.41	1.37
13	Z	506	CLA	C4B-NB	2.99	1.41	1.37
13	6	519	CLA	C4B-NB	2.99	1.41	1.37
13	a	509	CLA	C4B-NB	2.99	1.41	1.37
13	Z	512	CLA	C1D-ND	2.99	1.41	1.37
13	f	1215	CLA	C1D-ND	2.99	1.41	1.37
13	3	512	CLA	C1D-ND	2.98	1.41	1.37
13	c	504	CLA	C4B-NB	2.98	1.41	1.37
13	b	518	CLA	C4B-NB	2.98	1.41	1.37
13	s	509	CLA	C4B-NB	2.98	1.41	1.37
13	c	511	CLA	C4B-NB	2.98	1.41	1.37
13	d	504	CLA	C4B-NB	2.98	1.41	1.37
13	q	506	CLA	C4B-NB	2.98	1.41	1.37
13	1	506	CLA	C4B-NB	2.98	1.41	1.37
13	t	503	CLA	C4B-NB	2.98	1.41	1.37
13	f	1206	CLA	CMB-C2B	-2.98	1.44	1.50
13	A	1125	CLA	C1D-ND	2.98	1.41	1.37
13	4	518	CLA	C4B-NB	2.98	1.41	1.37
13	Z	518	CLA	C4B-NB	2.98	1.41	1.37
13	G	1119	CLA	C1D-ND	2.98	1.41	1.37
13	d	518	CLA	C4B-NB	2.98	1.41	1.37
13	6	518	CLA	C4B-NB	2.98	1.41	1.37
13	f	1226	CLA	C1B-NB	-2.98	1.33	1.37
13	3	517	CLA	C4B-NB	2.98	1.41	1.37
13	4	504	CLA	C4B-NB	2.98	1.41	1.37
13	B	1216	CLA	CMB-C2B	-2.98	1.44	1.50
13	5	518	CLA	C4B-NB	2.98	1.41	1.37
13	2	506	CLA	C4B-NB	2.97	1.41	1.37
13	r	517	CLA	C4B-NB	2.97	1.41	1.37
13	4	508	CLA	C4B-NB	2.97	1.41	1.37
13	e	1125	CLA	C1D-ND	2.97	1.41	1.37
13	b	508	CLA	C4B-NB	2.97	1.41	1.37
13	e	1134	CLA	C4B-NB	2.97	1.41	1.37
13	a	502	CLA	C4B-NB	2.97	1.41	1.37
13	e	1118	CLA	C1D-ND	2.97	1.41	1.37
13	q	516	CLA	C4B-NB	2.97	1.41	1.37
13	1	503	CLA	C4B-NB	2.97	1.41	1.37
13	6	511	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)
13	t	517	CLA	C4B-NB	2.97	1.41	1.37
13	3	502	CLA	C4B-NB	2.96	1.41	1.37
13	Y	509	CLA	C4B-NB	2.96	1.41	1.37
13	q	519	CLA	C1D-ND	2.96	1.41	1.37
13	Y	511	CLA	C4B-NB	2.96	1.41	1.37
13	3	504	CLA	C4B-NB	2.96	1.41	1.37
13	H	1226	CLA	C1B-NB	-2.96	1.34	1.37
13	f	1221	CLA	C1D-ND	2.96	1.41	1.37
13	r	506	CLA	C4B-NB	2.96	1.41	1.37
13	s	517	CLA	C4B-NB	2.96	1.41	1.37
13	v	504	CLA	C4B-NB	2.96	1.41	1.37
13	3	509	CLA	C4B-NB	2.96	1.41	1.37
13	t	508	CLA	CMB-C2B	-2.96	1.44	1.50
13	B	1226	CLA	C1B-NB	-2.96	1.34	1.37
13	4	510	CLA	C4B-NB	2.96	1.41	1.37
13	f	1228	CLA	C1D-ND	2.96	1.41	1.37
13	q	513	CLA	C4B-NB	2.96	1.41	1.37
13	2	501	CLA	C4B-NB	2.96	1.41	1.37
13	r	512	CLA	C1D-ND	2.96	1.41	1.37
13	6	509	CLA	C4B-NB	2.96	1.41	1.37
13	G	1118	CLA	C1D-ND	2.96	1.41	1.37
13	c	518	CLA	C4B-NB	2.96	1.41	1.37
13	1	516	CLA	C4B-NB	2.95	1.41	1.37
13	f	1205	CLA	C1D-ND	2.95	1.41	1.37
13	B	1230	CLA	C1D-ND	2.95	1.41	1.37
13	2	512	CLA	C1D-ND	2.95	1.41	1.37
13	c	510	CLA	C4B-NB	2.95	1.41	1.37
13	5	504	CLA	C4B-NB	2.95	1.41	1.37
13	q	511	CLA	C4B-NB	2.95	1.41	1.37
13	j	1302	CLA	C4B-NB	2.95	1.41	1.37
13	b	504	CLA	C4B-NB	2.95	1.41	1.37
13	G	1101	CLA	C1D-ND	2.95	1.41	1.37
13	q	503	CLA	C4B-NB	2.95	1.41	1.37
13	v	511	CLA	C4B-NB	2.95	1.41	1.37
13	2	517	CLA	C4B-NB	2.95	1.41	1.37
13	6	508	CLA	C4B-NB	2.95	1.41	1.37
13	s	504	CLA	C4B-NB	2.95	1.41	1.37
13	5	501	CLA	C4B-NB	2.95	1.41	1.37
13	c	506	CLA	C4B-NB	2.95	1.41	1.37
13	B	1224	CLA	C1D-ND	2.95	1.41	1.37
13	c	501	CLA	C4B-NB	2.95	1.41	1.37
13	d	508	CLA	C4B-NB	2.95	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	502	CLA	C4B-NB	2.95	1.41	1.37
13	R	1302	CLA	C1D-ND	2.94	1.41	1.37
13	e	1133	CLA	C1D-ND	2.94	1.41	1.37
13	d	509	CLA	C4B-NB	2.94	1.41	1.37
13	F	1302	CLA	C4B-NB	2.94	1.41	1.37
13	G	1112	CLA	C1D-ND	2.94	1.41	1.37
13	Y	516	CLA	C4B-NB	2.94	1.41	1.37
13	1	509	CLA	C4B-NB	2.94	1.41	1.37
13	1	511	CLA	C4B-NB	2.94	1.41	1.37
13	5	510	CLA	C4B-NB	2.94	1.41	1.37
13	G	1134	CLA	C4B-NB	2.94	1.41	1.37
13	Z	508	CLA	C4B-NB	2.94	1.41	1.37
13	b	508	CLA	CMB-C2B	-2.94	1.44	1.50
13	A	1119	CLA	C1D-ND	2.94	1.41	1.37
13	A	1134	CLA	C4B-NB	2.94	1.41	1.37
13	v	508	CLA	C4B-NB	2.94	1.41	1.37
13	H	1224	CLA	C1D-ND	2.94	1.41	1.37
13	H	1227	CLA	C1D-ND	2.94	1.41	1.37
13	H	1217	CLA	C1D-ND	2.94	1.41	1.37
13	d	502	CLA	C4B-NB	2.94	1.41	1.37
13	r	503	CLA	C4B-NB	2.94	1.41	1.37
13	t	510	CLA	C4B-NB	2.94	1.41	1.37
13	H	1221	CLA	C1D-ND	2.94	1.41	1.37
13	u	508	CLA	C4B-NB	2.94	1.41	1.37
13	e	1119	CLA	C1D-ND	2.94	1.41	1.37
20	Z	822	SQD	O47-C7	2.94	1.42	1.34
13	B	1205	CLA	C1D-ND	2.93	1.41	1.37
13	a	504	CLA	C4B-NB	2.93	1.41	1.37
13	a	517	CLA	C4B-NB	2.93	1.41	1.37
13	s	502	CLA	C4B-NB	2.93	1.41	1.37
13	r	508	CLA	C4B-NB	2.93	1.41	1.37
13	6	501	CLA	C4B-NB	2.93	1.41	1.37
13	4	508	CLA	CMB-C2B	-2.93	1.44	1.50
13	Z	517	CLA	C4B-NB	2.93	1.41	1.37
13	H	1205	CLA	C1D-ND	2.93	1.41	1.37
13	R	1301	CLA	C4B-NB	2.93	1.41	1.37
13	H	1238	CLA	C1D-ND	2.93	1.41	1.37
13	t	502	CLA	C4B-NB	2.93	1.41	1.37
13	d	507	CLA	C4B-NB	2.93	1.41	1.37
13	r	518	CLA	C4B-NB	2.93	1.41	1.37
13	A	1129	CLA	MG-NB	-2.93	2.00	2.05
13	A	1101	CLA	C1D-ND	2.92	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1219	CLA	C1D-ND	2.92	1.41	1.37
13	d	501	CLA	C4B-NB	2.92	1.41	1.37
13	c	508	CLA	C4B-NB	2.92	1.41	1.37
13	t	509	CLA	C4B-NB	2.92	1.41	1.37
13	A	1112	CLA	C1D-ND	2.92	1.41	1.37
13	A	1133	CLA	C1D-ND	2.92	1.41	1.37
13	u	512	CLA	C4B-NB	2.92	1.41	1.37
13	6	505	CLA	C4B-NB	2.92	1.41	1.37
13	r	502	CLA	C4B-NB	2.92	1.41	1.37
13	B	1238	CLA	C1D-ND	2.92	1.41	1.37
13	a	503	CLA	C4B-NB	2.92	1.41	1.37
13	r	516	CLA	C4B-NB	2.92	1.41	1.37
13	1	502	CLA	C4B-NB	2.92	1.41	1.37
13	5	508	CLA	C4B-NB	2.92	1.41	1.37
13	s	516	CLA	C4B-NB	2.92	1.41	1.37
13	B	1221	CLA	C1D-ND	2.92	1.41	1.37
13	6	502	CLA	C4B-NB	2.92	1.41	1.37
13	c	505	CLA	C4B-NB	2.92	1.41	1.37
13	v	505	CLA	C4B-NB	2.92	1.41	1.37
13	2	516	CLA	C4B-NB	2.91	1.41	1.37
13	A	1118	CLA	C1D-ND	2.91	1.41	1.37
13	5	505	CLA	C4B-NB	2.91	1.41	1.37
13	H	1021	CLA	C1D-ND	2.91	1.41	1.37
13	4	516	CLA	C4B-NB	2.91	1.41	1.37
13	G	1104	CLA	C1D-ND	2.91	1.41	1.37
13	v	501	CLA	C4B-NB	2.91	1.41	1.37
13	e	1129	CLA	MG-NB	-2.91	2.00	2.05
13	Y	503	CLA	C4B-NB	2.91	1.41	1.37
13	A	1104	CLA	C1D-ND	2.91	1.41	1.37
13	B	1227	CLA	C1D-ND	2.91	1.41	1.37
20	2	822	SQD	O47-C7	2.91	1.42	1.34
13	Z	516	CLA	C4B-NB	2.91	1.41	1.37
13	q	509	CLA	C4B-NB	2.91	1.41	1.37
13	u	510	CLA	C4B-NB	2.91	1.41	1.37
13	u	505	CLA	C4B-NB	2.91	1.41	1.37
13	Y	512	CLA	C4B-NB	2.91	1.41	1.37
13	d	505	CLA	C4B-NB	2.91	1.41	1.37
13	H	1230	CLA	C1D-ND	2.91	1.41	1.37
13	F	1301	CLA	C4B-NB	2.91	1.41	1.37
13	r	512	CLA	C4B-NB	2.91	1.41	1.37
13	b	516	CLA	C4B-NB	2.91	1.41	1.37
13	H	1228	CLA	C1D-ND	2.91	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1021	CLA	C1D-ND	2.90	1.41	1.37
13	q	502	CLA	C4B-NB	2.90	1.41	1.37
13	f	1224	CLA	C1D-ND	2.90	1.41	1.37
13	t	507	CLA	C4B-NB	2.90	1.41	1.37
13	Z	503	CLA	C4B-NB	2.90	1.41	1.37
13	3	503	CLA	C4B-NB	2.90	1.41	1.37
13	r	509	CLA	C4B-NB	2.90	1.41	1.37
13	2	508	CLA	C4B-NB	2.90	1.41	1.37
13	e	1110	CLA	C4B-NB	2.90	1.41	1.37
13	f	1238	CLA	C1D-ND	2.90	1.41	1.37
13	f	1230	CLA	C1D-ND	2.90	1.41	1.37
13	G	1129	CLA	MG-NB	-2.90	2.00	2.05
13	Z	512	CLA	C4B-NB	2.90	1.41	1.37
13	Y	502	CLA	C4B-NB	2.90	1.41	1.37
13	B	1228	CLA	C1D-ND	2.89	1.41	1.37
13	1	512	CLA	C4B-NB	2.89	1.41	1.37
13	e	1101	CLA	C1D-ND	2.89	1.41	1.37
13	Z	501	CLA	C4B-NB	2.89	1.41	1.37
13	s	510	CLA	C4B-NB	2.89	1.41	1.37
13	A	1102	CLA	C1D-ND	2.89	1.41	1.37
13	2	502	CLA	C4B-NB	2.89	1.41	1.37
20	r	822	SQD	O47-C7	2.89	1.42	1.34
13	2	503	CLA	C4B-NB	2.89	1.41	1.37
13	2	518	CLA	C4B-NB	2.89	1.41	1.37
13	3	516	CLA	C4B-NB	2.89	1.41	1.37
13	Y	518	CLA	C1D-ND	2.89	1.41	1.37
13	e	1104	CLA	C1D-ND	2.89	1.41	1.37
13	B	1217	CLA	C1D-ND	2.89	1.41	1.37
13	a	518	CLA	C4B-NB	2.89	1.41	1.37
13	A	1110	CLA	C4B-NB	2.89	1.41	1.37
13	G	1133	CLA	C1D-ND	2.89	1.41	1.37
13	f	1214	CLA	C4B-NB	2.89	1.41	1.37
13	2	512	CLA	C4B-NB	2.89	1.41	1.37
13	3	518	CLA	C4B-NB	2.89	1.41	1.37
13	Z	509	CLA	C4B-NB	2.88	1.41	1.37
13	e	1112	CLA	C1D-ND	2.88	1.41	1.37
13	2	509	CLA	C4B-NB	2.88	1.41	1.37
13	a	519	CLA	C4B-NB	2.88	1.41	1.37
13	b	509	CLA	C4B-NB	2.88	1.41	1.37
13	j	1301	CLA	C4B-NB	2.88	1.41	1.37
13	s	503	CLA	C4B-NB	2.88	1.41	1.37
13	B	1239	CLA	C4B-NB	2.88	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	509	CLA	C4B-NB	2.88	1.41	1.37
13	6	507	CLA	C4B-NB	2.88	1.41	1.37
20	s	822	SQD	O47-C7	2.88	1.42	1.34
13	G	1107	CLA	CMD-C2D	-2.88	1.44	1.50
13	a	510	CLA	C4B-NB	2.88	1.41	1.37
13	f	1227	CLA	C1D-ND	2.88	1.41	1.37
20	3	822	SQD	O47-C7	2.88	1.42	1.34
13	v	507	CLA	C4B-NB	2.87	1.41	1.37
13	f	1239	CLA	C4B-NB	2.87	1.41	1.37
13	3	519	CLA	C4B-NB	2.87	1.41	1.37
13	a	516	CLA	C4B-NB	2.87	1.41	1.37
13	A	1107	CLA	CMD-C2D	-2.87	1.44	1.50
13	e	1107	CLA	CMD-C2D	-2.87	1.44	1.50
13	3	510	CLA	C4B-NB	2.86	1.41	1.37
13	q	510	CLA	C4B-NB	2.86	1.41	1.37
13	r	510	CLA	C4B-NB	2.86	1.41	1.37
13	b	505	CLA	C4B-NB	2.86	1.41	1.37
13	B	1214	CLA	C4B-NB	2.86	1.41	1.37
13	1	518	CLA	C1D-ND	2.86	1.41	1.37
13	Z	502	CLA	C4B-NB	2.86	1.41	1.37
13	1	505	CLA	C4B-NB	2.86	1.41	1.37
13	q	512	CLA	C4B-NB	2.86	1.41	1.37
13	4	505	CLA	C4B-NB	2.86	1.41	1.37
13	H	1239	CLA	C4B-NB	2.86	1.41	1.37
13	G	1102	CLA	C1D-ND	2.86	1.41	1.37
13	G	1110	CLA	C4B-NB	2.86	1.41	1.37
13	4	507	CLA	C4B-NB	2.85	1.41	1.37
13	H	1219	CLA	C4B-NB	2.85	1.41	1.37
13	f	1226	CLA	C4B-NB	2.85	1.41	1.37
13	q	505	CLA	C4B-NB	2.85	1.41	1.37
20	u	822	SQD	O47-C7	2.85	1.42	1.34
13	t	516	CLA	C4B-NB	2.85	1.41	1.37
13	H	1226	CLA	C4B-NB	2.85	1.41	1.37
13	5	512	CLA	C4B-NB	2.85	1.41	1.37
13	e	1114	CLA	C4B-NB	2.85	1.41	1.37
13	3	513	CLA	C4B-NB	2.85	1.41	1.37
13	s	518	CLA	C4B-NB	2.85	1.41	1.37
13	Z	510	CLA	C4B-NB	2.85	1.41	1.37
13	a	512	CLA	C4B-NB	2.85	1.41	1.37
20	a	822	SQD	O47-C7	2.85	1.42	1.34
13	5	509	CLA	C4B-NB	2.84	1.41	1.37
20	5	822	SQD	O47-C7	2.84	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	505	CLA	C4B-NB	2.84	1.41	1.37
13	U	1105	CLA	C4B-NB	2.84	1.41	1.37
13	B	1226	CLA	C4B-NB	2.84	1.41	1.37
20	c	822	SQD	O47-C7	2.84	1.42	1.34
13	a	501	CLA	C1B-C2B	2.84	1.49	1.43
13	e	1102	CLA	C1D-ND	2.84	1.41	1.37
13	G	1129	CLA	C1D-ND	2.84	1.41	1.37
13	f	1021	CLA	C1D-ND	2.84	1.41	1.37
13	s	519	CLA	C4B-NB	2.84	1.41	1.37
13	c	509	CLA	C4B-NB	2.84	1.41	1.37
13	A	1114	CLA	C4B-NB	2.84	1.41	1.37
13	B	1234	CLA	MG-NB	-2.83	2.00	2.05
13	A	1108	CLA	C4B-NB	2.83	1.41	1.37
13	3	501	CLA	C1B-C2B	2.83	1.49	1.43
13	1	510	CLA	C4B-NB	2.83	1.41	1.37
13	2	519	CLA	C4B-NB	2.83	1.41	1.37
13	a	513	CLA	C4B-NB	2.83	1.41	1.37
13	e	1237	CLA	C4B-NB	2.83	1.41	1.37
13	s	507	CLA	C4B-NB	2.83	1.41	1.37
13	s	513	CLA	C4B-NB	2.83	1.41	1.37
13	K	1105	CLA	C4B-NB	2.83	1.41	1.37
13	H	1214	CLA	C4B-NB	2.83	1.41	1.37
13	H	1234	CLA	MG-NB	-2.83	2.00	2.05
13	e	1135	CLA	MG-NB	-2.83	2.00	2.05
13	f	1021	CLA	C1B-C2B	2.83	1.49	1.43
13	B	1219	CLA	C4B-NB	2.83	1.41	1.37
13	G	1114	CLA	C4B-NB	2.83	1.41	1.37
13	f	1217	CLA	C1D-ND	2.82	1.41	1.37
13	s	501	CLA	C1B-C2B	2.82	1.49	1.43
13	A	1136	CLA	C4B-NB	2.82	1.41	1.37
13	A	1135	CLA	MG-NB	-2.82	2.00	2.05
20	Y	822	SQD	O47-C7	2.82	1.42	1.34
13	c	512	CLA	C4B-NB	2.82	1.41	1.37
13	H	1239	CLA	CMB-C2B	-2.82	1.45	1.50
13	B	1216	CLA	C1D-ND	2.82	1.41	1.37
13	G	1106	CLA	C1D-ND	2.82	1.41	1.37
13	r	519	CLA	C4B-NB	2.82	1.41	1.37
13	B	1206	CLA	C1D-ND	2.82	1.41	1.37
13	L	1501	CLA	C4B-NB	2.82	1.41	1.37
13	f	1206	CLA	C1D-ND	2.82	1.41	1.37
13	s	512	CLA	C4B-NB	2.81	1.41	1.37
13	e	1136	CLA	C4B-NB	2.81	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1120	CLA	C1D-ND	2.81	1.41	1.37
13	e	1108	CLA	C4B-NB	2.81	1.41	1.37
13	f	1202	CLA	C4B-NB	2.81	1.41	1.37
13	u	509	CLA	C4B-NB	2.81	1.41	1.37
13	Y	510	CLA	C4B-NB	2.81	1.41	1.37
13	f	1240	CLA	C4B-NB	2.81	1.41	1.37
13	f	1202	CLA	C1D-ND	2.81	1.41	1.37
13	5	519	CLA	C4B-NB	2.81	1.41	1.37
13	G	1120	CLA	C1D-ND	2.81	1.41	1.37
20	1	822	SQD	O47-C7	2.81	1.42	1.34
20	q	822	SQD	O47-C7	2.81	1.42	1.34
13	A	1022	CLA	C1D-ND	2.81	1.41	1.37
13	G	1022	CLA	C1D-ND	2.81	1.41	1.37
13	G	1136	CLA	C4B-NB	2.81	1.41	1.37
13	q	508	CLA	C4B-NB	2.81	1.41	1.37
14	e	2001	PQN	C11-C12	2.80	1.55	1.50
13	H	1021	CLA	C1B-C2B	2.80	1.49	1.43
13	G	1108	CLA	C4B-NB	2.80	1.41	1.37
20	H	1852	SQD	O47-C45	-2.80	1.40	1.46
13	a	501	CLA	C4B-NB	2.80	1.41	1.37
13	B	1021	CLA	C1B-C2B	2.80	1.49	1.43
13	f	1234	CLA	MG-NB	-2.80	2.00	2.05
13	t	507	CLA	C1B-C2B	2.80	1.49	1.43
13	B	1202	CLA	C4B-NB	2.80	1.41	1.37
13	m	1105	CLA	C4B-NB	2.80	1.41	1.37
13	s	501	CLA	C4B-NB	2.80	1.41	1.37
13	b	507	CLA	C4B-NB	2.80	1.41	1.37
13	b	507	CLA	C1B-C2B	2.80	1.49	1.43
13	A	1237	CLA	C4B-NB	2.80	1.41	1.37
13	1	507	CLA	C4B-NB	2.80	1.41	1.37
13	q	505	CLA	C1B-C2B	2.80	1.49	1.43
13	3	512	CLA	C4B-NB	2.80	1.41	1.37
13	e	1022	CLA	C1D-ND	2.80	1.41	1.37
13	4	507	CLA	C1B-C2B	2.80	1.49	1.43
13	B	1240	CLA	C4B-NB	2.80	1.41	1.37
13	1	508	CLA	C4B-NB	2.80	1.41	1.37
13	H	1216	CLA	C1D-ND	2.80	1.41	1.37
13	Y	505	CLA	C4B-NB	2.80	1.41	1.37
13	q	507	CLA	C4B-NB	2.80	1.41	1.37
13	q	518	CLA	C1D-ND	2.80	1.41	1.37
13	2	510	CLA	C4B-NB	2.79	1.41	1.37
13	V	1501	CLA	C4B-NB	2.79	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1219	CLA	C4B-NB	2.79	1.41	1.37
13	e	1139	CLA	CMD-C2D	-2.79	1.45	1.50
13	Z	519	CLA	C4B-NB	2.79	1.41	1.37
13	u	507	CLA	C4B-NB	2.79	1.41	1.37
13	A	1140	CLA	C4B-NB	2.79	1.41	1.37
13	A	1106	CLA	C1D-ND	2.79	1.41	1.37
13	n	1501	CLA	C4B-NB	2.79	1.41	1.37
13	H	1234	CLA	C1D-ND	2.78	1.41	1.37
14	A	2001	PQN	C11-C12	2.78	1.54	1.50
13	A	1120	CLA	C1D-ND	2.78	1.41	1.37
13	f	1216	CLA	C1D-ND	2.78	1.41	1.37
20	B	1852	SQD	O47-C45	-2.78	1.40	1.46
13	G	1135	CLA	MG-NB	-2.78	2.00	2.05
13	u	505	CLA	C1B-C2B	2.78	1.49	1.43
13	s	508	CLA	CMB-C2B	-2.78	1.45	1.50
13	H	1206	CLA	C1D-ND	2.78	1.41	1.37
13	u	519	CLA	C4B-NB	2.78	1.41	1.37
13	Y	507	CLA	C4B-NB	2.78	1.41	1.37
13	f	1221	CLA	C4B-NB	2.78	1.41	1.37
13	5	505	CLA	C1B-C2B	2.78	1.49	1.43
13	H	1202	CLA	C4B-NB	2.78	1.41	1.37
13	A	1139	CLA	CMD-C2D	-2.78	1.45	1.50
13	5	507	CLA	C4B-NB	2.78	1.41	1.37
13	c	519	CLA	C4B-NB	2.78	1.41	1.37
13	B	1234	CLA	C1D-ND	2.78	1.41	1.37
13	B	1239	CLA	CMB-C2B	-2.78	1.45	1.50
13	G	1140	CLA	C4B-NB	2.78	1.41	1.37
13	3	508	CLA	CMB-C2B	-2.78	1.45	1.50
13	f	1239	CLA	CMB-C2B	-2.77	1.45	1.50
13	c	505	CLA	C1B-C2B	2.77	1.49	1.43
13	a	508	CLA	CMB-C2B	-2.77	1.45	1.50
13	A	1119	CLA	CMB-C2B	-2.77	1.45	1.50
13	Y	508	CLA	C4B-NB	2.77	1.41	1.37
13	t	517	CLA	C1B-C2B	2.77	1.49	1.43
13	G	1119	CLA	CMB-C2B	-2.77	1.45	1.50
13	B	1205	CLA	C4B-NB	2.77	1.41	1.37
14	G	2001	PQN	C11-C12	2.77	1.54	1.50
13	G	1121	CLA	CMD-C2D	-2.77	1.45	1.50
13	c	516	CLA	C1B-C2B	2.77	1.49	1.43
13	A	1101	CLA	C3B-C4B	2.77	1.50	1.42
13	e	1121	CLA	CMD-C2D	-2.77	1.45	1.50
13	Y	505	CLA	C1B-C2B	2.77	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1202	CLA	C1D-ND	2.77	1.41	1.37
13	3	501	CLA	C4B-NB	2.77	1.41	1.37
13	H	1205	CLA	C4B-NB	2.77	1.41	1.37
13	4	502	CLA	C1B-C2B	2.77	1.49	1.43
13	e	1119	CLA	CMB-C2B	-2.77	1.45	1.50
13	B	1221	CLA	C4B-NB	2.77	1.41	1.37
13	G	1128	CLA	MG-NB	-2.77	2.00	2.05
13	f	1234	CLA	C1D-ND	2.77	1.41	1.37
13	A	1129	CLA	C1D-ND	2.76	1.41	1.37
13	H	1240	CLA	C4B-NB	2.76	1.41	1.37
20	f	1852	SQD	O47-C45	-2.76	1.40	1.46
13	G	1139	CLA	CMD-C2D	-2.76	1.45	1.50
13	r	516	CLA	C1B-C2B	2.76	1.49	1.43
13	e	1140	CLA	C4B-NB	2.76	1.41	1.37
13	G	1103	CLA	CMC-C2C	-2.76	1.45	1.50
13	e	1106	CLA	C1D-ND	2.76	1.41	1.37
13	e	1103	CLA	CMC-C2C	-2.76	1.45	1.50
13	2	516	CLA	C1B-C2B	2.76	1.49	1.43
13	1	505	CLA	C1B-C2B	2.76	1.49	1.43
13	t	502	CLA	C1B-C2B	2.76	1.49	1.43
13	3	507	CLA	C4B-NB	2.76	1.41	1.37
13	c	507	CLA	C4B-NB	2.76	1.41	1.37
13	4	517	CLA	C1B-C2B	2.76	1.49	1.43
13	B	1204	CLA	C1D-ND	2.76	1.41	1.37
13	G	1101	CLA	C3B-C4B	2.76	1.50	1.42
13	e	1101	CLA	C3B-C4B	2.76	1.50	1.42
13	b	502	CLA	C1B-C2B	2.76	1.49	1.43
13	t	513	CLA	C1B-C2B	2.75	1.49	1.43
13	f	1205	CLA	C4B-NB	2.75	1.41	1.37
13	a	505	CLA	C4B-NB	2.75	1.41	1.37
13	q	518	CLA	C4B-NB	2.75	1.41	1.37
13	H	1221	CLA	C4B-NB	2.75	1.41	1.37
13	a	505	CLA	C1B-C2B	2.75	1.49	1.43
13	G	1114	CLA	CMB-C2B	-2.75	1.45	1.50
13	1	518	CLA	C4B-NB	2.75	1.41	1.37
13	e	1128	CLA	MG-NB	-2.75	2.00	2.05
13	s	516	CLA	C1B-C2B	2.75	1.49	1.43
13	c	502	CLA	C1B-C2B	2.75	1.49	1.43
13	e	1114	CLA	CMB-C2B	-2.75	1.45	1.50
13	e	1116	CLA	C4B-NB	2.75	1.41	1.37
13	3	505	CLA	C4B-NB	2.75	1.41	1.37
13	H	1204	CLA	C1D-ND	2.75	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	1401	CLA	C4B-NB	2.74	1.41	1.37
13	A	1121	CLA	CMD-C2D	-2.74	1.45	1.50
13	6	516	CLA	C1B-C2B	2.74	1.49	1.43
13	b	506	CLA	C1B-C2B	2.74	1.49	1.43
13	b	517	CLA	C1B-C2B	2.74	1.49	1.43
13	u	502	CLA	C1B-C2B	2.74	1.49	1.43
13	f	1229	CLA	C4B-NB	2.74	1.41	1.37
13	a	507	CLA	C1B-C2B	2.74	1.49	1.43
13	s	507	CLA	C1B-C2B	2.74	1.49	1.43
13	Z	516	CLA	C1B-C2B	2.74	1.49	1.43
13	a	507	CLA	C4B-NB	2.74	1.41	1.37
13	e	1128	CLA	C1D-ND	2.74	1.41	1.37
13	m	1401	CLA	C4B-NB	2.74	1.41	1.37
13	a	516	CLA	C1B-C2B	2.74	1.49	1.43
13	Z	505	CLA	C4B-NB	2.74	1.41	1.37
13	H	1021	CLA	CMD-C2D	-2.74	1.45	1.50
13	e	1102	CLA	C4B-NB	2.74	1.41	1.37
13	n	1502	CLA	C1D-ND	2.74	1.41	1.37
13	B	1209	CLA	C3B-C4B	2.74	1.50	1.42
13	A	1103	CLA	CMC-C2C	-2.74	1.45	1.50
13	G	1107	CLA	CMB-C2B	-2.73	1.45	1.50
13	f	1204	CLA	C1D-ND	2.73	1.41	1.37
13	4	506	CLA	C1B-C2B	2.73	1.49	1.43
13	5	502	CLA	C1B-C2B	2.73	1.49	1.43
13	s	505	CLA	C4B-NB	2.73	1.41	1.37
13	2	508	CLA	CMB-C2B	-2.73	1.45	1.50
13	e	1139	CLA	C4B-NB	2.73	1.41	1.37
13	A	1128	CLA	C1B-NB	-2.73	1.34	1.37
13	v	509	CLA	C1B-C2B	2.73	1.49	1.43
13	A	1128	CLA	MG-NB	-2.73	2.00	2.05
13	U	1401	CLA	C4B-NB	2.73	1.41	1.37
13	v	516	CLA	C1B-C2B	2.73	1.49	1.43
13	Z	508	CLA	CMB-C2B	-2.73	1.45	1.50
13	B	1226	CLA	MG-NB	-2.73	2.00	2.05
20	L	5216	SQD	O47-C7	2.73	1.42	1.34
13	6	509	CLA	C1B-C2B	2.73	1.49	1.43
13	d	516	CLA	C1B-C2B	2.73	1.49	1.43
13	3	505	CLA	C1B-C2B	2.73	1.49	1.43
13	H	1226	CLA	MG-NB	-2.73	2.00	2.05
13	V	1502	CLA	C1D-ND	2.73	1.41	1.37
13	e	1121	CLA	C4B-NB	2.73	1.41	1.37
13	5	516	CLA	C1B-C2B	2.73	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	502	CLA	C1B-C2B	2.73	1.49	1.43
13	A	1107	CLA	CMB-C2B	-2.73	1.45	1.50
13	A	1114	CLA	CMB-C2B	-2.73	1.45	1.50
13	H	1012	CLA	CHC-C1C	2.73	1.44	1.38
13	Y	518	CLA	C4B-NB	2.73	1.41	1.37
13	s	505	CLA	C1B-C2B	2.73	1.49	1.43
13	e	1139	CLA	C1D-ND	2.73	1.41	1.37
13	u	516	CLA	C1B-C2B	2.72	1.49	1.43
13	f	1209	CLA	C3B-C4B	2.72	1.50	1.42
13	A	1139	CLA	C4B-NB	2.72	1.41	1.37
13	3	516	CLA	C1B-C2B	2.72	1.49	1.43
13	f	1226	CLA	MG-NB	-2.72	2.00	2.05
13	t	506	CLA	C1B-C2B	2.72	1.49	1.43
13	G	1237	CLA	CMB-C2B	-2.72	1.45	1.50
13	2	505	CLA	C4B-NB	2.72	1.41	1.37
13	d	509	CLA	C1B-C2B	2.72	1.49	1.43
13	H	1209	CLA	C3B-C4B	2.72	1.50	1.42
13	q	503	CLA	C1B-C2B	2.72	1.49	1.43
13	G	1237	CLA	C4B-NB	2.72	1.41	1.37
13	r	508	CLA	CMB-C2B	-2.72	1.45	1.50
13	A	1128	CLA	C1D-ND	2.72	1.41	1.37
13	r	505	CLA	C4B-NB	2.72	1.41	1.37
13	f	1216	CLA	C4B-NB	2.72	1.41	1.37
20	V	5216	SQD	O47-C7	2.72	1.41	1.34
13	b	513	CLA	C1B-C2B	2.72	1.49	1.43
13	c	517	CLA	C1B-C2B	2.72	1.49	1.43
13	f	1021	CLA	CMD-C2D	-2.72	1.45	1.50
13	3	507	CLA	C1B-C2B	2.72	1.49	1.43
13	6	502	CLA	C1B-C2B	2.72	1.49	1.43
13	A	1013	CLA	CMB-C2B	-2.71	1.45	1.50
20	n	5216	SQD	O47-C7	2.71	1.41	1.34
13	A	1116	CLA	C4B-NB	2.71	1.41	1.37
13	e	1128	CLA	C1B-NB	-2.71	1.34	1.37
13	L	1502	CLA	C1D-ND	2.71	1.41	1.37
13	G	1013	CLA	CMB-C2B	-2.71	1.45	1.50
13	d	501	CLA	C1B-C2B	2.71	1.49	1.43
13	G	1102	CLA	C4B-NB	2.71	1.41	1.37
13	A	1237	CLA	CMB-C2B	-2.71	1.45	1.50
13	4	513	CLA	C1B-C2B	2.71	1.49	1.43
13	v	502	CLA	C1B-C2B	2.71	1.49	1.43
13	e	1107	CLA	CMB-C2B	-2.71	1.45	1.50
13	u	517	CLA	C1B-C2B	2.71	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1012	CLA	CHC-C1C	2.71	1.43	1.38
13	4	516	CLA	C1B-C2B	2.71	1.49	1.43
13	6	501	CLA	C1B-C2B	2.71	1.49	1.43
13	t	518	CLA	C1B-C2B	2.71	1.49	1.43
19	f	5002	LMG	O8-C9	-2.70	1.39	1.45
13	B	1229	CLA	C4B-NB	2.70	1.41	1.37
13	H	1202	CLA	C1D-ND	2.70	1.41	1.37
13	G	1013	CLA	C1B-NB	-2.70	1.34	1.37
13	e	1115	CLA	CMC-C2C	-2.70	1.45	1.50
13	e	1129	CLA	C1D-ND	2.70	1.41	1.37
13	G	1138	CLA	C4B-NB	2.70	1.41	1.37
13	1	508	CLA	CMB-C2B	-2.70	1.45	1.50
13	4	518	CLA	C1B-C2B	2.70	1.49	1.43
13	H	1207	CLA	C4B-NB	2.70	1.41	1.37
13	G	1128	CLA	C1B-NB	-2.70	1.34	1.37
13	u	501	CLA	C1B-C2B	2.70	1.49	1.43
13	r	507	CLA	C4B-NB	2.70	1.41	1.37
13	b	516	CLA	C1B-C2B	2.70	1.49	1.43
13	A	1102	CLA	C4B-NB	2.70	1.41	1.37
13	G	1116	CLA	C4B-NB	2.70	1.41	1.37
13	f	1221	CLA	CMD-C2D	-2.70	1.45	1.50
13	t	516	CLA	C1B-C2B	2.70	1.49	1.43
13	B	1021	CLA	CMD-C2D	-2.70	1.45	1.50
13	G	1139	CLA	C4B-NB	2.70	1.41	1.37
13	b	518	CLA	C1B-C2B	2.70	1.49	1.43
13	c	506	CLA	C1B-C2B	2.70	1.49	1.43
13	v	505	CLA	C1B-C2B	2.70	1.49	1.43
13	5	517	CLA	C1B-C2B	2.70	1.49	1.43
13	t	501	CLA	C1B-C2B	2.69	1.49	1.43
13	4	501	CLA	C1B-C2B	2.69	1.49	1.43
13	Y	508	CLA	CMB-C2B	-2.69	1.45	1.50
13	1	517	CLA	C1B-C2B	2.69	1.49	1.43
13	5	501	CLA	C1B-C2B	2.69	1.49	1.43
13	q	517	CLA	C1B-C2B	2.69	1.49	1.43
13	G	1128	CLA	C1D-ND	2.69	1.41	1.37
13	1	503	CLA	C1B-C2B	2.69	1.49	1.43
13	Z	505	CLA	C1B-C2B	2.69	1.49	1.43
13	F	1302	CLA	C1B-C2B	2.69	1.49	1.43
13	Y	503	CLA	C1B-C2B	2.69	1.49	1.43
13	Z	507	CLA	C1B-C2B	2.69	1.49	1.43
13	B	1225	CLA	C1D-ND	2.69	1.41	1.37
13	5	503	CLA	C1B-C2B	2.69	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1012	CLA	CHC-C1C	2.69	1.43	1.38
13	B	1012	CLA	C4B-NB	2.69	1.41	1.37
13	v	501	CLA	C1B-C2B	2.69	1.49	1.43
13	e	1013	CLA	CMB-C2B	-2.69	1.45	1.50
13	2	507	CLA	C1B-C2B	2.69	1.49	1.43
13	q	508	CLA	CMB-C2B	-2.69	1.45	1.50
13	6	505	CLA	C1B-C2B	2.69	1.49	1.43
13	A	1121	CLA	C4B-NB	2.69	1.41	1.37
20	H	1852	SQD	O48-C23	2.69	1.41	1.33
13	2	505	CLA	C1B-C2B	2.69	1.49	1.43
13	u	506	CLA	C1B-C2B	2.69	1.49	1.43
13	t	509	CLA	C1B-C2B	2.69	1.49	1.43
13	j	1302	CLA	C1B-C2B	2.69	1.49	1.43
13	b	501	CLA	C1B-C2B	2.68	1.49	1.43
13	4	509	CLA	C1B-C2B	2.68	1.49	1.43
13	f	1204	CLA	C1B-C2B	2.68	1.49	1.43
13	Y	517	CLA	C1B-C2B	2.68	1.49	1.43
13	c	501	CLA	C1B-C2B	2.68	1.49	1.43
13	A	1115	CLA	CMC-C2C	-2.68	1.45	1.50
13	5	506	CLA	C1B-C2B	2.68	1.49	1.43
13	A	1138	CLA	C4B-NB	2.68	1.41	1.37
13	H	1216	CLA	C4B-NB	2.68	1.41	1.37
13	Z	507	CLA	C4B-NB	2.68	1.41	1.37
13	e	1237	CLA	CMB-C2B	-2.68	1.45	1.50
13	H	1204	CLA	C1B-C2B	2.68	1.49	1.43
13	c	510	CLA	C1B-C2B	2.68	1.49	1.43
13	u	503	CLA	C1B-C2B	2.68	1.49	1.43
13	R	1302	CLA	C1B-C2B	2.68	1.49	1.43
13	B	1225	CLA	CMD-C2D	-2.68	1.45	1.50
13	t	503	CLA	C1B-C2B	2.68	1.49	1.43
13	H	1012	CLA	C4B-NB	2.68	1.41	1.37
13	e	1013	CLA	C1B-NB	-2.68	1.34	1.37
13	c	507	CLA	C1B-C2B	2.68	1.49	1.43
13	G	1111	CLA	C4B-NB	2.68	1.41	1.37
13	b	509	CLA	C1B-C2B	2.68	1.49	1.43
13	u	507	CLA	C1B-C2B	2.68	1.49	1.43
13	2	502	CLA	CMB-C2B	-2.68	1.45	1.50
13	f	1012	CLA	C4B-NB	2.67	1.41	1.37
13	5	507	CLA	C1B-C2B	2.67	1.49	1.43
13	6	503	CLA	C1B-C2B	2.67	1.49	1.43
13	s	517	CLA	C1B-C2B	2.67	1.49	1.43
13	A	1139	CLA	C1D-ND	2.67	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1201	CLA	C4B-NB	2.67	1.41	1.37
13	r	505	CLA	C1B-C2B	2.67	1.49	1.43
13	a	511	CLA	C1B-C2B	2.67	1.49	1.43
13	r	507	CLA	C1B-C2B	2.67	1.49	1.43
13	A	1013	CLA	C1B-NB	-2.67	1.34	1.37
13	H	1225	CLA	CMD-C2D	-2.67	1.45	1.50
13	d	503	CLA	C1B-C2B	2.67	1.49	1.43
13	d	517	CLA	C1B-C2B	2.67	1.49	1.43
13	B	1216	CLA	C4B-NB	2.67	1.41	1.37
13	G	1121	CLA	C4B-NB	2.67	1.41	1.37
13	G	1022	CLA	CMB-C2B	-2.67	1.45	1.50
13	b	512	CLA	C1B-C2B	2.67	1.49	1.43
13	d	505	CLA	C1B-C2B	2.67	1.49	1.43
13	4	503	CLA	C1B-C2B	2.67	1.49	1.43
13	H	1229	CLA	C4B-NB	2.67	1.41	1.37
13	r	502	CLA	CMB-C2B	-2.67	1.45	1.50
13	2	507	CLA	C4B-NB	2.67	1.41	1.37
13	b	503	CLA	C1B-C2B	2.67	1.49	1.43
13	d	507	CLA	C1B-C2B	2.67	1.49	1.43
13	B	1221	CLA	CMD-C2D	-2.67	1.45	1.50
13	B	1204	CLA	C1B-C2B	2.67	1.49	1.43
13	c	503	CLA	C1B-C2B	2.67	1.49	1.43
13	r	519	CLA	C1B-C2B	2.67	1.49	1.43
13	e	1129	CLA	CMD-C2D	-2.67	1.45	1.50
13	B	1207	CLA	C4B-NB	2.67	1.41	1.37
13	H	1221	CLA	CMD-C2D	-2.67	1.45	1.50
13	4	512	CLA	C1B-C2B	2.67	1.49	1.43
13	H	1225	CLA	C1D-ND	2.67	1.41	1.37
13	A	1135	CLA	CMD-C2D	-2.67	1.45	1.50
20	B	1852	SQD	O48-C23	2.67	1.41	1.33
13	4	504	CLA	C1B-C2B	2.67	1.49	1.43
13	G	1115	CLA	CMC-C2C	-2.66	1.45	1.50
13	v	503	CLA	C1B-C2B	2.66	1.49	1.43
19	B	5002	LMG	O8-C9	-2.66	1.39	1.45
13	Z	502	CLA	CMB-C2B	-2.66	1.45	1.50
13	3	503	CLA	C1B-C2B	2.66	1.49	1.43
20	f	1852	SQD	O48-C23	2.66	1.41	1.33
13	G	1103	CLA	C1D-ND	2.66	1.41	1.37
13	B	1214	CLA	CMC-C2C	-2.66	1.45	1.50
13	b	504	CLA	C1B-C2B	2.66	1.49	1.43
13	e	1118	CLA	C4B-NB	2.66	1.41	1.37
13	l	1302	CLA	C4B-NB	2.66	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	519	CLA	C1B-C2B	2.66	1.49	1.43
13	5	510	CLA	C1B-C2B	2.66	1.49	1.43
13	6	517	CLA	C1B-C2B	2.66	1.49	1.43
13	T	1302	CLA	C4B-NB	2.66	1.41	1.37
13	e	1111	CLA	C4B-NB	2.66	1.41	1.37
13	a	519	CLA	C1B-C2B	2.66	1.49	1.43
13	A	1022	CLA	CMB-C2B	-2.66	1.45	1.50
13	s	513	CLA	C1B-C2B	2.65	1.49	1.43
13	t	510	CLA	C1B-C2B	2.65	1.49	1.43
13	G	1013	CLA	MG-NB	-2.65	2.00	2.05
17	A	5004	LHG	O7-C5	-2.65	1.40	1.46
13	H	1214	CLA	CMC-C2C	-2.65	1.45	1.50
13	Z	519	CLA	C1B-C2B	2.65	1.49	1.43
13	u	510	CLA	C1B-C2B	2.65	1.49	1.43
13	3	513	CLA	C1B-C2B	2.65	1.49	1.43
13	t	512	CLA	C1B-C2B	2.65	1.49	1.43
13	f	1207	CLA	C4B-NB	2.65	1.41	1.37
13	Y	507	CLA	C1B-C2B	2.65	1.49	1.43
13	v	513	CLA	C1B-C2B	2.65	1.49	1.43
17	G	5004	LHG	O7-C5	-2.65	1.40	1.46
13	e	1135	CLA	C1D-ND	2.65	1.41	1.37
13	b	505	CLA	C1B-C2B	2.65	1.49	1.43
13	a	513	CLA	C1B-C2B	2.65	1.49	1.43
13	6	507	CLA	C1B-C2B	2.65	1.49	1.43
13	s	511	CLA	C1B-C2B	2.65	1.49	1.43
13	v	507	CLA	C1B-C2B	2.65	1.49	1.43
13	A	1128	CLA	C4B-NB	2.65	1.41	1.37
13	q	507	CLA	C1B-C2B	2.65	1.49	1.43
19	H	5002	LMG	O8-C9	-2.65	1.39	1.45
13	J	1302	CLA	C4B-NB	2.65	1.41	1.37
13	e	1135	CLA	CMD-C2D	-2.64	1.45	1.50
13	e	1022	CLA	CMB-C2B	-2.64	1.45	1.50
13	f	1225	CLA	CMD-C2D	-2.64	1.45	1.50
13	B	1231	CLA	C1B-C2B	2.64	1.49	1.43
13	t	504	CLA	C1B-C2B	2.64	1.49	1.43
13	t	505	CLA	C1B-C2B	2.64	1.49	1.43
13	G	1120	CLA	C4B-NB	2.64	1.41	1.37
13	v	517	CLA	C1B-C2B	2.64	1.49	1.43
13	4	505	CLA	C1B-C2B	2.64	1.49	1.43
13	3	519	CLA	C1B-C2B	2.64	1.49	1.43
17	e	5004	LHG	O7-C5	-2.64	1.40	1.46
13	f	1214	CLA	CMC-C2C	-2.64	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1201	CLA	C4B-NB	2.64	1.41	1.37
13	e	1138	CLA	C4B-NB	2.64	1.41	1.37
13	G	1129	CLA	CMD-C2D	-2.64	1.45	1.50
13	A	1111	CLA	C4B-NB	2.64	1.41	1.37
13	s	519	CLA	C1B-C2B	2.64	1.49	1.43
13	e	1128	CLA	C4B-NB	2.64	1.41	1.37
13	3	517	CLA	C1B-C2B	2.64	1.49	1.43
13	4	510	CLA	C1B-C2B	2.64	1.49	1.43
13	H	1201	CLA	C4B-NB	2.64	1.41	1.37
13	b	510	CLA	C1B-C2B	2.64	1.49	1.43
13	A	1013	CLA	MG-NB	-2.64	2.00	2.05
13	r	517	CLA	C1B-C2B	2.64	1.49	1.43
13	s	503	CLA	C1B-C2B	2.64	1.49	1.43
13	H	1219	CLA	CMD-C2D	-2.64	1.45	1.50
13	G	1022	CLA	MG-NB	-2.64	2.00	2.05
13	A	1107	CLA	C4B-NB	2.64	1.41	1.37
13	G	1128	CLA	C4B-NB	2.64	1.41	1.37
13	2	517	CLA	C1B-C2B	2.64	1.49	1.43
13	A	1118	CLA	C4B-NB	2.63	1.41	1.37
13	Y	516	CLA	C1B-C2B	2.63	1.49	1.43
13	a	503	CLA	C1B-C2B	2.63	1.49	1.43
13	a	517	CLA	C1B-C2B	2.63	1.49	1.43
13	3	511	CLA	C1B-C2B	2.63	1.49	1.43
13	A	1129	CLA	CMD-C2D	-2.63	1.45	1.50
13	6	513	CLA	C1B-C2B	2.63	1.49	1.43
13	e	1136	CLA	C3B-C4B	2.63	1.50	1.42
13	f	1225	CLA	C1D-ND	2.63	1.41	1.37
13	A	1136	CLA	C3B-C4B	2.63	1.50	1.42
13	H	1205	CLA	CMD-C2D	-2.63	1.45	1.50
13	f	1231	CLA	C1B-C2B	2.63	1.49	1.43
13	J	1303	CLA	C4B-NB	2.63	1.41	1.37
13	G	1135	CLA	C1D-ND	2.63	1.41	1.37
13	H	1219	CLA	C1B-C2B	2.63	1.49	1.43
13	m	1105	CLA	C1B-C2B	2.63	1.49	1.43
13	r	505	CLA	CMD-C2D	-2.63	1.45	1.50
13	G	1135	CLA	CMD-C2D	-2.63	1.45	1.50
13	T	1303	CLA	C4B-NB	2.63	1.41	1.37
13	Z	505	CLA	CMD-C2D	-2.63	1.45	1.50
13	e	1022	CLA	MG-NB	-2.63	2.00	2.05
13	1	507	CLA	C1B-C2B	2.63	1.49	1.43
13	e	1013	CLA	MG-NB	-2.63	2.00	2.05
13	G	1139	CLA	C1D-ND	2.63	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1103	CLA	C1D-ND	2.63	1.41	1.37
13	T	1303	CLA	C1B-C2B	2.62	1.49	1.43
13	B	1219	CLA	C1B-C2B	2.62	1.49	1.43
13	1	516	CLA	C1B-C2B	2.62	1.49	1.43
13	d	513	CLA	C1B-C2B	2.62	1.49	1.43
13	B	1230	CLA	C4B-NB	2.62	1.41	1.37
13	H	1212	CLA	CMC-C2C	-2.62	1.45	1.50
13	A	1022	CLA	MG-NB	-2.62	2.00	2.05
13	c	518	CLA	C1B-C2B	2.62	1.49	1.43
13	f	1219	CLA	C1B-C2B	2.62	1.49	1.43
13	B	1205	CLA	CMD-C2D	-2.62	1.45	1.50
13	e	1107	CLA	C4B-NB	2.62	1.41	1.37
13	H	1231	CLA	C1B-C2B	2.62	1.49	1.43
13	v	506	CLA	C1B-C2B	2.62	1.49	1.43
13	H	1232	CLA	C4B-NB	2.62	1.41	1.37
13	2	505	CLA	CMD-C2D	-2.62	1.45	1.50
13	f	1218	CLA	C4B-NB	2.62	1.41	1.37
13	q	505	CLA	CMD-C2D	-2.62	1.45	1.50
13	G	1107	CLA	C4B-NB	2.62	1.41	1.37
13	d	519	CLA	C1B-C2B	2.62	1.49	1.43
13	q	504	CLA	C1B-C2B	2.62	1.49	1.43
13	f	1205	CLA	CMD-C2D	-2.61	1.45	1.50
13	A	1135	CLA	C1D-ND	2.61	1.41	1.37
13	6	519	CLA	C1B-C2B	2.61	1.49	1.43
13	G	1118	CLA	C4B-NB	2.61	1.41	1.37
13	d	506	CLA	C1B-C2B	2.61	1.49	1.43
13	f	1230	CLA	C4B-NB	2.61	1.41	1.37
13	f	1227	CLA	C4B-NB	2.61	1.41	1.37
17	V	5221	LHG	O7-C5	-2.61	1.40	1.46
13	1	504	CLA	C1B-C2B	2.61	1.49	1.43
13	l	1303	CLA	C1B-C2B	2.61	1.49	1.43
13	Z	517	CLA	C1B-C2B	2.61	1.49	1.43
13	f	1219	CLA	CMD-C2D	-2.61	1.45	1.50
13	j	1301	CLA	C3B-C4B	2.61	1.50	1.42
13	B	1232	CLA	C4B-NB	2.61	1.41	1.37
13	B	1219	CLA	CMD-C2D	-2.61	1.45	1.50
13	Y	504	CLA	C1B-C2B	2.61	1.49	1.43
17	L	5221	LHG	O7-C5	-2.61	1.40	1.46
13	e	1121	CLA	C1B-C2B	2.61	1.49	1.43
13	6	511	CLA	C1B-C2B	2.60	1.49	1.43
13	s	502	CLA	C1B-C2B	2.60	1.49	1.43
13	d	512	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)
13	A	1120	CLA	C4B-NB	2.60	1.41	1.37
13	G	1801	CLA	C1B-C2B	2.60	1.49	1.43
13	e	1124	CLA	C4B-NB	2.60	1.41	1.37
13	3	518	CLA	C1B-C2B	2.60	1.49	1.43
13	e	1011	CLA	C1B-C2B	2.60	1.49	1.43
13	u	513	CLA	C1B-C2B	2.60	1.49	1.43
13	A	1119	CLA	MG-NB	-2.60	2.00	2.05
13	G	1136	CLA	C3B-C4B	2.60	1.50	1.42
13	G	1123	CLA	C1B-C2B	2.60	1.49	1.43
13	c	513	CLA	C1B-C2B	2.60	1.49	1.43
13	v	511	CLA	C1B-C2B	2.60	1.49	1.43
13	e	1119	CLA	MG-NB	-2.60	2.00	2.05
13	G	1121	CLA	C1B-C2B	2.60	1.49	1.43
13	a	502	CLA	C1B-C2B	2.60	1.49	1.43
13	1	502	CLA	C1B-C2B	2.60	1.49	1.43
13	c	504	CLA	C1B-C2B	2.60	1.49	1.43
13	f	1218	CLA	C1B-C2B	2.60	1.49	1.43
13	u	518	CLA	C1B-C2B	2.60	1.49	1.43
13	A	1121	CLA	C1B-C2B	2.60	1.49	1.43
13	A	1801	CLA	C1B-C2B	2.60	1.49	1.43
13	5	518	CLA	C1B-C2B	2.60	1.49	1.43
13	6	512	CLA	C1B-C2B	2.60	1.49	1.43
13	s	518	CLA	C1B-C2B	2.60	1.49	1.43
13	A	1103	CLA	C1D-ND	2.60	1.41	1.37
13	K	1105	CLA	C1B-C2B	2.60	1.49	1.43
13	5	504	CLA	C1B-C2B	2.60	1.49	1.43
13	e	1120	CLA	C4B-NB	2.60	1.41	1.37
13	v	519	CLA	C1B-C2B	2.60	1.49	1.43
13	H	1211	CLA	C4B-NB	2.60	1.41	1.37
13	J	1303	CLA	C1B-C2B	2.59	1.49	1.43
13	H	1230	CLA	C4B-NB	2.59	1.41	1.37
13	q	519	CLA	MG-NB	-2.59	2.00	2.05
13	e	1118	CLA	C1B-C2B	2.59	1.49	1.43
13	s	505	CLA	CMD-C2D	-2.59	1.45	1.50
13	A	1118	CLA	C1B-C2B	2.59	1.49	1.43
13	U	1105	CLA	C1B-C2B	2.59	1.49	1.43
13	e	1801	CLA	C1B-C2B	2.59	1.49	1.43
13	u	504	CLA	C1B-C2B	2.59	1.49	1.43
13	B	1218	CLA	C4B-NB	2.59	1.41	1.37
13	G	1119	CLA	MG-NB	-2.59	2.00	2.05
13	H	1227	CLA	C4B-NB	2.59	1.41	1.37
13	a	512	CLA	C1B-C2B	2.59	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	518	CLA	C1B-C2B	2.59	1.49	1.43
13	A	1011	CLA	C1B-C2B	2.59	1.49	1.43
13	1	519	CLA	MG-NB	-2.59	2.00	2.05
13	6	506	CLA	C1B-C2B	2.58	1.49	1.43
13	d	510	CLA	C1B-C2B	2.58	1.49	1.43
13	V	1502	CLA	C4B-NB	2.58	1.41	1.37
13	G	1124	CLA	C4B-NB	2.58	1.41	1.37
13	G	1011	CLA	C1B-C2B	2.58	1.49	1.43
13	f	1226	CLA	C1D-ND	2.58	1.41	1.37
13	q	506	CLA	C1B-C2B	2.58	1.49	1.43
13	q	516	CLA	C1B-C2B	2.58	1.49	1.43
13	f	1232	CLA	C4B-NB	2.58	1.41	1.37
13	F	1301	CLA	C3B-C4B	2.58	1.50	1.42
19	T	5104	LMG	O7-C8	-2.58	1.40	1.46
13	H	1217	CLA	CMD-C2D	-2.58	1.45	1.50
13	a	504	CLA	C1B-C2B	2.58	1.49	1.43
13	V	1503	CLA	C4B-NB	2.58	1.41	1.37
13	3	502	CLA	C1B-C2B	2.58	1.49	1.43
13	v	512	CLA	C1B-C2B	2.58	1.49	1.43
13	B	1212	CLA	CMC-C2C	-2.58	1.45	1.50
13	1	501	CLA	C1B-C2B	2.58	1.49	1.43
13	Y	502	CLA	C1B-C2B	2.58	1.49	1.43
13	r	503	CLA	C1B-C2B	2.58	1.49	1.43
13	H	1223	CLA	C1B-C2B	2.58	1.49	1.43
13	e	1112	CLA	C4B-NB	2.58	1.41	1.37
13	e	1137	CLA	C4B-NB	2.58	1.41	1.37
13	Y	519	CLA	MG-NB	-2.58	2.00	2.05
13	d	504	CLA	C1B-C2B	2.58	1.49	1.43
13	a	505	CLA	CMD-C2D	-2.58	1.45	1.50
13	B	1218	CLA	C1B-C2B	2.58	1.49	1.43
13	v	504	CLA	C1B-C2B	2.58	1.49	1.43
13	6	504	CLA	C1B-C2B	2.58	1.49	1.43
13	A	1124	CLA	C4B-NB	2.58	1.41	1.37
13	B	1227	CLA	C4B-NB	2.58	1.41	1.37
13	6	510	CLA	C1B-C2B	2.58	1.49	1.43
13	q	502	CLA	C1B-C2B	2.58	1.49	1.43
13	L	1503	CLA	C4B-NB	2.57	1.41	1.37
13	n	1502	CLA	C4B-NB	2.57	1.41	1.37
13	Y	513	CLA	C1B-C2B	2.57	1.49	1.43
13	d	511	CLA	C1B-C2B	2.57	1.49	1.43
13	Y	509	CLA	C1B-C2B	2.57	1.49	1.43
13	3	504	CLA	C1B-C2B	2.57	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1107	CLA	MG-NB	-2.57	2.00	2.05
13	3	505	CLA	CMD-C2D	-2.57	1.45	1.50
13	H	1218	CLA	C1B-C2B	2.57	1.49	1.43
17	n	5221	LHG	O7-C5	-2.57	1.40	1.46
13	G	1118	CLA	C1B-C2B	2.57	1.49	1.43
13	G	1109	CLA	C1B-C2B	2.57	1.49	1.43
13	B	1223	CLA	C1B-C2B	2.57	1.49	1.43
13	f	1214	CLA	CMB-C2B	-2.57	1.45	1.50
13	1	505	CLA	CMD-C2D	-2.57	1.45	1.50
13	5	513	CLA	C1B-C2B	2.56	1.49	1.43
13	Y	501	CLA	C1B-C2B	2.56	1.49	1.43
13	A	1123	CLA	C1B-C2B	2.56	1.49	1.43
13	e	1109	CLA	C1B-C2B	2.56	1.49	1.43
13	2	503	CLA	C1B-C2B	2.56	1.49	1.43
13	H	1217	CLA	C4B-NB	2.56	1.41	1.37
13	H	1216	CLA	MG-NB	-2.56	2.00	2.05
13	1	506	CLA	C1B-C2B	2.56	1.49	1.43
13	m	1401	CLA	C1B-C2B	2.56	1.49	1.43
13	3	512	CLA	C1B-C2B	2.56	1.49	1.43
13	H	1203	CLA	MG-NB	-2.56	2.00	2.05
13	B	1217	CLA	CMD-C2D	-2.56	1.45	1.50
13	B	1211	CLA	C1B-C2B	2.56	1.49	1.43
13	f	1212	CLA	CMC-C2C	-2.56	1.45	1.50
13	5	509	CLA	C1B-C2B	2.56	1.49	1.43
13	H	1215	CLA	CMB-C2B	-2.56	1.45	1.50
13	e	1013	CLA	CMD-C2D	-2.56	1.45	1.50
13	e	1107	CLA	MG-NB	-2.56	2.00	2.05
13	e	1123	CLA	C1B-C2B	2.56	1.49	1.43
13	l	1302	CLA	C1B-C2B	2.56	1.49	1.43
13	A	1112	CLA	C4B-NB	2.56	1.41	1.37
13	G	1112	CLA	C4B-NB	2.56	1.41	1.37
13	1	509	CLA	C1B-C2B	2.56	1.49	1.43
13	f	1223	CLA	C1B-C2B	2.56	1.49	1.43
13	q	501	CLA	C1B-C2B	2.56	1.49	1.43
13	r	518	CLA	C1B-C2B	2.56	1.49	1.43
13	R	1301	CLA	C3B-C4B	2.56	1.50	1.42
13	G	1113	CLA	C4B-NB	2.56	1.41	1.37
13	A	1137	CLA	C3B-C4B	2.56	1.50	1.42
13	Z	504	CLA	C1B-C2B	2.56	1.49	1.43
13	B	1214	CLA	CMB-C2B	-2.55	1.45	1.50
13	Y	505	CLA	CMD-C2D	-2.55	1.45	1.50
13	n	1503	CLA	C4B-NB	2.55	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1137	CLA	C4B-NB	2.55	1.41	1.37
13	q	509	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1217	CLA	C4B-NB	2.55	1.41	1.37
13	s	504	CLA	C1B-C2B	2.55	1.49	1.43
13	l	1303	CLA	C4B-NB	2.55	1.41	1.37
13	B	1226	CLA	C1D-ND	2.55	1.41	1.37
19	J	5104	LMG	O7-C8	-2.55	1.40	1.46
13	A	1103	CLA	CMD-C2D	-2.55	1.45	1.50
13	B	1211	CLA	C4B-NB	2.55	1.41	1.37
13	U	1401	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1230	CLA	C1B-C2B	2.55	1.49	1.43
13	G	1129	CLA	CMB-C2B	-2.55	1.45	1.50
14	B	2002	PQN	C10-C5	-2.55	1.36	1.40
13	A	1011	CLA	CMD-C2D	-2.55	1.45	1.50
14	e	2001	PQN	C10-C5	-2.55	1.36	1.40
13	A	1109	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1215	CLA	MG-NB	-2.55	2.00	2.05
13	K	1401	CLA	C1B-C2B	2.55	1.49	1.43
13	f	1203	CLA	MG-NB	-2.54	2.00	2.05
13	f	1217	CLA	CMD-C2D	-2.54	1.45	1.50
13	f	1211	CLA	C1B-C2B	2.54	1.49	1.43
13	B	1234	CLA	MG-ND	-2.54	2.00	2.05
13	e	1103	CLA	CMD-C2D	-2.54	1.45	1.50
13	s	512	CLA	C1B-C2B	2.54	1.49	1.43
13	H	1234	CLA	MG-ND	-2.54	2.00	2.05
13	H	1226	CLA	C1D-ND	2.54	1.41	1.37
13	e	1129	CLA	CMB-C2B	-2.54	1.45	1.50
13	c	509	CLA	C1B-C2B	2.54	1.49	1.43
13	v	510	CLA	C1B-C2B	2.54	1.49	1.43
13	H	1217	CLA	MG-NB	-2.54	2.00	2.05
13	s	509	CLA	C1B-C2B	2.54	1.49	1.43
13	e	1137	CLA	C3B-C4B	2.54	1.50	1.42
13	f	1211	CLA	C4B-NB	2.54	1.41	1.37
13	r	504	CLA	C1B-C2B	2.54	1.49	1.43
13	e	1011	CLA	CMD-C2D	-2.54	1.45	1.50
13	1	513	CLA	C1B-C2B	2.54	1.49	1.43
13	B	1203	CLA	MG-NB	-2.54	2.00	2.05
13	2	509	CLA	C1B-C2B	2.54	1.49	1.43
13	H	1211	CLA	C1B-C2B	2.54	1.49	1.43
13	B	1216	CLA	MG-NB	-2.54	2.00	2.05
13	e	1013	CLA	CMC-C2C	-2.54	1.45	1.50
13	L	1502	CLA	C4B-NB	2.54	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1012	CLA	C1D-ND	2.54	1.41	1.37
13	3	509	CLA	C1B-C2B	2.54	1.49	1.43
13	H	1230	CLA	C1B-C2B	2.54	1.49	1.43
13	2	504	CLA	C1B-C2B	2.54	1.49	1.43
13	a	509	CLA	C1B-C2B	2.54	1.49	1.43
13	T	1302	CLA	C1B-C2B	2.54	1.49	1.43
13	2	518	CLA	C1B-C2B	2.53	1.49	1.43
13	a	506	CLA	C1B-C2B	2.53	1.49	1.43
13	e	1022	CLA	CMD-C2D	-2.53	1.45	1.50
13	A	1013	CLA	CMD-C2D	-2.53	1.45	1.50
13	f	1230	CLA	C1B-C2B	2.53	1.49	1.43
13	f	1217	CLA	C4B-NB	2.53	1.41	1.37
13	Z	503	CLA	C1B-C2B	2.53	1.49	1.43
13	3	510	CLA	C1B-C2B	2.53	1.49	1.43
13	Y	506	CLA	C1B-C2B	2.53	1.49	1.43
13	G	1131	CLA	C4B-NB	2.53	1.41	1.37
13	u	509	CLA	C1B-C2B	2.53	1.49	1.43
13	a	510	CLA	C1B-C2B	2.53	1.49	1.43
13	n	1503	CLA	C1B-C2B	2.53	1.49	1.43
13	G	1127	CLA	MG-NB	-2.53	2.00	2.05
13	J	1302	CLA	C1B-C2B	2.53	1.49	1.43
19	l	5104	LMG	O7-C8	-2.53	1.40	1.46
13	e	1113	CLA	C1B-C2B	2.53	1.49	1.43
13	B	1240	CLA	CMD-C2D	-2.53	1.45	1.50
13	Z	518	CLA	C1B-C2B	2.53	1.49	1.43
13	Z	509	CLA	C1B-C2B	2.53	1.49	1.43
13	q	510	CLA	C1B-C2B	2.53	1.49	1.43
17	G	5005	LHG	O7-C5	-2.53	1.40	1.46
13	B	1238	CLA	MG-NB	-2.53	2.00	2.05
14	f	2002	PQN	C10-C5	-2.53	1.36	1.40
13	A	1113	CLA	C1B-C2B	2.53	1.49	1.43
13	s	510	CLA	C1B-C2B	2.53	1.49	1.43
13	f	1215	CLA	MG-NB	-2.53	2.00	2.05
13	A	1137	CLA	C4B-NB	2.53	1.41	1.37
13	A	1129	CLA	CMB-C2B	-2.52	1.45	1.50
13	H	1214	CLA	CMB-C2B	-2.52	1.45	1.50
13	B	1215	CLA	CMB-C2B	-2.52	1.45	1.50
13	H	1220	CLA	CMC-C2C	-2.52	1.45	1.50
13	f	1234	CLA	MG-ND	-2.52	2.00	2.05
13	H	1218	CLA	C4B-NB	2.52	1.41	1.37
13	q	513	CLA	C1B-C2B	2.52	1.49	1.43
17	A	5005	LHG	O7-C5	-2.52	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1217	CLA	MG-NB	-2.52	2.00	2.05
13	H	1210	CLA	CMC-C2C	-2.52	1.45	1.50
13	f	1208	CLA	C1B-C2B	2.52	1.49	1.43
13	d	513	CLA	C3B-C4B	2.52	1.50	1.42
13	H	1238	CLA	MG-NB	-2.52	2.00	2.05
13	V	1503	CLA	C1B-C2B	2.52	1.49	1.43
13	G	1119	CLA	C4B-NB	2.52	1.41	1.37
13	d	518	CLA	C1B-C2B	2.52	1.49	1.43
13	G	1137	CLA	C3B-C4B	2.52	1.50	1.42
13	G	1107	CLA	MG-NB	-2.52	2.00	2.05
13	G	1013	CLA	CMD-C2D	-2.52	1.45	1.50
13	B	1208	CLA	C1B-C2B	2.52	1.49	1.43
13	Y	510	CLA	C1B-C2B	2.52	1.49	1.43
13	A	1131	CLA	C4B-NB	2.52	1.41	1.37
13	G	1124	CLA	CMD-C2D	-2.52	1.45	1.50
13	A	1127	CLA	MG-NB	-2.52	2.00	2.05
13	6	518	CLA	C1B-C2B	2.52	1.49	1.43
13	r	509	CLA	C1B-C2B	2.52	1.49	1.43
13	L	1503	CLA	C1B-C2B	2.52	1.49	1.43
13	G	1110	CLA	C3B-C4B	2.52	1.50	1.42
13	Z	501	CLA	C1B-C2B	2.52	1.49	1.43
13	q	519	CLA	C4B-NB	2.52	1.41	1.37
13	G	1118	CLA	CMD-C2D	-2.52	1.45	1.50
13	2	501	CLA	C1B-C2B	2.51	1.49	1.43
13	G	1103	CLA	CMD-C2D	-2.51	1.45	1.50
13	q	519	CLA	CMC-C2C	-2.51	1.45	1.50
13	e	1127	CLA	MG-NB	-2.51	2.00	2.05
13	6	513	CLA	C3B-C4B	2.51	1.50	1.42
13	v	513	CLA	C3B-C4B	2.51	1.50	1.42
13	c	512	CLA	C1B-C2B	2.51	1.49	1.43
13	H	1206	CLA	MG-NB	-2.51	2.00	2.05
13	H	1240	CLA	CMD-C2D	-2.51	1.45	1.50
13	A	1113	CLA	C4B-NB	2.51	1.41	1.37
13	G	1139	CLA	CHC-C1C	2.51	1.43	1.38
13	A	1118	CLA	CMD-C2D	-2.51	1.45	1.50
13	2	513	CLA	C1B-C2B	2.51	1.49	1.43
13	H	1215	CLA	MG-NB	-2.51	2.00	2.05
13	f	1238	CLA	MG-NB	-2.51	2.00	2.05
14	H	2002	PQN	C10-C5	-2.51	1.36	1.40
13	r	513	CLA	C3B-C4B	2.51	1.50	1.42
13	B	1210	CLA	CMC-C2C	-2.51	1.45	1.50
13	H	1021	CLA	CMC-C2C	-2.51	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	519	CLA	C4B-NB	2.51	1.41	1.37
13	e	1118	CLA	CMD-C2D	-2.51	1.45	1.50
13	n	1501	CLA	C1B-C2B	2.51	1.49	1.43
13	e	1110	CLA	C3B-C4B	2.51	1.50	1.42
13	2	510	CLA	C1B-C2B	2.51	1.49	1.43
13	A	1022	CLA	CMD-C2D	-2.51	1.45	1.50
13	B	1217	CLA	MG-NB	-2.51	2.00	2.05
13	1	510	CLA	C1B-C2B	2.51	1.49	1.43
13	f	1240	CLA	CMD-C2D	-2.51	1.45	1.50
17	e	5005	LHG	O7-C5	-2.51	1.40	1.46
13	Z	510	CLA	C1B-C2B	2.51	1.49	1.43
13	G	1013	CLA	CMC-C2C	-2.51	1.45	1.50
13	e	1117	CLA	C4B-NB	2.50	1.41	1.37
13	G	1013	CLA	C3B-C4B	2.50	1.50	1.42
13	G	1022	CLA	CMD-C2D	-2.50	1.45	1.50
13	3	506	CLA	C1B-C2B	2.50	1.49	1.43
13	G	1103	CLA	C4B-NB	2.50	1.41	1.37
13	H	1208	CLA	C1B-C2B	2.50	1.49	1.43
13	f	1216	CLA	MG-NB	-2.50	2.00	2.05
13	e	1120	CLA	C1B-C2B	2.50	1.49	1.43
13	e	1013	CLA	C3B-C4B	2.50	1.50	1.42
13	B	1208	CLA	C4B-NB	2.50	1.41	1.37
13	e	1113	CLA	C4B-NB	2.50	1.41	1.37
13	G	1011	CLA	CMD-C2D	-2.50	1.45	1.50
13	f	1220	CLA	C1B-C2B	2.50	1.49	1.43
13	r	513	CLA	C1B-C2B	2.50	1.49	1.43
14	A	2001	PQN	C10-C5	-2.50	1.36	1.40
13	e	1131	CLA	C4B-NB	2.50	1.41	1.37
13	A	1110	CLA	C3B-C4B	2.50	1.50	1.42
13	f	1210	CLA	CMC-C2C	-2.50	1.45	1.50
13	B	1206	CLA	MG-NB	-2.50	2.00	2.05
13	A	1013	CLA	CMC-C2C	-2.49	1.45	1.50
13	H	1226	CLA	MG-ND	-2.49	2.00	2.05
13	G	1104	CLA	C1B-C2B	2.49	1.49	1.43
13	r	501	CLA	C1B-C2B	2.49	1.49	1.43
13	B	1220	CLA	CMC-C2C	-2.49	1.45	1.50
13	5	512	CLA	C1B-C2B	2.49	1.49	1.43
13	v	518	CLA	C1B-C2B	2.49	1.49	1.43
13	G	1113	CLA	C1B-C2B	2.49	1.49	1.43
13	f	1212	CLA	C1B-C2B	2.49	1.49	1.43
13	1	519	CLA	C4B-NB	2.49	1.41	1.37
13	A	1124	CLA	CMD-C2D	-2.49	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1125	CLA	C4B-NB	2.49	1.41	1.37
13	f	1223	CLA	CMC-C2C	-2.49	1.45	1.50
13	B	1012	CLA	C1D-ND	2.49	1.41	1.37
13	G	1011	CLA	C4B-NB	2.49	1.41	1.37
13	G	1123	CLA	C4B-NB	2.49	1.41	1.37
13	A	1119	CLA	C4B-NB	2.49	1.41	1.37
13	A	1013	CLA	C3B-C4B	2.49	1.50	1.42
13	2	512	CLA	C1B-C2B	2.49	1.49	1.43
13	B	1021	CLA	CMC-C2C	-2.49	1.45	1.50
13	H	1224	CLA	C1B-C2B	2.49	1.49	1.43
13	f	1215	CLA	CMB-C2B	-2.49	1.45	1.50
13	f	1215	CLA	C4B-NB	2.49	1.41	1.37
13	G	1117	CLA	C4B-NB	2.49	1.41	1.37
13	B	1226	CLA	MG-ND	-2.49	2.00	2.05
13	Z	513	CLA	C1B-C2B	2.49	1.49	1.43
13	c	511	CLA	C1B-C2B	2.49	1.49	1.43
13	u	511	CLA	C1B-C2B	2.49	1.49	1.43
13	2	511	CLA	C1B-C2B	2.49	1.49	1.43
13	t	511	CLA	C1B-C2B	2.49	1.49	1.43
13	2	513	CLA	C3B-C4B	2.49	1.50	1.42
13	G	1103	CLA	C1B-C2B	2.48	1.49	1.43
14	H	2002	PQN	C11-C12	2.48	1.54	1.50
13	f	1206	CLA	MG-NB	-2.48	2.00	2.05
13	q	506	CLA	C3B-C4B	2.48	1.50	1.42
14	G	2001	PQN	C10-C5	-2.48	1.36	1.40
13	5	511	CLA	C1B-C2B	2.48	1.49	1.43
13	r	510	CLA	C1B-C2B	2.48	1.49	1.43
13	B	1240	CLA	C1B-C2B	2.48	1.49	1.43
13	s	506	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1115	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1122	CLA	C1B-C2B	2.48	1.49	1.43
13	G	1116	CLA	C1B-C2B	2.48	1.49	1.43
13	f	1021	CLA	CMC-C2C	-2.48	1.45	1.50
13	Z	511	CLA	C1B-C2B	2.48	1.49	1.43
13	Z	513	CLA	C3B-C4B	2.48	1.50	1.42
13	e	1139	CLA	CHC-C1C	2.48	1.43	1.38
13	Y	506	CLA	C3B-C4B	2.48	1.50	1.42
13	A	1122	CLA	C1B-C2B	2.48	1.48	1.43
13	e	1122	CLA	C1B-C2B	2.48	1.48	1.43
14	f	2002	PQN	C11-C12	2.48	1.54	1.50
13	4	511	CLA	C1B-C2B	2.48	1.48	1.43
13	r	512	CLA	C1B-C2B	2.48	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	506	CLA	CMB-C2B	-2.48	1.45	1.50
13	H	1212	CLA	C1B-C2B	2.48	1.48	1.43
13	e	1115	CLA	C1B-C2B	2.48	1.48	1.43
13	A	1139	CLA	CHC-C1C	2.48	1.43	1.38
14	H	2002	PQN	C5-C4	-2.48	1.43	1.48
13	1	506	CLA	C3B-C4B	2.48	1.50	1.42
13	A	1104	CLA	C1B-C2B	2.48	1.48	1.43
13	Y	519	CLA	C1B-C2B	2.48	1.48	1.43
13	e	1111	CLA	CMC-C2C	-2.48	1.45	1.50
13	L	1501	CLA	C1B-C2B	2.48	1.48	1.43
13	1	512	CLA	C1B-C2B	2.48	1.48	1.43
13	b	511	CLA	C1B-C2B	2.48	1.48	1.43
13	H	1215	CLA	C4B-NB	2.48	1.41	1.37
13	q	511	CLA	C1B-C2B	2.48	1.48	1.43
13	e	1124	CLA	CMD-C2D	-2.48	1.45	1.50
13	5	508	CLA	C1B-C2B	2.48	1.48	1.43
13	f	1213	CLA	C4B-NB	2.48	1.41	1.37
13	f	1220	CLA	CMC-C2C	-2.48	1.45	1.50
13	f	1224	CLA	C1B-C2B	2.48	1.48	1.43
13	q	512	CLA	C1B-C2B	2.48	1.48	1.43
13	A	1103	CLA	C4B-NB	2.47	1.41	1.37
13	U	1103	CLA	MG-NB	-2.47	2.00	2.05
13	B	1224	CLA	C1B-C2B	2.47	1.48	1.43
13	e	1103	CLA	C4B-NB	2.47	1.41	1.37
13	1	519	CLA	CMC-C2C	-2.47	1.45	1.50
13	A	1115	CLA	C1B-C2B	2.47	1.48	1.43
13	B	1223	CLA	CMC-C2C	-2.47	1.45	1.50
13	G	1134	CLA	C3B-C4B	2.47	1.49	1.42
13	H	1205	CLA	CMC-C2C	-2.47	1.45	1.50
13	r	517	CLA	CMC-C2C	-2.47	1.45	1.50
14	f	2002	PQN	C5-C4	-2.47	1.43	1.48
13	u	512	CLA	C1B-C2B	2.47	1.48	1.43
13	f	1226	CLA	MG-ND	-2.47	2.00	2.05
13	B	1222	CLA	CHC-C1C	2.47	1.43	1.38
13	H	1240	CLA	C1B-C2B	2.47	1.48	1.43
13	f	1222	CLA	CHC-C1C	2.47	1.43	1.38
13	f	1227	CLA	CMB-C2B	-2.47	1.45	1.50
13	Z	512	CLA	C1B-C2B	2.47	1.48	1.43
13	u	519	CLA	C1B-C2B	2.47	1.48	1.43
13	H	1012	CLA	C1D-ND	2.47	1.41	1.37
13	A	1116	CLA	C1B-C2B	2.47	1.48	1.43
13	1	511	CLA	C1B-C2B	2.47	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	519	CLA	C1B-C2B	2.47	1.48	1.43
13	e	1114	CLA	C3B-C4B	2.47	1.49	1.42
13	e	1104	CLA	C1B-C2B	2.47	1.48	1.43
13	Z	506	CLA	CMB-C2B	-2.47	1.45	1.50
13	H	1222	CLA	CHC-C1C	2.47	1.43	1.38
13	t	519	CLA	MG-NB	-2.47	2.00	2.05
13	A	1120	CLA	C1B-C2B	2.47	1.48	1.43
13	f	1240	CLA	C1B-C2B	2.47	1.48	1.43
13	A	1117	CLA	C4B-NB	2.47	1.41	1.37
13	e	1119	CLA	C4B-NB	2.47	1.41	1.37
13	2	506	CLA	CMB-C2B	-2.47	1.45	1.50
13	H	1223	CLA	CMC-C2C	-2.47	1.45	1.50
13	B	1220	CLA	C1B-C2B	2.47	1.48	1.43
13	5	519	CLA	C1B-C2B	2.47	1.48	1.43
13	e	1103	CLA	C1B-C2B	2.47	1.48	1.43
13	e	1134	CLA	C1B-C2B	2.47	1.48	1.43
14	B	2002	PQN	C5-C4	-2.47	1.43	1.48
13	e	1116	CLA	C1B-C2B	2.47	1.48	1.43
13	B	1222	CLA	C4B-NB	2.47	1.41	1.37
13	H	1227	CLA	CMB-C2B	-2.46	1.45	1.50
13	V	1501	CLA	C1B-C2B	2.46	1.48	1.43
13	B	1205	CLA	CMC-C2C	-2.46	1.45	1.50
13	B	1012	CLA	C3B-C4B	2.46	1.49	1.42
13	G	1134	CLA	C1B-C2B	2.46	1.48	1.43
13	m	1103	CLA	C4B-NB	2.46	1.41	1.37
13	H	1012	CLA	MG-NB	-2.46	2.00	2.05
13	A	1134	CLA	C3B-C4B	2.46	1.49	1.42
13	A	1123	CLA	C4B-NB	2.46	1.41	1.37
13	f	1232	CLA	MG-NB	-2.46	2.00	2.05
13	f	1012	CLA	C3B-C4B	2.46	1.49	1.42
13	B	1215	CLA	C4B-NB	2.46	1.41	1.37
13	G	1125	CLA	C4B-NB	2.46	1.41	1.37
13	A	1103	CLA	C1B-C2B	2.46	1.48	1.43
13	A	1114	CLA	C3B-C4B	2.46	1.49	1.42
13	b	519	CLA	MG-NB	-2.46	2.00	2.05
13	f	1212	CLA	C4B-NB	2.46	1.41	1.37
13	B	1230	CLA	CMC-C2C	-2.46	1.45	1.50
13	Y	511	CLA	C1B-C2B	2.46	1.48	1.43
14	B	2002	PQN	C11-C12	2.46	1.54	1.50
13	H	1220	CLA	C1B-C2B	2.46	1.48	1.43
13	4	519	CLA	MG-NB	-2.46	2.00	2.05
13	e	1022	CLA	MG-ND	-2.46	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	519	CLA	C1B-C2B	2.46	1.48	1.43
13	4	519	CLA	C4B-NB	2.46	1.41	1.37
13	H	1212	CLA	C4B-NB	2.46	1.41	1.37
13	Z	517	CLA	CMC-C2C	-2.46	1.45	1.50
13	6	508	CLA	C1B-C2B	2.46	1.48	1.43
13	u	508	CLA	C1B-C2B	2.46	1.48	1.43
13	B	1213	CLA	C4B-NB	2.46	1.41	1.37
13	t	519	CLA	C1B-C2B	2.46	1.48	1.43
13	H	1012	CLA	C3B-C4B	2.46	1.49	1.42
13	e	1106	CLA	C4B-NB	2.46	1.41	1.37
13	H	1239	CLA	C1B-C2B	2.46	1.48	1.43
13	f	1228	CLA	C4B-NB	2.46	1.41	1.37
13	A	1111	CLA	CMC-C2C	-2.45	1.45	1.50
13	B	1212	CLA	C4B-NB	2.45	1.41	1.37
13	A	1134	CLA	C1B-C2B	2.45	1.48	1.43
13	r	502	CLA	C1B-C2B	2.45	1.48	1.43
13	B	1228	CLA	C4B-NB	2.45	1.41	1.37
13	B	1212	CLA	C1B-C2B	2.45	1.48	1.43
13	f	1204	CLA	MG-NB	-2.45	2.00	2.05
13	H	1208	CLA	C4B-NB	2.45	1.41	1.37
13	f	1207	CLA	C1B-C2B	2.45	1.48	1.43
13	r	511	CLA	C1B-C2B	2.45	1.48	1.43
13	e	1125	CLA	C4B-NB	2.45	1.41	1.37
13	G	1140	CLA	CMB-C2B	-2.45	1.45	1.50
13	f	1239	CLA	C1B-C2B	2.45	1.48	1.43
13	H	1230	CLA	CMC-C2C	-2.45	1.45	1.50
13	A	1122	CLA	C4B-NB	2.45	1.41	1.37
13	A	1022	CLA	MG-ND	-2.45	2.00	2.05
13	B	1232	CLA	MG-NB	-2.45	2.00	2.05
13	Y	518	CLA	MG-NB	-2.45	2.00	2.05
13	e	1123	CLA	C4B-NB	2.45	1.41	1.37
13	f	1230	CLA	CMB-C2B	-2.45	1.45	1.50
13	B	1012	CLA	MG-NB	-2.45	2.00	2.05
13	q	519	CLA	C1B-C2B	2.45	1.48	1.43
13	f	1205	CLA	CMC-C2C	-2.45	1.45	1.50
13	B	1230	CLA	CMB-C2B	-2.44	1.45	1.50
13	A	1011	CLA	C4B-NB	2.44	1.41	1.37
13	G	1120	CLA	C1B-C2B	2.44	1.48	1.43
13	G	1111	CLA	CMC-C2C	-2.44	1.45	1.50
13	G	1114	CLA	C3B-C4B	2.44	1.49	1.42
13	f	1208	CLA	C4B-NB	2.44	1.41	1.37
13	K	1103	CLA	C1B-C2B	2.44	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1227	CLA	CMB-C2B	-2.44	1.45	1.50
13	H	1232	CLA	MG-NB	-2.44	2.00	2.05
13	G	1101	CLA	CMD-C2D	-2.44	1.45	1.50
13	Y	519	CLA	C4B-NB	2.44	1.41	1.37
13	c	508	CLA	C1B-C2B	2.44	1.48	1.43
13	A	1101	CLA	CMD-C2D	-2.44	1.45	1.50
13	f	1222	CLA	C4B-NB	2.44	1.41	1.37
13	2	517	CLA	CMC-C2C	-2.44	1.45	1.50
13	c	508	CLA	CMB-C2B	-2.44	1.45	1.50
13	H	1204	CLA	MG-NB	-2.44	2.00	2.05
13	2	502	CLA	C1B-C2B	2.44	1.48	1.43
13	A	1140	CLA	CMB-C2B	-2.44	1.45	1.50
13	f	1229	CLA	CHC-C1C	2.44	1.43	1.38
13	U	1103	CLA	C1B-C2B	2.44	1.48	1.43
13	m	1103	CLA	MG-NB	-2.44	2.00	2.05
13	H	1230	CLA	CMB-C2B	-2.44	1.45	1.50
17	e	5008	LHG	O7-C5	-2.44	1.40	1.46
13	B	1204	CLA	MG-NB	-2.44	2.01	2.05
13	Y	519	CLA	CMC-C2C	-2.44	1.45	1.50
13	f	1230	CLA	CMC-C2C	-2.44	1.45	1.50
13	e	1134	CLA	C3B-C4B	2.44	1.49	1.42
13	q	518	CLA	MG-NB	-2.44	2.01	2.05
13	B	1207	CLA	C1B-C2B	2.44	1.48	1.43
13	4	519	CLA	C1B-C2B	2.44	1.48	1.43
13	G	1122	CLA	C4B-NB	2.44	1.41	1.37
13	B	1238	CLA	CMB-C2B	-2.44	1.45	1.50
13	5	508	CLA	CMB-C2B	-2.44	1.45	1.50
13	b	519	CLA	C4B-NB	2.44	1.41	1.37
13	Y	512	CLA	C1B-C2B	2.43	1.48	1.43
13	G	1022	CLA	MG-ND	-2.43	2.01	2.05
13	H	1228	CLA	C4B-NB	2.43	1.41	1.37
13	e	1011	CLA	C4B-NB	2.43	1.41	1.37
13	e	1022	CLA	C4B-NB	2.43	1.41	1.37
13	f	1238	CLA	C4B-NB	2.43	1.41	1.37
13	B	1239	CLA	C1B-C2B	2.43	1.48	1.43
13	H	1213	CLA	C4B-NB	2.43	1.41	1.37
13	G	1237	CLA	C1B-C2B	2.43	1.48	1.43
13	e	1122	CLA	C4B-NB	2.43	1.41	1.37
13	G	1117	CLA	CMB-C2B	-2.43	1.45	1.50
13	A	1106	CLA	MG-NB	-2.43	2.01	2.05
13	d	508	CLA	C1B-C2B	2.43	1.48	1.43
13	1	518	CLA	MG-NB	-2.43	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	502	CLA	C1B-C2B	2.43	1.48	1.43
13	m	1103	CLA	C1B-C2B	2.43	1.48	1.43
13	K	1103	CLA	MG-NB	-2.43	2.01	2.05
13	f	1235	CLA	MG-NB	-2.43	2.01	2.05
13	G	1128	CLA	CMD-C2D	-2.43	1.45	1.50
13	H	1222	CLA	C4B-NB	2.43	1.41	1.37
13	A	1102	CLA	CHC-C1C	2.43	1.43	1.38
13	f	1238	CLA	CMB-C2B	-2.43	1.45	1.50
13	A	1237	CLA	C1B-C2B	2.43	1.48	1.43
13	H	1207	CLA	C1B-C2B	2.43	1.48	1.43
13	G	1106	CLA	MG-NB	-2.43	2.01	2.05
13	e	1140	CLA	CMB-C2B	-2.43	1.45	1.50
13	v	508	CLA	C1B-C2B	2.43	1.48	1.43
13	B	1225	CLA	MG-NB	-2.43	2.01	2.05
13	e	1102	CLA	C1B-C2B	2.43	1.48	1.43
13	e	1106	CLA	MG-NB	-2.43	2.01	2.05
13	e	1128	CLA	CMD-C2D	-2.43	1.45	1.50
13	f	1012	CLA	MG-NB	-2.43	2.01	2.05
13	f	1225	CLA	MG-NB	-2.43	2.01	2.05
13	b	519	CLA	CMC-C2C	-2.43	1.45	1.50
13	G	1102	CLA	CHC-C1C	2.43	1.43	1.38
13	e	1125	CLA	C1B-C2B	2.42	1.48	1.43
13	t	516	CLA	C3B-C4B	2.42	1.49	1.42
13	A	1102	CLA	C1B-C2B	2.42	1.48	1.43
13	G	1022	CLA	C4B-NB	2.42	1.41	1.37
13	b	519	CLA	C1B-C2B	2.42	1.48	1.43
13	6	508	CLA	CMB-C2B	-2.42	1.45	1.50
13	d	508	CLA	CMB-C2B	-2.42	1.45	1.50
13	G	1125	CLA	C1B-C2B	2.42	1.48	1.43
13	H	1225	CLA	MG-NB	-2.42	2.01	2.05
13	d	505	CLA	CMD-C2D	-2.42	1.45	1.50
13	B	1205	CLA	CMB-C2B	-2.42	1.45	1.50
13	f	1236	CLA	C1B-C2B	2.42	1.48	1.43
13	a	506	CLA	CMB-C2B	-2.42	1.45	1.50
13	f	1205	CLA	CMB-C2B	-2.42	1.45	1.50
13	A	1125	CLA	C1B-C2B	2.42	1.48	1.43
13	e	1237	CLA	C1B-C2B	2.42	1.48	1.43
13	f	1234	CLA	CMD-C2D	-2.42	1.45	1.50
13	u	508	CLA	CMB-C2B	-2.42	1.45	1.50
13	A	1106	CLA	C4B-NB	2.42	1.41	1.37
13	G	1101	CLA	CMC-C2C	-2.42	1.45	1.50
13	f	1205	CLA	C1B-C2B	2.42	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1102	CLA	C1B-C2B	2.42	1.48	1.43
13	B	1236	CLA	C1B-C2B	2.42	1.48	1.43
13	H	1235	CLA	CMB-C2B	-2.42	1.45	1.50
13	e	1109	CLA	CMC-C2C	-2.42	1.45	1.50
13	H	1236	CLA	C1B-C2B	2.42	1.48	1.43
13	H	1206	CLA	C4B-NB	2.42	1.41	1.37
13	f	1232	CLA	CMB-C2B	-2.42	1.45	1.50
13	e	1109	CLA	C4B-NB	2.41	1.41	1.37
13	f	1220	CLA	C4B-NB	2.41	1.41	1.37
17	A	5008	LHG	O7-C5	-2.41	1.40	1.46
17	A	5009	LHG	O7-C5	-2.41	1.40	1.46
13	H	1220	CLA	C4B-NB	2.41	1.41	1.37
13	B	1229	CLA	CHC-C1C	2.41	1.43	1.38
13	B	1229	CLA	C1D-ND	2.41	1.41	1.37
13	H	1229	CLA	C1D-ND	2.41	1.41	1.37
13	B	1234	CLA	CMD-C2D	-2.41	1.45	1.50
13	f	1235	CLA	CMB-C2B	-2.41	1.45	1.50
13	4	516	CLA	C3B-C4B	2.41	1.49	1.42
13	3	506	CLA	CMB-C2B	-2.41	1.45	1.50
13	e	1107	CLA	C1D-ND	2.41	1.41	1.37
13	G	1022	CLA	CMC-C2C	-2.41	1.45	1.50
17	G	5009	LHG	O7-C5	-2.41	1.40	1.46
13	H	1234	CLA	CMD-C2D	-2.41	1.45	1.50
13	5	513	CLA	C3B-C4B	2.41	1.49	1.42
13	c	513	CLA	C3B-C4B	2.41	1.49	1.42
13	H	1229	CLA	C3B-C4B	2.41	1.49	1.42
13	G	1131	CLA	C1B-C2B	2.41	1.48	1.43
13	A	1117	CLA	CMB-C2B	-2.41	1.45	1.50
13	A	1101	CLA	CMC-C2C	-2.41	1.45	1.50
13	e	1022	CLA	CMC-C2C	-2.41	1.45	1.50
13	v	505	CLA	CMD-C2D	-2.41	1.45	1.50
13	B	1235	CLA	MG-NB	-2.41	2.01	2.05
13	b	516	CLA	C3B-C4B	2.41	1.49	1.42
13	K	1103	CLA	C4B-NB	2.41	1.41	1.37
13	e	1101	CLA	CMD-C2D	-2.41	1.45	1.50
13	A	1128	CLA	CMD-C2D	-2.41	1.45	1.50
17	e	5009	LHG	O7-C5	-2.41	1.40	1.46
13	H	1205	CLA	CMB-C2B	-2.41	1.45	1.50
13	6	505	CLA	CMD-C2D	-2.41	1.45	1.50
13	e	1102	CLA	CHC-C1C	2.41	1.43	1.38
13	A	1022	CLA	CMC-C2C	-2.41	1.45	1.50
13	V	1503	CLA	CMD-C2D	-2.41	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	1224	CLA	CMD-C2D	-2.41	1.45	1.50
13	A	1022	CLA	C4B-NB	2.41	1.41	1.37
13	A	1115	CLA	C4B-NB	2.40	1.41	1.37
13	G	1801	CLA	C4B-NB	2.40	1.41	1.37
13	e	1105	CLA	C4B-NB	2.40	1.41	1.37
13	A	1109	CLA	CMC-C2C	-2.40	1.45	1.50
13	L	1503	CLA	CMD-C2D	-2.40	1.45	1.50
13	u	513	CLA	CHC-C1C	2.40	1.43	1.38
13	B	1220	CLA	C4B-NB	2.40	1.41	1.37
13	G	1123	CLA	CMD-C2D	-2.40	1.45	1.50
13	f	1206	CLA	C4B-NB	2.40	1.41	1.37
13	B	1229	CLA	C3B-C4B	2.40	1.49	1.42
13	A	1104	CLA	MG-NB	-2.40	2.01	2.05
13	G	1107	CLA	C1D-ND	2.40	1.41	1.37
13	U	1103	CLA	C4B-NB	2.40	1.41	1.37
13	e	1127	CLA	C4B-NB	2.40	1.41	1.37
13	H	1023	CLA	CMD-C2D	-2.40	1.45	1.50
13	v	508	CLA	CMB-C2B	-2.40	1.45	1.50
13	G	1117	CLA	MG-NB	-2.40	2.01	2.05
13	H	1235	CLA	MG-NB	-2.40	2.01	2.05
13	A	1107	CLA	C1D-ND	2.40	1.41	1.37
13	e	1101	CLA	CMC-C2C	-2.40	1.45	1.50
13	B	1235	CLA	CMB-C2B	-2.40	1.45	1.50
13	H	1223	CLA	CMD-C2D	-2.40	1.45	1.50
13	u	513	CLA	C3B-C4B	2.40	1.49	1.42
13	G	1135	CLA	C1B-C2B	2.40	1.48	1.43
13	e	1125	CLA	MG-NB	-2.40	2.01	2.05
13	1	518	CLA	C1B-C2B	2.40	1.48	1.43
13	e	1139	CLA	C1B-C2B	2.40	1.48	1.43
13	A	1125	CLA	MG-NB	-2.40	2.01	2.05
13	G	1115	CLA	C4B-NB	2.40	1.41	1.37
13	A	1139	CLA	C1B-C2B	2.40	1.48	1.43
13	e	1117	CLA	MG-NB	-2.40	2.01	2.05
13	v	516	CLA	C3B-C4B	2.40	1.49	1.42
13	A	1127	CLA	CMD-C2D	-2.40	1.45	1.50
13	H	1238	CLA	CMB-C2B	-2.40	1.45	1.50
13	q	518	CLA	C1B-C2B	2.40	1.48	1.43
13	H	1203	CLA	C4B-NB	2.40	1.41	1.37
13	G	1109	CLA	CMC-C2C	-2.39	1.45	1.50
17	G	5007	LHG	O7-C5	-2.39	1.41	1.46
13	H	1229	CLA	CHC-C1C	2.39	1.43	1.38
13	A	1105	CLA	C4B-NB	2.39	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1127	CLA	CMD-C2D	-2.39	1.45	1.50
13	B	1206	CLA	C4B-NB	2.39	1.41	1.37
13	n	1503	CLA	CMD-C2D	-2.39	1.45	1.50
13	G	1125	CLA	MG-NB	-2.39	2.01	2.05
13	e	1117	CLA	CMB-C2B	-2.39	1.45	1.50
13	G	1106	CLA	CMB-C2B	-2.39	1.45	1.50
13	G	1139	CLA	C3B-C4B	2.39	1.49	1.42
13	H	1236	CLA	C3B-C4B	2.39	1.49	1.42
13	4	519	CLA	CMC-C2C	-2.39	1.45	1.50
13	G	1106	CLA	C4B-NB	2.39	1.41	1.37
13	B	1205	CLA	C1B-C2B	2.39	1.48	1.43
13	H	1230	CLA	CMD-C2D	-2.39	1.45	1.50
13	B	1236	CLA	C3B-C4B	2.39	1.49	1.42
13	e	1115	CLA	C4B-NB	2.39	1.41	1.37
13	B	1223	CLA	CMD-C2D	-2.39	1.45	1.50
13	H	1232	CLA	CMB-C2B	-2.39	1.45	1.50
13	f	1223	CLA	CMD-C2D	-2.39	1.45	1.50
13	q	502	CLA	CMD-C2D	-2.39	1.45	1.50
13	Y	518	CLA	C1B-C2B	2.39	1.48	1.43
13	B	1238	CLA	C4B-NB	2.39	1.41	1.37
13	t	513	CLA	C3B-C4B	2.39	1.49	1.42
13	G	1135	CLA	MG-ND	-2.39	2.01	2.05
13	A	1139	CLA	C3B-C4B	2.39	1.49	1.42
13	B	1224	CLA	CMD-C2D	-2.39	1.45	1.50
13	G	1133	CLA	C4B-NB	2.39	1.41	1.37
13	G	1139	CLA	C1B-C2B	2.39	1.48	1.43
13	e	1108	CLA	C1B-C2B	2.39	1.48	1.43
13	q	518	CLA	CMD-C2D	-2.38	1.45	1.50
13	A	1117	CLA	MG-NB	-2.38	2.01	2.05
13	G	1104	CLA	MG-NB	-2.38	2.01	2.05
13	A	1135	CLA	C1B-C2B	2.38	1.48	1.43
13	A	1106	CLA	CMB-C2B	-2.38	1.45	1.50
13	1	502	CLA	CMD-C2D	-2.38	1.45	1.50
13	m	1105	CLA	CMD-C2D	-2.38	1.45	1.50
13	u	518	CLA	C3B-C4B	2.38	1.49	1.42
13	G	1013	CLA	C4B-NB	2.38	1.41	1.37
13	G	1109	CLA	C4B-NB	2.38	1.41	1.37
13	f	1203	CLA	C4B-NB	2.38	1.41	1.37
13	f	1229	CLA	C3B-C4B	2.38	1.49	1.42
13	B	1210	CLA	C1B-C2B	2.38	1.48	1.43
13	A	1127	CLA	C4B-NB	2.38	1.41	1.37
13	d	516	CLA	C3B-C4B	2.38	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	5008	LHG	O7-C5	-2.38	1.41	1.46
13	A	1131	CLA	C1B-C2B	2.38	1.48	1.43
13	e	1127	CLA	CMD-C2D	-2.38	1.45	1.50
13	G	1801	CLA	MG-NB	-2.38	2.01	2.05
13	A	1108	CLA	C1B-C2B	2.38	1.48	1.43
13	e	1132	CLA	C1B-C2B	2.38	1.48	1.43
13	H	1201	CLA	C1B-C2B	2.38	1.48	1.43
13	r	512	CLA	C3B-C4B	2.38	1.49	1.42
13	t	519	CLA	CMC-C2C	-2.38	1.45	1.50
13	H	1217	CLA	C1B-C2B	2.38	1.48	1.43
13	2	512	CLA	C3B-C4B	2.38	1.49	1.42
13	Z	512	CLA	C3B-C4B	2.38	1.49	1.42
13	6	516	CLA	C3B-C4B	2.38	1.49	1.42
13	G	1108	CLA	C1B-C2B	2.38	1.48	1.43
13	G	1105	CLA	C4B-NB	2.38	1.41	1.37
13	f	1023	CLA	CMD-C2D	-2.38	1.45	1.50
13	H	1238	CLA	C4B-NB	2.38	1.41	1.37
13	G	1133	CLA	CMB-C2B	-2.38	1.45	1.50
13	b	504	CLA	C3B-C4B	2.38	1.49	1.42
13	b	513	CLA	C3B-C4B	2.38	1.49	1.42
13	u	509	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1232	CLA	CMB-C2B	-2.37	1.45	1.50
13	A	1132	CLA	C1B-C2B	2.37	1.48	1.43
13	A	1109	CLA	C4B-NB	2.37	1.41	1.37
13	H	1023	CLA	C1D-ND	2.37	1.41	1.37
13	A	1123	CLA	CMD-C2D	-2.37	1.45	1.50
13	1	512	CLA	MG-NB	-2.37	2.01	2.05
13	A	1013	CLA	C4B-NB	2.37	1.41	1.37
13	H	1205	CLA	C1B-C2B	2.37	1.48	1.43
13	e	1106	CLA	CMB-C2B	-2.37	1.45	1.50
13	B	1235	CLA	C4B-NB	2.37	1.41	1.37
13	e	1111	CLA	MG-NB	-2.37	2.01	2.05
13	f	1229	CLA	C1D-ND	2.37	1.41	1.37
13	f	1236	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1207	CLA	CMD-C2D	-2.37	1.45	1.50
13	5	509	CLA	C3B-C4B	2.37	1.49	1.42
13	H	1206	CLA	C1B-C2B	2.37	1.48	1.43
13	v	504	CLA	C3B-C4B	2.37	1.49	1.42
13	c	518	CLA	C3B-C4B	2.37	1.49	1.42
13	K	1105	CLA	CMD-C2D	-2.37	1.45	1.50
13	Y	518	CLA	CMD-C2D	-2.37	1.45	1.50
13	s	506	CLA	CMB-C2B	-2.37	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1139	CLA	C3B-C4B	2.37	1.49	1.42
13	e	1135	CLA	C1B-C2B	2.37	1.48	1.43
13	r	512	CLA	CMD-C2D	-2.37	1.45	1.50
13	s	509	CLA	C3B-C4B	2.37	1.49	1.42
13	H	1235	CLA	C4B-NB	2.37	1.41	1.37
13	e	1131	CLA	C1B-C2B	2.37	1.48	1.43
13	f	1201	CLA	C1B-C2B	2.37	1.48	1.43
13	B	1023	CLA	CMD-C2D	-2.37	1.45	1.50
13	6	506	CLA	C3B-C4B	2.37	1.49	1.42
13	t	506	CLA	C3B-C4B	2.37	1.49	1.42
13	4	513	CLA	C3B-C4B	2.37	1.49	1.42
13	d	504	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1230	CLA	CMD-C2D	-2.37	1.45	1.50
13	2	506	CLA	C1B-C2B	2.37	1.48	1.43
13	4	506	CLA	C3B-C4B	2.37	1.49	1.42
13	b	506	CLA	C3B-C4B	2.37	1.49	1.42
17	A	5007	LHG	O7-C5	-2.36	1.41	1.46
13	G	1138	CLA	C3B-C4B	2.36	1.49	1.42
13	1	518	CLA	CMD-C2D	-2.36	1.45	1.50
13	H	1207	CLA	CMD-C2D	-2.36	1.45	1.50
13	u	505	CLA	CMD-C2D	-2.36	1.45	1.50
13	G	1132	CLA	C1B-C2B	2.36	1.48	1.43
13	6	504	CLA	C3B-C4B	2.36	1.49	1.42
13	B	1217	CLA	C1B-C2B	2.36	1.48	1.43
13	A	1135	CLA	MG-ND	-2.36	2.01	2.05
13	G	1120	CLA	MG-NB	-2.36	2.01	2.05
13	e	1135	CLA	MG-ND	-2.36	2.01	2.05
13	2	509	CLA	C3B-C4B	2.36	1.49	1.42
17	V	5218	LHG	O7-C5	-2.36	1.41	1.46
13	f	1224	CLA	C4B-NB	2.36	1.41	1.37
13	5	518	CLA	C3B-C4B	2.36	1.49	1.42
13	d	506	CLA	C3B-C4B	2.36	1.49	1.42
13	t	504	CLA	C3B-C4B	2.36	1.49	1.42
13	3	509	CLA	C3B-C4B	2.36	1.49	1.42
13	Y	502	CLA	CMB-C2B	-2.36	1.45	1.50
13	q	502	CLA	CMB-C2B	-2.36	1.45	1.50
13	Z	506	CLA	C1B-C2B	2.36	1.48	1.43
13	r	506	CLA	C1B-C2B	2.36	1.48	1.43
13	3	512	CLA	MG-NB	-2.36	2.01	2.05
13	c	509	CLA	C3B-C4B	2.36	1.49	1.42
13	B	1201	CLA	C1B-C2B	2.36	1.48	1.43
13	e	1124	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)
13	f	1230	CLA	CMD-C2D	-2.36	1.45	1.50
13	e	1104	CLA	MG-NB	-2.36	2.01	2.05
13	B	1203	CLA	C4B-NB	2.36	1.41	1.37
13	2	512	CLA	CMD-C2D	-2.36	1.45	1.50
13	a	509	CLA	C3B-C4B	2.36	1.49	1.42
13	5	505	CLA	CMD-C2D	-2.36	1.45	1.50
13	s	511	CLA	CMB-C2B	-2.36	1.45	1.50
13	G	1129	CLA	MG-ND	-2.36	2.01	2.05
13	A	1133	CLA	C4B-NB	2.36	1.41	1.37
13	v	506	CLA	C3B-C4B	2.36	1.49	1.42
13	f	1210	CLA	C1B-C2B	2.36	1.48	1.43
13	B	1206	CLA	C1B-C2B	2.36	1.48	1.43
17	n	5218	LHG	O7-C5	-2.36	1.41	1.46
13	B	1211	CLA	CMD-C2D	-2.36	1.45	1.50
13	H	1224	CLA	CMC-C2C	-2.36	1.45	1.50
13	G	1127	CLA	C4B-NB	2.36	1.41	1.37
13	1	502	CLA	CMB-C2B	-2.36	1.45	1.50
13	f	1012	CLA	CMC-C2C	-2.36	1.45	1.50
13	5	513	CLA	CHC-C1C	2.36	1.43	1.38
13	c	506	CLA	C3B-C4B	2.36	1.49	1.42
13	H	1224	CLA	CMD-C2D	-2.36	1.45	1.50
13	f	1023	CLA	C1D-ND	2.36	1.41	1.37
13	f	1217	CLA	C1B-C2B	2.36	1.48	1.43
13	A	1138	CLA	C3B-C4B	2.36	1.49	1.42
13	d	519	CLA	C3B-C4B	2.36	1.49	1.42
13	u	505	CLA	C3B-C4B	2.36	1.49	1.42
13	t	511	CLA	CMD-C2D	-2.35	1.45	1.50
13	5	506	CLA	C3B-C4B	2.35	1.49	1.42
17	L	5218	LHG	O7-C5	-2.35	1.41	1.46
13	e	1801	CLA	MG-NB	-2.35	2.01	2.05
13	A	1133	CLA	CMB-C2B	-2.35	1.45	1.50
13	t	501	CLA	C3B-C4B	2.35	1.49	1.42
13	f	1211	CLA	CMD-C2D	-2.35	1.45	1.50
13	A	1801	CLA	MG-NB	-2.35	2.01	2.05
13	H	1210	CLA	C1B-C2B	2.35	1.48	1.43
13	H	1201	CLA	CMD-C2D	-2.35	1.45	1.50
13	H	1211	CLA	CMD-C2D	-2.35	1.45	1.50
13	u	506	CLA	C3B-C4B	2.35	1.49	1.42
13	B	1213	CLA	C1B-C2B	2.35	1.48	1.43
13	4	508	CLA	MG-NB	-2.35	2.01	2.05
13	4	504	CLA	C3B-C4B	2.35	1.49	1.42
13	H	1213	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)
13	e	1133	CLA	C4B-NB	2.35	1.40	1.37
13	f	1023	CLA	CHC-C1C	2.35	1.43	1.38
13	a	511	CLA	CMB-C2B	-2.35	1.46	1.50
13	f	1207	CLA	CMD-C2D	-2.35	1.46	1.50
17	e	5002	LHG	P-O6	2.35	1.68	1.59
13	c	513	CLA	CHC-C1C	2.35	1.43	1.38
13	s	512	CLA	MG-NB	-2.35	2.01	2.05
13	e	1140	CLA	CMC-C2C	-2.35	1.46	1.50
13	B	1021	CLA	MG-NB	-2.35	2.01	2.05
13	f	1021	CLA	MG-NB	-2.35	2.01	2.05
13	Y	502	CLA	CMD-C2D	-2.35	1.46	1.50
13	f	1212	CLA	CMD-C2D	-2.35	1.46	1.50
13	b	501	CLA	C3B-C4B	2.35	1.49	1.42
13	e	1140	CLA	C3B-C4B	2.35	1.49	1.42
13	f	1224	CLA	CMC-C2C	-2.35	1.46	1.50
13	a	512	CLA	MG-NB	-2.35	2.01	2.05
13	t	508	CLA	MG-NB	-2.35	2.01	2.05
13	Z	512	CLA	CMD-C2D	-2.35	1.46	1.50
13	A	1124	CLA	C1B-C2B	2.35	1.48	1.43
13	f	1206	CLA	C1B-C2B	2.35	1.48	1.43
13	e	1138	CLA	C3B-C4B	2.35	1.49	1.42
13	4	501	CLA	C3B-C4B	2.35	1.49	1.42
13	G	1801	CLA	CAA-C2A	-2.35	1.49	1.54
13	6	512	CLA	C3B-C4B	2.35	1.49	1.42
13	a	508	CLA	C3B-C4B	2.35	1.49	1.42
13	e	1123	CLA	CMD-C2D	-2.35	1.46	1.50
13	6	519	CLA	C3B-C4B	2.35	1.49	1.42
13	e	1133	CLA	CMB-C2B	-2.35	1.46	1.50
13	U	1105	CLA	CMD-C2D	-2.35	1.46	1.50
13	c	505	CLA	CMD-C2D	-2.35	1.46	1.50
13	A	1801	CLA	CAA-C2A	-2.35	1.49	1.54
13	G	1111	CLA	MG-NB	-2.34	2.01	2.05
13	A	1140	CLA	C3B-C4B	2.34	1.49	1.42
13	B	1224	CLA	CMC-C2C	-2.34	1.46	1.50
13	Z	509	CLA	C3B-C4B	2.34	1.49	1.42
13	B	1012	CLA	CMC-C2C	-2.34	1.46	1.50
13	4	511	CLA	CMD-C2D	-2.34	1.46	1.50
13	b	508	CLA	MG-NB	-2.34	2.01	2.05
17	e	5007	LHG	O7-C5	-2.34	1.41	1.46
13	H	1206	CLA	C1B-NB	-2.34	1.34	1.37
13	r	511	CLA	C3B-C4B	2.34	1.49	1.42
13	A	1108	CLA	CMB-C2B	-2.34	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	502	CLA	CMD-C2D	-2.34	1.46	1.50
13	G	1140	CLA	CMC-C2C	-2.34	1.46	1.50
13	H	1212	CLA	CMD-C2D	-2.34	1.46	1.50
13	f	1235	CLA	C1B-C2B	2.34	1.48	1.43
13	d	509	CLA	C3B-C4B	2.34	1.49	1.42
13	s	502	CLA	CMD-C2D	-2.34	1.46	1.50
13	A	1120	CLA	MG-NB	-2.34	2.01	2.05
13	G	1108	CLA	CMB-C2B	-2.34	1.46	1.50
13	3	508	CLA	C3B-C4B	2.34	1.49	1.42
13	G	1140	CLA	C3B-C4B	2.34	1.49	1.42
13	Z	511	CLA	C3B-C4B	2.34	1.49	1.42
13	f	1235	CLA	C4B-NB	2.34	1.40	1.37
13	j	1301	CLA	CMB-C2B	-2.34	1.46	1.50
13	e	1126	CLA	C4B-NB	2.34	1.40	1.37
13	A	1110	CLA	CMD-C2D	-2.34	1.46	1.50
13	q	518	CLA	CMB-C2B	-2.34	1.46	1.50
13	b	511	CLA	CMB-C2B	-2.34	1.46	1.50
13	v	512	CLA	C3B-C4B	2.34	1.49	1.42
13	A	1126	CLA	C4B-NB	2.34	1.40	1.37
13	B	1223	CLA	C4B-NB	2.34	1.40	1.37
13	A	1116	CLA	MG-NB	-2.34	2.01	2.05
13	A	1140	CLA	CMC-C2C	-2.34	1.46	1.50
13	G	1124	CLA	C1B-C2B	2.34	1.48	1.43
13	B	1224	CLA	C4B-NB	2.34	1.40	1.37
13	e	1116	CLA	MG-NB	-2.34	2.01	2.05
13	G	1122	CLA	CMC-C2C	-2.34	1.46	1.50
13	G	1237	CLA	CMD-C2D	-2.34	1.46	1.50
13	j	1302	CLA	CMB-C2B	-2.34	1.46	1.50
13	r	501	CLA	CMD-C2D	-2.34	1.46	1.50
13	t	511	CLA	CMB-C2B	-2.34	1.46	1.50
13	c	517	CLA	C3B-C4B	2.34	1.49	1.42
13	H	1228	CLA	MG-NB	-2.34	2.01	2.05
13	e	1122	CLA	CMC-C2C	-2.34	1.46	1.50
13	A	1801	CLA	C4B-NB	2.33	1.40	1.37
13	A	1112	CLA	CHC-C1C	2.33	1.43	1.38
13	s	513	CLA	C3B-C4B	2.33	1.49	1.42
13	A	1122	CLA	CMC-C2C	-2.33	1.46	1.50
13	A	1104	CLA	C4B-NB	2.33	1.40	1.37
13	B	1023	CLA	C1D-ND	2.33	1.40	1.37
13	B	1221	CLA	C1B-NB	-2.33	1.34	1.37
13	G	1125	CLA	CMC-C2C	-2.33	1.46	1.50
13	3	511	CLA	CMB-C2B	-2.33	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	513	CLA	C3B-C4B	2.33	1.49	1.42
13	1	506	CLA	CHC-C1C	2.33	1.43	1.38
13	f	1201	CLA	C3B-C4B	2.33	1.49	1.42
13	a	502	CLA	CMD-C2D	-2.33	1.46	1.50
17	A	5002	LHG	P-O6	2.33	1.68	1.59
13	B	1201	CLA	C3B-C4B	2.33	1.49	1.42
13	Y	512	CLA	MG-NB	-2.33	2.01	2.05
13	F	1302	CLA	CMB-C2B	-2.33	1.46	1.50
13	q	512	CLA	CMD-C2D	-2.33	1.46	1.50
13	r	508	CLA	CMC-C2C	-2.33	1.46	1.50
13	u	512	CLA	C3B-C4B	2.33	1.49	1.42
13	H	1021	CLA	C4B-NB	2.33	1.40	1.37
13	e	1013	CLA	C4B-NB	2.33	1.40	1.37
13	q	506	CLA	CHC-C1C	2.33	1.43	1.38
13	q	512	CLA	MG-NB	-2.33	2.01	2.05
13	B	1238	CLA	CMD-C2D	-2.33	1.46	1.50
13	f	1206	CLA	C1B-NB	-2.33	1.34	1.37
13	A	1111	CLA	MG-NB	-2.33	2.01	2.05
13	Z	509	CLA	CHC-C1C	2.33	1.43	1.38
13	e	1112	CLA	CHC-C1C	2.33	1.43	1.38
13	v	509	CLA	C3B-C4B	2.33	1.49	1.42
13	r	502	CLA	MG-NB	-2.33	2.01	2.05
13	R	1301	CLA	C1B-C2B	2.33	1.48	1.43
13	r	509	CLA	C3B-C4B	2.33	1.49	1.42
13	b	511	CLA	CMD-C2D	-2.33	1.46	1.50
13	s	502	CLA	CMB-C2B	-2.33	1.46	1.50
13	H	1221	CLA	C3B-C4B	2.33	1.49	1.42
17	G	5002	LHG	P-O6	2.33	1.68	1.59
13	c	505	CLA	C3B-C4B	2.33	1.49	1.42
13	q	513	CLA	C3B-C4B	2.33	1.49	1.42
13	f	1228	CLA	MG-NB	-2.33	2.01	2.05
13	2	511	CLA	C3B-C4B	2.33	1.49	1.42
13	5	505	CLA	C3B-C4B	2.33	1.49	1.42
13	A	1128	CLA	MG-ND	-2.33	2.01	2.05
13	T	1303	CLA	CMD-C2D	-2.33	1.46	1.50
13	G	1136	CLA	C1B-C2B	2.33	1.48	1.43
13	A	1102	CLA	C3B-C4B	2.33	1.49	1.42
13	G	1130	CLA	C1B-C2B	2.33	1.48	1.43
13	e	1801	CLA	C4B-NB	2.33	1.40	1.37
13	s	508	CLA	C3B-C4B	2.33	1.49	1.42
13	v	519	CLA	C3B-C4B	2.33	1.49	1.42
13	H	1021	CLA	MG-NB	-2.33	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	509	CLA	C3B-C4B	2.33	1.49	1.42
13	d	504	CLA	CHC-C1C	2.33	1.43	1.38
13	A	1126	CLA	CMD-C2D	-2.33	1.46	1.50
13	B	1212	CLA	CMD-C2D	-2.33	1.46	1.50
13	B	1228	CLA	MG-NB	-2.32	2.01	2.05
13	e	1110	CLA	CMD-C2D	-2.32	1.46	1.50
13	B	1221	CLA	C3B-C4B	2.32	1.49	1.42
13	G	1112	CLA	C3B-C4B	2.32	1.49	1.42
13	2	502	CLA	MG-NB	-2.32	2.01	2.05
13	v	510	CLA	C3B-C4B	2.32	1.49	1.42
13	Y	518	CLA	CMB-C2B	-2.32	1.46	1.50
13	6	504	CLA	CHC-C1C	2.32	1.43	1.38
13	G	1102	CLA	C3B-C4B	2.32	1.49	1.42
13	Y	509	CLA	C3B-C4B	2.32	1.49	1.42
13	B	1201	CLA	CMD-C2D	-2.32	1.46	1.50
13	3	513	CLA	C3B-C4B	2.32	1.49	1.42
13	5	517	CLA	C3B-C4B	2.32	1.49	1.42
13	c	511	CLA	C3B-C4B	2.32	1.49	1.42
13	c	512	CLA	C3B-C4B	2.32	1.49	1.42
13	c	516	CLA	C3B-C4B	2.32	1.49	1.42
13	f	1023	CLA	MG-NB	-2.32	2.01	2.05
13	e	1128	CLA	MG-ND	-2.32	2.01	2.05
13	e	1129	CLA	MG-ND	-2.32	2.01	2.05
13	4	512	CLA	C3B-C4B	2.32	1.49	1.42
13	v	518	CLA	C3B-C4B	2.32	1.49	1.42
13	4	511	CLA	CMB-C2B	-2.32	1.46	1.50
13	H	1201	CLA	C3B-C4B	2.32	1.49	1.42
13	f	1221	CLA	C3B-C4B	2.32	1.49	1.42
13	A	1129	CLA	MG-ND	-2.32	2.01	2.05
13	a	502	CLA	CMB-C2B	-2.32	1.46	1.50
13	e	1108	CLA	CMB-C2B	-2.32	1.46	1.50
13	r	509	CLA	CHC-C1C	2.32	1.43	1.38
13	f	1223	CLA	C4B-NB	2.32	1.40	1.37
13	B	1206	CLA	C1B-NB	-2.32	1.34	1.37
13	j	1301	CLA	C1B-C2B	2.32	1.48	1.43
13	G	1111	CLA	C3B-C4B	2.32	1.49	1.42
13	K	1103	CLA	CMB-C2B	-2.32	1.46	1.50
13	3	502	CLA	CMB-C2B	-2.32	1.46	1.50
13	A	1237	CLA	CMD-C2D	-2.32	1.46	1.50
13	f	1209	CLA	CMD-C2D	-2.32	1.46	1.50
13	B	1023	CLA	CHC-C1C	2.32	1.43	1.38
13	v	516	CLA	CHC-C1C	2.32	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	1301	CLA	C1B-C2B	2.32	1.48	1.43
13	H	1012	CLA	CMC-C2C	-2.32	1.46	1.50
13	e	1237	CLA	CMD-C2D	-2.32	1.46	1.50
13	5	512	CLA	C3B-C4B	2.32	1.49	1.42
13	Y	513	CLA	C3B-C4B	2.32	1.49	1.42
13	q	510	CLA	C3B-C4B	2.32	1.49	1.42
13	B	1023	CLA	MG-NB	-2.32	2.01	2.05
13	G	1013	CLA	CHC-C1C	2.32	1.43	1.38
13	1	512	CLA	CMD-C2D	-2.32	1.46	1.50
13	R	1302	CLA	CMB-C2B	-2.32	1.46	1.50
13	G	1126	CLA	C4B-NB	2.32	1.40	1.37
13	f	1215	CLA	C1B-NB	-2.32	1.34	1.37
13	G	1126	CLA	CMD-C2D	-2.32	1.46	1.50
13	H	1210	CLA	CMD-C2D	-2.32	1.46	1.50
13	e	1120	CLA	MG-NB	-2.32	2.01	2.05
13	5	516	CLA	C3B-C4B	2.32	1.49	1.42
13	H	1216	CLA	CMC-C2C	-2.32	1.46	1.50
13	G	1118	CLA	MG-NB	-2.32	2.01	2.05
13	G	1133	CLA	MG-NB	-2.32	2.01	2.05
13	H	1023	CLA	MG-NB	-2.32	2.01	2.05
13	f	1213	CLA	C1B-C2B	2.32	1.48	1.43
13	f	1235	CLA	CMC-C2C	-2.32	1.46	1.50
13	d	516	CLA	CHC-C1C	2.32	1.43	1.38
13	e	1104	CLA	C4B-NB	2.32	1.40	1.37
13	A	1136	CLA	C1B-C2B	2.32	1.48	1.43
13	B	1231	CLA	CMD-C2D	-2.32	1.46	1.50
13	Z	511	CLA	CMB-C2B	-2.32	1.46	1.50
13	e	1113	CLA	CMD-C2D	-2.32	1.46	1.50
13	e	1131	CLA	CMC-C2C	-2.32	1.46	1.50
13	d	512	CLA	C3B-C4B	2.32	1.49	1.42
13	e	1111	CLA	C3B-C4B	2.32	1.49	1.42
13	A	1125	CLA	CMC-C2C	-2.32	1.46	1.50
13	B	1021	CLA	C4B-NB	2.32	1.40	1.37
13	A	1101	CLA	C1B-C2B	2.32	1.48	1.43
13	L	1502	CLA	C1B-C2B	2.32	1.48	1.43
13	H	1235	CLA	C1B-C2B	2.32	1.48	1.43
13	e	1136	CLA	C1B-C2B	2.32	1.48	1.43
13	e	1102	CLA	C3B-C4B	2.32	1.49	1.42
13	u	517	CLA	C3B-C4B	2.32	1.49	1.42
13	1	518	CLA	CMB-C2B	-2.32	1.46	1.50
13	Y	512	CLA	CMD-C2D	-2.31	1.46	1.50
13	f	1222	CLA	C3B-C4B	2.31	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	509	CLA	CHC-C1C	2.31	1.43	1.38
13	d	508	CLA	C3B-C4B	2.31	1.49	1.42
13	K	1401	CLA	CMB-C2B	-2.31	1.46	1.50
13	A	1105	CLA	C1B-C2B	2.31	1.48	1.43
13	6	502	CLA	CMB-C2B	-2.31	1.46	1.50
13	e	1130	CLA	C1B-C2B	2.31	1.48	1.43
13	c	510	CLA	C3B-C4B	2.31	1.49	1.42
13	A	1112	CLA	C3B-C4B	2.31	1.49	1.42
13	1	513	CLA	C3B-C4B	2.31	1.49	1.42
13	5	511	CLA	C3B-C4B	2.31	1.49	1.42
13	H	1221	CLA	CHC-C1C	2.31	1.43	1.38
13	V	1502	CLA	C1B-C2B	2.31	1.48	1.43
13	e	1101	CLA	C1B-C2B	2.31	1.48	1.43
13	e	1105	CLA	C1B-C2B	2.31	1.48	1.43
13	B	1219	CLA	CMB-C2B	-2.31	1.46	1.50
13	H	1213	CLA	CMD-C2D	-2.31	1.46	1.50
13	e	1138	CLA	C1B-C2B	2.31	1.48	1.43
13	v	508	CLA	C3B-C4B	2.31	1.49	1.42
13	e	1126	CLA	CMD-C2D	-2.31	1.46	1.50
13	B	1227	CLA	MG-NB	-2.31	2.01	2.05
13	H	1221	CLA	C1B-NB	-2.31	1.34	1.37
13	Y	506	CLA	CHC-C1C	2.31	1.43	1.38
13	B	1222	CLA	C3B-C4B	2.31	1.49	1.42
13	H	1231	CLA	CMD-C2D	-2.31	1.46	1.50
13	u	516	CLA	C3B-C4B	2.31	1.49	1.42
13	A	1111	CLA	C3B-C4B	2.31	1.49	1.42
13	f	1216	CLA	CMC-C2C	-2.31	1.46	1.50
13	6	516	CLA	CHC-C1C	2.31	1.43	1.38
13	2	501	CLA	CMD-C2D	-2.31	1.46	1.50
13	H	1219	CLA	CMB-C2B	-2.31	1.46	1.50
13	G	1124	CLA	C3B-C4B	2.31	1.49	1.42
13	Z	502	CLA	MG-NB	-2.31	2.01	2.05
13	A	1130	CLA	C3B-C4B	2.31	1.49	1.42
13	e	1011	CLA	CMB-C2B	-2.31	1.46	1.50
13	d	506	CLA	CHC-C1C	2.31	1.43	1.38
13	n	1502	CLA	C1B-C2B	2.31	1.48	1.43
13	e	1112	CLA	C3B-C4B	2.31	1.49	1.42
13	G	1110	CLA	CMD-C2D	-2.31	1.46	1.50
13	f	1238	CLA	CMD-C2D	-2.31	1.46	1.50
13	5	510	CLA	C3B-C4B	2.31	1.49	1.42
13	H	1222	CLA	C3B-C4B	2.31	1.49	1.42
13	u	511	CLA	C3B-C4B	2.31	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1106	CLA	CMD-C2D	-2.31	1.46	1.50
13	Z	506	CLA	C3B-C4B	2.31	1.49	1.42
13	f	1219	CLA	CMB-C2B	-2.31	1.46	1.50
13	b	510	CLA	C3B-C4B	2.31	1.49	1.42
13	B	1235	CLA	C1B-C2B	2.30	1.48	1.43
13	6	510	CLA	C3B-C4B	2.30	1.49	1.42
13	a	517	CLA	C3B-C4B	2.30	1.49	1.42
13	d	510	CLA	C3B-C4B	2.30	1.49	1.42
13	G	1128	CLA	MG-ND	-2.30	2.01	2.05
13	f	1227	CLA	MG-NB	-2.30	2.01	2.05
13	t	512	CLA	C3B-C4B	2.30	1.49	1.42
13	A	1131	CLA	CMC-C2C	-2.30	1.46	1.50
13	2	508	CLA	CMC-C2C	-2.30	1.46	1.50
13	m	1103	CLA	CMC-C2C	-2.30	1.46	1.50
13	3	510	CLA	C3B-C4B	2.30	1.49	1.42
13	m	1401	CLA	MG-NB	-2.30	2.01	2.05
13	d	502	CLA	CMB-C2B	-2.30	1.46	1.50
13	4	510	CLA	C3B-C4B	2.30	1.49	1.42
13	G	1130	CLA	C3B-C4B	2.30	1.49	1.42
13	G	1133	CLA	C1B-C2B	2.30	1.48	1.43
13	A	1138	CLA	C1B-C2B	2.30	1.48	1.43
13	q	509	CLA	C3B-C4B	2.30	1.49	1.42
13	s	510	CLA	C3B-C4B	2.30	1.49	1.42
13	e	1106	CLA	CMD-C2D	-2.30	1.46	1.50
13	m	1103	CLA	CMB-C2B	-2.30	1.46	1.50
13	B	1221	CLA	CHC-C1C	2.30	1.43	1.38
13	a	510	CLA	C3B-C4B	2.30	1.49	1.42
13	e	1801	CLA	CAA-C2A	-2.30	1.49	1.54
13	H	1225	CLA	CMC-C2C	-2.30	1.46	1.50
13	H	1235	CLA	CMC-C2C	-2.30	1.46	1.50
13	G	1130	CLA	CHC-C1C	2.30	1.43	1.38
13	H	1227	CLA	MG-NB	-2.30	2.01	2.05
13	G	1105	CLA	C1B-C2B	2.30	1.48	1.43
13	d	517	CLA	C3B-C4B	2.30	1.49	1.42
13	B	1209	CLA	CMD-C2D	-2.30	1.46	1.50
13	U	1401	CLA	CMB-C2B	-2.30	1.46	1.50
13	G	1112	CLA	CHC-C1C	2.30	1.43	1.38
13	U	1401	CLA	C3B-C4B	2.30	1.49	1.42
13	G	1116	CLA	MG-NB	-2.30	2.01	2.05
13	e	1801	CLA	CMC-C2C	-2.30	1.46	1.50
13	r	511	CLA	CMB-C2B	-2.30	1.46	1.50
13	b	516	CLA	CHC-C1C	2.30	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1235	CLA	CMC-C2C	-2.30	1.46	1.50
13	G	1104	CLA	C4B-NB	2.30	1.40	1.37
13	G	1131	CLA	CMC-C2C	-2.30	1.46	1.50
13	s	517	CLA	C3B-C4B	2.30	1.49	1.42
13	G	1138	CLA	C1B-C2B	2.30	1.48	1.43
13	G	1801	CLA	CMC-C2C	-2.30	1.46	1.50
13	K	1401	CLA	C3B-C4B	2.30	1.49	1.42
13	2	503	CLA	C3B-C4B	2.30	1.49	1.42
13	6	518	CLA	C3B-C4B	2.30	1.49	1.42
13	t	517	CLA	C3B-C4B	2.30	1.49	1.42
13	R	1301	CLA	CMB-C2B	-2.30	1.46	1.50
13	1	511	CLA	C3B-C4B	2.30	1.49	1.42
13	2	504	CLA	C3B-C4B	2.30	1.49	1.42
13	A	1132	CLA	C4B-NB	2.30	1.40	1.37
13	A	1133	CLA	MG-NB	-2.30	2.01	2.05
13	2	513	CLA	CHC-C1C	2.30	1.43	1.38
13	c	503	CLA	C3B-C4B	2.30	1.49	1.42
13	e	1131	CLA	CMD-C2D	-2.30	1.46	1.50
13	Z	503	CLA	C3B-C4B	2.30	1.49	1.42
13	t	510	CLA	C3B-C4B	2.30	1.49	1.42
13	6	506	CLA	CHC-C1C	2.30	1.43	1.38
13	q	518	CLA	CMC-C2C	-2.30	1.46	1.50
13	f	1221	CLA	CHC-C1C	2.30	1.43	1.38
13	G	1140	CLA	C1B-C2B	2.30	1.48	1.43
13	1	509	CLA	C3B-C4B	2.29	1.49	1.42
13	B	1213	CLA	CMD-C2D	-2.29	1.46	1.50
13	e	1122	CLA	CMD-C2D	-2.29	1.46	1.50
13	e	1130	CLA	CHC-C1C	2.29	1.43	1.38
13	u	510	CLA	C3B-C4B	2.29	1.49	1.42
13	1	518	CLA	CMC-C2C	-2.29	1.46	1.50
13	Z	501	CLA	CMD-C2D	-2.29	1.46	1.50
13	Z	507	CLA	CMD-C2D	-2.29	1.46	1.50
13	f	1213	CLA	CMD-C2D	-2.29	1.46	1.50
13	b	512	CLA	C3B-C4B	2.29	1.49	1.42
13	m	1401	CLA	C3B-C4B	2.29	1.49	1.42
13	F	1301	CLA	CMB-C2B	-2.29	1.46	1.50
13	A	1111	CLA	C1B-C2B	2.29	1.48	1.43
13	s	513	CLA	CHC-C1C	2.29	1.43	1.38
13	3	517	CLA	C3B-C4B	2.29	1.49	1.42
13	b	503	CLA	C3B-C4B	2.29	1.49	1.42
13	e	1138	CLA	CMD-C2D	-2.29	1.46	1.50
13	e	1101	CLA	CMB-C2B	-2.29	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	511	CLA	C3B-C4B	2.29	1.49	1.42
13	A	1130	CLA	C1B-C2B	2.29	1.48	1.43
13	A	1801	CLA	CMC-C2C	-2.29	1.46	1.50
13	6	508	CLA	C3B-C4B	2.29	1.49	1.42
13	6	517	CLA	C3B-C4B	2.29	1.49	1.42
13	f	1231	CLA	CMD-C2D	-2.29	1.46	1.50
13	m	1401	CLA	CMB-C2B	-2.29	1.46	1.50
13	b	511	CLA	C3B-C4B	2.29	1.49	1.42
13	H	1023	CLA	CHC-C1C	2.29	1.43	1.38
13	e	1140	CLA	MG-NB	-2.29	2.01	2.05
13	e	1125	CLA	CMC-C2C	-2.29	1.46	1.50
13	G	1111	CLA	C1B-C2B	2.29	1.48	1.43
13	H	1224	CLA	C4B-NB	2.29	1.40	1.37
13	Z	504	CLA	C3B-C4B	2.29	1.49	1.42
13	Z	510	CLA	C3B-C4B	2.29	1.49	1.42
13	G	1139	CLA	MG-NB	-2.29	2.01	2.05
13	G	1011	CLA	CMB-C2B	-2.29	1.46	1.50
14	e	2001	PQN	C11-C3	2.29	1.55	1.51
13	r	513	CLA	CHC-C1C	2.29	1.43	1.38
13	r	506	CLA	CMC-C2C	-2.29	1.46	1.50
13	s	511	CLA	C3B-C4B	2.29	1.49	1.42
13	2	510	CLA	C3B-C4B	2.29	1.49	1.42
13	d	518	CLA	C3B-C4B	2.29	1.49	1.42
13	t	513	CLA	CHC-C1C	2.29	1.43	1.38
13	v	504	CLA	CHC-C1C	2.29	1.43	1.38
13	G	1013	CLA	C1D-ND	2.29	1.40	1.37
13	G	1122	CLA	CMD-C2D	-2.29	1.46	1.50
13	H	1012	CLA	CMD-C2D	-2.29	1.46	1.50
13	e	1110	CLA	CMC-C2C	-2.29	1.46	1.50
13	v	502	CLA	CMB-C2B	-2.29	1.46	1.50
13	4	517	CLA	C3B-C4B	2.29	1.49	1.42
13	f	1226	CLA	CHC-C4B	-2.29	1.34	1.39
13	d	518	CLA	CHC-C1C	2.29	1.43	1.38
13	e	1116	CLA	CMD-C2D	-2.29	1.46	1.50
13	q	519	CLA	CMB-C2B	-2.29	1.46	1.50
13	e	1133	CLA	C1B-C2B	2.29	1.48	1.43
13	B	1225	CLA	C4B-NB	2.29	1.40	1.37
13	2	506	CLA	C3B-C4B	2.29	1.49	1.42
13	3	506	CLA	C3B-C4B	2.29	1.49	1.42
13	H	1238	CLA	CMD-C2D	-2.29	1.46	1.50
13	Y	508	CLA	CMC-C2C	-2.29	1.46	1.50
13	r	501	CLA	CMC-C2C	-2.29	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1101	CLA	C1B-C2B	2.29	1.48	1.43
13	B	1215	CLA	C1B-NB	-2.29	1.34	1.37
13	e	1124	CLA	C3B-C4B	2.29	1.49	1.42
13	1	510	CLA	CHC-C1C	2.29	1.43	1.38
13	d	513	CLA	CHC-C1C	2.29	1.43	1.38
13	r	504	CLA	C3B-C4B	2.29	1.49	1.42
13	e	1125	CLA	CMB-C2B	-2.29	1.46	1.50
13	H	1215	CLA	C1B-NB	-2.29	1.34	1.37
13	A	1130	CLA	CHC-C1C	2.29	1.43	1.38
13	u	519	CLA	CHC-C1C	2.29	1.43	1.38
13	v	506	CLA	CHC-C1C	2.29	1.43	1.38
13	A	1125	CLA	CMB-C2B	-2.29	1.46	1.50
13	G	1138	CLA	CMD-C2D	-2.29	1.46	1.50
13	f	1223	CLA	MG-NB	-2.29	2.01	2.05
13	1	510	CLA	C3B-C4B	2.29	1.49	1.42
13	6	513	CLA	CHC-C1C	2.28	1.43	1.38
13	q	510	CLA	CHC-C1C	2.28	1.43	1.38
13	U	1103	CLA	CMB-C2B	-2.28	1.46	1.50
13	3	518	CLA	C3B-C4B	2.28	1.49	1.42
13	Y	503	CLA	C3B-C4B	2.28	1.49	1.42
13	Y	511	CLA	C3B-C4B	2.28	1.49	1.42
13	r	503	CLA	C3B-C4B	2.28	1.49	1.42
13	A	1113	CLA	CMD-C2D	-2.28	1.46	1.50
13	A	1122	CLA	CMD-C2D	-2.28	1.46	1.50
13	A	1101	CLA	CMB-C2B	-2.28	1.46	1.50
13	A	1133	CLA	C1B-C2B	2.28	1.48	1.43
13	v	518	CLA	CHC-C1C	2.28	1.43	1.38
13	B	1210	CLA	CMD-C2D	-2.28	1.46	1.50
13	H	1209	CLA	CMD-C2D	-2.28	1.46	1.50
13	f	1225	CLA	CMC-C2C	-2.28	1.46	1.50
13	f	1221	CLA	C1B-NB	-2.28	1.34	1.37
13	H	1023	CLA	C3B-C4B	2.28	1.49	1.42
13	d	519	CLA	CHC-C1C	2.28	1.43	1.38
13	t	516	CLA	CHC-C1C	2.28	1.43	1.38
13	5	503	CLA	C3B-C4B	2.28	1.49	1.42
13	G	1101	CLA	CMB-C2B	-2.28	1.46	1.50
13	j	1302	CLA	CMD-C2D	-2.28	1.46	1.50
13	4	513	CLA	CHC-C1C	2.28	1.43	1.38
13	a	518	CLA	C3B-C4B	2.28	1.49	1.42
13	r	508	CLA	MG-NB	-2.28	2.01	2.05
13	G	1106	CLA	CMD-C2D	-2.28	1.46	1.50
13	G	1128	CLA	CMC-C2C	-2.28	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	1303	CLA	CMD-C2D	-2.28	1.46	1.50
13	f	1021	CLA	C4B-NB	2.28	1.40	1.37
13	2	507	CLA	CMD-C2D	-2.28	1.46	1.50
13	2	513	CLA	CMC-C2C	-2.28	1.46	1.50
13	G	1113	CLA	CMD-C2D	-2.28	1.46	1.50
13	n	1502	CLA	C3B-C4B	2.28	1.49	1.42
13	B	1216	CLA	CMC-C2C	-2.28	1.46	1.50
13	J	1303	CLA	CMD-C2D	-2.28	1.46	1.50
13	2	511	CLA	CMB-C2B	-2.28	1.46	1.50
13	H	1225	CLA	CMB-C2B	-2.28	1.46	1.50
13	f	1210	CLA	CMD-C2D	-2.28	1.46	1.50
13	e	1139	CLA	MG-NB	-2.28	2.01	2.05
13	Z	502	CLA	CMD-C2D	-2.28	1.46	1.50
13	e	1125	CLA	CMD-C2D	-2.28	1.46	1.50
13	e	1110	CLA	C1B-C2B	2.28	1.48	1.43
13	Z	508	CLA	MG-NB	-2.28	2.01	2.05
13	n	1502	CLA	CHC-C1C	2.28	1.43	1.38
13	B	1240	CLA	MG-NB	-2.28	2.01	2.05
13	u	503	CLA	C3B-C4B	2.28	1.49	1.42
13	A	1112	CLA	CMC-C2C	-2.28	1.46	1.50
13	H	1223	CLA	C4B-NB	2.28	1.40	1.37
13	6	518	CLA	CHC-C1C	2.28	1.43	1.38
13	e	1130	CLA	C3B-C4B	2.28	1.49	1.42
13	e	1112	CLA	CMC-C2C	-2.28	1.46	1.50
13	B	1023	CLA	C3B-C4B	2.28	1.49	1.42
13	H	1210	CLA	C3B-C4B	2.28	1.49	1.42
13	A	1124	CLA	C3B-C4B	2.28	1.49	1.42
13	B	1226	CLA	CHC-C4B	-2.28	1.34	1.39
13	r	518	CLA	C3B-C4B	2.28	1.49	1.42
13	4	512	CLA	CMB-C2B	-2.28	1.46	1.50
13	G	1129	CLA	CMC-C2C	-2.28	1.46	1.50
13	f	1201	CLA	CMD-C2D	-2.28	1.46	1.50
13	4	503	CLA	C3B-C4B	2.28	1.49	1.42
13	f	1012	CLA	CMD-C2D	-2.28	1.46	1.50
13	H	1205	CLA	MG-NB	-2.28	2.01	2.05
13	H	1202	CLA	C1B-C2B	2.28	1.48	1.43
13	Y	512	CLA	C3B-C4B	2.28	1.49	1.42
13	A	1013	CLA	C1D-ND	2.28	1.40	1.37
13	r	513	CLA	CMC-C2C	-2.28	1.46	1.50
13	2	518	CLA	C3B-C4B	2.28	1.49	1.42
13	3	511	CLA	C3B-C4B	2.28	1.49	1.42
13	r	510	CLA	C3B-C4B	2.28	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	517	CLA	C3B-C4B	2.28	1.49	1.42
13	A	1140	CLA	C1B-C2B	2.28	1.48	1.43
13	A	1128	CLA	CMC-C2C	-2.28	1.46	1.50
13	B	1225	CLA	CMC-C2C	-2.28	1.46	1.50
13	e	1128	CLA	CMC-C2C	-2.28	1.46	1.50
13	t	511	CLA	C3B-C4B	2.27	1.49	1.42
13	U	1103	CLA	CMC-C2C	-2.27	1.46	1.50
13	2	510	CLA	CHC-C1C	2.27	1.43	1.38
13	Y	518	CLA	CMC-C2C	-2.27	1.46	1.50
13	e	1111	CLA	C1B-C2B	2.27	1.48	1.43
13	s	506	CLA	C3B-C4B	2.27	1.49	1.42
13	f	1202	CLA	C1B-C2B	2.27	1.48	1.43
13	4	510	CLA	CHC-C1C	2.27	1.43	1.38
13	c	519	CLA	CHC-C1C	2.27	1.43	1.38
13	4	511	CLA	C3B-C4B	2.27	1.49	1.42
13	a	504	CLA	C3B-C4B	2.27	1.49	1.42
13	s	518	CLA	C3B-C4B	2.27	1.49	1.42
13	a	511	CLA	C3B-C4B	2.27	1.49	1.42
13	u	501	CLA	C3B-C4B	2.27	1.49	1.42
13	A	1011	CLA	CMB-C2B	-2.27	1.46	1.50
13	A	1138	CLA	CMD-C2D	-2.27	1.46	1.50
13	G	1140	CLA	CMD-C2D	-2.27	1.46	1.50
13	t	503	CLA	CMD-C2D	-2.27	1.46	1.50
13	A	1139	CLA	MG-NB	-2.27	2.01	2.05
13	2	512	CLA	MG-NB	-2.27	2.01	2.05
13	q	517	CLA	C3B-C4B	2.27	1.49	1.42
13	r	507	CLA	CMD-C2D	-2.27	1.46	1.50
13	A	1013	CLA	CHC-C1C	2.27	1.43	1.38
13	6	519	CLA	CHC-C1C	2.27	1.43	1.38
13	e	1140	CLA	C1B-C2B	2.27	1.48	1.43
13	F	1302	CLA	CMD-C2D	-2.27	1.46	1.50
13	V	1502	CLA	CMD-C2D	-2.27	1.46	1.50
13	e	1132	CLA	C4B-NB	2.27	1.40	1.37
13	B	1012	CLA	CMD-C2D	-2.27	1.46	1.50
13	1	508	CLA	CMC-C2C	-2.27	1.46	1.50
13	2	506	CLA	CMC-C2C	-2.27	1.46	1.50
13	1	505	CLA	C3B-C4B	2.27	1.49	1.42
13	q	505	CLA	C3B-C4B	2.27	1.49	1.42
13	G	1123	CLA	MG-NB	-2.27	2.01	2.05
13	e	1013	CLA	C1D-ND	2.27	1.40	1.37
13	s	516	CLA	C3B-C4B	2.27	1.49	1.42
13	A	1110	CLA	C1B-C2B	2.27	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	508	CLA	CMC-C2C	-2.27	1.46	1.50
13	r	510	CLA	CHC-C1C	2.27	1.43	1.38
13	G	1125	CLA	CMB-C2B	-2.27	1.46	1.50
13	Z	513	CLA	CMC-C2C	-2.27	1.46	1.50
13	q	508	CLA	CMC-C2C	-2.27	1.46	1.50
13	2	502	CLA	CMD-C2D	-2.27	1.46	1.50
13	e	1104	CLA	CMD-C2D	-2.27	1.46	1.50
13	e	1114	CLA	MG-NB	-2.27	2.01	2.05
13	1	512	CLA	C3B-C4B	2.27	1.49	1.42
13	3	516	CLA	C3B-C4B	2.27	1.49	1.42
13	Y	505	CLA	C3B-C4B	2.27	1.49	1.42
13	4	516	CLA	CHC-C1C	2.27	1.43	1.38
13	r	506	CLA	C3B-C4B	2.27	1.49	1.42
13	B	1235	CLA	CMD-C2D	-2.27	1.46	1.50
13	L	1502	CLA	CHC-C1C	2.27	1.43	1.38
13	1	519	CLA	CMB-C2B	-2.27	1.46	1.50
13	H	1240	CLA	MG-NB	-2.27	2.01	2.05
13	b	517	CLA	C3B-C4B	2.27	1.49	1.42
13	t	503	CLA	C3B-C4B	2.27	1.49	1.42
13	Y	510	CLA	CHC-C1C	2.27	1.43	1.38
13	G	1112	CLA	CMC-C2C	-2.27	1.46	1.50
13	5	501	CLA	C3B-C4B	2.27	1.49	1.42
13	e	1125	CLA	C3B-C4B	2.27	1.49	1.42
13	B	1205	CLA	MG-NB	-2.27	2.01	2.05
13	Z	512	CLA	MG-NB	-2.27	2.01	2.05
13	R	1302	CLA	CMD-C2D	-2.27	1.46	1.50
13	f	1228	CLA	CMD-C2D	-2.27	1.46	1.50
13	G	1132	CLA	C4B-NB	2.27	1.40	1.37
13	1	503	CLA	C3B-C4B	2.27	1.49	1.42
13	a	506	CLA	C3B-C4B	2.27	1.49	1.42
13	Z	513	CLA	CHC-C1C	2.26	1.43	1.38
13	e	1119	CLA	CMD-C2D	-2.26	1.46	1.50
13	r	502	CLA	CMD-C2D	-2.26	1.46	1.50
13	2	501	CLA	CMC-C2C	-2.26	1.46	1.50
13	f	1219	CLA	MG-NB	-2.26	2.01	2.05
13	q	512	CLA	C3B-C4B	2.26	1.49	1.42
13	f	1225	CLA	C4B-NB	2.26	1.40	1.37
13	H	1226	CLA	CHC-C4B	-2.26	1.34	1.39
13	B	1214	CLA	C1B-C2B	2.26	1.48	1.43
13	B	1219	CLA	MG-NB	-2.26	2.01	2.05
13	j	1301	CLA	MG-NB	-2.26	2.01	2.05
13	q	508	CLA	MG-NB	-2.26	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1214	CLA	C1B-C2B	2.26	1.48	1.43
13	G	1106	CLA	CMC-C2C	-2.26	1.46	1.50
13	G	1126	CLA	MG-NB	-2.26	2.01	2.05
13	B	1228	CLA	CMD-C2D	-2.26	1.46	1.50
13	Z	506	CLA	CMC-C2C	-2.26	1.46	1.50
13	R	1301	CLA	MG-NB	-2.26	2.01	2.05
13	A	1116	CLA	CMD-C2D	-2.26	1.46	1.50
13	G	1130	CLA	CMB-C2B	-2.26	1.46	1.50
13	K	1103	CLA	CMC-C2C	-2.26	1.46	1.50
13	e	1136	CLA	CMD-C2D	-2.26	1.46	1.50
13	3	513	CLA	CHC-C1C	2.26	1.43	1.38
13	c	509	CLA	CHC-C1C	2.26	1.43	1.38
13	L	1502	CLA	C3B-C4B	2.26	1.49	1.42
13	Y	516	CLA	C3B-C4B	2.26	1.49	1.42
13	Z	518	CLA	C3B-C4B	2.26	1.49	1.42
13	a	516	CLA	C3B-C4B	2.26	1.49	1.42
13	q	508	CLA	C3B-C4B	2.26	1.49	1.42
13	K	1401	CLA	MG-NB	-2.26	2.01	2.05
13	U	1103	CLA	CMD-C2D	-2.26	1.46	1.50
13	b	512	CLA	CMB-C2B	-2.26	1.46	1.50
13	A	1119	CLA	CMC-C2C	-2.26	1.46	1.50
13	e	1137	CLA	CMB-C2B	-2.26	1.46	1.50
13	G	1119	CLA	CMD-C2D	-2.26	1.46	1.50
13	v	519	CLA	CHC-C1C	2.26	1.43	1.38
13	A	1125	CLA	CMD-C2D	-2.26	1.46	1.50
13	1	501	CLA	CMD-C2D	-2.26	1.46	1.50
13	A	1118	CLA	MG-NB	-2.26	2.01	2.05
13	r	512	CLA	MG-NB	-2.26	2.01	2.05
13	A	1125	CLA	C3B-C4B	2.26	1.49	1.42
13	Y	517	CLA	C3B-C4B	2.26	1.49	1.42
13	B	1206	CLA	CMD-C2D	-2.26	1.46	1.50
13	e	1137	CLA	CMC-C2C	-2.26	1.46	1.50
13	e	1123	CLA	MG-NB	-2.26	2.01	2.05
13	Y	508	CLA	C3B-C4B	2.26	1.49	1.42
13	q	503	CLA	C3B-C4B	2.26	1.49	1.42
13	a	512	CLA	CMD-C2D	-2.26	1.46	1.50
13	B	1210	CLA	C3B-C4B	2.26	1.49	1.42
13	G	1125	CLA	C3B-C4B	2.26	1.49	1.42
13	A	1126	CLA	MG-NB	-2.26	2.01	2.05
13	u	510	CLA	CHC-C1C	2.26	1.43	1.38
13	A	1113	CLA	CMC-C2C	-2.26	1.46	1.50
13	q	510	CLA	MG-NB	-2.26	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V	1502	CLA	CHC-C1C	2.26	1.43	1.38
13	Z	519	CLA	CHC-C1C	2.26	1.43	1.38
13	f	1227	CLA	CHC-C1C	2.26	1.43	1.38
13	G	1110	CLA	C1B-C2B	2.26	1.48	1.43
13	n	1501	CLA	CMB-C2B	-2.26	1.46	1.50
13	3	504	CLA	C3B-C4B	2.26	1.49	1.42
13	G	1122	CLA	CMB-C2B	-2.26	1.46	1.50
13	q	516	CLA	CHC-C1C	2.26	1.43	1.38
13	L	1501	CLA	CMB-C2B	-2.25	1.46	1.50
13	H	1231	CLA	CMC-C2C	-2.25	1.46	1.50
13	q	501	CLA	CMD-C2D	-2.25	1.46	1.50
13	e	1133	CLA	MG-NB	-2.25	2.01	2.05
13	f	1214	CLA	C1B-C2B	2.25	1.48	1.43
13	Y	510	CLA	C3B-C4B	2.25	1.49	1.42
13	H	1202	CLA	CMC-C2C	-2.25	1.46	1.50
13	t	512	CLA	CMB-C2B	-2.25	1.46	1.50
13	v	513	CLA	CHC-C1C	2.25	1.43	1.38
13	u	518	CLA	CMD-C2D	-2.25	1.46	1.50
13	u	512	CLA	MG-NB	-2.25	2.01	2.05
13	q	501	CLA	C3B-C4B	2.25	1.49	1.42
13	c	518	CLA	CMD-C2D	-2.25	1.46	1.50
13	l	1302	CLA	CMB-C2B	-2.25	1.46	1.50
13	q	504	CLA	C3B-C4B	2.25	1.49	1.42
13	A	1119	CLA	C3B-C4B	2.25	1.49	1.42
13	e	1119	CLA	C3B-C4B	2.25	1.49	1.42
13	f	1221	CLA	CMB-C2B	-2.25	1.46	1.50
13	f	1205	CLA	MG-NB	-2.25	2.01	2.05
13	b	506	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1127	CLA	C1B-C2B	2.25	1.48	1.43
13	3	512	CLA	CMD-C2D	-2.25	1.46	1.50
13	H	1206	CLA	CMD-C2D	-2.25	1.46	1.50
13	H	1235	CLA	CMD-C2D	-2.25	1.46	1.50
13	e	1140	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	2001	PQN	C11-C3	2.25	1.55	1.51
13	H	1213	CLA	MG-NB	-2.25	2.01	2.05
13	f	1234	CLA	CMC-C2C	-2.25	1.46	1.50
13	5	519	CLA	CHC-C1C	2.25	1.43	1.38
13	G	1131	CLA	CMD-C2D	-2.25	1.46	1.50
13	V	1501	CLA	CMB-C2B	-2.25	1.46	1.50
13	t	506	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1140	CLA	MG-NB	-2.25	2.01	2.05
13	5	512	CLA	MG-NB	-2.25	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1110	CLA	CMC-C2C	-2.25	1.46	1.50
13	A	1137	CLA	CMB-C2B	-2.25	1.46	1.50
13	G	1132	CLA	CMD-C2D	-2.25	1.46	1.50
13	B	1202	CLA	C1B-C2B	2.25	1.48	1.43
13	B	1227	CLA	CHC-C1C	2.25	1.43	1.38
13	f	1213	CLA	MG-NB	-2.25	2.01	2.05
14	G	2001	PQN	C11-C3	2.25	1.55	1.51
13	A	1119	CLA	CMD-C2D	-2.25	1.46	1.50
13	A	1132	CLA	CMD-C2D	-2.25	1.46	1.50
13	G	1137	CLA	CMB-C2B	-2.25	1.46	1.50
13	f	1207	CLA	CMC-C2C	-2.25	1.46	1.50
13	G	1119	CLA	C3B-C4B	2.25	1.49	1.42
13	f	1210	CLA	C3B-C4B	2.25	1.49	1.42
13	G	1125	CLA	CMD-C2D	-2.25	1.46	1.50
13	H	1209	CLA	C1B-C2B	2.25	1.48	1.43
13	1	517	CLA	C3B-C4B	2.25	1.49	1.42
13	4	506	CLA	CHC-C1C	2.25	1.43	1.38
13	b	513	CLA	CHC-C1C	2.25	1.43	1.38
13	G	1140	CLA	MG-NB	-2.25	2.01	2.05
13	f	1221	CLA	MG-NB	-2.25	2.01	2.05
13	Y	501	CLA	CMD-C2D	-2.25	1.46	1.50
13	e	1136	CLA	CMC-C2C	-2.25	1.46	1.50
13	b	510	CLA	CHC-C1C	2.25	1.43	1.38
13	4	505	CLA	CMD-C2D	-2.25	1.46	1.50
13	f	1023	CLA	C3B-C4B	2.25	1.49	1.42
13	v	505	CLA	C3B-C4B	2.25	1.49	1.42
13	u	509	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1114	CLA	MG-NB	-2.25	2.01	2.05
13	H	1227	CLA	C1B-C2B	2.25	1.48	1.43
13	5	518	CLA	CHC-C1C	2.25	1.43	1.38
13	d	505	CLA	C3B-C4B	2.25	1.49	1.42
13	a	509	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1131	CLA	CMD-C2D	-2.25	1.46	1.50
13	A	1140	CLA	CMD-C2D	-2.25	1.46	1.50
13	e	1127	CLA	C1B-C2B	2.25	1.48	1.43
13	f	1204	CLA	C4B-NB	2.25	1.40	1.37
13	V	1502	CLA	C3B-C4B	2.25	1.49	1.42
13	1	516	CLA	CHC-C1C	2.25	1.43	1.38
13	c	519	CLA	MG-NB	-2.25	2.01	2.05
13	Z	501	CLA	CMC-C2C	-2.25	1.46	1.50
13	B	1234	CLA	CMC-C2C	-2.25	1.46	1.50
13	L	1502	CLA	CMD-C2D	-2.25	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	504	CLA	CMD-C2D	-2.25	1.46	1.50
13	e	1113	CLA	CMC-C2C	-2.25	1.46	1.50
13	f	1209	CLA	C1B-C2B	2.25	1.48	1.43
13	G	1134	CLA	CMD-C2D	-2.25	1.46	1.50
13	f	1206	CLA	CMD-C2D	-2.25	1.46	1.50
13	1	504	CLA	C3B-C4B	2.24	1.49	1.42
13	B	1213	CLA	MG-NB	-2.24	2.01	2.05
13	B	1225	CLA	CMB-C2B	-2.24	1.46	1.50
13	A	1114	CLA	C1B-NB	-2.24	1.34	1.37
13	A	1137	CLA	CMC-C2C	-2.24	1.46	1.50
13	q	511	CLA	CMB-C2B	-2.24	1.46	1.50
13	d	503	CLA	C3B-C4B	2.24	1.49	1.42
13	A	1121	CLA	CMB-C2B	-2.24	1.46	1.50
13	A	1136	CLA	CMC-C2C	-2.24	1.46	1.50
13	G	1114	CLA	MG-NB	-2.24	2.01	2.05
13	1	511	CLA	CMB-C2B	-2.24	1.46	1.50
13	Z	503	CLA	CMD-C2D	-2.24	1.46	1.50
13	a	504	CLA	CMD-C2D	-2.24	1.46	1.50
13	u	504	CLA	C3B-C4B	2.24	1.49	1.42
13	H	1219	CLA	MG-NB	-2.24	2.01	2.05
13	T	1303	CLA	MG-NB	-2.24	2.01	2.05
13	5	519	CLA	C3B-C4B	2.24	1.49	1.42
13	u	519	CLA	C3B-C4B	2.24	1.49	1.42
13	Z	510	CLA	CHC-C1C	2.24	1.43	1.38
13	G	1137	CLA	CMC-C2C	-2.24	1.46	1.50
13	e	1126	CLA	MG-NB	-2.24	2.01	2.05
13	B	1216	CLA	CMD-C2D	-2.24	1.46	1.50
13	2	508	CLA	MG-NB	-2.24	2.01	2.05
13	s	519	CLA	C3B-C4B	2.24	1.49	1.42
13	A	1104	CLA	CMD-C2D	-2.24	1.46	1.50
13	A	1134	CLA	CMD-C2D	-2.24	1.46	1.50
13	B	1213	CLA	CMC-C2C	-2.24	1.46	1.50
13	e	1106	CLA	CMC-C2C	-2.24	1.46	1.50
13	A	1121	CLA	MG-NB	-2.24	2.01	2.05
13	B	1215	CLA	C1B-C2B	2.24	1.48	1.43
13	4	503	CLA	CMD-C2D	-2.24	1.46	1.50
13	b	519	CLA	CMB-C2B	-2.24	1.46	1.50
13	J	1303	CLA	MG-NB	-2.24	2.01	2.05
13	1	508	CLA	C3B-C4B	2.24	1.49	1.42
13	6	503	CLA	C3B-C4B	2.24	1.49	1.42
13	A	1106	CLA	CMC-C2C	-2.24	1.46	1.50
13	2	503	CLA	CMD-C2D	-2.24	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	518	CLA	CMD-C2D	-2.24	1.46	1.50
13	Z	501	CLA	C3B-C4B	2.24	1.49	1.42
13	H	1215	CLA	C1B-C2B	2.24	1.48	1.43
13	H	1221	CLA	MG-NB	-2.24	2.01	2.05
13	A	1133	CLA	CMD-C2D	-2.24	1.46	1.50
13	G	1121	CLA	CMB-C2B	-2.24	1.46	1.50
13	H	1216	CLA	CMD-C2D	-2.24	1.46	1.50
13	s	504	CLA	CMD-C2D	-2.24	1.46	1.50
13	b	512	CLA	MG-NB	-2.24	2.01	2.05
13	c	501	CLA	C3B-C4B	2.24	1.49	1.42
13	G	1104	CLA	CMD-C2D	-2.24	1.46	1.50
13	G	1131	CLA	CMB-C2B	-2.24	1.46	1.50
13	j	1301	CLA	CMD-C2D	-2.24	1.46	1.50
13	e	1013	CLA	CHC-C1C	2.24	1.43	1.38
13	B	1223	CLA	MG-NB	-2.24	2.01	2.05
13	G	1132	CLA	MG-NB	-2.24	2.01	2.05
13	A	1104	CLA	CMC-C2C	-2.24	1.46	1.50
13	H	1203	CLA	CMC-C2C	-2.24	1.46	1.50
13	H	1228	CLA	CMD-C2D	-2.24	1.46	1.50
13	e	1122	CLA	CMB-C2B	-2.24	1.46	1.50
13	f	1211	CLA	CMC-C2C	-2.24	1.46	1.50
13	q	511	CLA	CHC-C1C	2.24	1.43	1.38
13	b	505	CLA	CMD-C2D	-2.24	1.46	1.50
13	e	1132	CLA	CMD-C2D	-2.24	1.46	1.50
13	6	510	CLA	CHC-C1C	2.24	1.43	1.38
13	2	516	CLA	C3B-C4B	2.24	1.49	1.42
13	G	1127	CLA	C1B-C2B	2.24	1.48	1.43
13	A	1129	CLA	CMC-C2C	-2.24	1.46	1.50
13	3	506	CLA	CMC-C2C	-2.24	1.46	1.50
13	G	1116	CLA	CMD-C2D	-2.24	1.46	1.50
13	c	518	CLA	CHC-C1C	2.24	1.43	1.38
13	v	510	CLA	CHC-C1C	2.24	1.43	1.38
13	1	508	CLA	MG-NB	-2.24	2.01	2.05
13	c	502	CLA	C3B-C4B	2.24	1.49	1.42
13	H	1234	CLA	C1B-NB	-2.24	1.34	1.37
13	A	1116	CLA	CMC-C2C	-2.24	1.46	1.50
13	e	1133	CLA	CMD-C2D	-2.24	1.46	1.50
13	f	1240	CLA	MG-NB	-2.24	2.01	2.05
13	u	502	CLA	C3B-C4B	2.24	1.49	1.42
13	G	1116	CLA	CMC-C2C	-2.24	1.46	1.50
13	G	1132	CLA	CMC-C2C	-2.24	1.46	1.50
13	4	504	CLA	CHC-C1C	2.24	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	504	CLA	CHC-C1C	2.24	1.43	1.38
13	t	510	CLA	CHC-C1C	2.24	1.43	1.38
13	H	1204	CLA	C4B-NB	2.24	1.40	1.37
13	e	1118	CLA	MG-NB	-2.24	2.01	2.05
13	a	513	CLA	CHC-C1C	2.24	1.43	1.38
13	A	1122	CLA	CMB-C2B	-2.24	1.46	1.50
13	Y	511	CLA	CMB-C2B	-2.24	1.46	1.50
13	e	1129	CLA	CMC-C2C	-2.24	1.46	1.50
13	q	504	CLA	CMD-C2D	-2.24	1.46	1.50
13	6	505	CLA	C3B-C4B	2.24	1.49	1.42
13	B	1221	CLA	MG-NB	-2.24	2.01	2.05
13	c	519	CLA	C3B-C4B	2.24	1.49	1.42
13	T	1302	CLA	CMD-C2D	-2.23	1.46	1.50
13	t	518	CLA	CMD-C2D	-2.23	1.46	1.50
13	v	511	CLA	CMB-C2B	-2.23	1.46	1.50
13	Y	511	CLA	CHC-C1C	2.23	1.43	1.38
13	c	510	CLA	CHC-C1C	2.23	1.43	1.38
13	5	504	CLA	C3B-C4B	2.23	1.49	1.42
13	A	1123	CLA	MG-NB	-2.23	2.01	2.05
13	e	1106	CLA	MG-ND	-2.23	2.01	2.05
13	A	1130	CLA	CMB-C2B	-2.23	1.46	1.50
13	f	1213	CLA	CMC-C2C	-2.23	1.46	1.50
13	3	503	CLA	C3B-C4B	2.23	1.49	1.42
13	Y	512	CLA	CHC-C1C	2.23	1.43	1.38
13	3	519	CLA	C3B-C4B	2.23	1.49	1.42
13	B	1209	CLA	CMC-C2C	-2.23	1.46	1.50
13	1	504	CLA	CMD-C2D	-2.23	1.46	1.50
13	H	1227	CLA	CHC-C1C	2.23	1.43	1.38
13	s	509	CLA	CHC-C1C	2.23	1.43	1.38
13	B	1214	CLA	MG-NB	-2.23	2.01	2.05
13	B	1202	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	1224	CLA	CMB-C2B	-2.23	1.46	1.50
13	J	1302	CLA	CMB-C2B	-2.23	1.46	1.50
13	Y	503	CLA	CMD-C2D	-2.23	1.46	1.50
13	K	1103	CLA	CMD-C2D	-2.23	1.46	1.50
13	3	518	CLA	CHC-C1C	2.23	1.43	1.38
13	1	516	CLA	C3B-C4B	2.23	1.49	1.42
13	Y	504	CLA	C3B-C4B	2.23	1.49	1.42
13	Z	516	CLA	C3B-C4B	2.23	1.49	1.42
13	H	1023	CLA	MG-ND	-2.23	2.01	2.05
13	Z	517	CLA	MG-NB	-2.23	2.01	2.05
13	H	1207	CLA	CMC-C2C	-2.23	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	519	CLA	CMB-C2B	-2.23	1.46	1.50
13	r	503	CLA	CMD-C2D	-2.23	1.46	1.50
13	a	518	CLA	CHC-C1C	2.23	1.43	1.38
13	U	1401	CLA	MG-NB	-2.23	2.01	2.05
13	a	508	CLA	MG-NB	-2.23	2.01	2.05
13	e	1138	CLA	CMB-C2B	-2.23	1.46	1.50
13	B	1205	CLA	C3B-C4B	2.23	1.49	1.42
13	4	519	CLA	CMB-C2B	-2.23	1.46	1.50
13	s	504	CLA	C3B-C4B	2.23	1.49	1.42
13	2	519	CLA	CHC-C1C	2.23	1.43	1.38
13	q	516	CLA	C3B-C4B	2.23	1.49	1.42
13	A	1106	CLA	MG-ND	-2.23	2.01	2.05
13	q	502	CLA	MG-NB	-2.23	2.01	2.05
13	B	1231	CLA	CMC-C2C	-2.23	1.46	1.50
13	b	503	CLA	CMD-C2D	-2.23	1.46	1.50
13	e	1130	CLA	CMB-C2B	-2.23	1.46	1.50
13	f	1205	CLA	C3B-C4B	2.23	1.49	1.42
13	n	1502	CLA	CMD-C2D	-2.23	1.46	1.50
13	b	519	CLA	C3B-C4B	2.23	1.49	1.42
13	5	509	CLA	CHC-C1C	2.23	1.43	1.38
13	6	511	CLA	C3B-C4B	2.23	1.49	1.42
13	f	1209	CLA	CMC-C2C	-2.23	1.46	1.50
13	e	1121	CLA	CMB-C2B	-2.23	1.46	1.50
13	1	501	CLA	C3B-C4B	2.23	1.49	1.42
13	e	1114	CLA	C1B-NB	-2.23	1.34	1.37
13	f	1215	CLA	C1B-C2B	2.23	1.48	1.43
13	4	508	CLA	CMC-C2C	-2.23	1.46	1.50
13	6	502	CLA	CMD-C2D	-2.23	1.46	1.50
13	H	1201	CLA	CMC-C2C	-2.23	1.46	1.50
13	e	1104	CLA	CMC-C2C	-2.23	1.46	1.50
13	Y	516	CLA	CHC-C1C	2.23	1.43	1.38
13	r	519	CLA	CHC-C1C	2.23	1.43	1.38
13	t	519	CLA	C3B-C4B	2.23	1.49	1.42
13	f	1202	CLA	CMC-C2C	-2.23	1.46	1.50
13	e	1122	CLA	MG-NB	-2.23	2.01	2.05
13	H	1228	CLA	C1B-C2B	2.23	1.48	1.43
13	H	1225	CLA	C4B-NB	2.23	1.40	1.37
13	4	519	CLA	C3B-C4B	2.23	1.49	1.42
13	r	516	CLA	C3B-C4B	2.23	1.49	1.42
13	G	1122	CLA	MG-NB	-2.23	2.01	2.05
13	u	518	CLA	CHC-C1C	2.23	1.42	1.38
13	B	1221	CLA	CMB-C2B	-2.23	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1207	CLA	CMB-C2B	-2.23	1.46	1.50
13	f	1202	CLA	CMD-C2D	-2.23	1.46	1.50
13	v	511	CLA	C3B-C4B	2.23	1.49	1.42
13	3	512	CLA	CMB-C2B	-2.23	1.46	1.50
13	f	1207	CLA	CMB-C2B	-2.23	1.46	1.50
13	a	519	CLA	C3B-C4B	2.22	1.49	1.42
13	B	1209	CLA	C1B-C2B	2.22	1.48	1.43
13	G	1110	CLA	CMB-C2B	-2.22	1.46	1.50
13	H	1021	CLA	CMB-C2B	-2.22	1.46	1.50
13	H	1206	CLA	CMC-C2C	-2.22	1.46	1.50
13	u	511	CLA	CMB-C2B	-2.22	1.46	1.50
13	B	1212	CLA	MG-NB	-2.22	2.01	2.05
13	A	1111	CLA	CHC-C1C	2.22	1.42	1.38
13	3	519	CLA	CHC-C1C	2.22	1.42	1.38
13	a	512	CLA	CMB-C2B	-2.22	1.46	1.50
13	d	502	CLA	CMD-C2D	-2.22	1.46	1.50
13	F	1301	CLA	MG-NB	-2.22	2.01	2.05
13	f	1227	CLA	C1B-C2B	2.22	1.48	1.43
13	e	1120	CLA	CMB-C2B	-2.22	1.46	1.50
13	f	1234	CLA	C1B-NB	-2.22	1.34	1.37
13	u	508	CLA	C3B-C4B	2.22	1.49	1.42
13	s	502	CLA	MG-NB	-2.22	2.01	2.05
13	H	1209	CLA	CMB-C2B	-2.22	1.46	1.50
13	f	1229	CLA	C1B-NB	-2.22	1.34	1.37
13	4	502	CLA	C3B-C4B	2.22	1.49	1.42
13	1	511	CLA	CHC-C1C	2.22	1.42	1.38
13	e	1116	CLA	CHC-C1C	2.22	1.42	1.38
13	c	502	CLA	CMB-C2B	-2.22	1.46	1.50
13	Y	508	CLA	MG-NB	-2.22	2.01	2.05
13	l	1303	CLA	MG-NB	-2.22	2.01	2.05
13	f	1234	CLA	C3B-C4B	2.22	1.49	1.42
13	A	1132	CLA	CMB-C2B	-2.22	1.46	1.50
13	A	1136	CLA	CMD-C2D	-2.22	1.46	1.50
13	G	1132	CLA	CMB-C2B	-2.22	1.46	1.50
13	f	1203	CLA	CMD-C2D	-2.22	1.46	1.50
13	n	1502	CLA	MG-NB	-2.22	2.01	2.05
13	5	510	CLA	CHC-C1C	2.22	1.42	1.38
13	H	1205	CLA	C3B-C4B	2.22	1.49	1.42
13	1	503	CLA	CMD-C2D	-2.22	1.46	1.50
13	G	1104	CLA	CMC-C2C	-2.22	1.46	1.50
13	G	1108	CLA	CMD-C2D	-2.22	1.46	1.50
13	e	1116	CLA	CMC-C2C	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	508	CLA	C3B-C4B	2.22	1.49	1.42
13	B	1227	CLA	C1B-C2B	2.22	1.48	1.43
13	3	509	CLA	CHC-C1C	2.22	1.42	1.38
13	t	509	CLA	C3B-C4B	2.22	1.49	1.42
13	B	1023	CLA	MG-ND	-2.22	2.01	2.05
13	f	1202	CLA	C3B-C4B	2.22	1.49	1.42
13	G	1136	CLA	CMC-C2C	-2.22	1.46	1.50
13	H	1209	CLA	CMC-C2C	-2.22	1.46	1.50
13	Y	504	CLA	CMD-C2D	-2.22	1.46	1.50
13	f	1206	CLA	CMC-C2C	-2.22	1.46	1.50
13	A	1134	CLA	CHC-C1C	2.22	1.42	1.38
13	s	503	CLA	C3B-C4B	2.22	1.49	1.42
13	5	519	CLA	MG-NB	-2.22	2.01	2.05
13	G	1121	CLA	MG-NB	-2.22	2.01	2.05
13	A	1131	CLA	CMB-C2B	-2.22	1.46	1.50
13	B	1201	CLA	CMC-C2C	-2.22	1.46	1.50
13	G	1116	CLA	CHC-C1C	2.22	1.42	1.38
13	q	512	CLA	CMB-C2B	-2.22	1.46	1.50
13	2	501	CLA	C3B-C4B	2.22	1.49	1.42
13	c	512	CLA	MG-NB	-2.22	2.01	2.05
13	H	1211	CLA	CMC-C2C	-2.22	1.46	1.50
13	e	1119	CLA	CMC-C2C	-2.22	1.46	1.50
13	u	511	CLA	CMD-C2D	-2.22	1.46	1.50
13	f	1234	CLA	CHC-C1C	2.22	1.42	1.38
13	t	504	CLA	CHC-C1C	2.22	1.42	1.38
13	A	1111	CLA	CMD-C2D	-2.22	1.46	1.50
13	u	507	CLA	CMD-C2D	-2.22	1.46	1.50
13	6	512	CLA	CHC-C1C	2.22	1.42	1.38
13	a	510	CLA	CHC-C1C	2.22	1.42	1.38
13	3	508	CLA	MG-NB	-2.22	2.01	2.05
13	G	1119	CLA	CMC-C2C	-2.22	1.46	1.50
13	H	1202	CLA	CMD-C2D	-2.22	1.46	1.50
13	Y	512	CLA	CMB-C2B	-2.22	1.46	1.50
13	3	504	CLA	MG-NB	-2.22	2.01	2.05
13	c	504	CLA	C3B-C4B	2.22	1.49	1.42
13	v	503	CLA	C3B-C4B	2.22	1.49	1.42
13	G	1134	CLA	CMB-C2B	-2.22	1.46	1.50
13	t	502	CLA	CMB-C2B	-2.22	1.46	1.50
13	H	1223	CLA	C3B-C4B	2.22	1.49	1.42
13	Z	505	CLA	C3B-C4B	2.22	1.49	1.42
13	Y	519	CLA	MG-ND	-2.22	2.01	2.05
13	4	518	CLA	CMD-C2D	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	519	CLA	CMD-C2D	-2.22	1.46	1.50
13	G	1138	CLA	CMC-C2C	-2.22	1.46	1.50
13	Y	517	CLA	CMD-C2D	-2.22	1.46	1.50
13	f	1203	CLA	CMC-C2C	-2.22	1.46	1.50
13	r	509	CLA	CMC-C2C	-2.22	1.46	1.50
13	T	1302	CLA	C3B-C4B	2.22	1.49	1.42
13	t	502	CLA	C3B-C4B	2.22	1.49	1.42
13	B	1207	CLA	CMC-C2C	-2.22	1.46	1.50
13	1	517	CLA	CMD-C2D	-2.22	1.46	1.50
13	G	1133	CLA	CMD-C2D	-2.22	1.46	1.50
13	4	505	CLA	C3B-C4B	2.22	1.49	1.42
13	f	1229	CLA	C1B-C2B	2.22	1.48	1.43
13	1	510	CLA	MG-NB	-2.22	2.01	2.05
13	4	512	CLA	MG-NB	-2.22	2.01	2.05
13	1	507	CLA	MG-NB	-2.21	2.01	2.05
13	e	1111	CLA	CMD-C2D	-2.21	1.46	1.50
13	s	512	CLA	CMD-C2D	-2.21	1.46	1.50
13	t	508	CLA	CMD-C2D	-2.21	1.46	1.50
13	3	516	CLA	CHC-C1C	2.21	1.42	1.38
13	v	512	CLA	CHC-C1C	2.21	1.42	1.38
13	B	1204	CLA	C4B-NB	2.21	1.40	1.37
13	B	1234	CLA	C1B-NB	-2.21	1.35	1.37
13	B	1203	CLA	CMD-C2D	-2.21	1.46	1.50
13	f	1225	CLA	CMB-C2B	-2.21	1.46	1.50
13	d	510	CLA	CHC-C1C	2.21	1.42	1.38
13	Y	508	CLA	C1B-C2B	2.21	1.48	1.43
13	5	502	CLA	CMB-C2B	-2.21	1.46	1.50
13	m	1401	CLA	CMC-C2C	-2.21	1.46	1.50
13	B	1234	CLA	C3B-C4B	2.21	1.49	1.42
13	H	1207	CLA	C3B-C4B	2.21	1.49	1.42
13	B	1234	CLA	CHC-C1C	2.21	1.42	1.38
13	s	510	CLA	CHC-C1C	2.21	1.42	1.38
13	2	508	CLA	C3B-C4B	2.21	1.49	1.42
13	b	502	CLA	C3B-C4B	2.21	1.49	1.42
13	T	1302	CLA	CMB-C2B	-2.21	1.46	1.50
13	f	1021	CLA	CMB-C2B	-2.21	1.46	1.50
13	t	519	CLA	CMB-C2B	-2.21	1.46	1.50
13	e	1139	CLA	MG-ND	-2.21	2.01	2.05
13	f	1217	CLA	CMB-C2B	-2.21	1.46	1.50
13	f	1212	CLA	MG-NB	-2.21	2.01	2.05
13	s	508	CLA	MG-NB	-2.21	2.01	2.05
13	v	509	CLA	CHC-C1C	2.21	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1234	CLA	C3B-C4B	2.21	1.49	1.42
13	v	502	CLA	CMD-C2D	-2.21	1.46	1.50
13	f	1207	CLA	C3B-C4B	2.21	1.49	1.42
13	r	505	CLA	C3B-C4B	2.21	1.49	1.42
13	L	1502	CLA	MG-NB	-2.21	2.01	2.05
13	d	512	CLA	CHC-C1C	2.21	1.42	1.38
13	B	1203	CLA	C1B-C2B	2.21	1.48	1.43
13	B	1211	CLA	CMC-C2C	-2.21	1.46	1.50
13	1	508	CLA	CMD-C2D	-2.21	1.46	1.50
13	3	503	CLA	CMD-C2D	-2.21	1.46	1.50
13	m	1103	CLA	CMD-C2D	-2.21	1.46	1.50
13	r	509	CLA	CMB-C2B	-2.21	1.46	1.50
13	t	508	CLA	CMC-C2C	-2.21	1.46	1.50
13	A	1138	CLA	CMB-C2B	-2.21	1.46	1.50
13	G	1138	CLA	CMB-C2B	-2.21	1.46	1.50
13	b	519	CLA	CMD-C2D	-2.21	1.46	1.50
13	B	1239	CLA	MG-NB	-2.21	2.01	2.05
13	Y	501	CLA	C3B-C4B	2.21	1.49	1.42
13	B	1202	CLA	CMC-C2C	-2.21	1.46	1.50
13	6	511	CLA	CMB-C2B	-2.21	1.46	1.50
13	f	1239	CLA	CMD-C2D	-2.21	1.46	1.50
13	t	519	CLA	CMD-C2D	-2.21	1.46	1.50
13	H	1212	CLA	CMB-C2B	-2.21	1.46	1.50
13	H	1236	CLA	CMB-C2B	-2.21	1.46	1.50
13	R	1301	CLA	CMD-C2D	-2.21	1.46	1.50
13	f	1208	CLA	CMD-C2D	-2.21	1.46	1.50
13	f	1235	CLA	CMD-C2D	-2.21	1.46	1.50
13	H	1214	CLA	MG-NB	-2.21	2.01	2.05
13	s	518	CLA	CHC-C1C	2.21	1.42	1.38
13	G	1110	CLA	CMC-C2C	-2.21	1.46	1.50
13	4	509	CLA	C3B-C4B	2.21	1.49	1.42
13	G	1114	CLA	C1B-NB	-2.21	1.35	1.37
13	B	1228	CLA	C1B-C2B	2.21	1.48	1.43
13	A	1138	CLA	CHC-C1C	2.21	1.42	1.38
13	H	1234	CLA	CHC-C1C	2.21	1.42	1.38
13	q	512	CLA	CHC-C1C	2.21	1.42	1.38
13	5	507	CLA	CMD-C2D	-2.21	1.46	1.50
13	G	1113	CLA	CMC-C2C	-2.21	1.46	1.50
13	H	1224	CLA	CMB-C2B	-2.21	1.46	1.50
13	1	502	CLA	MG-NB	-2.21	2.01	2.05
13	5	508	CLA	C3B-C4B	2.21	1.49	1.42
13	r	501	CLA	C3B-C4B	2.21	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1203	CLA	CMD-C2D	-2.21	1.46	1.50
13	2	505	CLA	C3B-C4B	2.21	1.49	1.42
13	6	509	CLA	CHC-C1C	2.21	1.42	1.38
13	G	1111	CLA	CHC-C1C	2.21	1.42	1.38
13	d	509	CLA	CHC-C1C	2.21	1.42	1.38
13	A	1108	CLA	CMD-C2D	-2.21	1.46	1.50
13	5	511	CLA	CMB-C2B	-2.21	1.46	1.50
13	V	1502	CLA	CMC-C2C	-2.21	1.46	1.50
13	c	511	CLA	CMB-C2B	-2.21	1.46	1.50
13	q	511	CLA	MG-NB	-2.21	2.01	2.05
13	s	512	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1118	CLA	CMB-C2B	-2.21	1.46	1.50
13	B	1239	CLA	CMD-C2D	-2.21	1.46	1.50
13	G	1105	CLA	CMB-C2B	-2.21	1.46	1.50
13	s	506	CLA	CMC-C2C	-2.21	1.46	1.50
13	b	505	CLA	C3B-C4B	2.21	1.49	1.42
13	2	506	CLA	MG-NB	-2.21	2.01	2.05
13	f	1239	CLA	MG-NB	-2.21	2.01	2.05
13	a	503	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1105	CLA	CMB-C2B	-2.21	1.46	1.50
13	A	1134	CLA	CMB-C2B	-2.21	1.46	1.50
13	G	1124	CLA	CMB-C2B	-2.21	1.46	1.50
13	v	518	CLA	CMD-C2D	-2.21	1.46	1.50
20	f	1852	SQD	O2-C2	-2.21	1.37	1.43
13	e	1237	CLA	MG-NB	-2.21	2.01	2.05
13	s	504	CLA	MG-NB	-2.21	2.01	2.05
13	a	519	CLA	CHC-C1C	2.21	1.42	1.38
13	e	1111	CLA	CHC-C1C	2.21	1.42	1.38
13	A	1124	CLA	CMB-C2B	-2.21	1.46	1.50
13	a	506	CLA	CMC-C2C	-2.21	1.46	1.50
13	d	511	CLA	CMB-C2B	-2.21	1.46	1.50
13	e	1105	CLA	CMB-C2B	-2.21	1.46	1.50
13	a	504	CLA	MG-NB	-2.21	2.01	2.05
13	B	1202	CLA	C3B-C4B	2.21	1.49	1.42
13	f	1229	CLA	MG-NB	-2.21	2.01	2.05
13	B	1209	CLA	CHC-C1C	2.21	1.42	1.38
13	3	510	CLA	CHC-C1C	2.21	1.42	1.38
13	B	1209	CLA	CMB-C2B	-2.21	1.46	1.50
13	B	1236	CLA	CMB-C2B	-2.21	1.46	1.50
13	4	502	CLA	CMB-C2B	-2.21	1.46	1.50
13	H	1234	CLA	CMC-C2C	-2.21	1.46	1.50
13	t	505	CLA	CMD-C2D	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1134	CLA	CHC-C1C	2.21	1.42	1.38
13	J	1302	CLA	CMD-C2D	-2.21	1.46	1.50
13	H	1239	CLA	CMD-C2D	-2.21	1.46	1.50
13	e	1118	CLA	CMB-C2B	-2.21	1.46	1.50
13	f	1224	CLA	CMB-C2B	-2.21	1.46	1.50
13	R	1302	CLA	C3B-C4B	2.21	1.49	1.42
13	U	1105	CLA	C3B-C4B	2.21	1.49	1.42
13	G	1106	CLA	MG-ND	-2.20	2.01	2.05
13	B	1207	CLA	C3B-C4B	2.20	1.49	1.42
13	F	1302	CLA	C3B-C4B	2.20	1.49	1.42
13	H	1232	CLA	C3B-C4B	2.20	1.49	1.42
13	A	1138	CLA	CMC-C2C	-2.20	1.46	1.50
13	s	519	CLA	CHC-C1C	2.20	1.42	1.38
13	B	1207	CLA	CMB-C2B	-2.20	1.46	1.50
13	F	1301	CLA	CMD-C2D	-2.20	1.46	1.50
13	G	1105	CLA	CMC-C2C	-2.20	1.46	1.50
13	e	1134	CLA	CMD-C2D	-2.20	1.46	1.50
13	f	1201	CLA	CMC-C2C	-2.20	1.46	1.50
13	5	502	CLA	C3B-C4B	2.20	1.49	1.42
13	4	505	CLA	MG-NB	-2.20	2.01	2.05
13	A	1126	CLA	C3B-C4B	2.20	1.49	1.42
13	2	504	CLA	CMD-C2D	-2.20	1.46	1.50
13	a	503	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	506	CLA	CMB-C2B	-2.20	1.46	1.50
17	f	1855	LHG	P-O6	2.20	1.68	1.59
13	H	1203	CLA	C1B-C2B	2.20	1.48	1.43
13	G	1126	CLA	C3B-C4B	2.20	1.49	1.42
13	a	505	CLA	MG-NB	-2.20	2.01	2.05
13	H	1209	CLA	CHC-C1C	2.20	1.42	1.38
13	u	501	CLA	CHC-C1C	2.20	1.42	1.38
13	H	1213	CLA	CMC-C2C	-2.20	1.46	1.50
13	f	1216	CLA	CMD-C2D	-2.20	1.46	1.50
13	e	1123	CLA	C1B-NB	-2.20	1.35	1.37
17	n	5218	LHG	P-O6	2.20	1.68	1.59
13	B	1208	CLA	CMD-C2D	-2.20	1.46	1.50
13	Z	519	CLA	CMB-C2B	-2.20	1.46	1.50
13	e	1134	CLA	CMB-C2B	-2.20	1.46	1.50
13	s	512	CLA	CMB-C2B	-2.20	1.46	1.50
13	H	1202	CLA	C3B-C4B	2.20	1.49	1.42
13	B	1223	CLA	C3B-C4B	2.20	1.49	1.42
13	c	508	CLA	C3B-C4B	2.20	1.49	1.42
13	A	1132	CLA	MG-NB	-2.20	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1222	CLA	MG-NB	-2.20	2.01	2.05
13	H	1214	CLA	CHC-C1C	2.20	1.42	1.38
13	A	1110	CLA	CMB-C2B	-2.20	1.46	1.50
13	1	512	CLA	CMB-C2B	-2.20	1.46	1.50
13	f	1209	CLA	CMB-C2B	-2.20	1.46	1.50
13	3	512	CLA	C3B-C4B	2.20	1.49	1.42
13	b	507	CLA	C3B-C4B	2.20	1.49	1.42
13	H	1222	CLA	MG-NB	-2.20	2.01	2.05
13	A	1116	CLA	CHC-C1C	2.20	1.42	1.38
13	1	512	CLA	CHC-C1C	2.20	1.42	1.38
13	G	1136	CLA	CMD-C2D	-2.20	1.46	1.50
13	4	518	CLA	C3B-C4B	2.20	1.49	1.42
13	e	1138	CLA	CHC-C1C	2.20	1.42	1.38
13	s	503	CLA	CMD-C2D	-2.20	1.46	1.50
13	H	1211	CLA	C3B-C4B	2.20	1.49	1.42
13	l	1302	CLA	C3B-C4B	2.20	1.49	1.42
13	A	1123	CLA	C1B-NB	-2.20	1.35	1.37
13	B	1203	CLA	CMC-C2C	-2.20	1.46	1.50
13	B	1206	CLA	CMC-C2C	-2.20	1.46	1.50
13	e	1124	CLA	CMB-C2B	-2.20	1.46	1.50
13	r	504	CLA	CMD-C2D	-2.20	1.46	1.50
13	d	511	CLA	C3B-C4B	2.20	1.49	1.42
13	G	1140	CLA	CHC-C1C	2.20	1.42	1.38
13	f	1231	CLA	CMC-C2C	-2.20	1.46	1.50
17	V	5218	LHG	P-O6	2.20	1.68	1.59
13	B	1021	CLA	CMB-C2B	-2.20	1.46	1.50
13	2	509	CLA	CMB-C2B	-2.20	1.46	1.50
13	V	1501	CLA	CMC-C2C	-2.20	1.46	1.50
13	e	1136	CLA	CMB-C2B	-2.20	1.46	1.50
13	f	1218	CLA	CMD-C2D	-2.20	1.46	1.50
13	u	502	CLA	CMB-C2B	-2.20	1.46	1.50
13	a	516	CLA	CHC-C1C	2.20	1.42	1.38
13	H	1212	CLA	MG-NB	-2.20	2.01	2.05
13	f	1210	CLA	C4B-NB	2.20	1.40	1.37
13	f	1228	CLA	C1B-C2B	2.20	1.48	1.43
13	s	516	CLA	CHC-C1C	2.20	1.42	1.38
13	Y	510	CLA	MG-NB	-2.20	2.01	2.05
13	Z	507	CLA	MG-NB	-2.20	2.01	2.05
13	b	509	CLA	C3B-C4B	2.20	1.49	1.42
13	e	1132	CLA	CMB-C2B	-2.20	1.46	1.50
13	1	519	CLA	MG-ND	-2.20	2.01	2.05
13	e	1121	CLA	MG-NB	-2.20	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	518	CLA	CMD-C2D	-2.20	1.46	1.50
13	e	1108	CLA	CMD-C2D	-2.20	1.46	1.50
13	e	1138	CLA	CMC-C2C	-2.20	1.46	1.50
13	f	1230	CLA	MG-NB	-2.20	2.01	2.05
13	f	1023	CLA	C4B-NB	2.20	1.40	1.37
13	2	509	CLA	CMC-C2C	-2.20	1.46	1.50
13	a	504	CLA	CHC-C1C	2.20	1.42	1.38
13	A	1139	CLA	MG-ND	-2.20	2.01	2.05
13	2	517	CLA	MG-NB	-2.20	2.01	2.05
13	r	507	CLA	MG-NB	-2.20	2.01	2.05
13	2	517	CLA	CMD-C2D	-2.20	1.46	1.50
13	H	1223	CLA	MG-NB	-2.20	2.01	2.05
13	L	1502	CLA	CMC-C2C	-2.20	1.46	1.50
13	f	1222	CLA	CMC-C2C	-2.20	1.46	1.50
13	r	519	CLA	CMC-C2C	-2.20	1.46	1.50
13	r	508	CLA	C1B-C2B	2.20	1.48	1.43
17	L	5218	LHG	P-O6	2.20	1.68	1.59
13	6	501	CLA	C3B-C4B	2.20	1.49	1.42
17	B	1855	LHG	P-O6	2.20	1.68	1.59
13	f	1203	CLA	C1B-C2B	2.20	1.48	1.43
13	2	518	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	508	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	518	CLA	CMD-C2D	-2.20	1.46	1.50
13	e	1120	CLA	CMD-C2D	-2.20	1.46	1.50
13	s	503	CLA	CHC-C1C	2.20	1.42	1.38
13	f	1023	CLA	MG-ND	-2.20	2.01	2.05
13	H	1213	CLA	C3B-C4B	2.20	1.49	1.42
13	r	508	CLA	C3B-C4B	2.20	1.49	1.42
13	G	1117	CLA	CMD-C2D	-2.19	1.46	1.50
13	Z	517	CLA	CMD-C2D	-2.19	1.46	1.50
17	H	1855	LHG	P-O6	2.19	1.68	1.59
13	A	1132	CLA	CMC-C2C	-2.19	1.46	1.50
13	4	508	CLA	CMD-C2D	-2.19	1.46	1.50
13	q	503	CLA	CMD-C2D	-2.19	1.46	1.50
13	f	1232	CLA	C3B-C4B	2.19	1.49	1.42
13	G	1138	CLA	CHC-C1C	2.19	1.42	1.38
13	3	502	CLA	MG-NB	-2.19	2.01	2.05
13	a	518	CLA	CMD-C2D	-2.19	1.46	1.50
13	5	501	CLA	CHC-C1C	2.19	1.42	1.38
13	A	1130	CLA	MG-NB	-2.19	2.01	2.05
13	1	511	CLA	MG-NB	-2.19	2.01	2.05
13	v	509	CLA	CMD-C2D	-2.19	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	507	CLA	MG-NB	-2.19	2.01	2.05
13	f	1222	CLA	C1B-C2B	2.19	1.48	1.43
13	a	508	CLA	CMD-C2D	-2.19	1.46	1.50
13	d	509	CLA	CMD-C2D	-2.19	1.46	1.50
13	q	507	CLA	CMD-C2D	-2.19	1.46	1.50
13	Z	504	CLA	CMD-C2D	-2.19	1.46	1.50
13	b	502	CLA	CMD-C2D	-2.19	1.46	1.50
13	q	517	CLA	CMD-C2D	-2.19	1.46	1.50
13	t	506	CLA	CMB-C2B	-2.19	1.46	1.50
13	v	512	CLA	CMD-C2D	-2.19	1.46	1.50
13	b	518	CLA	C3B-C4B	2.19	1.49	1.42
13	f	1223	CLA	C3B-C4B	2.19	1.49	1.42
13	G	1111	CLA	CMD-C2D	-2.19	1.46	1.50
13	G	1136	CLA	CMB-C2B	-2.19	1.46	1.50
13	s	518	CLA	CMB-C2B	-2.19	1.46	1.50
13	2	519	CLA	C3B-C4B	2.19	1.49	1.42
13	Y	507	CLA	MG-NB	-2.19	2.01	2.05
13	f	1201	CLA	MG-NB	-2.19	2.01	2.05
13	e	1110	CLA	CMB-C2B	-2.19	1.46	1.50
13	f	1236	CLA	CMB-C2B	-2.19	1.46	1.50
13	t	505	CLA	C3B-C4B	2.19	1.49	1.42
13	u	505	CLA	CHC-C1C	2.19	1.42	1.38
13	f	1222	CLA	MG-NB	-2.19	2.01	2.05
13	t	507	CLA	C3B-C4B	2.19	1.49	1.42
13	b	508	CLA	CMC-C2C	-2.19	1.46	1.50
13	e	1130	CLA	CMC-C2C	-2.19	1.46	1.50
13	V	1502	CLA	MG-NB	-2.19	2.01	2.05
13	m	1105	CLA	C3B-C4B	2.19	1.49	1.42
13	5	512	CLA	CHC-C1C	2.19	1.42	1.38
13	G	1130	CLA	MG-NB	-2.19	2.01	2.05
13	Z	506	CLA	MG-NB	-2.19	2.01	2.05
13	r	517	CLA	MG-NB	-2.19	2.01	2.05
13	u	504	CLA	MG-NB	-2.19	2.01	2.05
13	3	508	CLA	CMD-C2D	-2.19	1.46	1.50
13	3	504	CLA	CHC-C1C	2.19	1.42	1.38
13	f	1214	CLA	CHC-C1C	2.19	1.42	1.38
13	A	1108	CLA	MG-NB	-2.19	2.01	2.05
13	B	1213	CLA	C3B-C4B	2.19	1.49	1.42
13	e	1132	CLA	CMC-C2C	-2.19	1.46	1.50
13	r	517	CLA	CMD-C2D	-2.19	1.46	1.50
13	c	506	CLA	CHC-C1C	2.19	1.42	1.38
13	e	1131	CLA	C3B-C4B	2.19	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	501	CLA	MG-NB	-2.19	2.01	2.05
13	e	1108	CLA	MG-NB	-2.19	2.01	2.05
13	B	1234	CLA	C4B-NB	2.19	1.40	1.37
13	Z	501	CLA	CMB-C2B	-2.19	1.46	1.50
13	e	1126	CLA	C3B-C4B	2.19	1.49	1.42
13	1	513	CLA	CHC-C1C	2.19	1.42	1.38
13	3	511	CLA	CHC-C1C	2.19	1.42	1.38
13	u	519	CLA	MG-NB	-2.19	2.01	2.05
13	2	508	CLA	C1B-C2B	2.19	1.48	1.43
13	H	1221	CLA	CMB-C2B	-2.19	1.46	1.50
13	Y	504	CLA	CMB-C2B	-2.19	1.46	1.50
13	6	517	CLA	CHC-C1C	2.19	1.42	1.38
13	4	507	CLA	C3B-C4B	2.19	1.49	1.42
13	A	1122	CLA	MG-NB	-2.19	2.01	2.05
13	G	1102	CLA	CMB-C2B	-2.19	1.46	1.50
13	q	508	CLA	CMD-C2D	-2.19	1.46	1.50
20	B	1852	SQD	O2-C2	-2.19	1.37	1.43
13	3	505	CLA	MG-NB	-2.19	2.01	2.05
13	f	1213	CLA	C3B-C4B	2.19	1.49	1.42
13	G	1134	CLA	CHC-C1C	2.19	1.42	1.38
13	a	503	CLA	CHC-C1C	2.19	1.42	1.38
13	u	503	CLA	CHC-C1C	2.19	1.42	1.38
13	B	1219	CLA	C3B-C4B	2.19	1.49	1.42
13	3	509	CLA	CMD-C2D	-2.19	1.46	1.50
13	d	512	CLA	CMD-C2D	-2.19	1.46	1.50
13	e	1130	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1131	CLA	C3B-C4B	2.19	1.49	1.42
13	B	1232	CLA	C3B-C4B	2.19	1.49	1.42
13	Z	519	CLA	C3B-C4B	2.19	1.49	1.42
13	q	505	CLA	MG-NB	-2.19	2.01	2.05
13	H	1217	CLA	CMB-C2B	-2.19	1.46	1.50
13	u	506	CLA	CHC-C1C	2.19	1.42	1.38
13	J	1302	CLA	C3B-C4B	2.19	1.49	1.42
13	B	1201	CLA	MG-NB	-2.19	2.01	2.05
13	Y	508	CLA	CMD-C2D	-2.19	1.46	1.50
13	Z	508	CLA	C1B-C2B	2.19	1.48	1.43
13	c	507	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1105	CLA	CMC-C2C	-2.18	1.46	1.50
13	e	1130	CLA	MG-NB	-2.18	2.01	2.05
13	v	512	CLA	MG-NB	-2.18	2.01	2.05
13	B	1211	CLA	C3B-C4B	2.18	1.49	1.42
13	G	1131	CLA	C3B-C4B	2.18	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	518	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	509	CLA	CMD-C2D	-2.18	1.46	1.50
13	d	508	CLA	MG-NB	-2.18	2.01	2.05
13	e	1132	CLA	MG-NB	-2.18	2.01	2.05
13	H	1234	CLA	C4B-NB	2.18	1.40	1.37
13	1	508	CLA	C1B-C2B	2.18	1.48	1.43
13	e	1237	CLA	CMC-C2C	-2.18	1.46	1.50
13	s	508	CLA	CMC-C2C	-2.18	1.46	1.50
13	5	507	CLA	MG-NB	-2.18	2.01	2.05
13	5	511	CLA	MG-NB	-2.18	2.01	2.05
13	H	1229	CLA	MG-NB	-2.18	2.01	2.05
13	b	505	CLA	MG-NB	-2.18	2.01	2.05
13	v	501	CLA	C3B-C4B	2.18	1.49	1.42
13	j	1302	CLA	C3B-C4B	2.18	1.49	1.42
13	A	1130	CLA	CMC-C2C	-2.18	1.46	1.50
13	5	511	CLA	CMD-C2D	-2.18	1.46	1.50
13	G	1102	CLA	CMC-C2C	-2.18	1.46	1.50
13	q	519	CLA	MG-ND	-2.18	2.01	2.05
13	u	512	CLA	CHC-C1C	2.18	1.42	1.38
13	t	512	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	1237	CLA	MG-NB	-2.18	2.01	2.05
13	5	511	CLA	CHC-C1C	2.18	1.42	1.38
13	u	511	CLA	CHC-C1C	2.18	1.42	1.38
13	v	517	CLA	CHC-C1C	2.18	1.42	1.38
13	G	1139	CLA	CMB-C2B	-2.18	1.46	1.50
13	H	1218	CLA	CMD-C2D	-2.18	1.46	1.50
13	e	1131	CLA	CMB-C2B	-2.18	1.46	1.50
13	G	1126	CLA	C1B-C2B	2.18	1.48	1.43
13	t	518	CLA	C3B-C4B	2.18	1.49	1.42
13	2	507	CLA	MG-NB	-2.18	2.01	2.05
13	t	505	CLA	MG-NB	-2.18	2.01	2.05
13	Y	513	CLA	CHC-C1C	2.18	1.42	1.38
13	H	1231	CLA	C4B-NB	2.18	1.40	1.37
13	B	1218	CLA	CMD-C2D	-2.18	1.46	1.50
16	G	4002	BCR	C30-C25	-2.18	1.51	1.53
13	4	512	CLA	CMD-C2D	-2.18	1.46	1.50
13	s	505	CLA	MG-NB	-2.18	2.01	2.05
13	K	1105	CLA	C3B-C4B	2.18	1.49	1.42
13	6	518	CLA	CMD-C2D	-2.18	1.46	1.50
13	e	1105	CLA	CMC-C2C	-2.18	1.46	1.50
13	q	501	CLA	CMB-C2B	-2.18	1.46	1.50
13	s	509	CLA	CMD-C2D	-2.18	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	516	CLA	MG-NB	-2.18	2.01	2.05
13	f	1214	CLA	MG-NB	-2.18	2.01	2.05
13	a	511	CLA	CHC-C1C	2.18	1.42	1.38
13	G	1123	CLA	C1B-NB	-2.18	1.35	1.37
13	B	1222	CLA	CMC-C2C	-2.18	1.46	1.50
13	B	1229	CLA	MG-NB	-2.18	2.01	2.05
13	B	1217	CLA	CMB-C2B	-2.18	1.46	1.50
13	1	501	CLA	CMB-C2B	-2.18	1.46	1.50
13	d	501	CLA	C3B-C4B	2.18	1.49	1.42
13	G	1115	CLA	CMD-C2D	-2.18	1.46	1.50
13	B	1229	CLA	C1B-C2B	2.18	1.48	1.43
13	Y	511	CLA	MG-NB	-2.18	2.01	2.05
13	c	511	CLA	CHC-C1C	2.18	1.42	1.38
13	H	1228	CLA	CMC-C2C	-2.18	1.46	1.50
13	e	1117	CLA	CMD-C2D	-2.18	1.46	1.50
13	e	1801	CLA	CMB-C2B	-2.18	1.46	1.50
13	f	1213	CLA	C1B-NB	-2.18	1.35	1.37
13	B	1240	CLA	C3B-C4B	2.18	1.49	1.42
13	B	1230	CLA	MG-NB	-2.18	2.01	2.05
13	t	511	CLA	MG-NB	-2.18	2.01	2.05
20	H	1852	SQD	O2-C2	-2.18	1.37	1.43
13	6	508	CLA	MG-NB	-2.18	2.01	2.05
13	6	512	CLA	MG-NB	-2.18	2.01	2.05
13	f	1209	CLA	CHC-C1C	2.18	1.42	1.38
13	a	512	CLA	C3B-C4B	2.18	1.49	1.42
13	f	1219	CLA	C3B-C4B	2.18	1.49	1.42
13	G	1130	CLA	CMC-C2C	-2.18	1.46	1.50
13	q	508	CLA	C1B-C2B	2.18	1.48	1.43
13	T	1302	CLA	MG-NB	-2.18	2.01	2.05
13	a	502	CLA	MG-NB	-2.18	2.01	2.05
13	A	1801	CLA	CMB-C2B	-2.18	1.46	1.50
13	4	506	CLA	CMB-C2B	-2.18	1.46	1.50
13	f	1220	CLA	CMB-C2B	-2.18	1.46	1.50
13	c	501	CLA	CHC-C1C	2.18	1.42	1.38
17	V	5221	LHG	P-O6	2.18	1.67	1.59
13	n	1502	CLA	CMC-C2C	-2.18	1.46	1.50
13	s	508	CLA	CMD-C2D	-2.18	1.46	1.50
13	Z	511	CLA	CHC-C1C	2.18	1.42	1.38
13	H	1239	CLA	MG-NB	-2.18	2.01	2.05
13	1	507	CLA	CMD-C2D	-2.18	1.46	1.50
13	d	517	CLA	CHC-C1C	2.18	1.42	1.38
13	H	1229	CLA	C1B-C2B	2.18	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1126	CLA	C1B-C2B	2.18	1.48	1.43
13	G	1103	CLA	CMB-C2B	-2.17	1.46	1.50
13	r	518	CLA	CMB-C2B	-2.17	1.46	1.50
13	H	1219	CLA	C3B-C4B	2.17	1.49	1.42
13	f	1211	CLA	C3B-C4B	2.17	1.49	1.42
13	R	1302	CLA	MG-NB	-2.17	2.01	2.05
13	c	504	CLA	MG-NB	-2.17	2.01	2.05
13	a	510	CLA	CMD-C2D	-2.17	1.46	1.50
13	f	1212	CLA	CMB-C2B	-2.17	1.46	1.50
13	q	517	CLA	CHC-C1C	2.17	1.42	1.38
13	r	519	CLA	C3B-C4B	2.17	1.49	1.42
13	B	1231	CLA	C4B-NB	2.17	1.40	1.37
13	H	1222	CLA	CMB-C2B	-2.17	1.46	1.50
13	b	502	CLA	CMB-C2B	-2.17	1.46	1.50
13	G	1126	CLA	CHC-C1C	2.17	1.42	1.38
13	t	512	CLA	MG-NB	-2.17	2.01	2.05
13	A	1237	CLA	CMC-C2C	-2.17	1.46	1.50
13	r	506	CLA	MG-NB	-2.17	2.01	2.05
13	u	507	CLA	MG-NB	-2.17	2.01	2.05
13	H	1222	CLA	CMC-C2C	-2.17	1.46	1.50
13	d	518	CLA	CMD-C2D	-2.17	1.46	1.50
13	b	501	CLA	CHC-C1C	2.17	1.42	1.38
13	A	1124	CLA	MG-NB	-2.17	2.01	2.05
13	H	1225	CLA	C3B-C4B	2.17	1.49	1.42
13	G	1112	CLA	CMD-C2D	-2.17	1.46	1.50
13	e	1112	CLA	CMD-C2D	-2.17	1.46	1.50
13	t	502	CLA	CMD-C2D	-2.17	1.46	1.50
13	A	1120	CLA	CMB-C2B	-2.17	1.46	1.50
13	3	511	CLA	CMD-C2D	-2.17	1.46	1.50
13	G	1118	CLA	CMB-C2B	-2.17	1.46	1.50
13	Z	509	CLA	CMC-C2C	-2.17	1.46	1.50
13	q	519	CLA	CMD-C2D	-2.17	1.46	1.50
19	f	5002	LMG	O1-C7	-2.17	1.40	1.43
13	r	504	CLA	CHC-C1C	2.17	1.42	1.38
13	c	507	CLA	MG-NB	-2.17	2.01	2.05
13	c	505	CLA	CHC-C1C	2.17	1.42	1.38
13	f	1240	CLA	C3B-C4B	2.17	1.49	1.42
13	G	1124	CLA	MG-NB	-2.17	2.01	2.05
13	u	508	CLA	MG-NB	-2.17	2.01	2.05
13	A	1117	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	1212	CLA	CMB-C2B	-2.17	1.46	1.50
13	5	506	CLA	CHC-C1C	2.17	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	512	CLA	CHC-C1C	2.17	1.42	1.38
13	G	1112	CLA	MG-NB	-2.17	2.01	2.05
13	K	1401	CLA	CMC-C2C	-2.17	1.46	1.50
13	A	1116	CLA	C3B-C4B	2.17	1.49	1.42
13	f	1231	CLA	C4B-NB	2.17	1.40	1.37
13	3	503	CLA	CHC-C1C	2.17	1.42	1.38
13	2	519	CLA	CMB-C2B	-2.17	1.46	1.50
13	1	505	CLA	MG-NB	-2.17	2.01	2.05
13	G	1124	CLA	CHC-C1C	2.17	1.42	1.38
13	6	509	CLA	CMD-C2D	-2.17	1.46	1.50
13	e	1124	CLA	CHC-C1C	2.17	1.42	1.38
13	2	519	CLA	CMC-C2C	-2.17	1.46	1.50
13	r	518	CLA	CMD-C2D	-2.17	1.46	1.50
13	G	1108	CLA	MG-NB	-2.17	2.01	2.05
13	q	513	CLA	CHC-C1C	2.17	1.42	1.38
13	3	505	CLA	C3B-C4B	2.17	1.49	1.42
13	1	504	CLA	MG-NB	-2.17	2.01	2.05
13	Y	502	CLA	MG-NB	-2.17	2.01	2.05
13	c	502	CLA	CHC-C1C	2.17	1.42	1.38
13	B	1229	CLA	C1B-NB	-2.17	1.35	1.37
13	5	501	CLA	CMC-C2C	-2.17	1.46	1.50
13	Z	519	CLA	CMC-C2C	-2.17	1.46	1.50
13	a	508	CLA	CMC-C2C	-2.17	1.46	1.50
13	H	1229	CLA	CMD-C2D	-2.17	1.46	1.50
13	l	1302	CLA	CMD-C2D	-2.17	1.46	1.50
13	J	1302	CLA	MG-NB	-2.17	2.01	2.05
13	d	519	CLA	MG-NB	-2.17	2.01	2.05
13	f	1225	CLA	C3B-C4B	2.17	1.49	1.42
13	v	518	CLA	MG-NB	-2.17	2.01	2.05
13	4	501	CLA	CHC-C1C	2.17	1.42	1.38
13	A	1115	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	1228	CLA	CMC-C2C	-2.17	1.46	1.50
13	c	518	CLA	CMB-C2B	-2.17	1.46	1.50
13	l	1302	CLA	MG-NB	-2.17	2.01	2.05
13	a	505	CLA	C3B-C4B	2.17	1.49	1.42
13	B	1023	CLA	C4B-NB	2.17	1.40	1.37
13	Z	509	CLA	CMD-C2D	-2.17	1.46	1.50
13	u	502	CLA	CMD-C2D	-2.17	1.46	1.50
13	H	1201	CLA	MG-NB	-2.17	2.01	2.05
13	A	1114	CLA	CMD-C2D	-2.17	1.46	1.50
13	H	1208	CLA	CMD-C2D	-2.17	1.46	1.50
13	Y	501	CLA	CMB-C2B	-2.17	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	513	CLA	CMB-C2B	-2.17	1.46	1.50
13	e	1102	CLA	CMC-C2C	-2.17	1.46	1.50
13	r	519	CLA	CMB-C2B	-2.17	1.46	1.50
16	A	4002	BCR	C30-C25	-2.16	1.51	1.53
13	G	1125	CLA	CHC-C1C	2.16	1.42	1.38
13	B	1222	CLA	C1B-C2B	2.16	1.48	1.43
19	f	5002	LMG	O7-C8	-2.16	1.41	1.46
13	G	1115	CLA	CMB-C2B	-2.16	1.46	1.50
13	c	512	CLA	CMB-C2B	-2.16	1.46	1.50
13	e	1139	CLA	CMB-C2B	-2.16	1.46	1.50
13	A	1124	CLA	CHC-C1C	2.16	1.42	1.38
13	G	1114	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1116	CLA	C3B-C4B	2.16	1.49	1.42
13	4	503	CLA	CHC-C1C	2.16	1.42	1.38
13	t	511	CLA	CHC-C1C	2.16	1.42	1.38
13	c	508	CLA	MG-NB	-2.16	2.01	2.05
13	B	1214	CLA	CHC-C1C	2.16	1.42	1.38
13	s	511	CLA	CHC-C1C	2.16	1.42	1.38
13	B	1227	CLA	CMD-C2D	-2.16	1.46	1.50
13	U	1105	CLA	CMB-C2B	-2.16	1.46	1.50
13	u	518	CLA	CMB-C2B	-2.16	1.46	1.50
13	c	511	CLA	MG-NB	-2.16	2.01	2.05
13	V	1503	CLA	CHC-C1C	2.16	1.42	1.38
13	e	1140	CLA	CHC-C1C	2.16	1.42	1.38
13	f	1228	CLA	CMC-C2C	-2.16	1.46	1.50
13	1	501	CLA	MG-NB	-2.16	2.01	2.05
13	4	511	CLA	MG-NB	-2.16	2.01	2.05
13	v	508	CLA	MG-NB	-2.16	2.01	2.05
13	B	1220	CLA	CMB-C2B	-2.16	1.46	1.50
13	2	513	CLA	CMB-C2B	-2.16	1.46	1.50
13	3	508	CLA	CMC-C2C	-2.16	1.46	1.50
13	a	507	CLA	CMD-C2D	-2.16	1.46	1.50
13	s	518	CLA	CMD-C2D	-2.16	1.46	1.50
13	s	504	CLA	CHC-C1C	2.16	1.42	1.38
17	n	5221	LHG	P-O6	2.16	1.67	1.59
13	A	1126	CLA	C1B-C2B	2.16	1.48	1.43
13	A	1112	CLA	CMD-C2D	-2.16	1.46	1.50
13	b	512	CLA	CMD-C2D	-2.16	1.46	1.50
13	c	501	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	1115	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	1108	CLA	C3B-C4B	2.16	1.49	1.42
13	e	1105	CLA	MG-NB	-2.16	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	504	CLA	CHC-C1C	2.16	1.42	1.38
13	3	518	CLA	CMB-C2B	-2.16	1.46	1.50
13	G	1139	CLA	MG-ND	-2.16	2.01	2.05
13	u	511	CLA	MG-NB	-2.16	2.01	2.05
13	A	1102	CLA	CMC-C2C	-2.16	1.46	1.50
13	4	502	CLA	CMD-C2D	-2.16	1.46	1.50
19	B	5002	LMG	O1-C7	-2.16	1.40	1.43
19	H	5002	LMG	O1-C7	-2.16	1.40	1.43
13	H	1218	CLA	CMB-C2B	-2.16	1.46	1.50
13	2	511	CLA	CHC-C1C	2.16	1.42	1.38
13	A	1120	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1237	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	1114	CLA	CMD-C2D	-2.16	1.46	1.50
13	B	1210	CLA	C4B-NB	2.16	1.40	1.37
16	k	4018	BCR	C1-C6	-2.16	1.51	1.53
13	Y	507	CLA	CMD-C2D	-2.16	1.46	1.50
13	Z	509	CLA	CMB-C2B	-2.16	1.46	1.50
13	r	501	CLA	CMB-C2B	-2.16	1.46	1.50
13	u	512	CLA	CMD-C2D	-2.16	1.46	1.50
13	c	511	CLA	CMD-C2D	-2.16	1.46	1.50
13	f	1222	CLA	CMB-C2B	-2.16	1.46	1.50
13	H	1240	CLA	C3B-C4B	2.16	1.49	1.42
13	e	1116	CLA	C3B-C4B	2.16	1.49	1.42
17	L	5221	LHG	P-O6	2.16	1.67	1.59
13	q	501	CLA	MG-NB	-2.16	2.01	2.05
13	r	510	CLA	MG-NB	-2.16	2.01	2.05
13	2	508	CLA	CMD-C2D	-2.16	1.46	1.50
13	u	508	CLA	CMD-C2D	-2.16	1.46	1.50
13	f	1218	CLA	MG-NB	-2.16	2.01	2.05
13	2	509	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	1801	CLA	CMB-C2B	-2.16	1.46	1.50
13	A	1139	CLA	CMB-C2B	-2.16	1.46	1.50
13	5	508	CLA	CMC-C2C	-2.16	1.46	1.50
13	f	1227	CLA	CMC-C2C	-2.16	1.46	1.50
13	A	1140	CLA	CHC-C1C	2.16	1.42	1.38
13	v	517	CLA	MG-NB	-2.16	2.01	2.05
13	B	1222	CLA	CMB-C2B	-2.16	1.46	1.50
13	6	512	CLA	CMD-C2D	-2.16	1.46	1.50
13	H	1204	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	1108	CLA	CHC-C1C	2.16	1.42	1.38
13	c	512	CLA	CMD-C2D	-2.16	1.46	1.50
13	u	501	CLA	CMC-C2C	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	503	CLA	CHC-C1C	2.16	1.42	1.38
13	A	1130	CLA	CMD-C2D	-2.16	1.46	1.50
13	f	1012	CLA	CMB-C2B	-2.16	1.46	1.50
13	q	516	CLA	CMD-C2D	-2.16	1.46	1.50
13	B	1012	CLA	CMB-C2B	-2.16	1.46	1.50
13	H	1222	CLA	CMD-C2D	-2.16	1.46	1.50
13	q	504	CLA	CMB-C2B	-2.16	1.46	1.50
13	e	1115	CLA	MG-NB	-2.16	2.01	2.05
13	A	1103	CLA	CMB-C2B	-2.15	1.46	1.50
13	A	1136	CLA	CMB-C2B	-2.15	1.46	1.50
13	2	501	CLA	CMB-C2B	-2.15	1.46	1.50
13	5	508	CLA	CMD-C2D	-2.15	1.46	1.50
13	e	1121	CLA	CMC-C2C	-2.15	1.46	1.50
13	6	518	CLA	MG-NB	-2.15	2.01	2.05
13	b	511	CLA	MG-NB	-2.15	2.01	2.05
13	H	1238	CLA	C3B-C4B	2.15	1.49	1.42
13	B	1232	CLA	C1B-NB	-2.15	1.35	1.37
13	G	1107	CLA	MG-ND	-2.15	2.01	2.05
13	H	1230	CLA	MG-NB	-2.15	2.01	2.05
13	r	511	CLA	CHC-C1C	2.15	1.42	1.38
13	G	1108	CLA	C3B-C4B	2.15	1.49	1.42
13	L	1501	CLA	CMC-C2C	-2.15	1.46	1.50
13	5	508	CLA	MG-NB	-2.15	2.01	2.05
13	e	1112	CLA	MG-NB	-2.15	2.01	2.05
13	1	517	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1213	CLA	C1B-NB	-2.15	1.35	1.37
13	6	508	CLA	CMD-C2D	-2.15	1.46	1.50
13	m	1105	CLA	CMB-C2B	-2.15	1.46	1.50
13	e	1124	CLA	MG-NB	-2.15	2.01	2.05
13	b	511	CLA	CHC-C1C	2.15	1.42	1.38
13	s	505	CLA	C3B-C4B	2.15	1.49	1.42
13	K	1105	CLA	CMB-C2B	-2.15	1.46	1.50
13	H	1227	CLA	CMC-C2C	-2.15	1.46	1.50
13	A	1101	CLA	MG-NB	-2.15	2.01	2.05
13	2	519	CLA	MG-NB	-2.15	2.01	2.05
13	e	1126	CLA	CHC-C1C	2.15	1.42	1.38
13	Z	512	CLA	CMB-C2B	-2.15	1.46	1.50
13	c	502	CLA	CMD-C2D	-2.15	1.46	1.50
13	t	507	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	1112	CLA	MG-NB	-2.15	2.01	2.05
13	q	504	CLA	MG-NB	-2.15	2.01	2.05
13	f	1240	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)
13	s	510	CLA	CMD-C2D	-2.15	1.46	1.50
13	u	508	CLA	CMC-C2C	-2.15	1.46	1.50
13	J	1303	CLA	CMC-C2C	-2.15	1.46	1.50
13	Y	519	CLA	CMD-C2D	-2.15	1.46	1.50
13	Z	506	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1225	CLA	C3B-C4B	2.15	1.49	1.42
13	B	1204	CLA	CMC-C2C	-2.15	1.46	1.50
13	H	1207	CLA	MG-NB	-2.15	2.01	2.05
13	d	518	CLA	MG-NB	-2.15	2.01	2.05
13	A	1126	CLA	CHC-C1C	2.15	1.42	1.38
13	5	503	CLA	CHC-C1C	2.15	1.42	1.38
13	5	502	CLA	CMD-C2D	-2.15	1.46	1.50
13	d	502	CLA	MG-NB	-2.15	2.01	2.05
13	r	506	CLA	CHC-C1C	2.15	1.42	1.38
13	2	517	CLA	C3B-C4B	2.15	1.49	1.42
13	B	1234	CLA	CMB-C2B	-2.15	1.46	1.50
13	3	507	CLA	CMD-C2D	-2.15	1.46	1.50
13	v	502	CLA	C3B-C4B	2.15	1.49	1.42
13	f	1205	CLA	MG-ND	-2.15	2.01	2.05
13	3	517	CLA	CHC-C1C	2.15	1.42	1.38
13	H	1012	CLA	CMB-C2B	-2.15	1.46	1.50
13	Y	517	CLA	CHC-C1C	2.15	1.42	1.38
13	t	501	CLA	CHC-C1C	2.15	1.42	1.38
20	a	822	SQD	O2-C2	-2.15	1.37	1.43
13	u	519	CLA	CMC-C2C	-2.15	1.46	1.50
13	v	508	CLA	CMC-C2C	-2.15	1.46	1.50
13	e	1108	CLA	C3B-C4B	2.15	1.49	1.42
13	f	1229	CLA	CMD-C2D	-2.15	1.46	1.50
13	r	508	CLA	CMD-C2D	-2.15	1.46	1.50
13	2	518	CLA	CHC-C1C	2.15	1.42	1.38
13	5	504	CLA	MG-NB	-2.15	2.01	2.05
13	2	518	CLA	CMB-C2B	-2.15	1.46	1.50
13	s	501	CLA	CMC-C2C	-2.15	1.46	1.50
13	H	1213	CLA	C1B-NB	-2.15	1.35	1.37
13	U	1401	CLA	CMC-C2C	-2.15	1.46	1.50
17	e	5003	LHG	O7-C5	-2.15	1.41	1.46
13	b	503	CLA	CHC-C1C	2.15	1.42	1.38
13	G	1106	CLA	C1B-C2B	2.15	1.48	1.43
13	Z	518	CLA	MG-NB	-2.15	2.01	2.05
13	Z	517	CLA	C3B-C4B	2.15	1.49	1.42
13	H	1229	CLA	C1B-NB	-2.15	1.35	1.37
13	f	1023	CLA	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)
13	B	1227	CLA	CMC-C2C	-2.15	1.46	1.50
13	G	1120	CLA	CMB-C2B	-2.15	1.46	1.50
13	H	1234	CLA	CMB-C2B	-2.15	1.46	1.50
17	A	5003	LHG	O7-C5	-2.15	1.41	1.46
13	4	511	CLA	CHC-C1C	2.15	1.42	1.38
13	A	1105	CLA	MG-NB	-2.15	2.01	2.05
13	G	1115	CLA	MG-NB	-2.15	2.01	2.05
13	f	1210	CLA	CMB-C2B	-2.15	1.46	1.50
13	1	519	CLA	CMD-C2D	-2.15	1.46	1.50
13	3	517	CLA	CMD-C2D	-2.15	1.46	1.50
13	f	1204	CLA	CMD-C2D	-2.15	1.46	1.50
13	t	503	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1208	CLA	MG-NB	-2.15	2.01	2.05
13	H	1218	CLA	MG-NB	-2.15	2.01	2.05
13	Y	505	CLA	MG-NB	-2.15	2.01	2.05
13	H	1232	CLA	C1B-NB	-2.15	1.35	1.37
13	e	1115	CLA	CMB-C2B	-2.15	1.46	1.50
13	n	1501	CLA	CMC-C2C	-2.15	1.46	1.50
13	t	509	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	1238	CLA	C3B-C4B	2.15	1.49	1.42
13	1	502	CLA	C3B-C4B	2.15	1.49	1.42
13	a	501	CLA	C3B-C4B	2.15	1.49	1.42
13	5	505	CLA	CHC-C1C	2.14	1.42	1.38
13	6	502	CLA	C3B-C4B	2.14	1.49	1.42
13	B	1204	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	1218	CLA	CMB-C2B	-2.14	1.46	1.50
13	v	508	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	1207	CLA	MG-NB	-2.14	2.01	2.05
13	Z	505	CLA	MG-NB	-2.14	2.01	2.05
13	e	1110	CLA	MG-NB	-2.14	2.01	2.05
13	A	1117	CLA	C1B-C2B	2.14	1.48	1.43
13	L	1503	CLA	CMC-C2C	-2.14	1.46	1.50
13	2	512	CLA	CMB-C2B	-2.14	1.46	1.50
13	f	1221	CLA	CMC-C2C	-2.14	1.46	1.50
13	c	504	CLA	CHC-C1C	2.14	1.42	1.38
13	s	517	CLA	CHC-C1C	2.14	1.42	1.38
13	A	1112	CLA	CMB-C2B	-2.14	1.46	1.50
13	B	1229	CLA	CMD-C2D	-2.14	1.46	1.50
13	3	510	CLA	CMD-C2D	-2.14	1.46	1.50
13	H	1227	CLA	CMD-C2D	-2.14	1.46	1.50
13	Z	504	CLA	CMB-C2B	-2.14	1.46	1.50
13	d	508	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)
13	f	1215	CLA	CMD-C2D	-2.14	1.46	1.50
13	s	501	CLA	C3B-C4B	2.14	1.49	1.42
13	b	517	CLA	CHC-C1C	2.14	1.42	1.38
13	A	1110	CLA	MG-NB	-2.14	2.01	2.05
13	2	505	CLA	MG-NB	-2.14	2.01	2.05
13	v	519	CLA	MG-NB	-2.14	2.01	2.05
13	n	1503	CLA	CMC-C2C	-2.14	1.46	1.50
13	r	519	CLA	MG-NB	-2.14	2.01	2.05
13	G	1121	CLA	CMC-C2C	-2.14	1.46	1.50
13	s	502	CLA	C3B-C4B	2.14	1.49	1.42
13	B	1213	CLA	CHC-C1C	2.14	1.42	1.38
13	d	512	CLA	MG-NB	-2.14	2.01	2.05
13	K	1401	CLA	CMD-C2D	-2.14	1.46	1.50
13	H	1220	CLA	CMB-C2B	-2.14	1.46	1.50
13	V	1501	CLA	CMD-C2D	-2.14	1.46	1.50
13	c	508	CLA	CMC-C2C	-2.14	1.46	1.50
13	f	1204	CLA	CMC-C2C	-2.14	1.46	1.50
13	v	506	CLA	CMB-C2B	-2.14	1.46	1.50
13	H	1023	CLA	C4B-NB	2.14	1.40	1.37
13	G	1022	CLA	C1B-C2B	2.14	1.48	1.43
13	B	1208	CLA	CMB-C2B	-2.14	1.46	1.50
13	c	509	CLA	CMD-C2D	-2.14	1.46	1.50
13	e	1112	CLA	CMB-C2B	-2.14	1.46	1.50
13	H	1222	CLA	C1B-C2B	2.14	1.48	1.43
13	B	1222	CLA	CMD-C2D	-2.14	1.46	1.50
13	f	1224	CLA	MG-NB	-2.14	2.01	2.05
13	H	1207	CLA	CHC-C1C	2.14	1.42	1.38
13	A	1102	CLA	CMB-C2B	-2.14	1.46	1.50
13	5	512	CLA	CMD-C2D	-2.14	1.46	1.50
13	5	518	CLA	CMB-C2B	-2.14	1.46	1.50
13	c	513	CLA	CMB-C2B	-2.14	1.46	1.50
13	f	1236	CLA	CMD-C2D	-2.14	1.46	1.50
13	3	502	CLA	C3B-C4B	2.14	1.49	1.42
13	2	511	CLA	CMD-C2D	-2.14	1.46	1.50
13	T	1303	CLA	CMC-C2C	-2.14	1.46	1.50
13	f	1227	CLA	CMD-C2D	-2.14	1.46	1.50
13	6	517	CLA	MG-NB	-2.14	2.01	2.05
13	c	508	CLA	CMD-C2D	-2.14	1.46	1.50
13	c	517	CLA	CMD-C2D	-2.14	1.46	1.50
13	s	511	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	1107	CLA	MG-ND	-2.14	2.01	2.05
13	B	1218	CLA	MG-NB	-2.14	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	504	CLA	MG-NB	-2.14	2.01	2.05
13	d	502	CLA	C3B-C4B	2.14	1.49	1.42
13	A	1121	CLA	CMC-C2C	-2.14	1.46	1.50
13	5	519	CLA	CMC-C2C	-2.14	1.46	1.50
13	c	519	CLA	CMC-C2C	-2.14	1.46	1.50
13	s	509	CLA	CMB-C2B	-2.14	1.46	1.50
13	v	507	CLA	C3B-C4B	2.14	1.49	1.42
13	s	508	CLA	C1B-C2B	2.14	1.48	1.43
13	G	1104	CLA	CMB-C2B	-2.14	1.46	1.50
13	a	511	CLA	CMD-C2D	-2.14	1.46	1.50
13	f	1232	CLA	CMC-C2C	-2.14	1.46	1.50
13	e	1107	CLA	MG-ND	-2.14	2.01	2.05
13	G	1111	CLA	CMB-C2B	-2.14	1.46	1.50
13	G	1112	CLA	CMB-C2B	-2.14	1.46	1.50
13	V	1503	CLA	CMC-C2C	-2.14	1.46	1.50
13	r	513	CLA	CMB-C2B	-2.14	1.46	1.50
13	q	502	CLA	C3B-C4B	2.14	1.49	1.42
14	G	2001	PQN	C10-C1	-2.14	1.44	1.48
13	t	508	CLA	C1B-C2B	2.14	1.48	1.43
13	1	504	CLA	CMB-C2B	-2.14	1.46	1.50
13	c	509	CLA	CMC-C2C	-2.14	1.46	1.50
13	e	1103	CLA	CMB-C2B	-2.14	1.46	1.50
13	n	1501	CLA	C3B-C4B	2.14	1.49	1.42
13	A	1115	CLA	CMB-C2B	-2.14	1.46	1.50
13	f	1214	CLA	CMD-C2D	-2.14	1.46	1.50
13	Z	519	CLA	MG-NB	-2.14	2.01	2.05
13	f	1207	CLA	MG-NB	-2.14	2.01	2.05
13	r	505	CLA	MG-NB	-2.14	2.01	2.05
13	A	1106	CLA	C1B-C2B	2.14	1.48	1.43
13	L	1501	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	1108	CLA	CHC-C1C	2.14	1.42	1.38
13	v	505	CLA	CHC-C1C	2.14	1.42	1.38
13	G	1237	CLA	MG-NB	-2.14	2.01	2.05
13	H	1208	CLA	MG-NB	-2.14	2.01	2.05
13	Y	513	CLA	MG-NB	-2.14	2.01	2.05
13	A	1107	CLA	C1B-C2B	2.14	1.48	1.43
13	A	1022	CLA	C1B-C2B	2.14	1.48	1.43
13	L	1501	CLA	C3B-C4B	2.14	1.49	1.42
13	B	1210	CLA	CMB-C2B	-2.14	1.46	1.50
13	e	1104	CLA	CMB-C2B	-2.14	1.46	1.50
20	3	822	SQD	O2-C2	-2.14	1.37	1.43
13	H	1204	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)
13	r	512	CLA	CMB-C2B	-2.14	1.46	1.50
13	Z	510	CLA	MG-NB	-2.14	2.01	2.05
13	B	1240	CLA	CMB-C2B	-2.13	1.46	1.50
13	f	1226	CLA	CMC-C2C	-2.13	1.46	1.50
13	q	507	CLA	CMB-C2B	-2.13	1.46	1.50
13	r	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	f	1202	CLA	MG-NB	-2.13	2.01	2.05
13	3	501	CLA	C3B-C4B	2.13	1.49	1.42
13	H	1208	CLA	CMB-C2B	-2.13	1.46	1.50
13	5	504	CLA	CHC-C1C	2.13	1.42	1.38
13	3	506	CLA	MG-NB	-2.13	2.01	2.05
13	H	1216	CLA	C3B-C4B	2.13	1.49	1.42
13	V	1501	CLA	C3B-C4B	2.13	1.49	1.42
13	U	1401	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	1801	CLA	C1B-NB	-2.13	1.35	1.37
13	s	507	CLA	MG-NB	-2.13	2.01	2.05
13	e	1107	CLA	C1B-C2B	2.13	1.48	1.43
13	f	1238	CLA	C3B-C4B	2.13	1.49	1.42
13	Z	508	CLA	CMD-C2D	-2.13	1.46	1.50
13	e	1117	CLA	C1B-C2B	2.13	1.48	1.43
13	Z	516	CLA	CMD-C2D	-2.13	1.46	1.50
13	5	506	CLA	MG-NB	-2.13	2.01	2.05
13	5	513	CLA	CMB-C2B	-2.13	1.46	1.50
13	G	1120	CLA	CMD-C2D	-2.13	1.46	1.50
13	l	1303	CLA	CMC-C2C	-2.13	1.46	1.50
13	q	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	f	1203	CLA	CHC-C1C	2.13	1.42	1.38
13	v	501	CLA	CHC-C1C	2.13	1.42	1.38
13	B	1221	CLA	CMC-C2C	-2.13	1.46	1.50
13	5	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	519	CLA	CMC-C2C	-2.13	1.46	1.50
13	u	504	CLA	CMB-C2B	-2.13	1.46	1.50
13	5	502	CLA	CHC-C1C	2.13	1.42	1.38
13	F	1302	CLA	MG-NB	-2.13	2.01	2.05
13	H	1210	CLA	MG-NB	-2.13	2.01	2.05
13	u	518	CLA	MG-NB	-2.13	2.01	2.05
13	v	509	CLA	MG-NB	-2.13	2.01	2.05
13	f	1234	CLA	C4B-NB	2.13	1.40	1.37
13	3	517	CLA	CMC-C2C	-2.13	1.46	1.50
13	G	1107	CLA	CMC-C2C	-2.13	1.46	1.50
13	b	518	CLA	CMB-C2B	-2.13	1.46	1.50
13	5	516	CLA	CHC-C1C	2.13	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	v	503	CLA	CHC-C1C	2.13	1.42	1.38
16	e	4002	BCR	C30-C25	-2.13	1.51	1.53
13	H	1202	CLA	MG-NB	-2.13	2.01	2.05
13	e	1131	CLA	MG-NB	-2.13	2.01	2.05
13	f	1236	CLA	MG-NB	-2.13	2.01	2.05
13	q	517	CLA	MG-NB	-2.13	2.01	2.05
13	B	1236	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	1125	CLA	CHC-C1C	2.13	1.42	1.38
13	L	1503	CLA	CHC-C1C	2.13	1.42	1.38
13	A	1113	CLA	MG-NB	-2.13	2.01	2.05
13	d	504	CLA	MG-NB	-2.13	2.01	2.05
13	j	1302	CLA	MG-NB	-2.13	2.01	2.05
13	Z	518	CLA	CHC-C1C	2.13	1.42	1.38
13	e	1022	CLA	C1B-C2B	2.13	1.48	1.43
13	2	510	CLA	MG-NB	-2.13	2.01	2.05
13	A	1107	CLA	CMC-C2C	-2.13	1.46	1.50
13	4	507	CLA	CMD-C2D	-2.13	1.46	1.50
13	6	511	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	1130	CLA	CMD-C2D	-2.13	1.46	1.50
13	s	507	CLA	CMD-C2D	-2.13	1.46	1.50
13	s	517	CLA	CMC-C2C	-2.13	1.46	1.50
13	v	511	CLA	CMD-C2D	-2.13	1.46	1.50
13	6	519	CLA	MG-NB	-2.13	2.01	2.05
13	v	501	CLA	MG-NB	-2.13	2.01	2.05
13	v	519	CLA	CMC-C2C	-2.13	1.46	1.50
13	d	507	CLA	C3B-C4B	2.13	1.48	1.42
13	2	501	CLA	CHC-C1C	2.13	1.42	1.38
13	c	517	CLA	CHC-C1C	2.13	1.42	1.38
13	B	1204	CLA	MG-ND	-2.13	2.01	2.05
13	2	516	CLA	MG-NB	-2.13	2.01	2.05
13	f	1208	CLA	CMB-C2B	-2.13	1.46	1.50
13	Y	502	CLA	C3B-C4B	2.13	1.48	1.42
13	5	502	CLA	MG-NB	-2.13	2.01	2.05
13	G	1113	CLA	MG-NB	-2.13	2.01	2.05
13	t	507	CLA	MG-NB	-2.13	2.01	2.05
13	A	1111	CLA	CMB-C2B	-2.13	1.46	1.50
13	a	517	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	1117	CLA	C1B-C2B	2.13	1.48	1.43
13	Z	501	CLA	CHC-C1C	2.13	1.42	1.38
13	b	518	CLA	CHC-C1C	2.13	1.42	1.38
13	q	509	CLA	CHC-C1C	2.13	1.42	1.38
13	u	502	CLA	CHC-C1C	2.13	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1210	CLA	MG-NB	-2.13	2.01	2.05
13	3	501	CLA	CMC-C2C	-2.13	1.46	1.50
13	2	518	CLA	MG-NB	-2.13	2.01	2.05
13	a	513	CLA	MG-NB	-2.13	2.01	2.05
13	d	511	CLA	MG-NB	-2.13	2.01	2.05
13	2	510	CLA	CMD-C2D	-2.13	1.46	1.50
13	4	517	CLA	CHC-C1C	2.13	1.42	1.38
13	B	1214	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	1226	CLA	CMC-C2C	-2.13	1.46	1.50
13	B	1232	CLA	CMD-C2D	-2.13	1.46	1.50
17	G	5003	LHG	O7-C5	-2.13	1.41	1.46
13	6	505	CLA	CHC-C1C	2.13	1.42	1.38
13	t	517	CLA	CHC-C1C	2.13	1.42	1.38
13	A	1115	CLA	MG-NB	-2.13	2.01	2.05
13	a	506	CLA	MG-NB	-2.13	2.01	2.05
13	6	507	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	1216	CLA	C3B-C4B	2.13	1.48	1.42
13	A	1131	CLA	MG-NB	-2.13	2.01	2.05
13	H	1221	CLA	CMC-C2C	-2.13	1.46	1.50
13	m	1401	CLA	CMD-C2D	-2.13	1.46	1.50
13	q	504	CLA	CMC-C2C	-2.13	1.46	1.50
13	r	518	CLA	MG-NB	-2.13	2.01	2.05
13	4	508	CLA	C3B-C4B	2.13	1.48	1.42
13	f	1216	CLA	C3B-C4B	2.13	1.48	1.42
13	q	504	CLA	CHC-C1C	2.13	1.42	1.38
13	n	1503	CLA	C3B-C4B	2.13	1.48	1.42
13	3	504	CLA	CMB-C2B	-2.13	1.46	1.50
13	H	1232	CLA	CMD-C2D	-2.13	1.46	1.50
13	f	1222	CLA	CMD-C2D	-2.13	1.46	1.50
13	u	512	CLA	CMB-C2B	-2.13	1.46	1.50
13	v	502	CLA	MG-NB	-2.13	2.01	2.05
13	2	517	CLA	CHC-C1C	2.12	1.42	1.38
13	e	1101	CLA	CHC-C1C	2.12	1.42	1.38
13	u	504	CLA	CHC-C1C	2.12	1.42	1.38
13	H	1210	CLA	CMB-C2B	-2.12	1.46	1.50
13	s	519	CLA	CMC-C2C	-2.12	1.46	1.50
13	u	517	CLA	CMD-C2D	-2.12	1.46	1.50
13	3	508	CLA	C1B-C2B	2.12	1.48	1.43
20	s	822	SQD	O2-C2	-2.12	1.37	1.43
13	6	518	CLA	CMB-C2B	-2.12	1.46	1.50
13	u	513	CLA	CMB-C2B	-2.12	1.46	1.50
13	G	1013	CLA	MG-ND	-2.12	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	507	CLA	MG-NB	-2.12	2.01	2.05
13	6	507	CLA	C3B-C4B	2.12	1.48	1.42
13	G	1105	CLA	C3B-C4B	2.12	1.48	1.42
13	3	519	CLA	CMC-C2C	-2.12	1.46	1.50
13	a	517	CLA	CMC-C2C	-2.12	1.46	1.50
13	c	516	CLA	CMD-C2D	-2.12	1.46	1.50
13	H	1210	CLA	C4B-NB	2.12	1.40	1.37
13	G	1801	CLA	C3B-C4B	2.12	1.48	1.42
13	6	504	CLA	MG-NB	-2.12	2.01	2.05
13	f	1203	CLA	MG-ND	-2.12	2.01	2.05
13	4	518	CLA	CHC-C1C	2.12	1.42	1.38
13	d	505	CLA	CHC-C1C	2.12	1.42	1.38
13	q	509	CLA	CMB-C2B	-2.12	1.46	1.50
13	V	1501	CLA	MG-NB	-2.12	2.01	2.05
13	Y	504	CLA	CHC-C1C	2.12	1.42	1.38
13	5	509	CLA	CMC-C2C	-2.12	1.46	1.50
13	5	512	CLA	CMB-C2B	-2.12	1.46	1.50
13	H	1214	CLA	CMD-C2D	-2.12	1.46	1.50
13	H	1220	CLA	CMD-C2D	-2.12	1.46	1.50
13	f	1229	CLA	CMC-C2C	-2.12	1.46	1.50
13	q	516	CLA	MG-NB	-2.12	2.01	2.05
13	B	1232	CLA	CHC-C1C	2.12	1.42	1.38
13	6	503	CLA	CHC-C1C	2.12	1.42	1.38
13	Z	504	CLA	CHC-C1C	2.12	1.42	1.38
20	2	822	SQD	O2-C2	-2.12	1.37	1.43
13	a	518	CLA	CMC-C2C	-2.12	1.46	1.50
13	e	1102	CLA	CMB-C2B	-2.12	1.46	1.50
13	A	1013	CLA	MG-ND	-2.12	2.01	2.05
13	B	1205	CLA	MG-ND	-2.12	2.01	2.05
13	1	513	CLA	MG-NB	-2.12	2.01	2.05
19	B	5002	LMG	O7-C8	-2.12	1.41	1.46
13	5	517	CLA	CHC-C1C	2.12	1.42	1.38
13	G	1110	CLA	CHC-C1C	2.12	1.42	1.38
13	n	1503	CLA	CHC-C1C	2.12	1.42	1.38
13	r	501	CLA	CHC-C1C	2.12	1.42	1.38
13	A	1104	CLA	CMB-C2B	-2.12	1.46	1.50
13	Z	507	CLA	CMB-C2B	-2.12	1.46	1.50
13	c	513	CLA	CMD-C2D	-2.12	1.46	1.50
13	d	511	CLA	CMD-C2D	-2.12	1.46	1.50
13	f	1220	CLA	CMD-C2D	-2.12	1.46	1.50
13	s	506	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	1203	CLA	CMB-C2B	-2.12	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	504	CLA	CMB-C2B	-2.12	1.46	1.50
13	a	518	CLA	CMB-C2B	-2.12	1.46	1.50
13	b	508	CLA	C3B-C4B	2.12	1.48	1.42
13	6	502	CLA	MG-NB	-2.12	2.01	2.05
13	G	1110	CLA	MG-NB	-2.12	2.01	2.05
13	r	517	CLA	C3B-C4B	2.12	1.48	1.42
13	1	509	CLA	CHC-C1C	2.12	1.42	1.38
13	2	506	CLA	CHC-C1C	2.12	1.42	1.38
13	f	1213	CLA	CHC-C1C	2.12	1.42	1.38
13	1	509	CLA	CMD-C2D	-2.12	1.46	1.50
13	c	504	CLA	CMB-C2B	-2.12	1.46	1.50
13	d	506	CLA	CMB-C2B	-2.12	1.46	1.50
13	d	518	CLA	CMB-C2B	-2.12	1.46	1.50
13	s	519	CLA	CMD-C2D	-2.12	1.46	1.50
13	H	1225	CLA	C1B-C2B	2.12	1.48	1.43
13	r	518	CLA	CHC-C1C	2.12	1.42	1.38
13	e	1105	CLA	C3B-C4B	2.12	1.48	1.42
13	a	511	CLA	MG-NB	-2.12	2.01	2.05
13	s	513	CLA	MG-NB	-2.12	2.01	2.05
13	H	1203	CLA	CHC-C1C	2.12	1.42	1.38
13	e	1125	CLA	CHC-C1C	2.12	1.42	1.38
13	f	1232	CLA	CHC-C1C	2.12	1.42	1.38
13	L	1503	CLA	C3B-C4B	2.12	1.48	1.42
13	H	1203	CLA	CMB-C2B	-2.12	1.46	1.50
13	Y	511	CLA	CMD-C2D	-2.12	1.46	1.50
13	f	1232	CLA	CMD-C2D	-2.12	1.46	1.50
13	u	513	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	1203	CLA	CHC-C1C	2.12	1.42	1.38
13	B	1207	CLA	CHC-C1C	2.12	1.42	1.38
13	G	1109	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	1105	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	1104	CLA	C3B-C4B	2.12	1.48	1.42
13	u	506	CLA	MG-NB	-2.12	2.01	2.05
13	1	509	CLA	CMB-C2B	-2.12	1.46	1.50
13	3	507	CLA	CMB-C2B	-2.12	1.46	1.50
13	5	517	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	1111	CLA	CMB-C2B	-2.12	1.46	1.50
13	f	1234	CLA	CMB-C2B	-2.12	1.46	1.50
13	B	1224	CLA	MG-NB	-2.12	2.01	2.05
13	B	1225	CLA	MG-ND	-2.12	2.01	2.05
13	G	1105	CLA	MG-NB	-2.12	2.01	2.05
13	b	507	CLA	MG-NB	-2.12	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	510	CLA	MG-NB	-2.12	2.01	2.05
13	e	1011	CLA	MG-NB	-2.12	2.01	2.05
13	e	1801	CLA	C3B-C4B	2.12	1.48	1.42
13	3	507	CLA	MG-NB	-2.12	2.01	2.05
13	A	1108	CLA	CMC-C2C	-2.12	1.46	1.50
13	1	511	CLA	CMD-C2D	-2.12	1.46	1.50
16	I	4018	BCR	C1-C6	-2.12	1.51	1.53
13	1	516	CLA	MG-NB	-2.12	2.01	2.05
13	f	1208	CLA	MG-NB	-2.12	2.01	2.05
13	f	1210	CLA	MG-NB	-2.12	2.01	2.05
13	f	1225	CLA	MG-ND	-2.12	2.01	2.05
13	H	1214	CLA	C3B-C4B	2.12	1.48	1.42
13	Z	503	CLA	CHC-C1C	2.12	1.42	1.38
13	Y	506	CLA	CMC-C2C	-2.12	1.46	1.50
13	Z	510	CLA	CMD-C2D	-2.12	1.46	1.50
13	f	1218	CLA	CMB-C2B	-2.12	1.46	1.50
13	f	1228	CLA	CMB-C2B	-2.12	1.46	1.50
13	q	501	CLA	CMC-C2C	-2.12	1.46	1.50
13	r	511	CLA	CMD-C2D	-2.12	1.46	1.50
13	v	511	CLA	MG-NB	-2.12	2.01	2.05
13	Z	511	CLA	CMD-C2D	-2.12	1.46	1.50
13	6	511	CLA	CHC-C1C	2.12	1.42	1.38
20	r	822	SQD	O2-C2	-2.12	1.37	1.43
13	c	506	CLA	MG-NB	-2.12	2.01	2.05
13	u	519	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	502	CLA	C3B-C4B	2.12	1.48	1.42
13	e	1123	CLA	C3B-C4B	2.12	1.48	1.42
13	f	1225	CLA	CHC-C1C	2.12	1.42	1.38
13	4	508	CLA	C1B-C2B	2.12	1.48	1.43
20	Z	822	SQD	O2-C2	-2.12	1.37	1.43
13	e	1801	CLA	C1B-NB	-2.12	1.35	1.37
13	e	1013	CLA	MG-ND	-2.12	2.01	2.05
13	n	1501	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	1201	CLA	CHC-C1C	2.12	1.42	1.38
13	1	504	CLA	CHC-C1C	2.12	1.42	1.38
13	G	1103	CLA	C3B-C4B	2.12	1.48	1.42
13	L	1501	CLA	MG-NB	-2.12	2.01	2.05
13	4	507	CLA	MG-NB	-2.12	2.01	2.05
13	Z	518	CLA	CMB-C2B	-2.11	1.46	1.50
13	s	504	CLA	CMB-C2B	-2.11	1.46	1.50
13	c	516	CLA	CHC-C1C	2.11	1.42	1.38
13	G	1132	CLA	C3B-C4B	2.11	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	516	CLA	MG-NB	-2.11	2.01	2.05
13	c	519	CLA	CMD-C2D	-2.11	1.46	1.50
13	q	511	CLA	CMD-C2D	-2.11	1.46	1.50
13	v	517	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1203	CLA	MG-ND	-2.11	2.01	2.05
13	3	513	CLA	MG-NB	-2.11	2.01	2.05
13	3	506	CLA	CMD-C2D	-2.11	1.46	1.50
13	s	517	CLA	CMD-C2D	-2.11	1.46	1.50
13	G	1108	CLA	CHC-C1C	2.11	1.42	1.38
13	u	516	CLA	CHC-C1C	2.11	1.42	1.38
13	A	1105	CLA	C3B-C4B	2.11	1.48	1.42
13	Z	504	CLA	MG-NB	-2.11	2.01	2.05
13	d	506	CLA	MG-NB	-2.11	2.01	2.05
13	1	501	CLA	CMC-C2C	-2.11	1.46	1.50
13	1	516	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1023	CLA	C1B-NB	-2.11	1.35	1.37
13	B	1225	CLA	CHC-C1C	2.11	1.42	1.38
13	H	1203	CLA	MG-ND	-2.11	2.01	2.05
13	c	517	CLA	MG-NB	-2.11	2.01	2.05
13	d	517	CLA	MG-NB	-2.11	2.01	2.05
13	b	510	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	513	CLA	CMC-C2C	-2.11	1.46	1.50
13	H	1225	CLA	CHC-C1C	2.11	1.42	1.38
13	B	1214	CLA	C3B-C4B	2.11	1.48	1.42
13	J	1303	CLA	C3B-C4B	2.11	1.48	1.42
13	G	1104	CLA	C3B-C4B	2.11	1.48	1.42
13	2	517	CLA	CMB-C2B	-2.11	1.46	1.50
13	3	518	CLA	CMC-C2C	-2.11	1.46	1.50
13	a	509	CLA	CMC-C2C	-2.11	1.46	1.50
13	a	519	CLA	CMB-C2B	-2.11	1.46	1.50
13	c	506	CLA	CMB-C2B	-2.11	1.46	1.50
13	v	507	CLA	CMD-C2D	-2.11	1.46	1.50
13	Y	517	CLA	MG-NB	-2.11	2.01	2.05
13	6	512	CLA	CMB-C2B	-2.11	1.46	1.50
13	H	1215	CLA	CMC-C2C	-2.11	1.46	1.50
13	e	1103	CLA	C3B-C4B	2.11	1.48	1.42
13	G	1123	CLA	CMC-C2C	-2.11	1.46	1.50
13	H	1229	CLA	CMC-C2C	-2.11	1.46	1.50
13	r	510	CLA	CMD-C2D	-2.11	1.46	1.50
19	H	5002	LMG	O7-C8	-2.11	1.41	1.46
13	d	512	CLA	CMB-C2B	-2.11	1.46	1.50
13	H	1213	CLA	CHC-C1C	2.11	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	508	CLA	C3B-C4B	2.11	1.48	1.42
13	2	504	CLA	CMB-C2B	-2.11	1.46	1.50
13	f	1203	CLA	CMB-C2B	-2.11	1.46	1.50
13	v	518	CLA	CMB-C2B	-2.11	1.46	1.50
13	6	501	CLA	MG-NB	-2.11	2.01	2.05
13	A	1801	CLA	C3B-C4B	2.11	1.48	1.42
13	A	1117	CLA	CMC-C2C	-2.11	1.46	1.50
13	1	506	CLA	CMC-C2C	-2.11	1.46	1.50
13	3	503	CLA	CMB-C2B	-2.11	1.46	1.50
13	5	519	CLA	CMD-C2D	-2.11	1.46	1.50
13	Y	509	CLA	CMD-C2D	-2.11	1.46	1.50
13	H	1231	CLA	CHC-C1C	2.11	1.42	1.38
13	b	508	CLA	C1B-C2B	2.11	1.48	1.43
13	5	513	CLA	CMD-C2D	-2.11	1.46	1.50
13	c	513	CLA	CMC-C2C	-2.11	1.46	1.50
13	B	1202	CLA	MG-NB	-2.11	2.01	2.05
13	5	517	CLA	MG-NB	-2.11	2.01	2.05
13	d	503	CLA	CHC-C1C	2.11	1.42	1.38
13	A	1105	CLA	CMD-C2D	-2.11	1.46	1.50
13	G	1109	CLA	CMB-C2B	-2.11	1.46	1.50
13	a	519	CLA	CMD-C2D	-2.11	1.46	1.50
13	q	506	CLA	CMC-C2C	-2.11	1.46	1.50
13	f	1201	CLA	CHC-C1C	2.11	1.42	1.38
13	f	1227	CLA	C3B-C4B	2.11	1.48	1.42
13	a	513	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	507	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	1107	CLA	CMC-C2C	-2.11	1.46	1.50
13	u	509	CLA	CMC-C2C	-2.11	1.46	1.50
13	A	1011	CLA	MG-NB	-2.11	2.01	2.05
13	3	511	CLA	MG-NB	-2.11	2.01	2.05
13	A	1104	CLA	C3B-C4B	2.11	1.48	1.42
13	q	503	CLA	CHC-C1C	2.11	1.42	1.38
13	2	507	CLA	CMB-C2B	-2.11	1.46	1.50
13	4	518	CLA	CMB-C2B	-2.11	1.46	1.50
13	6	508	CLA	CMC-C2C	-2.11	1.46	1.50
13	u	509	CLA	CMD-C2D	-2.11	1.46	1.50
13	6	511	CLA	MG-NB	-2.11	2.01	2.05
13	H	1201	CLA	CHC-C1C	2.11	1.42	1.38
13	H	1202	CLA	CHC-C1C	2.11	1.42	1.38
13	V	1503	CLA	C3B-C4B	2.11	1.48	1.42
13	1	504	CLA	CMC-C2C	-2.11	1.46	1.50
13	H	1240	CLA	CMB-C2B	-2.11	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	503	CLA	CMB-C2B	-2.11	1.46	1.50
13	c	502	CLA	MG-NB	-2.11	2.01	2.05
13	Z	517	CLA	CHC-C1C	2.11	1.42	1.38
13	3	509	CLA	CMB-C2B	-2.11	1.46	1.50
13	Y	504	CLA	CMC-C2C	-2.11	1.46	1.50
13	b	513	CLA	CMD-C2D	-2.11	1.46	1.50
13	d	519	CLA	CMC-C2C	-2.11	1.46	1.50
13	a	507	CLA	C3B-C4B	2.11	1.48	1.42
16	S	4018	BCR	C1-C6	-2.11	1.51	1.53
13	f	1218	CLA	C3B-C4B	2.11	1.48	1.42
13	a	504	CLA	CMB-C2B	-2.11	1.46	1.50
13	d	501	CLA	CMD-C2D	-2.11	1.46	1.50
13	s	507	CLA	CMB-C2B	-2.11	1.46	1.50
13	r	504	CLA	MG-NB	-2.11	2.01	2.05
13	r	513	CLA	MG-NB	-2.11	2.01	2.05
13	B	1225	CLA	C1B-C2B	2.11	1.48	1.43
13	r	517	CLA	CHC-C1C	2.11	1.42	1.38
13	H	1220	CLA	C3B-C4B	2.11	1.48	1.42
13	H	1218	CLA	CMC-C2C	-2.11	1.46	1.50
13	e	1120	CLA	CMC-C2C	-2.11	1.46	1.50
13	e	1127	CLA	CMC-C2C	-2.11	1.46	1.50
13	f	1238	CLA	CMC-C2C	-2.11	1.46	1.50
13	l	1303	CLA	C3B-C4B	2.11	1.48	1.42
13	H	1226	CLA	CMC-C2C	-2.11	1.46	1.50
13	Y	507	CLA	CMB-C2B	-2.11	1.46	1.50
13	d	503	CLA	CMD-C2D	-2.11	1.46	1.50
13	A	1103	CLA	C3B-C4B	2.11	1.48	1.42
13	1	503	CLA	CHC-C1C	2.10	1.42	1.38
13	d	508	CLA	CHC-C1C	2.10	1.42	1.38
13	A	1109	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	513	CLA	CMD-C2D	-2.10	1.46	1.50
13	H	1204	CLA	MG-ND	-2.10	2.01	2.05
13	d	510	CLA	MG-NB	-2.10	2.01	2.05
13	e	1109	CLA	MG-NB	-2.10	2.01	2.05
13	t	518	CLA	CHC-C1C	2.10	1.42	1.38
13	e	1106	CLA	C1B-C2B	2.10	1.48	1.43
13	6	506	CLA	CMB-C2B	-2.10	1.46	1.50
13	c	516	CLA	CMB-C2B	-2.10	1.46	1.50
13	e	1126	CLA	CMC-C2C	-2.10	1.46	1.50
13	v	512	CLA	CMB-C2B	-2.10	1.46	1.50
13	5	510	CLA	MG-NB	-2.10	2.01	2.05
13	e	1132	CLA	CHC-C1C	2.10	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	u	517	CLA	CHC-C1C	2.10	1.42	1.38
13	r	516	CLA	CMD-C2D	-2.10	1.46	1.50
13	2	504	CLA	MG-NB	-2.10	2.01	2.05
13	3	518	CLA	MG-NB	-2.10	2.01	2.05
13	U	1105	CLA	MG-NB	-2.10	2.01	2.05
13	Y	509	CLA	CHC-C1C	2.10	1.42	1.38
13	1	507	CLA	CMB-C2B	-2.10	1.46	1.50
13	3	519	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	506	CLA	CMD-C2D	-2.10	1.46	1.50
13	l	1303	CLA	CMB-C2B	-2.10	1.46	1.50
13	u	510	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	1107	CLA	C1B-C2B	2.10	1.48	1.43
13	u	513	CLA	MG-NB	-2.10	2.01	2.05
13	H	1240	CLA	CHC-C1C	2.10	1.42	1.38
13	B	1229	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	1217	CLA	MG-ND	-2.10	2.01	2.05
13	5	506	CLA	CMB-C2B	-2.10	1.46	1.50
13	Z	506	CLA	CMD-C2D	-2.10	1.46	1.50
13	t	518	CLA	CMB-C2B	-2.10	1.46	1.50
13	A	1123	CLA	C3B-C4B	2.10	1.48	1.42
13	Y	509	CLA	CMB-C2B	-2.10	1.46	1.50
13	f	1225	CLA	C1B-C2B	2.10	1.48	1.43
13	s	506	CLA	MG-NB	-2.10	2.01	2.05
13	a	517	CLA	CHC-C1C	2.10	1.42	1.38
13	u	503	CLA	CMD-C2D	-2.10	1.46	1.50
13	Z	511	CLA	MG-NB	-2.10	2.01	2.05
13	v	505	CLA	MG-NB	-2.10	2.01	2.05
13	d	508	CLA	CMC-C2C	-2.10	1.46	1.50
13	G	1123	CLA	C3B-C4B	2.10	1.48	1.42
13	6	506	CLA	MG-NB	-2.10	2.01	2.05
13	G	1101	CLA	MG-NB	-2.10	2.01	2.05
13	2	516	CLA	CHC-C1C	2.10	1.42	1.38
13	3	505	CLA	CHC-C1C	2.10	1.42	1.38
13	f	1207	CLA	CHC-C1C	2.10	1.42	1.38
13	q	501	CLA	CHC-C1C	2.10	1.42	1.38
13	G	1108	CLA	CMC-C2C	-2.10	1.46	1.50
13	u	506	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	1236	CLA	MG-NB	-2.10	2.01	2.05
13	u	510	CLA	MG-NB	-2.10	2.01	2.05
13	b	505	CLA	CHC-C1C	2.10	1.42	1.38
13	f	1202	CLA	CHC-C1C	2.10	1.42	1.38
13	2	516	CLA	CMD-C2D	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1126	CLA	CMB-C2B	-2.10	1.46	1.50
13	H	1236	CLA	CMD-C2D	-2.10	1.46	1.50
13	r	516	CLA	MG-NB	-2.10	2.01	2.05
13	A	1123	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	1232	CLA	CMC-C2C	-2.10	1.46	1.50
13	6	508	CLA	CHC-C1C	2.10	1.42	1.38
13	3	501	CLA	CMD-C2D	-2.10	1.46	1.50
13	4	517	CLA	CMC-C2C	-2.10	1.46	1.50
13	H	1228	CLA	CMB-C2B	-2.10	1.46	1.50
13	Z	517	CLA	CMB-C2B	-2.10	1.46	1.50
13	a	507	CLA	CMB-C2B	-2.10	1.46	1.50
13	t	510	CLA	CMD-C2D	-2.10	1.46	1.50
13	t	513	CLA	CMC-C2C	-2.10	1.46	1.50
13	G	1011	CLA	MG-NB	-2.10	2.01	2.05
13	H	1224	CLA	MG-NB	-2.10	2.01	2.05
13	e	1119	CLA	MG-ND	-2.10	2.01	2.05
13	e	1101	CLA	MG-NB	-2.10	2.01	2.05
13	s	510	CLA	MG-NB	-2.10	2.01	2.05
13	6	501	CLA	CHC-C1C	2.10	1.42	1.38
13	A	1113	CLA	CMB-C2B	-2.10	1.46	1.50
13	J	1303	CLA	CMB-C2B	-2.10	1.46	1.50
13	H	1238	CLA	CMC-C2C	-2.10	1.46	1.50
13	a	503	CLA	CMB-C2B	-2.10	1.46	1.50
13	s	513	CLA	CMD-C2D	-2.10	1.46	1.50
13	R	1301	CLA	CHC-C1C	2.10	1.42	1.38
13	d	511	CLA	CHC-C1C	2.10	1.42	1.38
13	v	504	CLA	MG-NB	-2.10	2.01	2.05
13	G	1113	CLA	CMB-C2B	-2.10	1.46	1.50
13	e	1120	CLA	C3B-C4B	2.10	1.48	1.42
13	Y	505	CLA	CHC-C1C	2.10	1.42	1.38
13	B	1220	CLA	CMD-C2D	-2.10	1.46	1.50
13	4	510	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	1227	CLA	C3B-C4B	2.10	1.48	1.42
13	1	505	CLA	CHC-C1C	2.10	1.42	1.38
13	a	519	CLA	MG-NB	-2.10	2.01	2.05
13	u	517	CLA	MG-NB	-2.10	2.01	2.05
13	B	1218	CLA	CMC-C2C	-2.10	1.46	1.50
13	s	518	CLA	CMC-C2C	-2.10	1.46	1.50
13	A	1120	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	1215	CLA	CMD-C2D	-2.10	1.46	1.50
13	T	1302	CLA	CMC-C2C	-2.10	1.46	1.50
13	s	516	CLA	CMD-C2D	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1205	CLA	MG-ND	-2.10	2.01	2.05
13	m	1105	CLA	MG-NB	-2.10	2.01	2.05
13	H	1232	CLA	CHC-C1C	2.10	1.42	1.38
13	3	513	CLA	CMD-C2D	-2.10	1.46	1.50
13	6	503	CLA	CMD-C2D	-2.10	1.46	1.50
13	u	513	CLA	CMC-C2C	-2.10	1.46	1.50
13	2	503	CLA	CHC-C1C	2.10	1.42	1.38
13	a	505	CLA	CHC-C1C	2.10	1.42	1.38
13	A	1109	CLA	MG-NB	-2.10	2.01	2.05
13	e	1113	CLA	MG-NB	-2.10	2.01	2.05
13	5	513	CLA	CMC-C2C	-2.09	1.46	1.50
13	e	1113	CLA	CMB-C2B	-2.09	1.46	1.50
13	e	1117	CLA	CMC-C2C	-2.09	1.46	1.50
13	r	517	CLA	CMB-C2B	-2.09	1.46	1.50
13	n	1501	CLA	MG-NB	-2.09	2.01	2.05
13	A	1109	CLA	CMD-C2D	-2.09	1.46	1.50
13	4	509	CLA	CMB-C2B	-2.09	1.46	1.50
13	6	517	CLA	CMD-C2D	-2.09	1.46	1.50
13	G	1117	CLA	CMC-C2C	-2.09	1.46	1.50
13	q	509	CLA	CMC-C2C	-2.09	1.46	1.50
13	3	519	CLA	MG-NB	-2.09	2.01	2.05
14	A	2001	PQN	C10-C1	-2.09	1.44	1.48
13	H	1227	CLA	C3B-C4B	2.09	1.48	1.42
13	B	1023	CLA	C1B-C2B	2.09	1.48	1.43
13	e	1109	CLA	CMB-C2B	-2.09	1.46	1.50
13	A	1101	CLA	CHC-C1C	2.09	1.42	1.38
13	G	1101	CLA	CHC-C1C	2.09	1.42	1.38
13	u	502	CLA	MG-NB	-2.09	2.01	2.05
13	H	1225	CLA	MG-ND	-2.09	2.01	2.05
13	H	1236	CLA	MG-NB	-2.09	2.01	2.05
13	2	502	CLA	C3B-C4B	2.09	1.48	1.42
13	H	1230	CLA	C3B-C4B	2.09	1.48	1.42
13	5	516	CLA	CMD-C2D	-2.09	1.46	1.50
13	s	509	CLA	CMC-C2C	-2.09	1.46	1.50
13	e	1127	CLA	CHC-C1C	2.09	1.42	1.38
13	H	1023	CLA	C1B-NB	-2.09	1.35	1.37
13	f	1232	CLA	C1B-NB	-2.09	1.35	1.37
13	G	1118	CLA	CMC-C2C	-2.09	1.46	1.50
13	t	505	CLA	CHC-C1C	2.09	1.42	1.38
13	B	1215	CLA	CMC-C2C	-2.09	1.46	1.50
13	1	517	CLA	CMB-C2B	-2.09	1.46	1.50
13	4	513	CLA	CMC-C2C	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1127	CLA	CHC-C1C	2.09	1.42	1.38
13	B	1206	CLA	MG-ND	-2.09	2.01	2.05
13	c	503	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	1230	CLA	C3B-C4B	2.09	1.48	1.42
13	5	510	CLA	CMD-C2D	-2.09	1.46	1.50
13	c	503	CLA	CMB-C2B	-2.09	1.46	1.50
13	d	507	CLA	CMD-C2D	-2.09	1.46	1.50
13	t	504	CLA	CMD-C2D	-2.09	1.46	1.50
13	s	505	CLA	CHC-C1C	2.09	1.42	1.38
20	t	822	SQD	O2-C2	-2.09	1.37	1.43
13	a	508	CLA	C1B-C2B	2.09	1.48	1.43
13	f	1232	CLA	C1B-C2B	2.09	1.48	1.43
13	e	1126	CLA	CMB-C2B	-2.09	1.46	1.50
13	q	513	CLA	CMB-C2B	-2.09	1.46	1.50
13	s	517	CLA	CMB-C2B	-2.09	1.46	1.50
13	G	1801	CLA	C1B-NB	-2.09	1.35	1.37
13	U	1105	CLA	C3C-C2C	2.09	1.41	1.36
13	b	502	CLA	CHC-C1C	2.09	1.42	1.38
13	c	501	CLA	MG-NB	-2.09	2.01	2.05
13	Y	501	CLA	CMC-C2C	-2.09	1.46	1.50
13	Y	516	CLA	CMD-C2D	-2.09	1.46	1.50
13	a	501	CLA	CMC-C2C	-2.09	1.46	1.50
13	f	1231	CLA	CHC-C1C	2.09	1.42	1.38
13	H	1218	CLA	C3B-C4B	2.09	1.48	1.42
13	q	503	CLA	MG-NB	-2.09	2.01	2.05
13	6	519	CLA	CMC-C2C	-2.09	1.46	1.50
13	b	516	CLA	CMD-C2D	-2.09	1.46	1.50
13	u	516	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	1102	CLA	MG-NB	-2.09	2.01	2.05
13	H	1206	CLA	MG-ND	-2.09	2.01	2.05
13	s	518	CLA	MG-NB	-2.09	2.01	2.05
13	v	506	CLA	MG-NB	-2.09	2.01	2.05
13	r	502	CLA	C3B-C4B	2.09	1.48	1.42
13	K	1105	CLA	MG-NB	-2.09	2.01	2.05
13	f	1218	CLA	CMC-C2C	-2.09	1.46	1.50
13	5	501	CLA	MG-NB	-2.09	2.01	2.05
13	t	518	CLA	MG-NB	-2.09	2.01	2.05
13	a	516	CLA	CMD-C2D	-2.09	1.46	1.50
13	l	1302	CLA	CMC-C2C	-2.09	1.46	1.50
13	4	518	CLA	MG-NB	-2.09	2.01	2.05
13	5	518	CLA	MG-NB	-2.09	2.01	2.05
13	e	1102	CLA	MG-NB	-2.09	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	507	CLA	C3B-C4B	2.09	1.48	1.42
13	Z	502	CLA	C3B-C4B	2.09	1.48	1.42
13	U	1401	CLA	CHC-C1C	2.09	1.42	1.38
13	v	508	CLA	CHC-C1C	2.09	1.42	1.38
13	1	513	CLA	CMB-C2B	-2.09	1.46	1.50
13	3	509	CLA	CMC-C2C	-2.09	1.46	1.50
13	H	1201	CLA	CMB-C2B	-2.09	1.46	1.50
13	Y	517	CLA	CMC-C2C	-2.09	1.46	1.50
13	u	506	CLA	CMB-C2B	-2.09	1.46	1.50
13	v	511	CLA	CHC-C1C	2.09	1.42	1.38
13	s	516	CLA	MG-NB	-2.09	2.01	2.05
13	v	507	CLA	MG-NB	-2.09	2.01	2.05
13	3	517	CLA	CMB-C2B	-2.09	1.46	1.50
13	r	504	CLA	CMB-C2B	-2.09	1.46	1.50
13	v	503	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	1238	CLA	CMC-C2C	-2.09	1.46	1.50
13	A	1132	CLA	C3B-C4B	2.09	1.48	1.42
13	T	1303	CLA	C3B-C4B	2.09	1.48	1.42
13	Z	516	CLA	CHC-C1C	2.09	1.42	1.38
13	d	501	CLA	CHC-C1C	2.09	1.42	1.38
13	G	1131	CLA	MG-NB	-2.09	2.01	2.05
13	H	1231	CLA	MG-NB	-2.09	2.01	2.05
13	f	1204	CLA	MG-ND	-2.09	2.01	2.05
13	e	1109	CLA	CMD-C2D	-2.09	1.46	1.50
13	v	503	CLA	MG-NB	-2.09	2.01	2.05
13	t	517	CLA	CMC-C2C	-2.09	1.46	1.50
13	A	1105	CLA	CHC-C1C	2.08	1.42	1.38
13	d	507	CLA	MG-NB	-2.08	2.01	2.05
13	e	1137	CLA	MG-NB	-2.08	2.01	2.05
13	f	1221	CLA	MG-ND	-2.08	2.01	2.05
13	s	501	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	2001	PQN	C5-C4	-2.08	1.44	1.48
13	d	501	CLA	MG-NB	-2.08	2.01	2.05
13	A	1118	CLA	CMC-C2C	-2.08	1.46	1.50
13	e	1108	CLA	CMC-C2C	-2.08	1.46	1.50
13	f	1230	CLA	C3B-C4B	2.08	1.48	1.42
13	A	1110	CLA	CHC-C1C	2.08	1.42	1.38
13	A	1137	CLA	C1B-C2B	2.08	1.48	1.43
13	e	1137	CLA	C1B-C2B	2.08	1.48	1.43
13	5	513	CLA	MG-NB	-2.08	2.01	2.05
13	b	513	CLA	MG-NB	-2.08	2.01	2.05
13	f	1214	CLA	C3B-C4B	2.08	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	501	CLA	MG-NB	-2.08	2.01	2.05
13	L	1502	CLA	CMB-C2B	-2.08	1.46	1.50
13	5	516	CLA	CMB-C2B	-2.08	1.46	1.50
13	u	517	CLA	CMB-C2B	-2.08	1.46	1.50
13	1	501	CLA	CHC-C1C	2.08	1.42	1.38
13	A	1119	CLA	MG-ND	-2.08	2.01	2.05
13	4	513	CLA	CMD-C2D	-2.08	1.46	1.50
13	H	1213	CLA	CMB-C2B	-2.08	1.46	1.50
13	r	516	CLA	CHC-C1C	2.08	1.42	1.38
13	t	502	CLA	CHC-C1C	2.08	1.42	1.38
13	1	510	CLA	CMD-C2D	-2.08	1.46	1.50
13	5	503	CLA	CMD-C2D	-2.08	1.46	1.50
13	6	510	CLA	CMD-C2D	-2.08	1.46	1.50
13	G	1114	CLA	CMC-C2C	-2.08	1.46	1.50
13	e	1118	CLA	CMC-C2C	-2.08	1.46	1.50
13	v	506	CLA	CMC-C2C	-2.08	1.46	1.50
13	F	1301	CLA	CHC-C1C	2.08	1.42	1.38
13	b	519	CLA	CHC-C1C	2.08	1.42	1.38
13	c	513	CLA	MG-NB	-2.08	2.01	2.05
13	G	1120	CLA	CMC-C2C	-2.08	1.46	1.50
13	Z	510	CLA	CMC-C2C	-2.08	1.46	1.50
13	e	1114	CLA	CMC-C2C	-2.08	1.46	1.50
13	q	517	CLA	CMB-C2B	-2.08	1.46	1.50
13	G	1137	CLA	C1B-C2B	2.08	1.48	1.43
13	B	1202	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1240	CLA	CHC-C1C	2.08	1.42	1.38
13	3	519	CLA	CMB-C2B	-2.08	1.46	1.50
13	f	1217	CLA	MG-ND	-2.08	2.01	2.05
13	B	1218	CLA	C3B-C4B	2.08	1.48	1.42
13	J	1302	CLA	CMC-C2C	-2.08	1.46	1.50
13	4	501	CLA	CMB-C2B	-2.08	1.46	1.50
13	1	517	CLA	MG-NB	-2.08	2.01	2.05
13	G	1102	CLA	MG-NB	-2.08	2.01	2.05
13	f	1206	CLA	MG-ND	-2.08	2.01	2.05
13	q	513	CLA	MG-NB	-2.08	2.01	2.05
13	B	1213	CLA	CMB-C2B	-2.08	1.46	1.50
13	T	1303	CLA	CMB-C2B	-2.08	1.46	1.50
13	Z	513	CLA	CMD-C2D	-2.08	1.46	1.50
13	f	1201	CLA	CMB-C2B	-2.08	1.46	1.50
13	v	510	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	1120	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1228	CLA	CMB-C2B	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	n	1502	CLA	CMB-C2B	-2.08	1.46	1.50
13	e	1117	CLA	C1B-NB	-2.08	1.35	1.37
13	G	1237	CLA	C3B-C4B	2.08	1.48	1.42
13	s	503	CLA	MG-NB	-2.08	2.01	2.05
13	4	505	CLA	CHC-C1C	2.08	1.42	1.38
13	3	516	CLA	CMD-C2D	-2.08	1.46	1.50
13	Y	510	CLA	CMD-C2D	-2.08	1.46	1.50
13	Y	517	CLA	CMB-C2B	-2.08	1.46	1.50
13	d	503	CLA	CMB-C2B	-2.08	1.46	1.50
13	6	510	CLA	MG-NB	-2.08	2.01	2.05
13	H	1232	CLA	C1B-C2B	2.08	1.48	1.43
13	G	1127	CLA	CHC-C1C	2.08	1.42	1.38
13	m	1401	CLA	CHC-C1C	2.08	1.42	1.38
13	4	506	CLA	CMD-C2D	-2.08	1.46	1.50
13	G	1105	CLA	CMD-C2D	-2.08	1.46	1.50
13	c	501	CLA	CMD-C2D	-2.08	1.46	1.50
13	u	503	CLA	CMB-C2B	-2.08	1.46	1.50
13	B	1203	CLA	C3B-C4B	2.08	1.48	1.42
13	4	506	CLA	MG-NB	-2.08	2.01	2.05
13	B	1232	CLA	C1B-C2B	2.08	1.48	1.43
13	A	1127	CLA	CMC-C2C	-2.08	1.46	1.50
13	q	513	CLA	CMC-C2C	-2.08	1.46	1.50
13	H	1023	CLA	C1B-C2B	2.08	1.48	1.43
13	t	513	CLA	MG-NB	-2.08	2.01	2.05
13	1	513	CLA	CMC-C2C	-2.08	1.46	1.50
13	Y	509	CLA	CMC-C2C	-2.08	1.46	1.50
13	s	513	CLA	CMB-C2B	-2.08	1.46	1.50
13	5	502	CLA	CMC-C2C	-2.08	1.46	1.50
13	t	506	CLA	CMD-C2D	-2.08	1.46	1.50
13	6	505	CLA	MG-NB	-2.08	2.01	2.05
13	4	509	CLA	CMD-C2D	-2.08	1.46	1.50
13	4	504	CLA	CMD-C2D	-2.08	1.46	1.50
13	5	517	CLA	CMC-C2C	-2.08	1.46	1.50
13	3	516	CLA	MG-NB	-2.08	2.01	2.05
13	3	517	CLA	MG-NB	-2.08	2.01	2.05
13	4	519	CLA	CHC-C1C	2.08	1.42	1.38
14	e	2001	PQN	C10-C1	-2.08	1.44	1.48
13	B	1231	CLA	MG-NB	-2.08	2.01	2.05
13	B	1220	CLA	C3B-C4B	2.08	1.48	1.42
13	2	519	CLA	CMD-C2D	-2.08	1.46	1.50
13	a	509	CLA	CMB-C2B	-2.08	1.46	1.50
13	r	513	CLA	CMD-C2D	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	510	CLA	MG-NB	-2.08	2.01	2.05
13	a	510	CLA	MG-NB	-2.08	2.01	2.05
13	s	511	CLA	MG-NB	-2.08	2.01	2.05
13	d	517	CLA	CMD-C2D	-2.07	1.46	1.50
13	t	509	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	1220	CLA	C3B-C4B	2.07	1.48	1.42
13	G	1117	CLA	MG-ND	-2.07	2.01	2.05
13	L	1503	CLA	CMB-C2B	-2.07	1.46	1.50
13	3	513	CLA	CMB-C2B	-2.07	1.46	1.50
13	V	1503	CLA	CMB-C2B	-2.07	1.46	1.50
13	q	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	s	519	CLA	CMB-C2B	-2.07	1.46	1.50
13	u	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	511	CLA	MG-NB	-2.07	2.01	2.05
13	G	1119	CLA	MG-ND	-2.07	2.01	2.05
13	G	1113	CLA	C3B-C4B	2.07	1.48	1.42
13	A	1114	CLA	CMC-C2C	-2.07	1.46	1.50
13	4	516	CLA	CMD-C2D	-2.07	1.46	1.50
13	6	501	CLA	CMD-C2D	-2.07	1.46	1.50
13	c	510	CLA	CMD-C2D	-2.07	1.46	1.50
13	r	510	CLA	CMC-C2C	-2.07	1.46	1.50
13	u	510	CLA	CMB-C2B	-2.07	1.46	1.50
13	f	1240	CLA	CHC-C1C	2.07	1.42	1.38
13	a	517	CLA	MG-NB	-2.07	2.01	2.05
13	f	1023	CLA	C1B-C2B	2.07	1.48	1.43
13	5	510	CLA	CMB-C2B	-2.07	1.46	1.50
13	a	501	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	1203	CLA	C3B-C4B	2.07	1.48	1.42
13	G	1120	CLA	C3B-C4B	2.07	1.48	1.42
13	A	1126	CLA	CMC-C2C	-2.07	1.46	1.50
13	5	503	CLA	CMB-C2B	-2.07	1.46	1.50
13	6	510	CLA	CMB-C2B	-2.07	1.46	1.50
13	H	1215	CLA	CMD-C2D	-2.07	1.46	1.50
13	d	510	CLA	CMB-C2B	-2.07	1.46	1.50
13	t	513	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	1120	CLA	C3B-C4B	2.07	1.48	1.42
14	e	2001	PQN	C5-C4	-2.07	1.44	1.48
13	b	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	e	1102	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	1132	CLA	C3B-C4B	2.07	1.48	1.42
13	s	507	CLA	C3B-C4B	2.07	1.48	1.42
13	2	504	CLA	CMC-C2C	-2.07	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	509	CLA	CMB-C2B	-2.07	1.46	1.50
13	c	507	CLA	CMB-C2B	-2.07	1.46	1.50
13	B	1231	CLA	CHC-C1C	2.07	1.42	1.38
13	b	518	CLA	MG-NB	-2.07	2.01	2.05
13	G	1127	CLA	C3B-C4B	2.07	1.48	1.42
13	Y	513	CLA	CMB-C2B	-2.07	1.46	1.50
13	e	1134	CLA	CMC-C2C	-2.07	1.46	1.50
13	t	517	CLA	CMD-C2D	-2.07	1.46	1.50
13	3	501	CLA	CHC-C1C	2.07	1.42	1.38
13	H	1217	CLA	MG-ND	-2.07	2.01	2.05
13	Z	503	CLA	MG-NB	-2.07	2.01	2.05
13	e	1132	CLA	MG-ND	-2.07	2.01	2.05
13	b	509	CLA	CMD-C2D	-2.07	1.46	1.50
13	v	501	CLA	CMC-C2C	-2.07	1.46	1.50
13	Y	503	CLA	CHC-C1C	2.07	1.42	1.38
13	e	1105	CLA	CHC-C1C	2.07	1.42	1.38
13	A	1113	CLA	C3B-C4B	2.07	1.48	1.42
13	a	518	CLA	MG-NB	-2.07	2.01	2.05
13	f	1216	CLA	MG-ND	-2.07	2.01	2.05
13	b	504	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	1123	CLA	CMC-C2C	-2.07	1.46	1.50
13	v	506	CLA	CMD-C2D	-2.07	1.46	1.50
13	j	1301	CLA	CHC-C1C	2.07	1.42	1.38
20	5	822	SQD	O2-C2	-2.07	1.37	1.43
13	6	509	CLA	MG-NB	-2.07	2.01	2.05
13	1	509	CLA	CMC-C2C	-2.07	1.46	1.50
13	5	506	CLA	CMC-C2C	-2.07	1.46	1.50
13	Y	513	CLA	CMD-C2D	-2.07	1.46	1.50
13	Z	519	CLA	CMD-C2D	-2.07	1.46	1.50
13	q	505	CLA	CHC-C1C	2.07	1.42	1.38
13	c	518	CLA	MG-NB	-2.07	2.01	2.05
13	6	507	CLA	CMB-C2B	-2.07	1.46	1.50
13	Z	516	CLA	CMC-C2C	-2.07	1.46	1.50
13	c	502	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	501	CLA	CHC-C1C	2.07	1.42	1.38
13	A	1127	CLA	C3B-C4B	2.07	1.48	1.42
13	v	510	CLA	MG-NB	-2.07	2.01	2.05
13	A	1126	CLA	CMB-C2B	-2.07	1.46	1.50
13	H	1223	CLA	C1B-NB	-2.07	1.35	1.37
13	A	1117	CLA	MG-ND	-2.07	2.01	2.05
13	f	1238	CLA	CHC-C1C	2.07	1.42	1.38
13	m	1105	CLA	C3C-C2C	2.07	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	513	CLA	MG-NB	-2.07	2.01	2.05
13	G	1109	CLA	MG-NB	-2.07	2.01	2.05
13	r	509	CLA	MG-NB	-2.07	2.01	2.05
13	s	509	CLA	MG-NB	-2.07	2.01	2.05
13	B	1201	CLA	CMB-C2B	-2.07	1.46	1.50
13	6	513	CLA	CMB-C2B	-2.07	1.46	1.50
13	r	507	CLA	CMB-C2B	-2.07	1.46	1.50
13	e	1110	CLA	CHC-C1C	2.07	1.42	1.38
13	n	1503	CLA	MG-NB	-2.07	2.01	2.05
13	u	509	CLA	MG-NB	-2.07	2.01	2.05
13	1	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	u	507	CLA	CMB-C2B	-2.07	1.46	1.50
17	B	1842	LHG	O7-C5	-2.07	1.41	1.46
17	H	1842	LHG	O7-C5	-2.07	1.41	1.46
13	2	506	CLA	CMD-C2D	-2.07	1.46	1.50
13	Y	516	CLA	CMB-C2B	-2.07	1.46	1.50
13	r	507	CLA	CMC-C2C	-2.07	1.46	1.50
13	f	1212	CLA	C3B-C4B	2.07	1.48	1.42
13	A	1132	CLA	CHC-C1C	2.07	1.42	1.38
13	G	1105	CLA	CHC-C1C	2.07	1.42	1.38
13	r	503	CLA	CHC-C1C	2.07	1.42	1.38
13	H	1232	CLA	CMC-C2C	-2.07	1.46	1.50
13	b	501	CLA	CMB-C2B	-2.07	1.46	1.50
13	u	502	CLA	CMC-C2C	-2.07	1.46	1.50
13	G	1137	CLA	MG-NB	-2.07	2.01	2.05
13	a	512	CLA	MG-ND	-2.07	2.01	2.05
13	t	506	CLA	MG-NB	-2.07	2.01	2.05
13	f	1203	CLA	C1B-NB	-2.07	1.35	1.37
13	2	508	CLA	CHC-C1C	2.07	1.42	1.38
13	b	509	CLA	CMB-C2B	-2.07	1.46	1.50
13	q	506	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	1012	CLA	MG-ND	-2.07	2.01	2.05
13	B	1203	CLA	C1B-NB	-2.07	1.35	1.37
13	e	1113	CLA	C3B-C4B	2.07	1.48	1.42
13	b	506	CLA	CMD-C2D	-2.07	1.46	1.50
13	r	518	CLA	CMC-C2C	-2.07	1.46	1.50
13	A	1137	CLA	MG-NB	-2.07	2.01	2.05
13	6	503	CLA	MG-NB	-2.07	2.01	2.05
13	K	1401	CLA	CHC-C1C	2.06	1.42	1.38
13	H	1208	CLA	CHC-C1C	2.06	1.42	1.38
13	v	507	CLA	CMB-C2B	-2.06	1.46	1.50
13	A	1114	CLA	C1B-C2B	2.06	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1012	CLA	MG-ND	-2.06	2.01	2.05
14	H	2002	PQN	C11-C3	2.06	1.55	1.51
13	A	1117	CLA	C1B-NB	-2.06	1.35	1.37
13	A	1134	CLA	CMC-C2C	-2.06	1.46	1.50
13	d	506	CLA	CMC-C2C	-2.06	1.46	1.50
13	u	509	CLA	CMB-C2B	-2.06	1.46	1.50
20	V	5216	SQD	O2-C2	-2.06	1.37	1.43
13	G	1132	CLA	CHC-C1C	2.06	1.42	1.38
13	r	508	CLA	CHC-C1C	2.06	1.42	1.38
20	u	822	SQD	O2-C2	-2.06	1.37	1.43
13	Y	503	CLA	CMB-C2B	-2.06	1.46	1.50
13	u	507	CLA	C3B-C4B	2.06	1.48	1.42
13	Y	513	CLA	CMC-C2C	-2.06	1.46	1.50
13	r	503	CLA	CMC-C2C	-2.06	1.46	1.50
13	u	501	CLA	CMB-C2B	-2.06	1.46	1.50
13	t	513	CLA	CMB-C2B	-2.06	1.46	1.50
13	v	501	CLA	CMD-C2D	-2.06	1.46	1.50
13	s	501	CLA	MG-NB	-2.06	2.01	2.05
13	1	513	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	1215	CLA	CMC-C2C	-2.06	1.46	1.50
13	r	504	CLA	CMC-C2C	-2.06	1.46	1.50
17	f	1842	LHG	O7-C5	-2.06	1.41	1.46
13	e	1138	CLA	MG-NB	-2.06	2.01	2.05
13	u	501	CLA	MG-NB	-2.06	2.01	2.05
13	V	1502	CLA	CMB-C2B	-2.06	1.46	1.50
13	u	516	CLA	MG-NB	-2.06	2.01	2.05
13	G	1112	CLA	C1B-C2B	2.06	1.48	1.43
13	a	517	CLA	CMB-C2B	-2.06	1.46	1.50
13	q	513	CLA	CMD-C2D	-2.06	1.46	1.50
13	K	1105	CLA	C3C-C2C	2.06	1.41	1.36
13	B	1220	CLA	MG-NB	-2.06	2.01	2.05
13	3	508	CLA	CHC-C1C	2.06	1.42	1.38
13	Y	501	CLA	CHC-C1C	2.06	1.42	1.38
13	B	1221	CLA	C1B-C2B	2.06	1.48	1.43
13	G	1114	CLA	C1B-C2B	2.06	1.48	1.43
13	u	504	CLA	CMD-C2D	-2.06	1.46	1.50
13	G	1138	CLA	MG-NB	-2.06	2.01	2.05
13	r	503	CLA	MG-NB	-2.06	2.01	2.05
13	B	1202	CLA	C1B-NB	-2.06	1.35	1.37
13	s	508	CLA	CHC-C1C	2.06	1.42	1.38
13	1	503	CLA	MG-NB	-2.06	2.01	2.05
13	2	503	CLA	MG-NB	-2.06	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	509	CLA	MG-NB	-2.06	2.01	2.05
13	6	507	CLA	MG-NB	-2.06	2.01	2.05
13	b	510	CLA	MG-NB	-2.06	2.01	2.05
13	B	1216	CLA	CHC-C1C	2.06	1.42	1.38
13	n	1503	CLA	CMB-C2B	-2.06	1.46	1.50
13	r	516	CLA	CMB-C2B	-2.06	1.46	1.50
13	t	516	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	1202	CLA	C1B-NB	-2.06	1.35	1.37
13	A	1120	CLA	CHC-C1C	2.06	1.42	1.38
14	B	2002	PQN	C11-C3	2.06	1.55	1.51
13	c	510	CLA	CMB-C2B	-2.06	1.46	1.50
13	Z	508	CLA	CHC-C1C	2.06	1.42	1.38
13	e	1120	CLA	C1B-NB	-2.06	1.35	1.37
13	2	501	CLA	MG-NB	-2.06	2.01	2.05
13	a	503	CLA	MG-NB	-2.06	2.01	2.05
13	e	1117	CLA	MG-ND	-2.06	2.01	2.05
13	H	1216	CLA	CHC-C1C	2.06	1.42	1.38
13	4	501	CLA	MG-NB	-2.06	2.01	2.05
13	Z	516	CLA	CMB-C2B	-2.06	1.46	1.50
13	f	1228	CLA	C3B-C4B	2.06	1.48	1.42
13	Z	513	CLA	MG-NB	-2.06	2.01	2.05
13	G	1120	CLA	CHC-C1C	2.06	1.42	1.38
13	1	516	CLA	CMB-C2B	-2.06	1.46	1.50
13	6	516	CLA	CMD-C2D	-2.06	1.46	1.50
20	1	822	SQD	O2-C2	-2.06	1.37	1.43
13	3	503	CLA	MG-NB	-2.06	2.01	2.05
13	Z	501	CLA	MG-NB	-2.06	2.01	2.05
13	6	517	CLA	CMC-C2C	-2.06	1.46	1.50
13	v	510	CLA	CMB-C2B	-2.06	1.46	1.50
13	f	1221	CLA	C1B-C2B	2.06	1.48	1.43
13	G	1127	CLA	CMC-C2C	-2.05	1.46	1.50
13	d	516	CLA	CMD-C2D	-2.05	1.46	1.50
13	d	517	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	506	CLA	MG-NB	-2.05	2.01	2.05
13	2	510	CLA	CMC-C2C	-2.05	1.46	1.50
13	6	504	CLA	CMD-C2D	-2.05	1.46	1.50
13	c	506	CLA	CMD-C2D	-2.05	1.46	1.50
13	v	517	CLA	CMC-C2C	-2.05	1.46	1.50
13	e	1114	CLA	C1B-C2B	2.05	1.47	1.43
13	H	1203	CLA	C3B-C4B	2.05	1.48	1.42
13	f	1231	CLA	MG-NB	-2.05	2.01	2.05
13	r	506	CLA	CMD-C2D	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	2002	PQN	C11-C3	2.05	1.55	1.51
13	B	1212	CLA	C3B-C4B	2.05	1.48	1.42
20	Y	822	SQD	O2-C2	-2.05	1.37	1.43
13	t	510	CLA	MG-NB	-2.05	2.01	2.05
13	e	1133	CLA	CMC-C2C	-2.05	1.46	1.50
13	r	519	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	1138	CLA	MG-NB	-2.05	2.01	2.05
13	2	518	CLA	CMC-C2C	-2.05	1.46	1.50
13	5	517	CLA	CMB-C2B	-2.05	1.46	1.50
13	H	1202	CLA	CMB-C2B	-2.05	1.46	1.50
13	A	1237	CLA	C3B-C4B	2.05	1.48	1.42
13	4	501	CLA	CMD-C2D	-2.05	1.46	1.50
13	2	516	CLA	CMB-C2B	-2.05	1.46	1.50
13	Z	504	CLA	CMC-C2C	-2.05	1.46	1.50
13	B	1221	CLA	MG-ND	-2.05	2.01	2.05
13	4	513	CLA	MG-NB	-2.05	2.01	2.05
13	s	512	CLA	MG-ND	-2.05	2.01	2.05
13	d	507	CLA	CHC-C1C	2.05	1.42	1.38
13	e	1119	CLA	C1B-NB	-2.05	1.35	1.37
13	4	513	CLA	CMB-C2B	-2.05	1.46	1.50
13	5	507	CLA	CMB-C2B	-2.05	1.46	1.50
13	d	513	CLA	CMB-C2B	-2.05	1.46	1.50
13	u	519	CLA	CMB-C2B	-2.05	1.46	1.50
13	c	509	CLA	MG-NB	-2.05	2.01	2.05
20	4	822	SQD	O2-C2	-2.05	1.37	1.43
13	A	1102	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	1801	CLA	CMD-C2D	-2.05	1.46	1.50
13	5	506	CLA	CMD-C2D	-2.05	1.46	1.50
13	v	513	CLA	CMB-C2B	-2.05	1.46	1.50
13	6	506	CLA	CMC-C2C	-2.05	1.46	1.50
13	d	510	CLA	CMD-C2D	-2.05	1.46	1.50
13	q	510	CLA	CMD-C2D	-2.05	1.46	1.50
13	G	1119	CLA	C1B-NB	-2.05	1.35	1.37
13	b	518	CLA	CMC-C2C	-2.05	1.46	1.50
13	V	1503	CLA	MG-NB	-2.05	2.01	2.05
13	f	1216	CLA	CHC-C1C	2.05	1.42	1.38
13	4	517	CLA	CMD-C2D	-2.05	1.46	1.50
20	L	5216	SQD	O2-C2	-2.05	1.37	1.43
13	A	1115	CLA	CHC-C1C	2.05	1.42	1.38
13	c	507	CLA	C3B-C4B	2.05	1.48	1.42
13	Z	518	CLA	CMC-C2C	-2.05	1.46	1.50
13	t	501	CLA	MG-NB	-2.05	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	502	CLA	CHC-C1C	2.05	1.42	1.38
13	u	516	CLA	CMB-C2B	-2.05	1.46	1.50
13	G	1117	CLA	C1B-NB	-2.05	1.35	1.37
13	s	501	CLA	CHC-C1C	2.05	1.42	1.38
13	5	501	CLA	CMD-C2D	-2.05	1.46	1.50
13	t	518	CLA	CMC-C2C	-2.05	1.46	1.50
13	v	516	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	501	CLA	MG-NB	-2.05	2.01	2.05
13	B	1238	CLA	CHC-C1C	2.05	1.42	1.38
13	v	507	CLA	CHC-C1C	2.05	1.42	1.38
13	r	505	CLA	CHC-C1C	2.05	1.42	1.38
13	t	519	CLA	CHC-C1C	2.05	1.42	1.38
13	H	1221	CLA	MG-ND	-2.05	2.01	2.05
13	H	1224	CLA	C3B-C4B	2.05	1.48	1.42
13	A	1112	CLA	C1B-C2B	2.05	1.47	1.43
20	n	5216	SQD	O2-C2	-2.05	1.37	1.43
13	a	513	CLA	CMB-C2B	-2.05	1.46	1.50
13	5	509	CLA	MG-NB	-2.05	2.01	2.05
13	G	1102	CLA	CMD-C2D	-2.05	1.46	1.50
13	b	513	CLA	CMB-C2B	-2.05	1.46	1.50
13	d	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	e	1115	CLA	CHC-C1C	2.05	1.42	1.38
13	Y	509	CLA	MG-NB	-2.05	2.01	2.05
13	q	509	CLA	MG-NB	-2.05	2.01	2.05
20	d	822	SQD	O4-C4	-2.05	1.37	1.43
13	2	516	CLA	CMC-C2C	-2.05	1.46	1.50
13	d	505	CLA	MG-NB	-2.05	2.01	2.05
13	A	1117	CLA	C3B-C4B	2.05	1.48	1.42
13	s	505	CLA	CMC-C2C	-2.05	1.46	1.50
13	f	1220	CLA	MG-NB	-2.04	2.01	2.05
13	H	1228	CLA	C3B-C4B	2.04	1.48	1.42
13	5	501	CLA	CMB-C2B	-2.04	1.46	1.50
13	c	504	CLA	CMD-C2D	-2.04	1.46	1.50
13	c	509	CLA	CMB-C2B	-2.04	1.46	1.50
13	5	507	CLA	C3B-C4B	2.04	1.48	1.42
13	f	1213	CLA	CMB-C2B	-2.04	1.46	1.50
13	f	1217	CLA	CMC-C2C	-2.04	1.46	1.50
13	s	511	CLA	CMC-C2C	-2.04	1.46	1.50
13	s	517	CLA	MG-NB	-2.04	2.01	2.05
13	e	1127	CLA	C3B-C4B	2.04	1.48	1.42
13	H	1238	CLA	C1B-NB	-2.04	1.35	1.37
13	e	1129	CLA	C4B-NB	2.04	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	509	CLA	CMB-C2B	-2.04	1.46	1.50
13	B	1216	CLA	MG-ND	-2.04	2.01	2.05
13	Y	503	CLA	MG-NB	-2.04	2.01	2.05
13	a	516	CLA	MG-NB	-2.04	2.01	2.05
13	s	519	CLA	MG-NB	-2.04	2.01	2.05
13	H	1221	CLA	C1B-C2B	2.04	1.47	1.43
13	G	1134	CLA	CMC-C2C	-2.04	1.46	1.50
13	u	506	CLA	CMD-C2D	-2.04	1.46	1.50
13	v	503	CLA	CMB-C2B	-2.04	1.46	1.50
20	b	822	SQD	O2-C2	-2.04	1.37	1.43
13	q	507	CLA	C3B-C4B	2.04	1.48	1.42
13	A	1119	CLA	C1B-NB	-2.04	1.35	1.37
13	4	518	CLA	CMC-C2C	-2.04	1.46	1.50
13	6	501	CLA	CMC-C2C	-2.04	1.46	1.50
13	6	503	CLA	CMB-C2B	-2.04	1.46	1.50
13	6	513	CLA	CMD-C2D	-2.04	1.46	1.50
13	c	506	CLA	CMC-C2C	-2.04	1.46	1.50
13	q	510	CLA	CMB-C2B	-2.04	1.46	1.50
13	5	519	CLA	CMB-C2B	-2.04	1.46	1.50
13	f	1215	CLA	MG-ND	-2.04	2.01	2.05
13	d	501	CLA	CMC-C2C	-2.04	1.46	1.50
13	v	505	CLA	CMC-C2C	-2.04	1.46	1.50
13	H	1203	CLA	C1B-NB	-2.04	1.35	1.37
13	H	1212	CLA	C3B-C4B	2.04	1.48	1.42
13	G	1137	CLA	CMD-C2D	-2.04	1.46	1.50
13	t	501	CLA	CMB-C2B	-2.04	1.46	1.50
13	4	510	CLA	MG-NB	-2.04	2.01	2.05
13	c	517	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	1801	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	1129	CLA	C4B-NB	2.04	1.40	1.37
20	6	822	SQD	O4-C4	-2.04	1.37	1.43
20	d	822	SQD	O2-C2	-2.04	1.37	1.43
20	q	822	SQD	O2-C2	-2.04	1.37	1.43
13	L	1503	CLA	MG-NB	-2.04	2.01	2.05
13	5	516	CLA	MG-NB	-2.04	2.01	2.05
13	e	1133	CLA	MG-ND	-2.04	2.01	2.05
13	1	506	CLA	CMD-C2D	-2.04	1.46	1.50
13	H	1208	CLA	CMC-C2C	-2.04	1.46	1.50
13	j	1302	CLA	CMC-C2C	-2.04	1.46	1.50
13	G	1123	CLA	CMB-C2B	-2.04	1.46	1.50
13	e	1117	CLA	C3B-C4B	2.04	1.48	1.42
13	H	1202	CLA	C1B-NB	-2.04	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1220	CLA	MG-NB	-2.04	2.01	2.05
13	b	517	CLA	MG-NB	-2.04	2.01	2.05
13	A	1116	CLA	CMB-C2B	-2.04	1.46	1.50
13	c	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	r	510	CLA	CMB-C2B	-2.04	1.46	1.50
13	B	1235	CLA	CHC-C1C	2.04	1.42	1.38
13	a	512	CLA	CHC-C1C	2.04	1.42	1.38
13	B	1217	CLA	CMC-C2C	-2.04	1.46	1.50
13	1	503	CLA	CMB-C2B	-2.04	1.46	1.50
13	H	1223	CLA	CMB-C2B	-2.04	1.46	1.50
13	q	516	CLA	CMB-C2B	-2.04	1.46	1.50
13	e	1237	CLA	C3B-C4B	2.04	1.48	1.42
13	Z	510	CLA	CMB-C2B	-2.04	1.46	1.50
13	b	501	CLA	CMD-C2D	-2.04	1.46	1.50
13	u	501	CLA	CMD-C2D	-2.04	1.46	1.50
13	H	1215	CLA	MG-ND	-2.04	2.01	2.05
13	B	1228	CLA	C3B-C4B	2.04	1.48	1.42
13	A	1132	CLA	MG-ND	-2.04	2.01	2.05
13	d	509	CLA	MG-NB	-2.04	2.01	2.05
13	A	1109	CLA	C3B-C4B	2.04	1.48	1.42
20	c	822	SQD	O2-C2	-2.04	1.37	1.43
13	f	1228	CLA	CHC-C1C	2.04	1.42	1.38
13	F	1302	CLA	CMC-C2C	-2.04	1.46	1.50
13	G	1117	CLA	C3B-C4B	2.04	1.48	1.42
13	a	508	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1137	CLA	CMD-C2D	-2.04	1.46	1.50
13	2	510	CLA	CMB-C2B	-2.04	1.46	1.50
13	q	503	CLA	CMB-C2B	-2.04	1.46	1.50
20	a	822	SQD	O3-C3	-2.04	1.37	1.43
13	2	507	CLA	CMC-C2C	-2.04	1.46	1.50
13	d	504	CLA	CMD-C2D	-2.04	1.46	1.50
13	f	1219	CLA	CMC-C2C	-2.04	1.46	1.50
13	r	516	CLA	CMC-C2C	-2.04	1.46	1.50
13	4	517	CLA	MG-NB	-2.04	2.01	2.05
13	f	1235	CLA	C3B-C4B	2.04	1.48	1.42
16	c	523	BCR	C1-C6	-2.04	1.51	1.53
13	2	503	CLA	CMC-C2C	-2.03	1.46	1.50
13	6	506	CLA	CMD-C2D	-2.03	1.46	1.50
13	d	503	CLA	MG-NB	-2.03	2.01	2.05
13	G	1109	CLA	C3B-C4B	2.03	1.48	1.42
13	6	509	CLA	CMB-C2B	-2.03	1.46	1.50
13	3	501	CLA	MG-NB	-2.03	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	505	CLA	CMC-C2C	-2.03	1.46	1.50
13	H	1217	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	1116	CLA	CMB-C2B	-2.03	1.46	1.50
13	G	1126	CLA	CMC-C2C	-2.03	1.46	1.50
20	6	822	SQD	O2-C2	-2.03	1.37	1.43
13	2	505	CLA	CHC-C1C	2.03	1.42	1.38
13	B	1224	CLA	C3B-C4B	2.03	1.48	1.42
13	2	509	CLA	MG-NB	-2.03	2.01	2.05
13	G	1116	CLA	MG-ND	-2.03	2.01	2.05
13	v	516	CLA	MG-NB	-2.03	2.01	2.05
13	e	1118	CLA	C3B-C4B	2.03	1.48	1.42
20	b	822	SQD	O3-C3	-2.03	1.37	1.43
13	Y	510	CLA	CMC-C2C	-2.03	1.46	1.50
13	d	507	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	1221	CLA	CMA-C3A	-2.03	1.48	1.53
13	f	1204	CLA	C3B-C4B	2.03	1.48	1.42
13	B	1219	CLA	CMC-C2C	-2.03	1.46	1.50
13	5	504	CLA	CMD-C2D	-2.03	1.46	1.50
13	d	504	CLA	CMB-C2B	-2.03	1.46	1.50
13	H	1235	CLA	CHC-C1C	2.03	1.42	1.38
13	b	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	G	1115	CLA	CHC-C1C	2.03	1.42	1.38
17	e	5006	LHG	O7-C5	-2.03	1.41	1.46
13	B	1215	CLA	MG-ND	-2.03	2.01	2.05
13	B	1223	CLA	C1B-NB	-2.03	1.35	1.37
13	B	1202	CLA	CMB-C2B	-2.03	1.46	1.50
13	6	505	CLA	CMC-C2C	-2.03	1.46	1.50
13	6	507	CLA	CHC-C1C	2.03	1.42	1.38
13	B	1204	CLA	C3B-C4B	2.03	1.48	1.42
13	B	1221	CLA	CMA-C3A	-2.03	1.48	1.53
13	a	509	CLA	MG-NB	-2.03	2.01	2.05
13	B	1223	CLA	CMB-C2B	-2.03	1.46	1.50
13	3	511	CLA	CMC-C2C	-2.03	1.46	1.50
13	v	504	CLA	CMD-C2D	-2.03	1.46	1.50
13	v	509	CLA	CMB-C2B	-2.03	1.46	1.50
14	G	2001	PQN	C5-C4	-2.03	1.44	1.48
13	H	1021	CLA	MG-ND	-2.03	2.01	2.05
13	H	1236	CLA	CMC-C2C	-2.03	1.46	1.50
13	Z	502	CLA	CMC-C2C	-2.03	1.46	1.50
13	c	501	CLA	CMB-C2B	-2.03	1.46	1.50
13	e	1106	CLA	CHC-C1C	2.03	1.42	1.38
13	B	1235	CLA	C3B-C4B	2.03	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	1221	CLA	CMA-C3A	-2.03	1.48	1.53
13	r	501	CLA	MG-NB	-2.03	2.01	2.05
13	H	1235	CLA	C3B-C4B	2.03	1.48	1.42
13	s	502	CLA	CMC-C2C	-2.03	1.46	1.50
13	H	1012	CLA	MG-ND	-2.03	2.01	2.05
13	G	1107	CLA	C1B-NB	-2.03	1.35	1.37
13	a	511	CLA	CMC-C2C	-2.03	1.46	1.50
13	q	502	CLA	CMC-C2C	-2.03	1.46	1.50
13	A	1103	CLA	CHC-C1C	2.03	1.42	1.38
13	6	516	CLA	MG-NB	-2.03	2.01	2.05
13	1	510	CLA	CMB-C2B	-2.03	1.46	1.50
13	B	1238	CLA	C1B-NB	-2.03	1.35	1.37
13	q	505	CLA	CMB-C2B	-2.03	1.46	1.50
20	v	822	SQD	O2-C2	-2.03	1.37	1.43
13	G	1801	CLA	CMD-C2D	-2.03	1.46	1.50
13	v	513	CLA	CMD-C2D	-2.03	1.46	1.50
13	A	1107	CLA	C3B-C4B	2.03	1.48	1.42
13	e	1103	CLA	CHC-C1C	2.03	1.42	1.38
13	G	1118	CLA	C3B-C4B	2.03	1.48	1.42
20	4	822	SQD	O3-C3	-2.03	1.37	1.43
13	t	507	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	1208	CLA	CHC-C1C	2.03	1.42	1.38
13	d	512	CLA	CMC-C2C	-2.03	1.46	1.50
13	5	508	CLA	CHC-C1C	2.03	1.42	1.38
13	1	510	CLA	CMC-C2C	-2.02	1.46	1.50
13	H	1238	CLA	CHC-C1C	2.02	1.42	1.38
13	r	511	CLA	MG-NB	-2.02	2.01	2.05
17	G	5006	LHG	O7-C5	-2.02	1.41	1.46
13	A	1127	CLA	CMB-C2B	-2.02	1.46	1.50
13	Y	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	1208	CLA	CHC-C1C	2.02	1.42	1.38
20	b	822	SQD	O4-C4	-2.02	1.37	1.43
20	t	822	SQD	O3-C3	-2.02	1.37	1.43
13	3	504	CLA	CMC-C2C	-2.02	1.46	1.50
13	4	507	CLA	CMB-C2B	-2.02	1.46	1.50
13	f	1202	CLA	CMB-C2B	-2.02	1.46	1.50
13	3	506	CLA	CHC-C1C	2.02	1.42	1.38
13	e	1107	CLA	CHC-C1C	2.02	1.42	1.38
13	A	1118	CLA	C3B-C4B	2.02	1.48	1.42
13	1	507	CLA	C3B-C4B	2.02	1.48	1.42
20	3	822	SQD	O3-C3	-2.02	1.37	1.43
20	v	822	SQD	O4-C4	-2.02	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	507	CLA	C3B-C4B	2.02	1.48	1.42
13	Z	503	CLA	CMC-C2C	-2.02	1.46	1.50
13	e	1127	CLA	CMB-C2B	-2.02	1.46	1.50
13	A	1133	CLA	CMC-C2C	-2.02	1.46	1.50
13	A	1133	CLA	MG-ND	-2.02	2.01	2.05
13	e	1116	CLA	MG-ND	-2.02	2.01	2.05
13	G	1011	CLA	C3B-C4B	2.02	1.48	1.42
13	e	1109	CLA	C3B-C4B	2.02	1.48	1.42
20	s	822	SQD	O3-C3	-2.02	1.38	1.43
13	a	505	CLA	CMC-C2C	-2.02	1.46	1.50
13	t	517	CLA	MG-NB	-2.02	2.01	2.05
13	d	518	CLA	CMC-C2C	-2.02	1.46	1.50
13	e	1112	CLA	C1B-C2B	2.02	1.47	1.43
13	H	1204	CLA	CMB-C2B	-2.02	1.46	1.50
13	t	501	CLA	CMD-C2D	-2.02	1.46	1.50
13	f	1238	CLA	C1B-NB	-2.02	1.35	1.37
16	k	4018	BCR	C30-C25	-2.02	1.51	1.53
13	f	1217	CLA	C3B-C4B	2.02	1.48	1.42
13	G	1116	CLA	CMB-C2B	-2.02	1.46	1.50
13	t	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	1	509	CLA	MG-NB	-2.02	2.01	2.05
13	A	1106	CLA	CHC-C1C	2.02	1.42	1.38
13	A	1135	CLA	C1B-NB	-2.02	1.35	1.37
16	S	4018	BCR	C30-C25	-2.02	1.51	1.53
13	A	1011	CLA	C3B-C4B	2.02	1.48	1.42
13	e	1107	CLA	C3B-C4B	2.02	1.48	1.42
13	b	502	CLA	CMC-C2C	-2.02	1.46	1.50
13	d	505	CLA	CMC-C2C	-2.02	1.46	1.50
13	G	1107	CLA	C3B-C4B	2.02	1.48	1.42
13	H	1219	CLA	CMC-C2C	-2.02	1.46	1.50
13	3	502	CLA	CMC-C2C	-2.02	1.46	1.50
13	6	512	CLA	CMC-C2C	-2.02	1.46	1.50
13	d	517	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	1852	SQD	O4-C4	-2.02	1.38	1.43
13	4	502	CLA	MG-NB	-2.02	2.01	2.05
13	B	1240	CLA	CMC-C2C	-2.02	1.46	1.50
13	s	505	CLA	CMB-C2B	-2.02	1.46	1.50
13	t	517	CLA	CMB-C2B	-2.02	1.46	1.50
13	G	1106	CLA	CHC-C1C	2.02	1.42	1.38
13	B	1228	CLA	CHC-C1C	2.02	1.42	1.38
13	s	512	CLA	CHC-C1C	2.02	1.42	1.38
13	2	505	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)
13	5	505	CLA	CMC-C2C	-2.02	1.46	1.50
17	A	5006	LHG	O7-C5	-2.02	1.41	1.46
13	b	502	CLA	MG-NB	-2.02	2.01	2.05
13	t	504	CLA	MG-NB	-2.02	2.01	2.05
13	A	1123	CLA	CMB-C2B	-2.02	1.46	1.50
13	3	512	CLA	MG-ND	-2.02	2.01	2.05
13	d	516	CLA	MG-NB	-2.02	2.01	2.05
13	c	519	CLA	CMB-C2B	-2.01	1.46	1.50
13	f	1224	CLA	C3B-C4B	2.01	1.48	1.42
13	t	509	CLA	MG-NB	-2.01	2.01	2.05
13	3	502	CLA	CHC-C1C	2.01	1.42	1.38
13	d	511	CLA	CMC-C2C	-2.01	1.46	1.50
13	Z	509	CLA	MG-NB	-2.01	2.01	2.05
13	e	1011	CLA	C3B-C4B	2.01	1.48	1.42
13	H	1228	CLA	CHC-C1C	2.01	1.42	1.38
13	c	508	CLA	CHC-C1C	2.01	1.42	1.38
13	6	504	CLA	CMB-C2B	-2.01	1.46	1.50
13	r	507	CLA	C3B-C4B	2.01	1.48	1.42
13	e	1135	CLA	C1B-NB	-2.01	1.35	1.37
13	b	509	CLA	CHC-C1C	2.01	1.42	1.38
13	e	1113	CLA	CHC-C1C	2.01	1.42	1.38
13	Z	507	CLA	CMC-C2C	-2.01	1.46	1.50
13	r	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	H	1204	CLA	C3B-C4B	2.01	1.48	1.42
13	b	512	CLA	CHC-C1C	2.01	1.42	1.38
13	v	519	CLA	CMD-C2D	-2.01	1.46	1.50
13	6	513	CLA	CMC-C2C	-2.01	1.46	1.50
13	a	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	1135	CLA	CMB-C2B	-2.01	1.46	1.50
13	H	1240	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	1135	CLA	CMC-C2C	-2.01	1.46	1.50
13	H	1211	CLA	CMB-C2B	-2.01	1.46	1.50
13	d	506	CLA	CMD-C2D	-2.01	1.46	1.50
13	4	516	CLA	MG-NB	-2.01	2.01	2.05
13	H	1212	CLA	MG-ND	-2.01	2.01	2.05
13	B	1204	CLA	CMB-C2B	-2.01	1.46	1.50
13	B	1208	CLA	CMC-C2C	-2.01	1.46	1.50
13	6	519	CLA	CMB-C2B	-2.01	1.46	1.50
20	f	1852	SQD	O4-C4	-2.01	1.38	1.43
13	b	517	CLA	CMD-C2D	-2.01	1.46	1.50
13	v	513	CLA	CMC-C2C	-2.01	1.46	1.50
13	Z	505	CLA	CHC-C1C	2.01	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	1121	CLA	CHC-C1C	2.01	1.42	1.38
13	B	1217	CLA	C3B-C4B	2.01	1.48	1.42
13	c	516	CLA	MG-NB	-2.01	2.01	2.05
13	e	1137	CLA	CMD-C2D	-2.01	1.46	1.50
13	f	1223	CLA	CMB-C2B	-2.01	1.46	1.50
13	4	509	CLA	CHC-C1C	2.01	1.42	1.38
13	a	506	CLA	CHC-C1C	2.01	1.42	1.38
13	G	1127	CLA	CMB-C2B	-2.01	1.46	1.50
13	Y	506	CLA	CMD-C2D	-2.01	1.46	1.50
13	v	509	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	1129	CLA	C4B-NB	2.01	1.40	1.37
13	B	1021	CLA	MG-ND	-2.01	2.01	2.05
13	b	516	CLA	MG-NB	-2.01	2.01	2.05
13	1	508	CLA	CHC-C1C	2.01	1.42	1.38
13	e	1135	CLA	CMC-C2C	-2.01	1.46	1.50
13	t	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	510	CLA	CMB-C2B	-2.01	1.46	1.50
13	f	1211	CLA	CMB-C2B	-2.01	1.46	1.50
13	B	1218	CLA	CHC-C1C	2.01	1.42	1.38
13	4	517	CLA	CMB-C2B	-2.01	1.46	1.50
13	Y	511	CLA	CMC-C2C	-2.01	1.46	1.50
13	s	504	CLA	CMC-C2C	-2.01	1.46	1.50
13	4	509	CLA	MG-NB	-2.01	2.01	2.05
13	2	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	A	1104	CLA	CHC-C1C	2.01	1.42	1.38
13	A	1011	CLA	CMC-C2C	-2.01	1.46	1.50
13	1	502	CLA	CMC-C2C	-2.01	1.46	1.50
13	4	510	CLA	CMB-C2B	-2.01	1.46	1.50
13	e	1133	CLA	C3B-C4B	2.01	1.48	1.42
13	b	503	CLA	MG-NB	-2.01	2.01	2.05
13	c	505	CLA	MG-NB	-2.01	2.01	2.05
13	B	1236	CLA	CHC-C1C	2.01	1.42	1.38
13	A	1107	CLA	CHC-C1C	2.00	1.42	1.38
13	A	1107	CLA	C1B-NB	-2.00	1.35	1.37
13	A	1135	CLA	CMB-C2B	-2.00	1.46	1.50
13	e	1123	CLA	CMB-C2B	-2.00	1.46	1.50
13	G	1109	CLA	CHC-C1C	2.00	1.42	1.38
13	A	1135	CLA	CMC-C2C	-2.00	1.46	1.50
13	4	504	CLA	CMB-C2B	-2.00	1.46	1.50
13	H	1216	CLA	MG-ND	-2.00	2.01	2.05
13	b	507	CLA	CHC-C1C	2.00	1.42	1.38
13	3	516	CLA	CMB-C2B	-2.00	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	516	CLA	MG-NB	-2.00	2.01	2.05
13	G	1133	CLA	C3B-C4B	2.00	1.48	1.42
13	V	1501	CLA	CHC-C1C	2.00	1.42	1.38
13	G	1135	CLA	C1B-NB	-2.00	1.35	1.37
13	e	1129	CLA	C1B-C2B	2.00	1.47	1.43
13	G	1107	CLA	CHC-C1C	2.00	1.42	1.38
13	6	518	CLA	CMC-C2C	-2.00	1.46	1.50
13	1	518	CLA	MG-ND	-2.00	2.01	2.05
13	f	1021	CLA	MG-ND	-2.00	2.01	2.05
13	u	508	CLA	CHC-C1C	2.00	1.42	1.38
13	B	1236	CLA	CMC-C2C	-2.00	1.46	1.50
13	R	1302	CLA	CMC-C2C	-2.00	1.46	1.50
13	f	1240	CLA	CMC-C2C	-2.00	1.46	1.50
13	A	1113	CLA	CHC-C1C	2.00	1.42	1.38
13	Y	508	CLA	CHC-C1C	2.00	1.42	1.38
20	d	822	SQD	O3-C3	-2.00	1.38	1.43
13	G	1106	CLA	C1B-NB	-2.00	1.35	1.37
13	G	1115	CLA	C3B-C4B	2.00	1.48	1.42
13	c	510	CLA	CMC-C2C	-2.00	1.46	1.50
20	4	822	SQD	O4-C4	-2.00	1.38	1.43
13	A	1133	CLA	C3B-C4B	2.00	1.48	1.42
13	Z	507	CLA	C3B-C4B	2.00	1.48	1.42
13	6	511	CLA	CMC-C2C	-2.00	1.46	1.50
13	6	516	CLA	CMB-C2B	-2.00	1.46	1.50
13	b	507	CLA	CMB-C2B	-2.00	1.46	1.50
13	c	505	CLA	CMC-C2C	-2.00	1.46	1.50
13	d	507	CLA	CMC-C2C	-2.00	1.46	1.50
13	r	511	CLA	CMC-C2C	-2.00	1.46	1.50
13	G	1121	CLA	MG-ND	-2.00	2.01	2.05
13	3	512	CLA	CHC-C1C	2.00	1.42	1.38
13	q	508	CLA	CHC-C1C	2.00	1.42	1.38

All (6786) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1211	CLA	C4A-NA-C1A	8.92	110.75	106.68
13	B	1211	CLA	C4A-NA-C1A	8.81	110.70	106.68
13	f	1211	CLA	C4A-NA-C1A	8.77	110.68	106.68
14	f	2002	PQN	C11-C12-C13	-8.72	111.81	126.83
14	B	2002	PQN	C11-C12-C13	-8.72	111.81	126.83
14	H	2002	PQN	C11-C12-C13	-8.70	111.85	126.83
13	G	1120	CLA	C4A-NA-C1A	8.18	110.41	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1120	CLA	C4A-NA-C1A	8.15	110.40	106.68
13	A	1120	CLA	C4A-NA-C1A	8.15	110.39	106.68
13	G	1103	CLA	C4A-NA-C1A	8.14	110.39	106.68
13	A	1103	CLA	C4A-NA-C1A	8.12	110.38	106.68
13	A	1115	CLA	C4A-NA-C1A	8.09	110.37	106.68
13	e	1103	CLA	C4A-NA-C1A	8.06	110.36	106.68
13	e	1115	CLA	C4A-NA-C1A	8.06	110.36	106.68
13	B	1023	CLA	C4A-NA-C1A	8.05	110.35	106.68
13	G	1115	CLA	C4A-NA-C1A	8.05	110.35	106.68
13	f	1201	CLA	C4A-NA-C1A	8.04	110.34	106.68
13	H	1023	CLA	C4A-NA-C1A	8.03	110.34	106.68
13	B	1201	CLA	C4A-NA-C1A	8.02	110.34	106.68
13	H	1201	CLA	C4A-NA-C1A	8.02	110.34	106.68
13	f	1023	CLA	C4A-NA-C1A	7.97	110.32	106.68
13	1	518	CLA	C4A-NA-C1A	7.90	110.28	106.68
13	q	518	CLA	C4A-NA-C1A	7.88	110.28	106.68
13	f	1231	CLA	C4A-NA-C1A	7.85	110.26	106.68
13	B	1224	CLA	C4A-NA-C1A	7.84	110.25	106.68
13	f	1224	CLA	C4A-NA-C1A	7.81	110.24	106.68
13	f	1206	CLA	C4A-NA-C1A	7.80	110.24	106.68
13	B	1206	CLA	C4A-NA-C1A	7.79	110.23	106.68
13	A	1109	CLA	C4A-NA-C1A	7.78	110.23	106.68
13	Y	518	CLA	C4A-NA-C1A	7.76	110.22	106.68
13	G	1109	CLA	C4A-NA-C1A	7.76	110.22	106.68
13	H	1206	CLA	C4A-NA-C1A	7.74	110.21	106.68
13	B	1231	CLA	C4A-NA-C1A	7.73	110.20	106.68
13	e	1109	CLA	C4A-NA-C1A	7.72	110.20	106.68
13	H	1224	CLA	C4A-NA-C1A	7.71	110.20	106.68
13	f	1212	CLA	C4A-NA-C1A	7.68	110.18	106.68
13	H	1231	CLA	C4A-NA-C1A	7.68	110.18	106.68
13	H	1239	CLA	C4A-NA-C1A	7.68	110.18	106.68
14	e	2001	PQN	C11-C12-C13	-7.64	113.67	126.83
13	B	1213	CLA	C4A-NA-C1A	7.63	110.16	106.68
13	e	1125	CLA	C4A-NA-C1A	7.63	110.16	106.68
14	G	2001	PQN	C11-C12-C13	-7.62	113.70	126.83
13	B	1239	CLA	C4A-NA-C1A	7.62	110.16	106.68
13	B	1212	CLA	C4A-NA-C1A	7.61	110.15	106.68
13	V	1502	CLA	C4A-NA-C1A	7.60	110.15	106.68
14	A	2001	PQN	C11-C12-C13	-7.60	113.73	126.83
13	H	1212	CLA	C4A-NA-C1A	7.60	110.15	106.68
13	H	1213	CLA	C4A-NA-C1A	7.60	110.14	106.68
13	G	1105	CLA	C4A-NA-C1A	7.59	110.14	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	1502	CLA	C4A-NA-C1A	7.58	110.14	106.68
13	H	1235	CLA	C4A-NA-C1A	7.57	110.13	106.68
13	f	1213	CLA	C4A-NA-C1A	7.56	110.13	106.68
13	B	1235	CLA	C4A-NA-C1A	7.56	110.13	106.68
13	a	501	CLA	C4A-NA-C1A	7.56	110.13	106.68
13	4	502	CLA	C4A-NA-C1A	7.54	110.12	106.68
13	n	1502	CLA	C4A-NA-C1A	7.54	110.12	106.68
13	A	1125	CLA	C4A-NA-C1A	7.53	110.12	106.68
13	f	1214	CLA	C4A-NA-C1A	7.52	110.11	106.68
13	A	1105	CLA	C4A-NA-C1A	7.52	110.11	106.68
13	e	1113	CLA	C4A-NA-C1A	7.51	110.11	106.68
13	f	1239	CLA	C4A-NA-C1A	7.51	110.11	106.68
13	G	1125	CLA	C4A-NA-C1A	7.51	110.10	106.68
13	f	1235	CLA	C4A-NA-C1A	7.51	110.10	106.68
13	H	1208	CLA	C4A-NA-C1A	7.50	110.10	106.68
13	3	501	CLA	C4A-NA-C1A	7.49	110.10	106.68
13	t	502	CLA	C4A-NA-C1A	7.49	110.10	106.68
13	H	1228	CLA	C4A-NA-C1A	7.48	110.09	106.68
13	b	502	CLA	C4A-NA-C1A	7.48	110.09	106.68
13	A	1113	CLA	C4A-NA-C1A	7.47	110.09	106.68
13	e	1105	CLA	C4A-NA-C1A	7.47	110.09	106.68
13	f	1208	CLA	C4A-NA-C1A	7.45	110.08	106.68
13	s	501	CLA	C4A-NA-C1A	7.45	110.08	106.68
13	B	1228	CLA	C4A-NA-C1A	7.45	110.08	106.68
13	G	1113	CLA	C4A-NA-C1A	7.44	110.07	106.68
13	H	1214	CLA	C4A-NA-C1A	7.43	110.07	106.68
13	B	1208	CLA	C4A-NA-C1A	7.43	110.07	106.68
13	G	1137	CLA	C4A-NA-C1A	7.40	110.06	106.68
13	d	502	CLA	C4A-NA-C1A	7.40	110.06	106.68
13	f	1228	CLA	C4A-NA-C1A	7.40	110.06	106.68
13	6	502	CLA	C4A-NA-C1A	7.40	110.05	106.68
13	3	502	CLA	C4A-NA-C1A	7.39	110.05	106.68
13	G	1133	CLA	C4A-NA-C1A	7.39	110.05	106.68
13	V	1501	CLA	C4A-NA-C1A	7.38	110.05	106.68
13	a	502	CLA	C4A-NA-C1A	7.38	110.05	106.68
13	B	1214	CLA	C4A-NA-C1A	7.38	110.05	106.68
13	v	502	CLA	C4A-NA-C1A	7.37	110.04	106.68
13	L	1501	CLA	C4A-NA-C1A	7.36	110.03	106.68
13	n	1501	CLA	C4A-NA-C1A	7.35	110.03	106.68
13	f	1223	CLA	C4A-NA-C1A	7.35	110.03	106.68
13	A	1137	CLA	C4A-NA-C1A	7.33	110.02	106.68
13	B	1223	CLA	C4A-NA-C1A	7.31	110.02	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	1503	CLA	C4A-NA-C1A	7.31	110.01	106.68
13	B	1202	CLA	C4A-NA-C1A	7.31	110.01	106.68
13	t	517	CLA	C4A-NA-C1A	7.30	110.01	106.68
13	A	1133	CLA	C4A-NA-C1A	7.29	110.01	106.68
13	e	1138	CLA	C4A-NA-C1A	7.29	110.01	106.68
13	s	509	CLA	C4A-NA-C1A	7.29	110.01	106.68
13	A	1138	CLA	C4A-NA-C1A	7.29	110.00	106.68
13	c	501	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	f	1215	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	f	1218	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	B	1210	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	B	1215	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	2	502	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	e	1133	CLA	C4A-NA-C1A	7.28	110.00	106.68
13	s	502	CLA	C4A-NA-C1A	7.27	110.00	106.68
13	4	517	CLA	C4A-NA-C1A	7.27	110.00	106.68
13	H	1202	CLA	C4A-NA-C1A	7.27	109.99	106.68
13	H	1210	CLA	C4A-NA-C1A	7.27	109.99	106.68
13	G	1138	CLA	C4A-NA-C1A	7.26	109.99	106.68
13	l	1302	CLA	C4A-NA-C1A	7.26	109.99	106.68
13	H	1218	CLA	C4A-NA-C1A	7.25	109.99	106.68
13	3	509	CLA	C4A-NA-C1A	7.24	109.98	106.68
13	H	1223	CLA	C4A-NA-C1A	7.24	109.98	106.68
13	f	1210	CLA	C4A-NA-C1A	7.24	109.98	106.68
13	u	501	CLA	C4A-NA-C1A	7.24	109.98	106.68
13	e	1137	CLA	C4A-NA-C1A	7.24	109.98	106.68
13	H	1215	CLA	C4A-NA-C1A	7.23	109.98	106.68
13	a	519	CLA	C4A-NA-C1A	7.23	109.98	106.68
13	b	517	CLA	C4A-NA-C1A	7.23	109.98	106.68
13	5	501	CLA	C4A-NA-C1A	7.22	109.97	106.68
13	B	1218	CLA	C4A-NA-C1A	7.22	109.97	106.68
13	b	518	CLA	C4A-NA-C1A	7.22	109.97	106.68
13	r	501	CLA	C4A-NA-C1A	7.21	109.97	106.68
13	3	519	CLA	C4A-NA-C1A	7.20	109.97	106.68
13	e	1801	CLA	C4A-NA-C1A	7.20	109.97	106.68
13	A	1118	CLA	C4A-NA-C1A	7.20	109.96	106.68
13	H	1205	CLA	C4A-NA-C1A	7.20	109.96	106.68
13	r	502	CLA	C4A-NA-C1A	7.20	109.96	106.68
13	f	1202	CLA	C4A-NA-C1A	7.19	109.96	106.68
13	s	519	CLA	C4A-NA-C1A	7.19	109.96	106.68
13	r	516	CLA	C4A-NA-C1A	7.19	109.96	106.68
13	L	1503	CLA	C4A-NA-C1A	7.18	109.96	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	502	CLA	C4A-NA-C1A	7.18	109.95	106.68
13	u	502	CLA	C4A-NA-C1A	7.18	109.95	106.68
13	f	1209	CLA	C4A-NA-C1A	7.18	109.95	106.68
13	e	1112	CLA	C4A-NA-C1A	7.18	109.95	106.68
13	n	1503	CLA	C4A-NA-C1A	7.18	109.95	106.68
13	s	513	CLA	C4A-NA-C1A	7.17	109.95	106.68
16	n	4019	BCR	C24-C23-C22	-7.17	115.63	126.23
13	Y	502	CLA	C4A-NA-C1A	7.17	109.95	106.68
13	A	1112	CLA	C4A-NA-C1A	7.16	109.94	106.68
13	a	509	CLA	C4A-NA-C1A	7.16	109.94	106.68
16	L	4019	BCR	C24-C23-C22	-7.15	115.65	126.23
13	t	518	CLA	C4A-NA-C1A	7.15	109.94	106.68
13	B	1227	CLA	C4A-NA-C1A	7.15	109.94	106.68
13	G	1118	CLA	C4A-NA-C1A	7.15	109.94	106.68
13	Z	501	CLA	C4A-NA-C1A	7.15	109.94	106.68
13	f	1227	CLA	C4A-NA-C1A	7.15	109.94	106.68
13	H	1209	CLA	C4A-NA-C1A	7.14	109.94	106.68
13	a	513	CLA	C4A-NA-C1A	7.14	109.94	106.68
13	Z	516	CLA	C4A-NA-C1A	7.14	109.94	106.68
13	e	1118	CLA	C4A-NA-C1A	7.13	109.93	106.68
13	A	1123	CLA	C4A-NA-C1A	7.13	109.93	106.68
13	B	1209	CLA	C4A-NA-C1A	7.13	109.93	106.68
16	V	4019	BCR	C24-C23-C22	-7.13	115.69	126.23
13	Z	518	CLA	C4A-NA-C1A	7.13	109.93	106.68
13	A	1801	CLA	C4A-NA-C1A	7.13	109.93	106.68
13	2	501	CLA	C4A-NA-C1A	7.12	109.93	106.68
13	a	512	CLA	C4A-NA-C1A	7.12	109.93	106.68
13	b	501	CLA	C4A-NA-C1A	7.12	109.93	106.68
13	s	512	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	4	518	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	2	516	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	A	1101	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	e	1101	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	H	1227	CLA	C4A-NA-C1A	7.10	109.92	106.68
13	J	1302	CLA	C4A-NA-C1A	7.10	109.92	106.68
13	G	1104	CLA	C4A-NA-C1A	7.10	109.92	106.68
13	3	513	CLA	C4A-NA-C1A	7.10	109.92	106.68
13	G	1801	CLA	C4A-NA-C1A	7.10	109.92	106.68
13	e	1123	CLA	C4A-NA-C1A	7.10	109.92	106.68
13	5	502	CLA	C4A-NA-C1A	7.09	109.91	106.68
13	A	1117	CLA	C4A-NA-C1A	7.09	109.91	106.68
13	G	1112	CLA	C4A-NA-C1A	7.09	109.91	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1101	CLA	C4A-NA-C1A	7.09	109.91	106.68
13	G	1117	CLA	C4A-NA-C1A	7.08	109.91	106.68
13	c	507	CLA	C4A-NA-C1A	7.08	109.91	106.68
13	u	508	CLA	C4A-NA-C1A	7.08	109.91	106.68
13	A	1104	CLA	C4A-NA-C1A	7.08	109.91	106.68
13	1	502	CLA	C4A-NA-C1A	7.08	109.91	106.68
13	T	1302	CLA	C4A-NA-C1A	7.08	109.91	106.68
13	2	518	CLA	C4A-NA-C1A	7.07	109.91	106.68
13	G	1106	CLA	C4A-NA-C1A	7.07	109.91	106.68
13	t	506	CLA	C4A-NA-C1A	7.07	109.91	106.68
13	5	508	CLA	C4A-NA-C1A	7.07	109.91	106.68
13	e	1117	CLA	C4A-NA-C1A	7.07	109.91	106.68
13	v	501	CLA	C4A-NA-C1A	7.07	109.91	106.68
13	B	1205	CLA	C4A-NA-C1A	7.07	109.90	106.68
13	c	508	CLA	C4A-NA-C1A	7.07	109.90	106.68
13	G	1123	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	u	505	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	u	506	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	4	509	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	q	502	CLA	C4A-NA-C1A	7.05	109.90	106.68
13	r	518	CLA	C4A-NA-C1A	7.05	109.90	106.68
13	3	512	CLA	C4A-NA-C1A	7.04	109.89	106.68
13	t	509	CLA	C4A-NA-C1A	7.04	109.89	106.68
13	A	1106	CLA	C4A-NA-C1A	7.04	109.89	106.68
13	4	506	CLA	C4A-NA-C1A	7.04	109.89	106.68
13	B	1220	CLA	C4A-NA-C1A	7.04	109.89	106.68
13	e	1106	CLA	C4A-NA-C1A	7.03	109.89	106.68
13	b	509	CLA	C4A-NA-C1A	7.03	109.89	106.68
13	t	519	CLA	C4A-NA-C1A	7.03	109.89	106.68
13	A	1122	CLA	C4A-NA-C1A	7.02	109.88	106.68
13	5	507	CLA	C4A-NA-C1A	7.02	109.88	106.68
13	e	1122	CLA	C4A-NA-C1A	7.02	109.88	106.68
13	F	1302	CLA	C4A-NA-C1A	7.02	109.88	106.68
13	Y	509	CLA	C4A-NA-C1A	7.02	109.88	106.68
13	c	502	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	l	1303	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	c	505	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	r	507	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	5	505	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	R	1302	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	6	501	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	T	1303	CLA	C4A-NA-C1A	7.01	109.88	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	5	506	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	H	1220	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	4	501	CLA	C4A-NA-C1A	7.00	109.87	106.68
13	G	1122	CLA	C4A-NA-C1A	7.00	109.87	106.68
13	d	501	CLA	C4A-NA-C1A	7.00	109.87	106.68
13	q	505	CLA	C4A-NA-C1A	7.00	109.87	106.68
13	c	506	CLA	C4A-NA-C1A	7.00	109.87	106.68
13	J	1303	CLA	C4A-NA-C1A	6.99	109.87	106.68
13	a	507	CLA	C4A-NA-C1A	6.99	109.87	106.68
13	H	1207	CLA	C4A-NA-C1A	6.98	109.86	106.68
13	1	505	CLA	C4A-NA-C1A	6.98	109.86	106.68
13	1	509	CLA	C4A-NA-C1A	6.98	109.86	106.68
13	r	517	CLA	C4A-NA-C1A	6.97	109.86	106.68
13	3	518	CLA	C4A-NA-C1A	6.97	109.86	106.68
13	b	506	CLA	C4A-NA-C1A	6.96	109.86	106.68
13	e	1104	CLA	C4A-NA-C1A	6.96	109.86	106.68
13	u	507	CLA	C4A-NA-C1A	6.96	109.86	106.68
13	4	519	CLA	C4A-NA-C1A	6.96	109.85	106.68
13	q	509	CLA	C4A-NA-C1A	6.96	109.85	106.68
13	r	513	CLA	C4A-NA-C1A	6.96	109.85	106.68
13	s	518	CLA	C4A-NA-C1A	6.96	109.85	106.68
13	t	510	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	B	1230	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	G	1134	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	f	1205	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	2	507	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	b	519	CLA	C4A-NA-C1A	6.94	109.85	106.68
13	A	1134	CLA	C4A-NA-C1A	6.94	109.85	106.68
13	H	1230	CLA	C4A-NA-C1A	6.94	109.84	106.68
13	2	517	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	e	1134	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	f	1216	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	3	507	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	f	1230	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	t	501	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	e	1136	CLA	C4A-NA-C1A	6.92	109.84	106.68
13	j	1302	CLA	C4A-NA-C1A	6.92	109.84	106.68
13	q	513	CLA	C4A-NA-C1A	6.92	109.84	106.68
13	3	511	CLA	C4A-NA-C1A	6.92	109.84	106.68
13	e	1126	CLA	C4A-NA-C1A	6.92	109.84	106.68
13	f	1220	CLA	C4A-NA-C1A	6.92	109.84	106.68
13	q	504	CLA	C4A-NA-C1A	6.92	109.84	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	513	CLA	C4A-NA-C1A	6.92	109.83	106.68
13	Y	511	CLA	C4A-NA-C1A	6.92	109.83	106.68
13	2	504	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	Z	507	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	4	510	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	Z	513	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	b	510	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	b	512	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	q	507	CLA	C4A-NA-C1A	6.91	109.83	106.68
13	A	1136	CLA	C4A-NA-C1A	6.90	109.83	106.68
13	A	1126	CLA	C4A-NA-C1A	6.90	109.83	106.68
13	f	1021	CLA	C4A-NA-C1A	6.90	109.83	106.68
13	G	1126	CLA	C4A-NA-C1A	6.90	109.83	106.68
13	4	512	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	H	1221	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	Y	505	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	B	1021	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	2	513	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	Y	508	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	v	503	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	B	1207	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	1	504	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	1	511	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	e	1114	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	Z	504	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	s	511	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	A	1114	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	6	503	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	f	1207	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	t	513	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	B	1221	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	a	511	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	u	503	CLA	C4A-NA-C1A	6.87	109.81	106.68
13	G	1114	CLA	C4A-NA-C1A	6.86	109.81	106.68
13	d	512	CLA	C4A-NA-C1A	6.86	109.81	106.68
13	a	518	CLA	C4A-NA-C1A	6.86	109.81	106.68
13	r	504	CLA	C4A-NA-C1A	6.86	109.81	106.68
13	4	513	CLA	C4A-NA-C1A	6.86	109.81	106.68
13	5	503	CLA	C4A-NA-C1A	6.85	109.81	106.68
13	3	506	CLA	C4A-NA-C1A	6.85	109.81	106.68
13	t	512	CLA	C4A-NA-C1A	6.85	109.80	106.68
13	1	503	CLA	C4A-NA-C1A	6.84	109.80	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	508	CLA	C4A-NA-C1A	6.84	109.80	106.68
13	Z	517	CLA	C4A-NA-C1A	6.84	109.80	106.68
13	f	1221	CLA	C4A-NA-C1A	6.84	109.80	106.68
13	u	516	CLA	C4A-NA-C1A	6.83	109.80	106.68
13	1	513	CLA	C4A-NA-C1A	6.83	109.80	106.68
13	G	1136	CLA	C4A-NA-C1A	6.83	109.80	106.68
13	c	516	CLA	C4A-NA-C1A	6.83	109.80	106.68
13	6	506	CLA	C4A-NA-C1A	6.83	109.79	106.68
13	a	506	CLA	C4A-NA-C1A	6.83	109.79	106.68
13	s	504	CLA	C4A-NA-C1A	6.83	109.79	106.68
13	q	508	CLA	C4A-NA-C1A	6.82	109.79	106.68
13	q	511	CLA	C4A-NA-C1A	6.82	109.79	106.68
13	Y	504	CLA	C4A-NA-C1A	6.82	109.79	106.68
13	B	1232	CLA	C4A-NA-C1A	6.82	109.79	106.68
13	q	503	CLA	C4A-NA-C1A	6.81	109.79	106.68
13	K	1105	CLA	C4A-NA-C1A	6.81	109.79	106.68
13	s	506	CLA	C4A-NA-C1A	6.81	109.79	106.68
13	1	507	CLA	C4A-NA-C1A	6.81	109.78	106.68
13	t	504	CLA	C4A-NA-C1A	6.81	109.78	106.68
13	H	1021	CLA	C4A-NA-C1A	6.81	109.78	106.68
13	H	1204	CLA	C4A-NA-C1A	6.81	109.78	106.68
13	v	512	CLA	C4A-NA-C1A	6.81	109.78	106.68
13	f	1232	CLA	C4A-NA-C1A	6.80	109.78	106.68
13	6	507	CLA	C4A-NA-C1A	6.80	109.78	106.68
13	6	512	CLA	C4A-NA-C1A	6.79	109.78	106.68
13	c	503	CLA	C4A-NA-C1A	6.79	109.78	106.68
13	c	513	CLA	C4A-NA-C1A	6.79	109.78	106.68
13	B	1216	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	B	1204	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	d	503	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	s	507	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	Z	511	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	2	511	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	b	504	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	H	1232	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	Y	507	CLA	C4A-NA-C1A	6.77	109.77	106.68
13	Y	503	CLA	C4A-NA-C1A	6.77	109.77	106.68
13	5	516	CLA	C4A-NA-C1A	6.77	109.77	106.68
13	4	504	CLA	C4A-NA-C1A	6.77	109.77	106.68
13	f	1204	CLA	C4A-NA-C1A	6.77	109.77	106.68
13	t	507	CLA	C4A-NA-C1A	6.77	109.77	106.68
13	R	1301	CLA	C4A-NA-C1A	6.76	109.77	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	v	505	CLA	C4A-NA-C1A	6.76	109.77	106.68
13	U	1105	CLA	C4A-NA-C1A	6.76	109.76	106.68
13	r	509	CLA	C4A-NA-C1A	6.76	109.76	106.68
13	3	504	CLA	C4A-NA-C1A	6.75	109.76	106.68
13	v	506	CLA	C4A-NA-C1A	6.75	109.76	106.68
13	v	507	CLA	C4A-NA-C1A	6.74	109.75	106.68
13	Y	513	CLA	C4A-NA-C1A	6.74	109.75	106.68
13	d	506	CLA	C4A-NA-C1A	6.74	109.75	106.68
13	H	1216	CLA	C4A-NA-C1A	6.73	109.75	106.68
13	5	513	CLA	C4A-NA-C1A	6.73	109.75	106.68
13	r	511	CLA	C4A-NA-C1A	6.72	109.74	106.68
13	a	504	CLA	C4A-NA-C1A	6.71	109.74	106.68
13	m	1105	CLA	C4A-NA-C1A	6.71	109.74	106.68
13	5	510	CLA	C4A-NA-C1A	6.71	109.74	106.68
13	d	507	CLA	C4A-NA-C1A	6.71	109.74	106.68
13	d	505	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	e	2001	PQN	C15-C13-C12	-6.70	106.12	121.17
13	2	509	CLA	C4A-NA-C1A	6.70	109.74	106.68
13	1	501	CLA	C4A-NA-C1A	6.70	109.74	106.68
14	G	2001	PQN	C15-C13-C12	-6.70	106.13	121.17
13	6	505	CLA	C4A-NA-C1A	6.70	109.73	106.68
13	s	505	CLA	C4A-NA-C1A	6.70	109.73	106.68
13	G	1102	CLA	C4A-NA-C1A	6.70	109.73	106.68
13	a	510	CLA	C4A-NA-C1A	6.69	109.73	106.68
13	v	504	CLA	C4A-NA-C1A	6.69	109.73	106.68
13	4	507	CLA	C4A-NA-C1A	6.69	109.73	106.68
13	Z	509	CLA	C4A-NA-C1A	6.69	109.73	106.68
14	A	2001	PQN	C15-C13-C12	-6.68	106.16	121.17
13	F	1301	CLA	C4A-NA-C1A	6.68	109.73	106.68
13	5	504	CLA	C4A-NA-C1A	6.68	109.73	106.68
13	6	504	CLA	C4A-NA-C1A	6.68	109.73	106.68
13	b	503	CLA	C4A-NA-C1A	6.68	109.72	106.68
13	u	510	CLA	C4A-NA-C1A	6.67	109.72	106.68
13	c	519	CLA	C4A-NA-C1A	6.67	109.72	106.68
13	u	504	CLA	C4A-NA-C1A	6.67	109.72	106.68
13	c	510	CLA	C4A-NA-C1A	6.67	109.72	106.68
13	1	517	CLA	C4A-NA-C1A	6.66	109.72	106.68
13	m	1401	CLA	C4A-NA-C1A	6.66	109.72	106.68
13	d	504	CLA	C4A-NA-C1A	6.66	109.72	106.68
13	A	1102	CLA	C4A-NA-C1A	6.65	109.72	106.68
13	v	511	CLA	C4A-NA-C1A	6.65	109.72	106.68
13	u	513	CLA	C4A-NA-C1A	6.65	109.71	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	d	518	CLA	C4A-NA-C1A	6.65	109.71	106.68
13	e	1102	CLA	C4A-NA-C1A	6.65	109.71	106.68
13	4	503	CLA	C4A-NA-C1A	6.64	109.71	106.68
13	b	507	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	d	519	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	q	501	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	v	519	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	Z	505	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	r	506	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	6	519	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	3	510	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	u	509	CLA	C4A-NA-C1A	6.62	109.70	106.68
13	u	519	CLA	C4A-NA-C1A	6.62	109.70	106.68
13	Y	501	CLA	C4A-NA-C1A	6.62	109.70	106.68
13	e	1131	CLA	C4A-NA-C1A	6.62	109.70	106.68
13	c	509	CLA	C4A-NA-C1A	6.62	109.70	106.68
13	v	509	CLA	C4A-NA-C1A	6.62	109.70	106.68
13	6	511	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	G	1131	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	Y	517	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	u	511	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	2	505	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	3	505	CLA	C4A-NA-C1A	6.61	109.69	106.68
13	2	506	CLA	C4A-NA-C1A	6.60	109.69	106.68
13	e	1013	CLA	C4A-NA-C1A	6.60	109.69	106.68
13	j	1301	CLA	C4A-NA-C1A	6.60	109.69	106.68
13	c	511	CLA	C4A-NA-C1A	6.60	109.69	106.68
13	G	1013	CLA	C4A-NA-C1A	6.59	109.69	106.68
13	e	1110	CLA	C4A-NA-C1A	6.59	109.69	106.68
13	v	513	CLA	C4A-NA-C1A	6.59	109.69	106.68
13	d	508	CLA	C4A-NA-C1A	6.59	109.69	106.68
13	2	512	CLA	C4A-NA-C1A	6.59	109.68	106.68
13	a	505	CLA	C4A-NA-C1A	6.59	109.68	106.68
13	5	509	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	5	519	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	a	503	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	5	511	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	A	1013	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	c	504	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	Z	506	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	U	1401	CLA	C4A-NA-C1A	6.58	109.68	106.68
13	q	517	CLA	C4A-NA-C1A	6.58	109.68	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	K	1401	CLA	C4A-NA-C1A	6.57	109.68	106.68
13	v	517	CLA	C4A-NA-C1A	6.57	109.68	106.68
13	Y	519	CLA	C4A-NA-C1A	6.57	109.68	106.68
13	s	510	CLA	C4A-NA-C1A	6.57	109.68	106.68
13	t	503	CLA	C4A-NA-C1A	6.57	109.68	106.68
13	v	508	CLA	C4A-NA-C1A	6.57	109.68	106.68
13	a	517	CLA	C4A-NA-C1A	6.56	109.67	106.68
13	A	1131	CLA	C4A-NA-C1A	6.56	109.67	106.68
13	e	1119	CLA	C4A-NA-C1A	6.56	109.67	106.68
13	A	1110	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	3	517	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	6	517	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	r	512	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	3	503	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	6	508	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	v	518	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	Z	512	CLA	C4A-NA-C1A	6.54	109.66	106.68
13	q	506	CLA	C4A-NA-C1A	6.54	109.66	106.68
13	d	511	CLA	C4A-NA-C1A	6.54	109.66	106.68
13	c	518	CLA	C4A-NA-C1A	6.54	109.66	106.68
13	G	1237	CLA	C4A-NA-C1A	6.54	109.66	106.68
13	6	518	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	s	517	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	u	518	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	A	1237	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	6	509	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	d	509	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	6	513	CLA	C4A-NA-C1A	6.52	109.66	106.68
13	r	503	CLA	C4A-NA-C1A	6.52	109.65	106.68
13	s	503	CLA	C4A-NA-C1A	6.52	109.65	106.68
13	A	1119	CLA	C4A-NA-C1A	6.51	109.65	106.68
13	1	519	CLA	C4A-NA-C1A	6.51	109.65	106.68
13	B	1240	CLA	C4A-NA-C1A	6.51	109.65	106.68
13	2	503	CLA	C4A-NA-C1A	6.51	109.65	106.68
13	q	519	CLA	C4A-NA-C1A	6.50	109.65	106.68
13	G	1110	CLA	C4A-NA-C1A	6.50	109.64	106.68
13	r	505	CLA	C4A-NA-C1A	6.49	109.64	106.68
13	d	513	CLA	C4A-NA-C1A	6.49	109.64	106.68
13	H	1240	CLA	C4A-NA-C1A	6.49	109.64	106.68
13	5	518	CLA	C4A-NA-C1A	6.49	109.64	106.68
13	1	506	CLA	C4A-NA-C1A	6.49	109.64	106.68
13	1	512	CLA	C4A-NA-C1A	6.48	109.64	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1217	CLA	C4A-NA-C1A	6.48	109.64	106.68
13	f	1217	CLA	C4A-NA-C1A	6.48	109.64	106.68
13	f	1240	CLA	C4A-NA-C1A	6.48	109.64	106.68
13	t	511	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	H	2002	PQN	C15-C13-C12	-6.48	106.63	121.17
14	B	2002	PQN	C15-C13-C12	-6.48	106.63	121.17
13	d	517	CLA	C4A-NA-C1A	6.47	109.63	106.68
13	e	1237	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	f	2002	PQN	C15-C13-C12	-6.47	106.64	121.17
13	Y	512	CLA	C4A-NA-C1A	6.46	109.63	106.68
13	4	511	CLA	C4A-NA-C1A	6.46	109.63	106.68
13	Y	506	CLA	C4A-NA-C1A	6.46	109.62	106.68
13	B	1217	CLA	C4A-NA-C1A	6.45	109.62	106.68
13	q	512	CLA	C4A-NA-C1A	6.44	109.62	106.68
13	G	1119	CLA	C4A-NA-C1A	6.43	109.61	106.68
13	Z	503	CLA	C4A-NA-C1A	6.43	109.61	106.68
13	b	505	CLA	C4A-NA-C1A	6.42	109.61	106.68
13	b	511	CLA	C4A-NA-C1A	6.41	109.60	106.68
13	H	1236	CLA	C4A-NA-C1A	6.41	109.60	106.68
13	v	510	CLA	C4A-NA-C1A	6.40	109.60	106.68
13	G	1111	CLA	C4A-NA-C1A	6.40	109.60	106.68
13	2	508	CLA	C4A-NA-C1A	6.40	109.60	106.68
13	B	1236	CLA	C4A-NA-C1A	6.39	109.59	106.68
13	c	512	CLA	C4A-NA-C1A	6.39	109.59	106.68
13	f	1236	CLA	C4A-NA-C1A	6.39	109.59	106.68
13	u	512	CLA	C4A-NA-C1A	6.39	109.59	106.68
13	r	508	CLA	C4A-NA-C1A	6.36	109.58	106.68
13	e	1111	CLA	C4A-NA-C1A	6.36	109.58	106.68
13	3	516	CLA	C4A-NA-C1A	6.35	109.58	106.68
13	4	505	CLA	C4A-NA-C1A	6.35	109.58	106.68
13	t	505	CLA	C4A-NA-C1A	6.35	109.57	106.68
13	A	1111	CLA	C4A-NA-C1A	6.33	109.57	106.68
13	G	1116	CLA	C4A-NA-C1A	6.33	109.56	106.68
16	V	4020	BCR	C24-C23-C22	-6.32	116.88	126.23
16	L	4020	BCR	C24-C23-C22	-6.32	116.89	126.23
13	d	516	CLA	C4A-NA-C1A	6.32	109.56	106.68
13	5	512	CLA	C4A-NA-C1A	6.31	109.56	106.68
13	6	510	CLA	C4A-NA-C1A	6.31	109.56	106.68
13	e	1127	CLA	C4A-NA-C1A	6.31	109.56	106.68
16	n	4020	BCR	C24-C23-C22	-6.31	116.90	126.23
13	G	1121	CLA	C4A-NA-C1A	6.31	109.56	106.68
13	s	516	CLA	C4A-NA-C1A	6.31	109.56	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	508	CLA	C4A-NA-C1A	6.30	109.55	106.68
13	a	516	CLA	C4A-NA-C1A	6.30	109.55	106.68
13	G	1124	CLA	C4A-NA-C1A	6.30	109.55	106.68
13	q	510	CLA	C4A-NA-C1A	6.30	109.55	106.68
13	4	508	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	G	1127	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	A	1121	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	6	516	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	G	1129	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	f	1234	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	v	516	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	a	508	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	B	1234	CLA	C4A-NA-C1A	6.27	109.54	106.68
13	1	510	CLA	C4A-NA-C1A	6.26	109.53	106.68
13	A	1116	CLA	C4A-NA-C1A	6.25	109.53	106.68
13	A	1129	CLA	C4A-NA-C1A	6.25	109.53	106.68
13	A	1124	CLA	C4A-NA-C1A	6.25	109.53	106.68
13	u	517	CLA	C4A-NA-C1A	6.24	109.53	106.68
13	3	508	CLA	C4A-NA-C1A	6.24	109.53	106.68
13	b	508	CLA	C4A-NA-C1A	6.23	109.52	106.68
13	5	517	CLA	C4A-NA-C1A	6.23	109.52	106.68
13	A	1127	CLA	C4A-NA-C1A	6.22	109.52	106.68
13	e	1129	CLA	C4A-NA-C1A	6.22	109.52	106.68
13	t	508	CLA	C4A-NA-C1A	6.22	109.52	106.68
13	U	1103	CLA	C4A-NA-C1A	6.21	109.51	106.68
13	d	510	CLA	C4A-NA-C1A	6.21	109.51	106.68
13	H	1238	CLA	C4A-NA-C1A	6.21	109.51	106.68
13	e	1121	CLA	C4A-NA-C1A	6.20	109.51	106.68
13	B	1238	CLA	C4A-NA-C1A	6.20	109.51	106.68
13	c	517	CLA	C4A-NA-C1A	6.20	109.51	106.68
13	A	1135	CLA	C4A-NA-C1A	6.19	109.50	106.68
13	2	519	CLA	C4A-NA-C1A	6.19	109.50	106.68
13	e	1011	CLA	C4A-NA-C1A	6.18	109.50	106.68
13	e	1116	CLA	C4A-NA-C1A	6.18	109.50	106.68
13	Y	510	CLA	C4A-NA-C1A	6.18	109.50	106.68
13	A	1011	CLA	C4A-NA-C1A	6.17	109.50	106.68
13	G	1011	CLA	C4A-NA-C1A	6.17	109.50	106.68
13	m	1103	CLA	C4A-NA-C1A	6.17	109.50	106.68
13	s	508	CLA	C4A-NA-C1A	6.17	109.49	106.68
13	K	1103	CLA	C4A-NA-C1A	6.15	109.49	106.68
13	H	1234	CLA	C4A-NA-C1A	6.15	109.48	106.68
13	f	1238	CLA	C4A-NA-C1A	6.15	109.48	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	519	CLA	C4A-NA-C1A	6.15	109.48	106.68
13	B	1229	CLA	C4A-NA-C1A	6.14	109.48	106.68
13	e	1124	CLA	C4A-NA-C1A	6.13	109.48	106.68
13	G	1135	CLA	C4A-NA-C1A	6.11	109.47	106.68
13	e	1135	CLA	C4A-NA-C1A	6.11	109.47	106.68
13	A	1130	CLA	C4A-NA-C1A	6.11	109.47	106.68
13	f	1225	CLA	C4A-NA-C1A	6.11	109.47	106.68
13	H	1229	CLA	C4A-NA-C1A	6.10	109.46	106.68
13	r	519	CLA	C4A-NA-C1A	6.10	109.46	106.68
16	G	4007	BCR	C3-C4-C5	-6.10	103.18	114.06
13	f	1229	CLA	C4A-NA-C1A	6.10	109.46	106.68
13	e	1108	CLA	C4A-NA-C1A	6.09	109.46	106.68
13	H	1226	CLA	CMB-C2B-C1B	-6.09	116.14	125.42
16	A	4007	BCR	C3-C4-C5	-6.09	103.20	114.06
13	Z	510	CLA	C4A-NA-C1A	6.08	109.45	106.68
13	B	1226	CLA	CMB-C2B-C1B	-6.08	116.16	125.42
16	e	4007	BCR	C3-C4-C5	-6.08	103.22	114.06
13	t	516	CLA	C4A-NA-C1A	6.07	109.45	106.68
13	H	1226	CLA	C4A-NA-C1A	6.07	109.45	106.68
13	f	1203	CLA	C4A-NA-C1A	6.07	109.45	106.68
13	B	1226	CLA	C4A-NA-C1A	6.06	109.45	106.68
13	f	1226	CLA	CMB-C2B-C1B	-6.06	116.19	125.42
16	G	4008	BCR	C24-C23-C22	-6.06	117.27	126.23
13	B	1225	CLA	C4A-NA-C1A	6.06	109.44	106.68
13	b	516	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	G	1130	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	e	1107	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	B	1203	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	e	1130	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	4	516	CLA	C4A-NA-C1A	6.05	109.44	106.68
16	A	4008	BCR	C24-C23-C22	-6.05	117.29	126.23
13	A	1108	CLA	C4A-NA-C1A	6.04	109.43	106.68
13	H	1203	CLA	C4A-NA-C1A	6.04	109.43	106.68
16	e	4008	BCR	C24-C23-C22	-6.03	117.31	126.23
13	G	1107	CLA	C4A-NA-C1A	6.03	109.43	106.68
13	f	1226	CLA	C4A-NA-C1A	6.03	109.43	106.68
16	B	4010	BCR	C15-C14-C13	-6.02	118.84	127.28
16	f	4010	BCR	C15-C14-C13	-6.01	118.86	127.28
13	A	1107	CLA	C4A-NA-C1A	6.00	109.42	106.68
16	v	524	BCR	C7-C8-C9	-6.00	117.36	126.23
13	G	1108	CLA	C4A-NA-C1A	5.99	109.41	106.68
16	H	4010	BCR	C15-C14-C13	-5.99	118.88	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	510	CLA	C4A-NA-C1A	5.99	109.41	106.68
16	l	4013	BCR	C20-C21-C22	-5.97	118.90	127.28
16	J	4013	BCR	C20-C21-C22	-5.97	118.91	127.28
16	T	4013	BCR	C20-C21-C22	-5.97	118.91	127.28
13	r	510	CLA	C4A-NA-C1A	5.96	109.40	106.68
16	6	524	BCR	C7-C8-C9	-5.96	117.42	126.23
16	d	524	BCR	C7-C8-C9	-5.96	117.42	126.23
13	1	516	CLA	C4A-NA-C1A	5.94	109.39	106.68
13	H	1225	CLA	C4A-NA-C1A	5.94	109.39	106.68
13	q	516	CLA	C4A-NA-C1A	5.90	109.37	106.68
13	G	1140	CLA	C4A-NA-C1A	5.87	109.36	106.68
13	e	1022	CLA	C4A-NA-C1A	5.86	109.35	106.68
13	e	1140	CLA	C4A-NA-C1A	5.86	109.35	106.68
13	Y	516	CLA	C4A-NA-C1A	5.85	109.35	106.68
13	A	1022	CLA	C4A-NA-C1A	5.84	109.34	106.68
13	H	1222	CLA	C4A-NA-C1A	5.84	109.34	106.68
13	A	1140	CLA	C4A-NA-C1A	5.83	109.34	106.68
13	G	1022	CLA	C4A-NA-C1A	5.81	109.33	106.68
13	f	1219	CLA	C4A-NA-C1A	5.80	109.32	106.68
13	B	1219	CLA	C4A-NA-C1A	5.79	109.32	106.68
13	B	1222	CLA	C4A-NA-C1A	5.79	109.32	106.68
16	H	4006	BCR	C7-C8-C9	-5.79	117.68	126.23
16	B	4006	BCR	C7-C8-C9	-5.77	117.70	126.23
16	f	4006	BCR	C7-C8-C9	-5.75	117.73	126.23
13	f	1222	CLA	C4A-NA-C1A	5.74	109.30	106.68
13	H	1219	CLA	C4A-NA-C1A	5.73	109.29	106.68
13	e	1139	CLA	C4A-NA-C1A	5.70	109.28	106.68
13	G	1139	CLA	C4A-NA-C1A	5.62	109.24	106.68
13	A	1139	CLA	C4A-NA-C1A	5.57	109.22	106.68
13	A	1132	CLA	C4A-NA-C1A	5.53	109.20	106.68
13	G	1132	CLA	C4A-NA-C1A	5.48	109.18	106.68
13	G	1128	CLA	C4A-NA-C1A	5.45	109.17	106.68
16	B	4006	BCR	C24-C23-C22	-5.44	118.19	126.23
13	e	1132	CLA	C4A-NA-C1A	5.43	109.16	106.68
16	G	4008	BCR	C20-C21-C22	-5.42	119.67	127.28
16	H	4006	BCR	C24-C23-C22	-5.42	118.21	126.23
13	A	1128	CLA	C4A-NA-C1A	5.42	109.15	106.68
13	e	1128	CLA	C4A-NA-C1A	5.42	109.15	106.68
16	f	4006	BCR	C24-C23-C22	-5.41	118.23	126.23
16	A	4008	BCR	C20-C21-C22	-5.41	119.70	127.28
16	e	4008	BCR	C20-C21-C22	-5.40	119.71	127.28
16	H	4004	BCR	C20-C21-C22	-5.36	119.76	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4004	BCR	C20-C21-C22	-5.35	119.77	127.28
13	e	1013	CLA	CMB-C2B-C1B	-5.35	117.27	125.42
16	L	4022	BCR	C1-C6-C5	-5.34	115.34	122.64
13	A	1013	CLA	CMB-C2B-C1B	-5.34	117.29	125.42
16	B	4004	BCR	C20-C21-C22	-5.33	119.80	127.28
13	G	1013	CLA	CMB-C2B-C1B	-5.33	117.31	125.42
16	V	4022	BCR	C1-C6-C5	-5.32	115.36	122.64
16	n	4022	BCR	C1-C6-C5	-5.32	115.37	122.64
16	J	4015	BCR	C7-C8-C9	-5.29	118.40	126.23
13	e	1128	CLA	CMB-C2B-C1B	-5.29	117.37	125.42
16	l	4015	BCR	C7-C8-C9	-5.28	118.42	126.23
16	T	4015	BCR	C7-C8-C9	-5.28	118.42	126.23
13	A	1128	CLA	CMB-C2B-C1B	-5.27	117.39	125.42
13	G	1128	CLA	CMB-C2B-C1B	-5.26	117.41	125.42
16	R	4016	BCR	C15-C14-C13	-5.21	119.98	127.28
16	e	4011	BCR	C7-C8-C9	-5.20	118.54	126.23
16	j	4016	BCR	C15-C14-C13	-5.19	119.99	127.28
16	G	4011	BCR	C7-C8-C9	-5.19	118.56	126.23
16	A	4011	BCR	C7-C8-C9	-5.19	118.56	126.23
16	F	4016	BCR	C15-C14-C13	-5.19	120.00	127.28
16	H	4014	BCR	C24-C23-C22	-5.15	118.62	126.23
16	B	4014	BCR	C24-C23-C22	-5.14	118.63	126.23
16	l	4013	BCR	C16-C17-C18	-5.14	120.07	127.28
16	T	4013	BCR	C16-C17-C18	-5.11	120.11	127.28
14	A	2001	PQN	C14-C13-C12	-5.11	110.52	123.63
16	J	4013	BCR	C16-C17-C18	-5.10	120.12	127.28
16	f	4014	BCR	C24-C23-C22	-5.10	118.69	126.23
14	e	2001	PQN	C14-C13-C12	-5.09	110.55	123.63
14	G	2001	PQN	C14-C13-C12	-5.09	110.56	123.63
16	V	4219	BCR	C15-C14-C13	-5.09	120.14	127.28
16	n	4219	BCR	C15-C14-C13	-5.08	120.16	127.28
16	L	4219	BCR	C15-C14-C13	-5.06	120.18	127.28
13	q	516	CLA	CAC-C3C-C4C	5.05	131.36	124.79
14	H	2002	PQN	C14-C13-C12	-5.04	110.69	123.63
13	1	516	CLA	CAC-C3C-C4C	5.03	131.34	124.79
16	V	4022	BCR	C7-C8-C9	-5.03	118.79	126.23
14	B	2002	PQN	C14-C13-C12	-5.02	110.72	123.63
14	f	2002	PQN	C14-C13-C12	-5.02	110.74	123.63
16	n	4022	BCR	C7-C8-C9	-5.02	118.81	126.23
13	Y	516	CLA	CAC-C3C-C4C	5.02	131.32	124.79
16	G	4002	BCR	C16-C17-C18	-5.01	120.25	127.28
16	L	4022	BCR	C7-C8-C9	-5.01	118.83	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4002	BCR	C16-C17-C18	-4.99	120.28	127.28
16	A	4002	BCR	C16-C17-C18	-4.98	120.29	127.28
16	G	4007	BCR	C28-C27-C26	-4.96	105.21	114.06
16	A	4007	BCR	C28-C27-C26	-4.96	105.21	114.06
16	e	4007	BCR	C28-C27-C26	-4.96	105.22	114.06
13	s	516	CLA	CAC-C3C-C4C	4.95	131.23	124.79
13	3	516	CLA	CAC-C3C-C4C	4.95	131.22	124.79
13	a	516	CLA	CAC-C3C-C4C	4.94	131.22	124.79
13	H	1012	CLA	C4A-NA-C1A	4.91	108.92	106.68
13	f	1012	CLA	C4A-NA-C1A	4.90	108.92	106.68
13	G	1117	CLA	O2D-CGD-O1D	-4.87	114.38	123.85
13	A	1117	CLA	O2D-CGD-O1D	-4.85	114.40	123.85
13	e	1117	CLA	O2D-CGD-O1D	-4.85	114.41	123.85
13	B	1012	CLA	C4A-NA-C1A	4.85	108.89	106.68
16	G	4002	BCR	C7-C8-C9	-4.79	119.15	126.23
13	B	1023	CLA	CAC-C3C-C4C	4.78	131.01	124.79
16	A	4002	BCR	C7-C8-C9	-4.78	119.17	126.23
13	f	1023	CLA	CAC-C3C-C4C	4.76	130.99	124.79
16	e	4002	BCR	C7-C8-C9	-4.76	119.19	126.23
13	H	1023	CLA	CAC-C3C-C4C	4.75	130.97	124.79
16	u	522	BCR	C15-C14-C13	-4.74	120.63	127.28
16	a	524	BCR	C15-C14-C13	-4.74	120.64	127.28
16	c	522	BCR	C15-C14-C13	-4.72	120.65	127.28
16	5	522	BCR	C15-C14-C13	-4.72	120.66	127.28
16	s	524	BCR	C15-C14-C13	-4.72	120.66	127.28
16	3	524	BCR	C15-C14-C13	-4.71	120.67	127.28
16	f	4010	BCR	C15-C16-C17	-4.70	113.89	123.52
16	H	4010	BCR	C15-C16-C17	-4.70	113.89	123.52
16	B	4010	BCR	C15-C16-C17	-4.70	113.90	123.52
13	A	1011	CLA	O2D-CGD-CBD	4.69	119.43	111.23
16	V	4019	BCR	C7-C8-C9	-4.68	119.31	126.23
13	G	1011	CLA	O2D-CGD-CBD	4.68	119.41	111.23
16	H	4004	BCR	C15-C14-C13	-4.67	120.72	127.28
16	H	4010	BCR	C11-C10-C9	-4.67	120.72	127.28
16	V	4020	BCR	C16-C17-C18	-4.67	120.72	127.28
16	f	4004	BCR	C15-C14-C13	-4.67	120.73	127.28
16	B	4010	BCR	C11-C10-C9	-4.67	120.73	127.28
13	e	1011	CLA	O2D-CGD-CBD	4.67	119.39	111.23
16	B	4004	BCR	C15-C14-C13	-4.67	120.73	127.28
16	B	4014	BCR	C20-C21-C22	-4.65	120.75	127.28
16	f	4010	BCR	C11-C10-C9	-4.65	120.75	127.28
16	n	4020	BCR	C16-C17-C18	-4.65	120.75	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4020	BCR	C16-C17-C18	-4.65	120.75	127.28
16	s	523	BCR	C15-C14-C13	-4.65	120.76	127.28
16	3	523	BCR	C15-C14-C13	-4.65	120.76	127.28
16	j	4016	BCR	C11-C10-C9	-4.65	120.76	127.28
16	f	4014	BCR	C20-C21-C22	-4.65	120.76	127.28
16	H	4014	BCR	C20-C21-C22	-4.64	120.77	127.28
16	c	523	BCR	C15-C14-C13	-4.64	120.77	127.28
16	L	4019	BCR	C7-C8-C9	-4.64	119.37	126.23
16	5	523	BCR	C15-C14-C13	-4.64	120.77	127.28
16	e	4001	BCR	C16-C17-C18	-4.64	120.77	127.28
16	H	4004	BCR	C16-C17-C18	-4.64	120.77	127.28
16	F	4016	BCR	C11-C10-C9	-4.64	120.78	127.28
16	B	4004	BCR	C16-C17-C18	-4.63	120.78	127.28
16	n	4019	BCR	C7-C8-C9	-4.63	119.38	126.23
16	A	4003	BCR	C7-C8-C9	-4.63	119.39	126.23
16	A	4001	BCR	C16-C17-C18	-4.63	120.79	127.28
16	G	4003	BCR	C7-C8-C9	-4.62	119.40	126.23
16	H	4009	BCR	C7-C8-C9	-4.62	119.40	126.23
16	a	523	BCR	C15-C14-C13	-4.62	120.80	127.28
16	G	4001	BCR	C16-C17-C18	-4.62	120.80	127.28
16	u	523	BCR	C15-C14-C13	-4.62	120.80	127.28
16	f	4004	BCR	C16-C17-C18	-4.61	120.81	127.28
16	R	4016	BCR	C11-C10-C9	-4.61	120.82	127.28
16	e	4003	BCR	C7-C8-C9	-4.61	119.42	126.23
16	B	4009	BCR	C7-C8-C9	-4.60	119.44	126.23
16	Z	521	BCR	C28-C27-C26	-4.59	105.86	114.06
16	f	4009	BCR	C7-C8-C9	-4.59	119.44	126.23
20	b	822	SQD	O47-C7-C8	4.58	119.26	111.09
16	m	4104	BCR	C7-C8-C9	-4.58	119.45	126.23
16	r	521	BCR	C28-C27-C26	-4.58	105.89	114.06
16	f	4014	BCR	C16-C17-C18	-4.58	120.86	127.28
20	4	822	SQD	O47-C7-C8	4.58	119.25	111.09
16	B	4014	BCR	C16-C17-C18	-4.57	120.86	127.28
16	2	521	BCR	C28-C27-C26	-4.57	105.90	114.06
20	t	822	SQD	O47-C7-C8	4.57	119.24	111.09
16	v	521	BCR	C16-C17-C18	-4.57	120.87	127.28
16	6	521	BCR	C20-C21-C22	-4.56	120.88	127.28
16	K	4104	BCR	C7-C8-C9	-4.56	119.49	126.23
16	v	521	BCR	C20-C21-C22	-4.56	120.88	127.28
16	6	521	BCR	C16-C17-C18	-4.56	120.89	127.28
16	d	521	BCR	C16-C17-C18	-4.55	120.89	127.28
16	H	4014	BCR	C16-C17-C18	-4.54	120.91	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	521	BCR	C20-C21-C22	-4.53	120.92	127.28
16	s	522	BCR	C15-C14-C13	-4.53	120.93	127.28
16	U	4104	BCR	C7-C8-C9	-4.52	119.55	126.23
16	3	522	BCR	C15-C14-C13	-4.51	120.96	127.28
17	B	1842	LHG	O4-P-O5	4.51	133.40	112.44
17	f	1842	LHG	O4-P-O5	4.50	133.40	112.44
17	H	1842	LHG	O4-P-O5	4.50	133.39	112.44
16	a	522	BCR	C15-C14-C13	-4.50	120.97	127.28
16	3	522	BCR	C11-C10-C9	-4.49	120.98	127.28
16	A	4003	BCR	C16-C17-C18	-4.49	120.99	127.28
16	a	522	BCR	C11-C10-C9	-4.48	121.00	127.28
17	A	5006	LHG	O4-P-O5	4.48	133.28	112.44
16	S	4018	BCR	C24-C23-C22	-4.48	119.61	126.23
17	e	5006	LHG	O4-P-O5	4.48	133.27	112.44
16	l	4012	BCR	C20-C21-C22	-4.48	121.00	127.28
16	q	522	BCR	C11-C10-C9	-4.47	121.00	127.28
16	Y	522	BCR	C11-C10-C9	-4.47	121.01	127.28
17	e	5004	LHG	O4-P-O5	4.47	133.24	112.44
16	e	4003	BCR	C16-C17-C18	-4.47	121.02	127.28
17	G	5006	LHG	O4-P-O5	4.47	133.22	112.44
17	G	5004	LHG	O4-P-O5	4.47	133.22	112.44
17	A	5004	LHG	O4-P-O5	4.46	133.19	112.44
16	s	522	BCR	C11-C10-C9	-4.46	121.03	127.28
16	1	522	BCR	C11-C10-C9	-4.46	121.03	127.28
16	4	524	BCR	C15-C14-C13	-4.45	121.03	127.28
17	G	5009	LHG	O4-P-O5	4.45	133.14	112.44
16	I	4018	BCR	C24-C23-C22	-4.45	119.66	126.23
16	t	524	BCR	C15-C14-C13	-4.44	121.05	127.28
17	A	5009	LHG	O4-P-O5	4.44	133.12	112.44
17	e	5009	LHG	O4-P-O5	4.44	133.12	112.44
17	e	5003	LHG	O4-P-O5	4.44	133.11	112.44
17	G	5003	LHG	O4-P-O5	4.44	133.11	112.44
16	G	4003	BCR	C16-C17-C18	-4.44	121.06	127.28
17	A	5003	LHG	O4-P-O5	4.43	133.07	112.44
16	T	4012	BCR	C20-C21-C22	-4.43	121.07	127.28
20	q	822	SQD	O5-C5-C4	4.43	117.68	109.70
16	J	4012	BCR	C20-C21-C22	-4.43	121.07	127.28
20	1	822	SQD	O5-C5-C4	4.43	117.67	109.70
20	Y	822	SQD	O5-C5-C4	4.42	117.67	109.70
17	e	5002	LHG	O4-P-O5	4.42	133.01	112.44
16	b	524	BCR	C15-C14-C13	-4.42	121.08	127.28
17	A	5002	LHG	O4-P-O5	4.42	132.99	112.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	524	BCR	C15-C14-C13	-4.41	121.09	127.28
17	G	5002	LHG	O4-P-O5	4.41	132.97	112.44
17	L	5218	LHG	O4-P-O5	4.41	132.97	112.44
17	n	5218	LHG	O4-P-O5	4.41	132.96	112.44
16	k	4018	BCR	C24-C23-C22	-4.41	119.72	126.23
17	V	5218	LHG	O4-P-O5	4.41	132.95	112.44
20	H	1852	SQD	O5-C5-C4	4.41	117.64	109.70
16	c	524	BCR	C15-C14-C13	-4.40	121.10	127.28
16	f	4010	BCR	C3-C4-C5	-4.40	106.21	114.06
17	e	5008	LHG	O4-P-O5	4.40	132.90	112.44
16	6	524	BCR	C15-C14-C13	-4.40	121.11	127.28
16	B	4010	BCR	C3-C4-C5	-4.39	106.22	114.06
20	B	1852	SQD	O5-C5-C4	4.39	117.61	109.70
17	A	5008	LHG	O4-P-O5	4.39	132.87	112.44
17	G	5008	LHG	O4-P-O5	4.39	132.86	112.44
20	f	1852	SQD	O5-C5-C4	4.39	117.61	109.70
13	B	1232	CLA	CMB-C2B-C1B	-4.39	118.74	125.42
13	H	1232	CLA	CMB-C2B-C1B	-4.39	118.74	125.42
17	n	5220	LHG	O4-P-O5	4.38	132.83	112.44
16	1	524	BCR	C15-C14-C13	-4.38	121.13	127.28
16	H	4010	BCR	C3-C4-C5	-4.38	106.24	114.06
16	5	524	BCR	C15-C14-C13	-4.38	121.14	127.28
16	u	524	BCR	C15-C14-C13	-4.38	121.14	127.28
17	L	5220	LHG	O4-P-O5	4.38	132.81	112.44
13	f	1232	CLA	CMB-C2B-C1B	-4.38	118.75	125.42
16	v	524	BCR	C15-C14-C13	-4.38	121.14	127.28
16	l	4015	BCR	C15-C14-C13	-4.37	121.14	127.28
17	V	5220	LHG	O4-P-O5	4.37	132.79	112.44
16	T	4015	BCR	C15-C14-C13	-4.37	121.15	127.28
17	S	5001	LHG	O4-P-O5	4.37	132.76	112.44
17	I	5001	LHG	O4-P-O5	4.37	132.76	112.44
17	k	5001	LHG	O4-P-O5	4.36	132.75	112.44
16	J	4015	BCR	C15-C14-C13	-4.36	121.16	127.28
16	m	4104	BCR	C20-C21-C22	-4.36	121.16	127.28
16	q	524	BCR	C15-C14-C13	-4.35	121.17	127.28
16	v	522	BCR	C15-C14-C13	-4.35	121.18	127.28
13	H	1234	CLA	CMB-C2B-C1B	-4.35	118.80	125.42
16	j	4016	BCR	C24-C23-C22	-4.35	119.80	126.23
16	Y	524	BCR	C15-C14-C13	-4.35	121.18	127.28
13	B	1234	CLA	CMB-C2B-C1B	-4.35	118.80	125.42
17	G	5007	LHG	O4-P-O5	4.34	132.66	112.44
16	m	4104	BCR	C15-C14-C13	-4.34	121.19	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	5007	LHG	O4-P-O5	4.34	132.64	112.44
16	U	4104	BCR	C15-C14-C13	-4.34	121.19	127.28
17	A	5007	LHG	O4-P-O5	4.34	132.63	112.44
20	d	822	SQD	O47-C7-C8	4.34	118.82	111.09
16	U	4104	BCR	C20-C21-C22	-4.34	121.19	127.28
16	t	521	BCR	C7-C8-C9	-4.34	119.82	126.23
16	K	4104	BCR	C20-C21-C22	-4.34	121.20	127.28
16	Z	524	BCR	C15-C14-C13	-4.34	121.20	127.28
16	2	524	BCR	C15-C14-C13	-4.33	121.20	127.28
13	f	1234	CLA	CMB-C2B-C1B	-4.33	118.82	125.42
16	4	521	BCR	C7-C8-C9	-4.33	119.83	126.23
16	6	522	BCR	C15-C14-C13	-4.33	121.21	127.28
16	K	4104	BCR	C15-C14-C13	-4.32	121.21	127.28
17	e	5005	LHG	O4-P-O5	4.32	132.56	112.44
17	A	5005	LHG	O4-P-O5	4.32	132.56	112.44
16	d	522	BCR	C15-C14-C13	-4.32	121.22	127.28
17	e	5001	LHG	O4-P-O5	4.31	132.51	112.44
16	b	521	BCR	C7-C8-C9	-4.31	119.86	126.23
17	A	5001	LHG	O4-P-O5	4.31	132.50	112.44
17	G	5005	LHG	O4-P-O5	4.31	132.50	112.44
16	F	4016	BCR	C24-C23-C22	-4.31	119.86	126.23
17	G	5001	LHG	O4-P-O5	4.31	132.47	112.44
17	V	5221	LHG	O4-P-O5	4.31	132.47	112.44
16	r	524	BCR	C15-C14-C13	-4.31	121.24	127.28
17	n	5221	LHG	O4-P-O5	4.30	132.47	112.44
16	e	4008	BCR	C16-C17-C18	-4.30	121.24	127.28
20	6	822	SQD	O47-C7-C8	4.30	118.76	111.09
17	L	5221	LHG	O4-P-O5	4.30	132.45	112.44
16	R	4016	BCR	C24-C23-C22	-4.30	119.88	126.23
16	G	4007	BCR	C15-C14-C13	-4.30	121.25	127.28
17	H	1855	LHG	O4-P-O5	4.30	132.43	112.44
20	v	822	SQD	O47-C7-C8	4.30	118.75	111.09
17	f	1855	LHG	O4-P-O5	4.30	132.43	112.44
17	B	1855	LHG	O4-P-O5	4.29	132.42	112.44
16	n	4019	BCR	C15-C14-C13	-4.29	121.26	127.28
16	G	4008	BCR	C16-C17-C18	-4.29	121.26	127.28
16	5	521	BCR	C20-C21-C22	-4.29	121.27	127.28
16	e	4007	BCR	C15-C14-C13	-4.29	121.27	127.28
16	k	4018	BCR	C7-C8-C9	-4.29	119.89	126.23
16	u	521	BCR	C20-C21-C22	-4.28	121.27	127.28
16	e	4011	BCR	C28-C27-C26	-4.28	106.42	114.06
16	S	4018	BCR	C7-C8-C9	-4.28	119.90	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	c	521	BCR	C20-C21-C22	-4.28	121.28	127.28
16	A	4007	BCR	C15-C14-C13	-4.28	121.28	127.28
16	A	4008	BCR	C16-C17-C18	-4.28	121.28	127.28
16	2	521	BCR	C15-C14-C13	-4.28	121.28	127.28
16	L	4019	BCR	C15-C14-C13	-4.28	121.28	127.28
16	G	4011	BCR	C28-C27-C26	-4.28	106.43	114.06
16	A	4011	BCR	C28-C27-C26	-4.27	106.43	114.06
16	I	4018	BCR	C7-C8-C9	-4.27	119.92	126.23
16	r	521	BCR	C15-C14-C13	-4.26	121.30	127.28
16	n	4022	BCR	C4-C5-C6	-4.26	116.95	122.70
16	V	4019	BCR	C15-C14-C13	-4.26	121.31	127.28
16	s	522	BCR	C3-C4-C5	-4.26	106.47	114.06
16	a	522	BCR	C3-C4-C5	-4.25	106.48	114.06
16	q	521	BCR	C16-C17-C18	-4.25	121.32	127.28
20	n	5216	SQD	O9-S-O7	-4.25	100.01	113.82
20	V	5216	SQD	O9-S-O7	-4.25	100.01	113.82
16	3	522	BCR	C3-C4-C5	-4.25	106.48	114.06
20	L	5216	SQD	O9-S-O7	-4.24	100.02	113.82
16	f	4004	BCR	C24-C23-C22	-4.24	119.96	126.23
16	Z	521	BCR	C15-C14-C13	-4.24	121.34	127.28
16	V	4022	BCR	C4-C5-C6	-4.23	116.98	122.70
16	1	521	BCR	C16-C17-C18	-4.23	121.34	127.28
16	L	4022	BCR	C4-C5-C6	-4.22	117.00	122.70
16	T	4015	BCR	C16-C17-C18	-4.21	121.37	127.28
16	Y	521	BCR	C16-C17-C18	-4.21	121.37	127.28
16	H	4004	BCR	C24-C23-C22	-4.21	120.01	126.23
16	B	4004	BCR	C24-C23-C22	-4.21	120.01	126.23
13	e	1132	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
13	A	1132	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
16	t	521	BCR	C16-C17-C18	-4.20	121.39	127.28
16	J	4015	BCR	C16-C17-C18	-4.20	121.39	127.28
20	V	5216	SQD	O7-S-C6	4.20	113.02	106.76
13	G	1132	CLA	O2D-CGD-O1D	-4.19	115.69	123.85
16	l	4015	BCR	C16-C17-C18	-4.19	121.40	127.28
16	b	521	BCR	C16-C17-C18	-4.19	121.40	127.28
16	e	4008	BCR	C15-C14-C13	-4.19	121.40	127.28
13	e	1011	CLA	O2D-CGD-O1D	-4.19	115.70	123.85
16	n	4022	BCR	C11-C10-C9	-4.18	121.41	127.28
13	B	1209	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
13	G	1011	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
13	H	1209	CLA	O2D-CGD-O1D	-4.18	115.72	123.85
13	A	1011	CLA	O2D-CGD-O1D	-4.18	115.72	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	4	521	BCR	C16-C17-C18	-4.18	121.42	127.28
13	f	1209	CLA	O2D-CGD-O1D	-4.18	115.72	123.85
20	L	5216	SQD	O7-S-C6	4.17	112.99	106.76
16	G	4008	BCR	C15-C14-C13	-4.17	121.43	127.28
16	Y	524	BCR	C16-C17-C18	-4.17	121.43	127.28
16	A	4008	BCR	C15-C14-C13	-4.16	121.44	127.28
16	4	522	BCR	C15-C16-C17	-4.16	115.01	123.52
16	t	522	BCR	C15-C16-C17	-4.16	115.01	123.52
16	1	524	BCR	C16-C17-C18	-4.16	121.45	127.28
13	f	1209	CLA	O2D-CGD-CBD	4.15	118.48	111.23
16	r	521	BCR	C20-C21-C22	-4.15	121.46	127.28
20	n	5216	SQD	O7-S-C6	4.15	112.95	106.76
16	q	524	BCR	C16-C17-C18	-4.15	121.46	127.28
13	H	1209	CLA	O2D-CGD-CBD	4.14	118.48	111.23
16	L	4022	BCR	C11-C10-C9	-4.14	121.47	127.28
16	f	4010	BCR	C7-C8-C9	-4.14	120.11	126.23
16	b	522	BCR	C15-C16-C17	-4.14	115.05	123.52
16	H	4010	BCR	C7-C8-C9	-4.14	120.11	126.23
13	B	1209	CLA	O2D-CGD-CBD	4.14	118.46	111.23
16	B	4010	BCR	C7-C8-C9	-4.14	120.11	126.23
16	d	523	BCR	C15-C14-C13	-4.14	121.48	127.28
16	f	4010	BCR	C24-C23-C22	-4.13	120.12	126.23
16	2	521	BCR	C20-C21-C22	-4.13	121.49	127.28
20	H	1852	SQD	O47-C7-C8	4.13	120.41	111.48
16	4	522	BCR	C24-C23-C22	-4.12	120.14	126.23
16	6	523	BCR	C15-C14-C13	-4.12	121.50	127.28
16	H	4005	BCR	C7-C8-C9	-4.12	120.14	126.23
16	d	524	BCR	C16-C17-C18	-4.12	121.50	127.28
16	Z	521	BCR	C20-C21-C22	-4.12	121.50	127.28
16	H	4010	BCR	C24-C23-C22	-4.12	120.14	126.23
20	f	1852	SQD	O47-C7-C8	4.12	120.39	111.48
20	B	1852	SQD	O47-C7-C8	4.12	120.39	111.48
16	B	4010	BCR	C24-C23-C22	-4.12	120.15	126.23
16	V	4022	BCR	C11-C10-C9	-4.11	121.51	127.28
16	v	524	BCR	C16-C17-C18	-4.11	121.51	127.28
16	6	524	BCR	C16-C17-C18	-4.11	121.51	127.28
16	B	4005	BCR	C7-C8-C9	-4.11	120.16	126.23
16	f	4005	BCR	C7-C8-C9	-4.10	120.16	126.23
16	4	522	BCR	C15-C14-C13	-4.10	121.53	127.28
16	t	522	BCR	C24-C23-C22	-4.10	120.17	126.23
20	f	1852	SQD	C1-O5-C5	4.10	121.72	113.72
16	b	522	BCR	C15-C14-C13	-4.10	121.53	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	523	BCR	C15-C14-C13	-4.09	121.54	127.28
16	b	522	BCR	C24-C23-C22	-4.09	120.18	126.23
20	B	1852	SQD	C1-O5-C5	4.09	121.71	113.72
20	H	1852	SQD	C1-O5-C5	4.09	121.71	113.72
16	t	522	BCR	C15-C14-C13	-4.08	121.55	127.28
16	A	4002	BCR	C24-C23-C22	-4.07	120.22	126.23
13	e	1011	CLA	C1D-ND-C4D	-4.06	103.46	106.31
16	6	521	BCR	C24-C23-C22	-4.06	120.23	126.23
16	G	4002	BCR	C24-C23-C22	-4.06	120.23	126.23
16	e	4002	BCR	C24-C23-C22	-4.06	120.23	126.23
16	v	521	BCR	C24-C23-C22	-4.05	120.24	126.23
16	d	521	BCR	C24-C23-C22	-4.05	120.25	126.23
16	2	523	BCR	C7-C8-C9	-4.04	120.26	126.23
16	b	524	BCR	C33-C5-C6	-4.04	120.08	124.48
16	Z	523	BCR	C7-C8-C9	-4.03	120.27	126.23
16	Z	521	BCR	C24-C23-C22	-4.03	120.27	126.23
13	H	1021	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
16	r	523	BCR	C7-C8-C9	-4.03	120.28	126.23
16	Y	522	BCR	C15-C14-C13	-4.03	121.63	127.28
16	c	521	BCR	C15-C14-C13	-4.03	121.63	127.28
16	H	4009	BCR	C21-C20-C19	-4.03	111.53	123.20
13	A	1801	CLA	CAA-CBA-CGA	-4.03	101.75	112.49
16	r	521	BCR	C24-C23-C22	-4.03	120.28	126.23
13	e	1801	CLA	CAA-CBA-CGA	-4.02	101.76	112.49
13	G	1801	CLA	CAA-CBA-CGA	-4.02	101.76	112.49
16	1	522	BCR	C15-C14-C13	-4.02	121.64	127.28
20	B	1852	SQD	O7-S-C6	4.02	112.76	106.76
13	B	1021	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
16	B	4009	BCR	C21-C20-C19	-4.02	111.55	123.20
16	5	521	BCR	C15-C14-C13	-4.02	121.64	127.28
16	2	521	BCR	C24-C23-C22	-4.02	120.29	126.23
16	A	4001	BCR	C3-C4-C5	-4.02	106.89	114.06
13	f	1021	CLA	O2D-CGD-O1D	-4.02	116.03	123.85
16	q	522	BCR	C15-C14-C13	-4.02	121.65	127.28
13	G	1121	CLA	CAA-C2A-C3A	-4.02	102.15	113.00
16	4	524	BCR	C33-C5-C6	-4.01	120.11	124.48
16	e	4001	BCR	C3-C4-C5	-4.01	106.90	114.06
13	A	1121	CLA	CAA-C2A-C3A	-4.01	102.16	113.00
20	f	1852	SQD	O7-S-C6	4.01	112.75	106.76
16	f	4009	BCR	C21-C20-C19	-4.01	111.58	123.20
13	A	1011	CLA	C1D-ND-C4D	-4.01	103.50	106.31
13	e	1121	CLA	CAA-C2A-C3A	-4.01	102.17	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1117	CLA	O2D-CGD-CBD	4.01	118.24	111.23
16	u	521	BCR	C15-C14-C13	-4.00	121.66	127.28
20	H	1852	SQD	O7-S-C6	4.00	112.73	106.76
16	G	4001	BCR	C3-C4-C5	-4.00	106.92	114.06
16	e	4001	BCR	C20-C21-C22	-4.00	121.67	127.28
13	e	1117	CLA	O2D-CGD-CBD	4.00	118.22	111.23
16	L	4219	BCR	C16-C17-C18	-3.99	121.68	127.28
16	a	522	BCR	C7-C8-C9	-3.99	120.33	126.23
16	f	4005	BCR	C24-C23-C22	-3.99	120.33	126.23
13	f	1238	CLA	CMB-C2B-C1B	-3.99	119.35	125.42
13	A	1117	CLA	O2D-CGD-CBD	3.99	118.20	111.23
16	d	521	BCR	C7-C8-C9	-3.98	120.34	126.23
16	A	4001	BCR	C20-C21-C22	-3.98	121.70	127.28
16	q	521	BCR	C15-C14-C13	-3.98	121.70	127.28
16	t	524	BCR	C33-C5-C6	-3.98	120.15	124.48
16	G	4001	BCR	C15-C16-C17	-3.97	115.39	123.52
13	B	1238	CLA	CMB-C2B-C1B	-3.97	119.37	125.42
16	n	4219	BCR	C16-C17-C18	-3.97	121.71	127.28
13	H	1238	CLA	CMB-C2B-C1B	-3.97	119.37	125.42
13	G	1129	CLA	C3B-C4B-NB	-3.97	106.98	110.53
16	3	522	BCR	C7-C8-C9	-3.97	120.36	126.23
16	B	4005	BCR	C24-C23-C22	-3.97	120.36	126.23
16	Y	521	BCR	C15-C14-C13	-3.97	121.71	127.28
16	V	4219	BCR	C16-C17-C18	-3.97	121.71	127.28
16	H	4009	BCR	C15-C14-C13	-3.96	121.72	127.28
16	1	521	BCR	C15-C14-C13	-3.96	121.72	127.28
16	b	521	BCR	C15-C14-C13	-3.96	121.72	127.28
16	5	522	BCR	C11-C10-C9	-3.96	121.72	127.28
16	6	521	BCR	C7-C8-C9	-3.96	120.38	126.23
16	G	4001	BCR	C20-C21-C22	-3.96	121.73	127.28
16	e	4001	BCR	C15-C16-C17	-3.95	115.43	123.52
16	c	522	BCR	C11-C10-C9	-3.95	121.73	127.28
16	t	521	BCR	C15-C14-C13	-3.95	121.73	127.28
16	A	4001	BCR	C15-C16-C17	-3.95	115.44	123.52
13	Y	516	CLA	CBC-CAC-C3C	3.95	123.13	112.42
16	f	4009	BCR	C15-C14-C13	-3.95	121.74	127.28
16	H	4005	BCR	C24-C23-C22	-3.95	120.40	126.23
16	s	522	BCR	C7-C8-C9	-3.95	120.40	126.23
13	1	516	CLA	CBC-CAC-C3C	3.94	123.10	112.42
16	I	4018	BCR	C16-C17-C18	-3.94	121.76	127.28
16	f	4005	BCR	C15-C14-C13	-3.94	121.76	127.28
16	B	4009	BCR	C15-C14-C13	-3.94	121.76	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	522	BCR	C11-C10-C9	-3.94	121.76	127.28
16	e	4011	BCR	C20-C21-C22	-3.93	121.76	127.28
13	G	1011	CLA	C1D-ND-C4D	-3.93	103.55	106.31
16	v	521	BCR	C7-C8-C9	-3.93	120.42	126.23
16	4	521	BCR	C15-C14-C13	-3.93	121.76	127.28
16	B	4005	BCR	C15-C14-C13	-3.93	121.77	127.28
13	e	1139	CLA	C3B-C4B-NB	-3.93	107.02	110.53
16	S	4018	BCR	C16-C17-C18	-3.93	121.77	127.28
16	T	4013	BCR	C15-C14-C13	-3.93	121.77	127.28
16	k	4018	BCR	C16-C17-C18	-3.92	121.77	127.28
13	q	516	CLA	CBC-CAC-C3C	3.92	123.06	112.42
13	A	1129	CLA	C3B-C4B-NB	-3.92	107.03	110.53
16	H	4005	BCR	C15-C14-C13	-3.92	121.78	127.28
16	J	4013	BCR	C15-C14-C13	-3.92	121.78	127.28
20	V	5216	SQD	O47-C7-C8	3.92	119.96	111.48
20	n	5216	SQD	O47-C7-C8	3.92	119.96	111.48
13	H	1211	CLA	CHB-C4A-NA	3.92	130.06	124.40
20	L	5216	SQD	O47-C7-C8	3.92	119.96	111.48
16	A	4011	BCR	C20-C21-C22	-3.92	121.79	127.28
16	G	4011	BCR	C20-C21-C22	-3.92	121.79	127.28
16	G	4003	BCR	C3-C4-C5	-3.91	107.08	114.06
16	l	4013	BCR	C15-C14-C13	-3.91	121.80	127.28
16	j	4016	BCR	C7-C8-C9	-3.91	120.45	126.23
16	6	521	BCR	C11-C10-C9	-3.91	121.80	127.28
13	e	1129	CLA	C3B-C4B-NB	-3.90	107.05	110.53
13	A	1139	CLA	C3B-C4B-NB	-3.90	107.05	110.53
20	d	822	SQD	O9-S-O7	-3.89	101.16	113.82
13	B	1211	CLA	CHB-C4A-NA	3.89	130.01	124.40
16	W	4021	BCR	C11-C10-C9	-3.89	121.82	127.28
16	v	521	BCR	C11-C10-C9	-3.89	121.83	127.28
13	G	1139	CLA	C3B-C4B-NB	-3.89	107.06	110.53
20	6	822	SQD	O9-S-O7	-3.89	101.18	113.82
20	v	822	SQD	O9-S-O7	-3.89	101.18	113.82
16	o	4021	BCR	C11-C10-C9	-3.89	121.83	127.28
13	U	1103	CLA	C1-C2-C3	-3.88	120.48	126.76
20	3	822	SQD	O9-S-O7	-3.88	101.19	113.82
16	A	4003	BCR	C3-C4-C5	-3.88	107.13	114.06
16	d	521	BCR	C11-C10-C9	-3.88	121.83	127.28
16	c	521	BCR	C16-C17-C18	-3.88	121.84	127.28
20	a	822	SQD	O9-S-O7	-3.88	101.21	113.82
16	F	4016	BCR	C7-C8-C9	-3.88	120.50	126.23
16	b	524	BCR	C11-C10-C9	-3.88	121.84	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1211	CLA	CHB-C4A-NA	3.88	129.99	124.40
16	3	521	BCR	C16-C17-C18	-3.87	121.84	127.28
16	M	4021	BCR	C11-C10-C9	-3.87	121.85	127.28
16	4	523	BCR	C16-C17-C18	-3.87	121.85	127.28
16	H	4017	BCR	C24-C23-C22	-3.87	120.51	126.23
20	s	822	SQD	O9-S-O7	-3.87	101.23	113.82
16	t	523	BCR	C16-C17-C18	-3.87	121.85	127.28
16	R	4016	BCR	C7-C8-C9	-3.87	120.51	126.23
16	4	524	BCR	C11-C10-C9	-3.87	121.85	127.28
16	s	521	BCR	C16-C17-C18	-3.87	121.85	127.28
16	e	4003	BCR	C3-C4-C5	-3.87	107.16	114.06
16	t	524	BCR	C11-C10-C9	-3.86	121.86	127.28
16	T	4015	BCR	C20-C21-C22	-3.86	121.86	127.28
16	J	4015	BCR	C20-C21-C22	-3.86	121.87	127.28
13	K	1103	CLA	C1-C2-C3	-3.86	120.52	126.76
16	l	4015	BCR	C20-C21-C22	-3.85	121.87	127.28
16	o	4021	BCR	C24-C23-C22	-3.85	120.53	126.23
16	W	4021	BCR	C24-C23-C22	-3.85	120.54	126.23
13	m	1103	CLA	C1-C2-C3	-3.85	120.53	126.76
16	2	522	BCR	C15-C14-C13	-3.85	121.88	127.28
16	J	4013	BCR	C24-C23-C22	-3.85	120.54	126.23
16	V	4019	BCR	C16-C17-C18	-3.85	121.88	127.28
20	5	822	SQD	O9-S-O7	-3.85	101.31	113.82
16	v	521	BCR	C15-C14-C13	-3.85	121.88	127.28
16	M	4021	BCR	C24-C23-C22	-3.85	120.55	126.23
16	r	522	BCR	C15-C14-C13	-3.85	121.89	127.28
16	f	4017	BCR	C24-C23-C22	-3.84	120.55	126.23
20	u	822	SQD	O9-S-O7	-3.84	101.32	113.82
16	B	4017	BCR	C24-C23-C22	-3.84	120.55	126.23
20	c	822	SQD	O9-S-O7	-3.84	101.33	113.82
16	b	523	BCR	C16-C17-C18	-3.84	121.89	127.28
16	u	521	BCR	C16-C17-C18	-3.84	121.89	127.28
16	5	521	BCR	C16-C17-C18	-3.84	121.89	127.28
16	L	4019	BCR	C16-C17-C18	-3.84	121.89	127.28
16	Z	522	BCR	C15-C14-C13	-3.84	121.90	127.28
16	T	4013	BCR	C24-C23-C22	-3.84	120.56	126.23
16	a	521	BCR	C16-C17-C18	-3.83	121.90	127.28
20	b	822	SQD	O9-S-O7	-3.83	101.36	113.82
16	n	4219	BCR	C7-C8-C9	-3.83	120.57	126.23
16	d	521	BCR	C15-C14-C13	-3.83	121.90	127.28
16	n	4019	BCR	C16-C17-C18	-3.83	121.90	127.28
16	t	523	BCR	C15-C14-C13	-3.83	121.91	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	4219	BCR	C7-C8-C9	-3.83	120.57	126.23
20	t	822	SQD	O9-S-O7	-3.83	101.38	113.82
16	n	4219	BCR	C33-C5-C6	-3.83	120.31	124.48
16	Z	523	BCR	C15-C14-C13	-3.83	121.91	127.28
20	4	822	SQD	O9-S-O7	-3.83	101.38	113.82
13	e	1137	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
20	r	822	SQD	O9-S-O7	-3.82	101.39	113.82
16	6	521	BCR	C15-C14-C13	-3.82	121.92	127.28
16	r	523	BCR	C15-C14-C13	-3.82	121.92	127.28
13	G	1137	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
20	2	822	SQD	O9-S-O7	-3.81	101.42	113.82
16	2	521	BCR	C16-C17-C18	-3.81	121.93	127.28
16	m	4104	BCR	C38-C26-C25	-3.81	120.33	124.48
16	r	521	BCR	C16-C17-C18	-3.81	121.93	127.28
16	l	4013	BCR	C24-C23-C22	-3.81	120.60	126.23
20	Y	822	SQD	O9-S-O7	-3.81	101.43	113.82
16	Z	521	BCR	C16-C17-C18	-3.81	121.94	127.28
13	K	1401	CLA	CAA-C2A-C3A	-3.81	102.70	113.00
16	L	4219	BCR	C33-C5-C6	-3.81	120.33	124.48
16	B	4006	BCR	C15-C14-C13	-3.81	121.94	127.28
20	Z	822	SQD	O9-S-O7	-3.81	101.44	113.82
20	f	1852	SQD	O9-S-O7	-3.81	101.44	113.82
20	1	822	SQD	O9-S-O7	-3.81	101.45	113.82
16	L	4219	BCR	C7-C8-C9	-3.80	120.61	126.23
13	A	1137	CLA	O2D-CGD-O1D	-3.80	116.44	123.85
16	4	523	BCR	C15-C14-C13	-3.80	121.95	127.28
16	2	523	BCR	C15-C14-C13	-3.80	121.95	127.28
20	H	1852	SQD	O9-S-O7	-3.80	101.46	113.82
20	q	822	SQD	C4-C3-C2	3.80	117.50	110.83
13	U	1401	CLA	CAA-C2A-C3A	-3.80	102.73	113.00
16	f	4006	BCR	C15-C14-C13	-3.80	121.95	127.28
16	e	4007	BCR	C11-C10-C9	-3.80	121.95	127.28
20	B	1852	SQD	O9-S-O7	-3.80	101.47	113.82
13	m	1401	CLA	CAA-C2A-C3A	-3.80	102.74	113.00
16	1	521	BCR	C3-C4-C5	-3.80	107.28	114.06
16	Y	521	BCR	C3-C4-C5	-3.80	107.28	114.06
20	Y	822	SQD	C4-C3-C2	3.80	117.50	110.83
16	b	524	BCR	C16-C17-C18	-3.80	121.95	127.28
16	q	521	BCR	C3-C4-C5	-3.80	107.29	114.06
16	f	4005	BCR	C33-C5-C6	-3.79	120.34	124.48
16	v	521	BCR	C28-C27-C26	-3.79	107.29	114.06
20	q	822	SQD	O9-S-O7	-3.79	101.49	113.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	4104	BCR	C38-C26-C25	-3.79	120.35	124.48
16	a	521	BCR	C15-C14-C13	-3.79	121.97	127.28
16	b	523	BCR	C15-C14-C13	-3.78	121.97	127.28
16	v	524	BCR	C11-C10-C9	-3.78	121.97	127.28
16	q	522	BCR	C7-C8-C9	-3.78	120.64	126.23
16	H	4005	BCR	C33-C5-C6	-3.78	120.36	124.48
16	6	521	BCR	C28-C27-C26	-3.78	107.32	114.06
16	H	4006	BCR	C15-C14-C13	-3.78	121.98	127.28
16	d	521	BCR	C28-C27-C26	-3.78	107.32	114.06
20	1	822	SQD	C4-C3-C2	3.78	117.46	110.83
16	t	524	BCR	C16-C17-C18	-3.78	121.98	127.28
16	V	4219	BCR	C33-C5-C6	-3.77	120.36	124.48
16	4	524	BCR	C16-C17-C18	-3.77	121.98	127.28
16	A	4007	BCR	C11-C10-C9	-3.77	121.99	127.28
16	q	524	BCR	C33-C5-C6	-3.77	120.37	124.48
16	B	4005	BCR	C33-C5-C6	-3.77	120.37	124.48
16	3	521	BCR	C15-C14-C13	-3.77	122.00	127.28
16	1	522	BCR	C7-C8-C9	-3.76	120.67	126.23
16	s	521	BCR	C15-C14-C13	-3.76	122.01	127.28
20	1	822	SQD	O47-C7-C8	3.75	119.60	111.48
16	U	4104	BCR	C38-C26-C25	-3.75	120.39	124.48
20	q	822	SQD	O47-C7-C8	3.75	119.60	111.48
16	G	4002	BCR	C11-C10-C9	-3.75	122.02	127.28
16	Z	522	BCR	C11-C10-C9	-3.75	122.02	127.28
16	1	524	BCR	C33-C5-C6	-3.75	120.39	124.48
13	H	1221	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
16	a	521	BCR	C28-C27-C26	-3.75	107.37	114.06
13	B	1221	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
16	3	521	BCR	C28-C27-C26	-3.75	107.37	114.06
20	Y	822	SQD	O47-C7-C8	3.75	119.59	111.48
20	Z	822	SQD	O47-C7-C8	3.74	119.58	111.48
20	r	822	SQD	O47-C7-C8	3.74	119.58	111.48
16	s	521	BCR	C28-C27-C26	-3.74	107.38	114.06
16	2	522	BCR	C11-C10-C9	-3.74	122.03	127.28
16	6	524	BCR	C11-C10-C9	-3.74	122.03	127.28
16	Y	524	BCR	C33-C5-C6	-3.74	120.40	124.48
16	Y	522	BCR	C7-C8-C9	-3.74	120.70	126.23
16	d	524	BCR	C11-C10-C9	-3.74	122.04	127.28
16	G	4007	BCR	C11-C10-C9	-3.74	122.04	127.28
13	f	1221	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
16	a	521	BCR	C7-C8-C9	-3.73	120.71	126.23
20	2	822	SQD	O47-C7-C8	3.73	119.56	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	s	521	BCR	C7-C8-C9	-3.73	120.71	126.23
16	r	523	BCR	C16-C17-C18	-3.73	122.05	127.28
16	A	4002	BCR	C11-C10-C9	-3.73	122.05	127.28
16	r	522	BCR	C11-C10-C9	-3.73	122.05	127.28
16	B	4005	BCR	C11-C10-C9	-3.73	122.05	127.28
16	3	521	BCR	C7-C8-C9	-3.72	120.73	126.23
13	A	1132	CLA	O2D-CGD-CBD	3.72	117.74	111.23
16	H	4005	BCR	C11-C10-C9	-3.72	122.06	127.28
13	e	1132	CLA	O2D-CGD-CBD	3.72	117.74	111.23
16	B	4005	BCR	C20-C21-C22	-3.72	122.06	127.28
13	U	1105	CLA	CMC-C2C-C1C	-3.72	119.22	125.03
13	K	1105	CLA	CMC-C2C-C1C	-3.72	119.22	125.03
16	Z	523	BCR	C16-C17-C18	-3.72	122.07	127.28
16	f	4005	BCR	C20-C21-C22	-3.71	122.07	127.28
13	G	1132	CLA	O2D-CGD-CBD	3.71	117.72	111.23
16	2	523	BCR	C16-C17-C18	-3.71	122.07	127.28
16	H	4017	BCR	C10-C11-C12	-3.71	112.45	123.20
16	f	4005	BCR	C11-C10-C9	-3.71	122.08	127.28
16	B	4017	BCR	C10-C11-C12	-3.70	112.48	123.20
16	H	4005	BCR	C20-C21-C22	-3.70	122.09	127.28
13	m	1105	CLA	CMC-C2C-C1C	-3.70	119.26	125.03
16	v	522	BCR	C15-C16-C17	-3.70	115.95	123.52
16	W	4021	BCR	C38-C26-C25	-3.69	120.46	124.48
16	A	4003	BCR	C15-C14-C13	-3.69	122.10	127.28
16	G	4003	BCR	C15-C14-C13	-3.69	122.10	127.28
16	f	4017	BCR	C10-C11-C12	-3.69	112.51	123.20
16	A	4007	BCR	C27-C26-C25	-3.69	117.72	122.70
16	6	522	BCR	C15-C16-C17	-3.68	115.98	123.52
16	S	4018	BCR	C27-C26-C25	-3.68	117.73	122.70
16	d	522	BCR	C15-C16-C17	-3.67	116.00	123.52
16	G	4007	BCR	C27-C26-C25	-3.67	117.74	122.70
16	e	4002	BCR	C11-C10-C9	-3.67	122.13	127.28
16	e	4003	BCR	C15-C14-C13	-3.67	122.13	127.28
16	2	524	BCR	C16-C17-C18	-3.66	122.14	127.28
16	Y	524	BCR	C7-C8-C9	-3.66	120.82	126.23
16	l	4012	BCR	C3-C4-C5	-3.66	107.53	114.06
16	M	4021	BCR	C38-C26-C25	-3.66	120.49	124.48
16	l	4013	BCR	C2-C1-C6	3.66	115.75	110.44
13	e	1106	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
16	I	4018	BCR	C27-C26-C25	-3.66	117.76	122.70
16	J	4012	BCR	C3-C4-C5	-3.65	107.54	114.06
16	r	524	BCR	C16-C17-C18	-3.65	122.16	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4007	BCR	C27-C26-C25	-3.65	117.77	122.70
16	J	4013	BCR	C3-C4-C5	-3.65	107.55	114.06
16	k	4018	BCR	C27-C26-C25	-3.65	117.77	122.70
16	J	4013	BCR	C2-C1-C6	3.64	115.73	110.44
13	A	1106	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
16	o	4021	BCR	C15-C14-C13	-3.64	122.17	127.28
13	B	1012	CLA	CMB-C2B-C1B	-3.64	119.87	125.42
13	H	1012	CLA	CMB-C2B-C1B	-3.64	119.88	125.42
13	G	1106	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
16	l	4013	BCR	C3-C4-C5	-3.64	107.57	114.06
16	o	4021	BCR	C38-C26-C25	-3.64	120.52	124.48
16	T	4012	BCR	C3-C4-C5	-3.64	107.57	114.06
16	Z	524	BCR	C16-C17-C18	-3.64	122.18	127.28
16	T	4013	BCR	C2-C1-C6	3.63	115.72	110.44
16	G	4008	BCR	C7-C8-C9	-3.63	120.86	126.23
13	f	1012	CLA	CMB-C2B-C1B	-3.63	119.89	125.42
16	A	4008	BCR	C7-C8-C9	-3.63	120.86	126.23
16	1	524	BCR	C7-C8-C9	-3.63	120.86	126.23
16	t	521	BCR	C20-C21-C22	-3.63	122.19	127.28
16	v	522	BCR	C24-C23-C22	-3.63	120.87	126.23
16	Y	523	BCR	C15-C14-C13	-3.62	122.20	127.28
13	H	1221	CLA	CMB-C2B-C1B	-3.62	119.90	125.42
16	Z	521	BCR	C11-C10-C9	-3.62	122.20	127.28
16	2	521	BCR	C11-C10-C9	-3.62	122.20	127.28
16	T	4013	BCR	C3-C4-C5	-3.62	107.60	114.06
13	e	1126	CLA	CMB-C2B-C1B	-3.61	119.92	125.42
16	q	524	BCR	C7-C8-C9	-3.61	120.90	126.23
16	n	4020	BCR	C16-C15-C14	-3.61	116.14	123.52
16	6	524	BCR	C33-C5-C6	-3.61	120.55	124.48
16	L	4020	BCR	C16-C15-C14	-3.61	116.14	123.52
16	H	4017	BCR	C16-C17-C18	-3.61	122.22	127.28
13	B	1221	CLA	CMB-C2B-C1B	-3.60	119.93	125.42
16	e	4008	BCR	C7-C8-C9	-3.60	120.91	126.23
16	v	524	BCR	C33-C5-C6	-3.60	120.56	124.48
16	W	4021	BCR	C15-C14-C13	-3.60	122.23	127.28
16	6	522	BCR	C24-C23-C22	-3.60	120.91	126.23
16	M	4021	BCR	C15-C14-C13	-3.60	122.23	127.28
16	V	4020	BCR	C16-C15-C14	-3.60	116.16	123.52
13	A	1107	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
13	H	1229	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
16	r	521	BCR	C11-C10-C9	-3.60	122.24	127.28
13	f	1221	CLA	CMB-C2B-C1B	-3.59	119.95	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	523	BCR	C15-C14-C13	-3.59	122.24	127.28
16	d	522	BCR	C24-C23-C22	-3.59	120.92	126.23
13	B	1229	CLA	CMB-C2B-C1B	-3.59	119.95	125.42
13	A	1126	CLA	CMB-C2B-C1B	-3.59	119.95	125.42
16	b	521	BCR	C20-C21-C22	-3.59	122.24	127.28
16	H	4010	BCR	C39-C30-C25	-3.59	104.61	110.24
16	q	523	BCR	C15-C14-C13	-3.59	122.24	127.28
13	2	507	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
16	B	4010	BCR	C39-C30-C25	-3.59	104.62	110.24
16	d	524	BCR	C33-C5-C6	-3.59	120.57	124.48
16	4	521	BCR	C20-C21-C22	-3.59	122.25	127.28
13	Z	507	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
16	5	522	BCR	C24-C23-C22	-3.58	120.93	126.23
13	G	1126	CLA	CMB-C2B-C1B	-3.58	119.96	125.42
13	G	1107	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
16	f	4010	BCR	C39-C30-C25	-3.58	104.62	110.24
13	e	1107	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
13	e	1011	CLA	CGD-CBD-CAD	3.58	122.44	110.85
16	f	4017	BCR	C16-C17-C18	-3.58	122.26	127.28
16	B	4017	BCR	C16-C17-C18	-3.58	122.26	127.28
13	G	1011	CLA	CGD-CBD-CAD	3.58	122.43	110.85
13	f	1229	CLA	CMB-C2B-C1B	-3.58	119.97	125.42
13	G	1013	CLA	CAA-C2A-C1A	-3.58	100.25	111.97
13	A	1011	CLA	CGD-CBD-CAD	3.58	122.42	110.85
16	u	521	BCR	C28-C27-C26	-3.58	107.68	114.06
13	e	1013	CLA	CAA-C2A-C1A	-3.57	100.26	111.97
13	A	1013	CLA	CAA-C2A-C1A	-3.57	100.27	111.97
16	u	522	BCR	C24-C23-C22	-3.57	120.95	126.23
16	c	522	BCR	C24-C23-C22	-3.57	120.96	126.23
13	e	1137	CLA	O2D-CGD-CBD	3.57	117.46	111.23
13	B	1227	CLA	C3B-C4B-NB	-3.56	107.35	110.53
13	f	1227	CLA	C3B-C4B-NB	-3.56	107.35	110.53
16	H	4009	BCR	C3-C4-C5	-3.56	107.71	114.06
16	c	521	BCR	C7-C8-C9	-3.56	120.97	126.23
13	a	508	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
16	B	4014	BCR	C20-C19-C18	-3.56	116.61	126.36
13	G	1137	CLA	O2D-CGD-CBD	3.56	117.45	111.23
13	T	1302	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
16	5	521	BCR	C28-C27-C26	-3.56	107.72	114.06
16	H	4014	BCR	C20-C19-C18	-3.55	116.62	126.36
13	l	1302	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
13	3	508	CLA	CMB-C2B-C1B	-3.55	120.01	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	r	507	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
13	A	1137	CLA	O2D-CGD-CBD	3.55	117.43	111.23
16	v	523	BCR	C16-C17-C18	-3.55	122.30	127.28
16	c	521	BCR	C28-C27-C26	-3.55	107.73	114.06
16	f	4014	BCR	C20-C19-C18	-3.54	116.64	126.36
16	6	523	BCR	C16-C17-C18	-3.54	122.31	127.28
13	f	1222	CLA	O2D-CGD-O1D	-3.54	116.97	123.85
13	J	1302	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
16	q	521	BCR	C11-C10-C9	-3.53	122.32	127.28
16	B	4009	BCR	C3-C4-C5	-3.53	107.75	114.06
16	5	521	BCR	C7-C8-C9	-3.53	121.01	126.23
16	s	524	BCR	C7-C8-C9	-3.53	121.01	126.23
13	H	1227	CLA	C3B-C4B-NB	-3.53	107.38	110.53
16	J	4015	BCR	C32-C1-C6	-3.53	104.71	110.24
16	u	521	BCR	C7-C8-C9	-3.53	121.01	126.23
16	Y	521	BCR	C11-C10-C9	-3.53	122.33	127.28
13	B	1222	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
16	T	4015	BCR	C32-C1-C6	-3.53	104.71	110.24
16	n	4020	BCR	C15-C14-C13	-3.53	122.33	127.28
13	f	1216	CLA	C3B-C4B-NB	-3.52	107.38	110.53
13	u	519	CLA	C3B-C4B-NB	-3.52	107.38	110.53
16	1	521	BCR	C11-C10-C9	-3.52	122.34	127.28
16	v	521	BCR	C3-C4-C5	-3.52	107.78	114.06
16	t	524	BCR	C7-C8-C9	-3.52	121.03	126.23
16	l	4013	BCR	C11-C10-C9	-3.52	122.34	127.28
16	f	4009	BCR	C3-C4-C5	-3.52	107.78	114.06
13	s	508	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
16	d	523	BCR	C16-C17-C18	-3.52	122.35	127.28
16	L	4020	BCR	C15-C14-C13	-3.52	122.35	127.28
16	6	521	BCR	C3-C4-C5	-3.51	107.79	114.06
16	V	4020	BCR	C15-C14-C13	-3.51	122.35	127.28
16	d	521	BCR	C3-C4-C5	-3.51	107.79	114.06
16	d	522	BCR	C11-C10-C9	-3.51	122.36	127.28
16	e	4007	BCR	C20-C21-C22	-3.51	122.36	127.28
13	f	1226	CLA	C2D-C1D-ND	-3.51	106.65	110.13
16	3	524	BCR	C7-C8-C9	-3.51	121.04	126.23
16	l	4015	BCR	C32-C1-C6	-3.51	104.74	110.24
16	T	4013	BCR	C11-C10-C9	-3.51	122.36	127.28
16	B	4009	BCR	C24-C23-C22	-3.51	121.05	126.23
16	b	524	BCR	C7-C8-C9	-3.51	121.05	126.23
16	a	522	BCR	C28-C27-C26	-3.50	107.81	114.06
16	1	521	BCR	C28-C27-C26	-3.50	107.81	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4009	BCR	C24-C23-C22	-3.50	121.06	126.23
16	a	524	BCR	C7-C8-C9	-3.50	121.06	126.23
16	v	522	BCR	C11-C10-C9	-3.50	122.37	127.28
13	e	1101	CLA	C3B-C4B-NB	-3.50	107.41	110.53
16	4	524	BCR	C7-C8-C9	-3.50	121.06	126.23
16	3	522	BCR	C28-C27-C26	-3.50	107.82	114.06
16	Y	521	BCR	C28-C27-C26	-3.50	107.82	114.06
13	H	1222	CLA	O2D-CGD-O1D	-3.50	117.05	123.85
13	B	1216	CLA	C3B-C4B-NB	-3.49	107.41	110.53
16	f	4009	BCR	C24-C23-C22	-3.49	121.07	126.23
16	6	522	BCR	C11-C10-C9	-3.49	122.38	127.28
16	J	4013	BCR	C11-C10-C9	-3.49	122.38	127.28
16	G	4007	BCR	C20-C21-C22	-3.49	122.38	127.28
13	5	519	CLA	C3B-C4B-NB	-3.49	107.41	110.53
16	3	524	BCR	C33-C5-C6	-3.49	120.67	124.48
16	s	524	BCR	C33-C5-C6	-3.49	120.68	124.48
16	b	522	BCR	C28-C27-C26	-3.49	107.84	114.06
16	o	4021	BCR	C20-C21-C22	-3.49	122.39	127.28
16	M	4021	BCR	C20-C21-C22	-3.49	122.39	127.28
16	t	522	BCR	C28-C27-C26	-3.49	107.84	114.06
16	W	4021	BCR	C20-C21-C22	-3.48	122.39	127.28
13	H	1216	CLA	C3B-C4B-NB	-3.48	107.42	110.53
16	A	4007	BCR	C20-C21-C22	-3.48	122.39	127.28
16	a	521	BCR	C20-C21-C22	-3.48	122.39	127.28
13	t	507	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
13	f	1220	CLA	CAA-C2A-C1A	-3.48	100.56	111.97
16	H	4017	BCR	C15-C14-C13	-3.48	122.39	127.28
16	q	521	BCR	C28-C27-C26	-3.48	107.85	114.06
16	B	4009	BCR	C11-C10-C9	-3.48	122.40	127.28
13	b	507	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
16	4	522	BCR	C28-C27-C26	-3.48	107.85	114.06
16	s	522	BCR	C28-C27-C26	-3.48	107.85	114.06
13	B	1220	CLA	CAA-C2A-C1A	-3.48	100.58	111.97
13	4	507	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
16	G	4008	BCR	C33-C5-C6	-3.48	120.69	124.48
13	H	1220	CLA	CAA-C2A-C1A	-3.47	100.59	111.97
16	H	4009	BCR	C11-C10-C9	-3.47	122.41	127.28
13	H	1228	CLA	CMB-C2B-C1B	-3.47	120.13	125.42
13	B	1228	CLA	CMB-C2B-C1B	-3.47	120.13	125.42
16	H	4010	BCR	C16-C17-C18	-3.47	122.41	127.28
16	3	521	BCR	C20-C21-C22	-3.47	122.41	127.28
13	H	1012	CLA	C3B-C4B-NB	-3.47	107.43	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4008	BCR	C33-C5-C6	-3.47	120.70	124.48
16	B	4010	BCR	C16-C17-C18	-3.47	122.42	127.28
13	U	1105	CLA	CBC-CAC-C3C	3.46	121.81	112.42
13	q	519	CLA	C3B-C4B-NB	-3.46	107.44	110.53
13	B	1226	CLA	C2D-C1D-ND	-3.46	106.70	110.13
16	5	523	BCR	C15-C16-C17	-3.46	116.43	123.52
13	e	1112	CLA	C3B-C4B-NB	-3.46	107.44	110.53
16	A	4008	BCR	C33-C5-C6	-3.46	120.71	124.48
16	a	524	BCR	C33-C5-C6	-3.46	120.71	124.48
13	A	1101	CLA	C3B-C4B-NB	-3.46	107.44	110.53
20	u	822	SQD	O9-S-C6	3.46	111.92	106.76
16	f	4006	BCR	C33-C5-C6	-3.46	120.71	124.48
16	6	522	BCR	C3-C4-C5	-3.46	107.89	114.06
16	v	524	BCR	C20-C21-C22	-3.46	122.43	127.28
13	A	1112	CLA	C3B-C4B-NB	-3.46	107.44	110.53
16	d	522	BCR	C3-C4-C5	-3.46	107.89	114.06
16	6	524	BCR	C20-C21-C22	-3.45	122.43	127.28
16	f	4010	BCR	C16-C17-C18	-3.45	122.43	127.28
16	f	4017	BCR	C15-C14-C13	-3.45	122.43	127.28
13	f	1235	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
20	c	822	SQD	O9-S-C6	3.45	111.91	106.76
13	G	1101	CLA	C3B-C4B-NB	-3.45	107.45	110.53
13	c	519	CLA	C3B-C4B-NB	-3.45	107.45	110.53
16	v	522	BCR	C3-C4-C5	-3.45	107.90	114.06
13	f	1012	CLA	C3B-C4B-NB	-3.45	107.45	110.53
16	c	522	BCR	C7-C8-C9	-3.45	121.13	126.23
16	c	523	BCR	C15-C16-C17	-3.45	116.46	123.52
16	B	4017	BCR	C15-C14-C13	-3.45	122.44	127.28
13	B	1012	CLA	C3B-C4B-NB	-3.45	107.45	110.53
20	5	822	SQD	O9-S-C6	3.45	111.91	106.76
16	d	524	BCR	C20-C21-C22	-3.45	122.44	127.28
16	f	4009	BCR	C11-C10-C9	-3.45	122.44	127.28
16	s	521	BCR	C20-C21-C22	-3.45	122.44	127.28
16	B	4006	BCR	C33-C5-C6	-3.45	120.72	124.48
16	G	4007	BCR	C24-C23-C22	-3.45	121.13	126.23
16	5	522	BCR	C7-C8-C9	-3.45	121.13	126.23
13	H	1201	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
13	f	1228	CLA	CMB-C2B-C1B	-3.45	120.17	125.42
13	H	1235	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
13	K	1105	CLA	CBC-CAC-C3C	3.45	121.77	112.42
13	m	1105	CLA	CBC-CAC-C3C	3.45	121.77	112.42
13	G	1112	CLA	C3B-C4B-NB	-3.45	107.45	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1013	CLA	CMB-C2B-C3B	3.44	134.65	126.55
13	B	1235	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
16	u	523	BCR	C15-C16-C17	-3.44	116.47	123.52
13	A	1013	CLA	CMB-C2B-C3B	3.44	134.65	126.55
13	1	519	CLA	C3B-C4B-NB	-3.44	107.46	110.53
16	s	523	BCR	C7-C8-C9	-3.44	121.14	126.23
16	o	4021	BCR	C28-C27-C26	-3.44	107.92	114.06
16	A	4007	BCR	C24-C23-C22	-3.44	121.15	126.23
16	H	4006	BCR	C33-C5-C6	-3.44	120.73	124.48
20	n	5216	SQD	C4-C3-C2	3.44	116.87	110.83
16	W	4021	BCR	C28-C27-C26	-3.44	107.93	114.06
13	f	1201	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
16	c	521	BCR	C11-C10-C9	-3.44	122.46	127.28
16	U	4104	BCR	C16-C17-C18	-3.43	122.47	127.28
16	u	522	BCR	C7-C8-C9	-3.43	121.16	126.23
13	B	1201	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
16	3	523	BCR	C7-C8-C9	-3.43	121.16	126.23
13	A	1128	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
13	H	1202	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
16	r	522	BCR	C7-C8-C9	-3.43	121.17	126.23
16	M	4021	BCR	C28-C27-C26	-3.43	107.94	114.06
13	e	1128	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
16	e	4007	BCR	C24-C23-C22	-3.43	121.17	126.23
16	2	522	BCR	C7-C8-C9	-3.43	121.17	126.23
16	1	521	BCR	C20-C21-C22	-3.42	122.47	127.28
13	G	1013	CLA	CMB-C2B-C3B	3.42	134.60	126.55
13	F	1301	CLA	C3B-C4B-NB	-3.42	107.47	110.53
16	3	524	BCR	C16-C17-C18	-3.42	122.48	127.28
16	f	4006	BCR	C16-C17-C18	-3.42	122.48	127.28
20	L	5216	SQD	C4-C3-C2	3.42	116.83	110.83
13	B	1012	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
13	H	1227	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
13	A	1123	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
13	f	1227	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
13	H	1023	CLA	CMB-C2B-C1B	-3.42	120.22	125.42
16	Z	522	BCR	C7-C8-C9	-3.42	121.18	126.23
13	H	1234	CLA	CMB-C2B-C3B	3.42	134.59	126.55
20	c	822	SQD	O47-C7-C8	3.42	118.87	111.48
16	a	524	BCR	C16-C17-C18	-3.42	122.49	127.28
13	f	1202	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
13	Y	519	CLA	C3B-C4B-NB	-3.42	107.48	110.53
16	B	4006	BCR	C16-C17-C18	-3.41	122.49	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1135	CLA	C1-C2-C3	-3.41	120.60	126.20
13	B	1202	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
13	B	1023	CLA	CMB-C2B-C1B	-3.41	120.22	125.42
16	2	524	BCR	C7-C8-C9	-3.41	121.19	126.23
16	a	523	BCR	C7-C8-C9	-3.41	121.19	126.23
13	f	1012	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
16	K	4104	BCR	C16-C17-C18	-3.41	122.49	127.28
16	u	521	BCR	C11-C10-C9	-3.41	122.49	127.28
13	G	1135	CLA	C1-C2-C3	-3.41	120.61	126.20
16	T	4015	BCR	C11-C10-C9	-3.41	122.49	127.28
16	5	521	BCR	C11-C10-C9	-3.41	122.49	127.28
13	B	1234	CLA	CMB-C2B-C3B	3.41	134.57	126.55
13	j	1301	CLA	C3B-C4B-NB	-3.41	107.49	110.53
16	q	521	BCR	C20-C21-C22	-3.41	122.50	127.28
13	H	1012	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
20	V	5216	SQD	C4-C3-C2	3.41	116.81	110.83
13	G	1128	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
13	R	1301	CLA	C3B-C4B-NB	-3.41	107.49	110.53
13	H	1226	CLA	C2D-C1D-ND	-3.41	106.75	110.13
16	r	524	BCR	C7-C8-C9	-3.41	121.19	126.23
16	Z	524	BCR	C7-C8-C9	-3.41	121.20	126.23
13	G	1123	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
20	u	822	SQD	O47-C7-C8	3.40	118.84	111.48
13	B	1227	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
13	e	1123	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
16	e	4007	BCR	C16-C17-C18	-3.40	122.51	127.28
16	Y	521	BCR	C20-C21-C22	-3.40	122.51	127.28
20	5	822	SQD	O47-C7-C8	3.40	118.84	111.48
16	s	523	BCR	C11-C10-C9	-3.40	122.51	127.28
13	A	1135	CLA	C1-C2-C3	-3.40	120.63	126.20
13	H	1205	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
16	5	521	BCR	C24-C23-C22	-3.39	121.22	126.23
13	G	1013	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
16	m	4104	BCR	C16-C17-C18	-3.39	122.52	127.28
13	f	1234	CLA	CMB-C2B-C3B	3.39	134.52	126.55
16	s	524	BCR	C16-C17-C18	-3.39	122.53	127.28
13	f	1023	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
16	H	4014	BCR	C16-C15-C14	-3.39	116.59	123.52
16	J	4015	BCR	C11-C10-C9	-3.38	122.53	127.28
16	A	4007	BCR	C16-C17-C18	-3.38	122.53	127.28
16	a	523	BCR	C11-C10-C9	-3.38	122.53	127.28
16	s	522	BCR	C24-C23-C22	-3.38	121.23	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	4007	BCR	C16-C17-C18	-3.38	122.54	127.28
16	l	4015	BCR	C11-C10-C9	-3.38	122.54	127.28
16	f	4014	BCR	C16-C15-C14	-3.38	116.61	123.52
16	H	4006	BCR	C16-C17-C18	-3.38	122.54	127.28
13	B	1023	CLA	C3B-C4B-NB	-3.38	107.52	110.53
13	B	1205	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
16	B	4014	BCR	C16-C15-C14	-3.38	116.61	123.52
16	v	522	BCR	C28-C27-C26	-3.37	108.04	114.06
16	n	4219	BCR	C24-C23-C22	-3.37	121.24	126.23
16	u	521	BCR	C24-C23-C22	-3.37	121.24	126.23
13	f	1205	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
16	3	523	BCR	C11-C10-C9	-3.37	122.55	127.28
13	A	1013	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
13	H	1202	CLA	CMB-C2B-C1B	-3.37	120.29	125.42
13	f	1023	CLA	C3B-C4B-NB	-3.36	107.53	110.53
13	e	1013	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
13	f	1202	CLA	CMB-C2B-C1B	-3.36	120.30	125.42
16	d	522	BCR	C28-C27-C26	-3.36	108.06	114.06
16	L	4022	BCR	C20-C21-C22	-3.36	122.57	127.28
16	4	521	BCR	C11-C10-C9	-3.36	122.57	127.28
16	V	4219	BCR	C24-C23-C22	-3.36	121.27	126.23
16	6	522	BCR	C28-C27-C26	-3.36	108.07	114.06
13	f	1222	CLA	CAA-C2A-C1A	-3.36	100.98	111.97
13	G	1101	CLA	O2D-CGD-CBD	3.35	117.09	111.23
16	c	521	BCR	C24-C23-C22	-3.35	121.27	126.23
16	L	4219	BCR	C24-C23-C22	-3.35	121.28	126.23
16	V	4022	BCR	C20-C21-C22	-3.35	122.58	127.28
13	B	1222	CLA	CAA-C2A-C1A	-3.35	100.99	111.97
13	B	1214	CLA	C3B-C4B-NB	-3.35	107.54	110.53
13	H	1222	CLA	CAA-C2A-C1A	-3.35	101.00	111.97
16	n	4022	BCR	C20-C21-C22	-3.35	122.58	127.28
16	W	4021	BCR	C10-C11-C12	-3.35	113.51	123.20
16	Y	522	BCR	C24-C23-C22	-3.34	121.29	126.23
13	f	1214	CLA	C3B-C4B-NB	-3.34	107.55	110.53
16	1	522	BCR	C24-C23-C22	-3.34	121.29	126.23
13	B	1202	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
16	b	521	BCR	C11-C10-C9	-3.34	122.59	127.28
16	a	523	BCR	C16-C17-C18	-3.34	122.60	127.28
16	m	4104	BCR	C30-C25-C26	-3.34	118.07	122.64
16	a	522	BCR	C24-C23-C22	-3.34	121.30	126.23
16	m	4104	BCR	C11-C10-C9	-3.34	122.60	127.28
13	H	1023	CLA	C3B-C4B-NB	-3.34	107.55	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	521	BCR	C7-C8-C9	-3.34	121.30	126.23
16	t	521	BCR	C11-C10-C9	-3.33	122.60	127.28
16	q	521	BCR	C7-C8-C9	-3.33	121.31	126.23
13	A	1101	CLA	O2D-CGD-CBD	3.33	117.06	111.23
16	3	522	BCR	C24-C23-C22	-3.33	121.31	126.23
13	B	1204	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
16	U	4104	BCR	C11-C10-C9	-3.33	122.61	127.28
13	A	1101	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
16	a	521	BCR	C24-C23-C22	-3.33	121.31	126.23
16	5	522	BCR	C28-C27-C26	-3.33	108.12	114.06
13	e	1101	CLA	O2D-CGD-CBD	3.33	117.05	111.23
16	3	521	BCR	C24-C23-C22	-3.33	121.31	126.23
13	a	516	CLA	CBC-CAC-C3C	3.33	121.44	112.42
16	K	4104	BCR	C11-C10-C9	-3.32	122.61	127.28
13	Y	501	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
16	u	522	BCR	C28-C27-C26	-3.32	108.13	114.06
16	s	523	BCR	C16-C17-C18	-3.32	122.62	127.28
16	M	4021	BCR	C10-C11-C12	-3.32	113.58	123.20
13	G	1101	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
13	f	1204	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
16	Y	521	BCR	C7-C8-C9	-3.32	121.33	126.23
16	q	522	BCR	C24-C23-C22	-3.32	121.33	126.23
16	G	4001	BCR	C24-C23-C22	-3.32	121.33	126.23
16	c	522	BCR	C28-C27-C26	-3.32	108.14	114.06
13	H	1204	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
13	1	501	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
16	V	4219	BCR	C10-C11-C12	-3.31	113.60	123.20
16	o	4021	BCR	C10-C11-C12	-3.31	113.60	123.20
16	u	524	BCR	C16-C17-C18	-3.31	122.63	127.28
16	Z	524	BCR	C33-C5-C6	-3.31	120.87	124.48
16	K	4104	BCR	C30-C25-C26	-3.31	118.11	122.64
13	3	516	CLA	CBC-CAC-C3C	3.31	121.40	112.42
13	e	1101	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
16	q	523	BCR	C21-C20-C19	-3.31	113.61	123.20
13	s	516	CLA	CBC-CAC-C3C	3.31	121.39	112.42
13	H	1214	CLA	C3B-C4B-NB	-3.31	107.58	110.53
13	G	1106	CLA	O2A-CGA-O1A	-3.31	115.35	123.63
16	V	4022	BCR	C15-C14-C13	-3.31	122.64	127.28
16	n	4219	BCR	C10-C11-C12	-3.31	113.62	123.20
13	6	512	CLA	C3B-C4B-NB	-3.30	107.58	110.53
16	3	523	BCR	C16-C17-C18	-3.30	122.64	127.28
16	5	523	BCR	C10-C11-C12	-3.30	113.63	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	1502	CLA	C3B-C4B-NB	-3.30	107.58	110.53
16	L	4219	BCR	C10-C11-C12	-3.30	113.64	123.20
13	e	1106	CLA	O2A-CGA-O1A	-3.30	115.38	123.63
16	c	524	BCR	C16-C17-C18	-3.30	122.65	127.28
13	q	501	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
16	u	523	BCR	C10-C11-C12	-3.30	113.64	123.20
13	d	512	CLA	C3B-C4B-NB	-3.30	107.59	110.53
16	e	4001	BCR	C24-C23-C22	-3.30	121.36	126.23
16	n	4020	BCR	C20-C21-C22	-3.29	122.66	127.28
16	b	524	BCR	C20-C21-C22	-3.29	122.66	127.28
16	Y	523	BCR	C21-C20-C19	-3.29	113.66	123.20
13	A	1136	CLA	C3B-C4B-NB	-3.29	107.59	110.53
13	n	1502	CLA	C3B-C4B-NB	-3.29	107.59	110.53
16	1	523	BCR	C21-C20-C19	-3.29	113.66	123.20
16	A	4001	BCR	C24-C23-C22	-3.29	121.37	126.23
16	s	521	BCR	C24-C23-C22	-3.29	121.37	126.23
16	c	523	BCR	C10-C11-C12	-3.29	113.67	123.20
16	L	4020	BCR	C20-C21-C22	-3.29	122.67	127.28
13	A	1106	CLA	O2A-CGA-O1A	-3.29	115.40	123.63
16	r	524	BCR	C33-C5-C6	-3.29	120.90	124.48
16	Z	521	BCR	C7-C8-C9	-3.29	121.37	126.23
16	U	4104	BCR	C30-C25-C26	-3.29	118.15	122.64
13	t	519	CLA	C3B-C4B-NB	-3.29	107.60	110.53
13	v	512	CLA	C3B-C4B-NB	-3.29	107.60	110.53
16	2	524	BCR	C33-C5-C6	-3.29	120.90	124.48
16	5	524	BCR	C16-C17-C18	-3.28	122.67	127.28
13	B	1239	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
13	H	1239	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
16	r	521	BCR	C7-C8-C9	-3.28	121.38	126.23
13	f	1239	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
13	e	1136	CLA	C3B-C4B-NB	-3.28	107.60	110.53
16	V	4020	BCR	C20-C21-C22	-3.28	122.67	127.28
16	4	524	BCR	C20-C21-C22	-3.28	122.68	127.28
13	f	1230	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
16	t	524	BCR	C20-C21-C22	-3.28	122.68	127.28
13	2	519	CLA	C3B-C4B-NB	-3.28	107.60	110.53
13	B	1223	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
20	a	822	SQD	O47-C7-C8	3.28	118.57	111.48
13	f	1207	CLA	C3B-C4B-NB	-3.28	107.60	110.53
13	G	1135	CLA	CMB-C2B-C1B	-3.28	120.43	125.42
16	2	521	BCR	C7-C8-C9	-3.28	121.39	126.23
16	t	522	BCR	C20-C21-C22	-3.28	122.69	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4009	BCR	C33-C5-C6	-3.27	120.91	124.48
13	G	1118	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
14	f	2002	PQN	C14-C13-C15	-3.27	109.55	115.23
13	G	1136	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	4	522	BCR	C20-C21-C22	-3.27	122.69	127.28
13	r	519	CLA	C3B-C4B-NB	-3.27	107.61	110.53
13	f	1223	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
13	f	1213	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
13	H	1207	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	L	4022	BCR	C15-C14-C13	-3.27	122.70	127.28
13	e	1112	CLA	CHB-C4A-NA	3.26	129.11	124.40
16	q	522	BCR	C28-C27-C26	-3.26	108.23	114.06
13	e	1128	CLA	CHB-C1B-NB	3.26	128.95	124.05
20	c	822	SQD	C1-O5-C5	3.26	120.09	113.72
16	b	522	BCR	C20-C21-C22	-3.26	122.70	127.28
13	B	1230	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
13	G	1124	CLA	CAA-C2A-C1A	-3.26	101.29	111.97
20	3	822	SQD	O47-C7-C8	3.26	118.53	111.48
13	G	1110	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
13	A	1118	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
13	B	1213	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
13	B	1207	CLA	C3B-C4B-NB	-3.26	107.62	110.53
16	e	4007	BCR	C7-C8-C9	-3.26	121.42	126.23
13	Z	519	CLA	C3B-C4B-NB	-3.26	107.62	110.53
16	1	522	BCR	C28-C27-C26	-3.26	108.25	114.06
14	B	2002	PQN	C14-C13-C15	-3.26	109.58	115.23
13	H	1223	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
13	A	1135	CLA	CMB-C2B-C1B	-3.26	120.46	125.42
13	H	1213	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
13	A	1110	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
16	A	4007	BCR	C7-C8-C9	-3.25	121.42	126.23
13	G	1112	CLA	CHB-C4A-NA	3.25	129.09	124.40
13	A	1124	CLA	CAA-C2A-C1A	-3.25	101.32	111.97
13	L	1502	CLA	C3B-C4B-NB	-3.25	107.63	110.53
13	e	1102	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
16	n	4022	BCR	C15-C14-C13	-3.25	122.72	127.28
13	e	1124	CLA	CAA-C2A-C1A	-3.25	101.33	111.97
13	2	516	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
16	G	4007	BCR	C7-C8-C9	-3.25	121.43	126.23
13	e	1110	CLA	C3B-C4B-NB	-3.25	107.63	110.53
13	e	1135	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
13	G	1128	CLA	CHB-C1B-NB	3.25	128.92	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	d	501	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
13	G	1102	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
13	r	516	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
16	3	521	BCR	C11-C10-C9	-3.25	122.73	127.28
13	A	1102	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
16	H	4009	BCR	C33-C5-C6	-3.25	120.94	124.48
13	A	1128	CLA	CHB-C1B-NB	3.24	128.92	124.05
16	s	521	BCR	C11-C10-C9	-3.24	122.73	127.28
13	A	1112	CLA	CHB-C4A-NA	3.24	129.08	124.40
14	H	2002	PQN	C14-C13-C15	-3.24	109.60	115.23
16	1	524	BCR	C24-C23-C22	-3.24	121.44	126.23
20	s	822	SQD	O47-C7-C8	3.24	118.49	111.48
13	e	1110	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
13	G	1105	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
13	G	1140	CLA	C3B-C4B-NB	-3.24	107.64	110.53
13	e	1118	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
13	T	1303	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
13	J	1303	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
20	5	822	SQD	C1-O5-C5	3.24	120.04	113.72
16	Y	522	BCR	C28-C27-C26	-3.24	108.29	114.06
13	e	1105	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
16	a	521	BCR	C11-C10-C9	-3.23	122.74	127.28
13	A	1107	CLA	C3B-C4B-NB	-3.23	107.64	110.53
16	n	4219	BCR	C21-C20-C19	-3.23	113.83	123.20
13	Z	516	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
13	4	519	CLA	C3B-C4B-NB	-3.23	107.64	110.53
13	A	1105	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
13	c	512	CLA	C3B-C4B-NB	-3.23	107.65	110.53
13	H	1230	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
16	q	524	BCR	C24-C23-C22	-3.23	121.46	126.23
16	G	4011	BCR	C34-C9-C10	-3.23	117.59	122.82
13	B	1209	CLA	C3B-C4B-NB	-3.23	107.65	110.53
13	b	519	CLA	C3B-C4B-NB	-3.23	107.65	110.53
16	B	4009	BCR	C33-C5-C6	-3.23	120.97	124.48
16	L	4219	BCR	C21-C20-C19	-3.22	113.86	123.20
13	e	1139	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
16	e	4003	BCR	C20-C21-C22	-3.22	122.76	127.28
20	Y	822	SQD	O7-S-C6	3.22	111.57	106.76
16	V	4219	BCR	C21-C20-C19	-3.22	113.87	123.20
16	Y	524	BCR	C24-C23-C22	-3.22	121.47	126.23
20	b	822	SQD	O9-S-C6	3.22	111.56	106.76
13	Z	501	CLA	O2D-CGD-O1D	-3.22	117.58	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4014	BCR	C2-C1-C6	3.22	115.11	110.44
13	H	1232	CLA	CMB-C2B-C3B	3.22	134.12	126.55
20	1	822	SQD	C3-C4-C5	3.22	116.06	110.23
20	u	822	SQD	C1-O5-C5	3.22	120.00	113.72
20	t	822	SQD	O9-S-C6	3.22	111.56	106.76
13	G	1110	CLA	C3B-C4B-NB	-3.22	107.66	110.53
13	f	1209	CLA	C3B-C4B-NB	-3.22	107.66	110.53
16	G	4003	BCR	C20-C21-C22	-3.22	122.77	127.28
13	A	1139	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
16	u	523	BCR	C28-C27-C26	-3.21	108.32	114.06
16	e	4001	BCR	C2-C1-C6	3.21	115.11	110.44
13	G	1139	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
16	B	4014	BCR	C2-C1-C6	3.21	115.11	110.44
13	G	1107	CLA	C3B-C4B-NB	-3.21	107.66	110.53
13	G	1134	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
13	6	501	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
13	l	1303	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
13	e	1107	CLA	C3B-C4B-NB	-3.21	107.66	110.53
16	A	4011	BCR	C34-C9-C10	-3.21	117.62	122.82
16	G	4001	BCR	C11-C10-C9	-3.21	122.78	127.28
16	G	4001	BCR	C2-C1-C6	3.21	115.10	110.44
16	f	4014	BCR	C2-C1-C6	3.21	115.10	110.44
16	2	522	BCR	C28-C27-C26	-3.21	108.33	114.06
13	B	1232	CLA	CMB-C2B-C3B	3.21	134.09	126.55
16	d	524	BCR	C15-C16-C17	-3.21	116.96	123.52
13	2	501	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
16	A	4001	BCR	C2-C1-C6	3.21	115.09	110.44
13	f	1232	CLA	CMB-C2B-C3B	3.20	134.09	126.55
20	4	822	SQD	O9-S-C6	3.20	111.54	106.76
13	f	1215	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
16	J	4013	BCR	C32-C1-C6	-3.20	105.22	110.24
16	v	524	BCR	C15-C16-C17	-3.20	116.96	123.52
16	f	4004	BCR	C33-C5-C6	-3.20	120.99	124.48
20	1	822	SQD	O7-S-C6	3.20	111.54	106.76
13	A	1140	CLA	C3B-C4B-NB	-3.20	107.67	110.53
13	f	1226	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
14	G	2001	PQN	C14-C13-C15	-3.20	109.67	115.23
13	A	1134	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
16	A	4003	BCR	C20-C21-C22	-3.20	122.79	127.28
16	r	522	BCR	C28-C27-C26	-3.20	108.35	114.06
16	5	523	BCR	C28-C27-C26	-3.20	108.35	114.06
13	B	1226	CLA	O2D-CGD-O1D	-3.20	117.62	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	5	512	CLA	C3B-C4B-NB	-3.20	107.67	110.53
13	u	512	CLA	C3B-C4B-NB	-3.20	107.67	110.53
13	Y	508	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
16	e	4001	BCR	C11-C10-C9	-3.20	122.79	127.28
16	T	4013	BCR	C32-C1-C6	-3.20	105.22	110.24
16	v	522	BCR	C20-C21-C22	-3.20	122.79	127.28
16	6	524	BCR	C15-C16-C17	-3.20	116.97	123.52
13	G	1112	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
13	v	501	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
16	Y	522	BCR	C20-C21-C22	-3.20	122.79	127.28
16	A	4001	BCR	C11-C10-C9	-3.20	122.80	127.28
16	4	524	BCR	C1-C6-C5	-3.20	118.27	122.64
20	Y	822	SQD	C3-C4-C5	3.20	116.03	110.23
20	q	822	SQD	C3-C4-C5	3.20	116.03	110.23
13	H	1226	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
13	G	1137	CLA	CHB-C4A-NA	3.19	129.01	124.40
16	e	4011	BCR	C34-C9-C10	-3.19	117.64	122.82
13	G	1131	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
13	1	508	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
13	A	1112	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	f	1023	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	r	501	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	A	1110	CLA	C3B-C4B-NB	-3.19	107.68	110.53
13	e	1112	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
16	u	521	BCR	C3-C4-C5	-3.19	108.37	114.06
13	e	1134	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	H	1209	CLA	C3B-C4B-NB	-3.19	107.68	110.53
16	1	521	BCR	C24-C23-C22	-3.19	121.52	126.23
14	A	2001	PQN	C14-C13-C15	-3.19	109.69	115.23
16	H	4005	BCR	C16-C17-C18	-3.19	122.81	127.28
13	q	508	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
16	T	4012	BCR	C7-C8-C9	-3.19	121.52	126.23
13	A	1131	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	B	1215	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	G	1106	CLA	C3B-C4B-NB	-3.19	107.69	110.53
16	J	4012	BCR	C7-C8-C9	-3.19	121.52	126.23
16	f	4005	BCR	C16-C17-C18	-3.19	122.81	127.28
13	H	1215	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
16	5	521	BCR	C3-C4-C5	-3.19	108.38	114.06
16	l	4013	BCR	C32-C1-C6	-3.18	105.25	110.24
16	Z	522	BCR	C28-C27-C26	-3.18	108.38	114.06
16	Y	521	BCR	C24-C23-C22	-3.18	121.52	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	5	524	BCR	C33-C5-C6	-3.18	121.01	124.48
16	B	4005	BCR	C16-C17-C18	-3.18	122.81	127.28
16	1	522	BCR	C20-C21-C22	-3.18	122.81	127.28
16	b	523	BCR	C33-C5-C6	-3.18	121.01	124.48
20	H	1852	SQD	O6-C1-C2	3.18	113.11	108.27
16	b	524	BCR	C1-C6-C5	-3.18	118.29	122.64
16	c	523	BCR	C28-C27-C26	-3.18	108.38	114.06
20	B	1852	SQD	O6-C1-C2	3.18	113.10	108.27
13	A	1137	CLA	CHB-C4A-NA	3.18	128.99	124.40
16	2	522	BCR	C24-C23-C22	-3.18	121.53	126.23
16	Z	522	BCR	C24-C23-C22	-3.18	121.53	126.23
16	q	521	BCR	C24-C23-C22	-3.18	121.53	126.23
16	n	4019	BCR	C28-C27-C26	-3.18	108.39	114.06
20	q	822	SQD	O7-S-C6	3.18	111.50	106.76
13	B	1023	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
13	H	1202	CLA	CHB-C4A-NA	3.18	128.99	124.40
13	H	1023	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
13	B	1202	CLA	CHB-C4A-NA	3.18	128.99	124.40
13	Z	512	CLA	C3B-C4B-NB	-3.18	107.69	110.53
13	e	1119	CLA	CMB-C2B-C1B	-3.17	120.58	125.42
13	r	513	CLA	C3B-C4B-NB	-3.17	107.70	110.53
16	4	521	BCR	C24-C23-C22	-3.17	121.54	126.23
16	b	523	BCR	C24-C23-C22	-3.17	121.54	126.23
13	e	1137	CLA	CHB-C4A-NA	3.17	128.98	124.40
16	B	4004	BCR	C33-C5-C6	-3.17	121.02	124.48
16	H	4004	BCR	C33-C5-C6	-3.17	121.02	124.48
16	c	524	BCR	C33-C5-C6	-3.17	121.02	124.48
13	f	1207	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
16	V	4019	BCR	C28-C27-C26	-3.17	108.40	114.06
16	V	4022	BCR	C16-C17-C18	-3.17	122.83	127.28
16	q	522	BCR	C20-C21-C22	-3.17	122.83	127.28
14	e	2001	PQN	C14-C13-C15	-3.17	109.72	115.23
13	e	1131	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
16	b	521	BCR	C24-C23-C22	-3.17	121.54	126.23
16	Y	523	BCR	C28-C27-C26	-3.17	108.40	114.06
13	e	1106	CLA	C3B-C4B-NB	-3.17	107.70	110.53
13	e	1140	CLA	C3B-C4B-NB	-3.17	107.70	110.53
20	f	1852	SQD	O6-C1-C2	3.17	113.09	108.27
16	u	524	BCR	C33-C5-C6	-3.17	121.02	124.48
16	4	523	BCR	C33-C5-C6	-3.17	121.03	124.48
16	t	523	BCR	C24-C23-C22	-3.17	121.55	126.23
16	l	4013	BCR	C20-C19-C18	-3.17	117.67	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	6	522	BCR	C20-C21-C22	-3.17	122.83	127.28
13	A	1103	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
16	c	521	BCR	C3-C4-C5	-3.17	108.41	114.06
16	t	524	BCR	C1-C6-C5	-3.17	118.31	122.64
16	5	522	BCR	C38-C26-C25	-3.17	121.03	124.48
13	f	1202	CLA	CHB-C4A-NA	3.17	128.97	124.40
16	u	522	BCR	C38-C26-C25	-3.17	121.03	124.48
13	f	1221	CLA	CHB-C4A-NA	3.16	128.97	124.40
16	d	522	BCR	C20-C21-C22	-3.16	122.84	127.28
16	l	4012	BCR	C7-C8-C9	-3.16	121.56	126.23
16	r	522	BCR	C24-C23-C22	-3.16	121.56	126.23
16	L	4019	BCR	C28-C27-C26	-3.16	108.42	114.06
13	a	510	CLA	CHB-C4A-NA	3.16	128.97	124.40
16	L	4219	BCR	C15-C16-C17	-3.16	117.05	123.52
16	1	523	BCR	C28-C27-C26	-3.16	108.42	114.06
13	A	1119	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
13	f	1217	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
13	G	1116	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
16	t	523	BCR	C33-C5-C6	-3.16	121.04	124.48
16	4	523	BCR	C24-C23-C22	-3.16	121.56	126.23
13	f	1240	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
13	H	1205	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
13	G	1138	CLA	C3B-C4B-NB	-3.16	107.71	110.53
13	B	1221	CLA	CHB-C4A-NA	3.16	128.96	124.40
13	G	1119	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
20	r	822	SQD	O9-S-C6	3.16	111.47	106.76
13	A	1106	CLA	C3B-C4B-NB	-3.16	107.71	110.53
13	B	1217	CLA	O2D-CGD-O1D	-3.16	117.71	123.85
13	e	1103	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
16	n	4219	BCR	C15-C16-C17	-3.15	117.06	123.52
20	s	822	SQD	O9-S-C6	3.15	111.47	106.76
13	2	513	CLA	C3B-C4B-NB	-3.15	107.72	110.53
13	e	1137	CLA	C3B-C4B-NB	-3.15	107.72	110.53
16	b	522	BCR	C7-C8-C9	-3.15	121.57	126.23
16	f	4010	BCR	C28-C27-C26	-3.15	108.43	114.06
16	I	4018	BCR	C11-C10-C9	-3.15	122.86	127.28
13	B	1205	CLA	O2A-CGA-O1A	-3.15	115.74	123.63
16	k	4018	BCR	C11-C10-C9	-3.15	122.86	127.28
16	s	524	BCR	C15-C16-C17	-3.15	117.07	123.52
16	t	521	BCR	C24-C23-C22	-3.15	121.57	126.23
20	2	822	SQD	O9-S-C6	3.15	111.46	106.76
20	3	822	SQD	O9-S-C6	3.15	111.46	106.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	4219	BCR	C15-C16-C17	-3.15	117.08	123.52
16	4	522	BCR	C7-C8-C9	-3.15	121.58	126.23
13	Z	513	CLA	C3B-C4B-NB	-3.15	107.72	110.53
13	r	512	CLA	C3B-C4B-NB	-3.15	107.72	110.53
13	s	510	CLA	CHB-C4A-NA	3.15	128.94	124.40
16	q	523	BCR	C28-C27-C26	-3.15	108.44	114.06
13	G	1103	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
16	a	524	BCR	C15-C16-C17	-3.15	117.08	123.52
13	B	1207	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
13	3	510	CLA	CHB-C4A-NA	3.15	128.94	124.40
13	A	1116	CLA	CMB-C2B-C1B	-3.15	120.63	125.42
16	J	4013	BCR	C20-C19-C18	-3.14	117.74	126.36
16	t	521	BCR	C3-C4-C5	-3.14	108.45	114.06
13	f	1205	CLA	O2A-CGA-O1A	-3.14	115.76	123.63
16	T	4013	BCR	C20-C19-C18	-3.14	117.74	126.36
20	a	822	SQD	O9-S-C6	3.14	111.45	106.76
13	e	1126	CLA	CMB-C2B-C3B	3.14	133.94	126.55
16	L	4022	BCR	C16-C17-C18	-3.14	122.87	127.28
16	S	4018	BCR	C11-C10-C9	-3.14	122.87	127.28
13	H	1221	CLA	CHB-C4A-NA	3.14	128.93	124.40
13	2	512	CLA	C3B-C4B-NB	-3.14	107.73	110.53
16	t	522	BCR	C7-C8-C9	-3.14	121.59	126.23
16	3	524	BCR	C15-C16-C17	-3.14	117.10	123.52
16	n	4022	BCR	C16-C17-C18	-3.14	122.88	127.28
13	A	1137	CLA	C3B-C4B-NB	-3.14	107.73	110.53
13	e	1133	CLA	C3B-C4B-NB	-3.14	107.73	110.53
16	H	4010	BCR	C28-C27-C26	-3.14	108.46	114.06
13	B	1240	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
16	B	4010	BCR	C28-C27-C26	-3.14	108.46	114.06
13	e	1116	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
20	Z	822	SQD	O9-S-C6	3.13	111.44	106.76
13	G	1111	CLA	C3B-C4B-NB	-3.13	107.73	110.53
16	c	522	BCR	C20-C21-C22	-3.13	122.89	127.28
16	2	523	BCR	C28-C27-C26	-3.13	108.47	114.06
16	4	521	BCR	C3-C4-C5	-3.13	108.47	114.06
13	H	1207	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
16	r	523	BCR	C28-C27-C26	-3.13	108.48	114.06
16	u	522	BCR	C20-C21-C22	-3.13	122.89	127.28
13	H	1217	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
16	M	4021	BCR	C15-C16-C17	-3.13	117.12	123.52
16	W	4021	BCR	C15-C16-C17	-3.13	117.12	123.52
16	Z	523	BCR	C28-C27-C26	-3.13	108.48	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1138	CLA	C3B-C4B-NB	-3.13	107.74	110.53
16	o	4021	BCR	C15-C16-C17	-3.12	117.12	123.52
16	2	523	BCR	C33-C5-C6	-3.12	121.08	124.48
16	c	522	BCR	C38-C26-C25	-3.12	121.08	124.48
13	A	1126	CLA	CMB-C2B-C3B	3.12	133.89	126.55
13	f	1225	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
13	A	1111	CLA	C3B-C4B-NB	-3.12	107.75	110.53
16	c	521	BCR	C38-C26-C25	-3.12	121.08	124.48
16	a	523	BCR	C15-C16-C17	-3.12	117.14	123.52
13	G	1126	CLA	CMB-C2B-C3B	3.12	133.88	126.55
13	e	1138	CLA	C3B-C4B-NB	-3.12	107.75	110.53
16	b	521	BCR	C3-C4-C5	-3.11	108.50	114.06
13	H	1240	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
13	G	1136	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
13	Y	512	CLA	C3B-C4B-NB	-3.11	107.75	110.53
16	l	4015	BCR	C38-C26-C25	-3.11	121.09	124.48
13	H	1225	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
13	G	1137	CLA	C3B-C4B-NB	-3.11	107.76	110.53
13	G	1103	CLA	CHB-C4A-NA	3.11	128.88	124.40
16	T	4012	BCR	C11-C10-C9	-3.11	122.92	127.28
13	f	1214	CLA	CHB-C4A-NA	3.10	128.88	124.40
16	b	523	BCR	C28-C27-C26	-3.10	108.52	114.06
13	f	1219	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
13	A	1103	CLA	CHB-C4A-NA	3.10	128.88	124.40
16	3	523	BCR	C15-C16-C17	-3.10	117.17	123.52
16	s	523	BCR	C15-C16-C17	-3.10	117.17	123.52
13	e	1111	CLA	C3B-C4B-NB	-3.10	107.76	110.53
16	t	523	BCR	C28-C27-C26	-3.10	108.53	114.06
13	B	1225	CLA	CMB-C2B-C1B	-3.10	120.70	125.42
13	m	1401	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
13	V	1501	CLA	CHB-C4A-NA	3.10	128.87	124.40
16	H	4017	BCR	C21-C20-C19	-3.10	114.22	123.20
16	J	4012	BCR	C11-C10-C9	-3.10	122.94	127.28
16	5	522	BCR	C20-C21-C22	-3.10	122.94	127.28
16	5	521	BCR	C38-C26-C25	-3.10	121.11	124.48
13	l	1302	CLA	CHB-C4A-NA	3.10	128.87	124.40
13	G	1125	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
16	B	4017	BCR	C21-C20-C19	-3.09	114.24	123.20
20	v	822	SQD	O7-S-C6	3.09	111.37	106.76
13	A	1136	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
13	a	506	CLA	CMB-C2B-C1B	-3.09	120.71	125.42
13	s	512	CLA	C3B-C4B-NB	-3.09	107.77	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	t	521	BCR	C28-C27-C26	-3.09	108.55	114.06
16	Z	523	BCR	C33-C5-C6	-3.09	121.11	124.48
13	A	1125	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
13	f	1216	CLA	CHB-C4A-NA	3.09	128.86	124.40
17	V	5221	LHG	O8-C23-C24	3.09	121.25	111.83
16	S	4018	BCR	C15-C16-C17	-3.09	117.20	123.52
13	G	1125	CLA	C3B-C4B-NB	-3.09	107.77	110.53
13	K	1401	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
13	G	1133	CLA	C3B-C4B-NB	-3.09	107.77	110.53
17	L	5221	LHG	O8-C23-C24	3.09	121.25	111.83
20	r	822	SQD	O6-C1-C2	3.09	112.96	108.27
16	l	4012	BCR	C11-C10-C9	-3.09	122.95	127.28
17	n	5221	LHG	O8-C23-C24	3.08	121.24	111.83
16	f	4017	BCR	C21-C20-C19	-3.08	114.26	123.20
13	q	512	CLA	C3B-C4B-NB	-3.08	107.78	110.53
16	e	4011	BCR	C15-C14-C13	-3.08	122.95	127.28
16	4	523	BCR	C28-C27-C26	-3.08	108.56	114.06
20	6	822	SQD	O7-S-C6	3.08	111.36	106.76
13	Z	519	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
16	k	4018	BCR	C15-C16-C17	-3.08	117.21	123.52
13	e	1103	CLA	CHB-C4A-NA	3.08	128.85	124.40
13	f	1205	CLA	CBA-CAA-C2A	3.08	122.96	113.79
13	B	1219	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
20	q	822	SQD	C1-O5-C5	3.08	119.73	113.72
16	I	4018	BCR	C15-C16-C17	-3.08	117.22	123.52
16	4	521	BCR	C28-C27-C26	-3.08	108.56	114.06
16	r	523	BCR	C24-C23-C22	-3.08	121.68	126.23
16	A	4011	BCR	C15-C14-C13	-3.08	122.96	127.28
13	1	512	CLA	C3B-C4B-NB	-3.08	107.78	110.53
16	c	522	BCR	C33-C5-C6	-3.08	121.12	124.48
16	b	521	BCR	C28-C27-C26	-3.08	108.56	114.06
20	Y	822	SQD	C1-O5-C5	3.08	119.73	113.72
13	B	1218	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
16	Y	523	BCR	C15-C16-C17	-3.08	117.22	123.52
16	T	4015	BCR	C38-C26-C25	-3.08	121.12	124.48
16	2	523	BCR	C24-C23-C22	-3.08	121.68	126.23
13	L	1501	CLA	CHB-C4A-NA	3.08	128.84	124.40
13	B	1214	CLA	CHB-C4A-NA	3.08	128.84	124.40
13	e	1125	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
13	B	1205	CLA	CBA-CAA-C2A	3.08	122.94	113.79
13	H	1226	CLA	CMB-C2B-C3B	3.08	133.78	126.55
16	Z	523	BCR	C24-C23-C22	-3.08	121.69	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1130	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
13	e	1130	CLA	C3B-C4B-NB	-3.07	107.79	110.53
13	B	1202	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
13	H	1202	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
13	3	512	CLA	C3B-C4B-NB	-3.07	107.79	110.53
13	H	1214	CLA	CHB-C4A-NA	3.07	128.83	124.40
16	6	523	BCR	C33-C5-C6	-3.07	121.13	124.48
16	d	523	BCR	C7-C8-C9	-3.07	121.69	126.23
16	6	523	BCR	C7-C8-C9	-3.07	121.69	126.23
13	f	1202	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
13	G	1130	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
16	v	523	BCR	C33-C5-C6	-3.07	121.13	124.48
20	d	822	SQD	O7-S-C6	3.07	111.34	106.76
20	q	822	SQD	O6-C1-C2	3.07	112.93	108.27
13	B	1226	CLA	CMB-C2B-C3B	3.07	133.77	126.55
13	n	1501	CLA	CHB-C4A-NA	3.07	128.83	124.40
16	r	523	BCR	C33-C5-C6	-3.07	121.14	124.48
13	e	1136	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
16	u	521	BCR	C38-C26-C25	-3.07	121.14	124.48
13	H	1205	CLA	CBA-CAA-C2A	3.07	122.92	113.79
13	A	1133	CLA	C3B-C4B-NB	-3.07	107.79	110.53
13	H	1219	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
13	A	1125	CLA	C3B-C4B-NB	-3.07	107.79	110.53
16	1	523	BCR	C15-C16-C17	-3.07	117.25	123.52
13	f	1203	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
13	U	1401	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
20	2	822	SQD	O6-C1-C2	3.06	112.93	108.27
13	A	1104	CLA	CAA-C2A-C3A	-3.06	104.72	113.00
20	1	822	SQD	C1-O5-C5	3.06	119.70	113.72
16	J	4015	BCR	C38-C26-C25	-3.06	121.14	124.48
13	q	509	CLA	CHB-C4A-NA	3.06	128.82	124.40
16	G	4008	BCR	C11-C10-C9	-3.06	122.98	127.28
13	3	510	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
13	H	1218	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
13	f	1218	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
13	a	510	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
16	d	523	BCR	C24-C23-C22	-3.06	121.71	126.23
13	A	1130	CLA	C3B-C4B-NB	-3.06	107.80	110.53
13	3	506	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
16	A	4008	BCR	C11-C10-C9	-3.06	122.99	127.28
13	G	1130	CLA	C3B-C4B-NB	-3.06	107.80	110.53
13	H	1012	CLA	CMB-C2B-C3B	3.06	133.74	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1129	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
16	G	4011	BCR	C15-C14-C13	-3.06	122.99	127.28
13	e	1104	CLA	CAA-C2A-C3A	-3.06	104.74	113.00
13	e	1127	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
13	q	510	CLA	C3B-C4B-NB	-3.06	107.80	110.53
13	2	519	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
13	G	1104	CLA	CAA-C2A-C3A	-3.05	104.74	113.00
13	a	512	CLA	C3B-C4B-NB	-3.05	107.80	110.53
16	v	523	BCR	C7-C8-C9	-3.05	121.72	126.23
20	1	822	SQD	O6-C1-C2	3.05	112.91	108.27
13	f	1012	CLA	CMB-C2B-C3B	3.05	133.73	126.55
13	B	1216	CLA	CHB-C4A-NA	3.05	128.81	124.40
13	e	1129	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
13	e	1130	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
13	d	513	CLA	C3B-C4B-NB	-3.05	107.80	110.53
13	B	1012	CLA	CMB-C2B-C3B	3.05	133.73	126.55
13	s	506	CLA	CMB-C2B-C1B	-3.05	120.77	125.42
13	A	1124	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	u	512	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	A	1140	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	f	1226	CLA	CMB-C2B-C3B	3.05	133.73	126.55
13	A	1129	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
16	3	521	BCR	C3-C4-C5	-3.05	108.61	114.06
13	Y	509	CLA	CHB-C4A-NA	3.05	128.80	124.40
13	e	1140	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	G	1140	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
20	Z	822	SQD	O6-C1-C2	3.05	112.91	108.27
20	Y	822	SQD	O6-C1-C2	3.05	112.90	108.27
16	f	4006	BCR	C11-C10-C9	-3.05	123.00	127.28
13	T	1302	CLA	CHB-C4A-NA	3.05	128.80	124.40
13	G	1127	CLA	CMB-C2B-C1B	-3.05	120.78	125.42
16	s	521	BCR	C3-C4-C5	-3.05	108.62	114.06
13	f	1238	CLA	CMB-C2B-C3B	3.05	133.72	126.55
13	A	1127	CLA	CMB-C2B-C1B	-3.05	120.78	125.42
16	Z	523	BCR	C11-C10-C9	-3.05	123.00	127.28
16	V	4020	BCR	C7-C8-C9	-3.05	121.73	126.23
16	L	4020	BCR	C7-C8-C9	-3.05	121.73	126.23
16	u	522	BCR	C33-C5-C6	-3.05	121.16	124.48
16	v	523	BCR	C24-C23-C22	-3.04	121.73	126.23
16	5	522	BCR	C33-C5-C6	-3.04	121.16	124.48
13	G	1124	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
13	1	509	CLA	CHB-C4A-NA	3.04	128.79	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1238	CLA	CMB-C2B-C3B	3.04	133.71	126.55
13	c	512	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
13	G	1105	CLA	CMB-C2B-C1B	-3.04	120.79	125.42
20	Z	822	SQD	O7-S-C6	3.04	111.30	106.76
13	B	1203	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
13	s	519	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
13	K	1401	CLA	C3B-C4B-NB	-3.04	107.81	110.53
13	1	510	CLA	C3B-C4B-NB	-3.04	107.81	110.53
13	G	1135	CLA	C3B-C4B-NB	-3.04	107.81	110.53
13	H	1216	CLA	CHB-C4A-NA	3.04	128.79	124.40
13	5	512	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
13	A	1140	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
20	a	822	SQD	O7-S-C6	3.04	111.30	106.76
16	q	523	BCR	C15-C16-C17	-3.04	117.30	123.52
13	H	1214	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
13	s	510	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
16	e	4002	BCR	C16-C15-C14	-3.04	117.30	123.52
13	H	1238	CLA	CMB-C2B-C3B	3.04	133.70	126.55
16	6	523	BCR	C24-C23-C22	-3.04	121.74	126.23
13	H	1203	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
13	J	1302	CLA	CHB-C4A-NA	3.04	128.78	124.40
16	d	523	BCR	C33-C5-C6	-3.04	121.17	124.48
13	U	1401	CLA	C3B-C4B-NB	-3.04	107.82	110.53
13	G	1140	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
13	B	1214	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
13	r	519	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
16	a	521	BCR	C3-C4-C5	-3.04	108.64	114.06
13	e	1140	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
16	A	4002	BCR	C16-C15-C14	-3.04	117.31	123.52
16	n	4020	BCR	C7-C8-C9	-3.04	121.75	126.23
13	H	1232	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
13	e	1120	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
13	s	519	CLA	C3B-C4B-NB	-3.03	107.82	110.53
16	G	4002	BCR	C16-C15-C14	-3.03	117.32	123.52
13	A	1105	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
16	B	4006	BCR	C11-C10-C9	-3.03	123.03	127.28
13	G	1121	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
16	S	4018	BCR	C1-C6-C5	-3.03	118.50	122.64
20	2	822	SQD	O7-S-C6	3.03	111.28	106.76
13	e	1105	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
16	n	4020	BCR	C10-C11-C12	-3.03	114.43	123.20
16	A	4002	BCR	C20-C21-C22	-3.03	123.03	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	510	CLA	C3B-C4B-NB	-3.03	107.83	110.53
16	e	4008	BCR	C11-C10-C9	-3.03	123.03	127.28
13	3	519	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
16	t	522	BCR	C38-C26-C25	-3.02	121.18	124.48
16	L	4020	BCR	C10-C11-C12	-3.02	114.44	123.20
13	G	1133	CLA	CHB-C4A-NA	3.02	128.76	124.40
13	A	1113	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
20	3	822	SQD	O7-S-C6	3.02	111.27	106.76
16	4	522	BCR	C38-C26-C25	-3.02	121.19	124.48
16	r	523	BCR	C11-C10-C9	-3.02	123.04	127.28
16	e	4002	BCR	C20-C21-C22	-3.02	123.04	127.28
13	e	1124	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
13	e	1125	CLA	C3B-C4B-NB	-3.02	107.83	110.53
13	m	1401	CLA	C3B-C4B-NB	-3.02	107.83	110.53
13	G	1109	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
20	s	822	SQD	O7-S-C6	3.02	111.26	106.76
13	B	1235	CLA	CHB-C4A-NA	3.02	128.75	124.40
16	k	4018	BCR	C1-C6-C5	-3.02	118.51	122.64
13	H	1209	CLA	CHB-C4A-NA	3.02	128.75	124.40
13	H	1206	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
13	B	1234	CLA	C3B-C4B-NB	-3.01	107.84	110.53
13	H	1235	CLA	CHB-C4A-NA	3.01	128.75	124.40
13	A	1120	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
13	e	1113	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
13	f	1214	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
13	A	1109	CLA	O2A-CGA-O1A	-3.01	116.09	123.63
13	H	1234	CLA	C3B-C4B-NB	-3.01	107.84	110.53
13	A	1121	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
13	f	1226	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
13	f	1201	CLA	CMB-C2B-C1B	-3.01	120.83	125.42
16	u	523	BCR	C21-C20-C19	-3.01	114.48	123.20
16	b	522	BCR	C38-C26-C25	-3.01	121.20	124.48
13	A	1111	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
16	5	523	BCR	C21-C20-C19	-3.01	114.48	123.20
16	2	523	BCR	C11-C10-C9	-3.01	123.06	127.28
16	G	4002	BCR	C20-C21-C22	-3.01	123.06	127.28
13	H	1201	CLA	CMB-C2B-C1B	-3.01	120.84	125.42
13	f	1229	CLA	CMB-C2B-C3B	3.01	133.62	126.55
16	a	523	BCR	C24-C23-C22	-3.01	121.79	126.23
13	G	1113	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
13	a	519	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
16	V	4020	BCR	C10-C11-C12	-3.01	114.49	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1229	CLA	CMB-C2B-C3B	3.01	133.62	126.55
13	a	519	CLA	C3B-C4B-NB	-3.01	107.85	110.53
16	e	4002	BCR	C15-C14-C13	-3.00	123.06	127.28
16	G	4011	BCR	C8-C9-C10	3.00	123.73	119.01
13	a	504	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	A	1135	CLA	C3B-C4B-NB	-3.00	107.85	110.53
13	e	1135	CLA	C3B-C4B-NB	-3.00	107.85	110.53
13	Z	504	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	e	1121	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	f	1232	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	B	1220	CLA	CHB-C4A-NA	3.00	128.74	124.40
13	3	504	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
20	r	822	SQD	O7-S-C6	3.00	111.24	106.76
13	f	1223	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
13	A	1133	CLA	CHB-C4A-NA	3.00	128.73	124.40
13	B	1232	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	e	1111	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	A	4011	BCR	C8-C9-C10	3.00	123.73	119.01
13	e	1102	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
16	H	4006	BCR	C11-C10-C9	-3.00	123.07	127.28
13	A	1102	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
16	c	523	BCR	C21-C20-C19	-3.00	114.50	123.20
13	G	1108	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
13	B	1201	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
13	f	1209	CLA	CHB-C4A-NA	3.00	128.73	124.40
13	f	1234	CLA	C3B-C4B-NB	-3.00	107.85	110.53
16	s	523	BCR	C24-C23-C22	-3.00	121.80	126.23
13	f	1206	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
13	H	1229	CLA	CMB-C2B-C3B	3.00	133.60	126.55
13	B	1206	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
13	e	1133	CLA	CHB-C4A-NA	3.00	128.72	124.40
13	s	504	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
13	f	1235	CLA	CHB-C4A-NA	3.00	128.72	124.40
16	c	521	BCR	C30-C25-C26	-3.00	118.54	122.64
13	G	1111	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
16	v	522	BCR	C33-C5-C6	-2.99	121.22	124.48
13	r	504	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
13	B	1209	CLA	CHB-C4A-NA	2.99	128.72	124.40
13	b	509	CLA	CHB-C4A-NA	2.99	128.72	124.40
20	v	822	SQD	O9-S-C6	2.99	111.22	106.76
13	H	1220	CLA	CHB-C4A-NA	2.99	128.72	124.40
16	q	524	BCR	C11-C10-C9	-2.99	123.08	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	3	523	BCR	C24-C23-C22	-2.99	121.81	126.23
13	B	1229	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
16	A	4002	BCR	C15-C14-C13	-2.99	123.08	127.28
16	Y	524	BCR	C11-C10-C9	-2.99	123.08	127.28
16	e	4011	BCR	C8-C9-C10	2.99	123.71	119.01
13	v	513	CLA	C3B-C4B-NB	-2.99	107.86	110.53
13	B	1226	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
13	e	1109	CLA	O2A-CGA-O1A	-2.99	116.15	123.63
16	I	4018	BCR	C1-C6-C5	-2.99	118.55	122.64
13	3	519	CLA	C3B-C4B-NB	-2.99	107.86	110.53
13	f	1229	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	A	1108	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	H	1229	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	A	1102	CLA	C3B-C4B-NB	-2.99	107.86	110.53
13	G	1115	CLA	C3B-C4B-NB	-2.99	107.86	110.53
13	2	504	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	f	1231	CLA	CHB-C4A-NA	2.99	128.71	124.40
13	e	1118	CLA	C3B-C4B-NB	-2.98	107.87	110.53
13	f	1227	CLA	CHB-C4A-NA	2.98	128.71	124.40
13	6	513	CLA	C3B-C4B-NB	-2.98	107.87	110.53
13	V	1502	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
13	s	513	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
16	H	4014	BCR	C3-C4-C5	-2.98	108.74	114.06
13	e	1108	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
16	u	521	BCR	C30-C25-C26	-2.98	118.56	122.64
13	H	1226	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
16	H	4017	BCR	C34-C9-C8	2.98	122.64	118.09
13	B	1223	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
13	v	518	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	5	521	BCR	C30-C25-C26	-2.98	118.56	122.64
16	B	4014	BCR	C3-C4-C5	-2.98	108.74	114.06
13	G	1120	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
16	S	4018	BCR	C21-C20-C19	-2.98	114.57	123.20
16	Y	523	BCR	C16-C17-C18	-2.98	123.10	127.28
13	H	1223	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
16	j	4016	BCR	C28-C27-C26	-2.98	108.75	114.06
16	6	522	BCR	C33-C5-C6	-2.98	121.23	124.48
13	q	519	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
16	d	524	BCR	C24-C23-C22	-2.98	121.83	126.23
20	d	822	SQD	O9-S-C6	2.98	111.20	106.76
16	1	524	BCR	C11-C10-C9	-2.98	123.11	127.28
16	k	4018	BCR	C20-C21-C22	-2.98	123.11	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	F	4016	BCR	C28-C27-C26	-2.98	108.75	114.06
13	t	506	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
13	B	1227	CLA	CHB-C4A-NA	2.97	128.69	124.40
20	u	822	SQD	O5-C5-C4	2.97	115.06	109.70
16	G	4002	BCR	C15-C14-C13	-2.97	123.11	127.28
13	t	509	CLA	CHB-C4A-NA	2.97	128.69	124.40
16	1	522	BCR	C38-C26-C25	-2.97	121.24	124.48
16	t	524	BCR	C8-C7-C6	-2.97	119.05	127.00
20	6	822	SQD	O9-S-C6	2.97	111.20	106.76
13	a	513	CLA	CHB-C4A-NA	2.97	128.69	124.40
13	G	1102	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
16	k	4018	BCR	C21-C20-C19	-2.97	114.59	123.20
13	H	1228	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
16	R	4016	BCR	C28-C27-C26	-2.97	108.76	114.06
20	5	822	SQD	O5-C5-C4	2.97	115.05	109.70
16	f	4014	BCR	C3-C4-C5	-2.97	108.76	114.06
13	5	518	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	4	509	CLA	CHB-C4A-NA	2.97	128.69	124.40
13	n	1502	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
13	f	1220	CLA	CHB-C4A-NA	2.97	128.69	124.40
16	I	4018	BCR	C21-C20-C19	-2.97	114.60	123.20
13	e	1126	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
16	I	4018	BCR	C20-C21-C22	-2.97	123.12	127.28
16	v	524	BCR	C24-C23-C22	-2.97	121.84	126.23
13	H	1227	CLA	CHB-C4A-NA	2.97	128.68	124.40
13	A	1118	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	G	1108	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	2	502	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
16	b	524	BCR	C8-C7-C6	-2.97	119.08	127.00
13	u	518	CLA	C3B-C4B-NB	-2.97	107.88	110.53
16	6	524	BCR	C24-C23-C22	-2.96	121.85	126.23
16	4	524	BCR	C8-C7-C6	-2.96	119.08	127.00
16	B	4017	BCR	C34-C9-C8	2.96	122.62	118.09
20	c	822	SQD	O5-C5-C4	2.96	115.04	109.70
16	s	523	BCR	C33-C5-C6	-2.96	121.25	124.48
13	4	506	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	B	1228	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	b	506	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
16	W	4021	BCR	C20-C19-C18	-2.96	118.24	126.36
13	f	1234	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	1	519	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	u	507	CLA	O2D-CGD-O1D	-2.96	118.08	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1115	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	B	1220	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	B	1224	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	d	512	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
16	S	4018	BCR	C20-C21-C22	-2.96	123.13	127.28
13	e	1102	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	U	1105	CLA	CMC-C2C-C3C	2.96	134.15	126.15
13	B	1236	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	3	513	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
16	A	4008	BCR	C10-C11-C12	-2.96	114.63	123.20
13	A	1108	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	5	501	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	K	1105	CLA	CMC-C2C-C3C	2.96	134.14	126.15
13	r	502	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
13	c	509	CLA	CMB-C2B-C1B	-2.95	120.92	125.42
16	Y	522	BCR	C38-C26-C25	-2.95	121.26	124.48
16	a	523	BCR	C33-C5-C6	-2.95	121.26	124.48
13	B	1231	CLA	CHB-C4A-NA	2.95	128.66	124.40
13	5	507	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	a	513	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	e	1115	CLA	C3B-C4B-NB	-2.95	107.89	110.53
16	d	522	BCR	C33-C5-C6	-2.95	121.26	124.48
13	B	1234	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
16	M	4021	BCR	C20-C19-C18	-2.95	118.27	126.36
13	6	512	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	e	1108	CLA	C3B-C4B-NB	-2.95	107.90	110.53
13	f	1220	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	f	1228	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	Z	513	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	u	501	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	G	1102	CLA	C3B-C4B-NB	-2.95	107.90	110.53
13	B	1023	CLA	CMB-C2B-C3B	2.95	133.48	126.55
13	G	1126	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	H	1224	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	Z	502	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	f	1236	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	v	511	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	m	1105	CLA	CMC-C2C-C3C	2.95	134.12	126.15
13	G	1135	CLA	CMB-C2B-C3B	2.95	133.48	126.55
13	c	507	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
16	G	4008	BCR	C10-C11-C12	-2.95	114.67	123.20
16	f	4017	BCR	C34-C9-C8	2.95	122.59	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	1502	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	2	513	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
16	u	523	BCR	C16-C17-C18	-2.94	123.15	127.28
13	f	1224	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	d	518	CLA	C3B-C4B-NB	-2.94	107.90	110.53
16	1	523	BCR	C16-C17-C18	-2.94	123.15	127.28
13	Y	519	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	s	513	CLA	CHB-C4A-NA	2.94	128.65	124.40
19	f	5002	LMG	O6-C1-O1	-2.94	103.09	110.04
16	e	4008	BCR	C10-C11-C12	-2.94	114.68	123.20
13	e	1135	CLA	CMB-C2B-C3B	2.94	133.47	126.55
13	A	1126	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	c	518	CLA	C3B-C4B-NB	-2.94	107.90	110.53
16	q	522	BCR	C38-C26-C25	-2.94	121.28	124.48
16	o	4021	BCR	C20-C19-C18	-2.94	118.30	126.36
13	3	513	CLA	CHB-C4A-NA	2.94	128.64	124.40
13	H	1023	CLA	CMB-C2B-C3B	2.94	133.46	126.55
13	f	1023	CLA	CMB-C2B-C3B	2.94	133.46	126.55
13	H	1236	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
13	4	510	CLA	C3B-C4B-NB	-2.94	107.91	110.53
13	6	518	CLA	C3B-C4B-NB	-2.94	107.91	110.53
13	u	509	CLA	CMB-C2B-C1B	-2.94	120.95	125.42
13	b	510	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
16	3	523	BCR	C33-C5-C6	-2.94	121.28	124.48
13	H	1220	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
19	B	5002	LMG	O6-C1-O1	-2.94	103.11	110.04
13	r	511	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
13	c	510	CLA	C3B-C4B-NB	-2.94	107.91	110.53
13	f	1240	CLA	C3B-C4B-NB	-2.94	107.91	110.53
13	A	1135	CLA	CMB-C2B-C3B	2.94	133.46	126.55
13	B	1222	CLA	C3B-C4B-NB	-2.93	107.91	110.53
16	q	523	BCR	C16-C17-C18	-2.93	123.16	127.28
13	s	509	CLA	CHB-C4A-NA	2.93	128.63	124.40
13	q	508	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
16	f	4004	BCR	C11-C10-C9	-2.93	123.16	127.28
13	H	1231	CLA	CHB-C4A-NA	2.93	128.63	124.40
13	d	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	t	508	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	5	509	CLA	CMB-C2B-C1B	-2.93	120.95	125.42
13	b	508	CLA	CMB-C2B-C1B	-2.93	120.95	125.42
13	4	508	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	c	501	CLA	O2D-CGD-O1D	-2.93	118.14	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	2	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	Z	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	t	519	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	A	1123	CLA	CHB-C4A-NA	2.93	128.63	124.40
16	F	4016	BCR	C11-C12-C13	-2.93	118.33	126.36
13	Y	512	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
13	v	512	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
19	H	5002	LMG	O6-C1-O1	-2.93	103.12	110.04
16	A	4011	BCR	C20-C19-C18	-2.93	118.33	126.36
16	3	524	BCR	C24-C23-C22	-2.93	121.91	126.23
16	s	524	BCR	C24-C23-C22	-2.93	121.91	126.23
16	6	523	BCR	C28-C27-C26	-2.93	108.84	114.06
16	G	4011	BCR	C20-C19-C18	-2.93	118.34	126.36
16	R	4016	BCR	C11-C12-C13	-2.93	118.34	126.36
13	r	513	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
16	5	523	BCR	C16-C17-C18	-2.92	123.18	127.28
13	s	518	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	H	1234	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	d	503	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	e	1109	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
16	H	4004	BCR	C11-C10-C9	-2.92	123.18	127.28
16	f	4010	BCR	C8-C7-C6	-2.92	119.19	127.00
16	B	4004	BCR	C11-C10-C9	-2.92	123.18	127.28
13	Y	508	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	v	503	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
16	L	4019	BCR	C11-C10-C9	-2.92	123.18	127.28
16	V	4019	BCR	C11-C10-C9	-2.92	123.18	127.28
13	4	510	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	H	1213	CLA	CHB-C4A-NA	2.92	128.62	124.40
16	d	523	BCR	C28-C27-C26	-2.92	108.84	114.06
13	a	518	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	b	510	CLA	C3B-C4B-NB	-2.92	107.92	110.53
16	1	522	BCR	C33-C5-C6	-2.92	121.30	124.48
17	e	5002	LHG	O8-C23-C24	2.92	120.75	111.83
17	A	5002	LHG	O8-C23-C24	2.92	120.74	111.83
16	Y	522	BCR	C33-C5-C6	-2.92	121.30	124.48
13	3	509	CLA	CHB-C4A-NA	2.92	128.61	124.40
16	j	4016	BCR	C11-C12-C13	-2.92	118.36	126.36
13	3	518	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	b	519	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
13	H	1222	CLA	C3B-C4B-NB	-2.92	107.92	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	508	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
16	B	4010	BCR	C8-C7-C6	-2.92	119.21	127.00
13	Z	509	CLA	CHB-C4A-NA	2.92	128.61	124.40
16	n	4019	BCR	C11-C10-C9	-2.92	123.19	127.28
13	t	510	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
13	d	513	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
16	q	522	BCR	C3-C4-C5	-2.91	108.86	114.06
13	f	1222	CLA	C3B-C4B-NB	-2.91	107.93	110.53
13	r	508	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
16	c	523	BCR	C16-C17-C18	-2.91	123.19	127.28
13	Y	502	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
16	e	4011	BCR	C20-C19-C18	-2.91	118.38	126.36
13	b	508	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	t	510	CLA	C3B-C4B-NB	-2.91	107.93	110.53
16	H	4010	BCR	C8-C7-C6	-2.91	119.22	127.00
13	b	511	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
16	Y	522	BCR	C3-C4-C5	-2.91	108.86	114.06
13	1	512	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
16	v	523	BCR	C28-C27-C26	-2.91	108.87	114.06
13	A	1134	CLA	C3B-C4B-NB	-2.91	107.93	110.53
13	G	1121	CLA	CHB-C4A-NA	2.91	128.60	124.40
13	e	1123	CLA	CHB-C4A-NA	2.91	128.60	124.40
13	a	509	CLA	CHB-C4A-NA	2.91	128.60	124.40
13	a	518	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	4	508	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
13	s	518	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	G	1123	CLA	CHB-C4A-NA	2.91	128.60	124.40
16	a	524	BCR	C24-C23-C22	-2.91	121.93	126.23
17	G	5002	LHG	O8-C23-C24	2.91	120.70	111.83
13	t	508	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
13	4	519	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	a	508	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	6	503	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	B	1240	CLA	C3B-C4B-NB	-2.90	107.94	110.53
13	3	518	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
13	q	512	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
13	A	1237	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
16	q	523	BCR	C33-C5-C6	-2.90	121.32	124.48
13	4	511	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
16	f	4009	BCR	C15-C16-C17	-2.90	117.58	123.52
13	B	1213	CLA	CHB-C4A-NA	2.90	128.59	124.40
13	G	1118	CLA	C3B-C4B-NB	-2.90	107.94	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	l	4015	BCR	C2-C1-C6	2.90	114.65	110.44
16	1	522	BCR	C3-C4-C5	-2.90	108.89	114.06
16	1	522	BCR	C11-C12-C13	-2.90	118.41	126.36
13	s	506	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	q	502	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	B	1203	CLA	C3B-C4B-NB	-2.90	107.94	110.53
13	A	1109	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	A	1121	CLA	CHB-C4A-NA	2.90	128.58	124.40
13	r	509	CLA	CHB-C4A-NA	2.90	128.58	124.40
13	v	513	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
16	Y	522	BCR	C11-C12-C13	-2.90	118.42	126.36
16	G	4008	BCR	C16-C15-C14	-2.90	117.59	123.52
13	e	1135	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
16	A	4008	BCR	C16-C15-C14	-2.89	117.60	123.52
13	1	502	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	Z	508	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	b	512	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	H	1203	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	1	513	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	H	1240	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	b	505	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
16	H	4009	BCR	C15-C16-C17	-2.89	117.60	123.52
13	A	1122	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	4	512	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	4	518	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	2	508	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	e	1134	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	e	1237	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
16	e	4008	BCR	C16-C15-C14	-2.89	117.61	123.52
13	f	1226	CLA	CHB-C1B-NB	2.89	128.38	124.05
13	6	513	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	f	1203	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	t	511	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	H	1226	CLA	CHB-C1B-NB	2.89	128.38	124.05
13	3	508	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	a	506	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	f	1213	CLA	CHB-C4A-NA	2.89	128.56	124.40
13	s	508	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
13	2	509	CLA	CHB-C4A-NA	2.88	128.56	124.40
13	Y	513	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
16	5	521	BCR	C23-C24-C25	-2.88	119.29	127.00
13	v	518	CLA	O2D-CGD-O1D	-2.88	118.23	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	521	BCR	C23-C24-C25	-2.88	119.30	127.00
13	q	513	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
16	J	4015	BCR	C2-C1-C6	2.88	114.63	110.44
16	q	522	BCR	C11-C12-C13	-2.88	118.46	126.36
16	c	521	BCR	C23-C24-C25	-2.88	119.30	127.00
13	G	1122	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	t	512	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	6	519	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	c	511	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	A	1135	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	G	1237	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	e	1121	CLA	CHB-C4A-NA	2.88	128.56	124.40
16	q	523	BCR	C10-C11-C12	-2.88	114.86	123.20
13	d	507	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	H	1202	CLA	CMB-C2B-C3B	2.88	133.32	126.55
13	6	518	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	4	505	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
16	B	4009	BCR	C15-C16-C17	-2.88	117.63	123.52
13	B	1215	CLA	CMB-C2B-C1B	-2.88	121.04	125.42
13	B	1226	CLA	CHB-C1B-NB	2.88	128.37	124.05
13	G	1109	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	G	1105	CLA	CHB-C4A-NA	2.88	128.55	124.40
13	q	507	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	5	510	CLA	C3B-C4B-NB	-2.88	107.96	110.53
13	G	1134	CLA	C3B-C4B-NB	-2.88	107.96	110.53
13	3	506	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	B	1213	CLA	C1-C2-C3	-2.88	121.48	126.20
13	e	1105	CLA	CHB-C4A-NA	2.88	128.55	124.40
13	c	508	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	e	1122	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
13	Y	507	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
13	f	1213	CLA	C1-C2-C3	-2.87	121.49	126.20
13	u	510	CLA	C3B-C4B-NB	-2.87	107.97	110.53
13	H	1213	CLA	C1-C2-C3	-2.87	121.49	126.20
13	b	518	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
13	f	1215	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
13	A	1114	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	S	5001	LHG	O8-C23-C24	2.87	120.59	111.83
13	e	1114	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
16	d	522	BCR	C38-C26-C25	-2.87	121.35	124.48
13	5	508	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
13	t	505	CLA	O2D-CGD-O1D	-2.87	118.26	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	522	BCR	C33-C5-C6	-2.87	121.35	124.48
16	Y	523	BCR	C10-C11-C12	-2.87	114.89	123.20
13	6	516	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
13	u	508	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
16	c	521	BCR	C38-C26-C27	2.87	119.71	113.60
16	1	523	BCR	C10-C11-C12	-2.87	114.89	123.20
16	n	4022	BCR	C28-C27-C26	-2.87	108.94	114.06
13	A	1105	CLA	CHB-C4A-NA	2.87	128.54	124.40
13	1	507	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
13	d	516	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
16	5	521	BCR	C38-C26-C27	2.87	119.71	113.60
13	6	507	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	I	5001	LHG	O8-C23-C24	2.87	120.57	111.83
16	G	4008	BCR	C38-C26-C25	-2.87	121.36	124.48
13	u	511	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
13	e	1123	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
13	e	1237	CLA	C4-C3-C5	2.86	120.20	115.23
16	r	523	BCR	C20-C21-C22	-2.86	123.26	127.28
13	5	511	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	G	1135	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	t	518	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
16	A	4008	BCR	C38-C26-C25	-2.86	121.36	124.48
17	k	5001	LHG	O8-C23-C24	2.86	120.56	111.83
16	r	521	BCR	C3-C4-C5	-2.86	108.95	114.06
13	d	518	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	r	508	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
13	e	1110	CLA	CHB-C4A-NA	2.86	128.53	124.40
13	G	1114	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	2	508	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
16	6	522	BCR	C38-C26-C25	-2.86	121.36	124.48
13	A	1133	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	v	516	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
16	Z	521	BCR	C3-C4-C5	-2.86	108.95	114.06
13	A	1237	CLA	C4-C3-C5	2.86	120.19	115.23
16	V	4022	BCR	C28-C27-C26	-2.86	108.96	114.06
13	G	1237	CLA	C4-C3-C5	2.86	120.19	115.23
13	c	517	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	v	519	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
16	1	523	BCR	C33-C5-C6	-2.86	121.36	124.48
13	f	1202	CLA	CMB-C2B-C3B	2.86	133.27	126.55
13	t	512	CLA	C3B-C4B-NB	-2.86	107.98	110.53
16	H	4010	BCR	C20-C21-C22	-2.86	123.27	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	509	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	r	503	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	H	1215	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
16	Y	523	BCR	C33-C5-C6	-2.86	121.37	124.48
16	T	4015	BCR	C2-C1-C6	2.86	114.59	110.44
13	s	511	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	u	513	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	G	1130	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
13	B	1220	CLA	O2A-CGA-O1A	-2.86	116.49	123.63
16	v	522	BCR	C38-C26-C25	-2.85	121.37	124.48
13	B	1202	CLA	CMB-C2B-C3B	2.85	133.26	126.55
13	b	509	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
16	A	4002	BCR	C3-C4-C5	-2.85	108.97	114.06
13	d	519	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	a	519	CLA	CHB-C4A-NA	2.85	128.52	124.40
13	4	502	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	A	1138	CLA	C1-C2-C3	-2.85	121.52	126.20
13	H	1220	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
16	2	522	BCR	C33-C5-C6	-2.85	121.37	124.48
16	e	4008	BCR	C38-C26-C25	-2.85	121.37	124.48
13	G	1138	CLA	C1-C2-C3	-2.85	121.53	126.20
13	G	1104	CLA	CHB-C4A-NA	2.85	128.51	124.40
16	2	521	BCR	C3-C4-C5	-2.85	108.97	114.06
13	A	1123	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
13	a	507	CLA	CHB-C4A-NA	2.85	128.51	124.40
13	H	1023	CLA	CBC-CAC-C3C	2.85	120.14	112.42
13	e	1133	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	c	502	CLA	C3B-C4B-NB	-2.85	107.99	110.53
13	f	1220	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
13	u	517	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
13	Z	508	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
13	u	502	CLA	C3B-C4B-NB	-2.85	107.99	110.53
13	t	509	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
13	A	1136	CLA	CHB-C4A-NA	2.85	128.51	124.40
13	3	519	CLA	CHB-C4A-NA	2.85	128.51	124.40
16	r	522	BCR	C33-C5-C6	-2.85	121.38	124.48
13	d	504	CLA	C3B-C4B-NB	-2.85	107.99	110.53
16	L	4022	BCR	C28-C27-C26	-2.85	108.98	114.06
13	5	502	CLA	C3B-C4B-NB	-2.84	107.99	110.53
13	f	1201	CLA	CHB-C4A-NA	2.84	128.50	124.40
16	a	522	BCR	C20-C21-C22	-2.84	123.29	127.28
13	G	1133	CLA	O2D-CGD-O1D	-2.84	118.31	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4002	BCR	C3-C4-C5	-2.84	108.99	114.06
16	Z	522	BCR	C33-C5-C6	-2.84	121.38	124.48
13	5	513	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
13	G	1119	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
13	A	1115	CLA	CHB-C4A-NA	2.84	128.50	124.40
13	H	1023	CLA	CHB-C4A-NA	2.84	128.50	124.40
16	G	4002	BCR	C3-C4-C5	-2.84	108.99	114.06
13	f	1206	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
16	u	524	BCR	C15-C16-C17	-2.84	117.71	123.52
16	u	521	BCR	C38-C26-C27	2.84	119.65	113.60
13	c	509	CLA	CHB-C4A-NA	2.84	128.50	124.40
13	v	507	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
13	G	1123	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
13	5	517	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
16	Z	523	BCR	C20-C21-C22	-2.84	123.30	127.28
13	B	1023	CLA	CBC-CAC-C3C	2.84	120.11	112.42
13	2	503	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
13	b	502	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
16	3	522	BCR	C20-C21-C22	-2.84	123.30	127.28
13	Z	506	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
16	2	523	BCR	C20-C21-C22	-2.84	123.30	127.28
13	3	511	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
13	Y	503	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
13	e	1119	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
16	v	523	BCR	C10-C11-C12	-2.84	114.98	123.20
13	A	1130	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
13	e	1130	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
13	e	1115	CLA	CHB-C4A-NA	2.83	128.49	124.40
16	B	4010	BCR	C20-C21-C22	-2.83	123.30	127.28
13	n	1503	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
13	A	1104	CLA	CHB-C4A-NA	2.83	128.49	124.40
13	5	516	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
13	b	503	CLA	CHB-C4A-NA	2.83	128.49	124.40
13	f	1023	CLA	CBC-CAC-C3C	2.83	120.09	112.42
16	V	4219	BCR	C28-C27-C26	-2.83	109.01	114.06
13	3	507	CLA	CHB-C4A-NA	2.83	128.49	124.40
13	G	1115	CLA	CHB-C4A-NA	2.83	128.49	124.40
13	G	1136	CLA	CHB-C4A-NA	2.83	128.49	124.40
13	f	1212	CLA	CHB-C4A-NA	2.83	128.48	124.40
13	1	503	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
16	L	4219	BCR	C28-C27-C26	-2.83	109.01	114.06
13	c	513	CLA	O2D-CGD-O1D	-2.83	118.34	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1231	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	B	1023	CLA	CHB-C4A-NA	2.83	128.48	124.40
16	A	4001	BCR	C11-C12-C13	-2.83	118.61	126.36
16	5	524	BCR	C20-C21-C22	-2.83	123.31	127.28
13	A	1110	CLA	CHB-C4A-NA	2.83	128.48	124.40
13	s	519	CLA	CHB-C4A-NA	2.83	128.48	124.40
13	f	1201	CLA	C3B-C4B-NB	-2.83	108.01	110.53
16	u	524	BCR	C20-C21-C22	-2.83	123.31	127.28
13	t	502	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	6	505	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
13	e	1136	CLA	CHB-C4A-NA	2.83	128.48	124.40
16	c	524	BCR	C15-C16-C17	-2.83	117.74	123.52
16	6	523	BCR	C10-C11-C12	-2.83	115.01	123.20
13	f	1023	CLA	CHB-C4A-NA	2.83	128.48	124.40
16	e	4001	BCR	C11-C12-C13	-2.83	118.61	126.36
13	Z	503	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
13	v	505	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
13	H	1212	CLA	CHB-C4A-NA	2.83	128.48	124.40
13	H	1221	CLA	O2D-CGD-CBD	2.82	116.17	111.23
13	u	502	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	B	1201	CLA	CHB-C4A-NA	2.82	128.48	124.40
13	e	1138	CLA	C1-C2-C3	-2.82	121.57	126.20
13	2	506	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	5	502	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	a	517	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	Z	502	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	r	522	BCR	C21-C20-C19	-2.82	115.02	123.20
13	H	1221	CLA	CMB-C2B-C3B	2.82	133.19	126.55
13	t	511	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	4	523	BCR	C20-C21-C22	-2.82	123.32	127.28
13	r	506	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
16	2	522	BCR	C21-C20-C19	-2.82	115.02	123.20
13	c	503	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	L	1503	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	4	512	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	n	4219	BCR	C28-C27-C26	-2.82	109.03	114.06
13	c	516	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	b	822	SQD	O7-S-C6	2.82	110.97	106.76
13	A	1116	CLA	C3B-C4B-NB	-2.82	108.01	110.53
13	Y	517	CLA	C3B-C4B-NB	-2.82	108.01	110.53
13	b	511	CLA	CHB-C4A-NA	2.82	128.47	124.40
13	u	516	CLA	O2D-CGD-O1D	-2.82	118.36	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	523	BCR	C10-C11-C12	-2.82	115.03	123.20
13	a	511	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	c	502	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	B	1212	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	Z	522	BCR	C21-C20-C19	-2.82	115.03	123.20
13	G	1801	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
13	5	509	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	G	4001	BCR	C11-C12-C13	-2.82	118.64	126.36
13	B	1206	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
13	d	519	CLA	C3B-C4B-NB	-2.82	108.02	110.53
13	q	504	CLA	C3B-C4B-NB	-2.82	108.02	110.53
16	b	523	BCR	C20-C21-C22	-2.82	123.33	127.28
13	H	1201	CLA	CHB-C4A-NA	2.82	128.47	124.40
13	f	1218	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	R	4016	BCR	C16-C17-C18	-2.82	123.33	127.28
13	A	1119	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
13	G	1124	CLA	C3B-C4B-NB	-2.82	108.02	110.53
13	3	517	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
13	c	504	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
16	c	524	BCR	C20-C21-C22	-2.82	123.33	127.28
13	f	1221	CLA	CMB-C2B-C3B	2.81	133.17	126.55
13	f	1221	CLA	O2D-CGD-CBD	2.81	116.15	111.23
13	a	505	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	A	1127	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	B	1201	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	H	1201	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	H	1225	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	q	501	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	s	517	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	4	503	CLA	CHB-C4A-NA	2.81	128.46	124.40
16	1	524	BCR	C20-C21-C22	-2.81	123.33	127.28
16	5	524	BCR	C15-C16-C17	-2.81	117.76	123.52
13	B	1221	CLA	CMB-C2B-C3B	2.81	133.17	126.55
13	d	510	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	t	518	CLA	CHB-C4A-NA	2.81	128.46	124.40
16	f	4010	BCR	C20-C21-C22	-2.81	123.33	127.28
13	A	1801	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
13	q	503	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
17	n	5218	LHG	O8-C23-C24	2.81	120.41	111.83
13	B	1231	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	s	517	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
17	V	5218	LHG	O8-C23-C24	2.81	120.41	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1218	CLA	CHB-C4A-NA	2.81	128.46	124.40
13	4	511	CLA	CHB-C4A-NA	2.81	128.46	124.40
13	3	505	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	t	505	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	q	506	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
13	d	505	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	b	510	CLA	CHB-C4A-NA	2.81	128.46	124.40
13	v	501	CLA	CHB-C4A-NA	2.81	128.46	124.40
20	V	5216	SQD	O6-C1-C2	2.81	112.54	108.27
13	4	505	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	6	519	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	e	1127	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	q	506	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	u	503	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	u	822	SQD	O7-S-C6	2.81	110.95	106.76
13	5	513	CLA	C3B-C4B-NB	-2.81	108.02	110.53
16	H	4006	BCR	C15-C16-C17	-2.81	117.77	123.52
18	G	1848	LMU	C1B-O1B-C4'	-2.81	111.32	117.98
13	F	1302	CLA	CHB-C4A-NA	2.81	128.45	124.40
13	b	518	CLA	CHB-C4A-NA	2.81	128.45	124.40
13	B	1221	CLA	O2D-CGD-CBD	2.81	116.14	111.23
13	H	1218	CLA	CHB-C4A-NA	2.81	128.45	124.40
13	u	509	CLA	CHB-C4A-NA	2.81	128.45	124.40
18	e	1848	LMU	C1B-O1B-C4'	-2.81	111.32	117.98
13	4	516	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	5	822	SQD	O7-S-C6	2.81	110.95	106.76
20	c	822	SQD	O7-S-C6	2.81	110.95	106.76
17	L	5218	LHG	O8-C23-C24	2.81	120.39	111.83
13	f	1238	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	A	1117	CLA	C1-C2-C3	-2.81	121.60	126.20
16	k	4018	BCR	C4-C5-C6	-2.81	118.91	122.70
16	s	522	BCR	C20-C21-C22	-2.81	123.34	127.28
20	n	5216	SQD	O6-C1-C2	2.81	112.53	108.27
13	f	1230	CLA	O2D-CGD-CBD	2.81	116.14	111.23
13	e	1801	CLA	CMB-C2B-C1B	-2.81	121.15	125.42
16	I	4018	BCR	C4-C5-C6	-2.81	118.91	122.70
13	6	504	CLA	C3B-C4B-NB	-2.81	108.03	110.53
13	e	1116	CLA	C3B-C4B-NB	-2.81	108.03	110.53
13	1	506	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	d	506	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	v	506	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	v	517	CLA	O2D-CGD-O1D	-2.81	118.39	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	501	CLA	CHB-C4A-NA	2.80	128.45	124.40
18	A	1848	LMU	C1B-O1B-C4'	-2.80	111.33	117.98
13	H	1238	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	t	822	SQD	O7-S-C6	2.80	110.94	106.76
13	G	1131	CLA	CHB-C4A-NA	2.80	128.45	124.40
16	f	4006	BCR	C15-C16-C17	-2.80	117.78	123.52
16	F	4016	BCR	C16-C17-C18	-2.80	123.35	127.28
13	6	517	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
13	H	1231	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
13	B	1222	CLA	O2D-CGD-CBD	2.80	116.13	111.23
13	4	502	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	G	1110	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	V	1503	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
13	2	502	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	Y	504	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	a	502	CLA	CHB-C4A-NA	2.80	128.44	124.40
20	4	822	SQD	O7-S-C6	2.80	110.94	106.76
13	R	1302	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	b	512	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	t	516	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
13	f	1208	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
20	L	5216	SQD	O6-C1-C2	2.80	112.53	108.27
16	c	524	BCR	C8-C7-C6	-2.80	119.52	127.00
16	Y	524	BCR	C20-C21-C22	-2.80	123.35	127.28
13	2	511	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	4	518	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	1	517	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	Y	506	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
16	B	4006	BCR	C15-C16-C17	-2.80	117.79	123.52
13	3	502	CLA	CHB-C4A-NA	2.80	128.44	124.40
16	j	4016	BCR	C16-C17-C18	-2.80	123.35	127.28
13	1	506	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
13	u	513	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	Z	521	BCR	C33-C5-C6	-2.80	121.43	124.48
13	A	1011	CLA	C2A-C1A-CHA	2.80	128.72	123.87
13	R	1302	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	a	517	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	s	505	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
13	H	1228	CLA	CMB-C2B-C3B	2.80	133.13	126.55
13	s	511	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	e	1011	CLA	C2A-C1A-CHA	2.80	128.72	123.87
13	6	506	CLA	O2D-CGD-O1D	-2.80	118.41	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1222	CLA	O2D-CGD-CBD	2.80	116.12	111.23
13	6	510	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
16	c	523	BCR	C7-C8-C9	-2.80	122.10	126.23
13	a	509	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
17	A	5003	LHG	C11-C10-C9	-2.80	100.24	114.37
13	a	503	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
13	Y	508	CLA	CHB-C4A-NA	2.80	128.43	124.40
13	q	508	CLA	CHB-C4A-NA	2.80	128.43	124.40
13	r	516	CLA	CHB-C4A-NA	2.80	128.43	124.40
13	t	510	CLA	CHB-C4A-NA	2.80	128.43	124.40
13	f	1222	CLA	O2D-CGD-CBD	2.79	116.12	111.23
13	V	1502	CLA	CHB-C4A-NA	2.79	128.43	124.40
16	L	4019	BCR	C20-C21-C22	-2.79	123.36	127.28
13	e	1104	CLA	CHB-C4A-NA	2.79	128.43	124.40
13	B	1238	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	F	1302	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	s	503	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
16	b	524	BCR	C33-C5-C4	2.79	119.55	113.60
13	Y	506	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	t	502	CLA	CHB-C4A-NA	2.79	128.43	124.40
16	u	523	BCR	C7-C8-C9	-2.79	122.10	126.23
16	4	524	BCR	C33-C5-C4	2.79	119.55	113.60
17	e	5003	LHG	C11-C10-C9	-2.79	100.25	114.37
13	B	1225	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	J	4013	BCR	C16-C15-C14	-2.79	117.81	123.52
17	G	5003	LHG	C11-C10-C9	-2.79	100.25	114.37
13	e	1117	CLA	C1-C2-C3	-2.79	121.62	126.20
13	u	504	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	r	516	CLA	O2D-CGD-CBD	2.79	116.11	111.23
13	3	509	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
13	m	1103	CLA	CHB-C4A-NA	2.79	128.43	124.40
13	3	503	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	G	1131	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	H	1217	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	B	1208	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	u	505	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
16	5	523	BCR	C7-C8-C9	-2.79	122.11	126.23
13	e	1124	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	3	501	CLA	CHB-C4A-NA	2.79	128.43	124.40
13	5	504	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	r	502	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	l	4013	BCR	C16-C15-C14	-2.79	117.81	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	5	505	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	4	501	CLA	CHB-C4A-NA	2.79	128.43	124.40
13	u	506	CLA	CHB-C4A-NA	2.79	128.43	124.40
20	s	822	SQD	O6-C1-C2	2.79	112.51	108.27
13	5	503	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	t	501	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	3	511	CLA	CHB-C4A-NA	2.79	128.42	124.40
13	Z	511	CLA	CHB-C4A-NA	2.79	128.42	124.40
16	T	4013	BCR	C16-C15-C14	-2.79	117.81	123.52
13	f	1217	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	q	517	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	U	1103	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	Z	516	CLA	O2D-CGD-CBD	2.79	116.10	111.23
16	t	523	BCR	C20-C21-C22	-2.79	123.37	127.28
13	Z	507	CLA	CHB-C4A-NA	2.79	128.42	124.40
16	A	4001	BCR	C35-C13-C12	2.79	122.35	118.09
13	b	501	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	3	517	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	t	524	BCR	C33-C5-C4	2.79	119.54	113.60
13	H	1208	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	v	516	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	b	516	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
16	G	4011	BCR	C16-C17-C18	-2.79	123.37	127.28
16	q	524	BCR	C20-C21-C22	-2.79	123.37	127.28
13	5	510	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
13	B	1228	CLA	CMB-C2B-C3B	2.78	133.10	126.55
13	A	1131	CLA	CHB-C4A-NA	2.78	128.42	124.40
13	G	1116	CLA	C3B-C4B-NB	-2.78	108.04	110.53
13	v	510	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
13	1	504	CLA	C3B-C4B-NB	-2.78	108.05	110.53
13	v	504	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	5	524	BCR	C8-C7-C6	-2.78	119.56	127.00
13	Z	501	CLA	CHB-C4A-NA	2.78	128.42	124.40
13	r	507	CLA	CHB-C4A-NA	2.78	128.42	124.40
13	L	1501	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
16	e	4001	BCR	C35-C13-C12	2.78	122.34	118.09
14	G	2001	PQN	C11-C3-C2	-2.78	120.12	124.89
13	j	1302	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	r	511	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	u	519	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	j	1302	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	B	4010	BCR	C21-C20-C19	-2.78	115.14	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1206	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
20	3	822	SQD	O6-C1-C2	2.78	112.50	108.27
13	6	501	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	r	501	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	t	503	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	s	507	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	6	516	CLA	C3B-C4B-NB	-2.78	108.05	110.53
13	4	510	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	e	1131	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	B	1230	CLA	O2D-CGD-CBD	2.78	116.09	111.23
13	B	1217	CLA	C3B-C4B-NB	-2.78	108.05	110.53
13	c	505	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	s	509	CLA	CMB-C2B-C1B	-2.78	121.19	125.42
13	n	1501	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	u	510	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	2	516	CLA	O2D-CGD-CBD	2.78	116.08	111.23
13	n	1502	CLA	O2D-CGD-CBD	2.78	116.08	111.23
13	l	1302	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	f	4010	BCR	C21-C20-C19	-2.78	115.15	123.20
13	b	501	CLA	CHB-C4A-NA	2.78	128.41	124.40
13	H	1230	CLA	O2D-CGD-CBD	2.78	116.08	111.23
16	u	522	BCR	C15-C16-C17	-2.78	117.84	123.52
16	r	521	BCR	C33-C5-C6	-2.78	121.45	124.48
13	v	519	CLA	C3B-C4B-NB	-2.78	108.05	110.53
13	1	508	CLA	CHB-C4A-NA	2.78	128.41	124.40
16	H	4010	BCR	C21-C20-C19	-2.78	115.16	123.20
13	G	1011	CLA	C2A-C1A-CHA	2.78	128.68	123.87
13	d	517	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
16	n	4019	BCR	C20-C21-C22	-2.78	123.39	127.28
16	2	521	BCR	C33-C5-C6	-2.78	121.46	124.48
16	e	4011	BCR	C16-C17-C18	-2.77	123.39	127.28
13	2	507	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	Z	518	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	S	4018	BCR	C4-C5-C6	-2.77	118.95	122.70
13	4	501	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
16	e	4007	BCR	C15-C16-C17	-2.77	117.84	123.52
16	u	524	BCR	C8-C7-C6	-2.77	119.59	127.00
13	a	511	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	c	519	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	s	502	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	b	505	CLA	C3B-C4B-NB	-2.77	108.05	110.53
16	B	4014	BCR	C28-C27-C26	-2.77	109.11	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	516	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	K	1103	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	a	822	SQD	O6-C1-C2	2.77	112.48	108.27
13	m	1103	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
13	1	508	CLA	C4-C3-C5	2.77	120.04	115.23
13	H	1205	CLA	C1-C2-C3	-2.77	121.66	126.20
13	c	513	CLA	C3B-C4B-NB	-2.77	108.06	110.53
13	b	502	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	b	517	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
13	f	1228	CLA	CMB-C2B-C3B	2.77	133.07	126.55
13	u	501	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	c	510	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
16	f	4014	BCR	C28-C27-C26	-2.77	109.12	114.06
13	U	1103	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	d	501	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	G	1127	CLA	C3B-C4B-NB	-2.77	108.06	110.53
13	r	512	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
13	B	1208	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	L	1502	CLA	CHB-C4A-NA	2.77	128.40	124.40
13	6	507	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	U	4104	BCR	C15-C16-C17	-2.77	117.86	123.52
13	G	1117	CLA	C1-C2-C3	-2.77	121.66	126.20
16	3	522	BCR	C11-C12-C13	-2.77	118.78	126.36
16	s	522	BCR	C11-C12-C13	-2.77	118.78	126.36
13	T	1302	CLA	C3B-C4B-NB	-2.77	108.06	110.53
13	a	510	CLA	C3B-C4B-NB	-2.77	108.06	110.53
13	B	1211	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
13	s	501	CLA	CHB-C4A-NA	2.77	128.39	124.40
13	A	1113	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
19	f	5002	LMG	O1-C7-C8	-2.77	104.09	110.82
13	R	1302	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
13	a	512	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
13	2	512	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
13	V	1501	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
13	Z	516	CLA	CHB-C4A-NA	2.77	128.39	124.40
13	q	508	CLA	C4-C3-C5	2.77	120.03	115.23
13	e	1113	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
13	d	502	CLA	CHB-C4A-NA	2.76	128.39	124.40
13	f	1208	CLA	CHB-C4A-NA	2.76	128.39	124.40
13	Y	508	CLA	C4-C3-C5	2.76	120.03	115.23
13	5	501	CLA	CHB-C4A-NA	2.76	128.39	124.40
13	V	1502	CLA	O2D-CGD-CBD	2.76	116.06	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1205	CLA	C1-C2-C3	-2.76	121.67	126.20
13	F	1302	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	H	1212	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	3	510	CLA	C3B-C4B-NB	-2.76	108.06	110.53
13	3	512	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	s	512	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
16	f	4010	BCR	C10-C11-C12	-2.76	115.20	123.20
13	6	502	CLA	CHB-C4A-NA	2.76	128.39	124.40
13	6	502	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	r	518	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	t	517	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	H	1210	CLA	C3B-C4B-NB	-2.76	108.06	110.53
13	l	1303	CLA	CHB-C4A-NA	2.76	128.38	124.40
13	4	517	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	K	1103	CLA	CHB-C4A-NA	2.76	128.38	124.40
13	G	1121	CLA	C3B-C4B-NB	-2.76	108.07	110.53
13	2	501	CLA	CHB-C4A-NA	2.76	128.38	124.40
19	B	5002	LMG	O1-C7-C8	-2.76	104.11	110.82
16	u	522	BCR	C16-C17-C18	-2.76	123.41	127.28
16	m	4104	BCR	C15-C16-C17	-2.76	117.87	123.52
13	f	1212	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	A	2001	PQN	C11-C3-C2	-2.76	120.16	124.89
13	5	506	CLA	CHB-C4A-NA	2.76	128.38	124.40
13	5	508	CLA	CHB-C4A-NA	2.76	128.38	124.40
13	H	1228	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	s	521	BCR	C29-C30-C25	2.76	114.45	110.44
13	s	510	CLA	C3B-C4B-NB	-2.76	108.07	110.53
16	V	4019	BCR	C20-C21-C22	-2.76	123.41	127.28
16	c	522	BCR	C16-C17-C18	-2.76	123.41	127.28
16	G	4001	BCR	C35-C13-C12	2.76	122.30	118.09
13	L	1502	CLA	O2D-CGD-CBD	2.76	116.05	111.23
16	c	522	BCR	C15-C16-C17	-2.76	117.88	123.52
13	b	517	CLA	CHB-C4A-NA	2.76	128.38	124.40
13	v	502	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
13	Z	512	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
13	d	502	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	H	4014	BCR	C28-C27-C26	-2.76	109.14	114.06
13	H	1230	CLA	C3B-C4B-NB	-2.76	108.07	110.53
13	e	1121	CLA	C3B-C4B-NB	-2.76	108.07	110.53
13	c	506	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	K	4104	BCR	C15-C16-C17	-2.76	117.88	123.52
16	3	521	BCR	C29-C30-C25	2.76	114.44	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	v	502	CLA	CHB-C4A-NA	2.76	128.38	124.40
19	H	5002	LMG	O1-C7-C8	-2.76	104.12	110.82
13	e	1106	CLA	O2D-CGD-CBD	2.76	116.05	111.23
13	5	519	CLA	CHB-C4A-NA	2.76	128.38	124.40
13	t	501	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	H	4010	BCR	C33-C5-C6	-2.75	121.48	124.48
13	m	1401	CLA	O2D-CGD-CBD	2.75	116.05	111.23
13	j	1302	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
13	B	1210	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	d	507	CLA	CHB-C4A-NA	2.75	128.38	124.40
13	v	503	CLA	CHB-C4A-NA	2.75	128.38	124.40
16	A	4011	BCR	C16-C17-C18	-2.75	123.42	127.28
16	H	4010	BCR	C10-C11-C12	-2.75	115.22	123.20
16	a	521	BCR	C29-C30-C25	2.75	114.44	110.44
13	j	1301	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
16	c	522	BCR	C1-C6-C5	-2.75	118.87	122.64
13	3	504	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	4	513	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	a	511	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	f	1210	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	f	1234	CLA	CBC-CAC-C3C	2.75	119.88	112.42
16	4	523	BCR	C11-C10-C9	-2.75	123.42	127.28
16	B	4010	BCR	C33-C5-C6	-2.75	121.48	124.48
13	n	1502	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	B	1234	CLA	CBC-CAC-C3C	2.75	119.88	112.42
13	A	1106	CLA	O2D-CGD-CBD	2.75	116.04	111.23
13	G	1113	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
13	H	1211	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
13	A	1124	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	G	1119	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	s	511	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	6	503	CLA	CHB-C4A-NA	2.75	128.37	124.40
16	A	4007	BCR	C15-C16-C17	-2.75	117.89	123.52
16	5	522	BCR	C15-C16-C17	-2.75	117.89	123.52
13	H	1204	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	H	1208	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	1	501	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	a	503	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	r	510	CLA	C3B-C4B-NB	-2.75	108.07	110.53
13	u	506	CLA	C3B-C4B-NB	-2.75	108.07	110.53
16	f	4010	BCR	C33-C5-C6	-2.75	121.48	124.48
13	B	1212	CLA	O2D-CGD-O1D	-2.75	118.49	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	522	BCR	C11-C12-C13	-2.75	118.82	126.36
16	Z	524	BCR	C11-C10-C9	-2.75	123.42	127.28
16	B	4010	BCR	C10-C11-C12	-2.75	115.23	123.20
16	r	524	BCR	C11-C10-C9	-2.75	123.42	127.28
13	J	1303	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	d	516	CLA	C3B-C4B-NB	-2.75	108.08	110.53
20	V	5216	SQD	O9-S-C6	2.75	110.86	106.76
16	a	523	BCR	C21-C20-C19	-2.75	115.23	123.20
16	3	523	BCR	C21-C20-C19	-2.75	115.23	123.20
13	1	518	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	T	1303	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	f	1207	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	1	504	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	f	1211	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
13	B	1228	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	G	1117	CLA	CHB-C4A-NA	2.75	128.37	124.40
13	m	1105	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	A	1131	CLA	C3B-C4B-NB	-2.75	108.08	110.53
13	F	1301	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	c	508	CLA	CHB-C4A-NA	2.75	128.36	124.40
13	u	508	CLA	CHB-C4A-NA	2.75	128.36	124.40
13	A	1136	CLA	C1-C2-C3	-2.75	121.70	126.20
16	H	4014	BCR	C10-C11-C12	-2.75	115.24	123.20
16	s	523	BCR	C21-C20-C19	-2.75	115.24	123.20
13	v	507	CLA	CHB-C4A-NA	2.75	128.36	124.40
13	B	1230	CLA	C3B-C4B-NB	-2.75	108.08	110.53
13	3	511	CLA	C3B-C4B-NB	-2.75	108.08	110.53
13	f	1225	CLA	C3B-C4B-NB	-2.75	108.08	110.53
13	G	1106	CLA	O2D-CGD-CBD	2.75	116.03	111.23
13	U	1401	CLA	O2D-CGD-CBD	2.75	116.03	111.23
13	q	510	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
13	b	513	CLA	C3B-C4B-NB	-2.74	108.08	110.53
13	2	518	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
13	Z	518	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
13	s	504	CLA	C3B-C4B-NB	-2.74	108.08	110.53
16	f	4004	BCR	C28-C27-C26	-2.74	109.16	114.06
16	2	524	BCR	C11-C10-C9	-2.74	123.43	127.28
13	f	1205	CLA	C1-C2-C3	-2.74	121.70	126.20
13	H	1234	CLA	CBC-CAC-C3C	2.74	119.86	112.42
13	c	501	CLA	CHB-C4A-NA	2.74	128.36	124.40
13	Y	504	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
16	5	522	BCR	C16-C17-C18	-2.74	123.43	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c	507	CLA	CHB-C4A-NA	2.74	128.36	124.40
16	B	4014	BCR	C10-C11-C12	-2.74	115.26	123.20
16	B	4004	BCR	C28-C27-C26	-2.74	109.17	114.06
20	L	5216	SQD	O9-S-C6	2.74	110.85	106.76
13	4	504	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
13	B	1207	CLA	CHB-C4A-NA	2.74	128.35	124.40
13	f	1225	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
13	a	504	CLA	C3B-C4B-NB	-2.74	108.08	110.53
13	5	507	CLA	CHB-C4A-NA	2.74	128.35	124.40
14	e	2001	PQN	C11-C3-C2	-2.74	120.19	124.89
13	K	1105	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	5	518	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	c	518	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
16	H	4010	BCR	C38-C26-C25	-2.74	121.50	124.48
17	G	5004	LHG	O8-C23-C24	2.74	120.18	111.83
13	e	1136	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
13	q	504	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	e	5005	LHG	C11-C10-C9	-2.74	100.53	114.37
13	t	513	CLA	C3B-C4B-NB	-2.74	108.09	110.53
13	q	518	CLA	CHB-C4A-NA	2.74	128.35	124.40
13	a	502	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	G	1104	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	B	1205	CLA	CHB-C4A-NA	2.74	128.35	124.40
13	H	1207	CLA	CHB-C4A-NA	2.74	128.35	124.40
13	B	1225	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	4	517	CLA	CHB-C4A-NA	2.73	128.35	124.40
13	e	1117	CLA	CHB-C4A-NA	2.73	128.35	124.40
16	m	4104	BCR	C3-C4-C5	-2.73	109.18	114.06
13	1	517	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	r	505	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	5	506	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	G	1011	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	2	513	CLA	CHB-C4A-NA	2.73	128.35	124.40
13	2	518	CLA	CHB-C4A-NA	2.73	128.35	124.40
13	q	507	CLA	CHB-C4A-NA	2.73	128.35	124.40
13	K	1401	CLA	O2D-CGD-CBD	2.73	116.01	111.23
13	u	518	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
17	A	5005	LHG	C11-C10-C9	-2.73	100.55	114.37
13	3	518	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	s	518	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	t	517	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	A	1136	CLA	O2A-CGA-O1A	-2.73	116.79	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	524	BCR	C1-C6-C5	-2.73	118.90	122.64
13	H	1205	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	f	1228	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	e	1120	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	r	518	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	3	502	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	6	509	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	s	502	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	4	513	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	Z	513	CLA	CHB-C4A-NA	2.73	128.34	124.40
16	G	4007	BCR	C15-C16-C17	-2.73	117.93	123.52
16	b	523	BCR	C11-C10-C9	-2.73	123.45	127.28
13	G	1122	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	t	504	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
16	r	521	BCR	C29-C30-C25	2.73	114.41	110.44
16	U	4104	BCR	C3-C4-C5	-2.73	109.19	114.06
16	q	523	BCR	C24-C23-C22	-2.73	122.20	126.23
13	G	1120	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	J	1302	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	e	1131	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	t	513	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	B	1204	CLA	CHB-C4A-NA	2.73	128.34	124.40
16	T	4012	BCR	C33-C5-C6	-2.73	121.51	124.48
20	2	822	SQD	C4-C3-C2	2.73	115.62	110.83
13	G	1237	CLA	C6-C5-C3	2.73	120.12	113.47
17	G	5005	LHG	C11-C10-C9	-2.73	100.57	114.37
13	e	1136	CLA	C1-C2-C3	-2.73	121.73	126.20
13	d	517	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	s	501	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
16	n	4020	BCR	C3-C4-C5	-2.73	109.19	114.06
13	3	501	CLA	CMB-C2B-C1B	-2.73	121.27	125.42
13	e	1122	CLA	CHB-C4A-NA	2.73	128.34	124.40
13	b	504	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	f	1230	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	G	1136	CLA	C1-C2-C3	-2.73	121.73	126.20
13	1	510	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
16	f	4014	BCR	C10-C11-C12	-2.73	115.30	123.20
13	e	1104	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
13	G	1136	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
13	c	506	CLA	C3B-C4B-NB	-2.73	108.10	110.53
13	q	517	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
13	A	1117	CLA	CHB-C4A-NA	2.73	128.33	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	517	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
16	5	522	BCR	C1-C6-C5	-2.73	118.91	122.64
13	4	513	CLA	CHB-C4A-NA	2.72	128.33	124.40
13	c	516	CLA	CHB-C4A-NA	2.72	128.33	124.40
16	K	4104	BCR	C3-C4-C5	-2.72	109.20	114.06
13	R	1301	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	H	1221	CLA	C3B-C4B-NB	-2.72	108.10	110.53
13	Z	510	CLA	C3B-C4B-NB	-2.72	108.10	110.53
16	J	4012	BCR	C33-C5-C6	-2.72	121.51	124.48
13	d	509	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	2	510	CLA	C3B-C4B-NB	-2.72	108.10	110.53
13	3	503	CLA	C3B-C4B-NB	-2.72	108.10	110.53
13	H	1205	CLA	C3B-C4B-NB	-2.72	108.10	110.53
16	l	4012	BCR	C33-C5-C6	-2.72	121.51	124.48
13	H	1225	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
17	A	5004	LHG	O8-C23-C24	2.72	120.13	111.83
13	A	1122	CLA	CHB-C4A-NA	2.72	128.33	124.40
13	H	1219	CLA	C3B-C4B-NB	-2.72	108.10	110.53
13	a	501	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
20	s	822	SQD	O5-C5-C4	2.72	114.60	109.70
13	Y	510	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	Y	511	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
16	H	4004	BCR	C28-C27-C26	-2.72	109.20	114.06
20	Z	822	SQD	C4-C3-C2	2.72	115.61	110.83
13	c	506	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	d	503	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	u	516	CLA	CHB-C4A-NA	2.72	128.32	124.40
16	Z	521	BCR	C29-C30-C25	2.72	114.39	110.44
13	A	1104	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
20	n	5216	SQD	O9-S-C6	2.72	110.82	106.76
13	B	1229	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	V	1503	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	f	1229	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	u	504	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	3	822	SQD	O5-C5-C4	2.72	114.60	109.70
17	e	5004	LHG	O8-C23-C24	2.72	120.12	111.83
13	A	1237	CLA	C6-C5-C3	2.72	120.09	113.47
13	5	503	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	s	503	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	r	513	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	t	507	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	4	516	CLA	C3B-C4B-NB	-2.72	108.10	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	r	516	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	a	822	SQD	O5-C5-C4	2.72	114.59	109.70
13	4	506	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	G	1116	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	e	1237	CLA	C6-C5-C3	2.72	120.08	113.47
13	u	507	CLA	CHB-C4A-NA	2.72	128.32	124.40
16	L	4020	BCR	C3-C4-C5	-2.72	109.21	114.06
13	s	503	CLA	C3B-C4B-NB	-2.72	108.11	110.53
16	t	523	BCR	C11-C10-C9	-2.72	123.47	127.28
16	f	4006	BCR	C31-C1-C6	-2.72	105.98	110.24
13	2	505	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
13	q	511	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
16	V	4020	BCR	C3-C4-C5	-2.72	109.21	114.06
13	H	1217	CLA	CHB-C4A-NA	2.71	128.32	124.40
13	e	1106	CLA	C1-C2-C3	-2.71	121.75	126.20
16	B	4006	BCR	C31-C1-C6	-2.71	105.99	110.24
13	A	1121	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	5	504	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	b	516	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	v	509	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
13	b	504	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
13	c	504	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	U	1105	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
16	1	523	BCR	C24-C23-C22	-2.71	122.22	126.23
13	b	513	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	f	1204	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	H	1213	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	u	511	CLA	C3B-C4B-NB	-2.71	108.11	110.53
16	f	4010	BCR	C38-C26-C25	-2.71	121.53	124.48
16	f	4017	BCR	C33-C5-C6	-2.71	121.53	124.48
13	5	516	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	H	1229	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	t	506	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	H	1210	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
13	Z	505	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
13	b	513	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
13	e	1127	CLA	CMB-C2B-C3B	2.71	132.93	126.55
16	J	4012	BCR	C23-C22-C21	2.71	123.27	119.01
13	Z	504	CLA	C3B-C4B-NB	-2.71	108.11	110.53
16	H	4006	BCR	C31-C1-C6	-2.71	105.99	110.24
13	u	510	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	B	1205	CLA	C3B-C4B-NB	-2.71	108.11	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	v	517	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	1	507	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	q	503	CLA	CHB-C4A-NA	2.71	128.31	124.40
16	2	521	BCR	C29-C30-C25	2.71	114.37	110.44
16	Y	524	BCR	C1-C6-C5	-2.71	118.94	122.64
13	G	1111	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	Y	511	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	u	518	CLA	CHB-C4A-NA	2.71	128.31	124.40
13	3	516	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
13	2	510	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
13	r	511	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	5	506	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
13	q	518	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
16	u	522	BCR	C1-C6-C5	-2.71	118.94	122.64
20	r	822	SQD	C4-C3-C2	2.71	115.58	110.83
16	s	521	BCR	C33-C5-C6	-2.70	121.53	124.48
18	1	902	LMU	O5'-C5'-C4'	2.70	114.57	109.70
13	t	504	CLA	CHB-C4A-NA	2.70	128.30	124.40
18	Y	902	LMU	O5'-C5'-C4'	2.70	114.57	109.70
13	Y	507	CLA	CHB-C4A-NA	2.70	128.30	124.40
13	6	517	CLA	C3B-C4B-NB	-2.70	108.12	110.53
13	f	1205	CLA	CHB-C4A-NA	2.70	128.30	124.40
16	1	524	BCR	C1-C6-C5	-2.70	118.94	122.64
13	e	1119	CLA	C3B-C4B-NB	-2.70	108.12	110.53
13	1	503	CLA	CHB-C4A-NA	2.70	128.30	124.40
13	f	1217	CLA	CHB-C4A-NA	2.70	128.30	124.40
13	u	503	CLA	CHB-C4A-NA	2.70	128.30	124.40
13	A	1106	CLA	C1-C2-C3	-2.70	121.77	126.20
13	r	506	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
13	r	510	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
13	t	516	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	T	4012	BCR	C23-C22-C21	2.70	123.25	119.01
13	A	1127	CLA	CMB-C2B-C3B	2.70	132.90	126.55
13	A	1120	CLA	CHB-C4A-NA	2.70	128.29	124.40
13	L	1503	CLA	CHB-C4A-NA	2.70	128.29	124.40
13	A	1011	CLA	C3B-C4B-NB	-2.70	108.12	110.53
13	1	511	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
13	1	518	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
13	s	516	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
16	5	523	BCR	C33-C5-C6	-2.70	121.54	124.48
13	2	510	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
13	a	518	CLA	CHB-C4A-NA	2.70	128.29	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1205	CLA	C3B-C4B-NB	-2.70	108.12	110.53
13	c	503	CLA	CHB-C4A-NA	2.70	128.29	124.40
13	Y	518	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
13	G	1127	CLA	CMB-C2B-C3B	2.70	132.89	126.55
13	2	504	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	B	4010	BCR	C38-C26-C25	-2.70	121.54	124.48
13	u	506	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
16	H	4017	BCR	C20-C21-C22	-2.70	123.50	127.28
13	Y	518	CLA	CHB-C4A-NA	2.70	128.29	124.40
18	q	902	LMU	O5'-C5'-C4'	2.70	114.56	109.70
16	B	4017	BCR	C33-C5-C6	-2.70	121.54	124.48
13	Y	503	CLA	CHB-C4A-NA	2.69	128.29	124.40
13	r	510	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
13	G	1106	CLA	C1-C2-C3	-2.69	121.78	126.20
13	1	511	CLA	CHB-C4A-NA	2.69	128.29	124.40
13	G	1013	CLA	CAA-CBA-CGA	-2.69	105.56	113.21
13	A	1138	CLA	CHB-C4A-NA	2.69	128.29	124.40
13	n	1503	CLA	CHB-C4A-NA	2.69	128.29	124.40
13	u	511	CLA	CHB-C4A-NA	2.69	128.29	124.40
13	a	516	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
13	a	513	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	e	1013	CLA	CAA-CBA-CGA	-2.69	105.56	113.21
13	A	1119	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	3	513	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	t	513	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	f	4009	BCR	C33-C5-C4	2.69	119.33	113.60
13	5	518	CLA	CHB-C4A-NA	2.69	128.28	124.40
13	a	503	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	H	4004	BCR	C20-C19-C18	-2.69	118.99	126.36
13	4	504	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	Y	501	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	f	1213	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	A	1022	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
16	H	4017	BCR	C33-C5-C6	-2.69	121.55	124.48
13	G	1116	CLA	CMB-C2B-C3B	2.69	132.87	126.55
13	A	1116	CLA	CHB-C4A-NA	2.69	128.28	124.40
13	B	1217	CLA	CHB-C4A-NA	2.69	128.28	124.40
13	e	1127	CLA	CHB-C4A-NA	2.69	128.28	124.40
13	4	504	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	V	4020	BCR	C37-C22-C21	-2.69	118.46	122.82
13	Z	506	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
13	4	507	CLA	CHB-C4A-NA	2.69	128.28	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c	511	CLA	CHB-C4A-NA	2.69	128.28	124.40
13	e	1138	CLA	CHB-C4A-NA	2.69	128.28	124.40
13	B	1210	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
13	b	501	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	2	506	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
16	s	522	BCR	C15-C16-C17	-2.69	118.02	123.52
16	c	524	BCR	C11-C10-C9	-2.69	123.51	127.28
13	G	1022	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
13	5	510	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	3	522	BCR	C15-C16-C17	-2.69	118.02	123.52
13	A	1118	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	L	4020	BCR	C37-C22-C21	-2.69	118.47	122.82
18	e	1848	LMU	C2'-C3'-C4'	2.68	115.77	109.68
13	A	1104	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
13	e	1104	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
16	f	4017	BCR	C20-C21-C22	-2.68	123.51	127.28
13	e	1125	CLA	CHB-C4A-NA	2.68	128.27	124.40
13	A	1013	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
16	G	4011	BCR	C10-C11-C12	-2.68	115.42	123.20
13	B	1221	CLA	C3B-C4B-NB	-2.68	108.13	110.53
13	4	501	CLA	C3B-C4B-NB	-2.68	108.13	110.53
13	v	506	CLA	C3B-C4B-NB	-2.68	108.13	110.53
16	B	4017	BCR	C20-C21-C22	-2.68	123.51	127.28
13	3	503	CLA	CHB-C4A-NA	2.68	128.27	124.40
13	Z	510	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
18	A	1848	LMU	C2'-C3'-C4'	2.68	115.77	109.68
13	e	1116	CLA	CMB-C2B-C3B	2.68	132.86	126.55
13	d	504	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
13	3	517	CLA	CHB-C4A-NA	2.68	128.27	124.40
13	q	511	CLA	CHB-C4A-NA	2.68	128.27	124.40
19	f	5002	LMG	O7-C10-O9	-2.68	117.44	123.70
13	e	1237	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	c	518	CLA	CHB-C4A-NA	2.68	128.27	124.40
13	r	517	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
13	A	1116	CLA	CMB-C2B-C3B	2.68	132.85	126.55
13	B	1213	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	2	516	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	b	506	CLA	CHB-C4A-NA	2.68	128.27	124.40
16	1	522	BCR	C23-C24-C25	-2.68	119.84	127.00
16	3	521	BCR	C33-C5-C6	-2.68	121.56	124.48
13	e	1114	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	6	504	CLA	O2D-CGD-O1D	-2.68	118.63	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	d	506	CLA	CHB-C4A-NA	2.68	128.27	124.40
16	n	4020	BCR	C37-C22-C21	-2.68	118.48	122.82
16	Y	523	BCR	C24-C23-C22	-2.68	122.27	126.23
13	r	503	CLA	CHB-C4A-NA	2.68	128.26	124.40
13	s	517	CLA	CHB-C4A-NA	2.68	128.26	124.40
13	Z	510	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
19	B	5002	LMG	O7-C10-O9	-2.68	117.44	123.70
16	f	4004	BCR	C20-C19-C18	-2.68	119.03	126.36
13	t	504	CLA	C3B-C4B-NB	-2.68	108.14	110.53
16	Y	522	BCR	C23-C24-C25	-2.68	119.85	127.00
13	B	1219	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	6	506	CLA	CHB-C4A-NA	2.67	128.26	124.40
13	1	516	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
13	Y	516	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
16	B	4004	BCR	C20-C19-C18	-2.67	119.03	126.36
13	e	1132	CLA	CAC-C3C-C4C	2.67	128.27	124.79
13	G	1104	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
13	t	501	CLA	C3B-C4B-NB	-2.67	108.14	110.53
13	A	1111	CLA	CHB-C4A-NA	2.67	128.26	124.40
13	a	501	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
13	G	1132	CLA	CAC-C3C-C4C	2.67	128.27	124.79
13	f	1223	CLA	CHB-C4A-NA	2.67	128.25	124.40
16	c	523	BCR	C33-C5-C6	-2.67	121.57	124.48
13	A	1127	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	G	1138	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	v	504	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
16	a	522	BCR	C15-C16-C17	-2.67	118.06	123.52
13	2	503	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	A	1114	CLA	C3B-C4B-NB	-2.67	108.15	110.53
13	B	1232	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	Z	510	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	a	517	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	b	519	CLA	CHB-C4A-NA	2.67	128.25	124.40
16	1	524	BCR	C15-C16-C17	-2.67	118.06	123.52
16	u	523	BCR	C33-C5-C6	-2.67	121.57	124.48
13	5	511	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	r	510	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	v	506	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	b	504	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	e	1118	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	3	501	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
18	G	1848	LMU	C2'-C3'-C4'	2.67	115.73	109.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	4011	BCR	C10-C11-C12	-2.67	115.47	123.20
13	c	510	CLA	CHB-C4A-NA	2.67	128.25	124.40
16	q	522	BCR	C23-C24-C25	-2.67	119.88	127.00
13	A	1125	CLA	CHB-C4A-NA	2.67	128.25	124.40
13	e	1022	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
13	f	1210	CLA	C1-C2-C3	-2.67	121.83	126.20
13	2	517	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
13	b	507	CLA	CHB-C4A-NA	2.67	128.25	124.40
16	f	4014	BCR	C34-C9-C8	2.67	122.16	118.09
16	Y	524	BCR	C15-C16-C17	-2.67	118.06	123.52
17	A	5001	LHG	C20-C19-C18	-2.67	100.90	114.37
13	H	1213	CLA	O2D-CGD-CBD	2.67	115.89	111.23
13	G	1114	CLA	C3B-C4B-NB	-2.66	108.15	110.53
13	H	1021	CLA	C3B-C4B-NB	-2.66	108.15	110.53
13	4	519	CLA	CHB-C4A-NA	2.66	128.25	124.40
16	a	521	BCR	C33-C5-C6	-2.66	121.58	124.48
17	e	5001	LHG	C20-C19-C18	-2.66	100.90	114.37
13	s	501	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
16	e	4011	BCR	C10-C11-C12	-2.66	115.48	123.20
16	m	4104	BCR	C30-C25-C24	2.66	122.87	115.65
16	B	4014	BCR	C34-C9-C8	2.66	122.16	118.09
13	G	1125	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	v	511	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	Z	517	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
13	a	507	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
13	f	1210	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
13	s	513	CLA	C3B-C4B-NB	-2.66	108.15	110.53
13	B	1210	CLA	CHB-C4A-NA	2.66	128.24	124.40
17	G	5001	LHG	C20-C19-C18	-2.66	100.92	114.37
13	G	1127	CLA	CHB-C4A-NA	2.66	128.24	124.40
16	B	4005	BCR	C28-C27-C26	-2.66	109.31	114.06
13	s	507	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
13	s	504	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	2	504	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	f	1232	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	v	519	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	d	506	CLA	C3B-C4B-NB	-2.66	108.16	110.53
13	H	1210	CLA	C1-C2-C3	-2.66	121.84	126.20
13	f	1213	CLA	O2D-CGD-CBD	2.66	115.88	111.23
13	B	1210	CLA	C1-C2-C3	-2.66	121.84	126.20
13	b	505	CLA	CHB-C4A-NA	2.66	128.24	124.40
19	H	5002	LMG	O7-C10-O9	-2.66	117.49	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1229	CLA	CHD-C1D-ND	-2.66	121.06	124.80
13	f	1229	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	l	4012	BCR	C23-C22-C21	2.66	123.19	119.01
13	H	1210	CLA	CHB-C4A-NA	2.66	128.24	124.40
16	4	523	BCR	C7-C8-C9	-2.66	122.30	126.23
13	A	1132	CLA	CAC-C3C-C4C	2.66	128.25	124.79
13	G	1113	CLA	CHB-C4A-NA	2.66	128.23	124.40
16	B	4009	BCR	C33-C5-C4	2.66	119.26	113.60
13	r	504	CLA	C3B-C4B-NB	-2.66	108.16	110.53
13	e	1111	CLA	CHB-C4A-NA	2.66	128.23	124.40
13	H	1201	CLA	CMB-C2B-C3B	2.66	132.80	126.55
13	3	507	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
16	f	4005	BCR	C28-C27-C26	-2.66	109.32	114.06
13	B	1021	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	2	517	CLA	C3B-C4B-NB	-2.65	108.16	110.53
16	q	524	BCR	C15-C16-C17	-2.65	118.09	123.52
13	f	1204	CLA	O2D-CGD-CBD	2.65	115.87	111.23
13	Z	503	CLA	CHB-C4A-NA	2.65	128.23	124.40
16	K	4104	BCR	C30-C25-C24	2.65	122.85	115.65
13	B	1213	CLA	O2D-CGD-CBD	2.65	115.87	111.23
13	2	502	CLA	CHB-C4A-NA	2.65	128.23	124.40
13	Z	504	CLA	CHB-C4A-NA	2.65	128.23	124.40
13	A	1237	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	Y	511	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	f	1201	CLA	CMB-C2B-C3B	2.65	132.79	126.55
13	d	519	CLA	CHB-C4A-NA	2.65	128.23	124.40
16	5	524	BCR	C11-C10-C9	-2.65	123.56	127.28
16	b	523	BCR	C7-C8-C9	-2.65	122.31	126.23
13	G	1127	CLA	C1-C2-C3	-2.65	121.85	126.20
13	5	511	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	e	1011	CLA	C3B-C4B-NB	-2.65	108.16	110.53
20	f	1852	SQD	C44-O6-C1	2.65	119.48	113.80
16	H	4009	BCR	C33-C5-C4	2.65	119.25	113.60
13	u	513	CLA	CHB-C4A-NA	2.65	128.23	124.40
13	Z	509	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
13	d	510	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	2	509	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
13	q	516	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
13	6	519	CLA	CHB-C4A-NA	2.65	128.22	124.40
16	Y	524	BCR	C8-C7-C6	-2.65	119.92	127.00
16	q	524	BCR	C33-C5-C4	2.65	119.25	113.60
13	B	1229	CLA	CHD-C1D-ND	-2.65	121.07	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	506	CLA	C3B-C4B-NB	-2.65	108.17	110.53
13	B	1204	CLA	O2D-CGD-CBD	2.65	115.86	111.23
16	v	523	BCR	C20-C21-C22	-2.65	123.56	127.28
13	f	1219	CLA	C3B-C4B-NB	-2.65	108.17	110.53
13	f	1221	CLA	C3B-C4B-NB	-2.65	108.17	110.53
16	H	4005	BCR	C28-C27-C26	-2.65	109.33	114.06
16	u	522	BCR	C38-C26-C27	2.65	119.24	113.60
16	H	4014	BCR	C34-C9-C8	2.65	122.13	118.09
13	G	1237	CLA	C3B-C4B-NB	-2.65	108.17	110.53
13	Z	516	CLA	C3B-C4B-NB	-2.65	108.17	110.53
13	c	511	CLA	C3B-C4B-NB	-2.65	108.17	110.53
13	f	1210	CLA	CHB-C4A-NA	2.65	128.22	124.40
13	t	519	CLA	CHB-C4A-NA	2.65	128.22	124.40
16	f	4009	BCR	C16-C17-C18	-2.65	123.57	127.28
16	u	524	BCR	C11-C10-C9	-2.65	123.57	127.28
13	f	1230	CLA	CAA-C2A-C3A	-2.65	105.85	113.00
13	2	510	CLA	CHB-C4A-NA	2.65	128.22	124.40
13	6	511	CLA	CHB-C4A-NA	2.65	128.22	124.40
13	d	518	CLA	CHB-C4A-NA	2.65	128.22	124.40
13	H	1223	CLA	CMB-C2B-C3B	2.65	132.77	126.55
13	G	1013	CLA	CHB-C4A-NA	2.65	128.22	124.40
16	1	524	BCR	C21-C20-C19	-2.65	115.54	123.20
13	3	504	CLA	CHB-C4A-NA	2.64	128.22	124.40
13	G	1118	CLA	CHB-C4A-NA	2.64	128.22	124.40
13	a	504	CLA	CHB-C4A-NA	2.64	128.22	124.40
13	B	1223	CLA	CMB-C2B-C3B	2.64	132.77	126.55
13	H	1230	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
13	H	1232	CLA	CHB-C4A-NA	2.64	128.22	124.40
13	Y	509	CLA	CMB-C2B-C1B	-2.64	121.39	125.42
13	B	1230	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
20	B	1852	SQD	C44-O6-C1	2.64	119.46	113.80
16	U	4104	BCR	C30-C25-C24	2.64	122.82	115.65
13	Y	501	CLA	CHB-C4A-NA	2.64	128.21	124.40
13	f	1223	CLA	CMB-C2B-C3B	2.64	132.77	126.55
13	1	511	CLA	C3B-C4B-NB	-2.64	108.17	110.53
13	Z	517	CLA	C3B-C4B-NB	-2.64	108.17	110.53
13	r	517	CLA	C3B-C4B-NB	-2.64	108.17	110.53
16	1	524	BCR	C33-C5-C4	2.64	119.23	113.60
13	2	511	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	H	1852	SQD	C44-O6-C1	2.64	119.45	113.80
13	6	504	CLA	CHB-C4A-NA	2.64	128.21	124.40
13	e	1013	CLA	CHB-C4A-NA	2.64	128.21	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	505	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
13	Y	509	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
13	r	509	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
16	r	523	BCR	C21-C20-C19	-2.64	115.55	123.20
13	d	511	CLA	CHB-C4A-NA	2.64	128.21	124.40
16	5	522	BCR	C38-C26-C27	2.64	119.22	113.60
13	B	1203	CLA	CHB-C4A-NA	2.64	128.21	124.40
16	1	524	BCR	C8-C7-C6	-2.64	119.95	127.00
13	A	1113	CLA	CHB-C4A-NA	2.64	128.21	124.40
13	e	1116	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	A	5008	LHG	C11-C10-C9	-2.64	101.04	114.37
16	q	524	BCR	C21-C20-C19	-2.64	115.56	123.20
13	B	1201	CLA	CMB-C2B-C3B	2.64	132.75	126.55
13	A	1013	CLA	CHB-C4A-NA	2.64	128.20	124.40
13	v	510	CLA	C3B-C4B-NB	-2.64	108.18	110.53
16	b	522	BCR	C33-C5-C6	-2.64	121.61	124.48
13	r	504	CLA	CHB-C4A-NA	2.64	128.20	124.40
13	1	505	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
13	5	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	H	1225	CLA	CMB-C2B-C3B	2.63	132.75	126.55
16	t	522	BCR	C33-C5-C6	-2.63	121.61	124.48
13	H	1223	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	f	1203	CLA	CHB-C4A-NA	2.63	128.20	124.40
16	Z	523	BCR	C21-C20-C19	-2.63	115.57	123.20
13	1	501	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	A	1106	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
13	B	1223	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	4	505	CLA	CHB-C4A-NA	2.63	128.20	124.40
17	e	5008	LHG	C11-C10-C9	-2.63	101.06	114.37
13	H	1204	CLA	O2D-CGD-CBD	2.63	115.83	111.23
16	2	523	BCR	C21-C20-C19	-2.63	115.58	123.20
17	G	5008	LHG	C11-C10-C9	-2.63	101.07	114.37
13	q	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	v	504	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	6	510	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	4	522	BCR	C33-C5-C6	-2.63	121.61	124.48
16	Y	524	BCR	C21-C20-C19	-2.63	115.58	123.20
16	q	524	BCR	C8-C7-C6	-2.63	119.97	127.00
13	r	509	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
13	q	501	CLA	CHB-C4A-NA	2.63	128.19	124.40
13	e	1127	CLA	C1-C2-C3	-2.63	121.89	126.20
13	A	1106	CLA	CHB-C4A-NA	2.63	128.19	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	c	522	BCR	C38-C26-C27	2.63	119.20	113.60
13	1	509	CLA	CMB-C2B-C1B	-2.63	121.42	125.42
13	c	513	CLA	CHB-C4A-NA	2.63	128.19	124.40
13	d	504	CLA	CHB-C4A-NA	2.63	128.19	124.40
13	B	1225	CLA	CMB-C2B-C3B	2.63	132.73	126.55
13	G	1106	CLA	CMB-C2B-C1B	-2.63	121.42	125.42
20	Z	822	SQD	O5-C5-C4	2.63	114.43	109.70
16	r	524	BCR	C21-C20-C19	-2.63	115.59	123.20
13	5	504	CLA	CHB-C4A-NA	2.62	128.19	124.40
13	A	1135	CLA	CHB-C4A-NA	2.62	128.19	124.40
13	u	504	CLA	CHB-C4A-NA	2.62	128.19	124.40
13	4	506	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	H	1203	CLA	CHB-C4A-NA	2.62	128.19	124.40
16	t	523	BCR	C7-C8-C9	-2.62	122.36	126.23
13	A	1127	CLA	C1-C2-C3	-2.62	121.90	126.20
16	B	4009	BCR	C10-C11-C12	-2.62	115.60	123.20
16	Y	524	BCR	C33-C5-C4	2.62	119.19	113.60
16	B	4009	BCR	C16-C17-C18	-2.62	123.60	127.28
13	H	1227	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
13	e	1106	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
13	f	1021	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	q	509	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
16	2	524	BCR	C21-C20-C19	-2.62	115.61	123.20
17	H	1842	LHG	O8-C23-C24	2.62	119.83	111.83
16	l	4015	BCR	C24-C23-C22	-2.62	122.36	126.23
13	e	1113	CLA	CHB-C4A-NA	2.62	128.18	124.40
16	G	4011	BCR	C23-C24-C25	-2.62	120.00	127.00
13	r	505	CLA	C1-C2-C3	-2.62	121.91	126.20
16	Z	524	BCR	C21-C20-C19	-2.62	115.61	123.20
13	b	518	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	q	505	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
13	Z	502	CLA	CHB-C4A-NA	2.62	128.18	124.40
16	5	521	BCR	C27-C26-C25	-2.62	119.17	122.70
13	c	504	CLA	CHB-C4A-NA	2.62	128.18	124.40
13	1	509	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
13	v	517	CLA	CHB-C4A-NA	2.62	128.18	124.40
13	c	509	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
13	q	511	CLA	C3B-C4B-NB	-2.62	108.19	110.53
16	c	523	BCR	C20-C21-C22	-2.62	123.61	127.28
13	f	1225	CLA	CMB-C2B-C3B	2.62	132.70	126.55
13	B	1224	CLA	CHB-C4A-NA	2.62	128.17	124.40
13	5	502	CLA	CHB-C4A-NA	2.62	128.17	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1138	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
16	6	523	BCR	C20-C21-C22	-2.61	123.61	127.28
20	5	822	SQD	C44-O6-C1	2.61	119.40	113.80
13	u	502	CLA	CHB-C4A-NA	2.61	128.17	124.40
13	a	516	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	G	1011	CLA	C4D-C3D-CAD	-2.61	105.27	108.11
13	t	506	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	e	1011	CLA	C4D-C3D-CAD	-2.61	105.27	108.11
16	d	523	BCR	C20-C21-C22	-2.61	123.62	127.28
20	v	822	SQD	C1-O5-C5	2.61	118.82	113.72
13	e	1106	CLA	CHB-C4A-NA	2.61	128.17	124.40
16	c	523	BCR	C34-C9-C8	2.61	122.08	118.09
13	q	509	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
20	c	822	SQD	C44-O6-C1	2.61	119.39	113.80
20	u	822	SQD	C44-O6-C1	2.61	119.39	113.80
13	1	513	CLA	CHB-C4A-NA	2.61	128.17	124.40
13	B	1227	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
20	r	822	SQD	O5-C5-C4	2.61	114.40	109.70
16	a	524	BCR	C20-C21-C22	-2.61	123.62	127.28
13	e	1135	CLA	CHB-C4A-NA	2.61	128.17	124.40
13	t	505	CLA	CHB-C4A-NA	2.61	128.17	124.40
20	2	822	SQD	O5-C5-C4	2.61	114.40	109.70
17	B	1842	LHG	O8-C23-C24	2.61	119.79	111.83
20	s	822	SQD	O48-C23-C24	2.61	119.79	111.83
13	f	1215	CLA	CHB-C4A-NA	2.61	128.16	124.40
16	L	4020	BCR	C34-C9-C8	2.61	122.07	118.09
13	3	509	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
13	6	517	CLA	CHB-C4A-NA	2.61	128.16	124.40
13	v	518	CLA	CHB-C4A-NA	2.61	128.16	124.40
20	3	822	SQD	O48-C23-C24	2.61	119.79	111.83
13	H	1224	CLA	CHB-C4A-NA	2.61	128.16	124.40
16	f	4009	BCR	C10-C11-C12	-2.61	115.64	123.20
13	f	1227	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
13	G	1106	CLA	CHB-C4A-NA	2.61	128.16	124.40
13	G	1138	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
13	u	519	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
13	t	518	CLA	C3B-C4B-NB	-2.61	108.20	110.53
17	f	1842	LHG	O8-C23-C24	2.61	119.78	111.83
13	s	509	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
16	A	4011	BCR	C23-C24-C25	-2.61	120.04	127.00
16	V	4020	BCR	C34-C9-C8	2.61	122.07	118.09
13	2	509	CLA	O2D-CGD-O1D	-2.61	118.78	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	501	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	d	509	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	e	1126	CLA	CHB-C4A-NA	2.60	128.16	124.40
13	e	1138	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
13	A	1102	CLA	CMB-C2B-C3B	2.60	132.68	126.55
20	d	822	SQD	C1-O5-C5	2.60	118.81	113.72
13	f	1219	CLA	O2D-CGD-CBD	2.60	115.78	111.23
16	c	521	BCR	C27-C26-C25	-2.60	119.19	122.70
13	T	1303	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
13	4	518	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	H	4009	BCR	C10-C11-C12	-2.60	115.66	123.20
13	r	502	CLA	CHB-C4A-NA	2.60	128.16	124.40
13	H	1220	CLA	CAA-CBA-CGA	-2.60	105.82	113.21
13	B	1215	CLA	CHB-C4A-NA	2.60	128.16	124.40
13	f	1224	CLA	CHB-C4A-NA	2.60	128.16	124.40
13	5	519	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
13	a	509	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
13	H	1239	CLA	CHB-C4A-NA	2.60	128.15	124.40
16	e	4011	BCR	C23-C24-C25	-2.60	120.05	127.00
20	a	822	SQD	O48-C23-C24	2.60	119.77	111.83
13	G	1130	CLA	CHB-C4A-NA	2.60	128.15	124.40
16	H	4009	BCR	C16-C17-C18	-2.60	123.63	127.28
13	e	1103	CLA	CAC-C3C-C4C	2.60	128.17	124.79
13	u	501	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	1	521	BCR	C33-C5-C6	-2.60	121.65	124.48
16	d	522	BCR	C11-C12-C13	-2.60	119.23	126.36
16	Y	522	BCR	C38-C26-C27	2.60	119.14	113.60
16	v	522	BCR	C11-C12-C13	-2.60	119.23	126.36
13	J	1303	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
13	u	509	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
13	r	501	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	3	524	BCR	C20-C21-C22	-2.60	123.63	127.28
16	u	521	BCR	C27-C26-C25	-2.60	119.19	122.70
16	L	4020	BCR	C38-C26-C25	-2.60	121.65	124.48
16	s	524	BCR	C20-C21-C22	-2.60	123.64	127.28
13	6	518	CLA	CHB-C4A-NA	2.60	128.15	124.40
13	5	509	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
13	Y	513	CLA	CHB-C4A-NA	2.60	128.15	124.40
16	q	521	BCR	C33-C5-C6	-2.60	121.65	124.48
13	e	1102	CLA	CMB-C2B-C3B	2.60	132.66	126.55
16	G	4007	BCR	C29-C30-C25	2.60	114.21	110.44
13	3	516	CLA	C3B-C4B-NB	-2.60	108.21	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Z	509	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	t	522	BCR	C1-C6-C5	-2.60	119.09	122.64
13	B	1220	CLA	CAA-CBA-CGA	-2.60	105.84	113.21
13	f	1231	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
20	6	822	SQD	C1-O5-C5	2.59	118.79	113.72
13	2	505	CLA	C1-C2-C3	-2.59	121.95	126.20
13	1	504	CLA	CHB-C4A-NA	2.59	128.14	124.40
13	G	1135	CLA	CHB-C4A-NA	2.59	128.14	124.40
13	Z	505	CLA	C1-C2-C3	-2.59	121.95	126.20
16	u	523	BCR	C34-C9-C8	2.59	122.05	118.09
16	6	523	BCR	C15-C16-C17	-2.59	118.21	123.52
16	b	522	BCR	C1-C6-C5	-2.59	119.09	122.64
13	A	1130	CLA	CHB-C4A-NA	2.59	128.14	124.40
20	Y	822	SQD	O9-S-C6	2.59	110.63	106.76
16	e	4007	BCR	C29-C30-C25	2.59	114.20	110.44
13	A	1126	CLA	CHB-C4A-NA	2.59	128.14	124.40
20	1	822	SQD	O9-S-C6	2.59	110.62	106.76
13	b	506	CLA	C3B-C4B-NB	-2.59	108.22	110.53
13	G	1102	CLA	CMB-C2B-C3B	2.59	132.64	126.55
13	r	517	CLA	CHB-C4A-NA	2.59	128.14	124.40
16	A	4007	BCR	C29-C30-C25	2.59	114.20	110.44
13	s	516	CLA	CHB-C4A-NA	2.59	128.14	124.40
16	6	522	BCR	C11-C12-C13	-2.59	119.26	126.36
16	5	523	BCR	C34-C9-C8	2.59	122.04	118.09
13	d	517	CLA	CHB-C4A-NA	2.59	128.14	124.40
13	Z	501	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	v	523	BCR	C15-C16-C17	-2.59	118.22	123.52
13	G	1126	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	H	2002	PQN	C11-C3-C2	-2.59	120.45	124.89
13	l	1303	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
13	6	508	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
14	f	2002	PQN	C11-C3-C2	-2.59	120.46	124.89
13	H	1215	CLA	CHB-C4A-NA	2.59	128.13	124.40
13	Y	504	CLA	CHB-C4A-NA	2.59	128.13	124.40
13	A	1011	CLA	C4D-C3D-CAD	-2.59	105.30	108.11
13	c	502	CLA	CHB-C4A-NA	2.59	128.13	124.40
16	1	522	BCR	C38-C26-C27	2.59	119.11	113.60
13	f	1220	CLA	CAA-CBA-CGA	-2.59	105.87	113.21
20	5	822	SQD	O48-C23-C24	2.58	119.00	111.15
16	J	4015	BCR	C24-C23-C22	-2.58	122.41	126.23
13	r	508	CLA	CHB-C4A-NA	2.58	128.13	124.40
20	u	822	SQD	O48-C23-C24	2.58	119.00	111.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	3	523	BCR	C20-C21-C22	-2.58	123.65	127.28
13	a	516	CLA	CHB-C4A-NA	2.58	128.13	124.40
13	B	1219	CLA	O2D-CGD-CBD	2.58	115.75	111.23
16	U	4104	BCR	C24-C23-C22	-2.58	122.41	126.23
13	3	516	CLA	CHB-C4A-NA	2.58	128.13	124.40
13	t	516	CLA	CHB-C4A-NA	2.58	128.13	124.40
13	Z	511	CLA	C3B-C4B-NB	-2.58	108.22	110.53
16	n	4020	BCR	C34-C9-C8	2.58	122.03	118.09
13	H	1224	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
16	s	523	BCR	C20-C21-C22	-2.58	123.66	127.28
13	c	519	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
13	A	1129	CLA	CHB-C4A-NA	2.58	128.13	124.40
17	A	5008	LHG	O8-C23-C24	2.58	119.71	111.83
17	e	5001	LHG	O8-C23-C24	2.58	119.71	111.83
13	G	1115	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
13	Z	509	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	B	2002	PQN	C11-C3-C2	-2.58	120.46	124.89
13	q	504	CLA	CHB-C4A-NA	2.58	128.13	124.40
16	n	4020	BCR	C38-C26-C25	-2.58	121.67	124.48
18	H	1843	LMU	O5B-C5B-C4B	2.58	114.35	109.70
17	G	5008	LHG	O8-C23-C24	2.58	119.71	111.83
13	B	1239	CLA	CHB-C4A-NA	2.58	128.12	124.40
18	B	1843	LMU	O5B-C5B-C4B	2.58	114.35	109.70
13	H	1219	CLA	O2D-CGD-CBD	2.58	115.74	111.23
13	1	517	CLA	CHB-C4A-NA	2.58	128.12	124.40
13	v	508	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
17	A	5007	LHG	O8-C23-C24	2.58	119.70	111.83
17	G	5007	LHG	O8-C23-C24	2.58	119.70	111.83
13	f	1234	CLA	CHB-C1B-NB	2.58	127.92	124.05
13	H	1201	CLA	O2D-CGD-CBD	2.58	115.74	111.23
16	4	522	BCR	C1-C6-C5	-2.58	119.11	122.64
13	G	1101	CLA	CHB-C4A-NA	2.58	128.12	124.40
13	B	1231	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
20	c	822	SQD	O48-C23-C24	2.58	118.97	111.15
13	d	516	CLA	CHB-C4A-NA	2.58	128.12	124.40
17	A	5001	LHG	O8-C23-C24	2.58	119.69	111.83
17	e	5007	LHG	O8-C23-C24	2.58	119.69	111.83
20	q	822	SQD	O48-C23-C24	2.58	119.69	111.83
16	H	4017	BCR	C8-C9-C10	-2.58	114.96	119.01
13	2	509	CLA	C3B-C4B-NB	-2.58	108.23	110.53
13	6	509	CLA	C3B-C4B-NB	-2.58	108.23	110.53
17	G	5001	LHG	O8-C23-C24	2.58	119.69	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	522	BCR	C38-C26-C27	2.58	119.09	113.60
13	A	1022	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
13	B	1235	CLA	C3B-C4B-NB	-2.58	108.23	110.53
13	2	517	CLA	CHB-C4A-NA	2.57	128.12	124.40
13	4	516	CLA	CHB-C4A-NA	2.57	128.12	124.40
13	Y	517	CLA	CHB-C4A-NA	2.57	128.12	124.40
16	u	521	BCR	C33-C5-C6	-2.57	121.67	124.48
13	v	509	CLA	C3B-C4B-NB	-2.57	108.23	110.53
16	d	523	BCR	C15-C16-C17	-2.57	118.25	123.52
20	Y	822	SQD	O48-C23-C24	2.57	119.68	111.83
16	5	523	BCR	C20-C21-C22	-2.57	123.67	127.28
13	e	1135	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
13	H	1230	CLA	CAA-C2A-C1A	-2.57	103.54	111.97
13	e	1116	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
13	A	1103	CLA	CAC-C3C-C4C	2.57	128.14	124.79
13	f	1230	CLA	CAA-C2A-C1A	-2.57	103.54	111.97
13	A	1115	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
20	1	822	SQD	O48-C23-C24	2.57	119.68	111.83
16	V	4020	BCR	C38-C26-C25	-2.57	121.68	124.48
13	G	1102	CLA	CHB-C4A-NA	2.57	128.11	124.40
16	T	4015	BCR	C24-C23-C22	-2.57	122.43	126.23
16	m	4104	BCR	C24-C23-C22	-2.57	122.43	126.23
13	5	501	CLA	C3B-C4B-NB	-2.57	108.23	110.53
13	G	1132	CLA	C3B-C4B-NB	-2.57	108.23	110.53
13	A	1135	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
16	K	4104	BCR	C24-C23-C22	-2.57	122.43	126.23
13	B	1201	CLA	O2D-CGD-CBD	2.57	115.72	111.23
13	H	1231	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
13	A	1132	CLA	C3B-C4B-NB	-2.57	108.23	110.53
16	5	522	BCR	C11-C12-C13	-2.57	119.31	126.36
16	u	523	BCR	C20-C21-C22	-2.57	123.67	127.28
20	q	822	SQD	O9-S-C6	2.57	110.59	106.76
16	Y	521	BCR	C33-C5-C6	-2.57	121.68	124.48
13	B	1224	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
16	a	523	BCR	C20-C21-C22	-2.57	123.68	127.28
16	c	522	BCR	C11-C12-C13	-2.57	119.32	126.36
13	G	1135	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
13	G	1140	CLA	C2A-C1A-CHA	2.57	128.32	123.87
18	f	1843	LMU	O5B-C5B-C4B	2.57	114.33	109.70
13	f	1201	CLA	O2D-CGD-CBD	2.57	115.72	111.23
16	5	521	BCR	C33-C5-C6	-2.57	121.68	124.48
13	B	1230	CLA	CAA-C2A-C1A	-2.57	103.57	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1116	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
13	A	1140	CLA	C2A-C1A-CHA	2.57	128.32	123.87
13	d	508	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
16	v	523	BCR	C21-C20-C19	-2.56	115.77	123.20
17	e	5008	LHG	O8-C23-C24	2.56	119.66	111.83
13	e	1022	CLA	CMB-C2B-C1B	-2.56	121.51	125.42
18	B	1843	LMU	C1B-O1B-C4'	-2.56	111.90	117.98
16	3	522	BCR	C16-C17-C18	-2.56	123.68	127.28
13	e	1109	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	q	502	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	v	516	CLA	CHB-C4A-NA	2.56	128.10	124.40
16	f	4010	BCR	C31-C1-C6	-2.56	106.22	110.24
16	B	4014	BCR	C35-C13-C12	2.56	122.00	118.09
13	1	506	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	G	1129	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	b	516	CLA	CHB-C4A-NA	2.56	128.10	124.40
20	f	1852	SQD	O9-S-C6	2.56	110.58	106.76
13	v	508	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
13	b	511	CLA	C3B-C4B-NB	-2.56	108.24	110.53
13	s	516	CLA	C3B-C4B-NB	-2.56	108.24	110.53
16	s	522	BCR	C16-C17-C18	-2.56	123.68	127.28
20	H	1852	SQD	O8-S-C6	2.56	110.92	105.97
13	A	1109	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	f	1225	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	f	1238	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
13	e	1102	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	e	1130	CLA	CHB-C4A-NA	2.56	128.10	124.40
16	6	523	BCR	C21-C20-C19	-2.56	115.78	123.20
13	B	1234	CLA	CHB-C1B-NB	2.56	127.89	124.05
13	H	1236	CLA	C3B-C4B-NB	-2.56	108.24	110.53
13	c	501	CLA	C3B-C4B-NB	-2.56	108.24	110.53
16	f	4014	BCR	C35-C13-C12	2.56	122.00	118.09
13	f	1224	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
13	B	1206	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	Z	505	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	e	1103	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
18	f	1843	LMU	C1B-O1B-C4'	-2.56	111.91	117.98
16	s	524	BCR	C33-C5-C4	2.56	119.05	113.60
16	a	524	BCR	C11-C10-C9	-2.56	123.69	127.28
16	S	4018	BCR	C30-C25-C26	-2.56	119.14	122.64
13	2	508	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	G	1109	CLA	CHB-C4A-NA	2.56	128.09	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	502	CLA	CHB-C4A-NA	2.56	128.09	124.40
16	d	523	BCR	C21-C20-C19	-2.56	115.79	123.20
16	u	522	BCR	C11-C12-C13	-2.56	119.35	126.36
18	H	1843	LMU	C1B-O1B-C4'	-2.56	111.92	117.98
16	c	521	BCR	C20-C19-C18	-2.56	119.36	126.36
16	H	4010	BCR	C31-C1-C6	-2.56	106.23	110.24
13	U	1401	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	Z	517	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	e	1119	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	q	517	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	G	1022	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
13	e	1120	CLA	C3B-C4B-NB	-2.56	108.25	110.53
13	d	508	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
13	e	1115	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
16	3	524	BCR	C33-C5-C4	2.55	119.04	113.60
13	H	1206	CLA	CHB-C4A-NA	2.55	128.09	124.40
13	f	1239	CLA	CHB-C4A-NA	2.55	128.09	124.40
16	f	4009	BCR	C29-C30-C25	2.55	114.15	110.44
17	e	5001	LHG	C11-C10-C9	-2.55	101.46	114.37
13	6	508	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
16	2	524	BCR	C8-C7-C6	-2.55	120.18	127.00
16	s	522	BCR	C38-C26-C25	-2.55	121.70	124.48
13	H	1229	CLA	C3B-C4B-NB	-2.55	108.25	110.53
16	u	521	BCR	C20-C19-C18	-2.55	119.36	126.36
16	4	522	BCR	C38-C26-C27	2.55	119.04	113.60
16	B	4009	BCR	C29-C30-C25	2.55	114.15	110.44
13	B	1238	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
16	B	4010	BCR	C31-C1-C6	-2.55	106.24	110.24
13	f	1021	CLA	O1D-CGD-CBD	2.55	129.55	124.52
13	r	518	CLA	C3B-C4B-NB	-2.55	108.25	110.53
13	e	1129	CLA	CHB-C4A-NA	2.55	128.08	124.40
13	f	1234	CLA	CHB-C4A-NA	2.55	128.08	124.40
16	3	524	BCR	C11-C10-C9	-2.55	123.70	127.28
16	b	522	BCR	C38-C26-C27	2.55	119.03	113.60
13	B	1234	CLA	CHB-C4A-NA	2.55	128.08	124.40
16	B	4017	BCR	C8-C9-C10	-2.55	115.00	119.01
13	G	1116	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
20	d	822	SQD	C45-O47-C7	2.55	122.35	117.85
13	6	516	CLA	CHB-C4A-NA	2.55	128.08	124.40
20	B	1852	SQD	O9-S-C6	2.55	110.56	106.76
16	H	4014	BCR	C35-C13-C12	2.55	121.98	118.09
17	A	5001	LHG	C11-C10-C9	-2.55	101.48	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1128	CLA	CMB-C2B-C3B	2.55	132.54	126.55
13	B	1203	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
13	A	1119	CLA	CHB-C4A-NA	2.55	128.08	124.40
13	f	1206	CLA	CHB-C4A-NA	2.55	128.08	124.40
16	t	522	BCR	C38-C26-C27	2.55	119.03	113.60
20	b	822	SQD	C44-O6-C1	2.55	119.26	113.80
13	Y	511	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
16	H	4010	BCR	C33-C5-C4	2.55	119.03	113.60
17	A	5003	LHG	O8-C23-C24	2.55	119.60	111.83
13	A	1102	CLA	CHB-C4A-NA	2.55	128.08	124.40
13	A	1101	CLA	CHB-C4A-NA	2.55	128.08	124.40
13	H	1021	CLA	O1D-CGD-CBD	2.55	129.54	124.52
16	a	524	BCR	C33-C5-C4	2.55	119.03	113.60
16	V	4020	BCR	C11-C10-C9	-2.55	123.71	127.28
13	Y	506	CLA	CHB-C4A-NA	2.55	128.07	124.40
13	Z	508	CLA	CHB-C4A-NA	2.55	128.07	124.40
16	f	4010	BCR	C33-C5-C4	2.55	119.03	113.60
13	e	1132	CLA	C3B-C4B-NB	-2.55	108.26	110.53
13	t	511	CLA	C3B-C4B-NB	-2.55	108.26	110.53
16	5	521	BCR	C20-C19-C18	-2.55	119.38	126.36
13	f	1212	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
17	V	5220	LHG	O8-C23-C24	2.55	119.60	111.83
16	5	522	BCR	C23-C24-C25	-2.55	120.20	127.00
16	c	521	BCR	C33-C5-C6	-2.54	121.71	124.48
16	B	4010	BCR	C33-C5-C4	2.54	119.02	113.60
13	B	1021	CLA	O1D-CGD-CBD	2.54	129.54	124.52
16	Z	524	BCR	C8-C7-C6	-2.54	120.20	127.00
17	G	5001	LHG	C11-C10-C9	-2.54	101.51	114.37
13	H	1234	CLA	CHB-C1B-NB	2.54	127.86	124.05
17	G	5003	LHG	O8-C23-C24	2.54	119.59	111.83
16	u	522	BCR	C23-C24-C25	-2.54	120.20	127.00
13	1	502	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	H	1852	SQD	O9-S-C6	2.54	110.55	106.76
13	A	1122	CLA	C3B-C4B-NB	-2.54	108.26	110.53
13	H	1220	CLA	C3B-C4B-NB	-2.54	108.26	110.53
13	c	516	CLA	C3B-C4B-NB	-2.54	108.26	110.53
16	I	4018	BCR	C30-C25-C26	-2.54	119.16	122.64
13	G	1103	CLA	CAC-C3C-C4C	2.54	128.10	124.79
20	4	822	SQD	C44-O6-C1	2.54	119.25	113.80
13	e	1140	CLA	C2A-C1A-CHA	2.54	128.28	123.87
13	A	1103	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
13	q	506	CLA	CHB-C4A-NA	2.54	128.07	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	522	BCR	C38-C26-C25	-2.54	121.71	124.48
16	H	4009	BCR	C29-C30-C25	2.54	114.13	110.44
13	G	1103	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
16	L	4020	BCR	C11-C10-C9	-2.54	123.72	127.28
17	e	5003	LHG	O8-C23-C24	2.54	119.58	111.83
16	r	524	BCR	C8-C7-C6	-2.54	120.21	127.00
20	B	1852	SQD	O8-S-C6	2.54	110.88	105.97
13	u	505	CLA	CHB-C4A-NA	2.54	128.06	124.40
16	s	524	BCR	C11-C10-C9	-2.54	123.72	127.28
13	f	1203	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
20	6	822	SQD	C45-O47-C7	2.54	122.33	117.85
13	B	1212	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
13	c	505	CLA	CHB-C4A-NA	2.54	128.06	124.40
20	V	5216	SQD	O48-C23-C24	2.54	119.57	111.83
16	a	522	BCR	C16-C17-C18	-2.54	123.72	127.28
13	a	516	CLA	CAC-C3C-C2C	-2.54	122.90	127.56
13	B	1222	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
13	d	513	CLA	CHB-C4A-NA	2.54	128.06	124.40
20	n	5216	SQD	O48-C23-C24	2.54	119.57	111.83
13	2	505	CLA	CHB-C4A-NA	2.54	128.06	124.40
13	H	1234	CLA	CHB-C4A-NA	2.54	128.06	124.40
13	4	511	CLA	C3B-C4B-NB	-2.54	108.27	110.53
20	v	822	SQD	C45-O47-C7	2.53	122.32	117.85
13	H	1238	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
13	B	1225	CLA	CHB-C4A-NA	2.53	128.06	124.40
13	e	1134	CLA	O2D-CGD-CBD	2.53	115.66	111.23
16	e	4003	BCR	C38-C26-C25	-2.53	121.72	124.48
13	G	1128	CLA	CMB-C2B-C3B	2.53	132.51	126.55
13	q	516	CLA	CAC-C3C-C2C	-2.53	122.91	127.56
13	m	1401	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	f	1852	SQD	O8-S-C6	2.53	110.86	105.97
13	t	509	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
13	H	1235	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	3	516	CLA	CAC-C3C-C2C	-2.53	122.91	127.56
13	A	1128	CLA	CMB-C2B-C3B	2.53	132.50	126.55
13	4	512	CLA	CHB-C4A-NA	2.53	128.05	124.40
13	5	505	CLA	CHB-C4A-NA	2.53	128.05	124.40
13	4	509	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
20	t	822	SQD	C44-O6-C1	2.53	119.22	113.80
13	r	505	CLA	CHB-C4A-NA	2.53	128.05	124.40
13	B	1229	CLA	C3B-C4B-NB	-2.53	108.27	110.53
16	f	4017	BCR	C8-C9-C10	-2.53	115.03	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	5220	LHG	O8-C23-C24	2.53	119.55	111.83
13	v	509	CLA	CHB-C4A-NA	2.53	128.05	124.40
16	c	524	BCR	C7-C8-C9	-2.53	122.49	126.23
16	A	4003	BCR	C38-C26-C25	-2.53	121.72	124.48
13	b	512	CLA	CHB-C4A-NA	2.53	128.05	124.40
16	n	4020	BCR	C11-C10-C9	-2.53	123.73	127.28
16	e	4003	BCR	C21-C20-C19	-2.53	115.87	123.20
16	a	522	BCR	C33-C5-C6	-2.53	121.72	124.48
13	Y	518	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
17	e	5009	LHG	O8-C23-C24	2.53	119.54	111.83
13	f	1222	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
13	A	1102	CLA	O2D-CGD-CBD	2.53	115.65	111.23
13	b	509	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
13	r	509	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	e	1102	CLA	O2D-CGD-CBD	2.53	115.65	111.23
17	A	5009	LHG	O8-C23-C24	2.53	119.54	111.83
16	c	524	BCR	C10-C11-C12	-2.53	115.88	123.20
13	A	1134	CLA	O2D-CGD-CBD	2.53	115.65	111.23
13	K	1401	CLA	CHB-C4A-NA	2.53	128.04	124.40
16	e	4007	BCR	C4-C5-C6	-2.53	119.29	122.70
16	s	523	BCR	C28-C27-C26	-2.53	109.55	114.06
16	T	4012	BCR	C2-C1-C6	2.53	114.11	110.44
13	5	516	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	f	1235	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	r	522	BCR	C11-C12-C13	-2.52	119.44	126.36
17	G	5009	LHG	O8-C23-C24	2.52	119.53	111.83
16	2	522	BCR	C11-C12-C13	-2.52	119.44	126.36
20	L	5216	SQD	O48-C23-C24	2.52	119.53	111.83
16	A	4007	BCR	C4-C5-C6	-2.52	119.29	122.70
16	u	523	BCR	C8-C7-C6	-2.52	120.25	127.00
13	H	1212	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
13	e	1104	CLA	C3B-C4B-NB	-2.52	108.28	110.53
17	n	5220	LHG	O8-C23-C24	2.52	119.53	111.83
16	k	4018	BCR	C30-C25-C26	-2.52	119.19	122.64
13	a	505	CLA	CHB-C4A-NA	2.52	128.04	124.40
16	c	522	BCR	C23-C24-C25	-2.52	120.26	127.00
13	B	1236	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	c	512	CLA	CHB-C4A-NA	2.52	128.04	124.40
16	j	4016	BCR	C21-C20-C19	-2.52	115.89	123.20
13	H	1225	CLA	CHB-C4A-NA	2.52	128.04	124.40
13	u	512	CLA	CHB-C4A-NA	2.52	128.04	124.40
13	1	518	CLA	O2A-CGA-O1A	-2.52	117.32	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	5221	LHG	C20-C19-C18	-2.52	101.62	114.37
16	u	524	BCR	C10-C11-C12	-2.52	115.89	123.20
13	H	1203	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
16	R	4016	BCR	C21-C20-C19	-2.52	115.90	123.20
13	1	516	CLA	CAC-C3C-C2C	-2.52	122.93	127.56
16	l	4012	BCR	C2-C1-C6	2.52	114.10	110.44
16	W	4021	BCR	C38-C26-C27	2.52	118.97	113.60
13	G	1119	CLA	CHB-C4A-NA	2.52	128.03	124.40
13	s	516	CLA	CAC-C3C-C2C	-2.52	122.93	127.56
13	e	1101	CLA	CHB-C4A-NA	2.52	128.03	124.40
20	H	1852	SQD	C26-C25-C24	-2.52	103.88	113.13
16	A	4003	BCR	C21-C20-C19	-2.52	115.91	123.20
13	1	513	CLA	C3B-C4B-NB	-2.52	108.28	110.53
20	B	1852	SQD	C26-C25-C24	-2.52	103.88	113.13
13	v	508	CLA	CHB-C4A-NA	2.52	128.03	124.40
13	A	1120	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
13	G	1134	CLA	O2D-CGD-CBD	2.52	115.63	111.23
13	q	513	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	5	524	BCR	C10-C11-C12	-2.52	115.91	123.20
13	G	1102	CLA	O2D-CGD-CBD	2.52	115.63	111.23
16	3	522	BCR	C38-C26-C25	-2.52	121.74	124.48
17	L	5221	LHG	C20-C19-C18	-2.52	101.65	114.37
13	q	505	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	f	5002	LMG	O1-C1-C2	-2.52	104.45	108.27
16	Z	522	BCR	C11-C12-C13	-2.51	119.47	126.36
17	n	5221	LHG	C20-C19-C18	-2.51	101.66	114.37
13	B	1211	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
16	F	4016	BCR	C21-C20-C19	-2.51	115.92	123.20
13	1	511	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
20	f	1852	SQD	C26-C25-C24	-2.51	103.89	113.13
13	Y	516	CLA	CAC-C3C-C2C	-2.51	122.94	127.56
13	6	508	CLA	CHB-C4A-NA	2.51	128.03	124.40
16	3	523	BCR	C28-C27-C26	-2.51	109.57	114.06
13	q	511	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
13	B	1240	CLA	CHB-C4A-NA	2.51	128.03	124.40
16	G	4003	BCR	C21-C20-C19	-2.51	115.92	123.20
16	5	523	BCR	C8-C7-C6	-2.51	120.29	127.00
16	3	522	BCR	C33-C5-C6	-2.51	121.74	124.48
13	6	513	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	q	510	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	t	512	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	e	1114	CLA	CMB-C2B-C1B	-2.51	121.60	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	d	822	SQD	C4-C3-C2	2.51	115.24	110.83
13	B	1231	CLA	CMA-C3A-C2A	-2.51	104.28	113.98
16	c	523	BCR	C8-C7-C6	-2.51	120.29	127.00
13	2	518	CLA	C3B-C4B-NB	-2.51	108.29	110.53
13	6	511	CLA	C3B-C4B-NB	-2.51	108.29	110.53
13	G	1122	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	M	4021	BCR	C38-C26-C27	2.51	118.95	113.60
13	f	1211	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
13	f	1231	CLA	CMA-C3A-C2A	-2.51	104.29	113.98
19	B	5002	LMG	O1-C1-C2	-2.51	104.47	108.27
13	G	1120	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
13	q	516	CLA	C3B-C4B-NB	-2.51	108.29	110.53
17	A	5005	LHG	O8-C23-C24	2.51	119.48	111.83
19	T	5104	LMG	O1-C1-C2	-2.51	104.47	108.27
13	Y	513	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	J	4012	BCR	C2-C1-C6	2.51	114.08	110.44
16	4	521	BCR	C29-C30-C25	2.51	114.08	110.44
13	H	1240	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	e	1801	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	q	507	CLA	C2A-C1A-CHA	2.51	128.22	123.87
13	H	1222	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
20	6	822	SQD	C4-C3-C2	2.50	115.23	110.83
16	b	521	BCR	C29-C30-C25	2.50	114.08	110.44
17	G	5005	LHG	O8-C23-C24	2.50	119.47	111.83
17	n	5221	LHG	C27-C26-C25	-2.50	101.71	114.37
16	m	4104	BCR	C28-C27-C26	-2.50	109.59	114.06
16	r	524	BCR	C37-C22-C23	2.50	121.91	118.09
13	6	501	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	d	501	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	e	1120	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
13	H	1211	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
17	L	5221	LHG	C27-C26-C25	-2.50	101.72	114.37
19	H	5002	LMG	O1-C1-C2	-2.50	104.47	108.27
20	v	822	SQD	C4-C3-C2	2.50	115.22	110.83
16	d	521	BCR	C20-C19-C18	-2.50	119.50	126.36
13	A	1114	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	1	510	CLA	CHB-C4A-NA	2.50	128.01	124.40
16	G	4007	BCR	C4-C5-C6	-2.50	119.32	122.70
19	J	5104	LMG	O1-C1-C2	-2.50	104.47	108.27
13	q	518	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
16	M	4021	BCR	C33-C5-C6	-2.50	121.75	124.48
13	f	1229	CLA	C3B-C4B-NB	-2.50	108.30	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	505	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	v	513	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	t	508	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	H	1231	CLA	CMA-C3A-C2A	-2.50	104.32	113.98
13	f	1220	CLA	C3B-C4B-NB	-2.50	108.30	110.53
17	e	5005	LHG	O8-C23-C24	2.50	119.45	111.83
17	V	5221	LHG	C27-C26-C25	-2.50	101.74	114.37
16	6	521	BCR	C20-C19-C18	-2.50	119.51	126.36
16	5	524	BCR	C7-C8-C9	-2.50	122.54	126.23
16	s	522	BCR	C33-C5-C6	-2.50	121.76	124.48
13	A	1120	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	v	508	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	q	519	CLA	CHB-C4A-NA	2.50	128.00	124.40
16	o	4021	BCR	C38-C26-C27	2.50	118.92	113.60
13	f	1228	CLA	C1-C2-C3	-2.50	122.11	126.20
13	5	512	CLA	CHB-C4A-NA	2.50	128.00	124.40
13	e	1114	CLA	CHB-C4A-NA	2.50	128.00	124.40
16	d	524	BCR	C38-C26-C25	-2.50	121.76	124.48
13	2	506	CLA	CHB-C4A-NA	2.50	128.00	124.40
16	o	4021	BCR	C33-C5-C6	-2.50	121.76	124.48
13	1	505	CLA	CHB-C4A-NA	2.50	128.00	124.40
13	f	1240	CLA	CHB-C4A-NA	2.50	128.00	124.40
16	a	523	BCR	C28-C27-C26	-2.49	109.61	114.06
13	H	1217	CLA	O2D-CGD-CBD	2.49	115.59	111.23
16	A	4007	BCR	C2-C1-C6	2.49	114.06	110.44
16	e	4007	BCR	C2-C1-C6	2.49	114.06	110.44
13	B	1217	CLA	O2D-CGD-CBD	2.49	115.59	111.23
13	Y	516	CLA	C3B-C4B-NB	-2.49	108.30	110.53
16	l	4013	BCR	C29-C30-C25	2.49	114.06	110.44
20	6	822	SQD	O5-C5-C4	2.49	114.19	109.70
13	Y	505	CLA	CHB-C4A-NA	2.49	128.00	124.40
13	d	508	CLA	CHB-C4A-NA	2.49	128.00	124.40
13	s	505	CLA	CHB-C4A-NA	2.49	128.00	124.40
13	H	1228	CLA	C1-C2-C3	-2.49	122.11	126.20
13	B	1220	CLA	C3B-C4B-NB	-2.49	108.31	110.53
16	r	522	BCR	C1-C6-C5	-2.49	119.23	122.64
13	H	1216	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
13	B	1228	CLA	C1-C2-C3	-2.49	122.11	126.20
16	V	4019	BCR	C38-C26-C25	-2.49	121.77	124.48
13	d	508	CLA	C3B-C4B-NB	-2.49	108.31	110.53
13	f	1216	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
13	G	1114	CLA	CHB-C4A-NA	2.49	128.00	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1114	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
13	1	507	CLA	C2A-C1A-CHA	2.49	128.19	123.87
19	l	5104	LMG	O1-C1-C2	-2.49	104.49	108.27
13	1	516	CLA	C3B-C4B-NB	-2.49	108.31	110.53
13	e	1122	CLA	C3B-C4B-NB	-2.49	108.31	110.53
13	v	511	CLA	C3B-C4B-NB	-2.49	108.31	110.53
16	t	521	BCR	C29-C30-C25	2.49	114.06	110.44
13	u	516	CLA	C3B-C4B-NB	-2.49	108.31	110.53
13	r	506	CLA	CHB-C4A-NA	2.49	127.99	124.40
13	6	509	CLA	CHB-C4A-NA	2.49	127.99	124.40
16	n	4020	BCR	C31-C1-C6	-2.49	106.34	110.24
13	4	508	CLA	CHB-C4A-NA	2.49	127.99	124.40
16	u	524	BCR	C7-C8-C9	-2.49	122.56	126.23
13	e	1114	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
13	G	1801	CLA	CHB-C4A-NA	2.49	127.99	124.40
13	A	1104	CLA	C3B-C4B-NB	-2.49	108.31	110.53
13	f	1217	CLA	O2D-CGD-CBD	2.49	115.58	111.23
16	2	522	BCR	C3-C4-C5	-2.49	109.62	114.06
16	G	4007	BCR	C2-C1-C6	2.49	114.05	110.44
13	A	1123	CLA	C2A-C1A-CHA	2.49	128.18	123.87
13	r	507	CLA	C3B-C4B-NB	-2.49	108.31	110.53
16	A	4003	BCR	C24-C23-C22	-2.49	122.56	126.23
13	d	509	CLA	CHB-C4A-NA	2.48	127.99	124.40
13	Y	507	CLA	C2A-C1A-CHA	2.48	128.18	123.87
13	G	1120	CLA	C3B-C4B-NB	-2.48	108.31	110.53
13	H	1239	CLA	CAC-C3C-C4C	-2.48	121.56	124.79
20	V	5216	SQD	O5-C5-C4	2.48	114.17	109.70
16	G	4003	BCR	C38-C26-C25	-2.48	121.77	124.48
13	b	508	CLA	CHB-C4A-NA	2.48	127.98	124.40
13	f	1236	CLA	C3B-C4B-NB	-2.48	108.31	110.53
13	H	1234	CLA	CBA-CAA-C2A	-2.48	106.40	113.79
16	v	521	BCR	C20-C19-C18	-2.48	119.55	126.36
16	L	4020	BCR	C31-C1-C6	-2.48	106.35	110.24
20	d	822	SQD	O5-C5-C4	2.48	114.17	109.70
16	W	4021	BCR	C33-C5-C6	-2.48	121.78	124.48
16	n	4019	BCR	C38-C26-C25	-2.48	121.78	124.48
13	A	1801	CLA	CHB-C4A-NA	2.48	127.98	124.40
13	A	1114	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
13	Z	507	CLA	C3B-C4B-NB	-2.48	108.31	110.53
13	r	503	CLA	C3B-C4B-NB	-2.48	108.31	110.53
16	K	4104	BCR	C28-C27-C26	-2.48	109.63	114.06
13	f	1234	CLA	CBA-CAA-C2A	-2.48	106.41	113.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	6	524	BCR	C38-C26-C25	-2.48	121.78	124.48
20	v	822	SQD	C44-O6-C1	2.48	119.11	113.80
16	L	4019	BCR	C38-C26-C25	-2.48	121.78	124.48
13	e	1123	CLA	C2A-C1A-CHA	2.48	128.17	123.87
16	4	523	BCR	C21-C20-C19	-2.48	116.02	123.20
13	d	505	CLA	CHB-C4A-NA	2.48	127.98	124.40
13	u	507	CLA	C2A-C1A-CHA	2.48	128.17	123.87
16	U	4104	BCR	C10-C11-C12	-2.48	116.02	123.20
13	A	1111	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
16	Z	522	BCR	C3-C4-C5	-2.48	109.64	114.06
13	B	1216	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
20	d	822	SQD	C44-O6-C1	2.48	119.11	113.80
13	Y	510	CLA	CHB-C4A-NA	2.48	127.97	124.40
20	L	5216	SQD	O5-C5-C4	2.48	114.16	109.70
13	H	1231	CLA	CMB-C2B-C3B	2.48	132.37	126.55
16	G	4003	BCR	C24-C23-C22	-2.48	122.57	126.23
13	Z	506	CLA	CHB-C4A-NA	2.48	127.97	124.40
20	3	822	SQD	C44-O6-C1	2.48	119.10	113.80
16	V	4020	BCR	C31-C1-C6	-2.48	106.36	110.24
16	2	522	BCR	C1-C6-C5	-2.48	119.25	122.64
16	G	4007	BCR	C30-C25-C26	-2.48	119.25	122.64
16	e	4007	BCR	C30-C25-C26	-2.48	119.25	122.64
13	B	1239	CLA	CAC-C3C-C4C	-2.47	121.57	124.79
13	B	1234	CLA	CBA-CAA-C2A	-2.47	106.43	113.79
13	G	1114	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
13	B	1231	CLA	CMB-C2B-C3B	2.47	132.37	126.55
16	t	524	BCR	C1-C6-C7	2.47	122.36	115.65
17	A	5003	LHG	C20-C19-C18	-2.47	101.87	114.37
13	1	512	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	6	822	SQD	C44-O6-C1	2.47	119.10	113.80
20	s	822	SQD	C44-O6-C1	2.47	119.10	113.80
17	G	5003	LHG	C20-C19-C18	-2.47	101.87	114.37
13	s	504	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
17	e	5003	LHG	C20-C19-C18	-2.47	101.87	114.37
13	c	517	CLA	C3B-C4B-NB	-2.47	108.32	110.53
16	U	4104	BCR	C28-C27-C26	-2.47	109.65	114.06
13	q	506	CLA	CMB-C2B-C3B	2.47	132.36	126.55
13	2	519	CLA	CHB-C4A-NA	2.47	127.97	124.40
13	v	505	CLA	CHB-C4A-NA	2.47	127.97	124.40
13	G	1123	CLA	C2A-C1A-CHA	2.47	128.16	123.87
16	b	523	BCR	C21-C20-C19	-2.47	116.04	123.20
13	6	508	CLA	C3B-C4B-NB	-2.47	108.32	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	d	511	CLA	C3B-C4B-NB	-2.47	108.32	110.53
16	K	4104	BCR	C10-C11-C12	-2.47	116.04	123.20
13	H	1213	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
16	4	524	BCR	C1-C6-C7	2.47	122.35	115.65
16	T	4013	BCR	C29-C30-C25	2.47	114.03	110.44
13	G	1111	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
13	Z	501	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
13	1	519	CLA	CHB-C4A-NA	2.47	127.96	124.40
16	v	524	BCR	C38-C26-C25	-2.47	121.79	124.48
13	Z	518	CLA	C3B-C4B-NB	-2.47	108.33	110.53
13	e	1124	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
13	2	503	CLA	C3B-C4B-NB	-2.47	108.33	110.53
13	G	1114	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
20	n	5216	SQD	O5-C5-C4	2.47	114.14	109.70
16	e	4003	BCR	C24-C23-C22	-2.47	122.58	126.23
13	A	1123	CLA	CMB-C2B-C3B	2.47	132.35	126.55
13	R	1301	CLA	CHB-C4A-NA	2.47	127.96	124.40
13	G	1123	CLA	CMB-C2B-C3B	2.47	132.35	126.55
13	q	512	CLA	CHB-C4A-NA	2.47	127.96	124.40
20	v	822	SQD	O5-C5-C4	2.47	114.14	109.70
13	f	1204	CLA	C3B-C4B-NB	-2.47	108.33	110.53
16	t	523	BCR	C21-C20-C19	-2.47	116.06	123.20
13	e	1105	CLA	CMB-C2B-C3B	2.47	132.35	126.55
16	n	4020	BCR	C21-C20-C19	-2.46	116.06	123.20
17	V	5220	LHG	C11-C10-C9	-2.46	101.91	114.37
13	B	1213	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
13	5	508	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
13	f	1213	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
16	f	4006	BCR	C1-C6-C5	-2.46	119.27	122.64
13	5	517	CLA	C3B-C4B-NB	-2.46	108.33	110.53
13	v	501	CLA	C3B-C4B-NB	-2.46	108.33	110.53
13	r	501	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
13	Y	512	CLA	CHB-C4A-NA	2.46	127.95	124.40
13	e	1123	CLA	CMB-C2B-C3B	2.46	132.34	126.55
13	f	1226	CLA	C3B-C2B-C1B	2.46	110.07	107.17
13	e	1117	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
13	6	505	CLA	CHB-C4A-NA	2.46	127.95	124.40
16	H	4006	BCR	C1-C6-C5	-2.46	119.27	122.64
13	c	507	CLA	C2A-C1A-CHA	2.46	128.14	123.87
16	2	524	BCR	C37-C22-C23	2.46	121.85	118.09
13	2	501	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
17	L	5220	LHG	C11-C10-C9	-2.46	101.93	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1111	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
13	1	506	CLA	CMB-C2B-C3B	2.46	132.34	126.55
16	B	4006	BCR	C1-C6-C5	-2.46	119.27	122.64
13	Z	519	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	e	2001	PQN	C2M-C2-C3	-2.46	120.41	124.45
16	J	4013	BCR	C29-C30-C25	2.46	114.01	110.44
14	A	2001	PQN	C2M-C2-C3	-2.46	120.41	124.45
20	a	822	SQD	C44-O6-C1	2.46	119.07	113.80
13	A	1117	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
13	A	1124	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
13	A	1105	CLA	CMB-C2B-C3B	2.46	132.33	126.55
16	m	4104	BCR	C10-C11-C12	-2.46	116.08	123.20
16	4	522	BCR	C36-C18-C19	2.46	121.84	118.09
16	b	522	BCR	C36-C18-C19	2.46	121.84	118.09
17	n	5220	LHG	C11-C10-C9	-2.46	101.94	114.37
13	B	1211	CLA	CMB-C2B-C3B	2.46	132.33	126.55
13	G	1105	CLA	CMB-C2B-C3B	2.46	132.33	126.55
13	u	508	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
17	G	5009	LHG	C11-C10-C9	-2.46	101.95	114.37
13	G	1117	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
16	A	4007	BCR	C38-C26-C27	2.46	118.83	113.60
13	f	1211	CLA	CMB-C2B-C3B	2.46	132.33	126.55
16	b	524	BCR	C1-C6-C7	2.46	122.31	115.65
13	H	1226	CLA	C3B-C2B-C1B	2.46	110.06	107.17
16	b	524	BCR	C3-C4-C5	-2.45	109.68	114.06
13	H	1211	CLA	CMB-C2B-C3B	2.45	132.32	126.55
13	Y	506	CLA	CMB-C2B-C3B	2.45	132.32	126.55
13	f	1231	CLA	CMB-C2B-C3B	2.45	132.32	126.55
13	3	506	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	e	4007	BCR	C38-C26-C27	2.45	118.83	113.60
16	A	4007	BCR	C30-C25-C26	-2.45	119.28	122.64
16	V	4020	BCR	C21-C20-C19	-2.45	116.09	123.20
17	A	5009	LHG	C11-C10-C9	-2.45	101.97	114.37
13	e	1134	CLA	CHB-C4A-NA	2.45	127.94	124.40
13	f	1239	CLA	CAC-C3C-C4C	-2.45	121.60	124.79
13	s	506	CLA	CHB-C4A-NA	2.45	127.94	124.40
13	U	1105	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	t	521	BCR	C33-C5-C6	-2.45	121.81	124.48
13	B	1226	CLA	C3B-C2B-C1B	2.45	110.06	107.17
13	G	1104	CLA	C3B-C4B-NB	-2.45	108.34	110.53
13	A	1134	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	n	4022	BCR	C29-C30-C25	2.45	114.00	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1215	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	r	522	BCR	C3-C4-C5	-2.45	109.69	114.06
13	G	1134	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	L	4020	BCR	C21-C20-C19	-2.45	116.10	123.20
16	4	521	BCR	C33-C5-C6	-2.45	121.81	124.48
16	b	521	BCR	C33-C5-C6	-2.45	121.81	124.48
13	5	507	CLA	C2A-C1A-CHA	2.45	128.12	123.87
13	5	509	CLA	CMB-C2B-C3B	2.45	132.31	126.55
13	3	504	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
16	t	522	BCR	C36-C18-C19	2.45	121.83	118.09
13	r	519	CLA	CHB-C4A-NA	2.45	127.93	124.40
13	3	502	CLA	C3B-C4B-NB	-2.45	108.35	110.53
13	4	517	CLA	C3B-C4B-NB	-2.45	108.35	110.53
13	Z	503	CLA	C3B-C4B-NB	-2.45	108.35	110.53
14	G	2001	PQN	C2M-C2-C3	-2.45	120.43	124.45
16	Z	522	BCR	C38-C26-C25	-2.45	121.81	124.48
13	a	504	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
16	G	4007	BCR	C38-C26-C27	2.45	118.81	113.60
13	a	506	CLA	CHB-C4A-NA	2.45	127.93	124.40
13	G	1801	CLA	CMB-C2B-C3B	2.45	132.30	126.55
16	B	4006	BCR	C37-C22-C21	-2.44	118.86	122.82
13	Y	519	CLA	CHB-C4A-NA	2.44	127.93	124.40
13	s	508	CLA	CHB-C4A-NA	2.44	127.93	124.40
13	B	1222	CLA	CMB-C2B-C3B	2.44	132.30	126.55
16	H	4006	BCR	C37-C22-C21	-2.44	118.86	122.82
17	e	5009	LHG	C11-C10-C9	-2.44	102.01	114.37
13	3	508	CLA	CHB-C4A-NA	2.44	127.93	124.40
13	G	1124	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
13	c	509	CLA	CMB-C2B-C3B	2.44	132.30	126.55
13	u	509	CLA	CMB-C2B-C3B	2.44	132.30	126.55
13	K	1105	CLA	CHB-C4A-NA	2.44	127.92	124.40
16	Z	522	BCR	C1-C6-C5	-2.44	119.30	122.64
13	A	1801	CLA	CMB-C2B-C3B	2.44	132.29	126.55
16	V	4022	BCR	C29-C30-C25	2.44	113.99	110.44
16	2	522	BCR	C38-C26-C25	-2.44	121.82	124.48
13	c	508	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
16	Z	524	BCR	C37-C22-C23	2.44	121.82	118.09
16	T	4013	BCR	C10-C11-C12	-2.44	116.13	123.20
13	f	1222	CLA	CMB-C2B-C3B	2.44	132.29	126.55
16	r	522	BCR	C38-C26-C25	-2.44	121.82	124.48
13	d	512	CLA	CHB-C4A-NA	2.44	127.92	124.40
13	a	509	CLA	C3B-C4B-NB	-2.44	108.35	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4022	BCR	C29-C30-C25	2.44	113.98	110.44
13	H	1210	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
13	b	503	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
16	Y	522	BCR	C15-C16-C17	-2.44	118.53	123.52
17	e	5006	LHG	O8-C23-C24	2.44	119.26	111.83
13	6	510	CLA	CHB-C4A-NA	2.44	127.92	124.40
16	1	523	BCR	C34-C9-C8	2.44	121.81	118.09
17	L	5218	LHG	C11-C10-C9	-2.44	102.06	114.37
16	1	522	BCR	C15-C16-C17	-2.43	118.54	123.52
16	t	524	BCR	C3-C4-C5	-2.43	109.71	114.06
13	B	1204	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	Y	523	BCR	C34-C9-C8	2.43	121.81	118.09
13	A	1013	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	f	1215	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	e	1129	CLA	O2D-CGD-CBD	2.43	115.48	111.23
16	J	4013	BCR	C10-C11-C12	-2.43	116.15	123.20
16	Z	523	BCR	C10-C11-C12	-2.43	116.15	123.20
16	l	4013	BCR	C10-C11-C12	-2.43	116.15	123.20
13	a	508	CLA	CHB-C4A-NA	2.43	127.91	124.40
17	A	5006	LHG	O8-C23-C24	2.43	119.25	111.83
13	F	1301	CLA	CHB-C4A-NA	2.43	127.91	124.40
17	H	1842	LHG	C11-C10-C9	-2.43	102.08	114.37
13	a	502	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	4	524	BCR	C3-C4-C5	-2.43	109.72	114.06
17	n	5218	LHG	C11-C10-C9	-2.43	102.08	114.37
13	G	1129	CLA	O2D-CGD-CBD	2.43	115.48	111.23
13	d	510	CLA	CHB-C4A-NA	2.43	127.91	124.40
16	Z	524	BCR	C20-C21-C22	-2.43	123.87	127.28
13	4	503	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
17	V	5218	LHG	C11-C10-C9	-2.43	102.09	114.37
13	A	1132	CLA	CHB-C4A-NA	2.43	127.91	124.40
13	G	1119	CLA	CHB-C1B-NB	2.43	127.69	124.05
13	a	505	CLA	C3B-C4B-NB	-2.43	108.36	110.53
17	B	1842	LHG	C11-C10-C9	-2.43	102.09	114.37
13	H	1222	CLA	CMB-C2B-C3B	2.43	132.26	126.55
13	A	1129	CLA	O2D-CGD-CBD	2.43	115.47	111.23
13	e	1801	CLA	CMB-C2B-C3B	2.43	132.26	126.55
13	f	1210	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
13	b	509	CLA	C2A-C1A-CHA	2.43	128.08	123.87
13	3	509	CLA	C3B-C4B-NB	-2.43	108.36	110.53
17	f	1842	LHG	C11-C10-C9	-2.43	102.10	114.37
13	B	1210	CLA	CAA-C2A-C3A	-2.43	106.44	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1013	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	H	1239	CLA	CMC-C2C-C3C	2.43	132.71	126.15
16	e	4011	BCR	C15-C16-C17	-2.42	118.56	123.52
13	H	1223	CLA	C3B-C4B-NB	-2.42	108.37	110.53
16	d	522	BCR	C30-C25-C26	-2.42	119.32	122.64
16	T	4015	BCR	C21-C20-C19	-2.42	116.18	123.20
16	3	523	BCR	C8-C7-C6	-2.42	120.53	127.00
13	B	1215	CLA	C3B-C4B-NB	-2.42	108.37	110.53
13	2	519	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
13	c	517	CLA	CHB-C4A-NA	2.42	127.90	124.40
13	5	517	CLA	CHB-C4A-NA	2.42	127.89	124.40
17	S	5001	LHG	C11-C10-C9	-2.42	102.13	114.37
16	2	524	BCR	C20-C21-C22	-2.42	123.88	127.28
13	2	507	CLA	C3B-C4B-NB	-2.42	108.37	110.53
16	q	522	BCR	C15-C16-C17	-2.42	118.57	123.52
13	1	501	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
16	s	523	BCR	C8-C7-C6	-2.42	120.53	127.00
16	a	523	BCR	C8-C7-C6	-2.42	120.53	127.00
16	R	4016	BCR	C33-C5-C6	-2.42	121.84	124.48
16	2	523	BCR	C10-C11-C12	-2.42	116.19	123.20
16	G	4002	BCR	C10-C11-C12	-2.42	116.19	123.20
17	k	5001	LHG	C11-C10-C9	-2.42	102.14	114.37
13	e	1107	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
13	r	519	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
13	e	1130	CLA	CMB-C2B-C3B	2.42	132.24	126.55
16	A	4008	BCR	C34-C9-C8	2.42	121.78	118.09
13	e	1125	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
13	H	1235	CLA	O2D-CGD-CBD	2.42	115.46	111.23
16	r	523	BCR	C10-C11-C12	-2.42	116.19	123.20
17	I	5001	LHG	C11-C10-C9	-2.42	102.15	114.37
13	Y	501	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
13	u	517	CLA	C3B-C4B-NB	-2.42	108.37	110.53
13	q	501	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
13	B	1239	CLA	CMC-C2C-C3C	2.42	132.68	126.15
13	Z	519	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
13	v	510	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	b	517	CLA	C3B-C4B-NB	-2.42	108.37	110.53
20	5	822	SQD	C4-C3-C2	2.41	115.07	110.83
13	Z	508	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	F	4016	BCR	C33-C5-C6	-2.41	121.85	124.48
13	4	509	CLA	C2A-C1A-CHA	2.41	128.06	123.87
17	e	5004	LHG	C11-C10-C9	-2.41	102.17	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	5006	LHG	O8-C23-C24	2.41	119.19	111.83
13	A	1119	CLA	CHB-C1B-NB	2.41	127.67	124.05
17	G	5004	LHG	C11-C10-C9	-2.41	102.17	114.37
13	s	502	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	q	523	BCR	C34-C9-C8	2.41	121.77	118.09
13	t	503	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
13	e	1132	CLA	CHB-C4A-NA	2.41	127.88	124.40
13	u	517	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	A	5004	LHG	C11-C10-C9	-2.41	102.18	114.37
16	H	4009	BCR	C37-C22-C23	2.41	121.77	118.09
16	l	4015	BCR	C21-C20-C19	-2.41	116.21	123.20
16	f	4006	BCR	C37-C22-C21	-2.41	118.91	122.82
16	e	4008	BCR	C34-C9-C8	2.41	121.77	118.09
13	t	509	CLA	C2A-C1A-CHA	2.41	128.05	123.87
13	G	1125	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
16	q	523	BCR	C20-C21-C22	-2.41	123.90	127.28
13	G	1107	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
13	Z	518	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
16	J	4015	BCR	C21-C20-C19	-2.41	116.22	123.20
13	f	1239	CLA	CMC-C2C-C3C	2.41	132.67	126.15
13	t	507	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	Y	522	BCR	C16-C17-C18	-2.41	123.90	127.28
20	r	822	SQD	O48-C23-C24	2.41	119.18	111.83
16	Y	522	BCR	C30-C25-C26	-2.41	119.34	122.64
13	e	1013	CLA	C3B-C4B-NB	-2.41	108.38	110.53
20	2	822	SQD	O48-C23-C24	2.41	119.18	111.83
13	v	512	CLA	CHB-C4A-NA	2.41	127.88	124.40
16	1	522	BCR	C30-C25-C26	-2.41	119.35	122.64
13	3	505	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	t	517	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	6	512	CLA	CHB-C4A-NA	2.41	127.87	124.40
13	G	1130	CLA	CMB-C2B-C3B	2.41	132.21	126.55
13	H	1202	CLA	O2D-CGD-CBD	2.41	115.44	111.23
20	u	822	SQD	C4-C3-C2	2.41	115.05	110.83
16	A	4002	BCR	C10-C11-C12	-2.41	116.23	123.20
16	B	4009	BCR	C37-C22-C23	2.41	121.76	118.09
13	m	1105	CLA	CHB-C4A-NA	2.40	127.87	124.40
20	Z	822	SQD	O48-C23-C24	2.40	119.17	111.83
13	v	503	CLA	C3B-C4B-NB	-2.40	108.38	110.53
16	f	4009	BCR	C36-C18-C19	2.40	121.76	118.09
20	a	822	SQD	C4-C3-C2	2.40	115.05	110.83
13	A	1107	CLA	O2A-CGA-O1A	-2.40	117.62	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	522	BCR	C30-C25-C26	-2.40	119.35	122.64
13	r	518	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
17	A	5007	LHG	C11-C10-C9	-2.40	102.22	114.37
13	B	1202	CLA	O2D-CGD-CBD	2.40	115.43	111.23
13	B	1223	CLA	C3B-C4B-NB	-2.40	108.39	110.53
20	s	822	SQD	C4-C3-C2	2.40	115.04	110.83
16	G	4008	BCR	C34-C9-C8	2.40	121.75	118.09
13	G	1132	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	f	1236	CLA	CHB-C4A-NA	2.40	127.86	124.40
16	r	524	BCR	C20-C21-C22	-2.40	123.91	127.28
19	T	5104	LMG	O2-C2-C1	-2.40	104.36	110.08
20	3	822	SQD	C4-C3-C2	2.40	115.04	110.83
17	G	5007	LHG	C11-C10-C9	-2.40	102.24	114.37
16	f	4010	BCR	C36-C18-C19	2.40	121.75	118.09
13	K	1103	CLA	C3B-C4B-NB	-2.40	108.39	110.53
13	2	508	CLA	C3B-C4B-NB	-2.40	108.39	110.53
13	s	509	CLA	C3B-C4B-NB	-2.40	108.39	110.53
13	f	1236	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
16	A	4011	BCR	C15-C16-C17	-2.40	118.61	123.52
13	d	504	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
17	e	5007	LHG	C11-C10-C9	-2.40	102.24	114.37
13	f	1235	CLA	O2D-CGD-CBD	2.40	115.42	111.23
16	G	4011	BCR	C15-C16-C17	-2.40	118.61	123.52
13	e	1140	CLA	CBA-CAA-C2A	2.40	120.93	113.79
16	r	522	BCR	C15-C16-C17	-2.40	118.61	123.52
13	A	1130	CLA	CMB-C2B-C3B	2.40	132.19	126.55
16	c	524	BCR	C21-C20-C19	-2.40	116.26	123.20
16	u	524	BCR	C21-C20-C19	-2.40	116.26	123.20
13	A	1124	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	j	1301	CLA	CHB-C4A-NA	2.40	127.86	124.40
16	H	4009	BCR	C36-C18-C19	2.40	121.75	118.09
16	f	4010	BCR	C4-C5-C6	-2.40	119.47	122.70
13	A	1140	CLA	CBA-CAA-C2A	2.39	120.92	113.79
16	Z	522	BCR	C15-C16-C17	-2.39	118.62	123.52
13	H	1238	CLA	CHB-C4A-NA	2.39	127.86	124.40
16	f	4009	BCR	C37-C22-C23	2.39	121.75	118.09
13	f	1202	CLA	C3B-C4B-NB	-2.39	108.39	110.53
13	A	1125	CLA	CMB-C2B-C1B	-2.39	121.77	125.42
16	H	4010	BCR	C4-C5-C6	-2.39	119.47	122.70
13	B	1235	CLA	O2D-CGD-CBD	2.39	115.41	111.23
16	B	4009	BCR	C36-C18-C19	2.39	121.74	118.09
16	4	523	BCR	C10-C11-C12	-2.39	116.27	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	508	CLA	C3B-C4B-NB	-2.39	108.39	110.53
16	V	4219	BCR	C20-C21-C22	-2.39	123.92	127.28
13	G	1107	CLA	CHB-C4A-NA	2.39	127.85	124.40
20	c	822	SQD	C4-C3-C2	2.39	115.03	110.83
16	6	522	BCR	C30-C25-C26	-2.39	119.37	122.64
16	B	4010	BCR	C4-C5-C6	-2.39	119.47	122.70
13	G	1126	CLA	C2A-C1A-CHA	2.39	128.01	123.87
16	1	522	BCR	C16-C17-C18	-2.39	123.93	127.28
13	H	1204	CLA	C3B-C4B-NB	-2.39	108.40	110.53
13	s	508	CLA	C3B-C4B-NB	-2.39	108.40	110.53
16	e	4002	BCR	C10-C11-C12	-2.39	116.28	123.20
13	A	1118	CLA	O2D-CGD-CBD	2.39	115.41	111.23
16	t	523	BCR	C10-C11-C12	-2.39	116.28	123.20
13	2	518	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
13	B	1236	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
13	b	503	CLA	C3B-C4B-NB	-2.39	108.40	110.53
16	5	524	BCR	C21-C20-C19	-2.39	116.28	123.20
16	H	4010	BCR	C23-C24-C25	-2.39	120.62	127.00
13	A	1126	CLA	C2A-C1A-CHA	2.39	128.01	123.87
13	e	1801	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
13	G	1118	CLA	O2D-CGD-CBD	2.39	115.40	111.23
16	e	4003	BCR	C10-C11-C12	-2.39	116.28	123.20
16	f	4010	BCR	C23-C24-C25	-2.39	120.62	127.00
19	J	5104	LMG	O2-C2-C1	-2.39	104.39	110.08
13	H	1236	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
13	B	1221	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
13	4	507	CLA	C3B-C4B-NB	-2.38	108.40	110.53
16	j	4016	BCR	C33-C5-C6	-2.38	121.88	124.48
13	G	1140	CLA	CBA-CAA-C2A	2.38	120.89	113.79
13	b	510	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
16	f	4006	BCR	C3-C4-C5	-2.38	109.80	114.06
16	H	4006	BCR	C21-C20-C19	-2.38	116.29	123.20
13	H	1221	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
13	b	507	CLA	O2D-CGD-CBD	2.38	115.40	111.23
13	G	1130	CLA	C1-C2-C3	-2.38	122.29	126.20
13	B	1236	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	G	1124	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	6	504	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
13	q	516	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	e	1118	CLA	O2D-CGD-CBD	2.38	115.39	111.23
13	f	1202	CLA	O2D-CGD-CBD	2.38	115.39	111.23
13	G	1121	CLA	C1-C2-C3	-2.38	122.30	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	522	BCR	C16-C17-C18	-2.38	123.94	127.28
16	B	4010	BCR	C23-C24-C25	-2.38	120.64	127.00
13	A	1125	CLA	CAA-CBA-CGA	-2.38	106.45	113.21
13	H	1236	CLA	CHB-C4A-NA	2.38	127.83	124.40
13	A	1022	CLA	C4D-C3D-CAD	-2.38	105.52	108.11
16	G	4003	BCR	C10-C11-C12	-2.38	116.30	123.20
16	q	522	BCR	C1-C6-C7	2.38	122.11	115.65
13	b	507	CLA	C3B-C4B-NB	-2.38	108.41	110.53
13	s	505	CLA	C3B-C4B-NB	-2.38	108.41	110.53
13	e	1126	CLA	C2A-C1A-CHA	2.38	128.00	123.87
16	B	4006	BCR	C21-C20-C19	-2.38	116.31	123.20
16	T	4013	BCR	C35-C13-C12	2.38	121.72	118.09
13	t	503	CLA	C3B-C4B-NB	-2.38	108.41	110.53
16	2	522	BCR	C15-C16-C17	-2.38	118.65	123.52
13	A	1121	CLA	C1-C2-C3	-2.38	122.30	126.20
16	b	523	BCR	C10-C11-C12	-2.38	116.31	123.20
13	H	1216	CLA	CHB-C1B-NB	2.38	127.62	124.05
16	d	523	BCR	C33-C5-C4	2.38	118.67	113.60
13	e	1130	CLA	C1-C2-C3	-2.38	122.30	126.20
13	3	508	CLA	C3B-C4B-NB	-2.38	108.41	110.53
13	U	1103	CLA	C3B-C4B-NB	-2.38	108.41	110.53
16	J	4013	BCR	C35-C13-C12	2.38	121.72	118.09
13	e	1022	CLA	C4D-C3D-CAD	-2.38	105.53	108.11
13	A	1130	CLA	C1-C2-C3	-2.38	122.30	126.20
13	B	1202	CLA	C3B-C4B-NB	-2.38	108.41	110.53
13	A	1128	CLA	C3B-C2B-C1B	2.38	109.97	107.17
13	G	1125	CLA	CAA-CBA-CGA	-2.38	106.46	113.21
16	B	4006	BCR	C3-C4-C5	-2.37	109.82	114.06
13	e	1125	CLA	CAA-CBA-CGA	-2.37	106.47	113.21
16	A	4003	BCR	C10-C11-C12	-2.37	116.32	123.20
13	e	1119	CLA	CHB-C1B-NB	2.37	127.61	124.05
16	B	4010	BCR	C36-C18-C19	2.37	121.72	118.09
13	A	1801	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
16	5	522	BCR	C1-C6-C7	2.37	122.09	115.65
13	G	1801	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
13	4	510	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
16	1	522	BCR	C1-C6-C7	2.37	122.09	115.65
16	Y	522	BCR	C1-C6-C7	2.37	122.09	115.65
13	n	1501	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
13	e	1124	CLA	CHB-C4A-NA	2.37	127.82	124.40
13	m	1103	CLA	C3B-C4B-NB	-2.37	108.41	110.53
19	f	5002	LMG	C38-C37-C36	-2.37	102.38	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	507	CLA	O2D-CGD-CBD	2.37	115.38	111.23
13	1	516	CLA	CHB-C4A-NA	2.37	127.82	124.40
16	v	523	BCR	C33-C5-C4	2.37	118.65	113.60
16	H	4006	BCR	C3-C4-C5	-2.37	109.83	114.06
16	L	4219	BCR	C20-C21-C22	-2.37	123.95	127.28
19	B	5002	LMG	C38-C37-C36	-2.37	102.39	114.37
13	1	503	CLA	C3B-C4B-NB	-2.37	108.41	110.53
16	Y	521	BCR	C2-C1-C6	2.37	113.88	110.44
16	e	4003	BCR	C11-C10-C9	-2.37	123.95	127.28
16	Z	524	BCR	C15-C16-C17	-2.37	118.67	123.52
19	l	5104	LMG	O2-C2-C1	-2.37	104.43	110.08
13	f	1234	CLA	CAC-C3C-C4C	2.37	127.87	124.79
13	v	504	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
16	n	4219	BCR	C20-C21-C22	-2.37	123.96	127.28
16	6	523	BCR	C33-C5-C4	2.37	118.64	113.60
13	Z	509	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
13	q	508	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
16	f	4005	BCR	C15-C16-C17	-2.37	118.67	123.52
13	L	1501	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
13	f	1221	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
13	t	510	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
13	A	1128	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
13	6	503	CLA	C3B-C4B-NB	-2.37	108.42	110.53
16	s	524	BCR	C23-C24-C25	-2.37	120.68	127.00
16	H	4004	BCR	C15-C16-C17	-2.37	118.68	123.52
13	B	1238	CLA	CHB-C4A-NA	2.37	127.81	124.40
13	6	516	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
16	3	524	BCR	C23-C24-C25	-2.36	120.68	127.00
13	a	501	CLA	CMB-C2B-C3B	2.36	132.11	126.55
16	u	522	BCR	C1-C6-C7	2.36	122.06	115.65
19	H	5002	LMG	C38-C37-C36	-2.36	102.42	114.37
13	d	516	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
13	f	1238	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
13	e	1128	CLA	C4B-C3B-C2B	-2.36	104.36	107.30
16	2	524	BCR	C15-C16-C17	-2.36	118.68	123.52
16	T	4013	BCR	C7-C8-C9	-2.36	122.74	126.23
13	4	503	CLA	C3B-C4B-NB	-2.36	108.42	110.53
16	s	524	BCR	C34-C9-C8	2.36	121.70	118.09
16	f	4006	BCR	C21-C20-C19	-2.36	116.36	123.20
16	c	522	BCR	C1-C6-C7	2.36	122.06	115.65
13	G	1022	CLA	C4D-C3D-CAD	-2.36	105.54	108.11
16	1	521	BCR	C2-C1-C6	2.36	113.87	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	4219	BCR	C36-C18-C19	2.36	121.69	118.09
13	e	1237	CLA	CHB-C4A-NA	2.36	127.81	124.40
13	H	1238	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
13	2	503	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
16	V	4219	BCR	C36-C18-C19	2.36	121.69	118.09
16	d	522	BCR	C38-C26-C27	2.36	118.63	113.60
16	H	4005	BCR	C15-C16-C17	-2.36	118.69	123.52
16	B	4005	BCR	C15-C16-C17	-2.36	118.69	123.52
13	B	1238	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
16	Y	523	BCR	C20-C21-C22	-2.36	123.97	127.28
13	t	507	CLA	O2D-CGD-CBD	2.36	115.35	111.23
16	B	4004	BCR	C15-C16-C17	-2.36	118.70	123.52
13	A	1107	CLA	CHB-C4A-NA	2.36	127.80	124.40
13	6	501	CLA	C1-C2-C3	-2.36	122.34	126.20
13	e	1117	CLA	C3B-C4B-NB	-2.36	108.43	110.53
16	T	4012	BCR	C1-C6-C7	2.36	122.04	115.65
13	1	508	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
13	r	508	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
16	q	522	BCR	C30-C25-C26	-2.36	119.42	122.64
13	v	516	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
13	e	1121	CLA	C1-C2-C3	-2.35	122.34	126.20
13	H	1202	CLA	C3B-C4B-NB	-2.35	108.43	110.53
13	f	1218	CLA	C3B-C4B-NB	-2.35	108.43	110.53
13	G	1128	CLA	C4B-C3B-C2B	-2.35	104.37	107.30
16	q	521	BCR	C2-C1-C6	2.35	113.86	110.44
13	3	501	CLA	CMB-C2B-C3B	2.35	132.09	126.55
13	e	1113	CLA	CMB-C2B-C3B	2.35	132.09	126.55
13	V	1501	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
13	H	1227	CLA	O2D-CGD-CBD	2.35	115.34	111.23
16	l	4013	BCR	C7-C8-C9	-2.35	122.75	126.23
13	f	1223	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	6	522	BCR	C38-C26-C27	2.35	118.61	113.60
16	v	524	BCR	C21-C20-C19	-2.35	116.38	123.20
13	A	1237	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	A	1113	CLA	CMB-C2B-C3B	2.35	132.09	126.55
16	1	523	BCR	C20-C21-C22	-2.35	123.98	127.28
13	B	1218	CLA	C3B-C4B-NB	-2.35	108.43	110.53
13	r	508	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	L	4219	BCR	C36-C18-C19	2.35	121.68	118.09
13	G	1128	CLA	C3B-C2B-C1B	2.35	109.94	107.17
13	e	1128	CLA	C3B-C2B-C1B	2.35	109.94	107.17
13	d	501	CLA	C1-C2-C3	-2.35	122.34	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	s	822	SQD	C1-O5-C5	2.35	118.31	113.72
13	f	1216	CLA	CHB-C1B-NB	2.35	127.58	124.05
16	v	521	BCR	C33-C5-C6	-2.35	121.92	124.48
13	Y	508	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
13	r	503	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
13	d	503	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	J	4012	BCR	C1-C6-C7	2.35	122.02	115.65
16	H	4010	BCR	C36-C18-C19	2.35	121.68	118.09
16	c	523	BCR	C37-C22-C23	2.35	121.68	118.09
13	2	510	CLA	CMB-C2B-C3B	2.35	132.08	126.55
16	k	4018	BCR	C33-C5-C4	2.35	118.61	113.60
13	q	503	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	W	4021	BCR	C30-C25-C24	2.35	122.02	115.65
13	2	509	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
13	H	1234	CLA	CAC-C3C-C4C	2.35	127.84	124.79
13	B	1216	CLA	CHB-C1B-NB	2.35	127.57	124.05
13	e	1107	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	a	524	BCR	C21-C20-C19	-2.35	116.40	123.20
16	a	524	BCR	C23-C24-C25	-2.35	120.73	127.00
13	Z	508	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
13	B	1234	CLA	CAC-C3C-C4C	2.35	127.84	124.79
13	2	508	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
16	f	4006	BCR	C34-C9-C10	-2.35	119.02	122.82
13	A	1022	CLA	CMB-C2B-C3B	2.35	132.07	126.55
13	s	501	CLA	CMB-C2B-C3B	2.35	132.07	126.55
16	M	4021	BCR	C30-C25-C24	2.35	122.01	115.65
13	A	1117	CLA	C3B-C4B-NB	-2.35	108.44	110.53
16	f	4004	BCR	C15-C16-C17	-2.34	118.72	123.52
16	l	4013	BCR	C35-C13-C12	2.34	121.67	118.09
19	B	5002	LMG	C40-C39-C38	-2.34	102.52	114.37
16	B	4006	BCR	C34-C9-C10	-2.34	119.02	122.82
13	r	509	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
16	r	524	BCR	C15-C16-C17	-2.34	118.72	123.52
19	H	5002	LMG	C40-C39-C38	-2.34	102.52	114.37
13	s	508	CLA	CHB-C1B-NB	2.34	127.56	124.05
13	r	510	CLA	CMB-C2B-C3B	2.34	132.06	126.55
19	f	5002	LMG	C40-C39-C38	-2.34	102.53	114.37
13	f	1238	CLA	CHB-C4A-NA	2.34	127.78	124.40
16	o	4021	BCR	C30-C25-C24	2.34	122.00	115.65
16	I	4018	BCR	C33-C5-C4	2.34	118.59	113.60
13	f	1227	CLA	O2D-CGD-CBD	2.34	115.32	111.23
16	3	524	BCR	C21-C20-C19	-2.34	116.42	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	6	524	BCR	C21-C20-C19	-2.34	116.42	123.20
16	d	524	BCR	C21-C20-C19	-2.34	116.42	123.20
16	u	523	BCR	C37-C22-C23	2.34	121.66	118.09
16	d	521	BCR	C33-C5-C6	-2.34	121.93	124.48
13	K	1103	CLA	C5-C3-C4	2.34	119.97	114.59
13	Z	506	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	v	501	CLA	C1-C2-C3	-2.34	122.36	126.20
16	r	523	BCR	C15-C16-C17	-2.34	118.73	123.52
16	J	4013	BCR	C7-C8-C9	-2.34	122.77	126.23
13	B	1240	CLA	C1-C2-C3	-2.34	122.36	126.20
16	v	522	BCR	C38-C26-C27	2.34	118.58	113.60
13	Y	516	CLA	CHB-C4A-NA	2.34	127.78	124.40
13	U	1103	CLA	C5-C3-C4	2.34	119.97	114.59
16	3	524	BCR	C34-C9-C8	2.34	121.66	118.09
16	a	524	BCR	C34-C9-C8	2.34	121.66	118.09
16	V	4019	BCR	C10-C11-C12	-2.34	116.42	123.20
13	e	1105	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
13	H	1225	CLA	C1-C2-C3	-2.34	122.37	126.20
16	l	4012	BCR	C1-C6-C7	2.34	121.99	115.65
13	G	1113	CLA	CMB-C2B-C3B	2.34	132.05	126.55
13	Z	503	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
13	G	1237	CLA	CHB-C4A-NA	2.34	127.77	124.40
16	s	524	BCR	C21-C20-C19	-2.34	116.43	123.20
16	6	521	BCR	C33-C5-C6	-2.34	121.93	124.48
20	5	822	SQD	O8-S-C6	2.34	110.48	105.97
20	u	822	SQD	O8-S-C6	2.34	110.48	105.97
16	S	4018	BCR	C33-C5-C4	2.34	118.58	113.60
13	B	1225	CLA	C1-C2-C3	-2.34	122.37	126.20
13	G	1022	CLA	CMB-C2B-C3B	2.34	132.04	126.55
13	B	1227	CLA	O2D-CGD-CBD	2.33	115.31	111.23
13	Y	502	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	L	4019	BCR	C10-C11-C12	-2.33	116.44	123.20
16	5	523	BCR	C37-C22-C23	2.33	121.65	118.09
13	Z	510	CLA	CMB-C2B-C3B	2.33	132.04	126.55
13	e	1022	CLA	CMB-C2B-C3B	2.33	132.04	126.55
13	H	1240	CLA	C1-C2-C3	-2.33	122.38	126.20
20	c	822	SQD	O8-S-C6	2.33	110.47	105.97
16	H	4006	BCR	C34-C9-C10	-2.33	119.04	122.82
16	V	4019	BCR	C15-C16-C17	-2.33	118.75	123.52
16	1	521	BCR	C29-C30-C25	2.33	113.82	110.44
16	2	523	BCR	C15-C16-C17	-2.33	118.75	123.52
16	n	4019	BCR	C15-C16-C17	-2.33	118.75	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	4019	BCR	C33-C5-C6	-2.33	121.94	124.48
16	3	523	BCR	C33-C5-C4	2.33	118.56	113.60
13	G	1105	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
20	6	822	SQD	O8-S-C6	2.33	110.47	105.97
13	1	502	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	H	1208	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	s	510	CLA	C2A-C1A-CHA	2.33	127.91	123.87
16	Y	521	BCR	C29-C30-C25	2.33	113.82	110.44
13	B	1234	CLA	O2D-CGD-CBD	2.33	115.30	111.23
20	3	822	SQD	C1-O5-C5	2.33	118.27	113.72
16	e	4002	BCR	C33-C5-C6	-2.33	121.94	124.48
13	G	1109	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	f	1208	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	m	1103	CLA	C5-C3-C4	2.33	119.94	114.59
13	Z	507	CLA	C2A-C1A-CHA	2.33	127.91	123.87
13	d	507	CLA	C2A-C1A-CHA	2.33	127.91	123.87
13	B	1208	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	G	1117	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	H	1218	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	L	4019	BCR	C15-C16-C17	-2.33	118.76	123.52
13	2	507	CLA	C2A-C1A-CHA	2.33	127.90	123.87
13	f	1240	CLA	C1-C2-C3	-2.33	122.39	126.20
16	A	4003	BCR	C11-C10-C9	-2.33	124.02	127.28
13	6	507	CLA	C2A-C1A-CHA	2.33	127.90	123.87
16	a	523	BCR	C33-C5-C4	2.33	118.55	113.60
13	v	507	CLA	C2A-C1A-CHA	2.33	127.90	123.87
16	l	4012	BCR	C28-C27-C26	-2.32	109.91	114.06
16	n	4019	BCR	C10-C11-C12	-2.32	116.47	123.20
13	2	502	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
13	f	1222	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	3	509	CLA	CMB-C2B-C3B	2.32	132.02	126.55
13	a	506	CLA	CMB-C2B-C3B	2.32	132.02	126.55
16	n	4022	BCR	C24-C23-C22	-2.32	122.80	126.23
20	d	822	SQD	O8-S-C6	2.32	110.46	105.97
13	s	510	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
13	A	1140	CLA	O2D-CGD-CBD	2.32	115.29	111.23
13	f	1225	CLA	C1-C2-C3	-2.32	122.39	126.20
16	L	4019	BCR	C33-C5-C6	-2.32	121.95	124.48
13	e	1140	CLA	O2D-CGD-CBD	2.32	115.29	111.23
13	r	502	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
16	A	4001	BCR	C34-C9-C8	2.32	121.63	118.09
13	a	510	CLA	O2A-CGA-O1A	-2.32	117.82	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	503	CLA	C3B-C4B-NB	-2.32	108.46	110.53
13	q	502	CLA	C3B-C4B-NB	-2.32	108.46	110.53
16	u	522	BCR	C3-C4-C5	-2.32	109.92	114.06
13	H	1222	CLA	CHB-C4A-NA	2.32	127.75	124.40
20	a	822	SQD	C1-O5-C5	2.32	118.25	113.72
16	s	523	BCR	C33-C5-C4	2.32	118.54	113.60
13	a	501	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
16	G	4001	BCR	C34-C9-C8	2.32	121.63	118.09
17	V	5221	LHG	C11-C10-C9	-2.32	102.64	114.37
13	a	509	CLA	CMB-C2B-C3B	2.32	132.01	126.55
13	3	501	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
16	d	523	BCR	C8-C7-C6	-2.32	120.80	127.00
13	G	1140	CLA	O2D-CGD-CBD	2.32	115.28	111.23
13	f	1234	CLA	O2D-CGD-CBD	2.32	115.28	111.23
16	Z	523	BCR	C15-C16-C17	-2.32	118.77	123.52
16	5	522	BCR	C30-C25-C26	-2.32	119.47	122.64
13	G	1113	CLA	C3B-C4B-NB	-2.32	108.46	110.53
16	S	4018	BCR	C38-C26-C27	2.32	118.54	113.60
16	Z	524	BCR	C33-C5-C4	2.32	118.54	113.60
13	f	1218	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
13	H	1238	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
13	V	1501	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
16	R	4016	BCR	C16-C15-C14	-2.32	118.78	123.52
13	A	1105	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
16	A	4008	BCR	C38-C26-C27	2.32	118.54	113.60
16	e	4001	BCR	C34-C9-C8	2.32	121.63	118.09
17	L	5221	LHG	C11-C10-C9	-2.32	102.66	114.37
13	B	1222	CLA	CHB-C4A-NA	2.32	127.74	124.40
16	5	522	BCR	C3-C4-C5	-2.32	109.93	114.06
13	n	1501	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
16	J	4012	BCR	C28-C27-C26	-2.32	109.93	114.06
20	4	822	SQD	O5-C5-C4	2.32	113.87	109.70
13	Z	502	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
16	A	4002	BCR	C33-C5-C6	-2.31	121.96	124.48
13	Z	511	CLA	CMB-C2B-C1B	-2.31	121.89	125.42
13	s	501	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
13	3	510	CLA	C2A-C1A-CHA	2.31	127.88	123.87
16	T	4012	BCR	C28-C27-C26	-2.31	109.93	114.06
20	v	822	SQD	O8-S-C6	2.31	110.44	105.97
16	6	523	BCR	C8-C7-C6	-2.31	120.82	127.00
13	s	509	CLA	CMB-C2B-C3B	2.31	131.99	126.55
16	e	4008	BCR	C38-C26-C27	2.31	118.53	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	j	4016	BCR	C16-C15-C14	-2.31	118.79	123.52
16	J	4012	BCR	C10-C11-C12	-2.31	116.50	123.20
20	t	822	SQD	O5-C5-C4	2.31	113.86	109.70
17	n	5221	LHG	C11-C10-C9	-2.31	102.68	114.37
20	b	822	SQD	C1-O5-C5	2.31	118.23	113.72
17	A	5009	LHG	C20-C19-C18	-2.31	102.69	114.37
13	L	1501	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
13	2	511	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
13	r	511	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
16	T	4012	BCR	C10-C11-C12	-2.31	116.50	123.20
16	u	522	BCR	C30-C25-C26	-2.31	119.48	122.64
13	B	1238	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
16	l	4012	BCR	C10-C11-C12	-2.31	116.51	123.20
16	V	4019	BCR	C33-C5-C6	-2.31	121.96	124.48
19	H	5002	LMG	C42-C41-C40	-2.31	102.69	114.37
13	r	519	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
20	t	822	SQD	C1-O5-C5	2.31	118.23	113.72
13	a	502	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
13	r	507	CLA	C2A-C1A-CHA	2.31	127.87	123.87
16	G	4003	BCR	C11-C10-C9	-2.31	124.04	127.28
16	2	524	BCR	C33-C5-C4	2.31	118.52	113.60
13	3	510	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
13	3	508	CLA	CHB-C1B-NB	2.31	127.51	124.05
20	r	822	SQD	C44-O6-C1	2.31	118.74	113.80
17	e	5009	LHG	C20-C19-C18	-2.31	102.70	114.37
13	B	1219	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
20	b	822	SQD	O5-C5-C4	2.31	113.86	109.70
16	F	4016	BCR	C16-C15-C14	-2.31	118.80	123.52
16	V	4022	BCR	C24-C23-C22	-2.31	122.82	126.23
13	H	1210	CLA	CBC-CAC-C3C	2.31	118.67	112.42
13	H	1218	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
16	k	4018	BCR	C38-C26-C27	2.31	118.51	113.60
13	Z	519	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
16	a	524	BCR	C27-C26-C25	-2.31	119.59	122.70
13	f	1238	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
16	K	4104	BCR	C38-C26-C27	2.31	118.51	113.60
16	3	524	BCR	C27-C26-C25	-2.31	119.59	122.70
13	H	1219	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
13	H	1221	CLA	C2A-C1A-CHA	2.30	127.87	123.87
16	I	4018	BCR	C38-C26-C27	2.30	118.51	113.60
16	G	4008	BCR	C38-C26-C27	2.30	118.51	113.60
17	G	5009	LHG	C20-C19-C18	-2.30	102.72	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1109	CLA	C3B-C4B-NB	-2.30	108.47	110.53
13	c	503	CLA	C3B-C4B-NB	-2.30	108.47	110.53
16	A	4011	BCR	C29-C30-C25	2.30	113.79	110.44
13	f	1210	CLA	CBC-CAC-C3C	2.30	118.67	112.42
20	2	822	SQD	C44-O6-C1	2.30	118.74	113.80
19	B	5002	LMG	C42-C41-C40	-2.30	102.72	114.37
19	f	5002	LMG	C42-C41-C40	-2.30	102.72	114.37
16	v	523	BCR	C8-C7-C6	-2.30	120.84	127.00
16	c	522	BCR	C3-C4-C5	-2.30	109.95	114.06
16	S	4018	BCR	C10-C11-C12	-2.30	116.53	123.20
16	Y	522	BCR	C27-C26-C25	-2.30	119.59	122.70
13	H	1228	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
13	2	519	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
19	H	5002	LMG	O2-C2-C1	-2.30	104.59	110.08
13	3	502	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
13	a	510	CLA	C2A-C1A-CHA	2.30	127.86	123.87
13	2	506	CLA	C3B-C4B-NB	-2.30	108.47	110.53
16	U	4104	BCR	C38-C26-C27	2.30	118.50	113.60
13	3	506	CLA	CMB-C2B-C3B	2.30	131.96	126.55
16	G	4002	BCR	C33-C5-C6	-2.30	121.97	124.48
13	f	1228	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
13	q	505	CLA	C1-C2-C3	-2.30	122.43	126.20
19	f	5002	LMG	O2-C2-C1	-2.30	104.59	110.08
13	c	509	CLA	C3B-C4B-NB	-2.30	108.48	110.53
13	s	507	CLA	C3B-C4B-NB	-2.30	108.48	110.53
13	B	1218	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
13	s	502	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
16	f	4004	BCR	C10-C11-C12	-2.30	116.54	123.20
16	k	4018	BCR	C10-C11-C12	-2.30	116.54	123.20
20	4	822	SQD	C1-O5-C5	2.30	118.21	113.72
13	A	1013	CLA	CHB-C1B-NB	2.30	127.50	124.05
13	1	509	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	I	4018	BCR	C10-C11-C12	-2.30	116.54	123.20
16	H	4004	BCR	C10-C11-C12	-2.30	116.54	123.20
13	d	505	CLA	C1-C2-C3	-2.30	122.43	126.20
16	e	4011	BCR	C29-C30-C25	2.30	113.78	110.44
16	r	524	BCR	C33-C5-C4	2.30	118.49	113.60
13	j	1301	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
16	B	4004	BCR	C10-C11-C12	-2.30	116.55	123.20
16	m	4104	BCR	C38-C26-C27	2.30	118.49	113.60
19	B	5002	LMG	O2-C2-C1	-2.30	104.60	110.08
16	q	521	BCR	C29-C30-C25	2.30	113.78	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	507	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	L	4022	BCR	C29-C28-C27	-2.30	106.23	111.28
13	Y	509	CLA	C3B-C4B-NB	-2.30	108.48	110.53
13	A	1117	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
16	M	4021	BCR	C3-C4-C5	-2.29	109.96	114.06
16	c	522	BCR	C33-C5-C4	2.29	118.49	113.60
13	H	1234	CLA	O2D-CGD-CBD	2.29	115.24	111.23
13	G	1117	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
20	Z	822	SQD	C44-O6-C1	2.29	118.71	113.80
13	H	1240	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
13	e	1117	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
13	f	1232	CLA	CHB-C1B-NB	2.29	127.49	124.05
13	s	506	CLA	CMB-C2B-C3B	2.29	131.94	126.55
13	B	1210	CLA	CBC-CAC-C3C	2.29	118.64	112.42
16	5	522	BCR	C33-C5-C4	2.29	118.48	113.60
13	1	505	CLA	C1-C2-C3	-2.29	122.44	126.20
13	Y	505	CLA	C1-C2-C3	-2.29	122.44	126.20
16	s	524	BCR	C1-C6-C5	-2.29	119.50	122.64
13	B	1232	CLA	CHB-C1B-NB	2.29	127.49	124.05
13	f	1221	CLA	C2A-C1A-CHA	2.29	127.84	123.87
13	e	1109	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	n	1501	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	G	1013	CLA	CHB-C1B-NB	2.29	127.49	124.05
13	A	1022	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
16	L	4022	BCR	C24-C23-C22	-2.29	122.84	126.23
13	A	1107	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
13	e	1104	CLA	CMB-C2B-C3B	2.29	131.94	126.55
13	G	1107	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
13	A	1113	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	b	502	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	L	1503	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
13	n	1503	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
13	H	1215	CLA	CMB-C2B-C3B	2.29	131.94	126.55
13	f	1219	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
16	V	4022	BCR	C29-C28-C27	-2.29	106.24	111.28
13	e	1013	CLA	CHB-C1B-NB	2.29	127.48	124.05
16	u	522	BCR	C33-C5-C4	2.29	118.48	113.60
13	e	1107	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
13	B	1228	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
16	H	4006	BCR	C29-C30-C25	2.29	113.76	110.44
13	v	505	CLA	C1-C2-C3	-2.29	122.45	126.20
13	B	1221	CLA	C2A-C1A-CHA	2.29	127.84	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	s	524	BCR	C27-C26-C25	-2.29	119.61	122.70
16	l	4012	BCR	C16-C17-C18	-2.29	124.07	127.28
13	B	1215	CLA	CMB-C2B-C3B	2.29	131.93	126.55
13	f	1210	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
13	e	1022	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
16	W	4021	BCR	C3-C4-C5	-2.29	109.98	114.06
13	R	1301	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
13	B	1012	CLA	O2D-CGD-CBD	2.29	115.23	111.23
17	e	5006	LHG	O8-C23-O10	-2.29	117.91	123.63
16	3	524	BCR	C1-C6-C5	-2.29	119.51	122.64
16	Y	524	BCR	C37-C22-C23	2.29	121.58	118.09
13	6	505	CLA	C1-C2-C3	-2.29	122.45	126.20
13	5	509	CLA	C3B-C4B-NB	-2.29	108.49	110.53
13	r	506	CLA	C3B-C4B-NB	-2.29	108.49	110.53
16	f	4006	BCR	C29-C30-C25	2.29	113.76	110.44
13	s	512	CLA	CHB-C4A-NA	2.29	127.70	124.40
13	B	1240	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
13	B	1222	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
13	f	1222	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
16	c	522	BCR	C21-C20-C19	-2.29	116.58	123.20
17	A	5006	LHG	O8-C23-O10	-2.29	117.91	123.63
13	A	1139	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
13	5	503	CLA	C3B-C4B-NB	-2.28	108.49	110.53
13	F	1301	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
16	B	4006	BCR	C29-C30-C25	2.28	113.76	110.44
17	e	5007	LHG	C18-C17-C16	-2.28	102.83	114.37
13	f	1240	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
13	G	1121	CLA	C2A-C1A-CHA	2.28	127.83	123.87
16	n	4022	BCR	C29-C28-C27	-2.28	106.26	111.28
13	V	1503	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
13	3	512	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	B	1210	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
17	G	5007	LHG	C18-C17-C16	-2.28	102.84	114.37
16	B	4009	BCR	C8-C7-C6	-2.28	120.90	127.00
16	q	524	BCR	C37-C22-C23	2.28	121.57	118.09
13	H	1201	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
20	t	822	SQD	C4-C3-C2	2.28	114.83	110.83
17	G	5005	LHG	C18-C17-C16	-2.28	102.84	114.37
16	c	522	BCR	C30-C25-C26	-2.28	119.52	122.64
16	1	524	BCR	C37-C22-C23	2.28	121.57	118.09
17	A	5007	LHG	C18-C17-C16	-2.28	102.84	114.37
13	e	1113	CLA	C3B-C4B-NB	-2.28	108.50	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	4012	BCR	C16-C17-C18	-2.28	124.08	127.28
13	f	1012	CLA	O2D-CGD-CBD	2.28	115.21	111.23
16	G	4011	BCR	C29-C30-C25	2.28	113.75	110.44
13	G	1123	CLA	O2D-CGD-CBD	2.28	115.21	111.23
13	A	1107	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
16	a	524	BCR	C1-C6-C5	-2.28	119.52	122.64
13	a	512	CLA	CHB-C4A-NA	2.28	127.69	124.40
17	A	5005	LHG	C18-C17-C16	-2.28	102.86	114.37
16	H	4009	BCR	C8-C7-C6	-2.28	120.91	127.00
16	q	522	BCR	C27-C26-C25	-2.28	119.63	122.70
17	e	5005	LHG	C18-C17-C16	-2.28	102.86	114.37
13	a	508	CLA	CHB-C1B-NB	2.28	127.46	124.05
16	J	4012	BCR	C16-C17-C18	-2.28	124.09	127.28
20	H	1852	SQD	O48-C23-C24	2.28	118.77	111.83
13	e	1128	CLA	O2D-CGD-CBD	2.28	115.21	111.23
13	H	1222	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
20	B	1852	SQD	O48-C23-C24	2.28	118.77	111.83
16	u	522	BCR	C21-C20-C19	-2.28	116.61	123.20
16	5	522	BCR	C21-C20-C19	-2.27	116.61	123.20
13	A	1123	CLA	O2D-CGD-CBD	2.27	115.21	111.23
13	A	1128	CLA	O2D-CGD-CBD	2.27	115.21	111.23
13	A	1104	CLA	CMB-C2B-C3B	2.27	131.90	126.55
13	4	502	CLA	C3B-C4B-NB	-2.27	108.50	110.53
13	a	507	CLA	C3B-C4B-NB	-2.27	108.50	110.53
13	G	1139	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
13	G	1107	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
13	f	1212	CLA	O2D-CGD-CBD	2.27	115.20	111.23
13	e	1139	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
16	T	4015	BCR	C10-C11-C12	-2.27	116.62	123.20
13	A	1121	CLA	C2A-C1A-CHA	2.27	127.81	123.87
13	B	1201	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
17	G	5003	LHG	C18-C17-C16	-2.27	102.89	114.37
16	t	522	BCR	C21-C20-C19	-2.27	116.62	123.20
17	A	5003	LHG	C18-C17-C16	-2.27	102.89	114.37
13	u	509	CLA	C3B-C4B-NB	-2.27	108.50	110.53
13	G	1104	CLA	CMB-C2B-C3B	2.27	131.89	126.55
13	G	1022	CLA	CAA-CBA-CGA	-2.27	106.76	113.21
13	f	1215	CLA	CMB-C2B-C3B	2.27	131.89	126.55
16	f	4009	BCR	C8-C7-C6	-2.27	120.94	127.00
17	A	5007	LHG	C27-C26-C25	-2.27	102.90	114.37
17	e	5003	LHG	C18-C17-C16	-2.27	102.90	114.37
20	f	1852	SQD	O48-C23-C24	2.27	118.75	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	5007	LHG	C27-C26-C25	-2.27	102.90	114.37
13	c	502	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
16	4	522	BCR	C3-C4-C5	-2.27	110.01	114.06
16	b	522	BCR	C21-C20-C19	-2.27	116.63	123.20
20	4	822	SQD	C4-C3-C2	2.27	114.81	110.83
13	H	1210	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
13	L	1501	CLA	C3B-C4B-NB	-2.27	108.51	110.53
13	q	509	CLA	C3B-C4B-NB	-2.27	108.51	110.53
17	e	5007	LHG	C27-C26-C25	-2.27	102.91	114.37
13	H	1226	CLA	CAC-C3C-C4C	2.27	127.74	124.79
13	H	1232	CLA	CHB-C1B-NB	2.27	127.45	124.05
13	H	1212	CLA	O2D-CGD-CBD	2.27	115.19	111.23
16	1	522	BCR	C27-C26-C25	-2.27	119.64	122.70
20	b	822	SQD	C4-C3-C2	2.26	114.81	110.83
16	4	522	BCR	C21-C20-C19	-2.26	116.64	123.20
13	3	508	CLA	CMB-C2B-C3B	2.26	131.88	126.55
17	G	5006	LHG	O8-C23-O10	-2.26	117.96	123.63
19	l	5104	LMG	C6-C5-C4	-2.26	107.46	113.02
13	s	508	CLA	CMB-C2B-C3B	2.26	131.88	126.55
16	o	4021	BCR	C3-C4-C5	-2.26	110.02	114.06
13	e	1104	CLA	O1D-CGD-CBD	2.26	128.98	124.52
13	e	1121	CLA	C2A-C1A-CHA	2.26	127.79	123.87
13	e	1022	CLA	C3B-C4B-NB	-2.26	108.51	110.53
19	J	5104	LMG	C6-C5-C4	-2.26	107.46	113.02
20	1	822	SQD	C44-O6-C1	2.26	118.65	113.80
13	H	1217	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
13	B	1212	CLA	O2D-CGD-CBD	2.26	115.18	111.23
20	B	1852	SQD	C4-C3-C2	2.26	114.80	110.83
16	a	524	BCR	C8-C7-C6	-2.26	120.96	127.00
13	f	1234	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
13	f	1201	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
16	6	523	BCR	C34-C9-C8	2.26	121.54	118.09
16	v	524	BCR	C10-C11-C12	-2.26	116.65	123.20
13	e	1115	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
13	u	502	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
13	B	1023	CLA	CAC-C3C-C2C	-2.26	123.41	127.56
16	5	524	BCR	C38-C26-C25	-2.26	122.02	124.48
16	n	4019	BCR	C21-C20-C19	-2.26	116.65	123.20
13	G	1104	CLA	O1D-CGD-CBD	2.26	128.97	124.52
13	G	1128	CLA	O2D-CGD-CBD	2.26	115.18	111.23
20	f	1852	SQD	C4-C3-C2	2.26	114.80	110.83
16	b	522	BCR	C3-C4-C5	-2.26	110.03	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	524	BCR	C38-C26-C25	-2.26	122.02	124.48
13	H	1012	CLA	O2D-CGD-CBD	2.26	115.18	111.23
13	f	1023	CLA	CAC-C3C-C2C	-2.26	123.41	127.56
13	f	1239	CLA	CAC-C3C-C2C	2.26	131.71	127.56
13	5	502	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
13	A	1115	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
13	H	1234	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
16	l	4013	BCR	C4-C5-C6	-2.26	119.65	122.70
16	q	523	BCR	C37-C22-C23	2.26	121.54	118.09
13	B	1234	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
13	B	1226	CLA	CAC-C3C-C4C	2.26	127.73	124.79
16	H	4004	BCR	C29-C30-C25	2.26	113.72	110.44
13	e	1103	CLA	C3B-C4B-NB	-2.26	108.52	110.53
20	Y	822	SQD	C44-O6-C1	2.26	118.64	113.80
13	H	1224	CLA	CMB-C2B-C3B	2.26	131.86	126.55
20	H	1852	SQD	O6-C44-C45	2.26	116.31	110.82
16	l	4015	BCR	C10-C11-C12	-2.26	116.66	123.20
13	f	1226	CLA	CAC-C3C-C4C	2.26	127.72	124.79
16	3	524	BCR	C8-C7-C6	-2.26	120.97	127.00
13	t	502	CLA	C3B-C4B-NB	-2.25	108.52	110.53
13	e	1107	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
13	e	1123	CLA	O2D-CGD-CBD	2.25	115.17	111.23
16	c	524	BCR	C38-C26-C25	-2.25	122.03	124.48
16	L	4019	BCR	C21-C20-C19	-2.25	116.67	123.20
13	J	1303	CLA	CAA-C2A-C1A	2.25	119.36	111.97
16	4	522	BCR	C23-C24-C25	-2.25	120.98	127.00
20	f	1852	SQD	O6-C44-C45	2.25	116.30	110.82
16	e	4007	BCR	C10-C11-C12	-2.25	116.67	123.20
20	H	1852	SQD	C4-C3-C2	2.25	114.78	110.83
19	T	5104	LMG	C6-C5-C4	-2.25	107.49	113.02
13	G	1115	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
20	q	822	SQD	C44-O6-C1	2.25	118.62	113.80
16	J	4015	BCR	C10-C11-C12	-2.25	116.68	123.20
13	B	1203	CLA	CMB-C2B-C3B	2.25	131.84	126.55
16	d	524	BCR	C10-C11-C12	-2.25	116.68	123.20
16	1	523	BCR	C37-C22-C23	2.25	121.53	118.09
13	T	1303	CLA	CAA-C2A-C1A	2.25	119.35	111.97
16	V	4022	BCR	C3-C4-C5	-2.25	110.04	114.06
13	J	1303	CLA	O2D-CGD-CBD	2.25	115.16	111.23
13	H	1023	CLA	CAC-C3C-C2C	-2.25	123.42	127.56
13	A	1104	CLA	O1D-CGD-CBD	2.25	128.96	124.52
16	s	524	BCR	C8-C7-C6	-2.25	120.99	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1852	SQD	O6-C44-C45	2.25	116.29	110.82
16	V	4019	BCR	C21-C20-C19	-2.25	116.68	123.20
16	c	524	BCR	C33-C5-C4	2.25	118.39	113.60
13	f	1203	CLA	CMB-C2B-C3B	2.25	131.84	126.55
13	a	508	CLA	CMB-C2B-C3B	2.25	131.84	126.55
16	5	524	BCR	C33-C5-C4	2.25	118.39	113.60
13	B	1239	CLA	CAC-C3C-C2C	2.25	131.69	127.56
19	T	5104	LMG	C1-C2-C3	-2.25	105.28	110.01
13	a	510	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
13	H	1239	CLA	CAC-C3C-C2C	2.25	131.69	127.56
13	l	1303	CLA	CAA-C2A-C1A	2.25	119.34	111.97
16	t	522	BCR	C23-C24-C25	-2.25	121.00	127.00
13	v	502	CLA	C3B-C4B-NB	-2.25	108.53	110.53
16	3	524	BCR	C37-C22-C23	2.25	121.52	118.09
13	A	1138	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
17	H	1855	LHG	C20-C19-C18	-2.25	103.02	114.37
16	u	524	BCR	C33-C5-C4	2.25	118.38	113.60
13	A	1140	CLA	CHA-C1A-NA	-2.25	121.31	126.39
13	u	503	CLA	C3B-C4B-NB	-2.24	108.53	110.53
17	e	5006	LHG	C27-C26-C25	-2.24	103.02	114.37
16	q	523	BCR	C27-C26-C25	-2.24	119.67	122.70
16	f	4009	BCR	C1-C6-C5	-2.24	119.57	122.64
13	B	1217	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
13	G	1108	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
16	v	523	BCR	C34-C9-C8	2.24	121.52	118.09
16	G	4008	BCR	C20-C19-C18	-2.24	120.21	126.36
17	f	1855	LHG	C20-C19-C18	-2.24	103.03	114.37
13	e	1138	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
13	A	1022	CLA	C3B-C4B-NB	-2.24	108.53	110.53
13	T	1303	CLA	O2D-CGD-CBD	2.24	115.15	111.23
17	G	5006	LHG	C27-C26-C25	-2.24	103.03	114.37
16	t	522	BCR	C3-C4-C5	-2.24	110.06	114.06
17	A	5006	LHG	C27-C26-C25	-2.24	103.03	114.37
17	B	1855	LHG	C20-C19-C18	-2.24	103.03	114.37
16	d	523	BCR	C34-C9-C8	2.24	121.51	118.09
13	B	1224	CLA	CMB-C2B-C3B	2.24	131.82	126.55
13	s	510	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
13	G	1140	CLA	CHA-C1A-NA	-2.24	121.31	126.39
13	A	1127	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
13	H	1203	CLA	CMB-C2B-C3B	2.24	131.82	126.55
13	H	1226	CLA	CHC-C1C-NC	2.24	127.69	124.31
16	A	4008	BCR	C20-C19-C18	-2.24	120.22	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	6	524	BCR	C10-C11-C12	-2.24	116.71	123.20
16	H	4009	BCR	C1-C6-C5	-2.24	119.57	122.64
13	l	1302	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	A	4007	BCR	C10-C11-C12	-2.24	116.71	123.20
13	H	1231	CLA	C1-C2-C3	-2.24	122.53	126.20
13	G	1127	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
13	v	509	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
13	A	1135	CLA	O2D-CGD-CBD	2.24	115.14	111.23
16	J	4013	BCR	C4-C5-C6	-2.24	119.68	122.70
13	f	1236	CLA	O2D-CGD-CBD	2.24	115.14	111.23
13	6	509	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
13	T	1302	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
16	a	524	BCR	C37-C22-C23	2.24	121.51	118.09
16	L	4022	BCR	C3-C4-C5	-2.24	110.07	114.06
13	H	1213	CLA	CMB-C2B-C3B	2.24	131.81	126.55
13	f	1217	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
13	e	1127	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
13	J	1302	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
16	A	4002	BCR	C23-C24-C25	-2.24	121.02	127.00
16	t	522	BCR	C30-C25-C26	-2.24	119.58	122.64
16	b	522	BCR	C23-C24-C25	-2.24	121.03	127.00
20	5	822	SQD	O6-C1-C2	2.24	111.67	108.27
16	s	524	BCR	C37-C22-C23	2.24	121.50	118.09
16	s	522	BCR	C38-C26-C27	2.24	118.36	113.60
13	t	507	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
13	e	1135	CLA	O2D-CGD-CBD	2.23	115.14	111.23
16	a	522	BCR	C38-C26-C27	2.23	118.36	113.60
13	f	1224	CLA	CMB-C2B-C3B	2.23	131.80	126.55
16	A	4008	BCR	C30-C25-C26	-2.23	119.58	122.64
13	f	1239	CLA	CMC-C2C-C1C	-2.23	121.55	125.03
16	T	4013	BCR	C4-C5-C6	-2.23	119.69	122.70
13	6	502	CLA	C3B-C4B-NB	-2.23	108.54	110.53
13	G	1106	CLA	CMB-C2B-C3B	2.23	131.80	126.55
16	n	4022	BCR	C3-C4-C5	-2.23	110.08	114.06
17	e	5009	LHG	C27-C26-C25	-2.23	103.08	114.37
16	G	4007	BCR	C10-C11-C12	-2.23	116.73	123.20
13	4	507	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
13	B	1230	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	G	1138	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	G	4002	BCR	C23-C24-C25	-2.23	121.04	127.00
16	W	4021	BCR	C36-C18-C19	2.23	121.50	118.09
16	f	4010	BCR	C20-C19-C18	-2.23	120.25	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	3	522	BCR	C38-C26-C27	2.23	118.35	113.60
13	q	505	CLA	C3B-C4B-NB	-2.23	108.54	110.53
16	e	4002	BCR	C23-C24-C25	-2.23	121.04	127.00
13	d	518	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
13	H	1230	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	J	5104	LMG	C1-C2-C3	-2.23	105.32	110.01
13	f	1229	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
13	B	1239	CLA	CMC-C2C-C1C	-2.23	121.55	125.03
13	B	1213	CLA	CMB-C2B-C3B	2.23	131.79	126.55
16	f	4010	BCR	C11-C12-C13	-2.23	120.25	126.36
13	f	1230	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	Z	509	CLA	CMB-C2B-C3B	2.23	131.79	126.55
16	A	4001	BCR	C8-C7-C6	-2.23	121.04	127.00
16	B	4004	BCR	C29-C30-C25	2.23	113.68	110.44
16	B	4010	BCR	C20-C19-C18	-2.23	120.25	126.36
20	c	822	SQD	O6-C1-C2	2.23	111.66	108.27
13	G	1103	CLA	C3B-C4B-NB	-2.23	108.54	110.53
16	G	4001	BCR	C8-C7-C6	-2.23	121.05	127.00
13	Y	509	CLA	CMB-C2B-C3B	2.23	131.79	126.55
13	B	1231	CLA	C1-C2-C3	-2.23	122.55	126.20
17	A	5003	LHG	C27-C26-C25	-2.23	103.11	114.37
13	q	509	CLA	CMB-C2B-C3B	2.23	131.79	126.55
16	Y	523	BCR	C37-C22-C23	2.23	121.49	118.09
20	u	822	SQD	O6-C1-C2	2.23	111.65	108.27
16	B	4009	BCR	C1-C6-C5	-2.23	119.59	122.64
13	3	510	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
13	d	509	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
13	v	518	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
13	l	1303	CLA	O2D-CGD-CBD	2.22	115.12	111.23
13	b	507	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
16	f	4004	BCR	C29-C30-C25	2.22	113.67	110.44
16	n	4020	BCR	C33-C5-C6	-2.22	122.06	124.48
13	V	1501	CLA	C3B-C4B-NB	-2.22	108.55	110.53
17	A	5009	LHG	C27-C26-C25	-2.22	103.13	114.37
17	G	5003	LHG	C27-C26-C25	-2.22	103.13	114.37
13	3	509	CLA	C2A-C1A-CHA	2.22	127.72	123.87
13	s	509	CLA	C2A-C1A-CHA	2.22	127.72	123.87
16	Y	523	BCR	C36-C18-C19	2.22	121.48	118.09
13	G	1135	CLA	O2D-CGD-CBD	2.22	115.12	111.23
16	e	4008	BCR	C20-C19-C18	-2.22	120.27	126.36
17	e	5003	LHG	C27-C26-C25	-2.22	103.13	114.37
16	e	4002	BCR	C38-C26-C25	-2.22	122.06	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	509	CLA	CMB-C2B-C3B	2.22	131.78	126.55
13	B	1226	CLA	CHC-C1C-NC	2.22	127.66	124.31
16	q	523	BCR	C11-C10-C9	-2.22	124.16	127.28
13	H	1239	CLA	CMC-C2C-C1C	-2.22	121.56	125.03
13	H	1229	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
13	1	505	CLA	C3B-C4B-NB	-2.22	108.55	110.53
13	f	1231	CLA	C1-C2-C3	-2.22	122.56	126.20
13	2	509	CLA	CMB-C2B-C3B	2.22	131.77	126.55
13	e	1140	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	l	5104	LMG	C1-C2-C3	-2.22	105.34	110.01
13	6	518	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
13	Y	509	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
13	r	509	CLA	CMB-C2B-C3B	2.22	131.77	126.55
17	V	5218	LHG	C27-C26-C25	-2.22	103.15	114.37
13	f	1213	CLA	CMB-C2B-C3B	2.22	131.77	126.55
13	b	511	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
13	e	1108	CLA	CHB-C4A-NA	2.22	127.60	124.40
16	M	4021	BCR	C36-C18-C19	2.22	121.48	118.09
18	Y	902	LMU	C1'-C2'-C3'	2.22	114.68	110.01
13	A	1108	CLA	CHB-C4A-NA	2.22	127.60	124.40
20	L	5216	SQD	O8-S-C6	2.22	110.25	105.97
16	e	4001	BCR	C8-C7-C6	-2.22	121.07	127.00
13	f	1240	CLA	O1D-CGD-CBD	2.22	128.89	124.52
16	H	4010	BCR	C20-C19-C18	-2.22	120.28	126.36
13	f	1234	CLA	C3A-C2A-C1A	2.22	104.66	101.34
16	e	4008	BCR	C30-C25-C26	-2.22	119.61	122.64
17	G	5009	LHG	C27-C26-C25	-2.22	103.16	114.37
17	f	1855	LHG	C11-C10-C9	-2.22	103.16	114.37
16	3	523	BCR	C36-C18-C19	2.22	121.47	118.09
16	a	523	BCR	C1-C6-C5	-2.22	119.61	122.64
13	l	1303	CLA	C2A-C1A-CHA	2.22	127.71	123.87
16	a	522	BCR	C2-C1-C6	2.22	113.66	110.44
13	B	1229	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
13	B	1236	CLA	O2D-CGD-CBD	2.22	115.10	111.23
17	L	5218	LHG	C27-C26-C25	-2.22	103.17	114.37
13	G	1129	CLA	CMB-C2B-C3B	2.22	131.76	126.55
17	B	1855	LHG	C11-C10-C9	-2.21	103.17	114.37
13	T	1303	CLA	C2A-C1A-CHA	2.21	127.71	123.87
17	H	1855	LHG	C11-C10-C9	-2.21	103.18	114.37
16	L	4019	BCR	C40-C30-C25	-2.21	106.77	110.24
17	n	5218	LHG	C27-C26-C25	-2.21	103.18	114.37
13	b	503	CLA	O2A-CGA-O1A	-2.21	118.09	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	q	509	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
16	Y	523	BCR	C7-C8-C9	-2.21	122.96	126.23
13	A	1106	CLA	CMB-C2B-C3B	2.21	131.75	126.55
16	n	4019	BCR	C40-C30-C25	-2.21	106.77	110.24
16	1	523	BCR	C27-C26-C25	-2.21	119.71	122.70
13	A	1108	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
20	V	5216	SQD	O8-S-C6	2.21	110.24	105.97
16	I	4018	BCR	C35-C13-C12	2.21	121.47	118.09
13	e	1108	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
13	f	1239	CLA	O2D-CGD-CBD	2.21	115.10	111.23
16	Z	522	BCR	C23-C24-C25	-2.21	121.09	127.00
16	H	4010	BCR	C11-C12-C13	-2.21	120.30	126.36
16	f	4014	BCR	C15-C14-C13	-2.21	124.18	127.28
16	B	4010	BCR	C11-C12-C13	-2.21	120.30	126.36
13	H	1206	CLA	O1D-CGD-CBD	2.21	128.88	124.52
16	3	523	BCR	C1-C6-C5	-2.21	119.61	122.64
16	c	522	BCR	C27-C26-C25	-2.21	119.72	122.70
13	a	509	CLA	C2A-C1A-CHA	2.21	127.70	123.87
13	1	509	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
13	d	502	CLA	C3B-C4B-NB	-2.21	108.56	110.53
16	u	522	BCR	C27-C26-C25	-2.21	119.72	122.70
16	V	4019	BCR	C40-C30-C25	-2.21	106.78	110.24
20	V	5216	SQD	C44-O6-C1	2.21	118.53	113.80
13	B	1231	CLA	C3B-C4B-NB	-2.21	108.56	110.53
16	Y	523	BCR	C27-C26-C25	-2.21	119.72	122.70
20	n	5216	SQD	C44-O6-C1	2.21	118.53	113.80
13	t	511	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
13	f	1226	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
16	A	4002	BCR	C27-C26-C25	-2.21	119.72	122.70
20	n	5216	SQD	O8-S-C6	2.21	110.24	105.97
13	B	1239	CLA	O2D-CGD-CBD	2.21	115.09	111.23
16	G	4002	BCR	C27-C26-C25	-2.21	119.72	122.70
13	b	503	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
16	G	4002	BCR	C38-C26-C25	-2.21	122.08	124.48
13	G	1105	CLA	C3B-C4B-NB	-2.21	108.56	110.53
13	4	503	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
13	e	1112	CLA	O2D-CGD-CBD	2.21	115.09	111.23
16	B	4014	BCR	C15-C14-C13	-2.21	124.18	127.28
16	G	4008	BCR	C30-C25-C26	-2.21	119.62	122.64
13	B	1216	CLA	C1-C2-C3	-2.21	122.58	126.20
13	r	505	CLA	C3B-C4B-NB	-2.21	108.56	110.53
16	S	4018	BCR	C35-C13-C12	2.21	121.46	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	523	BCR	C36-C18-C19	2.21	121.46	118.09
16	b	522	BCR	C30-C25-C26	-2.21	119.62	122.64
13	t	503	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
13	e	1115	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
13	f	1216	CLA	C1-C2-C3	-2.20	122.58	126.20
13	f	1221	CLA	C6-C7-C8	-2.20	108.64	115.97
16	L	4020	BCR	C33-C5-C6	-2.20	122.08	124.48
16	4	521	BCR	C20-C19-C18	-2.20	120.32	126.36
13	Z	505	CLA	C3B-C4B-NB	-2.20	108.56	110.53
13	f	1206	CLA	O1D-CGD-CBD	2.20	128.86	124.52
19	B	5002	LMG	O3-C3-C2	-2.20	105.18	110.38
13	B	1234	CLA	C3A-C2A-C1A	2.20	104.64	101.34
16	f	4009	BCR	C4-C5-C6	-2.20	119.73	122.70
19	f	5002	LMG	O3-C3-C2	-2.20	105.18	110.38
13	A	1103	CLA	C1-C2-C3	-2.20	122.59	126.20
13	e	1129	CLA	CMB-C2B-C3B	2.20	131.73	126.55
13	B	1221	CLA	C6-C7-C8	-2.20	108.65	115.97
13	H	1221	CLA	C6-C7-C8	-2.20	108.65	115.97
16	4	522	BCR	C30-C25-C26	-2.20	119.63	122.64
16	1	523	BCR	C7-C8-C9	-2.20	122.98	126.23
13	H	1226	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	3	522	BCR	C2-C1-C6	2.20	113.64	110.44
13	B	1219	CLA	CHB-C4A-NA	2.20	127.58	124.40
13	H	1216	CLA	C1-C2-C3	-2.20	122.59	126.20
16	k	4018	BCR	C35-C13-C12	2.20	121.45	118.09
13	G	1022	CLA	C3B-C4B-NB	-2.20	108.56	110.53
13	G	1101	CLA	CAA-CBA-CGA	-2.20	106.96	113.21
13	B	1226	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	H	1240	CLA	O1D-CGD-CBD	2.20	128.86	124.52
13	A	1011	CLA	CHA-C1A-NA	-2.20	121.41	126.39
13	U	1105	CLA	C3B-C4B-NB	-2.20	108.57	110.53
13	G	1104	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	u	509	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	A	1111	CLA	CMB-C2B-C3B	2.20	131.72	126.55
16	2	522	BCR	C23-C24-C25	-2.20	121.12	127.00
13	e	1011	CLA	CHA-C1A-NA	-2.20	121.41	126.39
13	6	507	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
16	r	522	BCR	C30-C25-C26	-2.20	119.63	122.64
13	J	1303	CLA	C2A-C1A-CHA	2.20	127.68	123.87
13	B	1206	CLA	O1D-CGD-CBD	2.20	128.86	124.52
16	r	522	BCR	C23-C24-C25	-2.20	121.12	127.00
16	s	523	BCR	C36-C18-C19	2.20	121.45	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	r	524	BCR	C1-C6-C5	-2.20	119.63	122.64
13	e	1106	CLA	CMB-C2B-C3B	2.20	131.72	126.55
13	A	1237	CLA	CAC-C3C-C4C	2.20	127.65	124.79
13	G	1123	CLA	CHA-C1A-NA	-2.20	121.41	126.39
13	T	1302	CLA	O2D-CGD-CBD	2.20	115.07	111.23
13	A	1115	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
13	G	1108	CLA	CHB-C4A-NA	2.20	127.57	124.40
13	A	1101	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
13	A	1129	CLA	CMB-C2B-C3B	2.20	131.72	126.55
16	1	523	BCR	C36-C18-C19	2.20	121.44	118.09
16	d	522	BCR	C36-C18-C19	2.20	121.44	118.09
16	o	4021	BCR	C36-C18-C19	2.20	121.44	118.09
13	4	503	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
13	H	1224	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
13	G	1111	CLA	CMB-C2B-C3B	2.20	131.72	126.55
13	5	509	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
13	e	1105	CLA	C3B-C4B-NB	-2.20	108.57	110.53
13	B	1240	CLA	O1D-CGD-CBD	2.20	128.85	124.52
13	Z	504	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
16	t	521	BCR	C20-C19-C18	-2.20	120.34	126.36
16	V	4020	BCR	C33-C5-C6	-2.20	122.09	124.48
13	r	504	CLA	CAA-C2A-C3A	-2.20	107.07	113.00
16	s	522	BCR	C2-C1-C6	2.20	113.63	110.44
13	e	1101	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
13	4	511	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
13	v	507	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
13	A	1123	CLA	CHA-C1A-NA	-2.19	121.42	126.39
13	G	1112	CLA	CMB-C2B-C3B	2.19	131.71	126.55
13	e	1111	CLA	CMB-C2B-C3B	2.19	131.71	126.55
13	A	1103	CLA	C3B-C4B-NB	-2.19	108.57	110.53
16	f	4014	BCR	C31-C1-C6	-2.19	106.80	110.24
16	5	522	BCR	C27-C26-C25	-2.19	119.74	122.70
13	e	1123	CLA	CHA-C1A-NA	-2.19	121.42	126.39
13	A	1117	CLA	CMB-C2B-C3B	2.19	131.71	126.55
13	H	1239	CLA	O2D-CGD-CBD	2.19	115.06	111.23
16	d	524	BCR	C37-C22-C23	2.19	121.44	118.09
13	G	1130	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
13	f	1224	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
13	J	1302	CLA	O2D-CGD-CBD	2.19	115.06	111.23
18	1	902	LMU	C1'-C2'-C3'	2.19	114.62	110.01
13	L	1501	CLA	C2A-C1A-CHA	2.19	127.67	123.87
13	A	1104	CLA	O2A-CGA-O1A	-2.19	118.14	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1229	CLA	C6-C7-C8	-2.19	108.68	115.97
13	G	1115	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
16	n	4022	BCR	C33-C5-C4	2.19	118.27	113.60
13	G	1110	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
13	l	1302	CLA	O2D-CGD-CBD	2.19	115.06	111.23
13	e	1011	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
13	A	1118	CLA	C2A-C1A-CHA	2.19	127.67	123.87
13	A	1136	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
13	f	1021	CLA	C2A-C1A-CHA	2.19	127.67	123.87
19	T	5104	LMG	O3-C3-C2	-2.19	105.21	110.38
13	2	505	CLA	C3B-C4B-NB	-2.19	108.57	110.53
13	G	1136	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
13	d	507	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
16	c	521	BCR	C2-C1-C6	2.19	113.62	110.44
13	G	1117	CLA	CMB-C2B-C3B	2.19	131.70	126.55
13	e	1117	CLA	CMB-C2B-C3B	2.19	131.70	126.55
13	e	1136	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
13	G	1107	CLA	O2D-CGD-CBD	2.19	115.06	111.23
17	G	5005	LHG	C27-C26-C25	-2.19	103.30	114.37
16	q	523	BCR	C7-C8-C9	-2.19	123.00	126.23
13	d	507	CLA	C3B-C4B-NB	-2.19	108.58	110.53
13	e	1111	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	e	1118	CLA	C2A-C1A-CHA	2.19	127.67	123.87
20	L	5216	SQD	C44-O6-C1	2.19	118.49	113.80
16	b	521	BCR	C20-C19-C18	-2.19	120.36	126.36
13	U	1401	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	H	1234	CLA	C3A-C2A-C1A	2.19	104.62	101.34
16	r	523	BCR	C37-C22-C23	2.19	121.43	118.09
16	v	522	BCR	C36-C18-C19	2.19	121.43	118.09
13	Y	504	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
13	Y	518	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
13	f	1231	CLA	C3B-C4B-NB	-2.19	108.58	110.53
13	H	1021	CLA	C2A-C1A-CHA	2.19	127.67	123.87
16	d	521	BCR	C2-C1-C6	2.19	113.62	110.44
13	f	1219	CLA	CHB-C4A-NA	2.19	127.56	124.40
16	H	4014	BCR	C15-C14-C13	-2.19	124.21	127.28
13	A	1110	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
13	A	1011	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	2	524	BCR	C1-C6-C5	-2.19	119.65	122.64
13	B	1224	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	B	4009	BCR	C4-C5-C6	-2.19	119.75	122.70
16	f	4006	BCR	C28-C27-C26	-2.19	110.16	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1110	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
13	q	504	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
17	e	5005	LHG	C27-C26-C25	-2.19	103.31	114.37
16	A	4007	BCR	C33-C5-C4	2.19	118.26	113.60
13	e	1140	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	A	1112	CLA	O2D-CGD-CBD	2.19	115.05	111.23
13	B	1021	CLA	C2A-C1A-CHA	2.19	127.66	123.87
13	f	1203	CLA	O1D-CGD-CBD	2.19	128.83	124.52
16	b	522	BCR	C27-C26-C25	-2.19	119.75	122.70
13	G	1011	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	2	504	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
16	B	4014	BCR	C31-C1-C6	-2.19	106.82	110.24
18	e	1849	LMU	O5'-C1'-C2'	2.19	114.86	110.37
16	6	524	BCR	C37-C22-C23	2.19	121.43	118.09
13	G	1011	CLA	CHA-C1A-NA	-2.19	121.44	126.39
16	2	522	BCR	C30-C25-C26	-2.18	119.65	122.64
17	A	5005	LHG	C27-C26-C25	-2.18	103.32	114.37
13	A	1101	CLA	CAA-C2A-C3A	-2.18	107.09	113.00
19	H	5002	LMG	O3-C3-C2	-2.18	105.23	110.38
16	e	4007	BCR	C33-C5-C4	2.18	118.25	113.60
13	e	1107	CLA	O2D-CGD-CBD	2.18	115.05	111.23
13	H	1229	CLA	C6-C7-C8	-2.18	108.70	115.97
13	G	1103	CLA	C1-C2-C3	-2.18	122.62	126.20
13	e	1101	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
13	c	509	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
16	s	523	BCR	C1-C6-C5	-2.18	119.65	122.64
13	B	1238	CLA	CHB-C1B-NB	2.18	127.33	124.05
13	G	1237	CLA	CAC-C3C-C4C	2.18	127.63	124.79
13	Y	505	CLA	C3B-C4B-NB	-2.18	108.58	110.53
13	e	1104	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	A	1115	CLA	C4-C3-C5	2.18	119.02	115.23
13	f	1229	CLA	C6-C7-C8	-2.18	108.71	115.97
13	a	509	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	1	523	BCR	C11-C10-C9	-2.18	124.22	127.28
13	f	1226	CLA	CHC-C1C-NC	2.18	127.60	124.31
13	A	1107	CLA	O2D-CGD-CBD	2.18	115.04	111.23
13	K	1401	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	Z	524	BCR	C1-C6-C5	-2.18	119.66	122.64
13	1	504	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
13	e	1137	CLA	C2A-C1A-CHA	2.18	127.65	123.87
16	4	522	BCR	C27-C26-C25	-2.18	119.76	122.70
16	e	4002	BCR	C27-C26-C25	-2.18	119.76	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1111	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	B	1203	CLA	O1D-CGD-CBD	2.18	128.82	124.52
13	4	517	CLA	C2A-C1A-CHA	2.18	127.65	123.87
13	G	1101	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
13	A	1140	CLA	CHB-C4A-NA	2.18	127.55	124.40
13	q	518	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
13	e	1115	CLA	C4-C3-C5	2.18	119.01	115.23
13	f	1012	CLA	C4-C3-C5	2.18	119.01	115.23
13	H	1236	CLA	O2D-CGD-CBD	2.18	115.04	111.23
16	q	523	BCR	C36-C18-C19	2.18	121.42	118.09
17	e	5001	LHG	C27-C26-C25	-2.18	103.35	114.37
13	G	1127	CLA	CAA-CBA-CGA	-2.18	107.02	113.21
16	G	4003	BCR	C16-C15-C14	-2.18	119.06	123.52
13	e	1120	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
18	q	902	LMU	C4'-C3'-C2'	2.18	114.66	110.83
13	A	1139	CLA	O2D-CGD-CBD	2.18	115.04	111.23
13	e	1130	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	t	503	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	H	1219	CLA	CHB-C4A-NA	2.18	127.54	124.40
16	A	4003	BCR	C16-C15-C14	-2.18	119.06	123.52
13	G	1118	CLA	C2A-C1A-CHA	2.18	127.65	123.87
13	Y	508	CLA	CMB-C2B-C3B	2.18	131.67	126.55
13	H	1238	CLA	CHB-C1B-NB	2.18	127.32	124.05
13	A	1112	CLA	CMB-C2B-C3B	2.18	131.67	126.55
13	G	1136	CLA	O1D-CGD-CBD	2.18	128.81	124.52
13	H	1203	CLA	O1D-CGD-CBD	2.18	128.81	124.52
16	s	522	BCR	C23-C24-C25	-2.18	121.18	127.00
13	H	1239	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	c	523	BCR	C23-C24-C25	-2.18	121.18	127.00
16	b	524	BCR	C15-C16-C17	-2.18	119.06	123.52
13	b	517	CLA	C2A-C1A-CHA	2.18	127.64	123.87
16	H	4010	BCR	C38-C26-C27	2.18	118.24	113.60
16	Y	523	BCR	C11-C10-C9	-2.18	124.23	127.28
16	Z	522	BCR	C30-C25-C26	-2.18	119.66	122.64
13	e	1237	CLA	CAC-C3C-C4C	2.18	127.62	124.79
16	u	523	BCR	C23-C24-C25	-2.18	121.19	127.00
16	f	4004	BCR	C34-C9-C8	2.18	121.41	118.09
13	G	1140	CLA	CHB-C4A-NA	2.18	127.54	124.40
13	H	1210	CLA	C3A-C2A-C1A	2.18	104.60	101.34
13	A	1127	CLA	CAA-CBA-CGA	-2.18	107.03	113.21
16	G	4007	BCR	C33-C5-C4	2.18	118.23	113.60
18	q	902	LMU	C1'-C2'-C3'	2.18	114.59	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	822	SQD	O8-S-C6	2.18	110.17	105.97
13	1	508	CLA	CMB-C2B-C3B	2.18	131.67	126.55
13	1	518	CLA	CAA-C2A-C3A	-2.18	107.12	113.00
17	G	5001	LHG	C27-C26-C25	-2.18	103.37	114.37
13	e	1139	CLA	O2D-CGD-CBD	2.17	115.03	111.23
13	A	1137	CLA	C2A-C1A-CHA	2.17	127.64	123.87
13	e	1119	CLA	CMB-C2B-C3B	2.17	131.66	126.55
20	a	822	SQD	O47-C7-O49	-2.17	118.62	123.70
20	s	822	SQD	O47-C7-O49	-2.17	118.62	123.70
13	A	1130	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
17	A	5001	LHG	C27-C26-C25	-2.17	103.38	114.37
16	v	521	BCR	C2-C1-C6	2.17	113.60	110.44
13	A	1111	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
13	A	1133	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
13	e	1133	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
13	G	1112	CLA	O2D-CGD-CBD	2.17	115.03	111.23
13	f	1239	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
18	A	1849	LMU	O5'-C1'-C2'	2.17	114.83	110.37
16	L	4022	BCR	C33-C5-C4	2.17	118.23	113.60
13	n	1501	CLA	C2A-C1A-CHA	2.17	127.64	123.87
19	J	5104	LMG	O3-C3-C2	-2.17	105.26	110.38
16	B	4004	BCR	C34-C9-C8	2.17	121.41	118.09
16	6	522	BCR	C36-C18-C19	2.17	121.41	118.09
13	B	1224	CLA	C1-C2-C3	-2.17	122.64	126.20
13	e	1103	CLA	C1-C2-C3	-2.17	122.64	126.20
16	5	523	BCR	C23-C24-C25	-2.17	121.20	127.00
16	5	521	BCR	C2-C1-C6	2.17	113.59	110.44
16	2	523	BCR	C16-C15-C14	-2.17	119.08	123.52
18	H	1843	LMU	C6B-C5B-C4B	-2.17	107.69	113.02
13	b	516	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
16	r	522	BCR	C38-C26-C27	2.17	118.22	113.60
16	t	522	BCR	C27-C26-C25	-2.17	119.77	122.70
16	4	524	BCR	C15-C16-C17	-2.17	119.08	123.52
13	m	1401	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
13	G	1139	CLA	O2D-CGD-CBD	2.17	115.02	111.23
13	V	1501	CLA	C2A-C1A-CHA	2.17	127.63	123.87
16	r	523	BCR	C16-C15-C14	-2.17	119.08	123.52
13	G	1133	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
13	H	1231	CLA	C3B-C4B-NB	-2.17	108.59	110.53
13	H	1224	CLA	C1-C2-C3	-2.17	122.64	126.20
16	B	4010	BCR	C38-C26-C27	2.17	118.22	113.60
13	e	1127	CLA	CAA-CBA-CGA	-2.17	107.05	113.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4006	BCR	C28-C27-C26	-2.17	110.19	114.06
16	6	521	BCR	C2-C1-C6	2.17	113.59	110.44
17	A	5008	LHG	C27-C26-C25	-2.17	103.40	114.37
16	H	4006	BCR	C28-C27-C26	-2.17	110.19	114.06
16	2	523	BCR	C37-C22-C23	2.17	121.40	118.09
16	Z	522	BCR	C38-C26-C27	2.17	118.22	113.60
13	1	518	CLA	C3B-C4B-NB	-2.17	108.59	110.53
13	6	507	CLA	C3B-C4B-NB	-2.17	108.59	110.53
13	f	1228	CLA	C3B-C4B-NB	-2.17	108.59	110.53
13	f	1224	CLA	C1-C2-C3	-2.17	122.64	126.20
16	e	4003	BCR	C16-C15-C14	-2.17	119.08	123.52
13	f	1213	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
20	3	822	SQD	O47-C7-O49	-2.17	118.64	123.70
13	B	1215	CLA	C1-C2-C3	-2.17	122.64	126.20
20	4	822	SQD	O8-S-C6	2.17	110.16	105.97
13	4	516	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
17	G	5008	LHG	C27-C26-C25	-2.17	103.41	114.37
16	t	524	BCR	C15-C16-C17	-2.17	119.08	123.52
16	u	523	BCR	C24-C23-C22	-2.17	123.03	126.23
18	f	1843	LMU	C6B-C5B-C4B	-2.17	107.70	113.02
16	q	524	BCR	C1-C6-C7	2.17	121.53	115.65
13	G	1125	CLA	CMB-C2B-C3B	2.17	131.65	126.55
13	e	1103	CLA	CMB-C2B-C3B	2.17	131.65	126.55
16	Z	523	BCR	C16-C15-C14	-2.17	119.09	123.52
13	A	1123	CLA	C3B-C4B-NB	-2.17	108.60	110.53
13	H	1232	CLA	C3B-C4B-NB	-2.17	108.60	110.53
13	f	1215	CLA	C1-C2-C3	-2.17	122.65	126.20
13	f	1221	CLA	CHA-C1A-NA	-2.17	121.49	126.39
16	c	523	BCR	C24-C23-C22	-2.17	123.03	126.23
18	B	1843	LMU	C6B-C5B-C4B	-2.17	107.70	113.02
16	Z	523	BCR	C37-C22-C23	2.17	121.40	118.09
16	v	524	BCR	C37-C22-C23	2.17	121.40	118.09
13	A	1105	CLA	C3B-C4B-NB	-2.17	108.60	110.53
16	2	522	BCR	C38-C26-C27	2.16	118.21	113.60
16	H	4014	BCR	C31-C1-C6	-2.16	106.85	110.24
17	e	5008	LHG	C27-C26-C25	-2.16	103.43	114.37
16	s	523	BCR	C3-C4-C5	-2.16	110.20	114.06
13	c	505	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	u	505	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	B	1239	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	A	4002	BCR	C38-C26-C25	-2.16	122.12	124.48
20	3	822	SQD	O8-S-C6	2.16	110.15	105.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	509	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	2	521	BCR	C20-C19-C18	-2.16	120.43	126.36
13	G	1115	CLA	C4-C3-C5	2.16	118.98	115.23
13	e	1112	CLA	CMB-C2B-C3B	2.16	131.64	126.55
16	H	4009	BCR	C4-C5-C6	-2.16	119.78	122.70
13	5	505	CLA	C3B-C4B-NB	-2.16	108.60	110.53
16	5	523	BCR	C33-C5-C4	2.16	118.21	113.60
16	t	522	BCR	C11-C10-C9	-2.16	124.25	127.28
13	f	1238	CLA	CHB-C1B-NB	2.16	127.29	124.05
13	t	516	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
13	a	502	CLA	C2A-C1A-CHA	2.16	127.62	123.87
16	n	4022	BCR	C21-C20-C19	-2.16	116.94	123.20
13	G	1112	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	B	1213	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	f	4006	BCR	C10-C11-C12	-2.16	116.94	123.20
18	G	1849	LMU	O5'-C1'-C2'	2.16	114.81	110.37
13	K	1105	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	Y	518	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	G	1137	CLA	C2A-C1A-CHA	2.16	127.62	123.87
16	a	522	BCR	C21-C20-C19	-2.16	116.94	123.20
13	G	1131	CLA	C1-C2-C3	-2.16	122.66	126.20
13	A	1120	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
20	t	822	SQD	O8-S-C6	2.16	110.14	105.97
13	d	506	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
20	H	1852	SQD	O47-C7-O49	-2.16	118.66	123.70
13	s	509	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	Z	521	BCR	C20-C19-C18	-2.16	120.44	126.36
13	K	1103	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
13	d	503	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
16	1	524	BCR	C1-C6-C7	2.16	121.51	115.65
16	u	521	BCR	C2-C1-C6	2.16	113.58	110.44
13	A	1131	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	B	1221	CLA	CHA-C1A-NA	-2.16	121.50	126.39
19	l	5104	LMG	O3-C3-C2	-2.16	105.29	110.38
13	t	517	CLA	C2A-C1A-CHA	2.16	127.61	123.87
16	t	523	BCR	C16-C15-C14	-2.16	119.10	123.52
13	n	1501	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	H	1228	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	t	509	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	v	507	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	s	502	CLA	C2A-C1A-CHA	2.16	127.61	123.87
13	G	1103	CLA	CMB-C2B-C3B	2.16	131.62	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	822	SQD	O8-S-C6	2.16	110.14	105.97
13	s	513	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
20	f	1852	SQD	O47-C7-O49	-2.16	118.66	123.70
16	V	4022	BCR	C33-C5-C4	2.16	118.19	113.60
13	m	1103	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
16	u	523	BCR	C33-C5-C4	2.16	118.19	113.60
16	Y	524	BCR	C1-C6-C7	2.16	121.50	115.65
13	G	1120	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
13	6	506	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
16	H	4006	BCR	C10-C11-C12	-2.16	116.95	123.20
13	G	1131	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
16	3	522	BCR	C21-C20-C19	-2.15	116.96	123.20
13	e	1131	CLA	C1-C2-C3	-2.15	122.67	126.20
13	e	1139	CLA	CHB-C4A-NA	2.15	127.51	124.40
13	H	1213	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
13	e	1131	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
20	s	822	SQD	O8-S-C6	2.15	110.13	105.97
16	c	524	BCR	C37-C22-C23	2.15	121.38	118.09
16	c	523	BCR	C33-C5-C4	2.15	118.19	113.60
13	B	1012	CLA	C4-C3-C5	2.15	118.97	115.23
13	f	1235	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
17	B	1855	LHG	C27-C26-C25	-2.15	103.48	114.37
13	U	1103	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
16	J	4012	BCR	C23-C24-C25	-2.15	121.25	127.00
13	v	503	CLA	C2A-C1A-CHA	2.15	127.60	123.87
18	1	902	LMU	C4'-C3'-C2'	2.15	114.61	110.83
13	v	503	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
16	L	4022	BCR	C21-C20-C19	-2.15	116.96	123.20
16	V	4022	BCR	C21-C20-C19	-2.15	116.96	123.20
13	3	502	CLA	C2A-C1A-CHA	2.15	127.60	123.87
13	A	1136	CLA	O1D-CGD-CBD	2.15	128.76	124.52
17	f	1855	LHG	C27-C26-C25	-2.15	103.49	114.37
13	q	508	CLA	CMB-C2B-C3B	2.15	131.61	126.55
16	a	523	BCR	C3-C4-C5	-2.15	110.22	114.06
16	b	522	BCR	C11-C10-C9	-2.15	124.26	127.28
16	r	522	BCR	C36-C18-C19	2.15	121.38	118.09
16	5	523	BCR	C24-C23-C22	-2.15	123.05	126.23
13	B	1023	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
13	A	1103	CLA	CMB-C2B-C3B	2.15	131.61	126.55
17	H	1855	LHG	C27-C26-C25	-2.15	103.49	114.37
16	B	4006	BCR	C10-C11-C12	-2.15	116.97	123.20
13	B	1235	CLA	O2A-CGA-O1A	-2.15	118.25	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4004	BCR	C34-C9-C8	2.15	121.37	118.09
13	A	1131	CLA	O1D-CGD-CBD	2.15	128.76	124.52
13	2	504	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	m	1105	CLA	C3B-C4B-NB	-2.15	108.61	110.53
13	6	503	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
13	G	1119	CLA	CMB-C2B-C3B	2.15	131.61	126.55
16	r	521	BCR	C20-C19-C18	-2.15	120.47	126.36
13	G	1140	CLA	CAA-C2A-C1A	2.15	119.02	111.97
13	f	1215	CLA	O2D-CGD-CBD	2.15	114.99	111.23
13	Y	509	CLA	C1-C2-C3	-2.15	122.68	126.20
13	H	1221	CLA	CHA-C1A-NA	-2.15	121.53	126.39
13	f	1021	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	b	508	CLA	CHB-C1B-NB	2.15	127.27	124.05
13	t	508	CLA	CHB-C1B-NB	2.15	127.27	124.05
16	3	522	BCR	C23-C24-C25	-2.15	121.26	127.00
16	3	523	BCR	C3-C4-C5	-2.15	110.23	114.06
13	A	1119	CLA	CMB-C2B-C3B	2.15	131.60	126.55
16	l	4012	BCR	C23-C24-C25	-2.15	121.26	127.00
16	G	4002	BCR	C38-C26-C27	2.15	118.17	113.60
13	e	1140	CLA	CAA-C2A-C1A	2.15	119.01	111.97
13	A	1118	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	s	522	BCR	C21-C20-C19	-2.15	116.98	123.20
16	4	523	BCR	C16-C15-C14	-2.15	119.13	123.52
13	Y	503	CLA	C2A-C1A-CHA	2.15	127.59	123.87
16	e	4008	BCR	C30-C25-C24	2.15	121.47	115.65
20	2	822	SQD	O8-S-C6	2.15	110.12	105.97
13	H	1209	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
13	Z	504	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
13	4	508	CLA	CHB-C1B-NB	2.15	127.27	124.05
16	4	522	BCR	C11-C10-C9	-2.15	124.27	127.28
16	H	4006	BCR	C20-C21-C22	-2.15	124.27	127.28
17	A	5002	LHG	C11-C10-C9	-2.15	103.52	114.37
13	H	1213	CLA	C2A-C1A-CHA	2.15	127.59	123.87
13	q	503	CLA	C2A-C1A-CHA	2.15	127.59	123.87
13	e	1120	CLA	CMB-C2B-C3B	2.14	131.59	126.55
13	A	1140	CLA	CAA-C2A-C1A	2.14	119.00	111.97
16	5	524	BCR	C37-C22-C23	2.14	121.36	118.09
17	G	5002	LHG	C11-C10-C9	-2.14	103.53	114.37
13	H	1012	CLA	C4-C3-C5	2.14	118.95	115.23
13	q	518	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	H	1235	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	2	522	BCR	C36-C18-C19	2.14	121.36	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	f	4010	BCR	C38-C26-C27	2.14	118.17	113.60
13	e	1118	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	a	522	BCR	C23-C24-C25	-2.14	121.27	127.00
13	Y	506	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	Y	519	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
17	S	5001	LHG	C27-C26-C25	-2.14	103.54	114.37
20	r	822	SQD	O8-S-C6	2.14	110.11	105.97
13	A	1112	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
13	H	1023	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
13	1	503	CLA	C2A-C1A-CHA	2.14	127.58	123.87
13	3	513	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	r	518	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	H	1215	CLA	C1-C2-C3	-2.14	122.69	126.20
20	Y	822	SQD	O48-C23-O10	-2.14	118.27	123.63
13	e	1124	CLA	CMB-C2B-C3B	2.14	131.59	126.55
13	A	1116	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	G	1124	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
17	e	5002	LHG	C11-C10-C9	-2.14	103.55	114.37
13	L	1501	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
13	B	1228	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	e	1123	CLA	C3B-C4B-NB	-2.14	108.62	110.53
16	H	4004	BCR	C39-C30-C25	-2.14	106.89	110.24
13	e	1125	CLA	CMB-C2B-C3B	2.14	131.58	126.55
13	a	513	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	f	1023	CLA	O2D-CGD-CBD	2.14	114.97	111.23
20	B	1852	SQD	O47-C7-O49	-2.14	118.70	123.70
13	A	1124	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
16	B	4009	BCR	C20-C21-C22	-2.14	124.28	127.28
17	V	5221	LHG	C18-C17-C16	-2.14	103.56	114.37
16	e	4002	BCR	C38-C26-C27	2.14	118.15	113.60
17	I	5001	LHG	C27-C26-C25	-2.14	103.56	114.37
16	H	4009	BCR	C20-C21-C22	-2.14	124.28	127.28
13	A	1120	CLA	CMB-C2B-C3B	2.14	131.58	126.55
13	G	1131	CLA	O1D-CGD-CBD	2.14	128.73	124.52
17	n	5221	LHG	C18-C17-C16	-2.14	103.57	114.37
13	Z	518	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	1	822	SQD	O48-C23-O10	-2.14	118.28	123.63
17	L	5221	LHG	C18-C17-C16	-2.14	103.57	114.37
16	A	4008	BCR	C30-C25-C24	2.14	121.44	115.65
13	A	1125	CLA	CMB-C2B-C3B	2.14	131.57	126.55
16	B	4006	BCR	C20-C21-C22	-2.14	124.28	127.28
13	q	509	CLA	C1-C2-C3	-2.14	122.70	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	u	507	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	e	1116	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	A	1124	CLA	CMB-C2B-C3B	2.14	131.57	126.55
16	b	523	BCR	C16-C15-C14	-2.14	119.15	123.52
13	2	518	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
13	e	1119	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
13	e	1124	CLA	CAA-C2A-C3A	-2.14	107.23	113.00
20	q	822	SQD	O48-C23-O10	-2.14	118.29	123.63
13	G	1123	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	d	508	CLA	O2A-CGA-O1A	-2.13	117.84	123.33
13	m	1103	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	A	1126	CLA	C3B-C4B-NB	-2.13	108.62	110.53
18	Y	902	LMU	C4'-C3'-C2'	2.13	114.58	110.83
13	f	1226	CLA	CHD-C1D-C2D	2.13	129.93	125.49
20	Z	822	SQD	O8-S-C6	2.13	110.09	105.97
13	G	1118	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	H	1023	CLA	CMD-C2D-C3D	2.13	132.58	127.69
13	A	1131	CLA	C1-C2-C3	-2.13	122.70	126.20
13	G	1130	CLA	CHB-C1B-NB	2.13	127.25	124.05
13	V	1501	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
16	T	4012	BCR	C23-C24-C25	-2.13	121.30	127.00
17	A	5001	LHG	C18-C17-C16	-2.13	103.59	114.37
17	G	5001	LHG	C18-C17-C16	-2.13	103.59	114.37
13	5	507	CLA	C3B-C4B-NB	-2.13	108.63	110.53
16	v	521	BCR	C16-C15-C14	-2.13	119.16	123.52
13	e	1136	CLA	O1D-CGD-CBD	2.13	128.72	124.52
13	A	1119	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	G	1119	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	u	524	BCR	C37-C22-C23	2.13	121.34	118.09
16	f	4009	BCR	C20-C21-C22	-2.13	124.29	127.28
13	B	1210	CLA	C3A-C2A-C1A	2.13	104.53	101.34
13	B	1209	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	v	506	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
13	B	1021	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	a	518	CLA	C1-C2-C3	-2.13	122.71	126.20
16	R	4016	BCR	C20-C21-C22	-2.13	124.29	127.28
16	f	4004	BCR	C39-C30-C25	-2.13	106.90	110.24
13	f	1210	CLA	C3A-C2A-C1A	2.13	104.53	101.34
13	G	1124	CLA	CMB-C2B-C3B	2.13	131.56	126.55
17	H	1842	LHG	C27-C26-C25	-2.13	103.60	114.37
17	k	5001	LHG	C27-C26-C25	-2.13	103.60	114.37
16	q	524	BCR	C10-C11-C12	-2.13	117.03	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	e	5001	LHG	C18-C17-C16	-2.13	103.60	114.37
13	A	1139	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	Z	512	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	f	1023	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
13	1	509	CLA	C1-C2-C3	-2.13	122.71	126.20
13	e	1112	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
13	e	1131	CLA	O1D-CGD-CBD	2.13	128.72	124.52
13	3	518	CLA	C1-C2-C3	-2.13	122.71	126.20
16	f	4009	BCR	C19-C18-C17	-2.13	115.66	119.01
13	G	1116	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
17	B	1842	LHG	C27-C26-C25	-2.13	103.61	114.37
13	A	1125	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
13	B	1215	CLA	O2D-CGD-CBD	2.13	114.95	111.23
16	Y	524	BCR	C3-C4-C5	-2.13	110.26	114.06
16	B	4004	BCR	C39-C30-C25	-2.13	106.91	110.24
17	f	1842	LHG	C27-C26-C25	-2.13	103.61	114.37
16	G	4008	BCR	C30-C25-C24	2.13	121.42	115.65
16	j	4016	BCR	C20-C21-C22	-2.13	124.30	127.28
13	6	508	CLA	O2A-CGA-O1A	-2.13	117.86	123.33
13	G	1120	CLA	CMB-C2B-C3B	2.13	131.55	126.55
16	B	4009	BCR	C19-C18-C17	-2.13	115.66	119.01
16	B	4006	BCR	C33-C5-C4	2.13	118.13	113.60
13	G	1022	CLA	C1D-ND-C4D	2.13	107.80	106.31
17	e	5009	LHG	C18-C17-C16	-2.13	103.62	114.37
16	1	524	BCR	C10-C11-C12	-2.13	117.04	123.20
13	B	1023	CLA	CMD-C2D-C3D	2.13	132.56	127.69
17	G	5009	LHG	C18-C17-C16	-2.13	103.62	114.37
13	U	1103	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	H	4006	BCR	C33-C5-C4	2.13	118.13	113.60
17	A	5009	LHG	C18-C17-C16	-2.13	103.62	114.37
13	r	504	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	A	4002	BCR	C38-C26-C27	2.13	118.13	113.60
16	B	4009	BCR	C28-C27-C26	-2.13	110.27	114.06
13	G	1126	CLA	C3B-C4B-NB	-2.13	108.63	110.53
13	f	1232	CLA	C3B-C4B-NB	-2.13	108.63	110.53
13	2	512	CLA	CHB-C4A-NA	2.12	127.47	124.40
20	1	822	SQD	O8-S-C6	2.12	110.07	105.97
13	c	501	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
16	6	521	BCR	C16-C15-C14	-2.12	119.17	123.52
13	B	1232	CLA	C3B-C4B-NB	-2.12	108.63	110.53
13	e	1130	CLA	CHB-C1B-NB	2.12	127.23	124.05
16	Z	522	BCR	C36-C18-C19	2.12	121.33	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	524	BCR	C10-C11-C12	-2.12	117.05	123.20
13	G	1139	CLA	CHB-C4A-NA	2.12	127.46	124.40
13	u	503	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
13	6	503	CLA	C2A-C1A-CHA	2.12	127.55	123.87
16	f	4006	BCR	C33-C5-C4	2.12	118.12	113.60
13	G	1115	CLA	CMB-C2B-C3B	2.12	131.54	126.55
13	B	1213	CLA	C2A-C1A-CHA	2.12	127.55	123.87
16	l	4015	BCR	C16-C15-C14	-2.12	119.18	123.52
13	5	501	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
20	Y	822	SQD	O8-S-C6	2.12	110.07	105.97
13	e	1115	CLA	CMB-C2B-C3B	2.12	131.54	126.55
13	e	1132	CLA	CBC-CAC-C3C	2.12	118.17	112.42
13	f	1023	CLA	CMD-C2D-C3D	2.12	132.55	127.69
13	A	1132	CLA	CBC-CAC-C3C	2.12	118.17	112.42
13	K	1103	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
13	q	519	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	d	521	BCR	C16-C15-C14	-2.12	119.18	123.52
16	b	524	BCR	C28-C27-C26	-2.12	110.28	114.06
13	1	506	CLA	C3B-C4B-NB	-2.12	108.64	110.53
13	H	1224	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	a	524	BCR	C10-C11-C12	-2.12	117.06	123.20
17	G	5004	LHG	C27-C26-C25	-2.12	103.66	114.37
13	Y	507	CLA	CHA-C1A-NA	-2.12	121.59	126.39
13	H	1229	CLA	O2D-CGD-CBD	2.12	114.93	111.23
16	J	4015	BCR	C16-C15-C14	-2.12	119.18	123.52
13	s	518	CLA	C1-C2-C3	-2.12	122.73	126.20
13	f	1224	CLA	C3B-C4B-NB	-2.12	108.64	110.53
13	1	519	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	f	1209	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	e	1022	CLA	C1D-ND-C4D	2.12	107.80	106.31
13	c	503	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	v	508	CLA	O2A-CGA-O1A	-2.12	117.89	123.33
13	e	1125	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
13	H	1023	CLA	O2D-CGD-CBD	2.12	114.93	111.23
13	B	1226	CLA	CHD-C1D-C2D	2.12	129.89	125.49
16	f	4009	BCR	C28-C27-C26	-2.12	110.28	114.06
13	H	1239	CLA	C11-C10-C8	-2.12	108.93	115.97
13	5	503	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	G	1132	CLA	CBC-CAC-C3C	2.12	118.16	112.42
13	f	1229	CLA	O2D-CGD-CBD	2.12	114.93	111.23
13	G	1125	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
20	q	822	SQD	O8-S-C6	2.12	110.06	105.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	1234	CLA	C2A-C1A-CHA	2.12	127.54	123.87
16	T	4015	BCR	C16-C15-C14	-2.12	119.19	123.52
13	A	1130	CLA	CHB-C1B-NB	2.12	127.22	124.05
16	4	524	BCR	C28-C27-C26	-2.11	110.28	114.06
13	H	1021	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
16	r	522	BCR	C33-C5-C4	2.11	118.10	113.60
13	r	512	CLA	CHB-C4A-NA	2.11	127.45	124.40
13	H	1224	CLA	C2A-C1A-CHA	2.11	127.53	123.87
16	f	4006	BCR	C20-C21-C22	-2.11	124.31	127.28
13	s	507	CLA	C2A-C1A-CHA	2.11	127.53	123.87
13	3	507	CLA	C2A-C1A-CHA	2.11	127.53	123.87
16	F	4016	BCR	C36-C18-C19	2.11	121.31	118.09
13	f	1213	CLA	C2A-C1A-CHA	2.11	127.53	123.87
16	3	524	BCR	C10-C11-C12	-2.11	117.08	123.20
13	s	510	CLA	CHA-C1A-NA	-2.11	121.61	126.39
13	B	1224	CLA	C3B-C4B-NB	-2.11	108.64	110.53
13	c	507	CLA	C3B-C4B-NB	-2.11	108.64	110.53
13	v	504	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
16	Z	522	BCR	C33-C5-C4	2.11	118.10	113.60
13	6	504	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
16	j	4016	BCR	C36-C18-C19	2.11	121.31	118.09
16	s	524	BCR	C10-C11-C12	-2.11	117.08	123.20
13	A	1105	CLA	C3A-C2A-C1A	2.11	104.50	101.34
13	u	501	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
13	B	1239	CLA	C11-C10-C8	-2.11	108.95	115.97
16	1	524	BCR	C3-C4-C5	-2.11	110.29	114.06
13	4	509	CLA	C3B-C4B-NB	-2.11	108.65	110.53
13	1	507	CLA	CHA-C1A-NA	-2.11	121.61	126.39
13	q	507	CLA	CHA-C1A-NA	-2.11	121.61	126.39
17	A	5004	LHG	C27-C26-C25	-2.11	103.70	114.37
16	J	4015	BCR	C15-C16-C17	-2.11	119.20	123.52
16	T	4015	BCR	C37-C22-C23	2.11	121.31	118.09
16	b	522	BCR	C33-C5-C4	2.11	118.09	113.60
13	5	507	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
16	H	4006	BCR	C1-C6-C7	2.11	121.37	115.65
13	d	503	CLA	C2A-C1A-CHA	2.11	127.53	123.87
16	H	4009	BCR	C19-C18-C17	-2.11	115.69	119.01
17	e	5004	LHG	C27-C26-C25	-2.11	103.72	114.37
13	s	504	CLA	CMB-C2B-C3B	2.11	131.51	126.55
13	f	1021	CLA	CHB-C4A-NA	2.11	127.44	124.40
16	R	4016	BCR	C36-C18-C19	2.11	121.31	118.09
16	F	4016	BCR	C20-C21-C22	-2.11	124.32	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1801	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
13	G	1801	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
16	t	522	BCR	C33-C5-C4	2.11	118.09	113.60
13	u	507	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
16	q	524	BCR	C3-C4-C5	-2.11	110.30	114.06
13	A	1022	CLA	C1D-ND-C4D	2.11	107.79	106.31
13	G	1139	CLA	C11-C10-C8	-2.11	108.96	115.97
13	A	1115	CLA	CMB-C2B-C3B	2.11	131.50	126.55
19	l	5104	LMG	O6-C1-O1	-2.11	105.07	110.04
16	1	523	BCR	C23-C24-C25	-2.11	121.37	127.00
13	H	1226	CLA	CHD-C1D-C2D	2.11	129.87	125.49
13	G	1105	CLA	C3A-C2A-C1A	2.11	104.49	101.34
17	A	5002	LHG	C5-O7-C7	-2.11	112.76	117.80
13	e	1126	CLA	C3B-C4B-NB	-2.10	108.65	110.53
13	e	1801	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
17	e	5002	LHG	C5-O7-C7	-2.10	112.76	117.80
13	c	507	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
13	f	1239	CLA	C11-C10-C8	-2.10	108.97	115.97
13	H	1215	CLA	O2D-CGD-CBD	2.10	114.91	111.23
16	2	522	BCR	C33-C5-C4	2.10	118.08	113.60
13	s	507	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
13	G	1111	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
13	e	1111	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
17	G	5002	LHG	C5-O7-C7	-2.10	112.76	117.80
16	T	4015	BCR	C15-C16-C17	-2.10	119.22	123.52
16	H	4009	BCR	C28-C27-C26	-2.10	110.31	114.06
16	Y	523	BCR	C23-C24-C25	-2.10	121.38	127.00
16	l	4015	BCR	C15-C16-C17	-2.10	119.22	123.52
13	Y	502	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
13	B	1023	CLA	O2D-CGD-CBD	2.10	114.91	111.23
13	B	1234	CLA	C2A-C1A-CHA	2.10	127.52	123.87
13	a	507	CLA	C2A-C1A-CHA	2.10	127.52	123.87
13	e	1105	CLA	C3A-C2A-C1A	2.10	104.49	101.34
13	r	518	CLA	CMB-C2B-C3B	2.10	131.50	126.55
16	t	524	BCR	C28-C27-C26	-2.10	110.31	114.06
13	e	1139	CLA	C11-C10-C8	-2.10	108.98	115.97
13	d	504	CLA	CMB-C2B-C3B	2.10	131.49	126.55
16	B	4006	BCR	C1-C6-C7	2.10	121.35	115.65
13	A	1139	CLA	C11-C10-C8	-2.10	108.98	115.97
13	B	1229	CLA	O2D-CGD-CBD	2.10	114.90	111.23
16	Y	522	BCR	C21-C20-C19	-2.10	117.11	123.20
13	r	503	CLA	CMB-C2B-C3B	2.10	131.49	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1111	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
13	v	503	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	b	508	CLA	O2A-CGA-O1A	-2.10	117.93	123.33
16	l	4015	BCR	C37-C22-C23	2.10	121.30	118.09
13	u	508	CLA	C3B-C4B-NB	-2.10	108.66	110.53
16	4	522	BCR	C33-C5-C4	2.10	118.07	113.60
13	2	512	CLA	C1-C2-C3	-2.10	122.76	126.20
13	Y	508	CLA	CHC-C1C-NC	2.10	127.47	124.31
13	B	1224	CLA	C2A-C1A-CHA	2.10	127.51	123.87
13	3	507	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	d	504	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
16	J	4015	BCR	C37-C22-C23	2.10	121.29	118.09
16	q	523	BCR	C23-C24-C25	-2.10	121.40	127.00
13	Y	510	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
16	1	522	BCR	C21-C20-C19	-2.10	117.12	123.20
13	6	503	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	3	510	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	q	522	BCR	C21-C20-C19	-2.10	117.13	123.20
16	G	4008	BCR	C15-C16-C17	-2.10	119.23	123.52
16	A	4008	BCR	C15-C16-C17	-2.10	119.23	123.52
13	t	518	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
13	Z	518	CLA	CMB-C2B-C3B	2.10	131.48	126.55
13	Z	512	CLA	C1-C2-C3	-2.10	122.76	126.20
16	A	4001	BCR	C21-C20-C19	-2.09	117.13	123.20
13	2	503	CLA	CMB-C2B-C3B	2.09	131.48	126.55
13	r	512	CLA	C1-C2-C3	-2.09	122.77	126.20
19	T	5104	LMG	O6-C1-O1	-2.09	105.10	110.04
13	V	1503	CLA	CMB-C2B-C3B	2.09	131.47	126.55
13	a	510	CLA	CMB-C2B-C3B	2.09	131.47	126.55
16	e	4008	BCR	C15-C16-C17	-2.09	119.24	123.52
13	H	1230	CLA	CAA-CBA-CGA	-2.09	107.27	113.21
13	3	504	CLA	CMB-C2B-C3B	2.09	131.47	126.55
13	s	510	CLA	CMB-C2B-C3B	2.09	131.47	126.55
16	G	4001	BCR	C21-C20-C19	-2.09	117.14	123.20
19	J	5104	LMG	O6-C1-O1	-2.09	105.10	110.04
16	d	523	BCR	C11-C10-C9	-2.09	124.34	127.28
13	q	510	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
13	B	1021	CLA	CHB-C4A-NA	2.09	127.42	124.40
13	a	507	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	e	4001	BCR	C21-C20-C19	-2.09	117.14	123.20
13	Y	507	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
13	2	518	CLA	CMB-C2B-C3B	2.09	131.47	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	502	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	a	510	CLA	CHA-C1A-NA	-2.09	121.66	126.39
13	1	508	CLA	CHC-C1C-NC	2.09	127.46	124.31
16	H	4017	BCR	C8-C7-C6	-2.09	121.42	127.00
13	4	508	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
16	c	524	BCR	C34-C9-C8	2.09	121.28	118.09
16	H	4005	BCR	C33-C5-C4	2.09	118.05	113.60
16	t	524	BCR	C11-C12-C13	-2.09	120.64	126.36
16	u	524	BCR	C34-C9-C8	2.09	121.28	118.09
13	a	518	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	c	507	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
13	t	508	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
16	Y	522	BCR	C1-C6-C5	-2.09	119.78	122.64
13	5	518	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	f	4006	BCR	C1-C6-C7	2.09	121.31	115.65
16	B	4017	BCR	C8-C7-C6	-2.09	121.42	127.00
13	3	510	CLA	CMB-C2B-C3B	2.09	131.46	126.55
13	Y	501	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
13	A	1237	CLA	C11-C12-C13	-2.09	109.03	115.97
13	q	506	CLA	C3B-C4B-NB	-2.09	108.67	110.53
13	L	1503	CLA	CMB-C2B-C3B	2.09	131.46	126.55
16	t	524	BCR	C21-C20-C19	-2.09	117.16	123.20
13	e	1130	CLA	C16-C15-C13	-2.09	109.03	115.97
13	a	504	CLA	CMB-C2B-C3B	2.08	131.45	126.55
13	G	1112	CLA	C2A-C1A-CHA	2.08	127.48	123.87
13	G	1237	CLA	C11-C12-C13	-2.08	109.04	115.97
16	b	524	BCR	C21-C20-C19	-2.08	117.16	123.20
13	q	501	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
13	f	1023	CLA	C3A-C2A-C1A	2.08	104.46	101.34
13	B	1230	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
13	e	1237	CLA	C11-C12-C13	-2.08	109.04	115.97
13	d	503	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	s	518	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	1	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	4	518	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	Y	508	CLA	CHB-C1B-NB	2.08	127.17	124.05
13	A	1127	CLA	C2A-C1A-CHA	2.08	127.48	123.87
13	Z	510	CLA	C1-C2-C3	-2.08	122.78	126.20
13	f	1224	CLA	C2A-C1A-CHA	2.08	127.48	123.87
13	5	508	CLA	C3B-C4B-NB	-2.08	108.67	110.53
13	q	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	u	822	SQD	C45-O47-C7	2.08	122.78	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	r	511	CLA	C2A-C1A-CHA	2.08	127.48	123.87
13	1	501	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	q	502	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	d	524	BCR	C20-C19-C18	-2.08	120.66	126.36
13	q	508	CLA	CHC-C1C-NC	2.08	127.44	124.31
16	4	524	BCR	C21-C20-C19	-2.08	117.17	123.20
16	H	4017	BCR	C15-C16-C17	-2.08	119.26	123.52
13	G	1130	CLA	C16-C15-C13	-2.08	109.05	115.97
13	f	1230	CLA	CAA-CBA-CGA	-2.08	107.30	113.21
20	c	822	SQD	C45-O47-C7	2.08	122.77	117.80
16	3	522	BCR	C27-C26-C25	-2.08	119.89	122.70
16	f	4005	BCR	C33-C5-C4	2.08	118.03	113.60
13	2	511	CLA	C2A-C1A-CHA	2.08	127.47	123.87
13	A	1103	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
16	G	4008	BCR	C28-C27-C26	-2.08	110.35	114.06
16	5	524	BCR	C34-C9-C8	2.08	121.26	118.09
13	n	1503	CLA	CMB-C2B-C3B	2.08	131.44	126.55
16	4	524	BCR	C11-C12-C13	-2.08	120.67	126.36
13	H	1234	CLA	C2A-C1A-CHA	2.08	127.47	123.87
16	e	4003	BCR	C4-C5-C6	-2.08	119.90	122.70
13	Z	503	CLA	CMB-C2B-C3B	2.08	131.44	126.55
13	A	1130	CLA	C16-C15-C13	-2.08	109.06	115.97
13	5	507	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
13	c	518	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
13	s	519	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
13	u	518	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
20	5	822	SQD	C45-O47-C7	2.08	122.77	117.80
13	1	510	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
13	q	508	CLA	CHB-C1B-NB	2.08	127.16	124.05
13	Y	507	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	1	522	BCR	C36-C18-C19	2.08	121.26	118.09
13	B	1023	CLA	C3A-C2A-C1A	2.08	104.45	101.34
13	H	1023	CLA	C3A-C2A-C1A	2.08	104.45	101.34
16	b	524	BCR	C11-C12-C13	-2.08	120.67	126.36
13	H	1212	CLA	CMB-C2B-C3B	2.08	131.43	126.55
13	r	510	CLA	C1-C2-C3	-2.08	122.80	126.20
16	j	4016	BCR	C38-C26-C25	-2.08	122.22	124.48
13	6	504	CLA	CMB-C2B-C3B	2.08	131.43	126.55
13	Y	511	CLA	CMB-C2B-C3B	2.08	131.43	126.55
13	G	1103	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
13	3	518	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
16	H	4009	BCR	C16-C15-C14	-2.08	119.27	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	1103	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
16	f	4017	BCR	C8-C7-C6	-2.07	121.45	127.00
13	5	511	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
13	v	501	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
13	T	1303	CLA	CHA-C1A-NA	-2.07	121.69	126.39
13	e	1117	CLA	C7-C6-C5	-2.07	107.73	113.26
13	H	1021	CLA	CHB-C4A-NA	2.07	127.39	124.40
19	l	5104	LMG	O8-C28-O10	-2.07	118.44	123.63
16	B	4005	BCR	C33-C5-C4	2.07	118.02	113.60
13	e	1125	CLA	C3A-C2A-C1A	2.07	104.44	101.34
17	B	1855	LHG	C18-C17-C16	-2.07	103.89	114.37
16	V	4219	BCR	C16-C15-C14	-2.07	119.28	123.52
13	G	1130	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
16	1	522	BCR	C1-C6-C5	-2.07	119.80	122.64
13	r	506	CLA	CMB-C2B-C3B	2.07	131.42	126.55
13	G	1127	CLA	C2A-C1A-CHA	2.07	127.46	123.87
13	a	516	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
17	f	1855	LHG	C18-C17-C16	-2.07	103.90	114.37
13	B	1204	CLA	C11-C10-C8	-2.07	109.08	115.97
13	r	508	CLA	CHB-C1B-NB	2.07	127.16	124.05
16	Y	522	BCR	C36-C18-C19	2.07	121.25	118.09
13	v	505	CLA	C3B-C4B-NB	-2.07	108.68	110.53
16	v	524	BCR	C20-C19-C18	-2.07	120.69	126.36
16	v	523	BCR	C11-C10-C9	-2.07	124.38	127.28
16	A	4003	BCR	C4-C5-C6	-2.07	119.91	122.70
13	G	1135	CLA	CHC-C4B-NB	2.07	127.15	124.05
13	2	510	CLA	C1-C2-C3	-2.07	122.81	126.20
17	H	1855	LHG	C18-C17-C16	-2.07	103.91	114.37
13	b	509	CLA	C3B-C4B-NB	-2.07	108.68	110.53
13	q	519	CLA	O2D-CGD-CBD	2.07	114.84	111.23
13	6	501	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
13	q	507	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
13	H	1212	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	W	4021	BCR	C30-C25-C26	-2.07	119.81	122.64
13	B	1239	CLA	C2A-C1A-CHA	2.07	127.45	123.87
16	6	524	BCR	C20-C19-C18	-2.07	120.70	126.36
13	B	1212	CLA	CMB-C2B-C3B	2.07	131.41	126.55
13	u	507	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
13	e	1112	CLA	C2A-C1A-CHA	2.07	127.45	123.87
16	L	4219	BCR	C16-C15-C14	-2.07	119.29	123.52
13	f	1204	CLA	C11-C10-C8	-2.07	109.10	115.97
17	A	5005	LHG	O8-C23-O10	-2.07	118.46	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4017	BCR	C15-C16-C17	-2.07	119.29	123.52
16	6	523	BCR	C11-C10-C9	-2.07	124.38	127.28
13	G	1117	CLA	C7-C6-C5	-2.07	107.76	113.26
16	t	523	BCR	C34-C9-C8	2.07	121.24	118.09
13	f	1212	CLA	CMB-C2B-C3B	2.06	131.41	126.55
13	3	504	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
17	G	5005	LHG	O8-C23-O10	-2.06	118.46	123.63
13	c	511	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
13	2	506	CLA	CMB-C2B-C3B	2.06	131.41	126.55
13	Z	506	CLA	CMB-C2B-C3B	2.06	131.41	126.55
13	Y	519	CLA	O2D-CGD-CBD	2.06	114.84	111.23
13	u	511	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
13	Z	502	CLA	C2A-C1A-CHA	2.06	127.45	123.87
16	B	4005	BCR	C3-C4-C5	-2.06	110.38	114.06
17	A	5002	LHG	O10-C23-C24	-2.06	115.71	123.78
13	1	519	CLA	O2D-CGD-CBD	2.06	114.84	111.23
13	b	518	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
13	G	1125	CLA	C3A-C2A-C1A	2.06	104.43	101.34
13	B	1209	CLA	C1-C2-C3	-2.06	122.82	126.20
13	A	1112	CLA	C2A-C1A-CHA	2.06	127.45	123.87
16	A	4008	BCR	C28-C27-C26	-2.06	110.38	114.06
13	J	1303	CLA	CHA-C1A-NA	-2.06	121.72	126.39
13	c	508	CLA	C3B-C4B-NB	-2.06	108.69	110.53
13	H	1240	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
13	H	1204	CLA	C11-C10-C8	-2.06	109.11	115.97
13	a	504	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
16	a	522	BCR	C27-C26-C25	-2.06	119.92	122.70
13	A	1130	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
13	B	1210	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
16	v	522	BCR	C21-C20-C19	-2.06	117.23	123.20
16	q	522	BCR	C36-C18-C19	2.06	121.24	118.09
19	T	5104	LMG	O8-C28-O10	-2.06	118.47	123.63
13	e	1130	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
17	G	5002	LHG	O10-C23-C24	-2.06	115.72	123.78
13	l	1303	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	t	523	BCR	C15-C16-C17	-2.06	119.30	123.52
13	G	1129	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
13	Z	511	CLA	C2A-C1A-CHA	2.06	127.44	123.87
13	H	1228	CLA	O2D-CGD-CBD	2.06	114.83	111.23
13	f	1212	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	J	5104	LMG	O8-C28-O10	-2.06	118.48	123.63
13	s	504	CLA	CAA-C2A-C3A	-2.06	107.44	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1129	CLA	CHC-C4B-NB	2.06	127.14	124.05
13	c	511	CLA	C2A-C1A-CHA	2.06	127.44	123.87
13	e	1127	CLA	C2A-C1A-CHA	2.06	127.44	123.87
13	v	504	CLA	CMB-C2B-C3B	2.06	131.39	126.55
13	e	1124	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	G	4003	BCR	C4-C5-C6	-2.06	119.92	122.70
16	f	4009	BCR	C16-C15-C14	-2.06	119.31	123.52
13	A	1117	CLA	C7-C6-C5	-2.06	107.78	113.26
13	f	1210	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
16	s	522	BCR	C27-C26-C25	-2.06	119.92	122.70
13	e	1124	CLA	C2D-C1D-ND	-2.06	108.09	110.13
16	n	4219	BCR	C16-C15-C14	-2.06	119.31	123.52
13	B	1240	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
13	s	505	CLA	C1-C2-C3	-2.06	122.83	126.20
13	B	1212	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	3	501	CLA	C3B-C4B-NB	-2.06	108.69	110.53
13	q	511	CLA	C2A-C1A-CHA	2.06	127.44	123.87
13	u	509	CLA	C2A-C1A-CHA	2.06	127.44	123.87
16	F	4016	BCR	C38-C26-C25	-2.06	122.24	124.48
13	3	519	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
17	e	5005	LHG	O8-C23-O10	-2.06	118.48	123.63
13	1	511	CLA	CMB-C2B-C3B	2.06	131.39	126.55
13	2	508	CLA	CHB-C1B-NB	2.06	127.13	124.05
17	e	5002	LHG	O10-C23-C24	-2.06	115.74	123.78
13	s	501	CLA	C3B-C4B-NB	-2.06	108.69	110.53
13	c	509	CLA	C2A-C1A-CHA	2.06	127.43	123.87
20	c	822	SQD	O48-C23-O10	-2.06	118.49	123.63
13	A	1109	CLA	C1-C2-C3	-2.06	122.83	126.20
13	A	1125	CLA	C3A-C2A-C1A	2.05	104.42	101.34
13	1	507	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
13	H	1239	CLA	C2A-C1A-CHA	2.05	127.43	123.87
16	6	522	BCR	C21-C20-C19	-2.05	117.25	123.20
13	A	1135	CLA	CHC-C4B-NB	2.05	127.13	124.05
13	1	508	CLA	CHB-C1B-NB	2.05	127.13	124.05
13	6	505	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	B	1012	CLA	C11-C12-C13	-2.05	109.14	115.97
13	d	501	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
13	f	1228	CLA	O2D-CGD-CBD	2.05	114.82	111.23
16	s	523	BCR	C37-C22-C23	2.05	121.22	118.09
13	f	1012	CLA	C11-C12-C13	-2.05	109.14	115.97
13	Y	502	CLA	C1-C2-C3	-2.05	122.83	126.20
13	G	1124	CLA	C2D-C1D-ND	-2.05	108.09	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	822	SQD	O6-C1-C2	2.05	111.39	108.27
16	H	4010	BCR	C1-C6-C7	2.05	121.22	115.65
13	1	511	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	q	511	CLA	CMB-C2B-C3B	2.05	131.38	126.55
13	2	502	CLA	C2A-C1A-CHA	2.05	127.43	123.87
13	B	1228	CLA	O2D-CGD-CBD	2.05	114.82	111.23
13	v	505	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
16	b	523	BCR	C34-C9-C8	2.05	121.22	118.09
13	d	505	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	5	523	BCR	C11-C10-C9	-2.05	124.40	127.28
13	H	1209	CLA	C1-C2-C3	-2.05	122.83	126.20
13	e	1109	CLA	C1-C2-C3	-2.05	122.83	126.20
16	R	4016	BCR	C38-C26-C25	-2.05	122.25	124.48
16	d	522	BCR	C21-C20-C19	-2.05	117.25	123.20
13	f	1208	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	q	502	CLA	C1-C2-C3	-2.05	122.84	126.20
16	B	4009	BCR	C16-C15-C14	-2.05	119.32	123.52
16	4	523	BCR	C15-C16-C17	-2.05	119.32	123.52
20	4	822	SQD	O6-C1-C2	2.05	111.39	108.27
16	b	523	BCR	C15-C16-C17	-2.05	119.32	123.52
13	H	1208	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	t	822	SQD	O6-C1-C2	2.05	111.39	108.27
13	H	1012	CLA	C11-C12-C13	-2.05	109.15	115.97
13	f	1240	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
13	3	516	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
13	B	1214	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	H	1210	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
13	s	511	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
16	c	523	BCR	C11-C10-C9	-2.05	124.41	127.28
13	3	508	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	4	523	BCR	C34-C9-C8	2.05	121.22	118.09
16	c	524	BCR	C24-C23-C22	-2.05	123.20	126.23
13	f	1239	CLA	C2A-C1A-CHA	2.05	127.42	123.87
16	e	4008	BCR	C28-C27-C26	-2.05	110.40	114.06
16	f	4005	BCR	C3-C4-C5	-2.05	110.40	114.06
13	j	1301	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	a	503	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
16	B	4010	BCR	C1-C6-C7	2.05	121.20	115.65
13	A	1129	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
16	3	523	BCR	C37-C22-C23	2.05	121.22	118.09
13	1	508	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	a	505	CLA	C1-C2-C3	-2.05	122.84	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1235	CLA	CBA-CAA-C2A	2.05	119.88	113.79
13	B	1217	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	Y	511	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	B	1221	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
16	l	4012	BCR	C15-C16-C17	-2.05	119.33	123.52
16	b	524	BCR	C38-C26-C25	-2.05	122.25	124.48
13	a	501	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	2	523	BCR	C33-C5-C4	2.05	117.96	113.60
13	G	1124	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
20	5	822	SQD	O48-C23-O10	-2.05	118.51	123.63
17	G	5006	LHG	C11-C10-C9	-2.05	104.03	114.37
13	Y	501	CLA	O2D-CGD-CBD	2.04	114.81	111.23
13	a	519	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
13	H	1210	CLA	CAC-C3C-C4C	2.04	127.45	124.79
13	A	1124	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
20	u	822	SQD	O48-C23-O10	-2.04	118.51	123.63
13	Y	504	CLA	C2A-C1A-CHA	2.04	127.42	123.87
13	q	508	CLA	C3B-C4B-NB	-2.04	108.70	110.53
16	f	4017	BCR	C15-C16-C17	-2.04	119.34	123.52
16	G	4007	BCR	C8-C7-C6	-2.04	121.54	127.00
13	r	502	CLA	C2A-C1A-CHA	2.04	127.41	123.87
13	B	1208	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	r	522	BCR	C27-C26-C25	-2.04	119.94	122.70
16	n	4219	BCR	C34-C9-C8	2.04	121.21	118.09
17	A	5006	LHG	C11-C10-C9	-2.04	104.04	114.37
13	f	1221	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	t	524	BCR	C38-C26-C25	-2.04	122.25	124.48
13	s	516	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
13	e	1135	CLA	CHC-C4B-NB	2.04	127.11	124.05
16	V	4219	BCR	C34-C9-C8	2.04	121.21	118.09
16	T	4012	BCR	C15-C16-C17	-2.04	119.34	123.52
16	f	4010	BCR	C1-C6-C7	2.04	121.19	115.65
13	3	505	CLA	C1-C2-C3	-2.04	122.85	126.20
16	v	522	BCR	C2-C3-C4	-2.04	106.79	111.28
16	H	4005	BCR	C3-C4-C5	-2.04	110.41	114.06
13	G	1122	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	4	521	BCR	C10-C11-C12	-2.04	117.28	123.20
13	5	509	CLA	C2A-C1A-CHA	2.04	127.41	123.87
13	Y	503	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
13	H	1218	CLA	CMB-C2B-C3B	2.04	131.35	126.55
16	L	4219	BCR	C34-C9-C8	2.04	121.20	118.09
13	f	1209	CLA	C1-C2-C3	-2.04	122.85	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	511	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	H	1239	CLA	C3B-C4B-NB	-2.04	108.71	110.53
13	1	511	CLA	C2A-C1A-CHA	2.04	127.41	123.87
13	A	1129	CLA	CHC-C4B-NB	2.04	127.11	124.05
13	s	508	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	B	1218	CLA	CMB-C2B-C3B	2.04	131.35	126.55
13	4	503	CLA	CAC-C3C-C4C	2.04	127.44	124.79
16	e	4007	BCR	C8-C7-C6	-2.04	121.55	127.00
13	B	1210	CLA	CAC-C3C-C4C	2.04	127.44	124.79
13	e	1129	CLA	CHC-C4B-NB	2.04	127.11	124.05
13	5	511	CLA	C2A-C1A-CHA	2.04	127.40	123.87
13	b	502	CLA	C2A-C1A-CHA	2.04	127.40	123.87
13	q	511	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	Z	522	BCR	C27-C26-C25	-2.04	119.95	122.70
16	a	523	BCR	C37-C22-C23	2.04	121.20	118.09
13	G	1109	CLA	C1-C2-C3	-2.04	122.86	126.20
13	4	505	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	f	1202	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	s	503	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	1	507	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
16	n	4022	BCR	C15-C16-C17	-2.04	119.35	123.52
13	f	1214	CLA	C2A-C1A-CHA	2.04	127.40	123.87
13	u	511	CLA	C2A-C1A-CHA	2.04	127.40	123.87
13	H	1221	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	r	503	CLA	C2A-C1A-CHA	2.04	127.40	123.87
13	B	1235	CLA	CBA-CAA-C2A	2.04	119.85	113.79
13	1	502	CLA	C1-C2-C3	-2.04	122.86	126.20
17	e	5006	LHG	C11-C10-C9	-2.04	104.08	114.37
13	Z	513	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	Z	523	BCR	C33-C5-C4	2.04	117.94	113.60
13	f	1217	CLA	C2A-C1A-CHA	2.04	127.40	123.87
16	A	4007	BCR	C8-C7-C6	-2.04	121.56	127.00
13	q	507	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
13	3	503	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
16	6	522	BCR	C2-C3-C4	-2.04	106.80	111.28
13	e	1129	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
16	2	522	BCR	C27-C26-C25	-2.03	119.95	122.70
16	u	523	BCR	C11-C10-C9	-2.03	124.42	127.28
13	3	511	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
16	a	522	BCR	C30-C25-C26	-2.03	119.86	122.64
16	S	4018	BCR	C37-C22-C23	2.03	121.19	118.09
13	Z	508	CLA	CMB-C2B-C3B	2.03	131.33	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	511	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
13	a	508	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
13	b	503	CLA	CAC-C3C-C4C	2.03	127.44	124.79
13	e	1121	CLA	CHA-C1A-NA	-2.03	121.79	126.39
13	6	502	CLA	C1-C2-C3	-2.03	123.47	126.76
13	H	1214	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	d	522	BCR	C2-C3-C4	-2.03	106.81	111.28
13	G	1140	CLA	CHB-C1B-NB	2.03	127.10	124.05
13	Y	507	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
16	6	523	BCR	C1-C6-C5	-2.03	119.86	122.64
13	G	1121	CLA	CHA-C1A-NA	-2.03	121.79	126.39
13	t	502	CLA	C2A-C1A-CHA	2.03	127.39	123.87
13	r	508	CLA	CMB-C2B-C3B	2.03	131.33	126.55
16	r	523	BCR	C33-C5-C4	2.03	117.93	113.60
13	t	505	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	q	522	BCR	C1-C6-C5	-2.03	119.86	122.64
16	J	4012	BCR	C15-C16-C17	-2.03	119.36	123.52
13	H	1226	CLA	CHB-C4A-NA	2.03	127.33	124.40
16	A	4002	BCR	C20-C19-C18	-2.03	120.80	126.36
13	1	504	CLA	C2A-C1A-CHA	2.03	127.39	123.87
13	s	516	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	5	524	BCR	C24-C23-C22	-2.03	123.23	126.23
13	f	1210	CLA	CAC-C3C-C4C	2.03	127.43	124.79
13	t	503	CLA	CAC-C3C-C4C	2.03	127.43	124.79
13	e	1129	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	u	523	BCR	C36-C18-C19	2.03	121.19	118.09
16	M	4021	BCR	C30-C25-C26	-2.03	119.86	122.64
13	b	509	CLA	CHA-C1A-NA	-2.03	121.80	126.39
16	e	4002	BCR	C20-C19-C18	-2.03	120.80	126.36
13	F	1301	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	b	521	BCR	C10-C11-C12	-2.03	117.32	123.20
13	d	502	CLA	C1-C2-C3	-2.03	123.48	126.76
13	J	1303	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
13	6	505	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
13	2	508	CLA	CMB-C2B-C3B	2.03	131.32	126.55
13	q	504	CLA	C2A-C1A-CHA	2.03	127.39	123.87
13	f	1214	CLA	O2D-CGD-CBD	2.03	114.78	111.23
13	1	503	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	G	1121	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	f	1218	CLA	CMB-C2B-C3B	2.03	131.32	126.55
16	v	522	BCR	C23-C24-C25	-2.03	121.58	127.00
17	G	5009	LHG	C5-O7-C7	-2.03	112.94	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	522	BCR	C20-C21-C22	-2.03	124.44	127.28
13	H	1217	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	t	521	BCR	C10-C11-C12	-2.03	117.33	123.20
13	Z	503	CLA	C2A-C1A-CHA	2.03	127.38	123.87
13	A	1121	CLA	CHA-C1A-NA	-2.03	121.80	126.39
16	Y	523	BCR	C8-C7-C6	-2.03	121.58	127.00
13	H	1202	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
16	3	524	BCR	C30-C25-C26	-2.03	119.87	122.64
13	t	503	CLA	C2A-C1A-CHA	2.03	127.38	123.87
13	f	1235	CLA	CBA-CAA-C2A	2.03	119.82	113.79
13	A	1124	CLA	C2D-C1D-ND	-2.03	108.12	110.13
13	b	509	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
13	Y	508	CLA	C3B-C4B-NB	-2.03	108.72	110.53
13	Y	507	CLA	CMB-C2B-C3B	2.02	131.31	126.55
13	A	1122	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
16	o	4021	BCR	C30-C25-C26	-2.02	119.87	122.64
16	6	522	BCR	C23-C24-C25	-2.02	121.59	127.00
13	1	501	CLA	O2D-CGD-CBD	2.02	114.77	111.23
16	e	4002	BCR	C21-C20-C19	-2.02	117.34	123.20
13	b	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	G	4002	BCR	C20-C19-C18	-2.02	120.81	126.36
16	U	4104	BCR	C23-C24-C25	-2.02	121.59	127.00
13	Y	503	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
13	B	1239	CLA	C3B-C4B-NB	-2.02	108.72	110.53
16	2	523	BCR	C3-C4-C5	-2.02	110.45	114.06
13	1	503	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
16	4	524	BCR	C38-C26-C25	-2.02	122.28	124.48
13	2	503	CLA	C2A-C1A-CHA	2.02	127.38	123.87
13	3	516	CLA	C2A-C1A-CHA	2.02	127.38	123.87
16	a	524	BCR	C30-C25-C26	-2.02	119.87	122.64
16	L	4022	BCR	C15-C16-C17	-2.02	119.38	123.52
16	5	523	BCR	C36-C18-C19	2.02	121.18	118.09
13	A	1129	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	A	4002	BCR	C21-C20-C19	-2.02	117.34	123.20
20	b	822	SQD	C45-O47-C7	2.02	121.42	117.85
16	d	522	BCR	C23-C24-C25	-2.02	121.60	127.00
13	Z	508	CLA	CHB-C1B-NB	2.02	127.08	124.05
13	e	1129	CLA	CHB-C1B-NB	2.02	127.08	124.05
13	B	1226	CLA	CHB-C4A-NA	2.02	127.32	124.40
16	u	524	BCR	C24-C23-C22	-2.02	123.25	126.23
16	s	522	BCR	C30-C25-C26	-2.02	119.87	122.64
13	d	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	1023	CLA	C2A-C1A-CHA	2.02	127.37	123.87
13	6	511	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
16	c	523	BCR	C36-C18-C19	2.02	121.17	118.09
13	2	513	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	G	1129	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	q	513	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
17	n	5220	LHG	C27-C26-C25	-2.02	104.16	114.37
13	q	510	CLA	C4-C3-C5	2.02	118.73	115.23
13	B	1214	CLA	O2D-CGD-CBD	2.02	114.76	111.23
16	u	522	BCR	C30-C25-C24	2.02	121.13	115.65
20	t	822	SQD	C45-O47-C7	2.02	121.41	117.85
13	T	1303	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
16	1	523	BCR	C8-C7-C6	-2.02	121.60	127.00
13	R	1301	CLA	C2A-C1A-CHA	2.02	127.37	123.87
16	b	524	BCR	C24-C23-C22	-2.02	123.25	126.23
17	e	5009	LHG	C5-O7-C7	-2.02	112.96	117.80
13	J	1303	CLA	C3B-C4B-NB	-2.02	108.73	110.53
13	G	1136	CLA	CHB-C1B-NB	2.02	127.08	124.05
17	V	5220	LHG	C27-C26-C25	-2.02	104.17	114.37
13	H	1226	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
13	1	507	CLA	CMB-C2B-C3B	2.02	131.30	126.55
16	2	522	BCR	C20-C21-C22	-2.02	124.45	127.28
13	q	501	CLA	O2D-CGD-CBD	2.02	114.76	111.23
17	L	5220	LHG	C27-C26-C25	-2.02	104.17	114.37
13	e	1126	CLA	C16-C15-C13	-2.02	109.26	115.97
13	A	1130	CLA	O2D-CGD-CBD	2.02	114.76	111.23
13	e	1130	CLA	O2D-CGD-CBD	2.02	114.76	111.23
13	e	1122	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
13	d	505	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
13	a	516	CLA	C2A-C1A-CHA	2.02	127.37	123.87
13	q	507	CLA	CMB-C2B-C3B	2.02	131.29	126.55
19	B	5002	LMG	C3-C4-C5	-2.02	106.58	110.23
13	f	1205	CLA	O2D-CGD-CBD	2.02	114.75	111.23
16	B	4005	BCR	C10-C11-C12	-2.02	117.36	123.20
13	B	1202	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
13	A	1127	CLA	CHA-C1A-NA	-2.02	121.83	126.39
13	G	1140	CLA	C1-C2-C3	-2.02	122.89	126.20
13	6	505	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
13	G	1133	CLA	CMB-C2B-C3B	2.02	131.29	126.55
13	f	1226	CLA	CMC-C2C-C3C	2.01	131.60	126.15
13	1	510	CLA	C4-C3-C5	2.01	118.72	115.23
16	Z	523	BCR	C3-C4-C5	-2.01	110.46	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	5009	LHG	C5-O7-C7	-2.01	112.98	117.80
13	B	1218	CLA	C2A-C1A-CHA	2.01	127.36	123.87
16	d	523	BCR	C1-C6-C5	-2.01	119.88	122.64
16	m	4104	BCR	C23-C24-C25	-2.01	121.62	127.00
13	r	513	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
20	n	5216	SQD	O48-C23-O10	-2.01	118.59	123.63
13	Y	502	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
19	f	5002	LMG	C3-C4-C5	-2.01	106.58	110.23
13	H	1205	CLA	O2D-CGD-CBD	2.01	114.75	111.23
16	I	4018	BCR	C37-C22-C23	2.01	121.16	118.09
20	L	5216	SQD	C1-O5-C5	2.01	117.65	113.72
13	4	502	CLA	C2A-C1A-CHA	2.01	127.36	123.87
16	s	523	BCR	C10-C11-C12	-2.01	117.37	123.20
13	B	1226	CLA	CMC-C2C-C3C	2.01	131.59	126.15
13	G	1140	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	A	1140	CLA	CHB-C1B-NB	2.01	127.07	124.05
16	f	4005	BCR	C10-C11-C12	-2.01	117.37	123.20
13	e	1121	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	V	4020	BCR	C8-C9-C10	-2.01	115.84	119.01
13	q	503	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
13	t	509	CLA	CHA-C1A-NA	-2.01	121.84	126.39
13	f	1226	CLA	CHB-C4A-NA	2.01	127.30	124.40
16	W	4021	BCR	C1-C6-C7	2.01	121.11	115.65
13	c	506	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
19	H	5002	LMG	C3-C4-C5	-2.01	106.59	110.23
13	B	1205	CLA	O2D-CGD-CBD	2.01	114.75	111.23
13	n	1503	CLA	O2D-CGD-CBD	2.01	114.75	111.23
13	H	1215	CLA	C4-C3-C5	2.01	118.72	115.23
16	c	522	BCR	C30-C25-C24	2.01	121.10	115.65
13	f	1218	CLA	C2A-C1A-CHA	2.01	127.36	123.87
13	B	1226	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
13	a	501	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	V	4022	BCR	C15-C16-C17	-2.01	119.41	123.52
13	4	509	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	Z	507	CLA	O2D-CGD-CBD	2.01	114.74	111.23
16	r	522	BCR	C20-C21-C22	-2.01	124.46	127.28
13	q	503	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
13	b	503	CLA	C2A-C1A-CHA	2.01	127.35	123.87
16	3	522	BCR	C30-C25-C26	-2.01	119.89	122.64
13	A	1114	CLA	CHB-C1B-NB	2.01	127.06	124.05
16	r	523	BCR	C3-C4-C5	-2.01	110.47	114.06
13	B	1023	CLA	CHC-C1C-NC	2.01	127.34	124.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	509	CLA	CHA-C1A-NA	-2.01	121.84	126.39
13	G	1130	CLA	O2D-CGD-CBD	2.01	114.74	111.23
16	n	4022	BCR	C10-C11-C12	-2.01	117.38	123.20
16	s	524	BCR	C1-C6-C7	2.01	121.10	115.65
16	d	521	BCR	C38-C26-C25	-2.01	122.29	124.48
13	e	1140	CLA	CHB-C1B-NB	2.01	127.06	124.05
13	H	1214	CLA	O2D-CGD-CBD	2.01	114.74	111.23
13	f	1223	CLA	C2A-C1A-CHA	2.01	127.35	123.87
13	B	1210	CLA	CMB-C2B-C3B	2.01	131.27	126.55
13	4	508	CLA	C3B-C4B-NB	-2.01	108.74	110.53
13	T	1303	CLA	C3B-C4B-NB	-2.01	108.74	110.53
20	n	5216	SQD	C1-O5-C5	2.01	117.64	113.72
13	f	1226	CLA	CHA-C4D-ND	2.01	136.69	132.55
16	5	522	BCR	C30-C25-C24	2.01	121.09	115.65
13	s	501	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	K	4104	BCR	C23-C24-C25	-2.01	121.64	127.00
20	4	822	SQD	C45-O47-C7	2.01	121.39	117.85
13	l	1303	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	f	1210	CLA	CMB-C2B-C3B	2.01	131.27	126.55
16	M	4021	BCR	C1-C6-C7	2.01	121.09	115.65
16	a	523	BCR	C10-C11-C12	-2.01	117.39	123.20
13	B	1226	CLA	CHA-C4D-ND	2.01	136.69	132.55
13	A	1121	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
13	c	503	CLA	C2A-C1A-CHA	2.01	127.35	123.87
13	v	502	CLA	C1-C2-C3	-2.01	123.52	126.76
13	B	1212	CLA	C3B-C4B-NB	-2.01	108.74	110.53
13	H	1212	CLA	C3B-C4B-NB	-2.01	108.74	110.53
13	e	1121	CLA	O2D-CGD-CBD	2.00	114.73	111.23
13	3	501	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
13	B	1223	CLA	C2A-C1A-CHA	2.00	127.34	123.87
13	B	1210	CLA	O2D-CGD-CBD	2.00	114.73	111.23
16	q	523	BCR	C35-C13-C12	2.00	121.15	118.09
16	t	524	BCR	C24-C23-C22	-2.00	123.27	126.23
16	G	4002	BCR	C21-C20-C19	-2.00	117.39	123.20
13	H	1210	CLA	O2D-CGD-CBD	2.00	114.73	111.23
16	L	4022	BCR	C10-C11-C12	-2.00	117.40	123.20
16	3	523	BCR	C10-C11-C12	-2.00	117.40	123.20
13	1	513	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
13	G	1105	CLA	O1D-CGD-CBD	2.00	128.47	124.52
13	f	1210	CLA	O2D-CGD-CBD	2.00	114.73	111.23
16	L	4020	BCR	C8-C9-C10	-2.00	115.86	119.01
13	f	1226	CLA	CHC-C1C-C2C	-2.00	121.26	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	4005	BCR	C10-C11-C12	-2.00	117.40	123.20
16	q	523	BCR	C8-C7-C6	-2.00	121.65	127.00
13	5	506	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
16	r	524	BCR	C38-C26-C25	-2.00	122.30	124.48
13	m	1105	CLA	CAC-C3C-C2C	2.00	131.24	127.56
16	1	523	BCR	C35-C13-C12	2.00	121.14	118.09
13	A	1133	CLA	CMB-C2B-C3B	2.00	131.26	126.55
13	a	511	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
16	6	522	BCR	C27-C26-C25	-2.00	120.00	122.70
16	H	4017	BCR	C16-C15-C14	-2.00	119.42	123.52
13	f	1212	CLA	C3B-C4B-NB	-2.00	108.74	110.53
13	H	1226	CLA	CMC-C2C-C3C	2.00	131.56	126.15
16	v	523	BCR	C1-C6-C5	-2.00	119.90	122.64
13	f	1225	CLA	O2D-CGD-CBD	2.00	114.73	111.23
16	d	522	BCR	C27-C26-C25	-2.00	120.00	122.70
13	u	506	CLA	O2A-CGA-O1A	-2.00	118.19	123.33
13	f	1221	CLA	C6-C5-C3	-2.00	108.60	113.47

All (588) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1011	CLA	ND
13	A	1013	CLA	ND
13	A	1102	CLA	ND
13	A	1103	CLA	ND
13	A	1104	CLA	ND
13	A	1105	CLA	ND
13	A	1106	CLA	ND
13	A	1107	CLA	ND
13	A	1108	CLA	ND
13	A	1109	CLA	ND
13	A	1110	CLA	ND
13	A	1111	CLA	ND
13	A	1112	CLA	ND
13	A	1113	CLA	ND
13	A	1114	CLA	ND
13	A	1115	CLA	ND
13	A	1116	CLA	ND
13	A	1117	CLA	ND
13	A	1118	CLA	ND
13	A	1119	CLA	ND
13	A	1120	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	A	1121	CLA	ND
13	A	1122	CLA	ND
13	A	1123	CLA	ND
13	A	1124	CLA	ND
13	A	1125	CLA	ND
13	A	1126	CLA	ND
13	A	1127	CLA	ND
13	A	1128	CLA	ND
13	A	1129	CLA	ND
13	A	1131	CLA	ND
13	A	1132	CLA	ND
13	A	1133	CLA	ND
13	A	1134	CLA	ND
13	A	1135	CLA	ND
13	A	1136	CLA	ND
13	A	1137	CLA	ND
13	A	1138	CLA	ND
13	A	1139	CLA	ND
13	A	1140	CLA	ND
13	A	1237	CLA	ND
13	A	1801	CLA	ND
13	A	1022	CLA	ND
13	A	1101	CLA	ND
13	A	1130	CLA	ND
13	B	1012	CLA	ND
13	B	1021	CLA	ND
13	B	1023	CLA	ND
13	B	1201	CLA	ND
13	B	1202	CLA	ND
13	B	1203	CLA	ND
13	B	1204	CLA	ND
13	B	1205	CLA	ND
13	B	1206	CLA	ND
13	B	1208	CLA	ND
13	B	1209	CLA	ND
13	B	1210	CLA	ND
13	B	1211	CLA	ND
13	B	1212	CLA	ND
13	B	1213	CLA	ND
13	B	1214	CLA	ND
13	B	1215	CLA	ND
13	B	1216	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	B	1217	CLA	ND
13	B	1218	CLA	ND
13	B	1219	CLA	ND
13	B	1220	CLA	ND
13	B	1221	CLA	ND
13	B	1222	CLA	ND
13	B	1223	CLA	ND
13	B	1224	CLA	ND
13	B	1225	CLA	ND
13	B	1226	CLA	ND
13	B	1227	CLA	ND
13	B	1228	CLA	ND
13	B	1229	CLA	ND
13	B	1231	CLA	ND
13	B	1232	CLA	ND
13	B	1234	CLA	ND
13	B	1235	CLA	ND
13	B	1238	CLA	ND
13	B	1239	CLA	ND
13	B	1207	CLA	ND
13	B	1230	CLA	ND
13	F	1301	CLA	ND
13	F	1302	CLA	ND
13	J	1302	CLA	ND
13	J	1303	CLA	ND
13	K	1401	CLA	ND
13	K	1103	CLA	ND
13	K	1105	CLA	ND
13	L	1501	CLA	ND
13	L	1502	CLA	ND
13	L	1503	CLA	ND
13	1	501	CLA	ND
13	1	502	CLA	ND
13	1	503	CLA	ND
13	1	504	CLA	ND
13	1	505	CLA	ND
13	1	506	CLA	ND
13	1	507	CLA	ND
13	1	508	CLA	ND
13	1	509	CLA	ND
13	1	510	CLA	ND
13	1	511	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	1	512	CLA	ND
13	1	513	CLA	ND
13	1	516	CLA	ND
13	1	517	CLA	ND
13	1	518	CLA	ND
13	1	519	CLA	ND
13	2	501	CLA	ND
13	2	502	CLA	ND
13	2	503	CLA	ND
13	2	504	CLA	ND
13	2	505	CLA	ND
13	2	506	CLA	ND
13	2	507	CLA	ND
13	2	508	CLA	ND
13	2	509	CLA	ND
13	2	510	CLA	ND
13	2	511	CLA	ND
13	2	512	CLA	ND
13	2	513	CLA	ND
13	2	516	CLA	ND
13	2	517	CLA	ND
13	2	518	CLA	ND
13	2	519	CLA	ND
13	3	501	CLA	ND
13	3	502	CLA	ND
13	3	503	CLA	ND
13	3	504	CLA	ND
13	3	505	CLA	ND
13	3	506	CLA	ND
13	3	507	CLA	ND
13	3	508	CLA	ND
13	3	509	CLA	ND
13	3	510	CLA	ND
13	3	511	CLA	ND
13	3	512	CLA	ND
13	3	513	CLA	ND
13	3	516	CLA	ND
13	3	517	CLA	ND
13	3	518	CLA	ND
13	3	519	CLA	ND
13	4	501	CLA	ND
13	4	502	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	4	503	CLA	ND
13	4	504	CLA	ND
13	4	505	CLA	ND
13	4	506	CLA	ND
13	4	507	CLA	ND
13	4	508	CLA	ND
13	4	509	CLA	ND
13	4	510	CLA	ND
13	4	511	CLA	ND
13	4	512	CLA	ND
13	4	513	CLA	ND
13	4	516	CLA	ND
13	4	517	CLA	ND
13	4	518	CLA	ND
13	4	519	CLA	ND
13	5	501	CLA	ND
13	5	502	CLA	ND
13	5	503	CLA	ND
13	5	504	CLA	ND
13	5	505	CLA	ND
13	5	506	CLA	ND
13	5	507	CLA	ND
13	5	508	CLA	ND
13	5	509	CLA	ND
13	5	510	CLA	ND
13	5	511	CLA	ND
13	5	512	CLA	ND
13	5	513	CLA	ND
13	5	516	CLA	ND
13	5	517	CLA	ND
13	5	518	CLA	ND
13	5	519	CLA	ND
13	6	501	CLA	ND
13	6	502	CLA	ND
13	6	503	CLA	ND
13	6	504	CLA	ND
13	6	505	CLA	ND
13	6	506	CLA	ND
13	6	507	CLA	ND
13	6	508	CLA	ND
13	6	509	CLA	ND
13	6	510	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	6	511	CLA	ND
13	6	512	CLA	ND
13	6	513	CLA	ND
13	6	516	CLA	ND
13	6	517	CLA	ND
13	6	518	CLA	ND
13	6	519	CLA	ND
13	G	1011	CLA	ND
13	G	1013	CLA	ND
13	G	1102	CLA	ND
13	G	1103	CLA	ND
13	G	1104	CLA	ND
13	G	1105	CLA	ND
13	G	1106	CLA	ND
13	G	1107	CLA	ND
13	G	1108	CLA	ND
13	G	1109	CLA	ND
13	G	1110	CLA	ND
13	G	1111	CLA	ND
13	G	1112	CLA	ND
13	G	1113	CLA	ND
13	G	1114	CLA	ND
13	G	1115	CLA	ND
13	G	1116	CLA	ND
13	G	1117	CLA	ND
13	G	1118	CLA	ND
13	G	1119	CLA	ND
13	G	1120	CLA	ND
13	G	1121	CLA	ND
13	G	1122	CLA	ND
13	G	1123	CLA	ND
13	G	1124	CLA	ND
13	G	1125	CLA	ND
13	G	1126	CLA	ND
13	G	1127	CLA	ND
13	G	1128	CLA	ND
13	G	1129	CLA	ND
13	G	1131	CLA	ND
13	G	1132	CLA	ND
13	G	1133	CLA	ND
13	G	1134	CLA	ND
13	G	1135	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	G	1136	CLA	ND
13	G	1137	CLA	ND
13	G	1138	CLA	ND
13	G	1139	CLA	ND
13	G	1140	CLA	ND
13	G	1237	CLA	ND
13	G	1801	CLA	ND
13	G	1022	CLA	ND
13	G	1101	CLA	ND
13	G	1130	CLA	ND
13	H	1012	CLA	ND
13	H	1021	CLA	ND
13	H	1023	CLA	ND
13	H	1201	CLA	ND
13	H	1202	CLA	ND
13	H	1203	CLA	ND
13	H	1204	CLA	ND
13	H	1205	CLA	ND
13	H	1206	CLA	ND
13	H	1208	CLA	ND
13	H	1209	CLA	ND
13	H	1210	CLA	ND
13	H	1211	CLA	ND
13	H	1212	CLA	ND
13	H	1213	CLA	ND
13	H	1214	CLA	ND
13	H	1215	CLA	ND
13	H	1216	CLA	ND
13	H	1217	CLA	ND
13	H	1218	CLA	ND
13	H	1219	CLA	ND
13	H	1220	CLA	ND
13	H	1221	CLA	ND
13	H	1222	CLA	ND
13	H	1223	CLA	ND
13	H	1224	CLA	ND
13	H	1225	CLA	ND
13	H	1226	CLA	ND
13	H	1227	CLA	ND
13	H	1228	CLA	ND
13	H	1229	CLA	ND
13	H	1231	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	H	1232	CLA	ND
13	H	1234	CLA	ND
13	H	1235	CLA	ND
13	H	1238	CLA	ND
13	H	1239	CLA	ND
13	H	1207	CLA	ND
13	H	1230	CLA	ND
13	R	1301	CLA	ND
13	R	1302	CLA	ND
13	T	1302	CLA	ND
13	T	1303	CLA	ND
13	U	1401	CLA	ND
13	U	1103	CLA	ND
13	U	1105	CLA	ND
13	V	1501	CLA	ND
13	V	1502	CLA	ND
13	V	1503	CLA	ND
13	Y	501	CLA	ND
13	Y	502	CLA	ND
13	Y	503	CLA	ND
13	Y	504	CLA	ND
13	Y	505	CLA	ND
13	Y	506	CLA	ND
13	Y	507	CLA	ND
13	Y	508	CLA	ND
13	Y	509	CLA	ND
13	Y	510	CLA	ND
13	Y	511	CLA	ND
13	Y	512	CLA	ND
13	Y	513	CLA	ND
13	Y	516	CLA	ND
13	Y	517	CLA	ND
13	Y	518	CLA	ND
13	Y	519	CLA	ND
13	Z	501	CLA	ND
13	Z	502	CLA	ND
13	Z	503	CLA	ND
13	Z	504	CLA	ND
13	Z	505	CLA	ND
13	Z	506	CLA	ND
13	Z	507	CLA	ND
13	Z	508	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	Z	509	CLA	ND
13	Z	510	CLA	ND
13	Z	511	CLA	ND
13	Z	512	CLA	ND
13	Z	513	CLA	ND
13	Z	516	CLA	ND
13	Z	517	CLA	ND
13	Z	518	CLA	ND
13	Z	519	CLA	ND
13	a	501	CLA	ND
13	a	502	CLA	ND
13	a	503	CLA	ND
13	a	504	CLA	ND
13	a	505	CLA	ND
13	a	506	CLA	ND
13	a	507	CLA	ND
13	a	508	CLA	ND
13	a	509	CLA	ND
13	a	510	CLA	ND
13	a	511	CLA	ND
13	a	512	CLA	ND
13	a	513	CLA	ND
13	a	516	CLA	ND
13	a	517	CLA	ND
13	a	518	CLA	ND
13	a	519	CLA	ND
13	b	501	CLA	ND
13	b	502	CLA	ND
13	b	503	CLA	ND
13	b	504	CLA	ND
13	b	505	CLA	ND
13	b	506	CLA	ND
13	b	507	CLA	ND
13	b	508	CLA	ND
13	b	509	CLA	ND
13	b	510	CLA	ND
13	b	511	CLA	ND
13	b	512	CLA	ND
13	b	513	CLA	ND
13	b	516	CLA	ND
13	b	517	CLA	ND
13	b	518	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	b	519	CLA	ND
13	c	501	CLA	ND
13	c	502	CLA	ND
13	c	503	CLA	ND
13	c	504	CLA	ND
13	c	505	CLA	ND
13	c	506	CLA	ND
13	c	507	CLA	ND
13	c	508	CLA	ND
13	c	509	CLA	ND
13	c	510	CLA	ND
13	c	511	CLA	ND
13	c	512	CLA	ND
13	c	513	CLA	ND
13	c	516	CLA	ND
13	c	517	CLA	ND
13	c	518	CLA	ND
13	c	519	CLA	ND
13	d	501	CLA	ND
13	d	502	CLA	ND
13	d	503	CLA	ND
13	d	504	CLA	ND
13	d	505	CLA	ND
13	d	506	CLA	ND
13	d	507	CLA	ND
13	d	508	CLA	ND
13	d	509	CLA	ND
13	d	510	CLA	ND
13	d	511	CLA	ND
13	d	512	CLA	ND
13	d	513	CLA	ND
13	d	516	CLA	ND
13	d	517	CLA	ND
13	d	518	CLA	ND
13	d	519	CLA	ND
13	e	1011	CLA	ND
13	e	1013	CLA	ND
13	e	1102	CLA	ND
13	e	1103	CLA	ND
13	e	1104	CLA	ND
13	e	1105	CLA	ND
13	e	1106	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	e	1107	CLA	ND
13	e	1108	CLA	ND
13	e	1109	CLA	ND
13	e	1110	CLA	ND
13	e	1111	CLA	ND
13	e	1112	CLA	ND
13	e	1113	CLA	ND
13	e	1114	CLA	ND
13	e	1115	CLA	ND
13	e	1116	CLA	ND
13	e	1117	CLA	ND
13	e	1118	CLA	ND
13	e	1119	CLA	ND
13	e	1120	CLA	ND
13	e	1121	CLA	ND
13	e	1122	CLA	ND
13	e	1123	CLA	ND
13	e	1124	CLA	ND
13	e	1125	CLA	ND
13	e	1126	CLA	ND
13	e	1127	CLA	ND
13	e	1128	CLA	ND
13	e	1129	CLA	ND
13	e	1131	CLA	ND
13	e	1132	CLA	ND
13	e	1133	CLA	ND
13	e	1134	CLA	ND
13	e	1135	CLA	ND
13	e	1136	CLA	ND
13	e	1137	CLA	ND
13	e	1138	CLA	ND
13	e	1139	CLA	ND
13	e	1140	CLA	ND
13	e	1237	CLA	ND
13	e	1801	CLA	ND
13	e	1022	CLA	ND
13	e	1101	CLA	ND
13	e	1130	CLA	ND
13	f	1012	CLA	ND
13	f	1021	CLA	ND
13	f	1023	CLA	ND
13	f	1201	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	f	1202	CLA	ND
13	f	1203	CLA	ND
13	f	1204	CLA	ND
13	f	1205	CLA	ND
13	f	1206	CLA	ND
13	f	1208	CLA	ND
13	f	1209	CLA	ND
13	f	1210	CLA	ND
13	f	1211	CLA	ND
13	f	1212	CLA	ND
13	f	1213	CLA	ND
13	f	1214	CLA	ND
13	f	1215	CLA	ND
13	f	1216	CLA	ND
13	f	1217	CLA	ND
13	f	1218	CLA	ND
13	f	1219	CLA	ND
13	f	1220	CLA	ND
13	f	1221	CLA	ND
13	f	1222	CLA	ND
13	f	1223	CLA	ND
13	f	1224	CLA	ND
13	f	1225	CLA	ND
13	f	1226	CLA	ND
13	f	1227	CLA	ND
13	f	1228	CLA	ND
13	f	1229	CLA	ND
13	f	1231	CLA	ND
13	f	1232	CLA	ND
13	f	1234	CLA	ND
13	f	1235	CLA	ND
13	f	1238	CLA	ND
13	f	1239	CLA	ND
13	f	1207	CLA	ND
13	f	1230	CLA	ND
13	j	1301	CLA	ND
13	j	1302	CLA	ND
13	l	1302	CLA	ND
13	l	1303	CLA	ND
13	m	1401	CLA	ND
13	m	1103	CLA	ND
13	m	1105	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	n	1501	CLA	ND
13	n	1502	CLA	ND
13	n	1503	CLA	ND
13	q	501	CLA	ND
13	q	502	CLA	ND
13	q	503	CLA	ND
13	q	504	CLA	ND
13	q	505	CLA	ND
13	q	506	CLA	ND
13	q	507	CLA	ND
13	q	508	CLA	ND
13	q	509	CLA	ND
13	q	510	CLA	ND
13	q	511	CLA	ND
13	q	512	CLA	ND
13	q	513	CLA	ND
13	q	516	CLA	ND
13	q	517	CLA	ND
13	q	518	CLA	ND
13	q	519	CLA	ND
13	r	501	CLA	ND
13	r	502	CLA	ND
13	r	503	CLA	ND
13	r	504	CLA	ND
13	r	505	CLA	ND
13	r	506	CLA	ND
13	r	507	CLA	ND
13	r	508	CLA	ND
13	r	509	CLA	ND
13	r	510	CLA	ND
13	r	511	CLA	ND
13	r	512	CLA	ND
13	r	513	CLA	ND
13	r	516	CLA	ND
13	r	517	CLA	ND
13	r	518	CLA	ND
13	r	519	CLA	ND
13	s	501	CLA	ND
13	s	502	CLA	ND
13	s	503	CLA	ND
13	s	504	CLA	ND
13	s	505	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	s	506	CLA	ND
13	s	507	CLA	ND
13	s	508	CLA	ND
13	s	509	CLA	ND
13	s	510	CLA	ND
13	s	511	CLA	ND
13	s	512	CLA	ND
13	s	513	CLA	ND
13	s	516	CLA	ND
13	s	517	CLA	ND
13	s	518	CLA	ND
13	s	519	CLA	ND
13	t	501	CLA	ND
13	t	502	CLA	ND
13	t	503	CLA	ND
13	t	504	CLA	ND
13	t	505	CLA	ND
13	t	506	CLA	ND
13	t	507	CLA	ND
13	t	508	CLA	ND
13	t	509	CLA	ND
13	t	510	CLA	ND
13	t	511	CLA	ND
13	t	512	CLA	ND
13	t	513	CLA	ND
13	t	516	CLA	ND
13	t	517	CLA	ND
13	t	518	CLA	ND
13	t	519	CLA	ND
13	u	501	CLA	ND
13	u	502	CLA	ND
13	u	503	CLA	ND
13	u	504	CLA	ND
13	u	505	CLA	ND
13	u	506	CLA	ND
13	u	507	CLA	ND
13	u	508	CLA	ND
13	u	509	CLA	ND
13	u	510	CLA	ND
13	u	511	CLA	ND
13	u	512	CLA	ND
13	u	513	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
13	u	516	CLA	ND
13	u	517	CLA	ND
13	u	518	CLA	ND
13	u	519	CLA	ND
13	v	501	CLA	ND
13	v	502	CLA	ND
13	v	503	CLA	ND
13	v	504	CLA	ND
13	v	505	CLA	ND
13	v	506	CLA	ND
13	v	507	CLA	ND
13	v	508	CLA	ND
13	v	509	CLA	ND
13	v	510	CLA	ND
13	v	511	CLA	ND
13	v	512	CLA	ND
13	v	513	CLA	ND
13	v	516	CLA	ND
13	v	517	CLA	ND
13	v	518	CLA	ND
13	v	519	CLA	ND

All (8327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	C1A-C2A-CAA-CBA
13	A	1103	CLA	CAD-CBD-CGD-O1D
13	A	1103	CLA	CAD-CBD-CGD-O2D
13	A	1104	CLA	C1A-C2A-CAA-CBA
13	A	1104	CLA	C4-C3-C5-C6
13	A	1106	CLA	C3A-C2A-CAA-CBA
13	A	1106	CLA	CHA-CBD-CGD-O1D
13	A	1106	CLA	CHA-CBD-CGD-O2D
13	A	1107	CLA	C4B-C3B-CAB-CBB
13	A	1108	CLA	C1A-C2A-CAA-CBA
13	A	1108	CLA	C3A-C2A-CAA-CBA
13	A	1110	CLA	C1A-C2A-CAA-CBA
13	A	1110	CLA	C3A-C2A-CAA-CBA
13	A	1110	CLA	C2-C3-C5-C6
13	A	1110	CLA	C4-C3-C5-C6
13	A	1116	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1117	CLA	CBD-CGD-O2D-CED
13	A	1121	CLA	C2B-C3B-CAB-CBB
13	A	1121	CLA	C4B-C3B-CAB-CBB
13	A	1122	CLA	C2B-C3B-CAB-CBB
13	A	1122	CLA	C4B-C3B-CAB-CBB
13	A	1126	CLA	C1A-C2A-CAA-CBA
13	A	1126	CLA	C3A-C2A-CAA-CBA
13	A	1128	CLA	CHA-CBD-CGD-O1D
13	A	1128	CLA	CHA-CBD-CGD-O2D
13	A	1131	CLA	CBD-CGD-O2D-CED
13	A	1132	CLA	CHA-CBD-CGD-O1D
13	A	1132	CLA	CHA-CBD-CGD-O2D
13	A	1134	CLA	C1A-C2A-CAA-CBA
13	A	1137	CLA	CHA-CBD-CGD-O1D
13	A	1137	CLA	CHA-CBD-CGD-O2D
13	A	1139	CLA	C1A-C2A-CAA-CBA
13	A	1139	CLA	C3A-C2A-CAA-CBA
13	A	1139	CLA	CBD-CGD-O2D-CED
13	A	1140	CLA	C1A-C2A-CAA-CBA
13	A	1140	CLA	C2-C3-C5-C6
13	A	1140	CLA	C4-C3-C5-C6
13	A	1101	CLA	CHA-CBD-CGD-O1D
13	A	1101	CLA	CHA-CBD-CGD-O2D
13	B	1012	CLA	CAD-CBD-CGD-O1D
13	B	1012	CLA	CAD-CBD-CGD-O2D
13	B	1202	CLA	C1A-C2A-CAA-CBA
13	B	1202	CLA	C3A-C2A-CAA-CBA
13	B	1205	CLA	CHA-CBD-CGD-O1D
13	B	1205	CLA	CHA-CBD-CGD-O2D
13	B	1209	CLA	C1A-C2A-CAA-CBA
13	B	1209	CLA	C3A-C2A-CAA-CBA
13	B	1209	CLA	CHA-CBD-CGD-O1D
13	B	1209	CLA	CHA-CBD-CGD-O2D
13	B	1210	CLA	C1A-C2A-CAA-CBA
13	B	1210	CLA	C11-C12-C13-C15
13	B	1211	CLA	CHA-CBD-CGD-O2D
13	B	1213	CLA	CHA-CBD-CGD-O1D
13	B	1213	CLA	CHA-CBD-CGD-O2D
13	B	1214	CLA	C4B-C3B-CAB-CBB
13	B	1215	CLA	C1A-C2A-CAA-CBA
13	B	1215	CLA	C3A-C2A-CAA-CBA
13	B	1216	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1216	CLA	C4B-C3B-CAB-CBB
13	B	1217	CLA	C1A-C2A-CAA-CBA
13	B	1217	CLA	C3A-C2A-CAA-CBA
13	B	1220	CLA	C2B-C3B-CAB-CBB
13	B	1220	CLA	C4B-C3B-CAB-CBB
13	B	1221	CLA	C1A-C2A-CAA-CBA
13	B	1221	CLA	CHA-CBD-CGD-O1D
13	B	1221	CLA	CHA-CBD-CGD-O2D
13	B	1222	CLA	CHA-CBD-CGD-O1D
13	B	1222	CLA	CHA-CBD-CGD-O2D
13	B	1224	CLA	C1A-C2A-CAA-CBA
13	B	1224	CLA	C3A-C2A-CAA-CBA
13	B	1226	CLA	CHA-CBD-CGD-O1D
13	B	1226	CLA	CHA-CBD-CGD-O2D
13	B	1239	CLA	C4B-C3B-CAB-CBB
13	B	1240	CLA	C1A-C2A-CAA-CBA
13	B	1230	CLA	C1A-C2A-CAA-CBA
13	B	1230	CLA	C3A-C2A-CAA-CBA
13	B	1230	CLA	C2B-C3B-CAB-CBB
13	B	1230	CLA	C4B-C3B-CAB-CBB
13	F	1302	CLA	C1A-C2A-CAA-CBA
13	F	1302	CLA	C3A-C2A-CAA-CBA
13	J	1302	CLA	CAD-CBD-CGD-O1D
13	J	1302	CLA	CAD-CBD-CGD-O2D
13	J	1303	CLA	C1A-C2A-CAA-CBA
13	K	1401	CLA	C1A-C2A-CAA-CBA
13	K	1401	CLA	C4B-C3B-CAB-CBB
13	K	1103	CLA	C2B-C3B-CAB-CBB
13	K	1103	CLA	C4B-C3B-CAB-CBB
13	K	1105	CLA	C2B-C3B-CAB-CBB
13	K	1105	CLA	C4B-C3B-CAB-CBB
13	1	501	CLA	C4B-C3B-CAB-CBB
13	1	501	CLA	CAD-CBD-CGD-O1D
13	1	501	CLA	CAD-CBD-CGD-O2D
13	1	501	CLA	CBD-CGD-O2D-CED
13	1	504	CLA	C2B-C3B-CAB-CBB
13	1	504	CLA	C4B-C3B-CAB-CBB
13	1	506	CLA	CAD-CBD-CGD-O2D
13	1	507	CLA	CHA-CBD-CGD-O1D
13	1	507	CLA	CHA-CBD-CGD-O2D
13	1	508	CLA	C2-C3-C5-C6
13	1	508	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	1	510	CLA	CBD-CGD-O2D-CED
13	1	512	CLA	C4B-C3B-CAB-CBB
13	1	512	CLA	C3-C5-C6-C7
13	1	516	CLA	C1A-C2A-CAA-CBA
13	1	516	CLA	C3A-C2A-CAA-CBA
13	1	516	CLA	C2B-C3B-CAB-CBB
13	1	516	CLA	C4B-C3B-CAB-CBB
13	1	516	CLA	CAD-CBD-CGD-O1D
13	1	516	CLA	CAD-CBD-CGD-O2D
13	1	517	CLA	C2B-C3B-CAB-CBB
13	1	517	CLA	C4B-C3B-CAB-CBB
13	1	518	CLA	C2B-C3B-CAB-CBB
13	1	518	CLA	C4B-C3B-CAB-CBB
13	1	518	CLA	CHA-CBD-CGD-O1D
13	1	518	CLA	CHA-CBD-CGD-O2D
13	1	518	CLA	C2-C3-C5-C6
13	1	518	CLA	C4-C3-C5-C6
13	1	519	CLA	C2B-C3B-CAB-CBB
13	1	519	CLA	C4B-C3B-CAB-CBB
13	2	501	CLA	C4B-C3B-CAB-CBB
13	2	501	CLA	CBD-CGD-O2D-CED
13	2	506	CLA	C2-C3-C5-C6
13	2	506	CLA	C4-C3-C5-C6
13	2	507	CLA	CHA-CBD-CGD-O1D
13	2	507	CLA	CHA-CBD-CGD-O2D
13	2	507	CLA	C2-C3-C5-C6
13	2	507	CLA	C4-C3-C5-C6
13	2	513	CLA	CBD-CGD-O2D-CED
13	2	516	CLA	C4B-C3B-CAB-CBB
13	2	516	CLA	CHA-CBD-CGD-O1D
13	2	516	CLA	CHA-CBD-CGD-O2D
13	2	518	CLA	CAD-CBD-CGD-O2D
13	2	519	CLA	C2B-C3B-CAB-CBB
13	2	519	CLA	C4B-C3B-CAB-CBB
13	3	502	CLA	CHA-CBD-CGD-O1D
13	3	502	CLA	CHA-CBD-CGD-O2D
13	3	503	CLA	C2B-C3B-CAB-CBB
13	3	503	CLA	C4B-C3B-CAB-CBB
13	3	510	CLA	CAD-CBD-CGD-O1D
13	3	510	CLA	CAD-CBD-CGD-O2D
13	3	512	CLA	C4B-C3B-CAB-CBB
13	3	512	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	3	513	CLA	C1A-C2A-CAA-CBA
13	3	513	CLA	CBD-CGD-O2D-CED
13	3	516	CLA	CAD-CBD-CGD-O1D
13	3	516	CLA	CAD-CBD-CGD-O2D
13	3	517	CLA	C2B-C3B-CAB-CBB
13	3	517	CLA	C4B-C3B-CAB-CBB
13	3	517	CLA	CBD-CGD-O2D-CED
13	3	518	CLA	C2B-C3B-CAB-CBB
13	3	518	CLA	C4B-C3B-CAB-CBB
13	3	518	CLA	CAD-CBD-CGD-O2D
13	4	501	CLA	C4B-C3B-CAB-CBB
13	4	501	CLA	CBD-CGD-O2D-CED
13	4	501	CLA	O1D-CGD-O2D-CED
13	4	502	CLA	CHA-CBD-CGD-O1D
13	4	502	CLA	CHA-CBD-CGD-O2D
13	4	503	CLA	CHA-CBD-CGD-O2D
13	4	506	CLA	CHA-CBD-CGD-O2D
13	4	506	CLA	CBD-CGD-O2D-CED
13	4	507	CLA	CHA-CBD-CGD-O1D
13	4	507	CLA	CHA-CBD-CGD-O2D
13	4	510	CLA	CBD-CGD-O2D-CED
13	4	517	CLA	C1A-C2A-CAA-CBA
13	4	517	CLA	C3A-C2A-CAA-CBA
13	4	518	CLA	C2B-C3B-CAB-CBB
13	4	518	CLA	C4B-C3B-CAB-CBB
13	4	519	CLA	C4B-C3B-CAB-CBB
13	4	519	CLA	CAD-CBD-CGD-O1D
13	4	519	CLA	CAD-CBD-CGD-O2D
13	5	501	CLA	CBD-CGD-O2D-CED
13	5	504	CLA	CBD-CGD-O2D-CED
13	5	505	CLA	CHA-CBD-CGD-O2D
13	5	506	CLA	CAD-CBD-CGD-O2D
13	5	507	CLA	CBD-CGD-O2D-CED
13	5	511	CLA	CBD-CGD-O2D-CED
13	5	512	CLA	C4B-C3B-CAB-CBB
13	5	513	CLA	C2B-C3B-CAB-CBB
13	5	513	CLA	C4B-C3B-CAB-CBB
13	5	513	CLA	CBD-CGD-O2D-CED
13	5	516	CLA	C4B-C3B-CAB-CBB
13	5	517	CLA	C4B-C3B-CAB-CBB
13	5	517	CLA	CAD-CBD-CGD-O2D
13	5	518	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	5	518	CLA	C4B-C3B-CAB-CBB
13	5	519	CLA	CAD-CBD-CGD-O1D
13	5	519	CLA	CAD-CBD-CGD-O2D
13	6	501	CLA	CBD-CGD-O2D-CED
13	6	504	CLA	CAD-CBD-CGD-O2D
13	6	505	CLA	C6-C7-C8-C9
13	6	512	CLA	C4B-C3B-CAB-CBB
13	6	513	CLA	CBD-CGD-O2D-CED
13	6	516	CLA	CBD-CGD-O2D-CED
13	6	517	CLA	CAD-CBD-CGD-O1D
13	6	517	CLA	CAD-CBD-CGD-O2D
13	6	518	CLA	CAD-CBD-CGD-O2D
13	6	519	CLA	CHA-CBD-CGD-O2D
13	G	1102	CLA	C3A-C2A-CAA-CBA
13	G	1103	CLA	C1A-C2A-CAA-CBA
13	G	1103	CLA	CAD-CBD-CGD-O1D
13	G	1103	CLA	CAD-CBD-CGD-O2D
13	G	1104	CLA	C1A-C2A-CAA-CBA
13	G	1104	CLA	C4-C3-C5-C6
13	G	1106	CLA	C3A-C2A-CAA-CBA
13	G	1106	CLA	CHA-CBD-CGD-O1D
13	G	1106	CLA	CHA-CBD-CGD-O2D
13	G	1107	CLA	C4B-C3B-CAB-CBB
13	G	1108	CLA	C1A-C2A-CAA-CBA
13	G	1108	CLA	C3A-C2A-CAA-CBA
13	G	1110	CLA	C1A-C2A-CAA-CBA
13	G	1110	CLA	C3A-C2A-CAA-CBA
13	G	1110	CLA	C2-C3-C5-C6
13	G	1110	CLA	C4-C3-C5-C6
13	G	1116	CLA	C3A-C2A-CAA-CBA
13	G	1117	CLA	CBD-CGD-O2D-CED
13	G	1121	CLA	C2B-C3B-CAB-CBB
13	G	1121	CLA	C4B-C3B-CAB-CBB
13	G	1122	CLA	C2B-C3B-CAB-CBB
13	G	1122	CLA	C4B-C3B-CAB-CBB
13	G	1126	CLA	C1A-C2A-CAA-CBA
13	G	1126	CLA	C3A-C2A-CAA-CBA
13	G	1128	CLA	CHA-CBD-CGD-O1D
13	G	1128	CLA	CHA-CBD-CGD-O2D
13	G	1131	CLA	CBD-CGD-O2D-CED
13	G	1132	CLA	CHA-CBD-CGD-O1D
13	G	1132	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1134	CLA	C1A-C2A-CAA-CBA
13	G	1137	CLA	CHA-CBD-CGD-O1D
13	G	1137	CLA	CHA-CBD-CGD-O2D
13	G	1139	CLA	C1A-C2A-CAA-CBA
13	G	1139	CLA	C3A-C2A-CAA-CBA
13	G	1139	CLA	CBD-CGD-O2D-CED
13	G	1140	CLA	C1A-C2A-CAA-CBA
13	G	1140	CLA	C2-C3-C5-C6
13	G	1140	CLA	C4-C3-C5-C6
13	G	1101	CLA	CHA-CBD-CGD-O1D
13	G	1101	CLA	CHA-CBD-CGD-O2D
13	H	1012	CLA	CAD-CBD-CGD-O1D
13	H	1012	CLA	CAD-CBD-CGD-O2D
13	H	1202	CLA	C1A-C2A-CAA-CBA
13	H	1202	CLA	C3A-C2A-CAA-CBA
13	H	1205	CLA	CHA-CBD-CGD-O1D
13	H	1205	CLA	CHA-CBD-CGD-O2D
13	H	1209	CLA	C1A-C2A-CAA-CBA
13	H	1209	CLA	C3A-C2A-CAA-CBA
13	H	1209	CLA	CHA-CBD-CGD-O1D
13	H	1209	CLA	CHA-CBD-CGD-O2D
13	H	1210	CLA	C1A-C2A-CAA-CBA
13	H	1210	CLA	C11-C12-C13-C15
13	H	1211	CLA	CHA-CBD-CGD-O2D
13	H	1213	CLA	CHA-CBD-CGD-O1D
13	H	1213	CLA	CHA-CBD-CGD-O2D
13	H	1214	CLA	C4B-C3B-CAB-CBB
13	H	1215	CLA	C1A-C2A-CAA-CBA
13	H	1215	CLA	C3A-C2A-CAA-CBA
13	H	1216	CLA	C2B-C3B-CAB-CBB
13	H	1216	CLA	C4B-C3B-CAB-CBB
13	H	1217	CLA	C1A-C2A-CAA-CBA
13	H	1217	CLA	C3A-C2A-CAA-CBA
13	H	1220	CLA	C2B-C3B-CAB-CBB
13	H	1220	CLA	C4B-C3B-CAB-CBB
13	H	1221	CLA	C1A-C2A-CAA-CBA
13	H	1221	CLA	CHA-CBD-CGD-O1D
13	H	1221	CLA	CHA-CBD-CGD-O2D
13	H	1222	CLA	CHA-CBD-CGD-O1D
13	H	1222	CLA	CHA-CBD-CGD-O2D
13	H	1224	CLA	C1A-C2A-CAA-CBA
13	H	1224	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1226	CLA	CHA-CBD-CGD-O1D
13	H	1226	CLA	CHA-CBD-CGD-O2D
13	H	1239	CLA	C4B-C3B-CAB-CBB
13	H	1240	CLA	C1A-C2A-CAA-CBA
13	H	1230	CLA	C1A-C2A-CAA-CBA
13	H	1230	CLA	C3A-C2A-CAA-CBA
13	H	1230	CLA	C2B-C3B-CAB-CBB
13	H	1230	CLA	C4B-C3B-CAB-CBB
13	R	1302	CLA	C1A-C2A-CAA-CBA
13	R	1302	CLA	C3A-C2A-CAA-CBA
13	T	1302	CLA	CAD-CBD-CGD-O1D
13	T	1302	CLA	CAD-CBD-CGD-O2D
13	T	1303	CLA	C1A-C2A-CAA-CBA
13	U	1401	CLA	C1A-C2A-CAA-CBA
13	U	1401	CLA	C4B-C3B-CAB-CBB
13	U	1103	CLA	C2B-C3B-CAB-CBB
13	U	1103	CLA	C4B-C3B-CAB-CBB
13	U	1105	CLA	C2B-C3B-CAB-CBB
13	U	1105	CLA	C4B-C3B-CAB-CBB
13	Y	501	CLA	C4B-C3B-CAB-CBB
13	Y	501	CLA	CAD-CBD-CGD-O1D
13	Y	501	CLA	CAD-CBD-CGD-O2D
13	Y	501	CLA	CBD-CGD-O2D-CED
13	Y	504	CLA	C2B-C3B-CAB-CBB
13	Y	504	CLA	C4B-C3B-CAB-CBB
13	Y	506	CLA	CAD-CBD-CGD-O2D
13	Y	507	CLA	CHA-CBD-CGD-O1D
13	Y	507	CLA	CHA-CBD-CGD-O2D
13	Y	508	CLA	C2-C3-C5-C6
13	Y	508	CLA	C4-C3-C5-C6
13	Y	510	CLA	CBD-CGD-O2D-CED
13	Y	512	CLA	C4B-C3B-CAB-CBB
13	Y	512	CLA	C3-C5-C6-C7
13	Y	516	CLA	C1A-C2A-CAA-CBA
13	Y	516	CLA	C3A-C2A-CAA-CBA
13	Y	516	CLA	C2B-C3B-CAB-CBB
13	Y	516	CLA	C4B-C3B-CAB-CBB
13	Y	516	CLA	CAD-CBD-CGD-O1D
13	Y	516	CLA	CAD-CBD-CGD-O2D
13	Y	517	CLA	C2B-C3B-CAB-CBB
13	Y	517	CLA	C4B-C3B-CAB-CBB
13	Y	518	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Y	518	CLA	C4B-C3B-CAB-CBB
13	Y	518	CLA	CHA-CBD-CGD-O1D
13	Y	518	CLA	CHA-CBD-CGD-O2D
13	Y	518	CLA	C2-C3-C5-C6
13	Y	518	CLA	C4-C3-C5-C6
13	Y	519	CLA	C2B-C3B-CAB-CBB
13	Y	519	CLA	C4B-C3B-CAB-CBB
13	Z	501	CLA	C4B-C3B-CAB-CBB
13	Z	501	CLA	CBD-CGD-O2D-CED
13	Z	506	CLA	C2-C3-C5-C6
13	Z	506	CLA	C4-C3-C5-C6
13	Z	507	CLA	CHA-CBD-CGD-O1D
13	Z	507	CLA	CHA-CBD-CGD-O2D
13	Z	507	CLA	C2-C3-C5-C6
13	Z	507	CLA	C4-C3-C5-C6
13	Z	513	CLA	CBD-CGD-O2D-CED
13	Z	516	CLA	C4B-C3B-CAB-CBB
13	Z	516	CLA	CHA-CBD-CGD-O1D
13	Z	516	CLA	CHA-CBD-CGD-O2D
13	Z	518	CLA	CAD-CBD-CGD-O2D
13	Z	519	CLA	C2B-C3B-CAB-CBB
13	Z	519	CLA	C4B-C3B-CAB-CBB
13	a	502	CLA	CHA-CBD-CGD-O1D
13	a	502	CLA	CHA-CBD-CGD-O2D
13	a	503	CLA	C2B-C3B-CAB-CBB
13	a	503	CLA	C4B-C3B-CAB-CBB
13	a	510	CLA	CAD-CBD-CGD-O1D
13	a	510	CLA	CAD-CBD-CGD-O2D
13	a	512	CLA	C4B-C3B-CAB-CBB
13	a	512	CLA	CHA-CBD-CGD-O2D
13	a	513	CLA	C1A-C2A-CAA-CBA
13	a	513	CLA	CBD-CGD-O2D-CED
13	a	516	CLA	CAD-CBD-CGD-O2D
13	a	517	CLA	C2B-C3B-CAB-CBB
13	a	517	CLA	C4B-C3B-CAB-CBB
13	a	517	CLA	CBD-CGD-O2D-CED
13	a	518	CLA	C2B-C3B-CAB-CBB
13	a	518	CLA	C4B-C3B-CAB-CBB
13	a	518	CLA	CAD-CBD-CGD-O2D
13	b	501	CLA	C4B-C3B-CAB-CBB
13	b	501	CLA	CBD-CGD-O2D-CED
13	b	501	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	b	502	CLA	CHA-CBD-CGD-O1D
13	b	502	CLA	CHA-CBD-CGD-O2D
13	b	503	CLA	CHA-CBD-CGD-O2D
13	b	506	CLA	CHA-CBD-CGD-O2D
13	b	506	CLA	CBD-CGD-O2D-CED
13	b	507	CLA	CHA-CBD-CGD-O1D
13	b	507	CLA	CHA-CBD-CGD-O2D
13	b	510	CLA	CBD-CGD-O2D-CED
13	b	517	CLA	C1A-C2A-CAA-CBA
13	b	517	CLA	C3A-C2A-CAA-CBA
13	b	518	CLA	C2B-C3B-CAB-CBB
13	b	518	CLA	C4B-C3B-CAB-CBB
13	b	519	CLA	C4B-C3B-CAB-CBB
13	b	519	CLA	CAD-CBD-CGD-O1D
13	b	519	CLA	CAD-CBD-CGD-O2D
13	c	501	CLA	CBD-CGD-O2D-CED
13	c	504	CLA	CBD-CGD-O2D-CED
13	c	505	CLA	CHA-CBD-CGD-O2D
13	c	506	CLA	CAD-CBD-CGD-O2D
13	c	507	CLA	CBD-CGD-O2D-CED
13	c	511	CLA	CBD-CGD-O2D-CED
13	c	512	CLA	C4B-C3B-CAB-CBB
13	c	513	CLA	C2B-C3B-CAB-CBB
13	c	513	CLA	C4B-C3B-CAB-CBB
13	c	513	CLA	CBD-CGD-O2D-CED
13	c	516	CLA	C4B-C3B-CAB-CBB
13	c	517	CLA	C4B-C3B-CAB-CBB
13	c	517	CLA	CAD-CBD-CGD-O2D
13	c	518	CLA	C2B-C3B-CAB-CBB
13	c	518	CLA	C4B-C3B-CAB-CBB
13	c	519	CLA	CAD-CBD-CGD-O1D
13	c	519	CLA	CAD-CBD-CGD-O2D
13	d	501	CLA	CBD-CGD-O2D-CED
13	d	504	CLA	CAD-CBD-CGD-O2D
13	d	505	CLA	C6-C7-C8-C9
13	d	512	CLA	C4B-C3B-CAB-CBB
13	d	513	CLA	CBD-CGD-O2D-CED
13	d	516	CLA	CBD-CGD-O2D-CED
13	d	517	CLA	CAD-CBD-CGD-O1D
13	d	517	CLA	CAD-CBD-CGD-O2D
13	d	518	CLA	CAD-CBD-CGD-O2D
13	d	519	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1102	CLA	C3A-C2A-CAA-CBA
13	e	1103	CLA	C1A-C2A-CAA-CBA
13	e	1103	CLA	CAD-CBD-CGD-O1D
13	e	1103	CLA	CAD-CBD-CGD-O2D
13	e	1104	CLA	C1A-C2A-CAA-CBA
13	e	1104	CLA	C4-C3-C5-C6
13	e	1106	CLA	C3A-C2A-CAA-CBA
13	e	1106	CLA	CHA-CBD-CGD-O1D
13	e	1106	CLA	CHA-CBD-CGD-O2D
13	e	1107	CLA	C4B-C3B-CAB-CBB
13	e	1108	CLA	C1A-C2A-CAA-CBA
13	e	1108	CLA	C3A-C2A-CAA-CBA
13	e	1110	CLA	C1A-C2A-CAA-CBA
13	e	1110	CLA	C3A-C2A-CAA-CBA
13	e	1110	CLA	C2-C3-C5-C6
13	e	1110	CLA	C4-C3-C5-C6
13	e	1116	CLA	C3A-C2A-CAA-CBA
13	e	1117	CLA	CBD-CGD-O2D-CED
13	e	1121	CLA	C2B-C3B-CAB-CBB
13	e	1121	CLA	C4B-C3B-CAB-CBB
13	e	1122	CLA	C2B-C3B-CAB-CBB
13	e	1122	CLA	C4B-C3B-CAB-CBB
13	e	1126	CLA	C1A-C2A-CAA-CBA
13	e	1126	CLA	C3A-C2A-CAA-CBA
13	e	1128	CLA	CHA-CBD-CGD-O1D
13	e	1128	CLA	CHA-CBD-CGD-O2D
13	e	1131	CLA	CBD-CGD-O2D-CED
13	e	1132	CLA	CHA-CBD-CGD-O1D
13	e	1132	CLA	CHA-CBD-CGD-O2D
13	e	1134	CLA	C1A-C2A-CAA-CBA
13	e	1137	CLA	CHA-CBD-CGD-O1D
13	e	1137	CLA	CHA-CBD-CGD-O2D
13	e	1139	CLA	C1A-C2A-CAA-CBA
13	e	1139	CLA	C3A-C2A-CAA-CBA
13	e	1139	CLA	CBD-CGD-O2D-CED
13	e	1140	CLA	C1A-C2A-CAA-CBA
13	e	1140	CLA	C2-C3-C5-C6
13	e	1140	CLA	C4-C3-C5-C6
13	e	1101	CLA	CHA-CBD-CGD-O1D
13	e	1101	CLA	CHA-CBD-CGD-O2D
13	f	1012	CLA	CAD-CBD-CGD-O1D
13	f	1012	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1202	CLA	C1A-C2A-CAA-CBA
13	f	1202	CLA	C3A-C2A-CAA-CBA
13	f	1205	CLA	CHA-CBD-CGD-O1D
13	f	1205	CLA	CHA-CBD-CGD-O2D
13	f	1209	CLA	C1A-C2A-CAA-CBA
13	f	1209	CLA	C3A-C2A-CAA-CBA
13	f	1209	CLA	CHA-CBD-CGD-O1D
13	f	1209	CLA	CHA-CBD-CGD-O2D
13	f	1210	CLA	C1A-C2A-CAA-CBA
13	f	1210	CLA	C11-C12-C13-C15
13	f	1211	CLA	CHA-CBD-CGD-O2D
13	f	1213	CLA	CHA-CBD-CGD-O1D
13	f	1213	CLA	CHA-CBD-CGD-O2D
13	f	1214	CLA	C4B-C3B-CAB-CBB
13	f	1215	CLA	C1A-C2A-CAA-CBA
13	f	1215	CLA	C3A-C2A-CAA-CBA
13	f	1216	CLA	C2B-C3B-CAB-CBB
13	f	1216	CLA	C4B-C3B-CAB-CBB
13	f	1217	CLA	C1A-C2A-CAA-CBA
13	f	1217	CLA	C3A-C2A-CAA-CBA
13	f	1220	CLA	C2B-C3B-CAB-CBB
13	f	1220	CLA	C4B-C3B-CAB-CBB
13	f	1221	CLA	C1A-C2A-CAA-CBA
13	f	1221	CLA	CHA-CBD-CGD-O1D
13	f	1221	CLA	CHA-CBD-CGD-O2D
13	f	1222	CLA	CHA-CBD-CGD-O1D
13	f	1222	CLA	CHA-CBD-CGD-O2D
13	f	1224	CLA	C1A-C2A-CAA-CBA
13	f	1224	CLA	C3A-C2A-CAA-CBA
13	f	1226	CLA	CHA-CBD-CGD-O1D
13	f	1226	CLA	CHA-CBD-CGD-O2D
13	f	1239	CLA	C4B-C3B-CAB-CBB
13	f	1240	CLA	C1A-C2A-CAA-CBA
13	f	1230	CLA	C1A-C2A-CAA-CBA
13	f	1230	CLA	C3A-C2A-CAA-CBA
13	f	1230	CLA	C2B-C3B-CAB-CBB
13	f	1230	CLA	C4B-C3B-CAB-CBB
13	j	1302	CLA	C1A-C2A-CAA-CBA
13	j	1302	CLA	C3A-C2A-CAA-CBA
13	l	1302	CLA	CAD-CBD-CGD-O1D
13	l	1302	CLA	CAD-CBD-CGD-O2D
13	l	1303	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	m	1401	CLA	C1A-C2A-CAA-CBA
13	m	1401	CLA	C4B-C3B-CAB-CBB
13	m	1103	CLA	C2B-C3B-CAB-CBB
13	m	1103	CLA	C4B-C3B-CAB-CBB
13	m	1105	CLA	C2B-C3B-CAB-CBB
13	m	1105	CLA	C4B-C3B-CAB-CBB
13	q	501	CLA	C4B-C3B-CAB-CBB
13	q	501	CLA	CAD-CBD-CGD-O1D
13	q	501	CLA	CAD-CBD-CGD-O2D
13	q	501	CLA	CBD-CGD-O2D-CED
13	q	504	CLA	C2B-C3B-CAB-CBB
13	q	504	CLA	C4B-C3B-CAB-CBB
13	q	506	CLA	CAD-CBD-CGD-O2D
13	q	507	CLA	CHA-CBD-CGD-O1D
13	q	507	CLA	CHA-CBD-CGD-O2D
13	q	508	CLA	C2-C3-C5-C6
13	q	508	CLA	C4-C3-C5-C6
13	q	510	CLA	CBD-CGD-O2D-CED
13	q	512	CLA	C4B-C3B-CAB-CBB
13	q	512	CLA	C3-C5-C6-C7
13	q	516	CLA	C1A-C2A-CAA-CBA
13	q	516	CLA	C3A-C2A-CAA-CBA
13	q	516	CLA	C2B-C3B-CAB-CBB
13	q	516	CLA	C4B-C3B-CAB-CBB
13	q	516	CLA	CAD-CBD-CGD-O1D
13	q	516	CLA	CAD-CBD-CGD-O2D
13	q	517	CLA	C2B-C3B-CAB-CBB
13	q	517	CLA	C4B-C3B-CAB-CBB
13	q	518	CLA	C2B-C3B-CAB-CBB
13	q	518	CLA	C4B-C3B-CAB-CBB
13	q	518	CLA	CHA-CBD-CGD-O1D
13	q	518	CLA	CHA-CBD-CGD-O2D
13	q	518	CLA	C2-C3-C5-C6
13	q	518	CLA	C4-C3-C5-C6
13	q	519	CLA	C2B-C3B-CAB-CBB
13	q	519	CLA	C4B-C3B-CAB-CBB
13	r	501	CLA	C4B-C3B-CAB-CBB
13	r	501	CLA	CBD-CGD-O2D-CED
13	r	506	CLA	C2-C3-C5-C6
13	r	506	CLA	C4-C3-C5-C6
13	r	507	CLA	CHA-CBD-CGD-O1D
13	r	507	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	r	507	CLA	C2-C3-C5-C6
13	r	507	CLA	C4-C3-C5-C6
13	r	513	CLA	CBD-CGD-O2D-CED
13	r	516	CLA	C4B-C3B-CAB-CBB
13	r	516	CLA	CHA-CBD-CGD-O1D
13	r	516	CLA	CHA-CBD-CGD-O2D
13	r	518	CLA	CAD-CBD-CGD-O2D
13	r	519	CLA	C2B-C3B-CAB-CBB
13	r	519	CLA	C4B-C3B-CAB-CBB
13	s	502	CLA	CHA-CBD-CGD-O1D
13	s	502	CLA	CHA-CBD-CGD-O2D
13	s	503	CLA	C2B-C3B-CAB-CBB
13	s	503	CLA	C4B-C3B-CAB-CBB
13	s	510	CLA	CAD-CBD-CGD-O1D
13	s	510	CLA	CAD-CBD-CGD-O2D
13	s	512	CLA	C4B-C3B-CAB-CBB
13	s	512	CLA	CHA-CBD-CGD-O2D
13	s	513	CLA	C1A-C2A-CAA-CBA
13	s	513	CLA	CBD-CGD-O2D-CED
13	s	516	CLA	CAD-CBD-CGD-O1D
13	s	516	CLA	CAD-CBD-CGD-O2D
13	s	517	CLA	C2B-C3B-CAB-CBB
13	s	517	CLA	C4B-C3B-CAB-CBB
13	s	517	CLA	CBD-CGD-O2D-CED
13	s	518	CLA	C2B-C3B-CAB-CBB
13	s	518	CLA	C4B-C3B-CAB-CBB
13	s	518	CLA	CAD-CBD-CGD-O2D
13	t	501	CLA	C4B-C3B-CAB-CBB
13	t	501	CLA	CBD-CGD-O2D-CED
13	t	501	CLA	O1D-CGD-O2D-CED
13	t	502	CLA	CHA-CBD-CGD-O1D
13	t	502	CLA	CHA-CBD-CGD-O2D
13	t	503	CLA	CHA-CBD-CGD-O2D
13	t	506	CLA	CHA-CBD-CGD-O2D
13	t	506	CLA	CBD-CGD-O2D-CED
13	t	507	CLA	CHA-CBD-CGD-O1D
13	t	507	CLA	CHA-CBD-CGD-O2D
13	t	510	CLA	CBD-CGD-O2D-CED
13	t	517	CLA	C1A-C2A-CAA-CBA
13	t	517	CLA	C3A-C2A-CAA-CBA
13	t	518	CLA	C2B-C3B-CAB-CBB
13	t	518	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	t	519	CLA	C4B-C3B-CAB-CBB
13	t	519	CLA	CAD-CBD-CGD-O1D
13	t	519	CLA	CAD-CBD-CGD-O2D
13	u	501	CLA	CBD-CGD-O2D-CED
13	u	504	CLA	CBD-CGD-O2D-CED
13	u	505	CLA	CHA-CBD-CGD-O2D
13	u	506	CLA	CAD-CBD-CGD-O2D
13	u	507	CLA	CBD-CGD-O2D-CED
13	u	511	CLA	CBD-CGD-O2D-CED
13	u	512	CLA	C4B-C3B-CAB-CBB
13	u	513	CLA	C2B-C3B-CAB-CBB
13	u	513	CLA	C4B-C3B-CAB-CBB
13	u	513	CLA	CBD-CGD-O2D-CED
13	u	516	CLA	C4B-C3B-CAB-CBB
13	u	517	CLA	C4B-C3B-CAB-CBB
13	u	517	CLA	CAD-CBD-CGD-O2D
13	u	518	CLA	C2B-C3B-CAB-CBB
13	u	518	CLA	C4B-C3B-CAB-CBB
13	u	519	CLA	CAD-CBD-CGD-O1D
13	u	519	CLA	CAD-CBD-CGD-O2D
13	v	501	CLA	CBD-CGD-O2D-CED
13	v	504	CLA	CAD-CBD-CGD-O2D
13	v	505	CLA	C6-C7-C8-C9
13	v	512	CLA	C4B-C3B-CAB-CBB
13	v	513	CLA	CBD-CGD-O2D-CED
13	v	516	CLA	CBD-CGD-O2D-CED
13	v	517	CLA	CAD-CBD-CGD-O1D
13	v	517	CLA	CAD-CBD-CGD-O2D
13	v	518	CLA	CAD-CBD-CGD-O2D
13	v	519	CLA	CHA-CBD-CGD-O2D
16	A	4001	BCR	C11-C12-C13-C14
16	A	4008	BCR	C21-C22-C23-C24
16	A	4008	BCR	C37-C22-C23-C24
16	A	4008	BCR	C23-C24-C25-C26
16	B	4004	BCR	C7-C8-C9-C10
16	B	4004	BCR	C7-C8-C9-C34
16	B	4004	BCR	C21-C22-C23-C24
16	B	4004	BCR	C37-C22-C23-C24
16	B	4005	BCR	C7-C8-C9-C10
16	B	4005	BCR	C21-C22-C23-C24
16	B	4005	BCR	C37-C22-C23-C24
16	B	4010	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	B	4010	BCR	C37-C22-C23-C24
16	B	4014	BCR	C17-C18-C19-C20
16	B	4014	BCR	C21-C22-C23-C24
16	B	4014	BCR	C37-C22-C23-C24
16	J	4013	BCR	C17-C18-C19-C20
16	J	4012	BCR	C5-C6-C7-C8
16	J	4012	BCR	C11-C12-C13-C14
16	J	4012	BCR	C11-C12-C13-C35
16	K	4104	BCR	C21-C22-C23-C24
16	K	4104	BCR	C37-C22-C23-C24
16	L	4019	BCR	C7-C8-C9-C10
16	L	4019	BCR	C7-C8-C9-C34
16	L	4022	BCR	C7-C8-C9-C10
16	L	4022	BCR	C7-C8-C9-C34
16	M	4021	BCR	C5-C6-C7-C8
16	M	4021	BCR	C17-C18-C19-C20
16	1	521	BCR	C7-C8-C9-C10
16	1	521	BCR	C7-C8-C9-C34
16	1	522	BCR	C1-C6-C7-C8
16	1	522	BCR	C5-C6-C7-C8
16	1	522	BCR	C7-C8-C9-C10
16	1	522	BCR	C7-C8-C9-C34
16	1	523	BCR	C21-C22-C23-C24
16	2	521	BCR	C7-C8-C9-C10
16	2	521	BCR	C7-C8-C9-C34
16	2	522	BCR	C5-C6-C7-C8
16	2	522	BCR	C7-C8-C9-C10
16	2	523	BCR	C21-C22-C23-C24
16	3	521	BCR	C7-C8-C9-C34
16	3	522	BCR	C7-C8-C9-C10
16	3	522	BCR	C7-C8-C9-C34
16	4	521	BCR	C7-C8-C9-C10
16	5	521	BCR	C7-C8-C9-C10
16	5	521	BCR	C7-C8-C9-C34
16	5	521	BCR	C17-C18-C19-C20
16	5	521	BCR	C36-C18-C19-C20
16	5	522	BCR	C5-C6-C7-C8
16	5	522	BCR	C7-C8-C9-C10
16	5	523	BCR	C21-C22-C23-C24
16	6	522	BCR	C5-C6-C7-C8
16	6	524	BCR	C7-C8-C9-C10
16	G	4001	BCR	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	G	4008	BCR	C21-C22-C23-C24
16	G	4008	BCR	C37-C22-C23-C24
16	G	4008	BCR	C23-C24-C25-C26
16	H	4004	BCR	C7-C8-C9-C10
16	H	4004	BCR	C7-C8-C9-C34
16	H	4004	BCR	C21-C22-C23-C24
16	H	4004	BCR	C37-C22-C23-C24
16	H	4005	BCR	C7-C8-C9-C10
16	H	4005	BCR	C21-C22-C23-C24
16	H	4005	BCR	C37-C22-C23-C24
16	H	4010	BCR	C21-C22-C23-C24
16	H	4010	BCR	C37-C22-C23-C24
16	H	4014	BCR	C17-C18-C19-C20
16	H	4014	BCR	C21-C22-C23-C24
16	H	4014	BCR	C37-C22-C23-C24
16	T	4013	BCR	C17-C18-C19-C20
16	T	4012	BCR	C5-C6-C7-C8
16	T	4012	BCR	C11-C12-C13-C14
16	T	4012	BCR	C11-C12-C13-C35
16	U	4104	BCR	C21-C22-C23-C24
16	U	4104	BCR	C37-C22-C23-C24
16	V	4019	BCR	C7-C8-C9-C10
16	V	4019	BCR	C7-C8-C9-C34
16	V	4022	BCR	C7-C8-C9-C10
16	V	4022	BCR	C7-C8-C9-C34
16	W	4021	BCR	C5-C6-C7-C8
16	W	4021	BCR	C17-C18-C19-C20
16	Y	521	BCR	C7-C8-C9-C10
16	Y	521	BCR	C7-C8-C9-C34
16	Y	522	BCR	C1-C6-C7-C8
16	Y	522	BCR	C5-C6-C7-C8
16	Y	522	BCR	C7-C8-C9-C10
16	Y	522	BCR	C7-C8-C9-C34
16	Y	523	BCR	C21-C22-C23-C24
16	Z	521	BCR	C7-C8-C9-C10
16	Z	521	BCR	C7-C8-C9-C34
16	Z	522	BCR	C5-C6-C7-C8
16	Z	522	BCR	C7-C8-C9-C10
16	Z	523	BCR	C21-C22-C23-C24
16	a	521	BCR	C7-C8-C9-C34
16	a	522	BCR	C7-C8-C9-C10
16	a	522	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	b	521	BCR	C7-C8-C9-C10
16	c	521	BCR	C7-C8-C9-C10
16	c	521	BCR	C7-C8-C9-C34
16	c	521	BCR	C17-C18-C19-C20
16	c	521	BCR	C36-C18-C19-C20
16	c	522	BCR	C5-C6-C7-C8
16	c	522	BCR	C7-C8-C9-C10
16	c	523	BCR	C21-C22-C23-C24
16	d	522	BCR	C5-C6-C7-C8
16	d	524	BCR	C7-C8-C9-C10
16	e	4001	BCR	C11-C12-C13-C14
16	e	4008	BCR	C21-C22-C23-C24
16	e	4008	BCR	C37-C22-C23-C24
16	e	4008	BCR	C23-C24-C25-C26
16	f	4004	BCR	C7-C8-C9-C10
16	f	4004	BCR	C7-C8-C9-C34
16	f	4004	BCR	C21-C22-C23-C24
16	f	4004	BCR	C37-C22-C23-C24
16	f	4005	BCR	C7-C8-C9-C10
16	f	4005	BCR	C21-C22-C23-C24
16	f	4005	BCR	C37-C22-C23-C24
16	f	4010	BCR	C21-C22-C23-C24
16	f	4010	BCR	C37-C22-C23-C24
16	f	4014	BCR	C17-C18-C19-C20
16	f	4014	BCR	C21-C22-C23-C24
16	f	4014	BCR	C37-C22-C23-C24
16	l	4013	BCR	C17-C18-C19-C20
16	l	4012	BCR	C5-C6-C7-C8
16	l	4012	BCR	C11-C12-C13-C14
16	l	4012	BCR	C11-C12-C13-C35
16	m	4104	BCR	C21-C22-C23-C24
16	m	4104	BCR	C37-C22-C23-C24
16	n	4019	BCR	C7-C8-C9-C10
16	n	4019	BCR	C7-C8-C9-C34
16	n	4022	BCR	C7-C8-C9-C10
16	n	4022	BCR	C7-C8-C9-C34
16	o	4021	BCR	C5-C6-C7-C8
16	o	4021	BCR	C17-C18-C19-C20
16	q	521	BCR	C7-C8-C9-C10
16	q	521	BCR	C7-C8-C9-C34
16	q	522	BCR	C1-C6-C7-C8
16	q	522	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	q	522	BCR	C7-C8-C9-C10
16	q	522	BCR	C7-C8-C9-C34
16	q	523	BCR	C21-C22-C23-C24
16	r	521	BCR	C7-C8-C9-C10
16	r	521	BCR	C7-C8-C9-C34
16	r	522	BCR	C5-C6-C7-C8
16	r	522	BCR	C7-C8-C9-C10
16	r	523	BCR	C21-C22-C23-C24
16	s	521	BCR	C7-C8-C9-C34
16	s	522	BCR	C7-C8-C9-C10
16	s	522	BCR	C7-C8-C9-C34
16	t	521	BCR	C7-C8-C9-C10
16	u	521	BCR	C7-C8-C9-C10
16	u	521	BCR	C7-C8-C9-C34
16	u	521	BCR	C17-C18-C19-C20
16	u	521	BCR	C36-C18-C19-C20
16	u	522	BCR	C5-C6-C7-C8
16	u	522	BCR	C7-C8-C9-C10
16	u	523	BCR	C21-C22-C23-C24
16	v	522	BCR	C5-C6-C7-C8
16	v	524	BCR	C7-C8-C9-C10
17	A	5002	LHG	C3-O3-P-O6
17	A	5002	LHG	C4-O6-P-O5
17	A	5002	LHG	C8-C7-O7-C5
17	A	5004	LHG	O1-C1-C2-C3
17	A	5004	LHG	C1-C2-C3-O3
17	A	5004	LHG	C3-O3-P-O4
17	A	5004	LHG	C3-O3-P-O6
17	A	5004	LHG	C8-C7-O7-C5
17	A	5005	LHG	O1-C1-C2-C3
17	A	5005	LHG	O2-C2-C3-O3
17	A	5005	LHG	C3-O3-P-O5
17	A	5005	LHG	C3-O3-P-O6
17	A	5006	LHG	O1-C1-C2-C3
17	A	5006	LHG	C4-O6-P-O3
17	A	5006	LHG	C4-O6-P-O4
17	A	5007	LHG	O1-C1-C2-C3
17	A	5007	LHG	C3-O3-P-O4
17	A	5008	LHG	C4-O6-P-O3
17	A	5008	LHG	C4-O6-P-O4
17	A	5008	LHG	O7-C5-C6-O8
17	A	5009	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	5009	LHG	C3-O3-P-O4
17	A	5009	LHG	C3-O3-P-O5
17	A	5009	LHG	C3-O3-P-O6
17	A	5009	LHG	C4-O6-P-O3
17	A	5009	LHG	C4-O6-P-O4
17	A	5001	LHG	O1-C1-C2-C3
17	A	5003	LHG	C3-O3-P-O5
17	B	1842	LHG	O1-C1-C2-C3
17	B	1842	LHG	C3-O3-P-O5
17	B	1842	LHG	C3-O3-P-O6
17	B	1842	LHG	O9-C7-O7-C5
17	B	1842	LHG	C8-C7-O7-C5
17	B	1855	LHG	O1-C1-C2-C3
17	B	1855	LHG	C3-O3-P-O4
17	B	1855	LHG	C3-O3-P-O6
17	B	1855	LHG	C4-O6-P-O5
17	I	5001	LHG	C3-O3-P-O5
17	I	5001	LHG	C3-O3-P-O6
17	I	5001	LHG	C4-O6-P-O3
17	I	5001	LHG	C4-O6-P-O5
17	I	5001	LHG	O9-C7-O7-C5
17	I	5001	LHG	C8-C7-O7-C5
17	L	5218	LHG	O1-C1-C2-C3
17	L	5218	LHG	C3-O3-P-O4
17	L	5218	LHG	C3-O3-P-O5
17	L	5218	LHG	C3-O3-P-O6
17	L	5218	LHG	O7-C5-C6-O8
17	L	5218	LHG	O9-C7-O7-C5
17	L	5218	LHG	C8-C7-O7-C5
17	L	5220	LHG	O1-C1-C2-C3
17	L	5221	LHG	C3-O3-P-O4
17	L	5221	LHG	C3-O3-P-O5
17	L	5221	LHG	C4-O6-P-O3
17	L	5221	LHG	C4-O6-P-O4
17	L	5221	LHG	C4-O6-P-O5
17	G	5002	LHG	C3-O3-P-O6
17	G	5002	LHG	C4-O6-P-O5
17	G	5002	LHG	C8-C7-O7-C5
17	G	5004	LHG	O1-C1-C2-C3
17	G	5004	LHG	C1-C2-C3-O3
17	G	5004	LHG	C3-O3-P-O4
17	G	5004	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5004	LHG	C8-C7-O7-C5
17	G	5005	LHG	O1-C1-C2-C3
17	G	5005	LHG	O2-C2-C3-O3
17	G	5005	LHG	C3-O3-P-O6
17	G	5006	LHG	O1-C1-C2-C3
17	G	5006	LHG	C4-O6-P-O3
17	G	5006	LHG	C4-O6-P-O4
17	G	5007	LHG	O1-C1-C2-C3
17	G	5007	LHG	C3-O3-P-O4
17	G	5008	LHG	C4-O6-P-O3
17	G	5008	LHG	C4-O6-P-O4
17	G	5008	LHG	O7-C5-C6-O8
17	G	5009	LHG	O1-C1-C2-C3
17	G	5009	LHG	C3-O3-P-O4
17	G	5009	LHG	C3-O3-P-O5
17	G	5009	LHG	C3-O3-P-O6
17	G	5009	LHG	C4-O6-P-O3
17	G	5009	LHG	C4-O6-P-O4
17	G	5001	LHG	O1-C1-C2-C3
17	G	5003	LHG	C3-O3-P-O5
17	H	1842	LHG	O1-C1-C2-C3
17	H	1842	LHG	C3-O3-P-O5
17	H	1842	LHG	C3-O3-P-O6
17	H	1842	LHG	O9-C7-O7-C5
17	H	1842	LHG	C8-C7-O7-C5
17	H	1855	LHG	O1-C1-C2-C3
17	H	1855	LHG	C3-O3-P-O4
17	H	1855	LHG	C3-O3-P-O6
17	H	1855	LHG	C4-O6-P-O5
17	S	5001	LHG	C3-O3-P-O5
17	S	5001	LHG	C3-O3-P-O6
17	S	5001	LHG	C4-O6-P-O3
17	S	5001	LHG	C4-O6-P-O5
17	S	5001	LHG	O9-C7-O7-C5
17	S	5001	LHG	C8-C7-O7-C5
17	V	5218	LHG	O1-C1-C2-C3
17	V	5218	LHG	C3-O3-P-O4
17	V	5218	LHG	C3-O3-P-O5
17	V	5218	LHG	C3-O3-P-O6
17	V	5218	LHG	O7-C5-C6-O8
17	V	5218	LHG	O9-C7-O7-C5
17	V	5218	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	V	5220	LHG	O1-C1-C2-C3
17	V	5221	LHG	C3-O3-P-O4
17	V	5221	LHG	C3-O3-P-O5
17	V	5221	LHG	C4-O6-P-O3
17	V	5221	LHG	C4-O6-P-O4
17	V	5221	LHG	C4-O6-P-O5
17	e	5002	LHG	C3-O3-P-O6
17	e	5002	LHG	C4-O6-P-O5
17	e	5002	LHG	C8-C7-O7-C5
17	e	5004	LHG	O1-C1-C2-C3
17	e	5004	LHG	C1-C2-C3-O3
17	e	5004	LHG	C3-O3-P-O4
17	e	5004	LHG	C3-O3-P-O6
17	e	5004	LHG	C8-C7-O7-C5
17	e	5005	LHG	O1-C1-C2-C3
17	e	5005	LHG	O2-C2-C3-O3
17	e	5005	LHG	C3-O3-P-O5
17	e	5005	LHG	C3-O3-P-O6
17	e	5006	LHG	O1-C1-C2-C3
17	e	5006	LHG	C4-O6-P-O3
17	e	5006	LHG	C4-O6-P-O4
17	e	5007	LHG	O1-C1-C2-C3
17	e	5007	LHG	C3-O3-P-O4
17	e	5008	LHG	C4-O6-P-O3
17	e	5008	LHG	C4-O6-P-O4
17	e	5008	LHG	O7-C5-C6-O8
17	e	5009	LHG	O1-C1-C2-C3
17	e	5009	LHG	C3-O3-P-O4
17	e	5009	LHG	C3-O3-P-O5
17	e	5009	LHG	C3-O3-P-O6
17	e	5009	LHG	C4-O6-P-O3
17	e	5009	LHG	C4-O6-P-O4
17	e	5001	LHG	O1-C1-C2-C3
17	e	5003	LHG	C3-O3-P-O5
17	f	1842	LHG	O1-C1-C2-C3
17	f	1842	LHG	C3-O3-P-O5
17	f	1842	LHG	C3-O3-P-O6
17	f	1842	LHG	O9-C7-O7-C5
17	f	1842	LHG	C8-C7-O7-C5
17	f	1855	LHG	O1-C1-C2-C3
17	f	1855	LHG	C3-O3-P-O4
17	f	1855	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	f	1855	LHG	C4-O6-P-O5
17	k	5001	LHG	C3-O3-P-O5
17	k	5001	LHG	C3-O3-P-O6
17	k	5001	LHG	C4-O6-P-O3
17	k	5001	LHG	C4-O6-P-O5
17	k	5001	LHG	O9-C7-O7-C5
17	k	5001	LHG	C8-C7-O7-C5
17	n	5218	LHG	O1-C1-C2-C3
17	n	5218	LHG	C3-O3-P-O4
17	n	5218	LHG	C3-O3-P-O5
17	n	5218	LHG	C3-O3-P-O6
17	n	5218	LHG	O7-C5-C6-O8
17	n	5218	LHG	O9-C7-O7-C5
17	n	5218	LHG	C8-C7-O7-C5
17	n	5220	LHG	O1-C1-C2-C3
17	n	5221	LHG	C3-O3-P-O4
17	n	5221	LHG	C3-O3-P-O5
17	n	5221	LHG	C4-O6-P-O3
17	n	5221	LHG	C4-O6-P-O4
17	n	5221	LHG	C4-O6-P-O5
18	B	1843	LMU	C2'-C1'-O1'-C1
18	B	1843	LMU	O5'-C1'-O1'-C1
18	J	5105	LMU	C2-C1-O1'-C1'
18	H	1843	LMU	C2'-C1'-O1'-C1
18	H	1843	LMU	O5'-C1'-O1'-C1
18	T	5105	LMU	C2-C1-O1'-C1'
18	f	1843	LMU	C2'-C1'-O1'-C1
18	f	1843	LMU	O5'-C1'-O1'-C1
18	l	5105	LMU	C2-C1-O1'-C1'
19	J	5104	LMG	O7-C8-C9-O8
19	T	5104	LMG	O7-C8-C9-O8
19	l	5104	LMG	O7-C8-C9-O8
20	L	5216	SQD	O47-C45-C46-O48
20	L	5216	SQD	C5-C6-S-O7
20	1	822	SQD	O49-C7-O47-C45
20	2	822	SQD	O49-C7-O47-C45
20	2	822	SQD	C8-C7-O47-C45
20	3	822	SQD	O47-C45-C46-O48
20	3	822	SQD	O49-C7-O47-C45
20	3	822	SQD	C8-C7-O47-C45
20	4	822	SQD	C8-C7-O47-C45
20	6	822	SQD	C8-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	V	5216	SQD	O47-C45-C46-O48
20	V	5216	SQD	C5-C6-S-O7
20	Y	822	SQD	O49-C7-O47-C45
20	Z	822	SQD	O49-C7-O47-C45
20	Z	822	SQD	C8-C7-O47-C45
20	a	822	SQD	O47-C45-C46-O48
20	a	822	SQD	O49-C7-O47-C45
20	a	822	SQD	C8-C7-O47-C45
20	b	822	SQD	C8-C7-O47-C45
20	d	822	SQD	C8-C7-O47-C45
20	n	5216	SQD	O47-C45-C46-O48
20	n	5216	SQD	C5-C6-S-O7
20	q	822	SQD	O49-C7-O47-C45
20	r	822	SQD	O49-C7-O47-C45
20	r	822	SQD	C8-C7-O47-C45
20	s	822	SQD	O47-C45-C46-O48
20	s	822	SQD	O49-C7-O47-C45
20	s	822	SQD	C8-C7-O47-C45
20	t	822	SQD	C8-C7-O47-C45
20	v	822	SQD	C8-C7-O47-C45
13	B	1023	CLA	O1D-CGD-O2D-CED
13	1	503	CLA	O1D-CGD-O2D-CED
13	1	506	CLA	O1D-CGD-O2D-CED
13	3	503	CLA	O1D-CGD-O2D-CED
13	4	506	CLA	O1D-CGD-O2D-CED
13	5	506	CLA	O1D-CGD-O2D-CED
13	6	506	CLA	O1D-CGD-O2D-CED
13	H	1023	CLA	O1D-CGD-O2D-CED
13	Y	503	CLA	O1D-CGD-O2D-CED
13	Y	506	CLA	O1D-CGD-O2D-CED
13	a	503	CLA	O1D-CGD-O2D-CED
13	b	506	CLA	O1D-CGD-O2D-CED
13	c	506	CLA	O1D-CGD-O2D-CED
13	d	506	CLA	O1D-CGD-O2D-CED
13	f	1023	CLA	O1D-CGD-O2D-CED
13	q	503	CLA	O1D-CGD-O2D-CED
13	q	506	CLA	O1D-CGD-O2D-CED
13	s	503	CLA	O1D-CGD-O2D-CED
13	t	506	CLA	O1D-CGD-O2D-CED
13	u	506	CLA	O1D-CGD-O2D-CED
13	v	506	CLA	O1D-CGD-O2D-CED
20	4	822	SQD	O49-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	b	822	SQD	O49-C7-O47-C45
20	t	822	SQD	O49-C7-O47-C45
13	2	503	CLA	O1D-CGD-O2D-CED
13	3	510	CLA	O1D-CGD-O2D-CED
13	4	504	CLA	O1D-CGD-O2D-CED
13	5	503	CLA	O1D-CGD-O2D-CED
13	6	503	CLA	O1D-CGD-O2D-CED
13	Z	503	CLA	O1D-CGD-O2D-CED
13	a	510	CLA	O1D-CGD-O2D-CED
13	b	504	CLA	O1D-CGD-O2D-CED
13	c	503	CLA	O1D-CGD-O2D-CED
13	d	503	CLA	O1D-CGD-O2D-CED
13	r	503	CLA	O1D-CGD-O2D-CED
13	s	510	CLA	O1D-CGD-O2D-CED
13	t	504	CLA	O1D-CGD-O2D-CED
13	u	503	CLA	O1D-CGD-O2D-CED
13	v	503	CLA	O1D-CGD-O2D-CED
13	v	513	CLA	O1D-CGD-O2D-CED
20	6	822	SQD	O49-C7-O47-C45
20	d	822	SQD	O49-C7-O47-C45
20	v	822	SQD	O49-C7-O47-C45
13	A	1107	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	CBD-CGD-O2D-CED
13	A	1119	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	CBD-CGD-O2D-CED
13	A	1801	CLA	CBD-CGD-O2D-CED
13	B	1021	CLA	CBD-CGD-O2D-CED
13	B	1023	CLA	CBD-CGD-O2D-CED
13	B	1203	CLA	CBD-CGD-O2D-CED
13	B	1219	CLA	CBD-CGD-O2D-CED
13	B	1221	CLA	CBD-CGD-O2D-CED
13	B	1207	CLA	CBD-CGD-O2D-CED
13	F	1302	CLA	CBD-CGD-O2D-CED
13	K	1105	CLA	CBD-CGD-O2D-CED
13	1	503	CLA	CBD-CGD-O2D-CED
13	1	506	CLA	CBD-CGD-O2D-CED
13	1	516	CLA	CBD-CGD-O2D-CED
13	2	503	CLA	CBD-CGD-O2D-CED
13	2	506	CLA	CBD-CGD-O2D-CED
13	2	511	CLA	CBD-CGD-O2D-CED
13	3	503	CLA	CBD-CGD-O2D-CED
13	3	506	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	3	510	CLA	CBD-CGD-O2D-CED
13	3	516	CLA	CBD-CGD-O2D-CED
13	3	518	CLA	CBD-CGD-O2D-CED
13	3	519	CLA	CBD-CGD-O2D-CED
13	4	504	CLA	CBD-CGD-O2D-CED
13	4	517	CLA	CBD-CGD-O2D-CED
13	4	518	CLA	CBD-CGD-O2D-CED
13	5	503	CLA	CBD-CGD-O2D-CED
13	5	506	CLA	CBD-CGD-O2D-CED
13	5	508	CLA	CBD-CGD-O2D-CED
13	5	510	CLA	CBD-CGD-O2D-CED
13	5	517	CLA	CBD-CGD-O2D-CED
13	6	502	CLA	CBD-CGD-O2D-CED
13	6	503	CLA	CBD-CGD-O2D-CED
13	6	506	CLA	CBD-CGD-O2D-CED
13	6	509	CLA	CBD-CGD-O2D-CED
13	G	1107	CLA	CBD-CGD-O2D-CED
13	G	1108	CLA	CBD-CGD-O2D-CED
13	G	1119	CLA	CBD-CGD-O2D-CED
13	G	1120	CLA	CBD-CGD-O2D-CED
13	G	1801	CLA	CBD-CGD-O2D-CED
13	H	1021	CLA	CBD-CGD-O2D-CED
13	H	1023	CLA	CBD-CGD-O2D-CED
13	H	1203	CLA	CBD-CGD-O2D-CED
13	H	1219	CLA	CBD-CGD-O2D-CED
13	H	1221	CLA	CBD-CGD-O2D-CED
13	H	1207	CLA	CBD-CGD-O2D-CED
13	R	1302	CLA	CBD-CGD-O2D-CED
13	U	1105	CLA	CBD-CGD-O2D-CED
13	Y	503	CLA	CBD-CGD-O2D-CED
13	Y	506	CLA	CBD-CGD-O2D-CED
13	Y	516	CLA	CBD-CGD-O2D-CED
13	Z	503	CLA	CBD-CGD-O2D-CED
13	Z	506	CLA	CBD-CGD-O2D-CED
13	Z	511	CLA	CBD-CGD-O2D-CED
13	a	503	CLA	CBD-CGD-O2D-CED
13	a	506	CLA	CBD-CGD-O2D-CED
13	a	510	CLA	CBD-CGD-O2D-CED
13	a	516	CLA	CBD-CGD-O2D-CED
13	a	518	CLA	CBD-CGD-O2D-CED
13	a	519	CLA	CBD-CGD-O2D-CED
13	b	504	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	b	517	CLA	CBD-CGD-O2D-CED
13	b	518	CLA	CBD-CGD-O2D-CED
13	c	503	CLA	CBD-CGD-O2D-CED
13	c	506	CLA	CBD-CGD-O2D-CED
13	c	508	CLA	CBD-CGD-O2D-CED
13	c	510	CLA	CBD-CGD-O2D-CED
13	c	517	CLA	CBD-CGD-O2D-CED
13	d	502	CLA	CBD-CGD-O2D-CED
13	d	503	CLA	CBD-CGD-O2D-CED
13	d	506	CLA	CBD-CGD-O2D-CED
13	d	509	CLA	CBD-CGD-O2D-CED
13	e	1107	CLA	CBD-CGD-O2D-CED
13	e	1108	CLA	CBD-CGD-O2D-CED
13	e	1119	CLA	CBD-CGD-O2D-CED
13	e	1120	CLA	CBD-CGD-O2D-CED
13	e	1801	CLA	CBD-CGD-O2D-CED
13	f	1021	CLA	CBD-CGD-O2D-CED
13	f	1023	CLA	CBD-CGD-O2D-CED
13	f	1203	CLA	CBD-CGD-O2D-CED
13	f	1219	CLA	CBD-CGD-O2D-CED
13	f	1221	CLA	CBD-CGD-O2D-CED
13	f	1207	CLA	CBD-CGD-O2D-CED
13	j	1302	CLA	CBD-CGD-O2D-CED
13	m	1105	CLA	CBD-CGD-O2D-CED
13	q	503	CLA	CBD-CGD-O2D-CED
13	q	506	CLA	CBD-CGD-O2D-CED
13	q	516	CLA	CBD-CGD-O2D-CED
13	r	503	CLA	CBD-CGD-O2D-CED
13	r	506	CLA	CBD-CGD-O2D-CED
13	r	511	CLA	CBD-CGD-O2D-CED
13	s	503	CLA	CBD-CGD-O2D-CED
13	s	506	CLA	CBD-CGD-O2D-CED
13	s	510	CLA	CBD-CGD-O2D-CED
13	s	516	CLA	CBD-CGD-O2D-CED
13	s	518	CLA	CBD-CGD-O2D-CED
13	s	519	CLA	CBD-CGD-O2D-CED
13	t	504	CLA	CBD-CGD-O2D-CED
13	t	517	CLA	CBD-CGD-O2D-CED
13	t	518	CLA	CBD-CGD-O2D-CED
13	u	503	CLA	CBD-CGD-O2D-CED
13	u	506	CLA	CBD-CGD-O2D-CED
13	u	508	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	u	510	CLA	CBD-CGD-O2D-CED
13	u	517	CLA	CBD-CGD-O2D-CED
13	v	502	CLA	CBD-CGD-O2D-CED
13	v	503	CLA	CBD-CGD-O2D-CED
13	v	506	CLA	CBD-CGD-O2D-CED
13	v	509	CLA	CBD-CGD-O2D-CED
13	A	1109	CLA	O1A-CGA-O2A-C1
13	B	1209	CLA	O1A-CGA-O2A-C1
13	B	1217	CLA	O1A-CGA-O2A-C1
13	B	1219	CLA	O1A-CGA-O2A-C1
13	B	1227	CLA	O1A-CGA-O2A-C1
13	B	1207	CLA	O1A-CGA-O2A-C1
13	3	510	CLA	O1A-CGA-O2A-C1
13	6	505	CLA	O1A-CGA-O2A-C1
13	G	1109	CLA	O1A-CGA-O2A-C1
13	H	1209	CLA	O1A-CGA-O2A-C1
13	H	1217	CLA	O1A-CGA-O2A-C1
13	H	1219	CLA	O1A-CGA-O2A-C1
13	H	1227	CLA	O1A-CGA-O2A-C1
13	H	1207	CLA	O1A-CGA-O2A-C1
13	a	510	CLA	O1A-CGA-O2A-C1
13	d	505	CLA	O1A-CGA-O2A-C1
13	e	1109	CLA	O1A-CGA-O2A-C1
13	f	1209	CLA	O1A-CGA-O2A-C1
13	f	1217	CLA	O1A-CGA-O2A-C1
13	f	1219	CLA	O1A-CGA-O2A-C1
13	f	1227	CLA	O1A-CGA-O2A-C1
13	f	1207	CLA	O1A-CGA-O2A-C1
13	s	510	CLA	O1A-CGA-O2A-C1
13	v	505	CLA	O1A-CGA-O2A-C1
17	A	5006	LHG	O10-C23-O8-C6
17	I	5001	LHG	O10-C23-O8-C6
17	L	5221	LHG	O10-C23-O8-C6
17	G	5006	LHG	O10-C23-O8-C6
17	S	5001	LHG	O10-C23-O8-C6
17	V	5221	LHG	O10-C23-O8-C6
17	e	5006	LHG	O10-C23-O8-C6
17	k	5001	LHG	O10-C23-O8-C6
17	n	5221	LHG	O10-C23-O8-C6
13	6	513	CLA	O1D-CGD-O2D-CED
13	d	513	CLA	O1D-CGD-O2D-CED
13	6	519	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	d	519	CLA	CBA-CGA-O2A-C1
13	v	519	CLA	CBA-CGA-O2A-C1
13	K	1105	CLA	C4C-C3C-CAC-CBC
13	B	1021	CLA	O1D-CGD-O2D-CED
13	3	506	CLA	O1D-CGD-O2D-CED
13	H	1021	CLA	O1D-CGD-O2D-CED
13	a	506	CLA	O1D-CGD-O2D-CED
13	f	1021	CLA	O1D-CGD-O2D-CED
13	s	506	CLA	O1D-CGD-O2D-CED
13	A	1109	CLA	CBA-CGA-O2A-C1
13	A	1110	CLA	CBA-CGA-O2A-C1
13	B	1217	CLA	CBA-CGA-O2A-C1
13	B	1227	CLA	CBA-CGA-O2A-C1
13	6	505	CLA	CBA-CGA-O2A-C1
13	G	1109	CLA	CBA-CGA-O2A-C1
13	G	1110	CLA	CBA-CGA-O2A-C1
13	H	1217	CLA	CBA-CGA-O2A-C1
13	H	1227	CLA	CBA-CGA-O2A-C1
13	d	505	CLA	CBA-CGA-O2A-C1
13	e	1109	CLA	CBA-CGA-O2A-C1
13	e	1110	CLA	CBA-CGA-O2A-C1
13	f	1217	CLA	CBA-CGA-O2A-C1
13	f	1227	CLA	CBA-CGA-O2A-C1
13	v	505	CLA	CBA-CGA-O2A-C1
17	L	5221	LHG	C24-C23-O8-C6
17	V	5221	LHG	C24-C23-O8-C6
17	n	5221	LHG	C24-C23-O8-C6
13	J	1302	CLA	CBD-CGD-O2D-CED
13	4	511	CLA	CBD-CGD-O2D-CED
13	T	1302	CLA	CBD-CGD-O2D-CED
13	b	511	CLA	CBD-CGD-O2D-CED
13	l	1302	CLA	CBD-CGD-O2D-CED
13	t	511	CLA	CBD-CGD-O2D-CED
13	A	1110	CLA	O1A-CGA-O2A-C1
13	A	1114	CLA	O1A-CGA-O2A-C1
13	A	1119	CLA	O1A-CGA-O2A-C1
13	A	1140	CLA	O1A-CGA-O2A-C1
13	A	1130	CLA	O1A-CGA-O2A-C1
13	B	1202	CLA	O1A-CGA-O2A-C1
13	B	1206	CLA	O1A-CGA-O2A-C1
13	B	1240	CLA	O1A-CGA-O2A-C1
13	1	505	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	2	504	CLA	O1A-CGA-O2A-C1
13	2	505	CLA	O1A-CGA-O2A-C1
13	3	505	CLA	O1A-CGA-O2A-C1
13	4	505	CLA	O1A-CGA-O2A-C1
13	4	510	CLA	O1A-CGA-O2A-C1
13	5	505	CLA	O1A-CGA-O2A-C1
13	G	1110	CLA	O1A-CGA-O2A-C1
13	G	1114	CLA	O1A-CGA-O2A-C1
13	G	1119	CLA	O1A-CGA-O2A-C1
13	G	1140	CLA	O1A-CGA-O2A-C1
13	G	1130	CLA	O1A-CGA-O2A-C1
13	H	1202	CLA	O1A-CGA-O2A-C1
13	H	1206	CLA	O1A-CGA-O2A-C1
13	H	1240	CLA	O1A-CGA-O2A-C1
13	Y	505	CLA	O1A-CGA-O2A-C1
13	Z	504	CLA	O1A-CGA-O2A-C1
13	Z	505	CLA	O1A-CGA-O2A-C1
13	a	505	CLA	O1A-CGA-O2A-C1
13	b	505	CLA	O1A-CGA-O2A-C1
13	b	510	CLA	O1A-CGA-O2A-C1
13	c	505	CLA	O1A-CGA-O2A-C1
13	e	1110	CLA	O1A-CGA-O2A-C1
13	e	1114	CLA	O1A-CGA-O2A-C1
13	e	1119	CLA	O1A-CGA-O2A-C1
13	e	1140	CLA	O1A-CGA-O2A-C1
13	e	1130	CLA	O1A-CGA-O2A-C1
13	f	1202	CLA	O1A-CGA-O2A-C1
13	f	1206	CLA	O1A-CGA-O2A-C1
13	f	1240	CLA	O1A-CGA-O2A-C1
13	q	505	CLA	O1A-CGA-O2A-C1
13	r	504	CLA	O1A-CGA-O2A-C1
13	r	505	CLA	O1A-CGA-O2A-C1
13	s	505	CLA	O1A-CGA-O2A-C1
13	t	505	CLA	O1A-CGA-O2A-C1
13	t	510	CLA	O1A-CGA-O2A-C1
13	u	505	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	O10-C23-O8-C6
17	A	5009	LHG	O10-C23-O8-C6
17	B	1842	LHG	O10-C23-O8-C6
17	L	5218	LHG	O10-C23-O8-C6
17	L	5220	LHG	O10-C23-O8-C6
17	G	5002	LHG	O10-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5009	LHG	O10-C23-O8-C6
17	H	1842	LHG	O10-C23-O8-C6
17	V	5218	LHG	O10-C23-O8-C6
17	V	5220	LHG	O10-C23-O8-C6
17	e	5002	LHG	O10-C23-O8-C6
17	e	5009	LHG	O10-C23-O8-C6
17	f	1842	LHG	O10-C23-O8-C6
17	n	5218	LHG	O10-C23-O8-C6
17	n	5220	LHG	O10-C23-O8-C6
19	J	5104	LMG	O10-C28-O8-C9
19	T	5104	LMG	O10-C28-O8-C9
19	l	5104	LMG	O10-C28-O8-C9
20	2	822	SQD	O10-C23-O48-C46
20	Z	822	SQD	O10-C23-O48-C46
20	r	822	SQD	O10-C23-O48-C46
13	U	1105	CLA	C4C-C3C-CAC-CBC
13	m	1105	CLA	C4C-C3C-CAC-CBC
13	A	1139	CLA	O1D-CGD-O2D-CED
13	K	1105	CLA	O1D-CGD-O2D-CED
13	2	506	CLA	O1D-CGD-O2D-CED
13	3	517	CLA	O1D-CGD-O2D-CED
13	U	1105	CLA	O1D-CGD-O2D-CED
13	Z	506	CLA	O1D-CGD-O2D-CED
13	a	517	CLA	O1D-CGD-O2D-CED
13	e	1139	CLA	O1D-CGD-O2D-CED
13	m	1105	CLA	O1D-CGD-O2D-CED
13	r	506	CLA	O1D-CGD-O2D-CED
13	s	517	CLA	O1D-CGD-O2D-CED
13	1	510	CLA	O1D-CGD-O2D-CED
13	2	513	CLA	O1D-CGD-O2D-CED
13	4	510	CLA	O1D-CGD-O2D-CED
13	5	504	CLA	O1D-CGD-O2D-CED
13	5	511	CLA	O1D-CGD-O2D-CED
13	5	513	CLA	O1D-CGD-O2D-CED
13	6	501	CLA	O1D-CGD-O2D-CED
13	6	516	CLA	O1D-CGD-O2D-CED
13	G	1139	CLA	O1D-CGD-O2D-CED
13	Y	510	CLA	O1D-CGD-O2D-CED
13	Z	513	CLA	O1D-CGD-O2D-CED
13	b	510	CLA	O1D-CGD-O2D-CED
13	c	504	CLA	O1D-CGD-O2D-CED
13	c	511	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	c	513	CLA	O1D-CGD-O2D-CED
13	d	501	CLA	O1D-CGD-O2D-CED
13	d	516	CLA	O1D-CGD-O2D-CED
13	q	510	CLA	O1D-CGD-O2D-CED
13	r	513	CLA	O1D-CGD-O2D-CED
13	t	510	CLA	O1D-CGD-O2D-CED
13	u	504	CLA	O1D-CGD-O2D-CED
13	u	511	CLA	O1D-CGD-O2D-CED
13	u	513	CLA	O1D-CGD-O2D-CED
13	v	501	CLA	O1D-CGD-O2D-CED
13	v	516	CLA	O1D-CGD-O2D-CED
20	4	822	SQD	C24-C23-O48-C46
20	b	822	SQD	C24-C23-O48-C46
20	t	822	SQD	C24-C23-O48-C46
13	B	1239	CLA	CBD-CGD-O2D-CED
13	H	1239	CLA	CBD-CGD-O2D-CED
13	f	1239	CLA	CBD-CGD-O2D-CED
13	K	1105	CLA	C2C-C3C-CAC-CBC
13	U	1105	CLA	C2C-C3C-CAC-CBC
13	m	1105	CLA	C2C-C3C-CAC-CBC
17	A	5004	LHG	O9-C7-O7-C5
17	A	5007	LHG	O9-C7-O7-C5
17	A	5008	LHG	O9-C7-O7-C5
17	A	5009	LHG	O9-C7-O7-C5
17	B	1855	LHG	O9-C7-O7-C5
17	L	5220	LHG	O9-C7-O7-C5
17	G	5004	LHG	O9-C7-O7-C5
17	G	5007	LHG	O9-C7-O7-C5
17	G	5008	LHG	O9-C7-O7-C5
17	G	5009	LHG	O9-C7-O7-C5
17	H	1855	LHG	O9-C7-O7-C5
17	V	5220	LHG	O9-C7-O7-C5
17	e	5004	LHG	O9-C7-O7-C5
17	e	5007	LHG	O9-C7-O7-C5
17	e	5008	LHG	O9-C7-O7-C5
17	e	5009	LHG	O9-C7-O7-C5
17	f	1855	LHG	O9-C7-O7-C5
17	n	5220	LHG	O9-C7-O7-C5
13	A	1102	CLA	C3-C5-C6-C7
13	A	1116	CLA	C3-C5-C6-C7
13	A	1118	CLA	C3-C5-C6-C7
13	A	1121	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1122	CLA	C3-C5-C6-C7
13	A	1133	CLA	C3-C5-C6-C7
13	A	1136	CLA	C3-C5-C6-C7
13	A	1139	CLA	C3-C5-C6-C7
13	B	1216	CLA	C3-C5-C6-C7
13	B	1231	CLA	C3-C5-C6-C7
13	B	1239	CLA	C3-C5-C6-C7
13	J	1303	CLA	C3-C5-C6-C7
13	L	1503	CLA	C3-C5-C6-C7
13	1	502	CLA	C3-C5-C6-C7
13	1	505	CLA	C3-C5-C6-C7
13	1	510	CLA	C3-C5-C6-C7
13	1	511	CLA	C3-C5-C6-C7
13	1	518	CLA	C3-C5-C6-C7
13	2	505	CLA	C3-C5-C6-C7
13	2	511	CLA	C3-C5-C6-C7
13	3	508	CLA	C3-C5-C6-C7
13	3	513	CLA	C3-C5-C6-C7
13	5	501	CLA	C3-C5-C6-C7
13	6	501	CLA	C3-C5-C6-C7
13	6	505	CLA	C3-C5-C6-C7
13	G	1102	CLA	C3-C5-C6-C7
13	G	1116	CLA	C3-C5-C6-C7
13	G	1118	CLA	C3-C5-C6-C7
13	G	1121	CLA	C3-C5-C6-C7
13	G	1122	CLA	C3-C5-C6-C7
13	G	1133	CLA	C3-C5-C6-C7
13	G	1136	CLA	C3-C5-C6-C7
13	G	1139	CLA	C3-C5-C6-C7
13	H	1216	CLA	C3-C5-C6-C7
13	H	1231	CLA	C3-C5-C6-C7
13	H	1239	CLA	C3-C5-C6-C7
13	T	1303	CLA	C3-C5-C6-C7
13	V	1503	CLA	C3-C5-C6-C7
13	Y	502	CLA	C3-C5-C6-C7
13	Y	505	CLA	C3-C5-C6-C7
13	Y	510	CLA	C3-C5-C6-C7
13	Y	511	CLA	C3-C5-C6-C7
13	Y	518	CLA	C3-C5-C6-C7
13	Z	505	CLA	C3-C5-C6-C7
13	Z	511	CLA	C3-C5-C6-C7
13	a	508	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	513	CLA	C3-C5-C6-C7
13	c	501	CLA	C3-C5-C6-C7
13	d	501	CLA	C3-C5-C6-C7
13	d	505	CLA	C3-C5-C6-C7
13	e	1102	CLA	C3-C5-C6-C7
13	e	1116	CLA	C3-C5-C6-C7
13	e	1118	CLA	C3-C5-C6-C7
13	e	1121	CLA	C3-C5-C6-C7
13	e	1122	CLA	C3-C5-C6-C7
13	e	1133	CLA	C3-C5-C6-C7
13	e	1136	CLA	C3-C5-C6-C7
13	e	1139	CLA	C3-C5-C6-C7
13	f	1216	CLA	C3-C5-C6-C7
13	f	1231	CLA	C3-C5-C6-C7
13	f	1239	CLA	C3-C5-C6-C7
13	l	1303	CLA	C3-C5-C6-C7
13	n	1503	CLA	C3-C5-C6-C7
13	q	502	CLA	C3-C5-C6-C7
13	q	505	CLA	C3-C5-C6-C7
13	q	510	CLA	C3-C5-C6-C7
13	q	511	CLA	C3-C5-C6-C7
13	q	518	CLA	C3-C5-C6-C7
13	r	505	CLA	C3-C5-C6-C7
13	r	511	CLA	C3-C5-C6-C7
13	s	508	CLA	C3-C5-C6-C7
13	s	513	CLA	C3-C5-C6-C7
13	u	501	CLA	C3-C5-C6-C7
13	v	501	CLA	C3-C5-C6-C7
13	v	505	CLA	C3-C5-C6-C7
13	1	516	CLA	C2C-C3C-CAC-CBC
13	q	516	CLA	C2C-C3C-CAC-CBC
13	A	1117	CLA	O1D-CGD-O2D-CED
13	3	513	CLA	O1D-CGD-O2D-CED
13	5	501	CLA	O1D-CGD-O2D-CED
13	5	507	CLA	O1D-CGD-O2D-CED
13	G	1117	CLA	O1D-CGD-O2D-CED
13	c	501	CLA	O1D-CGD-O2D-CED
13	c	507	CLA	O1D-CGD-O2D-CED
13	e	1117	CLA	O1D-CGD-O2D-CED
13	s	513	CLA	O1D-CGD-O2D-CED
13	u	501	CLA	O1D-CGD-O2D-CED
13	u	507	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1114	CLA	CBA-CGA-O2A-C1
13	B	1209	CLA	CBA-CGA-O2A-C1
13	B	1219	CLA	CBA-CGA-O2A-C1
13	B	1207	CLA	CBA-CGA-O2A-C1
13	1	505	CLA	CBA-CGA-O2A-C1
13	2	505	CLA	CBA-CGA-O2A-C1
13	3	505	CLA	CBA-CGA-O2A-C1
13	3	510	CLA	CBA-CGA-O2A-C1
13	4	505	CLA	CBA-CGA-O2A-C1
13	4	510	CLA	CBA-CGA-O2A-C1
13	5	505	CLA	CBA-CGA-O2A-C1
13	G	1114	CLA	CBA-CGA-O2A-C1
13	H	1209	CLA	CBA-CGA-O2A-C1
13	H	1219	CLA	CBA-CGA-O2A-C1
13	H	1207	CLA	CBA-CGA-O2A-C1
13	Y	505	CLA	CBA-CGA-O2A-C1
13	Z	505	CLA	CBA-CGA-O2A-C1
13	a	505	CLA	CBA-CGA-O2A-C1
13	a	510	CLA	CBA-CGA-O2A-C1
13	b	505	CLA	CBA-CGA-O2A-C1
13	b	510	CLA	CBA-CGA-O2A-C1
13	c	502	CLA	CBA-CGA-O2A-C1
13	c	505	CLA	CBA-CGA-O2A-C1
13	e	1114	CLA	CBA-CGA-O2A-C1
13	f	1209	CLA	CBA-CGA-O2A-C1
13	f	1219	CLA	CBA-CGA-O2A-C1
13	f	1207	CLA	CBA-CGA-O2A-C1
13	q	505	CLA	CBA-CGA-O2A-C1
13	r	505	CLA	CBA-CGA-O2A-C1
13	s	505	CLA	CBA-CGA-O2A-C1
13	s	510	CLA	CBA-CGA-O2A-C1
13	t	505	CLA	CBA-CGA-O2A-C1
13	t	510	CLA	CBA-CGA-O2A-C1
13	u	505	CLA	CBA-CGA-O2A-C1
17	A	5006	LHG	C24-C23-O8-C6
17	A	5009	LHG	C24-C23-O8-C6
17	I	5001	LHG	C24-C23-O8-C6
17	L	5218	LHG	C24-C23-O8-C6
17	L	5220	LHG	C24-C23-O8-C6
17	G	5006	LHG	C24-C23-O8-C6
17	G	5009	LHG	C24-C23-O8-C6
17	S	5001	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	V	5218	LHG	C24-C23-O8-C6
17	V	5220	LHG	C24-C23-O8-C6
17	e	5006	LHG	C24-C23-O8-C6
17	e	5009	LHG	C24-C23-O8-C6
17	k	5001	LHG	C24-C23-O8-C6
17	n	5218	LHG	C24-C23-O8-C6
17	n	5220	LHG	C24-C23-O8-C6
13	A	1011	CLA	CBD-CGD-O2D-CED
13	A	1103	CLA	CBD-CGD-O2D-CED
13	A	1104	CLA	CBD-CGD-O2D-CED
13	A	1106	CLA	CBD-CGD-O2D-CED
13	A	1111	CLA	CBD-CGD-O2D-CED
13	A	1112	CLA	CBD-CGD-O2D-CED
13	A	1123	CLA	CBD-CGD-O2D-CED
13	A	1132	CLA	CBD-CGD-O2D-CED
13	B	1012	CLA	CBD-CGD-O2D-CED
13	B	1201	CLA	CBD-CGD-O2D-CED
13	B	1209	CLA	CBD-CGD-O2D-CED
13	B	1220	CLA	CBD-CGD-O2D-CED
13	B	1229	CLA	CBD-CGD-O2D-CED
13	B	1240	CLA	CBD-CGD-O2D-CED
13	J	1303	CLA	CBD-CGD-O2D-CED
13	2	504	CLA	CBD-CGD-O2D-CED
13	2	507	CLA	CBD-CGD-O2D-CED
13	4	507	CLA	CBD-CGD-O2D-CED
13	4	508	CLA	CBD-CGD-O2D-CED
13	6	511	CLA	CBD-CGD-O2D-CED
13	6	512	CLA	CBD-CGD-O2D-CED
13	6	518	CLA	CBD-CGD-O2D-CED
13	6	519	CLA	CBD-CGD-O2D-CED
13	G	1011	CLA	CBD-CGD-O2D-CED
13	G	1103	CLA	CBD-CGD-O2D-CED
13	G	1104	CLA	CBD-CGD-O2D-CED
13	G	1106	CLA	CBD-CGD-O2D-CED
13	G	1111	CLA	CBD-CGD-O2D-CED
13	G	1112	CLA	CBD-CGD-O2D-CED
13	G	1123	CLA	CBD-CGD-O2D-CED
13	G	1132	CLA	CBD-CGD-O2D-CED
13	H	1012	CLA	CBD-CGD-O2D-CED
13	H	1201	CLA	CBD-CGD-O2D-CED
13	H	1209	CLA	CBD-CGD-O2D-CED
13	H	1220	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1229	CLA	CBD-CGD-O2D-CED
13	H	1240	CLA	CBD-CGD-O2D-CED
13	T	1303	CLA	CBD-CGD-O2D-CED
13	Z	504	CLA	CBD-CGD-O2D-CED
13	Z	507	CLA	CBD-CGD-O2D-CED
13	b	507	CLA	CBD-CGD-O2D-CED
13	b	508	CLA	CBD-CGD-O2D-CED
13	d	511	CLA	CBD-CGD-O2D-CED
13	d	512	CLA	CBD-CGD-O2D-CED
13	d	518	CLA	CBD-CGD-O2D-CED
13	d	519	CLA	CBD-CGD-O2D-CED
13	e	1011	CLA	CBD-CGD-O2D-CED
13	e	1103	CLA	CBD-CGD-O2D-CED
13	e	1104	CLA	CBD-CGD-O2D-CED
13	e	1106	CLA	CBD-CGD-O2D-CED
13	e	1111	CLA	CBD-CGD-O2D-CED
13	e	1112	CLA	CBD-CGD-O2D-CED
13	e	1123	CLA	CBD-CGD-O2D-CED
13	e	1132	CLA	CBD-CGD-O2D-CED
13	f	1012	CLA	CBD-CGD-O2D-CED
13	f	1201	CLA	CBD-CGD-O2D-CED
13	f	1209	CLA	CBD-CGD-O2D-CED
13	f	1220	CLA	CBD-CGD-O2D-CED
13	f	1229	CLA	CBD-CGD-O2D-CED
13	f	1240	CLA	CBD-CGD-O2D-CED
13	l	1303	CLA	CBD-CGD-O2D-CED
13	r	504	CLA	CBD-CGD-O2D-CED
13	r	507	CLA	CBD-CGD-O2D-CED
13	t	507	CLA	CBD-CGD-O2D-CED
13	t	508	CLA	CBD-CGD-O2D-CED
13	v	511	CLA	CBD-CGD-O2D-CED
13	v	512	CLA	CBD-CGD-O2D-CED
13	v	518	CLA	CBD-CGD-O2D-CED
13	v	519	CLA	CBD-CGD-O2D-CED
17	A	5008	LHG	C8-C7-O7-C5
17	L	5220	LHG	C8-C7-O7-C5
17	G	5008	LHG	C8-C7-O7-C5
17	V	5220	LHG	C8-C7-O7-C5
17	e	5008	LHG	C8-C7-O7-C5
17	n	5220	LHG	C8-C7-O7-C5
20	1	822	SQD	C8-C7-O47-C45
20	5	822	SQD	C8-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	Y	822	SQD	C8-C7-O47-C45
20	c	822	SQD	C8-C7-O47-C45
20	q	822	SQD	C8-C7-O47-C45
20	u	822	SQD	C8-C7-O47-C45
13	Y	516	CLA	C2C-C3C-CAC-CBC
13	1	501	CLA	O1D-CGD-O2D-CED
13	2	501	CLA	O1D-CGD-O2D-CED
13	2	511	CLA	O1D-CGD-O2D-CED
13	3	518	CLA	O1D-CGD-O2D-CED
13	Y	501	CLA	O1D-CGD-O2D-CED
13	Z	501	CLA	O1D-CGD-O2D-CED
13	Z	511	CLA	O1D-CGD-O2D-CED
13	a	513	CLA	O1D-CGD-O2D-CED
13	a	518	CLA	O1D-CGD-O2D-CED
13	q	501	CLA	O1D-CGD-O2D-CED
13	r	501	CLA	O1D-CGD-O2D-CED
13	r	511	CLA	O1D-CGD-O2D-CED
13	s	518	CLA	O1D-CGD-O2D-CED
13	6	519	CLA	O1A-CGA-O2A-C1
13	d	519	CLA	O1A-CGA-O2A-C1
13	v	519	CLA	O1A-CGA-O2A-C1
13	3	516	CLA	C2C-C3C-CAC-CBC
13	a	516	CLA	C2C-C3C-CAC-CBC
13	s	516	CLA	C2C-C3C-CAC-CBC
13	A	1131	CLA	O1D-CGD-O2D-CED
13	G	1131	CLA	O1D-CGD-O2D-CED
13	e	1131	CLA	O1D-CGD-O2D-CED
13	A	1122	CLA	C4-C3-C5-C6
13	A	1134	CLA	C4-C3-C5-C6
13	A	1139	CLA	C4-C3-C5-C6
13	A	1237	CLA	C4-C3-C5-C6
13	B	1012	CLA	C4-C3-C5-C6
13	B	1212	CLA	C4-C3-C5-C6
13	1	507	CLA	C4-C3-C5-C6
13	2	501	CLA	C4-C3-C5-C6
13	2	518	CLA	C4-C3-C5-C6
13	5	501	CLA	C4-C3-C5-C6
13	6	501	CLA	C4-C3-C5-C6
13	G	1122	CLA	C4-C3-C5-C6
13	G	1134	CLA	C4-C3-C5-C6
13	G	1139	CLA	C4-C3-C5-C6
13	G	1237	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1012	CLA	C4-C3-C5-C6
13	H	1212	CLA	C4-C3-C5-C6
13	Y	507	CLA	C4-C3-C5-C6
13	Z	501	CLA	C4-C3-C5-C6
13	Z	518	CLA	C4-C3-C5-C6
13	c	501	CLA	C4-C3-C5-C6
13	d	501	CLA	C4-C3-C5-C6
13	e	1122	CLA	C4-C3-C5-C6
13	e	1133	CLA	C4-C3-C5-C6
13	e	1134	CLA	C4-C3-C5-C6
13	e	1139	CLA	C4-C3-C5-C6
13	e	1237	CLA	C4-C3-C5-C6
13	f	1012	CLA	C4-C3-C5-C6
13	f	1212	CLA	C4-C3-C5-C6
13	q	507	CLA	C4-C3-C5-C6
13	r	501	CLA	C4-C3-C5-C6
13	r	518	CLA	C4-C3-C5-C6
13	u	501	CLA	C4-C3-C5-C6
13	v	501	CLA	C4-C3-C5-C6
13	A	1104	CLA	C2-C3-C5-C6
13	A	1122	CLA	C2-C3-C5-C6
13	A	1134	CLA	C2-C3-C5-C6
13	A	1139	CLA	C2-C3-C5-C6
13	B	1012	CLA	C2-C3-C5-C6
13	B	1212	CLA	C2-C3-C5-C6
13	1	507	CLA	C2-C3-C5-C6
13	2	501	CLA	C2-C3-C5-C6
13	2	518	CLA	C2-C3-C5-C6
13	6	501	CLA	C2-C3-C5-C6
13	G	1104	CLA	C2-C3-C5-C6
13	G	1122	CLA	C2-C3-C5-C6
13	G	1134	CLA	C2-C3-C5-C6
13	G	1139	CLA	C2-C3-C5-C6
13	H	1012	CLA	C2-C3-C5-C6
13	H	1212	CLA	C2-C3-C5-C6
13	Y	507	CLA	C2-C3-C5-C6
13	Z	501	CLA	C2-C3-C5-C6
13	Z	518	CLA	C2-C3-C5-C6
13	d	501	CLA	C2-C3-C5-C6
13	e	1104	CLA	C2-C3-C5-C6
13	e	1122	CLA	C2-C3-C5-C6
13	e	1134	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1139	CLA	C2-C3-C5-C6
13	f	1012	CLA	C2-C3-C5-C6
13	f	1212	CLA	C2-C3-C5-C6
13	q	507	CLA	C2-C3-C5-C6
13	r	501	CLA	C2-C3-C5-C6
13	r	518	CLA	C2-C3-C5-C6
13	v	501	CLA	C2-C3-C5-C6
20	4	822	SQD	O10-C23-O48-C46
20	b	822	SQD	O10-C23-O48-C46
20	t	822	SQD	O10-C23-O48-C46
13	B	1219	CLA	O1D-CGD-O2D-CED
13	F	1302	CLA	O1D-CGD-O2D-CED
13	4	518	CLA	O1D-CGD-O2D-CED
13	H	1219	CLA	O1D-CGD-O2D-CED
13	R	1302	CLA	O1D-CGD-O2D-CED
13	b	518	CLA	O1D-CGD-O2D-CED
13	f	1219	CLA	O1D-CGD-O2D-CED
13	j	1302	CLA	O1D-CGD-O2D-CED
13	t	518	CLA	O1D-CGD-O2D-CED
13	B	1214	CLA	C2A-CAA-CBA-CGA
13	B	1221	CLA	C2A-CAA-CBA-CGA
13	3	516	CLA	C2A-CAA-CBA-CGA
13	5	507	CLA	C2A-CAA-CBA-CGA
13	6	503	CLA	C2A-CAA-CBA-CGA
13	H	1214	CLA	C2A-CAA-CBA-CGA
13	H	1221	CLA	C2A-CAA-CBA-CGA
13	a	516	CLA	C2A-CAA-CBA-CGA
13	c	507	CLA	C2A-CAA-CBA-CGA
13	d	503	CLA	C2A-CAA-CBA-CGA
13	f	1214	CLA	C2A-CAA-CBA-CGA
13	f	1221	CLA	C2A-CAA-CBA-CGA
13	s	516	CLA	C2A-CAA-CBA-CGA
13	u	507	CLA	C2A-CAA-CBA-CGA
13	v	503	CLA	C2A-CAA-CBA-CGA
13	A	1119	CLA	C3-C5-C6-C7
13	B	1206	CLA	C3-C5-C6-C7
13	2	501	CLA	C3-C5-C6-C7
13	3	505	CLA	C3-C5-C6-C7
13	3	507	CLA	C3-C5-C6-C7
13	4	505	CLA	C3-C5-C6-C7
13	5	505	CLA	C3-C5-C6-C7
13	5	511	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	5	518	CLA	C3-C5-C6-C7
13	G	1119	CLA	C3-C5-C6-C7
13	H	1206	CLA	C3-C5-C6-C7
13	Z	501	CLA	C3-C5-C6-C7
13	a	505	CLA	C3-C5-C6-C7
13	a	507	CLA	C3-C5-C6-C7
13	b	505	CLA	C3-C5-C6-C7
13	c	505	CLA	C3-C5-C6-C7
13	c	511	CLA	C3-C5-C6-C7
13	c	518	CLA	C3-C5-C6-C7
13	e	1119	CLA	C3-C5-C6-C7
13	f	1206	CLA	C3-C5-C6-C7
13	r	501	CLA	C3-C5-C6-C7
13	s	505	CLA	C3-C5-C6-C7
13	s	507	CLA	C3-C5-C6-C7
13	t	505	CLA	C3-C5-C6-C7
13	u	505	CLA	C3-C5-C6-C7
13	u	511	CLA	C3-C5-C6-C7
13	u	518	CLA	C3-C5-C6-C7
13	A	1119	CLA	CBA-CGA-O2A-C1
13	A	1122	CLA	CBA-CGA-O2A-C1
13	A	1129	CLA	CBA-CGA-O2A-C1
13	A	1135	CLA	CBA-CGA-O2A-C1
13	A	1140	CLA	CBA-CGA-O2A-C1
13	A	1130	CLA	CBA-CGA-O2A-C1
13	B	1202	CLA	CBA-CGA-O2A-C1
13	B	1206	CLA	CBA-CGA-O2A-C1
13	B	1240	CLA	CBA-CGA-O2A-C1
13	B	1230	CLA	CBA-CGA-O2A-C1
13	2	504	CLA	CBA-CGA-O2A-C1
13	4	502	CLA	CBA-CGA-O2A-C1
13	5	502	CLA	CBA-CGA-O2A-C1
13	G	1119	CLA	CBA-CGA-O2A-C1
13	G	1122	CLA	CBA-CGA-O2A-C1
13	G	1129	CLA	CBA-CGA-O2A-C1
13	G	1135	CLA	CBA-CGA-O2A-C1
13	G	1140	CLA	CBA-CGA-O2A-C1
13	G	1130	CLA	CBA-CGA-O2A-C1
13	H	1202	CLA	CBA-CGA-O2A-C1
13	H	1206	CLA	CBA-CGA-O2A-C1
13	H	1240	CLA	CBA-CGA-O2A-C1
13	H	1230	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Z	504	CLA	CBA-CGA-O2A-C1
13	b	502	CLA	CBA-CGA-O2A-C1
13	e	1119	CLA	CBA-CGA-O2A-C1
13	e	1122	CLA	CBA-CGA-O2A-C1
13	e	1129	CLA	CBA-CGA-O2A-C1
13	e	1135	CLA	CBA-CGA-O2A-C1
13	e	1140	CLA	CBA-CGA-O2A-C1
13	e	1130	CLA	CBA-CGA-O2A-C1
13	f	1202	CLA	CBA-CGA-O2A-C1
13	f	1206	CLA	CBA-CGA-O2A-C1
13	f	1240	CLA	CBA-CGA-O2A-C1
13	f	1230	CLA	CBA-CGA-O2A-C1
13	r	504	CLA	CBA-CGA-O2A-C1
13	u	502	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C24-C23-O8-C6
17	G	5002	LHG	C24-C23-O8-C6
17	e	5002	LHG	C24-C23-O8-C6
19	J	5104	LMG	C29-C28-O8-C9
19	T	5104	LMG	C29-C28-O8-C9
19	l	5104	LMG	C29-C28-O8-C9
20	2	822	SQD	C24-C23-O48-C46
20	3	822	SQD	C24-C23-O48-C46
20	Z	822	SQD	C24-C23-O48-C46
20	a	822	SQD	C24-C23-O48-C46
20	r	822	SQD	C24-C23-O48-C46
20	s	822	SQD	C24-C23-O48-C46
14	A	2001	PQN	C11-C12-C13-C14
14	B	2002	PQN	C11-C12-C13-C14
14	G	2001	PQN	C11-C12-C13-C14
14	H	2002	PQN	C11-C12-C13-C14
14	e	2001	PQN	C11-C12-C13-C14
14	f	2002	PQN	C11-C12-C13-C14
19	B	5002	LMG	O6-C5-C6-O5
19	H	5002	LMG	O6-C5-C6-O5
19	f	5002	LMG	O6-C5-C6-O5
13	A	1129	CLA	O1A-CGA-O2A-C1
13	B	1212	CLA	O1A-CGA-O2A-C1
13	B	1230	CLA	O1A-CGA-O2A-C1
13	G	1129	CLA	O1A-CGA-O2A-C1
13	H	1212	CLA	O1A-CGA-O2A-C1
13	H	1230	CLA	O1A-CGA-O2A-C1
13	e	1129	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1212	CLA	O1A-CGA-O2A-C1
13	f	1230	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	O10-C23-O8-C6
17	G	5001	LHG	O10-C23-O8-C6
17	e	5001	LHG	O10-C23-O8-C6
20	1	822	SQD	O10-C23-O48-C46
20	Y	822	SQD	O10-C23-O48-C46
20	q	822	SQD	O10-C23-O48-C46
17	A	5002	LHG	O9-C7-O7-C5
17	G	5002	LHG	O9-C7-O7-C5
17	e	5002	LHG	O9-C7-O7-C5
20	5	822	SQD	O49-C7-O47-C45
20	c	822	SQD	O49-C7-O47-C45
20	u	822	SQD	O49-C7-O47-C45
13	3	516	CLA	O1D-CGD-O2D-CED
13	a	516	CLA	O1D-CGD-O2D-CED
13	e	1107	CLA	O1D-CGD-O2D-CED
13	s	516	CLA	O1D-CGD-O2D-CED
13	A	1107	CLA	O1D-CGD-O2D-CED
13	A	1119	CLA	O1D-CGD-O2D-CED
13	6	509	CLA	O1D-CGD-O2D-CED
13	G	1107	CLA	O1D-CGD-O2D-CED
13	G	1119	CLA	O1D-CGD-O2D-CED
13	d	509	CLA	O1D-CGD-O2D-CED
13	e	1119	CLA	O1D-CGD-O2D-CED
13	v	509	CLA	O1D-CGD-O2D-CED
13	A	1107	CLA	C3-C5-C6-C7
13	A	1108	CLA	C3-C5-C6-C7
13	B	1205	CLA	C3-C5-C6-C7
13	B	1215	CLA	C3-C5-C6-C7
13	2	507	CLA	C3-C5-C6-C7
13	3	510	CLA	C3-C5-C6-C7
13	G	1107	CLA	C3-C5-C6-C7
13	G	1108	CLA	C3-C5-C6-C7
13	H	1205	CLA	C3-C5-C6-C7
13	H	1215	CLA	C3-C5-C6-C7
13	Z	507	CLA	C3-C5-C6-C7
13	a	510	CLA	C3-C5-C6-C7
13	e	1107	CLA	C3-C5-C6-C7
13	e	1108	CLA	C3-C5-C6-C7
13	f	1205	CLA	C3-C5-C6-C7
13	f	1215	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	r	507	CLA	C3-C5-C6-C7
13	s	510	CLA	C3-C5-C6-C7
13	A	1113	CLA	CBD-CGD-O2D-CED
13	3	504	CLA	CBD-CGD-O2D-CED
13	6	507	CLA	CBD-CGD-O2D-CED
13	G	1113	CLA	CBD-CGD-O2D-CED
13	a	504	CLA	CBD-CGD-O2D-CED
13	d	507	CLA	CBD-CGD-O2D-CED
13	e	1113	CLA	CBD-CGD-O2D-CED
13	s	504	CLA	CBD-CGD-O2D-CED
13	v	507	CLA	CBD-CGD-O2D-CED
17	A	5004	LHG	O2-C2-C3-O3
17	G	5004	LHG	O2-C2-C3-O3
17	e	5004	LHG	O2-C2-C3-O3
13	A	1108	CLA	O1D-CGD-O2D-CED
13	A	1801	CLA	O1D-CGD-O2D-CED
13	1	516	CLA	O1D-CGD-O2D-CED
13	4	517	CLA	O1D-CGD-O2D-CED
13	5	508	CLA	O1D-CGD-O2D-CED
13	5	510	CLA	O1D-CGD-O2D-CED
13	5	517	CLA	O1D-CGD-O2D-CED
13	G	1108	CLA	O1D-CGD-O2D-CED
13	G	1801	CLA	O1D-CGD-O2D-CED
13	H	1221	CLA	O1D-CGD-O2D-CED
13	Y	516	CLA	O1D-CGD-O2D-CED
13	b	517	CLA	O1D-CGD-O2D-CED
13	c	508	CLA	O1D-CGD-O2D-CED
13	c	510	CLA	O1D-CGD-O2D-CED
13	c	517	CLA	O1D-CGD-O2D-CED
13	e	1108	CLA	O1D-CGD-O2D-CED
13	e	1801	CLA	O1D-CGD-O2D-CED
13	f	1221	CLA	O1D-CGD-O2D-CED
13	q	516	CLA	O1D-CGD-O2D-CED
13	t	517	CLA	O1D-CGD-O2D-CED
13	u	508	CLA	O1D-CGD-O2D-CED
13	u	510	CLA	O1D-CGD-O2D-CED
13	u	517	CLA	O1D-CGD-O2D-CED
13	A	1108	CLA	CBA-CGA-O2A-C1
13	G	1108	CLA	CBA-CGA-O2A-C1
13	e	1108	CLA	CBA-CGA-O2A-C1
13	t	502	CLA	CBA-CGA-O2A-C1
17	B	1842	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	1842	LHG	C24-C23-O8-C6
17	f	1842	LHG	C24-C23-O8-C6
18	B	1843	LMU	O5B-C5B-C6B-O6B
18	H	1843	LMU	O5B-C5B-C6B-O6B
18	f	1843	LMU	O5B-C5B-C6B-O6B
13	A	1135	CLA	O1A-CGA-O2A-C1
13	5	502	CLA	O1A-CGA-O2A-C1
13	G	1135	CLA	O1A-CGA-O2A-C1
13	c	502	CLA	O1A-CGA-O2A-C1
13	e	1135	CLA	O1A-CGA-O2A-C1
13	u	502	CLA	O1A-CGA-O2A-C1
13	B	1221	CLA	O1D-CGD-O2D-CED
18	A	1848	LMU	O5B-C5B-C6B-O6B
18	G	1848	LMU	O5B-C5B-C6B-O6B
18	e	1848	LMU	O5B-C5B-C6B-O6B
13	A	1137	CLA	CBD-CGD-O2D-CED
13	B	1227	CLA	CBD-CGD-O2D-CED
13	2	519	CLA	CBD-CGD-O2D-CED
13	4	505	CLA	CBD-CGD-O2D-CED
13	6	517	CLA	CBD-CGD-O2D-CED
13	G	1137	CLA	CBD-CGD-O2D-CED
13	H	1227	CLA	CBD-CGD-O2D-CED
13	Z	519	CLA	CBD-CGD-O2D-CED
13	b	505	CLA	CBD-CGD-O2D-CED
13	d	517	CLA	CBD-CGD-O2D-CED
13	e	1137	CLA	CBD-CGD-O2D-CED
13	f	1227	CLA	CBD-CGD-O2D-CED
13	r	519	CLA	CBD-CGD-O2D-CED
13	t	505	CLA	CBD-CGD-O2D-CED
13	v	517	CLA	CBD-CGD-O2D-CED
13	G	1108	CLA	O1A-CGA-O2A-C1
13	e	1108	CLA	O1A-CGA-O2A-C1
19	B	5002	LMG	C4-C5-C6-O5
19	H	5002	LMG	C4-C5-C6-O5
19	f	5002	LMG	C4-C5-C6-O5
13	B	1203	CLA	O1D-CGD-O2D-CED
13	B	1207	CLA	O1D-CGD-O2D-CED
13	H	1203	CLA	O1D-CGD-O2D-CED
13	H	1207	CLA	O1D-CGD-O2D-CED
13	f	1203	CLA	O1D-CGD-O2D-CED
13	f	1207	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	1	508	CLA	C3-C5-C6-C7
13	G	1013	CLA	C3-C5-C6-C7
13	Y	508	CLA	C3-C5-C6-C7
13	e	1013	CLA	C3-C5-C6-C7
13	q	508	CLA	C3-C5-C6-C7
17	A	5006	LHG	C29-C30-C31-C32
17	G	5006	LHG	C29-C30-C31-C32
17	e	5006	LHG	C29-C30-C31-C32
17	B	1855	LHG	C5-C6-O8-C23
17	H	1855	LHG	C5-C6-O8-C23
17	f	1855	LHG	C5-C6-O8-C23
13	A	1013	CLA	CBD-CGD-O2D-CED
13	B	1226	CLA	CBD-CGD-O2D-CED
13	B	1232	CLA	CBD-CGD-O2D-CED
13	1	502	CLA	CBD-CGD-O2D-CED
13	4	513	CLA	CBD-CGD-O2D-CED
13	5	512	CLA	CBD-CGD-O2D-CED
13	G	1013	CLA	CBD-CGD-O2D-CED
13	H	1226	CLA	CBD-CGD-O2D-CED
13	H	1232	CLA	CBD-CGD-O2D-CED
13	Y	502	CLA	CBD-CGD-O2D-CED
13	b	513	CLA	CBD-CGD-O2D-CED
13	c	512	CLA	CBD-CGD-O2D-CED
13	e	1013	CLA	CBD-CGD-O2D-CED
13	f	1226	CLA	CBD-CGD-O2D-CED
13	f	1232	CLA	CBD-CGD-O2D-CED
13	q	502	CLA	CBD-CGD-O2D-CED
13	t	513	CLA	CBD-CGD-O2D-CED
13	u	512	CLA	CBD-CGD-O2D-CED
13	3	519	CLA	O1D-CGD-O2D-CED
13	6	502	CLA	O1D-CGD-O2D-CED
13	a	519	CLA	O1D-CGD-O2D-CED
13	d	502	CLA	O1D-CGD-O2D-CED
13	s	519	CLA	O1D-CGD-O2D-CED
13	v	502	CLA	O1D-CGD-O2D-CED
13	B	1212	CLA	CBA-CGA-O2A-C1
13	H	1212	CLA	CBA-CGA-O2A-C1
13	f	1212	CLA	CBA-CGA-O2A-C1
13	A	1115	CLA	C4-C3-C5-C6
13	A	1133	CLA	C4-C3-C5-C6
13	G	1115	CLA	C4-C3-C5-C6
13	G	1133	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1115	CLA	C4-C3-C5-C6
13	A	1115	CLA	C2-C3-C5-C6
13	A	1237	CLA	C2-C3-C5-C6
13	5	501	CLA	C2-C3-C5-C6
13	G	1115	CLA	C2-C3-C5-C6
13	G	1237	CLA	C2-C3-C5-C6
13	c	501	CLA	C2-C3-C5-C6
13	e	1115	CLA	C2-C3-C5-C6
13	e	1237	CLA	C2-C3-C5-C6
13	u	501	CLA	C2-C3-C5-C6
13	A	1108	CLA	O1A-CGA-O2A-C1
13	A	1122	CLA	O1A-CGA-O2A-C1
13	4	502	CLA	O1A-CGA-O2A-C1
13	G	1122	CLA	O1A-CGA-O2A-C1
13	e	1122	CLA	O1A-CGA-O2A-C1
13	t	502	CLA	O1A-CGA-O2A-C1
17	A	5005	LHG	O10-C23-O8-C6
17	G	5005	LHG	O10-C23-O8-C6
17	e	5005	LHG	O10-C23-O8-C6
13	G	1120	CLA	O1D-CGD-O2D-CED
13	e	1120	CLA	O1D-CGD-O2D-CED
13	B	1231	CLA	CBD-CGD-O2D-CED
13	3	511	CLA	CBD-CGD-O2D-CED
13	H	1231	CLA	CBD-CGD-O2D-CED
13	a	511	CLA	CBD-CGD-O2D-CED
13	f	1231	CLA	CBD-CGD-O2D-CED
13	s	511	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	O1D-CGD-O2D-CED
18	B	1843	LMU	C4B-C5B-C6B-O6B
18	H	1843	LMU	C4B-C5B-C6B-O6B
18	f	1843	LMU	C4B-C5B-C6B-O6B
13	A	1127	CLA	C2A-CAA-CBA-CGA
13	5	505	CLA	C2A-CAA-CBA-CGA
13	G	1127	CLA	C2A-CAA-CBA-CGA
13	c	505	CLA	C2A-CAA-CBA-CGA
13	e	1127	CLA	C2A-CAA-CBA-CGA
13	u	505	CLA	C2A-CAA-CBA-CGA
13	3	502	CLA	O1A-CGA-O2A-C1
13	a	502	CLA	O1A-CGA-O2A-C1
13	b	502	CLA	O1A-CGA-O2A-C1
13	s	502	CLA	O1A-CGA-O2A-C1
18	1	902	LMU	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	Y	902	LMU	O5'-C1'-O1'-C1
18	Z	901	LMU	O5'-C1'-O1'-C1
18	q	902	LMU	O5'-C1'-O1'-C1
18	r	901	LMU	O5'-C1'-O1'-C1
13	4	511	CLA	O1D-CGD-O2D-CED
13	b	511	CLA	O1D-CGD-O2D-CED
13	B	1234	CLA	CBA-CGA-O2A-C1
13	J	1303	CLA	CBA-CGA-O2A-C1
13	3	502	CLA	CBA-CGA-O2A-C1
13	H	1234	CLA	CBA-CGA-O2A-C1
13	T	1303	CLA	CBA-CGA-O2A-C1
13	a	502	CLA	CBA-CGA-O2A-C1
13	f	1234	CLA	CBA-CGA-O2A-C1
13	l	1303	CLA	CBA-CGA-O2A-C1
13	s	502	CLA	CBA-CGA-O2A-C1
13	A	1138	CLA	CBD-CGD-O2D-CED
13	B	1206	CLA	CBD-CGD-O2D-CED
13	B	1235	CLA	CBD-CGD-O2D-CED
13	K	1103	CLA	CBD-CGD-O2D-CED
13	1	507	CLA	CBD-CGD-O2D-CED
13	1	511	CLA	CBD-CGD-O2D-CED
13	1	512	CLA	CBD-CGD-O2D-CED
13	1	519	CLA	CBD-CGD-O2D-CED
13	6	510	CLA	CBD-CGD-O2D-CED
13	G	1138	CLA	CBD-CGD-O2D-CED
13	H	1206	CLA	CBD-CGD-O2D-CED
13	H	1235	CLA	CBD-CGD-O2D-CED
13	U	1103	CLA	CBD-CGD-O2D-CED
13	Y	507	CLA	CBD-CGD-O2D-CED
13	Y	511	CLA	CBD-CGD-O2D-CED
13	Y	512	CLA	CBD-CGD-O2D-CED
13	Y	519	CLA	CBD-CGD-O2D-CED
13	d	510	CLA	CBD-CGD-O2D-CED
13	e	1138	CLA	CBD-CGD-O2D-CED
13	f	1206	CLA	CBD-CGD-O2D-CED
13	f	1235	CLA	CBD-CGD-O2D-CED
13	m	1103	CLA	CBD-CGD-O2D-CED
13	q	507	CLA	CBD-CGD-O2D-CED
13	q	511	CLA	CBD-CGD-O2D-CED
13	q	512	CLA	CBD-CGD-O2D-CED
13	q	519	CLA	CBD-CGD-O2D-CED
13	v	510	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	1843	LMU	O5'-C5'-C6'-O6'
18	H	1843	LMU	O5'-C5'-C6'-O6'
18	f	1843	LMU	O5'-C5'-C6'-O6'
13	B	1239	CLA	O1D-CGD-O2D-CED
13	H	1239	CLA	O1D-CGD-O2D-CED
13	f	1239	CLA	O1D-CGD-O2D-CED
13	t	511	CLA	O1D-CGD-O2D-CED
18	A	1848	LMU	C4B-C5B-C6B-O6B
18	G	1848	LMU	C4B-C5B-C6B-O6B
18	e	1848	LMU	C4B-C5B-C6B-O6B
13	1	518	CLA	CBD-CGD-O2D-CED
13	2	516	CLA	CBD-CGD-O2D-CED
13	Y	518	CLA	CBD-CGD-O2D-CED
13	Z	516	CLA	CBD-CGD-O2D-CED
13	q	518	CLA	CBD-CGD-O2D-CED
13	r	516	CLA	CBD-CGD-O2D-CED
13	B	1234	CLA	O1A-CGA-O2A-C1
13	H	1234	CLA	O1A-CGA-O2A-C1
13	f	1234	CLA	O1A-CGA-O2A-C1
20	3	822	SQD	O10-C23-O48-C46
20	a	822	SQD	O10-C23-O48-C46
20	s	822	SQD	O10-C23-O48-C46
17	A	5005	LHG	C1-C2-C3-O3
17	G	5005	LHG	C1-C2-C3-O3
17	e	5005	LHG	C1-C2-C3-O3
13	A	1104	CLA	CBA-CGA-O2A-C1
13	A	1106	CLA	CBA-CGA-O2A-C1
13	A	1118	CLA	CBA-CGA-O2A-C1
13	A	1133	CLA	CBA-CGA-O2A-C1
13	A	1237	CLA	CBA-CGA-O2A-C1
13	B	1214	CLA	CBA-CGA-O2A-C1
13	B	1225	CLA	CBA-CGA-O2A-C1
13	B	1239	CLA	CBA-CGA-O2A-C1
13	K	1401	CLA	CBA-CGA-O2A-C1
13	2	502	CLA	CBA-CGA-O2A-C1
13	2	512	CLA	CBA-CGA-O2A-C1
13	6	518	CLA	CBA-CGA-O2A-C1
13	G	1104	CLA	CBA-CGA-O2A-C1
13	G	1106	CLA	CBA-CGA-O2A-C1
13	G	1118	CLA	CBA-CGA-O2A-C1
13	G	1133	CLA	CBA-CGA-O2A-C1
13	G	1237	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1214	CLA	CBA-CGA-O2A-C1
13	H	1225	CLA	CBA-CGA-O2A-C1
13	H	1239	CLA	CBA-CGA-O2A-C1
13	U	1401	CLA	CBA-CGA-O2A-C1
13	Z	502	CLA	CBA-CGA-O2A-C1
13	Z	512	CLA	CBA-CGA-O2A-C1
13	d	518	CLA	CBA-CGA-O2A-C1
13	e	1104	CLA	CBA-CGA-O2A-C1
13	e	1106	CLA	CBA-CGA-O2A-C1
13	e	1118	CLA	CBA-CGA-O2A-C1
13	e	1133	CLA	CBA-CGA-O2A-C1
13	e	1237	CLA	CBA-CGA-O2A-C1
13	f	1214	CLA	CBA-CGA-O2A-C1
13	f	1225	CLA	CBA-CGA-O2A-C1
13	f	1239	CLA	CBA-CGA-O2A-C1
13	m	1401	CLA	CBA-CGA-O2A-C1
13	r	502	CLA	CBA-CGA-O2A-C1
13	r	512	CLA	CBA-CGA-O2A-C1
13	v	518	CLA	CBA-CGA-O2A-C1
17	A	5001	LHG	C24-C23-O8-C6
17	G	5001	LHG	C24-C23-O8-C6
17	e	5001	LHG	C24-C23-O8-C6
20	L	5216	SQD	C24-C23-O48-C46
20	1	822	SQD	C24-C23-O48-C46
20	V	5216	SQD	C24-C23-O48-C46
20	Y	822	SQD	C24-C23-O48-C46
20	n	5216	SQD	C24-C23-O48-C46
20	q	822	SQD	C24-C23-O48-C46
13	A	1126	CLA	CBD-CGD-O2D-CED
13	A	1134	CLA	CBD-CGD-O2D-CED
13	B	1230	CLA	CBD-CGD-O2D-CED
13	5	502	CLA	CBD-CGD-O2D-CED
13	G	1126	CLA	CBD-CGD-O2D-CED
13	H	1230	CLA	CBD-CGD-O2D-CED
13	c	502	CLA	CBD-CGD-O2D-CED
13	e	1126	CLA	CBD-CGD-O2D-CED
13	e	1134	CLA	CBD-CGD-O2D-CED
13	f	1230	CLA	CBD-CGD-O2D-CED
13	u	502	CLA	CBD-CGD-O2D-CED
19	J	5104	LMG	C4-C5-C6-O5
19	T	5104	LMG	C4-C5-C6-O5
19	l	5104	LMG	C4-C5-C6-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	J	1302	CLA	O1D-CGD-O2D-CED
13	T	1302	CLA	O1D-CGD-O2D-CED
13	l	1302	CLA	O1D-CGD-O2D-CED
13	1	516	CLA	C4C-C3C-CAC-CBC
13	Y	516	CLA	C4C-C3C-CAC-CBC
13	q	516	CLA	C4C-C3C-CAC-CBC
18	B	1843	LMU	C4'-C5'-C6'-O6'
18	H	1843	LMU	C4'-C5'-C6'-O6'
18	f	1843	LMU	C4'-C5'-C6'-O6'
13	1	510	CLA	C4-C3-C5-C6
13	Y	510	CLA	C4-C3-C5-C6
13	q	510	CLA	C4-C3-C5-C6
13	A	1133	CLA	C2-C3-C5-C6
13	1	510	CLA	C2-C3-C5-C6
13	G	1133	CLA	C2-C3-C5-C6
13	Y	510	CLA	C2-C3-C5-C6
13	e	1133	CLA	C2-C3-C5-C6
13	q	510	CLA	C2-C3-C5-C6
13	A	1130	CLA	C3-C5-C6-C7
13	B	1204	CLA	C3-C5-C6-C7
13	4	503	CLA	C3-C5-C6-C7
13	G	1130	CLA	C3-C5-C6-C7
13	H	1204	CLA	C3-C5-C6-C7
13	b	503	CLA	C3-C5-C6-C7
13	e	1130	CLA	C3-C5-C6-C7
13	f	1204	CLA	C3-C5-C6-C7
13	t	503	CLA	C3-C5-C6-C7
13	3	507	CLA	CBD-CGD-O2D-CED
13	G	1134	CLA	CBD-CGD-O2D-CED
13	a	507	CLA	CBD-CGD-O2D-CED
13	s	507	CLA	CBD-CGD-O2D-CED
13	A	1116	CLA	C6-C7-C8-C9
13	A	1137	CLA	C6-C7-C8-C9
13	A	1139	CLA	C6-C7-C8-C9
13	B	1215	CLA	C6-C7-C8-C9
13	B	1215	CLA	C11-C12-C13-C14
13	B	1226	CLA	C14-C13-C15-C16
13	J	1303	CLA	C14-C13-C15-C16
13	3	505	CLA	C6-C7-C8-C9
13	G	1116	CLA	C6-C7-C8-C9
13	G	1137	CLA	C6-C7-C8-C9
13	G	1139	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1215	CLA	C6-C7-C8-C9
13	H	1215	CLA	C11-C12-C13-C14
13	H	1226	CLA	C14-C13-C15-C16
13	T	1303	CLA	C14-C13-C15-C16
13	a	505	CLA	C6-C7-C8-C9
13	e	1116	CLA	C6-C7-C8-C9
13	e	1137	CLA	C6-C7-C8-C9
13	e	1139	CLA	C6-C7-C8-C9
13	f	1215	CLA	C6-C7-C8-C9
13	f	1215	CLA	C11-C12-C13-C14
13	f	1226	CLA	C14-C13-C15-C16
13	l	1303	CLA	C14-C13-C15-C16
13	s	505	CLA	C6-C7-C8-C9
14	A	2001	PQN	C21-C22-C23-C24
14	G	2001	PQN	C21-C22-C23-C24
14	e	2001	PQN	C21-C22-C23-C24
13	A	1103	CLA	O1D-CGD-O2D-CED
13	A	1132	CLA	O1D-CGD-O2D-CED
13	B	1229	CLA	O1D-CGD-O2D-CED
13	6	519	CLA	O1D-CGD-O2D-CED
13	G	1103	CLA	O1D-CGD-O2D-CED
13	G	1111	CLA	O1D-CGD-O2D-CED
13	G	1132	CLA	O1D-CGD-O2D-CED
13	H	1229	CLA	O1D-CGD-O2D-CED
13	d	519	CLA	O1D-CGD-O2D-CED
13	e	1103	CLA	O1D-CGD-O2D-CED
13	e	1132	CLA	O1D-CGD-O2D-CED
13	f	1229	CLA	O1D-CGD-O2D-CED
13	f	1240	CLA	O1D-CGD-O2D-CED
13	v	519	CLA	O1D-CGD-O2D-CED
18	A	1849	LMU	C2'-C1'-O1'-C1
18	J	5105	LMU	C2'-C1'-O1'-C1
18	1	902	LMU	C2'-C1'-O1'-C1
18	2	901	LMU	C2'-C1'-O1'-C1
18	G	1849	LMU	C2'-C1'-O1'-C1
18	T	5105	LMU	C2'-C1'-O1'-C1
18	Y	902	LMU	C2'-C1'-O1'-C1
18	Z	901	LMU	C2'-C1'-O1'-C1
18	e	1849	LMU	C2'-C1'-O1'-C1
18	l	5105	LMU	C2'-C1'-O1'-C1
18	q	902	LMU	C2'-C1'-O1'-C1
18	r	901	LMU	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1111	CLA	O1D-CGD-O2D-CED
13	B	1012	CLA	O1D-CGD-O2D-CED
13	B	1240	CLA	O1D-CGD-O2D-CED
13	6	511	CLA	O1D-CGD-O2D-CED
13	6	518	CLA	O1D-CGD-O2D-CED
13	H	1012	CLA	O1D-CGD-O2D-CED
13	H	1240	CLA	O1D-CGD-O2D-CED
13	d	511	CLA	O1D-CGD-O2D-CED
13	d	518	CLA	O1D-CGD-O2D-CED
13	e	1111	CLA	O1D-CGD-O2D-CED
13	f	1012	CLA	O1D-CGD-O2D-CED
13	v	511	CLA	O1D-CGD-O2D-CED
13	v	518	CLA	O1D-CGD-O2D-CED
13	A	1118	CLA	O1A-CGA-O2A-C1
13	A	1133	CLA	O1A-CGA-O2A-C1
13	G	1118	CLA	O1A-CGA-O2A-C1
13	G	1133	CLA	O1A-CGA-O2A-C1
13	e	1118	CLA	O1A-CGA-O2A-C1
13	e	1133	CLA	O1A-CGA-O2A-C1
13	J	1303	CLA	O1D-CGD-O2D-CED
13	2	504	CLA	O1D-CGD-O2D-CED
13	T	1303	CLA	O1D-CGD-O2D-CED
13	Z	504	CLA	O1D-CGD-O2D-CED
13	l	1303	CLA	O1D-CGD-O2D-CED
13	r	504	CLA	O1D-CGD-O2D-CED
16	A	4001	BCR	C37-C22-C23-C24
16	A	4011	BCR	C37-C22-C23-C24
16	B	4005	BCR	C7-C8-C9-C34
16	B	4014	BCR	C36-C18-C19-C20
16	J	4013	BCR	C36-C18-C19-C20
16	J	4013	BCR	C37-C22-C23-C24
16	J	4012	BCR	C37-C22-C23-C24
16	M	4021	BCR	C11-C12-C13-C35
16	M	4021	BCR	C36-C18-C19-C20
16	1	523	BCR	C37-C22-C23-C24
16	2	522	BCR	C7-C8-C9-C34
16	2	523	BCR	C37-C22-C23-C24
16	3	523	BCR	C37-C22-C23-C24
16	4	521	BCR	C7-C8-C9-C34
16	4	523	BCR	C37-C22-C23-C24
16	5	522	BCR	C7-C8-C9-C34
16	5	523	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	6	523	BCR	C37-C22-C23-C24
16	6	524	BCR	C7-C8-C9-C34
16	G	4001	BCR	C37-C22-C23-C24
16	G	4011	BCR	C37-C22-C23-C24
16	H	4005	BCR	C7-C8-C9-C34
16	H	4014	BCR	C36-C18-C19-C20
16	T	4013	BCR	C36-C18-C19-C20
16	T	4013	BCR	C37-C22-C23-C24
16	T	4012	BCR	C37-C22-C23-C24
16	W	4021	BCR	C11-C12-C13-C35
16	W	4021	BCR	C36-C18-C19-C20
16	Y	523	BCR	C37-C22-C23-C24
16	Z	522	BCR	C7-C8-C9-C34
16	Z	523	BCR	C37-C22-C23-C24
16	a	523	BCR	C37-C22-C23-C24
16	b	521	BCR	C7-C8-C9-C34
16	b	523	BCR	C37-C22-C23-C24
16	c	522	BCR	C7-C8-C9-C34
16	c	523	BCR	C37-C22-C23-C24
16	d	523	BCR	C37-C22-C23-C24
16	d	524	BCR	C7-C8-C9-C34
16	e	4001	BCR	C37-C22-C23-C24
16	e	4011	BCR	C37-C22-C23-C24
16	f	4005	BCR	C7-C8-C9-C34
16	f	4014	BCR	C36-C18-C19-C20
16	l	4013	BCR	C36-C18-C19-C20
16	l	4013	BCR	C37-C22-C23-C24
16	l	4012	BCR	C37-C22-C23-C24
16	o	4021	BCR	C11-C12-C13-C35
16	o	4021	BCR	C36-C18-C19-C20
16	q	523	BCR	C37-C22-C23-C24
16	r	522	BCR	C7-C8-C9-C34
16	r	523	BCR	C37-C22-C23-C24
16	s	523	BCR	C37-C22-C23-C24
16	t	521	BCR	C7-C8-C9-C34
16	t	523	BCR	C37-C22-C23-C24
16	u	522	BCR	C7-C8-C9-C34
16	u	523	BCR	C37-C22-C23-C24
16	v	523	BCR	C37-C22-C23-C24
16	v	524	BCR	C7-C8-C9-C34
16	A	4011	BCR	C21-C22-C23-C24
16	J	4013	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	J	4012	BCR	C21-C22-C23-C24
16	3	521	BCR	C7-C8-C9-C10
16	G	4011	BCR	C21-C22-C23-C24
16	T	4013	BCR	C21-C22-C23-C24
16	T	4012	BCR	C21-C22-C23-C24
16	a	521	BCR	C7-C8-C9-C10
16	e	4011	BCR	C21-C22-C23-C24
16	l	4013	BCR	C21-C22-C23-C24
16	l	4012	BCR	C21-C22-C23-C24
16	s	521	BCR	C7-C8-C9-C10
13	A	1135	CLA	C3-C5-C6-C7
13	B	1217	CLA	C2A-CAA-CBA-CGA
13	G	1135	CLA	C3-C5-C6-C7
13	H	1217	CLA	C2A-CAA-CBA-CGA
13	e	1135	CLA	C3-C5-C6-C7
13	f	1217	CLA	C2A-CAA-CBA-CGA
13	A	1106	CLA	O1D-CGD-O2D-CED
13	B	1214	CLA	O1A-CGA-O2A-C1
13	B	1239	CLA	O1A-CGA-O2A-C1
13	2	502	CLA	O1A-CGA-O2A-C1
13	H	1214	CLA	O1A-CGA-O2A-C1
13	H	1239	CLA	O1A-CGA-O2A-C1
13	Z	502	CLA	O1A-CGA-O2A-C1
13	f	1214	CLA	O1A-CGA-O2A-C1
13	f	1239	CLA	O1A-CGA-O2A-C1
13	r	502	CLA	O1A-CGA-O2A-C1
13	B	1210	CLA	C3-C5-C6-C7
13	H	1210	CLA	C3-C5-C6-C7
13	f	1210	CLA	C3-C5-C6-C7
13	e	1124	CLA	CBD-CGD-O2D-CED
13	4	507	CLA	O1D-CGD-O2D-CED
13	G	1106	CLA	O1D-CGD-O2D-CED
13	e	1106	CLA	O1D-CGD-O2D-CED
13	J	1302	CLA	CBA-CGA-O2A-C1
13	1	502	CLA	CBA-CGA-O2A-C1
13	T	1302	CLA	CBA-CGA-O2A-C1
13	Y	502	CLA	CBA-CGA-O2A-C1
13	l	1302	CLA	CBA-CGA-O2A-C1
13	q	502	CLA	CBA-CGA-O2A-C1
19	B	5002	LMG	C29-C28-O8-C9
19	H	5002	LMG	C29-C28-O8-C9
19	f	5002	LMG	C29-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1023	CLA	C2C-C3C-CAC-CBC
13	f	1023	CLA	C2C-C3C-CAC-CBC
13	A	1112	CLA	O1D-CGD-O2D-CED
13	B	1201	CLA	O1D-CGD-O2D-CED
13	B	1209	CLA	O1D-CGD-O2D-CED
13	2	507	CLA	O1D-CGD-O2D-CED
13	G	1112	CLA	O1D-CGD-O2D-CED
13	H	1201	CLA	O1D-CGD-O2D-CED
13	H	1209	CLA	O1D-CGD-O2D-CED
13	Z	507	CLA	O1D-CGD-O2D-CED
13	b	507	CLA	O1D-CGD-O2D-CED
13	e	1112	CLA	O1D-CGD-O2D-CED
13	f	1201	CLA	O1D-CGD-O2D-CED
13	f	1209	CLA	O1D-CGD-O2D-CED
13	r	507	CLA	O1D-CGD-O2D-CED
13	t	507	CLA	O1D-CGD-O2D-CED
13	v	512	CLA	O1D-CGD-O2D-CED
13	A	1124	CLA	CBD-CGD-O2D-CED
13	G	1124	CLA	CBD-CGD-O2D-CED
13	B	1023	CLA	C2C-C3C-CAC-CBC
13	A	1115	CLA	C10-C11-C12-C13
13	B	1215	CLA	C10-C11-C12-C13
13	B	1220	CLA	C5-C6-C7-C8
13	B	1223	CLA	C8-C10-C11-C12
13	B	1225	CLA	C15-C16-C17-C18
13	L	1503	CLA	C5-C6-C7-C8
13	L	1503	CLA	C8-C10-C11-C12
13	2	510	CLA	C8-C10-C11-C12
13	G	1115	CLA	C10-C11-C12-C13
13	H	1215	CLA	C10-C11-C12-C13
13	H	1220	CLA	C5-C6-C7-C8
13	H	1223	CLA	C8-C10-C11-C12
13	H	1225	CLA	C15-C16-C17-C18
13	V	1503	CLA	C5-C6-C7-C8
13	V	1503	CLA	C8-C10-C11-C12
13	Z	510	CLA	C8-C10-C11-C12
13	e	1115	CLA	C10-C11-C12-C13
13	f	1215	CLA	C10-C11-C12-C13
13	f	1220	CLA	C5-C6-C7-C8
13	f	1223	CLA	C8-C10-C11-C12
13	f	1225	CLA	C15-C16-C17-C18
13	n	1503	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	n	1503	CLA	C8-C10-C11-C12
13	r	510	CLA	C8-C10-C11-C12
13	6	512	CLA	O1D-CGD-O2D-CED
13	d	512	CLA	O1D-CGD-O2D-CED
17	A	5004	LHG	O1-C1-C2-O2
17	A	5007	LHG	O1-C1-C2-O2
17	G	5004	LHG	O1-C1-C2-O2
17	G	5007	LHG	O1-C1-C2-O2
17	e	5004	LHG	O1-C1-C2-O2
17	e	5007	LHG	O1-C1-C2-O2
13	4	508	CLA	O1D-CGD-O2D-CED
13	b	508	CLA	O1D-CGD-O2D-CED
13	t	508	CLA	O1D-CGD-O2D-CED
13	A	1133	CLA	C8-C10-C11-C12
13	1	509	CLA	C10-C11-C12-C13
13	G	1133	CLA	C8-C10-C11-C12
13	Y	509	CLA	C10-C11-C12-C13
13	e	1133	CLA	C8-C10-C11-C12
13	q	509	CLA	C10-C11-C12-C13
13	2	510	CLA	CBD-CGD-O2D-CED
13	3	505	CLA	CBD-CGD-O2D-CED
13	4	509	CLA	CBD-CGD-O2D-CED
13	Z	510	CLA	CBD-CGD-O2D-CED
13	b	509	CLA	CBD-CGD-O2D-CED
13	r	510	CLA	CBD-CGD-O2D-CED
13	s	505	CLA	CBD-CGD-O2D-CED
13	t	509	CLA	CBD-CGD-O2D-CED
19	J	5104	LMG	O6-C5-C6-O5
19	T	5104	LMG	O6-C5-C6-O5
19	l	5104	LMG	O6-C5-C6-O5
13	B	1221	CLA	C11-C10-C8-C7
13	B	1230	CLA	C6-C7-C8-C10
13	F	1301	CLA	C11-C10-C8-C7
13	H	1221	CLA	C11-C10-C8-C7
13	H	1230	CLA	C6-C7-C8-C10
13	R	1301	CLA	C11-C10-C8-C7
13	f	1221	CLA	C11-C10-C8-C7
13	f	1230	CLA	C6-C7-C8-C10
13	j	1301	CLA	C11-C10-C8-C7
13	B	1217	CLA	C4-C3-C5-C6
13	L	1503	CLA	C4-C3-C5-C6
13	H	1217	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	V	1503	CLA	C4-C3-C5-C6
13	f	1217	CLA	C4-C3-C5-C6
13	n	1503	CLA	C4-C3-C5-C6
13	A	1106	CLA	C8-C10-C11-C12
13	G	1106	CLA	C8-C10-C11-C12
13	e	1106	CLA	C8-C10-C11-C12
17	B	1842	LHG	C23-C24-C25-C26
17	L	5220	LHG	C23-C24-C25-C26
17	V	5220	LHG	C23-C24-C25-C26
17	f	1842	LHG	C23-C24-C25-C26
17	n	5220	LHG	C23-C24-C25-C26
16	6	522	BCR	C9-C10-C11-C12
16	d	522	BCR	C9-C10-C11-C12
16	v	522	BCR	C9-C10-C11-C12
18	A	1849	LMU	O1'-C1-C2-C3
18	G	1849	LMU	O1'-C1-C2-C3
18	e	1849	LMU	O1'-C1-C2-C3
13	a	505	CLA	CBD-CGD-O2D-CED
13	A	1123	CLA	O1D-CGD-O2D-CED
13	G	1123	CLA	O1D-CGD-O2D-CED
13	e	1123	CLA	O1D-CGD-O2D-CED
13	A	1115	CLA	C3-C5-C6-C7
13	B	1219	CLA	C3-C5-C6-C7
13	2	518	CLA	C3-C5-C6-C7
13	4	509	CLA	C3-C5-C6-C7
13	G	1115	CLA	C3-C5-C6-C7
13	H	1219	CLA	C3-C5-C6-C7
13	Z	518	CLA	C3-C5-C6-C7
13	e	1115	CLA	C3-C5-C6-C7
13	f	1219	CLA	C3-C5-C6-C7
13	r	518	CLA	C3-C5-C6-C7
13	t	509	CLA	C3-C5-C6-C7
13	A	1116	CLA	C5-C6-C7-C8
13	A	1137	CLA	C5-C6-C7-C8
13	B	1214	CLA	C13-C15-C16-C17
13	3	510	CLA	C8-C10-C11-C12
13	G	1116	CLA	C5-C6-C7-C8
13	G	1137	CLA	C5-C6-C7-C8
13	H	1214	CLA	C13-C15-C16-C17
13	a	510	CLA	C8-C10-C11-C12
13	e	1116	CLA	C5-C6-C7-C8
13	e	1137	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1214	CLA	C13-C15-C16-C17
13	s	510	CLA	C8-C10-C11-C12
17	A	5008	LHG	C23-C24-C25-C26
17	A	5001	LHG	C23-C24-C25-C26
17	L	5220	LHG	C7-C8-C9-C10
17	G	5008	LHG	C23-C24-C25-C26
17	G	5001	LHG	C23-C24-C25-C26
17	H	1842	LHG	C23-C24-C25-C26
17	V	5218	LHG	C23-C24-C25-C26
17	V	5220	LHG	C7-C8-C9-C10
17	e	5008	LHG	C23-C24-C25-C26
17	e	5001	LHG	C23-C24-C25-C26
17	n	5218	LHG	C23-C24-C25-C26
17	n	5220	LHG	C7-C8-C9-C10
13	B	1225	CLA	O1A-CGA-O2A-C1
13	K	1401	CLA	O1A-CGA-O2A-C1
13	6	518	CLA	O1A-CGA-O2A-C1
13	H	1225	CLA	O1A-CGA-O2A-C1
13	U	1401	CLA	O1A-CGA-O2A-C1
13	d	518	CLA	O1A-CGA-O2A-C1
13	f	1225	CLA	O1A-CGA-O2A-C1
13	m	1401	CLA	O1A-CGA-O2A-C1
13	v	518	CLA	O1A-CGA-O2A-C1
17	B	1855	LHG	O10-C23-O8-C6
17	H	1855	LHG	O10-C23-O8-C6
17	f	1855	LHG	O10-C23-O8-C6
13	L	1503	CLA	CBD-CGD-O2D-CED
13	V	1503	CLA	CBD-CGD-O2D-CED
13	n	1503	CLA	CBD-CGD-O2D-CED
13	B	1220	CLA	O1D-CGD-O2D-CED
13	H	1220	CLA	O1D-CGD-O2D-CED
13	e	1104	CLA	O1D-CGD-O2D-CED
13	f	1220	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	C13-C15-C16-C17
13	A	1102	CLA	C13-C15-C16-C17
13	A	1137	CLA	C10-C11-C12-C13
13	B	1203	CLA	C8-C10-C11-C12
13	B	1227	CLA	C13-C15-C16-C17
13	L	1501	CLA	C8-C10-C11-C12
13	3	519	CLA	C5-C6-C7-C8
13	4	505	CLA	C15-C16-C17-C18
13	5	503	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1013	CLA	C13-C15-C16-C17
13	G	1102	CLA	C13-C15-C16-C17
13	G	1137	CLA	C10-C11-C12-C13
13	H	1203	CLA	C8-C10-C11-C12
13	H	1227	CLA	C13-C15-C16-C17
13	V	1501	CLA	C8-C10-C11-C12
13	a	519	CLA	C5-C6-C7-C8
13	b	505	CLA	C15-C16-C17-C18
13	c	503	CLA	C5-C6-C7-C8
13	e	1102	CLA	C13-C15-C16-C17
13	e	1125	CLA	C10-C11-C12-C13
13	e	1137	CLA	C10-C11-C12-C13
13	f	1203	CLA	C8-C10-C11-C12
13	f	1227	CLA	C13-C15-C16-C17
13	n	1501	CLA	C8-C10-C11-C12
13	s	519	CLA	C5-C6-C7-C8
13	t	505	CLA	C15-C16-C17-C18
13	u	503	CLA	C5-C6-C7-C8
13	3	516	CLA	C4C-C3C-CAC-CBC
13	a	516	CLA	C4C-C3C-CAC-CBC
13	A	1107	CLA	C2A-CAA-CBA-CGA
13	A	1108	CLA	C2A-CAA-CBA-CGA
13	A	1119	CLA	C2A-CAA-CBA-CGA
13	B	1012	CLA	C2A-CAA-CBA-CGA
13	B	1206	CLA	C2A-CAA-CBA-CGA
13	B	1228	CLA	C2A-CAA-CBA-CGA
13	B	1232	CLA	C2A-CAA-CBA-CGA
13	B	1238	CLA	C2A-CAA-CBA-CGA
13	F	1302	CLA	C2A-CAA-CBA-CGA
13	1	505	CLA	C2A-CAA-CBA-CGA
13	1	516	CLA	C2A-CAA-CBA-CGA
13	2	505	CLA	C2A-CAA-CBA-CGA
13	2	512	CLA	C2A-CAA-CBA-CGA
13	3	505	CLA	C2A-CAA-CBA-CGA
13	3	512	CLA	C2A-CAA-CBA-CGA
13	4	505	CLA	C2A-CAA-CBA-CGA
13	6	505	CLA	C2A-CAA-CBA-CGA
13	6	513	CLA	C2A-CAA-CBA-CGA
13	6	516	CLA	C2A-CAA-CBA-CGA
13	G	1107	CLA	C2A-CAA-CBA-CGA
13	G	1108	CLA	C2A-CAA-CBA-CGA
13	G	1119	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1012	CLA	C2A-CAA-CBA-CGA
13	H	1206	CLA	C2A-CAA-CBA-CGA
13	H	1228	CLA	C2A-CAA-CBA-CGA
13	H	1232	CLA	C2A-CAA-CBA-CGA
13	H	1238	CLA	C2A-CAA-CBA-CGA
13	R	1302	CLA	C2A-CAA-CBA-CGA
13	Y	505	CLA	C2A-CAA-CBA-CGA
13	Y	516	CLA	C2A-CAA-CBA-CGA
13	Z	505	CLA	C2A-CAA-CBA-CGA
13	Z	512	CLA	C2A-CAA-CBA-CGA
13	a	505	CLA	C2A-CAA-CBA-CGA
13	a	512	CLA	C2A-CAA-CBA-CGA
13	b	505	CLA	C2A-CAA-CBA-CGA
13	d	505	CLA	C2A-CAA-CBA-CGA
13	d	513	CLA	C2A-CAA-CBA-CGA
13	d	516	CLA	C2A-CAA-CBA-CGA
13	e	1107	CLA	C2A-CAA-CBA-CGA
13	e	1108	CLA	C2A-CAA-CBA-CGA
13	e	1119	CLA	C2A-CAA-CBA-CGA
13	f	1012	CLA	C2A-CAA-CBA-CGA
13	f	1206	CLA	C2A-CAA-CBA-CGA
13	f	1228	CLA	C2A-CAA-CBA-CGA
13	f	1232	CLA	C2A-CAA-CBA-CGA
13	f	1238	CLA	C2A-CAA-CBA-CGA
13	j	1302	CLA	C2A-CAA-CBA-CGA
13	q	505	CLA	C2A-CAA-CBA-CGA
13	q	516	CLA	C2A-CAA-CBA-CGA
13	r	505	CLA	C2A-CAA-CBA-CGA
13	r	512	CLA	C2A-CAA-CBA-CGA
13	s	505	CLA	C2A-CAA-CBA-CGA
13	s	512	CLA	C2A-CAA-CBA-CGA
13	t	505	CLA	C2A-CAA-CBA-CGA
13	v	505	CLA	C2A-CAA-CBA-CGA
13	v	513	CLA	C2A-CAA-CBA-CGA
13	A	1104	CLA	O1D-CGD-O2D-CED
13	G	1104	CLA	O1D-CGD-O2D-CED
13	s	516	CLA	C4C-C3C-CAC-CBC
13	A	1115	CLA	C5-C6-C7-C8
13	A	1125	CLA	C10-C11-C12-C13
13	A	1126	CLA	C15-C16-C17-C18
13	A	1101	CLA	C13-C15-C16-C17
13	B	1204	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1210	CLA	C8-C10-C11-C12
13	B	1213	CLA	C5-C6-C7-C8
13	B	1239	CLA	C15-C16-C17-C18
13	B	1207	CLA	C13-C15-C16-C17
13	2	505	CLA	C8-C10-C11-C12
13	3	505	CLA	C8-C10-C11-C12
13	5	501	CLA	C13-C15-C16-C17
13	5	505	CLA	C8-C10-C11-C12
13	G	1115	CLA	C5-C6-C7-C8
13	G	1125	CLA	C10-C11-C12-C13
13	G	1126	CLA	C15-C16-C17-C18
13	G	1101	CLA	C13-C15-C16-C17
13	H	1204	CLA	C5-C6-C7-C8
13	H	1210	CLA	C8-C10-C11-C12
13	H	1213	CLA	C5-C6-C7-C8
13	H	1239	CLA	C15-C16-C17-C18
13	H	1207	CLA	C13-C15-C16-C17
13	Z	505	CLA	C8-C10-C11-C12
13	a	505	CLA	C8-C10-C11-C12
13	c	501	CLA	C13-C15-C16-C17
13	c	505	CLA	C8-C10-C11-C12
13	e	1013	CLA	C13-C15-C16-C17
13	e	1115	CLA	C5-C6-C7-C8
13	e	1126	CLA	C15-C16-C17-C18
13	e	1101	CLA	C13-C15-C16-C17
13	f	1204	CLA	C5-C6-C7-C8
13	f	1210	CLA	C8-C10-C11-C12
13	f	1213	CLA	C5-C6-C7-C8
13	f	1239	CLA	C15-C16-C17-C18
13	f	1207	CLA	C13-C15-C16-C17
13	r	505	CLA	C8-C10-C11-C12
13	s	505	CLA	C8-C10-C11-C12
13	u	501	CLA	C13-C15-C16-C17
13	u	505	CLA	C8-C10-C11-C12
17	A	5006	LHG	C23-C24-C25-C26
17	A	5008	LHG	C7-C8-C9-C10
17	A	5009	LHG	C23-C24-C25-C26
17	L	5218	LHG	C23-C24-C25-C26
17	G	5006	LHG	C23-C24-C25-C26
17	G	5008	LHG	C7-C8-C9-C10
17	G	5009	LHG	C23-C24-C25-C26
17	e	5006	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	5008	LHG	C7-C8-C9-C10
17	e	5009	LHG	C23-C24-C25-C26
20	L	5216	SQD	C7-C8-C9-C10
20	1	822	SQD	C23-C24-C25-C26
20	V	5216	SQD	C7-C8-C9-C10
20	Y	822	SQD	C23-C24-C25-C26
20	n	5216	SQD	C7-C8-C9-C10
20	q	822	SQD	C23-C24-C25-C26
13	A	1106	CLA	O1A-CGA-O2A-C1
13	2	512	CLA	O1A-CGA-O2A-C1
13	G	1106	CLA	O1A-CGA-O2A-C1
13	Z	512	CLA	O1A-CGA-O2A-C1
13	e	1106	CLA	O1A-CGA-O2A-C1
13	r	512	CLA	O1A-CGA-O2A-C1
13	b	509	CLA	C3-C5-C6-C7
13	2	502	CLA	CBD-CGD-O2D-CED
13	Z	502	CLA	CBD-CGD-O2D-CED
13	r	502	CLA	CBD-CGD-O2D-CED
18	A	1849	LMU	O5'-C1'-O1'-C1
18	J	5105	LMU	O5'-C1'-O1'-C1
18	2	901	LMU	O5'-C1'-O1'-C1
18	G	1849	LMU	O5'-C1'-O1'-C1
18	T	5105	LMU	O5'-C1'-O1'-C1
18	e	1849	LMU	O5'-C1'-O1'-C1
18	l	5105	LMU	O5'-C1'-O1'-C1
13	A	1106	CLA	C5-C6-C7-C8
13	A	1106	CLA	C10-C11-C12-C13
13	A	1101	CLA	C10-C11-C12-C13
13	B	1012	CLA	C5-C6-C7-C8
13	B	1205	CLA	C13-C15-C16-C17
13	B	1219	CLA	C15-C16-C17-C18
13	B	1223	CLA	C13-C15-C16-C17
13	B	1240	CLA	C10-C11-C12-C13
13	L	1501	CLA	C10-C11-C12-C13
13	L	1503	CLA	C10-C11-C12-C13
13	1	505	CLA	C8-C10-C11-C12
13	1	509	CLA	C15-C16-C17-C18
13	1	510	CLA	C5-C6-C7-C8
13	2	502	CLA	C10-C11-C12-C13
13	3	513	CLA	C8-C10-C11-C12
13	3	513	CLA	C13-C15-C16-C17
13	G	1106	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1106	CLA	C10-C11-C12-C13
13	G	1101	CLA	C10-C11-C12-C13
13	H	1012	CLA	C5-C6-C7-C8
13	H	1205	CLA	C13-C15-C16-C17
13	H	1219	CLA	C15-C16-C17-C18
13	H	1223	CLA	C13-C15-C16-C17
13	H	1240	CLA	C10-C11-C12-C13
13	V	1501	CLA	C10-C11-C12-C13
13	V	1503	CLA	C10-C11-C12-C13
13	Y	505	CLA	C8-C10-C11-C12
13	Y	509	CLA	C15-C16-C17-C18
13	Y	510	CLA	C5-C6-C7-C8
13	Z	502	CLA	C10-C11-C12-C13
13	a	513	CLA	C8-C10-C11-C12
13	a	513	CLA	C13-C15-C16-C17
13	e	1106	CLA	C5-C6-C7-C8
13	e	1106	CLA	C10-C11-C12-C13
13	e	1101	CLA	C10-C11-C12-C13
13	f	1012	CLA	C5-C6-C7-C8
13	f	1205	CLA	C13-C15-C16-C17
13	f	1219	CLA	C15-C16-C17-C18
13	f	1223	CLA	C13-C15-C16-C17
13	f	1240	CLA	C10-C11-C12-C13
13	n	1501	CLA	C10-C11-C12-C13
13	n	1503	CLA	C10-C11-C12-C13
13	q	505	CLA	C8-C10-C11-C12
13	q	509	CLA	C15-C16-C17-C18
13	q	510	CLA	C5-C6-C7-C8
13	r	502	CLA	C10-C11-C12-C13
13	s	513	CLA	C8-C10-C11-C12
13	s	513	CLA	C13-C15-C16-C17
14	A	2001	PQN	C15-C16-C17-C18
14	G	2001	PQN	C15-C16-C17-C18
14	e	2001	PQN	C15-C16-C17-C18
17	A	5009	LHG	O2-C2-C3-O3
17	A	5003	LHG	O2-C2-C3-O3
17	B	1842	LHG	O2-C2-C3-O3
17	L	5220	LHG	O2-C2-C3-O3
17	G	5009	LHG	O2-C2-C3-O3
17	G	5003	LHG	O2-C2-C3-O3
17	H	1842	LHG	O2-C2-C3-O3
17	S	5001	LHG	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	V	5220	LHG	O2-C2-C3-O3
17	e	5009	LHG	O2-C2-C3-O3
17	e	5003	LHG	O2-C2-C3-O3
17	f	1842	LHG	O2-C2-C3-O3
17	n	5220	LHG	O2-C2-C3-O3
13	J	1303	CLA	O1A-CGA-O2A-C1
13	T	1303	CLA	O1A-CGA-O2A-C1
13	e	1237	CLA	O1A-CGA-O2A-C1
13	l	1303	CLA	O1A-CGA-O2A-C1
13	A	1104	CLA	C15-C16-C17-C18
13	B	1023	CLA	C10-C11-C12-C13
13	B	1214	CLA	C5-C6-C7-C8
13	3	509	CLA	C15-C16-C17-C18
13	5	509	CLA	C8-C10-C11-C12
13	G	1104	CLA	C15-C16-C17-C18
13	H	1023	CLA	C10-C11-C12-C13
13	H	1214	CLA	C5-C6-C7-C8
13	c	509	CLA	C8-C10-C11-C12
13	e	1104	CLA	C15-C16-C17-C18
13	f	1023	CLA	C10-C11-C12-C13
13	f	1214	CLA	C5-C6-C7-C8
13	u	509	CLA	C8-C10-C11-C12
18	2	901	LMU	O1'-C1-C2-C3
18	Z	901	LMU	O1'-C1-C2-C3
13	A	1113	CLA	O1D-CGD-O2D-CED
13	6	507	CLA	O1D-CGD-O2D-CED
13	G	1113	CLA	O1D-CGD-O2D-CED
13	e	1113	CLA	O1D-CGD-O2D-CED
18	r	901	LMU	O1'-C1-C2-C3
13	d	507	CLA	O1D-CGD-O2D-CED
13	v	507	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C8-C10-C11-C12
13	A	1137	CLA	C15-C16-C17-C18
13	2	509	CLA	C15-C16-C17-C18
13	4	505	CLA	C8-C10-C11-C12
13	6	505	CLA	C8-C10-C11-C12
13	G	1126	CLA	C8-C10-C11-C12
13	G	1137	CLA	C15-C16-C17-C18
13	Z	509	CLA	C15-C16-C17-C18
13	a	509	CLA	C15-C16-C17-C18
13	b	505	CLA	C8-C10-C11-C12
13	d	505	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1126	CLA	C8-C10-C11-C12
13	e	1137	CLA	C15-C16-C17-C18
13	r	509	CLA	C15-C16-C17-C18
13	s	509	CLA	C15-C16-C17-C18
13	t	505	CLA	C8-C10-C11-C12
13	v	505	CLA	C8-C10-C11-C12
14	A	2001	PQN	C18-C20-C21-C22
14	G	2001	PQN	C18-C20-C21-C22
14	e	2001	PQN	C18-C20-C21-C22
13	A	1128	CLA	CBD-CGD-O2D-CED
13	G	1128	CLA	CBD-CGD-O2D-CED
13	e	1128	CLA	CBD-CGD-O2D-CED
13	A	1237	CLA	O1A-CGA-O2A-C1
13	J	1302	CLA	O1A-CGA-O2A-C1
13	1	502	CLA	O1A-CGA-O2A-C1
13	G	1237	CLA	O1A-CGA-O2A-C1
13	T	1302	CLA	O1A-CGA-O2A-C1
13	Y	502	CLA	O1A-CGA-O2A-C1
13	l	1302	CLA	O1A-CGA-O2A-C1
13	q	502	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	C7-C8-C9-C10
17	L	5218	LHG	C7-C8-C9-C10
17	G	5002	LHG	C7-C8-C9-C10
17	V	5218	LHG	C7-C8-C9-C10
17	e	5002	LHG	C7-C8-C9-C10
17	n	5218	LHG	C7-C8-C9-C10
13	a	504	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C10-C11-C12-C13
13	1	510	CLA	C8-C10-C11-C12
13	6	505	CLA	C5-C6-C7-C8
13	G	1126	CLA	C10-C11-C12-C13
13	Y	510	CLA	C8-C10-C11-C12
13	d	505	CLA	C5-C6-C7-C8
13	e	1126	CLA	C10-C11-C12-C13
13	q	510	CLA	C8-C10-C11-C12
13	v	505	CLA	C5-C6-C7-C8
13	A	1134	CLA	CBA-CGA-O2A-C1
13	B	1215	CLA	CBA-CGA-O2A-C1
13	G	1134	CLA	CBA-CGA-O2A-C1
13	H	1215	CLA	CBA-CGA-O2A-C1
13	e	1134	CLA	CBA-CGA-O2A-C1
13	f	1215	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1224	CLA	CBD-CGD-O2D-CED
13	H	1224	CLA	CBD-CGD-O2D-CED
13	f	1224	CLA	CBD-CGD-O2D-CED
17	B	1855	LHG	C8-C7-O7-C5
17	H	1855	LHG	C8-C7-O7-C5
17	f	1855	LHG	C8-C7-O7-C5
13	A	1104	CLA	O1A-CGA-O2A-C1
13	G	1104	CLA	O1A-CGA-O2A-C1
13	e	1104	CLA	O1A-CGA-O2A-C1
13	A	1013	CLA	O1D-CGD-O2D-CED
13	A	1137	CLA	O1D-CGD-O2D-CED
13	3	504	CLA	O1D-CGD-O2D-CED
13	G	1013	CLA	O1D-CGD-O2D-CED
13	G	1137	CLA	O1D-CGD-O2D-CED
13	e	1013	CLA	O1D-CGD-O2D-CED
13	e	1137	CLA	O1D-CGD-O2D-CED
13	s	504	CLA	O1D-CGD-O2D-CED
13	A	1136	CLA	C8-C10-C11-C12
13	G	1136	CLA	C8-C10-C11-C12
13	A	1011	CLA	C3-C5-C6-C7
13	A	1128	CLA	C3-C5-C6-C7
13	G	1011	CLA	C3-C5-C6-C7
13	G	1128	CLA	C3-C5-C6-C7
13	e	1128	CLA	C3-C5-C6-C7
13	f	1217	CLA	C8-C10-C11-C12
16	4	522	BCR	C9-C10-C11-C12
16	4	522	BCR	C13-C14-C15-C16
16	b	522	BCR	C9-C10-C11-C12
16	b	522	BCR	C13-C14-C15-C16
16	t	522	BCR	C9-C10-C11-C12
16	t	522	BCR	C13-C14-C15-C16
13	B	1203	CLA	C5-C6-C7-C8
13	B	1208	CLA	C10-C11-C12-C13
13	B	1210	CLA	C10-C11-C12-C13
13	H	1203	CLA	C5-C6-C7-C8
13	H	1208	CLA	C10-C11-C12-C13
13	H	1210	CLA	C10-C11-C12-C13
13	e	1136	CLA	C8-C10-C11-C12
13	f	1210	CLA	C10-C11-C12-C13
17	A	5001	LHG	O9-C7-O7-C5
17	G	5001	LHG	O9-C7-O7-C5
17	e	5001	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	5009	LHG	C1-C2-C3-O3
17	A	5003	LHG	C1-C2-C3-O3
17	B	1842	LHG	C1-C2-C3-O3
17	L	5220	LHG	C1-C2-C3-O3
17	G	5009	LHG	C1-C2-C3-O3
17	G	5003	LHG	C1-C2-C3-O3
17	H	1842	LHG	C1-C2-C3-O3
17	V	5220	LHG	C1-C2-C3-O3
17	e	5009	LHG	C1-C2-C3-O3
17	e	5003	LHG	C1-C2-C3-O3
17	f	1842	LHG	C1-C2-C3-O3
17	n	5220	LHG	C1-C2-C3-O3
13	A	1134	CLA	C2A-CAA-CBA-CGA
13	B	1201	CLA	C2A-CAA-CBA-CGA
13	B	1203	CLA	C2A-CAA-CBA-CGA
13	B	1218	CLA	C2A-CAA-CBA-CGA
13	1	517	CLA	C2A-CAA-CBA-CGA
13	G	1134	CLA	C2A-CAA-CBA-CGA
13	H	1201	CLA	C2A-CAA-CBA-CGA
13	H	1203	CLA	C2A-CAA-CBA-CGA
13	H	1218	CLA	C2A-CAA-CBA-CGA
13	Y	517	CLA	C2A-CAA-CBA-CGA
13	e	1134	CLA	C2A-CAA-CBA-CGA
13	f	1201	CLA	C2A-CAA-CBA-CGA
13	f	1203	CLA	C2A-CAA-CBA-CGA
13	f	1218	CLA	C2A-CAA-CBA-CGA
13	q	517	CLA	C2A-CAA-CBA-CGA
13	v	516	CLA	C2A-CAA-CBA-CGA
13	6	517	CLA	O1D-CGD-O2D-CED
13	b	505	CLA	O1D-CGD-O2D-CED
13	d	517	CLA	O1D-CGD-O2D-CED
13	v	517	CLA	O1D-CGD-O2D-CED
13	A	1137	CLA	CBA-CGA-O2A-C1
13	G	1137	CLA	CBA-CGA-O2A-C1
13	e	1137	CLA	CBA-CGA-O2A-C1
17	A	5005	LHG	C24-C23-O8-C6
17	G	5005	LHG	C24-C23-O8-C6
17	e	5005	LHG	C24-C23-O8-C6
13	A	1013	CLA	C15-C16-C17-C18
13	A	1122	CLA	C8-C10-C11-C12
13	B	1225	CLA	C13-C15-C16-C17
13	F	1301	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	1	501	CLA	C15-C16-C17-C18
13	1	502	CLA	C8-C10-C11-C12
13	6	501	CLA	C8-C10-C11-C12
13	G	1013	CLA	C15-C16-C17-C18
13	G	1122	CLA	C8-C10-C11-C12
13	H	1225	CLA	C13-C15-C16-C17
13	R	1301	CLA	C13-C15-C16-C17
13	Y	501	CLA	C15-C16-C17-C18
13	Y	502	CLA	C8-C10-C11-C12
13	d	501	CLA	C8-C10-C11-C12
13	e	1013	CLA	C15-C16-C17-C18
13	e	1122	CLA	C8-C10-C11-C12
13	f	1203	CLA	C5-C6-C7-C8
13	f	1208	CLA	C10-C11-C12-C13
13	f	1225	CLA	C13-C15-C16-C17
13	j	1301	CLA	C13-C15-C16-C17
13	q	501	CLA	C15-C16-C17-C18
13	q	502	CLA	C8-C10-C11-C12
13	v	501	CLA	C8-C10-C11-C12
13	F	1301	CLA	C3-C5-C6-C7
13	R	1301	CLA	C3-C5-C6-C7
13	e	1011	CLA	C3-C5-C6-C7
13	j	1301	CLA	C3-C5-C6-C7
13	A	1011	CLA	O1D-CGD-O2D-CED
13	B	1226	CLA	O1D-CGD-O2D-CED
13	4	505	CLA	O1D-CGD-O2D-CED
13	H	1226	CLA	O1D-CGD-O2D-CED
13	f	1226	CLA	O1D-CGD-O2D-CED
13	t	505	CLA	O1D-CGD-O2D-CED
13	B	1221	CLA	C8-C10-C11-C12
13	H	1221	CLA	C8-C10-C11-C12
13	q	509	CLA	C8-C10-C11-C12
13	B	1239	CLA	C2C-C3C-CAC-CBC
13	H	1239	CLA	C2C-C3C-CAC-CBC
13	f	1239	CLA	C2C-C3C-CAC-CBC
13	G	1011	CLA	O1D-CGD-O2D-CED
13	e	1011	CLA	O1D-CGD-O2D-CED
18	A	1848	LMU	O5'-C5'-C6'-O6'
18	G	1848	LMU	O5'-C5'-C6'-O6'
18	e	1848	LMU	O5'-C5'-C6'-O6'
13	A	1109	CLA	C13-C15-C16-C17
13	A	1126	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1133	CLA	C10-C11-C12-C13
13	A	1137	CLA	C13-C15-C16-C17
13	B	1234	CLA	C10-C11-C12-C13
13	B	1235	CLA	C8-C10-C11-C12
13	1	509	CLA	C8-C10-C11-C12
13	2	507	CLA	C5-C6-C7-C8
13	3	505	CLA	C5-C6-C7-C8
13	G	1102	CLA	C15-C16-C17-C18
13	G	1109	CLA	C13-C15-C16-C17
13	G	1126	CLA	C5-C6-C7-C8
13	G	1133	CLA	C10-C11-C12-C13
13	G	1137	CLA	C13-C15-C16-C17
13	H	1234	CLA	C10-C11-C12-C13
13	H	1235	CLA	C8-C10-C11-C12
13	Y	509	CLA	C8-C10-C11-C12
13	Z	507	CLA	C5-C6-C7-C8
13	a	505	CLA	C5-C6-C7-C8
13	e	1109	CLA	C13-C15-C16-C17
13	e	1126	CLA	C5-C6-C7-C8
13	e	1133	CLA	C10-C11-C12-C13
13	e	1137	CLA	C13-C15-C16-C17
13	f	1221	CLA	C8-C10-C11-C12
13	f	1234	CLA	C10-C11-C12-C13
13	f	1235	CLA	C8-C10-C11-C12
13	r	507	CLA	C5-C6-C7-C8
13	s	505	CLA	C5-C6-C7-C8
13	B	1217	CLA	C8-C10-C11-C12
13	H	1217	CLA	C8-C10-C11-C12
13	A	1102	CLA	C15-C16-C17-C18
13	B	1208	CLA	C15-C16-C17-C18
13	B	1214	CLA	C10-C11-C12-C13
13	H	1208	CLA	C15-C16-C17-C18
13	H	1214	CLA	C10-C11-C12-C13
13	e	1102	CLA	C15-C16-C17-C18
13	f	1208	CLA	C15-C16-C17-C18
13	f	1214	CLA	C10-C11-C12-C13
13	3	509	CLA	C3-C5-C6-C7
13	a	509	CLA	C3-C5-C6-C7
13	s	509	CLA	C3-C5-C6-C7
17	A	5009	LHG	C8-C7-O7-C5
17	G	5009	LHG	C8-C7-O7-C5
17	e	5009	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	1	502	CLA	O1D-CGD-O2D-CED
13	2	519	CLA	O1D-CGD-O2D-CED
13	4	513	CLA	O1D-CGD-O2D-CED
13	Y	502	CLA	O1D-CGD-O2D-CED
13	Z	519	CLA	O1D-CGD-O2D-CED
13	b	513	CLA	O1D-CGD-O2D-CED
13	q	502	CLA	O1D-CGD-O2D-CED
13	r	519	CLA	O1D-CGD-O2D-CED
13	t	513	CLA	O1D-CGD-O2D-CED
20	B	1852	SQD	C2-C1-O6-C44
20	H	1852	SQD	C2-C1-O6-C44
20	f	1852	SQD	C2-C1-O6-C44
13	A	1139	CLA	C15-C16-C17-C18
13	2	518	CLA	C10-C11-C12-C13
13	G	1139	CLA	C15-C16-C17-C18
13	Z	518	CLA	C10-C11-C12-C13
13	e	1139	CLA	C15-C16-C17-C18
13	r	518	CLA	C10-C11-C12-C13
13	5	512	CLA	O1D-CGD-O2D-CED
13	u	512	CLA	O1D-CGD-O2D-CED
17	I	5001	LHG	O2-C2-C3-O3
17	k	5001	LHG	O2-C2-C3-O3
13	c	512	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C16-C17-C18-C20
13	G	1126	CLA	C16-C17-C18-C20
13	e	1126	CLA	C16-C17-C18-C20
13	c	509	CLA	C15-C16-C17-C18
13	5	509	CLA	C15-C16-C17-C18
13	u	509	CLA	C15-C16-C17-C18
14	B	2002	PQN	C15-C16-C17-C18
14	H	2002	PQN	C15-C16-C17-C18
14	f	2002	PQN	C15-C16-C17-C18
16	A	4001	BCR	C7-C8-C9-C34
16	A	4001	BCR	C11-C12-C13-C35
16	A	4011	BCR	C36-C18-C19-C20
16	B	4014	BCR	C7-C8-C9-C34
16	L	4019	BCR	C37-C22-C23-C24
16	3	524	BCR	C7-C8-C9-C34
16	4	521	BCR	C36-C18-C19-C20
16	4	524	BCR	C7-C8-C9-C34
16	6	522	BCR	C7-C8-C9-C34
16	G	4001	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	G	4001	BCR	C11-C12-C13-C35
16	G	4011	BCR	C36-C18-C19-C20
16	H	4014	BCR	C7-C8-C9-C34
16	V	4019	BCR	C37-C22-C23-C24
16	a	524	BCR	C7-C8-C9-C34
16	b	521	BCR	C36-C18-C19-C20
16	b	524	BCR	C7-C8-C9-C34
16	d	522	BCR	C7-C8-C9-C34
16	e	4001	BCR	C7-C8-C9-C34
16	e	4001	BCR	C11-C12-C13-C35
16	e	4011	BCR	C36-C18-C19-C20
16	f	4014	BCR	C7-C8-C9-C34
16	n	4019	BCR	C37-C22-C23-C24
16	s	524	BCR	C7-C8-C9-C34
16	t	521	BCR	C36-C18-C19-C20
16	t	524	BCR	C7-C8-C9-C34
16	v	522	BCR	C7-C8-C9-C34
17	L	5221	LHG	C5-C4-O6-P
17	V	5221	LHG	C5-C4-O6-P
17	n	5221	LHG	C5-C4-O6-P
16	L	4019	BCR	C21-C22-C23-C24
16	3	523	BCR	C21-C22-C23-C24
16	4	523	BCR	C21-C22-C23-C24
16	6	523	BCR	C21-C22-C23-C24
16	V	4019	BCR	C21-C22-C23-C24
16	a	523	BCR	C21-C22-C23-C24
16	b	523	BCR	C21-C22-C23-C24
16	d	523	BCR	C21-C22-C23-C24
16	n	4019	BCR	C21-C22-C23-C24
16	s	523	BCR	C21-C22-C23-C24
16	t	523	BCR	C21-C22-C23-C24
16	v	523	BCR	C21-C22-C23-C24
13	A	1137	CLA	O1A-CGA-O2A-C1
13	G	1137	CLA	O1A-CGA-O2A-C1
13	e	1137	CLA	O1A-CGA-O2A-C1
13	A	1116	CLA	C2A-CAA-CBA-CGA
13	B	1224	CLA	C2A-CAA-CBA-CGA
13	B	1207	CLA	C2A-CAA-CBA-CGA
13	G	1116	CLA	C2A-CAA-CBA-CGA
13	H	1224	CLA	C2A-CAA-CBA-CGA
13	H	1207	CLA	C2A-CAA-CBA-CGA
13	e	1116	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1224	CLA	C2A-CAA-CBA-CGA
13	f	1207	CLA	C2A-CAA-CBA-CGA
13	1	507	CLA	C10-C11-C12-C13
13	5	509	CLA	C13-C15-C16-C17
13	Y	507	CLA	C10-C11-C12-C13
13	c	509	CLA	C13-C15-C16-C17
13	q	507	CLA	C10-C11-C12-C13
13	u	509	CLA	C13-C15-C16-C17
17	A	5002	LHG	O1-C1-C2-C3
17	A	5008	LHG	O1-C1-C2-C3
17	L	5221	LHG	O1-C1-C2-C3
17	G	5002	LHG	O1-C1-C2-C3
17	G	5008	LHG	O1-C1-C2-C3
17	V	5221	LHG	O1-C1-C2-C3
17	e	5002	LHG	O1-C1-C2-C3
17	e	5008	LHG	O1-C1-C2-C3
17	n	5221	LHG	O1-C1-C2-C3
13	q	504	CLA	CBD-CGD-O2D-CED
13	H	1232	CLA	O1D-CGD-O2D-CED
20	5	822	SQD	C46-C45-O47-C7
20	6	822	SQD	C46-C45-O47-C7
20	c	822	SQD	C46-C45-O47-C7
20	d	822	SQD	C46-C45-O47-C7
20	u	822	SQD	C46-C45-O47-C7
20	v	822	SQD	C46-C45-O47-C7
17	A	5002	LHG	C28-C29-C30-C31
13	A	1105	CLA	C6-C7-C8-C9
13	B	1218	CLA	C11-C12-C13-C15
13	B	1239	CLA	C16-C17-C18-C20
13	B	1207	CLA	C16-C17-C18-C19
13	G	1105	CLA	C6-C7-C8-C9
13	H	1218	CLA	C11-C12-C13-C15
13	H	1239	CLA	C16-C17-C18-C20
13	Z	508	CLA	C6-C7-C8-C10
13	f	1218	CLA	C11-C12-C13-C15
13	f	1239	CLA	C16-C17-C18-C20
13	f	1207	CLA	C16-C17-C18-C19
17	G	5002	LHG	C28-C29-C30-C31
17	e	5002	LHG	C28-C29-C30-C31
13	B	1227	CLA	O1D-CGD-O2D-CED
13	B	1232	CLA	O1D-CGD-O2D-CED
13	H	1227	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1227	CLA	O1D-CGD-O2D-CED
13	f	1232	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	C3-C5-C6-C7
13	B	1218	CLA	C3-C5-C6-C7
13	H	1203	CLA	C3-C5-C6-C7
13	H	1218	CLA	C3-C5-C6-C7
13	f	1203	CLA	C3-C5-C6-C7
13	f	1218	CLA	C3-C5-C6-C7
13	1	504	CLA	CBD-CGD-O2D-CED
13	L	1503	CLA	C2-C3-C5-C6
13	V	1503	CLA	C2-C3-C5-C6
13	n	1503	CLA	C2-C3-C5-C6
13	3	511	CLA	O1D-CGD-O2D-CED
13	a	511	CLA	O1D-CGD-O2D-CED
13	s	511	CLA	O1D-CGD-O2D-CED
13	B	1232	CLA	CBA-CGA-O2A-C1
13	1	512	CLA	CBA-CGA-O2A-C1
13	H	1232	CLA	CBA-CGA-O2A-C1
13	Y	512	CLA	CBA-CGA-O2A-C1
13	f	1232	CLA	CBA-CGA-O2A-C1
13	q	512	CLA	CBA-CGA-O2A-C1
13	A	1103	CLA	C10-C11-C12-C13
13	A	1103	CLA	C15-C16-C17-C18
13	G	1103	CLA	C10-C11-C12-C13
13	G	1103	CLA	C15-C16-C17-C18
13	e	1103	CLA	C10-C11-C12-C13
13	e	1103	CLA	C15-C16-C17-C18
13	Y	504	CLA	CBD-CGD-O2D-CED
13	A	1118	CLA	C2-C1-O2A-CGA
13	J	1302	CLA	C2-C1-O2A-CGA
13	3	510	CLA	C2-C1-O2A-CGA
13	T	1302	CLA	C2-C1-O2A-CGA
13	a	510	CLA	C2-C1-O2A-CGA
13	e	1118	CLA	C2-C1-O2A-CGA
13	l	1302	CLA	C2-C1-O2A-CGA
13	s	510	CLA	C2-C1-O2A-CGA
13	A	1116	CLA	C11-C12-C13-C15
13	A	1140	CLA	C16-C17-C18-C20
13	B	1213	CLA	C16-C17-C18-C20
13	B	1222	CLA	C11-C12-C13-C15
13	B	1224	CLA	C11-C12-C13-C15
13	B	1238	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	2	508	CLA	C6-C7-C8-C10
13	6	505	CLA	C16-C17-C18-C20
13	G	1116	CLA	C11-C12-C13-C15
13	G	1140	CLA	C16-C17-C18-C20
13	H	1213	CLA	C16-C17-C18-C20
13	H	1222	CLA	C11-C12-C13-C15
13	H	1224	CLA	C11-C12-C13-C15
13	H	1238	CLA	C16-C17-C18-C19
13	H	1207	CLA	C16-C17-C18-C19
13	d	505	CLA	C16-C17-C18-C20
13	e	1105	CLA	C6-C7-C8-C9
13	e	1116	CLA	C11-C12-C13-C15
13	e	1140	CLA	C16-C17-C18-C20
13	f	1213	CLA	C16-C17-C18-C20
13	f	1222	CLA	C11-C12-C13-C15
13	f	1224	CLA	C11-C12-C13-C15
13	f	1238	CLA	C16-C17-C18-C19
13	r	508	CLA	C6-C7-C8-C10
13	v	505	CLA	C16-C17-C18-C20
14	A	2001	PQN	C26-C27-C28-C29
14	B	2002	PQN	C26-C27-C28-C30
14	G	2001	PQN	C26-C27-C28-C29
14	H	2002	PQN	C26-C27-C28-C30
14	e	2001	PQN	C26-C27-C28-C29
14	f	2002	PQN	C26-C27-C28-C30
13	B	1218	CLA	C8-C10-C11-C12
13	f	1218	CLA	C8-C10-C11-C12
17	G	5007	LHG	C32-C33-C34-C35
13	A	1122	CLA	CBD-CGD-O2D-CED
13	G	1122	CLA	CBD-CGD-O2D-CED
13	e	1122	CLA	CBD-CGD-O2D-CED
17	A	5002	LHG	C24-C25-C26-C27
17	A	5002	LHG	C30-C31-C32-C33
17	A	5007	LHG	C32-C33-C34-C35
17	A	5001	LHG	C15-C16-C17-C18
17	A	5001	LHG	C25-C26-C27-C28
17	B	1855	LHG	C12-C13-C14-C15
17	G	5002	LHG	C24-C25-C26-C27
17	G	5002	LHG	C30-C31-C32-C33
17	G	5009	LHG	C16-C17-C18-C19
17	G	5001	LHG	C15-C16-C17-C18
17	G	5001	LHG	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	1855	LHG	C12-C13-C14-C15
17	V	5221	LHG	C29-C30-C31-C32
17	e	5002	LHG	C24-C25-C26-C27
17	e	5002	LHG	C30-C31-C32-C33
17	e	5007	LHG	C32-C33-C34-C35
17	e	5009	LHG	C16-C17-C18-C19
17	e	5001	LHG	C15-C16-C17-C18
17	e	5001	LHG	C25-C26-C27-C28
17	f	1855	LHG	C12-C13-C14-C15
20	B	1852	SQD	C28-C29-C30-C31
20	f	1852	SQD	C28-C29-C30-C31
13	B	1231	CLA	O1D-CGD-O2D-CED
13	6	510	CLA	O1D-CGD-O2D-CED
13	H	1231	CLA	O1D-CGD-O2D-CED
13	H	1235	CLA	O1D-CGD-O2D-CED
13	d	510	CLA	O1D-CGD-O2D-CED
13	f	1231	CLA	O1D-CGD-O2D-CED
13	v	510	CLA	O1D-CGD-O2D-CED
13	H	1218	CLA	C8-C10-C11-C12
17	A	5009	LHG	C16-C17-C18-C19
17	L	5221	LHG	C29-C30-C31-C32
17	n	5221	LHG	C29-C30-C31-C32
19	B	5002	LMG	C29-C30-C31-C32
19	f	5002	LMG	C29-C30-C31-C32
20	3	822	SQD	C25-C26-C27-C28
20	H	1852	SQD	C28-C29-C30-C31
20	a	822	SQD	C25-C26-C27-C28
20	s	822	SQD	C25-C26-C27-C28
13	A	1134	CLA	O1A-CGA-O2A-C1
13	G	1134	CLA	O1A-CGA-O2A-C1
13	e	1134	CLA	O1A-CGA-O2A-C1
13	1	508	CLA	CBA-CGA-O2A-C1
13	Y	508	CLA	CBA-CGA-O2A-C1
13	q	508	CLA	CBA-CGA-O2A-C1
17	A	5005	LHG	C10-C11-C12-C13
17	A	5005	LHG	C14-C15-C16-C17
17	A	5003	LHG	C10-C11-C12-C13
17	G	5005	LHG	C10-C11-C12-C13
17	G	5005	LHG	C14-C15-C16-C17
17	G	5003	LHG	C10-C11-C12-C13
17	e	5005	LHG	C10-C11-C12-C13
17	e	5005	LHG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	5003	LHG	C10-C11-C12-C13
19	H	5002	LMG	C29-C30-C31-C32
17	A	5002	LHG	O1-C1-C2-O2
17	A	5005	LHG	O1-C1-C2-O2
17	A	5008	LHG	O1-C1-C2-O2
17	A	5009	LHG	O1-C1-C2-O2
17	B	1842	LHG	O1-C1-C2-O2
17	B	1855	LHG	O1-C1-C2-O2
17	L	5218	LHG	O1-C1-C2-O2
17	L	5220	LHG	O1-C1-C2-O2
17	G	5002	LHG	O1-C1-C2-O2
17	G	5005	LHG	O1-C1-C2-O2
17	G	5008	LHG	O1-C1-C2-O2
17	G	5009	LHG	O1-C1-C2-O2
17	H	1842	LHG	O1-C1-C2-O2
17	H	1855	LHG	O1-C1-C2-O2
17	V	5218	LHG	O1-C1-C2-O2
17	V	5220	LHG	O1-C1-C2-O2
17	e	5002	LHG	O1-C1-C2-O2
17	e	5005	LHG	O1-C1-C2-O2
17	e	5008	LHG	O1-C1-C2-O2
17	e	5009	LHG	O1-C1-C2-O2
17	f	1842	LHG	O1-C1-C2-O2
17	f	1855	LHG	O1-C1-C2-O2
17	n	5218	LHG	O1-C1-C2-O2
17	n	5220	LHG	O1-C1-C2-O2
18	1	902	LMU	C2-C1-O1'-C1'
18	Y	902	LMU	C2-C1-O1'-C1'
18	q	902	LMU	C2-C1-O1'-C1'
17	L	5218	LHG	C28-C29-C30-C31
17	V	5218	LHG	C28-C29-C30-C31
17	n	5218	LHG	C28-C29-C30-C31
18	A	1849	LMU	C4-C5-C6-C7
18	G	1849	LMU	C4-C5-C6-C7
18	e	1849	LMU	C4-C5-C6-C7
20	B	1852	SQD	C11-C10-C9-C8
20	H	1852	SQD	C11-C10-C9-C8
20	f	1852	SQD	C11-C10-C9-C8
13	B	1235	CLA	O1D-CGD-O2D-CED
13	1	507	CLA	O1D-CGD-O2D-CED
13	1	519	CLA	O1D-CGD-O2D-CED
13	G	1138	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Y	507	CLA	O1D-CGD-O2D-CED
13	Y	519	CLA	O1D-CGD-O2D-CED
13	f	1235	CLA	O1D-CGD-O2D-CED
13	q	507	CLA	O1D-CGD-O2D-CED
13	q	519	CLA	O1D-CGD-O2D-CED
13	A	1118	CLA	C4B-C3B-CAB-CBB
13	A	1129	CLA	C4B-C3B-CAB-CBB
13	A	1131	CLA	C4B-C3B-CAB-CBB
13	A	1132	CLA	C4B-C3B-CAB-CBB
13	A	1134	CLA	C4B-C3B-CAB-CBB
13	A	1138	CLA	C4B-C3B-CAB-CBB
13	A	1139	CLA	C4B-C3B-CAB-CBB
13	A	1237	CLA	C4B-C3B-CAB-CBB
13	B	1021	CLA	C4B-C3B-CAB-CBB
13	B	1219	CLA	C4B-C3B-CAB-CBB
13	B	1227	CLA	C4B-C3B-CAB-CBB
13	B	1235	CLA	C4B-C3B-CAB-CBB
13	B	1207	CLA	C4B-C3B-CAB-CBB
13	F	1302	CLA	C4B-C3B-CAB-CBB
13	J	1302	CLA	C4B-C3B-CAB-CBB
13	2	502	CLA	C4B-C3B-CAB-CBB
13	3	502	CLA	C4B-C3B-CAB-CBB
13	3	519	CLA	C4B-C3B-CAB-CBB
13	4	505	CLA	C4B-C3B-CAB-CBB
13	5	502	CLA	C4B-C3B-CAB-CBB
13	5	519	CLA	C4B-C3B-CAB-CBB
13	6	501	CLA	C4B-C3B-CAB-CBB
13	6	507	CLA	C4B-C3B-CAB-CBB
13	6	518	CLA	C4B-C3B-CAB-CBB
13	6	519	CLA	C4B-C3B-CAB-CBB
13	G	1118	CLA	C4B-C3B-CAB-CBB
13	G	1129	CLA	C4B-C3B-CAB-CBB
13	G	1131	CLA	C4B-C3B-CAB-CBB
13	G	1132	CLA	C4B-C3B-CAB-CBB
13	G	1134	CLA	C4B-C3B-CAB-CBB
13	G	1138	CLA	C4B-C3B-CAB-CBB
13	G	1139	CLA	C4B-C3B-CAB-CBB
13	G	1237	CLA	C4B-C3B-CAB-CBB
13	H	1021	CLA	C4B-C3B-CAB-CBB
13	H	1219	CLA	C4B-C3B-CAB-CBB
13	H	1227	CLA	C4B-C3B-CAB-CBB
13	H	1235	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1207	CLA	C4B-C3B-CAB-CBB
13	R	1302	CLA	C4B-C3B-CAB-CBB
13	T	1302	CLA	C4B-C3B-CAB-CBB
13	Z	502	CLA	C4B-C3B-CAB-CBB
13	a	502	CLA	C4B-C3B-CAB-CBB
13	a	519	CLA	C4B-C3B-CAB-CBB
13	b	505	CLA	C4B-C3B-CAB-CBB
13	c	502	CLA	C4B-C3B-CAB-CBB
13	c	519	CLA	C4B-C3B-CAB-CBB
13	d	501	CLA	C4B-C3B-CAB-CBB
13	d	507	CLA	C4B-C3B-CAB-CBB
13	d	518	CLA	C4B-C3B-CAB-CBB
13	d	519	CLA	C4B-C3B-CAB-CBB
13	e	1118	CLA	C4B-C3B-CAB-CBB
13	e	1129	CLA	C4B-C3B-CAB-CBB
13	e	1131	CLA	C4B-C3B-CAB-CBB
13	e	1132	CLA	C4B-C3B-CAB-CBB
13	e	1134	CLA	C4B-C3B-CAB-CBB
13	e	1138	CLA	C4B-C3B-CAB-CBB
13	e	1139	CLA	C4B-C3B-CAB-CBB
13	e	1237	CLA	C4B-C3B-CAB-CBB
13	f	1021	CLA	C4B-C3B-CAB-CBB
13	f	1219	CLA	C4B-C3B-CAB-CBB
13	f	1227	CLA	C4B-C3B-CAB-CBB
13	f	1235	CLA	C4B-C3B-CAB-CBB
13	f	1207	CLA	C4B-C3B-CAB-CBB
13	j	1302	CLA	C4B-C3B-CAB-CBB
13	l	1302	CLA	C4B-C3B-CAB-CBB
13	r	502	CLA	C4B-C3B-CAB-CBB
13	s	502	CLA	C4B-C3B-CAB-CBB
13	s	519	CLA	C4B-C3B-CAB-CBB
13	t	505	CLA	C4B-C3B-CAB-CBB
13	u	502	CLA	C4B-C3B-CAB-CBB
13	u	519	CLA	C4B-C3B-CAB-CBB
13	v	501	CLA	C4B-C3B-CAB-CBB
13	v	507	CLA	C4B-C3B-CAB-CBB
13	v	518	CLA	C4B-C3B-CAB-CBB
13	v	519	CLA	C4B-C3B-CAB-CBB
19	T	5104	LMG	C28-C29-C30-C31
17	H	1855	LHG	C11-C12-C13-C14
17	f	1855	LHG	C11-C12-C13-C14
18	2	901	LMU	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	Z	901	LMU	C2-C3-C4-C5
18	r	901	LMU	C2-C3-C4-C5
13	A	1105	CLA	C6-C7-C8-C10
13	A	1140	CLA	C16-C17-C18-C19
13	A	1101	CLA	C16-C17-C18-C19
13	B	1210	CLA	C16-C17-C18-C19
13	B	1213	CLA	C16-C17-C18-C19
13	B	1218	CLA	C11-C12-C13-C14
13	B	1224	CLA	C11-C12-C13-C14
13	B	1207	CLA	C16-C17-C18-C20
13	6	505	CLA	C16-C17-C18-C19
13	G	1105	CLA	C6-C7-C8-C10
13	G	1140	CLA	C16-C17-C18-C19
13	G	1101	CLA	C16-C17-C18-C19
13	H	1210	CLA	C16-C17-C18-C19
13	H	1213	CLA	C16-C17-C18-C19
13	H	1218	CLA	C11-C12-C13-C14
13	H	1224	CLA	C11-C12-C13-C14
13	H	1207	CLA	C16-C17-C18-C20
13	d	505	CLA	C16-C17-C18-C19
13	e	1105	CLA	C6-C7-C8-C10
13	e	1140	CLA	C16-C17-C18-C19
13	f	1210	CLA	C16-C17-C18-C19
13	f	1213	CLA	C16-C17-C18-C19
13	f	1218	CLA	C11-C12-C13-C14
13	f	1224	CLA	C11-C12-C13-C14
13	f	1207	CLA	C16-C17-C18-C20
13	v	505	CLA	C16-C17-C18-C19
13	A	1138	CLA	O1D-CGD-O2D-CED
13	1	511	CLA	O1D-CGD-O2D-CED
13	Y	511	CLA	O1D-CGD-O2D-CED
13	e	1138	CLA	O1D-CGD-O2D-CED
13	q	511	CLA	O1D-CGD-O2D-CED
13	1	518	CLA	C2A-CAA-CBA-CGA
13	5	518	CLA	C2A-CAA-CBA-CGA
13	Y	518	CLA	C2A-CAA-CBA-CGA
13	c	518	CLA	C2A-CAA-CBA-CGA
13	q	518	CLA	C2A-CAA-CBA-CGA
13	u	518	CLA	C2A-CAA-CBA-CGA
17	B	1855	LHG	C11-C12-C13-C14
19	J	5104	LMG	C11-C12-C13-C14
19	T	5104	LMG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	l	5104	LMG	C11-C12-C13-C14
13	B	1208	CLA	C8-C10-C11-C12
13	5	509	CLA	C10-C11-C12-C13
13	H	1208	CLA	C8-C10-C11-C12
13	c	509	CLA	C10-C11-C12-C13
13	f	1208	CLA	C8-C10-C11-C12
13	u	509	CLA	C10-C11-C12-C13
17	A	5007	LHG	C8-C7-O7-C5
17	G	5007	LHG	C8-C7-O7-C5
17	e	5007	LHG	C8-C7-O7-C5
19	J	5104	LMG	C11-C10-O7-C8
19	T	5104	LMG	C11-C10-O7-C8
19	l	5104	LMG	C11-C10-O7-C8
13	2	501	CLA	C6-C7-C8-C10
13	Z	501	CLA	C6-C7-C8-C10
13	r	501	CLA	C6-C7-C8-C10
18	H	1843	LMU	C5-C6-C7-C8
18	f	1843	LMU	C5-C6-C7-C8
19	J	5104	LMG	C28-C29-C30-C31
19	l	5104	LMG	C28-C29-C30-C31
13	4	509	CLA	C15-C16-C17-C18
13	b	509	CLA	C15-C16-C17-C18
13	t	509	CLA	C15-C16-C17-C18
17	L	5220	LHG	C27-C28-C29-C30
17	V	5220	LHG	C27-C28-C29-C30
17	f	1842	LHG	C27-C28-C29-C30
17	n	5220	LHG	C27-C28-C29-C30
18	B	1843	LMU	C5-C6-C7-C8
20	2	822	SQD	C10-C11-C12-C13
20	Z	822	SQD	C10-C11-C12-C13
20	r	822	SQD	C10-C11-C12-C13
13	2	512	CLA	C3-C5-C6-C7
13	Z	512	CLA	C3-C5-C6-C7
13	r	512	CLA	C3-C5-C6-C7
13	A	1103	CLA	C3A-C2A-CAA-CBA
13	A	1125	CLA	C3A-C2A-CAA-CBA
13	A	1134	CLA	C3A-C2A-CAA-CBA
13	A	1135	CLA	C3A-C2A-CAA-CBA
13	A	1140	CLA	C3A-C2A-CAA-CBA
13	A	1022	CLA	C3A-C2A-CAA-CBA
13	A	1101	CLA	C3A-C2A-CAA-CBA
13	B	1210	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1219	CLA	C3A-C2A-CAA-CBA
13	B	1221	CLA	C3A-C2A-CAA-CBA
13	K	1105	CLA	C3A-C2A-CAA-CBA
13	2	516	CLA	C3A-C2A-CAA-CBA
13	2	519	CLA	C3A-C2A-CAA-CBA
13	3	513	CLA	C3A-C2A-CAA-CBA
13	4	516	CLA	C3A-C2A-CAA-CBA
13	5	516	CLA	C3A-C2A-CAA-CBA
13	6	512	CLA	C3A-C2A-CAA-CBA
13	6	516	CLA	C3A-C2A-CAA-CBA
13	G	1103	CLA	C3A-C2A-CAA-CBA
13	G	1125	CLA	C3A-C2A-CAA-CBA
13	G	1134	CLA	C3A-C2A-CAA-CBA
13	G	1135	CLA	C3A-C2A-CAA-CBA
13	G	1140	CLA	C3A-C2A-CAA-CBA
13	G	1022	CLA	C3A-C2A-CAA-CBA
13	G	1101	CLA	C3A-C2A-CAA-CBA
13	H	1210	CLA	C3A-C2A-CAA-CBA
13	H	1219	CLA	C3A-C2A-CAA-CBA
13	H	1221	CLA	C3A-C2A-CAA-CBA
13	U	1105	CLA	C3A-C2A-CAA-CBA
13	Z	516	CLA	C3A-C2A-CAA-CBA
13	Z	519	CLA	C3A-C2A-CAA-CBA
13	a	513	CLA	C3A-C2A-CAA-CBA
13	b	516	CLA	C3A-C2A-CAA-CBA
13	c	516	CLA	C3A-C2A-CAA-CBA
13	d	512	CLA	C3A-C2A-CAA-CBA
13	d	516	CLA	C3A-C2A-CAA-CBA
13	e	1103	CLA	C3A-C2A-CAA-CBA
13	e	1125	CLA	C3A-C2A-CAA-CBA
13	e	1134	CLA	C3A-C2A-CAA-CBA
13	e	1135	CLA	C3A-C2A-CAA-CBA
13	e	1140	CLA	C3A-C2A-CAA-CBA
13	e	1022	CLA	C3A-C2A-CAA-CBA
13	e	1101	CLA	C3A-C2A-CAA-CBA
13	f	1210	CLA	C3A-C2A-CAA-CBA
13	f	1219	CLA	C3A-C2A-CAA-CBA
13	f	1221	CLA	C3A-C2A-CAA-CBA
13	m	1105	CLA	C3A-C2A-CAA-CBA
13	r	516	CLA	C3A-C2A-CAA-CBA
13	r	519	CLA	C3A-C2A-CAA-CBA
13	s	513	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	t	516	CLA	C3A-C2A-CAA-CBA
13	u	516	CLA	C3A-C2A-CAA-CBA
13	v	512	CLA	C3A-C2A-CAA-CBA
13	v	516	CLA	C3A-C2A-CAA-CBA
13	H	1206	CLA	O1D-CGD-O2D-CED
17	A	5003	LHG	C12-C13-C14-C15
17	B	1842	LHG	C27-C28-C29-C30
20	L	5216	SQD	C12-C13-C14-C15
20	V	5216	SQD	C12-C13-C14-C15
20	n	5216	SQD	C12-C13-C14-C15
13	B	1217	CLA	C2-C3-C5-C6
13	H	1217	CLA	C2-C3-C5-C6
13	f	1217	CLA	C2-C3-C5-C6
13	B	1205	CLA	CBD-CGD-O2D-CED
13	H	1205	CLA	CBD-CGD-O2D-CED
13	f	1205	CLA	CBD-CGD-O2D-CED
17	G	5003	LHG	C12-C13-C14-C15
17	H	1842	LHG	C27-C28-C29-C30
17	e	5003	LHG	C12-C13-C14-C15
13	A	1127	CLA	C15-C16-C17-C18
13	A	1101	CLA	C15-C16-C17-C18
13	B	1229	CLA	C15-C16-C17-C18
13	2	502	CLA	C8-C10-C11-C12
13	2	503	CLA	C8-C10-C11-C12
13	G	1127	CLA	C15-C16-C17-C18
13	G	1101	CLA	C15-C16-C17-C18
13	H	1229	CLA	C15-C16-C17-C18
13	Z	502	CLA	C8-C10-C11-C12
13	e	1101	CLA	C15-C16-C17-C18
13	f	1229	CLA	C15-C16-C17-C18
13	r	502	CLA	C8-C10-C11-C12
13	r	503	CLA	C8-C10-C11-C12
13	B	1206	CLA	O1D-CGD-O2D-CED
13	f	1206	CLA	O1D-CGD-O2D-CED
16	B	4010	BCR	C9-C10-C11-C12
16	2	522	BCR	C9-C10-C11-C12
16	H	4010	BCR	C9-C10-C11-C12
16	Z	522	BCR	C9-C10-C11-C12
16	f	4010	BCR	C9-C10-C11-C12
16	r	522	BCR	C9-C10-C11-C12
13	B	1238	CLA	C16-C17-C18-C20
13	1	505	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	6	501	CLA	C11-C12-C13-C14
13	H	1238	CLA	C16-C17-C18-C20
13	Y	505	CLA	C16-C17-C18-C20
13	d	501	CLA	C11-C12-C13-C14
13	e	1101	CLA	C16-C17-C18-C19
13	f	1238	CLA	C16-C17-C18-C20
13	q	505	CLA	C16-C17-C18-C20
13	v	501	CLA	C11-C12-C13-C14
18	1	902	LMU	C1-C2-C3-C4
18	Y	902	LMU	C1-C2-C3-C4
18	q	902	LMU	C1-C2-C3-C4
17	A	5007	LHG	C28-C29-C30-C31
17	G	5007	LHG	C28-C29-C30-C31
17	e	5007	LHG	C28-C29-C30-C31
13	e	1127	CLA	C15-C16-C17-C18
13	1	508	CLA	CBD-CGD-O2D-CED
13	Y	508	CLA	CBD-CGD-O2D-CED
13	q	508	CLA	CBD-CGD-O2D-CED
17	A	5004	LHG	C24-C25-C26-C27
17	e	5004	LHG	C24-C25-C26-C27
18	G	1848	LMU	C2-C3-C4-C5
18	e	1848	LMU	C2-C3-C4-C5
20	1	822	SQD	C12-C13-C14-C15
20	Y	822	SQD	C12-C13-C14-C15
13	A	1132	CLA	CBA-CGA-O2A-C1
13	3	513	CLA	CBA-CGA-O2A-C1
13	6	502	CLA	CBA-CGA-O2A-C1
13	G	1132	CLA	CBA-CGA-O2A-C1
13	a	513	CLA	CBA-CGA-O2A-C1
13	d	502	CLA	CBA-CGA-O2A-C1
13	e	1132	CLA	CBA-CGA-O2A-C1
13	s	513	CLA	CBA-CGA-O2A-C1
13	v	502	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C32-C33-C34-C35
17	I	5001	LHG	C26-C27-C28-C29
17	G	5002	LHG	C32-C33-C34-C35
17	S	5001	LHG	C26-C27-C28-C29
17	e	5002	LHG	C32-C33-C34-C35
20	q	822	SQD	C12-C13-C14-C15
13	4	501	CLA	C3-C5-C6-C7
13	b	501	CLA	C3-C5-C6-C7
13	t	501	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	5002	LHG	C23-C24-C25-C26
17	G	5002	LHG	C23-C24-C25-C26
17	e	5002	LHG	C23-C24-C25-C26
20	B	1852	SQD	C23-C24-C25-C26
20	H	1852	SQD	C23-C24-C25-C26
20	f	1852	SQD	C23-C24-C25-C26
13	Z	503	CLA	C8-C10-C11-C12
17	B	1855	LHG	C26-C27-C28-C29
17	I	5001	LHG	C29-C30-C31-C32
17	G	5004	LHG	C24-C25-C26-C27
17	H	1855	LHG	C26-C27-C28-C29
17	S	5001	LHG	C29-C30-C31-C32
17	f	1855	LHG	C26-C27-C28-C29
17	k	5001	LHG	C29-C30-C31-C32
18	A	1848	LMU	C2-C3-C4-C5
19	B	5002	LMG	C22-C23-C24-C25
19	H	5002	LMG	C22-C23-C24-C25
19	f	5002	LMG	C22-C23-C24-C25
20	1	822	SQD	C11-C10-C9-C8
20	Y	822	SQD	C11-C10-C9-C8
20	q	822	SQD	C11-C10-C9-C8
13	B	1215	CLA	O1A-CGA-O2A-C1
13	H	1215	CLA	O1A-CGA-O2A-C1
13	f	1215	CLA	O1A-CGA-O2A-C1
20	L	5216	SQD	O10-C23-O48-C46
20	V	5216	SQD	O10-C23-O48-C46
20	n	5216	SQD	O10-C23-O48-C46
17	L	5221	LHG	C32-C33-C34-C35
17	n	5221	LHG	C32-C33-C34-C35
13	U	1103	CLA	O1D-CGD-O2D-CED
17	V	5221	LHG	C32-C33-C34-C35
17	k	5001	LHG	C26-C27-C28-C29
20	1	822	SQD	C30-C31-C32-C33
20	q	822	SQD	C30-C31-C32-C33
13	H	1235	CLA	C5-C6-C7-C8
18	J	5105	LMU	C1-C2-C3-C4
18	T	5105	LMU	C1-C2-C3-C4
18	l	5105	LMU	C1-C2-C3-C4
13	K	1103	CLA	O1D-CGD-O2D-CED
13	1	512	CLA	O1D-CGD-O2D-CED
13	1	518	CLA	O1D-CGD-O2D-CED
13	Y	512	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Y	518	CLA	O1D-CGD-O2D-CED
13	m	1103	CLA	O1D-CGD-O2D-CED
13	q	512	CLA	O1D-CGD-O2D-CED
13	q	518	CLA	O1D-CGD-O2D-CED
17	B	1842	LHG	C32-C33-C34-C35
17	H	1842	LHG	C32-C33-C34-C35
17	f	1842	LHG	C32-C33-C34-C35
19	f	5002	LMG	C32-C33-C34-C35
20	Y	822	SQD	C30-C31-C32-C33
13	A	1115	CLA	C11-C12-C13-C15
13	e	1115	CLA	C11-C12-C13-C15
13	A	1107	CLA	C2B-C3B-CAB-CBB
13	A	1131	CLA	C2B-C3B-CAB-CBB
13	A	1134	CLA	C2B-C3B-CAB-CBB
13	A	1139	CLA	C2B-C3B-CAB-CBB
13	A	1237	CLA	C2B-C3B-CAB-CBB
13	B	1214	CLA	C2B-C3B-CAB-CBB
13	B	1219	CLA	C2B-C3B-CAB-CBB
13	B	1239	CLA	C2B-C3B-CAB-CBB
13	B	1207	CLA	C2B-C3B-CAB-CBB
13	F	1302	CLA	C2B-C3B-CAB-CBB
13	J	1302	CLA	C2B-C3B-CAB-CBB
13	K	1401	CLA	C2B-C3B-CAB-CBB
13	1	501	CLA	C2B-C3B-CAB-CBB
13	1	512	CLA	C2B-C3B-CAB-CBB
13	2	501	CLA	C2B-C3B-CAB-CBB
13	2	502	CLA	C2B-C3B-CAB-CBB
13	2	513	CLA	C2B-C3B-CAB-CBB
13	2	516	CLA	C2B-C3B-CAB-CBB
13	3	512	CLA	C2B-C3B-CAB-CBB
13	4	501	CLA	C2B-C3B-CAB-CBB
13	4	519	CLA	C2B-C3B-CAB-CBB
13	5	502	CLA	C2B-C3B-CAB-CBB
13	5	512	CLA	C2B-C3B-CAB-CBB
13	5	516	CLA	C2B-C3B-CAB-CBB
13	5	517	CLA	C2B-C3B-CAB-CBB
13	6	512	CLA	C2B-C3B-CAB-CBB
13	G	1107	CLA	C2B-C3B-CAB-CBB
13	G	1131	CLA	C2B-C3B-CAB-CBB
13	G	1134	CLA	C2B-C3B-CAB-CBB
13	G	1139	CLA	C2B-C3B-CAB-CBB
13	G	1237	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1214	CLA	C2B-C3B-CAB-CBB
13	H	1219	CLA	C2B-C3B-CAB-CBB
13	H	1239	CLA	C2B-C3B-CAB-CBB
13	H	1207	CLA	C2B-C3B-CAB-CBB
13	R	1302	CLA	C2B-C3B-CAB-CBB
13	T	1302	CLA	C2B-C3B-CAB-CBB
13	U	1401	CLA	C2B-C3B-CAB-CBB
13	Y	501	CLA	C2B-C3B-CAB-CBB
13	Y	512	CLA	C2B-C3B-CAB-CBB
13	Z	501	CLA	C2B-C3B-CAB-CBB
13	Z	502	CLA	C2B-C3B-CAB-CBB
13	Z	513	CLA	C2B-C3B-CAB-CBB
13	Z	516	CLA	C2B-C3B-CAB-CBB
13	a	512	CLA	C2B-C3B-CAB-CBB
13	b	501	CLA	C2B-C3B-CAB-CBB
13	b	519	CLA	C2B-C3B-CAB-CBB
13	c	502	CLA	C2B-C3B-CAB-CBB
13	c	512	CLA	C2B-C3B-CAB-CBB
13	c	516	CLA	C2B-C3B-CAB-CBB
13	c	517	CLA	C2B-C3B-CAB-CBB
13	d	512	CLA	C2B-C3B-CAB-CBB
13	e	1107	CLA	C2B-C3B-CAB-CBB
13	e	1131	CLA	C2B-C3B-CAB-CBB
13	e	1134	CLA	C2B-C3B-CAB-CBB
13	e	1139	CLA	C2B-C3B-CAB-CBB
13	e	1237	CLA	C2B-C3B-CAB-CBB
13	f	1214	CLA	C2B-C3B-CAB-CBB
13	f	1219	CLA	C2B-C3B-CAB-CBB
13	f	1239	CLA	C2B-C3B-CAB-CBB
13	f	1207	CLA	C2B-C3B-CAB-CBB
13	j	1302	CLA	C2B-C3B-CAB-CBB
13	l	1302	CLA	C2B-C3B-CAB-CBB
13	m	1401	CLA	C2B-C3B-CAB-CBB
13	q	501	CLA	C2B-C3B-CAB-CBB
13	q	512	CLA	C2B-C3B-CAB-CBB
13	r	501	CLA	C2B-C3B-CAB-CBB
13	r	502	CLA	C2B-C3B-CAB-CBB
13	r	513	CLA	C2B-C3B-CAB-CBB
13	r	516	CLA	C2B-C3B-CAB-CBB
13	s	512	CLA	C2B-C3B-CAB-CBB
13	t	501	CLA	C2B-C3B-CAB-CBB
13	t	519	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	u	502	CLA	C2B-C3B-CAB-CBB
13	u	512	CLA	C2B-C3B-CAB-CBB
13	u	516	CLA	C2B-C3B-CAB-CBB
13	u	517	CLA	C2B-C3B-CAB-CBB
13	v	512	CLA	C2B-C3B-CAB-CBB
16	A	4008	BCR	C23-C24-C25-C30
16	A	4011	BCR	C23-C24-C25-C26
16	A	4011	BCR	C23-C24-C25-C30
16	B	4004	BCR	C1-C6-C7-C8
16	B	4004	BCR	C5-C6-C7-C8
16	J	4012	BCR	C1-C6-C7-C8
16	J	4012	BCR	C23-C24-C25-C26
16	J	4012	BCR	C23-C24-C25-C30
16	L	4019	BCR	C23-C24-C25-C26
16	L	4019	BCR	C23-C24-C25-C30
16	M	4021	BCR	C1-C6-C7-C8
16	1	521	BCR	C1-C6-C7-C8
16	1	521	BCR	C5-C6-C7-C8
16	1	523	BCR	C1-C6-C7-C8
16	1	523	BCR	C5-C6-C7-C8
16	1	523	BCR	C23-C24-C25-C26
16	1	523	BCR	C23-C24-C25-C30
16	2	521	BCR	C1-C6-C7-C8
16	2	521	BCR	C5-C6-C7-C8
16	2	522	BCR	C1-C6-C7-C8
16	2	523	BCR	C23-C24-C25-C26
16	2	523	BCR	C23-C24-C25-C30
16	3	521	BCR	C1-C6-C7-C8
16	3	521	BCR	C5-C6-C7-C8
16	3	523	BCR	C23-C24-C25-C26
16	3	523	BCR	C23-C24-C25-C30
16	4	521	BCR	C1-C6-C7-C8
16	4	521	BCR	C5-C6-C7-C8
16	4	521	BCR	C23-C24-C25-C26
16	4	521	BCR	C23-C24-C25-C30
16	4	522	BCR	C1-C6-C7-C8
16	4	522	BCR	C5-C6-C7-C8
16	4	523	BCR	C23-C24-C25-C26
16	4	523	BCR	C23-C24-C25-C30
16	4	524	BCR	C23-C24-C25-C26
16	4	524	BCR	C23-C24-C25-C30
16	5	522	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	5	523	BCR	C23-C24-C25-C26
16	5	523	BCR	C23-C24-C25-C30
16	5	524	BCR	C23-C24-C25-C26
16	5	524	BCR	C23-C24-C25-C30
16	6	521	BCR	C1-C6-C7-C8
16	6	521	BCR	C5-C6-C7-C8
16	6	522	BCR	C1-C6-C7-C8
16	6	523	BCR	C23-C24-C25-C26
16	6	523	BCR	C23-C24-C25-C30
16	G	4008	BCR	C23-C24-C25-C30
16	G	4011	BCR	C23-C24-C25-C26
16	G	4011	BCR	C23-C24-C25-C30
16	H	4004	BCR	C1-C6-C7-C8
16	H	4004	BCR	C5-C6-C7-C8
16	T	4012	BCR	C1-C6-C7-C8
16	T	4012	BCR	C23-C24-C25-C26
16	T	4012	BCR	C23-C24-C25-C30
16	V	4019	BCR	C23-C24-C25-C26
16	V	4019	BCR	C23-C24-C25-C30
16	W	4021	BCR	C1-C6-C7-C8
16	Y	521	BCR	C1-C6-C7-C8
16	Y	521	BCR	C5-C6-C7-C8
16	Y	523	BCR	C1-C6-C7-C8
16	Y	523	BCR	C5-C6-C7-C8
16	Y	523	BCR	C23-C24-C25-C26
16	Y	523	BCR	C23-C24-C25-C30
16	Z	521	BCR	C1-C6-C7-C8
16	Z	521	BCR	C5-C6-C7-C8
16	Z	522	BCR	C1-C6-C7-C8
16	Z	523	BCR	C23-C24-C25-C26
16	Z	523	BCR	C23-C24-C25-C30
16	a	521	BCR	C1-C6-C7-C8
16	a	521	BCR	C5-C6-C7-C8
16	a	523	BCR	C23-C24-C25-C26
16	a	523	BCR	C23-C24-C25-C30
16	b	521	BCR	C1-C6-C7-C8
16	b	521	BCR	C5-C6-C7-C8
16	b	521	BCR	C23-C24-C25-C26
16	b	521	BCR	C23-C24-C25-C30
16	b	522	BCR	C1-C6-C7-C8
16	b	522	BCR	C5-C6-C7-C8
16	b	523	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	b	523	BCR	C23-C24-C25-C30
16	b	524	BCR	C23-C24-C25-C26
16	b	524	BCR	C23-C24-C25-C30
16	c	522	BCR	C1-C6-C7-C8
16	c	523	BCR	C23-C24-C25-C26
16	c	523	BCR	C23-C24-C25-C30
16	c	524	BCR	C23-C24-C25-C26
16	c	524	BCR	C23-C24-C25-C30
16	d	521	BCR	C1-C6-C7-C8
16	d	521	BCR	C5-C6-C7-C8
16	d	522	BCR	C1-C6-C7-C8
16	d	523	BCR	C23-C24-C25-C26
16	d	523	BCR	C23-C24-C25-C30
16	e	4008	BCR	C23-C24-C25-C30
16	e	4011	BCR	C23-C24-C25-C26
16	e	4011	BCR	C23-C24-C25-C30
16	f	4004	BCR	C1-C6-C7-C8
16	f	4004	BCR	C5-C6-C7-C8
16	l	4012	BCR	C1-C6-C7-C8
16	l	4012	BCR	C23-C24-C25-C26
16	l	4012	BCR	C23-C24-C25-C30
16	n	4019	BCR	C23-C24-C25-C26
16	n	4019	BCR	C23-C24-C25-C30
16	o	4021	BCR	C1-C6-C7-C8
16	q	521	BCR	C1-C6-C7-C8
16	q	521	BCR	C5-C6-C7-C8
16	q	523	BCR	C1-C6-C7-C8
16	q	523	BCR	C5-C6-C7-C8
16	q	523	BCR	C23-C24-C25-C30
16	r	521	BCR	C1-C6-C7-C8
16	r	521	BCR	C5-C6-C7-C8
16	r	522	BCR	C1-C6-C7-C8
16	r	523	BCR	C23-C24-C25-C26
16	r	523	BCR	C23-C24-C25-C30
16	s	521	BCR	C1-C6-C7-C8
16	s	521	BCR	C5-C6-C7-C8
16	s	523	BCR	C23-C24-C25-C26
16	s	523	BCR	C23-C24-C25-C30
16	t	521	BCR	C1-C6-C7-C8
16	t	521	BCR	C5-C6-C7-C8
16	t	521	BCR	C23-C24-C25-C26
16	t	521	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	t	522	BCR	C1-C6-C7-C8
16	t	522	BCR	C5-C6-C7-C8
16	t	523	BCR	C23-C24-C25-C26
16	t	523	BCR	C23-C24-C25-C30
16	t	524	BCR	C23-C24-C25-C26
16	t	524	BCR	C23-C24-C25-C30
16	u	522	BCR	C1-C6-C7-C8
16	u	523	BCR	C23-C24-C25-C26
16	u	523	BCR	C23-C24-C25-C30
16	u	524	BCR	C23-C24-C25-C26
16	u	524	BCR	C23-C24-C25-C30
16	v	521	BCR	C1-C6-C7-C8
16	v	521	BCR	C5-C6-C7-C8
16	v	522	BCR	C1-C6-C7-C8
16	v	523	BCR	C23-C24-C25-C26
16	v	523	BCR	C23-C24-C25-C30
13	A	1116	CLA	CBA-CGA-O2A-C1
13	G	1116	CLA	CBA-CGA-O2A-C1
13	e	1116	CLA	CBA-CGA-O2A-C1
17	e	5003	LHG	C24-C23-O8-C6
13	A	1127	CLA	C8-C10-C11-C12
13	B	1210	CLA	C5-C6-C7-C8
13	B	1235	CLA	C5-C6-C7-C8
13	G	1127	CLA	C8-C10-C11-C12
13	H	1210	CLA	C5-C6-C7-C8
13	e	1127	CLA	C8-C10-C11-C12
13	f	1210	CLA	C5-C6-C7-C8
13	f	1235	CLA	C5-C6-C7-C8
14	f	2002	PQN	C25-C26-C27-C28
20	6	822	SQD	C24-C23-O48-C46
20	d	822	SQD	C24-C23-O48-C46
20	v	822	SQD	C24-C23-O48-C46
17	A	5007	LHG	C11-C10-C9-C8
17	G	5007	LHG	C11-C10-C9-C8
17	e	5007	LHG	C11-C10-C9-C8
19	B	5002	LMG	C32-C33-C34-C35
19	H	5002	LMG	C32-C33-C34-C35
17	L	5221	LHG	C26-C27-C28-C29
13	A	1125	CLA	C2A-CAA-CBA-CGA
13	A	1022	CLA	C2A-CAA-CBA-CGA
13	K	1103	CLA	C2A-CAA-CBA-CGA
13	G	1125	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1022	CLA	C2A-CAA-CBA-CGA
13	U	1103	CLA	C2A-CAA-CBA-CGA
13	e	1125	CLA	C2A-CAA-CBA-CGA
13	e	1022	CLA	C2A-CAA-CBA-CGA
13	m	1103	CLA	C2A-CAA-CBA-CGA
14	B	2002	PQN	C25-C26-C27-C28
14	H	2002	PQN	C25-C26-C27-C28
17	L	5220	LHG	C10-C11-C12-C13
17	V	5220	LHG	C10-C11-C12-C13
17	V	5221	LHG	C26-C27-C28-C29
17	n	5220	LHG	C10-C11-C12-C13
17	n	5221	LHG	C26-C27-C28-C29
19	B	5002	LMG	C21-C22-C23-C24
19	f	5002	LMG	C21-C22-C23-C24
20	3	822	SQD	C27-C28-C29-C30
20	Y	822	SQD	C27-C28-C29-C30
20	a	822	SQD	C27-C28-C29-C30
20	s	822	SQD	C27-C28-C29-C30
13	B	1232	CLA	O1A-CGA-O2A-C1
13	1	512	CLA	O1A-CGA-O2A-C1
13	H	1232	CLA	O1A-CGA-O2A-C1
13	Y	512	CLA	O1A-CGA-O2A-C1
13	f	1232	CLA	O1A-CGA-O2A-C1
13	q	512	CLA	O1A-CGA-O2A-C1
13	v	502	CLA	O1A-CGA-O2A-C1
20	1	822	SQD	C27-C28-C29-C30
20	3	822	SQD	C9-C10-C11-C12
20	q	822	SQD	C27-C28-C29-C30
13	A	1124	CLA	C11-C10-C8-C7
13	B	1211	CLA	C11-C10-C8-C7
13	G	1124	CLA	C11-C10-C8-C7
13	H	1211	CLA	C11-C10-C8-C7
13	e	1124	CLA	C11-C10-C8-C7
13	f	1211	CLA	C11-C10-C8-C7
13	A	1130	CLA	C4-C3-C5-C6
13	L	1501	CLA	C4-C3-C5-C6
13	G	1137	CLA	C4-C3-C5-C6
13	G	1130	CLA	C4-C3-C5-C6
13	V	1501	CLA	C4-C3-C5-C6
13	e	1137	CLA	C4-C3-C5-C6
13	e	1130	CLA	C4-C3-C5-C6
13	n	1501	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	I	5001	LHG	C10-C11-C12-C13
17	L	5221	LHG	C28-C29-C30-C31
17	S	5001	LHG	C10-C11-C12-C13
17	k	5001	LHG	C10-C11-C12-C13
17	n	5221	LHG	C28-C29-C30-C31
19	H	5002	LMG	C21-C22-C23-C24
20	a	822	SQD	C9-C10-C11-C12
13	B	1219	CLA	C5-C6-C7-C8
13	f	1219	CLA	C5-C6-C7-C8
13	G	1115	CLA	C11-C12-C13-C15
17	A	5005	LHG	C24-C25-C26-C27
17	G	5005	LHG	C24-C25-C26-C27
17	V	5221	LHG	C28-C29-C30-C31
17	e	5005	LHG	C24-C25-C26-C27
20	3	822	SQD	C7-C8-C9-C10
20	s	822	SQD	C7-C8-C9-C10
13	A	1105	CLA	CBA-CGA-O2A-C1
13	B	1201	CLA	CBA-CGA-O2A-C1
13	L	1502	CLA	CBA-CGA-O2A-C1
13	3	507	CLA	CBA-CGA-O2A-C1
13	G	1105	CLA	CBA-CGA-O2A-C1
13	H	1201	CLA	CBA-CGA-O2A-C1
13	V	1502	CLA	CBA-CGA-O2A-C1
13	a	507	CLA	CBA-CGA-O2A-C1
13	e	1105	CLA	CBA-CGA-O2A-C1
13	f	1201	CLA	CBA-CGA-O2A-C1
13	n	1502	CLA	CBA-CGA-O2A-C1
13	s	507	CLA	CBA-CGA-O2A-C1
17	A	5003	LHG	C24-C23-O8-C6
17	G	5003	LHG	C24-C23-O8-C6
13	d	502	CLA	O1A-CGA-O2A-C1
13	A	1106	CLA	C6-C7-C8-C9
13	G	1106	CLA	C6-C7-C8-C9
13	e	1106	CLA	C6-C7-C8-C9
17	L	5220	LHG	C13-C14-C15-C16
17	G	5008	LHG	C13-C14-C15-C16
20	s	822	SQD	C9-C10-C11-C12
17	A	5008	LHG	C13-C14-C15-C16
17	L	5221	LHG	C25-C26-C27-C28
17	V	5220	LHG	C13-C14-C15-C16
17	V	5221	LHG	C11-C12-C13-C14
17	V	5221	LHG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	5008	LHG	C13-C14-C15-C16
17	n	5220	LHG	C13-C14-C15-C16
17	n	5221	LHG	C11-C12-C13-C14
17	n	5221	LHG	C25-C26-C27-C28
18	B	1843	LMU	C4-C5-C6-C7
18	H	1843	LMU	C4-C5-C6-C7
18	f	1843	LMU	C4-C5-C6-C7
20	B	1852	SQD	O5-C1-O6-C44
20	H	1852	SQD	O5-C1-O6-C44
20	f	1852	SQD	O5-C1-O6-C44
17	A	5001	LHG	C27-C28-C29-C30
17	L	5220	LHG	C9-C10-C11-C12
17	L	5221	LHG	C11-C12-C13-C14
17	L	5221	LHG	C17-C18-C19-C20
17	G	5001	LHG	C27-C28-C29-C30
17	V	5220	LHG	C9-C10-C11-C12
17	V	5221	LHG	C25-C26-C27-C28
17	e	5001	LHG	C27-C28-C29-C30
17	n	5220	LHG	C9-C10-C11-C12
17	n	5221	LHG	C17-C18-C19-C20
13	A	1117	CLA	C13-C15-C16-C17
13	A	1133	CLA	C13-C15-C16-C17
13	1	508	CLA	C5-C6-C7-C8
13	2	501	CLA	C10-C11-C12-C13
13	G	1117	CLA	C13-C15-C16-C17
13	G	1133	CLA	C13-C15-C16-C17
13	H	1219	CLA	C5-C6-C7-C8
13	Y	508	CLA	C5-C6-C7-C8
13	Z	501	CLA	C10-C11-C12-C13
13	e	1117	CLA	C13-C15-C16-C17
13	e	1133	CLA	C13-C15-C16-C17
13	q	508	CLA	C5-C6-C7-C8
13	r	501	CLA	C10-C11-C12-C13
13	6	502	CLA	O1A-CGA-O2A-C1
20	a	822	SQD	C7-C8-C9-C10
13	2	516	CLA	O1D-CGD-O2D-CED
13	r	516	CLA	O1D-CGD-O2D-CED
17	A	5008	LHG	C10-C11-C12-C13
17	G	5008	LHG	C10-C11-C12-C13
17	e	5008	LHG	C10-C11-C12-C13
16	1	522	BCR	C9-C10-C11-C12
16	Y	522	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	q	522	BCR	C9-C10-C11-C12
13	B	1239	CLA	C16-C17-C18-C19
13	H	1239	CLA	C16-C17-C18-C19
13	f	1239	CLA	C16-C17-C18-C19
17	A	5005	LHG	C8-C7-O7-C5
17	A	5001	LHG	C8-C7-O7-C5
17	G	5005	LHG	C8-C7-O7-C5
17	G	5001	LHG	C8-C7-O7-C5
17	e	5005	LHG	C8-C7-O7-C5
17	e	5001	LHG	C8-C7-O7-C5
17	A	5005	LHG	C23-C24-C25-C26
17	A	5006	LHG	C7-C8-C9-C10
17	G	5005	LHG	C23-C24-C25-C26
17	G	5006	LHG	C7-C8-C9-C10
17	e	5005	LHG	C23-C24-C25-C26
17	e	5006	LHG	C7-C8-C9-C10
13	2	513	CLA	C8-C10-C11-C12
13	Z	513	CLA	C8-C10-C11-C12
13	r	513	CLA	C8-C10-C11-C12
13	B	1215	CLA	CBD-CGD-O2D-CED
13	f	1215	CLA	CBD-CGD-O2D-CED
13	3	513	CLA	O1A-CGA-O2A-C1
13	s	513	CLA	O1A-CGA-O2A-C1
13	1	501	CLA	C13-C15-C16-C17
13	Y	501	CLA	C13-C15-C16-C17
13	q	501	CLA	C13-C15-C16-C17
16	B	4010	BCR	C11-C12-C13-C35
16	H	4010	BCR	C11-C12-C13-C35
16	f	4010	BCR	C11-C12-C13-C35
17	A	5007	LHG	C25-C26-C27-C28
17	A	5007	LHG	C33-C34-C35-C36
17	G	5007	LHG	C33-C34-C35-C36
17	e	5007	LHG	C25-C26-C27-C28
17	G	5007	LHG	C25-C26-C27-C28
13	A	1124	CLA	C3-C5-C6-C7
13	G	1124	CLA	C3-C5-C6-C7
13	e	1124	CLA	C3-C5-C6-C7
16	A	4001	BCR	C21-C22-C23-C24
16	G	4001	BCR	C21-C22-C23-C24
16	e	4001	BCR	C21-C22-C23-C24
13	B	1220	CLA	CBA-CGA-O2A-C1
13	1	518	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Y	518	CLA	CBA-CGA-O2A-C1
13	f	1220	CLA	CBA-CGA-O2A-C1
17	e	5007	LHG	C33-C34-C35-C36
13	A	1118	CLA	C2A-CAA-CBA-CGA
13	5	503	CLA	C2A-CAA-CBA-CGA
13	5	517	CLA	C2A-CAA-CBA-CGA
13	G	1118	CLA	C2A-CAA-CBA-CGA
13	c	503	CLA	C2A-CAA-CBA-CGA
13	c	517	CLA	C2A-CAA-CBA-CGA
13	e	1118	CLA	C2A-CAA-CBA-CGA
13	u	503	CLA	C2A-CAA-CBA-CGA
13	u	517	CLA	C2A-CAA-CBA-CGA
13	A	1124	CLA	C11-C10-C8-C9
13	G	1124	CLA	C11-C10-C8-C9
13	e	1124	CLA	C11-C10-C8-C9
13	A	1103	CLA	C16-C17-C18-C20
13	A	1116	CLA	C11-C12-C13-C14
13	A	1121	CLA	C6-C7-C8-C9
13	A	1121	CLA	C6-C7-C8-C10
13	A	1127	CLA	C16-C17-C18-C20
13	A	1101	CLA	C16-C17-C18-C20
13	B	1219	CLA	C16-C17-C18-C20
13	B	1222	CLA	C11-C12-C13-C14
13	L	1502	CLA	C16-C17-C18-C19
13	1	502	CLA	C11-C12-C13-C14
13	2	508	CLA	C6-C7-C8-C9
13	5	518	CLA	C6-C7-C8-C9
13	5	518	CLA	C6-C7-C8-C10
13	G	1103	CLA	C16-C17-C18-C20
13	G	1116	CLA	C11-C12-C13-C14
13	G	1121	CLA	C6-C7-C8-C9
13	G	1121	CLA	C6-C7-C8-C10
13	G	1127	CLA	C16-C17-C18-C20
13	G	1101	CLA	C16-C17-C18-C20
13	H	1219	CLA	C16-C17-C18-C20
13	H	1222	CLA	C11-C12-C13-C14
13	V	1502	CLA	C16-C17-C18-C19
13	Y	502	CLA	C11-C12-C13-C14
13	Z	508	CLA	C6-C7-C8-C9
13	c	518	CLA	C6-C7-C8-C9
13	c	518	CLA	C6-C7-C8-C10
13	d	501	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1103	CLA	C16-C17-C18-C20
13	e	1116	CLA	C11-C12-C13-C14
13	e	1121	CLA	C6-C7-C8-C9
13	e	1121	CLA	C6-C7-C8-C10
13	e	1127	CLA	C16-C17-C18-C20
13	e	1101	CLA	C16-C17-C18-C20
13	f	1219	CLA	C16-C17-C18-C20
13	f	1222	CLA	C11-C12-C13-C14
13	n	1502	CLA	C16-C17-C18-C19
13	q	502	CLA	C11-C12-C13-C14
13	r	508	CLA	C6-C7-C8-C9
13	u	518	CLA	C6-C7-C8-C9
13	u	518	CLA	C6-C7-C8-C10
14	B	2002	PQN	C26-C27-C28-C29
14	H	2002	PQN	C26-C27-C28-C29
14	f	2002	PQN	C26-C27-C28-C29
13	H	1215	CLA	CBD-CGD-O2D-CED
17	B	1842	LHG	C28-C29-C30-C31
17	L	5218	LHG	C11-C10-C9-C8
17	H	1842	LHG	C28-C29-C30-C31
17	V	5218	LHG	C11-C10-C9-C8
17	f	1842	LHG	C28-C29-C30-C31
17	n	5218	LHG	C11-C10-C9-C8
13	A	1137	CLA	C4-C3-C5-C6
13	B	1229	CLA	C4-C3-C5-C6
13	H	1229	CLA	C4-C3-C5-C6
13	f	1229	CLA	C4-C3-C5-C6
13	B	1229	CLA	C2-C3-C5-C6
13	H	1229	CLA	C2-C3-C5-C6
13	f	1229	CLA	C2-C3-C5-C6
17	A	5005	LHG	C13-C14-C15-C16
17	G	5005	LHG	C13-C14-C15-C16
17	e	5005	LHG	C13-C14-C15-C16
20	2	822	SQD	C9-C10-C11-C12
20	Z	822	SQD	C9-C10-C11-C12
20	r	822	SQD	C9-C10-C11-C12
13	Z	516	CLA	O1D-CGD-O2D-CED
13	B	1221	CLA	C5-C6-C7-C8
13	H	1221	CLA	C5-C6-C7-C8
13	f	1221	CLA	C5-C6-C7-C8
20	3	822	SQD	C10-C11-C12-C13
20	a	822	SQD	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	s	822	SQD	C10-C11-C12-C13
13	A	1132	CLA	O1A-CGA-O2A-C1
13	1	508	CLA	O1A-CGA-O2A-C1
13	G	1132	CLA	O1A-CGA-O2A-C1
13	Y	508	CLA	O1A-CGA-O2A-C1
13	a	513	CLA	O1A-CGA-O2A-C1
13	e	1132	CLA	O1A-CGA-O2A-C1
13	q	508	CLA	O1A-CGA-O2A-C1
13	A	1138	CLA	C8-C10-C11-C12
13	B	1218	CLA	C5-C6-C7-C8
13	1	518	CLA	C10-C11-C12-C13
13	G	1117	CLA	C8-C10-C11-C12
13	G	1138	CLA	C8-C10-C11-C12
13	H	1218	CLA	C5-C6-C7-C8
13	H	1207	CLA	C10-C11-C12-C13
13	Y	518	CLA	C10-C11-C12-C13
13	e	1138	CLA	C8-C10-C11-C12
13	f	1218	CLA	C5-C6-C7-C8
13	q	518	CLA	C10-C11-C12-C13
13	H	1220	CLA	CBA-CGA-O2A-C1
13	q	518	CLA	CBA-CGA-O2A-C1
20	5	822	SQD	C24-C23-O48-C46
20	u	822	SQD	C24-C23-O48-C46
19	B	5002	LMG	C23-C24-C25-C26
19	H	5002	LMG	C23-C24-C25-C26
19	f	5002	LMG	C23-C24-C25-C26
17	A	5006	LHG	O9-C7-O7-C5
17	G	5006	LHG	O9-C7-O7-C5
17	e	5006	LHG	O9-C7-O7-C5
17	A	5005	LHG	C16-C17-C18-C19
17	A	5001	LHG	C32-C33-C34-C35
17	G	5005	LHG	C16-C17-C18-C19
17	e	5005	LHG	C16-C17-C18-C19
13	A	1117	CLA	C8-C10-C11-C12
13	A	1137	CLA	C8-C10-C11-C12
13	B	1202	CLA	C13-C15-C16-C17
13	B	1216	CLA	C8-C10-C11-C12
13	B	1207	CLA	C10-C11-C12-C13
13	G	1137	CLA	C8-C10-C11-C12
13	H	1202	CLA	C13-C15-C16-C17
13	H	1216	CLA	C8-C10-C11-C12
13	e	1117	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1137	CLA	C8-C10-C11-C12
13	f	1202	CLA	C13-C15-C16-C17
13	f	1216	CLA	C8-C10-C11-C12
13	f	1207	CLA	C10-C11-C12-C13
13	6	501	CLA	C11-C12-C13-C15
13	v	501	CLA	C11-C12-C13-C15
17	G	5001	LHG	C32-C33-C34-C35
17	e	5001	LHG	C32-C33-C34-C35
17	L	5221	LHG	C14-C15-C16-C17
17	n	5221	LHG	C14-C15-C16-C17
20	V	5216	SQD	C18-C19-C20-C21
20	Y	822	SQD	C10-C11-C12-C13
20	q	822	SQD	C10-C11-C12-C13
19	B	5002	LMG	C28-C29-C30-C31
19	H	5002	LMG	C28-C29-C30-C31
13	A	1136	CLA	C10-C11-C12-C13
13	B	1210	CLA	C13-C15-C16-C17
13	G	1136	CLA	C10-C11-C12-C13
13	H	1210	CLA	C13-C15-C16-C17
13	e	1136	CLA	C10-C11-C12-C13
13	5	502	CLA	O1D-CGD-O2D-CED
13	c	502	CLA	O1D-CGD-O2D-CED
17	V	5221	LHG	C14-C15-C16-C17
20	L	5216	SQD	C18-C19-C20-C21
20	1	822	SQD	C10-C11-C12-C13
20	n	5216	SQD	C18-C19-C20-C21
17	A	5001	LHG	O7-C5-C6-O8
17	I	5001	LHG	O7-C5-C6-O8
17	G	5001	LHG	O7-C5-C6-O8
17	S	5001	LHG	O7-C5-C6-O8
17	e	5001	LHG	O7-C5-C6-O8
17	k	5001	LHG	O7-C5-C6-O8
19	B	5002	LMG	O7-C8-C9-O8
19	J	5104	LMG	O1-C7-C8-O7
19	H	5002	LMG	O7-C8-C9-O8
19	T	5104	LMG	O1-C7-C8-O7
19	f	5002	LMG	O7-C8-C9-O8
19	l	5104	LMG	O1-C7-C8-O7
20	1	822	SQD	O47-C45-C46-O48
20	Y	822	SQD	O47-C45-C46-O48
20	q	822	SQD	O47-C45-C46-O48
17	A	5001	LHG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	L	5221	LHG	C18-C19-C20-C21
17	G	5001	LHG	C29-C30-C31-C32
17	V	5221	LHG	C18-C19-C20-C21
17	e	5001	LHG	C29-C30-C31-C32
17	n	5221	LHG	C18-C19-C20-C21
13	u	502	CLA	O1D-CGD-O2D-CED
20	c	822	SQD	C24-C23-O48-C46
13	f	1210	CLA	C13-C15-C16-C17
13	s	507	CLA	O1D-CGD-O2D-CED
17	G	5002	LHG	C25-C26-C27-C28
17	e	5003	LHG	C11-C10-C9-C8
17	A	5002	LHG	C25-C26-C27-C28
17	A	5005	LHG	C9-C10-C11-C12
17	A	5009	LHG	C24-C25-C26-C27
17	A	5003	LHG	C11-C10-C9-C8
17	G	5004	LHG	C27-C28-C29-C30
17	G	5005	LHG	C9-C10-C11-C12
17	G	5009	LHG	C24-C25-C26-C27
17	G	5003	LHG	C11-C10-C9-C8
17	e	5002	LHG	C25-C26-C27-C28
17	e	5005	LHG	C9-C10-C11-C12
20	B	1852	SQD	C11-C12-C13-C14
20	H	1852	SQD	C11-C12-C13-C14
20	f	1852	SQD	C11-C12-C13-C14
13	G	1118	CLA	C2-C1-O2A-CGA
13	3	507	CLA	O1D-CGD-O2D-CED
13	a	507	CLA	O1D-CGD-O2D-CED
13	A	1136	CLA	C11-C12-C13-C15
13	1	505	CLA	C16-C17-C18-C19
13	G	1136	CLA	C11-C12-C13-C15
13	Y	505	CLA	C16-C17-C18-C19
13	e	1136	CLA	C11-C12-C13-C15
13	q	505	CLA	C16-C17-C18-C19
17	A	5004	LHG	C27-C28-C29-C30
17	e	5004	LHG	C27-C28-C29-C30
17	e	5009	LHG	C24-C25-C26-C27
13	B	1239	CLA	C4C-C3C-CAC-CBC
13	A	1108	CLA	C4-C3-C5-C6
13	B	1208	CLA	C4-C3-C5-C6
13	J	1303	CLA	C4-C3-C5-C6
13	G	1108	CLA	C4-C3-C5-C6
13	H	1208	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	T	1303	CLA	C4-C3-C5-C6
13	e	1108	CLA	C4-C3-C5-C6
13	f	1208	CLA	C4-C3-C5-C6
13	l	1303	CLA	C4-C3-C5-C6
13	B	1213	CLA	C3-C5-C6-C7
13	H	1213	CLA	C3-C5-C6-C7
13	f	1213	CLA	C3-C5-C6-C7
17	I	5001	LHG	C1-C2-C3-O3
17	S	5001	LHG	C1-C2-C3-O3
17	k	5001	LHG	C1-C2-C3-O3
13	H	1239	CLA	C4C-C3C-CAC-CBC
13	f	1239	CLA	C4C-C3C-CAC-CBC
17	A	5006	LHG	C25-C26-C27-C28
17	A	5003	LHG	C9-C10-C11-C12
17	G	5006	LHG	C25-C26-C27-C28
17	G	5003	LHG	C9-C10-C11-C12
17	e	5003	LHG	C9-C10-C11-C12
19	f	5002	LMG	C16-C17-C18-C19
13	A	1135	CLA	C2A-CAA-CBA-CGA
13	B	1023	CLA	C2A-CAA-CBA-CGA
13	1	501	CLA	C2A-CAA-CBA-CGA
13	3	501	CLA	C2A-CAA-CBA-CGA
13	4	501	CLA	C2A-CAA-CBA-CGA
13	6	518	CLA	C2A-CAA-CBA-CGA
13	G	1135	CLA	C2A-CAA-CBA-CGA
13	H	1023	CLA	C2A-CAA-CBA-CGA
13	Y	501	CLA	C2A-CAA-CBA-CGA
13	a	501	CLA	C2A-CAA-CBA-CGA
13	b	501	CLA	C2A-CAA-CBA-CGA
13	d	518	CLA	C2A-CAA-CBA-CGA
13	e	1135	CLA	C2A-CAA-CBA-CGA
13	f	1023	CLA	C2A-CAA-CBA-CGA
13	q	501	CLA	C2A-CAA-CBA-CGA
13	s	501	CLA	C2A-CAA-CBA-CGA
13	t	501	CLA	C2A-CAA-CBA-CGA
13	v	518	CLA	C2A-CAA-CBA-CGA
13	5	518	CLA	CBD-CGD-O2D-CED
13	c	518	CLA	CBD-CGD-O2D-CED
13	u	518	CLA	CBD-CGD-O2D-CED
13	3	511	CLA	CBA-CGA-O2A-C1
13	a	511	CLA	CBA-CGA-O2A-C1
13	s	511	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	5006	LHG	C25-C26-C27-C28
19	B	5002	LMG	C16-C17-C18-C19
19	H	5002	LMG	C16-C17-C18-C19
18	1	902	LMU	C2-C3-C4-C5
18	Y	902	LMU	C2-C3-C4-C5
18	q	902	LMU	C2-C3-C4-C5
13	A	1125	CLA	C13-C15-C16-C17
13	B	1223	CLA	C10-C11-C12-C13
13	2	509	CLA	C5-C6-C7-C8
13	3	505	CLA	C15-C16-C17-C18
13	G	1125	CLA	C13-C15-C16-C17
13	H	1223	CLA	C10-C11-C12-C13
13	Z	509	CLA	C5-C6-C7-C8
13	a	505	CLA	C15-C16-C17-C18
13	e	1125	CLA	C13-C15-C16-C17
13	f	1223	CLA	C10-C11-C12-C13
13	r	509	CLA	C5-C6-C7-C8
13	s	505	CLA	C15-C16-C17-C18
19	f	5002	LMG	C28-C29-C30-C31
17	e	5009	LHG	C9-C10-C11-C12
20	L	5216	SQD	C11-C12-C13-C14
20	n	5216	SQD	C11-C12-C13-C14
17	A	5009	LHG	C9-C10-C11-C12
17	G	5009	LHG	C9-C10-C11-C12
20	V	5216	SQD	C11-C12-C13-C14
13	A	1134	CLA	O1D-CGD-O2D-CED
13	G	1134	CLA	O1D-CGD-O2D-CED
13	H	1230	CLA	O1D-CGD-O2D-CED
13	e	1134	CLA	O1D-CGD-O2D-CED
13	f	1230	CLA	O1D-CGD-O2D-CED
17	A	5006	LHG	O1-C1-C2-O2
17	G	5006	LHG	O1-C1-C2-O2
17	e	5006	LHG	O1-C1-C2-O2
13	A	1105	CLA	O1A-CGA-O2A-C1
13	3	507	CLA	O1A-CGA-O2A-C1
13	G	1105	CLA	O1A-CGA-O2A-C1
13	G	1116	CLA	O1A-CGA-O2A-C1
13	a	507	CLA	O1A-CGA-O2A-C1
13	e	1105	CLA	O1A-CGA-O2A-C1
13	e	1116	CLA	O1A-CGA-O2A-C1
13	s	507	CLA	O1A-CGA-O2A-C1
19	B	5002	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	f	5002	LMG	O10-C28-O8-C9
13	A	1102	CLA	C1A-C2A-CAA-CBA
13	A	1106	CLA	C1A-C2A-CAA-CBA
13	A	1107	CLA	C1A-C2A-CAA-CBA
13	A	1113	CLA	C1A-C2A-CAA-CBA
13	A	1116	CLA	C1A-C2A-CAA-CBA
13	A	1118	CLA	C1A-C2A-CAA-CBA
13	A	1120	CLA	C1A-C2A-CAA-CBA
13	A	1122	CLA	C1A-C2A-CAA-CBA
13	A	1125	CLA	C1A-C2A-CAA-CBA
13	A	1128	CLA	C1A-C2A-CAA-CBA
13	A	1132	CLA	C1A-C2A-CAA-CBA
13	A	1135	CLA	C1A-C2A-CAA-CBA
13	A	1101	CLA	C1A-C2A-CAA-CBA
13	A	1130	CLA	C1A-C2A-CAA-CBA
13	B	1219	CLA	C1A-C2A-CAA-CBA
13	B	1225	CLA	C1A-C2A-CAA-CBA
13	B	1226	CLA	C1A-C2A-CAA-CBA
13	B	1227	CLA	C1A-C2A-CAA-CBA
13	B	1236	CLA	C1A-C2A-CAA-CBA
13	B	1239	CLA	C1A-C2A-CAA-CBA
13	K	1103	CLA	C1A-C2A-CAA-CBA
13	K	1105	CLA	C1A-C2A-CAA-CBA
13	L	1501	CLA	C1A-C2A-CAA-CBA
13	1	501	CLA	C1A-C2A-CAA-CBA
13	1	505	CLA	C1A-C2A-CAA-CBA
13	1	519	CLA	C1A-C2A-CAA-CBA
13	2	501	CLA	C1A-C2A-CAA-CBA
13	2	505	CLA	C1A-C2A-CAA-CBA
13	2	508	CLA	C1A-C2A-CAA-CBA
13	2	516	CLA	C1A-C2A-CAA-CBA
13	2	518	CLA	C1A-C2A-CAA-CBA
13	3	503	CLA	C1A-C2A-CAA-CBA
13	3	517	CLA	C1A-C2A-CAA-CBA
13	4	511	CLA	C1A-C2A-CAA-CBA
13	4	516	CLA	C1A-C2A-CAA-CBA
13	4	518	CLA	C1A-C2A-CAA-CBA
13	5	501	CLA	C1A-C2A-CAA-CBA
13	5	516	CLA	C1A-C2A-CAA-CBA
13	5	518	CLA	C1A-C2A-CAA-CBA
13	6	501	CLA	C1A-C2A-CAA-CBA
13	6	505	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	6	508	CLA	C1A-C2A-CAA-CBA
13	6	512	CLA	C1A-C2A-CAA-CBA
13	6	516	CLA	C1A-C2A-CAA-CBA
13	6	517	CLA	C1A-C2A-CAA-CBA
13	6	518	CLA	C1A-C2A-CAA-CBA
13	6	519	CLA	C1A-C2A-CAA-CBA
13	G	1102	CLA	C1A-C2A-CAA-CBA
13	G	1106	CLA	C1A-C2A-CAA-CBA
13	G	1107	CLA	C1A-C2A-CAA-CBA
13	G	1113	CLA	C1A-C2A-CAA-CBA
13	G	1116	CLA	C1A-C2A-CAA-CBA
13	G	1118	CLA	C1A-C2A-CAA-CBA
13	G	1120	CLA	C1A-C2A-CAA-CBA
13	G	1122	CLA	C1A-C2A-CAA-CBA
13	G	1125	CLA	C1A-C2A-CAA-CBA
13	G	1128	CLA	C1A-C2A-CAA-CBA
13	G	1132	CLA	C1A-C2A-CAA-CBA
13	G	1135	CLA	C1A-C2A-CAA-CBA
13	G	1101	CLA	C1A-C2A-CAA-CBA
13	G	1130	CLA	C1A-C2A-CAA-CBA
13	H	1219	CLA	C1A-C2A-CAA-CBA
13	H	1225	CLA	C1A-C2A-CAA-CBA
13	H	1226	CLA	C1A-C2A-CAA-CBA
13	H	1227	CLA	C1A-C2A-CAA-CBA
13	H	1236	CLA	C1A-C2A-CAA-CBA
13	H	1239	CLA	C1A-C2A-CAA-CBA
13	U	1103	CLA	C1A-C2A-CAA-CBA
13	U	1105	CLA	C1A-C2A-CAA-CBA
13	V	1501	CLA	C1A-C2A-CAA-CBA
13	Y	501	CLA	C1A-C2A-CAA-CBA
13	Y	505	CLA	C1A-C2A-CAA-CBA
13	Y	519	CLA	C1A-C2A-CAA-CBA
13	Z	501	CLA	C1A-C2A-CAA-CBA
13	Z	505	CLA	C1A-C2A-CAA-CBA
13	Z	508	CLA	C1A-C2A-CAA-CBA
13	Z	516	CLA	C1A-C2A-CAA-CBA
13	Z	518	CLA	C1A-C2A-CAA-CBA
13	a	503	CLA	C1A-C2A-CAA-CBA
13	a	517	CLA	C1A-C2A-CAA-CBA
13	b	511	CLA	C1A-C2A-CAA-CBA
13	b	516	CLA	C1A-C2A-CAA-CBA
13	b	518	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	c	501	CLA	C1A-C2A-CAA-CBA
13	c	516	CLA	C1A-C2A-CAA-CBA
13	c	518	CLA	C1A-C2A-CAA-CBA
13	d	501	CLA	C1A-C2A-CAA-CBA
13	d	505	CLA	C1A-C2A-CAA-CBA
13	d	508	CLA	C1A-C2A-CAA-CBA
13	d	512	CLA	C1A-C2A-CAA-CBA
13	d	516	CLA	C1A-C2A-CAA-CBA
13	d	517	CLA	C1A-C2A-CAA-CBA
13	d	518	CLA	C1A-C2A-CAA-CBA
13	d	519	CLA	C1A-C2A-CAA-CBA
13	e	1102	CLA	C1A-C2A-CAA-CBA
13	e	1106	CLA	C1A-C2A-CAA-CBA
13	e	1107	CLA	C1A-C2A-CAA-CBA
13	e	1113	CLA	C1A-C2A-CAA-CBA
13	e	1116	CLA	C1A-C2A-CAA-CBA
13	e	1118	CLA	C1A-C2A-CAA-CBA
13	e	1120	CLA	C1A-C2A-CAA-CBA
13	e	1122	CLA	C1A-C2A-CAA-CBA
13	e	1125	CLA	C1A-C2A-CAA-CBA
13	e	1128	CLA	C1A-C2A-CAA-CBA
13	e	1132	CLA	C1A-C2A-CAA-CBA
13	e	1135	CLA	C1A-C2A-CAA-CBA
13	e	1101	CLA	C1A-C2A-CAA-CBA
13	e	1130	CLA	C1A-C2A-CAA-CBA
13	f	1219	CLA	C1A-C2A-CAA-CBA
13	f	1225	CLA	C1A-C2A-CAA-CBA
13	f	1226	CLA	C1A-C2A-CAA-CBA
13	f	1227	CLA	C1A-C2A-CAA-CBA
13	f	1236	CLA	C1A-C2A-CAA-CBA
13	f	1239	CLA	C1A-C2A-CAA-CBA
13	m	1103	CLA	C1A-C2A-CAA-CBA
13	m	1105	CLA	C1A-C2A-CAA-CBA
13	n	1501	CLA	C1A-C2A-CAA-CBA
13	q	501	CLA	C1A-C2A-CAA-CBA
13	q	505	CLA	C1A-C2A-CAA-CBA
13	q	519	CLA	C1A-C2A-CAA-CBA
13	r	501	CLA	C1A-C2A-CAA-CBA
13	r	505	CLA	C1A-C2A-CAA-CBA
13	r	508	CLA	C1A-C2A-CAA-CBA
13	r	516	CLA	C1A-C2A-CAA-CBA
13	r	518	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	s	503	CLA	C1A-C2A-CAA-CBA
13	s	517	CLA	C1A-C2A-CAA-CBA
13	t	511	CLA	C1A-C2A-CAA-CBA
13	t	516	CLA	C1A-C2A-CAA-CBA
13	t	518	CLA	C1A-C2A-CAA-CBA
13	u	501	CLA	C1A-C2A-CAA-CBA
13	u	516	CLA	C1A-C2A-CAA-CBA
13	u	518	CLA	C1A-C2A-CAA-CBA
13	v	501	CLA	C1A-C2A-CAA-CBA
13	v	505	CLA	C1A-C2A-CAA-CBA
13	v	508	CLA	C1A-C2A-CAA-CBA
13	v	512	CLA	C1A-C2A-CAA-CBA
13	v	516	CLA	C1A-C2A-CAA-CBA
13	v	517	CLA	C1A-C2A-CAA-CBA
13	v	518	CLA	C1A-C2A-CAA-CBA
13	v	519	CLA	C1A-C2A-CAA-CBA
13	B	1230	CLA	O1D-CGD-O2D-CED
13	e	1126	CLA	O1D-CGD-O2D-CED
13	B	1222	CLA	C5-C6-C7-C8
13	H	1222	CLA	C5-C6-C7-C8
13	f	1222	CLA	C5-C6-C7-C8
13	A	1116	CLA	O1A-CGA-O2A-C1
19	H	5002	LMG	O10-C28-O8-C9
17	A	5009	LHG	C11-C12-C13-C14
17	G	5009	LHG	C11-C12-C13-C14
19	J	5104	LMG	C31-C32-C33-C34
19	T	5104	LMG	C31-C32-C33-C34
19	l	5104	LMG	C31-C32-C33-C34
14	A	2001	PQN	C25-C26-C27-C28
14	G	2001	PQN	C25-C26-C27-C28
14	e	2001	PQN	C25-C26-C27-C28
17	A	5005	LHG	O6-C4-C5-C6
17	G	5005	LHG	O6-C4-C5-C6
17	e	5005	LHG	O6-C4-C5-C6
17	A	5005	LHG	O9-C7-O7-C5
17	G	5005	LHG	O9-C7-O7-C5
17	e	5005	LHG	O9-C7-O7-C5
17	e	5009	LHG	C11-C12-C13-C14
13	A	1103	CLA	C12-C13-C15-C16
13	A	1106	CLA	C12-C13-C15-C16
13	A	1116	CLA	C6-C7-C8-C10
13	A	1123	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1127	CLA	C11-C12-C13-C15
13	A	1127	CLA	C12-C13-C15-C16
13	A	1132	CLA	C12-C13-C15-C16
13	A	1137	CLA	C6-C7-C8-C10
13	A	1137	CLA	C12-C13-C15-C16
13	A	1138	CLA	C12-C13-C15-C16
13	A	1237	CLA	C11-C10-C8-C7
13	A	1101	CLA	C11-C10-C8-C7
13	B	1203	CLA	C11-C10-C8-C7
13	B	1206	CLA	C6-C7-C8-C10
13	B	1231	CLA	C6-C7-C8-C10
13	F	1301	CLA	C12-C13-C15-C16
13	1	509	CLA	C11-C12-C13-C15
13	G	1103	CLA	C12-C13-C15-C16
13	G	1106	CLA	C12-C13-C15-C16
13	G	1116	CLA	C6-C7-C8-C10
13	G	1123	CLA	C11-C10-C8-C7
13	G	1127	CLA	C11-C12-C13-C15
13	G	1127	CLA	C12-C13-C15-C16
13	G	1132	CLA	C12-C13-C15-C16
13	G	1137	CLA	C6-C7-C8-C10
13	G	1137	CLA	C12-C13-C15-C16
13	G	1138	CLA	C12-C13-C15-C16
13	G	1237	CLA	C11-C10-C8-C7
13	G	1101	CLA	C11-C10-C8-C7
13	H	1203	CLA	C11-C10-C8-C7
13	H	1206	CLA	C6-C7-C8-C10
13	H	1231	CLA	C6-C7-C8-C10
13	R	1301	CLA	C12-C13-C15-C16
13	Y	509	CLA	C11-C12-C13-C15
13	e	1103	CLA	C12-C13-C15-C16
13	e	1106	CLA	C12-C13-C15-C16
13	e	1116	CLA	C6-C7-C8-C10
13	e	1123	CLA	C11-C10-C8-C7
13	e	1127	CLA	C11-C12-C13-C15
13	e	1127	CLA	C12-C13-C15-C16
13	e	1132	CLA	C12-C13-C15-C16
13	e	1137	CLA	C6-C7-C8-C10
13	e	1137	CLA	C12-C13-C15-C16
13	e	1138	CLA	C12-C13-C15-C16
13	e	1237	CLA	C11-C10-C8-C7
13	e	1101	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1203	CLA	C11-C10-C8-C7
13	f	1206	CLA	C6-C7-C8-C10
13	f	1231	CLA	C6-C7-C8-C10
13	j	1301	CLA	C12-C13-C15-C16
13	q	509	CLA	C11-C12-C13-C15
20	n	5216	SQD	C15-C16-C17-C18
13	A	1127	CLA	C16-C17-C18-C19
13	G	1127	CLA	C16-C17-C18-C19
13	e	1127	CLA	C16-C17-C18-C19
13	A	1131	CLA	C13-C15-C16-C17
13	B	1203	CLA	C13-C15-C16-C17
13	G	1125	CLA	C8-C10-C11-C12
13	G	1131	CLA	C13-C15-C16-C17
13	H	1203	CLA	C13-C15-C16-C17
13	e	1131	CLA	C13-C15-C16-C17
13	f	1203	CLA	C13-C15-C16-C17
13	f	1201	CLA	O1A-CGA-O2A-C1
20	L	5216	SQD	C15-C16-C17-C18
20	V	5216	SQD	C15-C16-C17-C18
13	A	1126	CLA	O1D-CGD-O2D-CED
13	e	1128	CLA	O1D-CGD-O2D-CED
18	B	1843	LMU	C7-C8-C9-C10
18	H	1843	LMU	C7-C8-C9-C10
18	f	1843	LMU	C7-C8-C9-C10
13	Z	508	CLA	CBD-CGD-O2D-CED
13	A	1125	CLA	C8-C10-C11-C12
13	B	1224	CLA	C10-C11-C12-C13
13	H	1224	CLA	C10-C11-C12-C13
13	e	1125	CLA	C8-C10-C11-C12
13	f	1224	CLA	C10-C11-C12-C13
17	A	5009	LHG	C27-C28-C29-C30
17	L	5221	LHG	C31-C32-C33-C34
17	V	5221	LHG	C31-C32-C33-C34
17	e	5009	LHG	C27-C28-C29-C30
17	n	5221	LHG	C31-C32-C33-C34
13	A	1132	CLA	C4-C3-C5-C6
13	G	1132	CLA	C4-C3-C5-C6
13	e	1132	CLA	C4-C3-C5-C6
14	B	2002	PQN	C14-C13-C15-C16
14	H	2002	PQN	C14-C13-C15-C16
14	f	2002	PQN	C14-C13-C15-C16
13	A	1124	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	4	519	CLA	C2-C3-C5-C6
13	G	1124	CLA	C2-C3-C5-C6
13	b	519	CLA	C2-C3-C5-C6
13	e	1124	CLA	C2-C3-C5-C6
13	t	519	CLA	C2-C3-C5-C6
17	G	5009	LHG	C27-C28-C29-C30
20	r	822	SQD	C16-C17-C18-C19
13	B	1201	CLA	O1A-CGA-O2A-C1
13	H	1201	CLA	O1A-CGA-O2A-C1
13	G	1128	CLA	O1D-CGD-O2D-CED
17	L	5220	LHG	C29-C30-C31-C32
17	V	5220	LHG	C29-C30-C31-C32
20	2	822	SQD	C16-C17-C18-C19
20	Z	822	SQD	C16-C17-C18-C19
13	2	508	CLA	CBD-CGD-O2D-CED
13	A	1128	CLA	O1D-CGD-O2D-CED
13	G	1126	CLA	O1D-CGD-O2D-CED
13	A	1121	CLA	C2A-CAA-CBA-CGA
13	L	1501	CLA	C2A-CAA-CBA-CGA
13	1	512	CLA	C2A-CAA-CBA-CGA
13	5	501	CLA	C2A-CAA-CBA-CGA
13	G	1121	CLA	C2A-CAA-CBA-CGA
13	V	1501	CLA	C2A-CAA-CBA-CGA
13	Y	512	CLA	C2A-CAA-CBA-CGA
13	c	501	CLA	C2A-CAA-CBA-CGA
13	e	1121	CLA	C2A-CAA-CBA-CGA
13	n	1501	CLA	C2A-CAA-CBA-CGA
13	q	512	CLA	C2A-CAA-CBA-CGA
13	u	501	CLA	C2A-CAA-CBA-CGA
13	A	1102	CLA	C14-C13-C15-C16
13	A	1107	CLA	C11-C12-C13-C14
13	A	1109	CLA	C11-C12-C13-C14
13	A	1127	CLA	C14-C13-C15-C16
13	A	1101	CLA	C11-C10-C8-C9
13	B	1215	CLA	C11-C10-C8-C9
13	B	1225	CLA	C14-C13-C15-C16
13	B	1231	CLA	C6-C7-C8-C9
13	F	1301	CLA	C14-C13-C15-C16
13	L	1501	CLA	C14-C13-C15-C16
13	1	507	CLA	C11-C10-C8-C9
13	1	509	CLA	C11-C12-C13-C14
13	2	501	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	2	510	CLA	C14-C13-C15-C16
13	3	507	CLA	C11-C10-C8-C9
13	4	505	CLA	C14-C13-C15-C16
13	G	1102	CLA	C14-C13-C15-C16
13	G	1107	CLA	C11-C12-C13-C14
13	G	1109	CLA	C11-C12-C13-C14
13	G	1127	CLA	C14-C13-C15-C16
13	G	1137	CLA	C14-C13-C15-C16
13	G	1101	CLA	C11-C10-C8-C9
13	H	1215	CLA	C11-C10-C8-C9
13	H	1225	CLA	C14-C13-C15-C16
13	H	1231	CLA	C6-C7-C8-C9
13	R	1301	CLA	C14-C13-C15-C16
13	V	1501	CLA	C14-C13-C15-C16
13	Y	507	CLA	C11-C10-C8-C9
13	Y	509	CLA	C11-C12-C13-C14
13	Z	501	CLA	C6-C7-C8-C9
13	Z	510	CLA	C14-C13-C15-C16
13	a	507	CLA	C11-C10-C8-C9
13	b	505	CLA	C14-C13-C15-C16
13	e	1102	CLA	C14-C13-C15-C16
13	e	1107	CLA	C11-C12-C13-C14
13	e	1109	CLA	C11-C12-C13-C14
13	e	1117	CLA	C11-C12-C13-C14
13	e	1127	CLA	C14-C13-C15-C16
13	e	1101	CLA	C11-C10-C8-C9
13	f	1215	CLA	C11-C10-C8-C9
13	f	1225	CLA	C14-C13-C15-C16
13	f	1231	CLA	C6-C7-C8-C9
13	j	1301	CLA	C14-C13-C15-C16
13	n	1501	CLA	C14-C13-C15-C16
13	q	507	CLA	C11-C10-C8-C9
13	q	509	CLA	C11-C12-C13-C14
13	r	501	CLA	C6-C7-C8-C9
13	r	510	CLA	C14-C13-C15-C16
13	s	507	CLA	C11-C10-C8-C9
13	t	505	CLA	C14-C13-C15-C16
17	n	5220	LHG	C29-C30-C31-C32
13	r	508	CLA	CBD-CGD-O2D-CED
20	1	822	SQD	C25-C26-C27-C28
20	Y	822	SQD	C25-C26-C27-C28
20	q	822	SQD	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	f	5002	LMG	C37-C38-C39-C40
20	f	1852	SQD	C25-C26-C27-C28
17	A	5002	LHG	C4-C5-C6-O8
17	A	5004	LHG	C4-C5-C6-O8
17	A	5001	LHG	C4-C5-C6-O8
17	L	5218	LHG	C4-C5-C6-O8
17	G	5002	LHG	C4-C5-C6-O8
17	G	5004	LHG	C4-C5-C6-O8
17	G	5001	LHG	C4-C5-C6-O8
17	V	5218	LHG	C4-C5-C6-O8
17	e	5002	LHG	C4-C5-C6-O8
17	e	5004	LHG	C4-C5-C6-O8
17	e	5001	LHG	C4-C5-C6-O8
17	n	5218	LHG	C4-C5-C6-O8
20	1	822	SQD	C44-C45-C46-O48
20	Y	822	SQD	C44-C45-C46-O48
20	q	822	SQD	C44-C45-C46-O48
19	B	5002	LMG	C37-C38-C39-C40
19	H	5002	LMG	C37-C38-C39-C40
20	B	1852	SQD	C25-C26-C27-C28
20	H	1852	SQD	C25-C26-C27-C28
13	2	510	CLA	O1D-CGD-O2D-CED
13	Z	510	CLA	O1D-CGD-O2D-CED
17	e	5006	LHG	C16-C17-C18-C19
13	5	501	CLA	C8-C10-C11-C12
13	c	501	CLA	C8-C10-C11-C12
13	u	501	CLA	C8-C10-C11-C12
17	A	5006	LHG	C16-C17-C18-C19
17	G	5006	LHG	C16-C17-C18-C19
13	r	510	CLA	O1D-CGD-O2D-CED
13	B	1210	CLA	CBA-CGA-O2A-C1
13	4	519	CLA	CBA-CGA-O2A-C1
13	5	518	CLA	CBA-CGA-O2A-C1
13	H	1210	CLA	CBA-CGA-O2A-C1
13	b	519	CLA	CBA-CGA-O2A-C1
13	c	518	CLA	CBA-CGA-O2A-C1
13	f	1210	CLA	CBA-CGA-O2A-C1
13	t	519	CLA	CBA-CGA-O2A-C1
13	u	518	CLA	CBA-CGA-O2A-C1
13	A	1136	CLA	C11-C12-C13-C14
13	G	1136	CLA	C11-C12-C13-C14
13	e	1136	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	1502	CLA	O1A-CGA-O2A-C1
13	V	1502	CLA	O1A-CGA-O2A-C1
13	n	1502	CLA	O1A-CGA-O2A-C1
17	S	5001	LHG	C31-C32-C33-C34
17	k	5001	LHG	C31-C32-C33-C34
20	3	822	SQD	C26-C27-C28-C29
20	a	822	SQD	C26-C27-C28-C29
20	s	822	SQD	C26-C27-C28-C29
13	4	509	CLA	O1D-CGD-O2D-CED
13	b	509	CLA	O1D-CGD-O2D-CED
13	t	509	CLA	O1D-CGD-O2D-CED
17	A	5007	LHG	C30-C31-C32-C33
17	I	5001	LHG	C31-C32-C33-C34
17	e	5007	LHG	C30-C31-C32-C33
18	A	1849	LMU	O5'-C5'-C6'-O6'
18	G	1849	LMU	O5'-C5'-C6'-O6'
18	e	1849	LMU	O5'-C5'-C6'-O6'
17	G	5007	LHG	C30-C31-C32-C33
13	A	1124	CLA	C4-C3-C5-C6
13	G	1124	CLA	C4-C3-C5-C6
13	e	1124	CLA	C4-C3-C5-C6
17	A	5006	LHG	C8-C7-O7-C5
17	G	5006	LHG	C8-C7-O7-C5
17	e	5006	LHG	C8-C7-O7-C5
13	A	1130	CLA	C2-C3-C5-C6
13	B	1208	CLA	C2-C3-C5-C6
13	B	1231	CLA	C2-C3-C5-C6
13	G	1130	CLA	C2-C3-C5-C6
13	H	1208	CLA	C2-C3-C5-C6
13	H	1231	CLA	C2-C3-C5-C6
13	e	1130	CLA	C2-C3-C5-C6
13	f	1208	CLA	C2-C3-C5-C6
13	f	1231	CLA	C2-C3-C5-C6
13	e	1111	CLA	CBA-CGA-O2A-C1
13	B	1204	CLA	C13-C15-C16-C17
13	B	1215	CLA	C13-C15-C16-C17
13	6	505	CLA	C13-C15-C16-C17
13	H	1204	CLA	C13-C15-C16-C17
13	H	1215	CLA	C13-C15-C16-C17
13	d	505	CLA	C13-C15-C16-C17
13	e	1126	CLA	C13-C15-C16-C17
13	f	1204	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1215	CLA	C13-C15-C16-C17
13	v	505	CLA	C13-C15-C16-C17
13	2	505	CLA	C16-C17-C18-C19
13	Z	505	CLA	C16-C17-C18-C19
13	r	505	CLA	C16-C17-C18-C19
13	r	505	CLA	C16-C17-C18-C20
17	H	1842	LHG	C29-C30-C31-C32
13	B	1220	CLA	O1A-CGA-O2A-C1
13	1	518	CLA	O1A-CGA-O2A-C1
13	3	511	CLA	O1A-CGA-O2A-C1
13	H	1220	CLA	O1A-CGA-O2A-C1
13	Y	518	CLA	O1A-CGA-O2A-C1
13	a	511	CLA	O1A-CGA-O2A-C1
13	f	1220	CLA	O1A-CGA-O2A-C1
13	q	518	CLA	O1A-CGA-O2A-C1
13	s	511	CLA	O1A-CGA-O2A-C1
13	A	1121	CLA	C5-C6-C7-C8
13	A	1126	CLA	C13-C15-C16-C17
13	1	502	CLA	C10-C11-C12-C13
13	G	1121	CLA	C5-C6-C7-C8
13	G	1126	CLA	C13-C15-C16-C17
13	Y	502	CLA	C10-C11-C12-C13
13	e	1121	CLA	C5-C6-C7-C8
13	q	502	CLA	C10-C11-C12-C13
17	A	5009	LHG	C28-C29-C30-C31
17	B	1842	LHG	C29-C30-C31-C32
17	G	5009	LHG	C28-C29-C30-C31
17	e	5009	LHG	C28-C29-C30-C31
17	f	1842	LHG	C29-C30-C31-C32
13	A	1129	CLA	C2A-CAA-CBA-CGA
13	G	1129	CLA	C2A-CAA-CBA-CGA
13	e	1129	CLA	C2A-CAA-CBA-CGA
17	A	5005	LHG	C31-C32-C33-C34
17	G	5005	LHG	C31-C32-C33-C34
17	e	5005	LHG	C31-C32-C33-C34
20	B	1852	SQD	C7-C8-C9-C10
20	H	1852	SQD	C7-C8-C9-C10
20	f	1852	SQD	C7-C8-C9-C10
17	A	5001	LHG	C10-C11-C12-C13
17	G	5001	LHG	C10-C11-C12-C13
13	A	1111	CLA	CBA-CGA-O2A-C1
13	B	1208	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	2	518	CLA	CBA-CGA-O2A-C1
13	G	1111	CLA	CBA-CGA-O2A-C1
13	H	1208	CLA	CBA-CGA-O2A-C1
13	Z	518	CLA	CBA-CGA-O2A-C1
13	f	1208	CLA	CBA-CGA-O2A-C1
13	r	518	CLA	CBA-CGA-O2A-C1
13	B	1214	CLA	O2A-C1-C2-C3
13	H	1214	CLA	O2A-C1-C2-C3
13	f	1214	CLA	O2A-C1-C2-C3
20	2	822	SQD	C46-C45-O47-C7
20	4	822	SQD	C46-C45-O47-C7
20	Z	822	SQD	C46-C45-O47-C7
20	b	822	SQD	C46-C45-O47-C7
20	r	822	SQD	C46-C45-O47-C7
20	t	822	SQD	C46-C45-O47-C7
17	A	5006	LHG	C24-C25-C26-C27
17	G	5006	LHG	C24-C25-C26-C27
17	e	5006	LHG	C24-C25-C26-C27
17	e	5001	LHG	C10-C11-C12-C13
13	A	1132	CLA	C5-C6-C7-C8
13	G	1132	CLA	C5-C6-C7-C8
13	e	1132	CLA	C5-C6-C7-C8
17	A	5008	LHG	C25-C26-C27-C28
17	G	5008	LHG	C25-C26-C27-C28
17	e	5008	LHG	C25-C26-C27-C28
20	3	822	SQD	C12-C13-C14-C15
20	a	822	SQD	C12-C13-C14-C15
20	s	822	SQD	C12-C13-C14-C15
13	2	505	CLA	C16-C17-C18-C20
13	Z	505	CLA	C16-C17-C18-C20
13	F	1301	CLA	C15-C16-C17-C18
13	j	1301	CLA	C15-C16-C17-C18
17	A	5008	LHG	C12-C13-C14-C15
17	G	5008	LHG	C12-C13-C14-C15
17	e	5008	LHG	C12-C13-C14-C15
13	2	502	CLA	O1D-CGD-O2D-CED
13	Z	502	CLA	O1D-CGD-O2D-CED
13	e	1124	CLA	O1D-CGD-O2D-CED
13	1	501	CLA	CBA-CGA-O2A-C1
13	2	513	CLA	CBA-CGA-O2A-C1
13	Y	501	CLA	CBA-CGA-O2A-C1
13	Z	513	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	r	513	CLA	CBA-CGA-O2A-C1
13	A	1124	CLA	O1D-CGD-O2D-CED
13	3	505	CLA	O1D-CGD-O2D-CED
13	G	1124	CLA	O1D-CGD-O2D-CED
13	r	502	CLA	O1D-CGD-O2D-CED
13	s	505	CLA	O1D-CGD-O2D-CED
17	B	1855	LHG	C19-C20-C21-C22
17	H	1855	LHG	C19-C20-C21-C22
18	B	1843	LMU	C11-C10-C9-C8
18	H	1843	LMU	C11-C10-C9-C8
18	f	1843	LMU	C11-C10-C9-C8
13	4	519	CLA	C4-C3-C5-C6
13	b	519	CLA	C4-C3-C5-C6
13	t	519	CLA	C4-C3-C5-C6
14	A	2001	PQN	C14-C13-C15-C16
14	G	2001	PQN	C14-C13-C15-C16
14	e	2001	PQN	C14-C13-C15-C16
13	A	1132	CLA	C2-C3-C5-C6
13	G	1132	CLA	C2-C3-C5-C6
13	e	1132	CLA	C2-C3-C5-C6
17	f	1855	LHG	C19-C20-C21-C22
17	e	5004	LHG	C26-C27-C28-C29
17	f	1855	LHG	C27-C28-C29-C30
17	A	5004	LHG	C26-C27-C28-C29
17	B	1855	LHG	C27-C28-C29-C30
17	L	5218	LHG	C9-C10-C11-C12
17	G	5004	LHG	C26-C27-C28-C29
17	H	1855	LHG	C27-C28-C29-C30
17	V	5218	LHG	C9-C10-C11-C12
17	n	5218	LHG	C9-C10-C11-C12
17	A	5006	LHG	O7-C5-C6-O8
17	G	5006	LHG	O7-C5-C6-O8
17	e	5006	LHG	O7-C5-C6-O8
13	q	501	CLA	CBA-CGA-O2A-C1
17	A	5005	LHG	C11-C10-C9-C8
17	G	5005	LHG	C11-C10-C9-C8
17	e	5005	LHG	C11-C10-C9-C8
13	a	505	CLA	O1D-CGD-O2D-CED
13	A	1108	CLA	C5-C6-C7-C8
13	G	1108	CLA	C5-C6-C7-C8
13	e	1108	CLA	C5-C6-C7-C8
13	2	519	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Z	519	CLA	C2A-CAA-CBA-CGA
13	r	519	CLA	C2A-CAA-CBA-CGA
13	J	1303	CLA	C13-C15-C16-C17
13	R	1301	CLA	C15-C16-C17-C18
13	T	1303	CLA	C13-C15-C16-C17
13	l	1303	CLA	C13-C15-C16-C17
13	A	1126	CLA	C16-C17-C18-C19
13	G	1126	CLA	C16-C17-C18-C19
13	e	1126	CLA	C16-C17-C18-C19
17	B	1855	LHG	C30-C31-C32-C33
17	H	1855	LHG	C30-C31-C32-C33
17	f	1855	LHG	C30-C31-C32-C33
13	A	1138	CLA	C13-C15-C16-C17
13	G	1138	CLA	C13-C15-C16-C17
13	e	1138	CLA	C13-C15-C16-C17
17	A	5005	LHG	C25-C26-C27-C28
17	e	5005	LHG	C25-C26-C27-C28
13	A	1103	CLA	CBA-CGA-O2A-C1
13	1	507	CLA	CBA-CGA-O2A-C1
13	3	508	CLA	CBA-CGA-O2A-C1
13	G	1103	CLA	CBA-CGA-O2A-C1
13	Y	507	CLA	CBA-CGA-O2A-C1
13	a	508	CLA	CBA-CGA-O2A-C1
13	e	1103	CLA	CBA-CGA-O2A-C1
13	q	507	CLA	CBA-CGA-O2A-C1
13	s	508	CLA	CBA-CGA-O2A-C1
17	G	5005	LHG	C25-C26-C27-C28
17	A	5004	LHG	C9-C10-C11-C12
17	e	5001	LHG	C9-C10-C11-C12
13	B	1231	CLA	C5-C6-C7-C8
13	H	1231	CLA	C5-C6-C7-C8
13	H	1230	CLA	C5-C6-C7-C8
13	f	1231	CLA	C5-C6-C7-C8
17	A	5001	LHG	C9-C10-C11-C12
17	G	5001	LHG	C9-C10-C11-C12
17	e	5004	LHG	C9-C10-C11-C12
13	L	1503	CLA	O1D-CGD-O2D-CED
13	V	1503	CLA	O1D-CGD-O2D-CED
13	n	1503	CLA	O1D-CGD-O2D-CED
13	1	509	CLA	C5-C6-C7-C8
13	2	502	CLA	C5-C6-C7-C8
13	Y	509	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Z	502	CLA	C5-C6-C7-C8
13	f	1240	CLA	C8-C10-C11-C12
13	q	509	CLA	C5-C6-C7-C8
13	r	502	CLA	C5-C6-C7-C8
13	B	1220	CLA	C6-C7-C8-C10
13	B	1227	CLA	C16-C17-C18-C20
13	H	1220	CLA	C6-C7-C8-C10
13	H	1227	CLA	C16-C17-C18-C20
13	f	1220	CLA	C6-C7-C8-C10
13	f	1227	CLA	C16-C17-C18-C20
17	G	5004	LHG	C9-C10-C11-C12
13	r	505	CLA	CBD-CGD-O2D-CED
13	A	1102	CLA	C4-C3-C5-C6
13	B	1231	CLA	C4-C3-C5-C6
13	G	1102	CLA	C4-C3-C5-C6
13	H	1231	CLA	C4-C3-C5-C6
13	e	1102	CLA	C4-C3-C5-C6
13	f	1231	CLA	C4-C3-C5-C6
13	B	1230	CLA	C5-C6-C7-C8
13	f	1230	CLA	C5-C6-C7-C8
18	B	1843	LMU	C2-C1-O1'-C1'
18	H	1843	LMU	C2-C1-O1'-C1'
18	f	1843	LMU	C2-C1-O1'-C1'
13	A	1106	CLA	C14-C13-C15-C16
13	A	1117	CLA	C11-C12-C13-C14
13	A	1125	CLA	C11-C12-C13-C14
13	A	1127	CLA	C11-C12-C13-C14
13	A	1128	CLA	C6-C7-C8-C9
13	A	1132	CLA	C14-C13-C15-C16
13	A	1137	CLA	C14-C13-C15-C16
13	A	1138	CLA	C14-C13-C15-C16
13	A	1237	CLA	C11-C10-C8-C9
13	B	1201	CLA	C6-C7-C8-C9
13	B	1206	CLA	C6-C7-C8-C9
13	B	1234	CLA	C6-C7-C8-C9
13	B	1235	CLA	C6-C7-C8-C9
13	B	1239	CLA	C14-C13-C15-C16
13	F	1301	CLA	C11-C10-C8-C9
13	L	1503	CLA	C6-C7-C8-C9
13	5	501	CLA	C11-C10-C8-C9
13	5	509	CLA	C11-C12-C13-C14
13	5	509	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1106	CLA	C14-C13-C15-C16
13	G	1117	CLA	C11-C12-C13-C14
13	G	1125	CLA	C11-C12-C13-C14
13	G	1127	CLA	C11-C12-C13-C14
13	G	1128	CLA	C6-C7-C8-C9
13	G	1132	CLA	C14-C13-C15-C16
13	G	1138	CLA	C14-C13-C15-C16
13	G	1237	CLA	C11-C10-C8-C9
13	H	1201	CLA	C6-C7-C8-C9
13	H	1206	CLA	C6-C7-C8-C9
13	H	1234	CLA	C6-C7-C8-C9
13	H	1235	CLA	C6-C7-C8-C9
13	H	1239	CLA	C14-C13-C15-C16
13	R	1301	CLA	C11-C10-C8-C9
13	V	1503	CLA	C6-C7-C8-C9
13	c	501	CLA	C11-C10-C8-C9
13	c	509	CLA	C11-C12-C13-C14
13	c	509	CLA	C14-C13-C15-C16
13	e	1106	CLA	C14-C13-C15-C16
13	e	1125	CLA	C11-C12-C13-C14
13	e	1127	CLA	C11-C12-C13-C14
13	e	1128	CLA	C6-C7-C8-C9
13	e	1132	CLA	C14-C13-C15-C16
13	e	1137	CLA	C14-C13-C15-C16
13	e	1138	CLA	C14-C13-C15-C16
13	e	1237	CLA	C11-C10-C8-C9
13	f	1201	CLA	C6-C7-C8-C9
13	f	1206	CLA	C6-C7-C8-C9
13	f	1234	CLA	C6-C7-C8-C9
13	f	1235	CLA	C6-C7-C8-C9
13	f	1239	CLA	C14-C13-C15-C16
13	j	1301	CLA	C11-C10-C8-C9
13	n	1503	CLA	C6-C7-C8-C9
13	u	501	CLA	C11-C10-C8-C9
13	u	509	CLA	C11-C12-C13-C14
13	u	509	CLA	C14-C13-C15-C16
14	A	2001	PQN	C19-C18-C20-C21
14	G	2001	PQN	C19-C18-C20-C21
14	e	2001	PQN	C19-C18-C20-C21
13	A	1103	CLA	C13-C15-C16-C17
13	A	1140	CLA	C15-C16-C17-C18
13	B	1240	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1140	CLA	C15-C16-C17-C18
13	H	1240	CLA	C8-C10-C11-C12
13	e	1140	CLA	C15-C16-C17-C18
17	L	5221	LHG	C2-C3-O3-P
17	V	5221	LHG	C2-C3-O3-P
17	n	5221	LHG	C2-C3-O3-P
13	A	1011	CLA	C4B-C3B-CAB-CBB
13	A	1112	CLA	C4B-C3B-CAB-CBB
13	A	1115	CLA	C4B-C3B-CAB-CBB
13	A	1140	CLA	C4B-C3B-CAB-CBB
13	B	1208	CLA	C4B-C3B-CAB-CBB
13	B	1217	CLA	C4B-C3B-CAB-CBB
13	B	1240	CLA	C4B-C3B-CAB-CBB
13	1	503	CLA	C4B-C3B-CAB-CBB
13	1	513	CLA	C4B-C3B-CAB-CBB
13	2	504	CLA	C4B-C3B-CAB-CBB
13	2	507	CLA	C4B-C3B-CAB-CBB
13	2	513	CLA	C4B-C3B-CAB-CBB
13	2	517	CLA	C4B-C3B-CAB-CBB
13	3	507	CLA	C4B-C3B-CAB-CBB
13	3	513	CLA	C4B-C3B-CAB-CBB
13	3	516	CLA	C4B-C3B-CAB-CBB
13	4	502	CLA	C4B-C3B-CAB-CBB
13	4	503	CLA	C4B-C3B-CAB-CBB
13	4	506	CLA	C4B-C3B-CAB-CBB
13	4	507	CLA	C4B-C3B-CAB-CBB
13	4	508	CLA	C4B-C3B-CAB-CBB
13	4	510	CLA	C4B-C3B-CAB-CBB
13	4	512	CLA	C4B-C3B-CAB-CBB
13	4	513	CLA	C4B-C3B-CAB-CBB
13	4	516	CLA	C4B-C3B-CAB-CBB
13	4	517	CLA	C4B-C3B-CAB-CBB
13	5	501	CLA	C4B-C3B-CAB-CBB
13	5	503	CLA	C4B-C3B-CAB-CBB
13	5	504	CLA	C4B-C3B-CAB-CBB
13	5	507	CLA	C4B-C3B-CAB-CBB
13	5	510	CLA	C4B-C3B-CAB-CBB
13	6	502	CLA	C4B-C3B-CAB-CBB
13	6	503	CLA	C4B-C3B-CAB-CBB
13	6	510	CLA	C4B-C3B-CAB-CBB
13	6	511	CLA	C4B-C3B-CAB-CBB
13	6	516	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	6	517	CLA	C4B-C3B-CAB-CBB
13	G	1011	CLA	C4B-C3B-CAB-CBB
13	G	1112	CLA	C4B-C3B-CAB-CBB
13	G	1115	CLA	C4B-C3B-CAB-CBB
13	G	1140	CLA	C4B-C3B-CAB-CBB
13	H	1208	CLA	C4B-C3B-CAB-CBB
13	H	1217	CLA	C4B-C3B-CAB-CBB
13	H	1240	CLA	C4B-C3B-CAB-CBB
13	Y	503	CLA	C4B-C3B-CAB-CBB
13	Y	513	CLA	C4B-C3B-CAB-CBB
13	Z	504	CLA	C4B-C3B-CAB-CBB
13	Z	507	CLA	C4B-C3B-CAB-CBB
13	Z	513	CLA	C4B-C3B-CAB-CBB
13	Z	517	CLA	C4B-C3B-CAB-CBB
13	a	507	CLA	C4B-C3B-CAB-CBB
13	a	513	CLA	C4B-C3B-CAB-CBB
13	a	516	CLA	C4B-C3B-CAB-CBB
13	b	502	CLA	C4B-C3B-CAB-CBB
13	b	503	CLA	C4B-C3B-CAB-CBB
13	b	506	CLA	C4B-C3B-CAB-CBB
13	b	507	CLA	C4B-C3B-CAB-CBB
13	b	508	CLA	C4B-C3B-CAB-CBB
13	b	510	CLA	C4B-C3B-CAB-CBB
13	b	512	CLA	C4B-C3B-CAB-CBB
13	b	513	CLA	C4B-C3B-CAB-CBB
13	b	516	CLA	C4B-C3B-CAB-CBB
13	b	517	CLA	C4B-C3B-CAB-CBB
13	c	501	CLA	C4B-C3B-CAB-CBB
13	c	503	CLA	C4B-C3B-CAB-CBB
13	c	504	CLA	C4B-C3B-CAB-CBB
13	c	507	CLA	C4B-C3B-CAB-CBB
13	c	510	CLA	C4B-C3B-CAB-CBB
13	d	502	CLA	C4B-C3B-CAB-CBB
13	d	503	CLA	C4B-C3B-CAB-CBB
13	d	510	CLA	C4B-C3B-CAB-CBB
13	d	511	CLA	C4B-C3B-CAB-CBB
13	d	516	CLA	C4B-C3B-CAB-CBB
13	d	517	CLA	C4B-C3B-CAB-CBB
13	e	1011	CLA	C4B-C3B-CAB-CBB
13	e	1112	CLA	C4B-C3B-CAB-CBB
13	e	1115	CLA	C4B-C3B-CAB-CBB
13	e	1140	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1208	CLA	C4B-C3B-CAB-CBB
13	f	1217	CLA	C4B-C3B-CAB-CBB
13	f	1240	CLA	C4B-C3B-CAB-CBB
13	q	503	CLA	C4B-C3B-CAB-CBB
13	q	513	CLA	C4B-C3B-CAB-CBB
13	r	504	CLA	C4B-C3B-CAB-CBB
13	r	507	CLA	C4B-C3B-CAB-CBB
13	r	513	CLA	C4B-C3B-CAB-CBB
13	r	517	CLA	C4B-C3B-CAB-CBB
13	s	507	CLA	C4B-C3B-CAB-CBB
13	s	513	CLA	C4B-C3B-CAB-CBB
13	s	516	CLA	C4B-C3B-CAB-CBB
13	t	502	CLA	C4B-C3B-CAB-CBB
13	t	503	CLA	C4B-C3B-CAB-CBB
13	t	506	CLA	C4B-C3B-CAB-CBB
13	t	507	CLA	C4B-C3B-CAB-CBB
13	t	508	CLA	C4B-C3B-CAB-CBB
13	t	510	CLA	C4B-C3B-CAB-CBB
13	t	512	CLA	C4B-C3B-CAB-CBB
13	t	513	CLA	C4B-C3B-CAB-CBB
13	t	516	CLA	C4B-C3B-CAB-CBB
13	t	517	CLA	C4B-C3B-CAB-CBB
13	u	501	CLA	C4B-C3B-CAB-CBB
13	u	503	CLA	C4B-C3B-CAB-CBB
13	u	504	CLA	C4B-C3B-CAB-CBB
13	u	507	CLA	C4B-C3B-CAB-CBB
13	u	510	CLA	C4B-C3B-CAB-CBB
13	v	502	CLA	C4B-C3B-CAB-CBB
13	v	503	CLA	C4B-C3B-CAB-CBB
13	v	510	CLA	C4B-C3B-CAB-CBB
13	v	511	CLA	C4B-C3B-CAB-CBB
13	v	516	CLA	C4B-C3B-CAB-CBB
13	v	517	CLA	C4B-C3B-CAB-CBB
13	G	1103	CLA	C13-C15-C16-C17
13	e	1103	CLA	C13-C15-C16-C17
19	H	5002	LMG	C41-C42-C43-C44
19	f	5002	LMG	C41-C42-C43-C44
13	B	1201	CLA	C11-C12-C13-C15
13	H	1201	CLA	C11-C12-C13-C15
17	G	5004	LHG	C31-C32-C33-C34
19	B	5002	LMG	C41-C42-C43-C44
13	4	518	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	b	518	CLA	C2A-CAA-CBA-CGA
13	t	518	CLA	C2A-CAA-CBA-CGA
20	6	822	SQD	C2-C1-O6-C44
20	d	822	SQD	C2-C1-O6-C44
20	v	822	SQD	C2-C1-O6-C44
17	A	5004	LHG	C31-C32-C33-C34
17	e	5004	LHG	C31-C32-C33-C34
17	e	5007	LHG	O6-C4-C5-C6
13	2	505	CLA	CBD-CGD-O2D-CED
13	A	1107	CLA	C11-C12-C13-C15
13	A	1109	CLA	C11-C12-C13-C15
13	A	1117	CLA	C11-C12-C13-C15
13	A	1125	CLA	C11-C12-C13-C15
13	A	1128	CLA	C6-C7-C8-C10
13	A	1139	CLA	C6-C7-C8-C10
13	A	1101	CLA	C11-C12-C13-C15
13	B	1201	CLA	C6-C7-C8-C10
13	B	1210	CLA	C6-C7-C8-C10
13	B	1214	CLA	C11-C12-C13-C15
13	B	1215	CLA	C11-C10-C8-C7
13	B	1217	CLA	C11-C10-C8-C7
13	B	1225	CLA	C12-C13-C15-C16
13	B	1234	CLA	C6-C7-C8-C10
13	B	1234	CLA	C11-C12-C13-C15
13	B	1235	CLA	C6-C7-C8-C10
13	B	1239	CLA	C12-C13-C15-C16
13	L	1501	CLA	C12-C13-C15-C16
13	1	507	CLA	C11-C10-C8-C7
13	2	510	CLA	C12-C13-C15-C16
13	3	507	CLA	C11-C10-C8-C7
13	4	505	CLA	C12-C13-C15-C16
13	5	501	CLA	C6-C7-C8-C10
13	5	501	CLA	C11-C10-C8-C7
13	5	509	CLA	C11-C12-C13-C15
13	5	509	CLA	C12-C13-C15-C16
13	6	501	CLA	C11-C10-C8-C7
13	6	505	CLA	C6-C7-C8-C10
13	G	1107	CLA	C11-C12-C13-C15
13	G	1109	CLA	C11-C12-C13-C15
13	G	1117	CLA	C11-C12-C13-C15
13	G	1125	CLA	C11-C12-C13-C15
13	G	1128	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1139	CLA	C6-C7-C8-C10
13	G	1101	CLA	C11-C12-C13-C15
13	H	1201	CLA	C6-C7-C8-C10
13	H	1210	CLA	C6-C7-C8-C10
13	H	1214	CLA	C11-C12-C13-C15
13	H	1215	CLA	C11-C10-C8-C7
13	H	1217	CLA	C11-C10-C8-C7
13	H	1225	CLA	C12-C13-C15-C16
13	H	1234	CLA	C6-C7-C8-C10
13	H	1234	CLA	C11-C12-C13-C15
13	H	1235	CLA	C6-C7-C8-C10
13	H	1239	CLA	C12-C13-C15-C16
13	V	1501	CLA	C12-C13-C15-C16
13	Y	507	CLA	C11-C10-C8-C7
13	Z	510	CLA	C12-C13-C15-C16
13	a	507	CLA	C11-C10-C8-C7
13	b	505	CLA	C12-C13-C15-C16
13	c	501	CLA	C6-C7-C8-C10
13	c	501	CLA	C11-C10-C8-C7
13	c	509	CLA	C11-C12-C13-C15
13	c	509	CLA	C12-C13-C15-C16
13	d	501	CLA	C11-C10-C8-C7
13	d	505	CLA	C6-C7-C8-C10
13	e	1107	CLA	C11-C12-C13-C15
13	e	1109	CLA	C11-C12-C13-C15
13	e	1117	CLA	C11-C12-C13-C15
13	e	1125	CLA	C11-C12-C13-C15
13	e	1128	CLA	C6-C7-C8-C10
13	e	1139	CLA	C6-C7-C8-C10
13	e	1101	CLA	C11-C12-C13-C15
13	f	1201	CLA	C6-C7-C8-C10
13	f	1210	CLA	C6-C7-C8-C10
13	f	1214	CLA	C11-C12-C13-C15
13	f	1215	CLA	C11-C10-C8-C7
13	f	1217	CLA	C11-C10-C8-C7
13	f	1225	CLA	C12-C13-C15-C16
13	f	1234	CLA	C6-C7-C8-C10
13	f	1234	CLA	C11-C12-C13-C15
13	f	1235	CLA	C6-C7-C8-C10
13	f	1239	CLA	C12-C13-C15-C16
13	n	1501	CLA	C12-C13-C15-C16
13	q	507	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	r	510	CLA	C12-C13-C15-C16
13	s	507	CLA	C11-C10-C8-C7
13	t	505	CLA	C12-C13-C15-C16
13	u	501	CLA	C6-C7-C8-C10
13	u	501	CLA	C11-C10-C8-C7
13	u	509	CLA	C12-C13-C15-C16
13	v	501	CLA	C11-C10-C8-C7
13	v	505	CLA	C6-C7-C8-C10
14	A	2001	PQN	C17-C18-C20-C21
14	A	2001	PQN	C22-C23-C25-C26
14	G	2001	PQN	C17-C18-C20-C21
14	G	2001	PQN	C22-C23-C25-C26
14	e	2001	PQN	C17-C18-C20-C21
14	e	2001	PQN	C22-C23-C25-C26
13	2	507	CLA	C10-C11-C12-C13
13	Z	507	CLA	C10-C11-C12-C13
13	r	507	CLA	C10-C11-C12-C13
17	G	5008	LHG	C26-C27-C28-C29
17	n	5218	LHG	C24-C25-C26-C27
17	A	5008	LHG	C26-C27-C28-C29
17	e	5008	LHG	C26-C27-C28-C29
13	Z	505	CLA	CBD-CGD-O2D-CED
13	f	1201	CLA	C11-C12-C13-C15
13	r	513	CLA	C16-C17-C18-C19
17	e	5005	LHG	C17-C18-C19-C20
17	L	5218	LHG	C24-C25-C26-C27
17	V	5218	LHG	C24-C25-C26-C27
19	B	5002	LMG	C30-C31-C32-C33
19	f	5002	LMG	C30-C31-C32-C33
13	5	518	CLA	O1A-CGA-O2A-C1
13	b	519	CLA	O1A-CGA-O2A-C1
13	c	518	CLA	O1A-CGA-O2A-C1
19	H	5002	LMG	C30-C31-C32-C33
17	A	5005	LHG	C17-C18-C19-C20
17	G	5005	LHG	C17-C18-C19-C20
13	A	1104	CLA	C3A-C2A-CAA-CBA
13	A	1119	CLA	C4-C3-C5-C6
13	B	1206	CLA	C3A-C2A-CAA-CBA
13	B	1227	CLA	C3A-C2A-CAA-CBA
13	B	1240	CLA	C3A-C2A-CAA-CBA
13	J	1303	CLA	C3A-C2A-CAA-CBA
13	3	517	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	6	517	CLA	C3A-C2A-CAA-CBA
13	G	1104	CLA	C3A-C2A-CAA-CBA
13	G	1119	CLA	C4-C3-C5-C6
13	H	1206	CLA	C3A-C2A-CAA-CBA
13	H	1227	CLA	C3A-C2A-CAA-CBA
13	H	1240	CLA	C3A-C2A-CAA-CBA
13	T	1303	CLA	C3A-C2A-CAA-CBA
13	a	517	CLA	C3A-C2A-CAA-CBA
13	d	517	CLA	C3A-C2A-CAA-CBA
13	e	1104	CLA	C3A-C2A-CAA-CBA
13	e	1119	CLA	C4-C3-C5-C6
13	f	1206	CLA	C3A-C2A-CAA-CBA
13	f	1227	CLA	C3A-C2A-CAA-CBA
13	f	1240	CLA	C3A-C2A-CAA-CBA
13	l	1303	CLA	C3A-C2A-CAA-CBA
13	s	517	CLA	C3A-C2A-CAA-CBA
13	v	517	CLA	C3A-C2A-CAA-CBA
13	3	507	CLA	C5-C6-C7-C8
13	a	507	CLA	C5-C6-C7-C8
13	e	1117	CLA	C15-C16-C17-C18
17	A	5004	LHG	C30-C31-C32-C33
17	G	5004	LHG	C30-C31-C32-C33
17	e	5004	LHG	C30-C31-C32-C33
20	B	1852	SQD	C12-C13-C14-C15
20	H	1852	SQD	C12-C13-C14-C15
13	B	1210	CLA	O1A-CGA-O2A-C1
13	4	519	CLA	O1A-CGA-O2A-C1
13	H	1210	CLA	O1A-CGA-O2A-C1
13	f	1210	CLA	O1A-CGA-O2A-C1
13	t	519	CLA	O1A-CGA-O2A-C1
13	u	518	CLA	O1A-CGA-O2A-C1
13	A	1117	CLA	C15-C16-C17-C18
13	G	1117	CLA	C15-C16-C17-C18
13	s	507	CLA	C5-C6-C7-C8
13	Y	504	CLA	O1D-CGD-O2D-CED
13	q	504	CLA	O1D-CGD-O2D-CED
20	f	1852	SQD	C12-C13-C14-C15
16	5	522	BCR	C9-C10-C11-C12
16	c	522	BCR	C9-C10-C11-C12
16	u	522	BCR	C9-C10-C11-C12
13	A	1104	CLA	C3-C5-C6-C7
13	A	1125	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1104	CLA	C3-C5-C6-C7
13	e	1104	CLA	C3-C5-C6-C7
13	2	513	CLA	C16-C17-C18-C19
13	2	513	CLA	C16-C17-C18-C20
13	Z	513	CLA	C16-C17-C18-C19
13	Z	513	CLA	C16-C17-C18-C20
13	r	513	CLA	C16-C17-C18-C20
16	3	524	BCR	C37-C22-C23-C24
16	T	4015	BCR	C7-C8-C9-C34
16	a	524	BCR	C37-C22-C23-C24
16	s	524	BCR	C37-C22-C23-C24
17	A	5004	LHG	C11-C10-C9-C8
17	G	5004	LHG	C11-C10-C9-C8
17	e	5004	LHG	C11-C10-C9-C8
19	B	5002	LMG	C35-C36-C37-C38
19	H	5002	LMG	C35-C36-C37-C38
13	J	1302	CLA	C10-C11-C12-C13
13	T	1302	CLA	C10-C11-C12-C13
13	l	1302	CLA	C10-C11-C12-C13
17	I	5001	LHG	C33-C34-C35-C36
17	S	5001	LHG	C33-C34-C35-C36
17	k	5001	LHG	C33-C34-C35-C36
13	A	1111	CLA	O1A-CGA-O2A-C1
13	G	1111	CLA	O1A-CGA-O2A-C1
13	e	1111	CLA	O1A-CGA-O2A-C1
13	1	504	CLA	O1D-CGD-O2D-CED
19	f	5002	LMG	C35-C36-C37-C38
17	B	1855	LHG	C13-C14-C15-C16
17	H	1855	LHG	C13-C14-C15-C16
17	f	1855	LHG	C13-C14-C15-C16
17	A	5003	LHG	C15-C16-C17-C18
17	G	5003	LHG	C15-C16-C17-C18
17	V	5220	LHG	C28-C29-C30-C31
17	e	5003	LHG	C15-C16-C17-C18
17	A	5005	LHG	C4-C5-C6-O8
17	A	5007	LHG	C4-C5-C6-O8
17	A	5009	LHG	C4-C5-C6-O8
17	I	5001	LHG	C4-C5-C6-O8
17	L	5220	LHG	C4-C5-C6-O8
17	G	5005	LHG	C4-C5-C6-O8
17	G	5007	LHG	C4-C5-C6-O8
17	G	5009	LHG	C4-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	S	5001	LHG	C4-C5-C6-O8
17	V	5220	LHG	C4-C5-C6-O8
17	e	5005	LHG	C4-C5-C6-O8
17	e	5007	LHG	C4-C5-C6-O8
17	e	5009	LHG	C4-C5-C6-O8
17	k	5001	LHG	C4-C5-C6-O8
17	n	5220	LHG	C4-C5-C6-O8
20	B	1852	SQD	O6-C44-C45-C46
20	4	822	SQD	C44-C45-C46-O48
20	6	822	SQD	C44-C45-C46-O48
20	H	1852	SQD	O6-C44-C45-C46
20	b	822	SQD	C44-C45-C46-O48
20	d	822	SQD	C44-C45-C46-O48
20	f	1852	SQD	O6-C44-C45-C46
20	t	822	SQD	C44-C45-C46-O48
20	v	822	SQD	C44-C45-C46-O48
17	A	5006	LHG	C14-C15-C16-C17
17	L	5220	LHG	C28-C29-C30-C31
17	G	5006	LHG	C14-C15-C16-C17
17	e	5006	LHG	C14-C15-C16-C17
17	A	5007	LHG	C35-C36-C37-C38
17	G	5007	LHG	C35-C36-C37-C38
17	e	5007	LHG	C35-C36-C37-C38
13	G	1125	CLA	C3-C5-C6-C7
13	e	1125	CLA	C3-C5-C6-C7
17	n	5220	LHG	C28-C29-C30-C31
13	B	1220	CLA	C6-C7-C8-C9
13	H	1220	CLA	C6-C7-C8-C9
13	f	1220	CLA	C6-C7-C8-C9
17	f	1842	LHG	C31-C32-C33-C34
18	J	5105	LMU	C3-C4-C5-C6
18	l	5105	LMU	C3-C4-C5-C6
18	2	901	LMU	C1-C2-C3-C4
18	Z	901	LMU	C1-C2-C3-C4
18	r	901	LMU	C1-C2-C3-C4
13	1	507	CLA	C8-C10-C11-C12
13	Y	507	CLA	C8-C10-C11-C12
13	q	507	CLA	C8-C10-C11-C12
17	B	1842	LHG	C31-C32-C33-C34
17	H	1842	LHG	C31-C32-C33-C34
18	T	5105	LMU	C3-C4-C5-C6
17	A	5001	LHG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5001	LHG	C31-C32-C33-C34
17	e	5001	LHG	C31-C32-C33-C34
13	1	518	CLA	CAA-CBA-CGA-O2A
13	Y	518	CLA	CAA-CBA-CGA-O2A
13	q	518	CLA	CAA-CBA-CGA-O2A
13	B	1227	CLA	C2-C3-C5-C6
13	H	1227	CLA	C2-C3-C5-C6
13	f	1227	CLA	C2-C3-C5-C6
13	B	1012	CLA	C3-C5-C6-C7
13	B	1227	CLA	C3-C5-C6-C7
13	H	1012	CLA	C3-C5-C6-C7
13	H	1227	CLA	C3-C5-C6-C7
13	f	1012	CLA	C3-C5-C6-C7
13	f	1227	CLA	C3-C5-C6-C7
13	f	1224	CLA	O1D-CGD-O2D-CED
13	B	1224	CLA	O1D-CGD-O2D-CED
13	H	1224	CLA	O1D-CGD-O2D-CED
13	1	501	CLA	C16-C17-C18-C19
13	1	501	CLA	C16-C17-C18-C20
13	Y	501	CLA	C16-C17-C18-C19
13	Y	501	CLA	C16-C17-C18-C20
13	q	501	CLA	C16-C17-C18-C19
13	q	501	CLA	C16-C17-C18-C20
17	B	1855	LHG	O6-C4-C5-O7
17	H	1855	LHG	O6-C4-C5-O7
17	f	1855	LHG	O6-C4-C5-O7
17	L	5221	LHG	C19-C20-C21-C22
17	V	5221	LHG	C19-C20-C21-C22
17	n	5221	LHG	C19-C20-C21-C22
16	B	4004	BCR	C23-C24-C25-C30
16	B	4005	BCR	C23-C24-C25-C30
16	B	4017	BCR	C1-C6-C7-C8
16	J	4015	BCR	C23-C24-C25-C30
16	1	521	BCR	C23-C24-C25-C26
16	1	521	BCR	C23-C24-C25-C30
16	2	524	BCR	C23-C24-C25-C30
16	H	4004	BCR	C23-C24-C25-C30
16	H	4005	BCR	C23-C24-C25-C30
16	H	4017	BCR	C1-C6-C7-C8
16	T	4015	BCR	C23-C24-C25-C30
16	Y	521	BCR	C23-C24-C25-C26
16	Y	521	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	Z	524	BCR	C23-C24-C25-C30
16	f	4004	BCR	C23-C24-C25-C30
16	f	4005	BCR	C23-C24-C25-C30
16	f	4017	BCR	C1-C6-C7-C8
16	l	4015	BCR	C23-C24-C25-C30
16	q	521	BCR	C23-C24-C25-C26
16	q	521	BCR	C23-C24-C25-C30
16	q	523	BCR	C23-C24-C25-C26
16	r	524	BCR	C23-C24-C25-C30
17	A	5004	LHG	C2-C3-O3-P
17	G	5004	LHG	C2-C3-O3-P
17	e	5004	LHG	C2-C3-O3-P
13	B	1211	CLA	C11-C10-C8-C9
13	5	505	CLA	C14-C13-C15-C16
13	H	1211	CLA	C11-C10-C8-C9
13	c	505	CLA	C14-C13-C15-C16
13	f	1211	CLA	C11-C10-C8-C9
13	u	505	CLA	C14-C13-C15-C16
17	A	5003	LHG	C25-C26-C27-C28
17	G	5003	LHG	C25-C26-C27-C28
17	e	5003	LHG	C25-C26-C27-C28
13	B	1208	CLA	O1A-CGA-O2A-C1
13	2	518	CLA	O1A-CGA-O2A-C1
13	H	1208	CLA	O1A-CGA-O2A-C1
13	Z	518	CLA	O1A-CGA-O2A-C1
13	f	1208	CLA	O1A-CGA-O2A-C1
13	r	518	CLA	O1A-CGA-O2A-C1
13	A	1122	CLA	C10-C11-C12-C13
13	A	1132	CLA	C13-C15-C16-C17
13	B	1206	CLA	C13-C15-C16-C17
13	B	1221	CLA	C13-C15-C16-C17
13	2	518	CLA	C8-C10-C11-C12
13	G	1122	CLA	C10-C11-C12-C13
13	G	1132	CLA	C13-C15-C16-C17
13	H	1206	CLA	C13-C15-C16-C17
13	H	1221	CLA	C13-C15-C16-C17
13	Z	518	CLA	C8-C10-C11-C12
13	e	1132	CLA	C13-C15-C16-C17
13	f	1206	CLA	C13-C15-C16-C17
13	f	1221	CLA	C13-C15-C16-C17
13	r	518	CLA	C8-C10-C11-C12
13	B	1227	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1227	CLA	C16-C17-C18-C19
13	f	1227	CLA	C16-C17-C18-C19
13	A	1111	CLA	C2A-CAA-CBA-CGA
13	3	518	CLA	C2A-CAA-CBA-CGA
13	G	1111	CLA	C2A-CAA-CBA-CGA
13	a	518	CLA	C2A-CAA-CBA-CGA
13	e	1106	CLA	C2A-CAA-CBA-CGA
13	e	1111	CLA	C2A-CAA-CBA-CGA
19	J	5104	LMG	C10-C11-C12-C13
19	T	5104	LMG	C10-C11-C12-C13
19	l	5104	LMG	C10-C11-C12-C13
13	A	1128	CLA	C5-C6-C7-C8
13	G	1128	CLA	C5-C6-C7-C8
13	e	1122	CLA	C10-C11-C12-C13
13	e	1128	CLA	C5-C6-C7-C8
17	A	5009	LHG	O7-C5-C6-O8
17	G	5009	LHG	O7-C5-C6-O8
17	e	5009	LHG	O7-C5-C6-O8
20	1	822	SQD	O6-C44-C45-O47
20	Y	822	SQD	O6-C44-C45-O47
20	q	822	SQD	O6-C44-C45-O47
17	f	1855	LHG	C24-C25-C26-C27
17	B	1855	LHG	C24-C25-C26-C27
17	H	1855	LHG	C24-C25-C26-C27
13	B	1205	CLA	O1D-CGD-O2D-CED
13	H	1205	CLA	O1D-CGD-O2D-CED
13	f	1205	CLA	O1D-CGD-O2D-CED
17	V	5221	LHG	C24-C25-C26-C27
13	A	1117	CLA	C4-C3-C5-C6
13	B	1227	CLA	C4-C3-C5-C6
13	J	1302	CLA	C4-C3-C5-C6
13	G	1117	CLA	C4-C3-C5-C6
13	H	1227	CLA	C4-C3-C5-C6
13	T	1302	CLA	C4-C3-C5-C6
13	e	1117	CLA	C4-C3-C5-C6
13	f	1227	CLA	C4-C3-C5-C6
13	l	1302	CLA	C4-C3-C5-C6
17	A	5009	LHG	C32-C33-C34-C35
17	L	5221	LHG	C24-C25-C26-C27
17	G	5009	LHG	C32-C33-C34-C35
17	e	5009	LHG	C32-C33-C34-C35
17	n	5221	LHG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1208	CLA	C13-C15-C16-C17
13	H	1208	CLA	C13-C15-C16-C17
13	f	1208	CLA	C13-C15-C16-C17
13	A	1119	CLA	C2-C3-C5-C6
13	J	1302	CLA	C2-C3-C5-C6
13	G	1119	CLA	C2-C3-C5-C6
13	T	1302	CLA	C2-C3-C5-C6
13	e	1119	CLA	C2-C3-C5-C6
13	l	1302	CLA	C2-C3-C5-C6
13	B	1210	CLA	C16-C17-C18-C20
13	H	1210	CLA	C16-C17-C18-C20
13	f	1210	CLA	C16-C17-C18-C20
17	A	5007	LHG	C15-C16-C17-C18
17	L	5220	LHG	C11-C10-C9-C8
17	G	5007	LHG	C15-C16-C17-C18
17	V	5220	LHG	C11-C10-C9-C8
17	e	5007	LHG	C15-C16-C17-C18
17	n	5220	LHG	C11-C10-C9-C8
13	Y	508	CLA	O1D-CGD-O2D-CED
13	A	1237	CLA	C3-C5-C6-C7
20	H	1852	SQD	C8-C7-O47-C45
13	A	1104	CLA	C14-C13-C15-C16
13	A	1106	CLA	C11-C12-C13-C14
13	B	1205	CLA	C14-C13-C15-C16
13	B	1210	CLA	C11-C12-C13-C14
13	B	1214	CLA	C11-C12-C13-C14
13	5	509	CLA	C11-C10-C8-C9
13	G	1104	CLA	C14-C13-C15-C16
13	G	1106	CLA	C11-C12-C13-C14
13	H	1205	CLA	C14-C13-C15-C16
13	H	1210	CLA	C11-C12-C13-C14
13	H	1214	CLA	C11-C12-C13-C14
13	R	1301	CLA	C6-C7-C8-C9
13	c	509	CLA	C11-C10-C8-C9
13	e	1104	CLA	C14-C13-C15-C16
13	e	1106	CLA	C11-C12-C13-C14
13	f	1205	CLA	C14-C13-C15-C16
13	f	1210	CLA	C11-C12-C13-C14
13	f	1214	CLA	C11-C12-C13-C14
13	j	1301	CLA	C6-C7-C8-C9
13	u	509	CLA	C11-C10-C8-C9
17	A	5006	LHG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5004	LHG	C25-C26-C27-C28
17	G	5006	LHG	C30-C31-C32-C33
17	e	5006	LHG	C30-C31-C32-C33
13	1	508	CLA	O1D-CGD-O2D-CED
13	q	508	CLA	O1D-CGD-O2D-CED
13	G	1237	CLA	C10-C11-C12-C13
13	e	1237	CLA	C10-C11-C12-C13
17	A	5004	LHG	C25-C26-C27-C28
17	e	5004	LHG	C25-C26-C27-C28
19	f	5002	LMG	C34-C35-C36-C37
13	A	1103	CLA	C16-C17-C18-C19
13	G	1103	CLA	C16-C17-C18-C19
13	e	1103	CLA	C16-C17-C18-C19
14	A	2001	PQN	C26-C27-C28-C30
14	G	2001	PQN	C26-C27-C28-C30
14	e	2001	PQN	C26-C27-C28-C30
13	G	1237	CLA	C3-C5-C6-C7
13	e	1237	CLA	C3-C5-C6-C7
19	B	5002	LMG	C34-C35-C36-C37
19	H	5002	LMG	C34-C35-C36-C37
13	A	1237	CLA	C10-C11-C12-C13
13	G	1106	CLA	C2A-CAA-CBA-CGA
20	3	822	SQD	C28-C29-C30-C31
13	r	513	CLA	O1A-CGA-O2A-C1
17	f	1855	LHG	C14-C15-C16-C17
17	B	1842	LHG	C34-C35-C36-C37
20	B	1852	SQD	C32-C33-C34-C35
20	H	1852	SQD	C32-C33-C34-C35
20	a	822	SQD	C28-C29-C30-C31
20	f	1852	SQD	C32-C33-C34-C35
20	s	822	SQD	C28-C29-C30-C31
17	A	5001	LHG	O1-C1-C2-O2
17	L	5221	LHG	O1-C1-C2-O2
17	G	5001	LHG	O1-C1-C2-O2
17	V	5221	LHG	O1-C1-C2-O2
17	e	5001	LHG	O1-C1-C2-O2
17	n	5221	LHG	O1-C1-C2-O2
13	B	1236	CLA	CBA-CGA-O2A-C1
13	4	518	CLA	CBA-CGA-O2A-C1
13	H	1236	CLA	CBA-CGA-O2A-C1
13	R	1301	CLA	CBA-CGA-O2A-C1
13	b	518	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1236	CLA	CBA-CGA-O2A-C1
13	t	518	CLA	CBA-CGA-O2A-C1
17	H	1855	LHG	C14-C15-C16-C17
16	J	4015	BCR	C15-C16-C17-C18
16	3	522	BCR	C9-C10-C11-C12
16	T	4015	BCR	C15-C16-C17-C18
16	a	522	BCR	C9-C10-C11-C12
16	l	4015	BCR	C15-C16-C17-C18
16	s	522	BCR	C9-C10-C11-C12
17	H	1842	LHG	C34-C35-C36-C37
17	f	1842	LHG	C34-C35-C36-C37
13	A	1102	CLA	C2-C3-C5-C6
13	G	1102	CLA	C2-C3-C5-C6
13	e	1102	CLA	C2-C3-C5-C6
13	A	1115	CLA	C11-C12-C13-C14
13	B	1219	CLA	C16-C17-C18-C19
13	G	1115	CLA	C11-C12-C13-C14
13	H	1219	CLA	C16-C17-C18-C19
13	e	1115	CLA	C11-C12-C13-C14
13	f	1219	CLA	C16-C17-C18-C19
17	B	1855	LHG	C14-C15-C16-C17
20	B	1852	SQD	C8-C7-O47-C45
20	f	1852	SQD	C8-C7-O47-C45
13	2	513	CLA	O1A-CGA-O2A-C1
13	Z	513	CLA	O1A-CGA-O2A-C1
17	V	5220	LHG	C30-C31-C32-C33
13	1	501	CLA	O1A-CGA-O2A-C1
13	e	1103	CLA	O1A-CGA-O2A-C1
13	A	1103	CLA	C3-C5-C6-C7
13	G	1103	CLA	C3-C5-C6-C7
13	e	1103	CLA	C3-C5-C6-C7
13	B	1224	CLA	CAA-CBA-CGA-O2A
13	H	1224	CLA	CAA-CBA-CGA-O2A
13	f	1224	CLA	CAA-CBA-CGA-O2A
13	F	1301	CLA	CBA-CGA-O2A-C1
13	j	1301	CLA	CBA-CGA-O2A-C1
17	L	5220	LHG	C30-C31-C32-C33
17	A	5002	LHG	O6-C4-C5-C6
17	A	5007	LHG	O6-C4-C5-C6
17	L	5218	LHG	O6-C4-C5-C6
17	G	5002	LHG	O6-C4-C5-C6
17	G	5007	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	V	5218	LHG	O6-C4-C5-C6
17	e	5002	LHG	O6-C4-C5-C6
17	n	5218	LHG	O6-C4-C5-C6
13	1	502	CLA	C11-C12-C13-C15
13	Y	502	CLA	C11-C12-C13-C15
13	q	502	CLA	C11-C12-C13-C15
17	n	5220	LHG	C30-C31-C32-C33
13	3	508	CLA	O1A-CGA-O2A-C1
13	s	508	CLA	O1A-CGA-O2A-C1
13	B	1224	CLA	C5-C6-C7-C8
13	H	1224	CLA	C5-C6-C7-C8
13	f	1224	CLA	C5-C6-C7-C8
16	J	4015	BCR	C7-C8-C9-C34
16	1	524	BCR	C11-C12-C13-C35
16	Y	524	BCR	C11-C12-C13-C35
16	Z	523	BCR	C7-C8-C9-C34
16	l	4015	BCR	C7-C8-C9-C34
16	q	524	BCR	C11-C12-C13-C35
13	A	1104	CLA	C12-C13-C15-C16
13	A	1106	CLA	C11-C12-C13-C15
13	A	1131	CLA	C12-C13-C15-C16
13	B	1012	CLA	C11-C10-C8-C7
13	B	1012	CLA	C12-C13-C15-C16
13	B	1203	CLA	C6-C7-C8-C10
13	B	1203	CLA	C11-C12-C13-C15
13	B	1206	CLA	C11-C10-C8-C7
13	B	1208	CLA	C6-C7-C8-C10
13	B	1226	CLA	C11-C12-C13-C15
13	B	1240	CLA	C11-C12-C13-C15
13	F	1301	CLA	C6-C7-C8-C10
13	1	510	CLA	C6-C7-C8-C10
13	2	507	CLA	C11-C10-C8-C7
13	3	505	CLA	C6-C7-C8-C10
13	3	513	CLA	C12-C13-C15-C16
13	4	501	CLA	C6-C7-C8-C10
13	G	1104	CLA	C12-C13-C15-C16
13	G	1106	CLA	C11-C12-C13-C15
13	G	1131	CLA	C12-C13-C15-C16
13	H	1012	CLA	C11-C10-C8-C7
13	H	1012	CLA	C12-C13-C15-C16
13	H	1203	CLA	C6-C7-C8-C10
13	H	1203	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1206	CLA	C11-C10-C8-C7
13	H	1208	CLA	C6-C7-C8-C10
13	H	1226	CLA	C11-C12-C13-C15
13	H	1240	CLA	C11-C12-C13-C15
13	R	1301	CLA	C6-C7-C8-C10
13	Y	510	CLA	C6-C7-C8-C10
13	Z	507	CLA	C11-C10-C8-C7
13	a	505	CLA	C6-C7-C8-C10
13	a	513	CLA	C12-C13-C15-C16
13	b	501	CLA	C6-C7-C8-C10
13	e	1104	CLA	C12-C13-C15-C16
13	e	1106	CLA	C11-C12-C13-C15
13	e	1131	CLA	C12-C13-C15-C16
13	f	1012	CLA	C11-C10-C8-C7
13	f	1012	CLA	C12-C13-C15-C16
13	f	1203	CLA	C6-C7-C8-C10
13	f	1203	CLA	C11-C12-C13-C15
13	f	1206	CLA	C11-C10-C8-C7
13	f	1208	CLA	C6-C7-C8-C10
13	f	1226	CLA	C11-C12-C13-C15
13	f	1240	CLA	C11-C12-C13-C15
13	j	1301	CLA	C6-C7-C8-C10
13	q	510	CLA	C6-C7-C8-C10
13	r	507	CLA	C11-C10-C8-C7
13	s	505	CLA	C6-C7-C8-C10
13	s	513	CLA	C12-C13-C15-C16
13	t	501	CLA	C6-C7-C8-C10
13	u	509	CLA	C11-C12-C13-C15
20	B	1852	SQD	C10-C11-C12-C13
20	H	1852	SQD	C10-C11-C12-C13
20	f	1852	SQD	C10-C11-C12-C13
16	A	4001	BCR	C7-C8-C9-C10
16	A	4011	BCR	C17-C18-C19-C20
16	B	4014	BCR	C7-C8-C9-C10
16	M	4021	BCR	C11-C12-C13-C14
16	3	524	BCR	C7-C8-C9-C10
16	4	524	BCR	C7-C8-C9-C10
16	6	522	BCR	C7-C8-C9-C10
16	G	4001	BCR	C7-C8-C9-C10
16	G	4011	BCR	C17-C18-C19-C20
16	H	4014	BCR	C7-C8-C9-C10
16	W	4021	BCR	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	a	524	BCR	C7-C8-C9-C10
16	b	524	BCR	C7-C8-C9-C10
16	d	522	BCR	C7-C8-C9-C10
16	e	4001	BCR	C7-C8-C9-C10
16	e	4011	BCR	C17-C18-C19-C20
16	f	4014	BCR	C7-C8-C9-C10
16	o	4021	BCR	C11-C12-C13-C14
16	s	524	BCR	C7-C8-C9-C10
16	t	524	BCR	C7-C8-C9-C10
16	v	522	BCR	C7-C8-C9-C10
13	6	503	CLA	CBA-CGA-O2A-C1
13	d	503	CLA	CBA-CGA-O2A-C1
13	v	503	CLA	CBA-CGA-O2A-C1
17	A	5009	LHG	C10-C11-C12-C13
17	G	5009	LHG	C10-C11-C12-C13
17	e	5009	LHG	C10-C11-C12-C13
13	A	1103	CLA	O1A-CGA-O2A-C1
13	G	1103	CLA	O1A-CGA-O2A-C1
13	Y	501	CLA	O1A-CGA-O2A-C1
13	a	508	CLA	O1A-CGA-O2A-C1
13	q	501	CLA	O1A-CGA-O2A-C1
20	L	5216	SQD	C5-C6-S-O8
20	4	822	SQD	C5-C6-S-O8
20	V	5216	SQD	C5-C6-S-O8
20	b	822	SQD	C5-C6-S-O8
20	n	5216	SQD	C5-C6-S-O8
20	t	822	SQD	C5-C6-S-O8
13	A	1106	CLA	C2A-CAA-CBA-CGA
13	A	1115	CLA	C2A-CAA-CBA-CGA
13	2	501	CLA	C2A-CAA-CBA-CGA
13	2	518	CLA	C2A-CAA-CBA-CGA
13	G	1115	CLA	C2A-CAA-CBA-CGA
13	Z	501	CLA	C2A-CAA-CBA-CGA
13	Z	518	CLA	C2A-CAA-CBA-CGA
13	e	1115	CLA	C2A-CAA-CBA-CGA
13	r	501	CLA	C2A-CAA-CBA-CGA
13	r	518	CLA	C2A-CAA-CBA-CGA
13	s	518	CLA	C2A-CAA-CBA-CGA
13	n	1502	CLA	C16-C17-C18-C20
13	B	1215	CLA	O1D-CGD-O2D-CED
19	J	5104	LMG	O9-C10-O7-C8
19	T	5104	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	l	5104	LMG	O9-C10-O7-C8
13	5	505	CLA	C4-C3-C5-C6
13	c	505	CLA	C4-C3-C5-C6
13	u	505	CLA	C4-C3-C5-C6
13	A	1117	CLA	C2-C3-C5-C6
13	L	1501	CLA	C2-C3-C5-C6
13	G	1117	CLA	C2-C3-C5-C6
13	V	1501	CLA	C2-C3-C5-C6
13	e	1117	CLA	C2-C3-C5-C6
13	B	1215	CLA	C5-C6-C7-C8
20	s	822	SQD	C11-C10-C9-C8
13	B	1217	CLA	C3-C5-C6-C7
13	2	506	CLA	C3-C5-C6-C7
13	H	1217	CLA	C3-C5-C6-C7
13	Z	506	CLA	C3-C5-C6-C7
13	f	1217	CLA	C3-C5-C6-C7
13	r	506	CLA	C3-C5-C6-C7
20	3	822	SQD	C11-C10-C9-C8
13	H	1215	CLA	O1D-CGD-O2D-CED
13	f	1215	CLA	O1D-CGD-O2D-CED
20	a	822	SQD	C11-C10-C9-C8
13	2	507	CLA	C13-C15-C16-C17
13	H	1215	CLA	C5-C6-C7-C8
13	Z	507	CLA	C13-C15-C16-C17
13	r	507	CLA	C13-C15-C16-C17
17	B	1855	LHG	C6-C5-O7-C7
17	H	1855	LHG	C6-C5-O7-C7
17	f	1855	LHG	C6-C5-O7-C7
13	1	507	CLA	O1A-CGA-O2A-C1
13	Y	507	CLA	O1A-CGA-O2A-C1
17	G	5008	LHG	C11-C12-C13-C14
13	B	1201	CLA	C11-C12-C13-C14
13	L	1502	CLA	C16-C17-C18-C20
13	V	1502	CLA	C16-C17-C18-C20
13	f	1201	CLA	C11-C12-C13-C14
17	A	5008	LHG	C11-C12-C13-C14
17	e	5008	LHG	C11-C12-C13-C14
20	L	5216	SQD	C31-C32-C33-C34
20	V	5216	SQD	C31-C32-C33-C34
20	n	5216	SQD	C31-C32-C33-C34
13	q	507	CLA	O1A-CGA-O2A-C1
13	f	1215	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	5002	LHG	O6-C4-C5-O7
17	L	5218	LHG	O6-C4-C5-O7
17	G	5002	LHG	O6-C4-C5-O7
17	V	5218	LHG	O6-C4-C5-O7
17	e	5002	LHG	O6-C4-C5-O7
17	n	5218	LHG	O6-C4-C5-O7
17	A	5008	LHG	C4-C5-C6-O8
17	G	5008	LHG	C4-C5-C6-O8
17	e	5008	LHG	C4-C5-C6-O8
19	J	5104	LMG	C7-C8-C9-O8
19	T	5104	LMG	C7-C8-C9-O8
19	l	5104	LMG	C7-C8-C9-O8
20	L	5216	SQD	C44-C45-C46-O48
20	1	822	SQD	O6-C44-C45-C46
20	V	5216	SQD	C44-C45-C46-O48
20	Y	822	SQD	O6-C44-C45-C46
20	n	5216	SQD	C44-C45-C46-O48
20	q	822	SQD	O6-C44-C45-C46
13	T	1303	CLA	C5-C6-C7-C8
13	H	1201	CLA	C11-C12-C13-C14
13	B	1202	CLA	C15-C16-C17-C18
13	J	1303	CLA	C5-C6-C7-C8
13	f	1202	CLA	C15-C16-C17-C18
13	B	1204	CLA	C4-C3-C5-C6
13	H	1204	CLA	C4-C3-C5-C6
13	f	1204	CLA	C4-C3-C5-C6
13	A	1108	CLA	C2-C3-C5-C6
13	A	1137	CLA	C2-C3-C5-C6
13	J	1303	CLA	C2-C3-C5-C6
13	G	1108	CLA	C2-C3-C5-C6
13	G	1137	CLA	C2-C3-C5-C6
13	e	1108	CLA	C2-C3-C5-C6
13	e	1137	CLA	C2-C3-C5-C6
13	l	1303	CLA	C2-C3-C5-C6
13	n	1501	CLA	C2-C3-C5-C6
13	H	1202	CLA	C15-C16-C17-C18
13	l	1303	CLA	C5-C6-C7-C8
13	4	518	CLA	O1A-CGA-O2A-C1
17	A	5007	LHG	C10-C11-C12-C13
17	G	5007	LHG	C10-C11-C12-C13
17	A	5003	LHG	C13-C14-C15-C16
17	e	5007	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	e	5003	LHG	C13-C14-C15-C16
17	A	5007	LHG	O7-C5-C6-O8
17	L	5220	LHG	O7-C5-C6-O8
17	G	5007	LHG	O7-C5-C6-O8
17	V	5220	LHG	O7-C5-C6-O8
17	e	5007	LHG	O7-C5-C6-O8
17	n	5220	LHG	O7-C5-C6-O8
20	B	1852	SQD	O6-C44-C45-O47
20	2	822	SQD	O47-C45-C46-O48
20	4	822	SQD	O47-C45-C46-O48
20	H	1852	SQD	O6-C44-C45-O47
20	Z	822	SQD	O47-C45-C46-O48
20	b	822	SQD	O47-C45-C46-O48
20	f	1852	SQD	O6-C44-C45-O47
20	r	822	SQD	O47-C45-C46-O48
20	t	822	SQD	O47-C45-C46-O48
13	2	518	CLA	C13-C15-C16-C17
13	Z	518	CLA	C13-C15-C16-C17
13	f	1219	CLA	C8-C10-C11-C12
13	r	518	CLA	C13-C15-C16-C17
13	A	1103	CLA	C14-C13-C15-C16
13	A	1109	CLA	C14-C13-C15-C16
13	A	1140	CLA	C6-C7-C8-C9
13	B	1012	CLA	C11-C10-C8-C9
13	B	1012	CLA	C14-C13-C15-C16
13	B	1214	CLA	C11-C10-C8-C9
13	B	1221	CLA	C11-C10-C8-C9
13	F	1301	CLA	C6-C7-C8-C9
13	1	510	CLA	C6-C7-C8-C9
13	3	513	CLA	C14-C13-C15-C16
13	5	501	CLA	C6-C7-C8-C9
13	G	1103	CLA	C14-C13-C15-C16
13	G	1109	CLA	C14-C13-C15-C16
13	G	1123	CLA	C11-C10-C8-C9
13	G	1140	CLA	C6-C7-C8-C9
13	H	1012	CLA	C11-C10-C8-C9
13	H	1012	CLA	C14-C13-C15-C16
13	H	1214	CLA	C11-C10-C8-C9
13	H	1221	CLA	C11-C10-C8-C9
13	Y	510	CLA	C6-C7-C8-C9
13	a	513	CLA	C14-C13-C15-C16
13	c	501	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1103	CLA	C14-C13-C15-C16
13	e	1109	CLA	C14-C13-C15-C16
13	e	1140	CLA	C6-C7-C8-C9
13	f	1012	CLA	C11-C10-C8-C9
13	f	1012	CLA	C14-C13-C15-C16
13	f	1214	CLA	C11-C10-C8-C9
13	f	1221	CLA	C11-C10-C8-C9
13	q	510	CLA	C6-C7-C8-C9
13	s	513	CLA	C14-C13-C15-C16
13	u	501	CLA	C6-C7-C8-C9
17	G	5009	LHG	C34-C35-C36-C37
17	G	5003	LHG	C13-C14-C15-C16
17	e	5009	LHG	C34-C35-C36-C37
20	1	822	SQD	C28-C29-C30-C31
20	Y	822	SQD	C28-C29-C30-C31
17	A	5009	LHG	C34-C35-C36-C37
17	f	1842	LHG	C30-C31-C32-C33
20	q	822	SQD	C28-C29-C30-C31
13	B	1236	CLA	O1A-CGA-O2A-C1
13	G	1125	CLA	O1A-CGA-O2A-C1
13	H	1236	CLA	O1A-CGA-O2A-C1
13	b	518	CLA	O1A-CGA-O2A-C1
13	e	1125	CLA	O1A-CGA-O2A-C1
13	f	1236	CLA	O1A-CGA-O2A-C1
13	t	518	CLA	O1A-CGA-O2A-C1
17	B	1842	LHG	C30-C31-C32-C33
17	H	1842	LHG	C30-C31-C32-C33
13	B	1219	CLA	C8-C10-C11-C12
13	G	1130	CLA	C5-C6-C7-C8
13	H	1219	CLA	C8-C10-C11-C12
13	5	518	CLA	O1D-CGD-O2D-CED
13	A	1130	CLA	C5-C6-C7-C8
13	e	1130	CLA	C5-C6-C7-C8
13	A	1125	CLA	O1A-CGA-O2A-C1
13	F	1301	CLA	O1A-CGA-O2A-C1
13	R	1301	CLA	O1A-CGA-O2A-C1
13	j	1301	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	C33-C34-C35-C36
17	G	5002	LHG	C33-C34-C35-C36
17	e	5002	LHG	C33-C34-C35-C36
16	J	4012	BCR	C9-C10-C11-C12
16	T	4012	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	c	518	CLA	O1D-CGD-O2D-CED
13	u	518	CLA	O1D-CGD-O2D-CED
13	A	1125	CLA	CBA-CGA-O2A-C1
13	B	1021	CLA	CBA-CGA-O2A-C1
13	4	509	CLA	CBA-CGA-O2A-C1
13	G	1125	CLA	CBA-CGA-O2A-C1
13	H	1021	CLA	CBA-CGA-O2A-C1
13	b	509	CLA	CBA-CGA-O2A-C1
13	e	1125	CLA	CBA-CGA-O2A-C1
13	f	1021	CLA	CBA-CGA-O2A-C1
17	A	5007	LHG	C34-C35-C36-C37
17	A	5001	LHG	C14-C15-C16-C17
17	e	5007	LHG	C34-C35-C36-C37
17	G	5007	LHG	C34-C35-C36-C37
17	e	5001	LHG	C14-C15-C16-C17
18	r	901	LMU	C5-C6-C7-C8
13	f	1223	CLA	CBD-CGD-O2D-CED
18	2	901	LMU	C5-C6-C7-C8
18	Z	901	LMU	C5-C6-C7-C8
17	G	5001	LHG	C14-C15-C16-C17
13	5	503	CLA	C4-C3-C5-C6
13	c	503	CLA	C4-C3-C5-C6
13	u	503	CLA	C4-C3-C5-C6
13	L	1502	CLA	C3-C5-C6-C7
13	V	1502	CLA	C3-C5-C6-C7
13	n	1502	CLA	C3-C5-C6-C7
13	T	1303	CLA	C2-C3-C5-C6
13	A	1123	CLA	C15-C16-C17-C18
13	e	1123	CLA	C15-C16-C17-C18
13	B	1223	CLA	CBD-CGD-O2D-CED
13	t	509	CLA	CBA-CGA-O2A-C1
13	G	1123	CLA	C15-C16-C17-C18
13	c	501	CLA	C15-C16-C17-C18
13	u	509	CLA	C5-C6-C7-C8
13	4	509	CLA	O1A-CGA-O2A-C1
13	b	509	CLA	O1A-CGA-O2A-C1
13	H	1223	CLA	CBD-CGD-O2D-CED
13	5	501	CLA	C15-C16-C17-C18
13	5	509	CLA	C5-C6-C7-C8
13	c	509	CLA	C5-C6-C7-C8
13	u	501	CLA	C15-C16-C17-C18
17	B	1855	LHG	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	5003	LHG	C23-C24-C25-C26
17	G	5003	LHG	C23-C24-C25-C26
17	e	5003	LHG	C23-C24-C25-C26
17	f	1855	LHG	C18-C19-C20-C21
13	t	509	CLA	O1A-CGA-O2A-C1
17	H	1855	LHG	C18-C19-C20-C21
13	2	508	CLA	O1D-CGD-O2D-CED
13	r	508	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	C16-C17-C18-C19
13	G	1013	CLA	C16-C17-C18-C19
13	e	1013	CLA	C16-C17-C18-C19
13	A	1122	CLA	O1D-CGD-O2D-CED
13	G	1122	CLA	O1D-CGD-O2D-CED
13	Z	508	CLA	O1D-CGD-O2D-CED
13	e	1122	CLA	O1D-CGD-O2D-CED
16	2	523	BCR	C7-C8-C9-C34
16	r	523	BCR	C7-C8-C9-C34
13	A	1110	CLA	C4B-C3B-CAB-CBB
13	A	1129	CLA	C1A-C2A-CAA-CBA
13	A	1022	CLA	C1A-C2A-CAA-CBA
13	B	1205	CLA	C4B-C3B-CAB-CBB
13	B	1236	CLA	C4B-C3B-CAB-CBB
13	1	508	CLA	C1A-C2A-CAA-CBA
13	2	512	CLA	C4B-C3B-CAB-CBB
13	3	501	CLA	C1A-C2A-CAA-CBA
13	3	516	CLA	C1A-C2A-CAA-CBA
13	4	501	CLA	C1A-C2A-CAA-CBA
13	5	503	CLA	C1A-C2A-CAA-CBA
13	6	513	CLA	C4B-C3B-CAB-CBB
13	G	1110	CLA	C4B-C3B-CAB-CBB
13	G	1129	CLA	C1A-C2A-CAA-CBA
13	G	1022	CLA	C1A-C2A-CAA-CBA
13	H	1205	CLA	C4B-C3B-CAB-CBB
13	H	1236	CLA	C4B-C3B-CAB-CBB
13	Y	508	CLA	C1A-C2A-CAA-CBA
13	Z	503	CLA	C1A-C2A-CAA-CBA
13	Z	512	CLA	C4B-C3B-CAB-CBB
13	a	501	CLA	C1A-C2A-CAA-CBA
13	a	516	CLA	C1A-C2A-CAA-CBA
13	b	501	CLA	C1A-C2A-CAA-CBA
13	c	503	CLA	C1A-C2A-CAA-CBA
13	d	513	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1110	CLA	C4B-C3B-CAB-CBB
13	e	1129	CLA	C1A-C2A-CAA-CBA
13	e	1022	CLA	C1A-C2A-CAA-CBA
13	f	1205	CLA	C4B-C3B-CAB-CBB
13	f	1236	CLA	C4B-C3B-CAB-CBB
13	q	508	CLA	C1A-C2A-CAA-CBA
13	r	512	CLA	C4B-C3B-CAB-CBB
13	s	501	CLA	C1A-C2A-CAA-CBA
13	s	516	CLA	C1A-C2A-CAA-CBA
13	t	501	CLA	C1A-C2A-CAA-CBA
13	u	503	CLA	C1A-C2A-CAA-CBA
13	v	513	CLA	C4B-C3B-CAB-CBB
13	L	1501	CLA	CBA-CGA-O2A-C1
13	V	1501	CLA	CBA-CGA-O2A-C1
13	A	1107	CLA	C4-C3-C5-C6
13	B	1202	CLA	C4-C3-C5-C6
13	G	1107	CLA	C4-C3-C5-C6
13	H	1202	CLA	C4-C3-C5-C6
13	f	1202	CLA	C4-C3-C5-C6
13	B	1212	CLA	C5-C6-C7-C8
13	H	1212	CLA	C5-C6-C7-C8
13	H	1223	CLA	C5-C6-C7-C8
13	e	1237	CLA	C5-C6-C7-C8
13	f	1212	CLA	C5-C6-C7-C8
16	3	524	BCR	C21-C22-C23-C24
16	4	521	BCR	C17-C18-C19-C20
16	a	524	BCR	C21-C22-C23-C24
16	b	521	BCR	C17-C18-C19-C20
16	s	524	BCR	C21-C22-C23-C24
16	t	521	BCR	C17-C18-C19-C20
16	l	4012	BCR	C9-C10-C11-C12
13	B	1023	CLA	C4C-C3C-CAC-CBC
13	6	503	CLA	O1A-CGA-O2A-C1
13	d	503	CLA	O1A-CGA-O2A-C1
13	A	1237	CLA	C5-C6-C7-C8
13	B	1223	CLA	C5-C6-C7-C8
13	G	1237	CLA	C5-C6-C7-C8
13	f	1223	CLA	C5-C6-C7-C8
13	f	1023	CLA	C4C-C3C-CAC-CBC
17	B	1855	LHG	O6-C4-C5-C6
17	H	1855	LHG	O6-C4-C5-C6
17	f	1855	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1108	CLA	C6-C7-C8-C9
20	B	1852	SQD	O49-C7-O47-C45
20	H	1852	SQD	O49-C7-O47-C45
20	f	1852	SQD	O49-C7-O47-C45
13	v	503	CLA	O1A-CGA-O2A-C1
13	G	1108	CLA	C6-C7-C8-C9
13	e	1108	CLA	C6-C7-C8-C9
17	A	5005	LHG	C12-C13-C14-C15
17	e	5005	LHG	C12-C13-C14-C15
13	A	1103	CLA	C11-C10-C8-C7
13	B	1208	CLA	C11-C12-C13-C15
13	B	1208	CLA	C12-C13-C15-C16
13	B	1234	CLA	C12-C13-C15-C16
13	J	1303	CLA	C6-C7-C8-C10
13	1	502	CLA	C11-C10-C8-C7
13	2	513	CLA	C11-C10-C8-C7
13	3	505	CLA	C12-C13-C15-C16
13	5	509	CLA	C11-C10-C8-C7
13	6	505	CLA	C11-C12-C13-C15
13	G	1103	CLA	C11-C10-C8-C7
13	H	1208	CLA	C11-C12-C13-C15
13	H	1208	CLA	C12-C13-C15-C16
13	H	1234	CLA	C12-C13-C15-C16
13	T	1303	CLA	C6-C7-C8-C10
13	Y	502	CLA	C11-C10-C8-C7
13	Z	513	CLA	C11-C10-C8-C7
13	a	505	CLA	C12-C13-C15-C16
13	c	509	CLA	C11-C10-C8-C7
13	d	505	CLA	C11-C12-C13-C15
13	e	1103	CLA	C11-C10-C8-C7
13	f	1208	CLA	C11-C12-C13-C15
13	f	1208	CLA	C12-C13-C15-C16
13	f	1234	CLA	C12-C13-C15-C16
13	l	1303	CLA	C6-C7-C8-C10
13	q	502	CLA	C11-C10-C8-C7
13	r	513	CLA	C11-C10-C8-C7
13	s	505	CLA	C12-C13-C15-C16
13	u	509	CLA	C11-C10-C8-C7
13	v	505	CLA	C11-C12-C13-C15
14	B	2002	PQN	C21-C22-C23-C25
14	H	2002	PQN	C21-C22-C23-C25
14	f	2002	PQN	C21-C22-C23-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1023	CLA	C4C-C3C-CAC-CBC
17	G	5005	LHG	C12-C13-C14-C15
13	A	1102	CLA	C16-C17-C18-C19
13	G	1102	CLA	C16-C17-C18-C19
13	e	1013	CLA	C16-C17-C18-C20
13	e	1102	CLA	C16-C17-C18-C19
13	2	505	CLA	O1D-CGD-O2D-CED
13	n	1501	CLA	CBA-CGA-O2A-C1
13	B	1234	CLA	C15-C16-C17-C18
13	H	1234	CLA	C15-C16-C17-C18
13	f	1234	CLA	C15-C16-C17-C18
13	H	1211	CLA	O1A-CGA-O2A-C1
13	r	505	CLA	O1D-CGD-O2D-CED
17	A	5009	LHG	C5-C4-O6-P
17	G	5009	LHG	C5-C4-O6-P
17	e	5009	LHG	C5-C4-O6-P
17	k	5001	LHG	C2-C3-O3-P
13	K	1401	CLA	C3A-C2A-CAA-CBA
13	U	1401	CLA	C3A-C2A-CAA-CBA
13	e	1107	CLA	C4-C3-C5-C6
13	m	1401	CLA	C3A-C2A-CAA-CBA
13	A	1013	CLA	C16-C17-C18-C20
13	G	1013	CLA	C16-C17-C18-C20
13	B	1211	CLA	O1A-CGA-O2A-C1
13	f	1211	CLA	O1A-CGA-O2A-C1
13	B	1213	CLA	CBA-CGA-O2A-C1
17	A	5005	LHG	O6-C4-C5-O7
17	A	5007	LHG	O6-C4-C5-O7
17	G	5005	LHG	O6-C4-C5-O7
17	G	5007	LHG	O6-C4-C5-O7
17	e	5005	LHG	O6-C4-C5-O7
17	e	5007	LHG	O6-C4-C5-O7
13	Z	505	CLA	O1D-CGD-O2D-CED
13	B	1213	CLA	C2A-CAA-CBA-CGA
13	2	517	CLA	C2A-CAA-CBA-CGA
13	H	1213	CLA	C2A-CAA-CBA-CGA
13	Y	513	CLA	C2A-CAA-CBA-CGA
13	Z	517	CLA	C2A-CAA-CBA-CGA
13	f	1213	CLA	C2A-CAA-CBA-CGA
13	r	517	CLA	C2A-CAA-CBA-CGA
13	A	1123	CLA	C11-C10-C8-C9
13	B	1203	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1203	CLA	C11-C12-C13-C14
13	B	1206	CLA	C11-C10-C8-C9
13	B	1208	CLA	C6-C7-C8-C9
13	B	1210	CLA	C6-C7-C8-C9
13	B	1217	CLA	C11-C10-C8-C9
13	B	1226	CLA	C11-C12-C13-C14
13	B	1240	CLA	C11-C12-C13-C14
13	2	507	CLA	C11-C10-C8-C9
13	4	501	CLA	C6-C7-C8-C9
13	H	1203	CLA	C6-C7-C8-C9
13	H	1203	CLA	C11-C12-C13-C14
13	H	1206	CLA	C11-C10-C8-C9
13	H	1208	CLA	C6-C7-C8-C9
13	H	1210	CLA	C6-C7-C8-C9
13	H	1226	CLA	C11-C12-C13-C14
13	H	1240	CLA	C11-C12-C13-C14
13	Z	507	CLA	C11-C10-C8-C9
13	b	501	CLA	C6-C7-C8-C9
13	d	501	CLA	C11-C10-C8-C9
13	e	1123	CLA	C11-C10-C8-C9
13	f	1203	CLA	C6-C7-C8-C9
13	f	1203	CLA	C11-C12-C13-C14
13	f	1206	CLA	C11-C10-C8-C9
13	f	1208	CLA	C6-C7-C8-C9
13	f	1210	CLA	C6-C7-C8-C9
13	f	1217	CLA	C11-C10-C8-C9
13	f	1226	CLA	C11-C12-C13-C14
13	f	1240	CLA	C11-C12-C13-C14
13	r	507	CLA	C11-C10-C8-C9
13	t	501	CLA	C6-C7-C8-C9
13	2	508	CLA	C5-C6-C7-C8
13	Z	508	CLA	C5-C6-C7-C8
13	a	501	CLA	C15-C16-C17-C18
13	r	508	CLA	C5-C6-C7-C8
13	3	510	CLA	C16-C17-C18-C19
13	a	510	CLA	C16-C17-C18-C19
13	s	510	CLA	C16-C17-C18-C19
13	B	1223	CLA	O1D-CGD-O2D-CED
13	f	1223	CLA	O1D-CGD-O2D-CED
13	f	1213	CLA	CBA-CGA-O2A-C1
13	A	1128	CLA	C10-C11-C12-C13
13	3	501	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1128	CLA	C10-C11-C12-C13
13	e	1128	CLA	C10-C11-C12-C13
13	s	501	CLA	C15-C16-C17-C18
13	H	1223	CLA	O1D-CGD-O2D-CED
17	A	5002	LHG	O7-C5-C6-O8
17	A	5004	LHG	O7-C5-C6-O8
17	A	5005	LHG	O7-C5-C6-O8
17	L	5221	LHG	O7-C5-C6-O8
17	G	5002	LHG	O7-C5-C6-O8
17	G	5004	LHG	O7-C5-C6-O8
17	G	5005	LHG	O7-C5-C6-O8
17	V	5221	LHG	O7-C5-C6-O8
17	e	5002	LHG	O7-C5-C6-O8
17	e	5004	LHG	O7-C5-C6-O8
17	e	5005	LHG	O7-C5-C6-O8
17	n	5221	LHG	O7-C5-C6-O8
20	3	822	SQD	O6-C44-C45-O47
20	6	822	SQD	O47-C45-C46-O48
20	a	822	SQD	O6-C44-C45-O47
20	d	822	SQD	O47-C45-C46-O48
20	s	822	SQD	O6-C44-C45-O47
20	v	822	SQD	O47-C45-C46-O48
13	H	1213	CLA	CBA-CGA-O2A-C1
17	A	5006	LHG	C4-C5-C6-O8
17	L	5221	LHG	C4-C5-C6-O8
17	G	5006	LHG	C4-C5-C6-O8
17	V	5221	LHG	C4-C5-C6-O8
17	e	5006	LHG	C4-C5-C6-O8
17	n	5221	LHG	C4-C5-C6-O8
20	L	5216	SQD	O6-C44-C45-C46
20	2	822	SQD	C44-C45-C46-O48
20	3	822	SQD	O6-C44-C45-C46
20	3	822	SQD	C44-C45-C46-O48
20	V	5216	SQD	O6-C44-C45-C46
20	Z	822	SQD	C44-C45-C46-O48
20	a	822	SQD	O6-C44-C45-C46
20	a	822	SQD	C44-C45-C46-O48
20	n	5216	SQD	O6-C44-C45-C46
20	r	822	SQD	C44-C45-C46-O48
20	s	822	SQD	O6-C44-C45-C46
20	s	822	SQD	C44-C45-C46-O48
17	n	5218	LHG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	5	505	CLA	C5-C6-C7-C8
13	c	505	CLA	C5-C6-C7-C8
13	u	505	CLA	C5-C6-C7-C8
13	A	1121	CLA	CAA-CBA-CGA-O2A
13	G	1121	CLA	CAA-CBA-CGA-O2A
13	e	1121	CLA	CAA-CBA-CGA-O2A
13	B	1204	CLA	C2-C3-C5-C6
13	H	1204	CLA	C2-C3-C5-C6
13	f	1204	CLA	C2-C3-C5-C6
17	L	5218	LHG	C30-C31-C32-C33
17	V	5218	LHG	C30-C31-C32-C33
13	A	1011	CLA	CAD-CBD-CGD-O2D
13	B	1207	CLA	CAD-CBD-CGD-O2D
13	K	1103	CLA	CAD-CBD-CGD-O2D
13	1	502	CLA	CAD-CBD-CGD-O2D
13	1	503	CLA	CAD-CBD-CGD-O2D
13	1	504	CLA	CAD-CBD-CGD-O2D
13	2	502	CLA	CAD-CBD-CGD-O2D
13	2	503	CLA	CAD-CBD-CGD-O2D
13	2	506	CLA	CAD-CBD-CGD-O2D
13	3	503	CLA	CAD-CBD-CGD-O2D
13	3	504	CLA	CAD-CBD-CGD-O2D
13	3	506	CLA	CAD-CBD-CGD-O2D
13	3	507	CLA	CAD-CBD-CGD-O2D
13	3	517	CLA	CAD-CBD-CGD-O2D
13	4	504	CLA	CAD-CBD-CGD-O2D
13	5	503	CLA	CAD-CBD-CGD-O2D
13	5	510	CLA	CAD-CBD-CGD-O2D
13	6	506	CLA	CAD-CBD-CGD-O2D
13	6	510	CLA	CAD-CBD-CGD-O2D
13	G	1011	CLA	CAD-CBD-CGD-O2D
13	H	1207	CLA	CAD-CBD-CGD-O2D
13	U	1103	CLA	CAD-CBD-CGD-O2D
13	Y	502	CLA	CAD-CBD-CGD-O2D
13	Y	503	CLA	CAD-CBD-CGD-O2D
13	Y	504	CLA	CAD-CBD-CGD-O2D
13	Z	502	CLA	CAD-CBD-CGD-O2D
13	Z	503	CLA	CAD-CBD-CGD-O2D
13	Z	506	CLA	CAD-CBD-CGD-O2D
13	a	503	CLA	CAD-CBD-CGD-O2D
13	a	504	CLA	CAD-CBD-CGD-O2D
13	a	506	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	507	CLA	CAD-CBD-CGD-O2D
13	a	517	CLA	CAD-CBD-CGD-O2D
13	b	504	CLA	CAD-CBD-CGD-O2D
13	c	503	CLA	CAD-CBD-CGD-O2D
13	c	510	CLA	CAD-CBD-CGD-O2D
13	d	506	CLA	CAD-CBD-CGD-O2D
13	d	510	CLA	CAD-CBD-CGD-O2D
13	e	1011	CLA	CAD-CBD-CGD-O2D
13	f	1207	CLA	CAD-CBD-CGD-O2D
13	m	1103	CLA	CAD-CBD-CGD-O2D
13	q	502	CLA	CAD-CBD-CGD-O2D
13	q	503	CLA	CAD-CBD-CGD-O2D
13	q	504	CLA	CAD-CBD-CGD-O2D
13	r	502	CLA	CAD-CBD-CGD-O2D
13	r	503	CLA	CAD-CBD-CGD-O2D
13	r	506	CLA	CAD-CBD-CGD-O2D
13	s	503	CLA	CAD-CBD-CGD-O2D
13	s	504	CLA	CAD-CBD-CGD-O2D
13	s	506	CLA	CAD-CBD-CGD-O2D
13	s	507	CLA	CAD-CBD-CGD-O2D
13	s	517	CLA	CAD-CBD-CGD-O2D
13	t	504	CLA	CAD-CBD-CGD-O2D
13	u	503	CLA	CAD-CBD-CGD-O2D
13	u	510	CLA	CAD-CBD-CGD-O2D
13	v	506	CLA	CAD-CBD-CGD-O2D
13	v	510	CLA	CAD-CBD-CGD-O2D
13	B	1211	CLA	CBA-CGA-O2A-C1
13	2	509	CLA	CBA-CGA-O2A-C1
13	H	1211	CLA	CBA-CGA-O2A-C1
13	Z	509	CLA	CBA-CGA-O2A-C1
13	f	1211	CLA	CBA-CGA-O2A-C1
13	r	509	CLA	CBA-CGA-O2A-C1
13	A	1102	CLA	C16-C17-C18-C20
13	G	1102	CLA	C16-C17-C18-C20
13	e	1102	CLA	C16-C17-C18-C20
13	e	1117	CLA	C16-C17-C18-C20
18	1	902	LMU	C3-C4-C5-C6
18	Y	902	LMU	C3-C4-C5-C6
18	q	902	LMU	C3-C4-C5-C6
13	1	513	CLA	C2A-CAA-CBA-CGA
13	q	513	CLA	C2A-CAA-CBA-CGA
13	B	1021	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	1501	CLA	O1A-CGA-O2A-C1
13	V	1501	CLA	O1A-CGA-O2A-C1
13	n	1501	CLA	O1A-CGA-O2A-C1
13	A	1011	CLA	CAD-CBD-CGD-O1D
13	A	1131	CLA	CHA-CBD-CGD-O1D
13	A	1801	CLA	CAD-CBD-CGD-O1D
13	B	1202	CLA	CAD-CBD-CGD-O1D
13	B	1211	CLA	CHA-CBD-CGD-O1D
13	B	1207	CLA	CAD-CBD-CGD-O1D
13	K	1103	CLA	CAD-CBD-CGD-O1D
13	1	502	CLA	CAD-CBD-CGD-O1D
13	1	503	CLA	CAD-CBD-CGD-O1D
13	1	504	CLA	CAD-CBD-CGD-O1D
13	1	506	CLA	CAD-CBD-CGD-O1D
13	2	502	CLA	CAD-CBD-CGD-O1D
13	2	503	CLA	CAD-CBD-CGD-O1D
13	2	506	CLA	CAD-CBD-CGD-O1D
13	2	518	CLA	CAD-CBD-CGD-O1D
13	3	503	CLA	CAD-CBD-CGD-O1D
13	3	504	CLA	CAD-CBD-CGD-O1D
13	3	506	CLA	CAD-CBD-CGD-O1D
13	3	507	CLA	CAD-CBD-CGD-O1D
13	3	512	CLA	CHA-CBD-CGD-O1D
13	3	517	CLA	CAD-CBD-CGD-O1D
13	3	518	CLA	CAD-CBD-CGD-O1D
13	3	519	CLA	CHA-CBD-CGD-O1D
13	3	519	CLA	CHA-CBD-CGD-O2D
13	4	503	CLA	CHA-CBD-CGD-O1D
13	4	504	CLA	CAD-CBD-CGD-O1D
13	4	506	CLA	CHA-CBD-CGD-O1D
13	4	510	CLA	CHA-CBD-CGD-O1D
13	4	510	CLA	CHA-CBD-CGD-O2D
13	4	512	CLA	CHA-CBD-CGD-O1D
13	4	512	CLA	CHA-CBD-CGD-O2D
13	4	517	CLA	CHA-CBD-CGD-O1D
13	4	517	CLA	CHA-CBD-CGD-O2D
13	4	518	CLA	CHA-CBD-CGD-O1D
13	4	518	CLA	CHA-CBD-CGD-O2D
13	5	503	CLA	CAD-CBD-CGD-O1D
13	5	505	CLA	CHA-CBD-CGD-O1D
13	5	506	CLA	CAD-CBD-CGD-O1D
13	5	507	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	5	507	CLA	CHA-CBD-CGD-O2D
13	5	510	CLA	CAD-CBD-CGD-O1D
13	5	512	CLA	CHA-CBD-CGD-O1D
13	5	512	CLA	CHA-CBD-CGD-O2D
13	5	517	CLA	CAD-CBD-CGD-O1D
13	5	518	CLA	CHA-CBD-CGD-O1D
13	5	518	CLA	CHA-CBD-CGD-O2D
13	6	503	CLA	CAD-CBD-CGD-O1D
13	6	504	CLA	CAD-CBD-CGD-O1D
13	6	506	CLA	CAD-CBD-CGD-O1D
13	6	510	CLA	CAD-CBD-CGD-O1D
13	6	512	CLA	CHA-CBD-CGD-O1D
13	6	512	CLA	CHA-CBD-CGD-O2D
13	6	518	CLA	CAD-CBD-CGD-O1D
13	6	519	CLA	CHA-CBD-CGD-O1D
13	G	1011	CLA	CAD-CBD-CGD-O1D
13	G	1131	CLA	CHA-CBD-CGD-O1D
13	G	1801	CLA	CAD-CBD-CGD-O1D
13	H	1202	CLA	CAD-CBD-CGD-O1D
13	H	1211	CLA	CHA-CBD-CGD-O1D
13	H	1207	CLA	CAD-CBD-CGD-O1D
13	U	1103	CLA	CAD-CBD-CGD-O1D
13	Y	502	CLA	CAD-CBD-CGD-O1D
13	Y	503	CLA	CAD-CBD-CGD-O1D
13	Y	504	CLA	CAD-CBD-CGD-O1D
13	Y	506	CLA	CAD-CBD-CGD-O1D
13	Z	502	CLA	CAD-CBD-CGD-O1D
13	Z	503	CLA	CAD-CBD-CGD-O1D
13	Z	506	CLA	CAD-CBD-CGD-O1D
13	Z	518	CLA	CAD-CBD-CGD-O1D
13	a	503	CLA	CAD-CBD-CGD-O1D
13	a	504	CLA	CAD-CBD-CGD-O1D
13	a	506	CLA	CAD-CBD-CGD-O1D
13	a	507	CLA	CAD-CBD-CGD-O1D
13	a	512	CLA	CHA-CBD-CGD-O1D
13	a	516	CLA	CAD-CBD-CGD-O1D
13	a	517	CLA	CAD-CBD-CGD-O1D
13	a	518	CLA	CAD-CBD-CGD-O1D
13	a	519	CLA	CHA-CBD-CGD-O1D
13	a	519	CLA	CHA-CBD-CGD-O2D
13	b	503	CLA	CHA-CBD-CGD-O1D
13	b	504	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	b	506	CLA	CHA-CBD-CGD-O1D
13	b	510	CLA	CHA-CBD-CGD-O1D
13	b	510	CLA	CHA-CBD-CGD-O2D
13	b	512	CLA	CHA-CBD-CGD-O1D
13	b	512	CLA	CHA-CBD-CGD-O2D
13	b	517	CLA	CHA-CBD-CGD-O1D
13	b	517	CLA	CHA-CBD-CGD-O2D
13	b	518	CLA	CHA-CBD-CGD-O1D
13	b	518	CLA	CHA-CBD-CGD-O2D
13	c	503	CLA	CAD-CBD-CGD-O1D
13	c	505	CLA	CHA-CBD-CGD-O1D
13	c	506	CLA	CAD-CBD-CGD-O1D
13	c	507	CLA	CHA-CBD-CGD-O1D
13	c	507	CLA	CHA-CBD-CGD-O2D
13	c	510	CLA	CAD-CBD-CGD-O1D
13	c	512	CLA	CHA-CBD-CGD-O1D
13	c	512	CLA	CHA-CBD-CGD-O2D
13	c	517	CLA	CAD-CBD-CGD-O1D
13	c	518	CLA	CHA-CBD-CGD-O1D
13	c	518	CLA	CHA-CBD-CGD-O2D
13	d	503	CLA	CAD-CBD-CGD-O1D
13	d	504	CLA	CAD-CBD-CGD-O1D
13	d	506	CLA	CAD-CBD-CGD-O1D
13	d	510	CLA	CAD-CBD-CGD-O1D
13	d	512	CLA	CHA-CBD-CGD-O1D
13	d	512	CLA	CHA-CBD-CGD-O2D
13	d	518	CLA	CAD-CBD-CGD-O1D
13	d	519	CLA	CHA-CBD-CGD-O1D
13	e	1011	CLA	CAD-CBD-CGD-O1D
13	e	1131	CLA	CHA-CBD-CGD-O1D
13	e	1801	CLA	CAD-CBD-CGD-O1D
13	f	1202	CLA	CAD-CBD-CGD-O1D
13	f	1211	CLA	CHA-CBD-CGD-O1D
13	f	1207	CLA	CAD-CBD-CGD-O1D
13	m	1103	CLA	CAD-CBD-CGD-O1D
13	q	502	CLA	CAD-CBD-CGD-O1D
13	q	503	CLA	CAD-CBD-CGD-O1D
13	q	504	CLA	CAD-CBD-CGD-O1D
13	q	506	CLA	CAD-CBD-CGD-O1D
13	r	502	CLA	CAD-CBD-CGD-O1D
13	r	503	CLA	CAD-CBD-CGD-O1D
13	r	506	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	r	518	CLA	CAD-CBD-CGD-O1D
13	s	503	CLA	CAD-CBD-CGD-O1D
13	s	504	CLA	CAD-CBD-CGD-O1D
13	s	506	CLA	CAD-CBD-CGD-O1D
13	s	507	CLA	CAD-CBD-CGD-O1D
13	s	512	CLA	CHA-CBD-CGD-O1D
13	s	517	CLA	CAD-CBD-CGD-O1D
13	s	518	CLA	CAD-CBD-CGD-O1D
13	s	519	CLA	CHA-CBD-CGD-O1D
13	s	519	CLA	CHA-CBD-CGD-O2D
13	t	503	CLA	CHA-CBD-CGD-O1D
13	t	504	CLA	CAD-CBD-CGD-O1D
13	t	506	CLA	CHA-CBD-CGD-O1D
13	t	510	CLA	CHA-CBD-CGD-O1D
13	t	510	CLA	CHA-CBD-CGD-O2D
13	t	512	CLA	CHA-CBD-CGD-O1D
13	t	512	CLA	CHA-CBD-CGD-O2D
13	t	517	CLA	CHA-CBD-CGD-O1D
13	t	517	CLA	CHA-CBD-CGD-O2D
13	t	518	CLA	CHA-CBD-CGD-O1D
13	t	518	CLA	CHA-CBD-CGD-O2D
13	u	503	CLA	CAD-CBD-CGD-O1D
13	u	505	CLA	CHA-CBD-CGD-O1D
13	u	506	CLA	CAD-CBD-CGD-O1D
13	u	507	CLA	CHA-CBD-CGD-O1D
13	u	507	CLA	CHA-CBD-CGD-O2D
13	u	510	CLA	CAD-CBD-CGD-O1D
13	u	512	CLA	CHA-CBD-CGD-O1D
13	u	512	CLA	CHA-CBD-CGD-O2D
13	u	517	CLA	CAD-CBD-CGD-O1D
13	u	518	CLA	CHA-CBD-CGD-O1D
13	u	518	CLA	CHA-CBD-CGD-O2D
13	v	503	CLA	CAD-CBD-CGD-O1D
13	v	504	CLA	CAD-CBD-CGD-O1D
13	v	506	CLA	CAD-CBD-CGD-O1D
13	v	510	CLA	CAD-CBD-CGD-O1D
13	v	512	CLA	CHA-CBD-CGD-O1D
13	v	512	CLA	CHA-CBD-CGD-O2D
13	v	518	CLA	CAD-CBD-CGD-O1D
13	v	519	CLA	CHA-CBD-CGD-O1D
16	A	4001	BCR	C13-C14-C15-C16
16	3	521	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	3	524	BCR	C9-C10-C11-C12
16	4	521	BCR	C13-C14-C15-C16
16	G	4001	BCR	C13-C14-C15-C16
16	a	521	BCR	C9-C10-C11-C12
16	a	524	BCR	C9-C10-C11-C12
16	b	521	BCR	C13-C14-C15-C16
16	e	4001	BCR	C13-C14-C15-C16
16	s	521	BCR	C9-C10-C11-C12
16	s	524	BCR	C9-C10-C11-C12
16	t	521	BCR	C13-C14-C15-C16
17	A	5002	LHG	C3-O3-P-O5
17	A	5002	LHG	C4-O6-P-O3
17	A	5002	LHG	C4-O6-P-O4
17	A	5001	LHG	C3-O3-P-O5
17	B	1855	LHG	C3-O3-P-O5
17	B	1855	LHG	C4-O6-P-O3
17	B	1855	LHG	C4-O6-P-O4
17	I	5001	LHG	C4-O6-P-O4
17	L	5221	LHG	C3-O3-P-O6
17	G	5002	LHG	C3-O3-P-O5
17	G	5002	LHG	C4-O6-P-O3
17	G	5002	LHG	C4-O6-P-O4
17	G	5005	LHG	C3-O3-P-O5
17	G	5001	LHG	C3-O3-P-O5
17	H	1855	LHG	C3-O3-P-O5
17	H	1855	LHG	C4-O6-P-O3
17	H	1855	LHG	C4-O6-P-O4
17	S	5001	LHG	C4-O6-P-O4
17	V	5221	LHG	C3-O3-P-O6
17	e	5002	LHG	C3-O3-P-O5
17	e	5002	LHG	C4-O6-P-O3
17	e	5002	LHG	C4-O6-P-O4
17	e	5001	LHG	C3-O3-P-O5
17	f	1855	LHG	C3-O3-P-O5
17	f	1855	LHG	C4-O6-P-O3
17	f	1855	LHG	C4-O6-P-O4
17	k	5001	LHG	C4-O6-P-O4
17	n	5221	LHG	C3-O3-P-O6
13	L	1501	CLA	C3-C5-C6-C7
13	V	1501	CLA	C3-C5-C6-C7
13	n	1501	CLA	C3-C5-C6-C7
13	A	1117	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1117	CLA	C16-C17-C18-C20
13	H	1021	CLA	O1A-CGA-O2A-C1
13	f	1021	CLA	O1A-CGA-O2A-C1
13	B	1224	CLA	C4-C3-C5-C6
13	H	1224	CLA	C4-C3-C5-C6
13	e	1022	CLA	C4-C3-C5-C6
13	f	1224	CLA	C4-C3-C5-C6
13	A	1118	CLA	C2B-C3B-CAB-CBB
13	A	1132	CLA	C2B-C3B-CAB-CBB
13	A	1138	CLA	C2B-C3B-CAB-CBB
13	A	1140	CLA	C2B-C3B-CAB-CBB
13	B	1205	CLA	C2B-C3B-CAB-CBB
13	B	1227	CLA	C2B-C3B-CAB-CBB
13	B	1235	CLA	C2B-C3B-CAB-CBB
13	3	502	CLA	C2B-C3B-CAB-CBB
13	3	519	CLA	C2B-C3B-CAB-CBB
13	4	502	CLA	C2B-C3B-CAB-CBB
13	4	505	CLA	C2B-C3B-CAB-CBB
13	4	508	CLA	C2B-C3B-CAB-CBB
13	4	512	CLA	C2B-C3B-CAB-CBB
13	5	519	CLA	C2B-C3B-CAB-CBB
13	6	501	CLA	C2B-C3B-CAB-CBB
13	6	503	CLA	C2B-C3B-CAB-CBB
13	6	513	CLA	C2B-C3B-CAB-CBB
13	6	518	CLA	C2B-C3B-CAB-CBB
13	6	519	CLA	C2B-C3B-CAB-CBB
13	G	1118	CLA	C2B-C3B-CAB-CBB
13	G	1132	CLA	C2B-C3B-CAB-CBB
13	G	1138	CLA	C2B-C3B-CAB-CBB
13	G	1140	CLA	C2B-C3B-CAB-CBB
13	H	1205	CLA	C2B-C3B-CAB-CBB
13	H	1227	CLA	C2B-C3B-CAB-CBB
13	H	1235	CLA	C2B-C3B-CAB-CBB
13	Z	512	CLA	C2B-C3B-CAB-CBB
13	a	502	CLA	C2B-C3B-CAB-CBB
13	a	519	CLA	C2B-C3B-CAB-CBB
13	b	502	CLA	C2B-C3B-CAB-CBB
13	b	505	CLA	C2B-C3B-CAB-CBB
13	b	508	CLA	C2B-C3B-CAB-CBB
13	b	512	CLA	C2B-C3B-CAB-CBB
13	c	519	CLA	C2B-C3B-CAB-CBB
13	d	501	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	d	513	CLA	C2B-C3B-CAB-CBB
13	d	518	CLA	C2B-C3B-CAB-CBB
13	d	519	CLA	C2B-C3B-CAB-CBB
13	e	1118	CLA	C2B-C3B-CAB-CBB
13	e	1132	CLA	C2B-C3B-CAB-CBB
13	e	1138	CLA	C2B-C3B-CAB-CBB
13	e	1140	CLA	C2B-C3B-CAB-CBB
13	f	1205	CLA	C2B-C3B-CAB-CBB
13	f	1227	CLA	C2B-C3B-CAB-CBB
13	f	1235	CLA	C2B-C3B-CAB-CBB
13	s	502	CLA	C2B-C3B-CAB-CBB
13	s	519	CLA	C2B-C3B-CAB-CBB
13	t	502	CLA	C2B-C3B-CAB-CBB
13	t	505	CLA	C2B-C3B-CAB-CBB
13	t	508	CLA	C2B-C3B-CAB-CBB
13	t	512	CLA	C2B-C3B-CAB-CBB
13	u	519	CLA	C2B-C3B-CAB-CBB
13	v	501	CLA	C2B-C3B-CAB-CBB
13	v	503	CLA	C2B-C3B-CAB-CBB
13	v	513	CLA	C2B-C3B-CAB-CBB
13	v	518	CLA	C2B-C3B-CAB-CBB
13	v	519	CLA	C2B-C3B-CAB-CBB
13	5	505	CLA	C2-C3-C5-C6
13	u	505	CLA	C2-C3-C5-C6
16	6	521	BCR	C7-C8-C9-C34
16	d	521	BCR	C7-C8-C9-C34
16	v	521	BCR	C7-C8-C9-C34
17	A	5005	LHG	C2-C3-O3-P
17	I	5001	LHG	C2-C3-O3-P
17	G	5005	LHG	C2-C3-O3-P
17	S	5001	LHG	C2-C3-O3-P
17	e	5005	LHG	C2-C3-O3-P
13	f	1234	CLA	C2C-C3C-CAC-CBC
13	B	1234	CLA	C5-C6-C7-C8
13	2	519	CLA	C5-C6-C7-C8
13	H	1234	CLA	C5-C6-C7-C8
13	Z	519	CLA	C5-C6-C7-C8
13	f	1234	CLA	C5-C6-C7-C8
13	r	505	CLA	C5-C6-C7-C8
13	r	519	CLA	C5-C6-C7-C8
13	H	1234	CLA	C2C-C3C-CAC-CBC
19	H	5002	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	f	5002	LMG	C39-C40-C41-C42
13	B	1234	CLA	C2C-C3C-CAC-CBC
19	B	5002	LMG	C39-C40-C41-C42
13	A	1116	CLA	C8-C10-C11-C12
13	B	1213	CLA	O1A-CGA-O2A-C1
13	f	1213	CLA	O1A-CGA-O2A-C1
13	2	505	CLA	C5-C6-C7-C8
13	G	1116	CLA	C8-C10-C11-C12
13	Z	505	CLA	C5-C6-C7-C8
13	e	1116	CLA	C8-C10-C11-C12
13	H	1213	CLA	O1A-CGA-O2A-C1
13	A	1022	CLA	C4-C3-C5-C6
13	G	1022	CLA	C4-C3-C5-C6
13	B	1228	CLA	CAA-CBA-CGA-O2A
13	H	1228	CLA	CAA-CBA-CGA-O2A
13	f	1228	CLA	CAA-CBA-CGA-O2A
13	c	505	CLA	C2-C3-C5-C6
17	A	5006	LHG	C32-C33-C34-C35
17	e	5006	LHG	C32-C33-C34-C35
17	L	5221	LHG	C13-C14-C15-C16
17	G	5006	LHG	C32-C33-C34-C35
17	n	5221	LHG	C13-C14-C15-C16
17	V	5221	LHG	C13-C14-C15-C16
17	V	5221	LHG	C15-C16-C17-C18
13	A	1103	CLA	C11-C10-C8-C9
13	A	1131	CLA	C14-C13-C15-C16
13	A	1138	CLA	C11-C10-C8-C9
13	A	1237	CLA	C6-C7-C8-C9
13	A	1101	CLA	C11-C12-C13-C14
13	B	1208	CLA	C11-C12-C13-C14
13	B	1223	CLA	C11-C12-C13-C14
13	B	1234	CLA	C11-C12-C13-C14
13	B	1230	CLA	C6-C7-C8-C9
13	5	501	CLA	C11-C12-C13-C14
13	5	505	CLA	C6-C7-C8-C9
13	6	501	CLA	C11-C10-C8-C9
13	G	1103	CLA	C11-C10-C8-C9
13	G	1131	CLA	C14-C13-C15-C16
13	G	1138	CLA	C11-C10-C8-C9
13	G	1237	CLA	C6-C7-C8-C9
13	G	1101	CLA	C11-C12-C13-C14
13	H	1208	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1217	CLA	C11-C10-C8-C9
13	H	1223	CLA	C11-C12-C13-C14
13	H	1234	CLA	C11-C12-C13-C14
13	H	1230	CLA	C6-C7-C8-C9
13	c	501	CLA	C11-C12-C13-C14
13	c	505	CLA	C6-C7-C8-C9
13	e	1103	CLA	C11-C10-C8-C9
13	e	1131	CLA	C14-C13-C15-C16
13	e	1138	CLA	C11-C10-C8-C9
13	e	1237	CLA	C6-C7-C8-C9
13	e	1101	CLA	C11-C12-C13-C14
13	f	1208	CLA	C11-C12-C13-C14
13	f	1223	CLA	C11-C12-C13-C14
13	f	1234	CLA	C11-C12-C13-C14
13	f	1230	CLA	C6-C7-C8-C9
13	u	501	CLA	C11-C12-C13-C14
13	u	505	CLA	C6-C7-C8-C9
13	v	501	CLA	C11-C10-C8-C9
14	A	2001	PQN	C24-C23-C25-C26
14	B	2002	PQN	C21-C22-C23-C24
14	G	2001	PQN	C24-C23-C25-C26
14	H	2002	PQN	C21-C22-C23-C24
14	e	2001	PQN	C24-C23-C25-C26
14	f	2002	PQN	C21-C22-C23-C24
17	L	5221	LHG	C15-C16-C17-C18
13	A	1138	CLA	C11-C10-C8-C7
13	B	1215	CLA	C11-C12-C13-C15
13	B	1239	CLA	C6-C7-C8-C10
13	5	501	CLA	C11-C12-C13-C15
13	G	1138	CLA	C11-C10-C8-C7
13	H	1215	CLA	C11-C12-C13-C15
13	H	1239	CLA	C6-C7-C8-C10
13	c	501	CLA	C11-C12-C13-C15
13	e	1138	CLA	C11-C10-C8-C7
13	f	1215	CLA	C11-C12-C13-C15
13	f	1239	CLA	C6-C7-C8-C10
13	u	501	CLA	C11-C12-C13-C15
17	n	5221	LHG	C15-C16-C17-C18
17	L	5218	LHG	C27-C28-C29-C30
17	V	5218	LHG	C27-C28-C29-C30
17	n	5218	LHG	C27-C28-C29-C30
20	5	822	SQD	O5-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	c	822	SQD	O5-C1-O6-C44
20	u	822	SQD	O5-C1-O6-C44
13	B	1021	CLA	C16-C17-C18-C20
13	H	1021	CLA	C16-C17-C18-C20
13	f	1021	CLA	C16-C17-C18-C20
13	B	1207	CLA	C15-C16-C17-C18
13	B	1229	CLA	CAA-CBA-CGA-O2A
13	H	1229	CLA	CAA-CBA-CGA-O2A
13	f	1229	CLA	CAA-CBA-CGA-O2A
13	2	509	CLA	O1A-CGA-O2A-C1
13	Z	509	CLA	O1A-CGA-O2A-C1
13	r	509	CLA	O1A-CGA-O2A-C1
13	H	1207	CLA	C15-C16-C17-C18
17	G	5002	LHG	C31-C32-C33-C34
13	f	1207	CLA	C15-C16-C17-C18
13	B	1210	CLA	C4-C3-C5-C6
13	H	1210	CLA	C4-C3-C5-C6
13	f	1210	CLA	C4-C3-C5-C6
17	A	5002	LHG	C31-C32-C33-C34
20	2	822	SQD	C14-C15-C16-C17
17	e	5002	LHG	C31-C32-C33-C34
20	Z	822	SQD	C14-C15-C16-C17
20	r	822	SQD	C14-C15-C16-C17
13	B	1205	CLA	CBA-CGA-O2A-C1
13	H	1205	CLA	CBA-CGA-O2A-C1
13	f	1205	CLA	CBA-CGA-O2A-C1
13	3	510	CLA	C16-C17-C18-C20
13	a	510	CLA	C16-C17-C18-C20
13	s	510	CLA	C16-C17-C18-C20
13	6	518	CLA	CAA-CBA-CGA-O2A
13	a	518	CLA	CAA-CBA-CGA-O2A
13	d	518	CLA	CAA-CBA-CGA-O2A
13	v	518	CLA	CAA-CBA-CGA-O2A
13	3	508	CLA	CBD-CGD-O2D-CED
13	a	508	CLA	CBD-CGD-O2D-CED
13	s	508	CLA	CBD-CGD-O2D-CED
13	B	1021	CLA	C16-C17-C18-C19
13	H	1021	CLA	C16-C17-C18-C19
13	f	1021	CLA	C16-C17-C18-C19
13	3	518	CLA	CAA-CBA-CGA-O2A
13	4	518	CLA	CAA-CBA-CGA-O2A
13	b	518	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	s	518	CLA	CAA-CBA-CGA-O2A
13	t	518	CLA	CAA-CBA-CGA-O2A
13	A	1132	CLA	C8-C10-C11-C12
19	B	5002	LMG	C7-C8-C9-O8
19	J	5104	LMG	O1-C7-C8-C9
19	H	5002	LMG	C7-C8-C9-O8
19	T	5104	LMG	O1-C7-C8-C9
19	f	5002	LMG	C7-C8-C9-O8
19	l	5104	LMG	O1-C7-C8-C9
13	G	1133	CLA	O1D-CGD-O2D-CED
13	G	1132	CLA	C8-C10-C11-C12
13	e	1132	CLA	C8-C10-C11-C12
13	G	1126	CLA	CAA-CBA-CGA-O2A
13	e	1126	CLA	CAA-CBA-CGA-O2A
13	A	1133	CLA	O1D-CGD-O2D-CED
16	f	4010	BCR	C11-C12-C13-C14
13	A	1126	CLA	CAA-CBA-CGA-O2A
19	J	5104	LMG	C8-C7-O1-C1
19	T	5104	LMG	C8-C7-O1-C1
19	l	5104	LMG	C8-C7-O1-C1
13	A	1128	CLA	O1A-CGA-O2A-C1
13	G	1128	CLA	O1A-CGA-O2A-C1
13	B	1212	CLA	C2A-CAA-CBA-CGA
13	H	1212	CLA	C2A-CAA-CBA-CGA
13	f	1212	CLA	C2A-CAA-CBA-CGA
13	H	1212	CLA	O1D-CGD-O2D-CED
13	e	1133	CLA	O1D-CGD-O2D-CED
16	A	4008	BCR	C19-C20-C21-C22
16	G	4008	BCR	C19-C20-C21-C22
16	e	4008	BCR	C19-C20-C21-C22
13	2	507	CLA	C16-C17-C18-C19
13	Z	507	CLA	C16-C17-C18-C19
13	r	507	CLA	C16-C17-C18-C19
18	A	1848	LMU	O5'-C1'-O1'-C1
18	G	1848	LMU	O5'-C1'-O1'-C1
18	e	1848	LMU	O5'-C1'-O1'-C1
19	J	5104	LMG	O6-C1-O1-C7
19	T	5104	LMG	O6-C1-O1-C7
19	l	5104	LMG	O6-C1-O1-C7
13	G	1022	CLA	C2-C3-C5-C6
13	e	1128	CLA	O1A-CGA-O2A-C1
13	B	1212	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	B	1223	CLA	C14-C13-C15-C16
13	B	1239	CLA	C6-C7-C8-C9
13	1	502	CLA	C11-C10-C8-C9
13	2	505	CLA	C6-C7-C8-C9
13	2	513	CLA	C11-C10-C8-C9
13	3	505	CLA	C14-C13-C15-C16
13	5	509	CLA	C6-C7-C8-C9
13	6	505	CLA	C11-C12-C13-C14
13	H	1223	CLA	C14-C13-C15-C16
13	H	1239	CLA	C6-C7-C8-C9
13	Y	502	CLA	C11-C10-C8-C9
13	Z	505	CLA	C6-C7-C8-C9
13	Z	513	CLA	C11-C10-C8-C9
13	a	505	CLA	C14-C13-C15-C16
13	c	509	CLA	C6-C7-C8-C9
13	d	505	CLA	C11-C12-C13-C14
13	f	1214	CLA	C14-C13-C15-C16
13	f	1223	CLA	C14-C13-C15-C16
13	f	1239	CLA	C6-C7-C8-C9
13	q	502	CLA	C11-C10-C8-C9
13	r	505	CLA	C6-C7-C8-C9
13	r	513	CLA	C11-C10-C8-C9
13	s	505	CLA	C14-C13-C15-C16
13	u	509	CLA	C6-C7-C8-C9
13	v	505	CLA	C11-C12-C13-C14
13	A	1128	CLA	CBA-CGA-O2A-C1
13	G	1128	CLA	CBA-CGA-O2A-C1
13	e	1128	CLA	CBA-CGA-O2A-C1
13	2	503	CLA	C13-C15-C16-C17
13	r	503	CLA	C13-C15-C16-C17
13	f	1212	CLA	O1D-CGD-O2D-CED
13	A	1106	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	C4B-C3B-CAB-CBB
13	L	1502	CLA	C4B-C3B-CAB-CBB
13	1	502	CLA	C4B-C3B-CAB-CBB
13	1	510	CLA	C4B-C3B-CAB-CBB
13	2	508	CLA	C4B-C3B-CAB-CBB
13	3	511	CLA	C4B-C3B-CAB-CBB
13	4	504	CLA	C4B-C3B-CAB-CBB
13	5	511	CLA	C4B-C3B-CAB-CBB
13	G	1106	CLA	C4B-C3B-CAB-CBB
13	R	1301	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	V	1502	CLA	C4B-C3B-CAB-CBB
13	Y	502	CLA	C4B-C3B-CAB-CBB
13	Y	510	CLA	C4B-C3B-CAB-CBB
13	a	511	CLA	C4B-C3B-CAB-CBB
13	b	504	CLA	C4B-C3B-CAB-CBB
13	c	511	CLA	C4B-C3B-CAB-CBB
13	e	1106	CLA	C4B-C3B-CAB-CBB
13	j	1301	CLA	C4B-C3B-CAB-CBB
13	n	1502	CLA	C4B-C3B-CAB-CBB
13	q	502	CLA	C4B-C3B-CAB-CBB
13	q	510	CLA	C4B-C3B-CAB-CBB
13	r	508	CLA	C4B-C3B-CAB-CBB
13	s	511	CLA	C4B-C3B-CAB-CBB
13	t	504	CLA	C4B-C3B-CAB-CBB
13	u	511	CLA	C4B-C3B-CAB-CBB
13	Z	503	CLA	C13-C15-C16-C17
13	e	1109	CLA	C15-C16-C17-C18
13	B	1228	CLA	CBA-CGA-O2A-C1
13	H	1228	CLA	CBA-CGA-O2A-C1
13	f	1228	CLA	CBA-CGA-O2A-C1
17	B	1855	LHG	C24-C23-O8-C6
17	H	1855	LHG	C24-C23-O8-C6
17	f	1855	LHG	C24-C23-O8-C6
13	4	508	CLA	CAA-CBA-CGA-O2A
13	b	508	CLA	CAA-CBA-CGA-O2A
13	t	508	CLA	CAA-CBA-CGA-O2A
18	A	1848	LMU	O1'-C1-C2-C3
18	G	1848	LMU	O1'-C1-C2-C3
18	e	1848	LMU	O1'-C1-C2-C3
17	A	5006	LHG	C28-C29-C30-C31
20	a	822	SQD	C11-C12-C13-C14
13	A	1022	CLA	C2-C3-C5-C6
13	e	1022	CLA	C2-C3-C5-C6
17	e	5006	LHG	C28-C29-C30-C31
20	3	822	SQD	C11-C12-C13-C14
20	s	822	SQD	C11-C12-C13-C14
17	G	5006	LHG	C28-C29-C30-C31
20	Y	822	SQD	O10-C23-C24-C25
17	A	5002	LHG	C9-C10-C11-C12
17	G	5002	LHG	C9-C10-C11-C12
17	e	5002	LHG	C9-C10-C11-C12
13	A	1107	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1131	CLA	C11-C12-C13-C15
13	B	1226	CLA	C11-C10-C8-C7
13	L	1501	CLA	C6-C7-C8-C10
13	3	513	CLA	C6-C7-C8-C10
13	G	1107	CLA	C11-C10-C8-C7
13	G	1131	CLA	C11-C12-C13-C15
13	H	1226	CLA	C11-C10-C8-C7
13	V	1501	CLA	C6-C7-C8-C10
13	a	513	CLA	C6-C7-C8-C10
13	e	1107	CLA	C11-C10-C8-C7
13	e	1131	CLA	C11-C12-C13-C15
13	f	1226	CLA	C11-C10-C8-C7
13	n	1501	CLA	C6-C7-C8-C10
13	s	513	CLA	C6-C7-C8-C10
14	B	2002	PQN	C17-C18-C20-C21
14	H	2002	PQN	C17-C18-C20-C21
14	f	2002	PQN	C17-C18-C20-C21
13	A	1109	CLA	C15-C16-C17-C18
13	3	510	CLA	C5-C6-C7-C8
13	G	1109	CLA	C15-C16-C17-C18
13	s	510	CLA	C5-C6-C7-C8
20	q	822	SQD	O10-C23-C24-C25
13	a	510	CLA	C5-C6-C7-C8
13	A	1117	CLA	C16-C17-C18-C19
13	G	1117	CLA	C16-C17-C18-C19
13	e	1117	CLA	C16-C17-C18-C19
20	1	822	SQD	O10-C23-C24-C25
17	L	5220	LHG	C25-C26-C27-C28
17	V	5220	LHG	C25-C26-C27-C28
17	n	5220	LHG	C25-C26-C27-C28
13	A	1135	CLA	C4-C3-C5-C6
13	B	1228	CLA	C3A-C2A-CAA-CBA
13	G	1135	CLA	C4-C3-C5-C6
13	H	1228	CLA	C3A-C2A-CAA-CBA
13	e	1135	CLA	C4-C3-C5-C6
13	f	1228	CLA	C3A-C2A-CAA-CBA
13	2	518	CLA	CAA-CBA-CGA-O2A
13	Z	518	CLA	CAA-CBA-CGA-O2A
13	r	518	CLA	CAA-CBA-CGA-O2A
13	B	1224	CLA	C2-C3-C5-C6
13	H	1224	CLA	C2-C3-C5-C6
13	f	1224	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	L	5216	SQD	C10-C11-C12-C13
20	V	5216	SQD	C10-C11-C12-C13
20	n	5216	SQD	C10-C11-C12-C13
20	q	822	SQD	C9-C10-C11-C12
20	1	822	SQD	C9-C10-C11-C12
16	A	4011	BCR	C11-C10-C9-C34
16	A	4011	BCR	C16-C17-C18-C36
16	B	4006	BCR	C11-C10-C9-C34
16	B	4006	BCR	C20-C21-C22-C37
16	F	4016	BCR	C35-C13-C14-C15
16	L	4020	BCR	C20-C21-C22-C37
16	G	4011	BCR	C11-C10-C9-C34
16	G	4011	BCR	C16-C17-C18-C36
16	H	4006	BCR	C11-C10-C9-C34
16	H	4006	BCR	C20-C21-C22-C37
16	R	4016	BCR	C35-C13-C14-C15
16	V	4020	BCR	C20-C21-C22-C37
16	e	4011	BCR	C11-C10-C9-C34
16	e	4011	BCR	C16-C17-C18-C36
16	f	4006	BCR	C11-C10-C9-C34
16	f	4006	BCR	C20-C21-C22-C37
16	j	4016	BCR	C35-C13-C14-C15
16	n	4020	BCR	C20-C21-C22-C37
13	G	1132	CLA	C2C-C3C-CAC-CBC
17	G	5003	LHG	C11-C12-C13-C14
17	e	5003	LHG	C11-C12-C13-C14
20	Y	822	SQD	C9-C10-C11-C12
13	l	1303	CLA	C15-C16-C17-C18
13	A	1132	CLA	C2C-C3C-CAC-CBC
13	e	1132	CLA	C2C-C3C-CAC-CBC
17	A	5003	LHG	C11-C12-C13-C14
13	6	510	CLA	CAA-CBA-CGA-O2A
13	d	510	CLA	CAA-CBA-CGA-O2A
13	v	510	CLA	CAA-CBA-CGA-O2A
13	A	1123	CLA	C13-C15-C16-C17
13	A	1237	CLA	C8-C10-C11-C12
13	J	1303	CLA	C15-C16-C17-C18
13	G	1237	CLA	C8-C10-C11-C12
13	e	1123	CLA	C13-C15-C16-C17
13	s	508	CLA	O1D-CGD-O2D-CED
13	B	1223	CLA	C2-C1-O2A-CGA
13	2	502	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1223	CLA	C2-C1-O2A-CGA
13	Z	502	CLA	C2-C1-O2A-CGA
13	f	1223	CLA	C2-C1-O2A-CGA
13	r	502	CLA	C2-C1-O2A-CGA
16	A	4011	BCR	C19-C20-C21-C22
16	1	522	BCR	C15-C16-C17-C18
16	4	521	BCR	C15-C16-C17-C18
16	6	521	BCR	C9-C10-C11-C12
16	G	4011	BCR	C19-C20-C21-C22
16	Y	522	BCR	C15-C16-C17-C18
16	b	521	BCR	C15-C16-C17-C18
16	d	521	BCR	C9-C10-C11-C12
16	e	4011	BCR	C19-C20-C21-C22
16	q	522	BCR	C15-C16-C17-C18
16	v	521	BCR	C9-C10-C11-C12
13	1	505	CLA	C13-C15-C16-C17
13	G	1123	CLA	C13-C15-C16-C17
13	Y	505	CLA	C13-C15-C16-C17
13	e	1237	CLA	C8-C10-C11-C12
13	q	505	CLA	C13-C15-C16-C17
13	q	518	CLA	C8-C10-C11-C12
13	t	508	CLA	CAA-CBA-CGA-O1A
13	1	518	CLA	C8-C10-C11-C12
13	T	1303	CLA	C15-C16-C17-C18
13	3	508	CLA	O1D-CGD-O2D-CED
13	G	1118	CLA	O1D-CGD-O2D-CED
13	4	508	CLA	CAA-CBA-CGA-O1A
13	v	517	CLA	CAA-CBA-CGA-O1A
16	B	4010	BCR	C11-C12-C13-C14
16	H	4010	BCR	C11-C12-C13-C14
13	A	1107	CLA	C2-C3-C5-C6
13	B	1202	CLA	C2-C3-C5-C6
13	G	1107	CLA	C2-C3-C5-C6
13	H	1202	CLA	C2-C3-C5-C6
13	e	1107	CLA	C2-C3-C5-C6
13	f	1202	CLA	C2-C3-C5-C6
13	A	1022	CLA	C16-C17-C18-C20
13	G	1022	CLA	C16-C17-C18-C20
13	e	1022	CLA	C16-C17-C18-C20
13	Y	518	CLA	C8-C10-C11-C12
17	V	5220	LHG	C26-C27-C28-C29
17	n	5220	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	4	513	CLA	C2A-CAA-CBA-CGA
13	b	513	CLA	C2A-CAA-CBA-CGA
13	t	513	CLA	C2A-CAA-CBA-CGA
13	3	512	CLA	CAA-CBA-CGA-O2A
13	6	517	CLA	CAA-CBA-CGA-O1A
13	a	512	CLA	CAA-CBA-CGA-O2A
13	b	508	CLA	CAA-CBA-CGA-O1A
13	d	517	CLA	CAA-CBA-CGA-O1A
13	s	512	CLA	CAA-CBA-CGA-O2A
13	A	1118	CLA	O1D-CGD-O2D-CED
17	L	5220	LHG	C26-C27-C28-C29
13	a	508	CLA	O1D-CGD-O2D-CED
13	H	1228	CLA	O1A-CGA-O2A-C1
13	A	1116	CLA	C11-C10-C8-C9
13	A	1124	CLA	C6-C7-C8-C9
13	B	1214	CLA	C14-C13-C15-C16
13	B	1229	CLA	C6-C7-C8-C9
13	J	1303	CLA	C6-C7-C8-C9
13	L	1501	CLA	C6-C7-C8-C9
13	1	505	CLA	C6-C7-C8-C9
13	1	510	CLA	C11-C12-C13-C14
13	2	518	CLA	C11-C10-C8-C9
13	3	513	CLA	C6-C7-C8-C9
13	G	1116	CLA	C11-C10-C8-C9
13	G	1124	CLA	C6-C7-C8-C9
13	H	1214	CLA	C14-C13-C15-C16
13	H	1229	CLA	C6-C7-C8-C9
13	T	1303	CLA	C6-C7-C8-C9
13	V	1501	CLA	C6-C7-C8-C9
13	Y	505	CLA	C6-C7-C8-C9
13	Y	510	CLA	C11-C12-C13-C14
13	Z	518	CLA	C11-C10-C8-C9
13	a	513	CLA	C6-C7-C8-C9
13	e	1116	CLA	C11-C10-C8-C9
13	e	1124	CLA	C6-C7-C8-C9
13	f	1229	CLA	C6-C7-C8-C9
13	l	1303	CLA	C6-C7-C8-C9
13	n	1501	CLA	C6-C7-C8-C9
13	q	505	CLA	C6-C7-C8-C9
13	q	510	CLA	C11-C12-C13-C14
13	r	518	CLA	C11-C10-C8-C9
13	s	513	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	J	5105	LMU	C5-C6-C7-C8
18	l	5105	LMU	C5-C6-C7-C8
18	T	5105	LMU	C5-C6-C7-C8
13	Y	503	CLA	C16-C17-C18-C19
13	1	503	CLA	C16-C17-C18-C19
13	q	503	CLA	C16-C17-C18-C19
13	e	1118	CLA	O1D-CGD-O2D-CED
16	t	521	BCR	C15-C16-C17-C18
13	K	1105	CLA	CAA-CBA-CGA-O2A
13	U	1105	CLA	CAA-CBA-CGA-O2A
13	d	510	CLA	CAA-CBA-CGA-O1A
13	m	1105	CLA	CAA-CBA-CGA-O2A
13	2	507	CLA	C16-C17-C18-C20
13	Z	507	CLA	C16-C17-C18-C20
13	r	507	CLA	C16-C17-C18-C20
13	G	1118	CLA	CBD-CGD-O2D-CED
13	A	1011	CLA	CAA-CBA-CGA-O2A
13	G	1011	CLA	CAA-CBA-CGA-O2A
13	e	1011	CLA	CAA-CBA-CGA-O2A
13	B	1228	CLA	O1A-CGA-O2A-C1
13	f	1228	CLA	O1A-CGA-O2A-C1
13	K	1105	CLA	CAA-CBA-CGA-O1A
13	6	510	CLA	CAA-CBA-CGA-O1A
13	U	1105	CLA	CAA-CBA-CGA-O1A
13	d	517	CLA	CAA-CBA-CGA-O2A
13	m	1105	CLA	CAA-CBA-CGA-O1A
13	t	512	CLA	CAA-CBA-CGA-O2A
13	v	510	CLA	CAA-CBA-CGA-O1A
13	f	1212	CLA	CBD-CGD-O2D-CED
13	A	1237	CLA	C2A-CAA-CBA-CGA
13	G	1237	CLA	C2A-CAA-CBA-CGA
13	e	1237	CLA	C2A-CAA-CBA-CGA
13	A	1111	CLA	C1A-C2A-CAA-CBA
13	B	1206	CLA	C1A-C2A-CAA-CBA
13	B	1212	CLA	C1A-C2A-CAA-CBA
13	B	1223	CLA	C1A-C2A-CAA-CBA
13	B	1228	CLA	C1A-C2A-CAA-CBA
13	B	1229	CLA	C1A-C2A-CAA-CBA
13	1	503	CLA	C1A-C2A-CAA-CBA
13	1	506	CLA	C1A-C2A-CAA-CBA
13	2	503	CLA	C1A-C2A-CAA-CBA
13	2	513	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	2	519	CLA	C1A-C2A-CAA-CBA
13	3	504	CLA	C1A-C2A-CAA-CBA
13	3	508	CLA	C1A-C2A-CAA-CBA
13	3	518	CLA	C1A-C2A-CAA-CBA
13	5	511	CLA	C1A-C2A-CAA-CBA
13	5	519	CLA	C1A-C2A-CAA-CBA
13	G	1111	CLA	C1A-C2A-CAA-CBA
13	H	1206	CLA	C1A-C2A-CAA-CBA
13	H	1212	CLA	C1A-C2A-CAA-CBA
13	H	1223	CLA	C1A-C2A-CAA-CBA
13	H	1228	CLA	C1A-C2A-CAA-CBA
13	H	1229	CLA	C1A-C2A-CAA-CBA
13	Y	503	CLA	C1A-C2A-CAA-CBA
13	Y	506	CLA	C1A-C2A-CAA-CBA
13	Z	513	CLA	C1A-C2A-CAA-CBA
13	Z	519	CLA	C1A-C2A-CAA-CBA
13	a	504	CLA	C1A-C2A-CAA-CBA
13	a	508	CLA	C1A-C2A-CAA-CBA
13	a	518	CLA	C1A-C2A-CAA-CBA
13	c	511	CLA	C1A-C2A-CAA-CBA
13	c	519	CLA	C1A-C2A-CAA-CBA
13	e	1111	CLA	C1A-C2A-CAA-CBA
13	f	1206	CLA	C1A-C2A-CAA-CBA
13	f	1212	CLA	C1A-C2A-CAA-CBA
13	f	1223	CLA	C1A-C2A-CAA-CBA
13	f	1228	CLA	C1A-C2A-CAA-CBA
13	f	1229	CLA	C1A-C2A-CAA-CBA
13	q	506	CLA	C1A-C2A-CAA-CBA
13	r	503	CLA	C1A-C2A-CAA-CBA
13	r	513	CLA	C1A-C2A-CAA-CBA
13	r	519	CLA	C1A-C2A-CAA-CBA
13	s	504	CLA	C1A-C2A-CAA-CBA
13	s	508	CLA	C1A-C2A-CAA-CBA
13	s	518	CLA	C1A-C2A-CAA-CBA
13	u	511	CLA	C1A-C2A-CAA-CBA
13	u	519	CLA	C1A-C2A-CAA-CBA
16	A	4011	BCR	C11-C10-C9-C8
16	A	4011	BCR	C16-C17-C18-C19
16	B	4006	BCR	C11-C10-C9-C8
16	B	4006	BCR	C20-C21-C22-C23
16	F	4016	BCR	C12-C13-C14-C15
16	L	4020	BCR	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	G	4011	BCR	C11-C10-C9-C8
16	G	4011	BCR	C16-C17-C18-C19
16	H	4006	BCR	C11-C10-C9-C8
16	H	4006	BCR	C20-C21-C22-C23
16	R	4016	BCR	C12-C13-C14-C15
16	V	4020	BCR	C20-C21-C22-C23
16	e	4011	BCR	C11-C10-C9-C8
16	e	4011	BCR	C16-C17-C18-C19
16	f	4006	BCR	C11-C10-C9-C8
16	f	4006	BCR	C20-C21-C22-C23
16	j	4016	BCR	C12-C13-C14-C15
16	n	4020	BCR	C20-C21-C22-C23
17	L	5220	LHG	C31-C32-C33-C34
17	V	5220	LHG	C31-C32-C33-C34
17	n	5220	LHG	C31-C32-C33-C34
13	4	512	CLA	CAA-CBA-CGA-O2A
13	6	517	CLA	CAA-CBA-CGA-O2A
13	b	512	CLA	CAA-CBA-CGA-O2A
13	v	517	CLA	CAA-CBA-CGA-O2A
13	A	1106	CLA	C2B-C3B-CAB-CBB
13	A	1109	CLA	C2B-C3B-CAB-CBB
13	A	1110	CLA	C2B-C3B-CAB-CBB
13	A	1111	CLA	C2B-C3B-CAB-CBB
13	A	1112	CLA	C2B-C3B-CAB-CBB
13	A	1115	CLA	C2B-C3B-CAB-CBB
13	A	1129	CLA	C2B-C3B-CAB-CBB
13	B	1021	CLA	C2B-C3B-CAB-CBB
13	B	1203	CLA	C2B-C3B-CAB-CBB
13	B	1210	CLA	C2B-C3B-CAB-CBB
13	B	1236	CLA	C2B-C3B-CAB-CBB
13	L	1501	CLA	C2B-C3B-CAB-CBB
13	1	510	CLA	C2B-C3B-CAB-CBB
13	1	513	CLA	C2B-C3B-CAB-CBB
13	2	504	CLA	C2B-C3B-CAB-CBB
13	2	507	CLA	C2B-C3B-CAB-CBB
13	2	511	CLA	C2B-C3B-CAB-CBB
13	2	512	CLA	C2B-C3B-CAB-CBB
13	2	517	CLA	C2B-C3B-CAB-CBB
13	3	507	CLA	C2B-C3B-CAB-CBB
13	4	503	CLA	C2B-C3B-CAB-CBB
13	4	507	CLA	C2B-C3B-CAB-CBB
13	4	510	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	4	511	CLA	C2B-C3B-CAB-CBB
13	4	516	CLA	C2B-C3B-CAB-CBB
13	4	517	CLA	C2B-C3B-CAB-CBB
13	5	503	CLA	C2B-C3B-CAB-CBB
13	5	504	CLA	C2B-C3B-CAB-CBB
13	5	507	CLA	C2B-C3B-CAB-CBB
13	5	508	CLA	C2B-C3B-CAB-CBB
13	5	510	CLA	C2B-C3B-CAB-CBB
13	6	502	CLA	C2B-C3B-CAB-CBB
13	6	507	CLA	C2B-C3B-CAB-CBB
13	6	508	CLA	C2B-C3B-CAB-CBB
13	6	510	CLA	C2B-C3B-CAB-CBB
13	6	516	CLA	C2B-C3B-CAB-CBB
13	6	517	CLA	C2B-C3B-CAB-CBB
13	G	1106	CLA	C2B-C3B-CAB-CBB
13	G	1109	CLA	C2B-C3B-CAB-CBB
13	G	1110	CLA	C2B-C3B-CAB-CBB
13	G	1111	CLA	C2B-C3B-CAB-CBB
13	G	1112	CLA	C2B-C3B-CAB-CBB
13	G	1115	CLA	C2B-C3B-CAB-CBB
13	G	1129	CLA	C2B-C3B-CAB-CBB
13	H	1021	CLA	C2B-C3B-CAB-CBB
13	H	1203	CLA	C2B-C3B-CAB-CBB
13	H	1210	CLA	C2B-C3B-CAB-CBB
13	H	1236	CLA	C2B-C3B-CAB-CBB
13	V	1501	CLA	C2B-C3B-CAB-CBB
13	Y	510	CLA	C2B-C3B-CAB-CBB
13	Y	513	CLA	C2B-C3B-CAB-CBB
13	Z	504	CLA	C2B-C3B-CAB-CBB
13	Z	507	CLA	C2B-C3B-CAB-CBB
13	Z	511	CLA	C2B-C3B-CAB-CBB
13	Z	517	CLA	C2B-C3B-CAB-CBB
13	a	507	CLA	C2B-C3B-CAB-CBB
13	a	513	CLA	C2B-C3B-CAB-CBB
13	b	503	CLA	C2B-C3B-CAB-CBB
13	b	507	CLA	C2B-C3B-CAB-CBB
13	b	510	CLA	C2B-C3B-CAB-CBB
13	b	511	CLA	C2B-C3B-CAB-CBB
13	b	516	CLA	C2B-C3B-CAB-CBB
13	b	517	CLA	C2B-C3B-CAB-CBB
13	c	503	CLA	C2B-C3B-CAB-CBB
13	c	504	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	c	507	CLA	C2B-C3B-CAB-CBB
13	c	508	CLA	C2B-C3B-CAB-CBB
13	d	502	CLA	C2B-C3B-CAB-CBB
13	d	503	CLA	C2B-C3B-CAB-CBB
13	d	507	CLA	C2B-C3B-CAB-CBB
13	d	508	CLA	C2B-C3B-CAB-CBB
13	d	510	CLA	C2B-C3B-CAB-CBB
13	d	516	CLA	C2B-C3B-CAB-CBB
13	d	517	CLA	C2B-C3B-CAB-CBB
13	e	1106	CLA	C2B-C3B-CAB-CBB
13	e	1109	CLA	C2B-C3B-CAB-CBB
13	e	1110	CLA	C2B-C3B-CAB-CBB
13	e	1111	CLA	C2B-C3B-CAB-CBB
13	e	1112	CLA	C2B-C3B-CAB-CBB
13	e	1115	CLA	C2B-C3B-CAB-CBB
13	e	1129	CLA	C2B-C3B-CAB-CBB
13	f	1021	CLA	C2B-C3B-CAB-CBB
13	f	1203	CLA	C2B-C3B-CAB-CBB
13	f	1210	CLA	C2B-C3B-CAB-CBB
13	f	1236	CLA	C2B-C3B-CAB-CBB
13	n	1501	CLA	C2B-C3B-CAB-CBB
13	q	510	CLA	C2B-C3B-CAB-CBB
13	q	513	CLA	C2B-C3B-CAB-CBB
13	r	504	CLA	C2B-C3B-CAB-CBB
13	r	507	CLA	C2B-C3B-CAB-CBB
13	r	511	CLA	C2B-C3B-CAB-CBB
13	r	512	CLA	C2B-C3B-CAB-CBB
13	r	517	CLA	C2B-C3B-CAB-CBB
13	s	507	CLA	C2B-C3B-CAB-CBB
13	t	503	CLA	C2B-C3B-CAB-CBB
13	t	507	CLA	C2B-C3B-CAB-CBB
13	t	510	CLA	C2B-C3B-CAB-CBB
13	t	511	CLA	C2B-C3B-CAB-CBB
13	t	513	CLA	C2B-C3B-CAB-CBB
13	t	516	CLA	C2B-C3B-CAB-CBB
13	t	517	CLA	C2B-C3B-CAB-CBB
13	u	503	CLA	C2B-C3B-CAB-CBB
13	u	504	CLA	C2B-C3B-CAB-CBB
13	u	507	CLA	C2B-C3B-CAB-CBB
13	u	508	CLA	C2B-C3B-CAB-CBB
13	u	510	CLA	C2B-C3B-CAB-CBB
13	v	502	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	v	507	CLA	C2B-C3B-CAB-CBB
13	v	508	CLA	C2B-C3B-CAB-CBB
13	v	510	CLA	C2B-C3B-CAB-CBB
13	v	516	CLA	C2B-C3B-CAB-CBB
13	v	517	CLA	C2B-C3B-CAB-CBB
16	B	4004	BCR	C23-C24-C25-C26
16	B	4005	BCR	C23-C24-C25-C26
16	B	4017	BCR	C5-C6-C7-C8
16	J	4015	BCR	C23-C24-C25-C26
16	L	4020	BCR	C23-C24-C25-C26
16	L	4020	BCR	C23-C24-C25-C30
16	L	4219	BCR	C1-C6-C7-C8
16	2	524	BCR	C23-C24-C25-C26
16	3	521	BCR	C23-C24-C25-C26
16	3	521	BCR	C23-C24-C25-C30
16	H	4004	BCR	C23-C24-C25-C26
16	H	4005	BCR	C23-C24-C25-C26
16	H	4017	BCR	C5-C6-C7-C8
16	T	4015	BCR	C23-C24-C25-C26
16	V	4020	BCR	C23-C24-C25-C26
16	V	4020	BCR	C23-C24-C25-C30
16	V	4219	BCR	C1-C6-C7-C8
16	Z	524	BCR	C23-C24-C25-C26
16	a	521	BCR	C23-C24-C25-C26
16	a	521	BCR	C23-C24-C25-C30
16	f	4004	BCR	C23-C24-C25-C26
16	f	4005	BCR	C23-C24-C25-C26
16	f	4017	BCR	C5-C6-C7-C8
16	l	4015	BCR	C23-C24-C25-C26
16	n	4020	BCR	C23-C24-C25-C26
16	n	4020	BCR	C23-C24-C25-C30
16	n	4219	BCR	C1-C6-C7-C8
16	r	524	BCR	C23-C24-C25-C26
16	s	521	BCR	C23-C24-C25-C26
16	s	521	BCR	C23-C24-C25-C30
13	a	512	CLA	CAA-CBA-CGA-O1A
13	3	518	CLA	CBA-CGA-O2A-C1
13	a	518	CLA	CBA-CGA-O2A-C1
13	s	518	CLA	CBA-CGA-O2A-C1
13	L	1501	CLA	C13-C15-C16-C17
13	V	1501	CLA	C13-C15-C16-C17
13	n	1501	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5009	LHG	C12-C13-C14-C15
17	A	5009	LHG	C12-C13-C14-C15
17	e	5009	LHG	C12-C13-C14-C15
13	A	1118	CLA	CBD-CGD-O2D-CED
13	B	1212	CLA	CBD-CGD-O2D-CED
13	H	1212	CLA	CBD-CGD-O2D-CED
17	S	5001	LHG	C24-C25-C26-C27
13	3	512	CLA	CAA-CBA-CGA-O1A
13	A	1106	CLA	C4-C3-C5-C6
13	A	1127	CLA	C4-C3-C5-C6
13	G	1106	CLA	C4-C3-C5-C6
13	e	1106	CLA	C4-C3-C5-C6
13	e	1127	CLA	C4-C3-C5-C6
17	k	5001	LHG	C24-C25-C26-C27
17	I	5001	LHG	C24-C25-C26-C27
19	B	5002	LMG	C40-C41-C42-C43
19	f	5002	LMG	C40-C41-C42-C43
13	e	1118	CLA	CBD-CGD-O2D-CED
18	l	5105	LMU	C2-C3-C4-C5
19	H	5002	LMG	C40-C41-C42-C43
13	4	512	CLA	CAA-CBA-CGA-O1A
13	b	512	CLA	CAA-CBA-CGA-O1A
13	s	512	CLA	CAA-CBA-CGA-O1A
13	t	512	CLA	CAA-CBA-CGA-O1A
18	J	5105	LMU	C2-C3-C4-C5
18	T	5105	LMU	C2-C3-C4-C5
13	B	1214	CLA	C12-C13-C15-C16
13	B	1215	CLA	C6-C7-C8-C10
13	B	1223	CLA	C12-C13-C15-C16
13	B	1229	CLA	C11-C10-C8-C7
13	J	1303	CLA	C12-C13-C15-C16
13	2	513	CLA	C12-C13-C15-C16
13	2	518	CLA	C11-C10-C8-C7
13	H	1214	CLA	C12-C13-C15-C16
13	H	1215	CLA	C6-C7-C8-C10
13	H	1223	CLA	C12-C13-C15-C16
13	H	1229	CLA	C11-C10-C8-C7
13	T	1303	CLA	C12-C13-C15-C16
13	Z	513	CLA	C12-C13-C15-C16
13	Z	518	CLA	C11-C10-C8-C7
13	f	1214	CLA	C12-C13-C15-C16
13	f	1215	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1223	CLA	C12-C13-C15-C16
13	f	1229	CLA	C11-C10-C8-C7
13	l	1303	CLA	C12-C13-C15-C16
13	r	513	CLA	C12-C13-C15-C16
13	r	518	CLA	C11-C10-C8-C7
13	B	1229	CLA	C16-C17-C18-C19
13	H	1229	CLA	C16-C17-C18-C19
13	f	1229	CLA	C16-C17-C18-C19
13	B	1204	CLA	C2A-CAA-CBA-CGA
13	B	1210	CLA	C2A-CAA-CBA-CGA
13	H	1204	CLA	C2A-CAA-CBA-CGA
13	H	1210	CLA	C2A-CAA-CBA-CGA
13	f	1204	CLA	C2A-CAA-CBA-CGA
13	f	1210	CLA	C2A-CAA-CBA-CGA
13	A	1022	CLA	C15-C16-C17-C18
13	G	1022	CLA	C15-C16-C17-C18
20	Z	822	SQD	C26-C27-C28-C29
17	L	5221	LHG	C16-C17-C18-C19
17	f	1842	LHG	C11-C10-C9-C8
17	n	5221	LHG	C16-C17-C18-C19
17	B	1842	LHG	C11-C10-C9-C8
20	r	822	SQD	C26-C27-C28-C29
13	e	1022	CLA	C15-C16-C17-C18
17	H	1842	LHG	C11-C10-C9-C8
17	V	5221	LHG	C16-C17-C18-C19
20	2	822	SQD	C26-C27-C28-C29
13	B	1222	CLA	C3-C5-C6-C7
13	H	1222	CLA	C3-C5-C6-C7
13	f	1222	CLA	C3-C5-C6-C7
17	e	5004	LHG	C28-C29-C30-C31
17	G	5004	LHG	C28-C29-C30-C31
17	A	5004	LHG	C28-C29-C30-C31
17	S	5001	LHG	C28-C29-C30-C31
17	k	5001	LHG	C28-C29-C30-C31
13	5	505	CLA	C12-C13-C15-C16
13	c	505	CLA	C12-C13-C15-C16
13	u	505	CLA	C12-C13-C15-C16
13	6	509	CLA	CAA-CBA-CGA-O2A
13	d	509	CLA	CAA-CBA-CGA-O2A
13	v	509	CLA	CAA-CBA-CGA-O2A
13	A	1126	CLA	C4-C3-C5-C6
13	B	1240	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1126	CLA	C4-C3-C5-C6
13	G	1127	CLA	C4-C3-C5-C6
13	H	1240	CLA	C4-C3-C5-C6
13	e	1126	CLA	C4-C3-C5-C6
17	I	5001	LHG	C28-C29-C30-C31
14	A	2001	PQN	C23-C25-C26-C27
14	G	2001	PQN	C23-C25-C26-C27
14	e	2001	PQN	C23-C25-C26-C27
13	A	1126	CLA	C2-C3-C5-C6
13	B	1210	CLA	C2-C3-C5-C6
13	G	1126	CLA	C2-C3-C5-C6
13	H	1210	CLA	C2-C3-C5-C6
13	e	1126	CLA	C2-C3-C5-C6
13	f	1210	CLA	C2-C3-C5-C6
13	3	501	CLA	C10-C11-C12-C13
13	a	501	CLA	C10-C11-C12-C13
13	s	501	CLA	C10-C11-C12-C13
13	a	518	CLA	O1A-CGA-O2A-C1
13	a	519	CLA	O1A-CGA-O2A-C1
13	1	507	CLA	C2A-CAA-CBA-CGA
13	B	1213	CLA	C6-C7-C8-C9
13	6	501	CLA	C6-C7-C8-C9
13	H	1213	CLA	C6-C7-C8-C9
13	d	501	CLA	C6-C7-C8-C9
13	f	1213	CLA	C6-C7-C8-C9
13	v	501	CLA	C6-C7-C8-C9
13	3	510	CLA	C13-C15-C16-C17
13	s	510	CLA	C13-C15-C16-C17
13	s	518	CLA	O1A-CGA-O2A-C1
13	a	510	CLA	C13-C15-C16-C17
13	3	519	CLA	O1A-CGA-O2A-C1
13	s	519	CLA	O1A-CGA-O2A-C1
17	e	5007	LHG	O10-C23-O8-C6
13	A	1013	CLA	C4-C3-C5-C6
13	2	513	CLA	C4-C3-C5-C6
13	G	1013	CLA	C4-C3-C5-C6
13	Z	513	CLA	C4-C3-C5-C6
13	e	1013	CLA	C4-C3-C5-C6
13	f	1240	CLA	C4-C3-C5-C6
13	r	513	CLA	C4-C3-C5-C6
17	L	5218	LHG	C5-C4-O6-P
17	V	5218	LHG	C5-C4-O6-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	n	5218	LHG	C5-C4-O6-P
13	5	503	CLA	C2-C3-C5-C6
13	c	503	CLA	C2-C3-C5-C6
13	u	503	CLA	C2-C3-C5-C6
13	3	518	CLA	O1A-CGA-O2A-C1
17	A	5007	LHG	O10-C23-O8-C6
17	G	5007	LHG	O10-C23-O8-C6
17	A	5004	LHG	C24-C23-O8-C6
17	G	5004	LHG	C24-C23-O8-C6
13	5	507	CLA	CAA-CBA-CGA-O2A
13	c	507	CLA	CAA-CBA-CGA-O2A
13	u	507	CLA	CAA-CBA-CGA-O2A
13	G	1109	CLA	C3-C5-C6-C7
13	J	1302	CLA	C2A-CAA-CBA-CGA
13	3	503	CLA	C2A-CAA-CBA-CGA
13	T	1302	CLA	C2A-CAA-CBA-CGA
13	Y	507	CLA	C2A-CAA-CBA-CGA
13	a	503	CLA	C2A-CAA-CBA-CGA
13	l	1302	CLA	C2A-CAA-CBA-CGA
13	q	507	CLA	C2A-CAA-CBA-CGA
13	s	503	CLA	C2A-CAA-CBA-CGA
13	f	1202	CLA	C16-C17-C18-C20
13	u	518	CLA	CAA-CBA-CGA-O2A
18	B	1843	LMU	C6-C7-C8-C9
13	d	507	CLA	CAA-CBA-CGA-O2A
13	v	507	CLA	CAA-CBA-CGA-O2A
18	H	1843	LMU	C6-C7-C8-C9
13	H	1226	CLA	C8-C10-C11-C12
18	f	1843	LMU	C6-C7-C8-C9
13	1	516	CLA	CAA-CBA-CGA-O2A
13	5	512	CLA	CAA-CBA-CGA-O2A
13	6	507	CLA	CAA-CBA-CGA-O2A
13	c	512	CLA	CAA-CBA-CGA-O2A
13	u	512	CLA	CAA-CBA-CGA-O2A
13	v	509	CLA	CAA-CBA-CGA-O1A
20	1	822	SQD	O48-C23-C24-C25
20	Y	822	SQD	O48-C23-C24-C25
20	q	822	SQD	O48-C23-C24-C25
13	A	1022	CLA	C16-C17-C18-C19
13	B	1202	CLA	C16-C17-C18-C20
13	G	1022	CLA	C16-C17-C18-C19
13	L	1501	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	n	1501	CLA	C15-C16-C17-C18
17	I	5001	LHG	C30-C31-C32-C33
17	S	5001	LHG	C30-C31-C32-C33
17	k	5001	LHG	C30-C31-C32-C33
13	A	1109	CLA	C4B-C3B-CAB-CBB
13	A	1124	CLA	C4B-C3B-CAB-CBB
13	B	1203	CLA	C4B-C3B-CAB-CBB
13	B	1210	CLA	C4B-C3B-CAB-CBB
13	1	508	CLA	C4B-C3B-CAB-CBB
13	2	511	CLA	C4B-C3B-CAB-CBB
13	5	508	CLA	C4B-C3B-CAB-CBB
13	6	504	CLA	C4B-C3B-CAB-CBB
13	6	508	CLA	C4B-C3B-CAB-CBB
13	G	1109	CLA	C4B-C3B-CAB-CBB
13	G	1124	CLA	C4B-C3B-CAB-CBB
13	H	1203	CLA	C4B-C3B-CAB-CBB
13	H	1210	CLA	C4B-C3B-CAB-CBB
13	Y	508	CLA	C4B-C3B-CAB-CBB
13	Z	508	CLA	C4B-C3B-CAB-CBB
13	Z	511	CLA	C4B-C3B-CAB-CBB
13	c	508	CLA	C4B-C3B-CAB-CBB
13	d	504	CLA	C4B-C3B-CAB-CBB
13	d	508	CLA	C4B-C3B-CAB-CBB
13	e	1109	CLA	C4B-C3B-CAB-CBB
13	e	1124	CLA	C4B-C3B-CAB-CBB
13	f	1203	CLA	C4B-C3B-CAB-CBB
13	f	1210	CLA	C4B-C3B-CAB-CBB
13	q	508	CLA	C4B-C3B-CAB-CBB
13	r	511	CLA	C4B-C3B-CAB-CBB
13	u	508	CLA	C4B-C3B-CAB-CBB
13	v	504	CLA	C4B-C3B-CAB-CBB
13	v	508	CLA	C4B-C3B-CAB-CBB
13	B	1226	CLA	C8-C10-C11-C12
13	V	1501	CLA	C15-C16-C17-C18
13	4	507	CLA	CAA-CBA-CGA-O2A
13	6	509	CLA	CAA-CBA-CGA-O1A
13	Y	516	CLA	CAA-CBA-CGA-O2A
13	b	507	CLA	CAA-CBA-CGA-O2A
13	d	509	CLA	CAA-CBA-CGA-O1A
13	q	516	CLA	CAA-CBA-CGA-O2A
13	t	507	CLA	CAA-CBA-CGA-O2A
17	A	5008	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5008	LHG	C9-C10-C11-C12
17	e	5008	LHG	C9-C10-C11-C12
17	e	5001	LHG	C24-C25-C26-C27
17	e	5004	LHG	C24-C23-O8-C6
13	5	518	CLA	CAA-CBA-CGA-O2A
13	c	518	CLA	CAA-CBA-CGA-O2A
13	f	1226	CLA	C8-C10-C11-C12
17	A	5001	LHG	C24-C25-C26-C27
17	G	5001	LHG	C24-C25-C26-C27
13	4	513	CLA	CAA-CBA-CGA-O2A
13	b	513	CLA	CAA-CBA-CGA-O2A
13	t	513	CLA	CAA-CBA-CGA-O2A
20	n	5216	SQD	C17-C18-C19-C20
13	H	1202	CLA	C16-C17-C18-C20
13	e	1022	CLA	C16-C17-C18-C19
20	L	5216	SQD	C17-C18-C19-C20
17	A	5001	LHG	C19-C20-C21-C22
17	G	5001	LHG	C19-C20-C21-C22
13	A	1109	CLA	C3-C5-C6-C7
13	e	1109	CLA	C3-C5-C6-C7
13	6	511	CLA	CAA-CBA-CGA-O2A
13	d	511	CLA	CAA-CBA-CGA-O2A
13	v	511	CLA	CAA-CBA-CGA-O2A
17	e	5001	LHG	C19-C20-C21-C22
20	V	5216	SQD	C17-C18-C19-C20
20	L	5216	SQD	O6-C44-C45-O47
20	V	5216	SQD	O6-C44-C45-O47
20	n	5216	SQD	O6-C44-C45-O47
13	5	510	CLA	CAA-CBA-CGA-O2A
13	6	512	CLA	CAA-CBA-CGA-O2A
13	c	510	CLA	CAA-CBA-CGA-O2A
13	u	510	CLA	CAA-CBA-CGA-O2A
18	T	5105	LMU	O1'-C1-C2-C3
13	2	513	CLA	C2-C3-C5-C6
13	Z	513	CLA	C2-C3-C5-C6
13	r	513	CLA	C2-C3-C5-C6
13	a	509	CLA	C5-C6-C7-C8
13	s	509	CLA	C5-C6-C7-C8
13	3	510	CLA	C12-C13-C15-C16
13	a	510	CLA	C12-C13-C15-C16
13	f	1226	CLA	C12-C13-C15-C16
13	s	510	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	2001	PQN	C21-C22-C23-C25
14	G	2001	PQN	C21-C22-C23-C25
14	e	2001	PQN	C21-C22-C23-C25
13	d	512	CLA	CAA-CBA-CGA-O2A
13	v	512	CLA	CAA-CBA-CGA-O2A
18	l	5105	LMU	O1'-C1-C2-C3
13	3	509	CLA	C5-C6-C7-C8
16	f	4009	BCR	C19-C20-C21-C22
18	J	5105	LMU	O1'-C1-C2-C3
13	5	510	CLA	CAA-CBA-CGA-O1A
13	c	510	CLA	CAA-CBA-CGA-O1A
13	u	510	CLA	CAA-CBA-CGA-O1A
13	a	519	CLA	CBA-CGA-O2A-C1
13	A	1111	CLA	C11-C12-C13-C14
13	A	1119	CLA	C6-C7-C8-C9
13	A	1133	CLA	C11-C12-C13-C14
13	B	1234	CLA	C14-C13-C15-C16
13	G	1111	CLA	C11-C12-C13-C14
13	G	1119	CLA	C6-C7-C8-C9
13	G	1133	CLA	C11-C12-C13-C14
13	H	1234	CLA	C14-C13-C15-C16
13	e	1111	CLA	C11-C12-C13-C14
13	e	1119	CLA	C6-C7-C8-C9
13	e	1133	CLA	C11-C12-C13-C14
13	f	1234	CLA	C14-C13-C15-C16
13	H	1228	CLA	CBD-CGD-O2D-CED
20	B	1852	SQD	C5-C6-S-O8
20	3	822	SQD	C5-C6-S-O8
20	H	1852	SQD	C5-C6-S-O8
20	a	822	SQD	C5-C6-S-O8
20	f	1852	SQD	C5-C6-S-O8
20	s	822	SQD	C5-C6-S-O8
13	A	1013	CLA	C2A-CAA-CBA-CGA
13	A	1137	CLA	C2A-CAA-CBA-CGA
13	B	1216	CLA	C2A-CAA-CBA-CGA
13	1	503	CLA	C2A-CAA-CBA-CGA
13	2	503	CLA	C2A-CAA-CBA-CGA
13	G	1013	CLA	C2A-CAA-CBA-CGA
13	G	1137	CLA	C2A-CAA-CBA-CGA
13	H	1216	CLA	C2A-CAA-CBA-CGA
13	Y	503	CLA	C2A-CAA-CBA-CGA
13	Z	503	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1013	CLA	C2A-CAA-CBA-CGA
13	e	1120	CLA	C2A-CAA-CBA-CGA
13	e	1137	CLA	C2A-CAA-CBA-CGA
13	f	1216	CLA	C2A-CAA-CBA-CGA
13	q	503	CLA	C2A-CAA-CBA-CGA
13	r	503	CLA	C2A-CAA-CBA-CGA
13	A	1105	CLA	C2-C1-O2A-CGA
13	A	1138	CLA	C2-C1-O2A-CGA
13	A	1237	CLA	C2-C1-O2A-CGA
13	G	1105	CLA	C2-C1-O2A-CGA
13	G	1138	CLA	C2-C1-O2A-CGA
13	G	1237	CLA	C2-C1-O2A-CGA
13	e	1105	CLA	C2-C1-O2A-CGA
13	e	1138	CLA	C2-C1-O2A-CGA
13	e	1237	CLA	C2-C1-O2A-CGA
13	H	1212	CLA	C3-C5-C6-C7
13	B	1201	CLA	C8-C10-C11-C12
13	H	1201	CLA	C8-C10-C11-C12
13	f	1201	CLA	C8-C10-C11-C12
13	A	1011	CLA	CBA-CGA-O2A-C1
13	3	519	CLA	CBA-CGA-O2A-C1
13	G	1011	CLA	CBA-CGA-O2A-C1
13	e	1011	CLA	CBA-CGA-O2A-C1
13	s	519	CLA	CBA-CGA-O2A-C1
13	A	1111	CLA	C3A-C2A-CAA-CBA
13	A	1118	CLA	C3A-C2A-CAA-CBA
13	G	1111	CLA	C3A-C2A-CAA-CBA
13	G	1118	CLA	C3A-C2A-CAA-CBA
13	e	1111	CLA	C3A-C2A-CAA-CBA
13	e	1118	CLA	C3A-C2A-CAA-CBA
13	q	512	CLA	C3A-C2A-CAA-CBA
13	2	516	CLA	CAA-CBA-CGA-O2A
13	5	517	CLA	CAA-CBA-CGA-O2A
13	6	507	CLA	CAA-CBA-CGA-O1A
13	Z	516	CLA	CAA-CBA-CGA-O2A
13	c	512	CLA	CAA-CBA-CGA-O1A
13	c	517	CLA	CAA-CBA-CGA-O2A
13	q	517	CLA	CAA-CBA-CGA-O2A
13	r	516	CLA	CAA-CBA-CGA-O2A
13	u	517	CLA	CAA-CBA-CGA-O2A
13	v	507	CLA	CAA-CBA-CGA-O1A
13	A	1133	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	1133	CLA	CBD-CGD-O2D-CED
13	B	1212	CLA	C3-C5-C6-C7
13	f	1212	CLA	C3-C5-C6-C7
13	1	518	CLA	CAA-CBA-CGA-O1A
13	q	518	CLA	CAA-CBA-CGA-O1A
13	1	517	CLA	CAA-CBA-CGA-O2A
13	Y	517	CLA	CAA-CBA-CGA-O2A
13	d	507	CLA	CAA-CBA-CGA-O1A
13	G	1126	CLA	O1A-CGA-O2A-C1
13	Y	518	CLA	CAA-CBA-CGA-O1A
13	4	513	CLA	CAA-CBA-CGA-O1A
13	5	512	CLA	CAA-CBA-CGA-O1A
13	5	513	CLA	CAA-CBA-CGA-O2A
13	6	504	CLA	CAA-CBA-CGA-O2A
13	6	516	CLA	CAA-CBA-CGA-O2A
13	c	507	CLA	CAA-CBA-CGA-O1A
13	c	513	CLA	CAA-CBA-CGA-O2A
13	d	504	CLA	CAA-CBA-CGA-O2A
13	d	516	CLA	CAA-CBA-CGA-O2A
13	u	512	CLA	CAA-CBA-CGA-O1A
13	u	513	CLA	CAA-CBA-CGA-O2A
13	v	504	CLA	CAA-CBA-CGA-O2A
16	B	4009	BCR	C19-C20-C21-C22
13	5	507	CLA	CAA-CBA-CGA-O1A
13	b	513	CLA	CAA-CBA-CGA-O1A
13	t	513	CLA	CAA-CBA-CGA-O1A
13	v	516	CLA	CAA-CBA-CGA-O2A
13	A	1120	CLA	C2A-CAA-CBA-CGA
13	G	1120	CLA	C2A-CAA-CBA-CGA
13	B	1228	CLA	CBD-CGD-O2D-CED
13	G	1123	CLA	C8-C10-C11-C12
13	6	511	CLA	CAA-CBA-CGA-O1A
13	d	511	CLA	CAA-CBA-CGA-O1A
13	t	507	CLA	CAA-CBA-CGA-O1A
13	u	507	CLA	CAA-CBA-CGA-O1A
13	v	511	CLA	CAA-CBA-CGA-O1A
13	A	1124	CLA	CBA-CGA-O2A-C1
13	G	1124	CLA	CBA-CGA-O2A-C1
13	H	1204	CLA	CBA-CGA-O2A-C1
13	e	1126	CLA	O1A-CGA-O2A-C1
13	1	516	CLA	CAA-CBA-CGA-O1A
13	4	507	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	b	507	CLA	CAA-CBA-CGA-O1A
13	q	516	CLA	CAA-CBA-CGA-O1A
17	e	5003	LHG	C26-C27-C28-C29
13	A	1011	CLA	O1A-CGA-O2A-C1
13	e	1011	CLA	O1A-CGA-O2A-C1
13	A	1123	CLA	C8-C10-C11-C12
13	e	1123	CLA	C8-C10-C11-C12
17	A	5003	LHG	C26-C27-C28-C29
13	B	1204	CLA	CBA-CGA-O2A-C1
13	e	1124	CLA	CBA-CGA-O2A-C1
13	f	1204	CLA	CBA-CGA-O2A-C1
13	Y	516	CLA	CAA-CBA-CGA-O1A
13	B	1228	CLA	O1D-CGD-O2D-CED
13	f	1228	CLA	CBD-CGD-O2D-CED
13	A	1126	CLA	O1A-CGA-O2A-C1
13	B	1205	CLA	O1A-CGA-O2A-C1
13	G	1011	CLA	O1A-CGA-O2A-C1
13	H	1205	CLA	O1A-CGA-O2A-C1
13	f	1205	CLA	O1A-CGA-O2A-C1
13	2	510	CLA	C13-C15-C16-C17
13	Z	510	CLA	C13-C15-C16-C17
13	r	510	CLA	C13-C15-C16-C17
17	G	5003	LHG	C26-C27-C28-C29
13	d	512	CLA	CAA-CBA-CGA-O1A
13	v	512	CLA	CAA-CBA-CGA-O1A
13	e	1127	CLA	O1A-CGA-O2A-C1
19	f	5002	LMG	C38-C39-C40-C41
13	H	1228	CLA	O1D-CGD-O2D-CED
13	Z	511	CLA	C4-C3-C5-C6
20	B	1852	SQD	O47-C7-C8-C9
20	H	1852	SQD	O47-C7-C8-C9
13	2	516	CLA	CAA-CBA-CGA-O1A
13	5	513	CLA	CAA-CBA-CGA-O1A
13	5	517	CLA	CAA-CBA-CGA-O1A
13	6	512	CLA	CAA-CBA-CGA-O1A
13	c	513	CLA	CAA-CBA-CGA-O1A
13	c	517	CLA	CAA-CBA-CGA-O1A
13	d	504	CLA	CAA-CBA-CGA-O1A
13	r	516	CLA	CAA-CBA-CGA-O1A
13	u	513	CLA	CAA-CBA-CGA-O1A
13	u	517	CLA	CAA-CBA-CGA-O1A
16	5	521	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	H	4009	BCR	C19-C20-C21-C22
16	c	521	BCR	C9-C10-C11-C12
16	u	521	BCR	C9-C10-C11-C12
19	B	5002	LMG	C38-C39-C40-C41
13	A	1127	CLA	O1A-CGA-O2A-C1
13	G	1127	CLA	O1A-CGA-O2A-C1
13	f	1228	CLA	O1D-CGD-O2D-CED
13	q	503	CLA	C15-C16-C17-C18
13	1	503	CLA	C15-C16-C17-C18
13	Y	503	CLA	C15-C16-C17-C18
19	H	5002	LMG	C38-C39-C40-C41
13	e	1133	CLA	CBD-CGD-O2D-CED
13	Z	516	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	CAA-CBA-CGA-O2A
13	G	1123	CLA	CAA-CBA-CGA-O2A
13	e	1123	CLA	CAA-CBA-CGA-O2A
17	H	1842	LHG	O7-C7-C8-C9
17	f	1842	LHG	O7-C7-C8-C9
13	Z	505	CLA	C13-C15-C16-C17
13	6	504	CLA	CAA-CBA-CGA-O1A
13	v	504	CLA	CAA-CBA-CGA-O1A
13	2	505	CLA	C13-C15-C16-C17
13	r	505	CLA	C13-C15-C16-C17
13	A	1122	CLA	C6-C7-C8-C9
13	A	1123	CLA	C11-C12-C13-C14
13	A	1237	CLA	C14-C13-C15-C16
13	B	1208	CLA	C14-C13-C15-C16
13	B	1216	CLA	C6-C7-C8-C9
13	G	1122	CLA	C6-C7-C8-C9
13	G	1123	CLA	C11-C12-C13-C14
13	G	1237	CLA	C14-C13-C15-C16
13	H	1208	CLA	C14-C13-C15-C16
13	H	1216	CLA	C6-C7-C8-C9
13	e	1122	CLA	C6-C7-C8-C9
13	e	1123	CLA	C11-C12-C13-C14
13	e	1237	CLA	C14-C13-C15-C16
13	f	1208	CLA	C14-C13-C15-C16
13	f	1216	CLA	C6-C7-C8-C9
13	3	519	CLA	CAA-CBA-CGA-O2A
13	a	519	CLA	CAA-CBA-CGA-O2A
13	s	519	CLA	CAA-CBA-CGA-O2A
17	B	1842	LHG	O7-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	3	822	SQD	O48-C23-C24-C25
20	a	822	SQD	O48-C23-C24-C25
20	f	1852	SQD	O47-C7-C8-C9
20	s	822	SQD	O48-C23-C24-C25
16	J	4015	BCR	C7-C8-C9-C10
16	2	523	BCR	C7-C8-C9-C10
16	6	521	BCR	C7-C8-C9-C10
16	T	4015	BCR	C7-C8-C9-C10
16	Z	523	BCR	C7-C8-C9-C10
16	d	521	BCR	C7-C8-C9-C10
16	l	4015	BCR	C7-C8-C9-C10
16	r	523	BCR	C7-C8-C9-C10
16	v	521	BCR	C7-C8-C9-C10
20	H	1852	SQD	C30-C31-C32-C33
13	u	505	CLA	O1D-CGD-O2D-CED
13	B	1224	CLA	CAA-CBA-CGA-O1A
13	H	1224	CLA	CAA-CBA-CGA-O1A
20	B	1852	SQD	C30-C31-C32-C33
20	f	1852	SQD	C30-C31-C32-C33
13	3	507	CLA	CAA-CBA-CGA-O2A
13	a	507	CLA	CAA-CBA-CGA-O2A
13	A	1133	CLA	C11-C12-C13-C15
13	A	1237	CLA	C12-C13-C15-C16
13	B	1213	CLA	C6-C7-C8-C10
13	B	1226	CLA	C12-C13-C15-C16
13	B	1229	CLA	C6-C7-C8-C10
13	2	505	CLA	C12-C13-C15-C16
13	6	501	CLA	C6-C7-C8-C10
13	G	1133	CLA	C11-C12-C13-C15
13	G	1237	CLA	C12-C13-C15-C16
13	H	1213	CLA	C6-C7-C8-C10
13	H	1226	CLA	C12-C13-C15-C16
13	H	1229	CLA	C6-C7-C8-C10
13	Z	505	CLA	C12-C13-C15-C16
13	d	501	CLA	C6-C7-C8-C10
13	e	1133	CLA	C11-C12-C13-C15
13	e	1237	CLA	C12-C13-C15-C16
13	f	1213	CLA	C6-C7-C8-C10
13	f	1229	CLA	C6-C7-C8-C10
13	r	505	CLA	C12-C13-C15-C16
13	v	501	CLA	C6-C7-C8-C10
13	A	1140	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	f	1224	CLA	CAA-CBA-CGA-O1A
13	v	516	CLA	CAA-CBA-CGA-O1A
13	A	1108	CLA	C2B-C3B-CAB-CBB
13	A	1124	CLA	C2B-C3B-CAB-CBB
13	A	1133	CLA	C2B-C3B-CAB-CBB
13	A	1130	CLA	C2B-C3B-CAB-CBB
13	B	1208	CLA	C2B-C3B-CAB-CBB
13	B	1217	CLA	C2B-C3B-CAB-CBB
13	B	1240	CLA	C2B-C3B-CAB-CBB
13	L	1502	CLA	C2B-C3B-CAB-CBB
13	1	502	CLA	C2B-C3B-CAB-CBB
13	1	503	CLA	C2B-C3B-CAB-CBB
13	1	508	CLA	C2B-C3B-CAB-CBB
13	2	508	CLA	C2B-C3B-CAB-CBB
13	3	505	CLA	C2B-C3B-CAB-CBB
13	3	510	CLA	C2B-C3B-CAB-CBB
13	3	511	CLA	C2B-C3B-CAB-CBB
13	3	513	CLA	C2B-C3B-CAB-CBB
13	3	516	CLA	C2B-C3B-CAB-CBB
13	4	504	CLA	C2B-C3B-CAB-CBB
13	4	506	CLA	C2B-C3B-CAB-CBB
13	4	513	CLA	C2B-C3B-CAB-CBB
13	5	501	CLA	C2B-C3B-CAB-CBB
13	5	506	CLA	C2B-C3B-CAB-CBB
13	5	511	CLA	C2B-C3B-CAB-CBB
13	6	504	CLA	C2B-C3B-CAB-CBB
13	6	511	CLA	C2B-C3B-CAB-CBB
13	G	1108	CLA	C2B-C3B-CAB-CBB
13	G	1124	CLA	C2B-C3B-CAB-CBB
13	G	1133	CLA	C2B-C3B-CAB-CBB
13	G	1130	CLA	C2B-C3B-CAB-CBB
13	H	1208	CLA	C2B-C3B-CAB-CBB
13	H	1217	CLA	C2B-C3B-CAB-CBB
13	H	1240	CLA	C2B-C3B-CAB-CBB
13	V	1502	CLA	C2B-C3B-CAB-CBB
13	Y	502	CLA	C2B-C3B-CAB-CBB
13	Y	503	CLA	C2B-C3B-CAB-CBB
13	Y	508	CLA	C2B-C3B-CAB-CBB
13	Z	508	CLA	C2B-C3B-CAB-CBB
13	a	505	CLA	C2B-C3B-CAB-CBB
13	a	510	CLA	C2B-C3B-CAB-CBB
13	a	511	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	516	CLA	C2B-C3B-CAB-CBB
13	b	504	CLA	C2B-C3B-CAB-CBB
13	b	506	CLA	C2B-C3B-CAB-CBB
13	b	513	CLA	C2B-C3B-CAB-CBB
13	c	501	CLA	C2B-C3B-CAB-CBB
13	c	506	CLA	C2B-C3B-CAB-CBB
13	c	510	CLA	C2B-C3B-CAB-CBB
13	c	511	CLA	C2B-C3B-CAB-CBB
13	d	504	CLA	C2B-C3B-CAB-CBB
13	d	511	CLA	C2B-C3B-CAB-CBB
13	e	1108	CLA	C2B-C3B-CAB-CBB
13	e	1124	CLA	C2B-C3B-CAB-CBB
13	e	1133	CLA	C2B-C3B-CAB-CBB
13	e	1130	CLA	C2B-C3B-CAB-CBB
13	f	1208	CLA	C2B-C3B-CAB-CBB
13	f	1217	CLA	C2B-C3B-CAB-CBB
13	f	1240	CLA	C2B-C3B-CAB-CBB
13	n	1502	CLA	C2B-C3B-CAB-CBB
13	q	502	CLA	C2B-C3B-CAB-CBB
13	q	503	CLA	C2B-C3B-CAB-CBB
13	q	508	CLA	C2B-C3B-CAB-CBB
13	r	508	CLA	C2B-C3B-CAB-CBB
13	s	505	CLA	C2B-C3B-CAB-CBB
13	s	510	CLA	C2B-C3B-CAB-CBB
13	s	511	CLA	C2B-C3B-CAB-CBB
13	s	513	CLA	C2B-C3B-CAB-CBB
13	s	516	CLA	C2B-C3B-CAB-CBB
13	t	504	CLA	C2B-C3B-CAB-CBB
13	t	506	CLA	C2B-C3B-CAB-CBB
13	u	501	CLA	C2B-C3B-CAB-CBB
13	u	506	CLA	C2B-C3B-CAB-CBB
13	u	511	CLA	C2B-C3B-CAB-CBB
13	v	504	CLA	C2B-C3B-CAB-CBB
13	v	511	CLA	C2B-C3B-CAB-CBB
16	L	4219	BCR	C5-C6-C7-C8
16	3	522	BCR	C1-C6-C7-C8
16	3	522	BCR	C5-C6-C7-C8
16	5	521	BCR	C5-C6-C7-C8
16	6	524	BCR	C5-C6-C7-C8
16	V	4219	BCR	C5-C6-C7-C8
16	a	522	BCR	C1-C6-C7-C8
16	a	522	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	c	521	BCR	C5-C6-C7-C8
16	d	524	BCR	C5-C6-C7-C8
16	n	4219	BCR	C5-C6-C7-C8
16	s	522	BCR	C1-C6-C7-C8
16	s	522	BCR	C5-C6-C7-C8
16	u	521	BCR	C5-C6-C7-C8
16	v	524	BCR	C5-C6-C7-C8
13	s	507	CLA	CAA-CBA-CGA-O2A
17	e	5007	LHG	C27-C28-C29-C30
13	A	1106	CLA	C2-C1-O2A-CGA
13	B	1219	CLA	C2-C1-O2A-CGA
13	3	505	CLA	C2-C1-O2A-CGA
13	5	505	CLA	C2-C1-O2A-CGA
13	6	505	CLA	C2-C1-O2A-CGA
13	G	1106	CLA	C2-C1-O2A-CGA
13	H	1219	CLA	C2-C1-O2A-CGA
13	a	505	CLA	C2-C1-O2A-CGA
13	c	505	CLA	C2-C1-O2A-CGA
13	d	505	CLA	C2-C1-O2A-CGA
13	e	1106	CLA	C2-C1-O2A-CGA
13	f	1219	CLA	C2-C1-O2A-CGA
13	s	505	CLA	C2-C1-O2A-CGA
13	u	505	CLA	C2-C1-O2A-CGA
13	v	505	CLA	C2-C1-O2A-CGA
13	6	516	CLA	CAA-CBA-CGA-O1A
13	d	516	CLA	CAA-CBA-CGA-O1A
17	A	5007	LHG	C27-C28-C29-C30
17	G	5007	LHG	C27-C28-C29-C30
13	B	1203	CLA	CAA-CBA-CGA-O2A
13	H	1203	CLA	CAA-CBA-CGA-O2A
13	f	1203	CLA	CAA-CBA-CGA-O2A
13	5	508	CLA	CAA-CBA-CGA-O2A
13	c	508	CLA	CAA-CBA-CGA-O2A
13	u	508	CLA	CAA-CBA-CGA-O2A
13	2	511	CLA	C4-C3-C5-C6
13	r	511	CLA	C4-C3-C5-C6
13	L	1501	CLA	CAA-CBA-CGA-O2A
13	V	1501	CLA	CAA-CBA-CGA-O2A
13	n	1501	CLA	CAA-CBA-CGA-O2A
18	G	1848	LMU	C7-C8-C9-C10
13	5	505	CLA	O1D-CGD-O2D-CED
13	e	1140	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	1855	LHG	C16-C17-C18-C19
17	f	1855	LHG	C16-C17-C18-C19
18	A	1848	LMU	C7-C8-C9-C10
17	A	5003	LHG	O7-C7-C8-C9
19	B	5002	LMG	O7-C10-C11-C12
19	f	5002	LMG	O7-C10-C11-C12
13	1	507	CLA	C3-C5-C6-C7
13	Y	507	CLA	C3-C5-C6-C7
13	q	507	CLA	C3-C5-C6-C7
17	B	1855	LHG	C16-C17-C18-C19
18	e	1848	LMU	C7-C8-C9-C10
13	f	1215	CLA	C15-C16-C17-C18
17	n	5218	LHG	C25-C26-C27-C28
17	L	5218	LHG	C25-C26-C27-C28
17	V	5218	LHG	C25-C26-C27-C28
13	A	1107	CLA	C8-C10-C11-C12
13	B	1215	CLA	C15-C16-C17-C18
13	G	1107	CLA	C8-C10-C11-C12
13	H	1215	CLA	C15-C16-C17-C18
13	e	1107	CLA	C8-C10-C11-C12
13	B	1206	CLA	CAA-CBA-CGA-O2A
13	H	1206	CLA	CAA-CBA-CGA-O2A
13	a	501	CLA	CAA-CBA-CGA-O2A
13	f	1206	CLA	CAA-CBA-CGA-O2A
17	G	5003	LHG	O7-C7-C8-C9
17	e	5003	LHG	O7-C7-C8-C9
19	H	5002	LMG	O7-C10-C11-C12
13	G	1140	CLA	O1D-CGD-O2D-CED
13	1	517	CLA	CAA-CBA-CGA-O1A
13	H	1023	CLA	C8-C10-C11-C12
19	J	5104	LMG	C29-C30-C31-C32
19	l	5104	LMG	C29-C30-C31-C32
20	1	822	SQD	C11-C12-C13-C14
20	Y	822	SQD	C11-C12-C13-C14
13	A	1237	CLA	CAA-CBA-CGA-O2A
13	3	501	CLA	CAA-CBA-CGA-O2A
13	4	519	CLA	CAA-CBA-CGA-O2A
13	5	501	CLA	CAA-CBA-CGA-O2A
13	G	1237	CLA	CAA-CBA-CGA-O2A
13	b	519	CLA	CAA-CBA-CGA-O2A
13	c	501	CLA	CAA-CBA-CGA-O2A
13	e	1237	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	s	501	CLA	CAA-CBA-CGA-O2A
13	t	519	CLA	CAA-CBA-CGA-O2A
13	u	501	CLA	CAA-CBA-CGA-O2A
17	G	5005	LHG	C33-C34-C35-C36
13	A	1135	CLA	C2-C3-C5-C6
13	G	1135	CLA	C2-C3-C5-C6
13	e	1135	CLA	C2-C3-C5-C6
19	T	5104	LMG	C29-C30-C31-C32
13	c	505	CLA	O1D-CGD-O2D-CED
13	5	505	CLA	CBD-CGD-O2D-CED
13	u	505	CLA	CBD-CGD-O2D-CED
20	q	822	SQD	C11-C12-C13-C14
17	A	5005	LHG	C33-C34-C35-C36
17	e	5005	LHG	C33-C34-C35-C36
13	v	501	CLA	C2A-CAA-CBA-CGA
13	Y	517	CLA	CAA-CBA-CGA-O1A
13	q	517	CLA	CAA-CBA-CGA-O1A
13	f	1023	CLA	C8-C10-C11-C12
13	1	501	CLA	CAA-CBA-CGA-O2A
13	U	1401	CLA	CAA-CBA-CGA-O2A
13	Y	501	CLA	CAA-CBA-CGA-O2A
13	m	1401	CLA	CAA-CBA-CGA-O2A
13	q	501	CLA	CAA-CBA-CGA-O2A
13	G	1127	CLA	CBA-CGA-O2A-C1
18	2	901	LMU	C2-C1-O1'-C1'
18	r	901	LMU	C2-C1-O1'-C1'
13	c	505	CLA	CBD-CGD-O2D-CED
13	B	1023	CLA	C8-C10-C11-C12
16	1	521	BCR	C36-C18-C19-C20
16	q	521	BCR	C36-C18-C19-C20
13	K	1401	CLA	CAA-CBA-CGA-O2A
17	L	5220	LHG	O8-C23-C24-C25
17	n	5220	LHG	O8-C23-C24-C25
13	A	1108	CLA	C4B-C3B-CAB-CBB
13	A	1111	CLA	C4B-C3B-CAB-CBB
13	A	1117	CLA	C4B-C3B-CAB-CBB
13	A	1133	CLA	C4B-C3B-CAB-CBB
13	A	1130	CLA	C4B-C3B-CAB-CBB
13	B	1012	CLA	C1A-C2A-CAA-CBA
13	L	1501	CLA	C4B-C3B-CAB-CBB
13	L	1502	CLA	C1A-C2A-CAA-CBA
13	1	507	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	1	512	CLA	C1A-C2A-CAA-CBA
13	1	518	CLA	C1A-C2A-CAA-CBA
13	3	505	CLA	C4B-C3B-CAB-CBB
13	3	510	CLA	C4B-C3B-CAB-CBB
13	4	502	CLA	C1A-C2A-CAA-CBA
13	4	511	CLA	C4B-C3B-CAB-CBB
13	5	505	CLA	C1A-C2A-CAA-CBA
13	5	506	CLA	C4B-C3B-CAB-CBB
13	6	506	CLA	C4B-C3B-CAB-CBB
13	G	1108	CLA	C4B-C3B-CAB-CBB
13	G	1111	CLA	C4B-C3B-CAB-CBB
13	G	1117	CLA	C4B-C3B-CAB-CBB
13	G	1133	CLA	C4B-C3B-CAB-CBB
13	G	1130	CLA	C4B-C3B-CAB-CBB
13	H	1012	CLA	C1A-C2A-CAA-CBA
13	V	1501	CLA	C4B-C3B-CAB-CBB
13	V	1502	CLA	C1A-C2A-CAA-CBA
13	Y	507	CLA	C4B-C3B-CAB-CBB
13	Y	512	CLA	C1A-C2A-CAA-CBA
13	Y	518	CLA	C1A-C2A-CAA-CBA
13	a	505	CLA	C4B-C3B-CAB-CBB
13	a	510	CLA	C4B-C3B-CAB-CBB
13	b	502	CLA	C1A-C2A-CAA-CBA
13	b	511	CLA	C4B-C3B-CAB-CBB
13	c	505	CLA	C1A-C2A-CAA-CBA
13	c	506	CLA	C4B-C3B-CAB-CBB
13	d	506	CLA	C4B-C3B-CAB-CBB
13	e	1108	CLA	C4B-C3B-CAB-CBB
13	e	1111	CLA	C4B-C3B-CAB-CBB
13	e	1117	CLA	C4B-C3B-CAB-CBB
13	e	1133	CLA	C4B-C3B-CAB-CBB
13	e	1130	CLA	C4B-C3B-CAB-CBB
13	f	1012	CLA	C1A-C2A-CAA-CBA
13	n	1501	CLA	C4B-C3B-CAB-CBB
13	n	1502	CLA	C1A-C2A-CAA-CBA
13	q	503	CLA	C1A-C2A-CAA-CBA
13	q	507	CLA	C4B-C3B-CAB-CBB
13	q	512	CLA	C1A-C2A-CAA-CBA
13	q	518	CLA	C1A-C2A-CAA-CBA
13	s	505	CLA	C4B-C3B-CAB-CBB
13	s	510	CLA	C4B-C3B-CAB-CBB
13	t	502	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	t	511	CLA	C4B-C3B-CAB-CBB
13	u	505	CLA	C1A-C2A-CAA-CBA
13	u	506	CLA	C4B-C3B-CAB-CBB
13	v	506	CLA	C4B-C3B-CAB-CBB
13	A	1127	CLA	CBA-CGA-O2A-C1
13	A	1133	CLA	C15-C16-C17-C18
20	6	822	SQD	O5-C1-O6-C44
20	d	822	SQD	O5-C1-O6-C44
20	v	822	SQD	O5-C1-O6-C44
13	B	1221	CLA	CAA-CBA-CGA-O2A
13	f	1221	CLA	CAA-CBA-CGA-O2A
16	Y	524	BCR	C11-C12-C13-C14
16	M	4021	BCR	C9-C10-C11-C12
16	2	522	BCR	C15-C16-C17-C18
16	W	4021	BCR	C9-C10-C11-C12
16	Z	522	BCR	C15-C16-C17-C18
16	o	4021	BCR	C9-C10-C11-C12
16	r	522	BCR	C15-C16-C17-C18
13	G	1133	CLA	C15-C16-C17-C18
17	L	5221	LHG	C7-C8-C9-C10
17	V	5221	LHG	C7-C8-C9-C10
17	A	5005	LHG	C32-C33-C34-C35
17	G	5005	LHG	C32-C33-C34-C35
18	Z	901	LMU	C3-C4-C5-C6
18	2	901	LMU	C3-C4-C5-C6
13	e	1127	CLA	CBA-CGA-O2A-C1
13	H	1023	CLA	C13-C15-C16-C17
13	e	1133	CLA	C15-C16-C17-C18
17	e	5005	LHG	C32-C33-C34-C35
18	r	901	LMU	C3-C4-C5-C6
13	A	1106	CLA	CAA-CBA-CGA-O2A
13	A	1107	CLA	CAA-CBA-CGA-O2A
13	A	1135	CLA	CAA-CBA-CGA-O2A
13	6	501	CLA	CAA-CBA-CGA-O2A
13	G	1106	CLA	CAA-CBA-CGA-O2A
13	G	1107	CLA	CAA-CBA-CGA-O2A
13	G	1135	CLA	CAA-CBA-CGA-O2A
13	H	1221	CLA	CAA-CBA-CGA-O2A
13	d	501	CLA	CAA-CBA-CGA-O2A
13	e	1106	CLA	CAA-CBA-CGA-O2A
13	e	1107	CLA	CAA-CBA-CGA-O2A
13	e	1135	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	v	501	CLA	CAA-CBA-CGA-O2A
17	V	5220	LHG	O8-C23-C24-C25
20	Z	822	SQD	C25-C26-C27-C28
13	A	1110	CLA	C2A-CAA-CBA-CGA
13	A	1117	CLA	C2A-CAA-CBA-CGA
13	6	501	CLA	C2A-CAA-CBA-CGA
13	G	1117	CLA	C2A-CAA-CBA-CGA
13	d	501	CLA	C2A-CAA-CBA-CGA
13	e	1110	CLA	C2A-CAA-CBA-CGA
13	e	1117	CLA	C2A-CAA-CBA-CGA
20	2	822	SQD	C25-C26-C27-C28
20	r	822	SQD	C25-C26-C27-C28
13	B	1023	CLA	C13-C15-C16-C17
13	f	1023	CLA	C13-C15-C16-C17
13	A	1124	CLA	O1A-CGA-O2A-C1
13	B	1204	CLA	O1A-CGA-O2A-C1
13	H	1204	CLA	O1A-CGA-O2A-C1
13	e	1124	CLA	O1A-CGA-O2A-C1
13	f	1204	CLA	O1A-CGA-O2A-C1
17	n	5221	LHG	C7-C8-C9-C10
13	A	1108	CLA	CAA-CBA-CGA-O2A
13	B	1219	CLA	CAA-CBA-CGA-O2A
13	4	501	CLA	CAA-CBA-CGA-O2A
13	G	1108	CLA	CAA-CBA-CGA-O2A
13	H	1219	CLA	CAA-CBA-CGA-O2A
13	b	501	CLA	CAA-CBA-CGA-O2A
13	e	1108	CLA	CAA-CBA-CGA-O2A
13	f	1219	CLA	CAA-CBA-CGA-O2A
13	t	501	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	O8-C23-C24-C25
17	G	5001	LHG	O8-C23-C24-C25
17	e	5001	LHG	O8-C23-C24-C25
20	B	1852	SQD	C5-C6-S-O7
20	3	822	SQD	C5-C6-S-O7
20	4	822	SQD	C5-C6-S-O7
20	H	1852	SQD	C5-C6-S-O7
20	a	822	SQD	C5-C6-S-O7
20	b	822	SQD	C5-C6-S-O7
20	f	1852	SQD	C5-C6-S-O7
20	s	822	SQD	C5-C6-S-O7
20	t	822	SQD	C5-C6-S-O7
13	A	1011	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	H	1229	CLA	C10-C11-C12-C13
13	e	1011	CLA	C8-C10-C11-C12
13	A	1107	CLA	C2-C1-O2A-CGA
13	B	1212	CLA	C2-C1-O2A-CGA
13	L	1502	CLA	C2-C1-O2A-CGA
13	1	511	CLA	C2-C1-O2A-CGA
13	3	511	CLA	C2-C1-O2A-CGA
13	G	1107	CLA	C2-C1-O2A-CGA
13	H	1212	CLA	C2-C1-O2A-CGA
13	V	1502	CLA	C2-C1-O2A-CGA
13	Y	511	CLA	C2-C1-O2A-CGA
13	a	511	CLA	C2-C1-O2A-CGA
13	e	1107	CLA	C2-C1-O2A-CGA
13	f	1212	CLA	C2-C1-O2A-CGA
13	n	1502	CLA	C2-C1-O2A-CGA
13	q	511	CLA	C2-C1-O2A-CGA
13	s	511	CLA	C2-C1-O2A-CGA
13	A	1011	CLA	C12-C13-C15-C16
13	A	1119	CLA	C6-C7-C8-C10
13	A	1119	CLA	C12-C13-C15-C16
13	A	1133	CLA	C12-C13-C15-C16
13	3	505	CLA	C11-C12-C13-C15
13	G	1011	CLA	C12-C13-C15-C16
13	G	1119	CLA	C6-C7-C8-C10
13	G	1119	CLA	C12-C13-C15-C16
13	G	1133	CLA	C12-C13-C15-C16
13	a	505	CLA	C11-C12-C13-C15
13	e	1011	CLA	C12-C13-C15-C16
13	e	1119	CLA	C6-C7-C8-C10
13	e	1119	CLA	C12-C13-C15-C16
13	e	1133	CLA	C12-C13-C15-C16
13	s	505	CLA	C11-C12-C13-C15
13	4	519	CLA	C5-C6-C7-C8
13	G	1011	CLA	C8-C10-C11-C12
13	b	519	CLA	C5-C6-C7-C8
13	t	519	CLA	C5-C6-C7-C8
17	e	5001	LHG	C28-C29-C30-C31
13	5	508	CLA	CAA-CBA-CGA-O1A
13	c	508	CLA	CAA-CBA-CGA-O1A
13	u	508	CLA	CAA-CBA-CGA-O1A
13	A	1126	CLA	O2A-C1-C2-C3
13	G	1126	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	e	1126	CLA	O2A-C1-C2-C3
17	A	5001	LHG	C28-C29-C30-C31
13	G	1124	CLA	O1A-CGA-O2A-C1
13	F	1302	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	C10-C11-C12-C13
13	A	1138	CLA	C15-C16-C17-C18
13	B	1229	CLA	C10-C11-C12-C13
13	G	1123	CLA	C10-C11-C12-C13
13	G	1138	CLA	C15-C16-C17-C18
13	e	1123	CLA	C10-C11-C12-C13
13	e	1138	CLA	C15-C16-C17-C18
13	f	1021	CLA	C13-C15-C16-C17
13	f	1229	CLA	C10-C11-C12-C13
17	G	5001	LHG	C28-C29-C30-C31
13	G	1110	CLA	C2A-CAA-CBA-CGA
13	B	1021	CLA	C13-C15-C16-C17
13	L	1502	CLA	C8-C10-C11-C12
13	H	1021	CLA	C13-C15-C16-C17
13	V	1502	CLA	C8-C10-C11-C12
13	n	1502	CLA	C8-C10-C11-C12
13	b	516	CLA	CAA-CBA-CGA-O1A
13	j	1302	CLA	CAA-CBA-CGA-O1A
17	A	5006	LHG	O8-C23-C24-C25
17	G	5006	LHG	O8-C23-C24-C25
13	e	1126	CLA	CBA-CGA-O2A-C1
13	4	516	CLA	CAA-CBA-CGA-O1A
13	R	1302	CLA	CAA-CBA-CGA-O1A
13	t	516	CLA	CAA-CBA-CGA-O1A
13	B	1012	CLA	C3A-C2A-CAA-CBA
13	B	1223	CLA	C3A-C2A-CAA-CBA
13	1	512	CLA	C3A-C2A-CAA-CBA
13	H	1012	CLA	C3A-C2A-CAA-CBA
13	H	1223	CLA	C3A-C2A-CAA-CBA
13	f	1012	CLA	C3A-C2A-CAA-CBA
13	f	1223	CLA	C3A-C2A-CAA-CBA
13	4	519	CLA	CAA-CBA-CGA-O1A
13	b	519	CLA	CAA-CBA-CGA-O1A
13	t	519	CLA	CAA-CBA-CGA-O1A
13	A	1126	CLA	CBA-CGA-O2A-C1
17	A	5001	LHG	O6-C4-C5-O7
17	G	5001	LHG	O6-C4-C5-O7
17	e	5001	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	5008	LHG	O7-C7-C8-C9
17	e	5006	LHG	O8-C23-C24-C25
13	B	1206	CLA	CAA-CBA-CGA-O1A
13	H	1206	CLA	CAA-CBA-CGA-O1A
17	A	5007	LHG	O9-C7-C8-C9
13	G	1126	CLA	CBA-CGA-O2A-C1
13	A	1119	CLA	C14-C13-C15-C16
13	B	1203	CLA	C11-C10-C8-C9
13	B	1229	CLA	C11-C10-C8-C9
13	G	1119	CLA	C14-C13-C15-C16
13	H	1203	CLA	C11-C10-C8-C9
13	H	1229	CLA	C11-C10-C8-C9
13	e	1119	CLA	C14-C13-C15-C16
13	f	1203	CLA	C11-C10-C8-C9
13	f	1229	CLA	C11-C10-C8-C9
13	3	501	CLA	CAA-CBA-CGA-O1A
13	3	519	CLA	CAA-CBA-CGA-O1A
13	a	519	CLA	CAA-CBA-CGA-O1A
13	f	1206	CLA	CAA-CBA-CGA-O1A
13	s	507	CLA	CAA-CBA-CGA-O1A
13	s	519	CLA	CAA-CBA-CGA-O1A
17	e	5007	LHG	O9-C7-C8-C9
16	I	4018	BCR	C15-C16-C17-C18
16	S	4018	BCR	C15-C16-C17-C18
16	k	4018	BCR	C15-C16-C17-C18
16	e	4011	BCR	C7-C8-C9-C34
13	3	505	CLA	C4-C3-C5-C6
13	a	505	CLA	C4-C3-C5-C6
13	s	505	CLA	C4-C3-C5-C6
13	3	507	CLA	CAA-CBA-CGA-O1A
13	s	501	CLA	CAA-CBA-CGA-O1A
17	G	5007	LHG	O9-C7-C8-C9
20	L	5216	SQD	O5-C5-C6-S
20	5	822	SQD	O5-C5-C6-S
20	6	822	SQD	O5-C5-C6-S
20	V	5216	SQD	O5-C5-C6-S
20	c	822	SQD	O5-C5-C6-S
20	d	822	SQD	O5-C5-C6-S
20	n	5216	SQD	O5-C5-C6-S
20	u	822	SQD	O5-C5-C6-S
20	v	822	SQD	O5-C5-C6-S
13	A	1123	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	501	CLA	CAA-CBA-CGA-O1A
13	a	507	CLA	CAA-CBA-CGA-O1A
13	e	1123	CLA	CAA-CBA-CGA-O1A
13	f	1203	CLA	CAA-CBA-CGA-O1A
13	5	519	CLA	CAA-CBA-CGA-O2A
13	c	519	CLA	CAA-CBA-CGA-O2A
17	A	5008	LHG	O7-C7-C8-C9
17	e	5008	LHG	O7-C7-C8-C9
16	1	524	BCR	C11-C12-C13-C14
16	q	524	BCR	C11-C12-C13-C14
20	5	822	SQD	O10-C23-C24-C25
20	c	822	SQD	O10-C23-C24-C25
20	u	822	SQD	O10-C23-C24-C25
13	B	1203	CLA	CAA-CBA-CGA-O1A
13	G	1123	CLA	CAA-CBA-CGA-O1A
13	H	1203	CLA	CAA-CBA-CGA-O1A
13	f	1221	CLA	CAA-CBA-CGA-O1A
20	f	1852	SQD	O49-C7-C8-C9
13	A	1108	CLA	CAA-CBA-CGA-O1A
13	A	1237	CLA	CAA-CBA-CGA-O1A
13	B	1219	CLA	CAA-CBA-CGA-O1A
13	B	1221	CLA	CAA-CBA-CGA-O1A
13	G	1108	CLA	CAA-CBA-CGA-O1A
13	G	1237	CLA	CAA-CBA-CGA-O1A
13	H	1219	CLA	CAA-CBA-CGA-O1A
13	H	1221	CLA	CAA-CBA-CGA-O1A
13	Y	501	CLA	CAA-CBA-CGA-O1A
13	e	1108	CLA	CAA-CBA-CGA-O1A
13	e	1237	CLA	CAA-CBA-CGA-O1A
13	f	1219	CLA	CAA-CBA-CGA-O1A
17	A	5008	LHG	O9-C7-C8-C9
17	B	1842	LHG	O9-C7-C8-C9
17	G	5008	LHG	O9-C7-C8-C9
17	H	1842	LHG	O9-C7-C8-C9
17	e	5008	LHG	O9-C7-C8-C9
17	f	1842	LHG	O9-C7-C8-C9
19	B	5002	LMG	O10-C28-C29-C30
19	H	5002	LMG	O10-C28-C29-C30
19	f	5002	LMG	O10-C28-C29-C30
20	B	1852	SQD	O49-C7-C8-C9
20	H	1852	SQD	O49-C7-C8-C9
20	s	822	SQD	O10-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	2	509	CLA	CAA-CBA-CGA-O2A
13	Z	509	CLA	CAA-CBA-CGA-O2A
13	r	509	CLA	CAA-CBA-CGA-O2A
13	u	519	CLA	CAA-CBA-CGA-O2A
13	A	1106	CLA	CAA-CBA-CGA-O1A
13	K	1401	CLA	CAA-CBA-CGA-O1A
13	1	501	CLA	CAA-CBA-CGA-O1A
13	U	1401	CLA	CAA-CBA-CGA-O1A
13	m	1401	CLA	CAA-CBA-CGA-O1A
13	q	501	CLA	CAA-CBA-CGA-O1A
20	3	822	SQD	O10-C23-C24-C25
20	a	822	SQD	O10-C23-C24-C25
17	A	5002	LHG	C5-C4-O6-P
17	G	5002	LHG	C5-C4-O6-P
17	e	5002	LHG	C5-C4-O6-P
19	B	5002	LMG	O8-C28-C29-C30
19	H	5002	LMG	O8-C28-C29-C30
19	f	5002	LMG	O8-C28-C29-C30
16	2	524	BCR	C9-C10-C11-C12
16	Z	524	BCR	C9-C10-C11-C12
13	A	1135	CLA	CAA-CBA-CGA-O1A
13	4	501	CLA	CAA-CBA-CGA-O1A
13	G	1106	CLA	CAA-CBA-CGA-O1A
13	G	1135	CLA	CAA-CBA-CGA-O1A
13	e	1106	CLA	CAA-CBA-CGA-O1A
13	e	1135	CLA	CAA-CBA-CGA-O1A
13	A	1102	CLA	CAD-CBD-CGD-O2D
13	A	1116	CLA	CAD-CBD-CGD-O2D
13	A	1801	CLA	CAD-CBD-CGD-O2D
13	B	1202	CLA	CAD-CBD-CGD-O2D
13	B	1218	CLA	CAD-CBD-CGD-O2D
13	K	1105	CLA	CAD-CBD-CGD-O2D
13	1	505	CLA	CAD-CBD-CGD-O2D
13	1	519	CLA	CAD-CBD-CGD-O2D
13	4	509	CLA	CAD-CBD-CGD-O2D
13	6	503	CLA	CAD-CBD-CGD-O2D
13	G	1102	CLA	CAD-CBD-CGD-O2D
13	G	1116	CLA	CAD-CBD-CGD-O2D
13	G	1801	CLA	CAD-CBD-CGD-O2D
13	H	1202	CLA	CAD-CBD-CGD-O2D
13	H	1218	CLA	CAD-CBD-CGD-O2D
13	U	1105	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Y	505	CLA	CAD-CBD-CGD-O2D
13	Y	519	CLA	CAD-CBD-CGD-O2D
13	b	509	CLA	CAD-CBD-CGD-O2D
13	d	503	CLA	CAD-CBD-CGD-O2D
13	e	1102	CLA	CAD-CBD-CGD-O2D
13	e	1116	CLA	CAD-CBD-CGD-O2D
13	e	1801	CLA	CAD-CBD-CGD-O2D
13	f	1202	CLA	CAD-CBD-CGD-O2D
13	f	1218	CLA	CAD-CBD-CGD-O2D
13	m	1105	CLA	CAD-CBD-CGD-O2D
13	q	505	CLA	CAD-CBD-CGD-O2D
13	q	519	CLA	CAD-CBD-CGD-O2D
13	t	509	CLA	CAD-CBD-CGD-O2D
13	v	503	CLA	CAD-CBD-CGD-O2D
13	2	510	CLA	CAA-CBA-CGA-O2A
13	Z	510	CLA	CAA-CBA-CGA-O2A
13	r	510	CLA	CAA-CBA-CGA-O2A
13	b	501	CLA	CAA-CBA-CGA-O1A
13	t	501	CLA	CAA-CBA-CGA-O1A
13	A	1237	CLA	C13-C15-C16-C17
13	e	1237	CLA	C13-C15-C16-C17
13	B	1207	CLA	C2-C1-O2A-CGA
13	5	511	CLA	C2-C1-O2A-CGA
13	H	1207	CLA	C2-C1-O2A-CGA
13	c	511	CLA	C2-C1-O2A-CGA
13	f	1207	CLA	C2-C1-O2A-CGA
13	u	511	CLA	C2-C1-O2A-CGA
13	L	1501	CLA	CAA-CBA-CGA-O1A
13	5	501	CLA	CAA-CBA-CGA-O1A
13	V	1501	CLA	CAA-CBA-CGA-O1A
13	H	1222	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	CAA-CBA-CGA-O2A
13	A	1137	CLA	CAA-CBA-CGA-O2A
13	G	1013	CLA	CAA-CBA-CGA-O2A
13	G	1137	CLA	CAA-CBA-CGA-O2A
13	H	1021	CLA	CAA-CBA-CGA-O2A
13	e	1137	CLA	CAA-CBA-CGA-O2A
13	f	1021	CLA	CAA-CBA-CGA-O2A
13	G	1237	CLA	C13-C15-C16-C17
13	d	501	CLA	CAA-CBA-CGA-O1A
13	u	501	CLA	CAA-CBA-CGA-O1A
13	u	505	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	1116	CLA	CAA-CBA-CGA-O2A
13	A	1125	CLA	CAA-CBA-CGA-O2A
13	B	1021	CLA	CAA-CBA-CGA-O2A
13	2	501	CLA	CAA-CBA-CGA-O2A
13	G	1116	CLA	CAA-CBA-CGA-O2A
13	G	1125	CLA	CAA-CBA-CGA-O2A
13	Z	501	CLA	CAA-CBA-CGA-O2A
13	e	1013	CLA	CAA-CBA-CGA-O2A
13	e	1116	CLA	CAA-CBA-CGA-O2A
13	e	1125	CLA	CAA-CBA-CGA-O2A
13	r	501	CLA	CAA-CBA-CGA-O2A
17	G	5007	LHG	O7-C7-C8-C9
13	c	505	CLA	C10-C11-C12-C13
13	4	516	CLA	CAA-CBA-CGA-O2A
13	b	516	CLA	CAA-CBA-CGA-O2A
13	t	516	CLA	CAA-CBA-CGA-O2A
13	6	501	CLA	CAA-CBA-CGA-O1A
13	c	501	CLA	CAA-CBA-CGA-O1A
13	n	1501	CLA	CAA-CBA-CGA-O1A
13	v	501	CLA	CAA-CBA-CGA-O1A
13	5	505	CLA	C10-C11-C12-C13
13	A	1103	CLA	CAA-CBA-CGA-O2A
13	A	1110	CLA	CAA-CBA-CGA-O2A
13	G	1103	CLA	CAA-CBA-CGA-O2A
13	e	1103	CLA	CAA-CBA-CGA-O2A
13	e	1110	CLA	CAA-CBA-CGA-O2A
17	A	5007	LHG	O7-C7-C8-C9
17	B	1855	LHG	O7-C7-C8-C9
17	H	1855	LHG	O7-C7-C8-C9
17	f	1855	LHG	O7-C7-C8-C9
13	B	1222	CLA	O1D-CGD-O2D-CED
13	F	1302	CLA	CAA-CBA-CGA-O2A
13	R	1302	CLA	CAA-CBA-CGA-O2A
13	j	1302	CLA	CAA-CBA-CGA-O2A
13	A	1107	CLA	CAA-CBA-CGA-O1A
13	G	1107	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

704 monomers are involved in 1558 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	6	519	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	1226	CLA	7	0
13	A	1114	CLA	1	0
13	Y	508	CLA	1	0
13	d	513	CLA	1	0
13	e	1128	CLA	5	0
13	B	1228	CLA	4	0
13	4	516	CLA	1	0
13	A	1111	CLA	1	0
13	B	1235	CLA	3	0
13	f	1226	CLA	6	0
16	r	524	BCR	7	0
13	H	1220	CLA	3	0
13	c	510	CLA	1	0
13	m	1103	CLA	2	0
13	U	1401	CLA	1	0
13	u	502	CLA	3	0
13	v	502	CLA	2	0
17	H	1842	LHG	2	0
13	e	1136	CLA	2	0
13	Y	518	CLA	2	0
13	B	1210	CLA	4	0
16	q	524	BCR	5	0
13	3	501	CLA	2	0
13	e	1114	CLA	1	0
16	u	521	BCR	4	0
13	f	1221	CLA	6	0
13	U	1105	CLA	1	0
13	G	1130	CLA	4	0
13	Y	502	CLA	7	0
13	2	517	CLA	1	0
13	A	1119	CLA	4	0
13	A	1011	CLA	4	0
13	G	1102	CLA	3	0
13	G	1103	CLA	4	0
13	3	506	CLA	1	0
16	H	4009	BCR	4	0
13	H	1218	CLA	2	0
13	t	513	CLA	1	0
16	v	521	BCR	2	0
13	H	1204	CLA	1	0
13	a	513	CLA	3	0
13	2	512	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	e	4002	BCR	3	0
16	u	524	BCR	3	0
13	A	1120	CLA	2	0
13	B	1223	CLA	1	0
13	H	1213	CLA	1	0
13	B	1214	CLA	2	0
16	f	4009	BCR	5	0
13	1	508	CLA	2	0
13	3	519	CLA	1	0
13	t	518	CLA	1	0
16	T	4012	BCR	6	0
13	n	1503	CLA	2	0
13	b	519	CLA	2	0
13	A	1135	CLA	2	0
17	G	5005	LHG	1	0
16	A	4011	BCR	4	0
13	b	517	CLA	2	0
13	5	513	CLA	1	0
13	H	1225	CLA	3	0
13	u	506	CLA	3	0
14	e	2001	PQN	2	0
13	r	517	CLA	1	0
13	G	1137	CLA	2	0
13	v	505	CLA	4	0
13	G	1135	CLA	3	0
13	Y	510	CLA	1	0
13	a	511	CLA	1	0
13	a	519	CLA	1	0
17	I	5001	LHG	1	0
13	1	507	CLA	3	0
16	H	4006	BCR	1	0
13	G	1136	CLA	2	0
16	l	4012	BCR	5	0
13	s	509	CLA	1	0
13	e	1119	CLA	5	0
16	t	523	BCR	3	0
13	A	1139	CLA	3	0
13	A	1013	CLA	7	0
13	1	503	CLA	4	0
16	Z	523	BCR	1	0
13	Z	507	CLA	2	0
13	G	1013	CLA	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	509	CLA	1	0
13	2	519	CLA	1	0
13	H	1236	CLA	4	0
13	r	503	CLA	4	0
16	s	524	BCR	4	0
13	f	1228	CLA	3	0
13	s	506	CLA	1	0
16	5	522	BCR	2	0
20	f	1852	SQD	8	0
13	1	502	CLA	7	0
13	Z	509	CLA	1	0
20	H	1852	SQD	10	0
13	B	1222	CLA	4	0
13	t	517	CLA	2	0
13	G	1138	CLA	2	0
13	B	1219	CLA	5	0
13	G	1022	CLA	3	0
16	1	524	BCR	5	0
16	H	4014	BCR	4	0
13	G	1104	CLA	7	0
13	H	1238	CLA	1	0
17	G	5002	LHG	2	0
16	a	524	BCR	6	0
13	d	519	CLA	2	0
20	r	822	SQD	1	0
16	c	523	BCR	1	0
16	B	4009	BCR	5	0
13	q	512	CLA	6	0
16	u	523	BCR	2	0
13	r	510	CLA	3	0
16	5	521	BCR	4	0
13	e	1107	CLA	2	0
13	q	502	CLA	7	0
13	s	513	CLA	2	0
13	B	1240	CLA	1	0
16	3	522	BCR	5	0
17	e	5005	LHG	1	0
17	n	5221	LHG	10	0
16	V	4022	BCR	6	0
16	2	522	BCR	2	0
17	L	5221	LHG	11	0
13	B	1012	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	d	822	SQD	1	0
13	H	1201	CLA	3	0
13	A	1130	CLA	4	0
17	B	1855	LHG	2	0
13	A	1129	CLA	2	0
16	M	4021	BCR	2	0
16	3	521	BCR	2	0
18	l	5105	LMU	2	0
13	1	513	CLA	1	0
13	t	512	CLA	2	0
13	e	1115	CLA	1	0
13	e	1123	CLA	2	0
13	s	519	CLA	1	0
13	H	1219	CLA	5	0
13	d	517	CLA	3	0
13	j	1301	CLA	3	0
13	A	1126	CLA	8	0
13	f	1213	CLA	1	0
16	e	4003	BCR	4	0
17	f	1842	LHG	2	0
13	G	1125	CLA	1	0
13	q	510	CLA	2	0
16	l	4015	BCR	4	0
13	B	1229	CLA	5	0
13	b	512	CLA	2	0
13	A	1106	CLA	2	0
13	6	505	CLA	4	0
13	B	1023	CLA	3	0
17	e	5006	LHG	1	0
13	1	510	CLA	2	0
16	o	4021	BCR	4	0
16	S	4018	BCR	5	0
16	Y	521	BCR	2	0
13	H	1203	CLA	3	0
20	Z	822	SQD	1	0
13	Z	506	CLA	5	0
16	v	522	BCR	4	0
13	e	1131	CLA	1	0
13	e	1126	CLA	9	0
13	d	511	CLA	1	0
17	G	5004	LHG	1	0
13	q	503	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	4010	BCR	6	0
16	n	4020	BCR	3	0
13	r	502	CLA	5	0
13	e	1137	CLA	4	0
13	5	511	CLA	1	0
13	V	1502	CLA	2	0
13	H	1207	CLA	6	0
13	H	1012	CLA	2	0
13	A	1128	CLA	5	0
13	r	505	CLA	4	0
16	a	523	BCR	2	0
13	H	1224	CLA	6	0
13	q	516	CLA	2	0
17	A	5007	LHG	1	0
13	e	1118	CLA	2	0
16	J	4015	BCR	3	0
13	v	519	CLA	2	0
16	c	521	BCR	5	0
13	B	1231	CLA	3	0
13	q	508	CLA	2	0
16	J	4013	BCR	6	0
13	G	1109	CLA	3	0
13	v	506	CLA	1	0
13	r	511	CLA	3	0
13	G	1107	CLA	2	0
14	A	2001	PQN	3	0
16	k	4018	BCR	4	0
17	e	5007	LHG	1	0
17	V	5220	LHG	2	0
13	b	518	CLA	1	0
13	a	509	CLA	1	0
13	H	1221	CLA	6	0
13	f	1012	CLA	2	0
13	a	517	CLA	1	0
13	c	506	CLA	3	0
13	B	1209	CLA	1	0
16	c	522	BCR	2	0
16	G	4007	BCR	5	0
13	f	1217	CLA	4	0
13	U	1103	CLA	2	0
16	f	4004	BCR	3	0
13	B	1239	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	n	5216	SQD	4	0
13	r	512	CLA	5	0
14	H	2002	PQN	4	0
13	B	1216	CLA	1	0
13	t	505	CLA	1	0
16	T	4013	BCR	6	0
13	t	503	CLA	1	0
13	A	1801	CLA	3	0
13	A	1118	CLA	2	0
13	m	1401	CLA	1	0
13	K	1105	CLA	1	0
16	5	524	BCR	3	0
16	A	4001	BCR	1	0
17	n	5220	LHG	2	0
17	G	5009	LHG	4	0
16	G	4003	BCR	3	0
17	L	5220	LHG	2	0
13	6	513	CLA	1	0
13	G	1121	CLA	2	0
13	3	511	CLA	2	0
13	c	503	CLA	3	0
13	f	1204	CLA	2	0
17	G	5007	LHG	1	0
13	G	1131	CLA	1	0
13	c	509	CLA	1	0
17	k	5001	LHG	1	0
17	A	5008	LHG	2	0
13	G	1108	CLA	1	0
13	b	509	CLA	2	0
16	e	4001	BCR	2	0
13	u	510	CLA	1	0
16	Y	524	BCR	5	0
13	1	519	CLA	1	0
13	B	1225	CLA	3	0
13	t	510	CLA	1	0
13	H	1239	CLA	2	0
16	A	4002	BCR	4	0
20	L	5216	SQD	4	0
13	F	1301	CLA	2	0
13	v	513	CLA	1	0
13	u	507	CLA	1	0
16	q	522	BCR	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	f	1219	CLA	4	0
13	G	1118	CLA	2	0
13	4	513	CLA	1	0
16	6	522	BCR	4	0
13	B	1204	CLA	1	0
13	d	502	CLA	2	0
13	2	518	CLA	2	0
13	H	1217	CLA	4	0
13	Y	507	CLA	3	0
13	d	505	CLA	4	0
13	s	511	CLA	1	0
13	b	502	CLA	2	0
13	G	1133	CLA	1	0
20	a	822	SQD	1	0
16	e	4011	BCR	3	0
13	a	506	CLA	1	0
16	4	521	BCR	1	0
16	Y	522	BCR	5	0
13	a	503	CLA	3	0
13	t	502	CLA	2	0
13	u	511	CLA	1	0
13	H	1228	CLA	4	0
17	A	5001	LHG	4	0
13	3	509	CLA	1	0
13	e	1111	CLA	1	0
13	3	512	CLA	2	0
13	V	1501	CLA	8	0
13	j	1302	CLA	1	0
13	A	1123	CLA	2	0
17	G	5006	LHG	1	0
17	A	5005	LHG	1	0
17	e	5003	LHG	1	0
20	2	822	SQD	1	0
13	J	1302	CLA	1	0
16	6	521	BCR	2	0
13	Z	511	CLA	4	0
13	5	503	CLA	3	0
13	A	1117	CLA	2	0
13	A	1124	CLA	1	0
13	f	1208	CLA	1	0
16	3	524	BCR	6	0
13	1	511	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	f	5002	LMG	7	0
13	R	1302	CLA	2	0
13	L	1503	CLA	1	0
16	n	4022	BCR	6	0
13	a	518	CLA	1	0
16	1	523	BCR	1	0
13	Z	505	CLA	2	0
16	b	523	BCR	2	0
13	a	510	CLA	3	0
16	c	524	BCR	3	0
13	B	1236	CLA	5	0
13	e	1109	CLA	3	0
20	3	822	SQD	1	0
13	B	1224	CLA	6	0
13	e	1117	CLA	3	0
13	e	1105	CLA	2	0
16	A	4003	BCR	2	0
13	1	505	CLA	8	0
13	G	1122	CLA	3	0
16	Y	523	BCR	1	0
13	Y	512	CLA	6	0
13	e	1101	CLA	3	0
13	3	513	CLA	3	0
16	d	524	BCR	8	0
13	a	507	CLA	2	0
13	Z	518	CLA	2	0
13	l	1303	CLA	3	0
16	R	4016	BCR	4	0
16	j	4016	BCR	3	0
13	B	1021	CLA	1	0
13	A	1116	CLA	2	0
16	H	4010	BCR	6	0
17	G	5003	LHG	1	0
17	A	5004	LHG	1	0
13	H	1227	CLA	3	0
13	a	505	CLA	3	0
13	V	1503	CLA	3	0
13	5	510	CLA	1	0
13	1	509	CLA	4	0
16	2	523	BCR	1	0
16	f	4010	BCR	5	0
13	s	507	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	v	524	BCR	6	0
13	T	1303	CLA	3	0
13	a	501	CLA	2	0
13	H	1214	CLA	2	0
16	b	521	BCR	2	0
13	H	1205	CLA	1	0
16	G	4002	BCR	3	0
13	H	1223	CLA	1	0
13	G	1114	CLA	1	0
16	V	4219	BCR	5	0
13	e	1139	CLA	2	0
13	3	505	CLA	2	0
13	e	1237	CLA	3	0
13	Y	519	CLA	1	0
13	f	1021	CLA	1	0
13	s	517	CLA	1	0
13	e	1108	CLA	2	0
17	H	1855	LHG	3	0
13	B	1215	CLA	3	0
13	2	510	CLA	2	0
16	T	4015	BCR	5	0
13	e	1110	CLA	1	0
13	B	1205	CLA	1	0
13	4	505	CLA	1	0
16	F	4016	BCR	5	0
13	G	1119	CLA	4	0
13	H	1212	CLA	1	0
13	B	1238	CLA	1	0
13	2	507	CLA	3	0
13	3	502	CLA	2	0
16	4	523	BCR	1	0
13	u	509	CLA	2	0
13	q	513	CLA	1	0
13	q	519	CLA	1	0
13	B	1226	CLA	5	0
17	B	1842	LHG	2	0
13	f	1212	CLA	1	0
16	s	523	BCR	3	0
13	4	501	CLA	2	0
13	f	1236	CLA	4	0
13	f	1227	CLA	3	0
13	Y	509	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	l	4013	BCR	6	0
13	Y	513	CLA	1	0
13	s	516	CLA	1	0
13	u	512	CLA	4	0
13	1	518	CLA	1	0
13	n	1502	CLA	2	0
17	f	1855	LHG	2	0
13	L	1502	CLA	2	0
16	G	4011	BCR	3	0
16	H	4004	BCR	3	0
20	6	822	SQD	1	0
13	v	501	CLA	3	0
16	d	521	BCR	2	0
13	e	1129	CLA	2	0
16	H	4005	BCR	2	0
13	A	1101	CLA	3	0
13	6	501	CLA	4	0
13	4	511	CLA	1	0
13	G	1111	CLA	1	0
13	6	502	CLA	2	0
13	e	1135	CLA	3	0
13	A	1102	CLA	4	0
13	A	1103	CLA	4	0
13	G	1112	CLA	1	0
13	e	1120	CLA	2	0
13	f	1225	CLA	3	0
13	n	1501	CLA	9	0
13	q	507	CLA	3	0
13	e	1130	CLA	4	0
13	d	512	CLA	4	0
13	Z	501	CLA	4	0
13	b	506	CLA	1	0
16	G	4008	BCR	1	0
18	T	5105	LMU	2	0
13	G	1237	CLA	4	0
13	G	1128	CLA	3	0
13	f	1220	CLA	4	0
13	e	1011	CLA	3	0
13	f	1224	CLA	6	0
13	b	513	CLA	1	0
16	Z	521	BCR	2	0
13	e	1106	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	4020	BCR	3	0
13	G	1139	CLA	2	0
13	H	1023	CLA	2	0
13	q	509	CLA	3	0
13	e	1122	CLA	3	0
13	e	1801	CLA	4	0
13	Y	504	CLA	1	0
13	Z	517	CLA	2	0
13	5	502	CLA	3	0
13	A	1137	CLA	3	0
13	G	1105	CLA	2	0
13	t	506	CLA	1	0
13	F	1302	CLA	2	0
19	B	5002	LMG	7	0
14	B	2002	PQN	2	0
13	r	507	CLA	3	0
16	q	521	BCR	1	0
13	B	1221	CLA	7	0
20	v	822	SQD	1	0
13	6	506	CLA	1	0
13	4	509	CLA	3	0
13	u	503	CLA	3	0
13	B	1212	CLA	1	0
16	H	4017	BCR	3	0
13	a	512	CLA	2	0
13	b	501	CLA	2	0
16	f	4017	BCR	5	0
13	H	1229	CLA	4	0
13	3	516	CLA	1	0
20	Y	822	SQD	5	0
13	q	504	CLA	1	0
16	d	522	BCR	9	0
13	t	501	CLA	2	0
13	B	1208	CLA	2	0
16	4	524	BCR	4	0
13	H	1235	CLA	4	0
16	f	4006	BCR	3	0
13	G	1123	CLA	2	0
13	e	1116	CLA	4	0
16	t	521	BCR	1	0
13	e	1104	CLA	7	0
13	c	511	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	t	509	CLA	3	0
13	e	1013	CLA	8	0
13	5	512	CLA	4	0
13	A	1022	CLA	4	0
13	5	506	CLA	3	0
13	Y	501	CLA	4	0
20	s	822	SQD	1	0
13	b	503	CLA	1	0
13	5	505	CLA	1	0
13	3	517	CLA	1	0
13	s	503	CLA	3	0
13	G	1120	CLA	2	0
13	A	1104	CLA	6	0
13	B	1202	CLA	2	0
13	B	1220	CLA	4	0
13	c	505	CLA	1	0
13	e	1103	CLA	4	0
13	A	1121	CLA	3	0
13	B	1234	CLA	2	0
13	3	518	CLA	1	0
13	H	1208	CLA	2	0
13	u	505	CLA	2	0
16	t	524	BCR	5	0
13	e	1022	CLA	4	0
13	G	1011	CLA	3	0
13	r	506	CLA	5	0
13	c	502	CLA	3	0
13	3	510	CLA	3	0
13	4	517	CLA	2	0
13	A	1108	CLA	2	0
13	Y	505	CLA	5	0
13	r	519	CLA	1	0
13	A	1115	CLA	1	0
13	2	511	CLA	3	0
13	c	501	CLA	4	0
13	f	1235	CLA	4	0
16	A	4007	BCR	5	0
16	6	523	BCR	2	0
13	u	501	CLA	4	0
16	b	524	BCR	4	0
13	Z	503	CLA	4	0
13	G	1140	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	1116	CLA	3	0
13	3	507	CLA	2	0
13	K	1103	CLA	2	0
13	H	1202	CLA	2	0
13	s	518	CLA	1	0
16	m	4104	BCR	5	0
13	J	1303	CLA	4	0
13	H	1234	CLA	4	0
13	d	501	CLA	3	0
13	s	510	CLA	4	0
16	a	522	BCR	2	0
13	2	501	CLA	4	0
13	A	1109	CLA	3	0
13	f	1215	CLA	2	0
13	q	511	CLA	3	0
13	a	516	CLA	1	0
20	V	5216	SQD	3	0
13	r	518	CLA	2	0
16	2	521	BCR	4	0
13	G	1129	CLA	1	0
16	e	4008	BCR	1	0
13	2	506	CLA	5	0
16	a	521	BCR	3	0
13	f	1239	CLA	3	0
13	s	505	CLA	2	0
16	B	4006	BCR	1	0
13	Y	511	CLA	3	0
13	4	518	CLA	1	0
13	Z	510	CLA	2	0
13	l	1302	CLA	1	0
18	A	1849	LMU	1	0
13	s	502	CLA	2	0
13	G	1126	CLA	8	0
16	q	523	BCR	1	0
17	e	5001	LHG	5	0
20	B	1852	SQD	7	0
13	s	501	CLA	2	0
13	B	1207	CLA	6	0
13	H	1021	CLA	2	0
13	G	1106	CLA	2	0
16	f	4005	BCR	1	0
20	q	822	SQD	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	m	1105	CLA	1	0
13	q	501	CLA	4	0
18	e	1849	LMU	1	0
16	s	521	BCR	3	0
17	e	5002	LHG	4	0
13	G	1801	CLA	2	0
16	n	4219	BCR	4	0
13	f	1229	CLA	4	0
13	e	1124	CLA	1	0
16	K	4104	BCR	7	0
13	a	502	CLA	2	0
16	A	4008	BCR	2	0
13	f	1201	CLA	3	0
13	f	1234	CLA	4	0
13	A	1105	CLA	2	0
13	Z	502	CLA	5	0
16	G	4001	BCR	2	0
13	B	1227	CLA	4	0
13	f	1206	CLA	1	0
13	B	1213	CLA	1	0
13	f	1218	CLA	2	0
13	r	513	CLA	1	0
13	t	511	CLA	1	0
13	4	510	CLA	1	0
13	A	1122	CLA	2	0
13	H	1216	CLA	2	0
16	V	4020	BCR	3	0
18	J	5105	LMU	2	0
13	K	1401	CLA	1	0
13	A	1107	CLA	1	0
13	G	1134	CLA	1	0
13	2	502	CLA	5	0
13	s	512	CLA	2	0
16	r	521	BCR	2	0
13	f	1216	CLA	1	0
17	G	5008	LHG	2	0
15	C	3002	SF4	1	0
16	Z	524	BCR	5	0
13	H	1222	CLA	4	0
20	1	822	SQD	4	0
13	f	1214	CLA	2	0
13	Z	512	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	6	524	BCR	8	0
17	A	5002	LHG	3	0
13	c	507	CLA	1	0
16	J	4012	BCR	4	0
16	I	4018	BCR	3	0
16	u	522	BCR	3	0
17	e	5009	LHG	4	0
16	n	4019	BCR	2	0
13	B	1206	CLA	2	0
13	B	1218	CLA	1	0
13	1	512	CLA	6	0
16	v	523	BCR	3	0
16	r	522	BCR	2	0
16	W	4021	BCR	4	0
13	3	503	CLA	4	0
19	H	5002	LMG	7	0
17	A	5009	LHG	4	0
17	A	5006	LHG	1	0
16	d	523	BCR	2	0
16	e	4007	BCR	4	0
13	6	511	CLA	1	0
13	B	1203	CLA	2	0
13	4	502	CLA	2	0
13	4	503	CLA	1	0
13	v	512	CLA	3	0
13	2	505	CLA	3	0
13	f	1210	CLA	4	0
16	L	4219	BCR	4	0
13	v	511	CLA	1	0
13	f	1222	CLA	4	0
16	B	4004	BCR	4	0
17	V	5221	LHG	9	0
13	B	1217	CLA	3	0
13	Y	517	CLA	1	0
13	2	503	CLA	4	0
16	B	4005	BCR	3	0
13	B	1201	CLA	2	0
13	A	1140	CLA	6	0
17	e	5004	LHG	1	0
16	f	4014	BCR	4	0
13	6	517	CLA	3	0
13	H	1206	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	5	501	CLA	4	0
13	G	1117	CLA	3	0
13	G	1124	CLA	1	0
13	e	1133	CLA	1	0
13	f	1238	CLA	1	0
16	Z	522	BCR	2	0
13	G	1101	CLA	4	0
16	r	523	BCR	2	0
13	q	505	CLA	24	0
13	f	1202	CLA	3	0
16	1	522	BCR	4	0
13	c	512	CLA	4	0
16	L	4022	BCR	5	0
13	1	501	CLA	4	0
13	A	1133	CLA	1	0
13	t	516	CLA	1	0
16	V	4019	BCR	1	0
13	5	507	CLA	1	0
13	r	501	CLA	4	0
13	H	1209	CLA	2	0
13	u	513	CLA	1	0
13	q	518	CLA	4	0
16	1	521	BCR	1	0
14	G	2001	PQN	3	0
13	v	517	CLA	2	0
13	e	1140	CLA	6	0
13	1	516	CLA	2	0
16	B	4014	BCR	4	0
13	b	516	CLA	1	0
13	Z	513	CLA	1	0
13	r	509	CLA	1	0
13	d	506	CLA	1	0
16	B	4017	BCR	6	0
13	A	1237	CLA	3	0
13	t	519	CLA	2	0
17	G	5001	LHG	4	0
16	s	522	BCR	1	0
13	Z	519	CLA	1	0
13	e	1102	CLA	2	0
13	f	1231	CLA	3	0
15	N	3002	SF4	1	0
13	H	1231	CLA	3	0

Continued on next page...

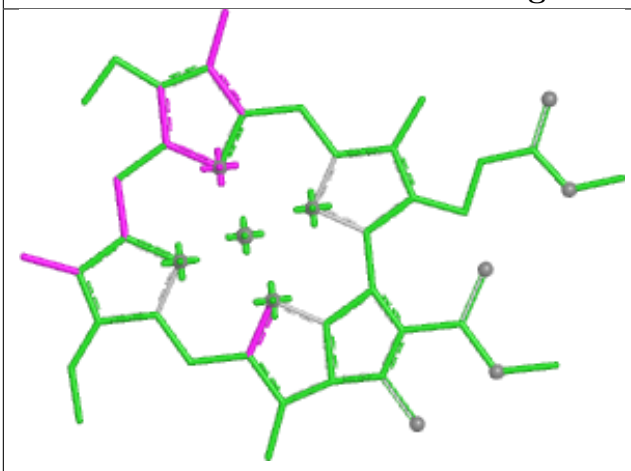
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	R	1301	CLA	1	0
13	6	512	CLA	4	0
13	e	1121	CLA	3	0
13	b	510	CLA	1	0
13	A	1138	CLA	2	0
13	f	1203	CLA	3	0
13	4	506	CLA	1	0
13	L	1501	CLA	8	0
13	f	1223	CLA	2	0
16	3	523	BCR	1	0
17	e	5008	LHG	2	0
13	A	1136	CLA	1	0
17	A	5003	LHG	2	0
16	U	4104	BCR	6	0
13	4	519	CLA	2	0
14	f	2002	PQN	3	0
16	2	524	BCR	6	0
13	f	1023	CLA	4	0
13	f	1207	CLA	8	0
13	e	1138	CLA	2	0
13	Y	503	CLA	4	0
13	Y	516	CLA	2	0
13	H	1215	CLA	4	0
15	g	3002	SF4	1	0
13	1	504	CLA	1	0
13	H	1210	CLA	4	0
13	4	512	CLA	2	0
13	c	513	CLA	1	0
13	f	1209	CLA	2	0
13	b	511	CLA	1	0
13	G	1110	CLA	1	0

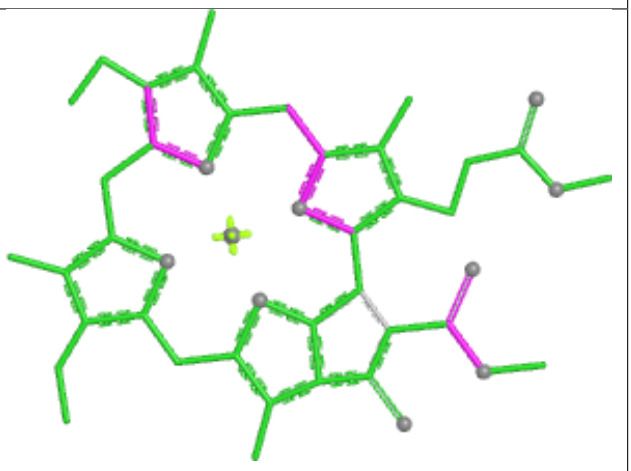
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

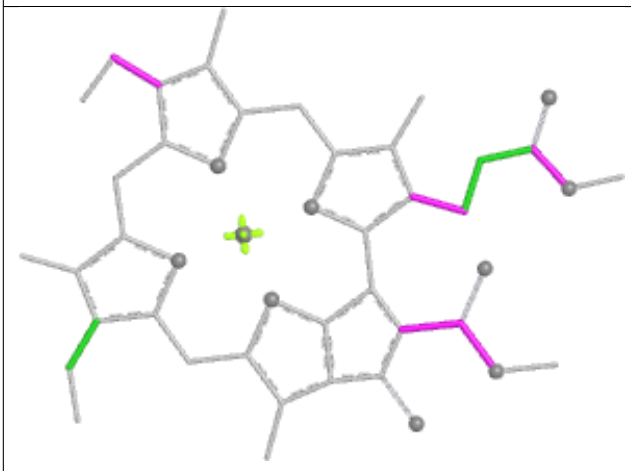
Ligand CLA 6 519



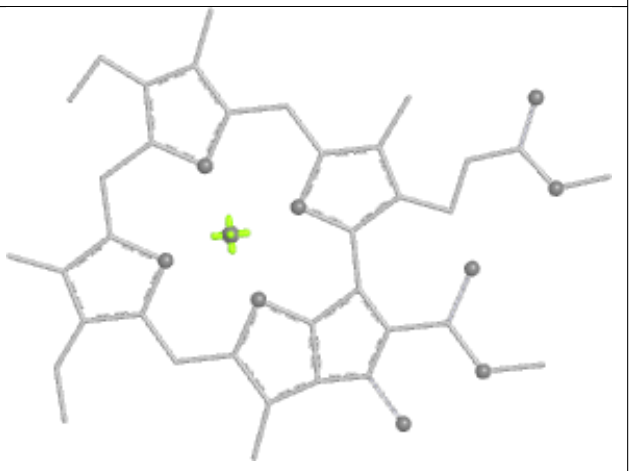
Bond lengths



Bond angles

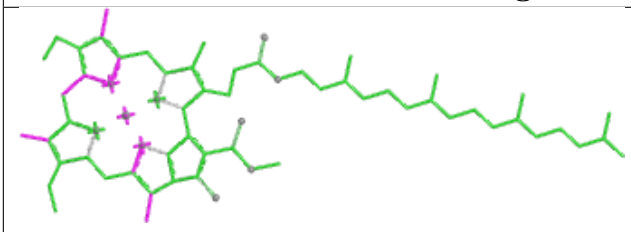


Torsions

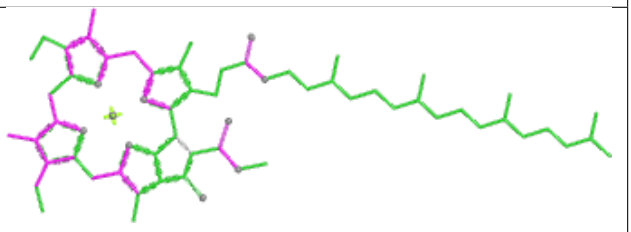


Rings

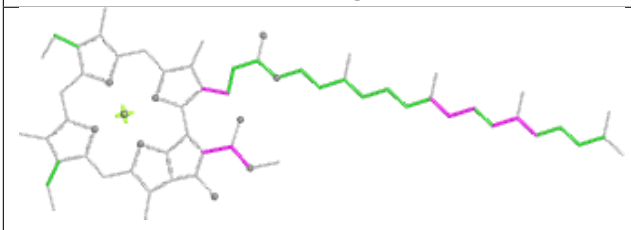
Ligand CLA H 1226



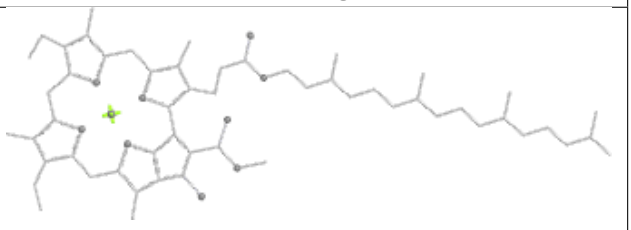
Bond lengths



Bond angles

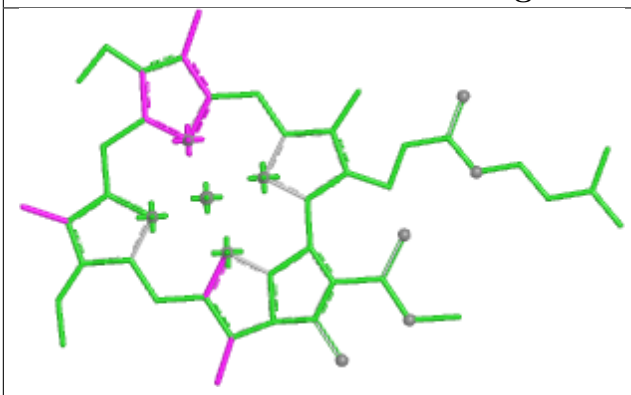


Torsions

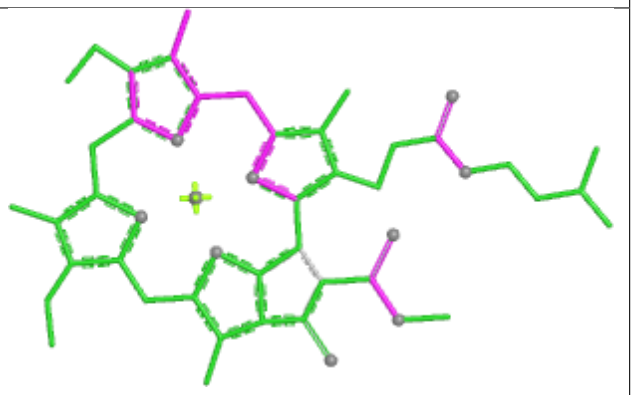


Rings

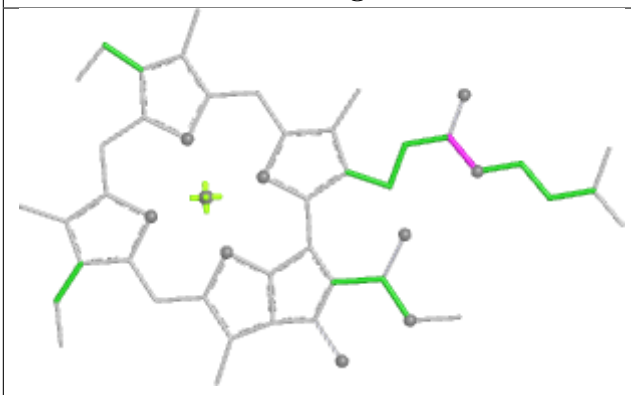
Ligand CLA A 1114



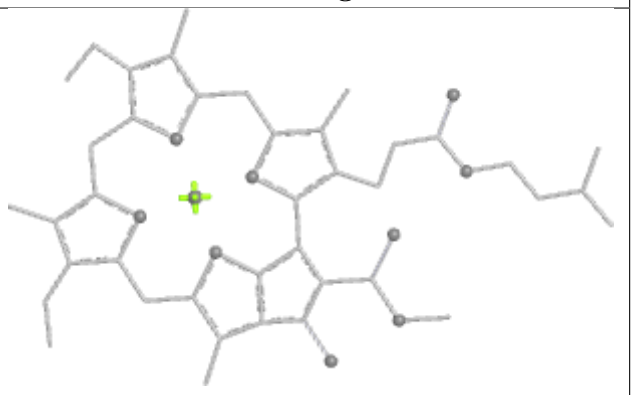
Bond lengths



Bond angles

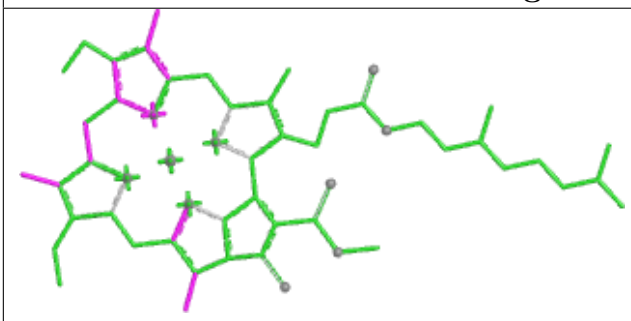


Torsions

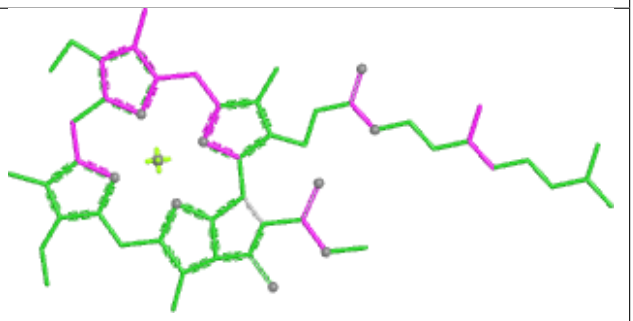


Rings

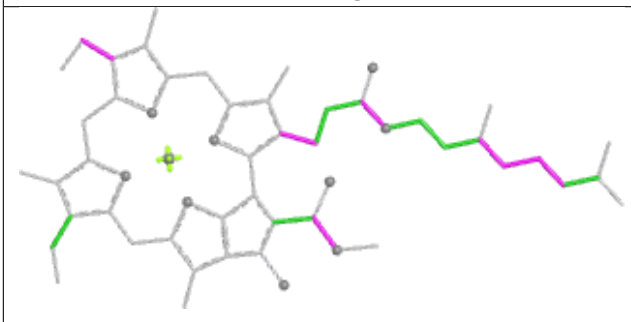
Ligand CLA Y 508



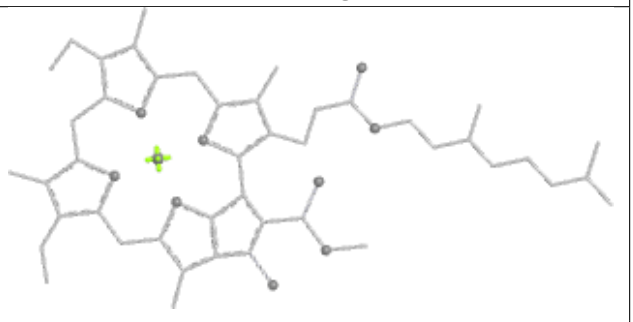
Bond lengths



Bond angles

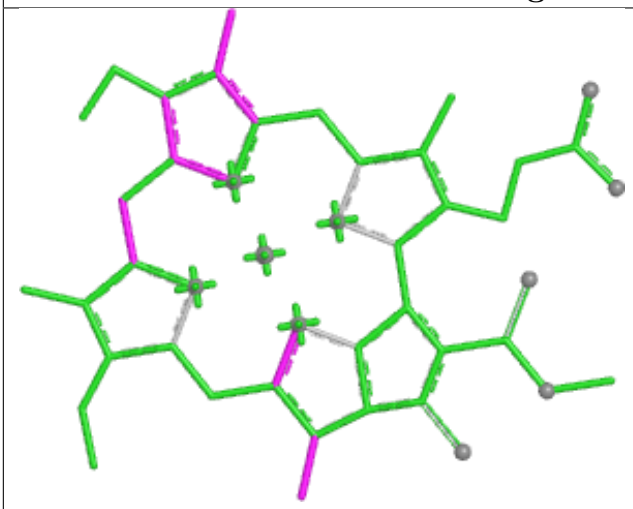


Torsions

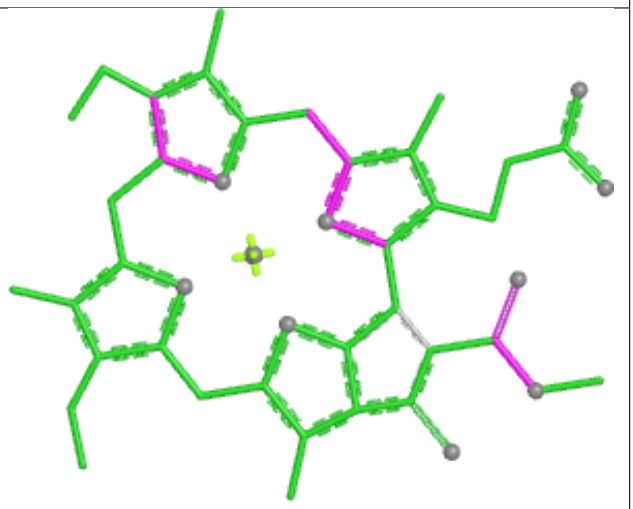


Rings

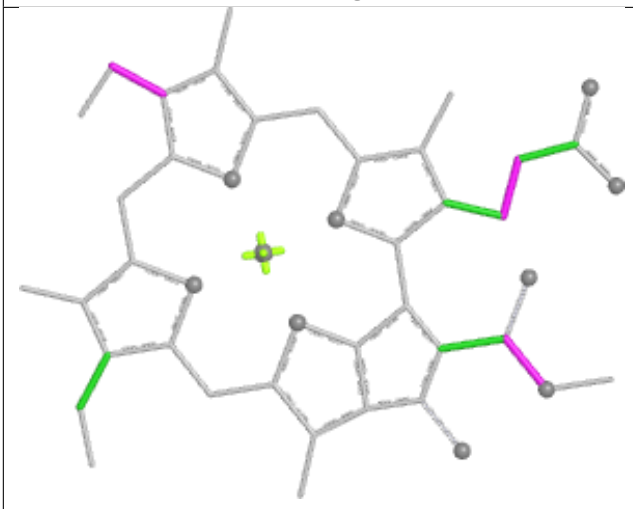
Ligand CLA d 513



Bond lengths



Bond angles

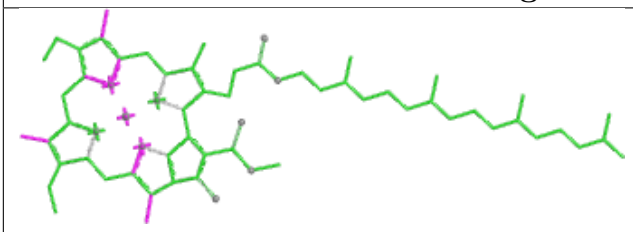


Torsions

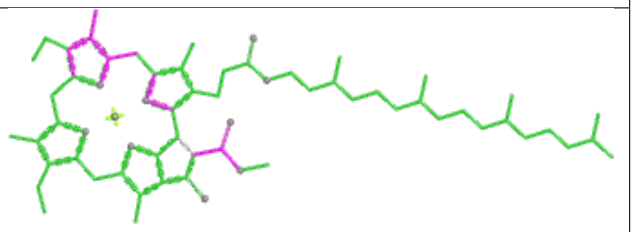


Rings

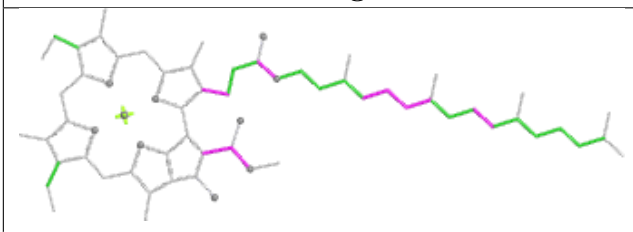
Ligand CLA e 1128



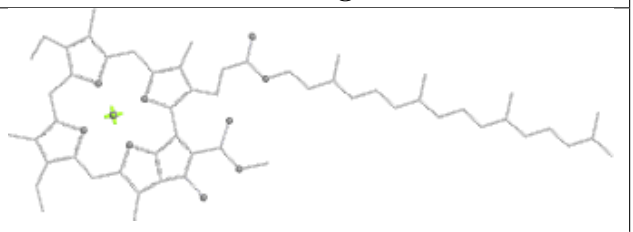
Bond lengths



Bond angles

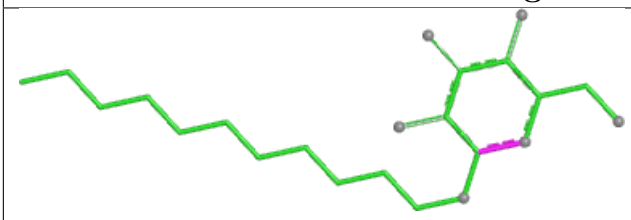


Torsions

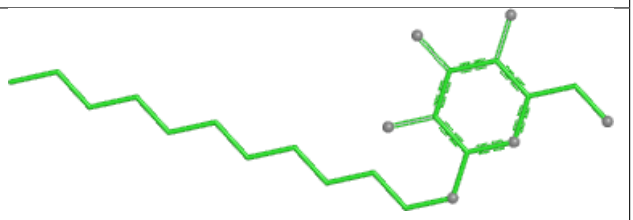


Rings

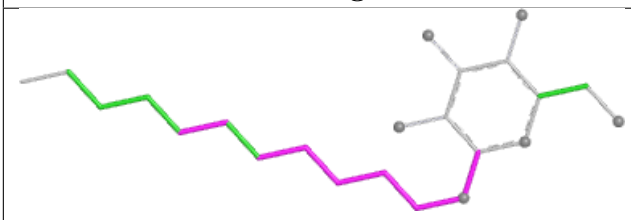
Ligand LMU 2 901



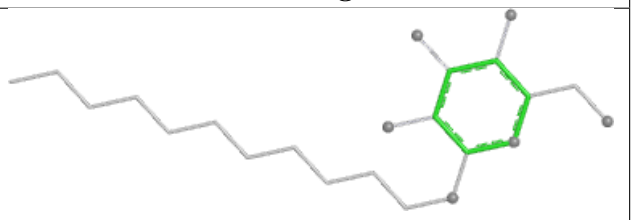
Bond lengths



Bond angles

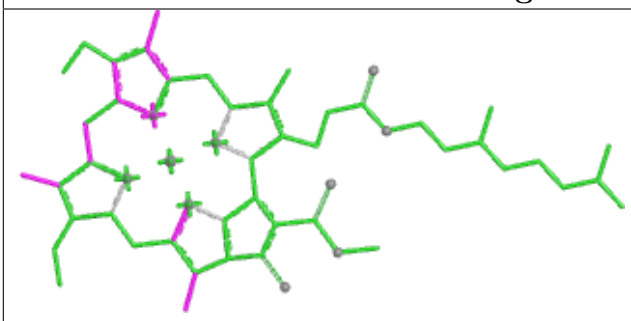


Torsions

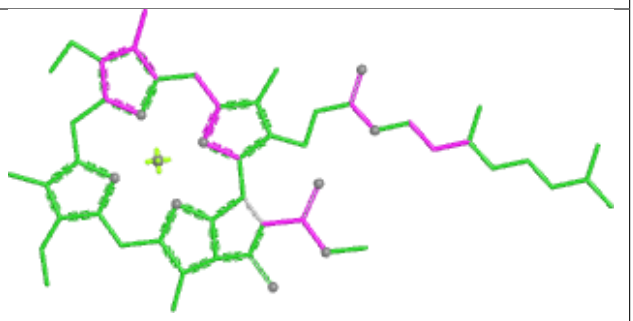


Rings

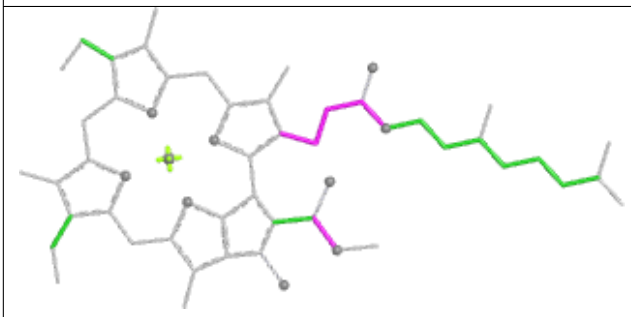
Ligand CLA B 1228



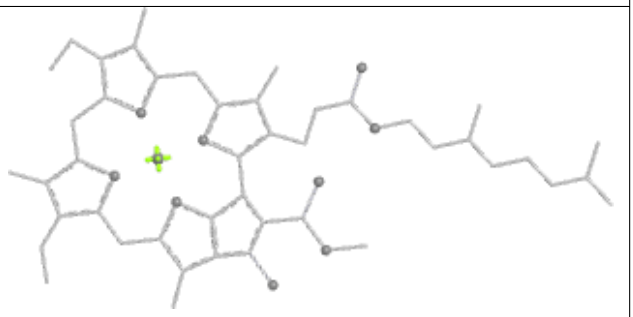
Bond lengths



Bond angles

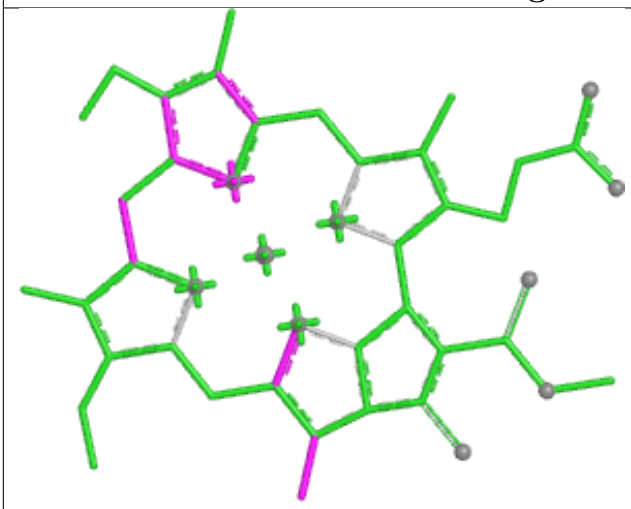


Torsions

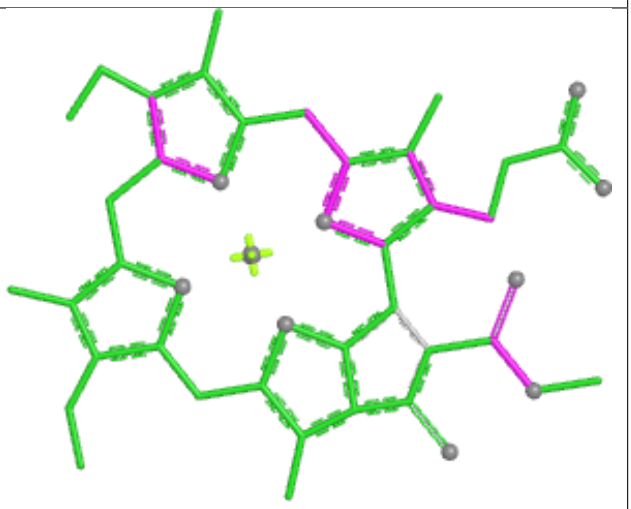


Rings

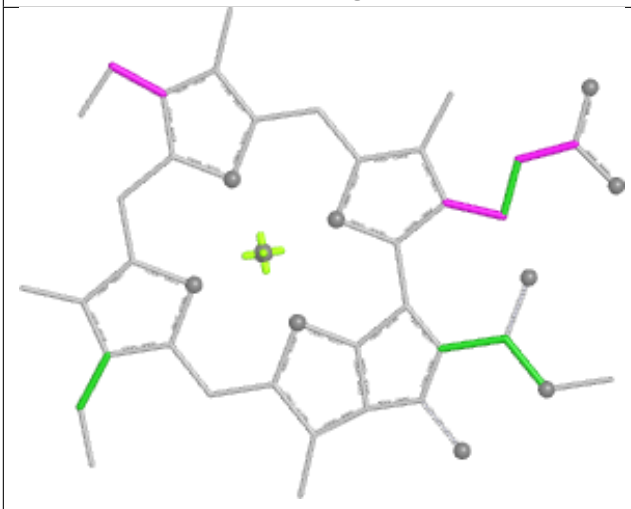
Ligand CLA 4 516



Bond lengths



Bond angles

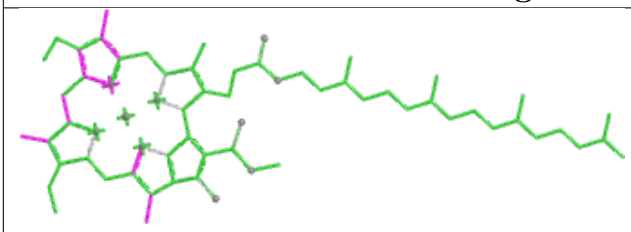


Torsions

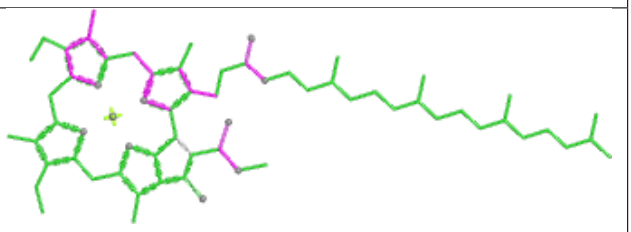


Rings

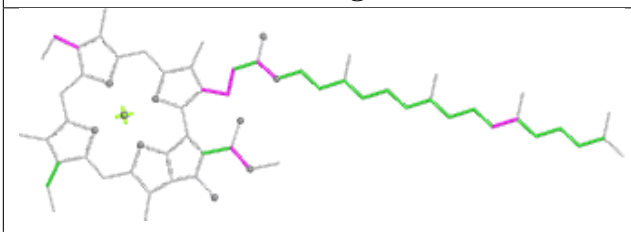
Ligand CLA A 1111



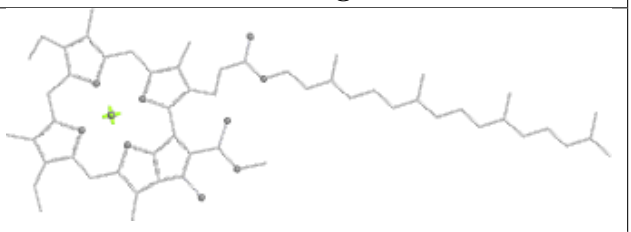
Bond lengths



Bond angles

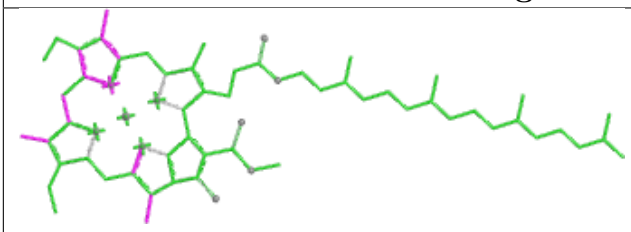


Torsions

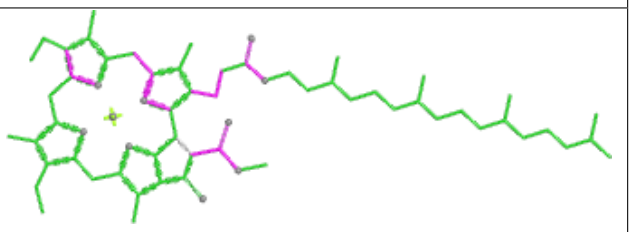


Rings

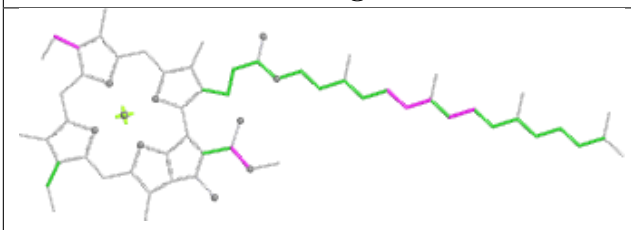
Ligand CLA B 1235



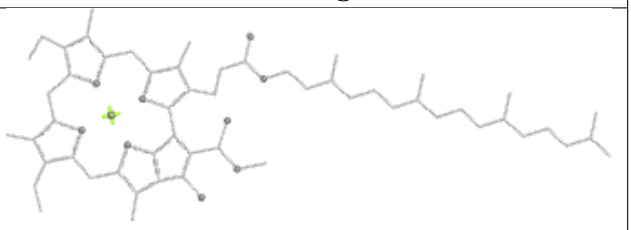
Bond lengths



Bond angles

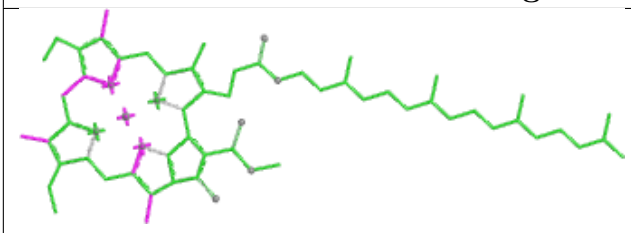


Torsions

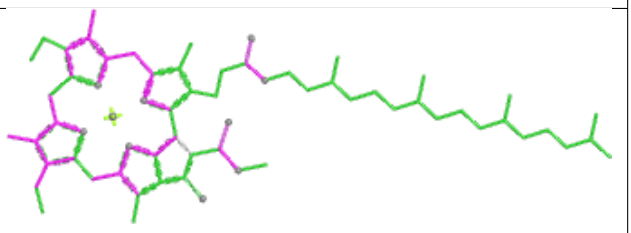


Rings

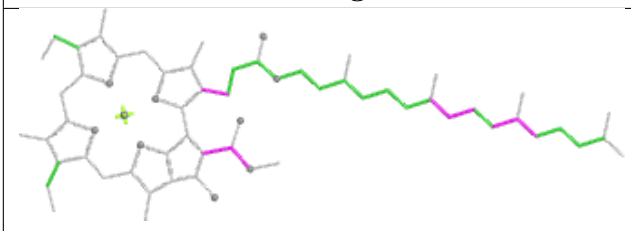
Ligand CLA f 1226



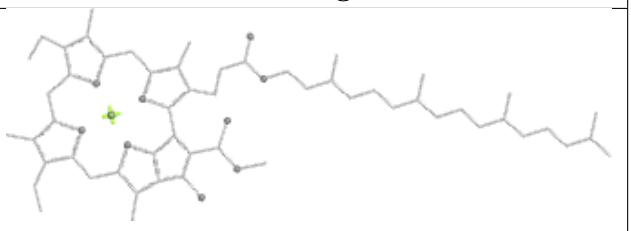
Bond lengths



Bond angles

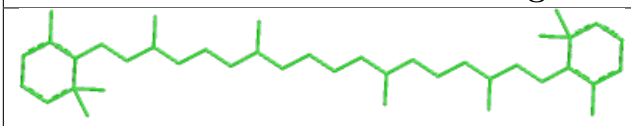


Torsions

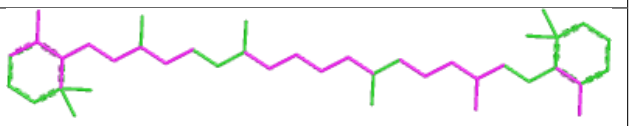


Rings

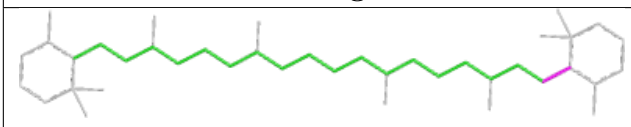
Ligand BCR r 524



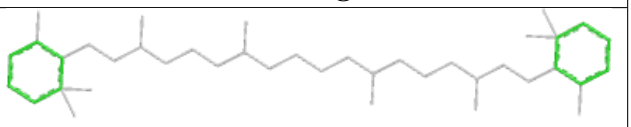
Bond lengths



Bond angles

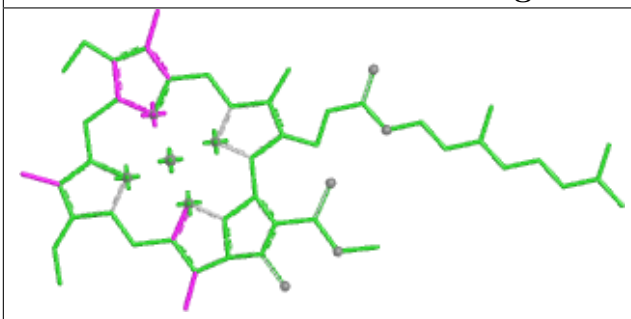


Torsions

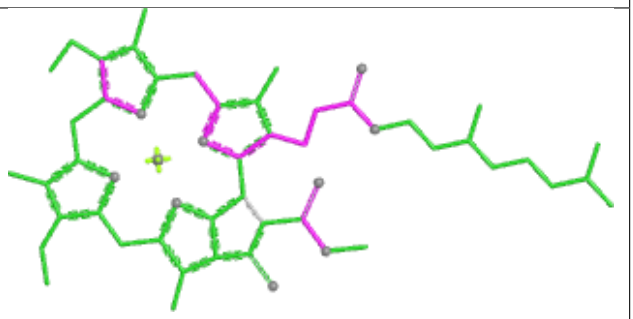


Rings

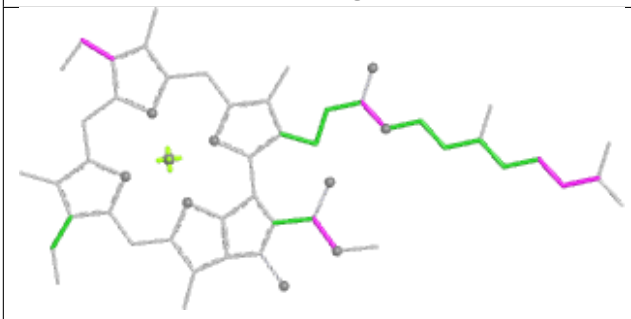
Ligand CLA H 1220



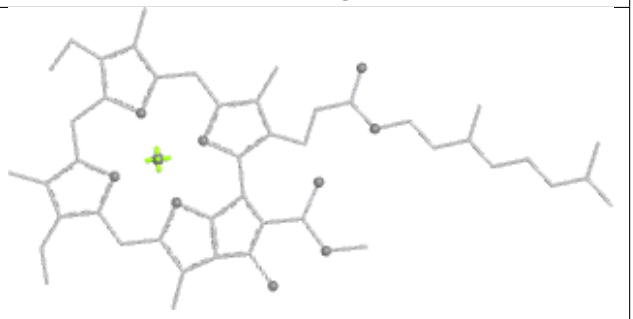
Bond lengths



Bond angles

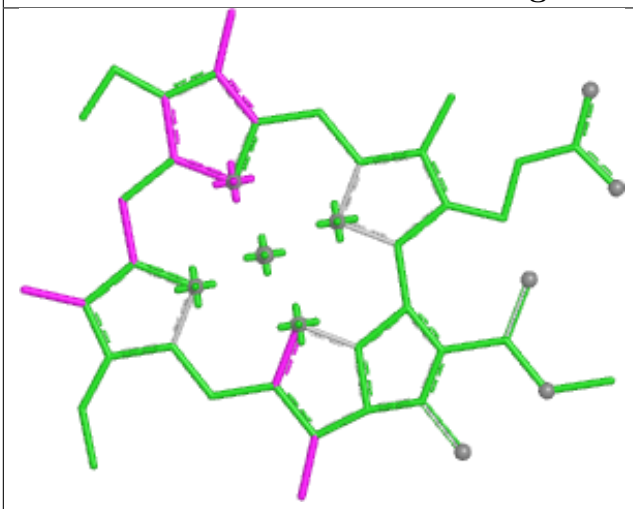


Torsions

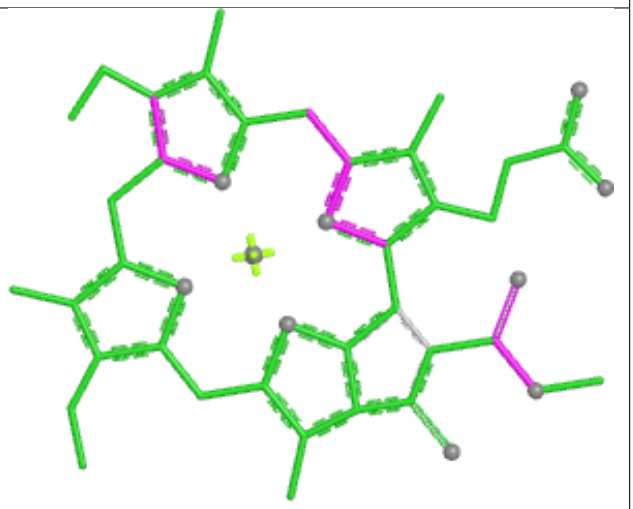


Rings

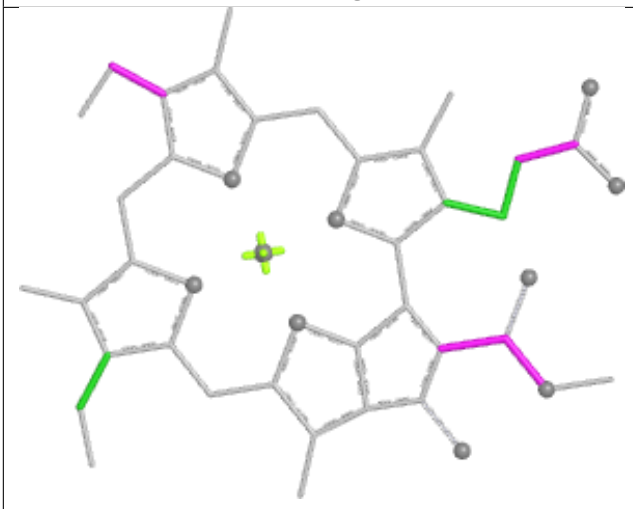
Ligand CLA c 510



Bond lengths



Bond angles

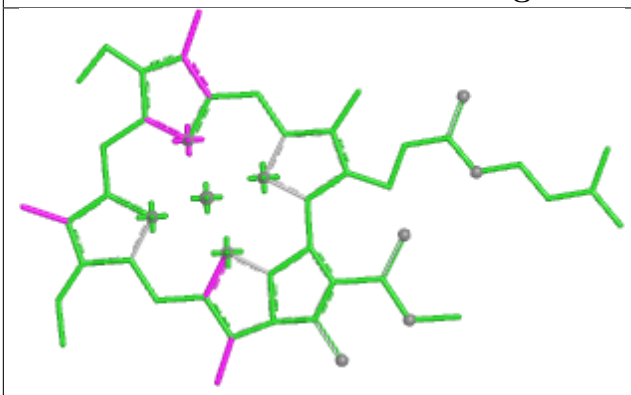


Torsions

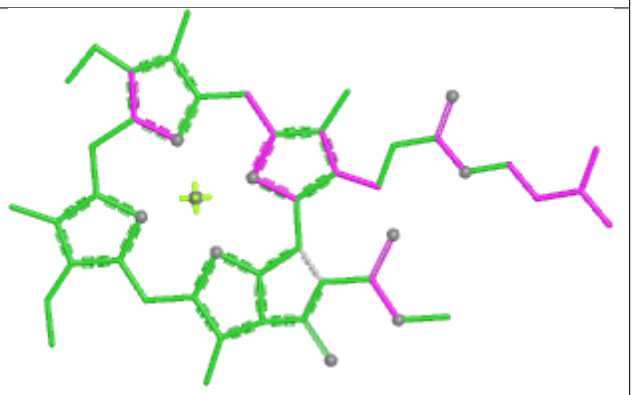


Rings

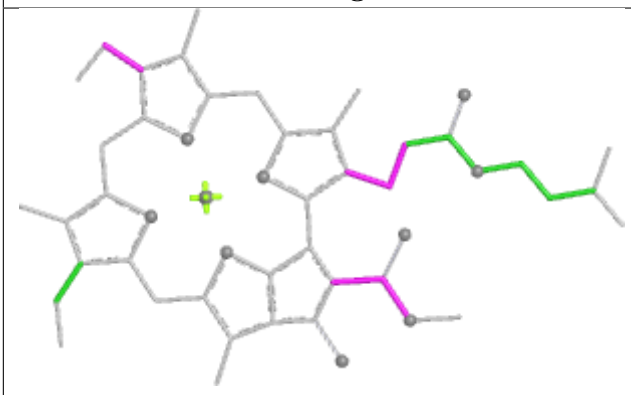
Ligand CLA m 1103



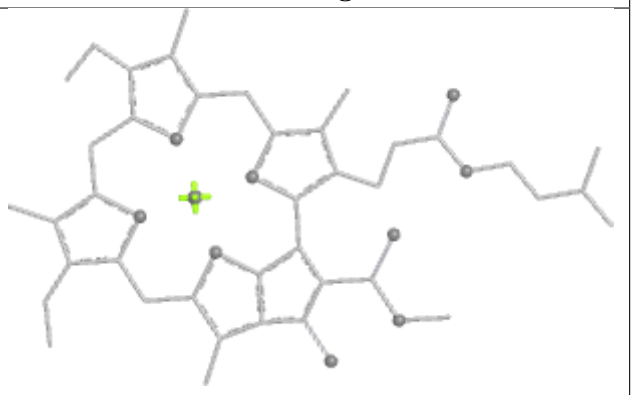
Bond lengths



Bond angles

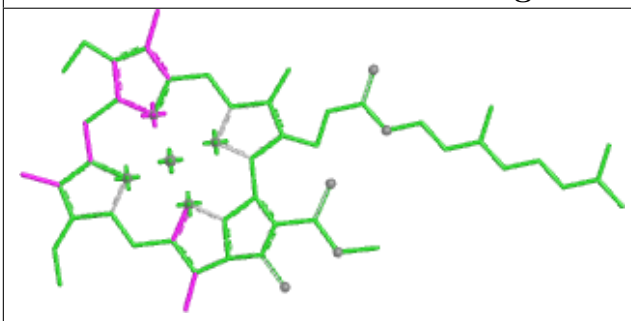


Torsions

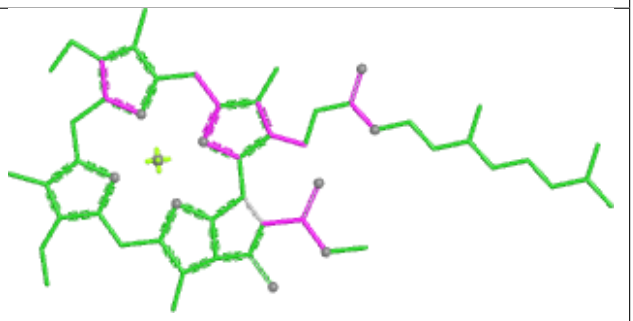


Rings

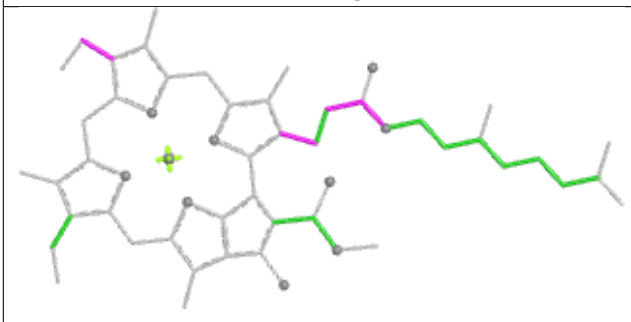
Ligand CLA U 1401



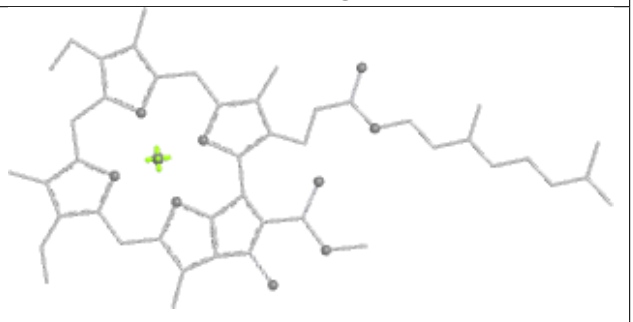
Bond lengths



Bond angles

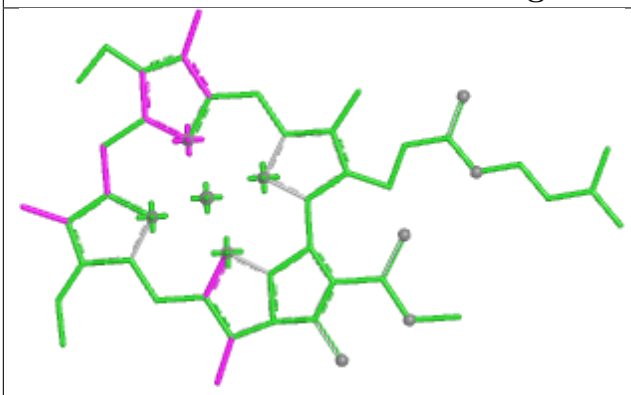


Torsions

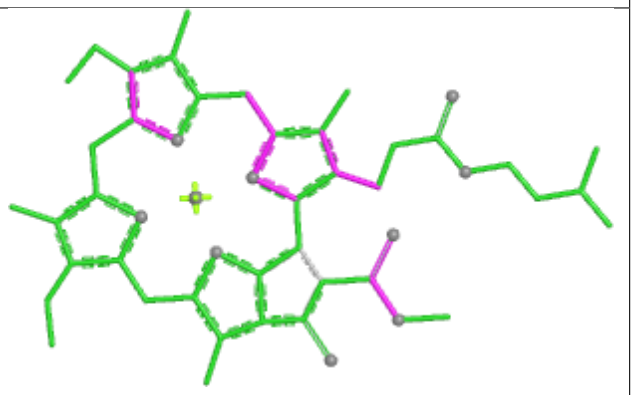


Rings

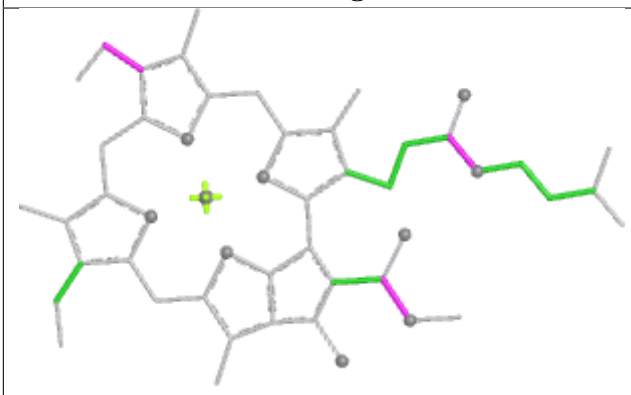
Ligand CLA u 502



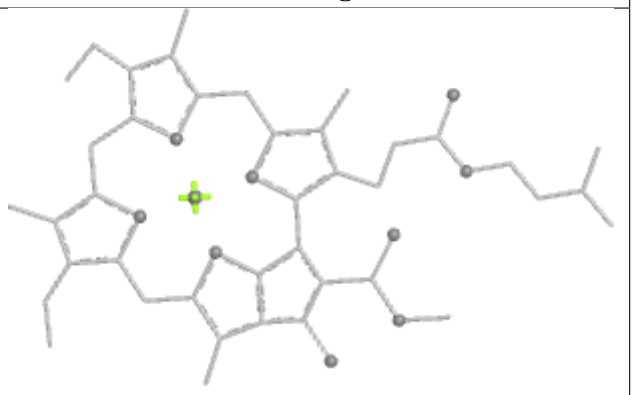
Bond lengths



Bond angles

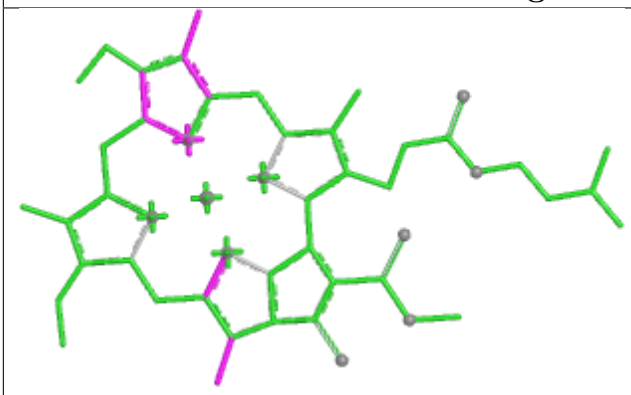


Torsions

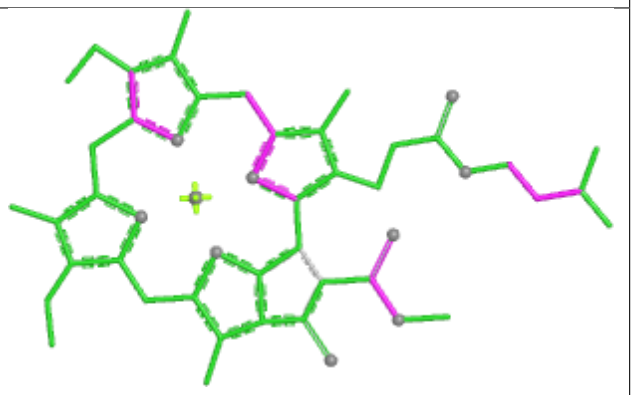


Rings

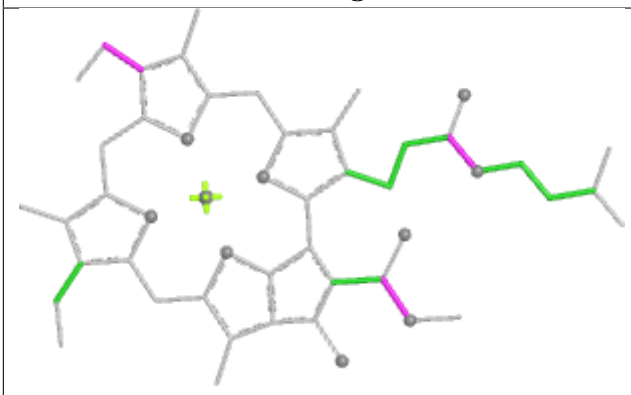
Ligand CLA v 502



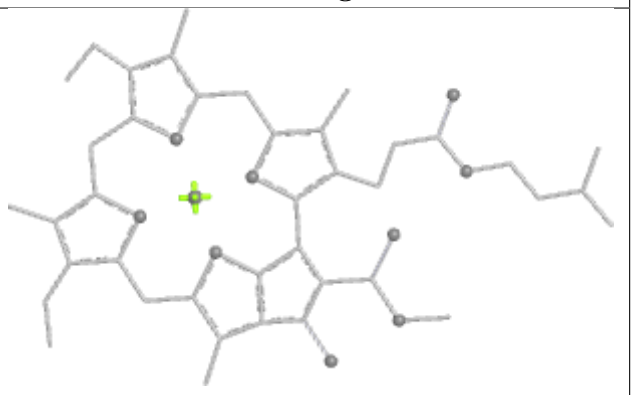
Bond lengths



Bond angles

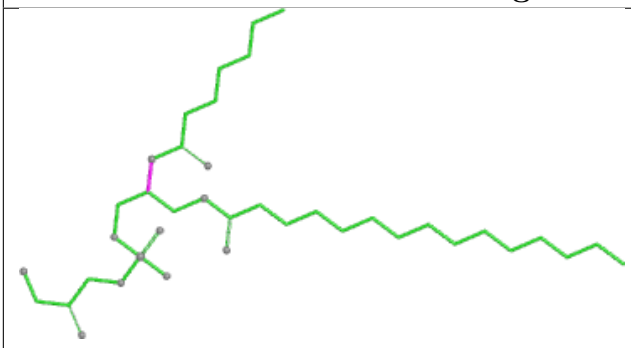


Torsions

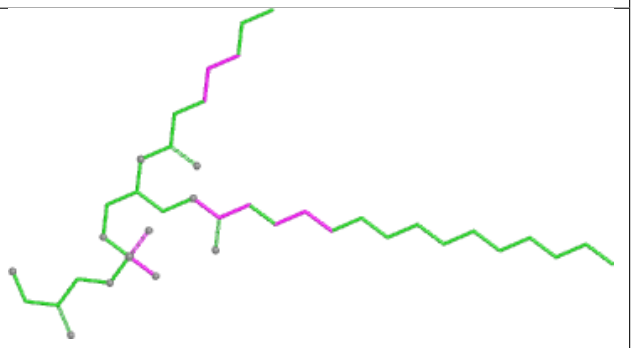


Rings

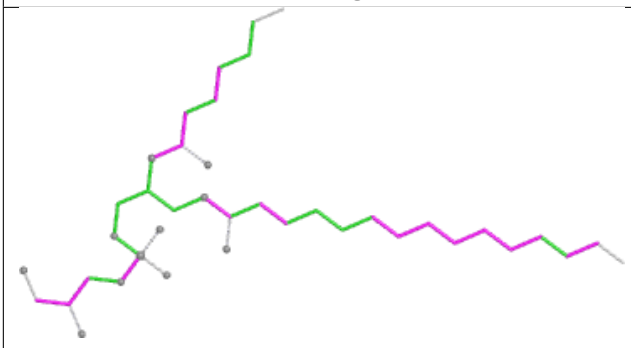
Ligand LHG H 1842



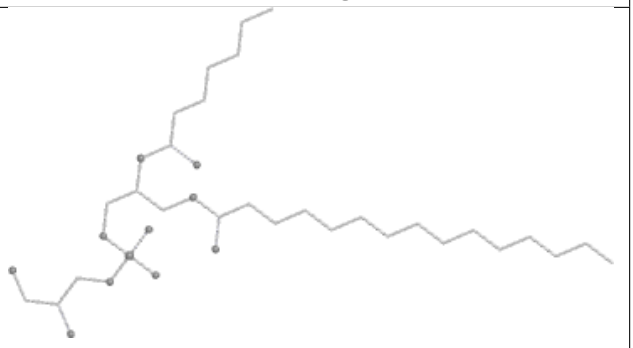
Bond lengths



Bond angles

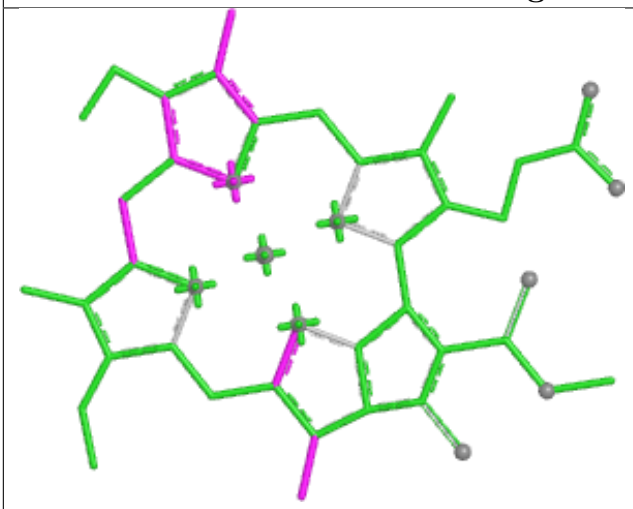


Torsions

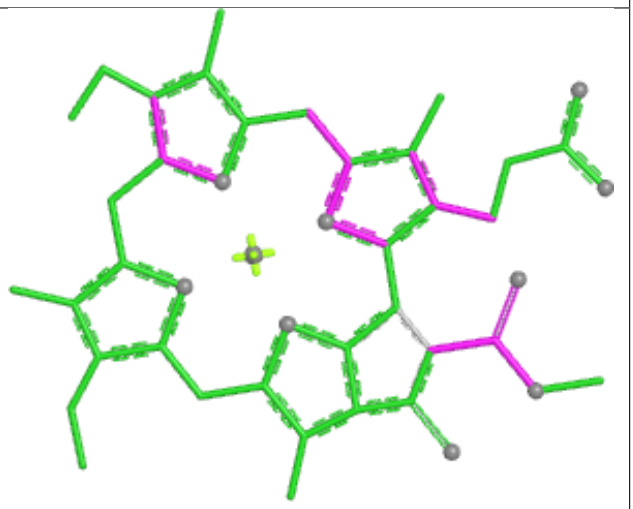


Rings

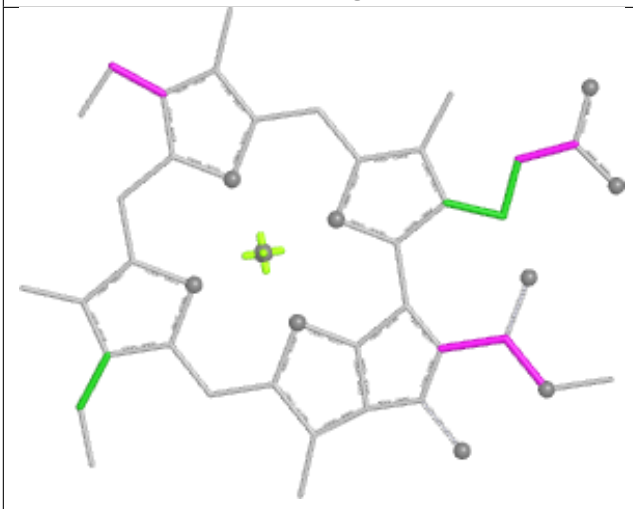
Ligand CLA b 507



Bond lengths



Bond angles

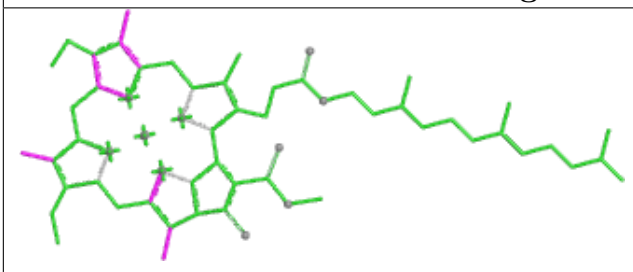


Torsions

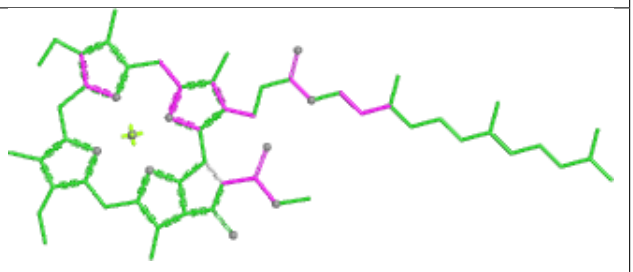


Rings

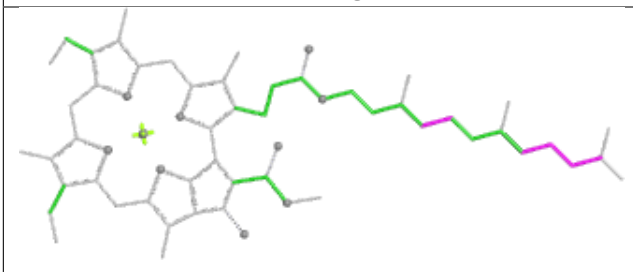
Ligand CLA e 1136



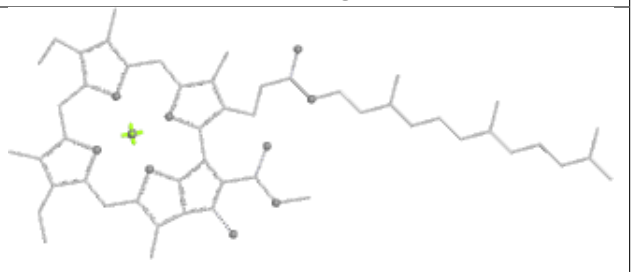
Bond lengths



Bond angles

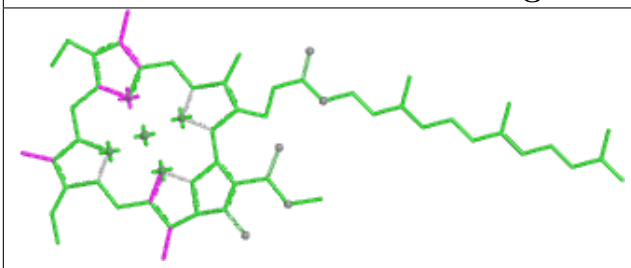


Torsions

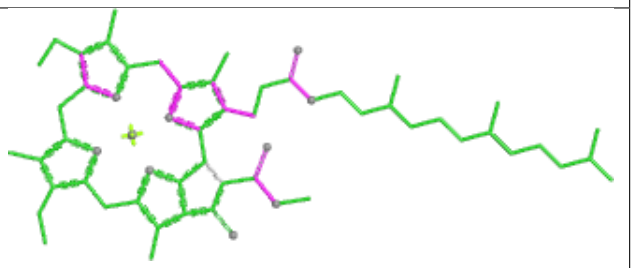


Rings

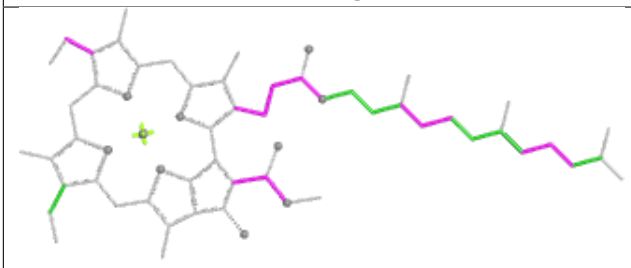
Ligand CLA Y 518



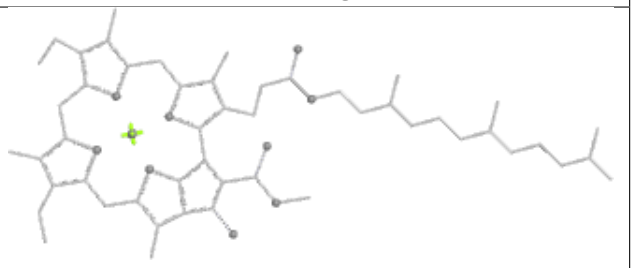
Bond lengths



Bond angles

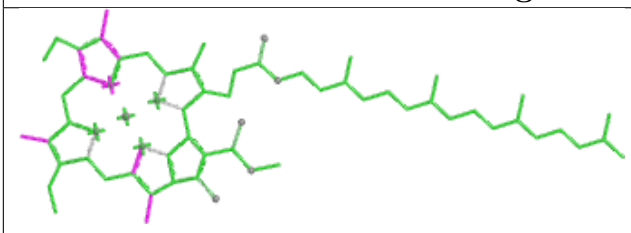


Torsions

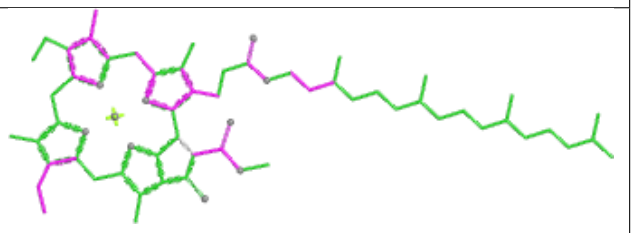


Rings

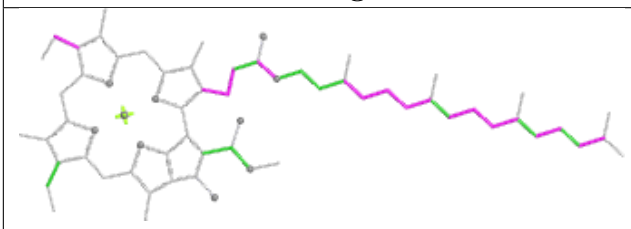
Ligand CLA B 1210



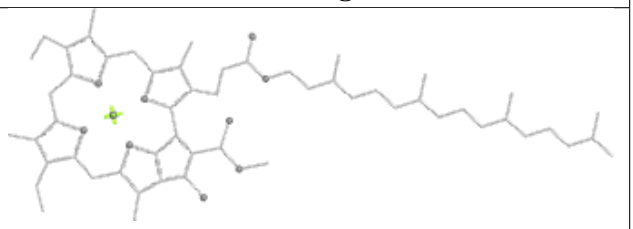
Bond lengths



Bond angles



Torsions

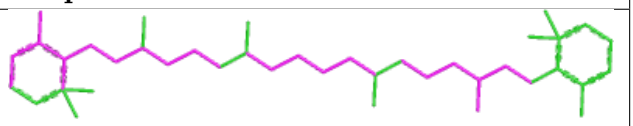


Rings

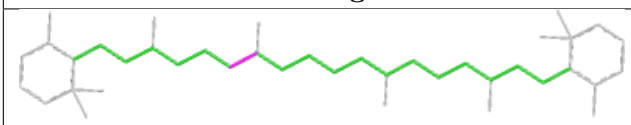
Ligand BCR q 524



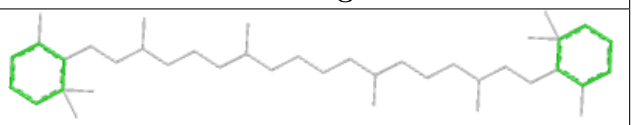
Bond lengths



Bond angles

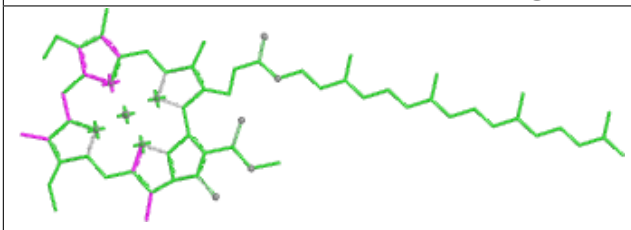


Torsions

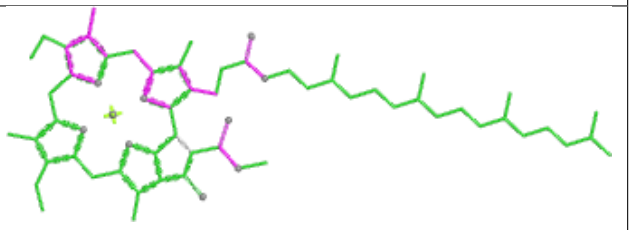


Rings

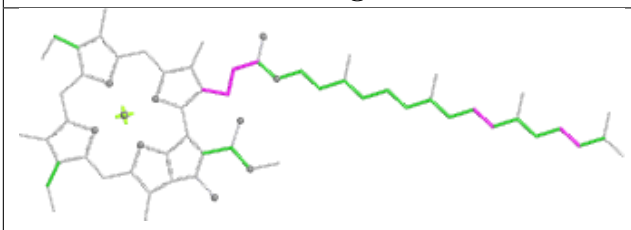
Ligand CLA 3 501



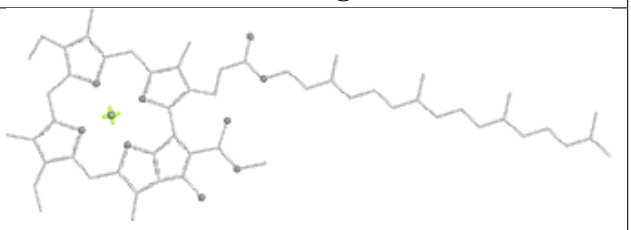
Bond lengths



Bond angles

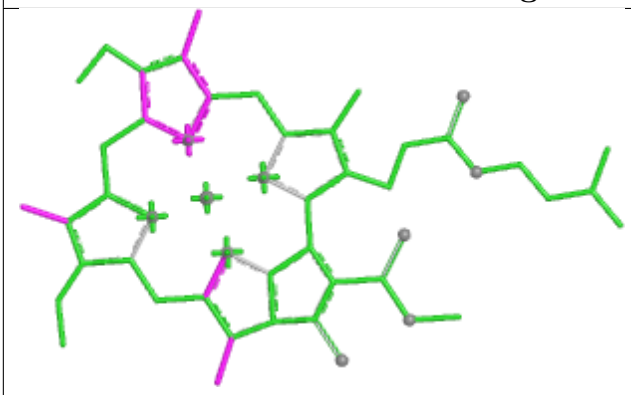


Torsions

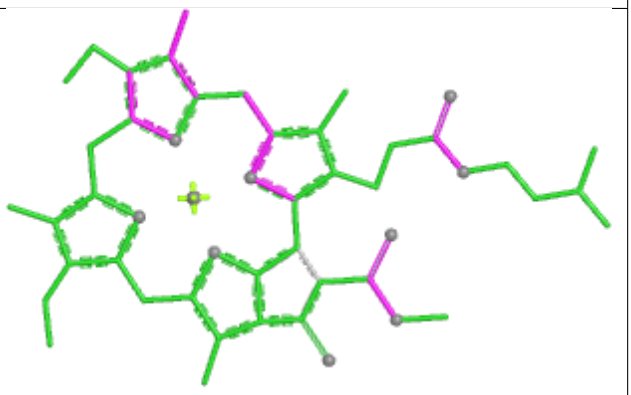


Rings

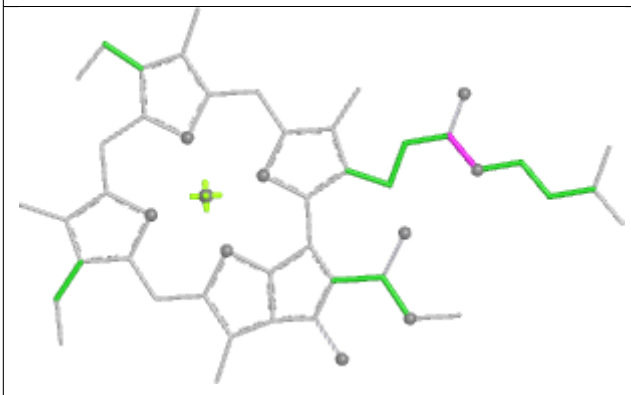
Ligand CLA e 1114



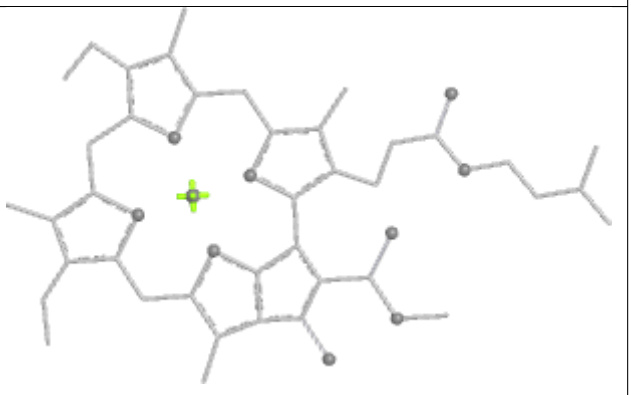
Bond lengths



Bond angles

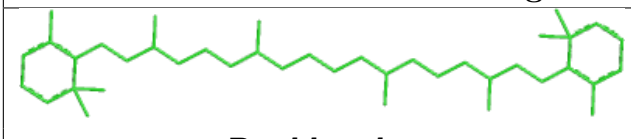


Torsions

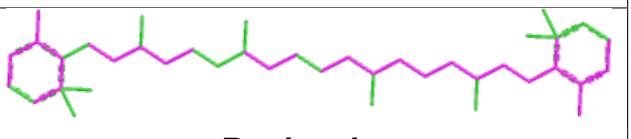


Rings

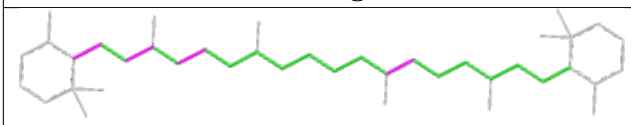
Ligand BCR u 521



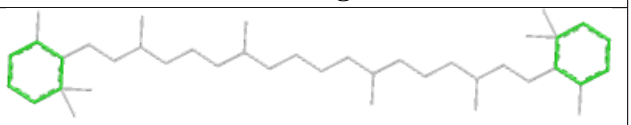
Bond lengths



Bond angles

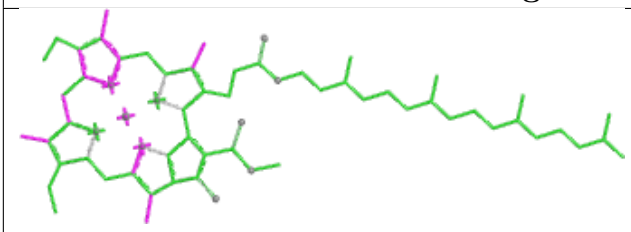


Torsions

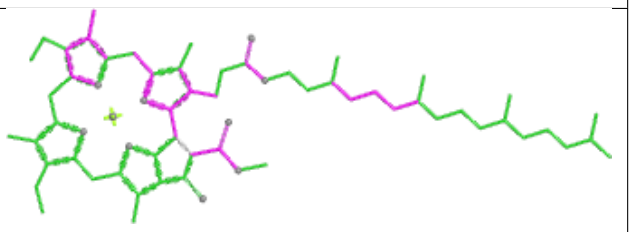


Rings

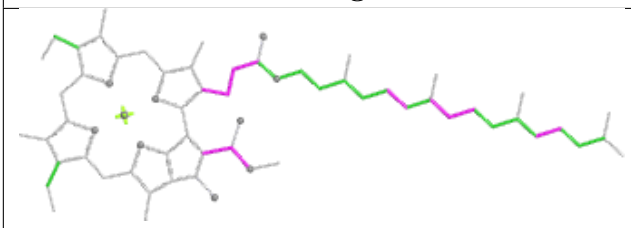
Ligand CLA f 1221



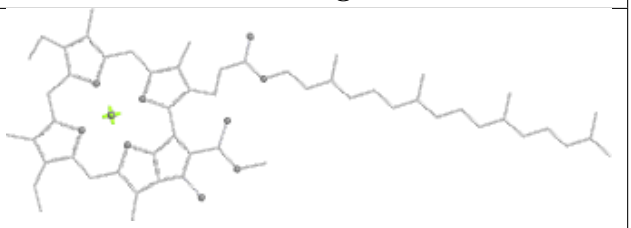
Bond lengths



Bond angles

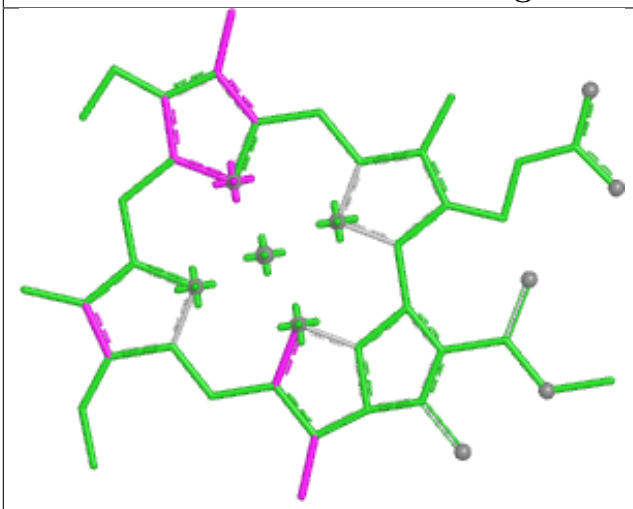


Torsions

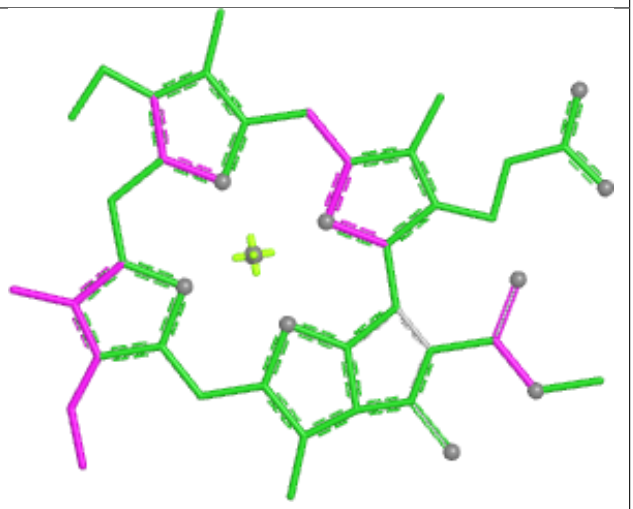


Rings

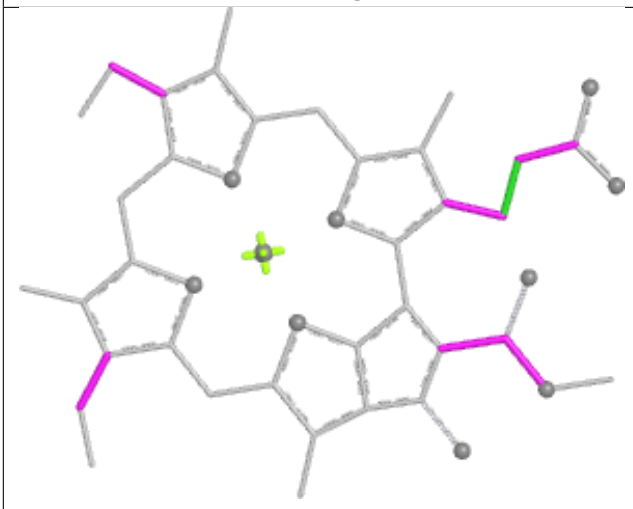
Ligand CLA U 1105



Bond lengths



Bond angles

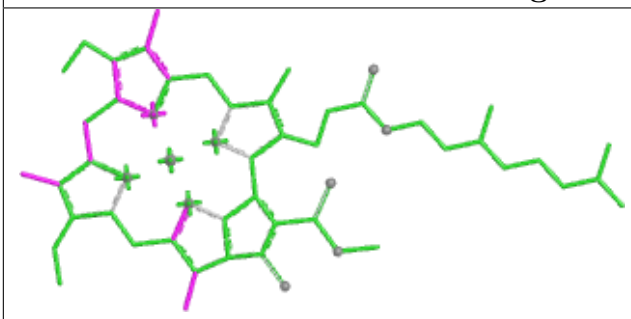


Torsions

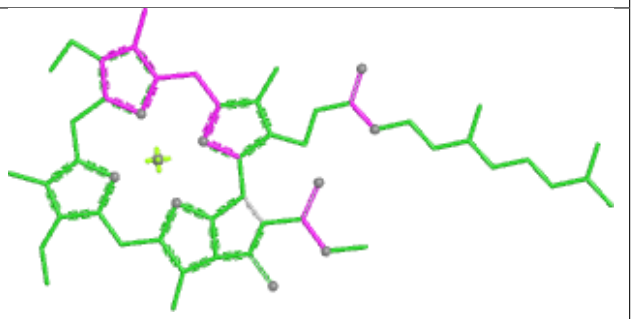


Rings

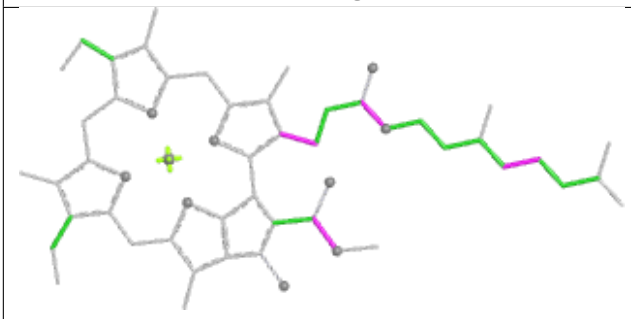
Ligand CLA s 508



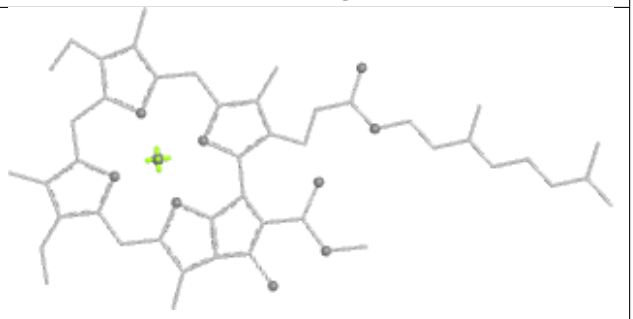
Bond lengths



Bond angles

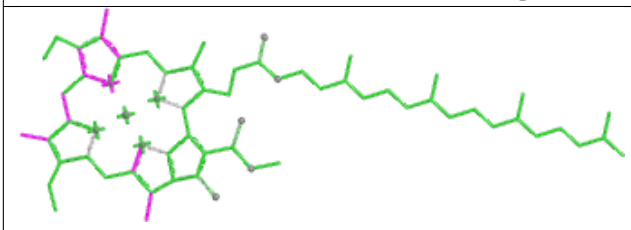


Torsions

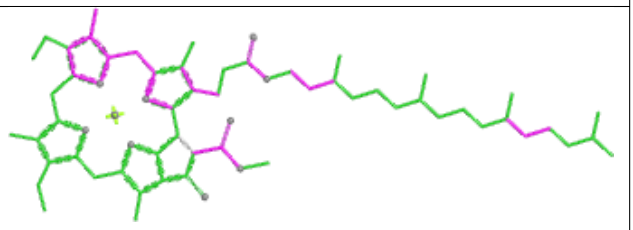


Rings

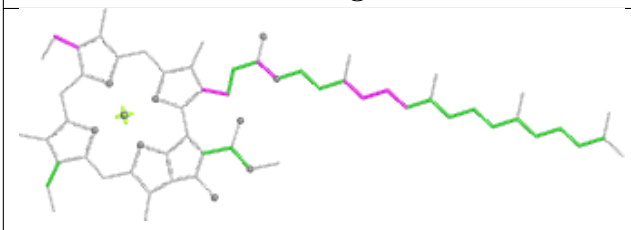
Ligand CLA G 1130



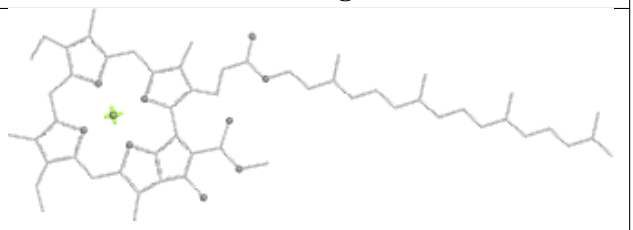
Bond lengths



Bond angles

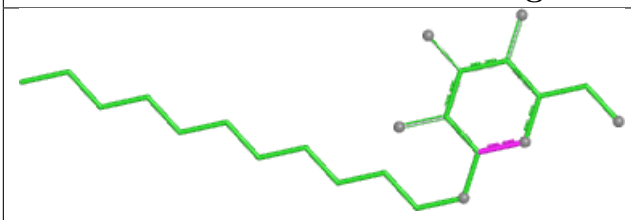


Torsions

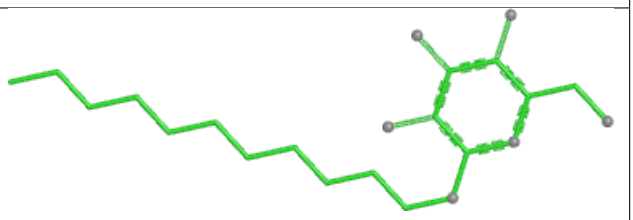


Rings

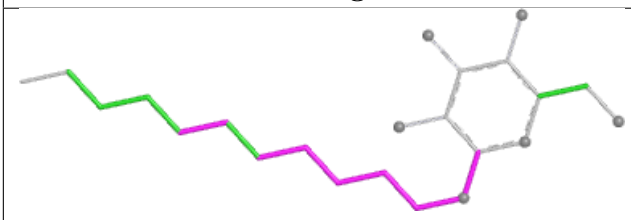
Ligand LMU r 901



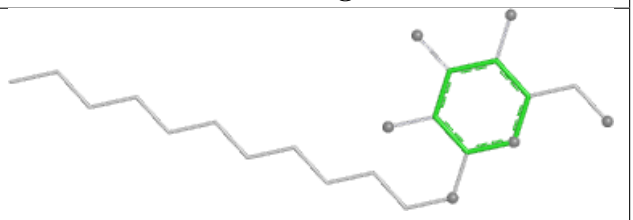
Bond lengths



Bond angles

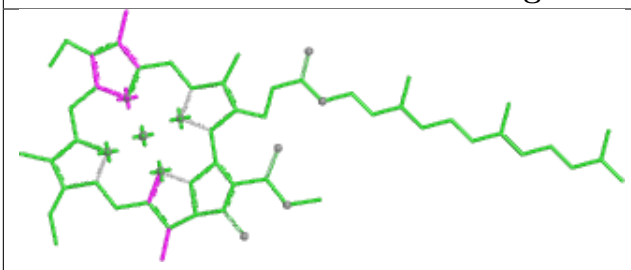


Torsions

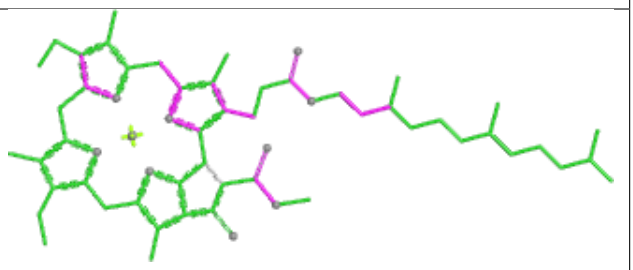


Rings

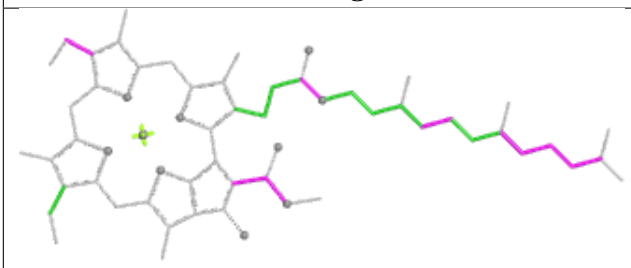
Ligand CLA Y 502



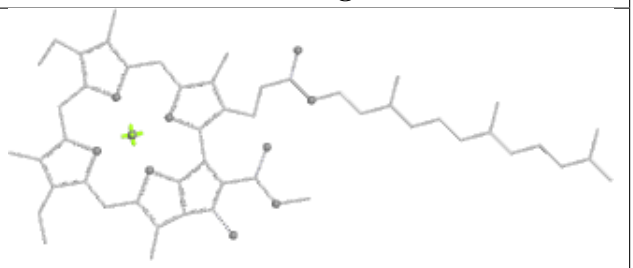
Bond lengths



Bond angles

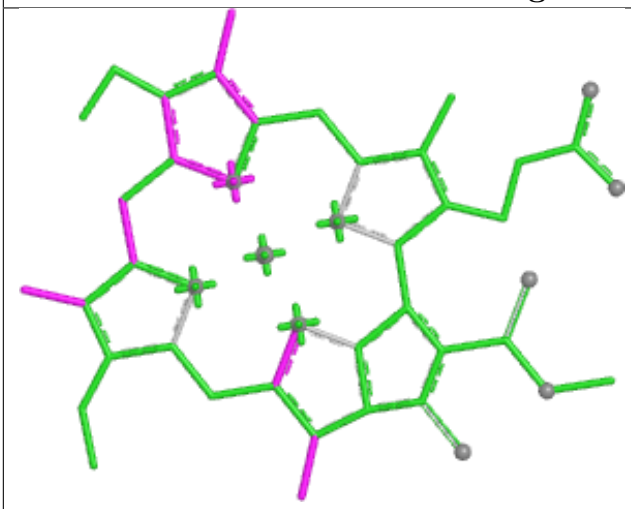


Torsions

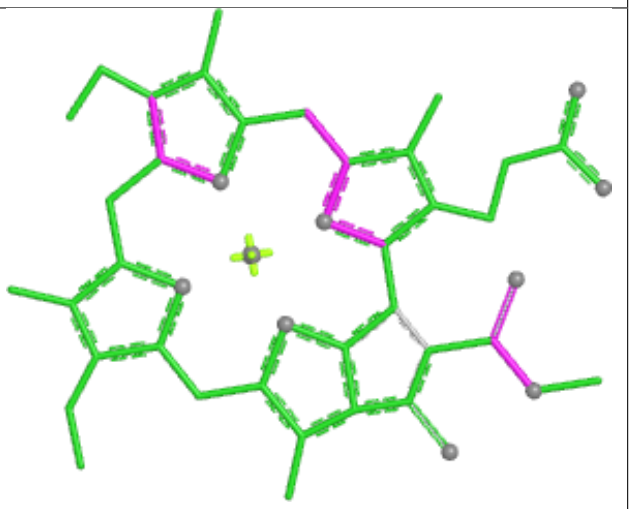


Rings

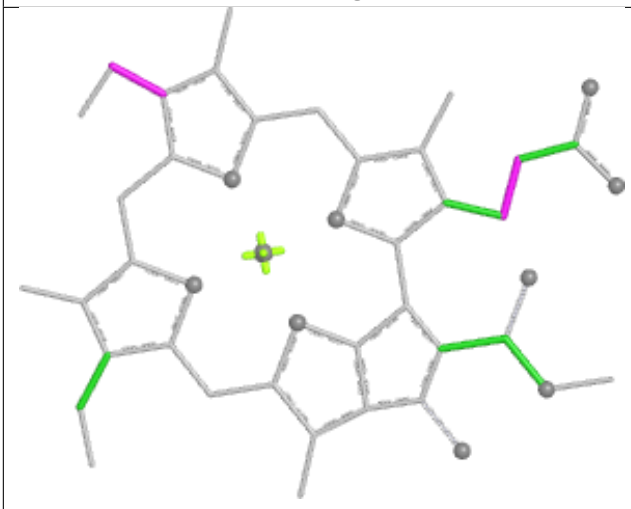
Ligand CLA 2 517



Bond lengths



Bond angles

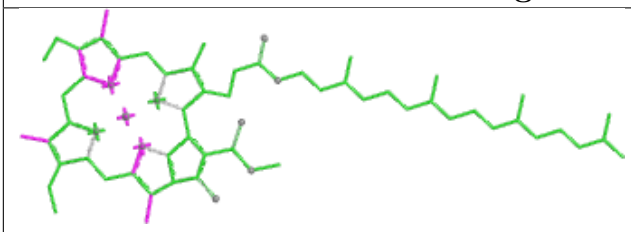


Torsions

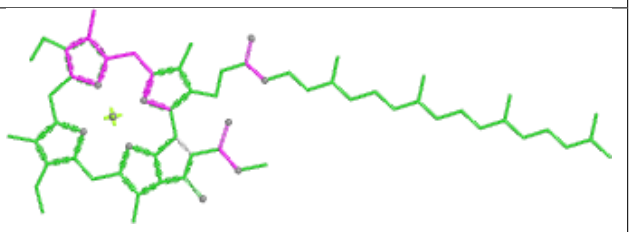


Rings

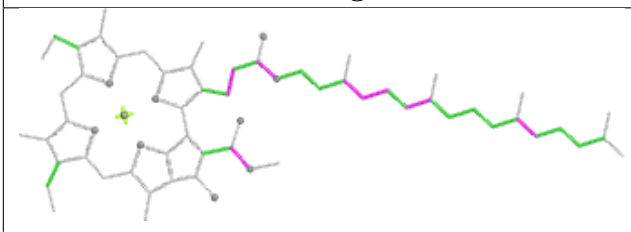
Ligand CLA A 1119



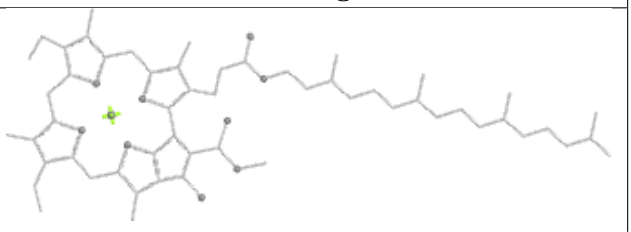
Bond lengths



Bond angles

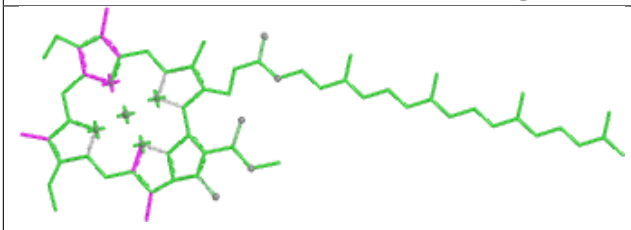


Torsions

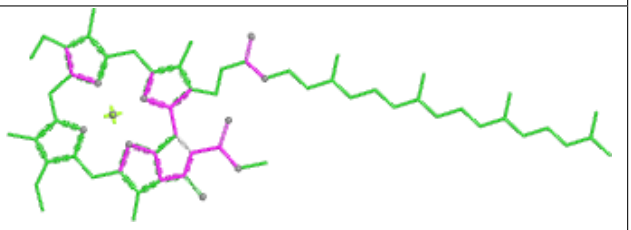


Rings

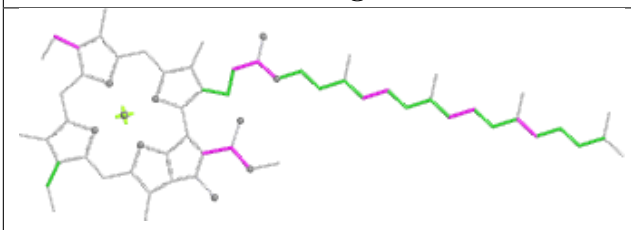
Ligand CLA A 1011



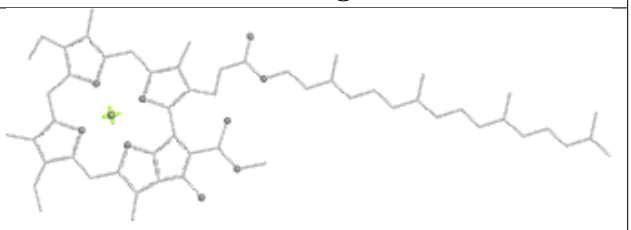
Bond lengths



Bond angles

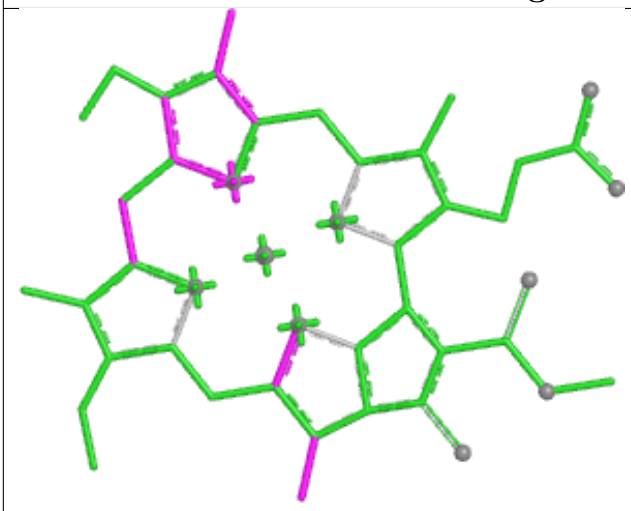


Torsions

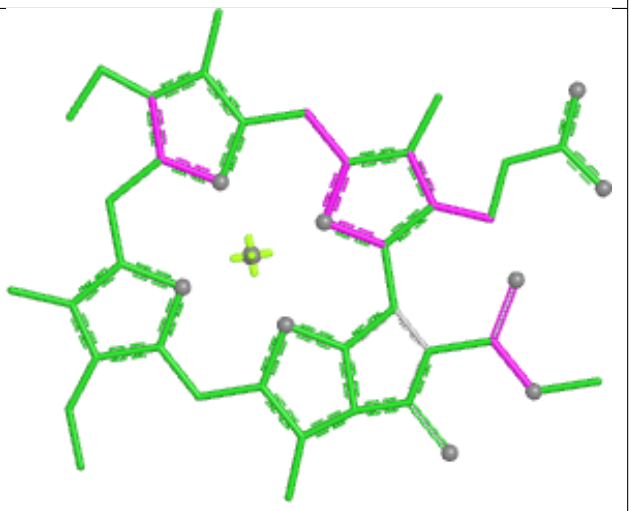


Rings

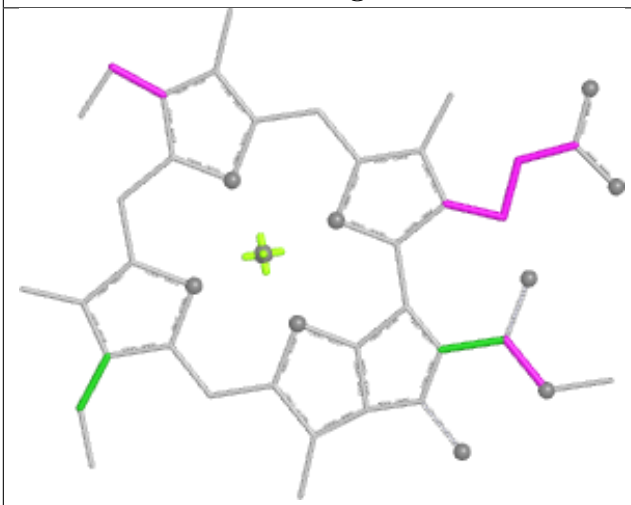
Ligand CLA 6 516



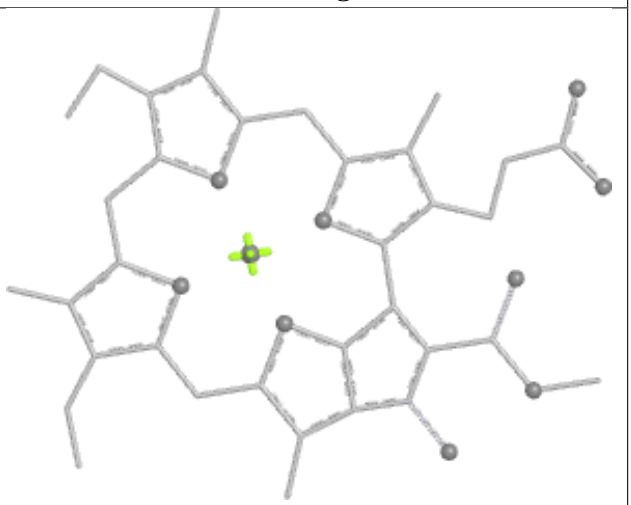
Bond lengths



Bond angles

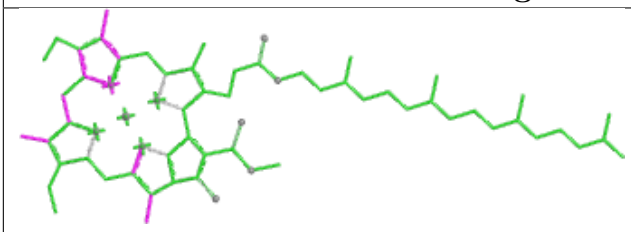


Torsions

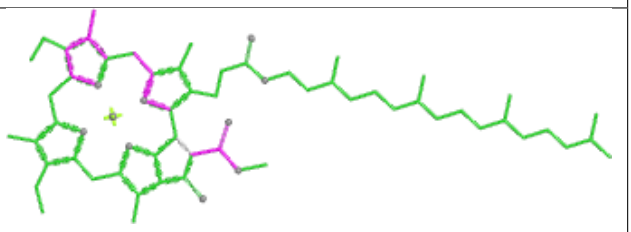


Rings

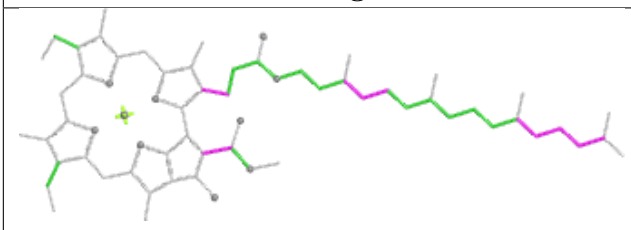
Ligand CLA G 1102



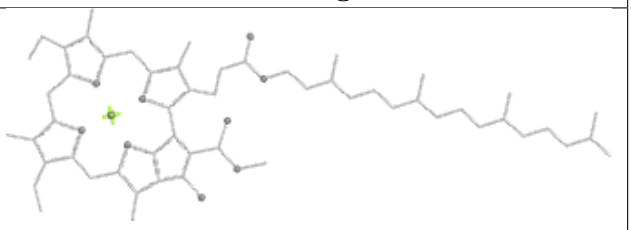
Bond lengths



Bond angles

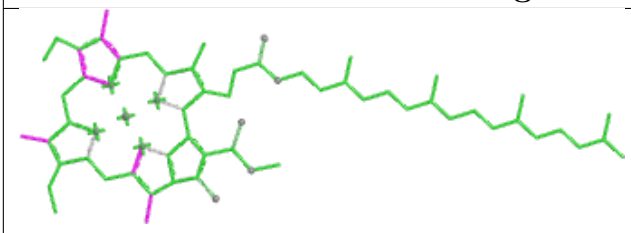


Torsions

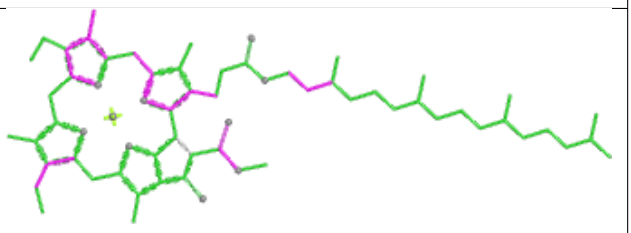


Rings

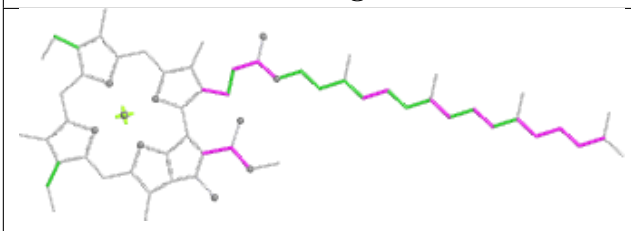
Ligand CLA G 1103



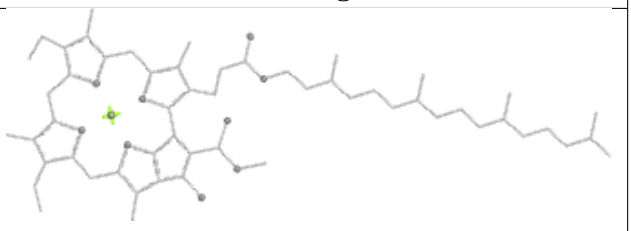
Bond lengths



Bond angles

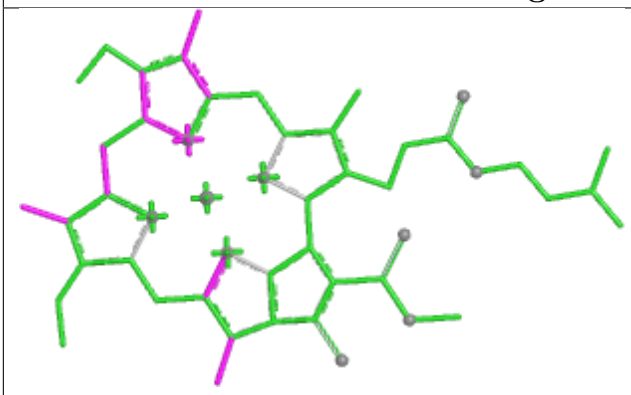


Torsions

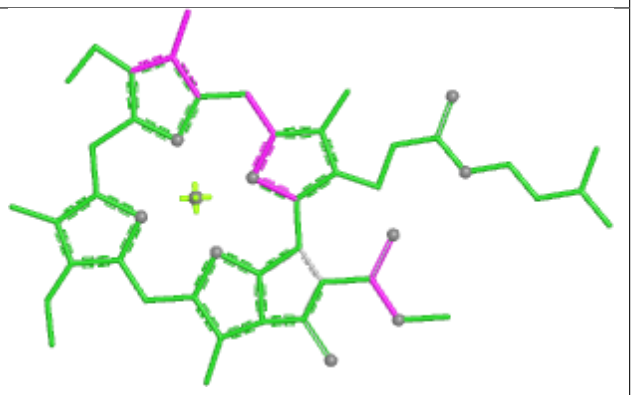


Rings

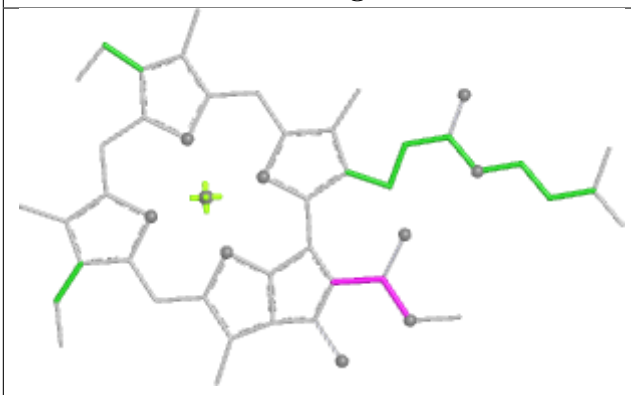
Ligand CLA 3 506



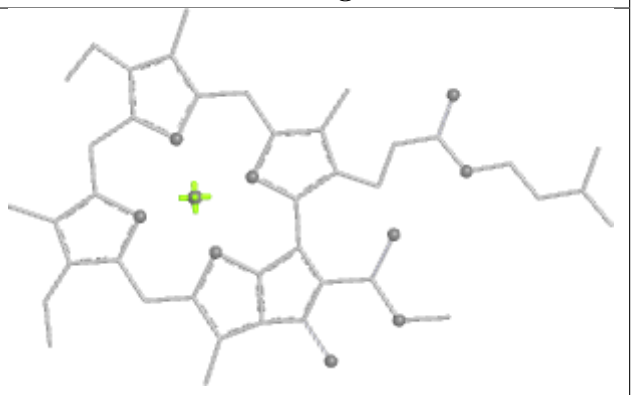
Bond lengths



Bond angles



Torsions

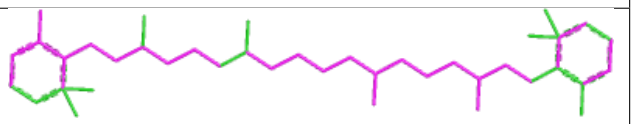


Rings

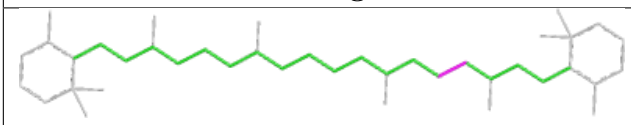
Ligand BCR H 4009



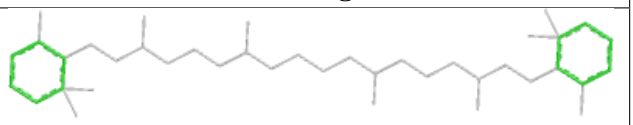
Bond lengths



Bond angles

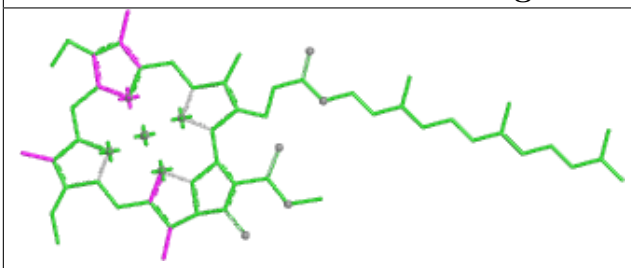


Torsions

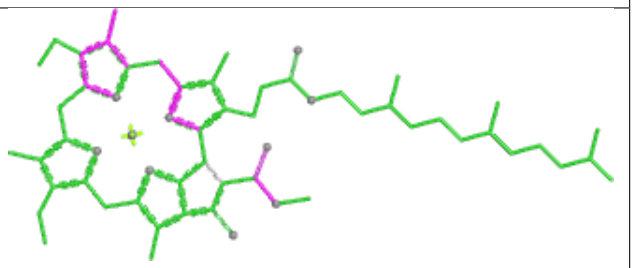


Rings

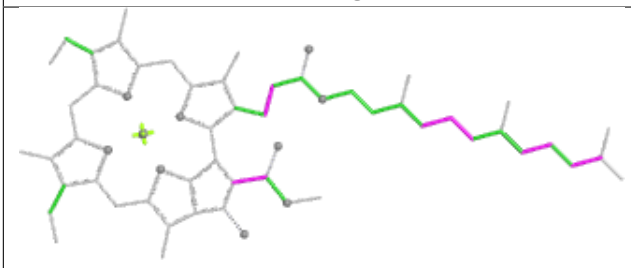
Ligand CLA H 1218



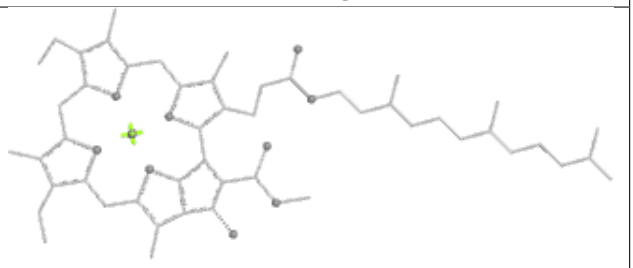
Bond lengths



Bond angles

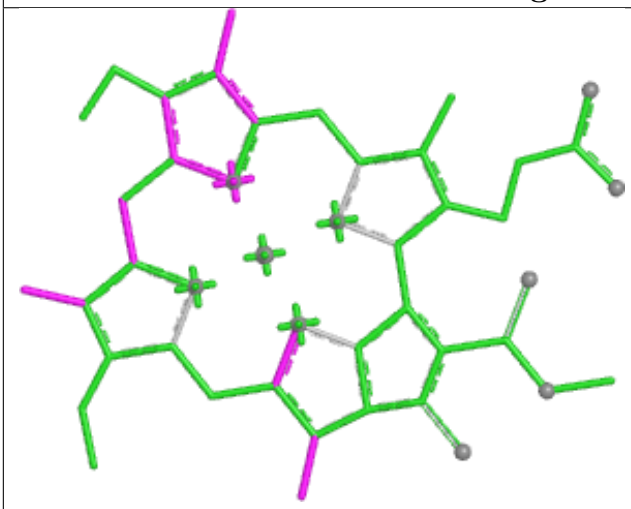


Torsions

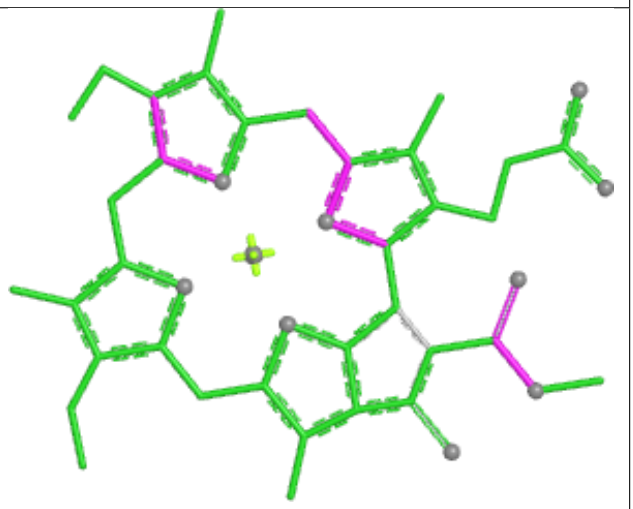


Rings

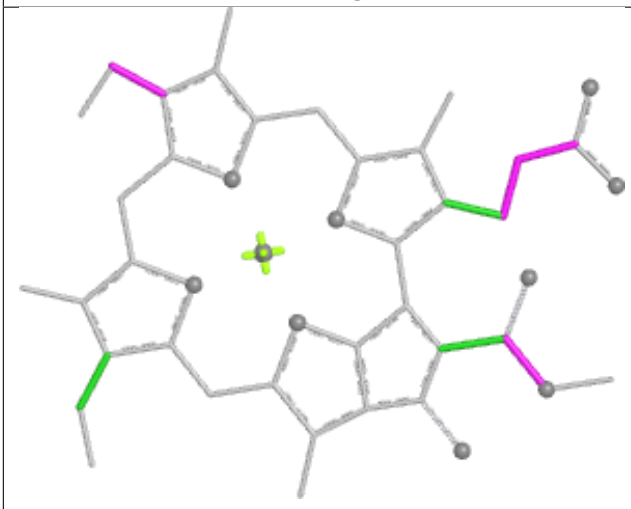
Ligand CLA t 513



Bond lengths



Bond angles

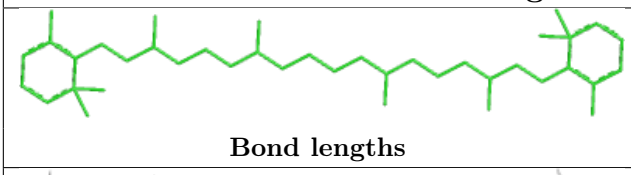


Torsions

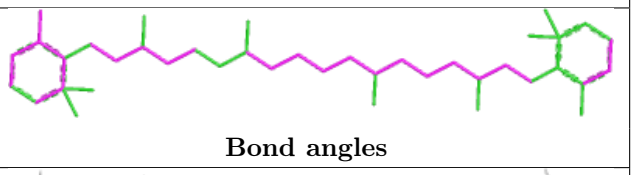


Rings

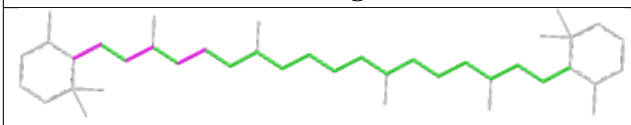
Ligand BCR v 521



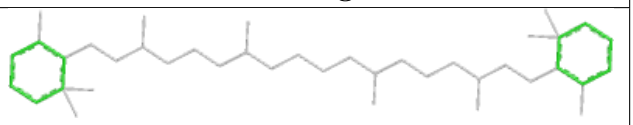
Bond lengths



Bond angles

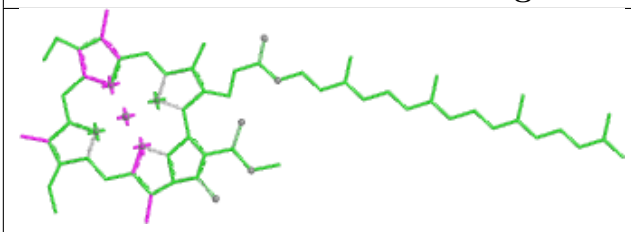


Torsions

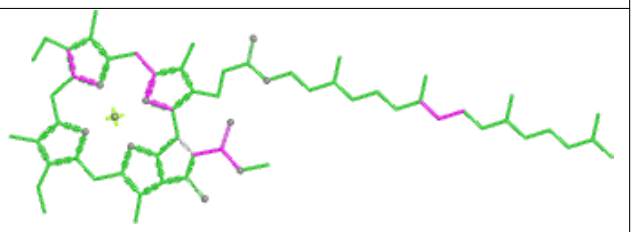


Rings

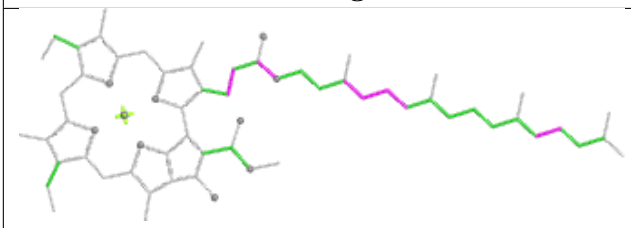
Ligand CLA H 1204



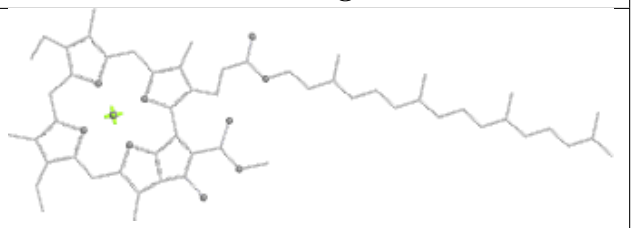
Bond lengths



Bond angles

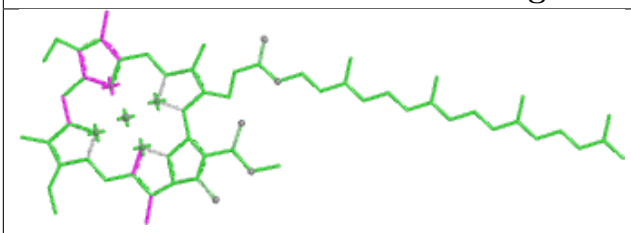


Torsions

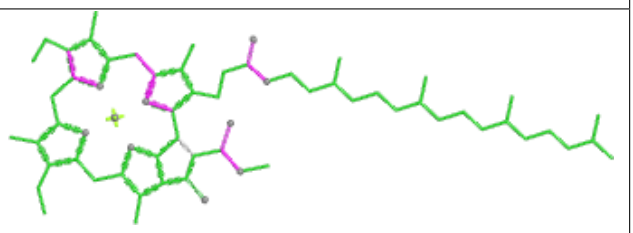


Rings

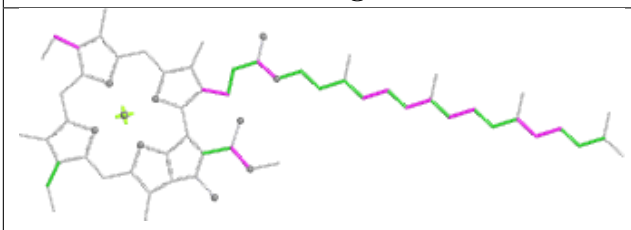
Ligand CLA a 513



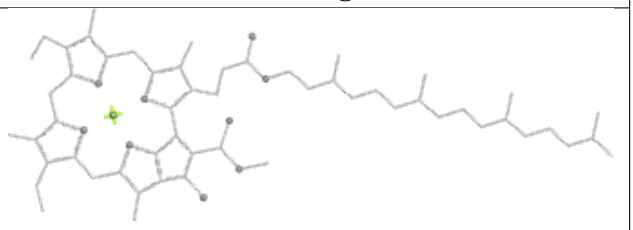
Bond lengths



Bond angles

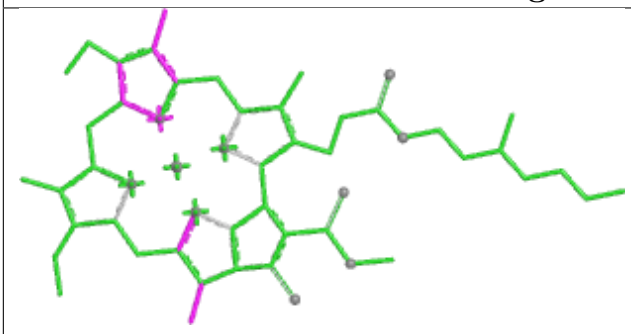


Torsions

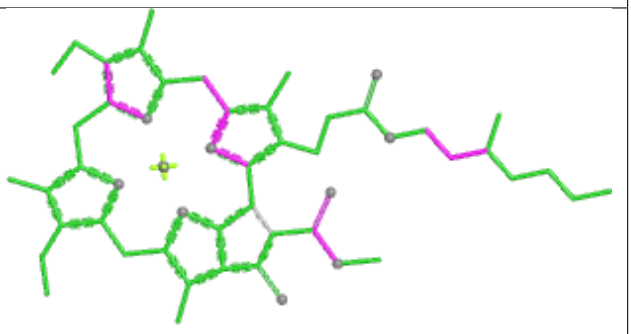


Rings

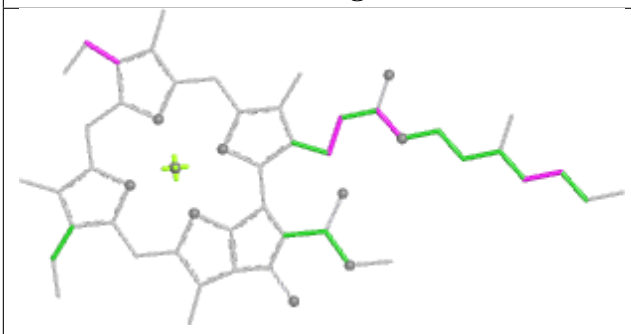
Ligand CLA 2 512



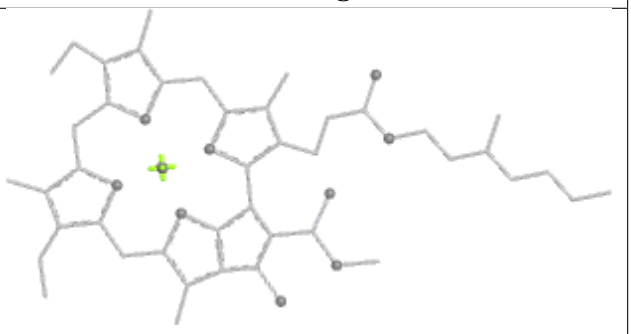
Bond lengths



Bond angles

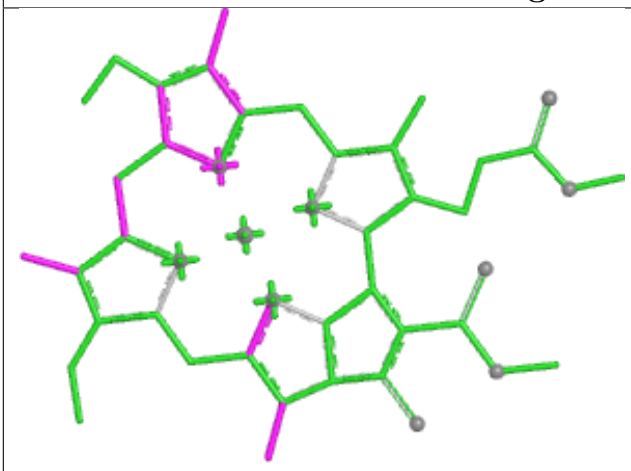


Torsions

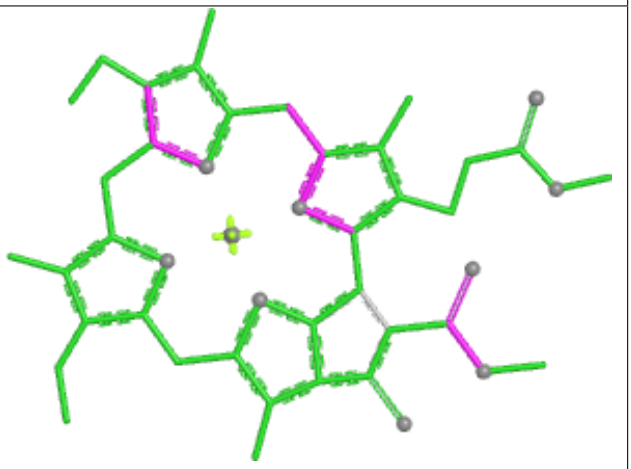


Rings

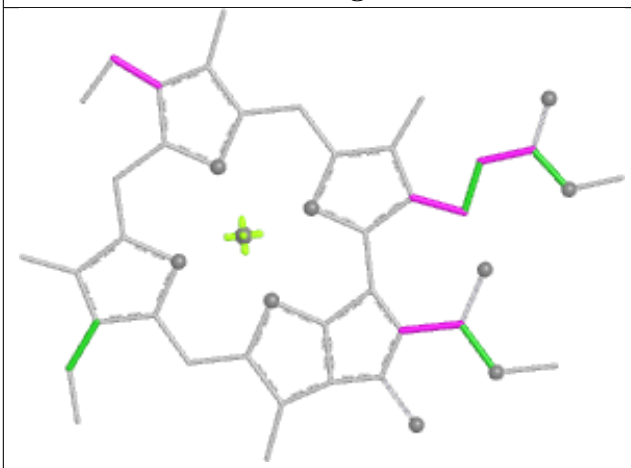
Ligand CLA 5 519



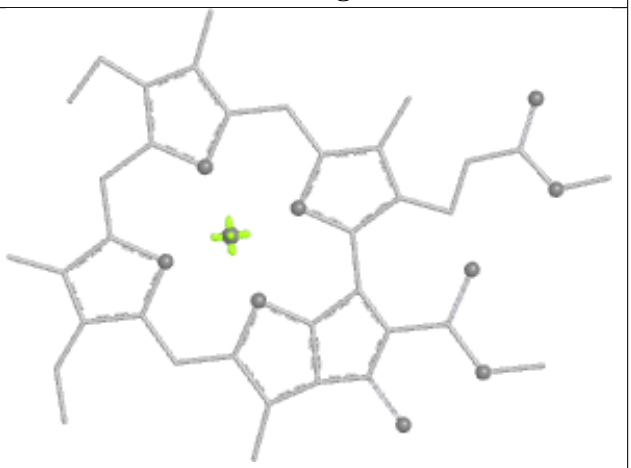
Bond lengths



Bond angles



Torsions

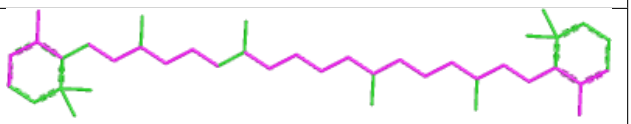


Rings

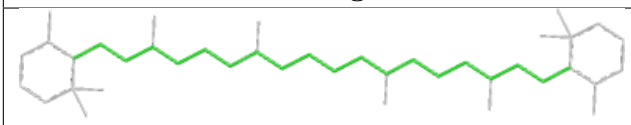
Ligand BCR e 4002



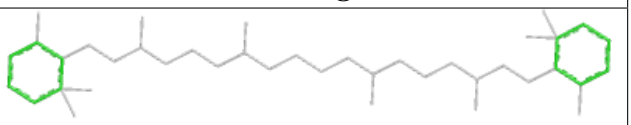
Bond lengths



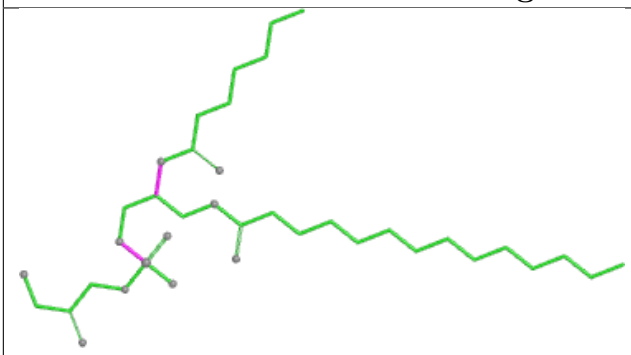
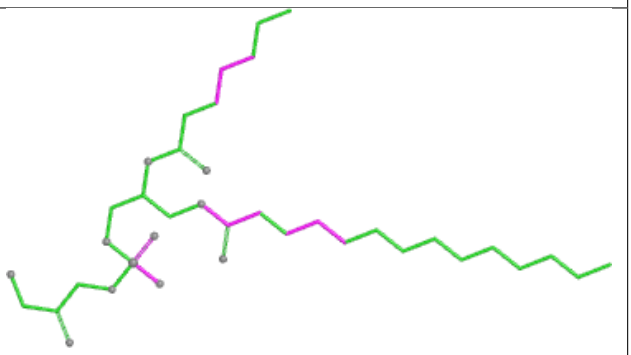
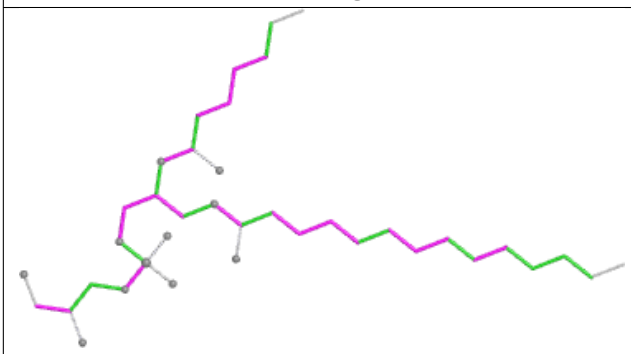
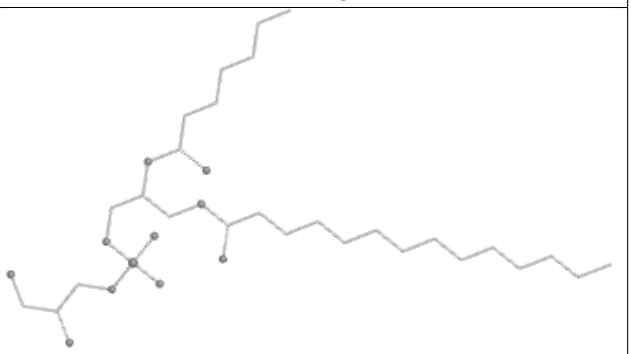
Bond angles

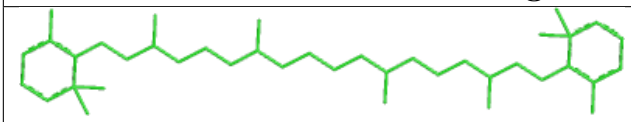
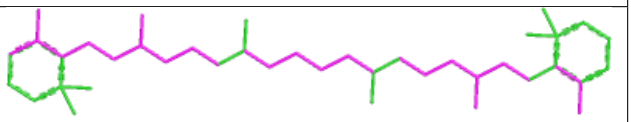
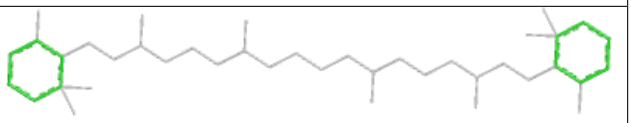


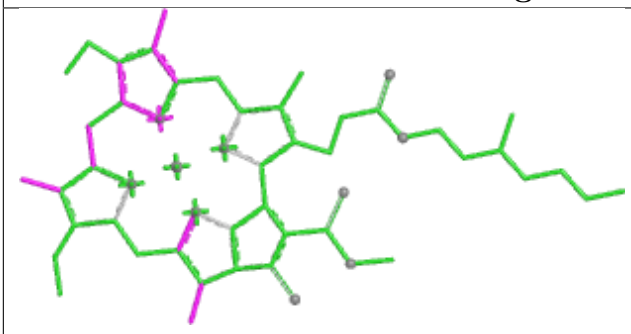
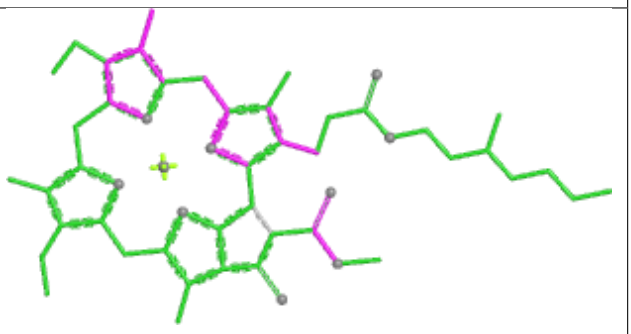
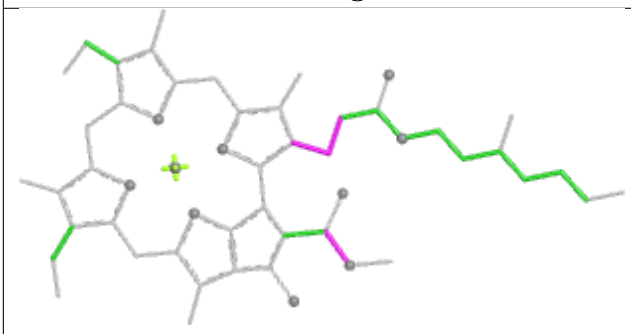
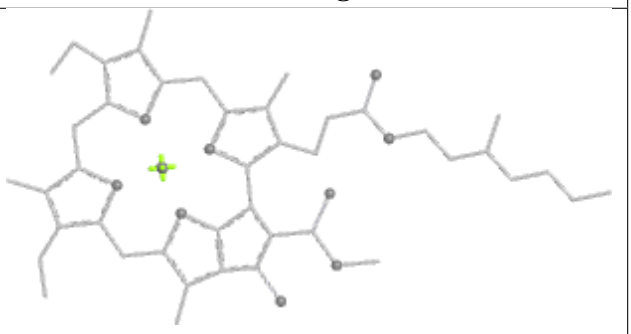
Torsions

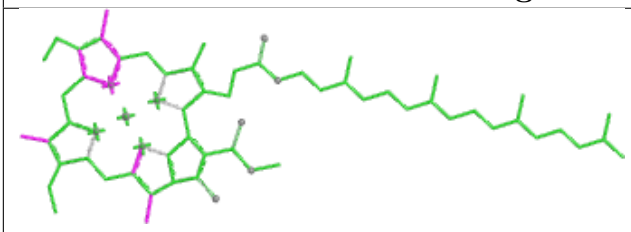
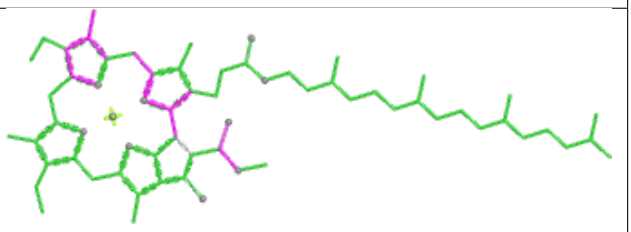
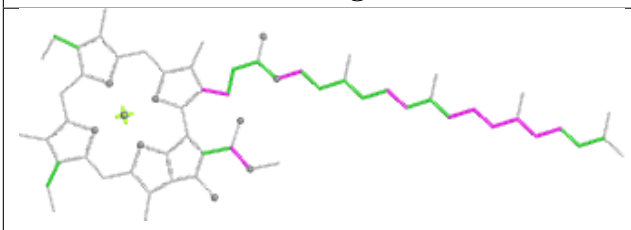
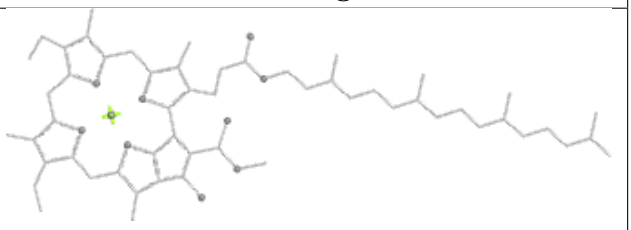


Rings

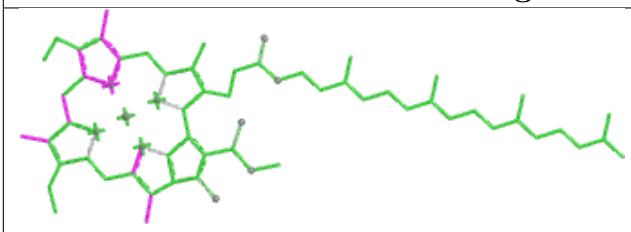
Ligand LHG n 5218	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR u 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

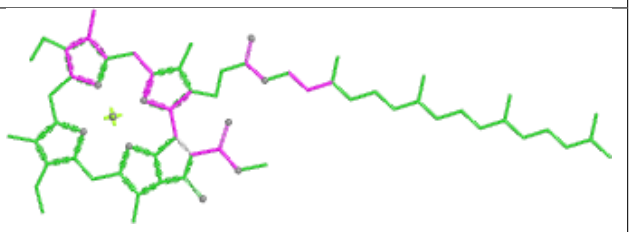
Ligand CLA A 1120	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

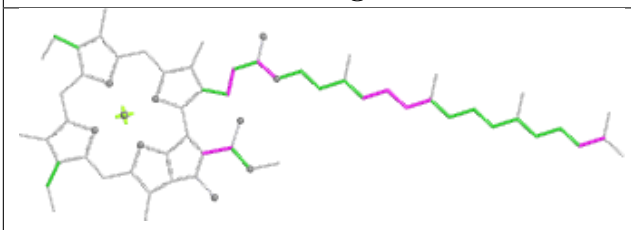
Ligand CLA H 1213



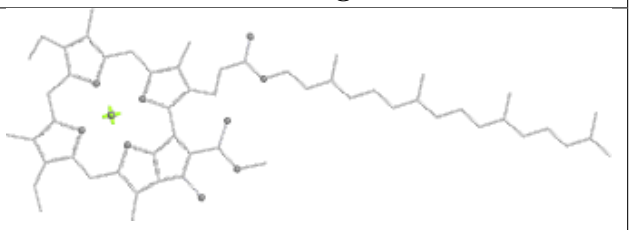
Bond lengths



Bond angles

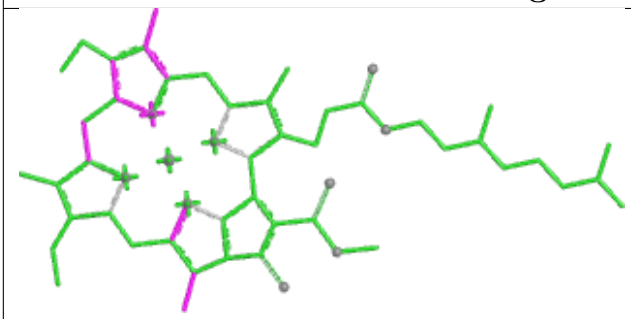


Torsions

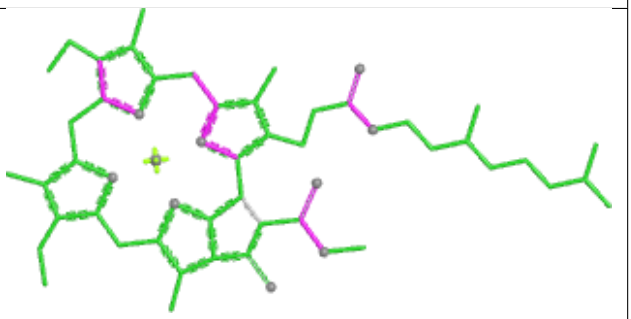


Rings

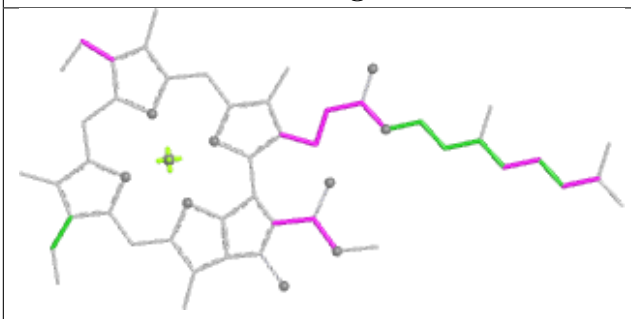
Ligand CLA c 518



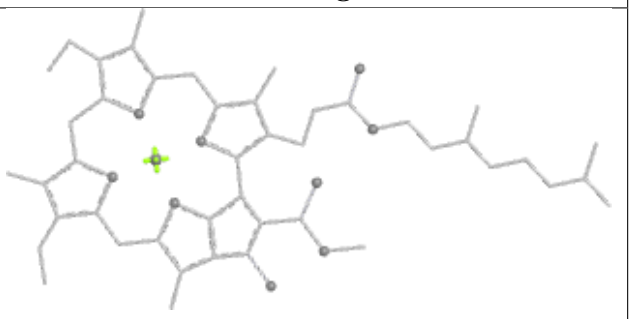
Bond lengths



Bond angles

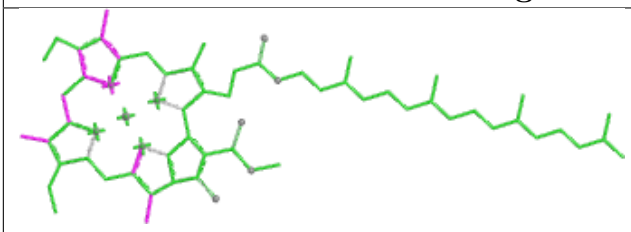


Torsions

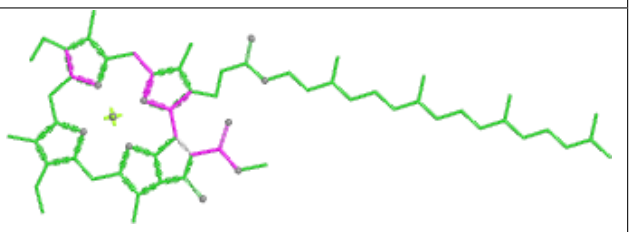


Rings

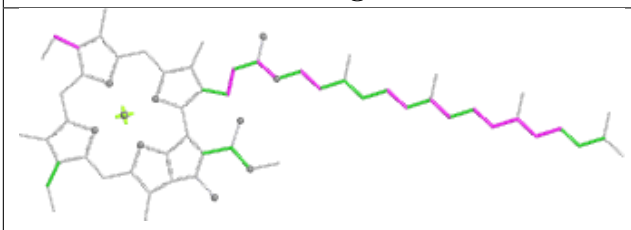
Ligand CLA B 1214



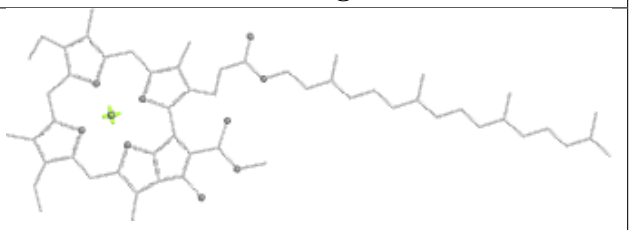
Bond lengths



Bond angles



Torsions



Rings

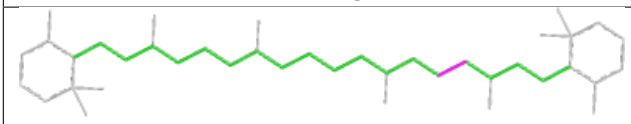
Ligand BCR f 4009



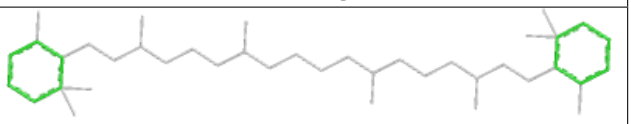
Bond lengths



Bond angles

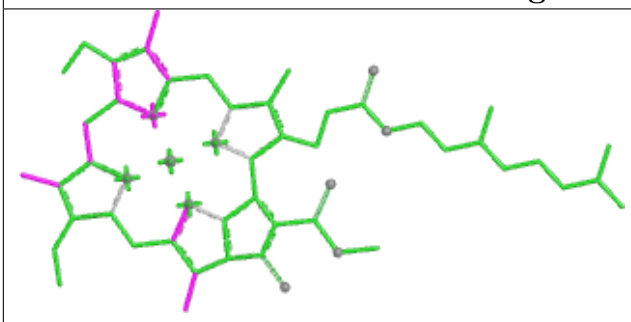


Torsions

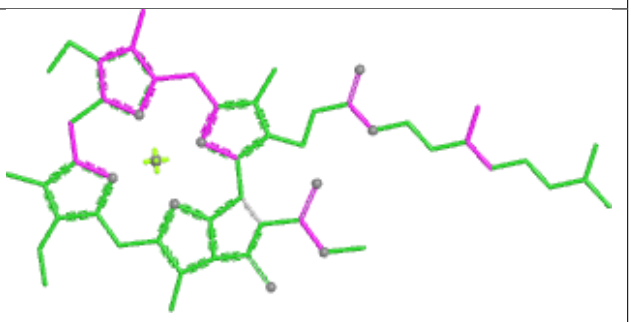


Rings

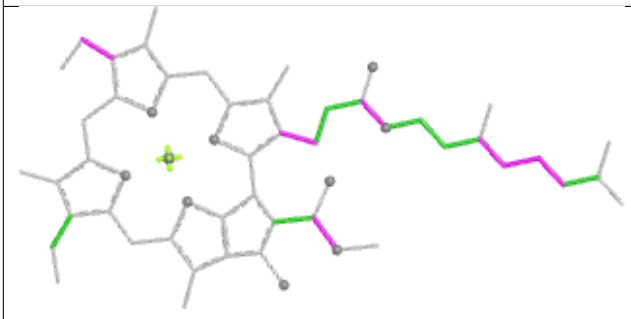
Ligand CLA 1 508



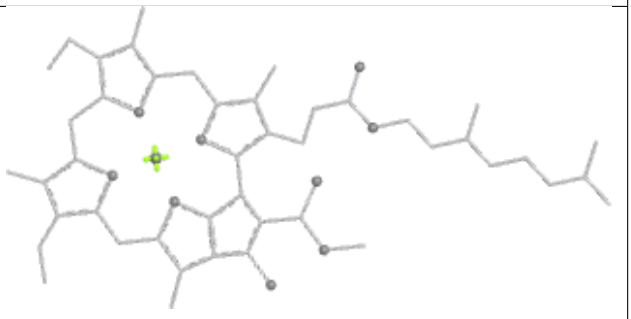
Bond lengths



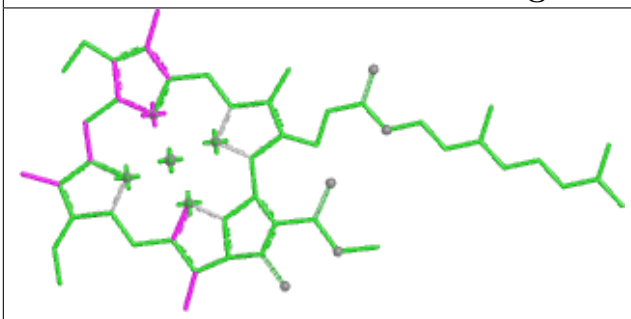
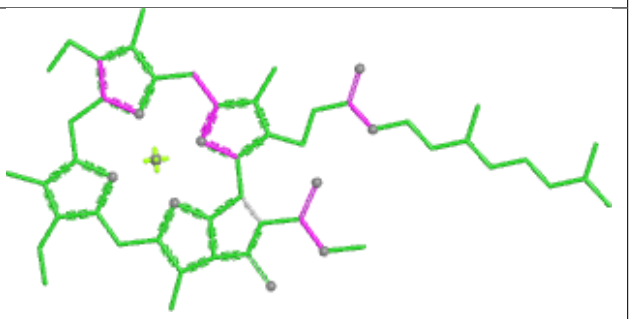
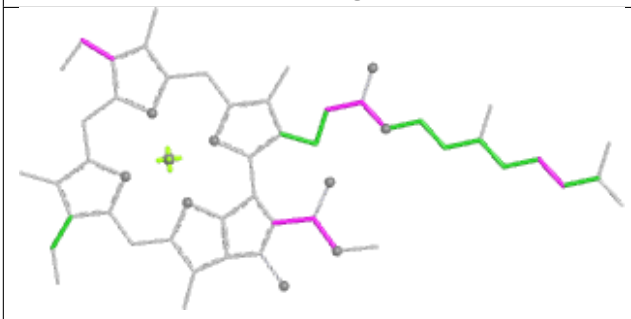
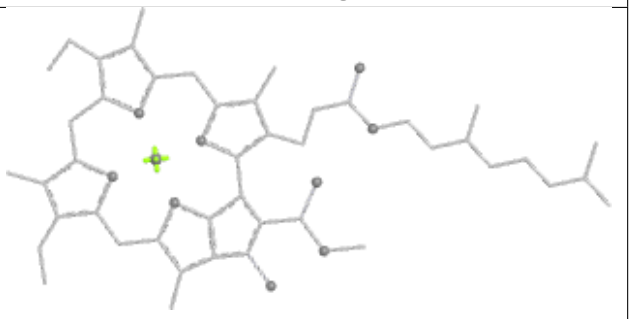
Bond angles

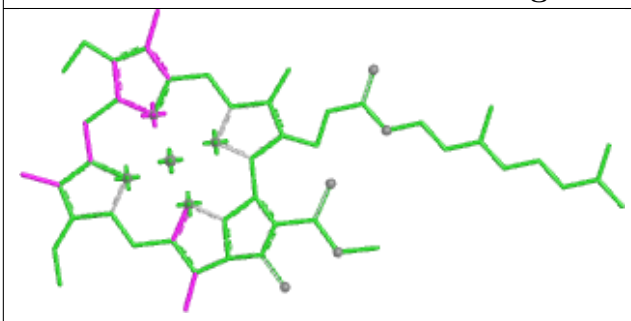
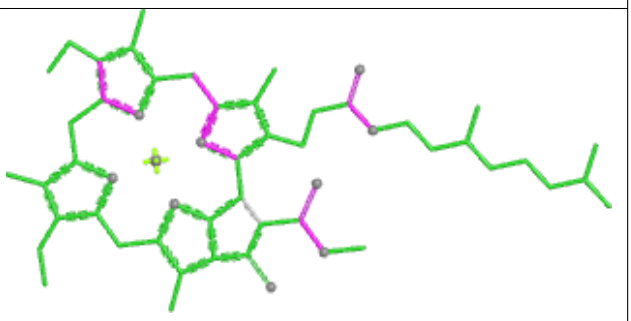
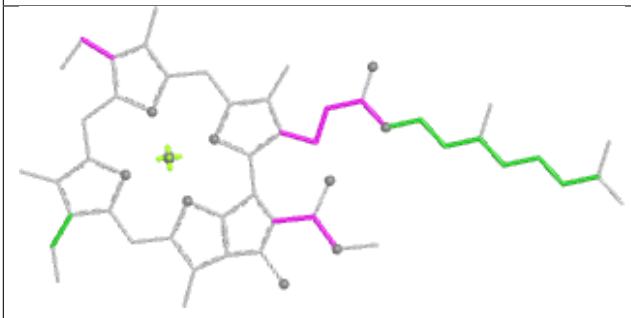
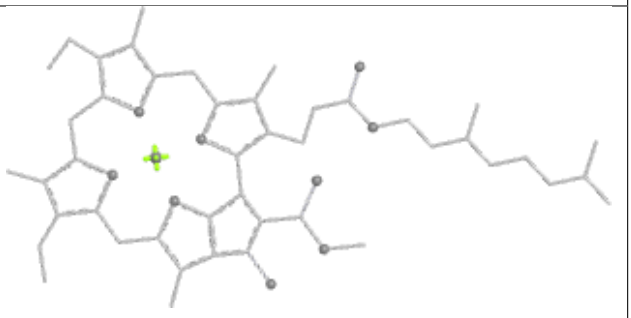


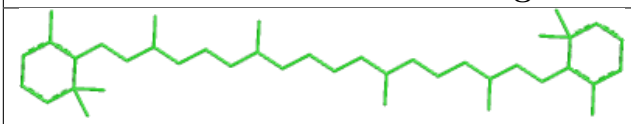
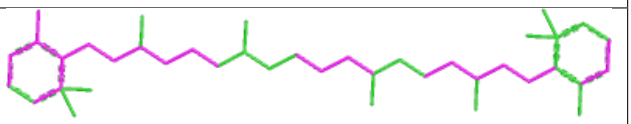
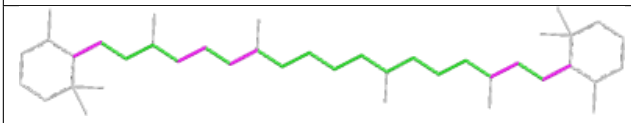
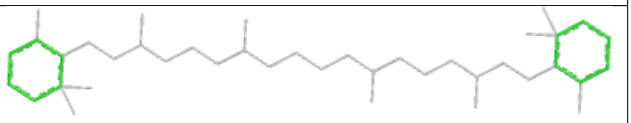
Torsions

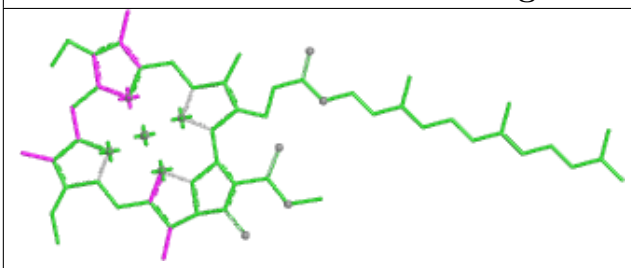
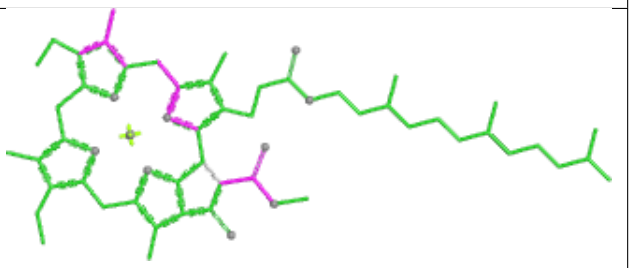
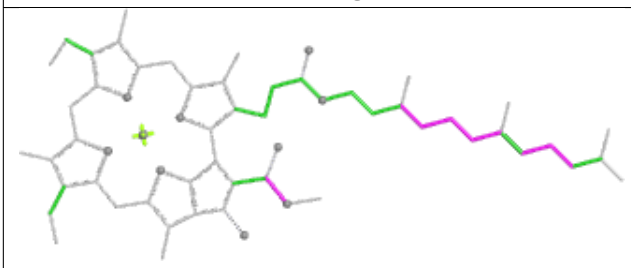
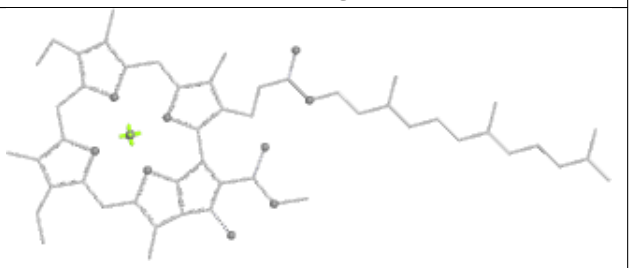


Rings

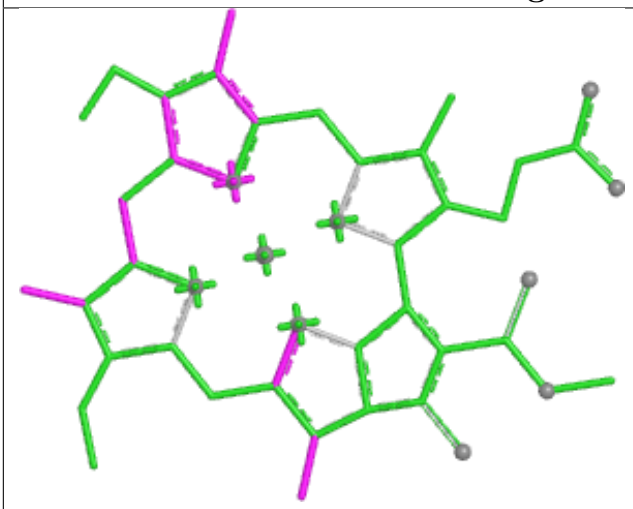
Ligand CLA 3 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA t 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

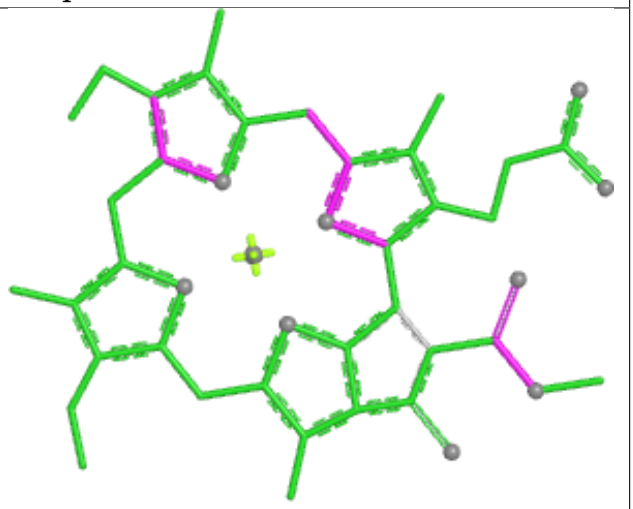
Ligand BCR T 4012	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 1503	
 Bond lengths	 Bond angles
 Torsions	 Rings

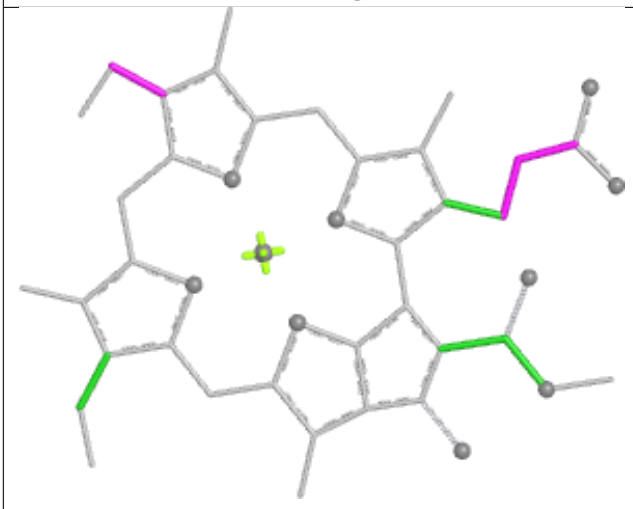
Ligand CLA q 517



Bond lengths



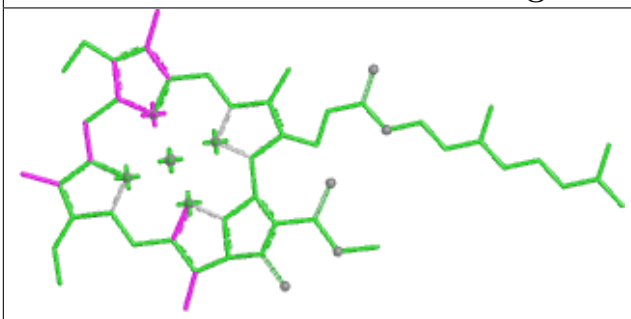
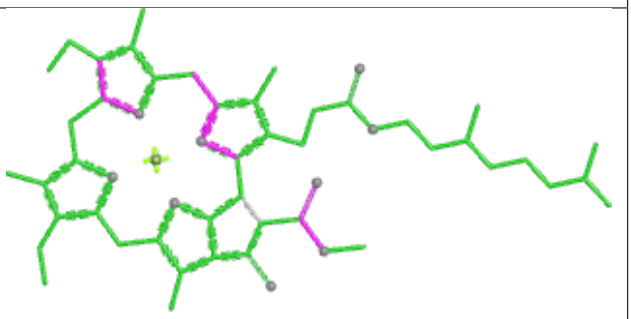
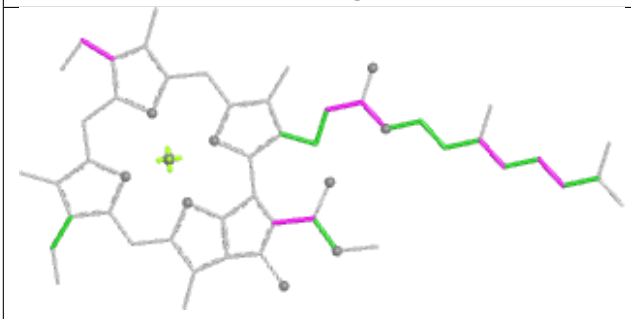
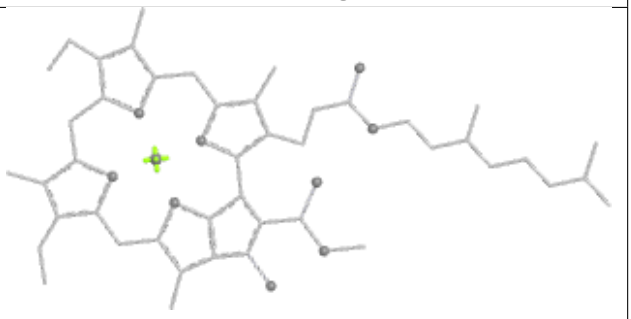
Bond angles

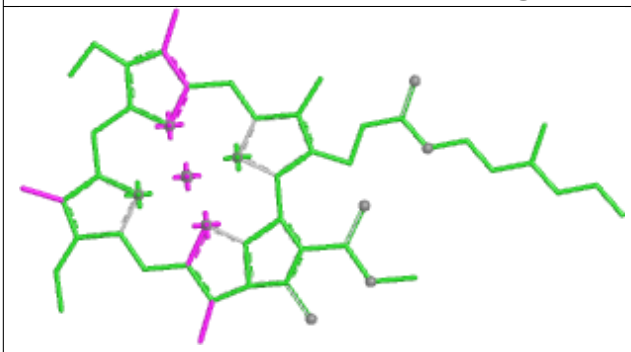
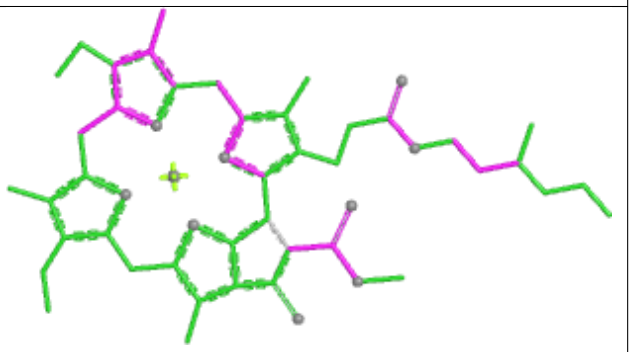
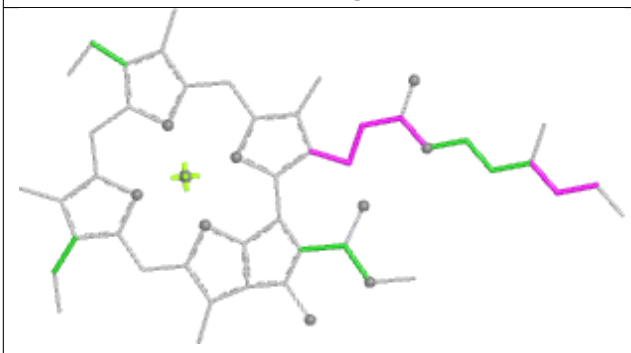
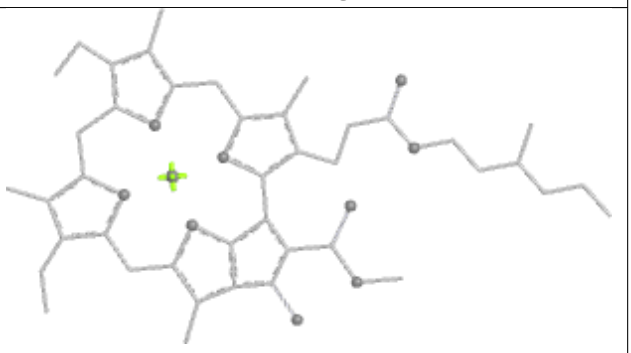


Torsions

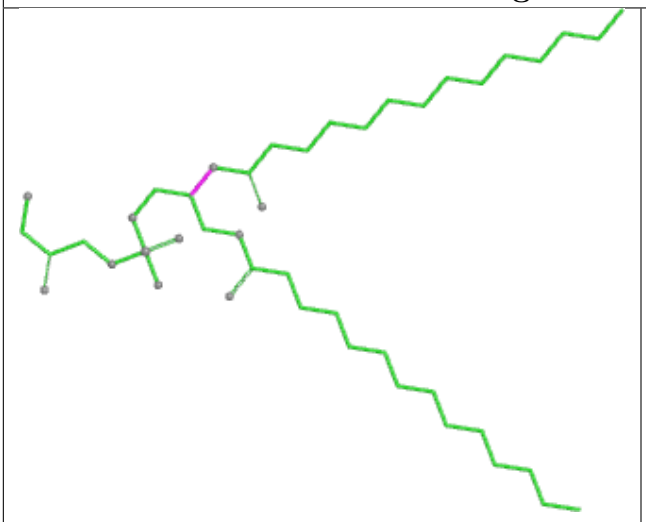


Rings

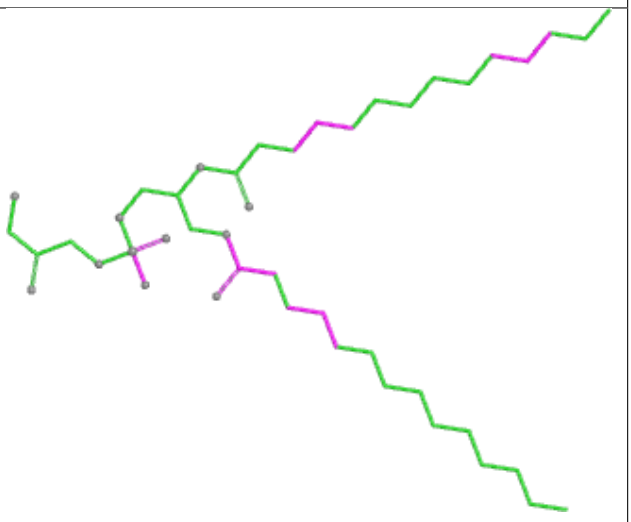
Ligand CLA b 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1135	
	
Bond lengths	Bond angles
	
Torsions	Rings

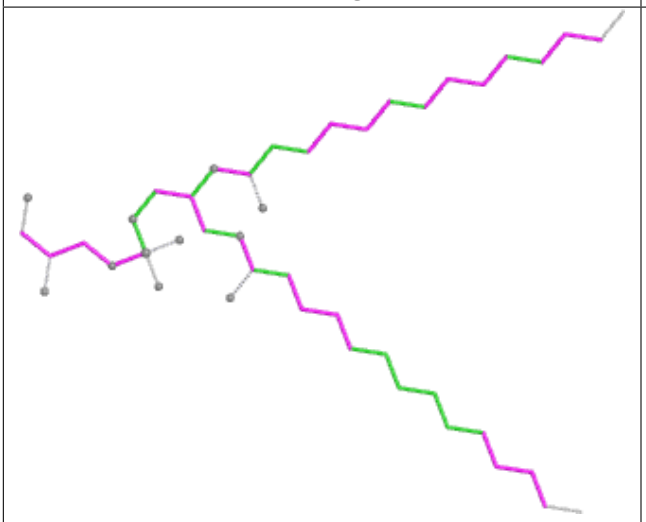
Ligand LHG G 5005



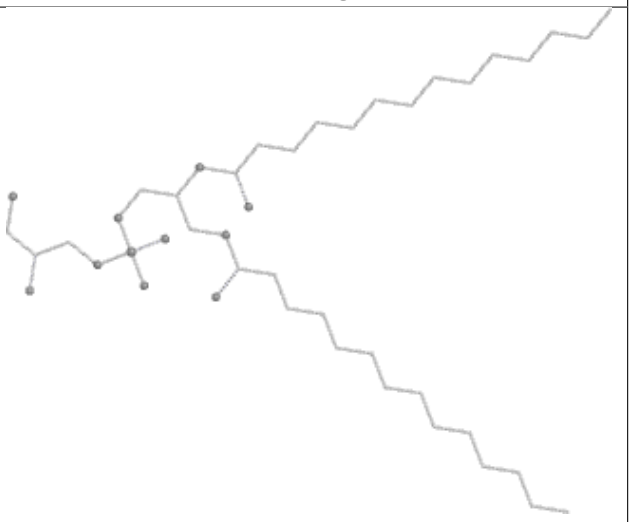
Bond lengths



Bond angles

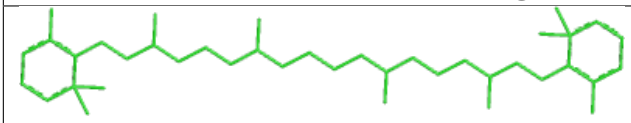


Torsions

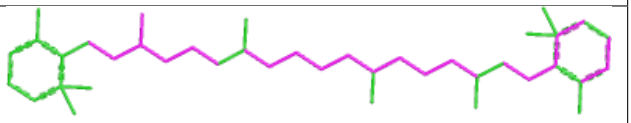


Rings

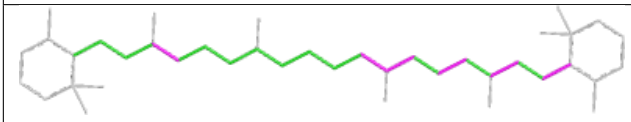
Ligand BCR A 4011



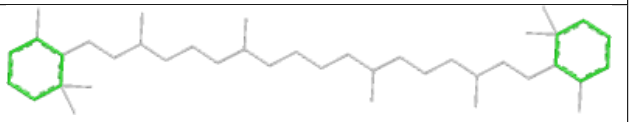
Bond lengths



Bond angles

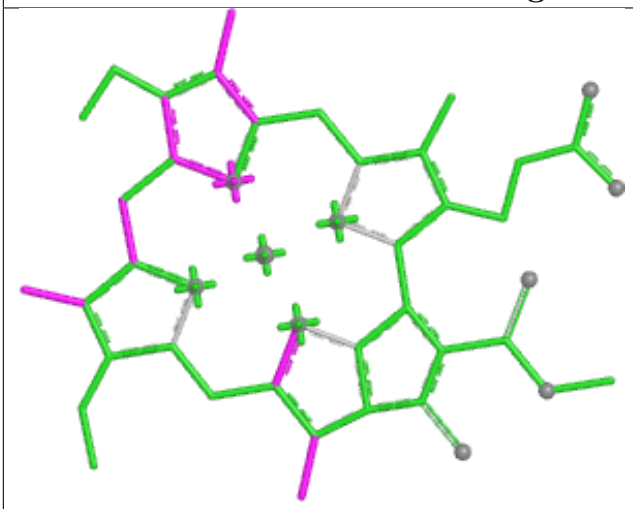


Torsions

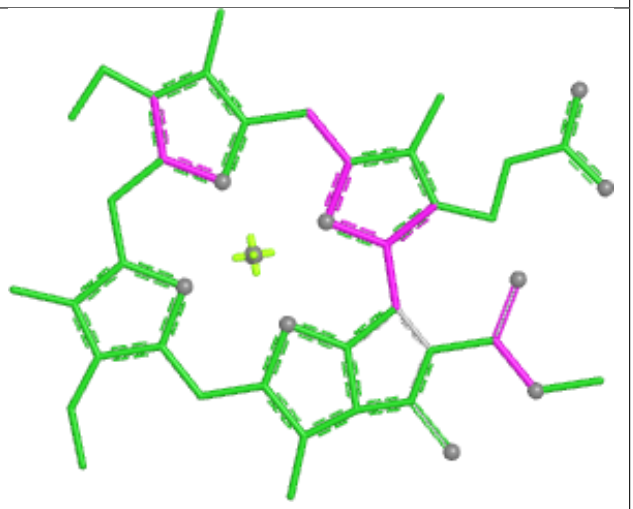


Rings

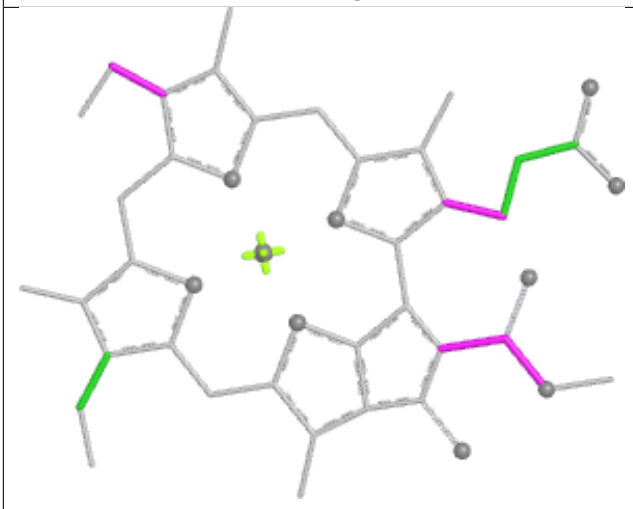
Ligand CLA b 517



Bond lengths



Bond angles

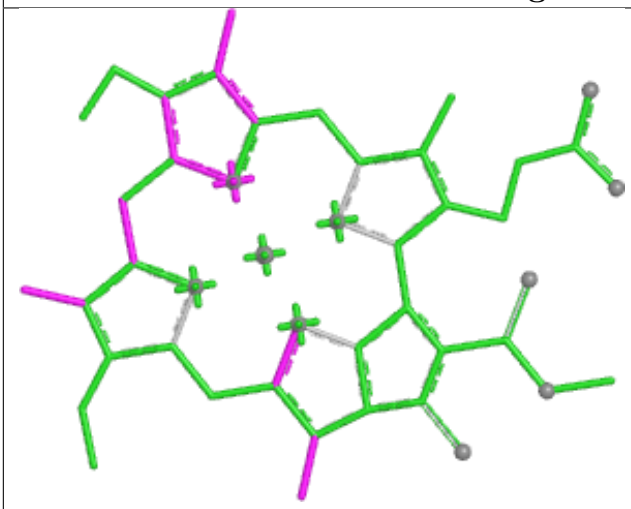


Torsions

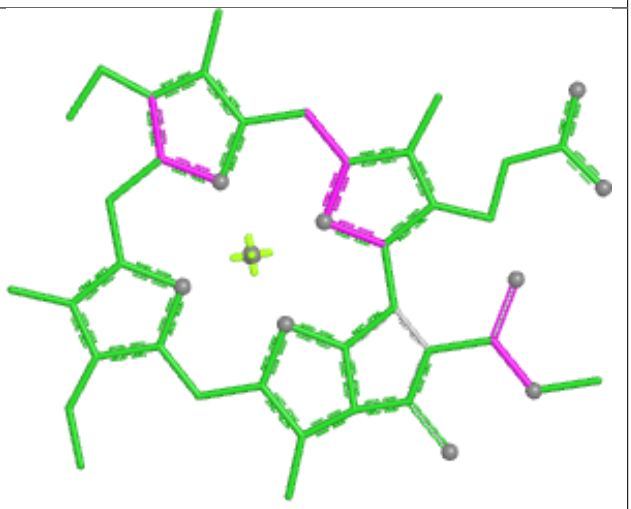


Rings

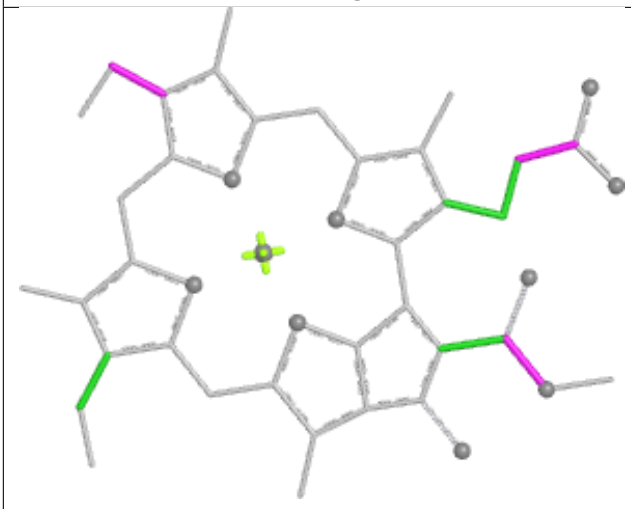
Ligand CLA 5 513



Bond lengths



Bond angles

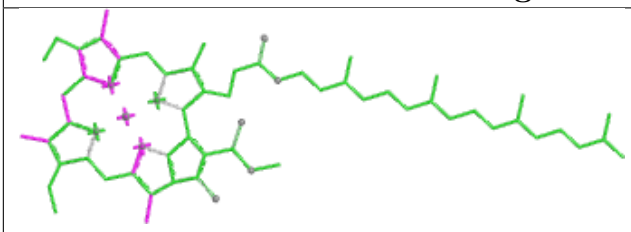


Torsions

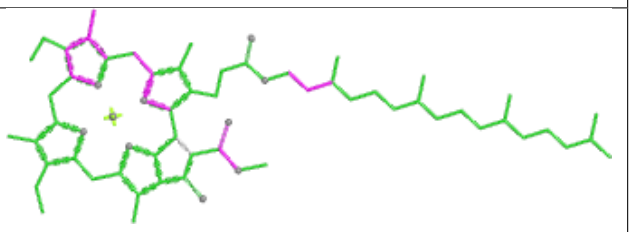


Rings

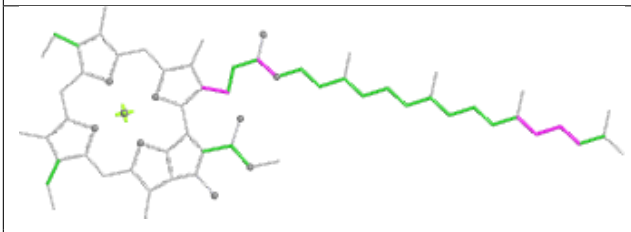
Ligand CLA H 1225



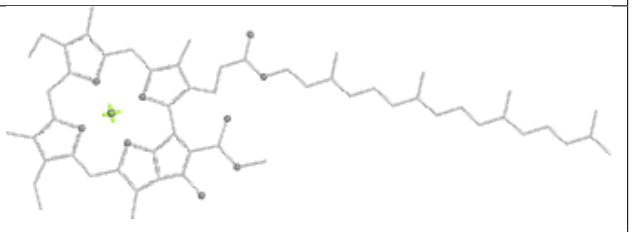
Bond lengths



Bond angles

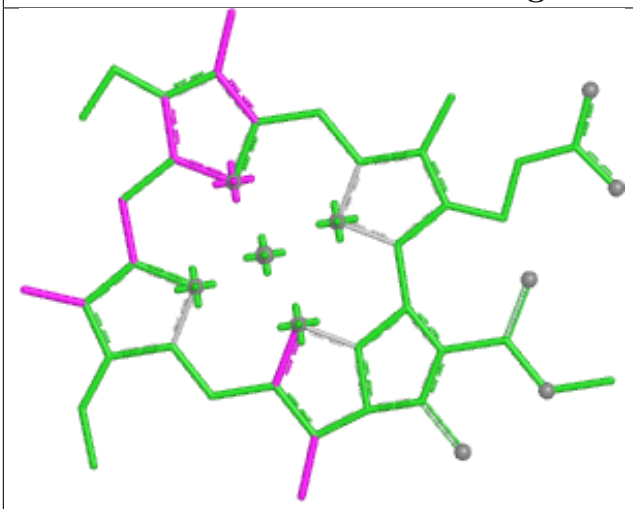


Torsions

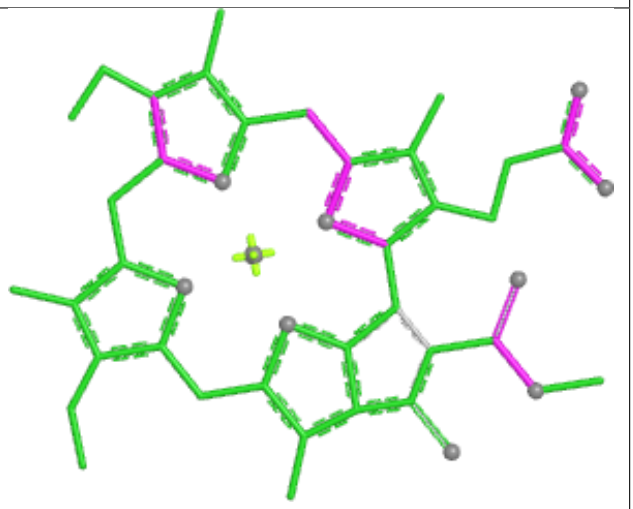


Rings

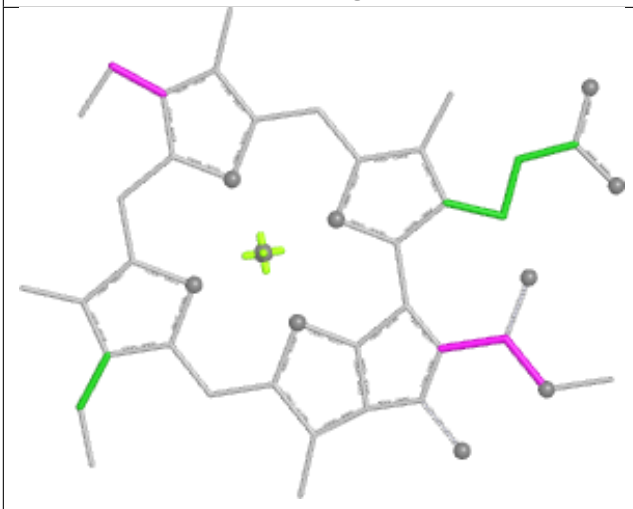
Ligand CLA u 506



Bond lengths



Bond angles

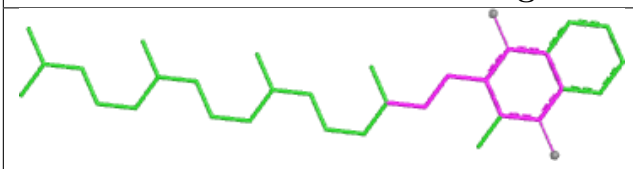


Torsions

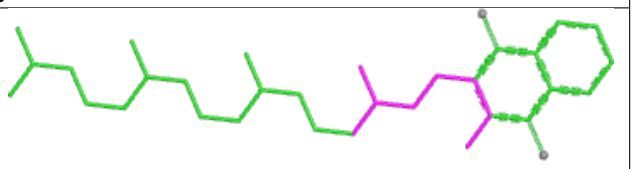


Rings

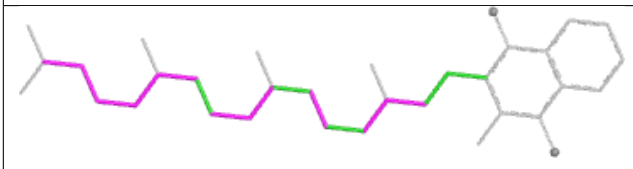
Ligand PQN e 2001



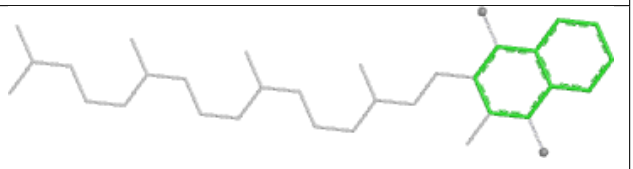
Bond lengths



Bond angles

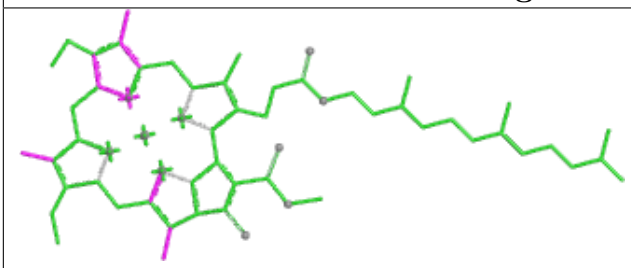


Torsions

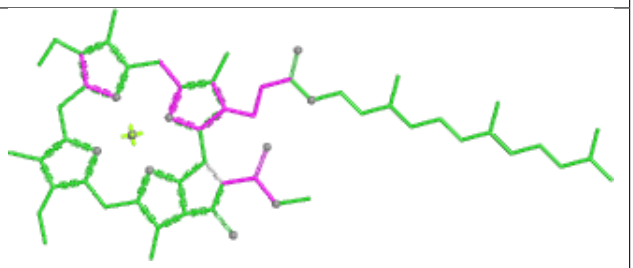


Rings

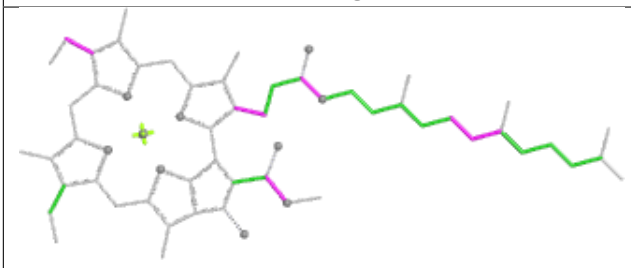
Ligand CLA B 1230



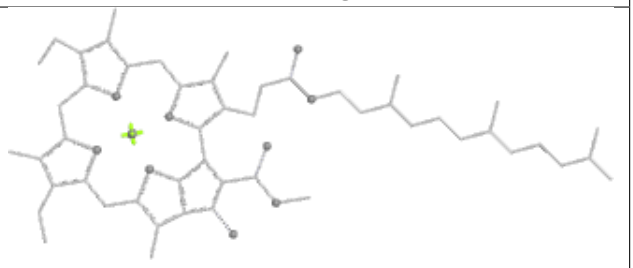
Bond lengths



Bond angles

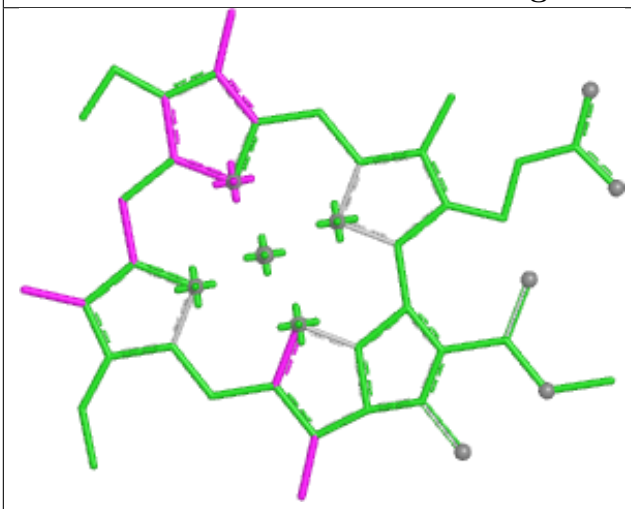


Torsions

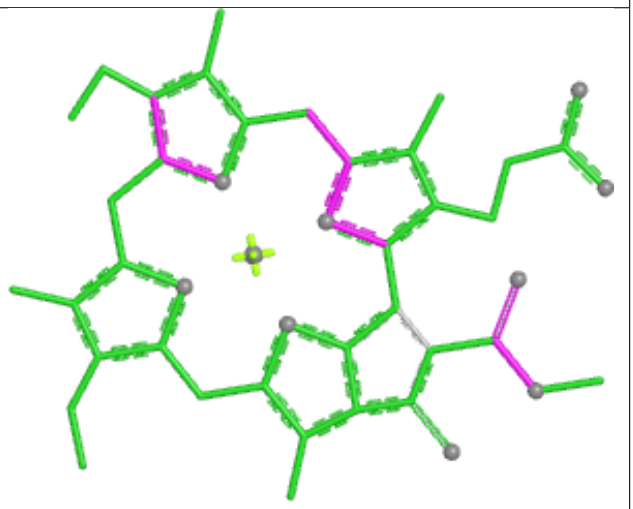


Rings

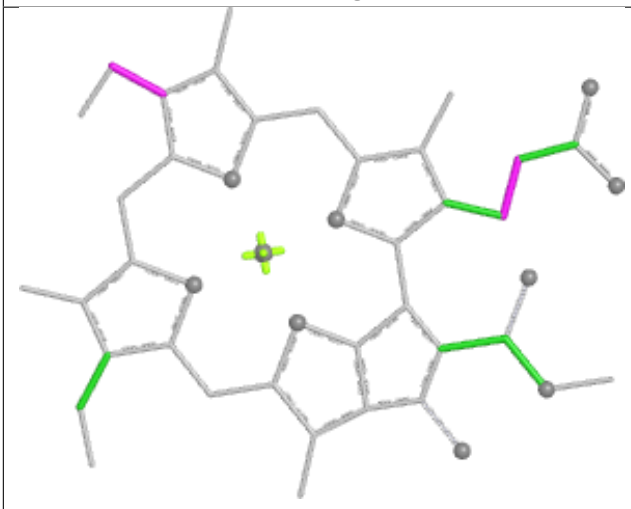
Ligand CLA r 517



Bond lengths



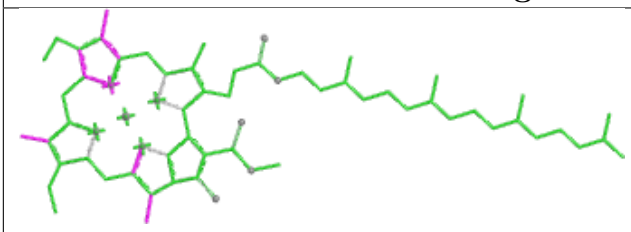
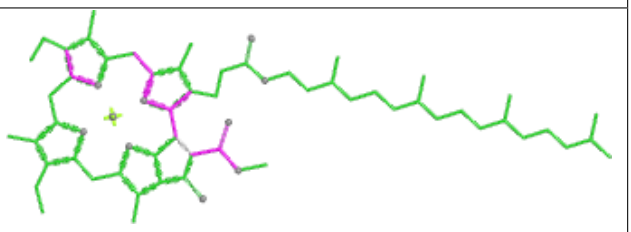
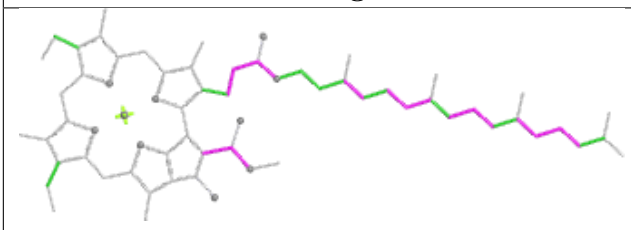
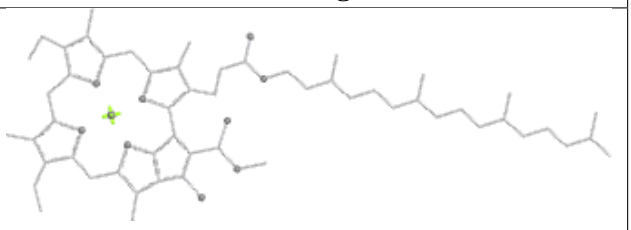
Bond angles

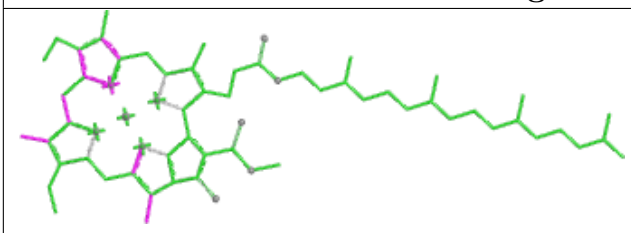
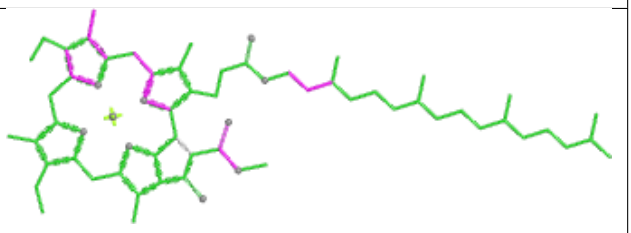
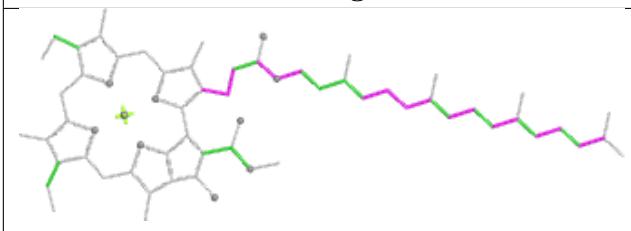
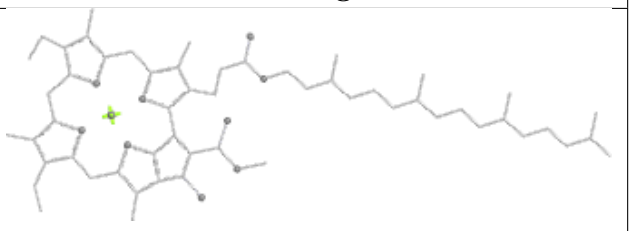


Torsions

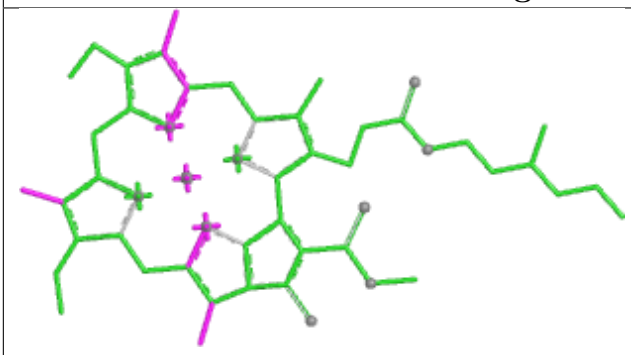


Rings

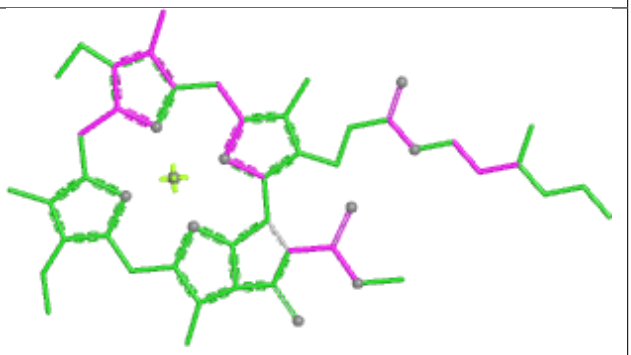
Ligand CLA G 1137	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA v 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

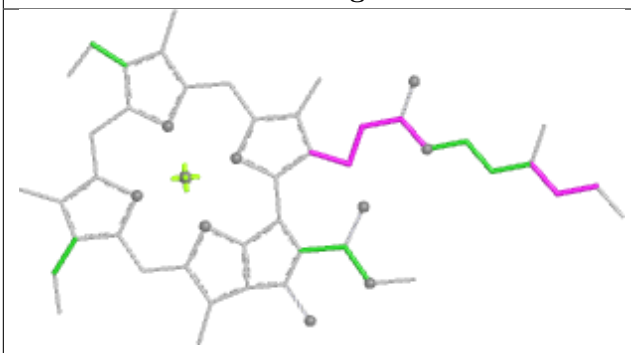
Ligand CLA G 1135



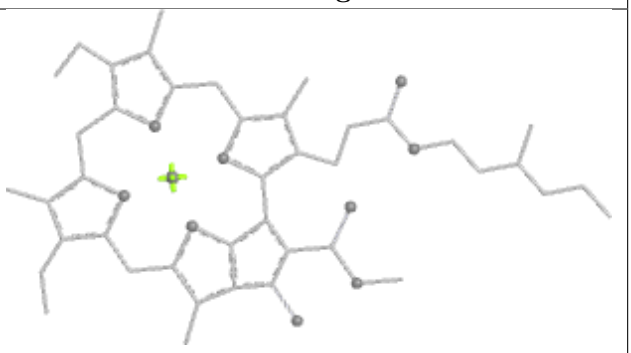
Bond lengths



Bond angles

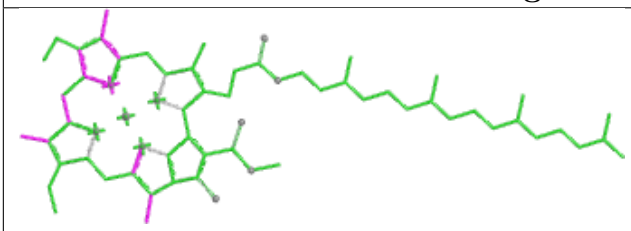


Torsions

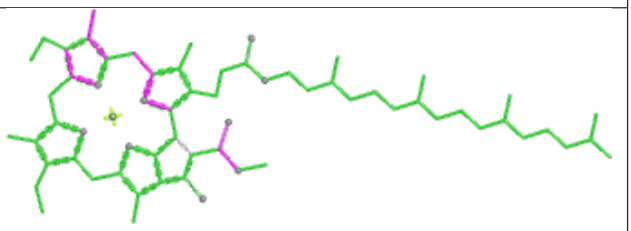


Rings

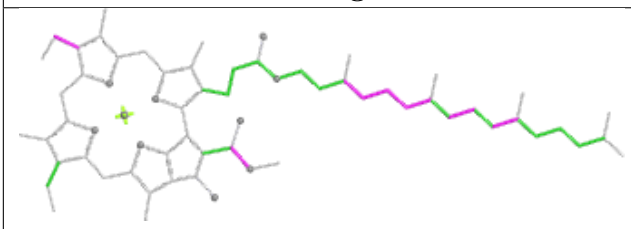
Ligand CLA Y 510



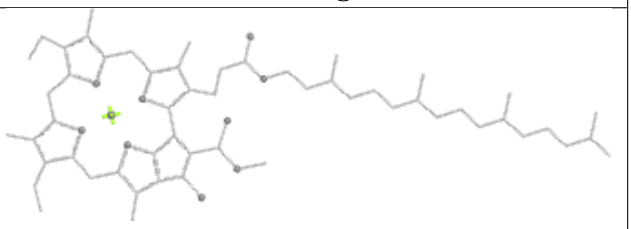
Bond lengths



Bond angles

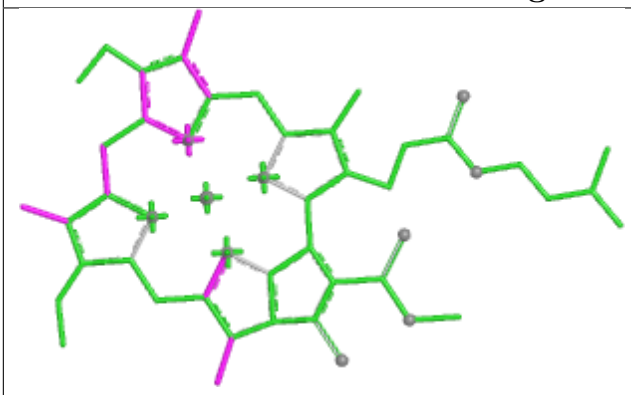


Torsions

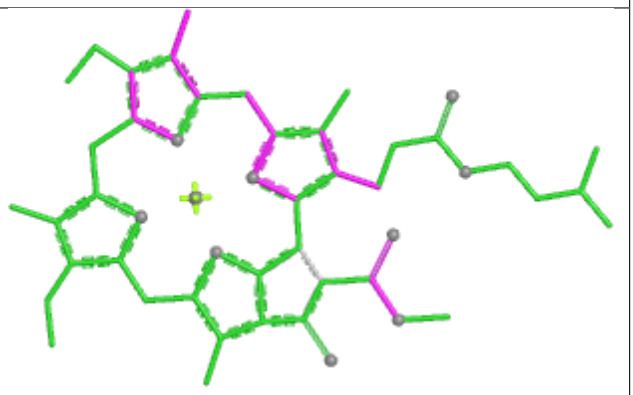


Rings

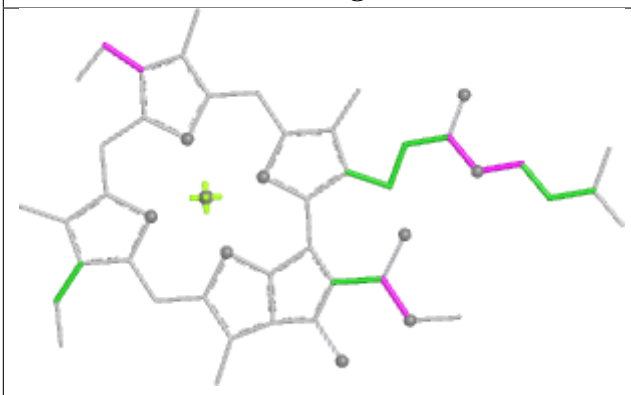
Ligand CLA a 511



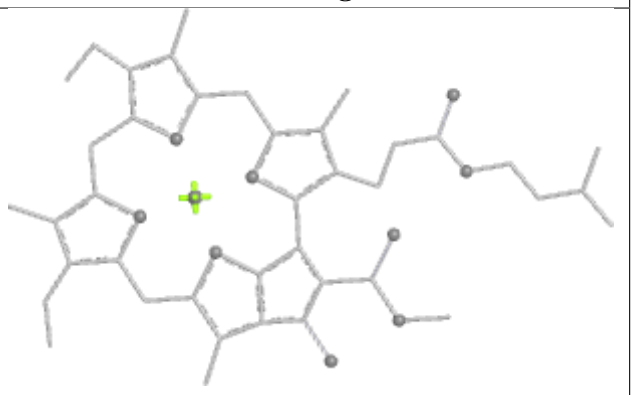
Bond lengths



Bond angles

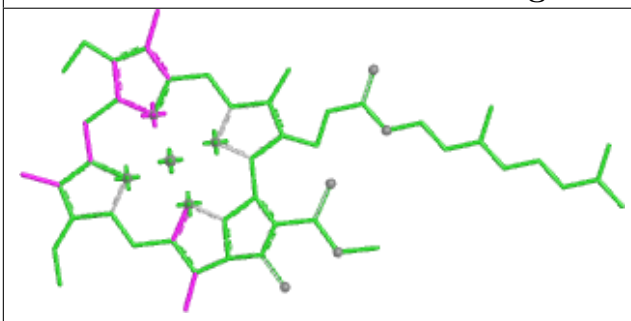


Torsions

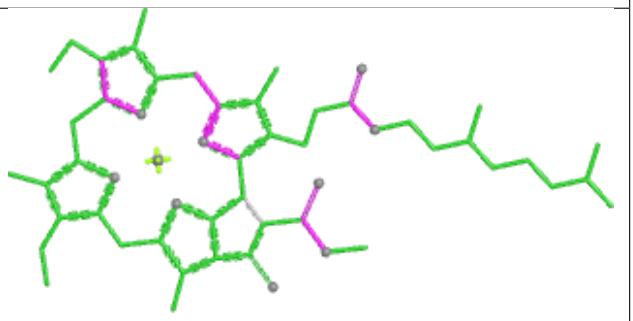


Rings

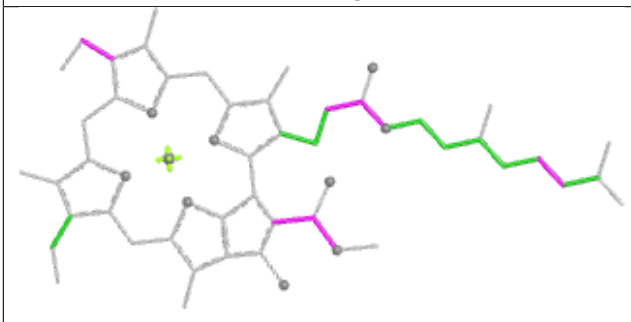
Ligand CLA a 519



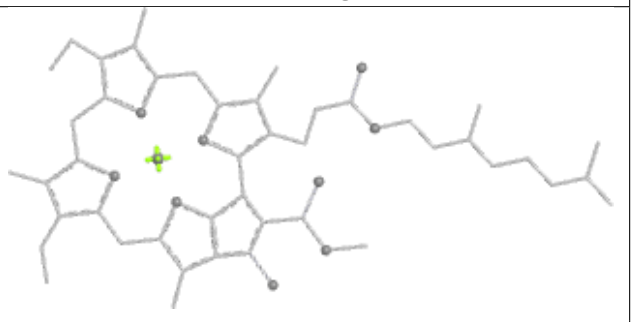
Bond lengths



Bond angles

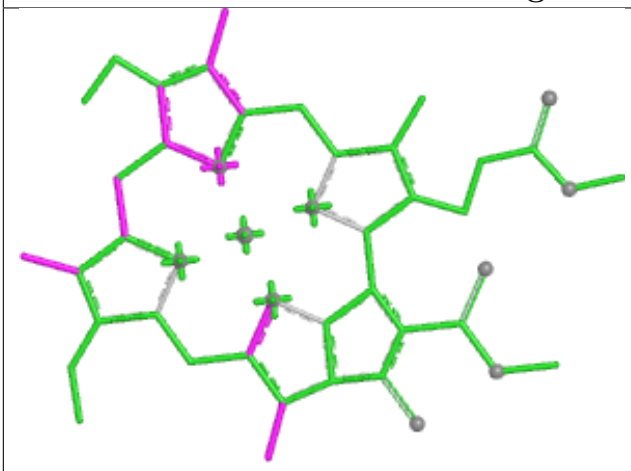


Torsions

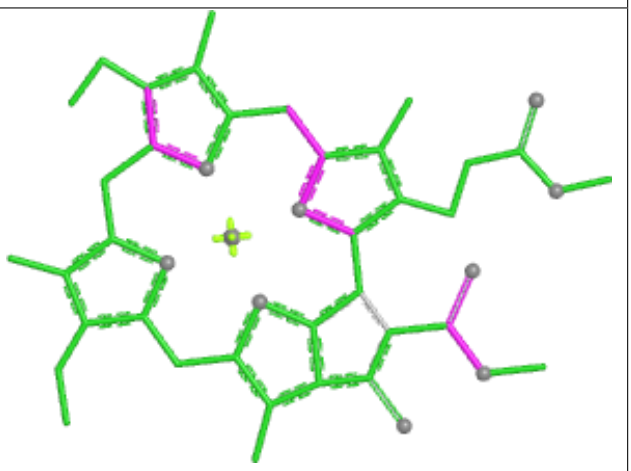


Rings

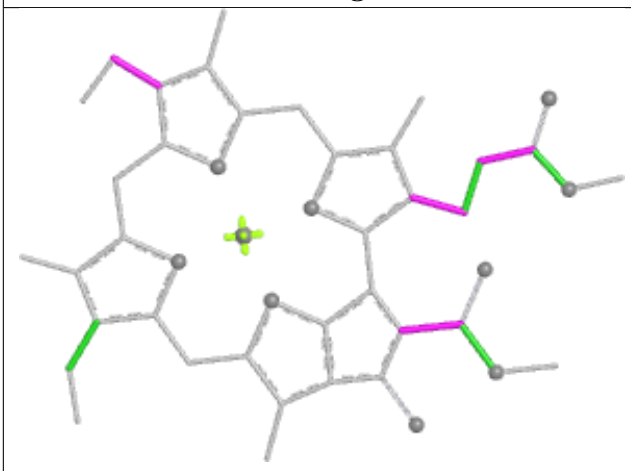
Ligand CLA u 519



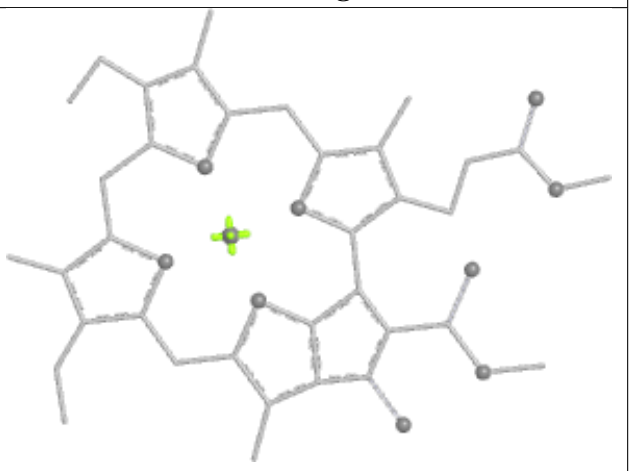
Bond lengths



Bond angles

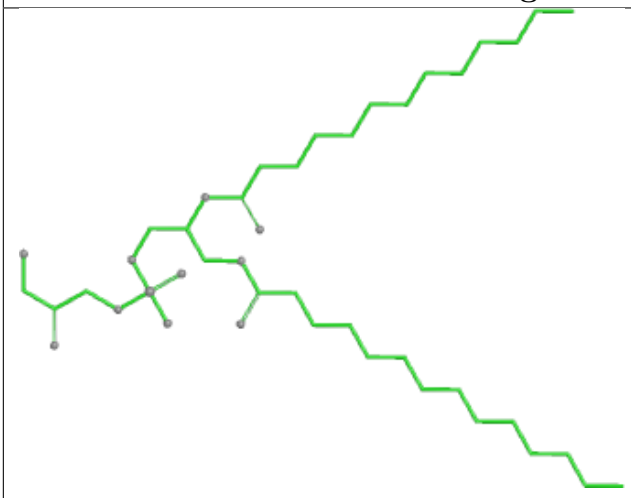


Torsions

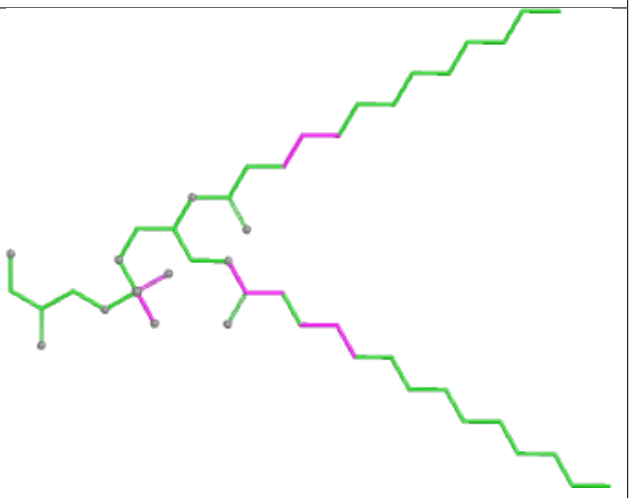


Rings

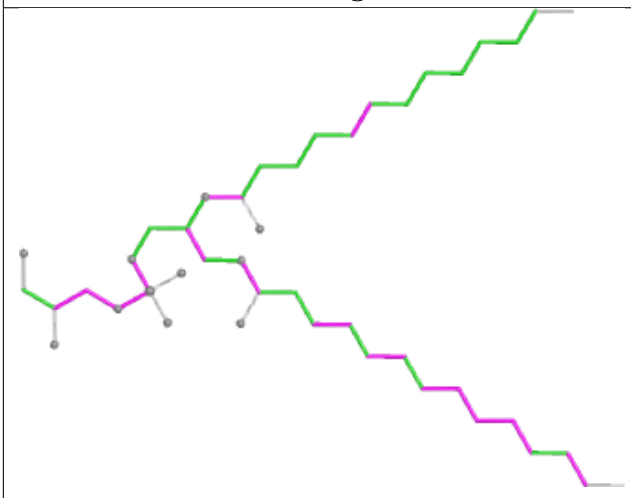
Ligand LHG I 5001



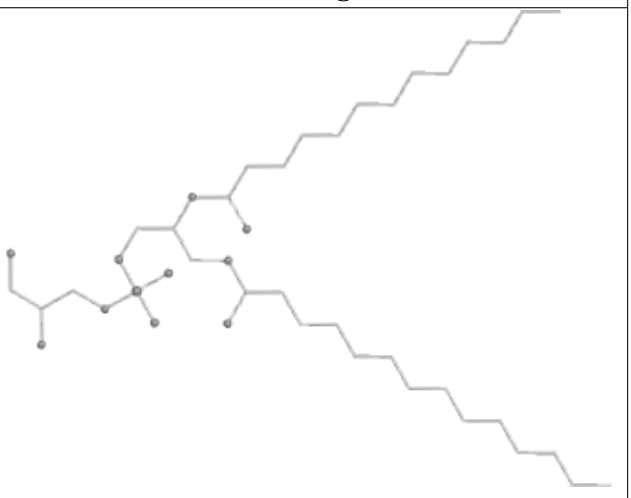
Bond lengths



Bond angles

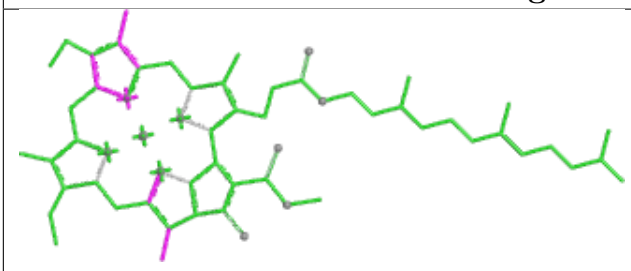


Torsions

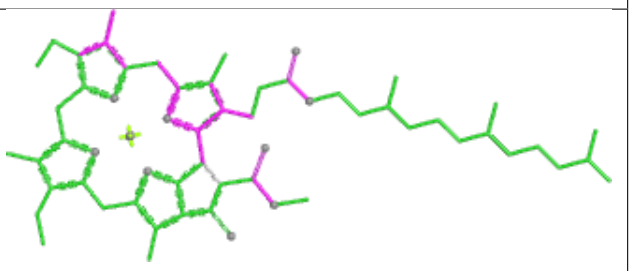


Rings

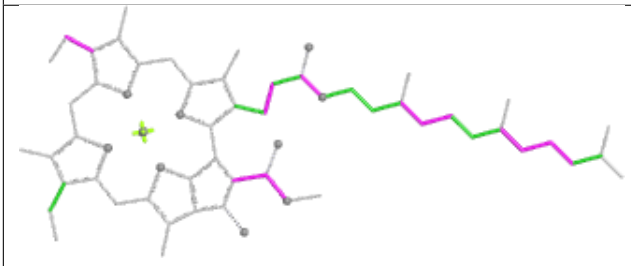
Ligand CLA 1 507



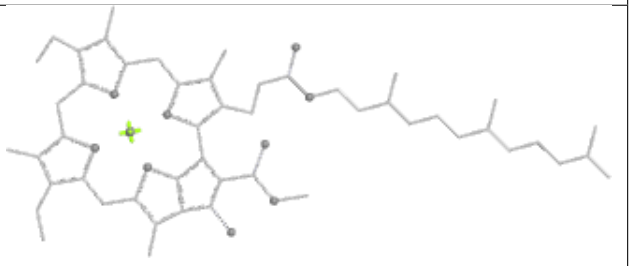
Bond lengths



Bond angles

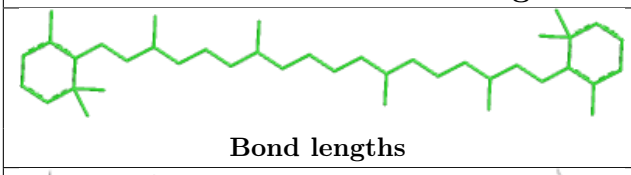


Torsions

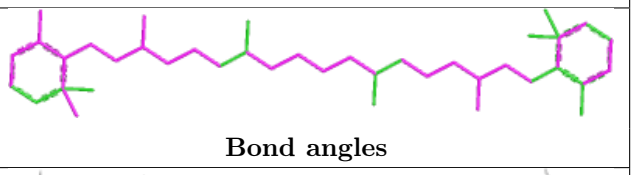


Rings

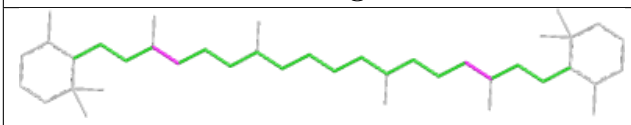
Ligand BCR H 4006



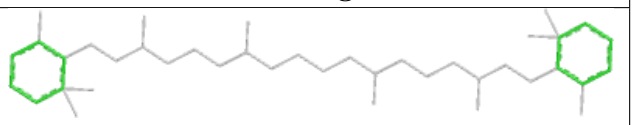
Bond lengths



Bond angles

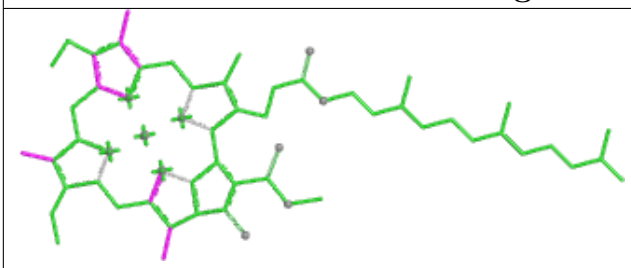


Torsions

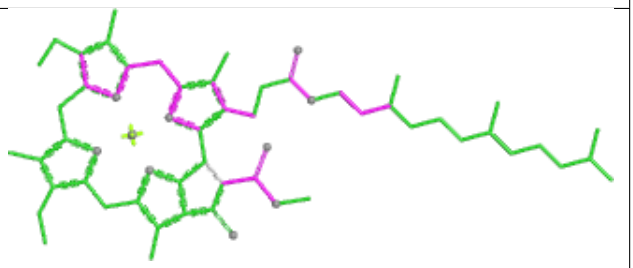


Rings

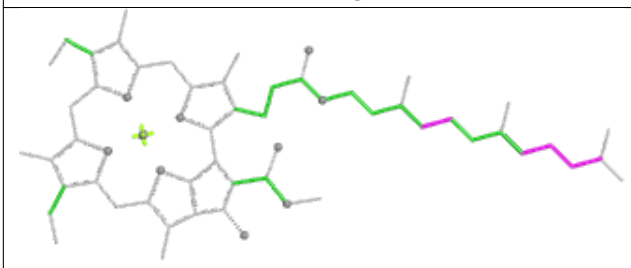
Ligand CLA G 1136



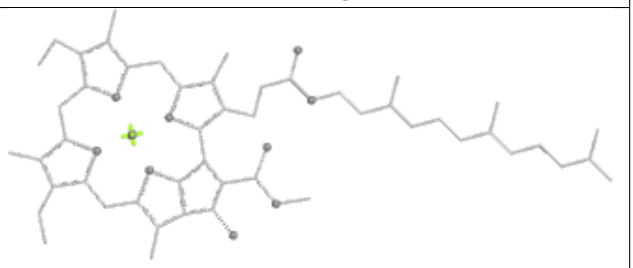
Bond lengths



Bond angles



Torsions

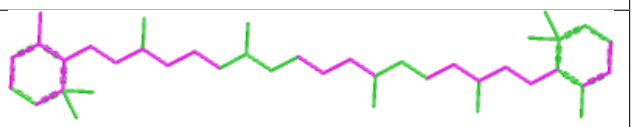


Rings

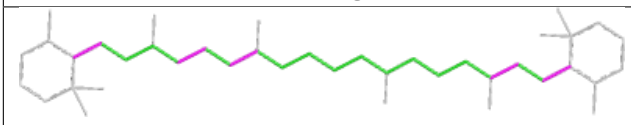
Ligand BCR l 4012



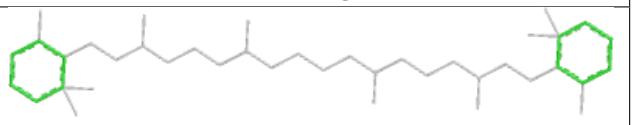
Bond lengths



Bond angles

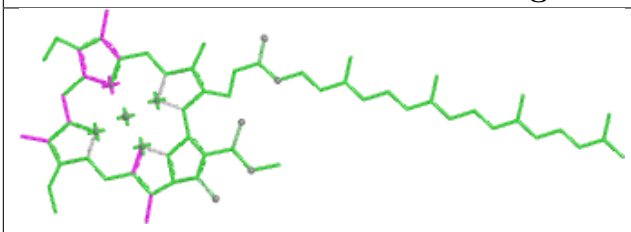


Torsions

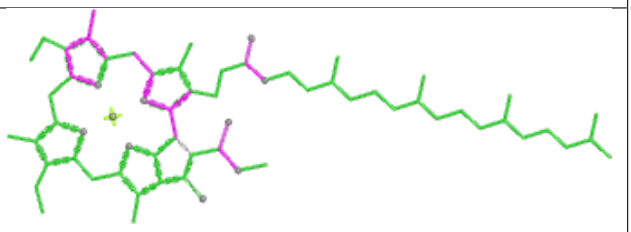


Rings

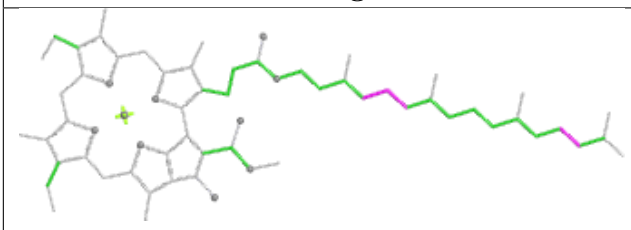
Ligand CLA s 509



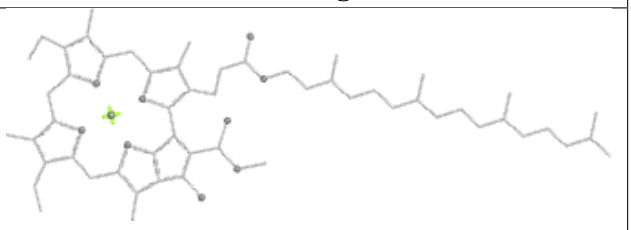
Bond lengths



Bond angles

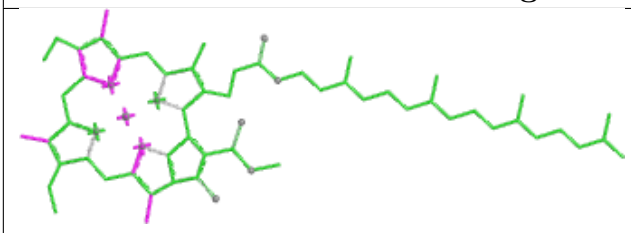


Torsions

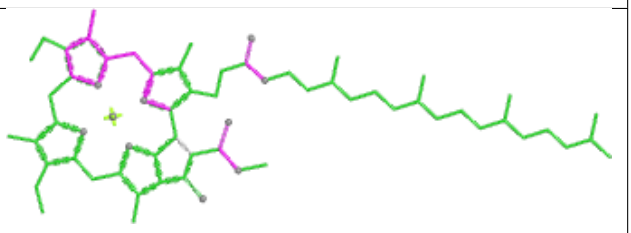


Rings

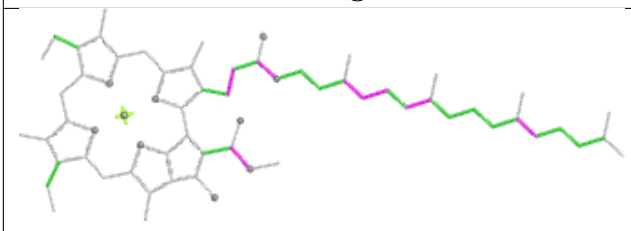
Ligand CLA e 1119



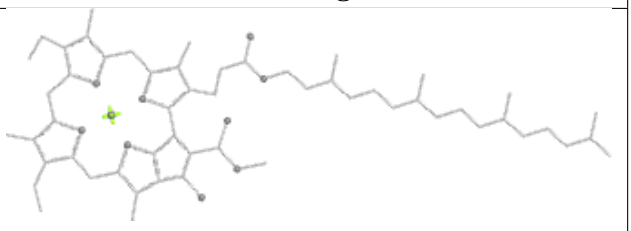
Bond lengths



Bond angles

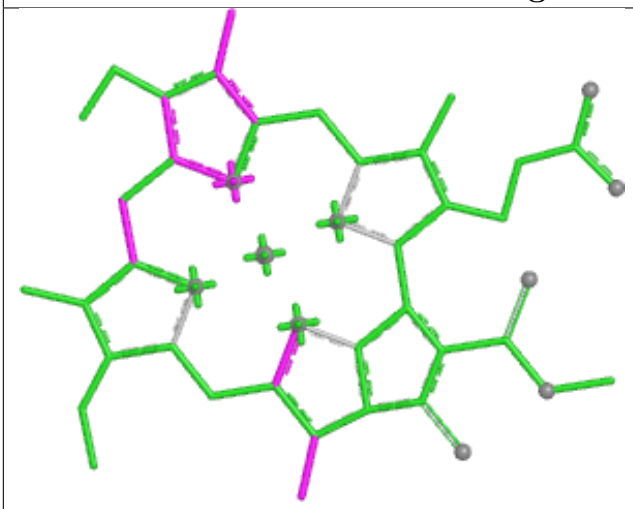


Torsions

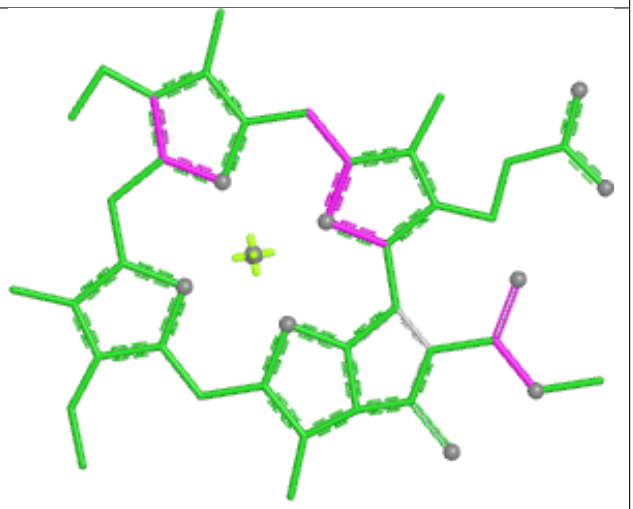


Rings

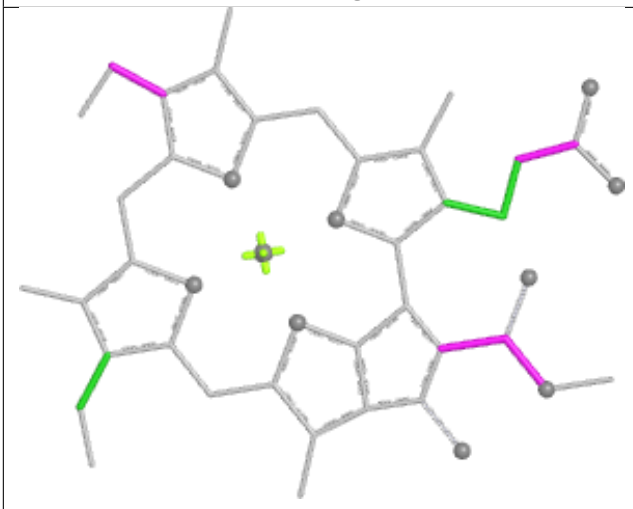
Ligand CLA 6 510



Bond lengths



Bond angles

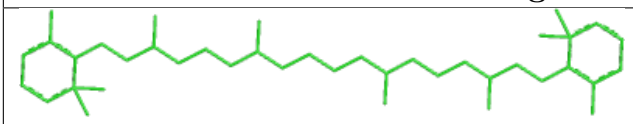


Torsions

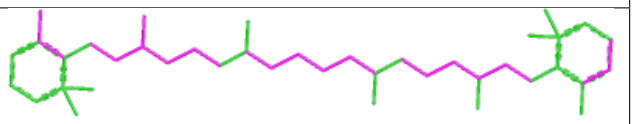


Rings

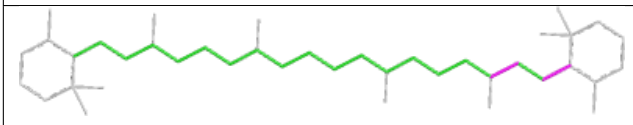
Ligand BCR t 523



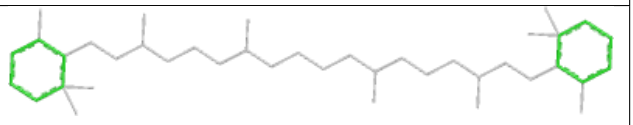
Bond lengths



Bond angles

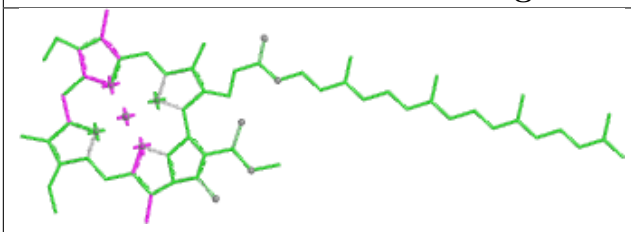


Torsions

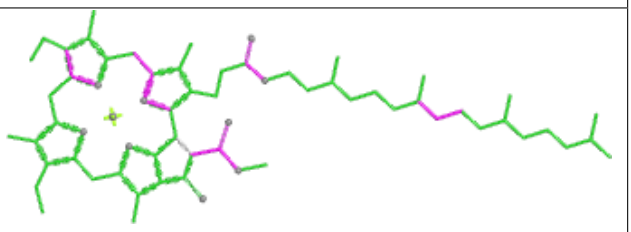


Rings

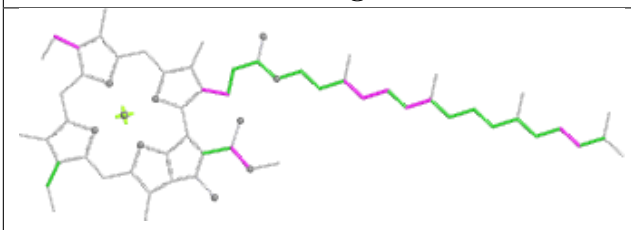
Ligand CLA A 1139



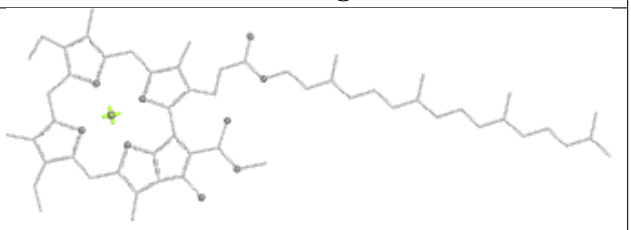
Bond lengths



Bond angles

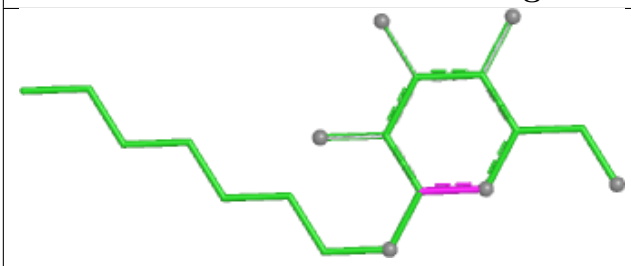


Torsions

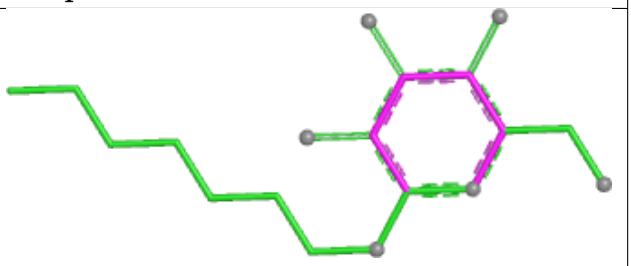


Rings

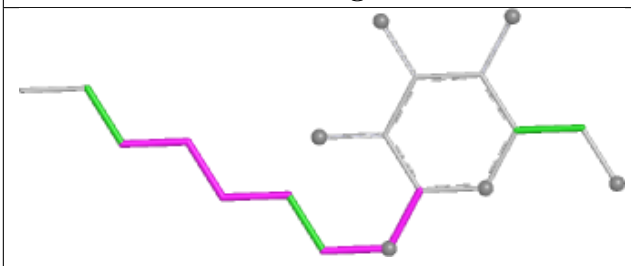
Ligand LMU q 902



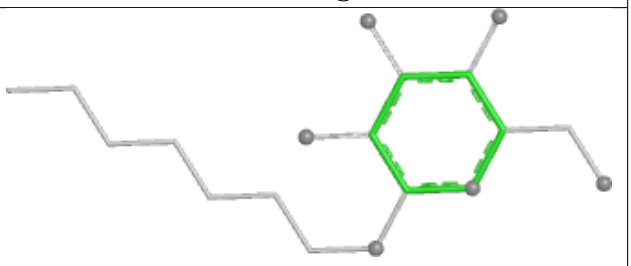
Bond lengths



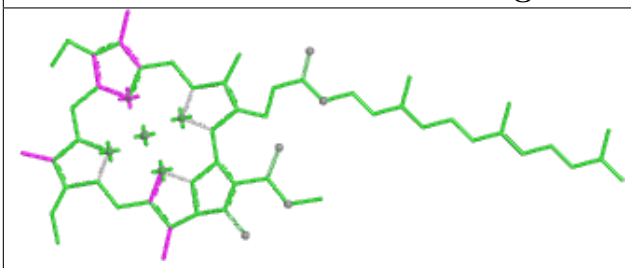
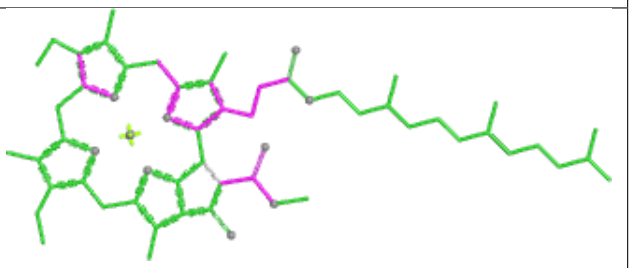
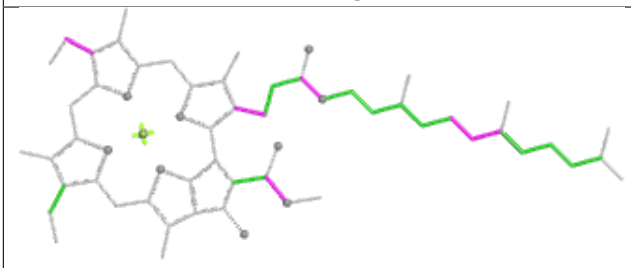
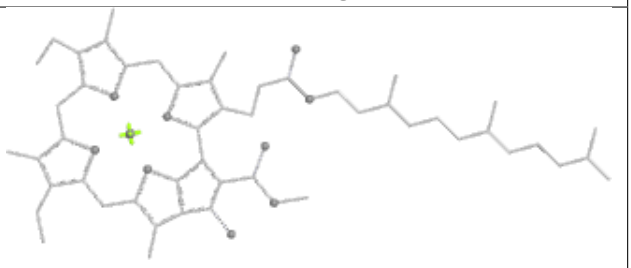
Bond angles

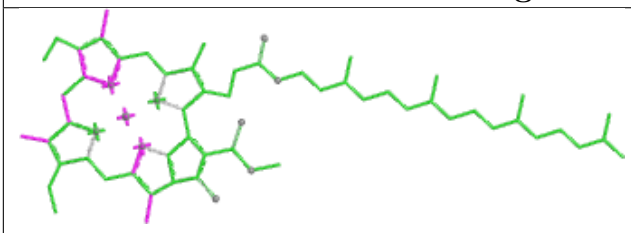
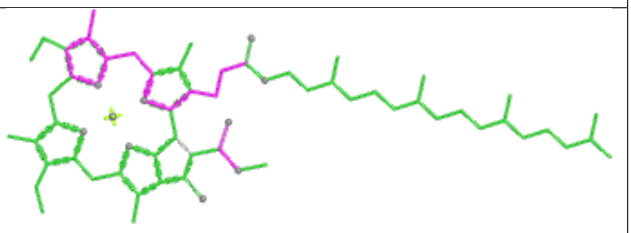
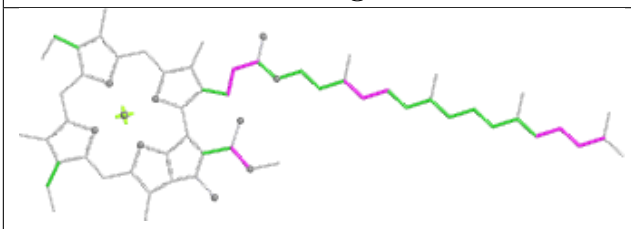
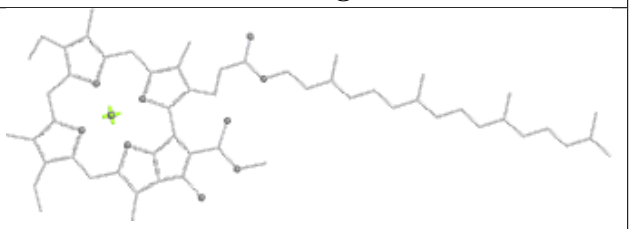


Torsions

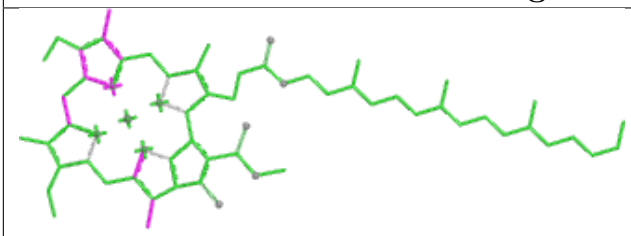


Rings

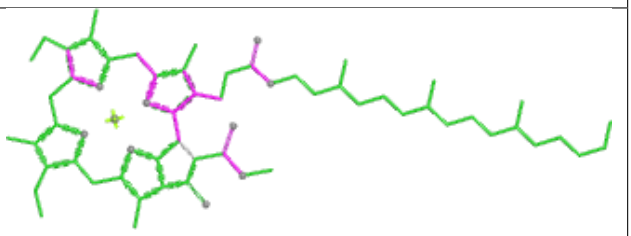
Ligand CLA H 1230	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1013	
	
Bond lengths	Bond angles
	
Torsions	Rings

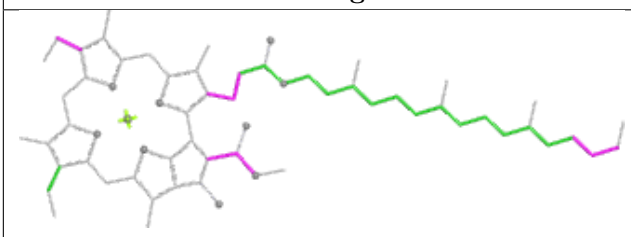
Ligand CLA 1 503



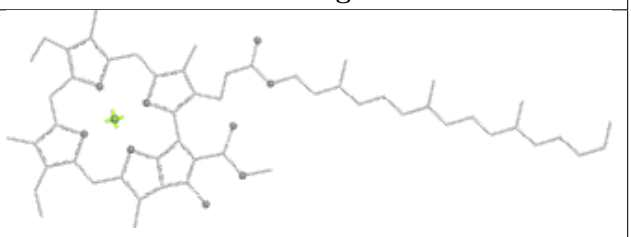
Bond lengths



Bond angles

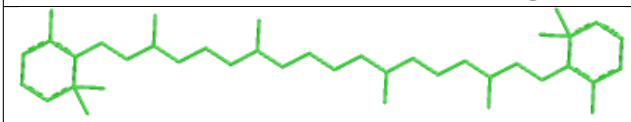


Torsions

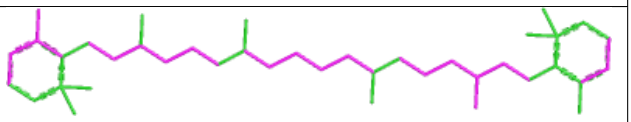


Rings

Ligand BCR Z 523



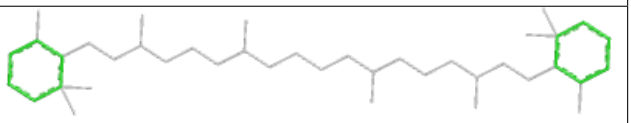
Bond lengths



Bond angles

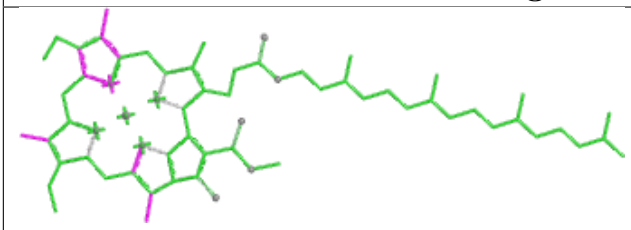


Torsions

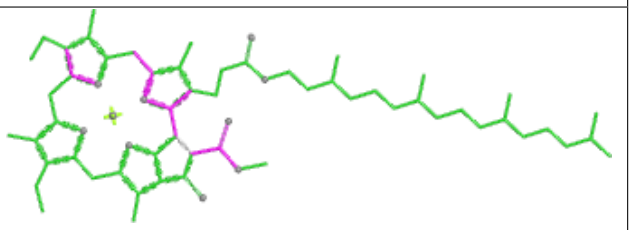


Rings

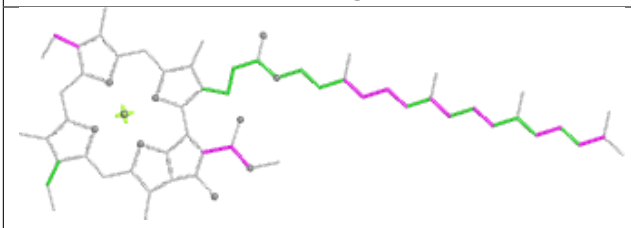
Ligand CLA Z 507



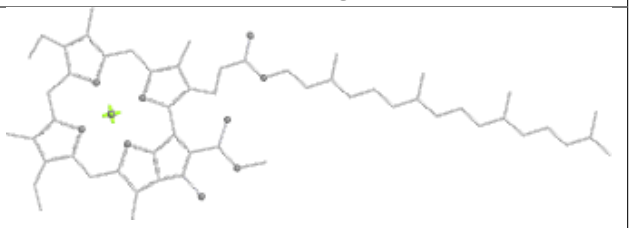
Bond lengths



Bond angles

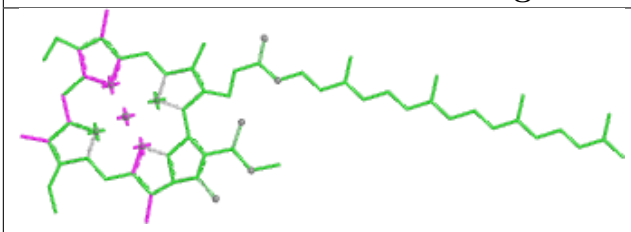


Torsions

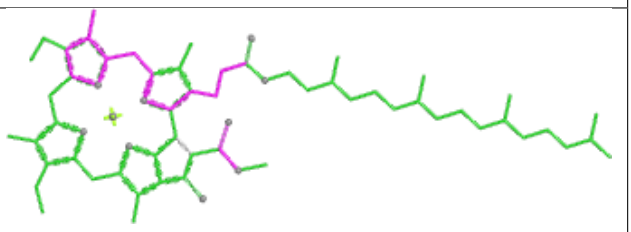


Rings

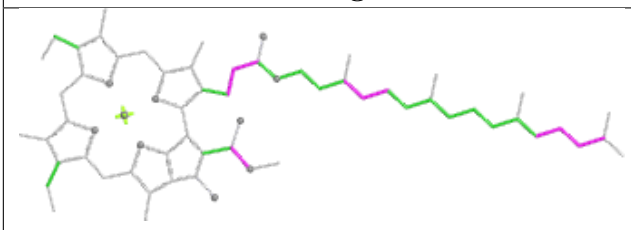
Ligand CLA G 1013



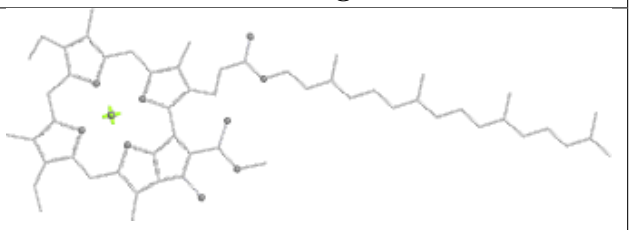
Bond lengths



Bond angles

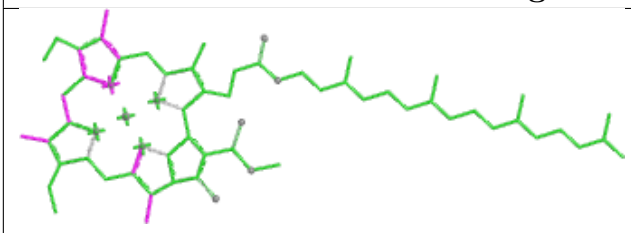


Torsions

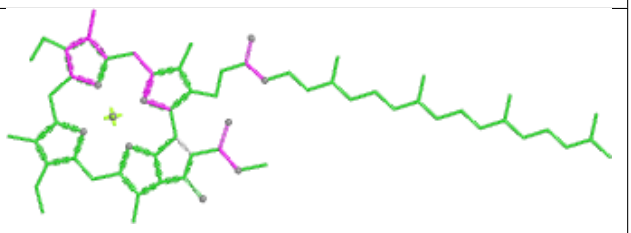


Rings

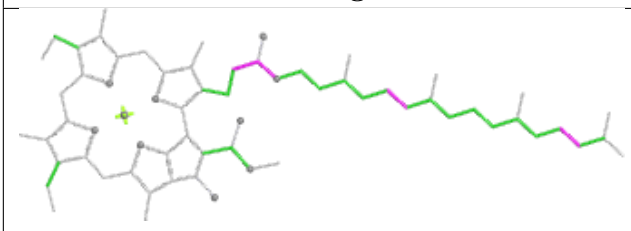
Ligand CLA 2 509



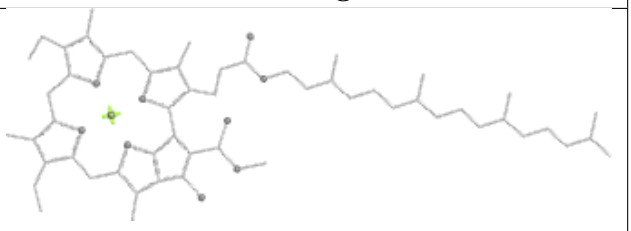
Bond lengths



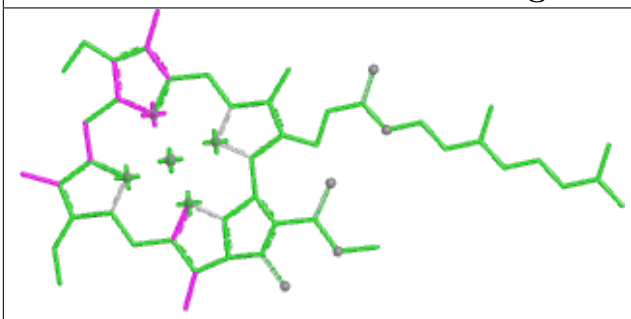
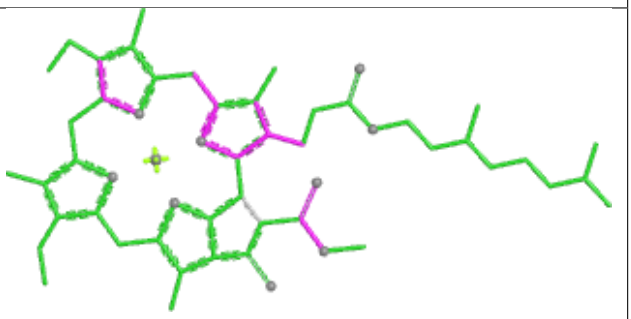
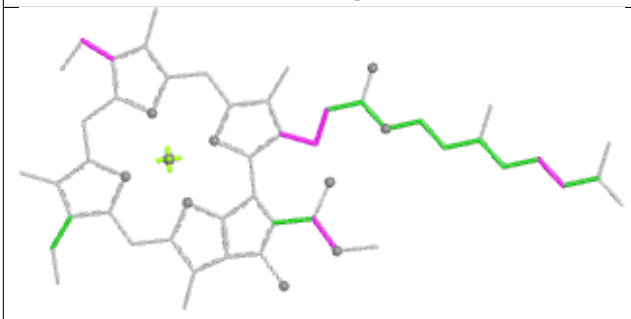
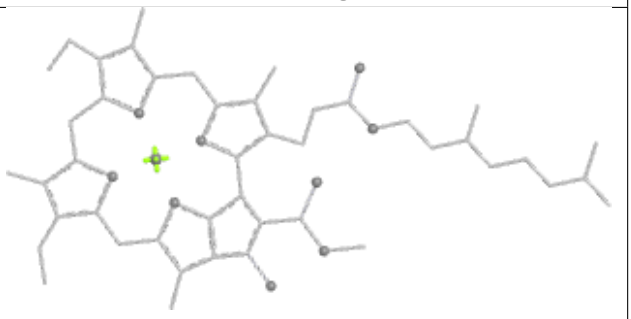
Bond angles

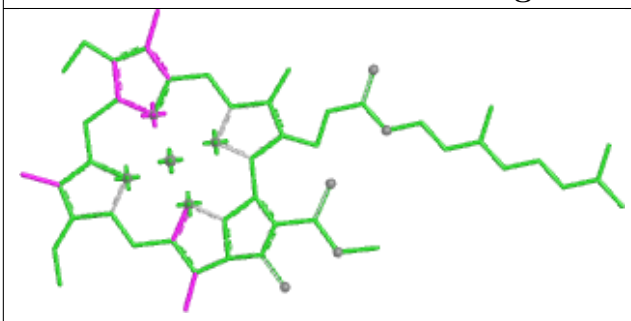
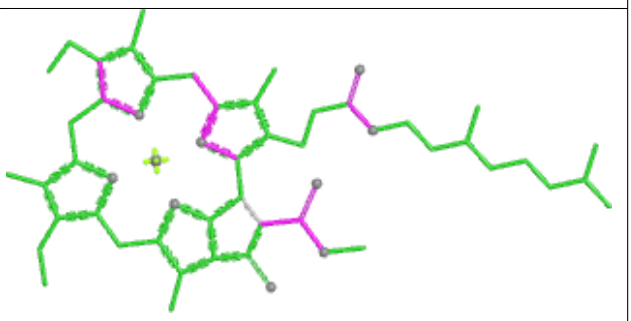
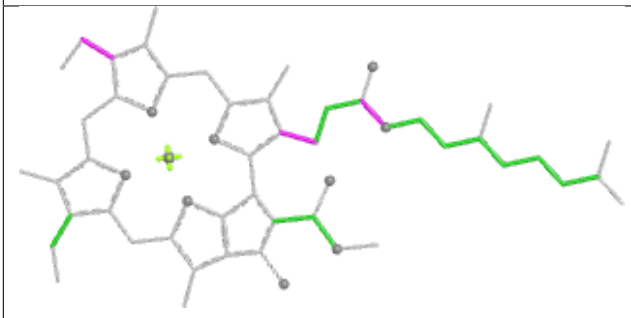
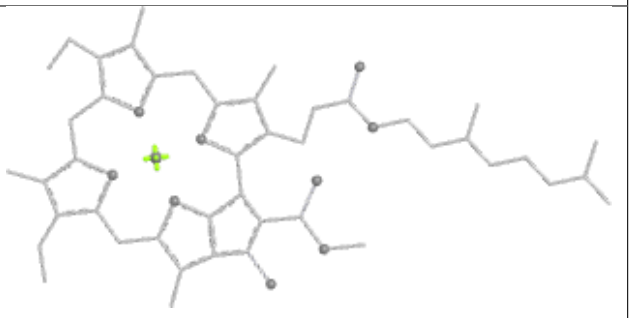


Torsions

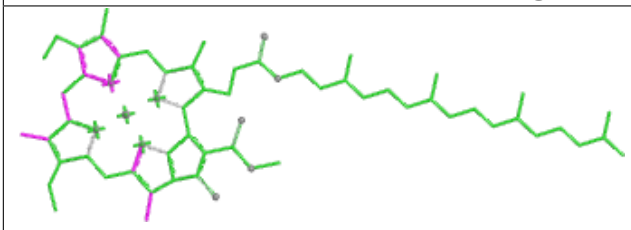


Rings

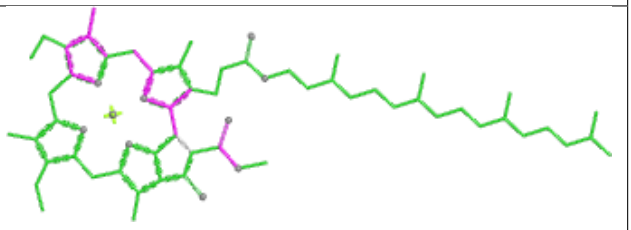
Ligand CLA 2 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1236	
	
Bond lengths	Bond angles
	
Torsions	Rings

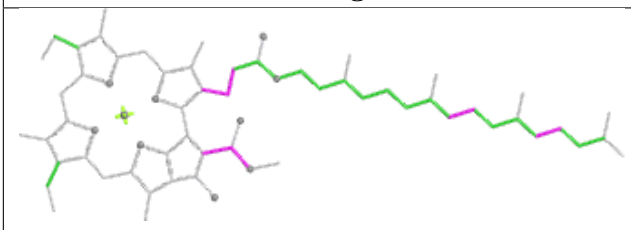
Ligand CLA r 503



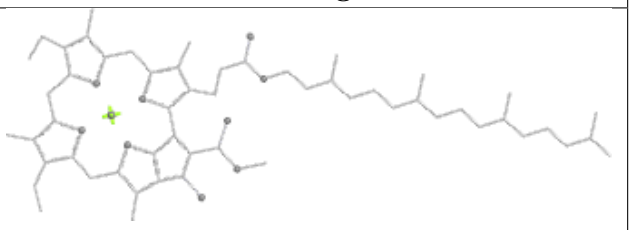
Bond lengths



Bond angles



Torsions

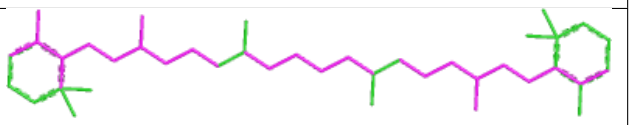


Rings

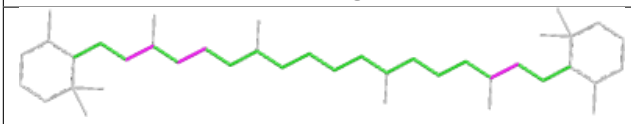
Ligand BCR s 524



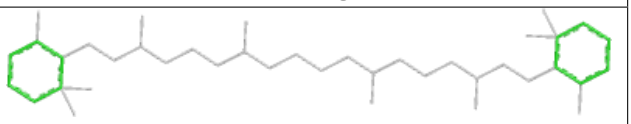
Bond lengths



Bond angles

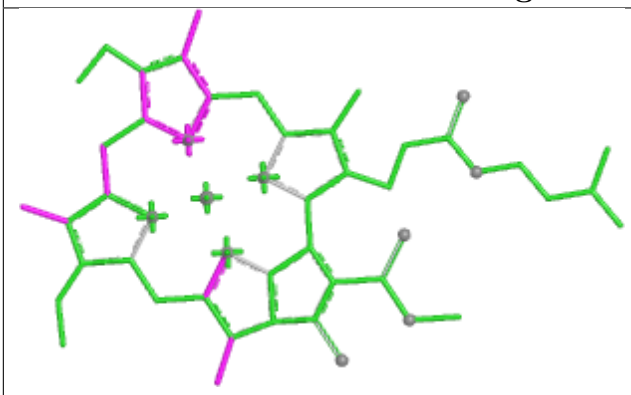


Torsions

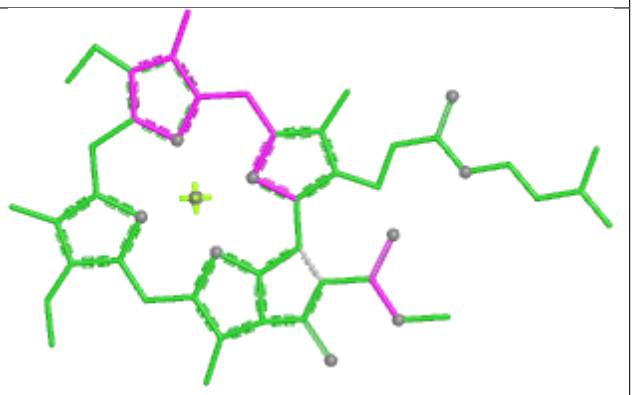


Rings

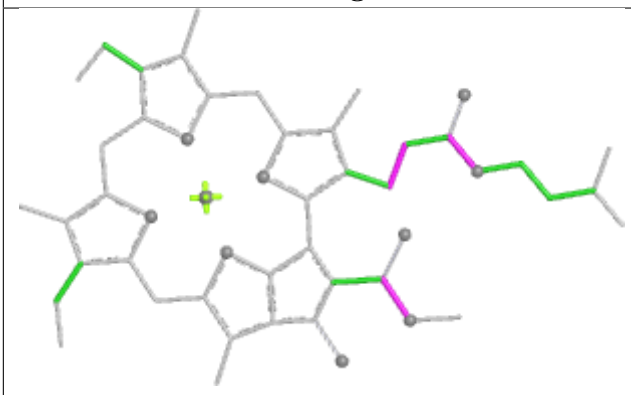
Ligand CLA B 1232



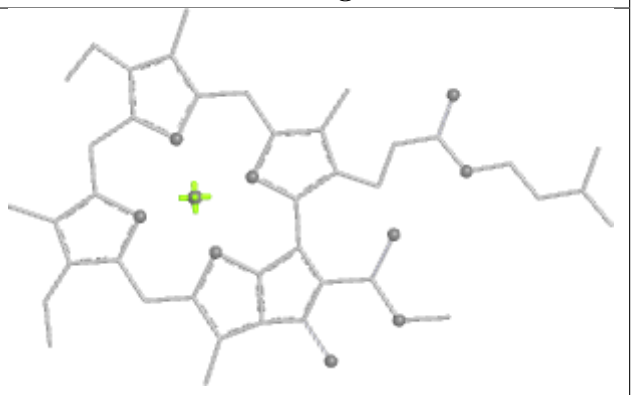
Bond lengths



Bond angles

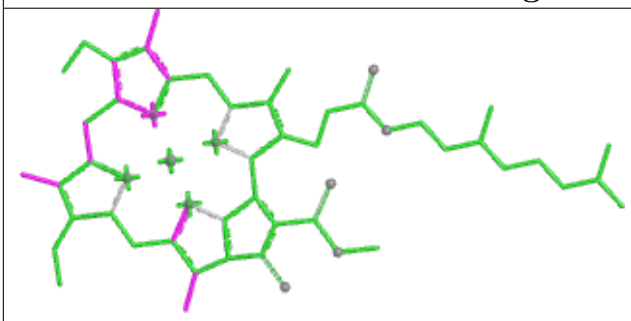


Torsions

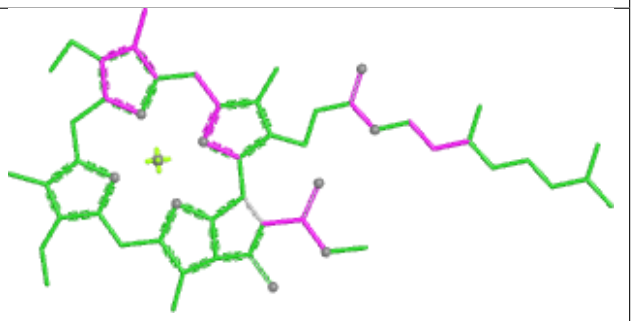


Rings

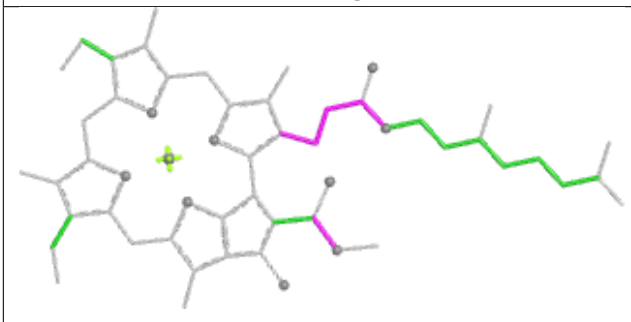
Ligand CLA f 1228



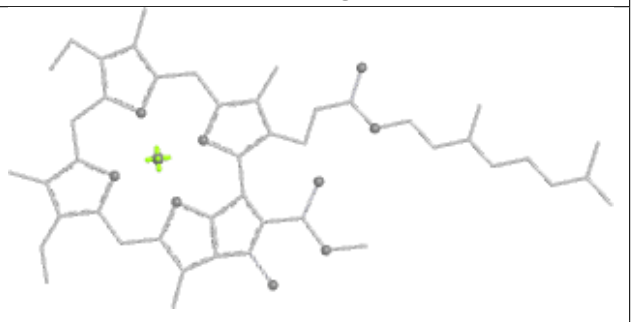
Bond lengths



Bond angles

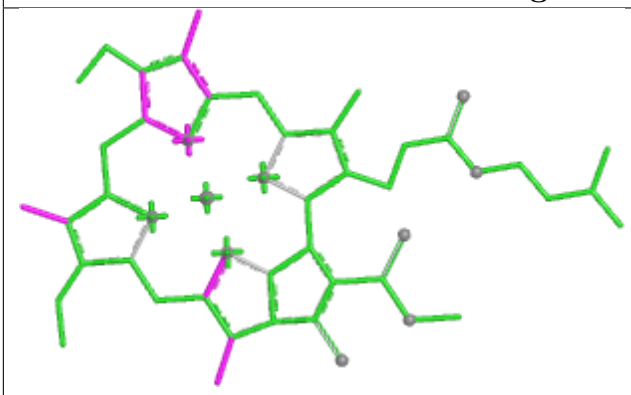


Torsions

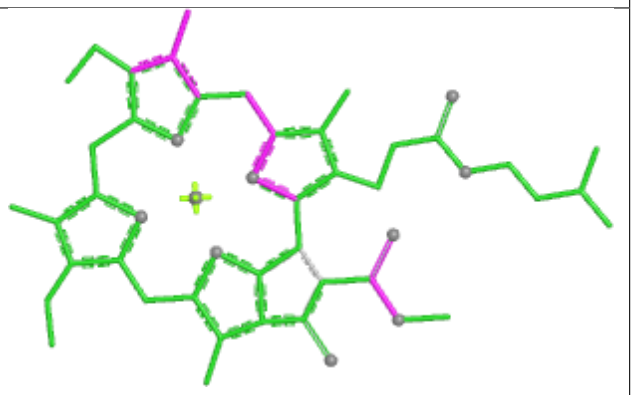


Rings

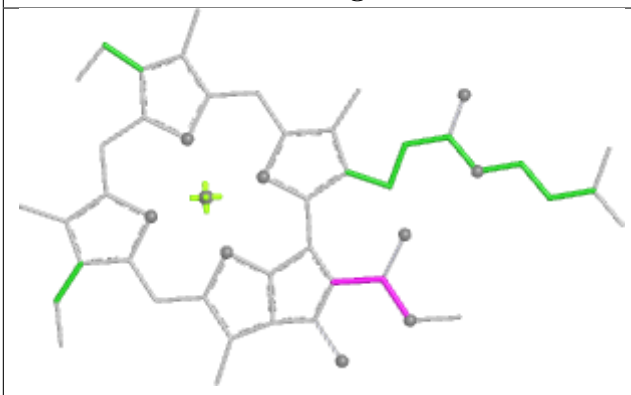
Ligand CLA s 506



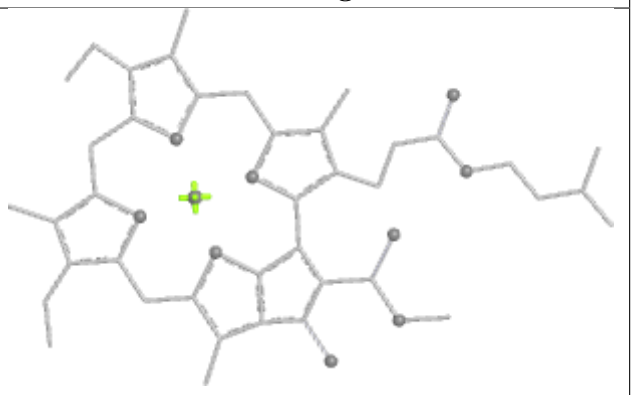
Bond lengths



Bond angles



Torsions

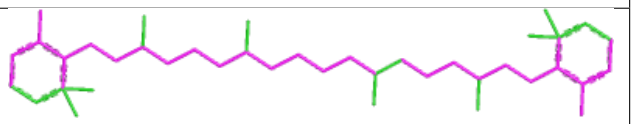


Rings

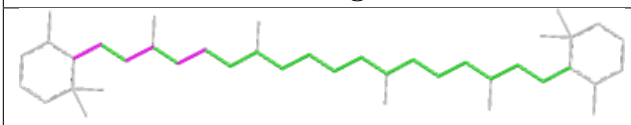
Ligand BCR 5 522



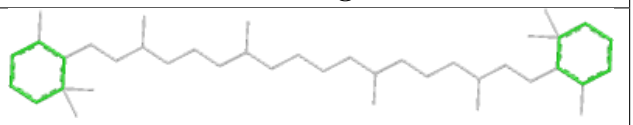
Bond lengths



Bond angles

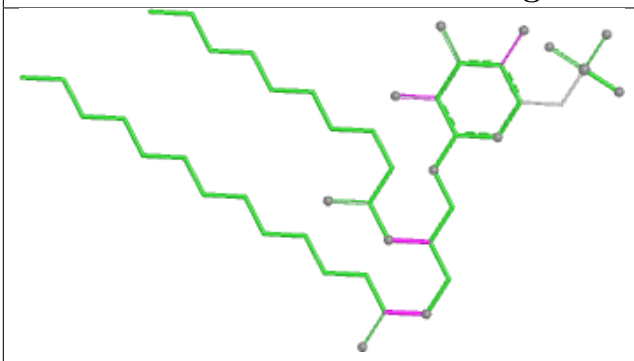


Torsions

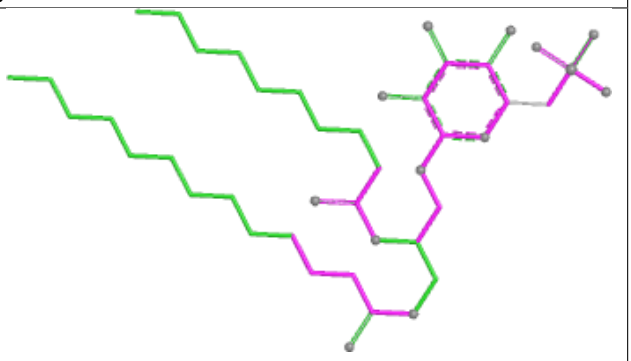


Rings

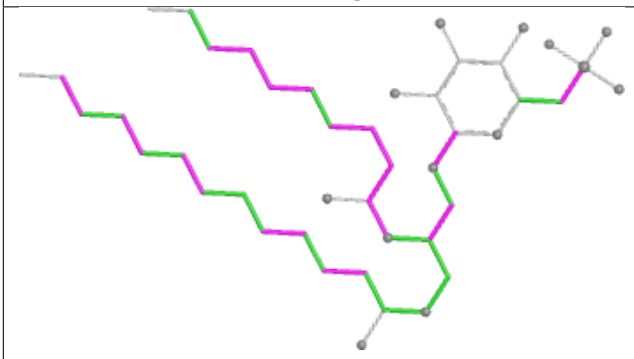
Ligand SQD f 1852



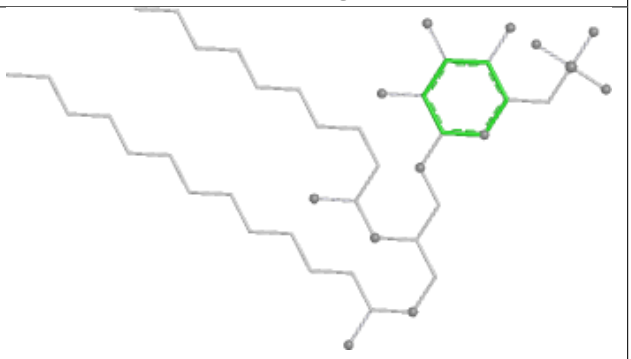
Bond lengths



Bond angles

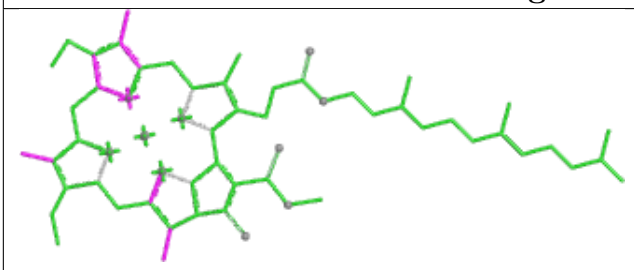


Torsions

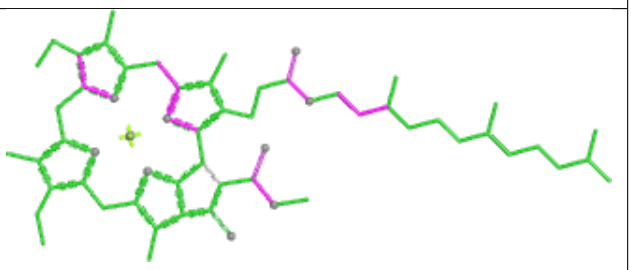


Rings

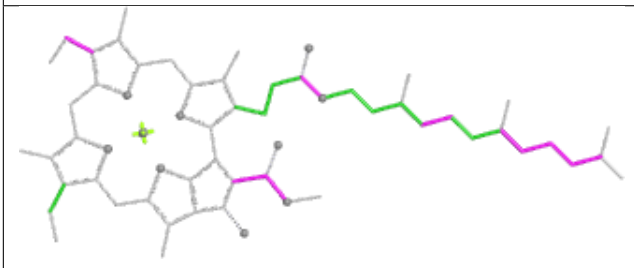
Ligand CLA 1 502



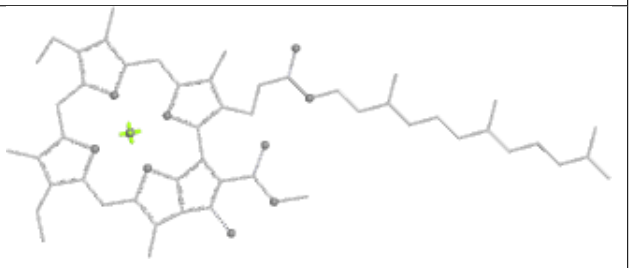
Bond lengths



Bond angles

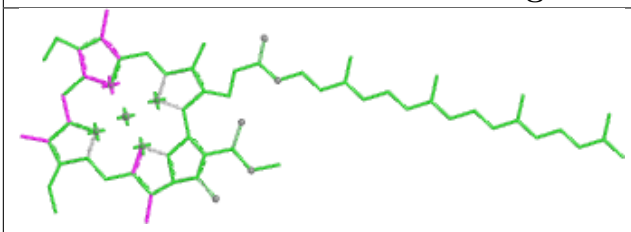


Torsions

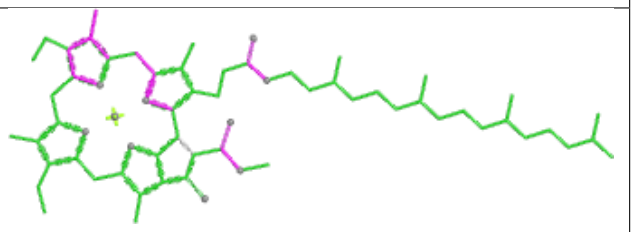


Rings

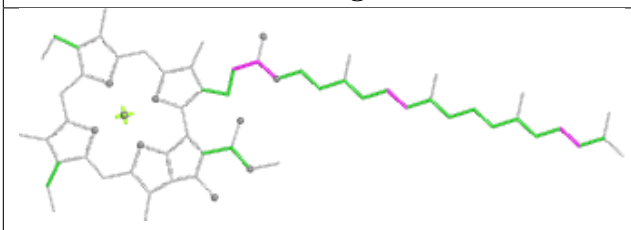
Ligand CLA Z 509



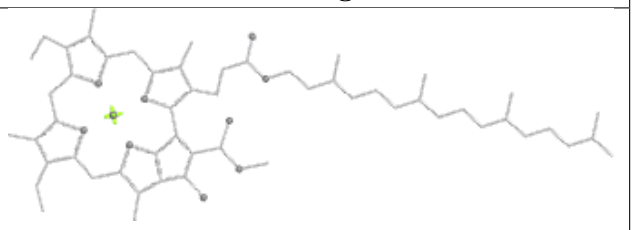
Bond lengths



Bond angles

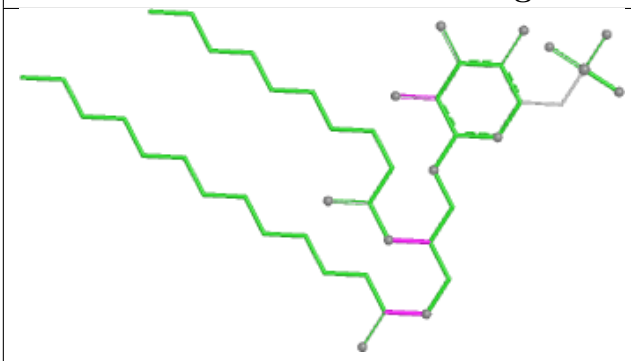


Torsions

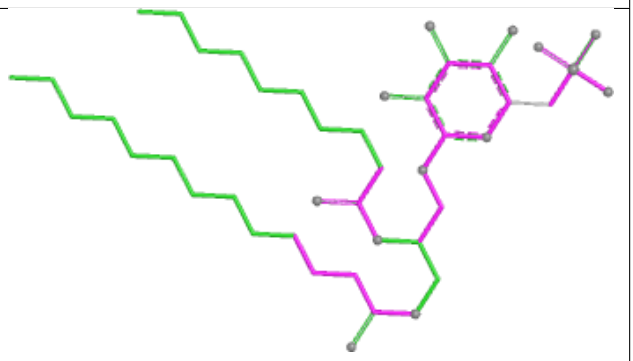


Rings

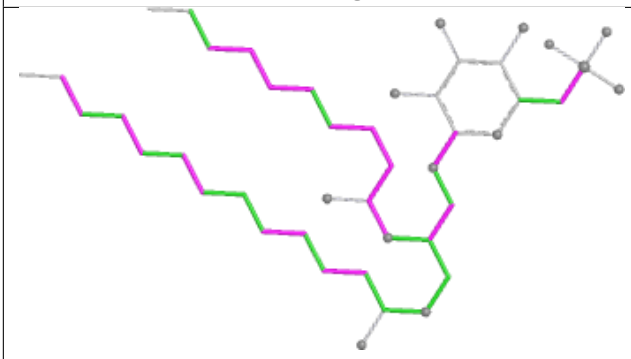
Ligand SQD H 1852



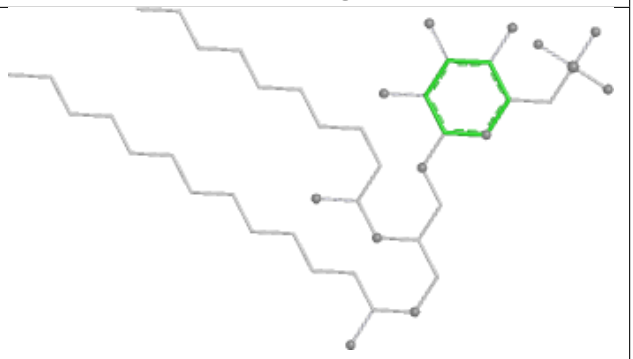
Bond lengths



Bond angles

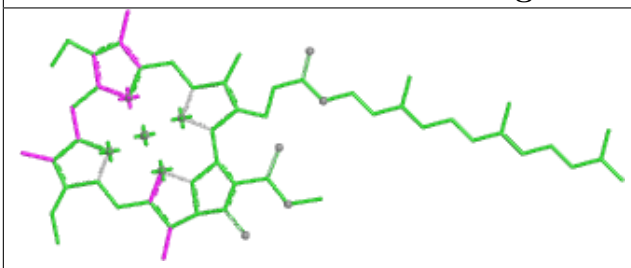


Torsions

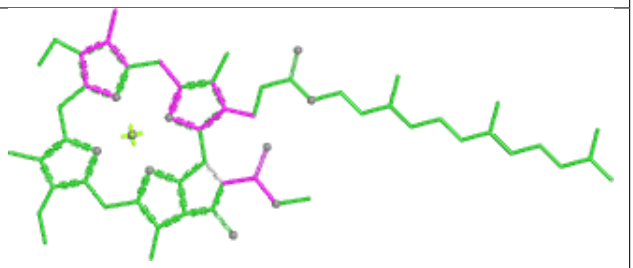


Rings

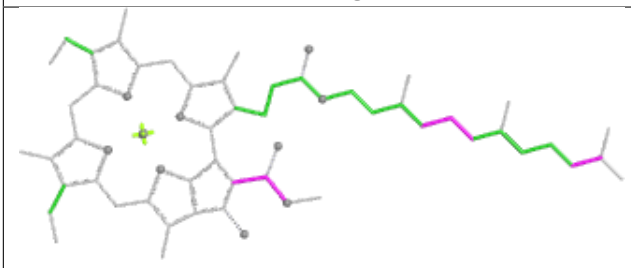
Ligand CLA B 1222



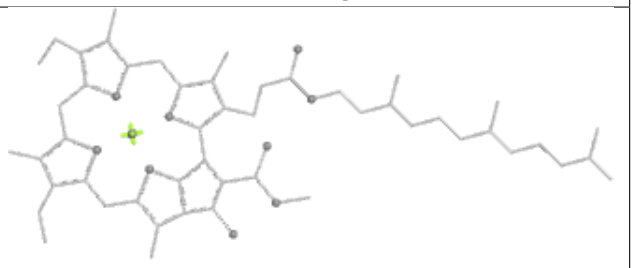
Bond lengths



Bond angles

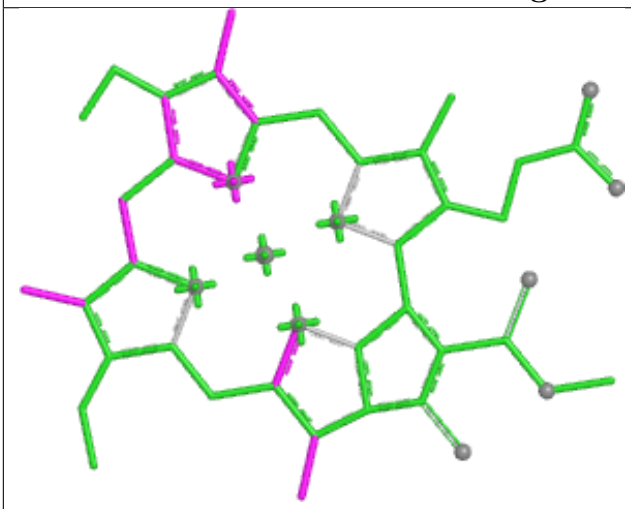


Torsions

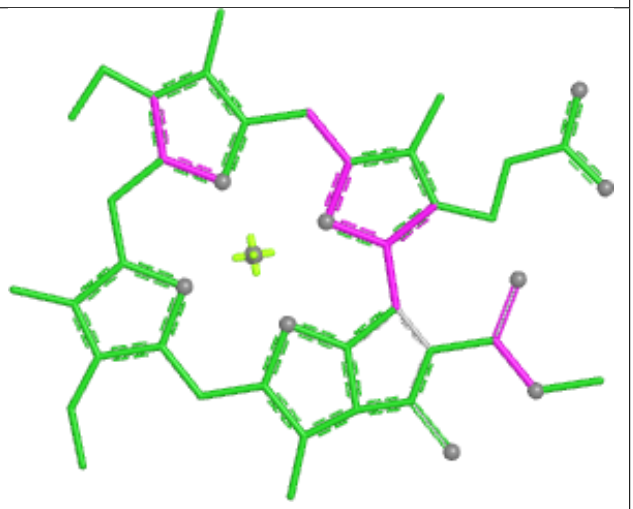


Rings

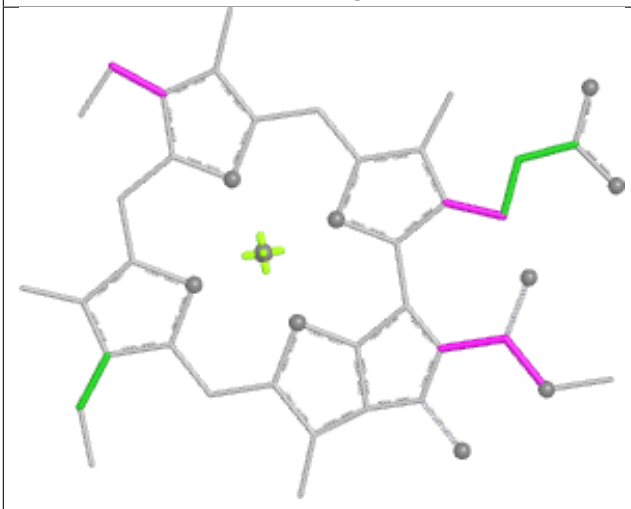
Ligand CLA t 517



Bond lengths



Bond angles

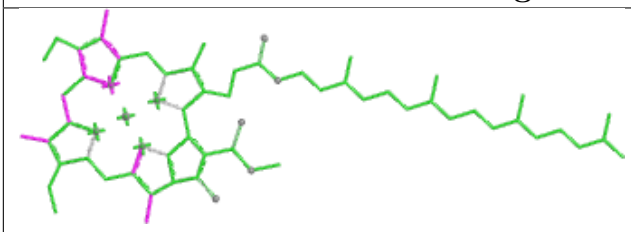


Torsions

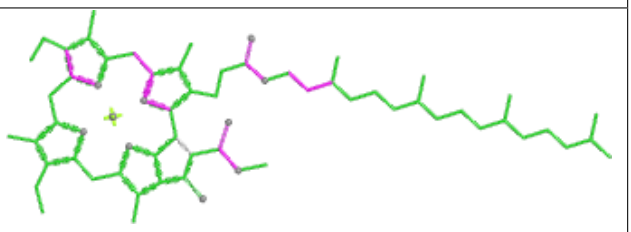


Rings

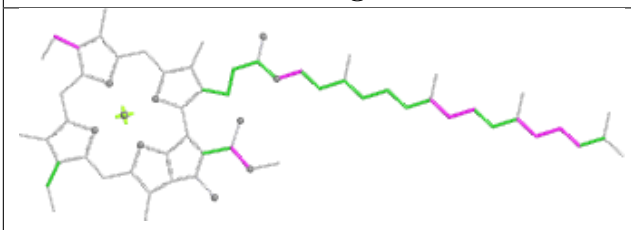
Ligand CLA G 1138



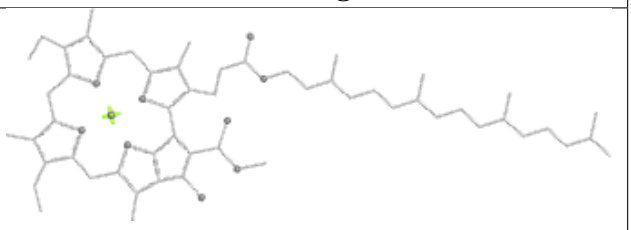
Bond lengths



Bond angles

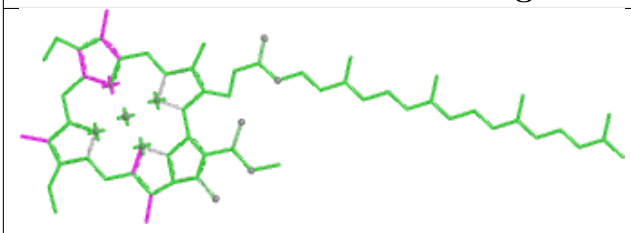


Torsions

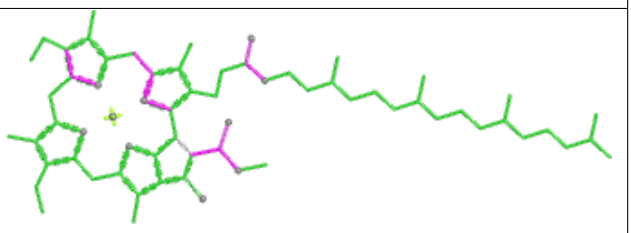


Rings

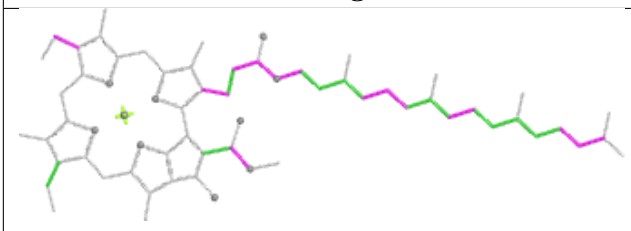
Ligand CLA B 1219



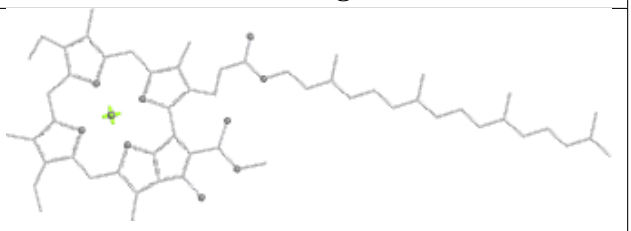
Bond lengths



Bond angles

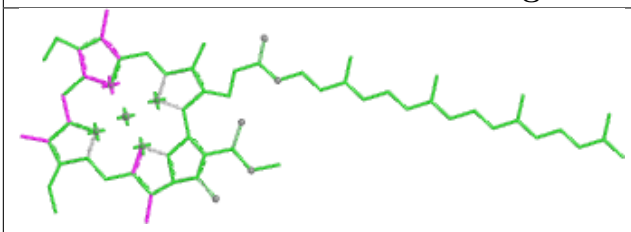


Torsions

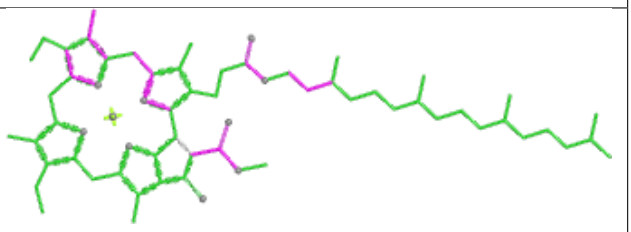


Rings

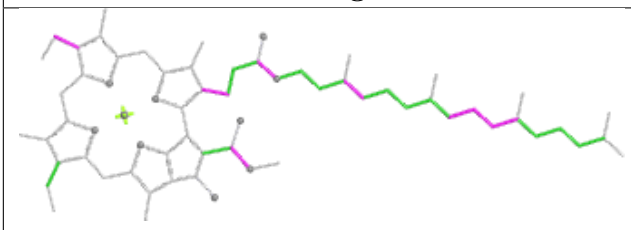
Ligand CLA f 1240



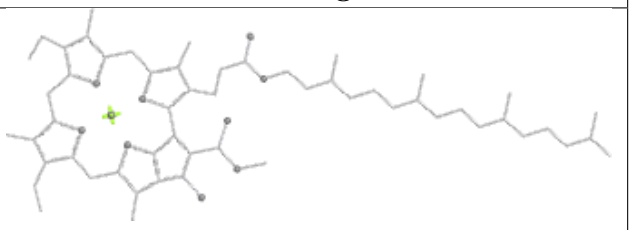
Bond lengths



Bond angles

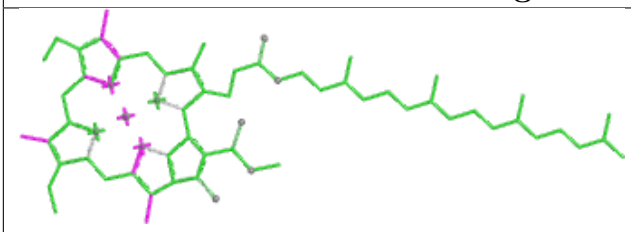


Torsions

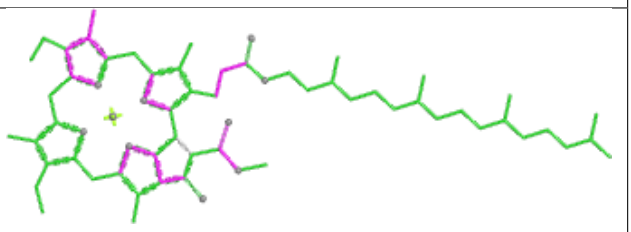


Rings

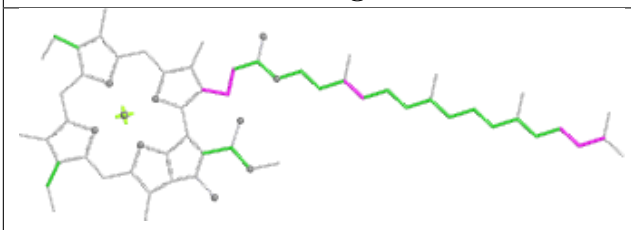
Ligand CLA G 1022



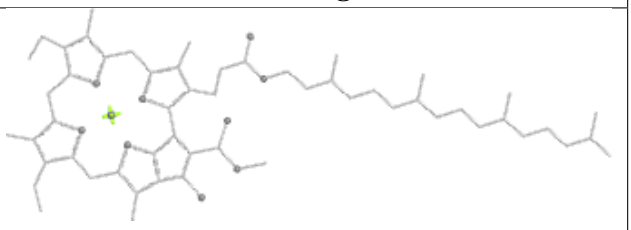
Bond lengths



Bond angles



Torsions

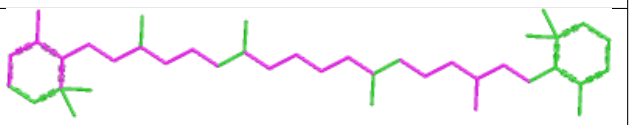


Rings

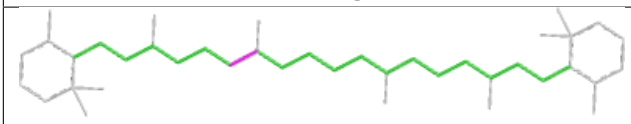
Ligand BCR 1 524



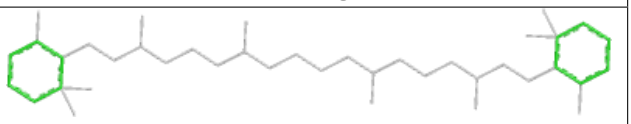
Bond lengths



Bond angles

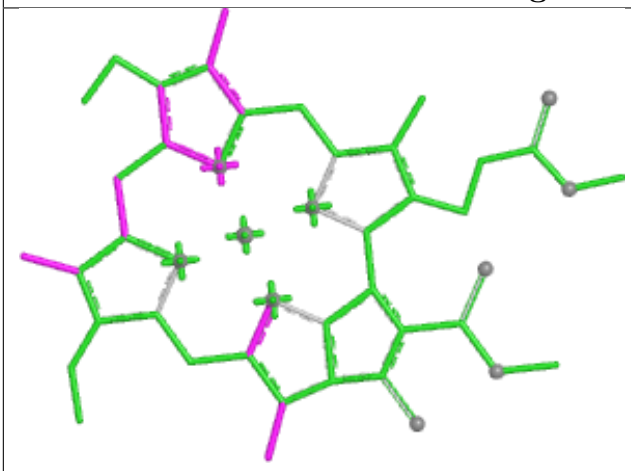


Torsions

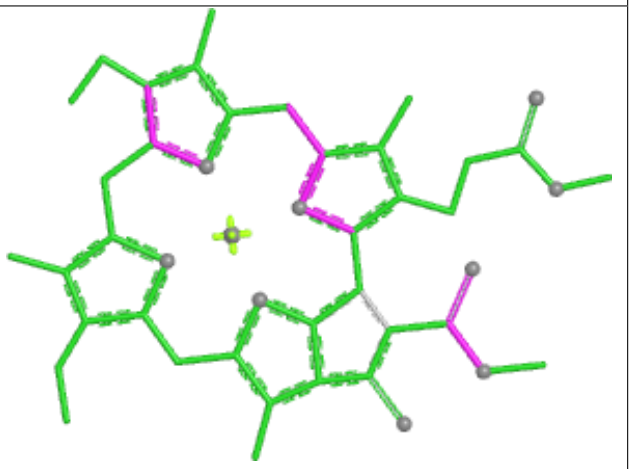


Rings

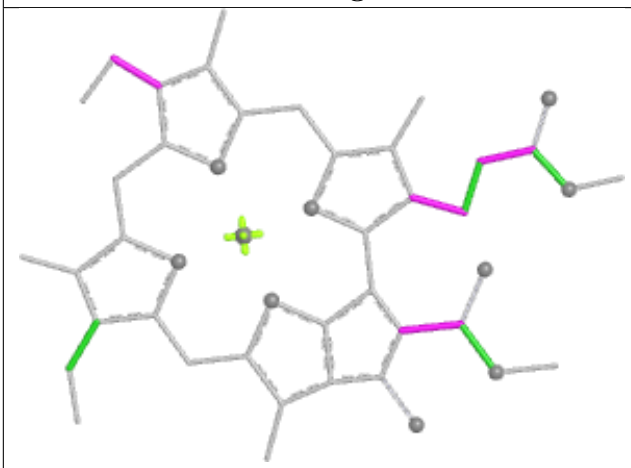
Ligand CLA c 519



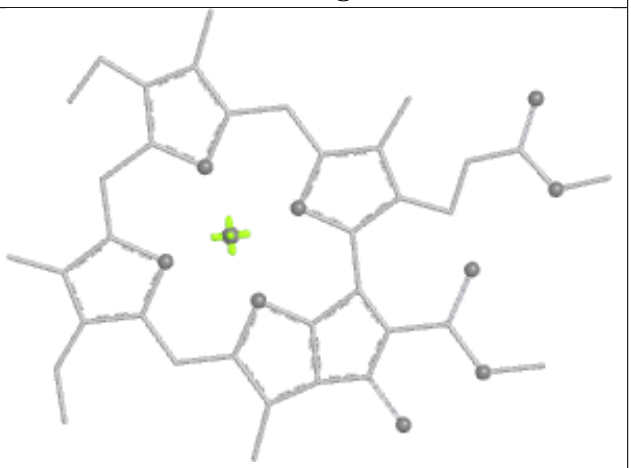
Bond lengths



Bond angles



Torsions

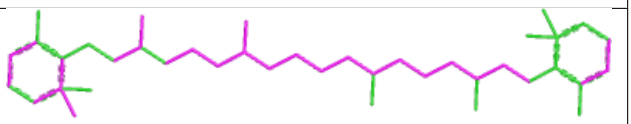


Rings

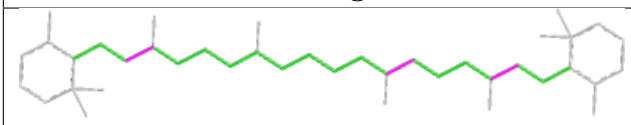
Ligand BCR H 4014



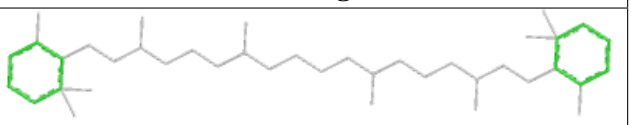
Bond lengths



Bond angles

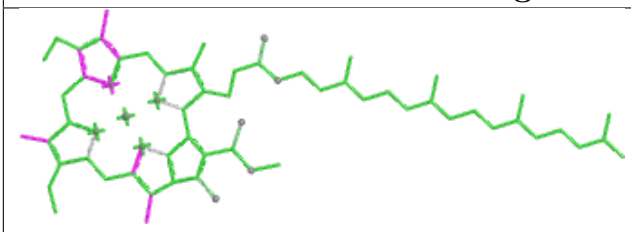


Torsions

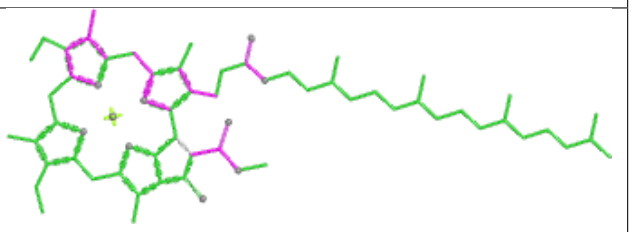


Rings

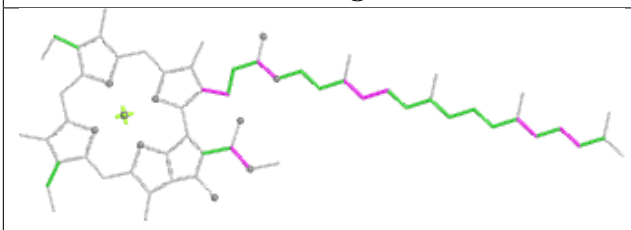
Ligand CLA G 1104



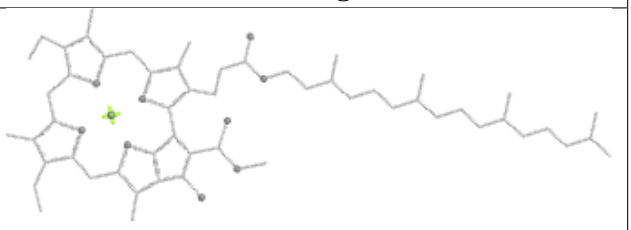
Bond lengths



Bond angles

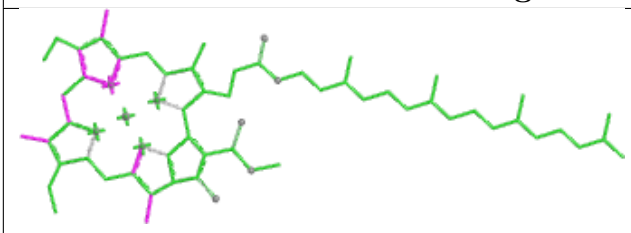


Torsions

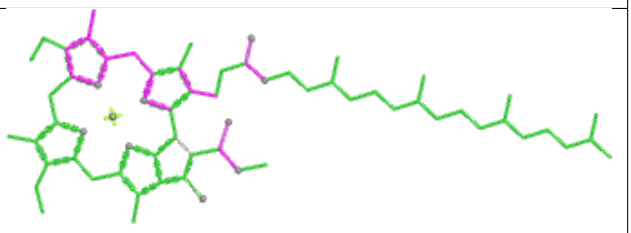


Rings

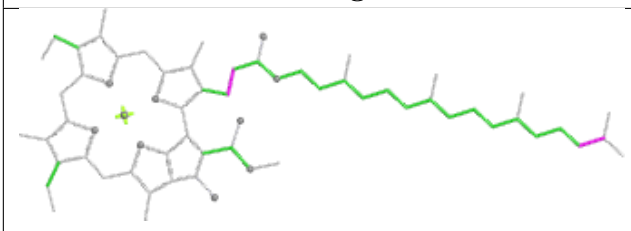
Ligand CLA H 1238



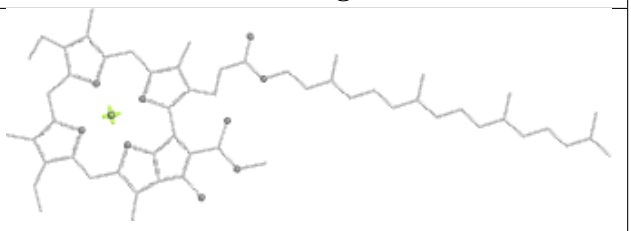
Bond lengths



Bond angles

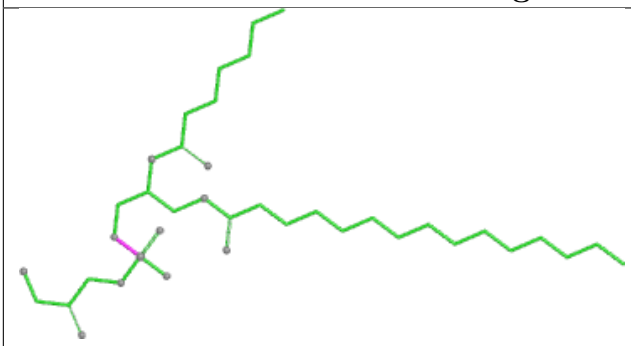


Torsions

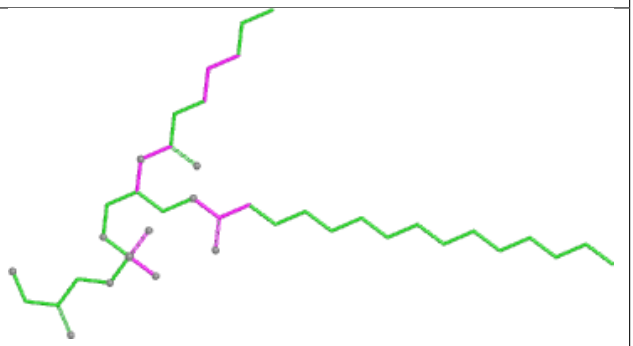


Rings

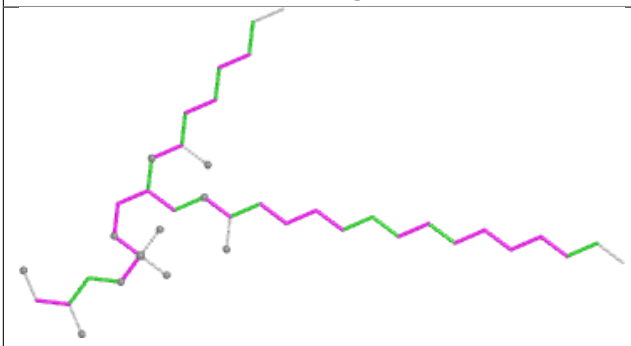
Ligand LHG G 5002



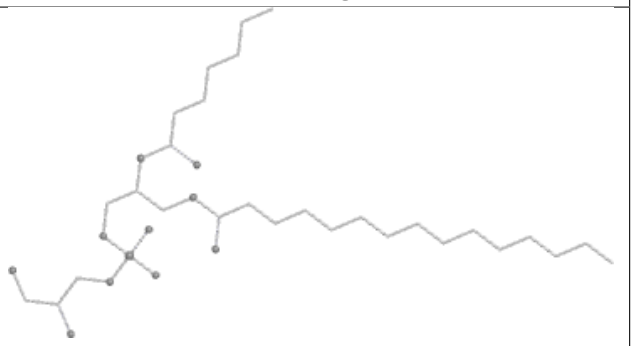
Bond lengths



Bond angles

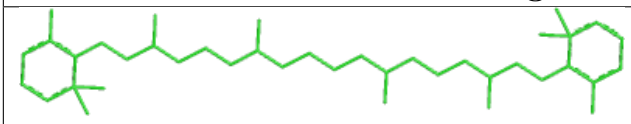


Torsions

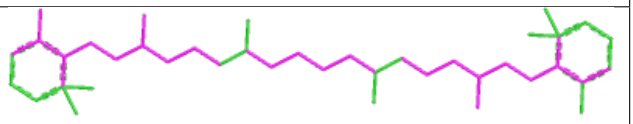


Rings

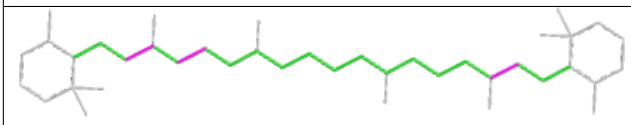
Ligand BCR a 524



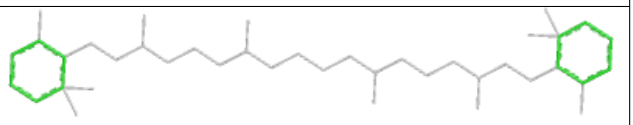
Bond lengths



Bond angles

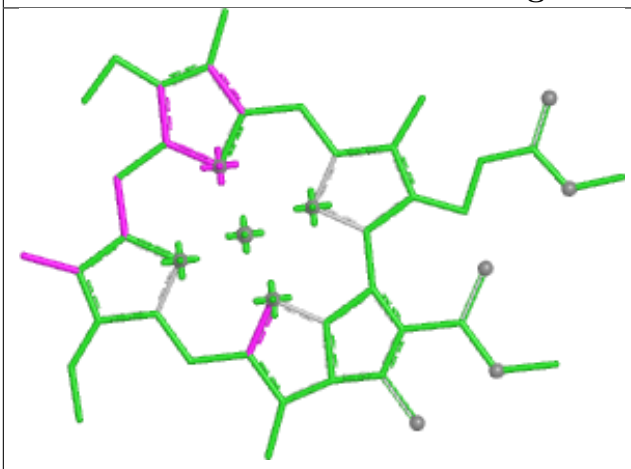


Torsions

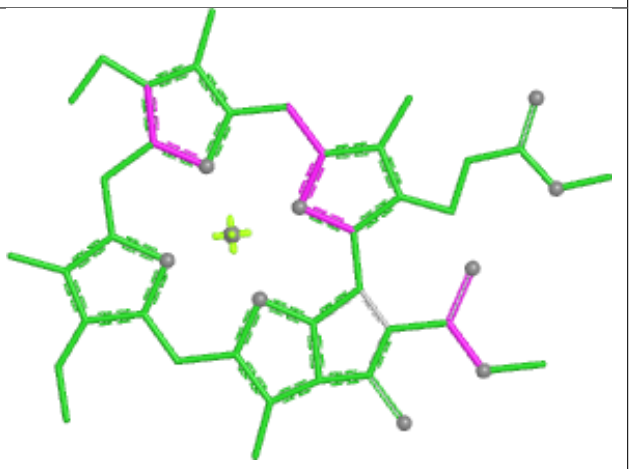


Rings

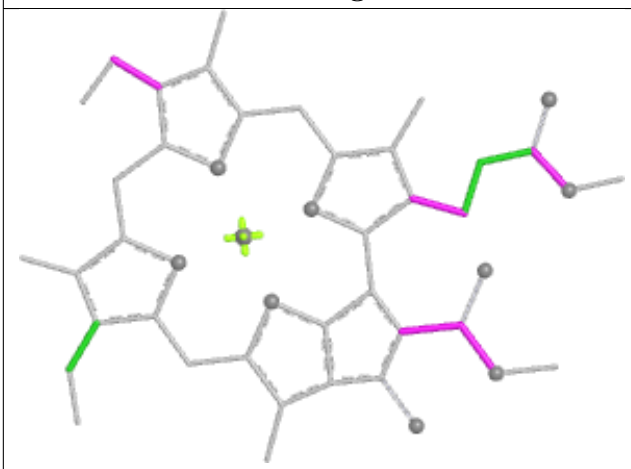
Ligand CLA d 519



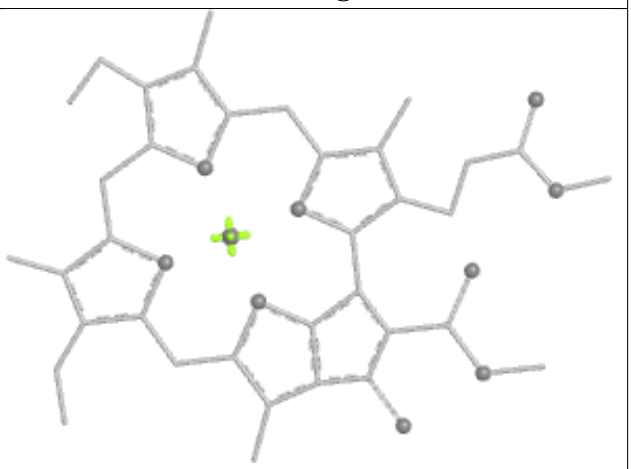
Bond lengths



Bond angles

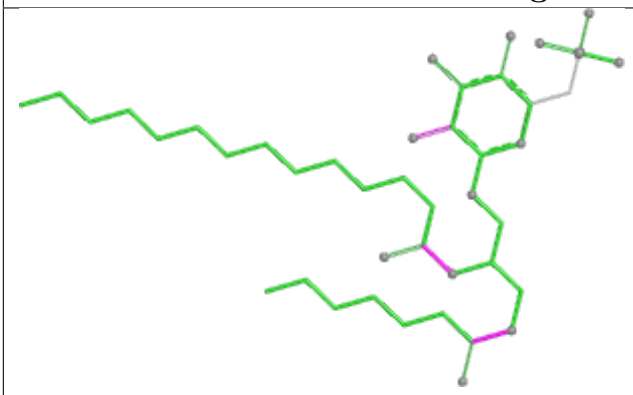


Torsions

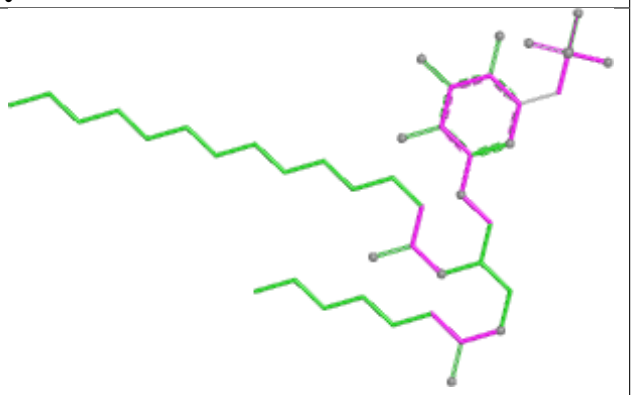


Rings

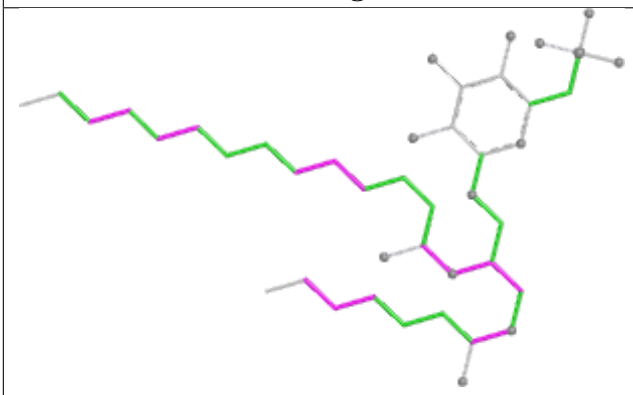
Ligand SQD r 822



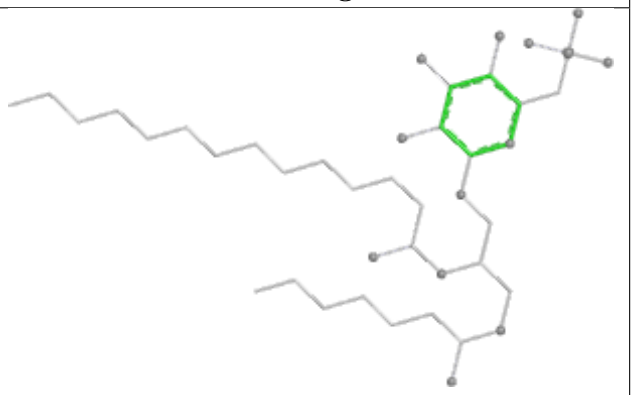
Bond lengths



Bond angles



Torsions



Rings

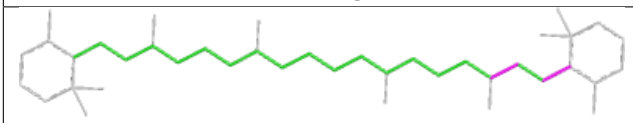
Ligand BCR c 523



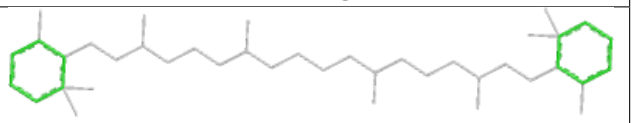
Bond lengths



Bond angles

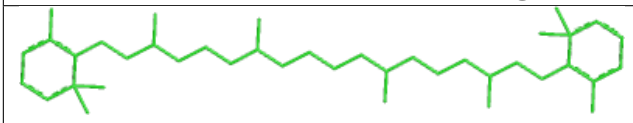


Torsions

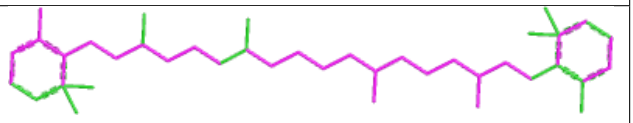


Rings

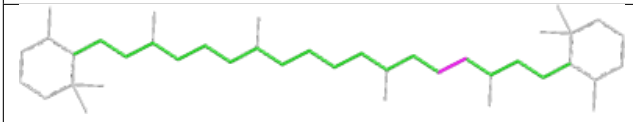
Ligand BCR B 4009



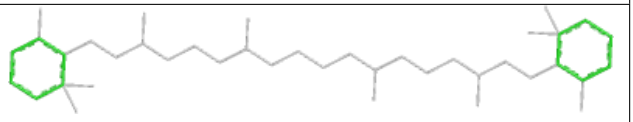
Bond lengths



Bond angles

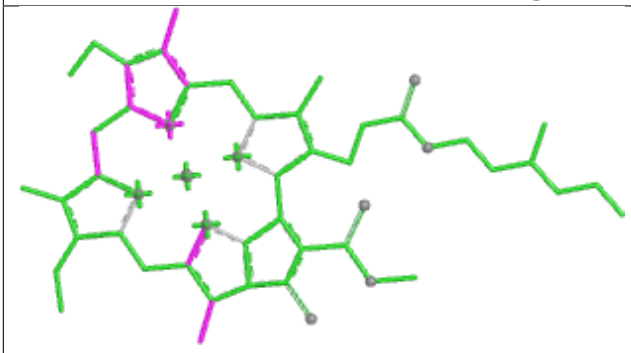


Torsions

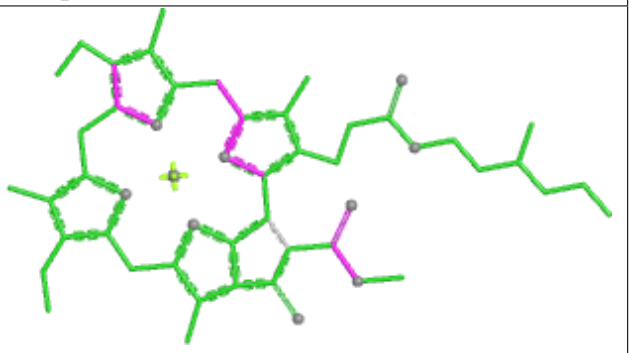


Rings

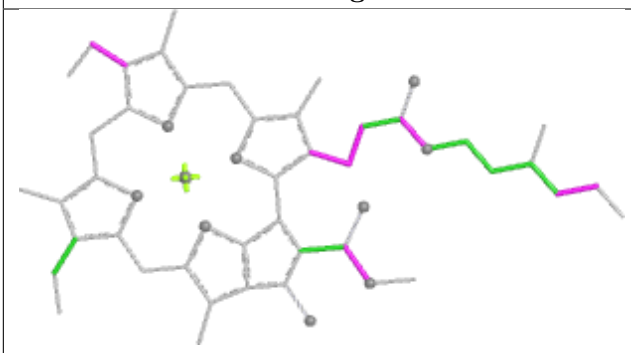
Ligand CLA q 512



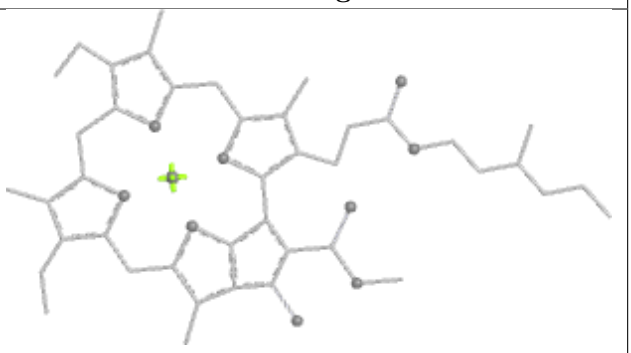
Bond lengths



Bond angles

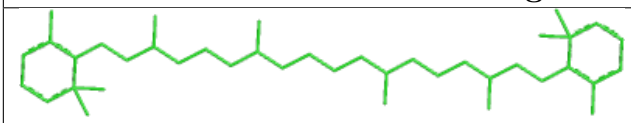


Torsions

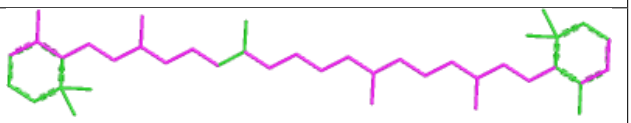


Rings

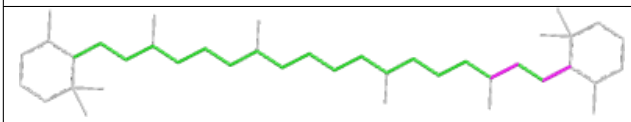
Ligand BCR u 523



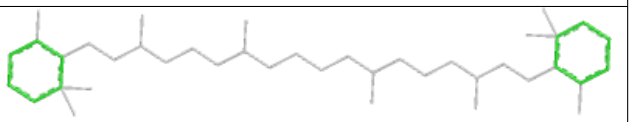
Bond lengths



Bond angles

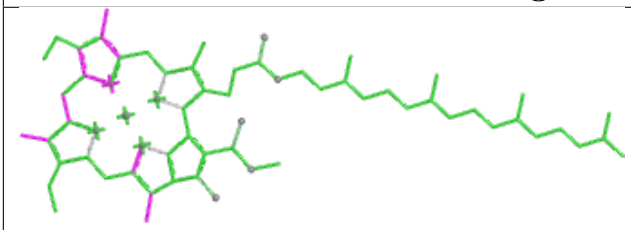


Torsions

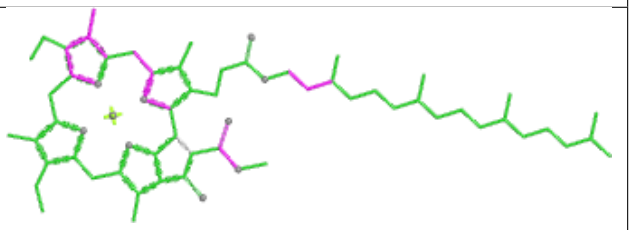


Rings

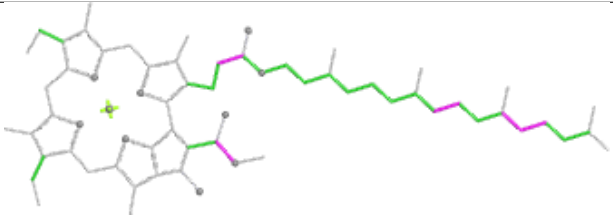
Ligand CLA r 510



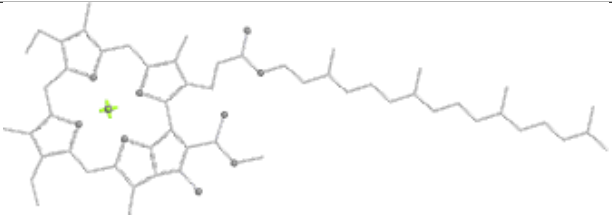
Bond lengths



Bond angles

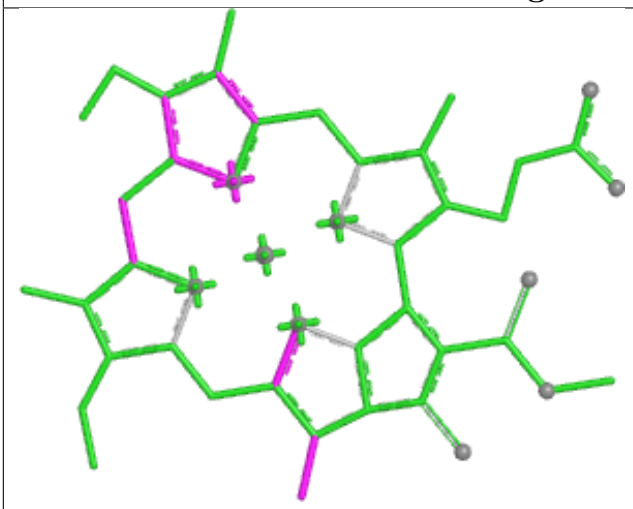


Torsions

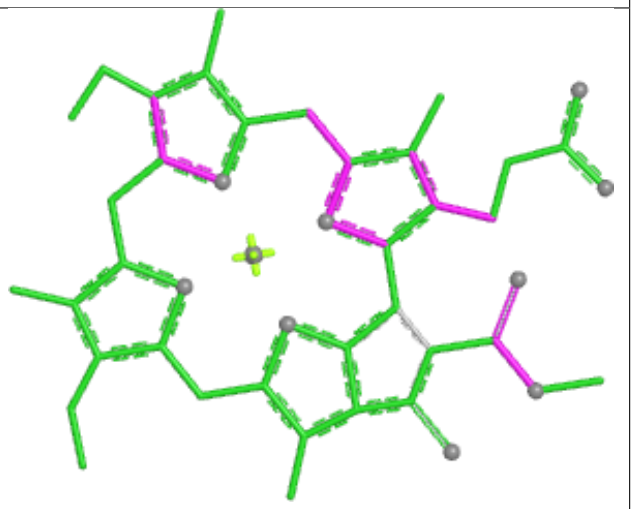


Rings

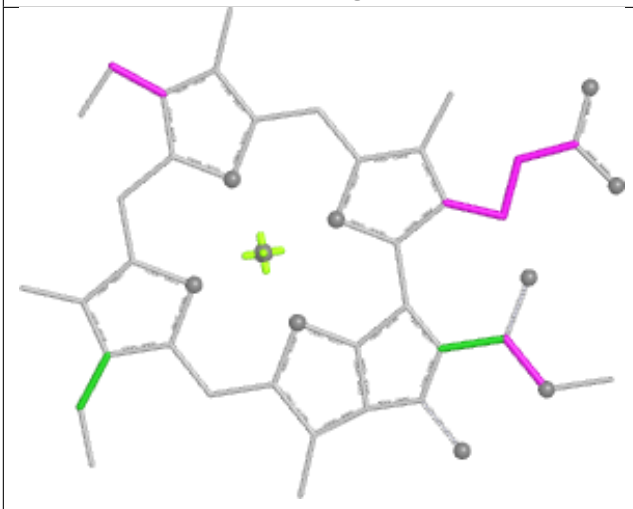
Ligand CLA v 516



Bond lengths



Bond angles

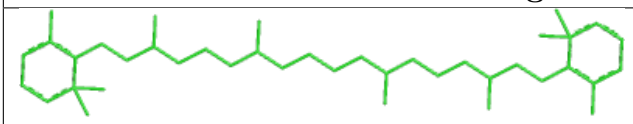


Torsions

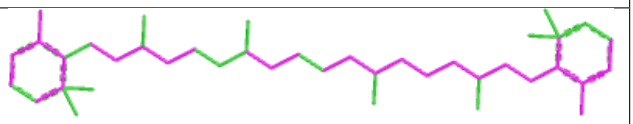


Rings

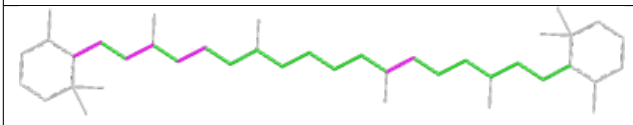
Ligand BCR 5 521



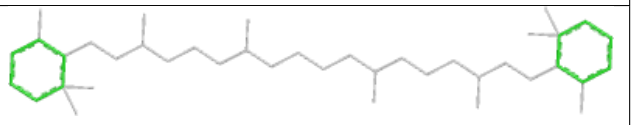
Bond lengths



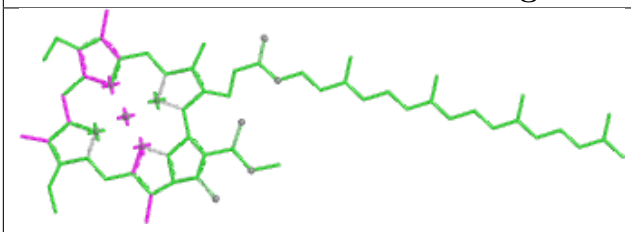
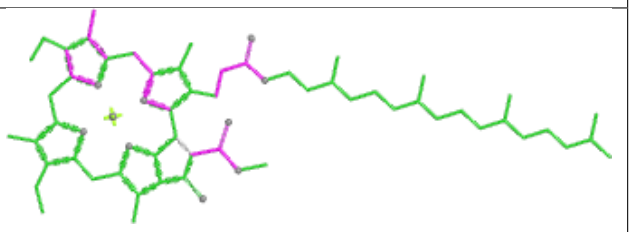
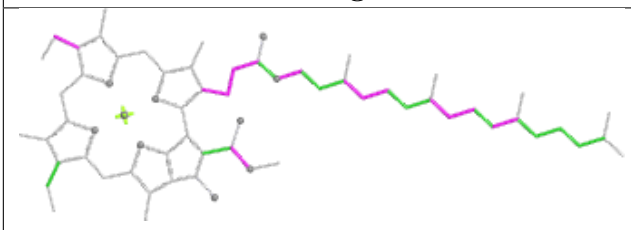
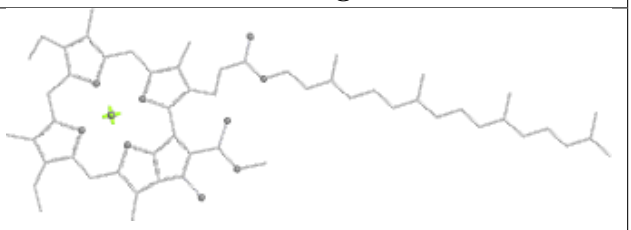
Bond angles

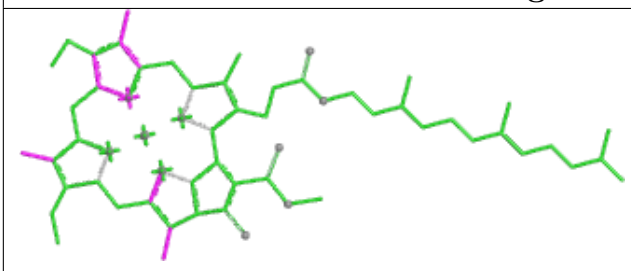
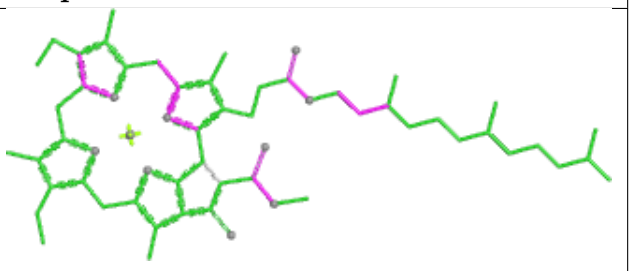
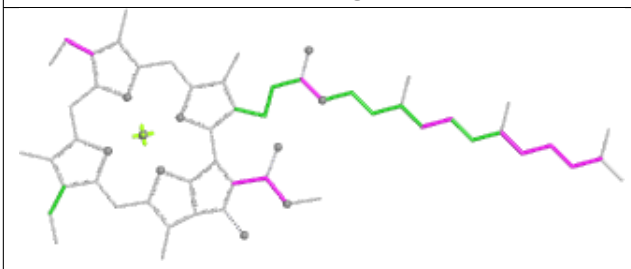
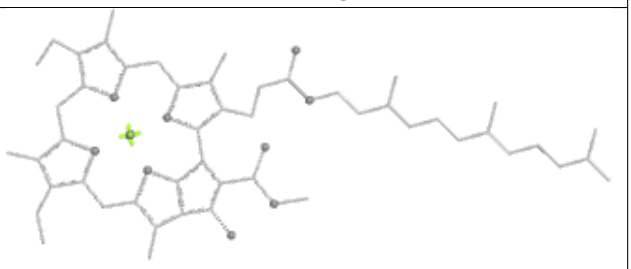


Torsions

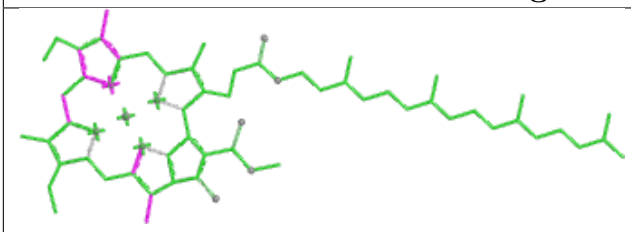


Rings

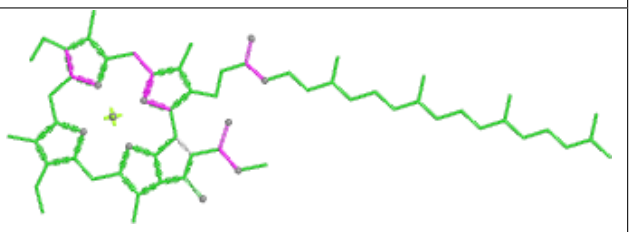
Ligand CLA e 1107	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

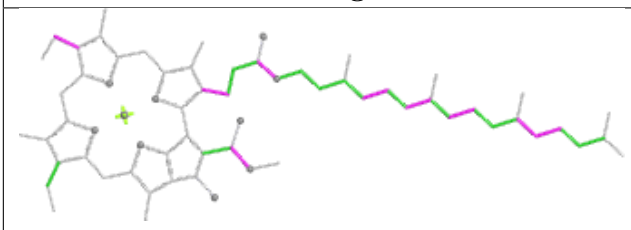
Ligand CLA s 513



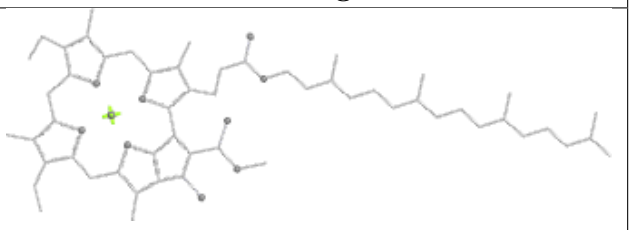
Bond lengths



Bond angles

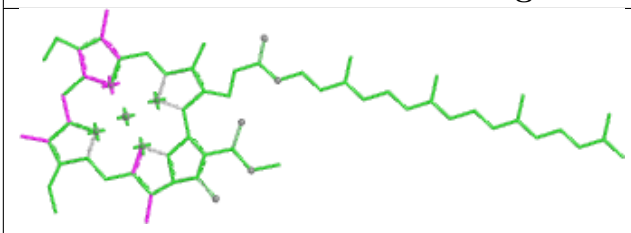


Torsions

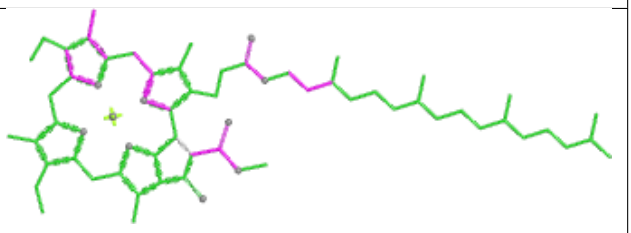


Rings

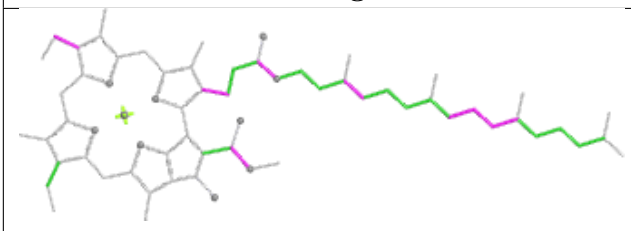
Ligand CLA B 1240



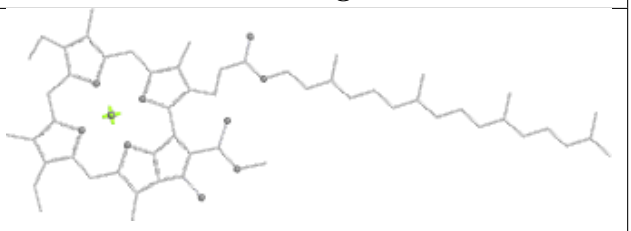
Bond lengths



Bond angles

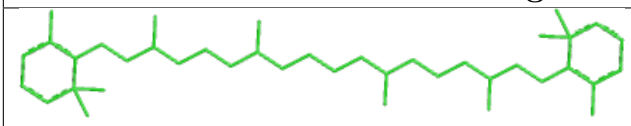


Torsions

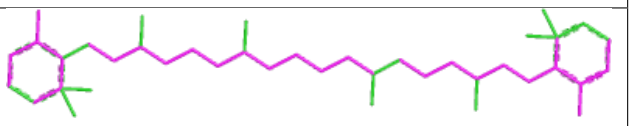


Rings

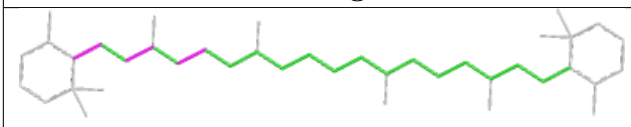
Ligand BCR 3 522



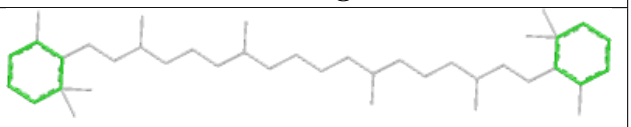
Bond lengths



Bond angles

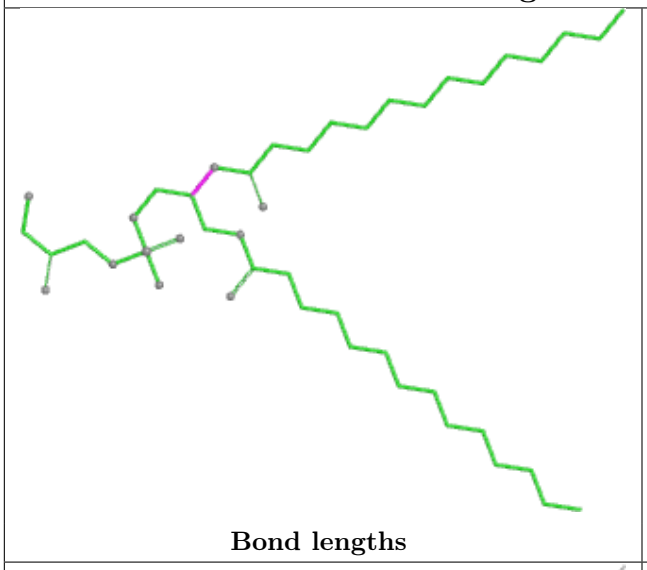


Torsions

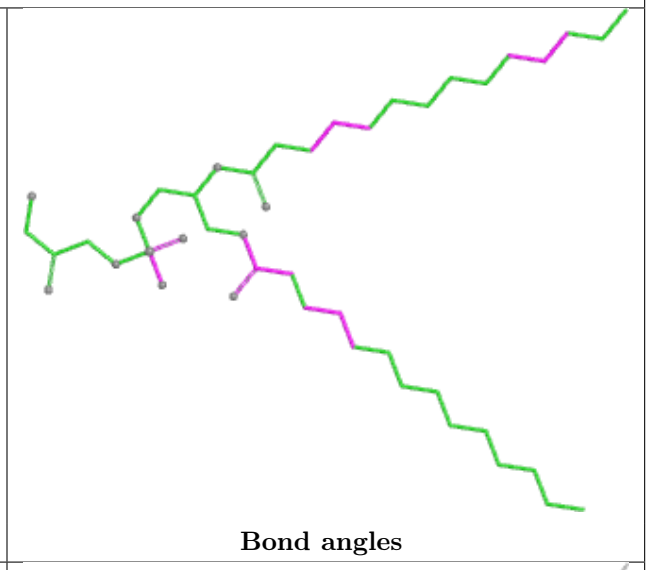


Rings

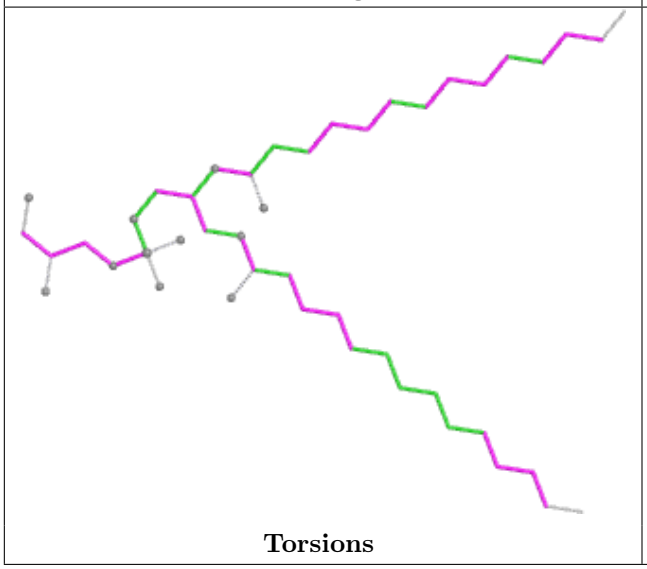
Ligand LHG e 5005



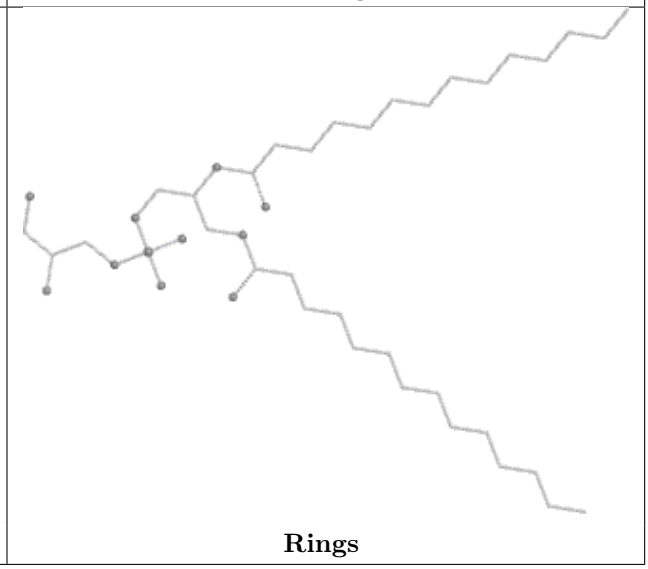
Bond lengths



Bond angles

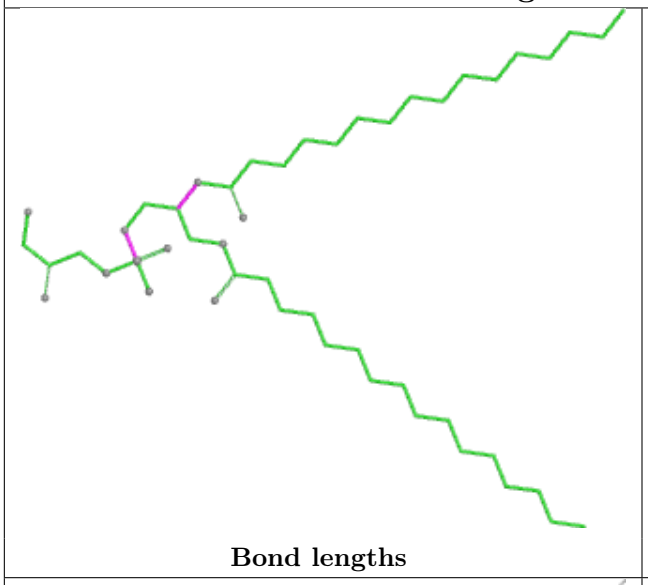


Torsions

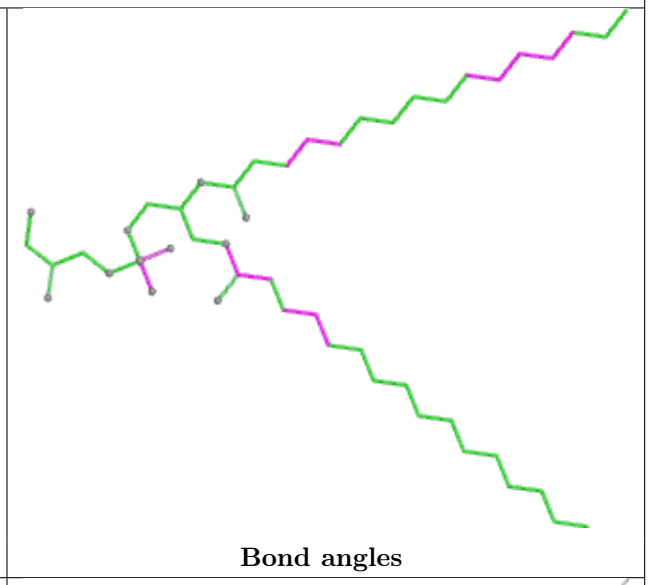


Rings

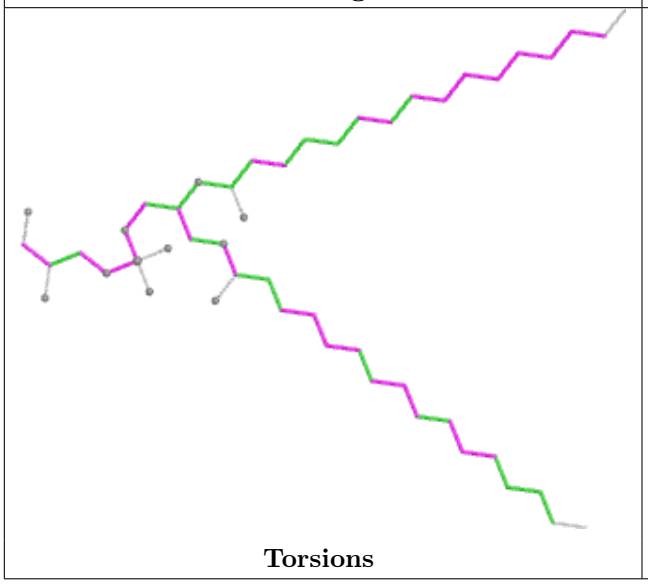
Ligand LHG n 5221



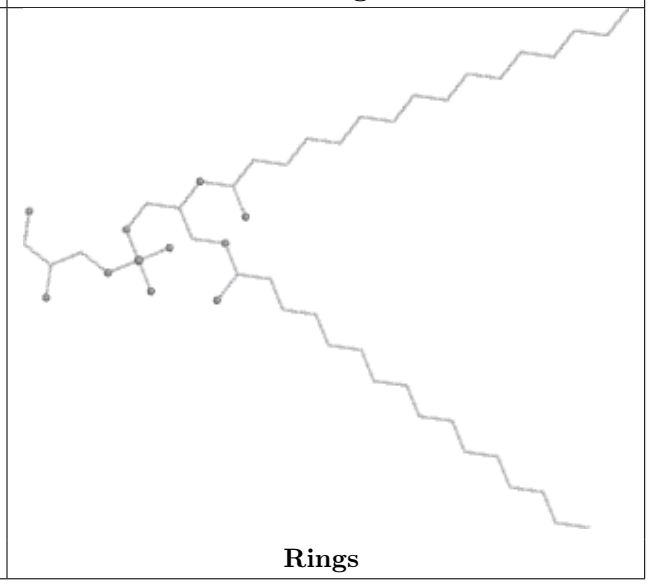
Bond lengths



Bond angles



Torsions

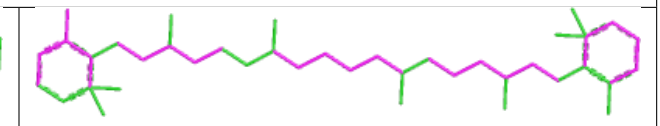


Rings

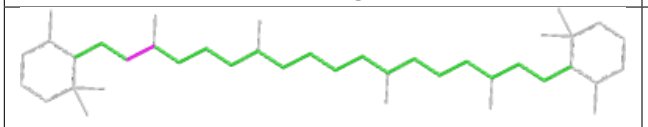
Ligand BCR V 4022



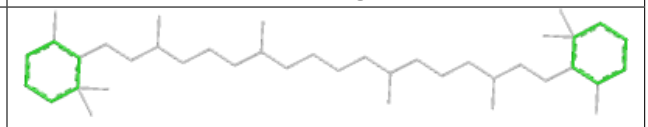
Bond lengths



Bond angles

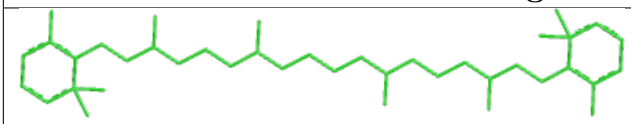


Torsions

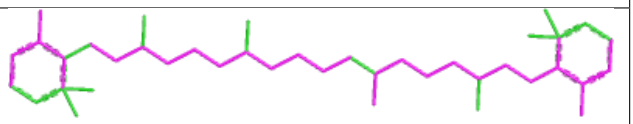


Rings

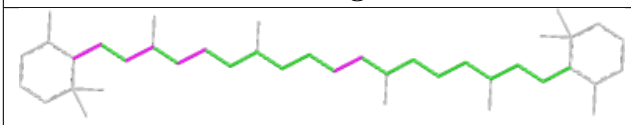
Ligand BCR 2 522



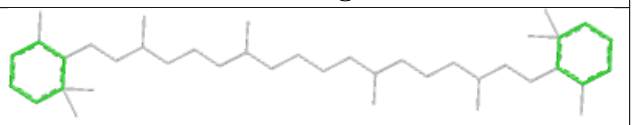
Bond lengths



Bond angles

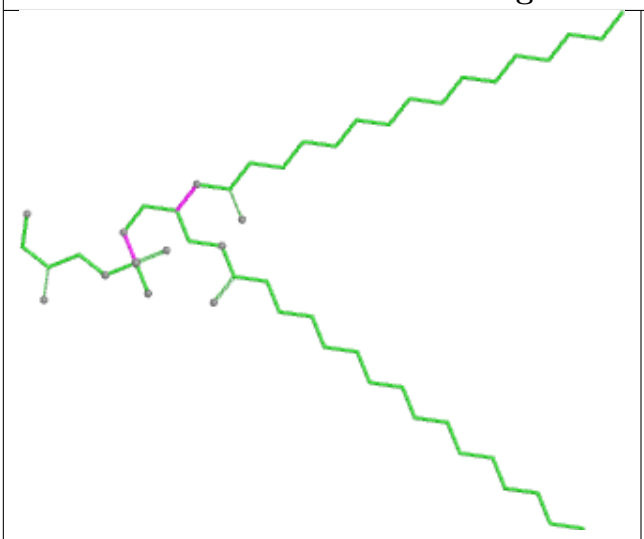


Torsions

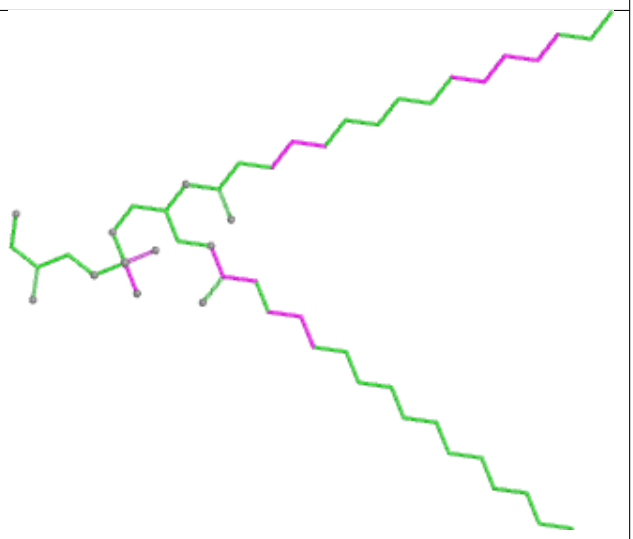


Rings

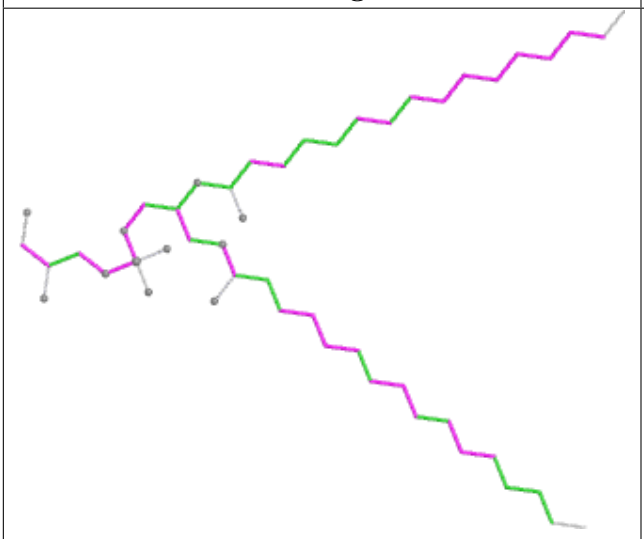
Ligand LHG L 5221



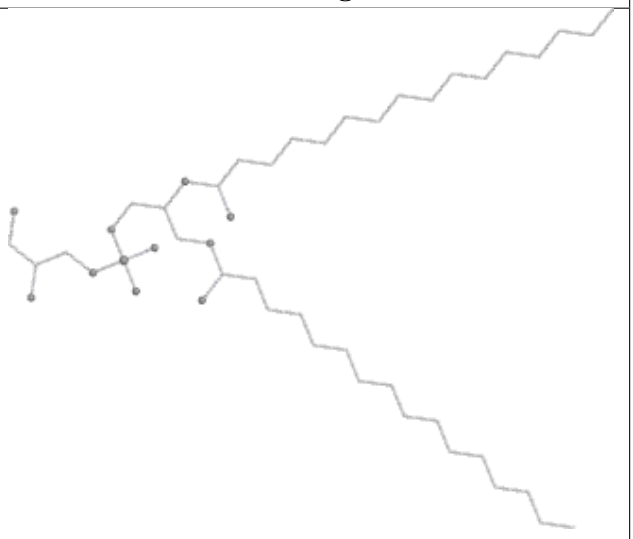
Bond lengths



Bond angles

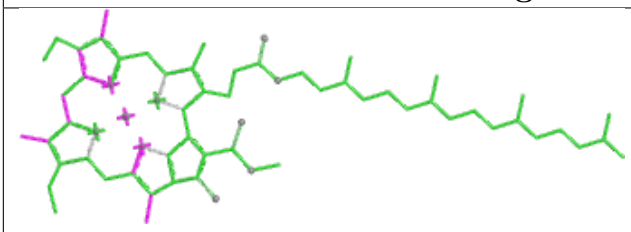


Torsions

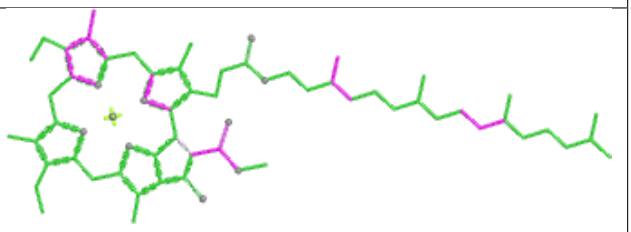


Rings

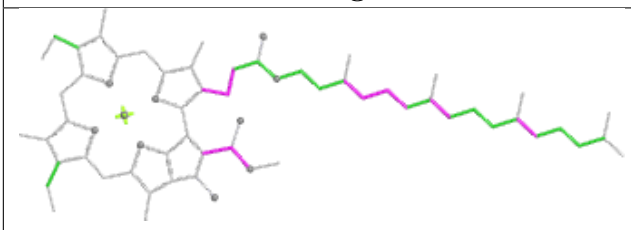
Ligand CLA B 1012



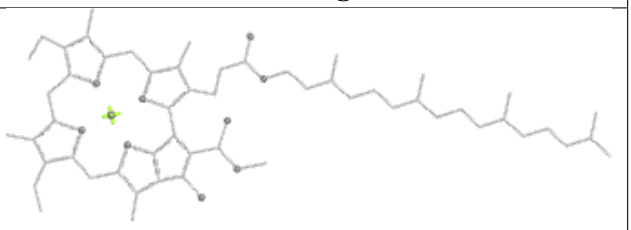
Bond lengths



Bond angles

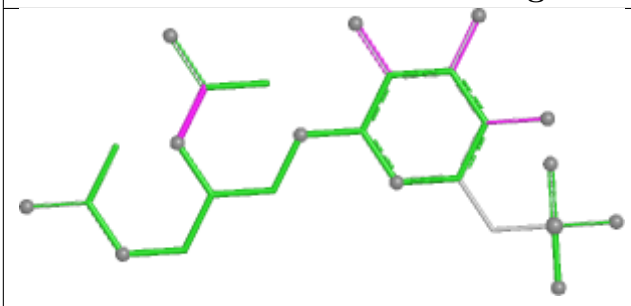


Torsions

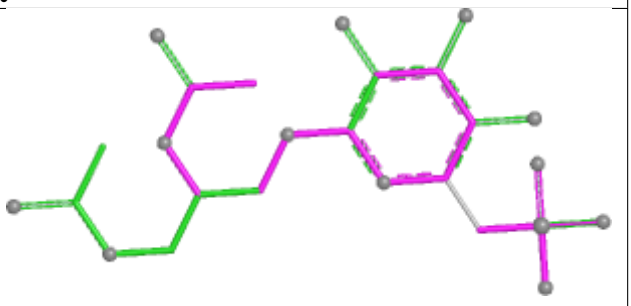


Rings

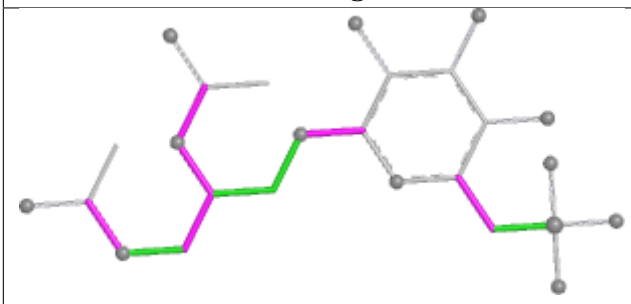
Ligand SQD d 822



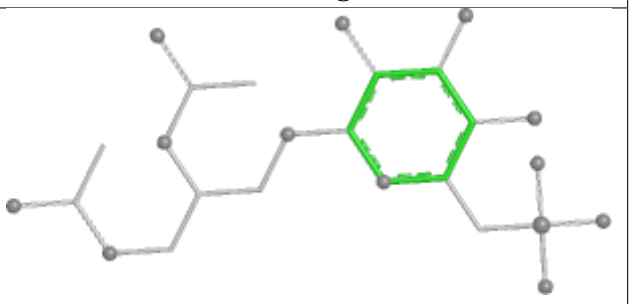
Bond lengths



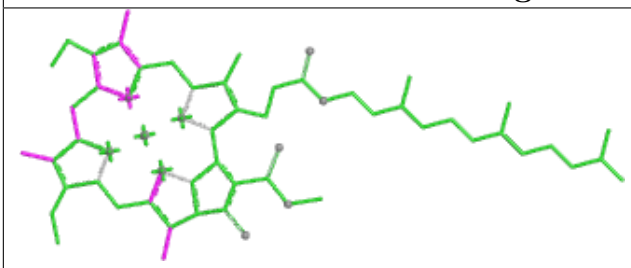
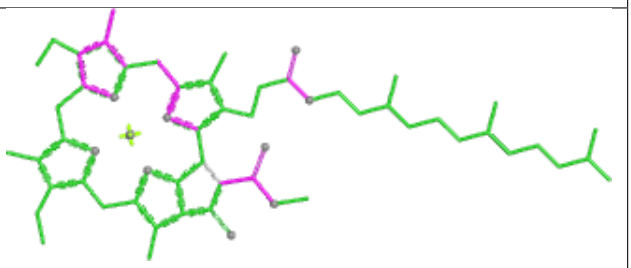
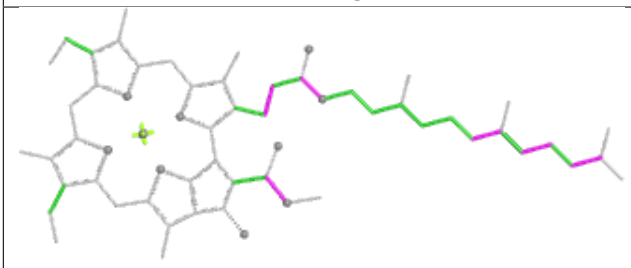
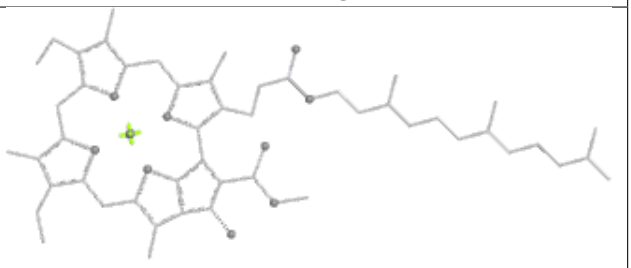
Bond angles

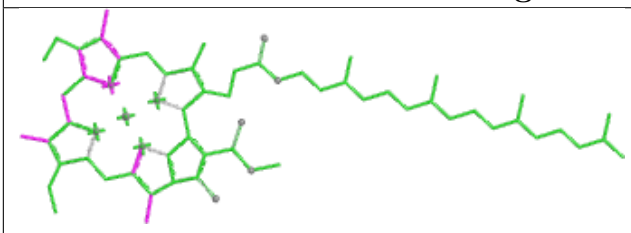
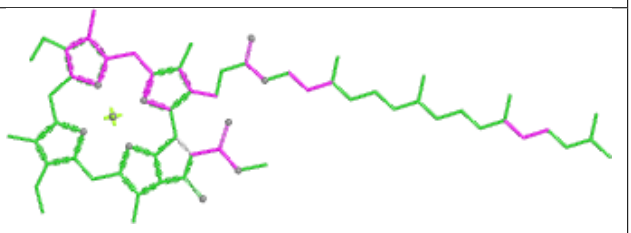
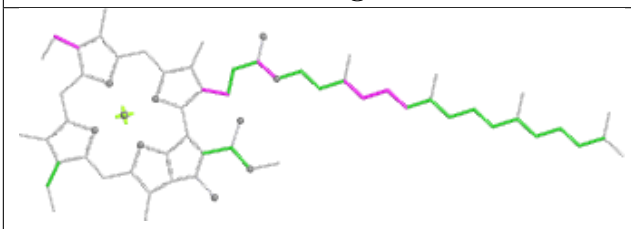
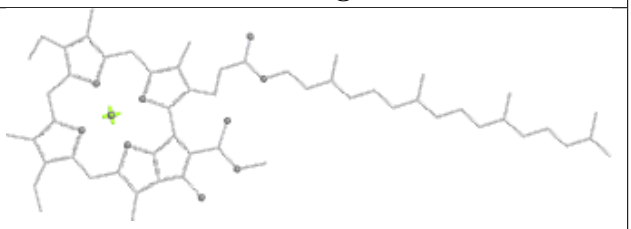


Torsions

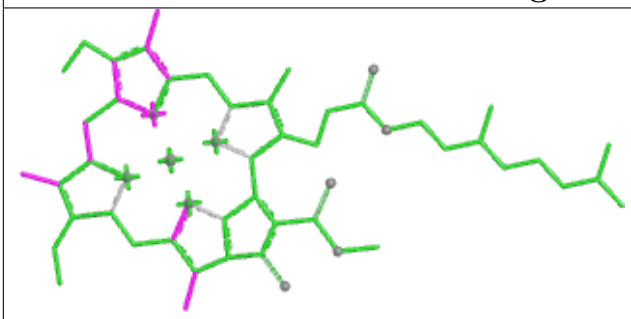


Rings

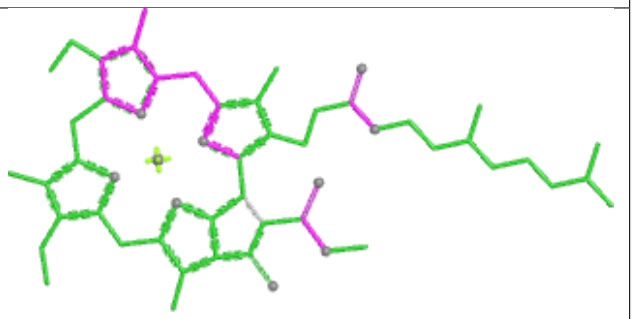
Ligand CLA H 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1130	
	
Bond lengths	Bond angles
	
Torsions	Rings

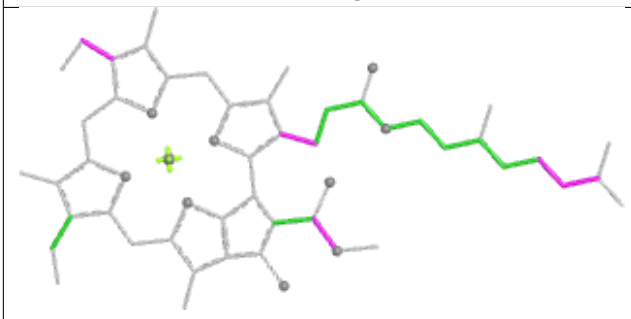
Ligand CLA r 508



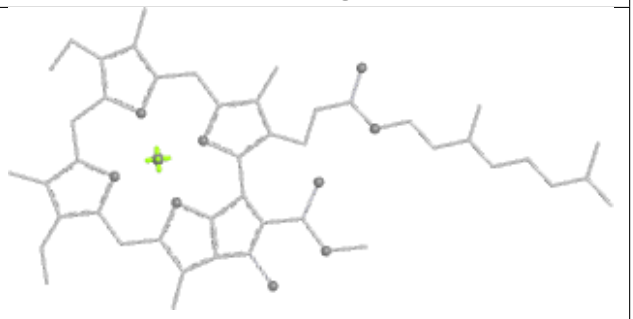
Bond lengths



Bond angles

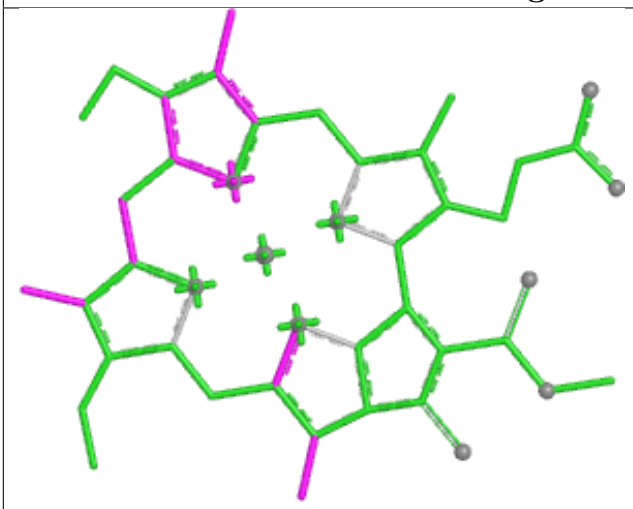


Torsions

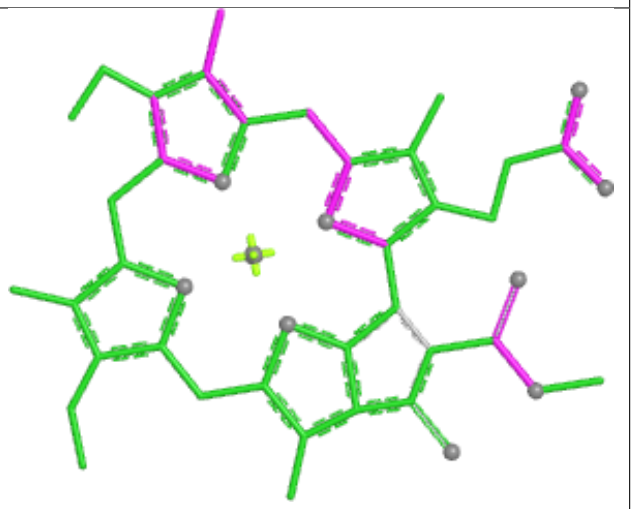


Rings

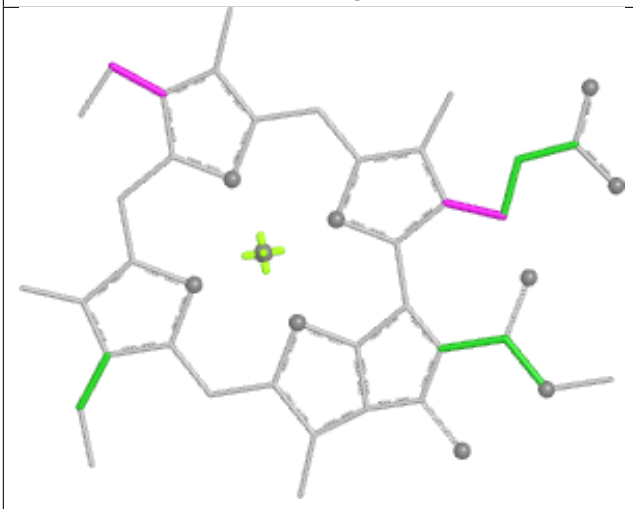
Ligand CLA v 508



Bond lengths



Bond angles

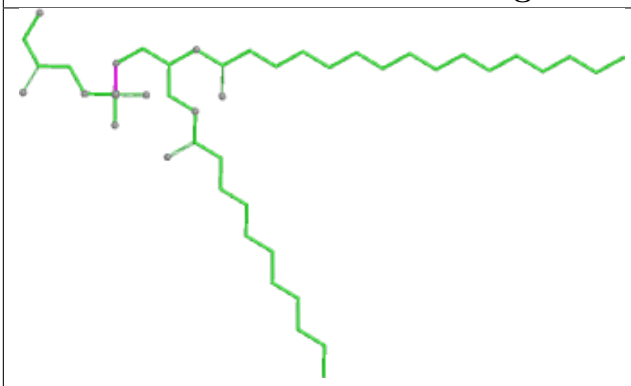


Torsions

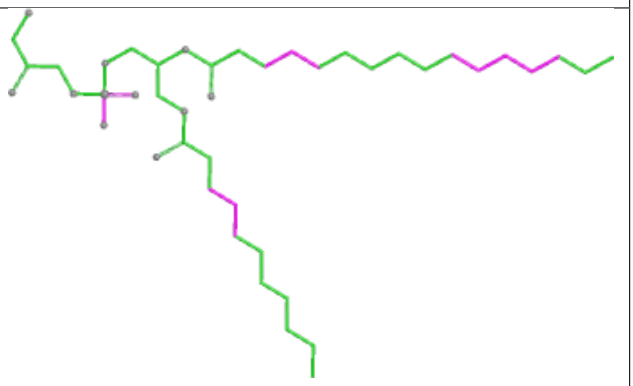


Rings

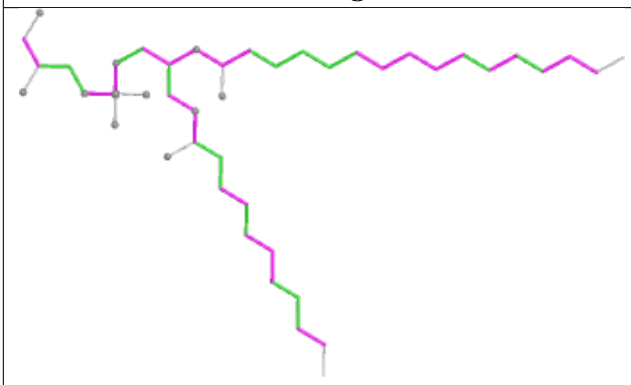
Ligand LHG B 1855



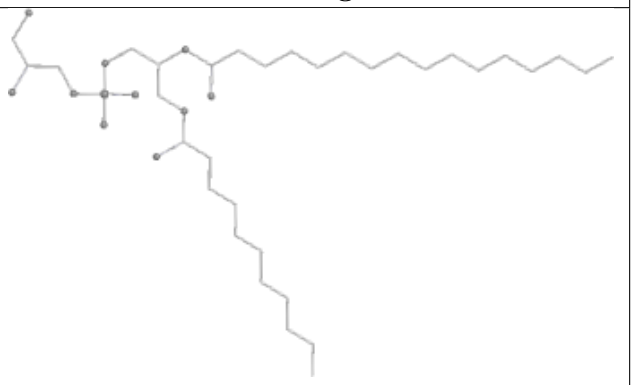
Bond lengths



Bond angles

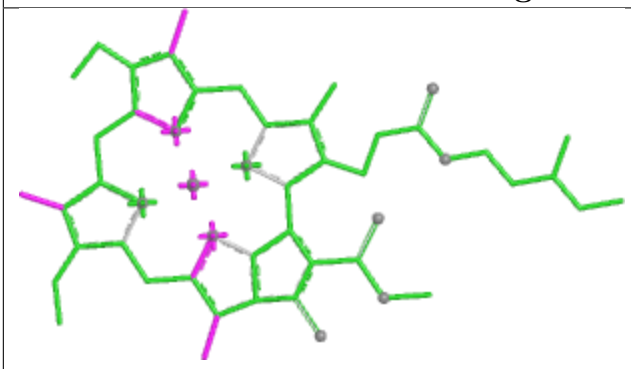


Torsions

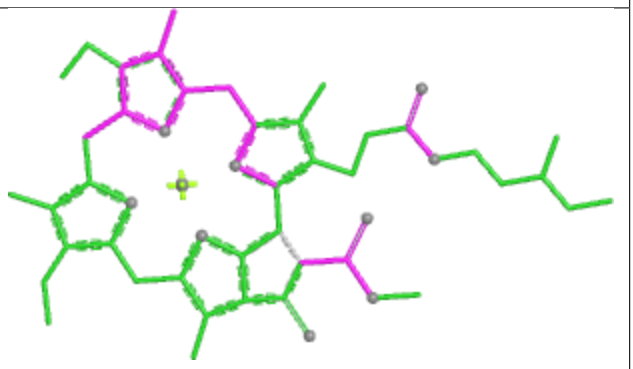


Rings

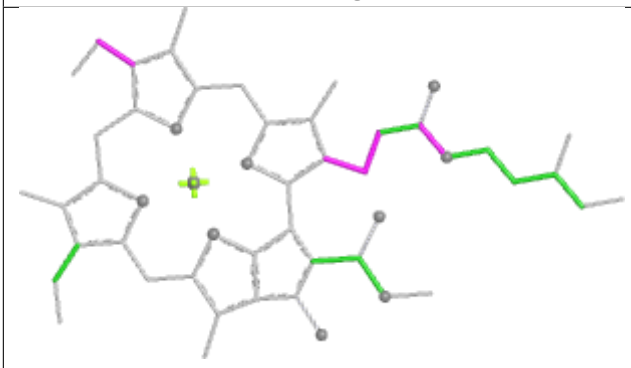
Ligand CLA A 1129



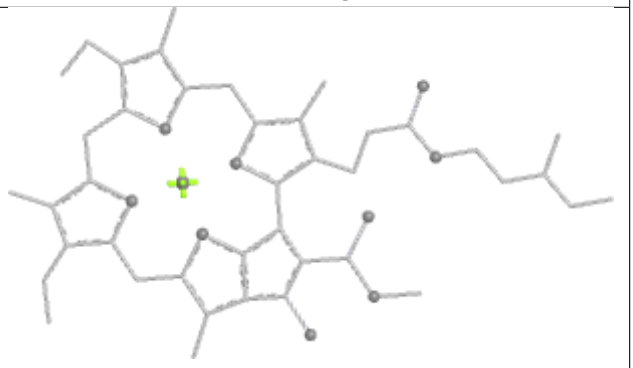
Bond lengths



Bond angles

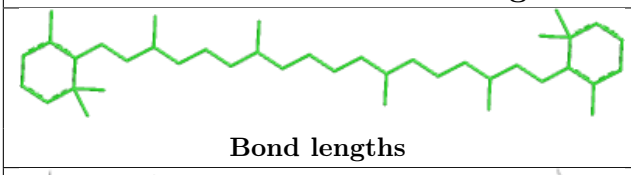


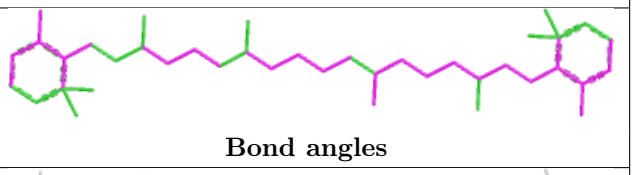
Torsions

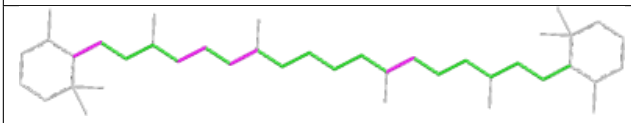


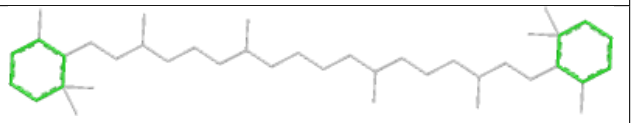
Rings

Ligand BCR M 4021


Bond lengths

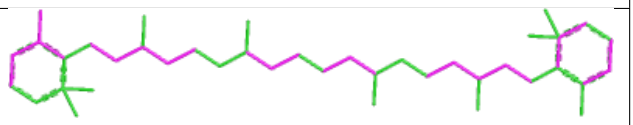

Bond angles

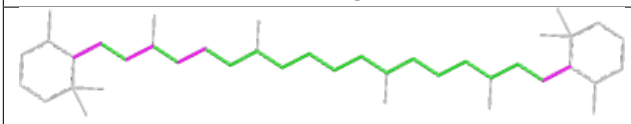

Torsions

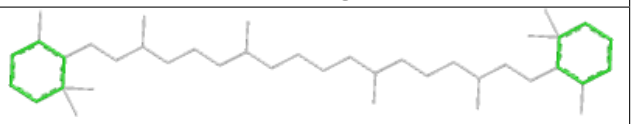

Rings

Ligand BCR 3 521

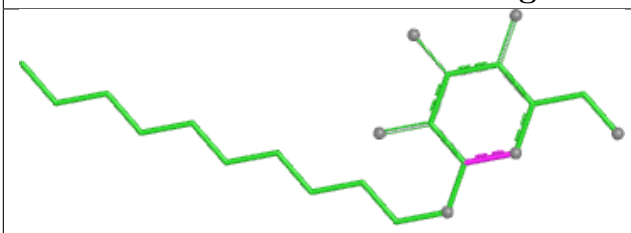

Bond lengths

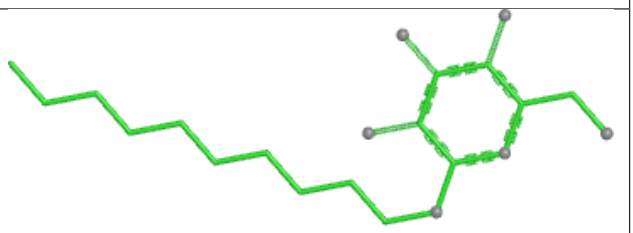

Bond angles

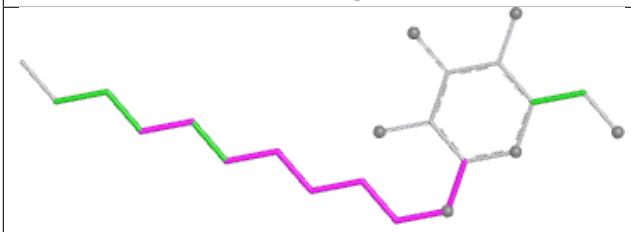

Torsions

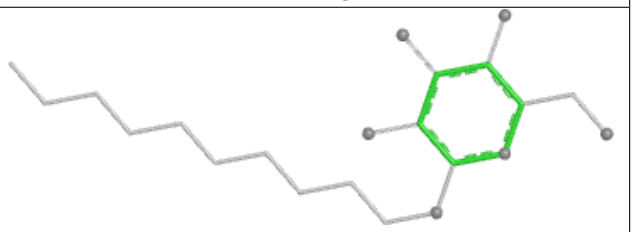

Rings

Ligand LMU l 5105

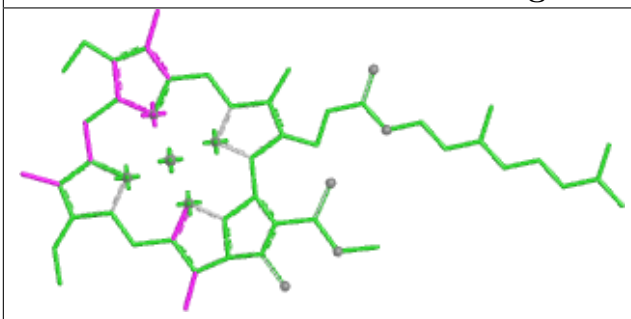

Bond lengths


Bond angles

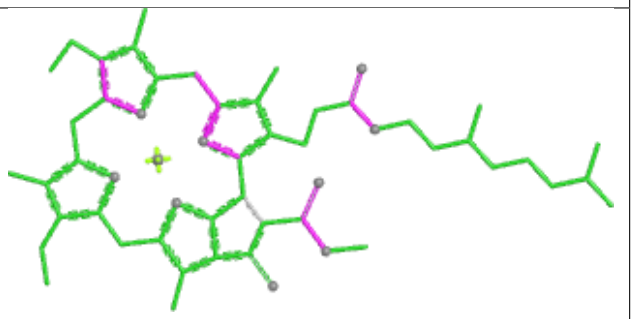

Torsions


Rings

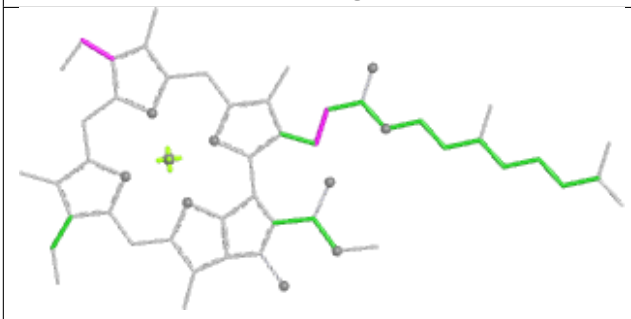
Ligand CLA 1 513



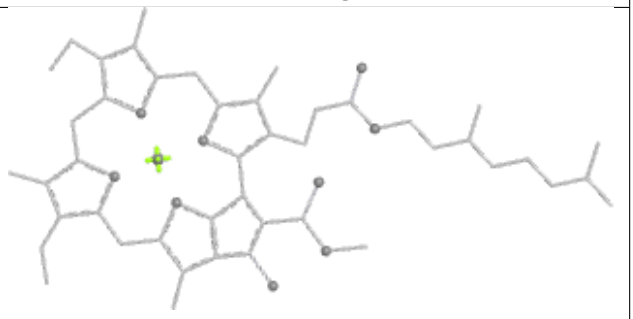
Bond lengths



Bond angles

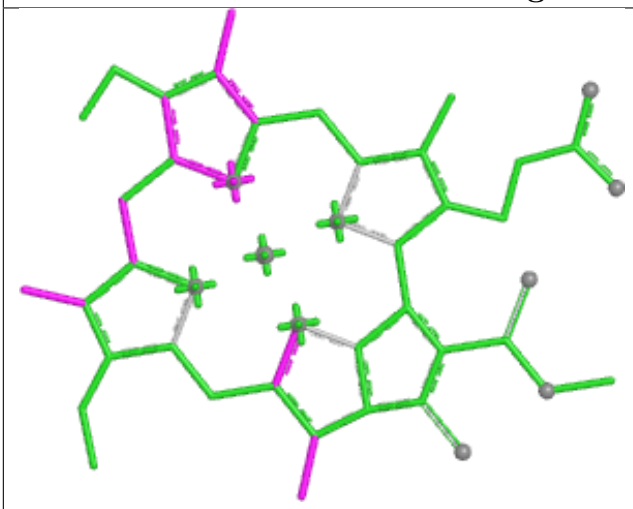


Torsions

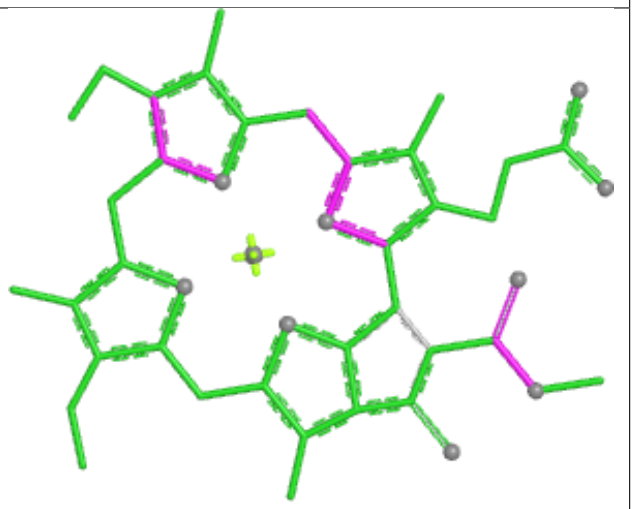


Rings

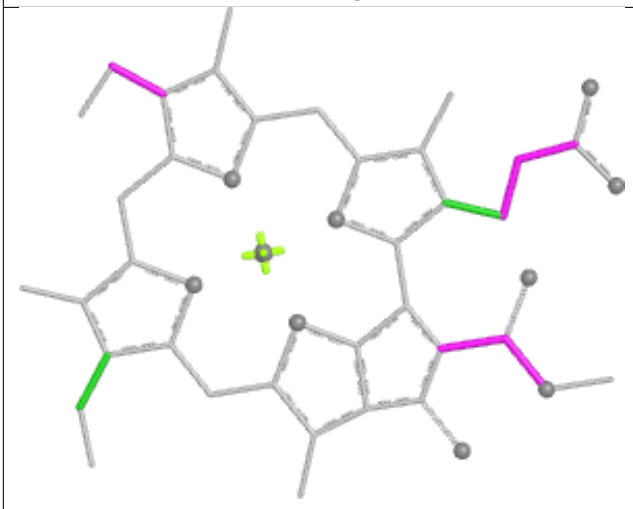
Ligand CLA u 517



Bond lengths



Bond angles

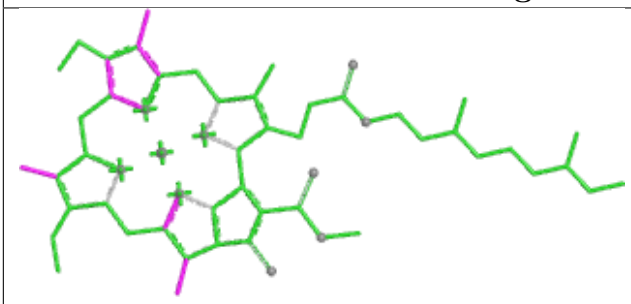


Torsions

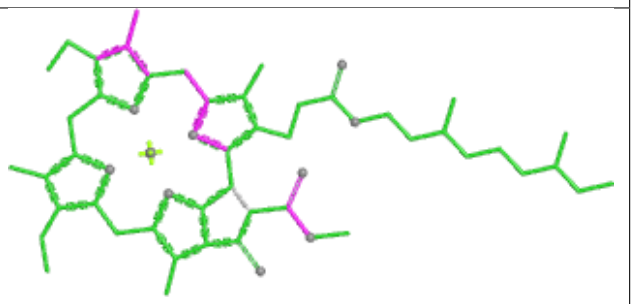


Rings

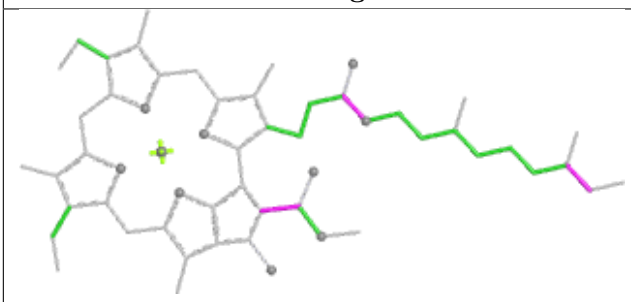
Ligand CLA H 1211



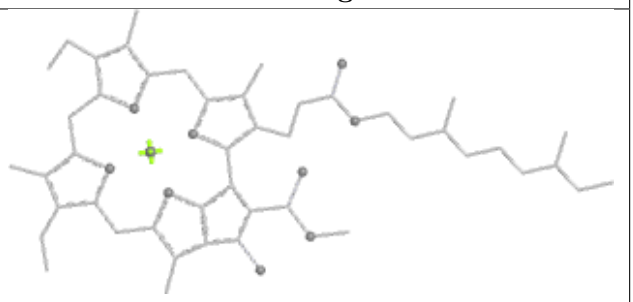
Bond lengths



Bond angles

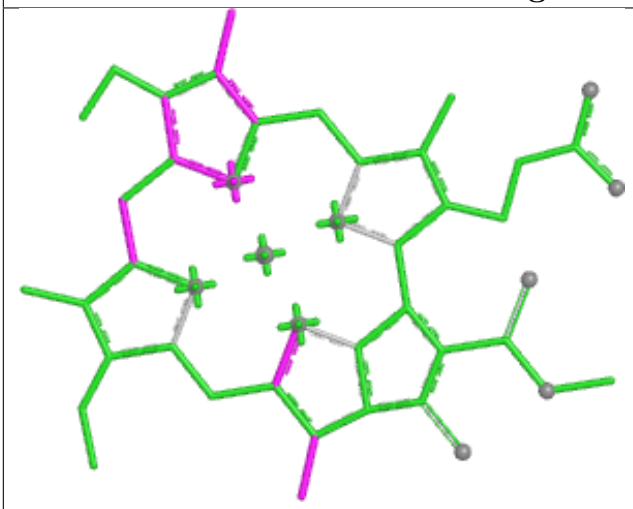


Torsions

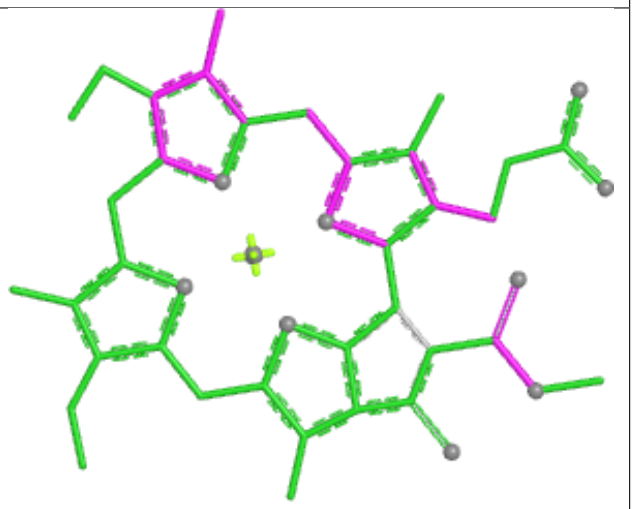


Rings

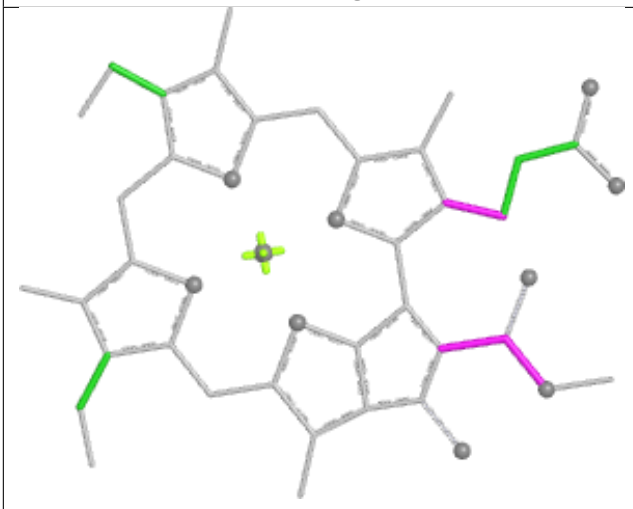
Ligand CLA a 504



Bond lengths



Bond angles

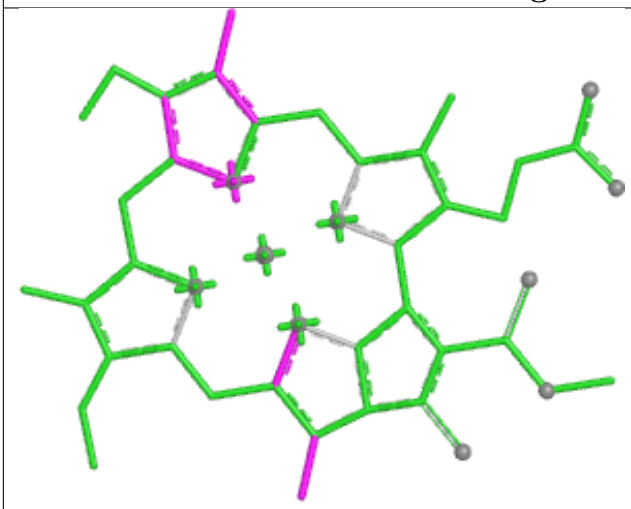


Torsions

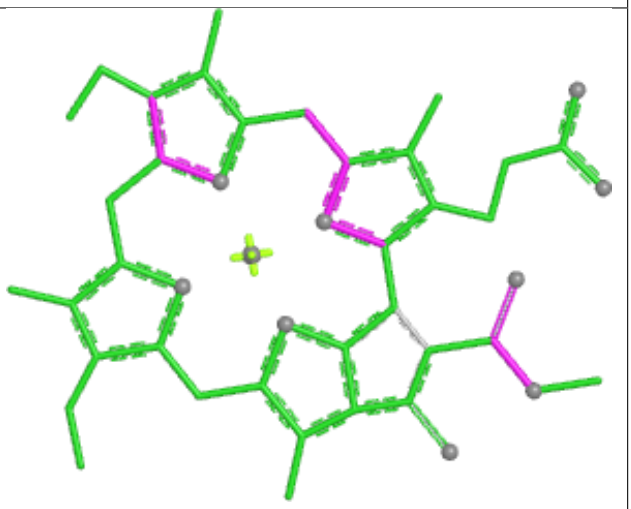


Rings

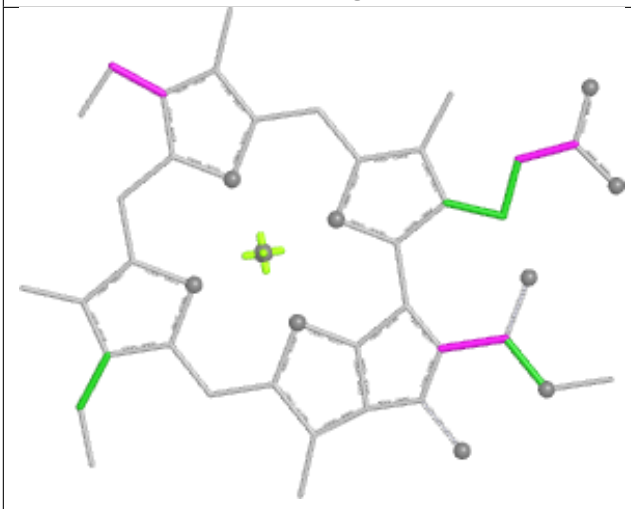
Ligand CLA t 512



Bond lengths



Bond angles

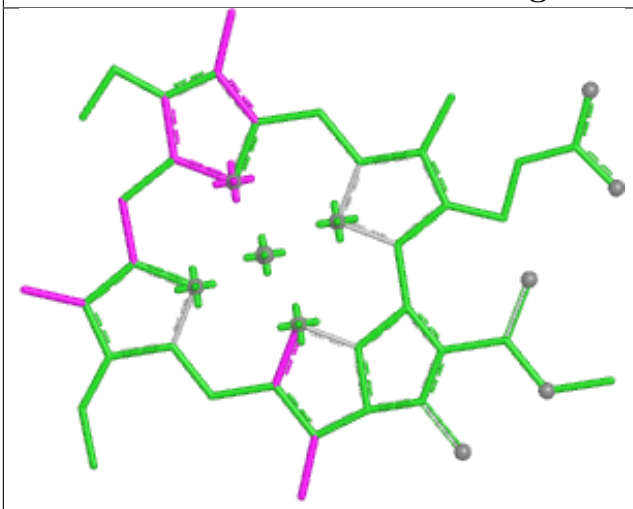


Torsions

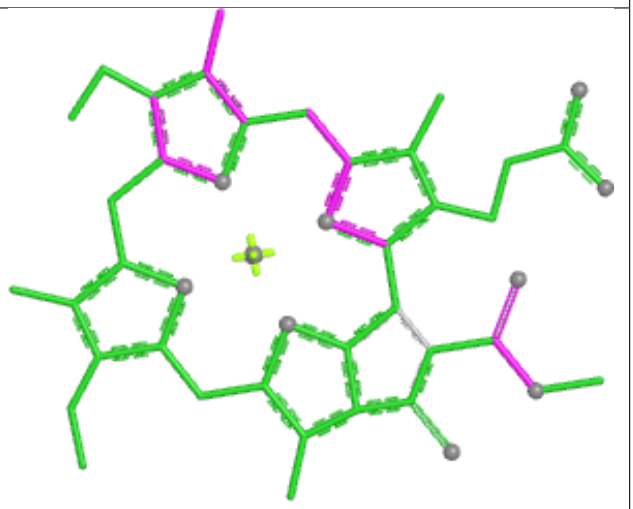


Rings

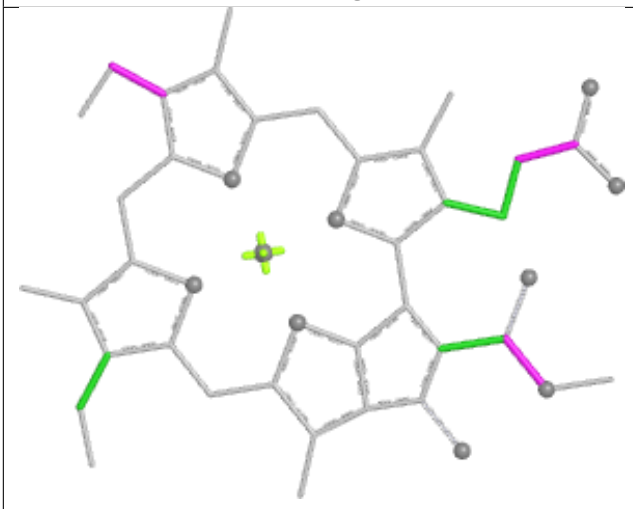
Ligand CLA c 508



Bond lengths



Bond angles

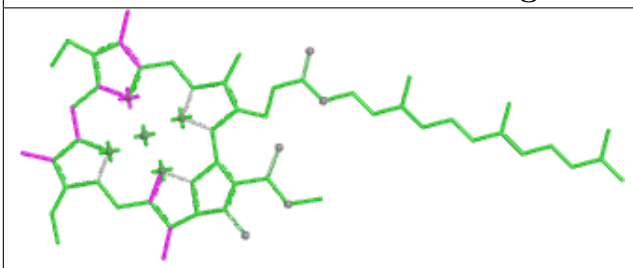


Torsions

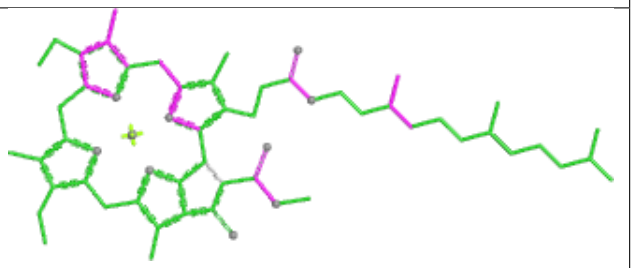


Rings

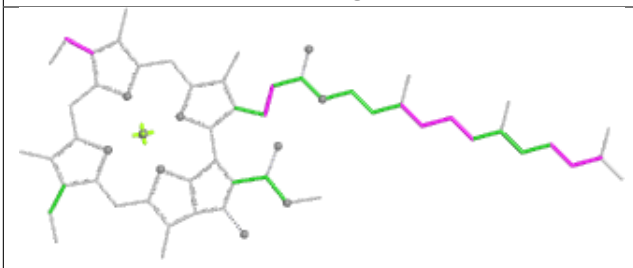
Ligand CLA e 1115



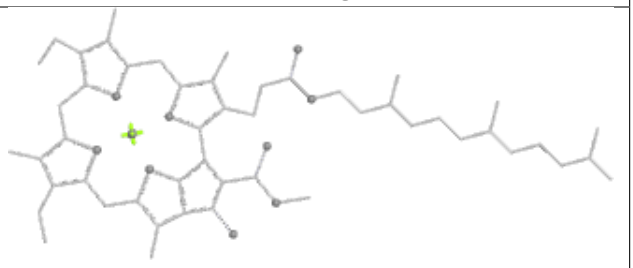
Bond lengths



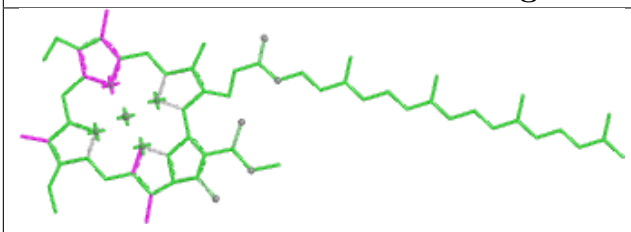
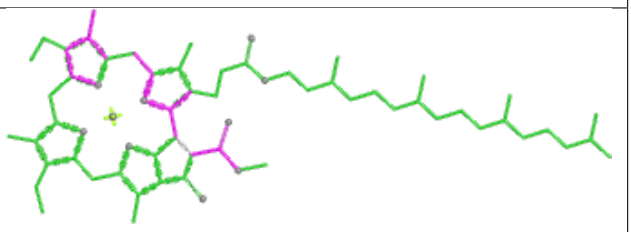
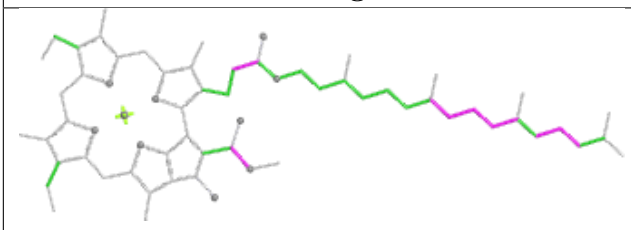
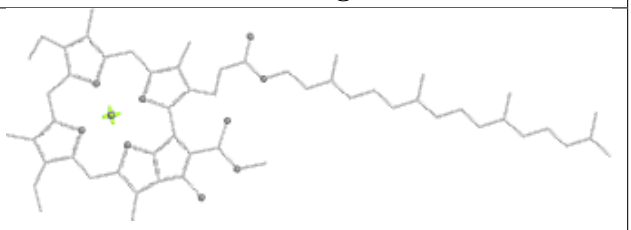
Bond angles

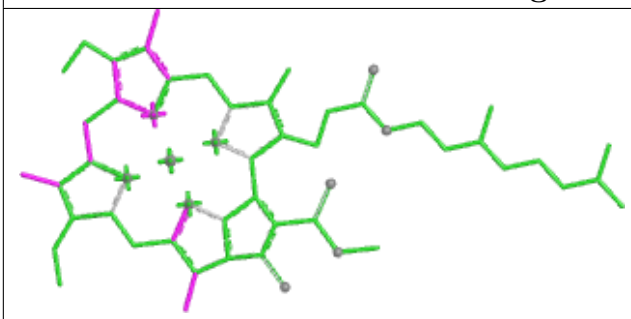
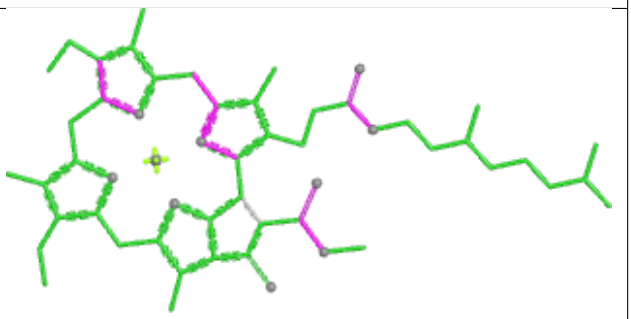
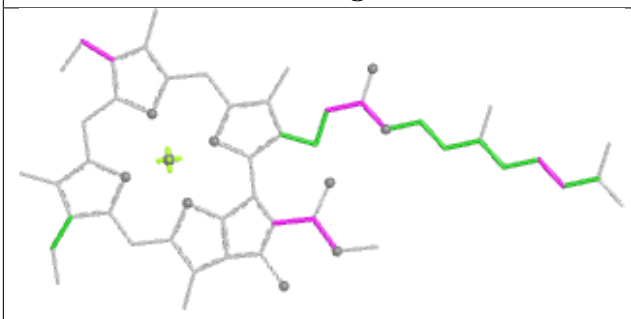
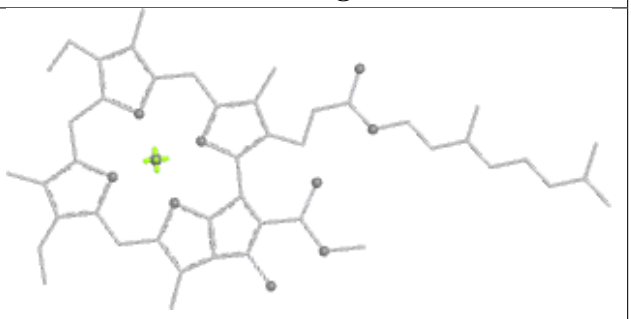


Torsions

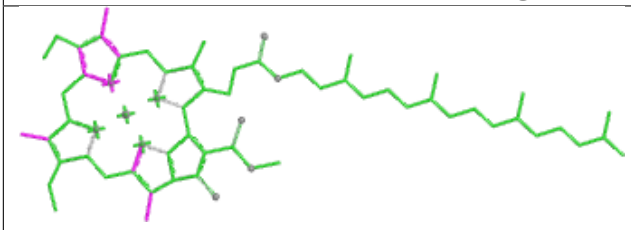


Rings

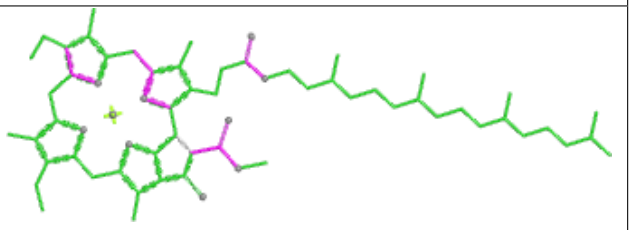
Ligand CLA e 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

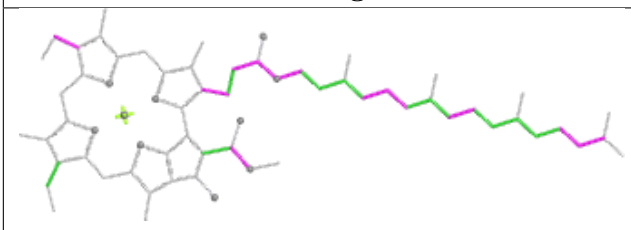
Ligand CLA H 1219



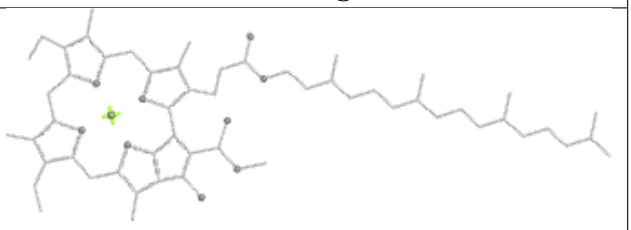
Bond lengths



Bond angles

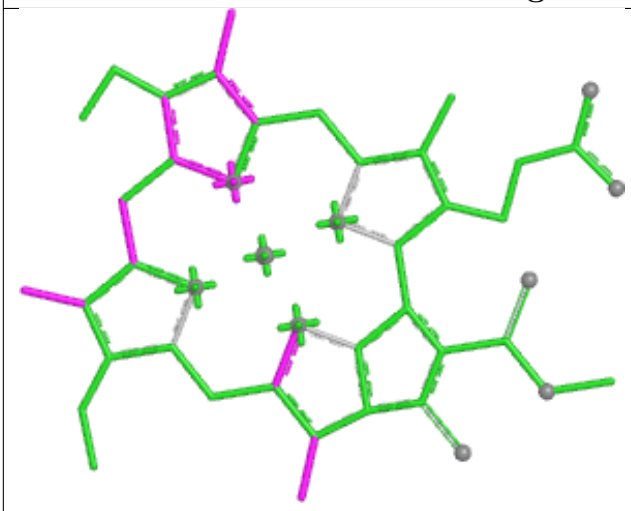


Torsions

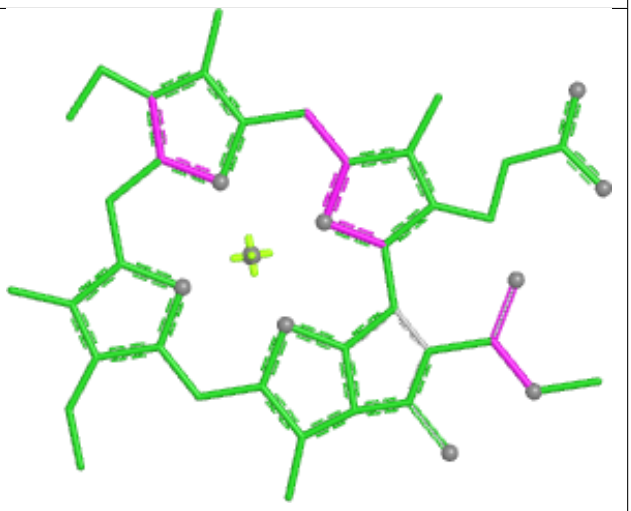


Rings

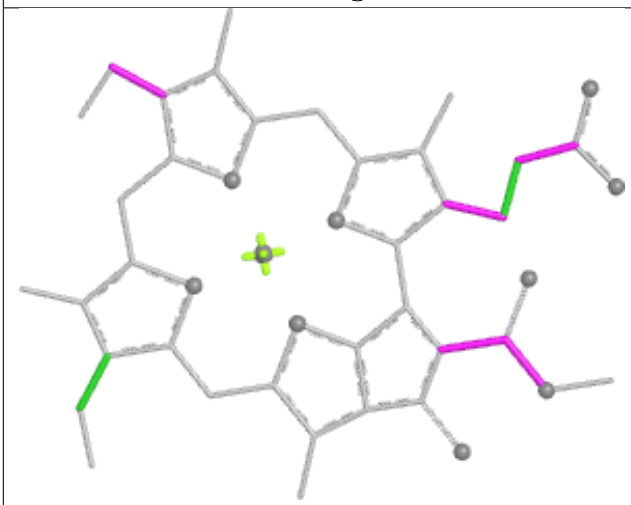
Ligand CLA d 517



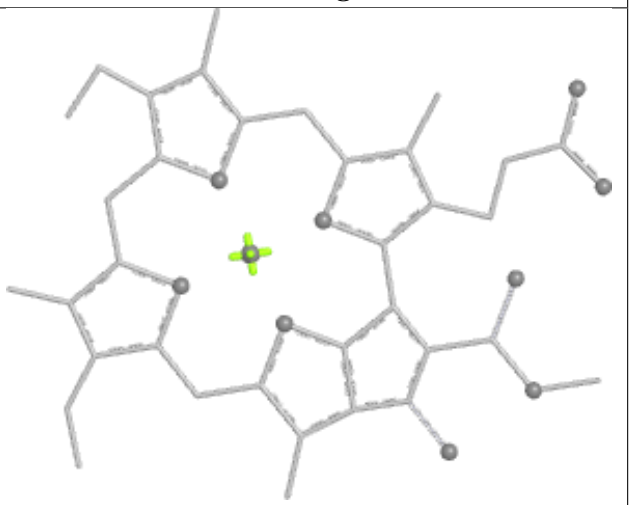
Bond lengths



Bond angles

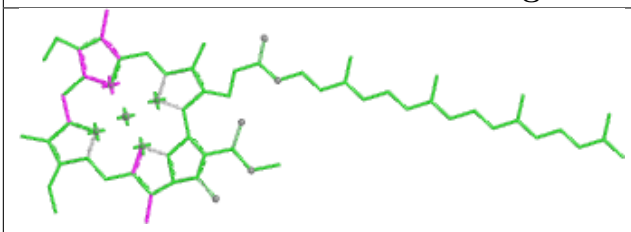


Torsions

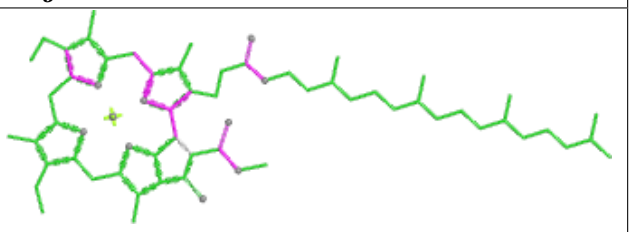


Rings

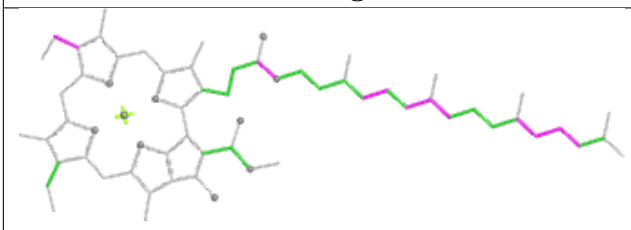
Ligand CLA j 1301



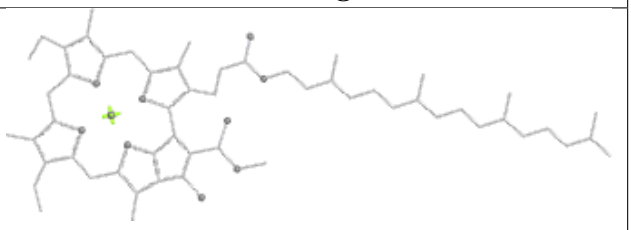
Bond lengths



Bond angles

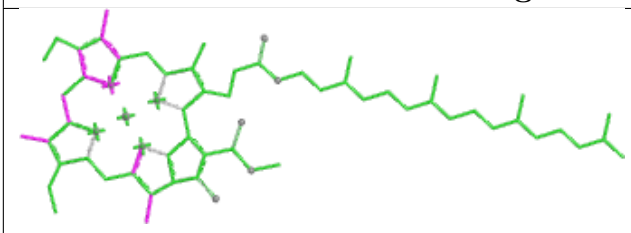


Torsions

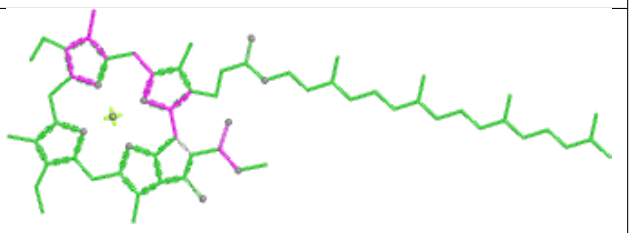


Rings

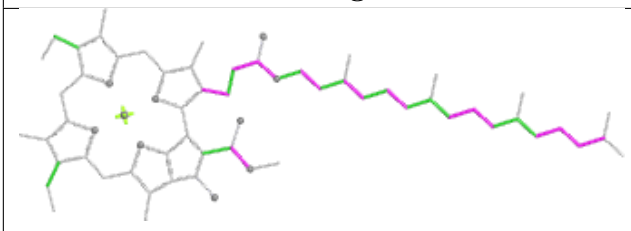
Ligand CLA A 1126



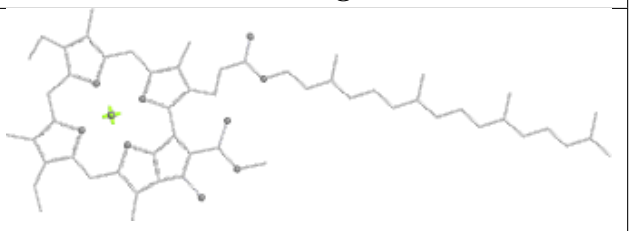
Bond lengths



Bond angles

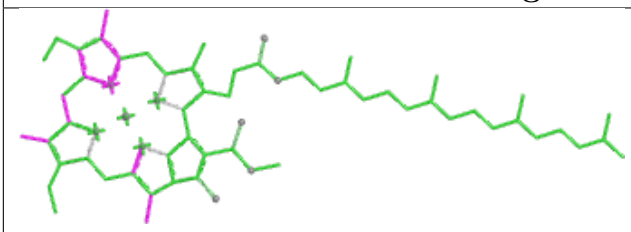


Torsions

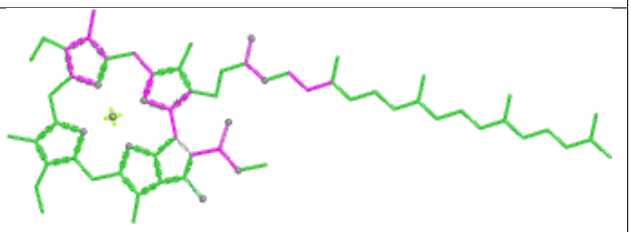


Rings

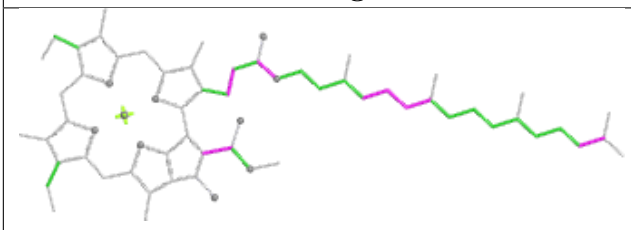
Ligand CLA f 1213



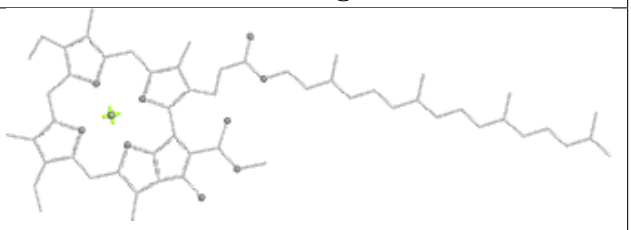
Bond lengths



Bond angles

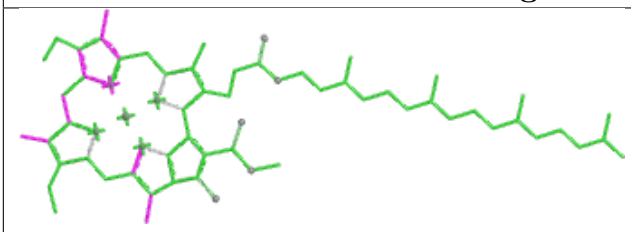


Torsions

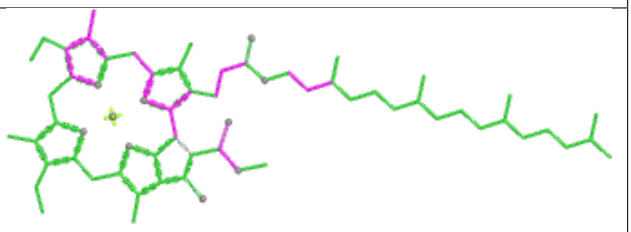


Rings

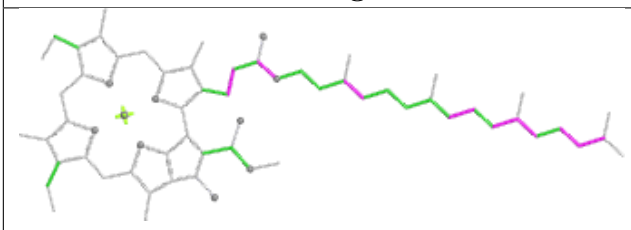
Ligand CLA e 1127



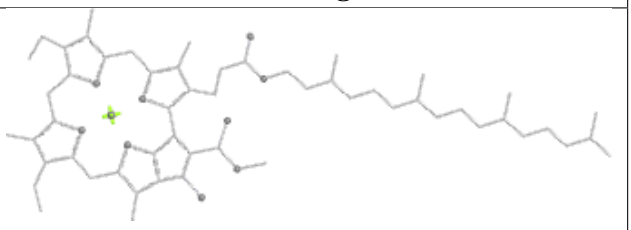
Bond lengths



Bond angles



Torsions

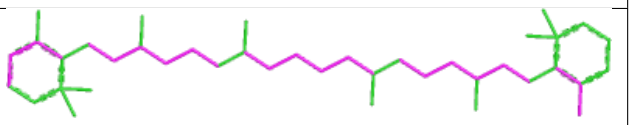


Rings

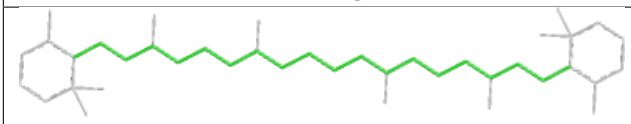
Ligand BCR e 4003



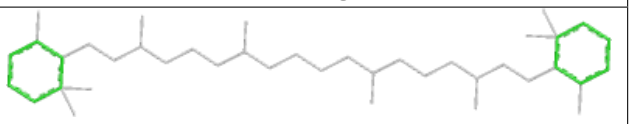
Bond lengths



Bond angles

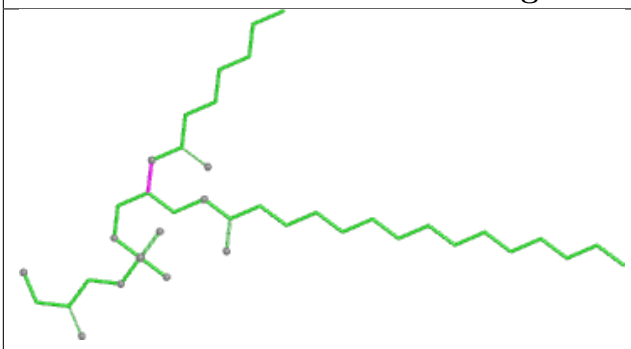


Torsions

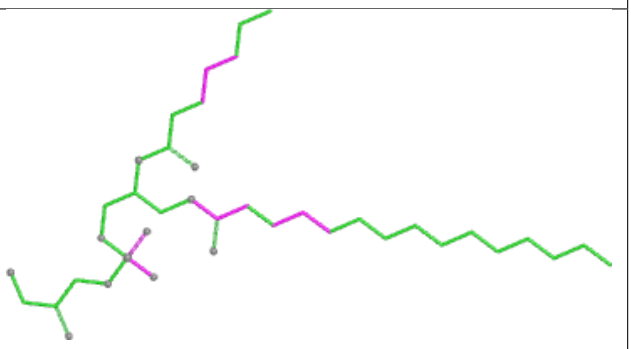


Rings

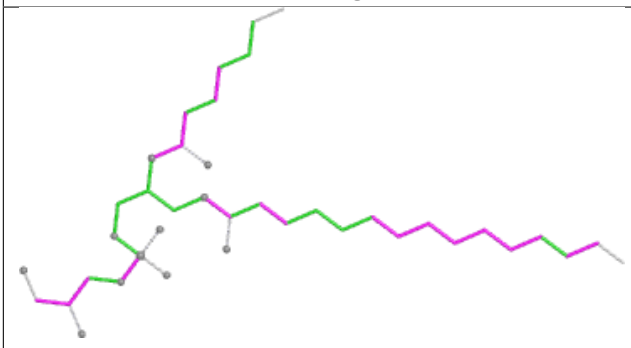
Ligand LHG f 1842



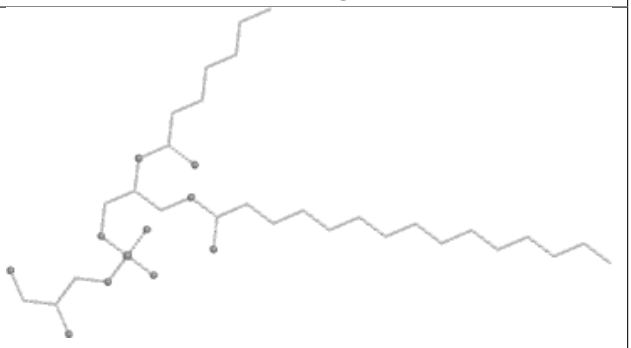
Bond lengths



Bond angles

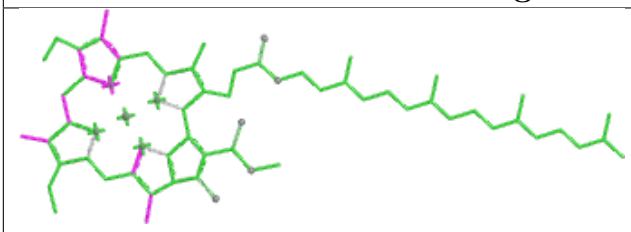


Torsions

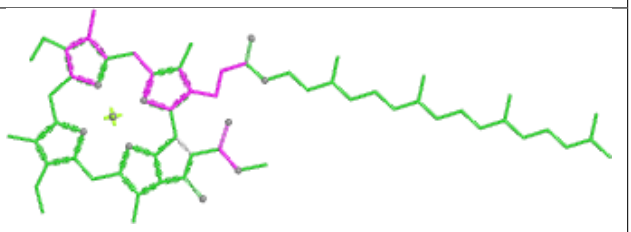


Rings

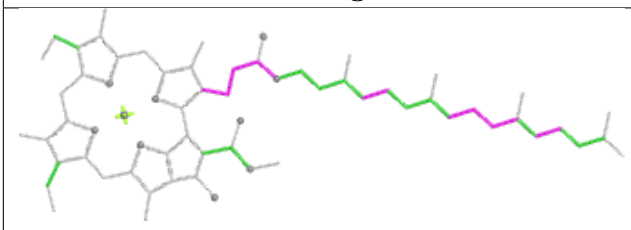
Ligand CLA G 1125



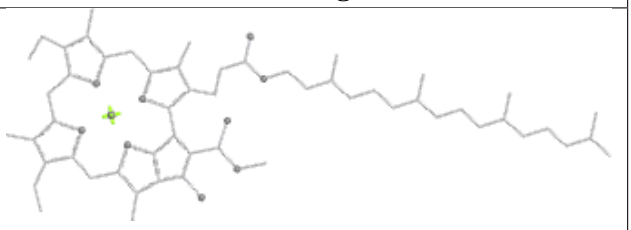
Bond lengths



Bond angles

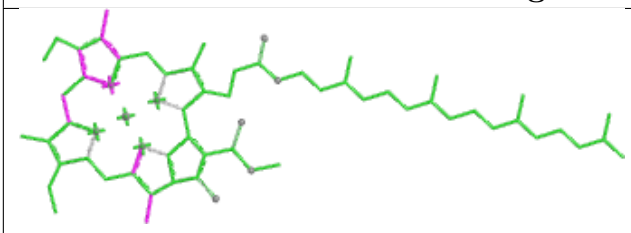


Torsions

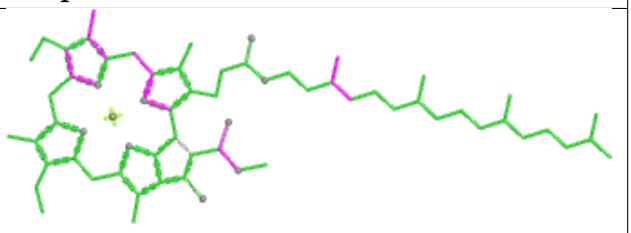


Rings

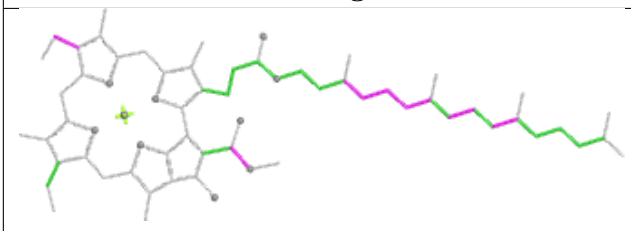
Ligand CLA q 510



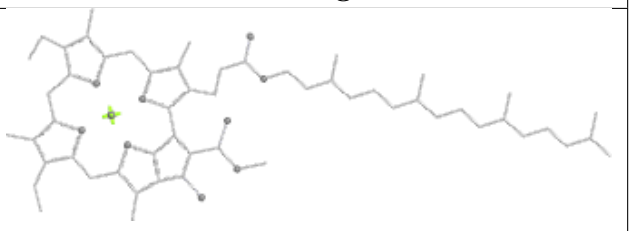
Bond lengths



Bond angles

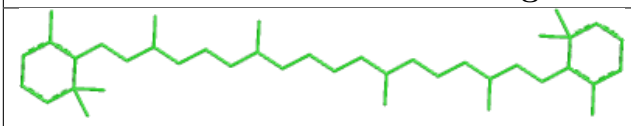


Torsions

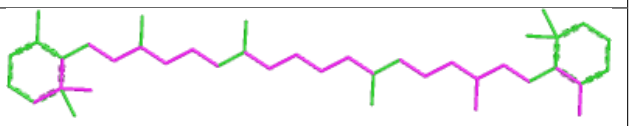


Rings

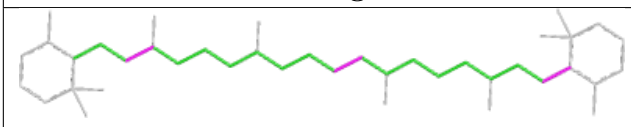
Ligand BCR l 4015



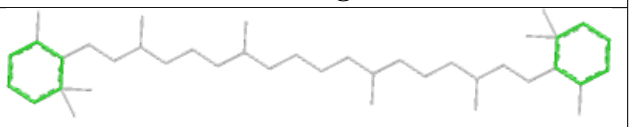
Bond lengths



Bond angles

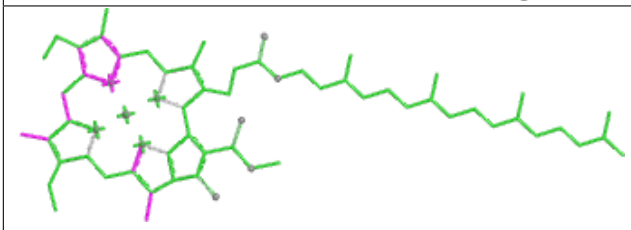


Torsions

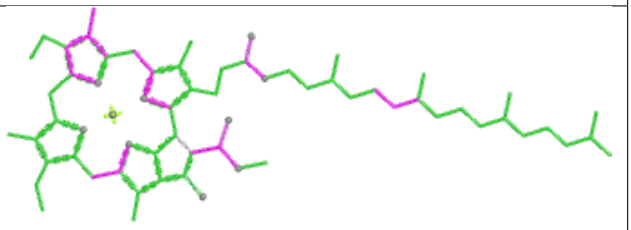


Rings

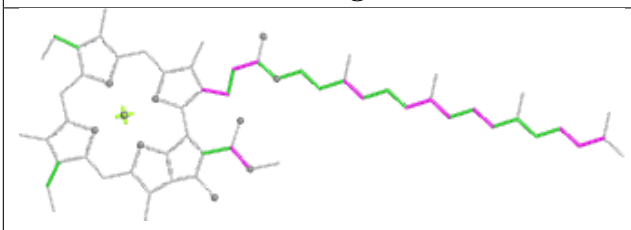
Ligand CLA B 1229



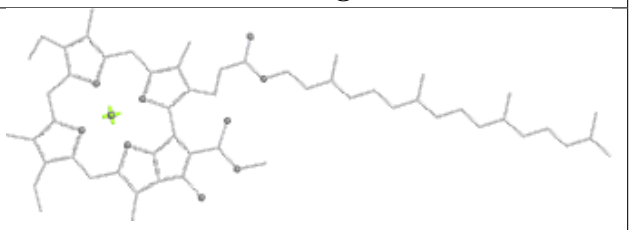
Bond lengths



Bond angles

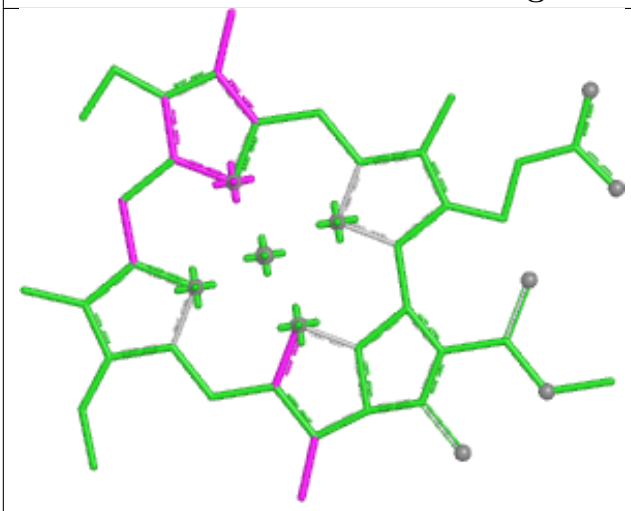


Torsions

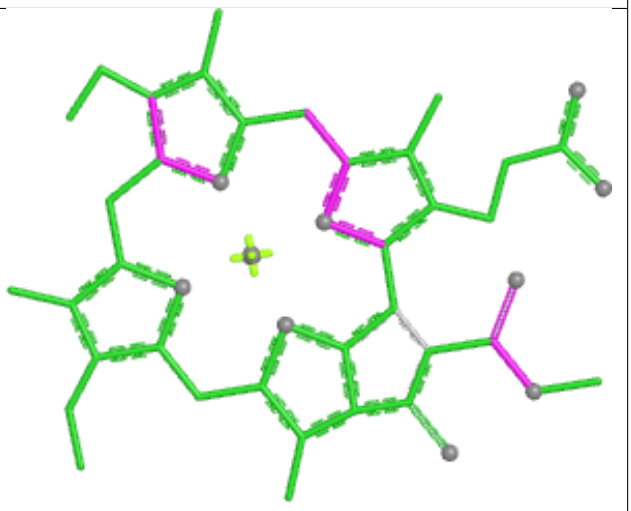


Rings

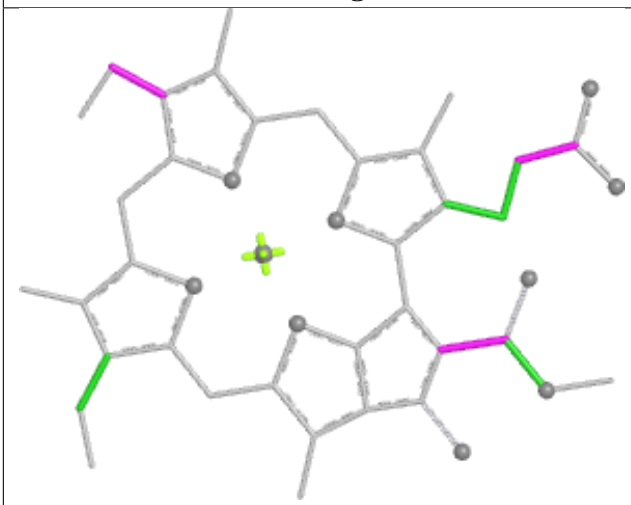
Ligand CLA b 512



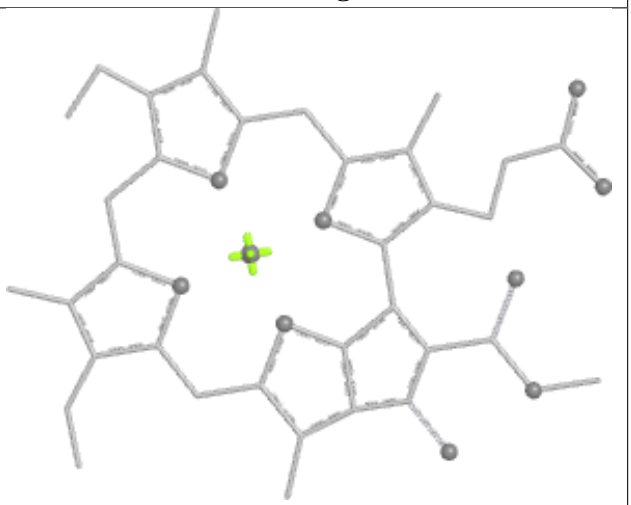
Bond lengths



Bond angles

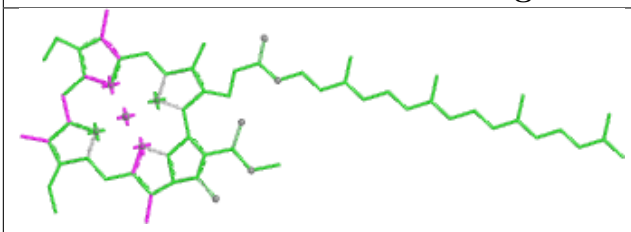


Torsions

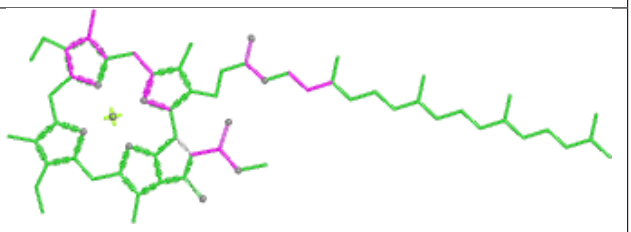


Rings

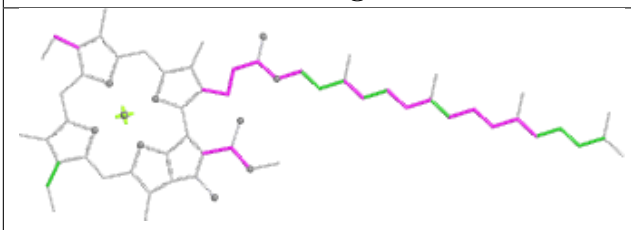
Ligand CLA A 1106



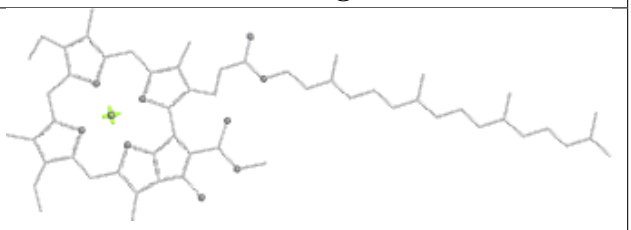
Bond lengths



Bond angles

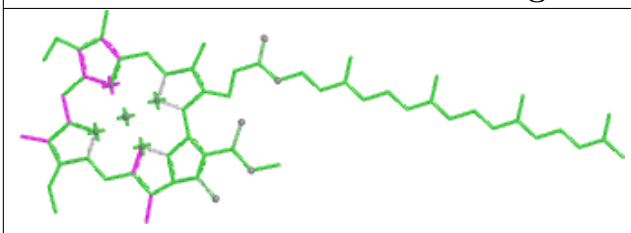


Torsions

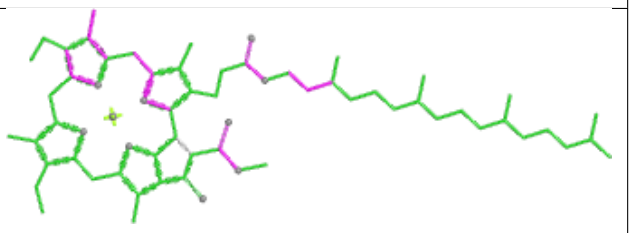


Rings

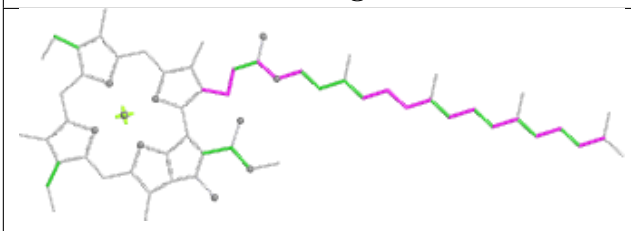
Ligand CLA 6 505



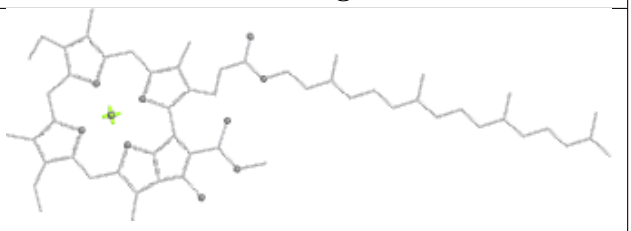
Bond lengths



Bond angles

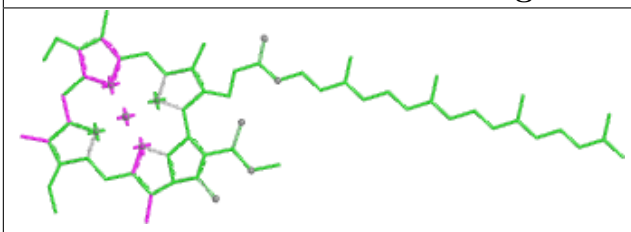


Torsions

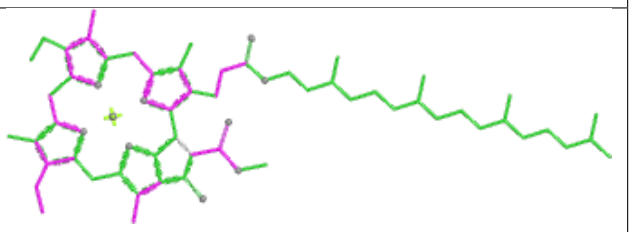


Rings

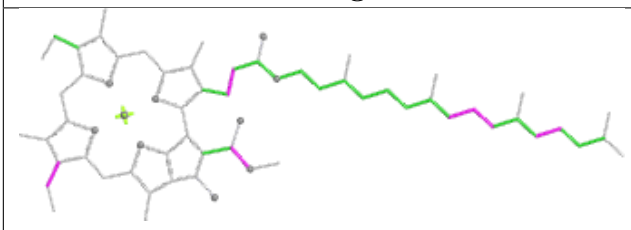
Ligand CLA B 1023



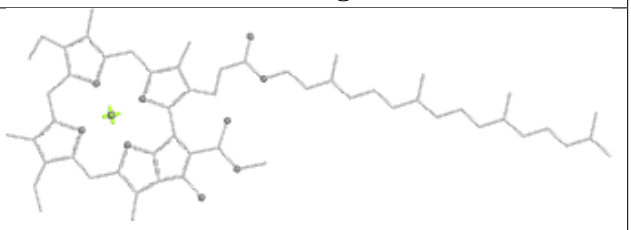
Bond lengths



Bond angles

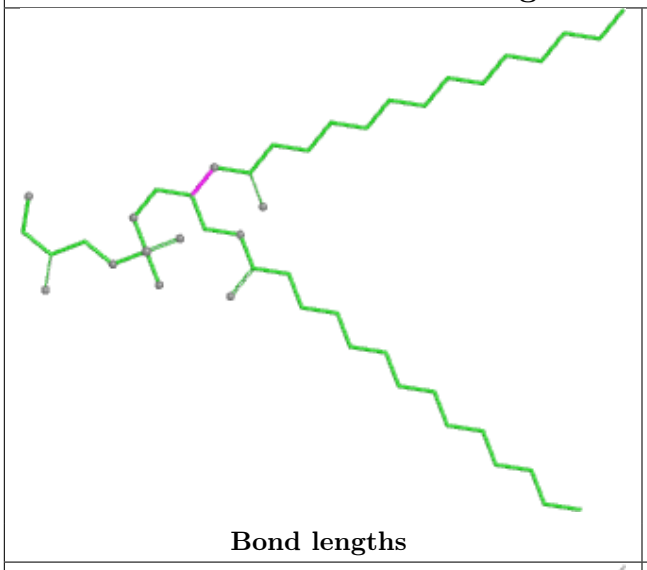


Torsions

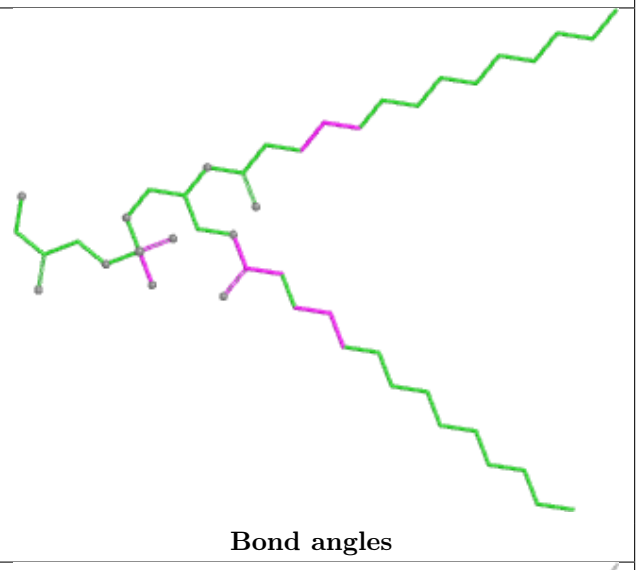


Rings

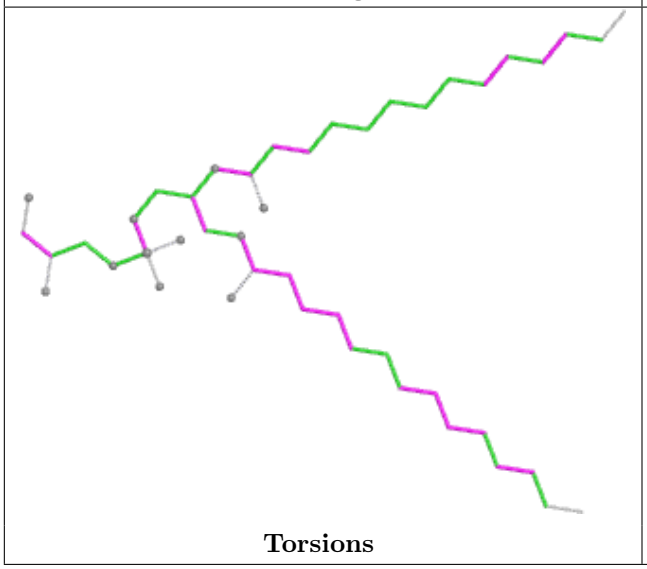
Ligand LHG e 5006



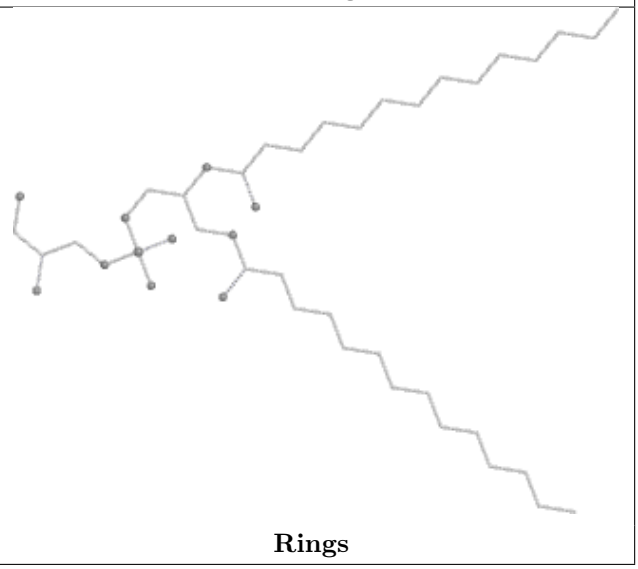
Bond lengths



Bond angles

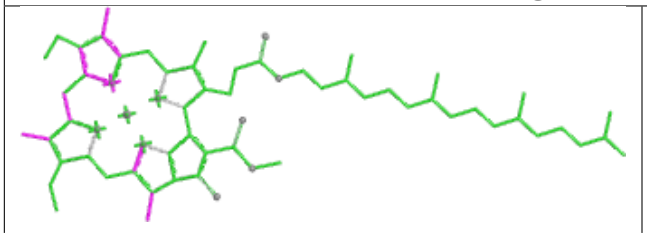


Torsions

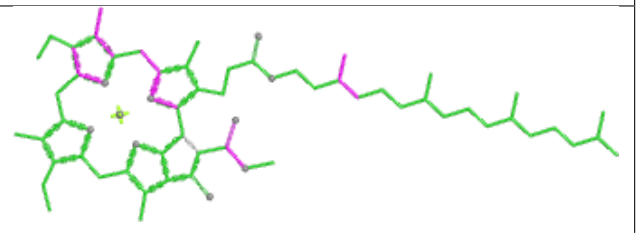


Rings

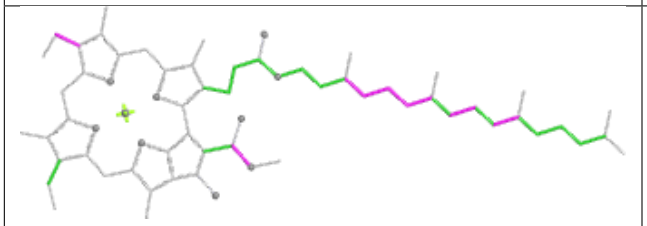
Ligand CLA 1 510



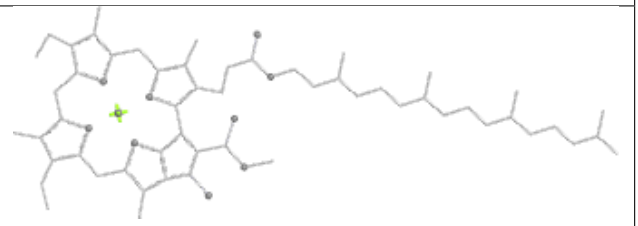
Bond lengths



Bond angles

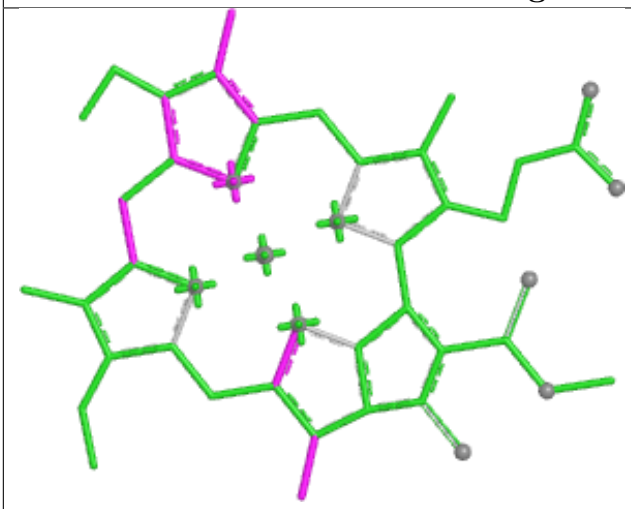


Torsions

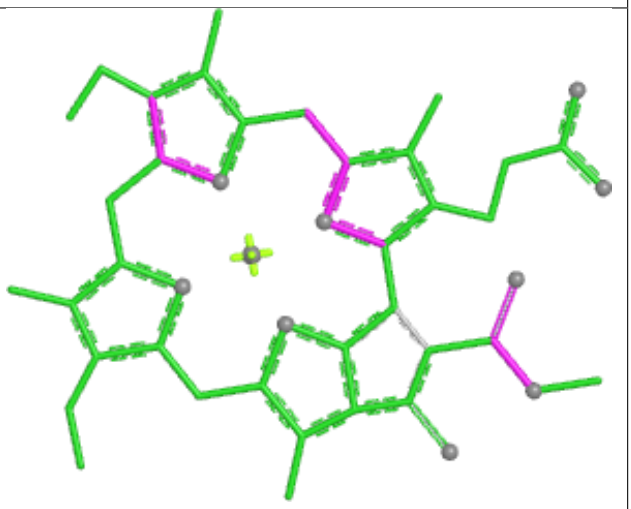


Rings

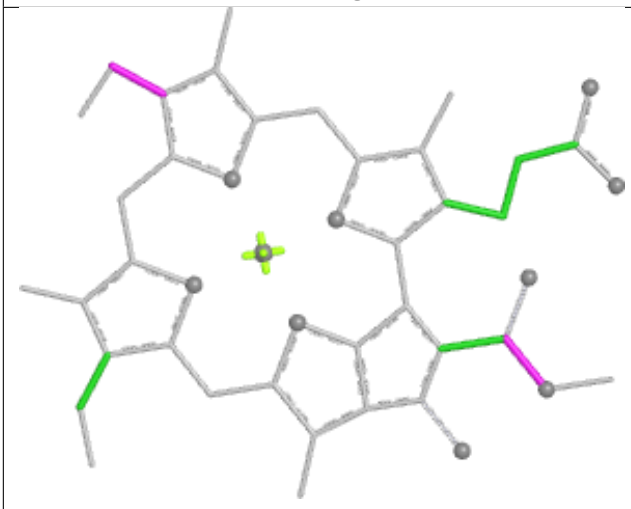
Ligand CLA 5 504



Bond lengths



Bond angles

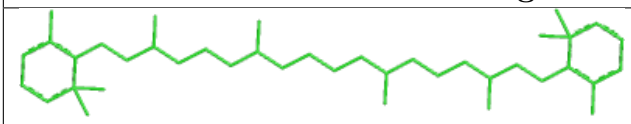


Torsions

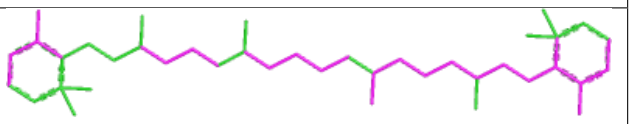


Rings

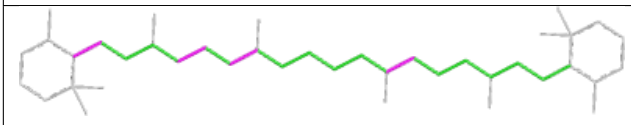
Ligand BCR o 4021



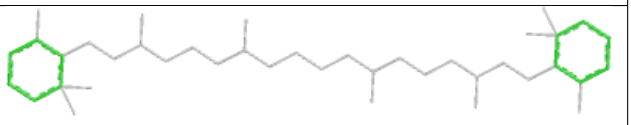
Bond lengths



Bond angles

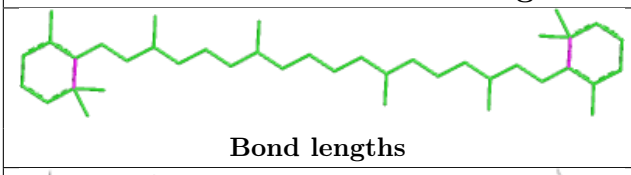


Torsions

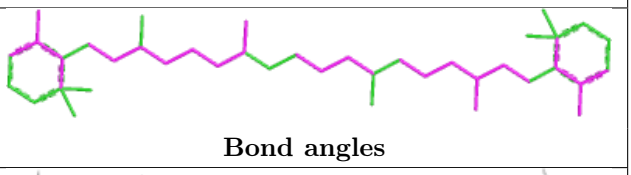


Rings

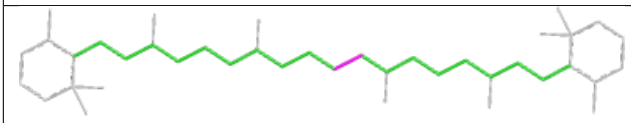
Ligand BCR S 4018



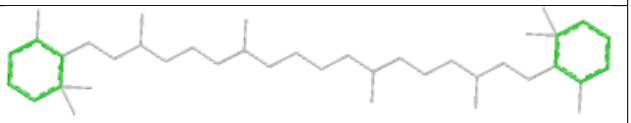
Bond lengths



Bond angles



Torsions

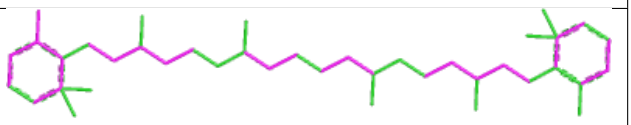


Rings

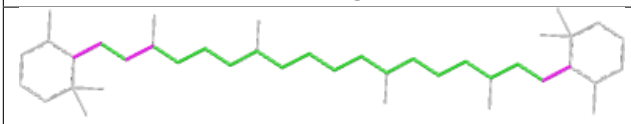
Ligand BCR Y 521



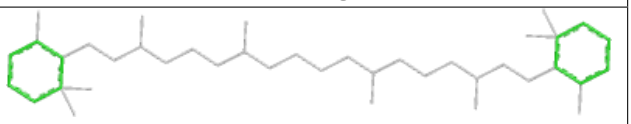
Bond lengths



Bond angles

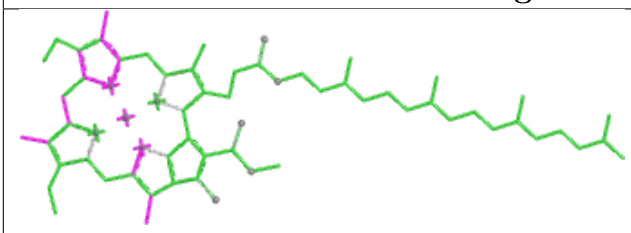


Torsions

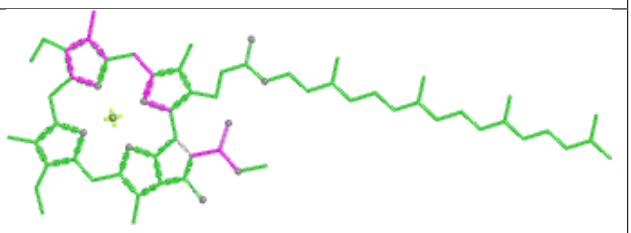


Rings

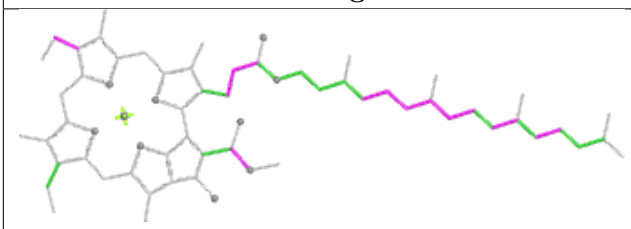
Ligand CLA H 1203



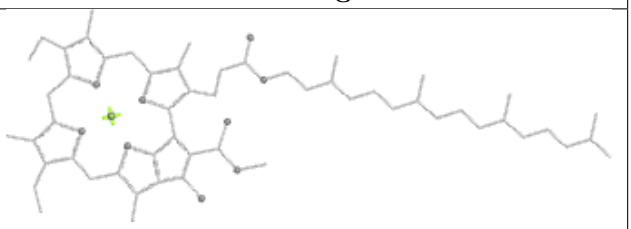
Bond lengths



Bond angles

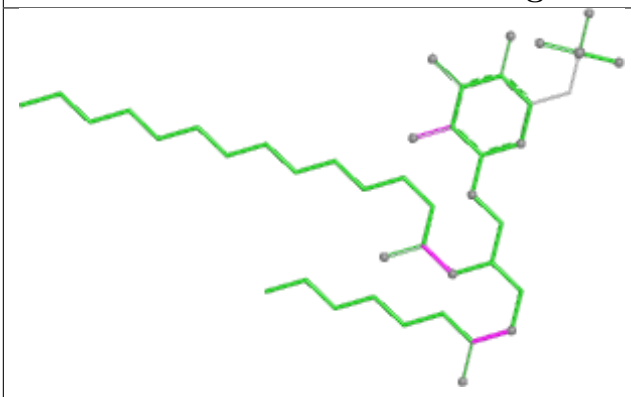


Torsions

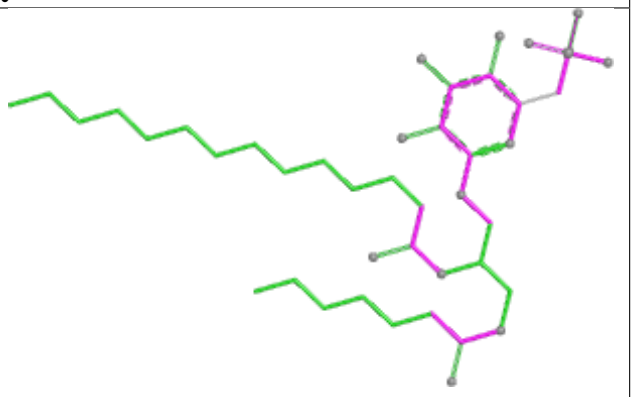


Rings

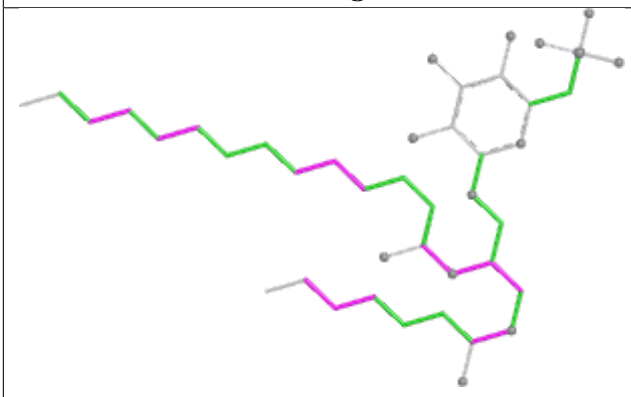
Ligand SQD Z 822



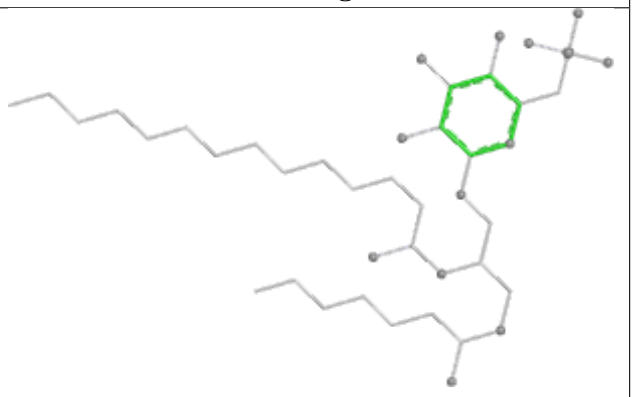
Bond lengths



Bond angles

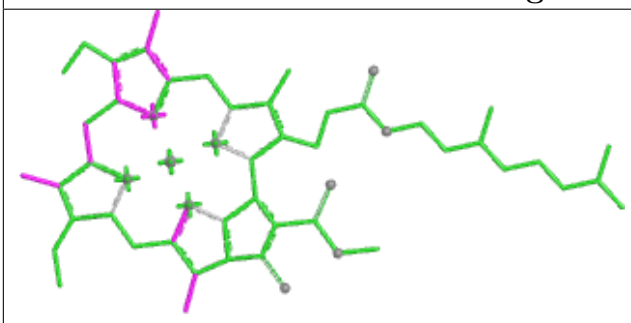


Torsions

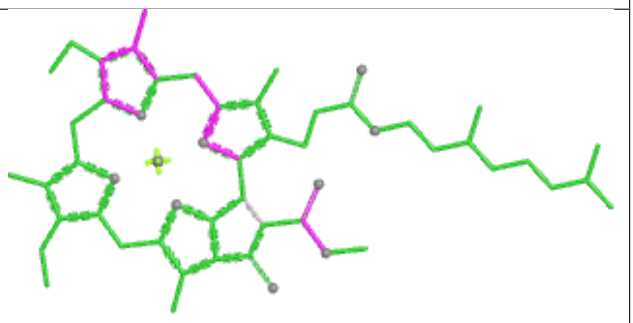


Rings

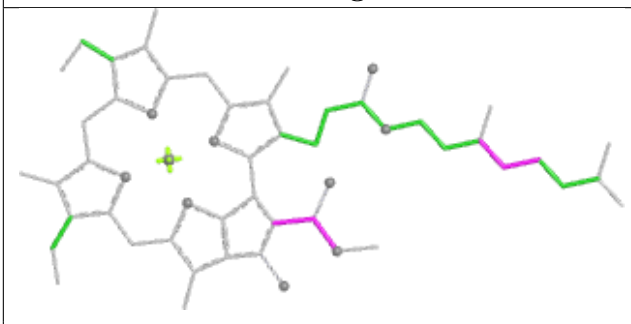
Ligand CLA Z 506



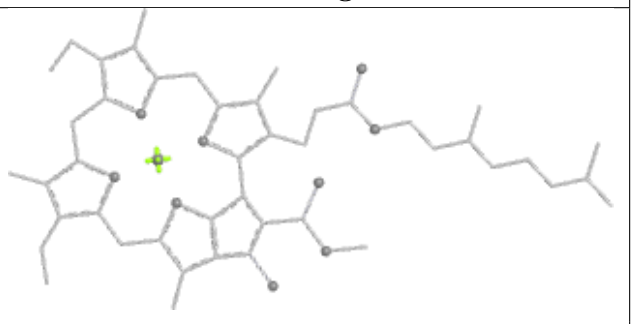
Bond lengths



Bond angles

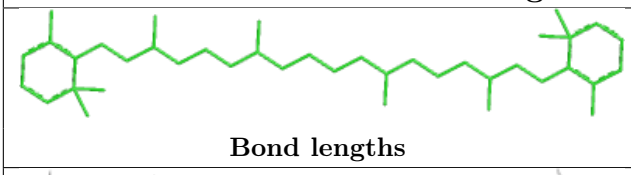


Torsions

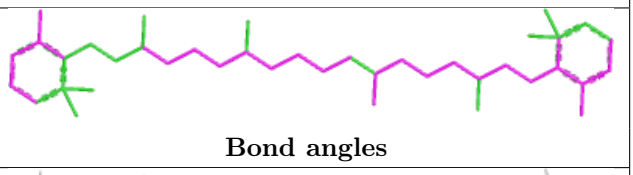


Rings

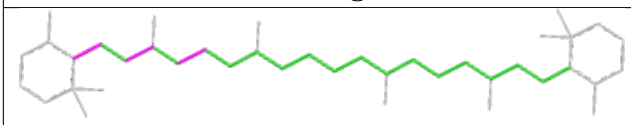
Ligand BCR v 522



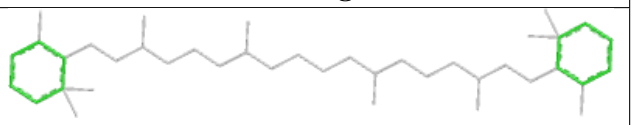
Bond lengths



Bond angles

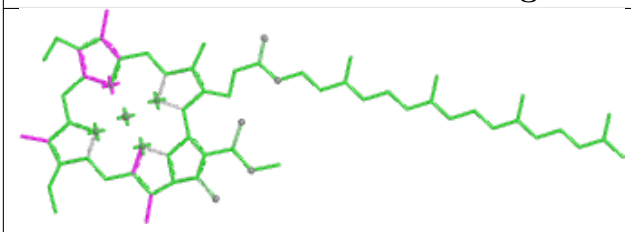


Torsions

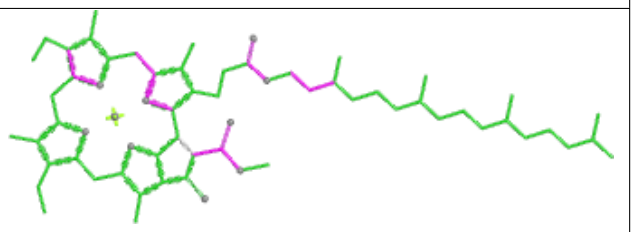


Rings

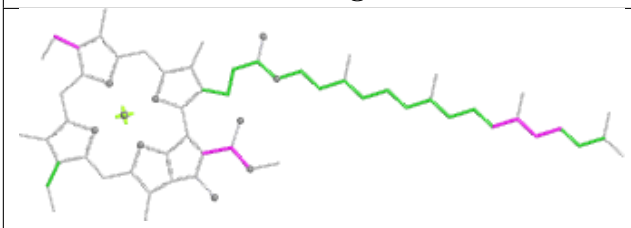
Ligand CLA e 1131



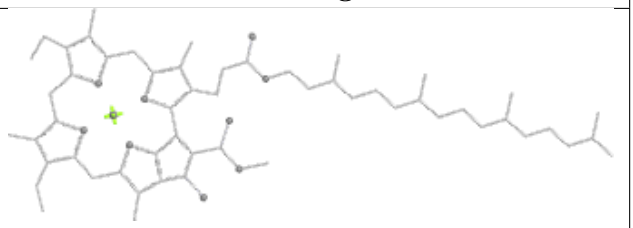
Bond lengths



Bond angles

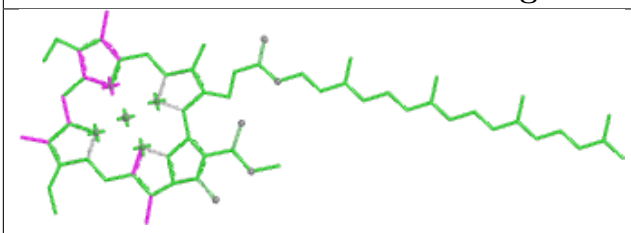


Torsions

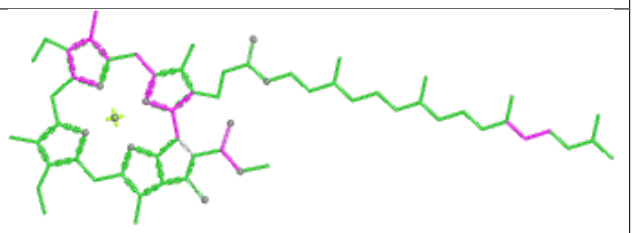


Rings

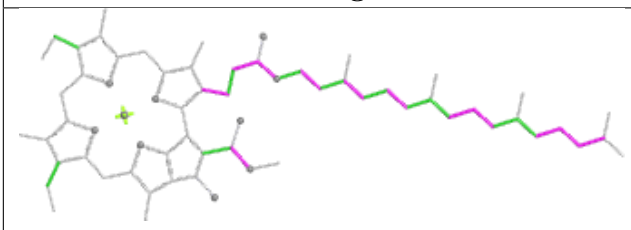
Ligand CLA e 1126



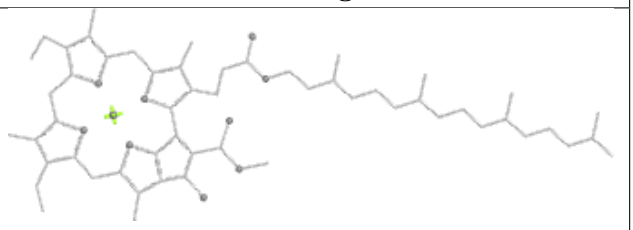
Bond lengths



Bond angles

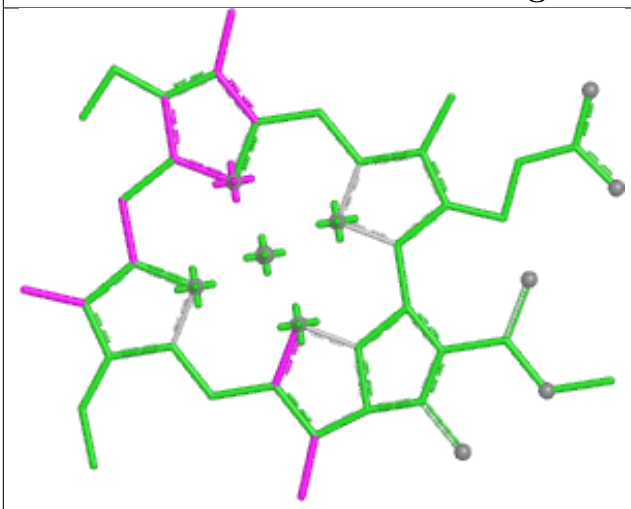


Torsions

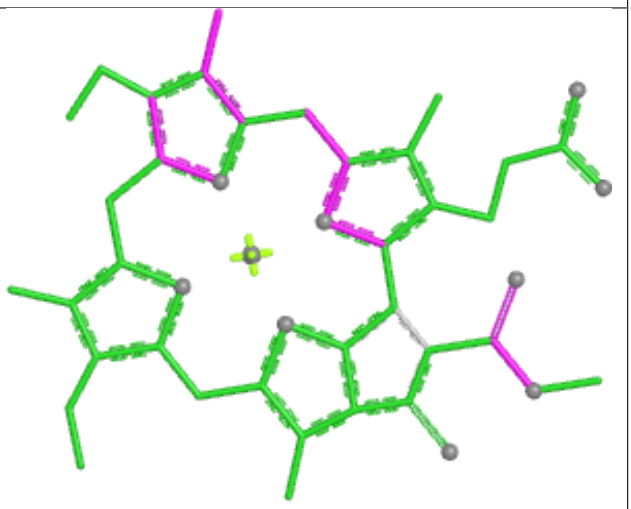


Rings

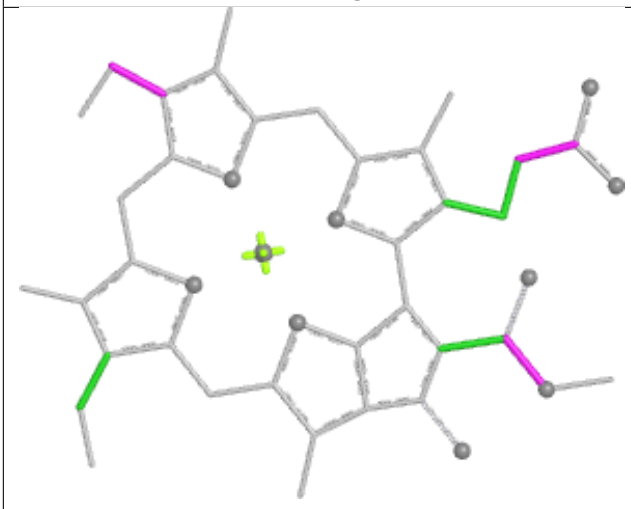
Ligand CLA 5 508



Bond lengths



Bond angles

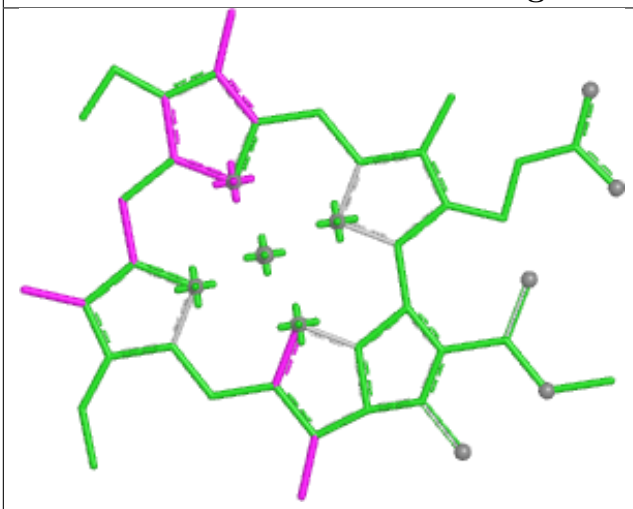


Torsions

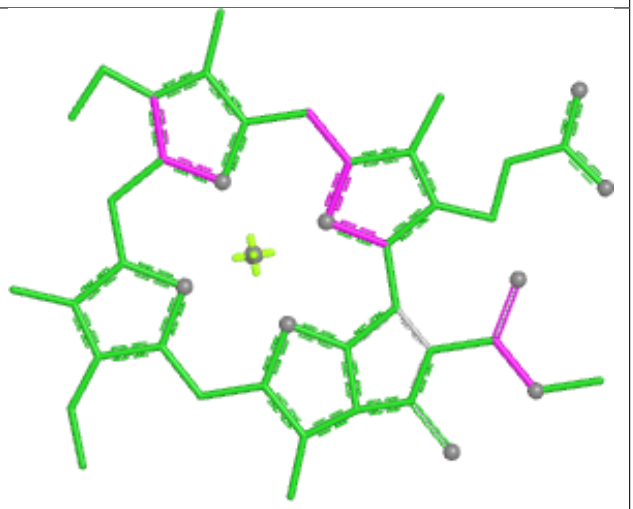


Rings

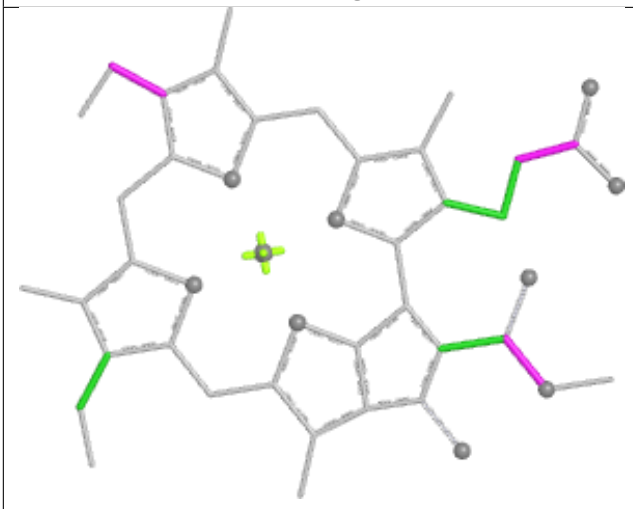
Ligand CLA d 511



Bond lengths



Bond angles

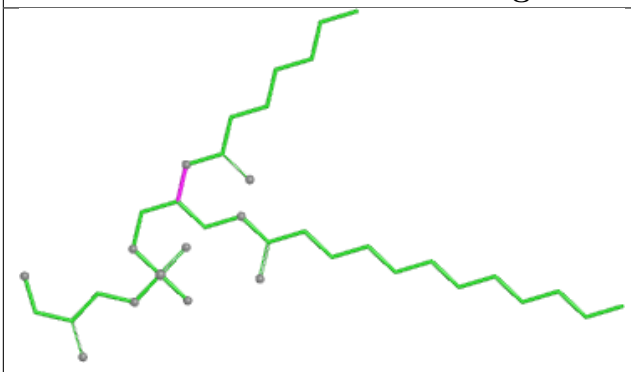


Torsions

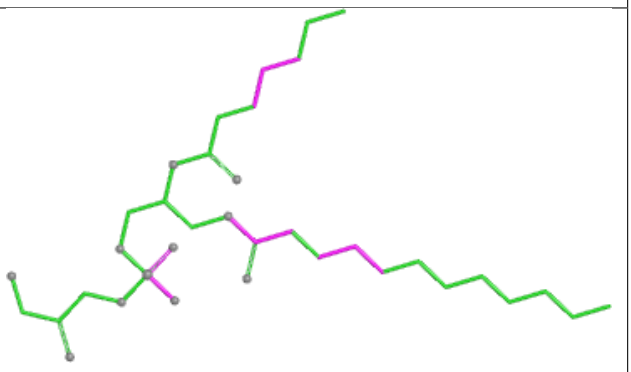


Rings

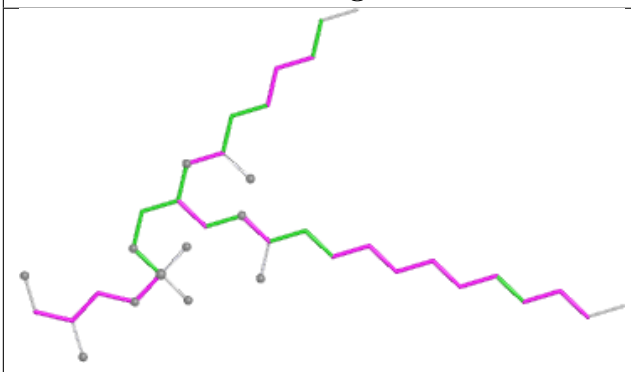
Ligand LHG G 5004



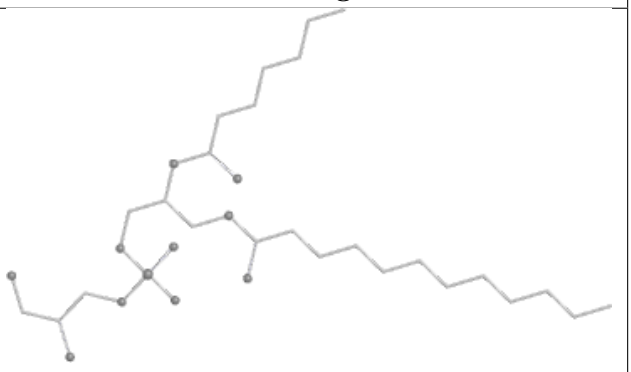
Bond lengths



Bond angles

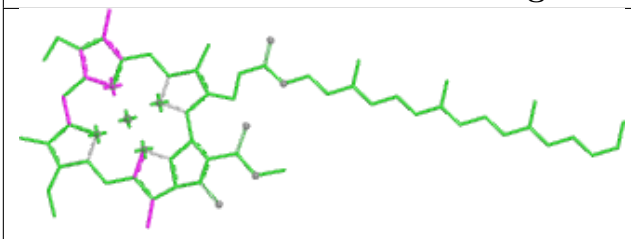


Torsions

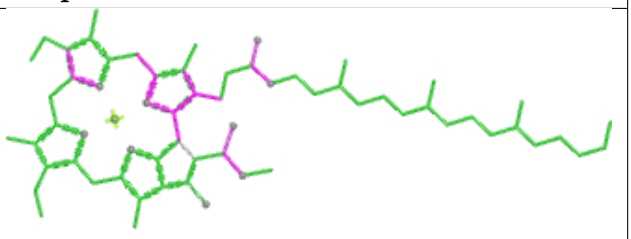


Rings

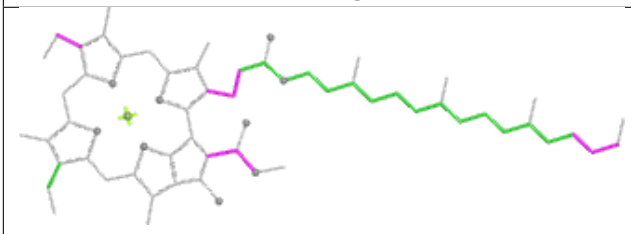
Ligand CLA q 503



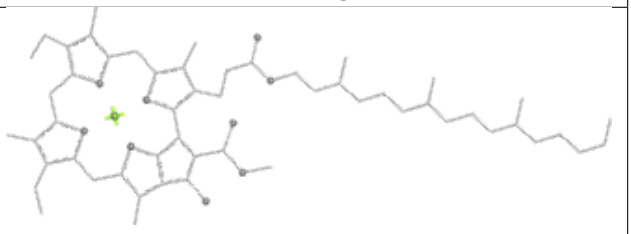
Bond lengths



Bond angles

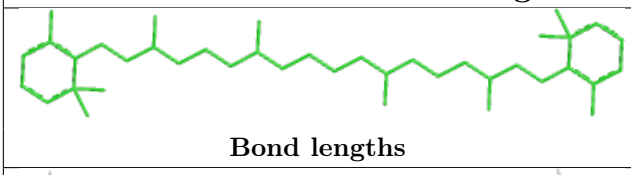


Torsions

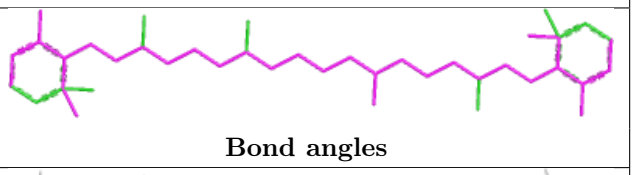


Rings

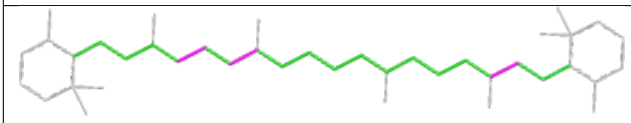
Ligand BCR B 4010



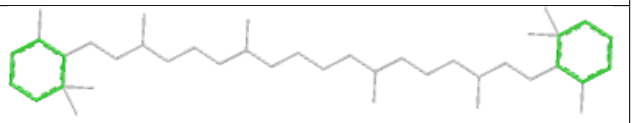
Bond lengths



Bond angles



Torsions

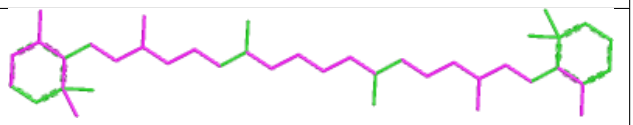


Rings

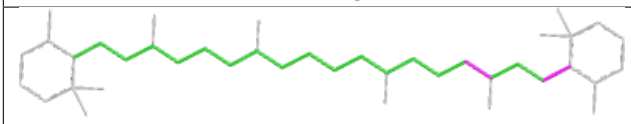
Ligand BCR n 4020



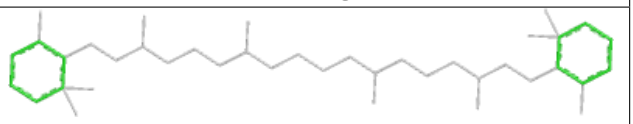
Bond lengths



Bond angles

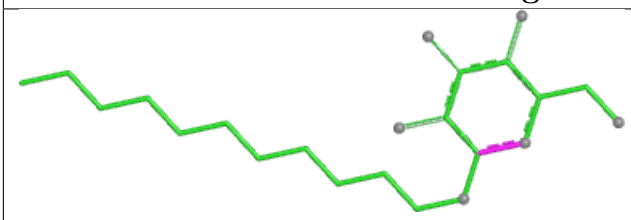


Torsions

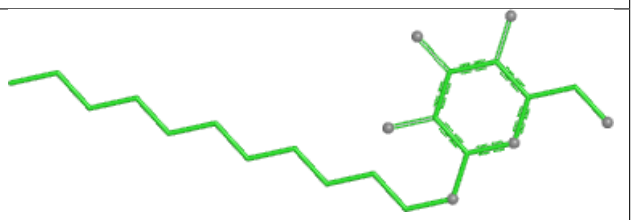


Rings

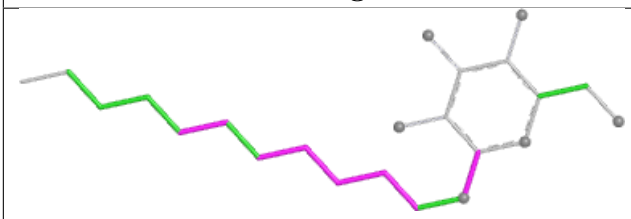
Ligand LMU Z 901



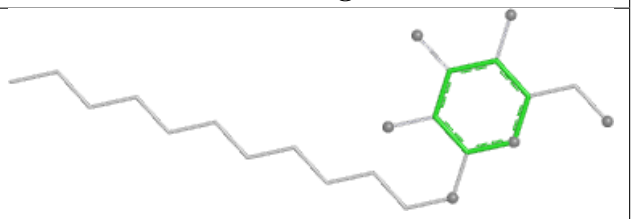
Bond lengths



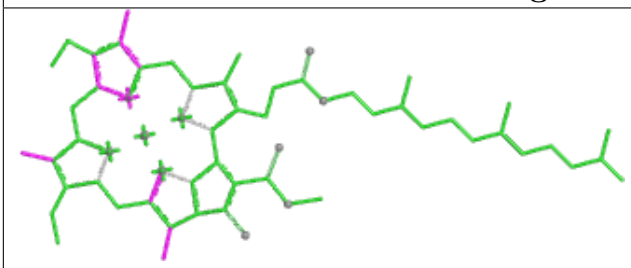
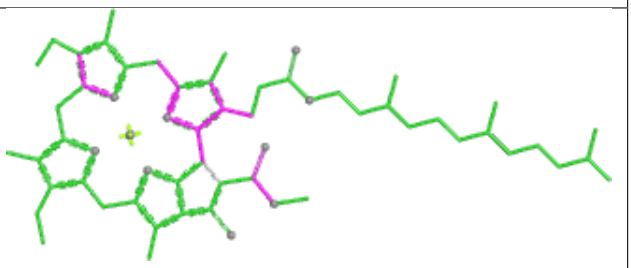
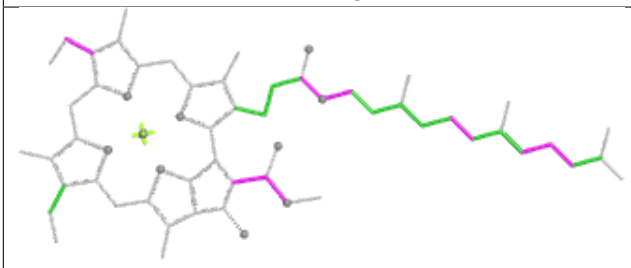
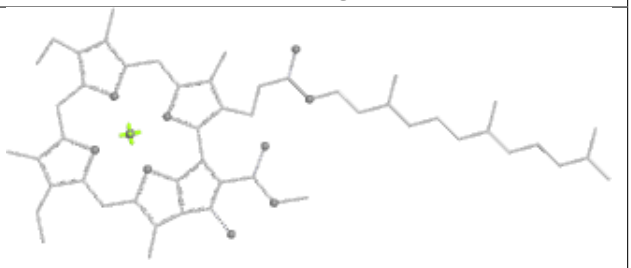
Bond angles

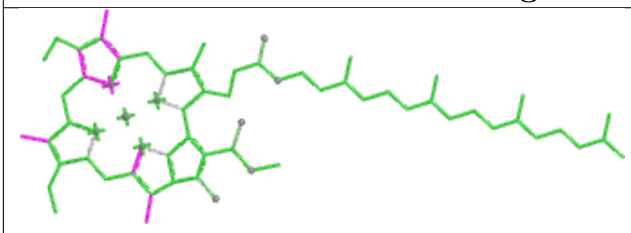
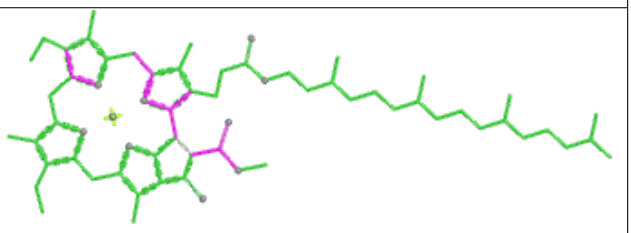
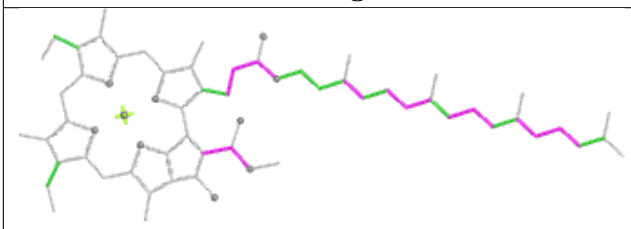
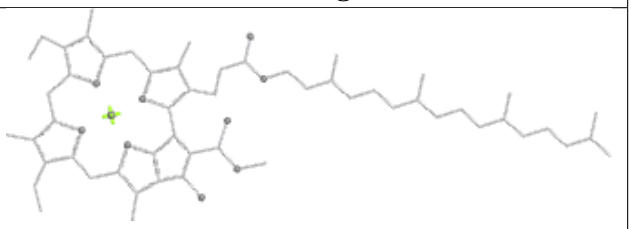


Torsions

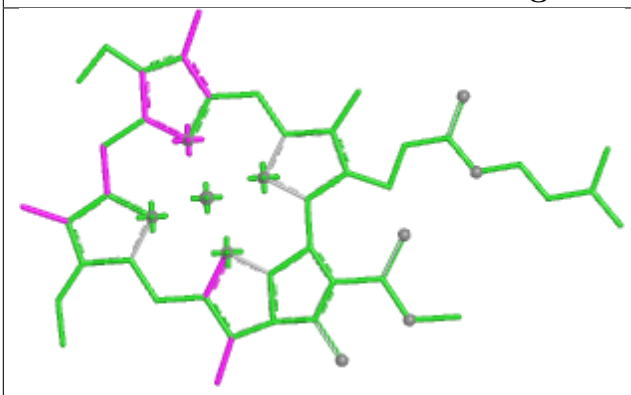


Rings

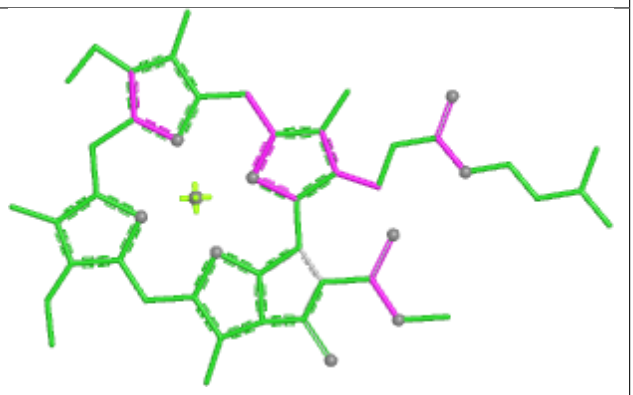
Ligand CLA r 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 1137	
	
Bond lengths	Bond angles
	
Torsions	Rings

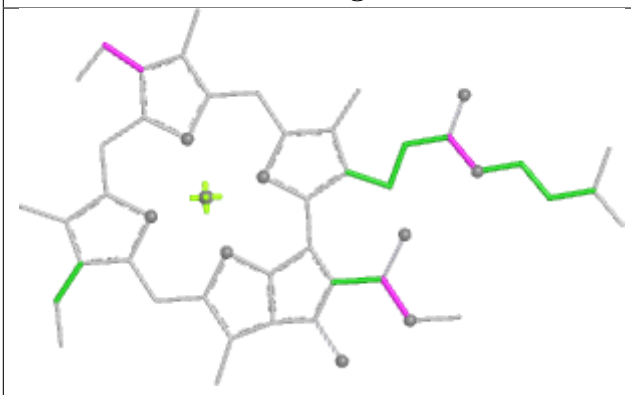
Ligand CLA r 504



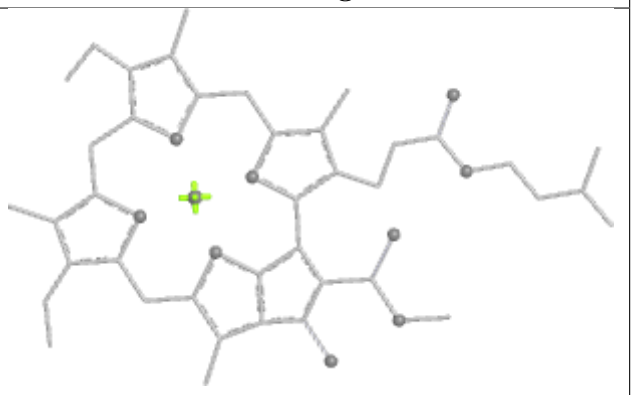
Bond lengths



Bond angles

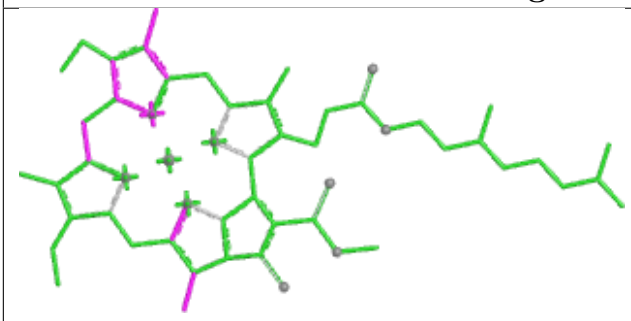


Torsions

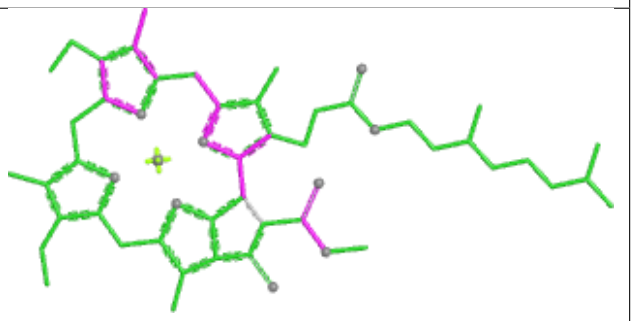


Rings

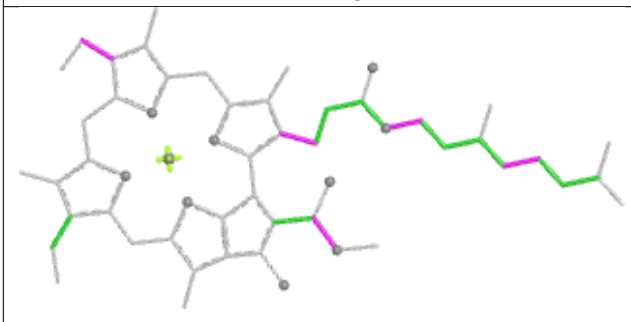
Ligand CLA 5 511



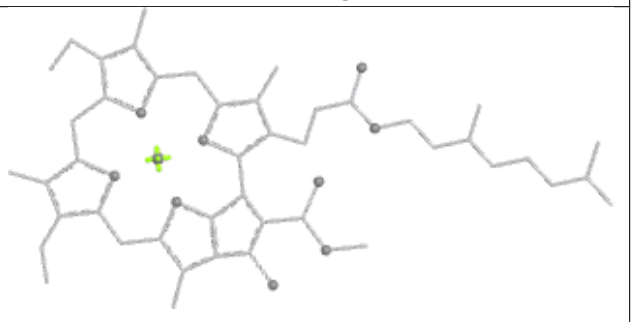
Bond lengths



Bond angles

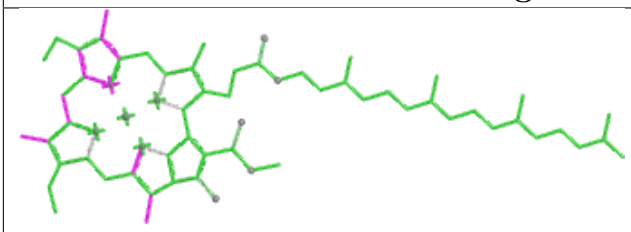


Torsions

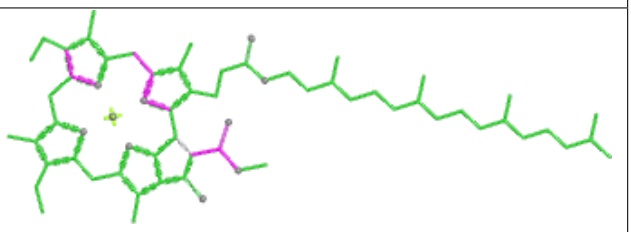


Rings

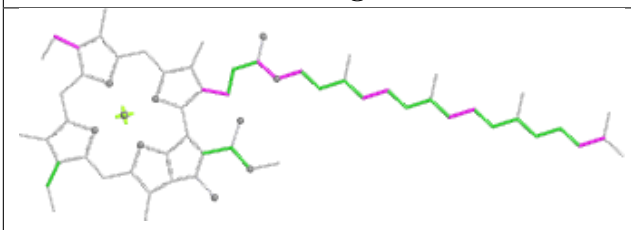
Ligand CLA V 1502



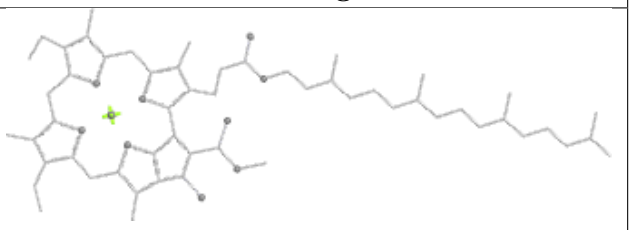
Bond lengths



Bond angles

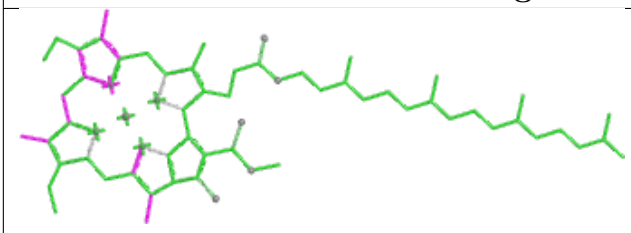


Torsions

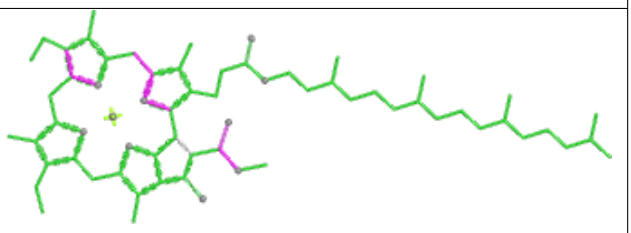


Rings

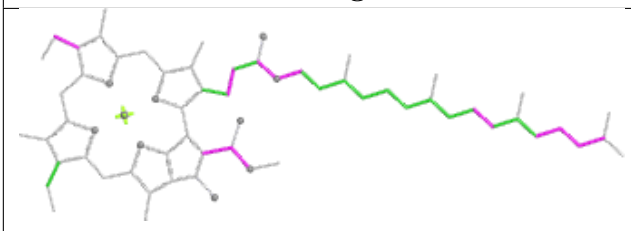
Ligand CLA H 1207



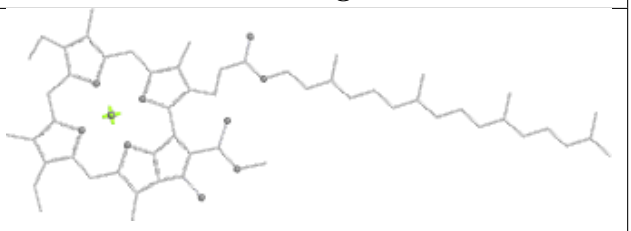
Bond lengths



Bond angles

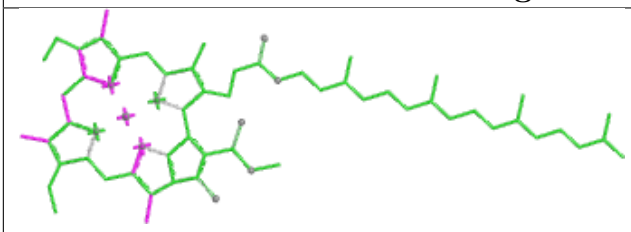


Torsions

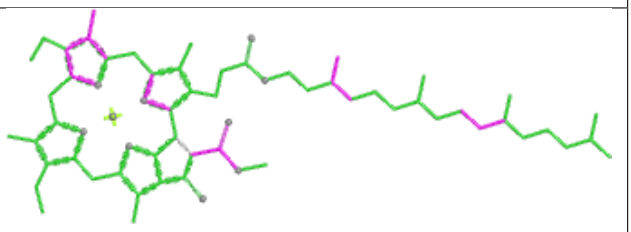


Rings

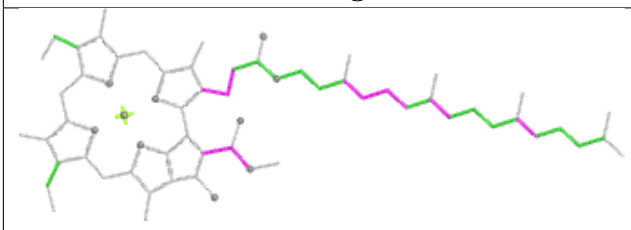
Ligand CLA H 1012



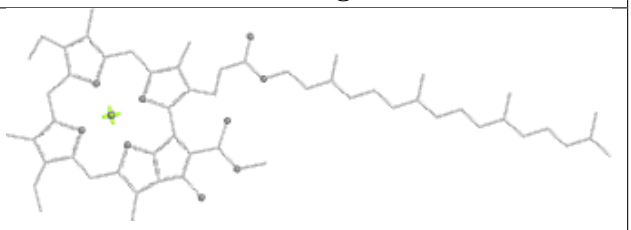
Bond lengths



Bond angles

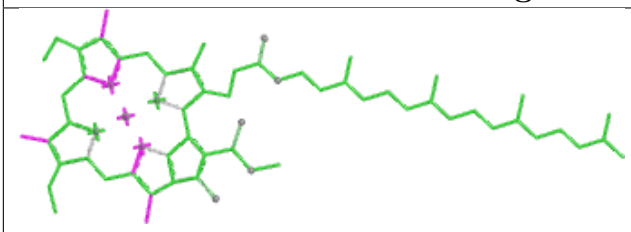


Torsions

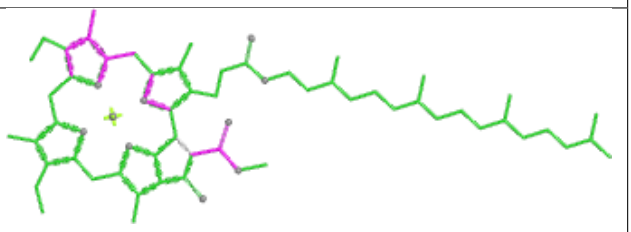


Rings

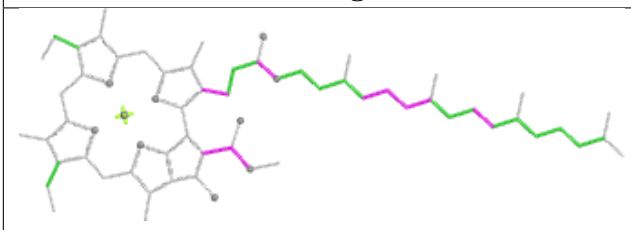
Ligand CLA A 1128



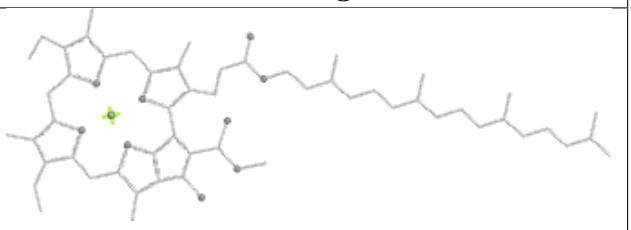
Bond lengths



Bond angles

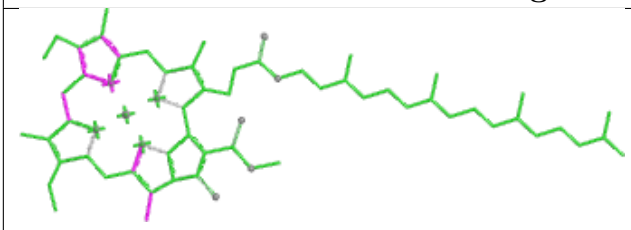


Torsions

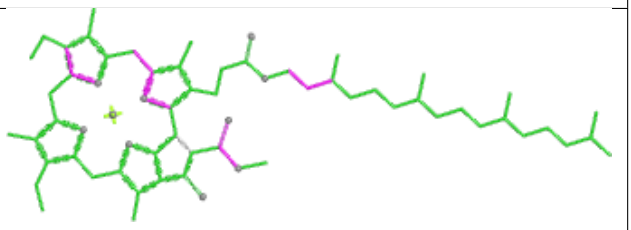


Rings

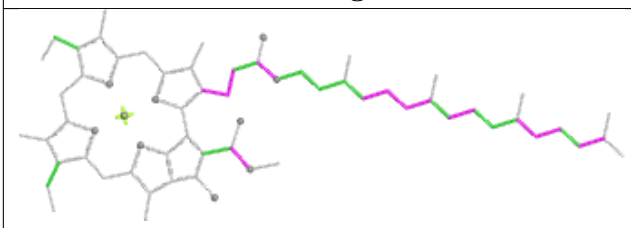
Ligand CLA r 505



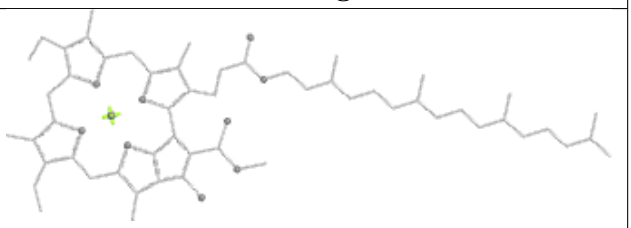
Bond lengths



Bond angles

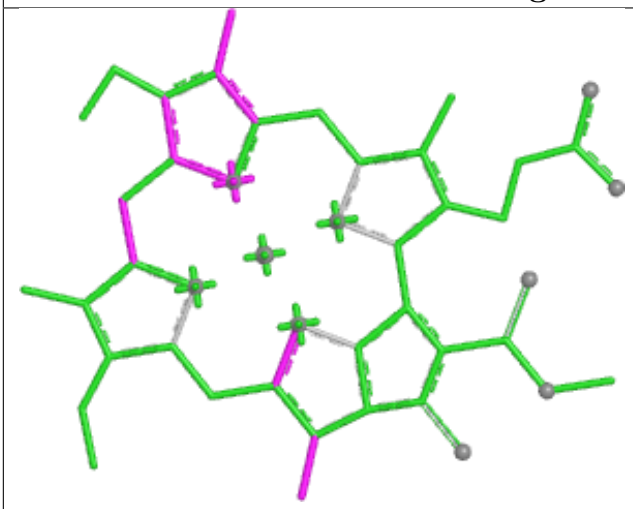


Torsions

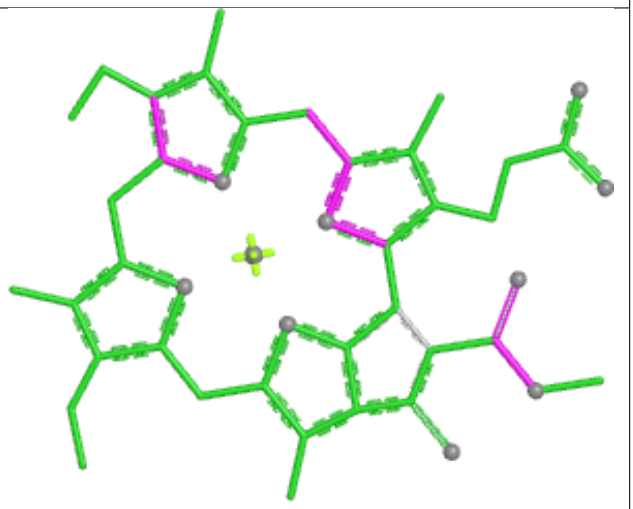


Rings

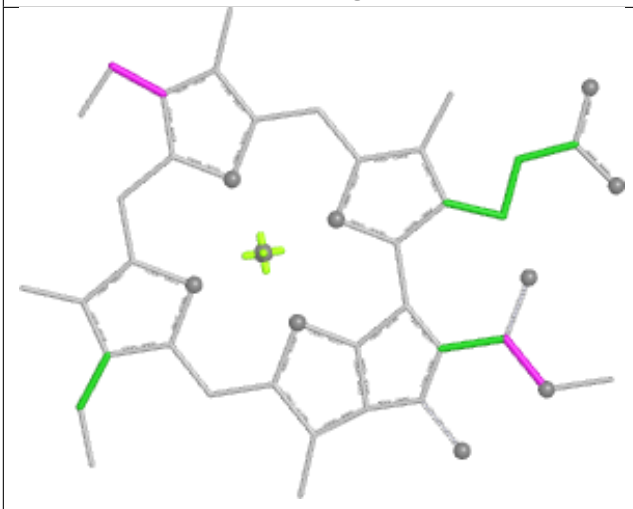
Ligand CLA c 504



Bond lengths



Bond angles

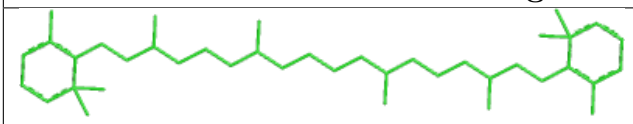


Torsions

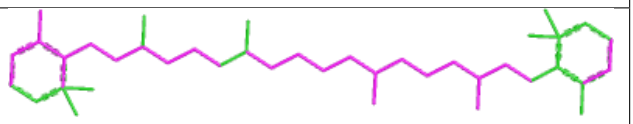


Rings

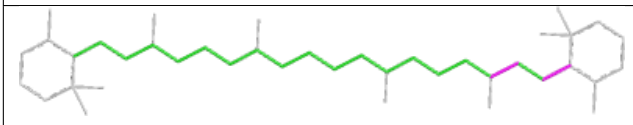
Ligand BCR a 523



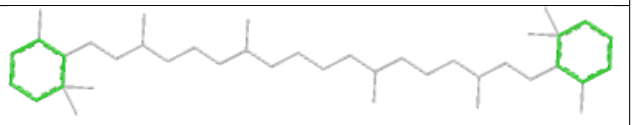
Bond lengths



Bond angles

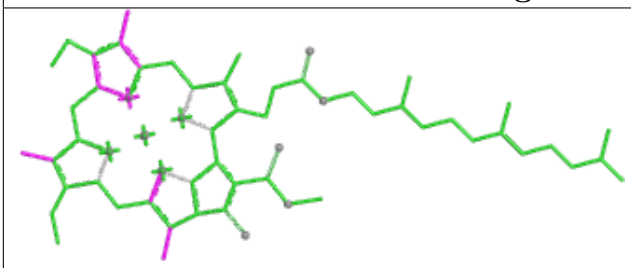


Torsions

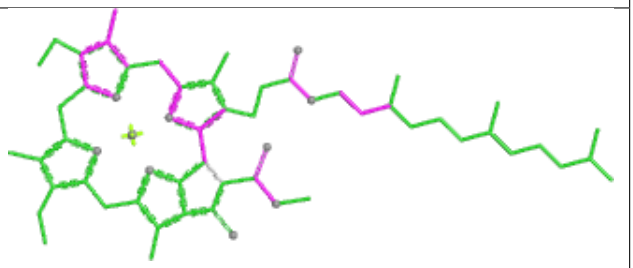


Rings

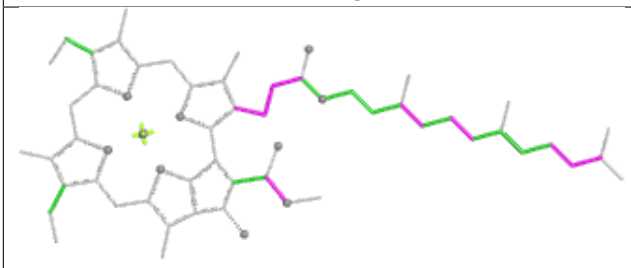
Ligand CLA H 1224



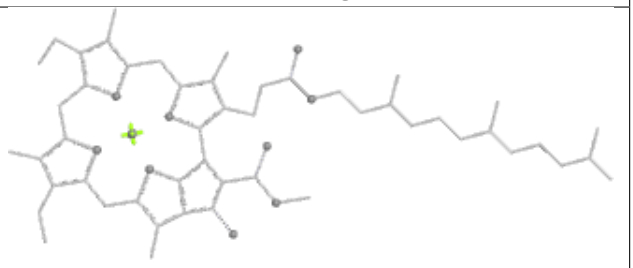
Bond lengths



Bond angles

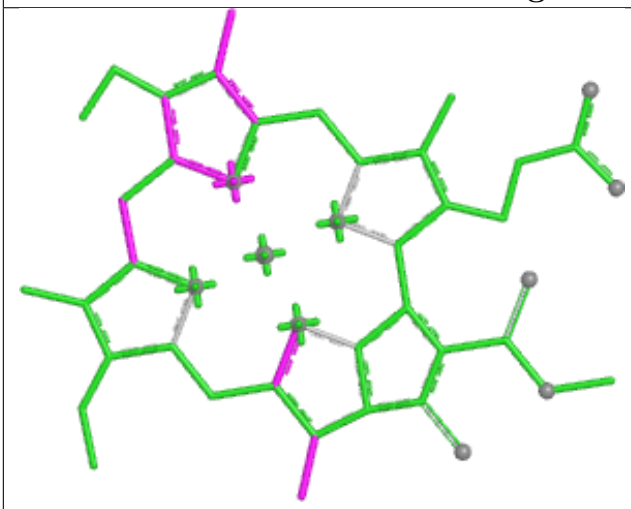


Torsions

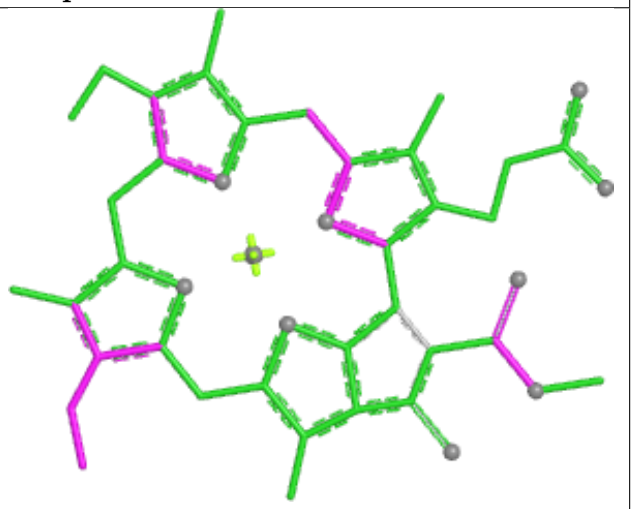


Rings

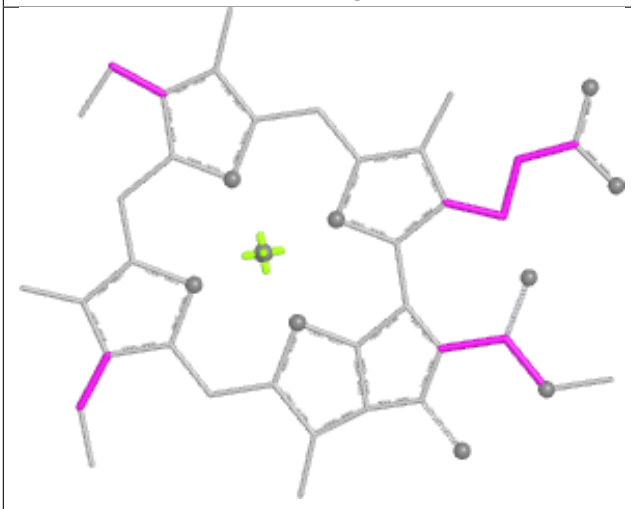
Ligand CLA q 516



Bond lengths



Bond angles

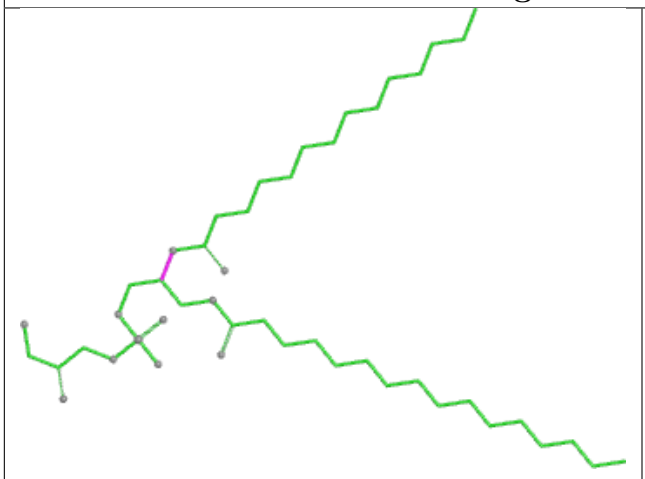


Torsions

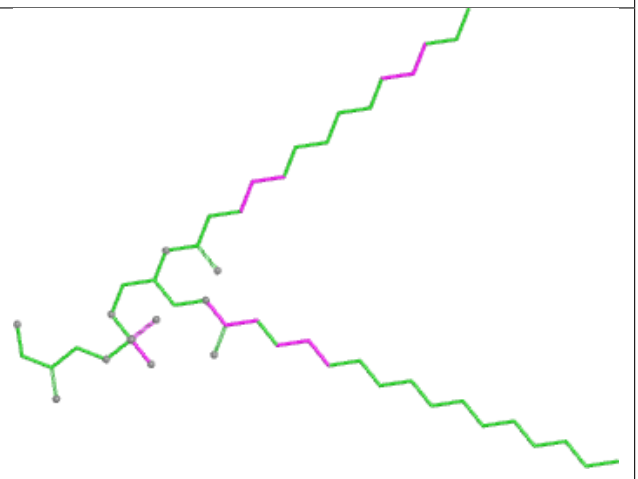


Rings

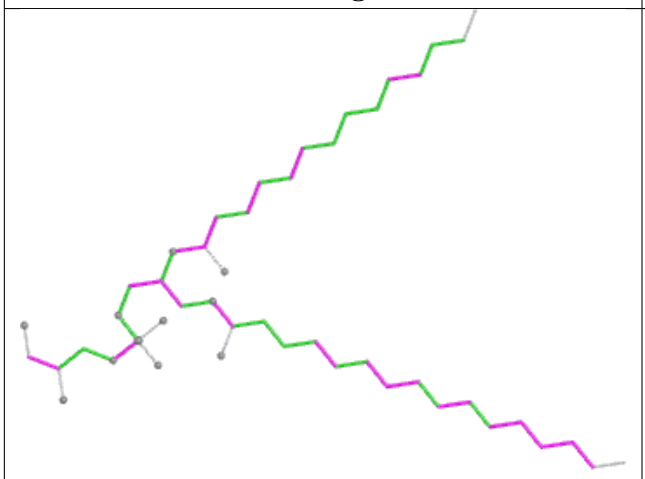
Ligand LHG A 5007



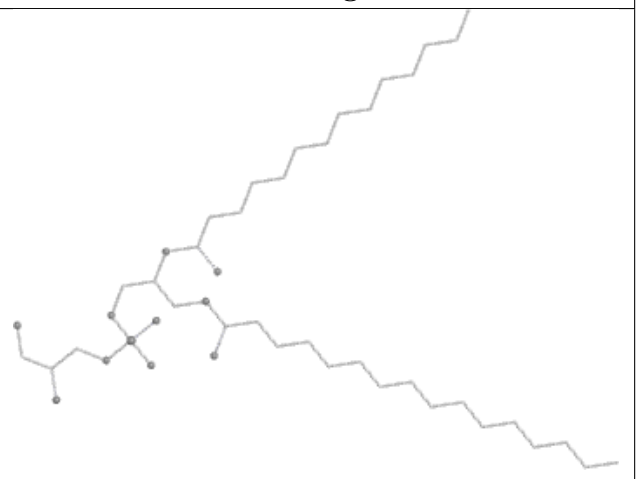
Bond lengths



Bond angles

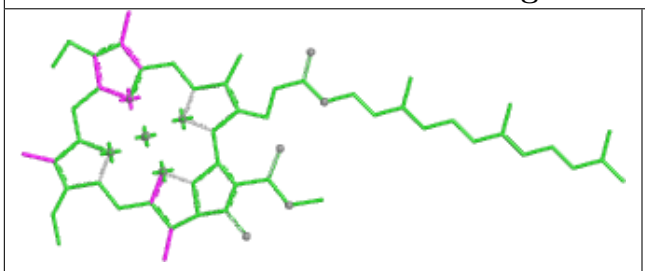


Torsions

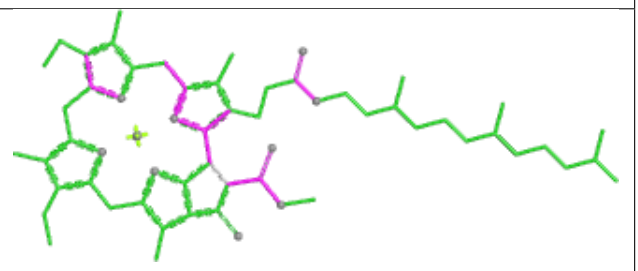


Rings

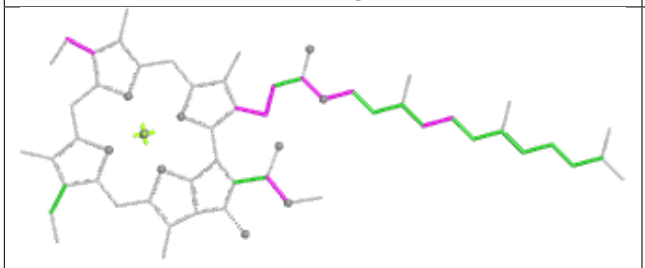
Ligand CLA e 1118



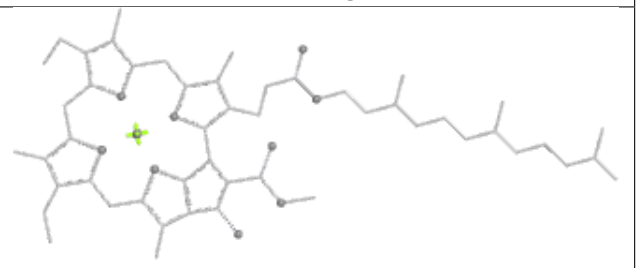
Bond lengths



Bond angles

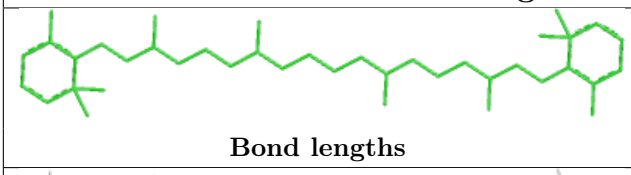


Torsions

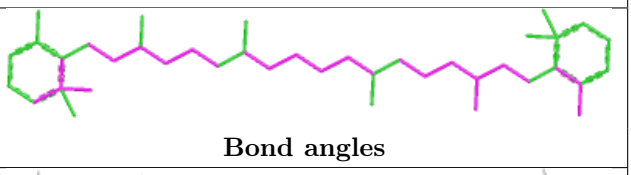


Rings

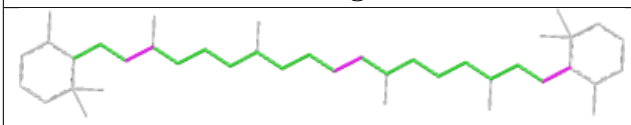
Ligand BCR J 4015



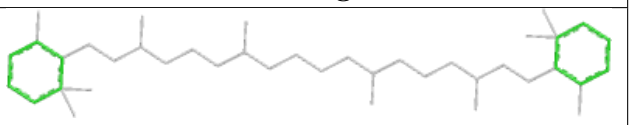
Bond lengths



Bond angles

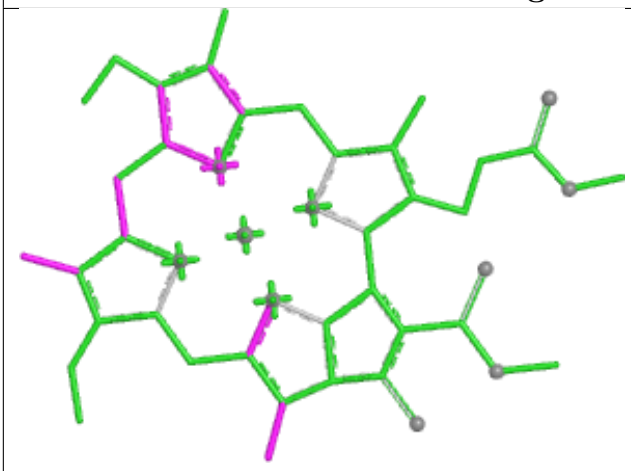


Torsions

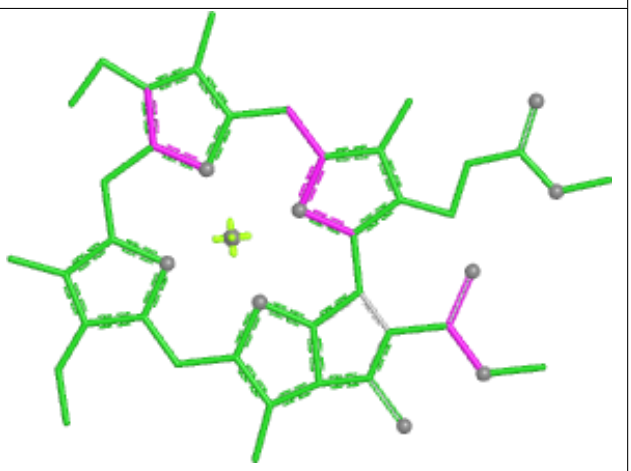


Rings

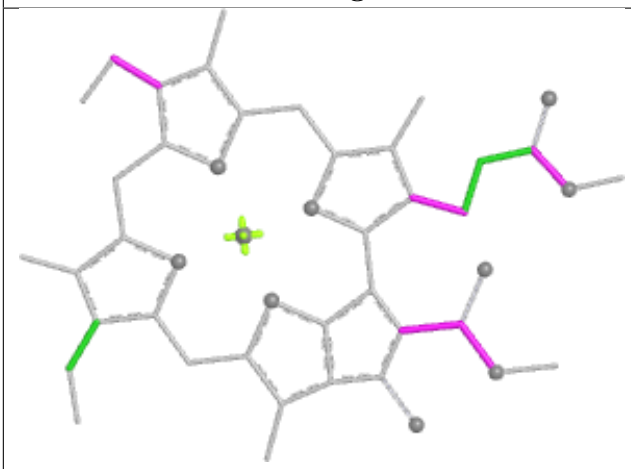
Ligand CLA v 519



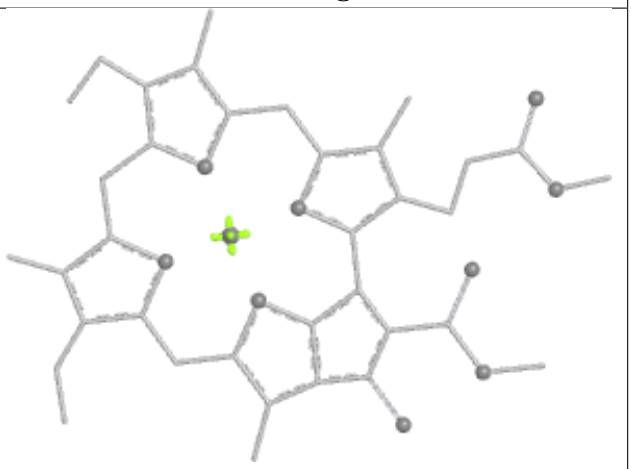
Bond lengths



Bond angles

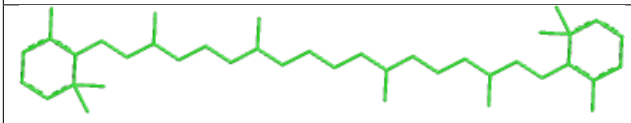


Torsions

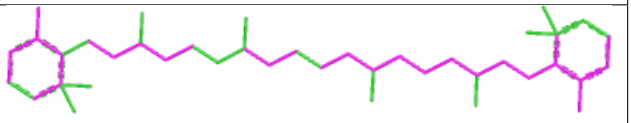


Rings

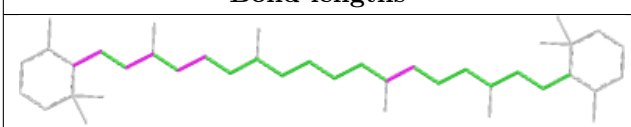
Ligand BCR c 521



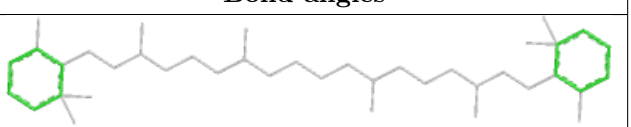
Bond lengths



Bond angles

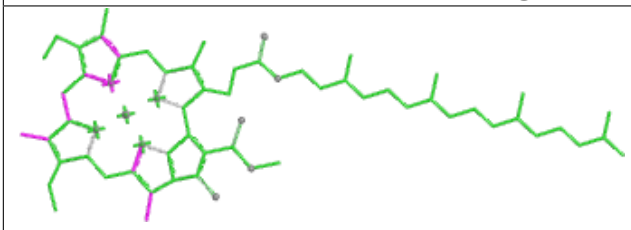


Torsions

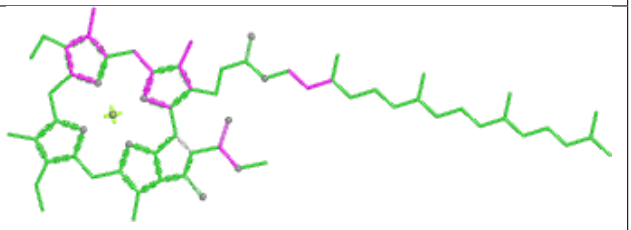


Rings

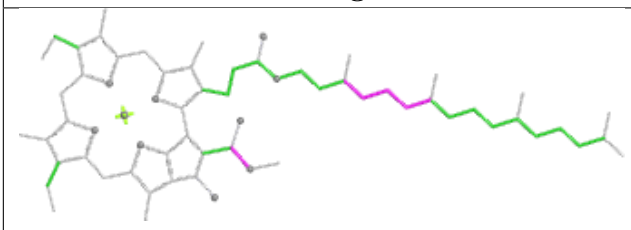
Ligand CLA B 1231



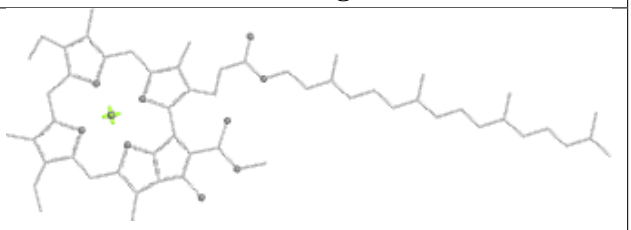
Bond lengths



Bond angles

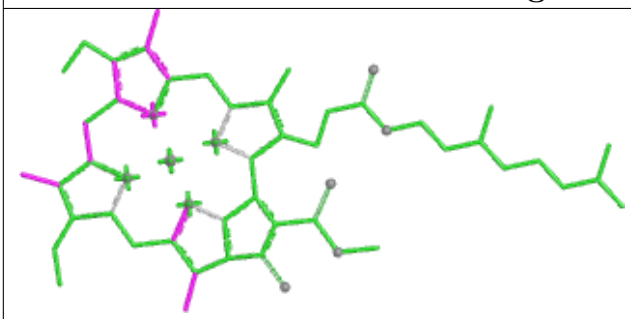


Torsions

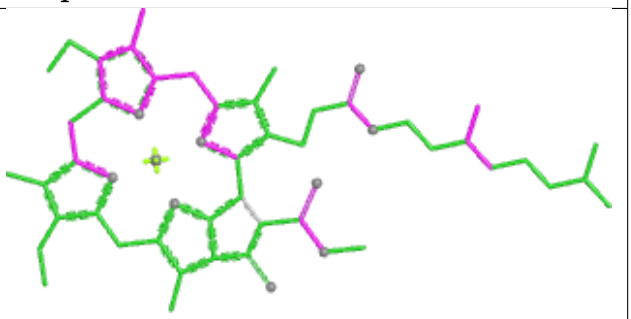


Rings

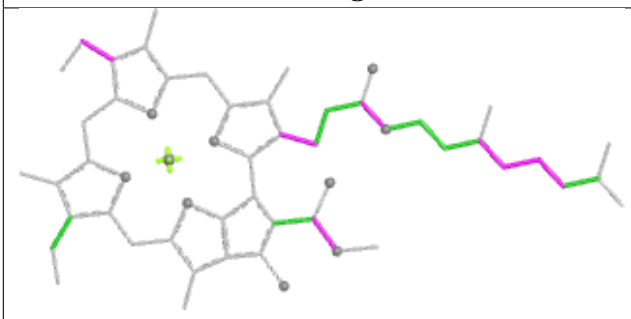
Ligand CLA q 508



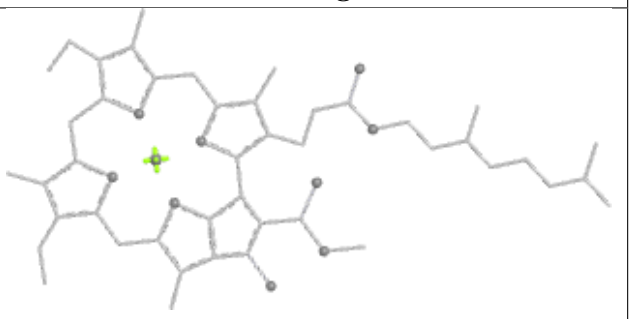
Bond lengths



Bond angles

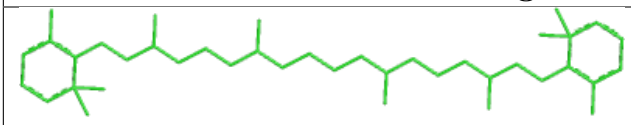


Torsions

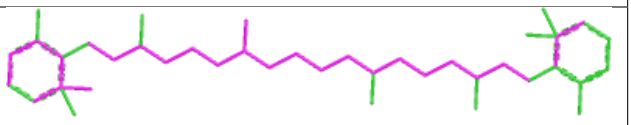


Rings

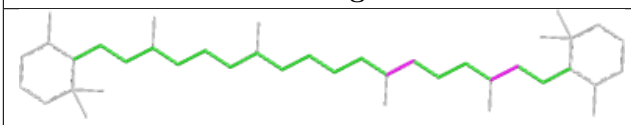
Ligand BCR J 4013



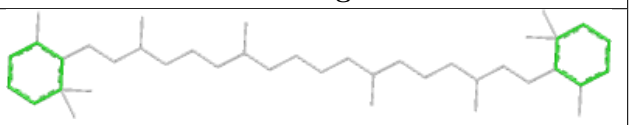
Bond lengths



Bond angles

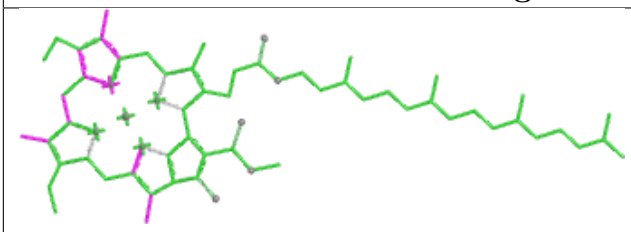


Torsions

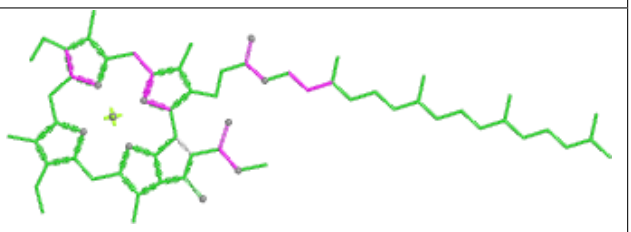


Rings

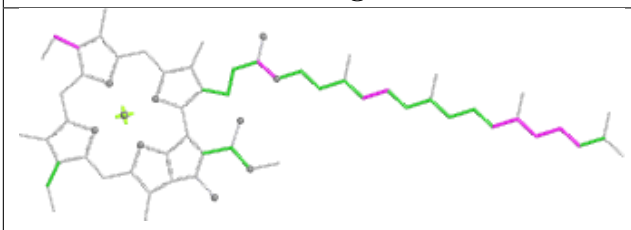
Ligand CLA G 1109



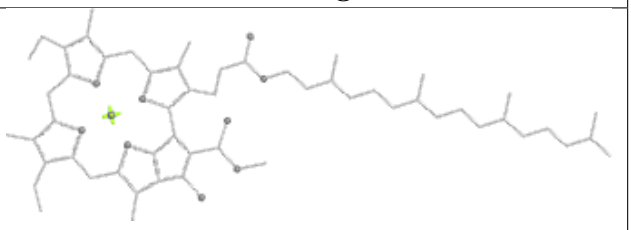
Bond lengths



Bond angles

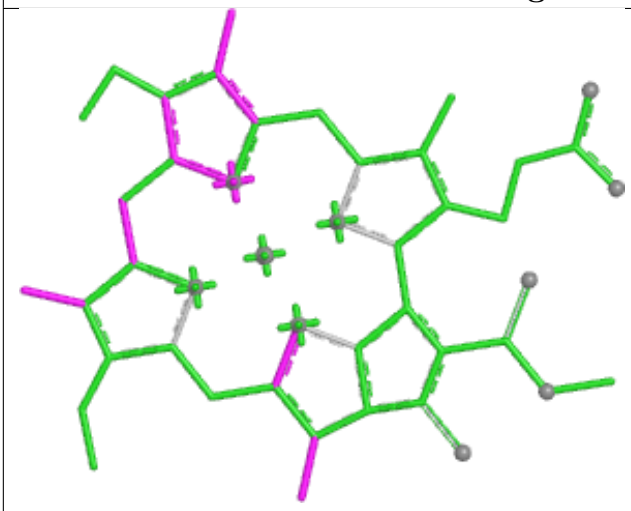


Torsions

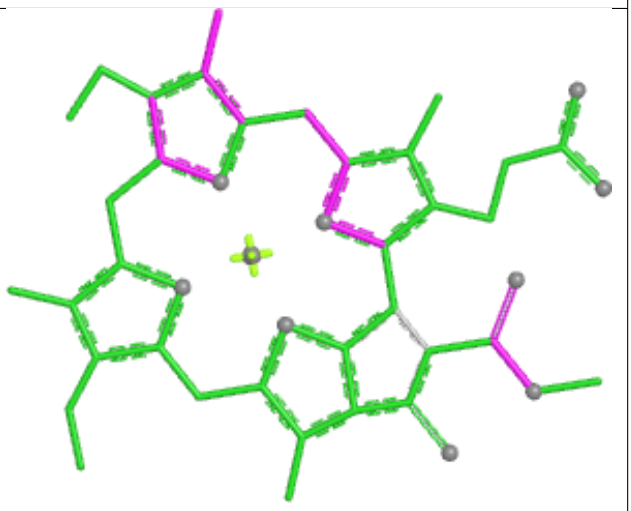


Rings

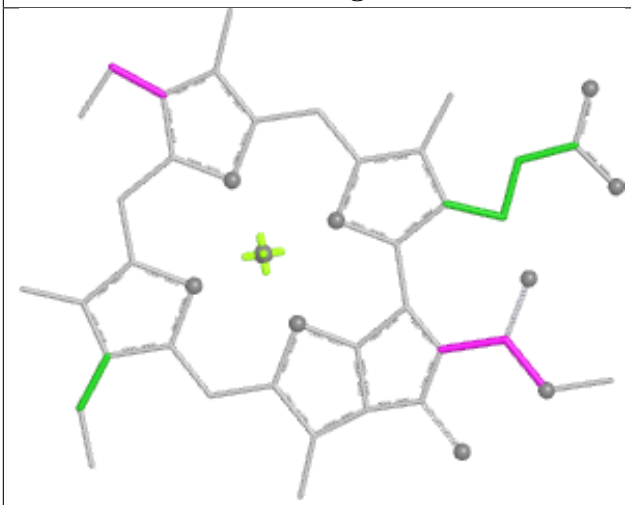
Ligand CLA v 506



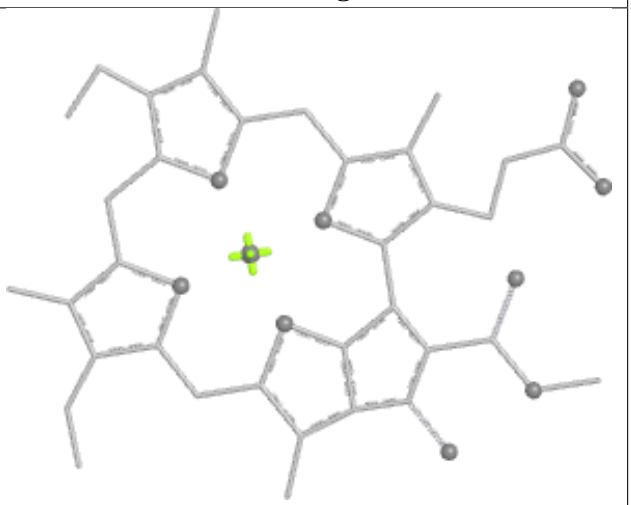
Bond lengths



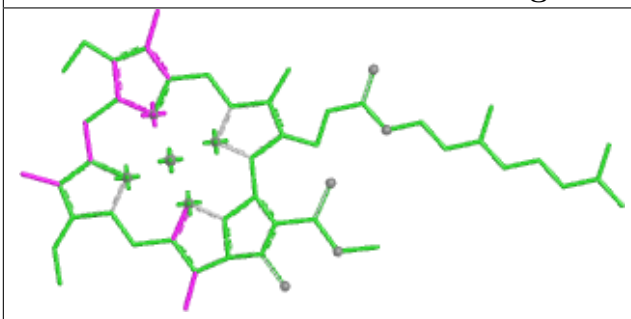
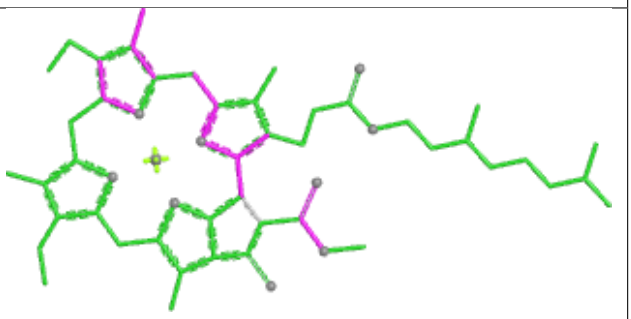
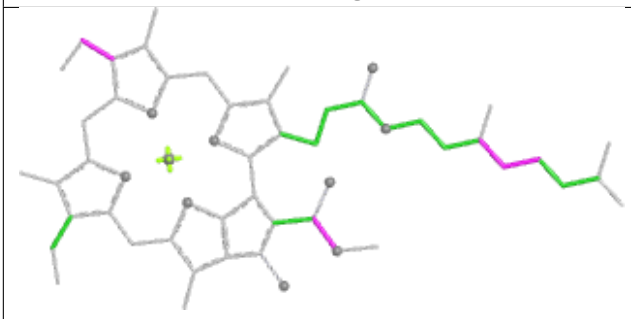
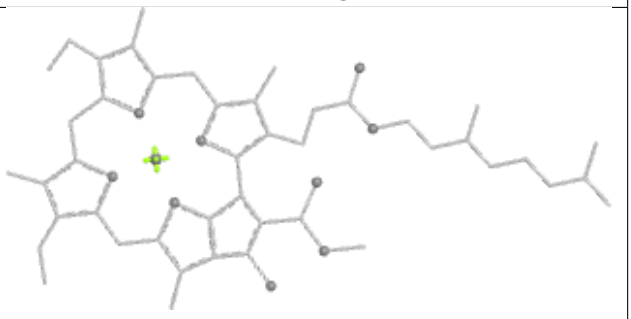
Bond angles

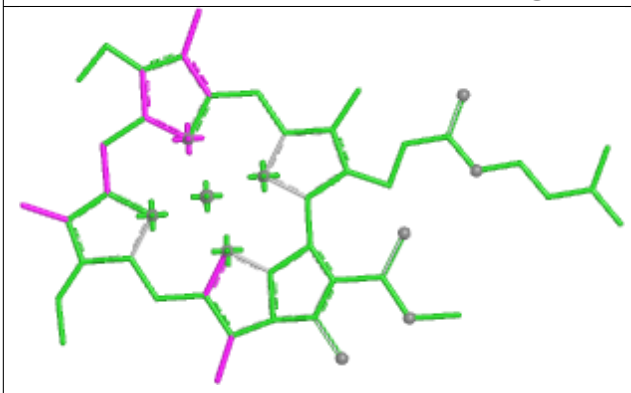
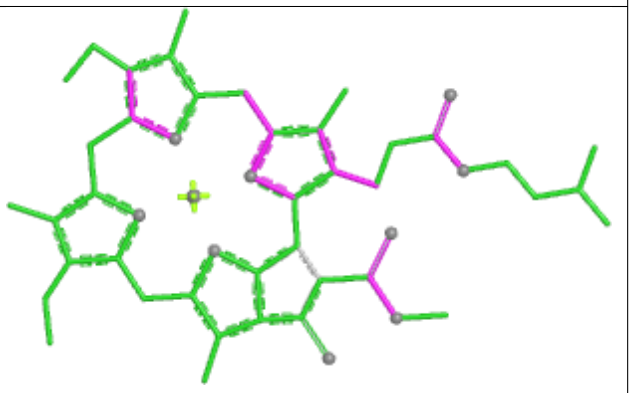
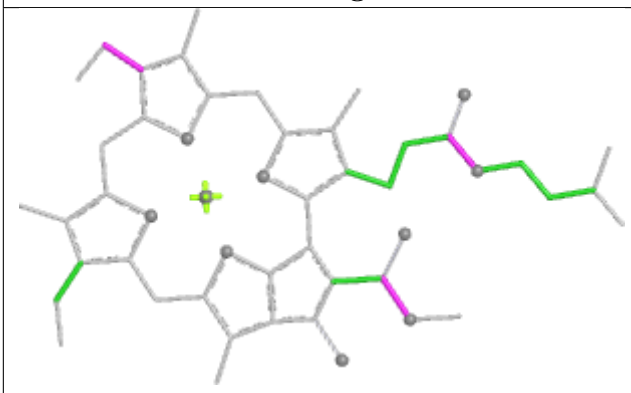
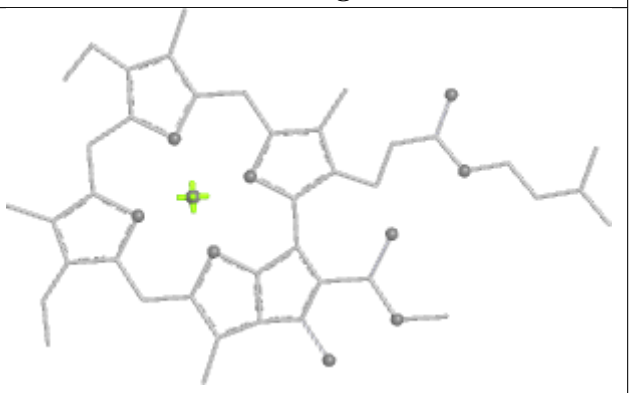


Torsions

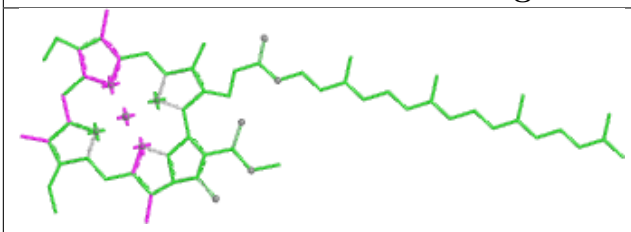


Rings

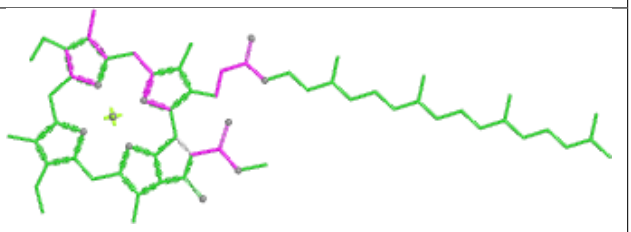
Ligand CLA r 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

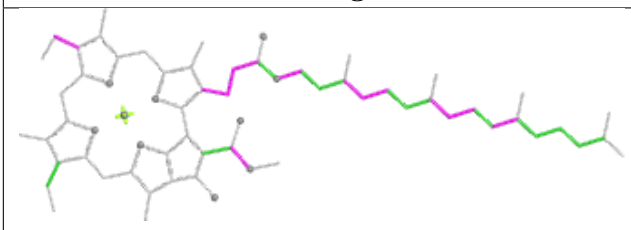
Ligand CLA G 1107



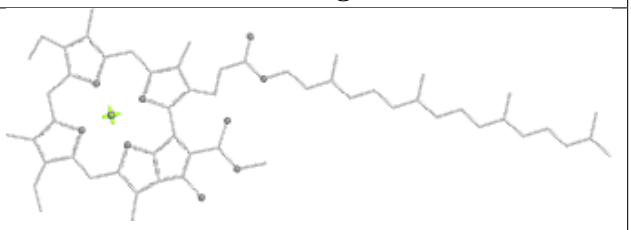
Bond lengths



Bond angles

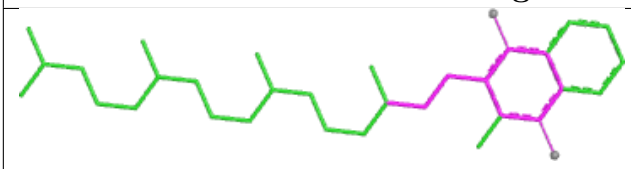


Torsions

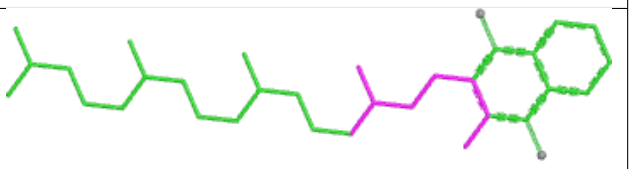


Rings

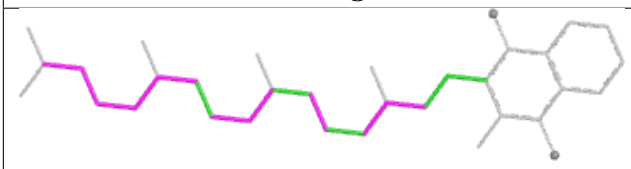
Ligand PQN A 2001



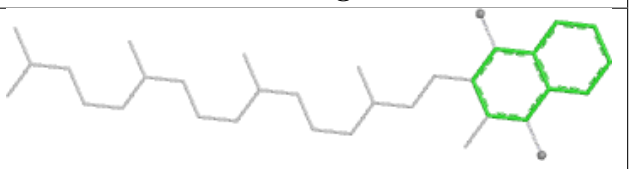
Bond lengths



Bond angles

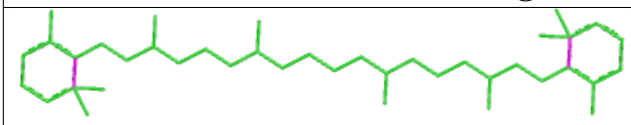


Torsions

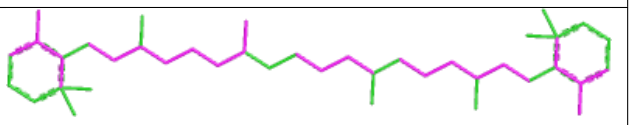


Rings

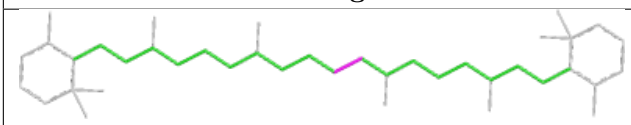
Ligand BCR k 4018



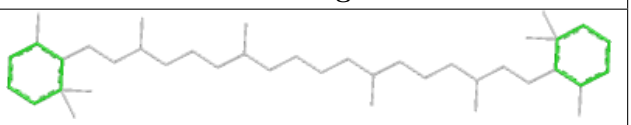
Bond lengths



Bond angles

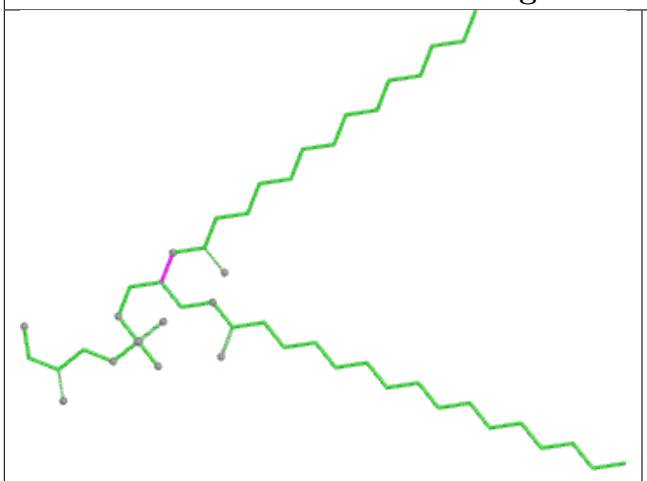


Torsions

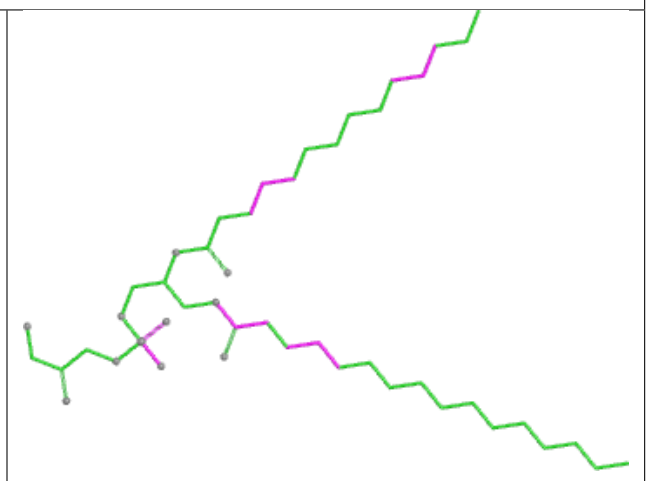


Rings

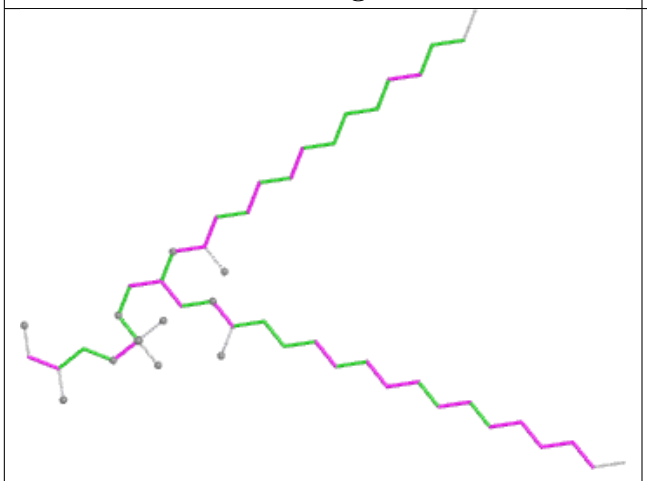
Ligand LHG e 5007



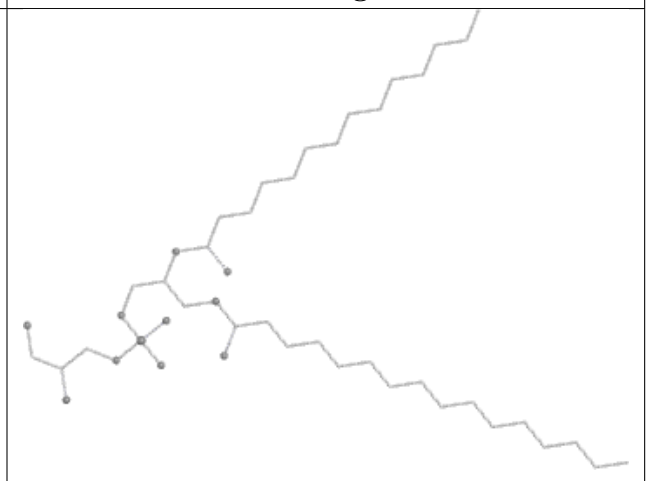
Bond lengths



Bond angles

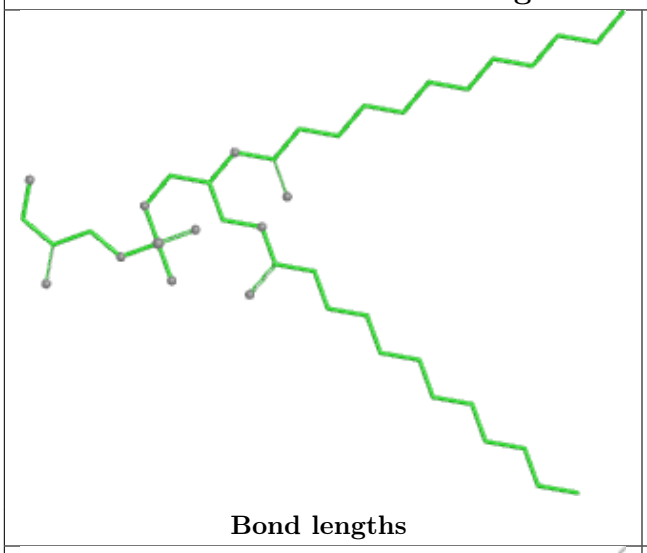


Torsions

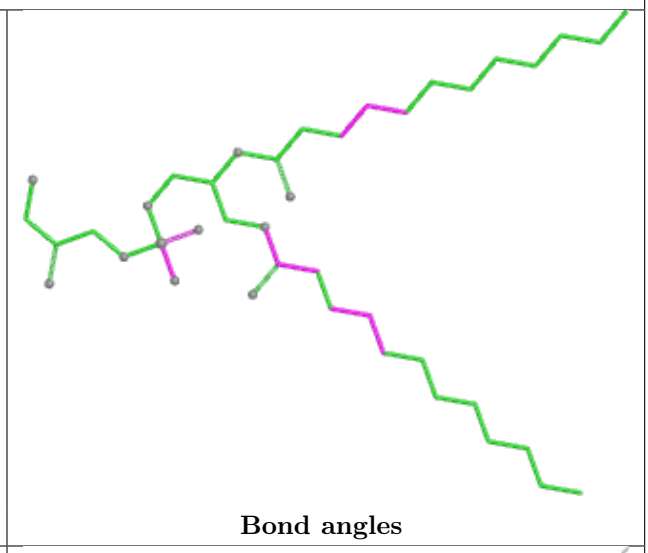


Rings

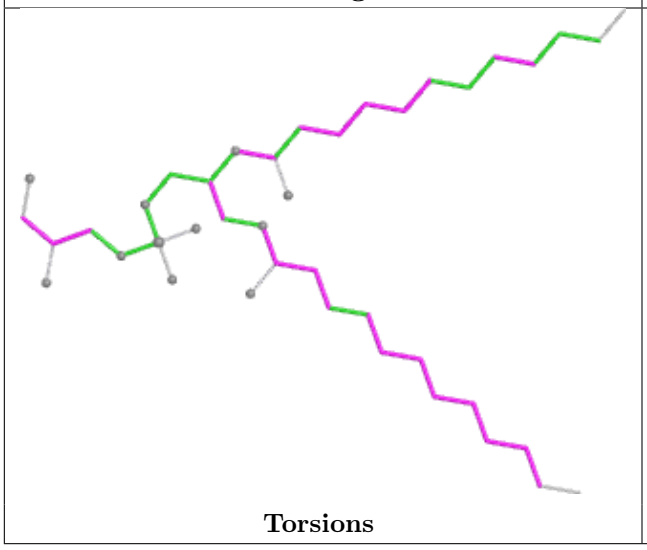
Ligand LHG V 5220



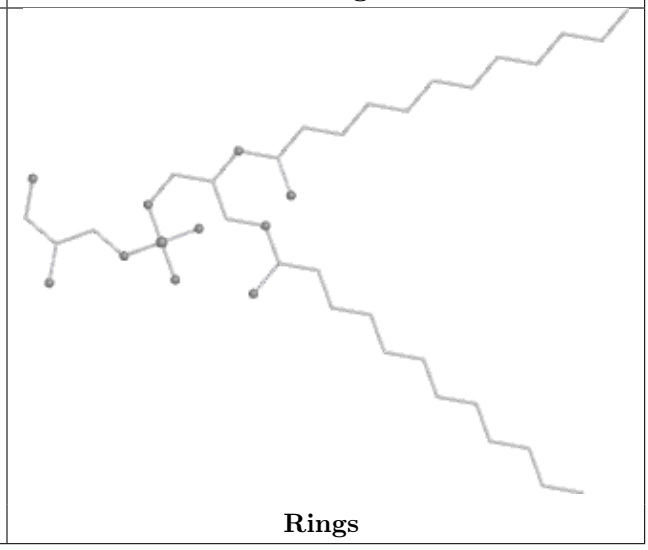
Bond lengths



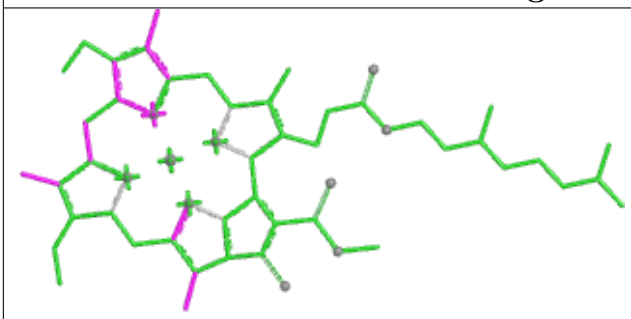
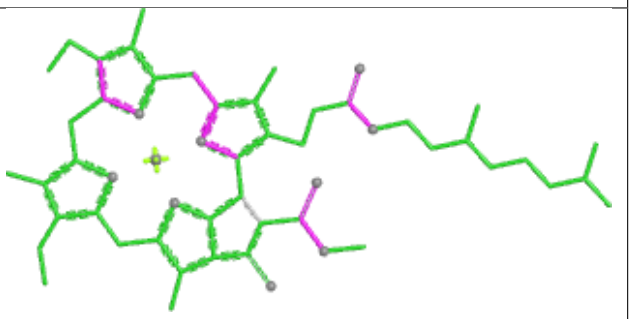
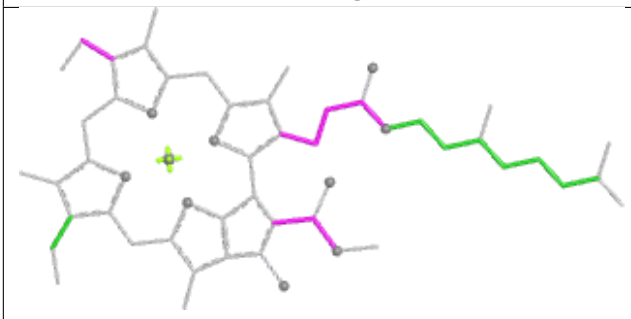
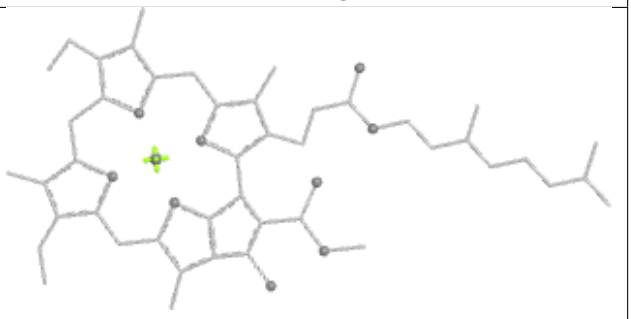
Bond angles

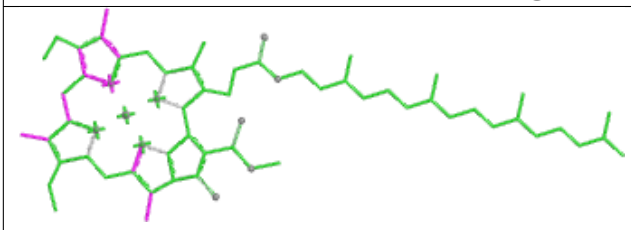
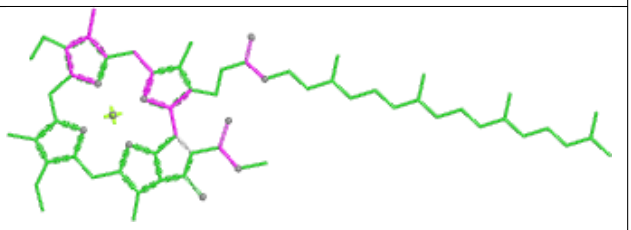
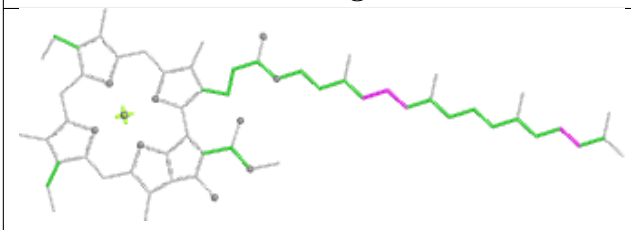
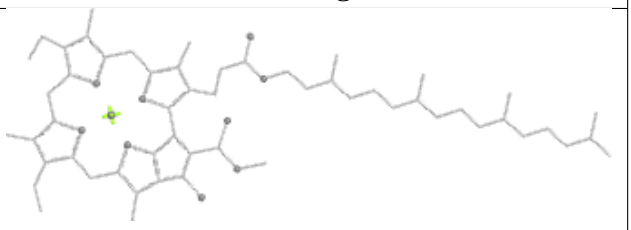


Torsions

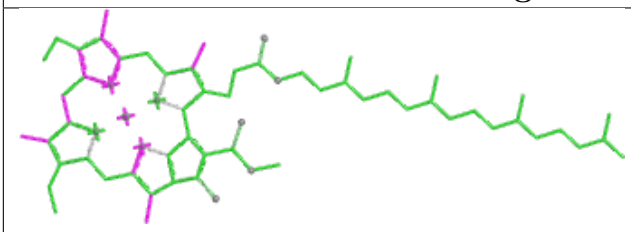


Rings

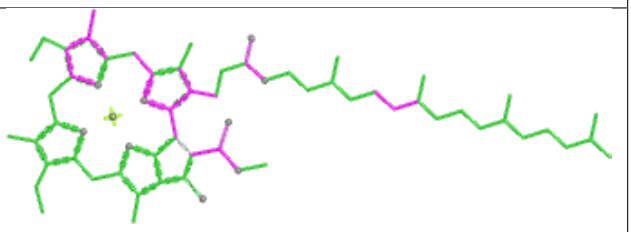
Ligand CLA b 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

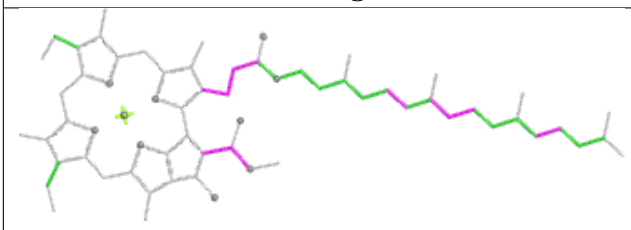
Ligand CLA H 1221



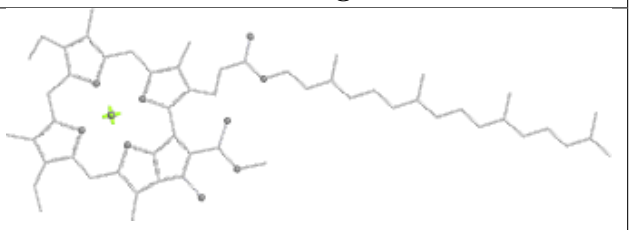
Bond lengths



Bond angles

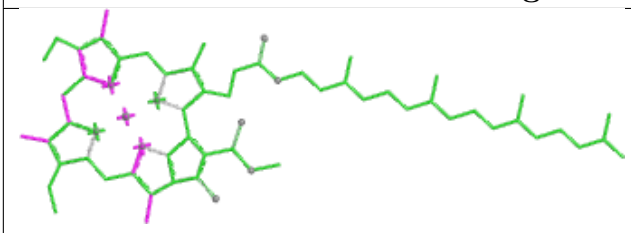


Torsions

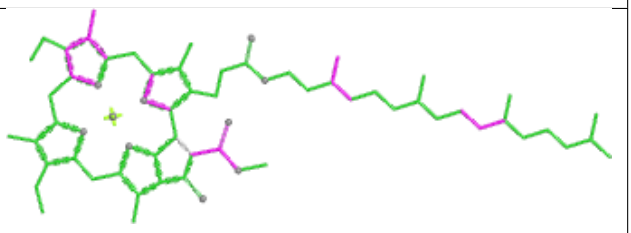


Rings

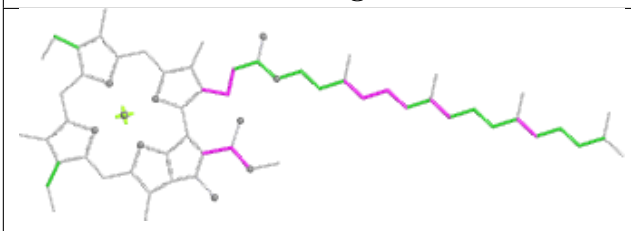
Ligand CLA f 1012



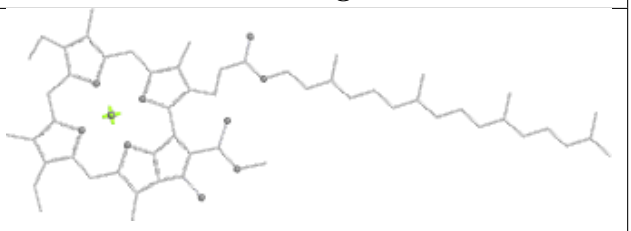
Bond lengths



Bond angles

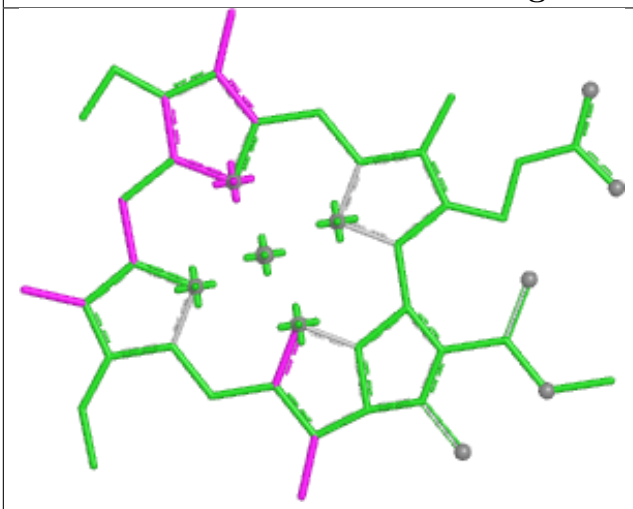


Torsions

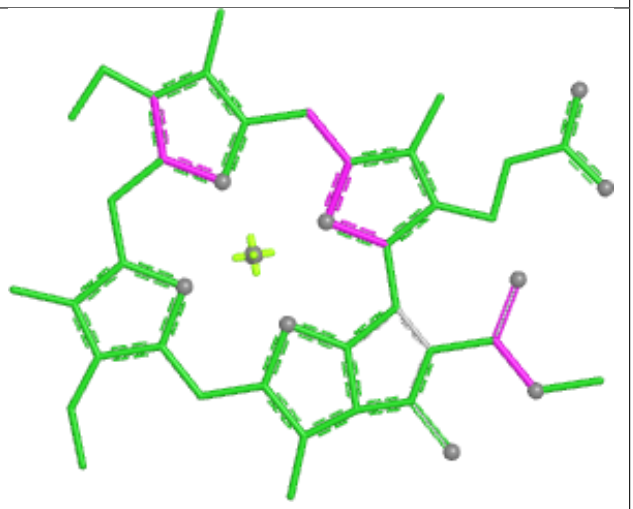


Rings

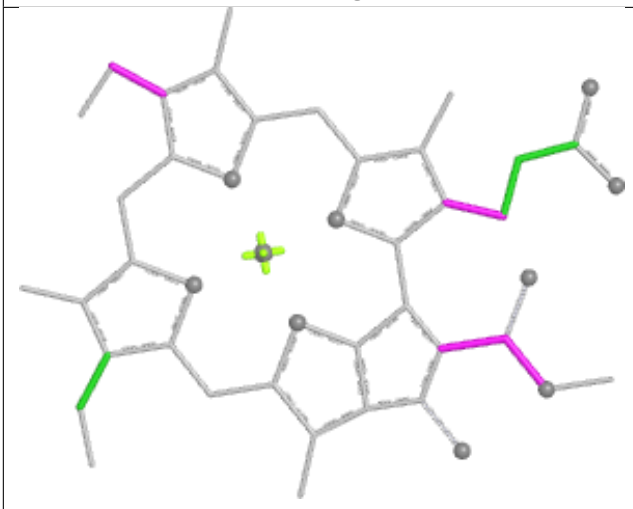
Ligand CLA a 517



Bond lengths



Bond angles

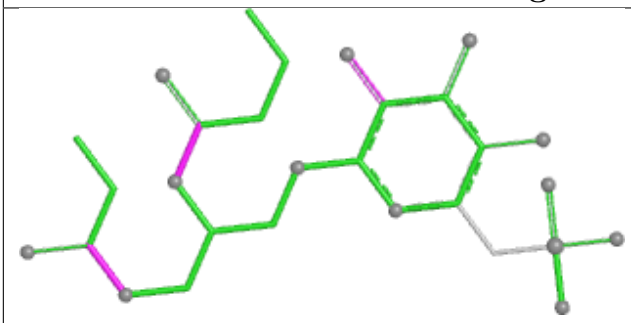


Torsions

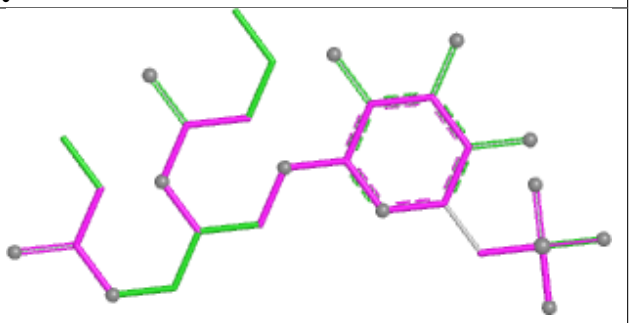


Rings

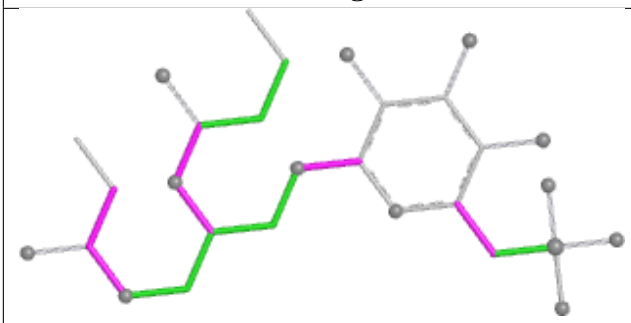
Ligand SQD c 822



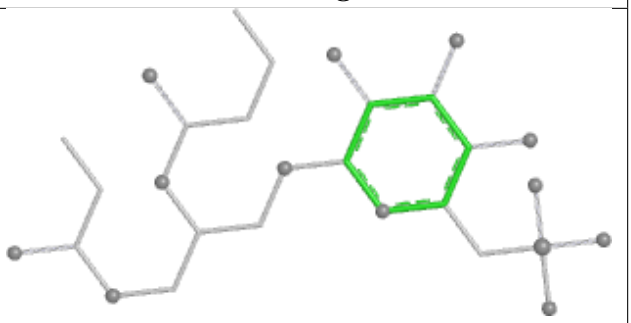
Bond lengths



Bond angles

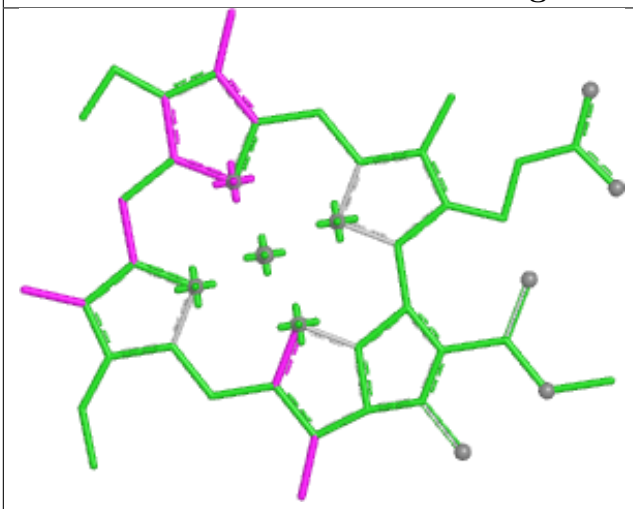


Torsions

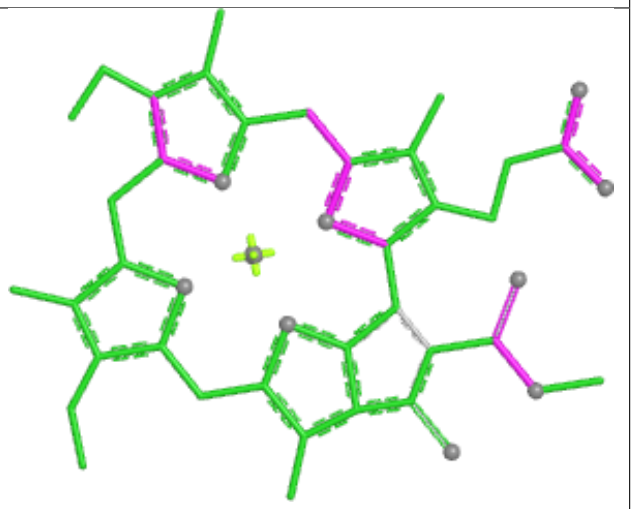


Rings

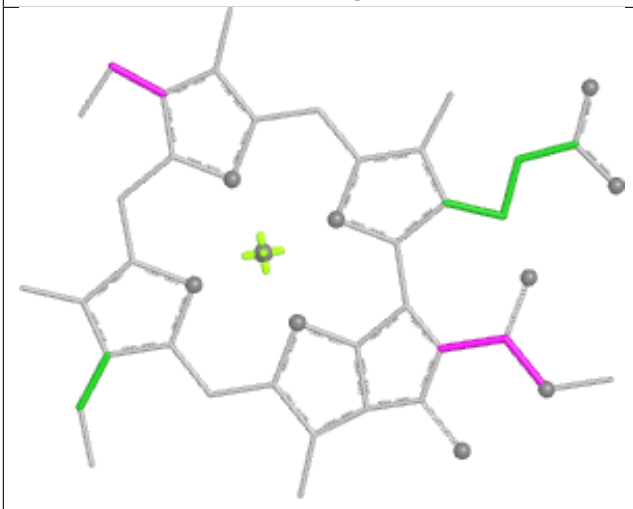
Ligand CLA c 506



Bond lengths



Bond angles

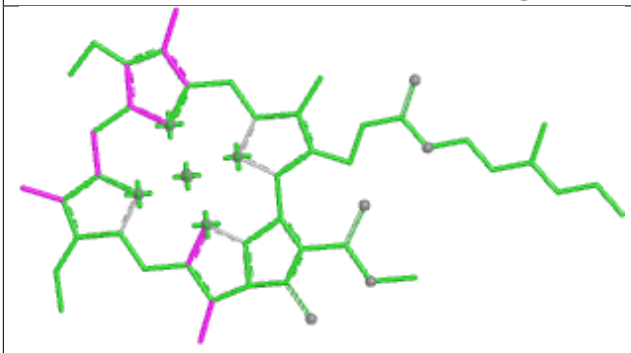


Torsions

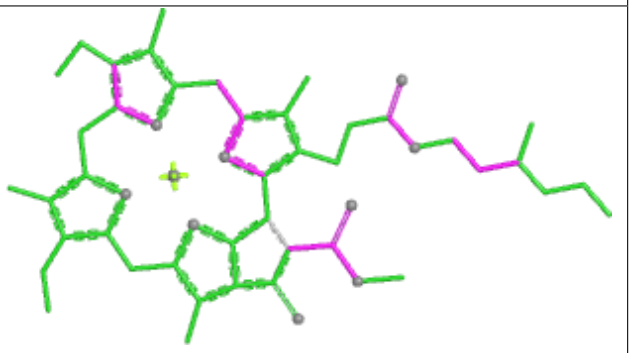


Rings

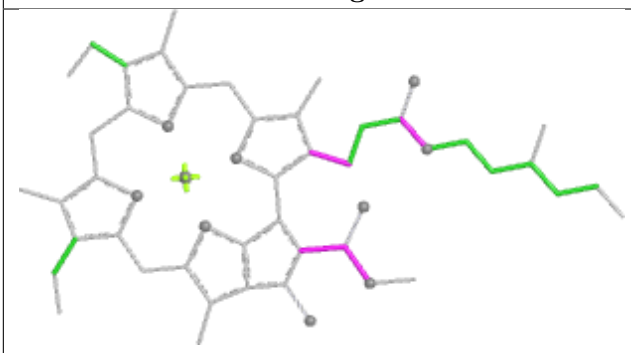
Ligand CLA B 1209



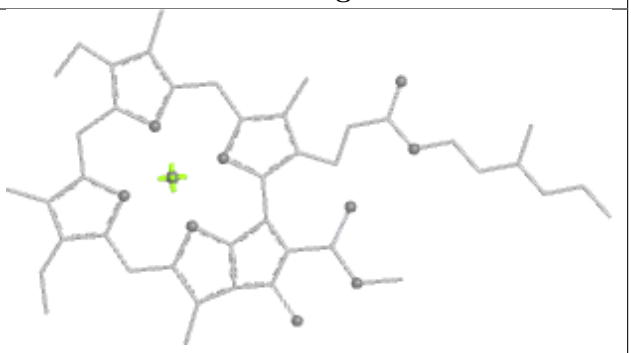
Bond lengths



Bond angles

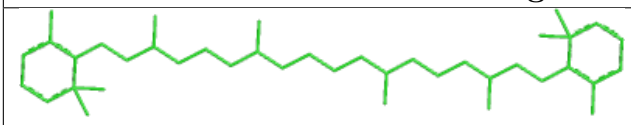


Torsions

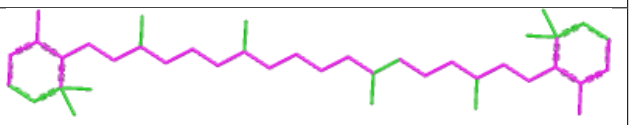


Rings

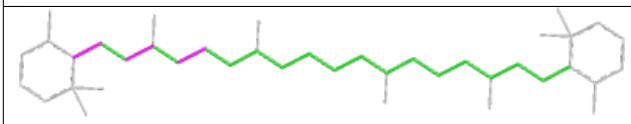
Ligand BCR c 522



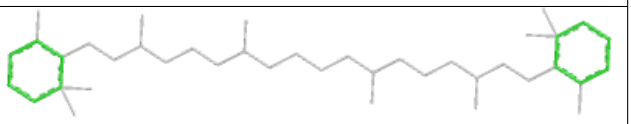
Bond lengths



Bond angles



Torsions

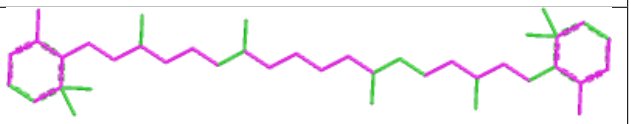


Rings

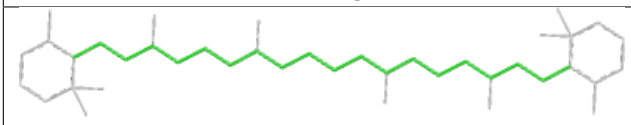
Ligand BCR G 4007



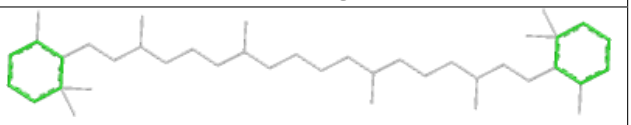
Bond lengths



Bond angles

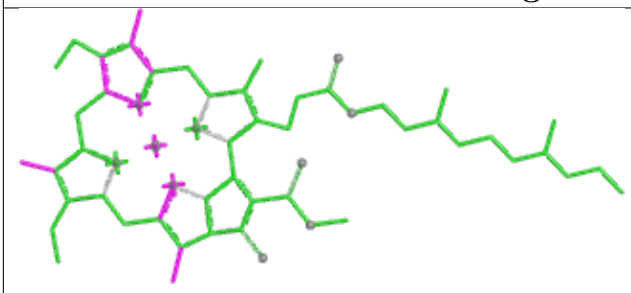


Torsions

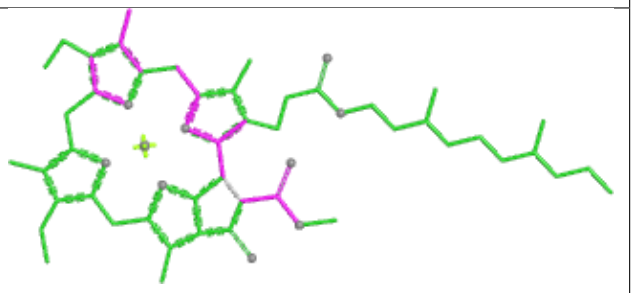


Rings

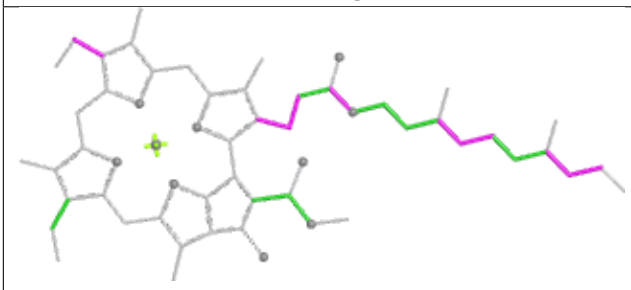
Ligand CLA f 1217



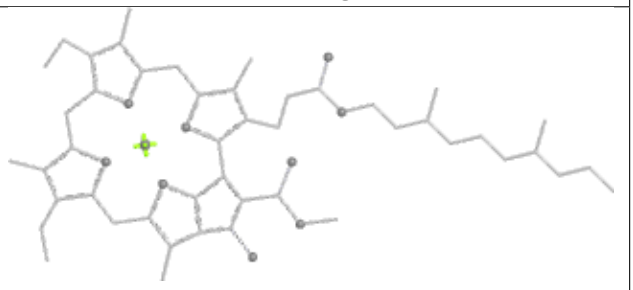
Bond lengths



Bond angles

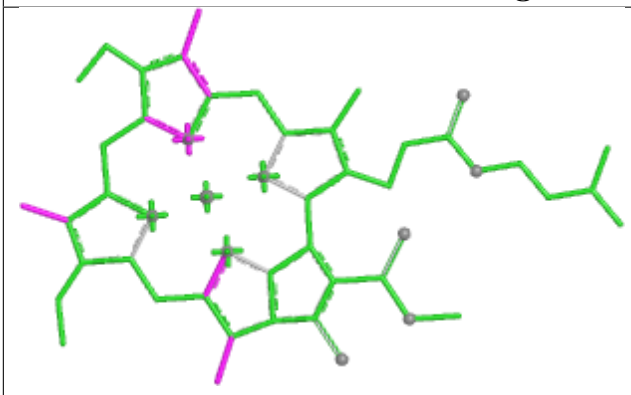


Torsions

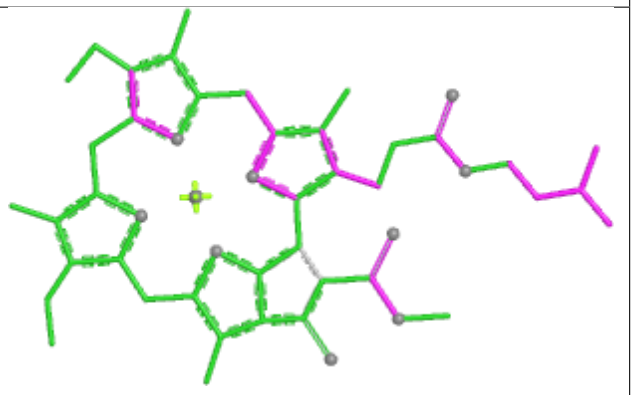


Rings

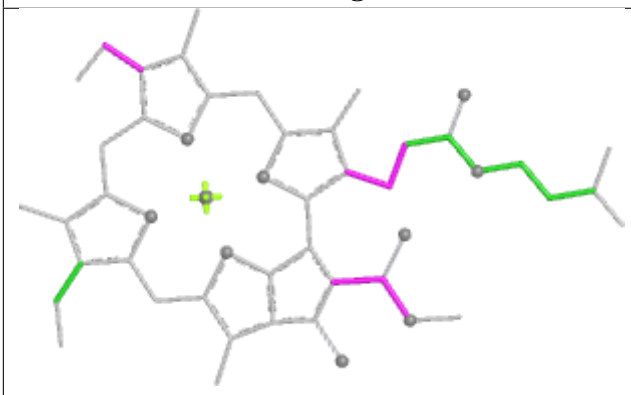
Ligand CLA U 1103



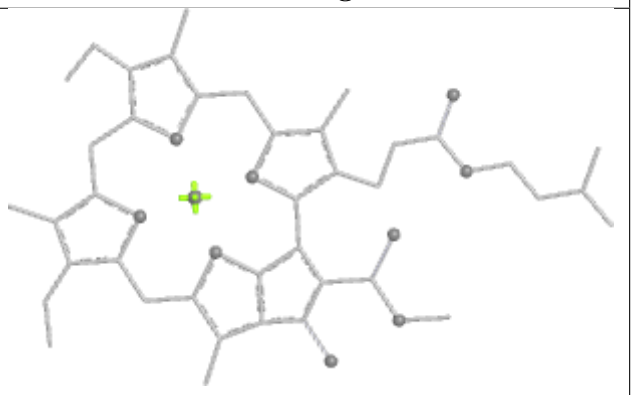
Bond lengths



Bond angles

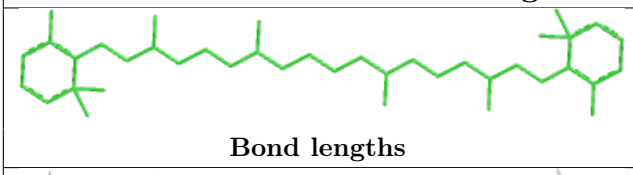


Torsions

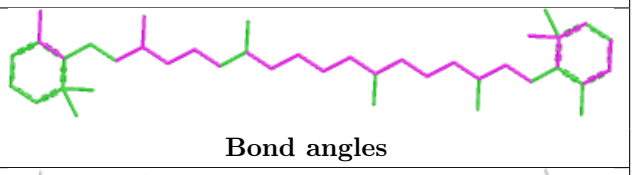


Rings

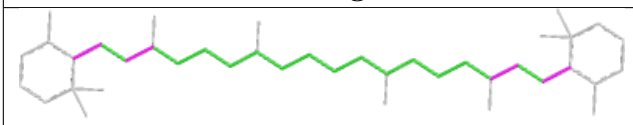
Ligand BCR f 4004



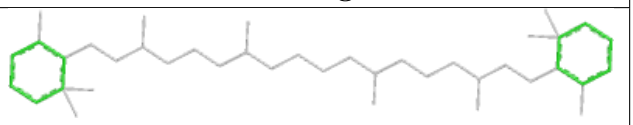
Bond lengths



Bond angles

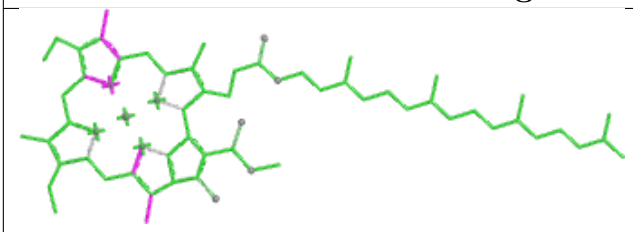


Torsions

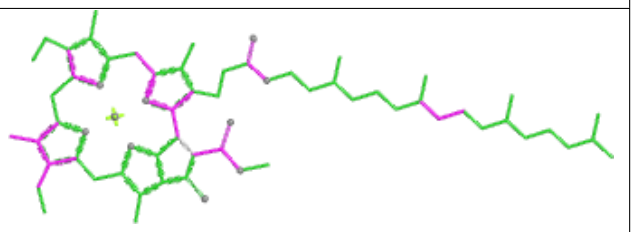


Rings

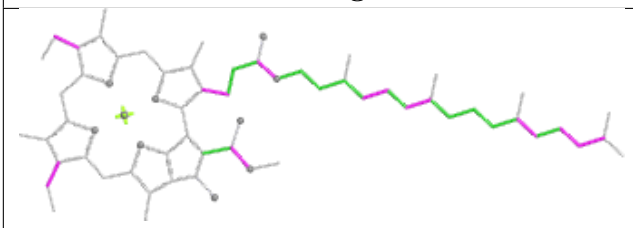
Ligand CLA B 1239



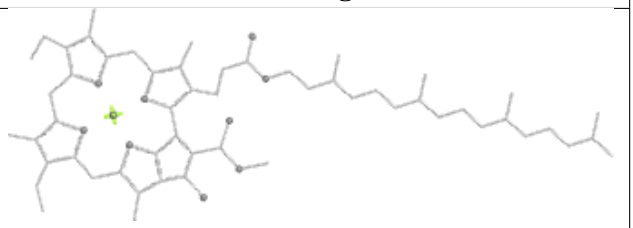
Bond lengths



Bond angles

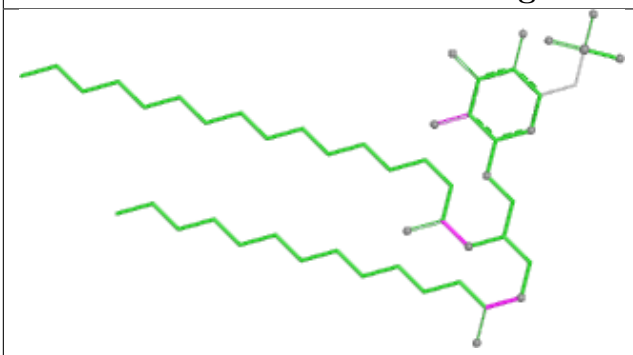


Torsions

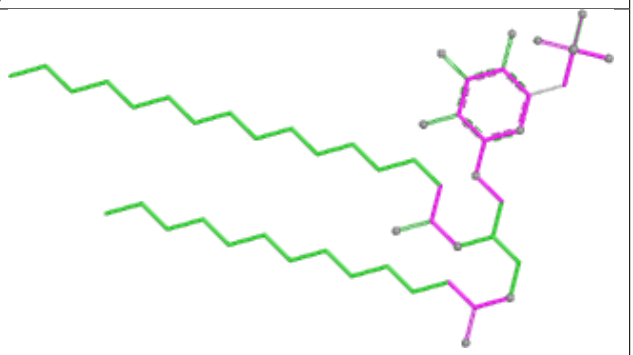


Rings

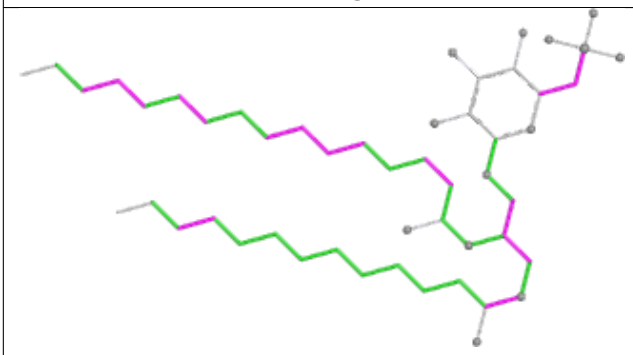
Ligand SQD n 5216



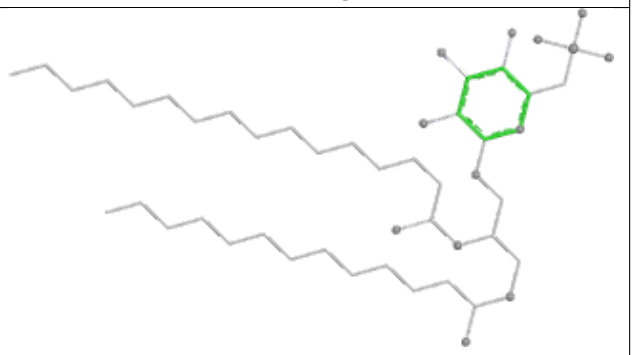
Bond lengths



Bond angles

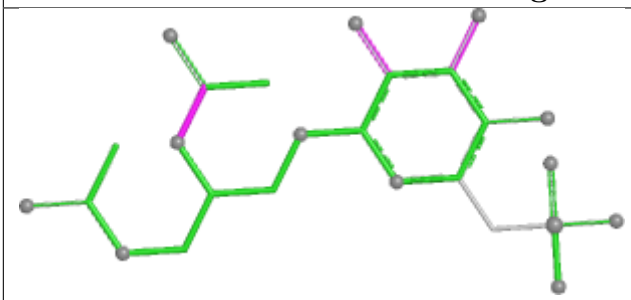


Torsions

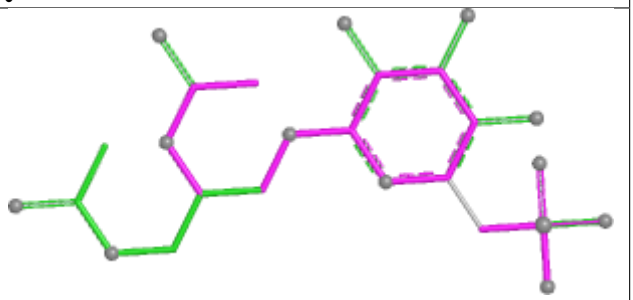


Rings

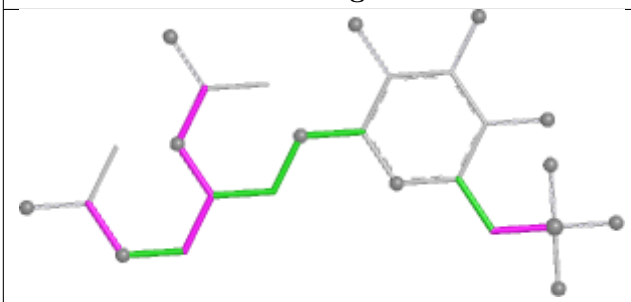
Ligand SQD t 822



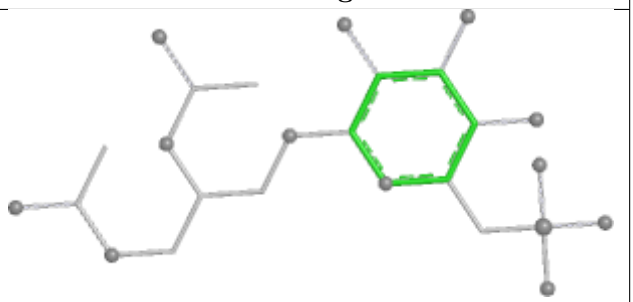
Bond lengths



Bond angles

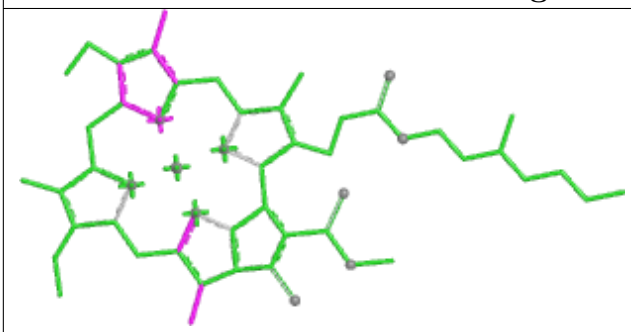


Torsions

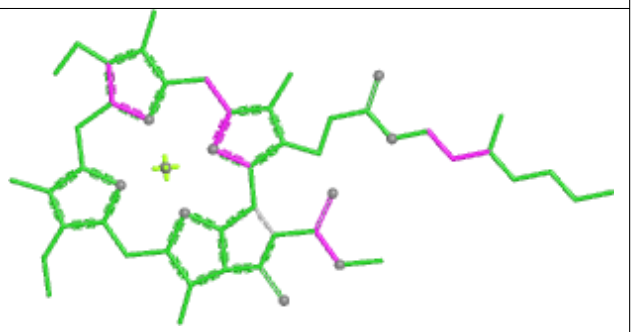


Rings

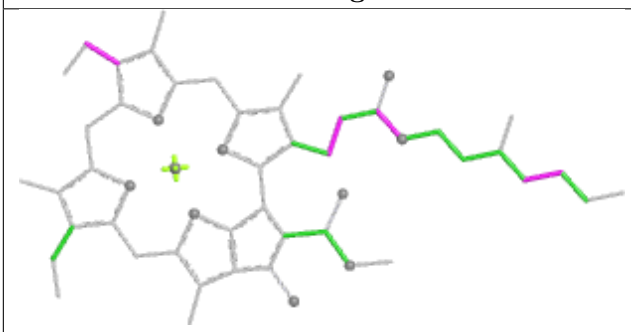
Ligand CLA r 512



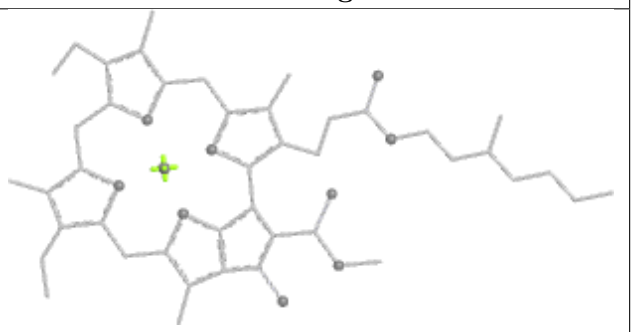
Bond lengths



Bond angles

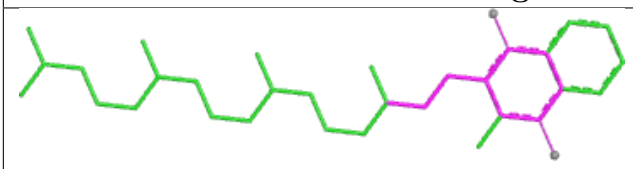


Torsions

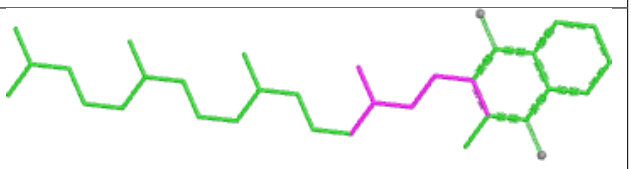


Rings

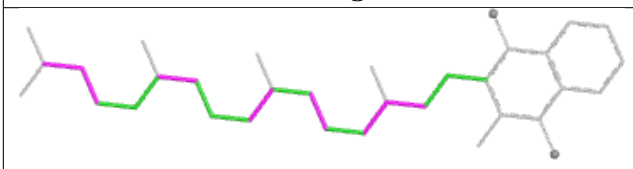
Ligand PQN H 2002



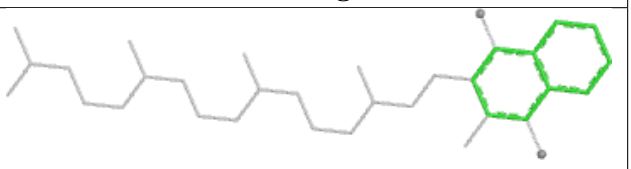
Bond lengths



Bond angles

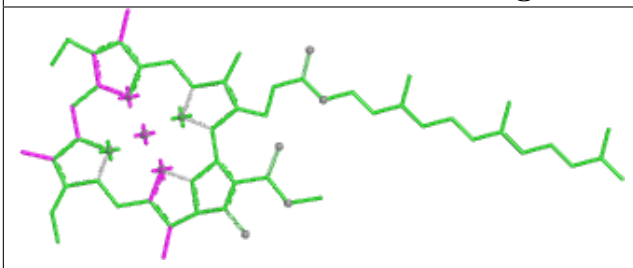


Torsions

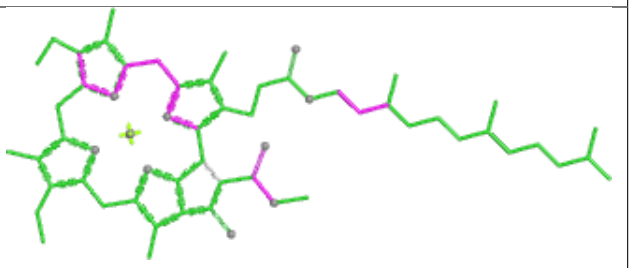


Rings

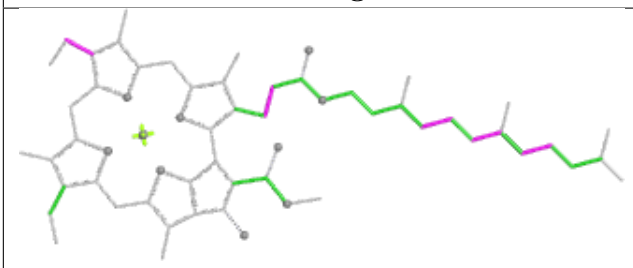
Ligand CLA B 1216



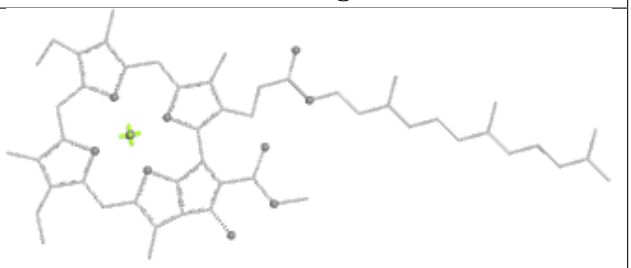
Bond lengths



Bond angles

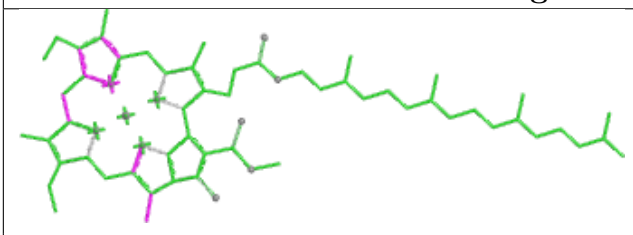


Torsions

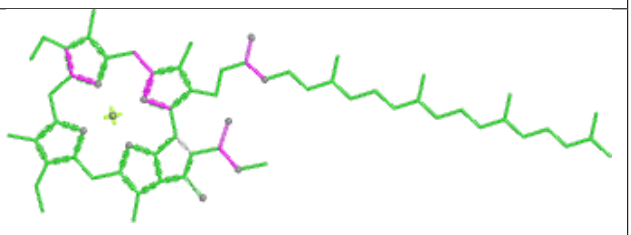


Rings

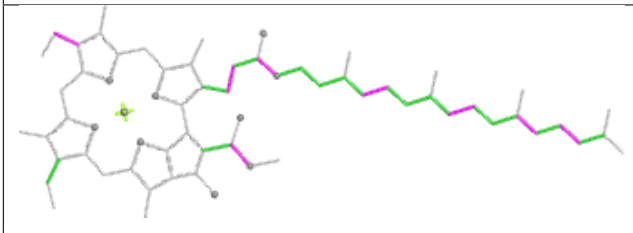
Ligand CLA t 505



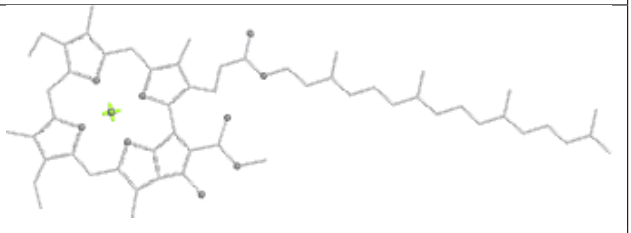
Bond lengths



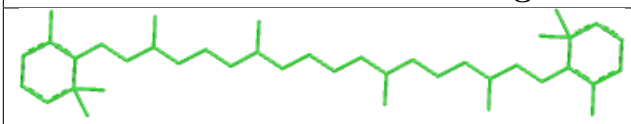
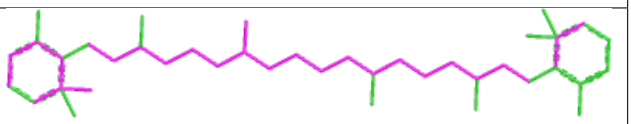
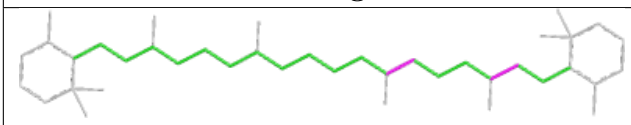
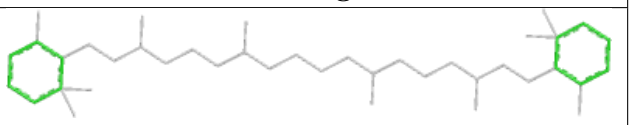
Bond angles

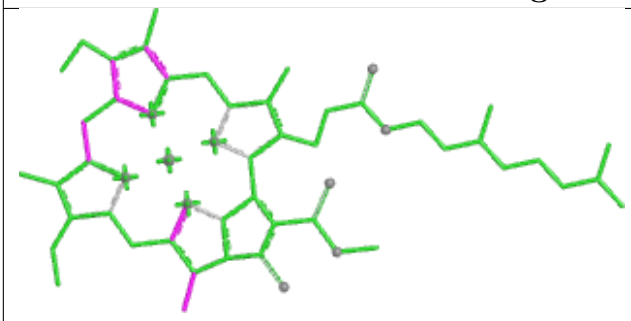
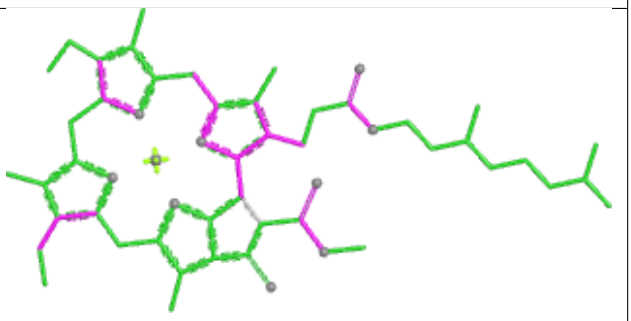
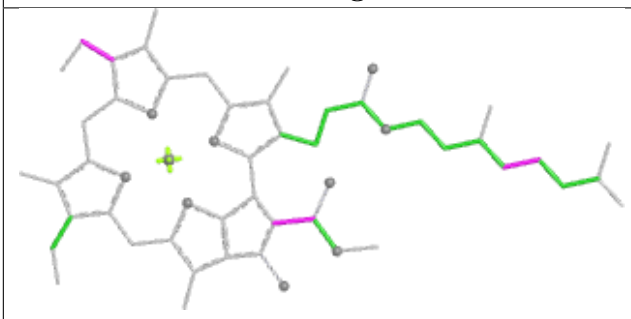
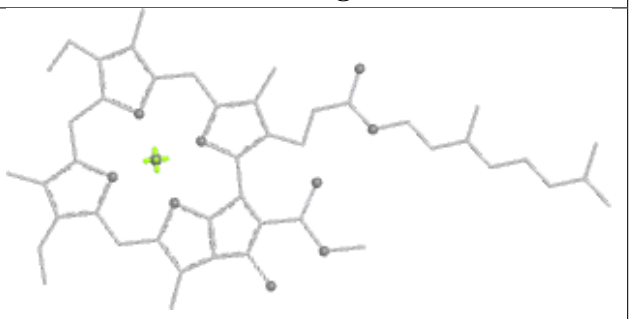


Torsions

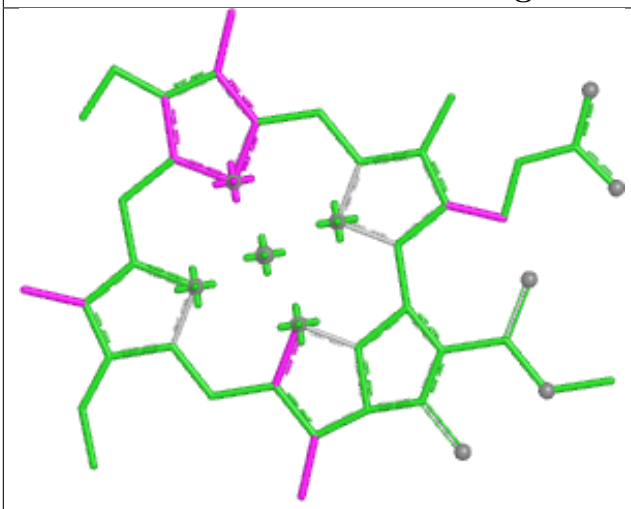


Rings

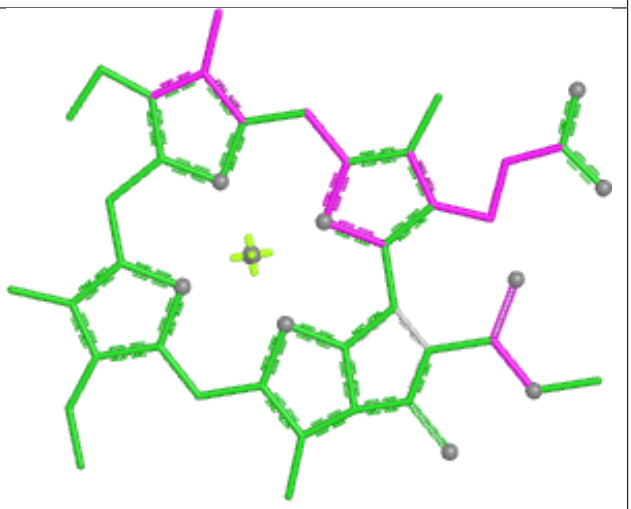
Ligand BCR T 4013	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA t 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

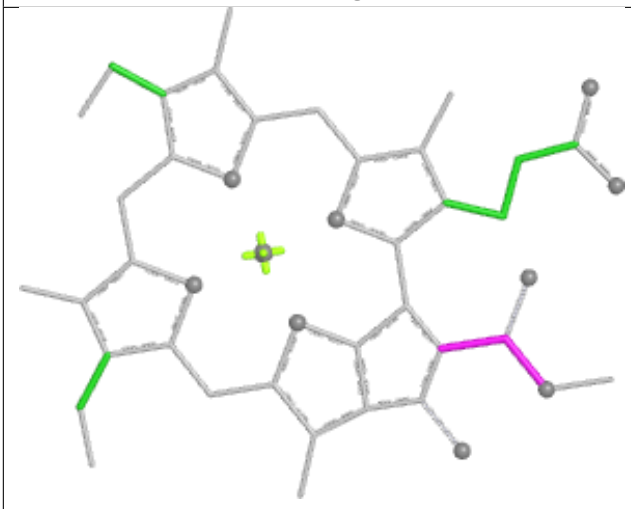
Ligand CLA A 1801



Bond lengths



Bond angles

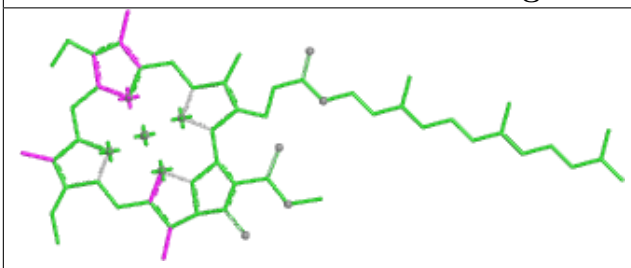


Torsions

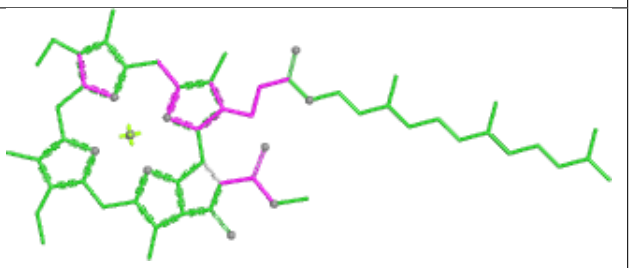


Rings

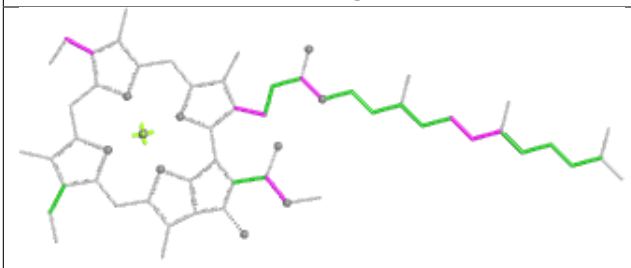
Ligand CLA f 1230



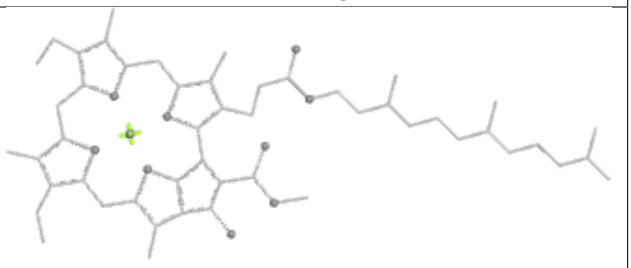
Bond lengths



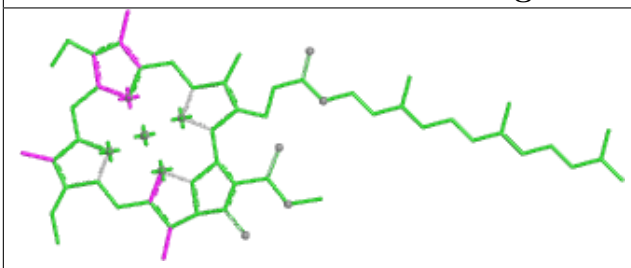
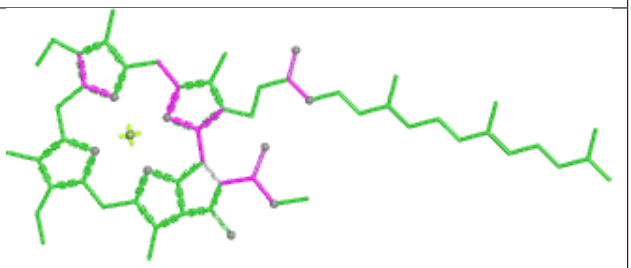
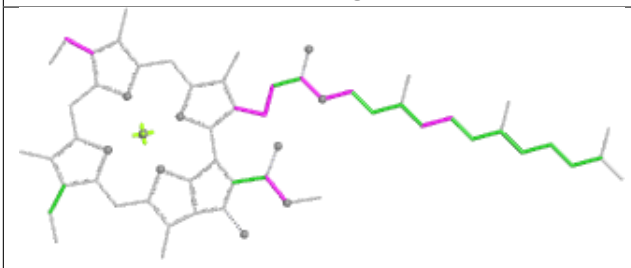
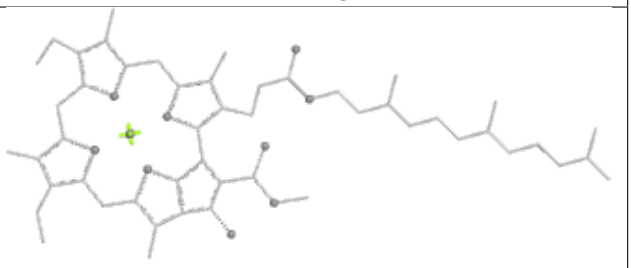
Bond angles

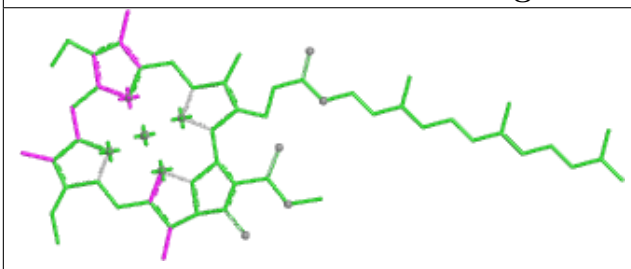
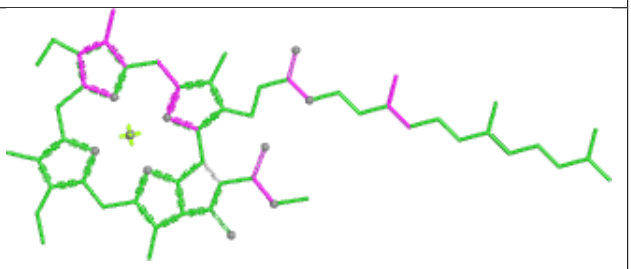
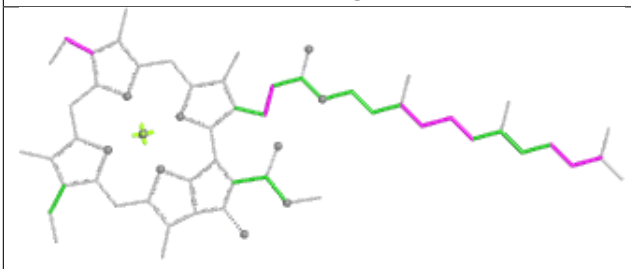
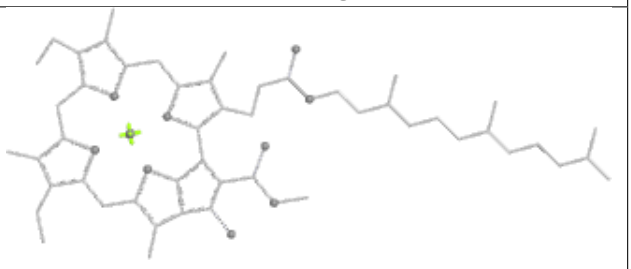


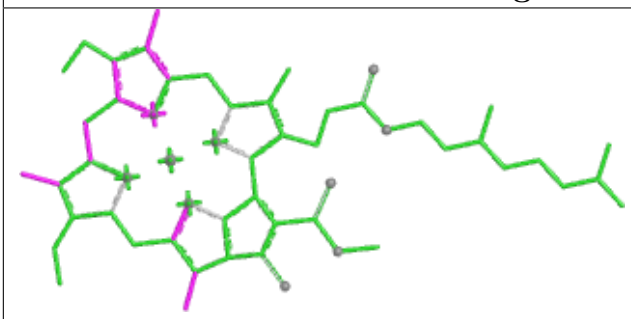
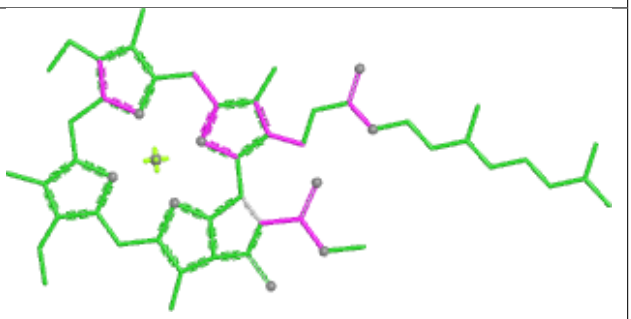
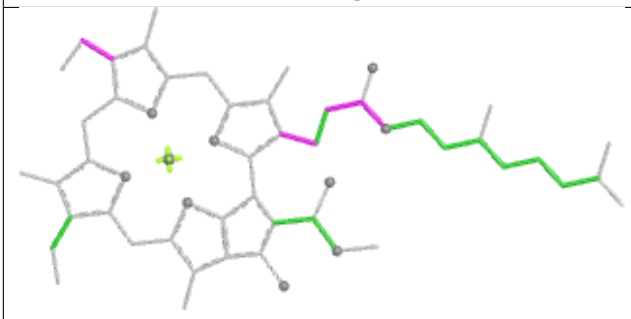
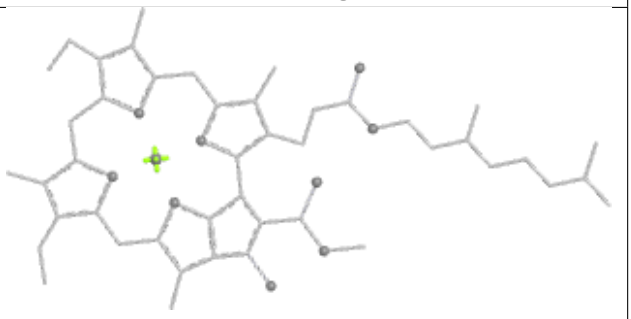
Torsions

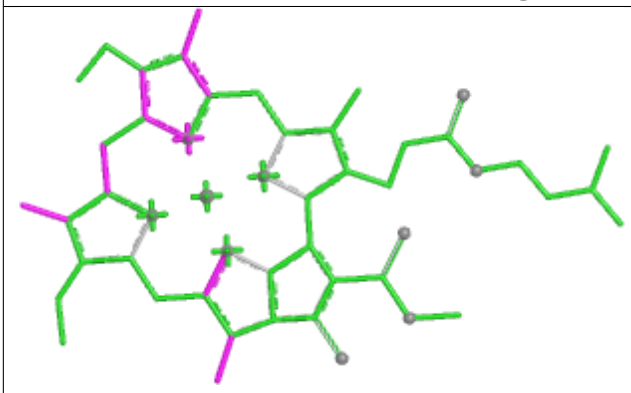
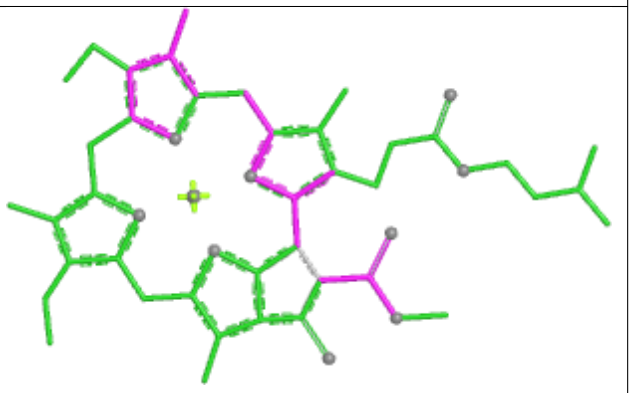
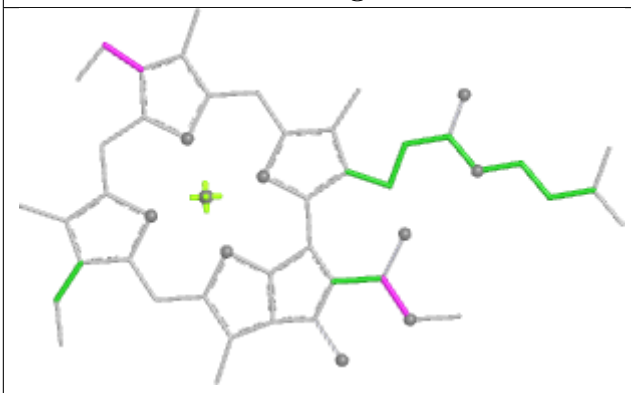
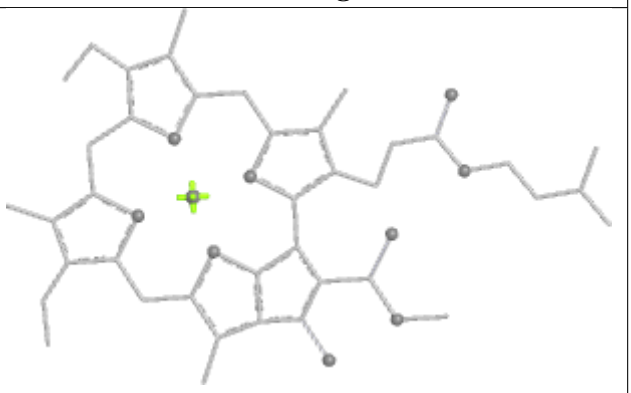


Rings

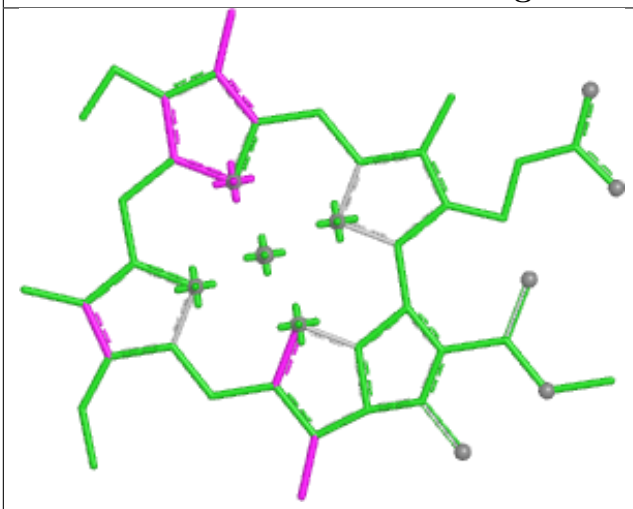
Ligand CLA A 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1115	
	
Bond lengths	Bond angles
	
Torsions	Rings

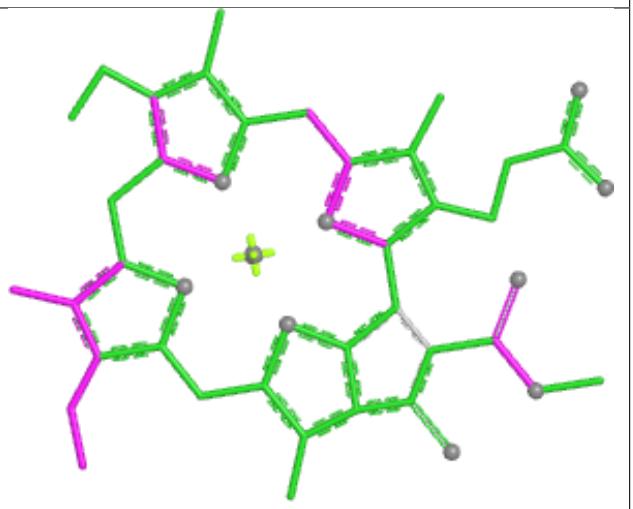
Ligand CLA m 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1112	
 Bond lengths	 Bond angles
 Torsions	 Rings

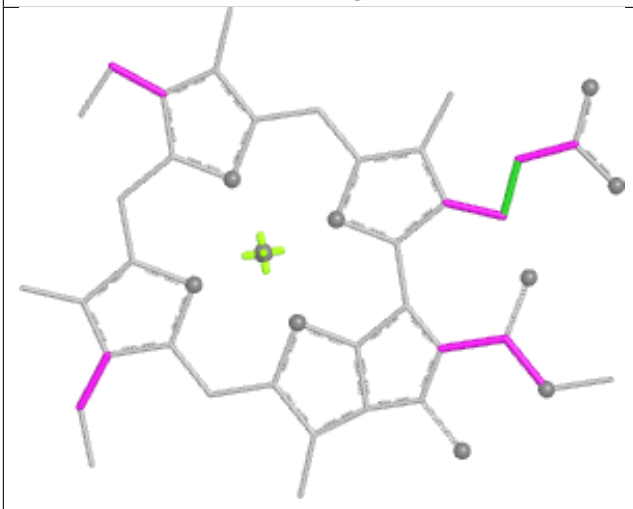
Ligand CLA K 1105



Bond lengths



Bond angles

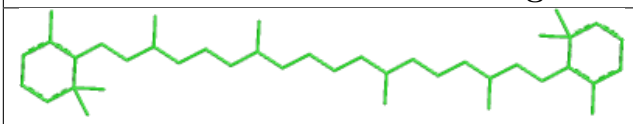


Torsions

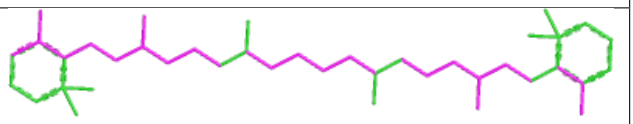


Rings

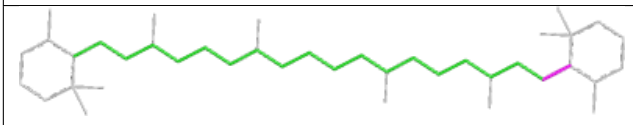
Ligand BCR 5 524



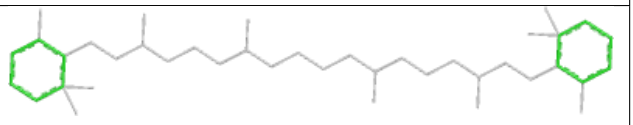
Bond lengths



Bond angles

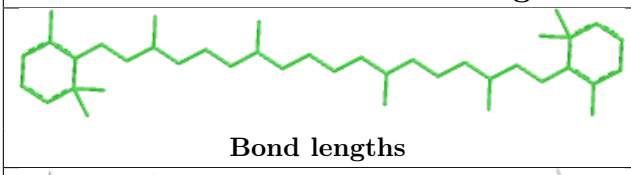


Torsions

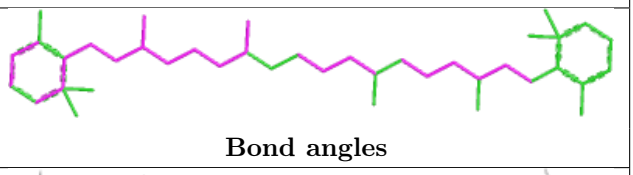


Rings

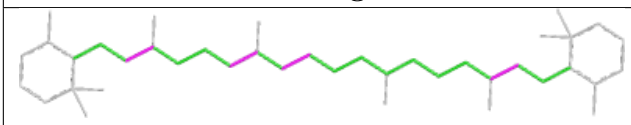
Ligand BCR A 4001



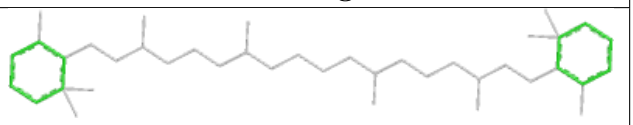
Bond lengths



Bond angles

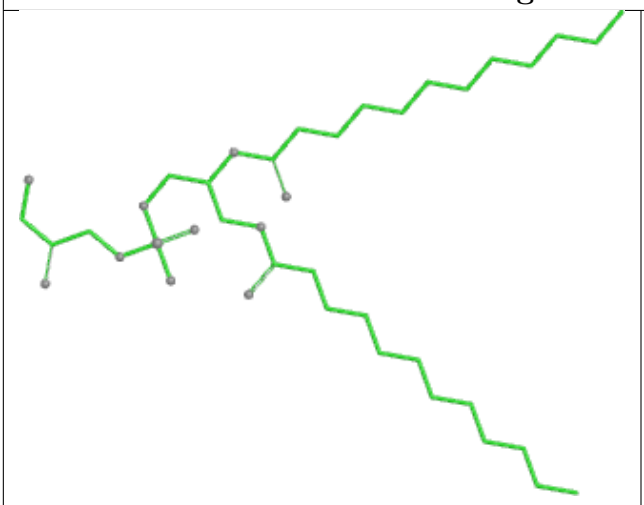


Torsions

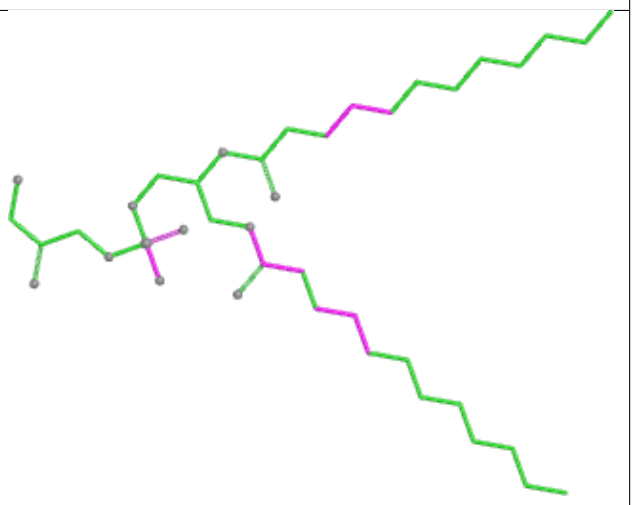


Rings

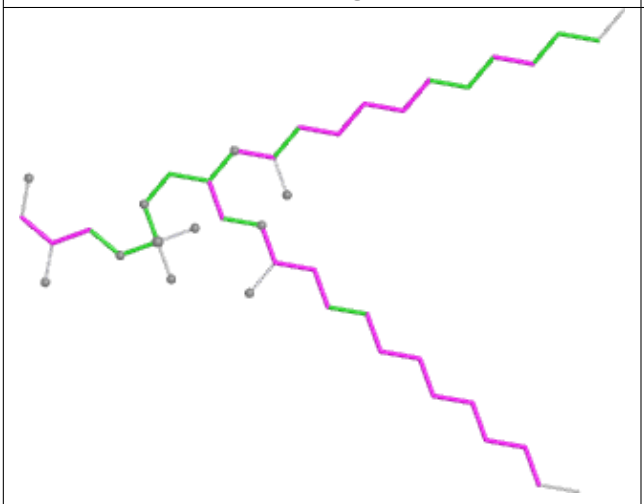
Ligand LHG n 5220



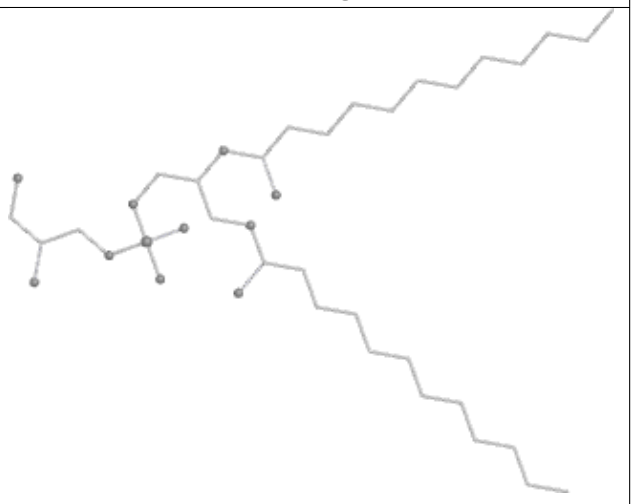
Bond lengths



Bond angles

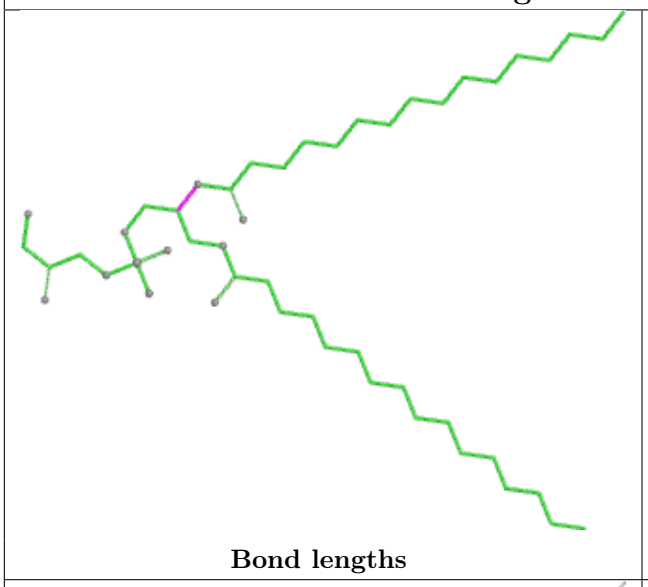


Torsions

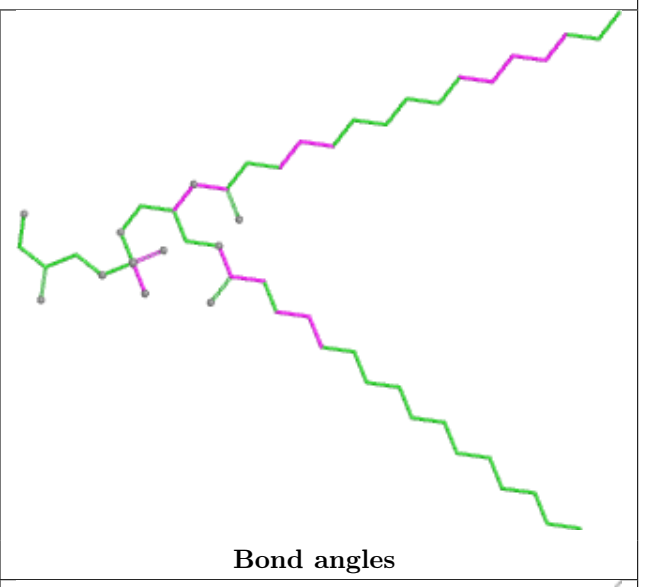


Rings

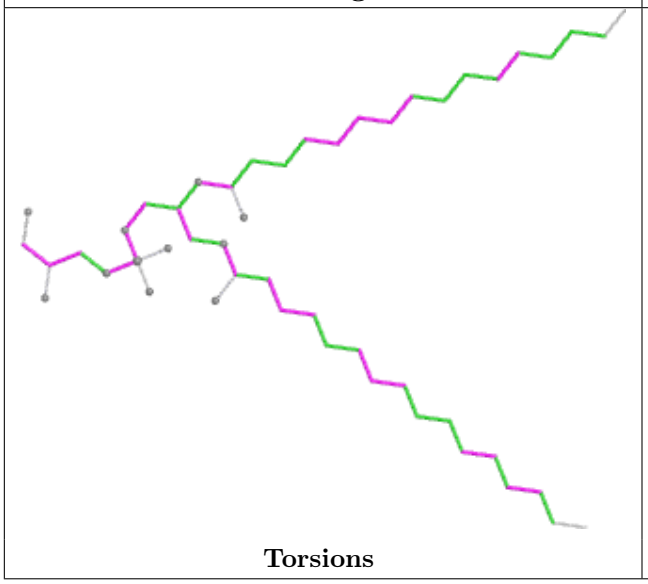
Ligand LHG G 5009



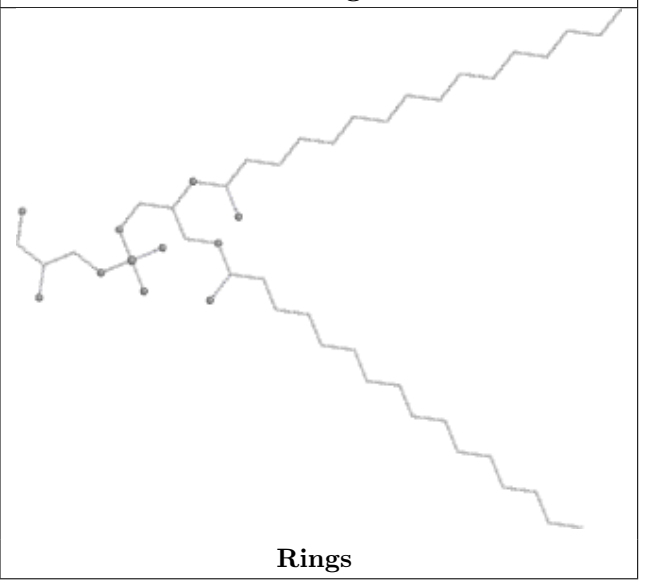
Bond lengths



Bond angles



Torsions

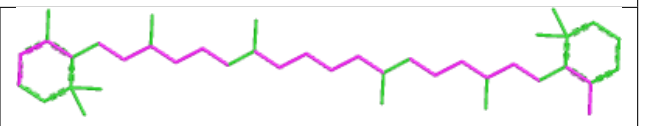


Rings

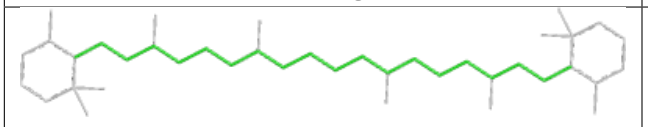
Ligand BCR G 4003



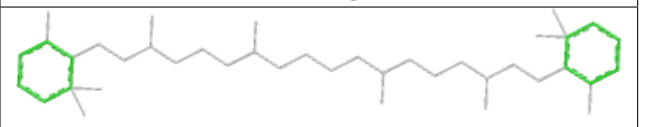
Bond lengths



Bond angles

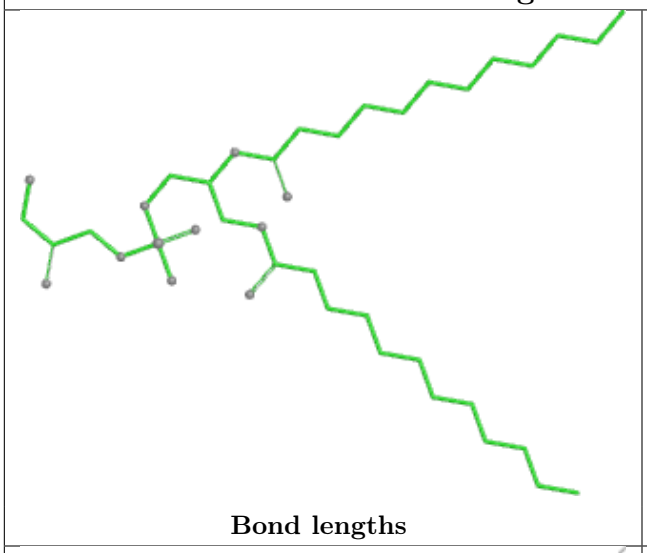


Torsions

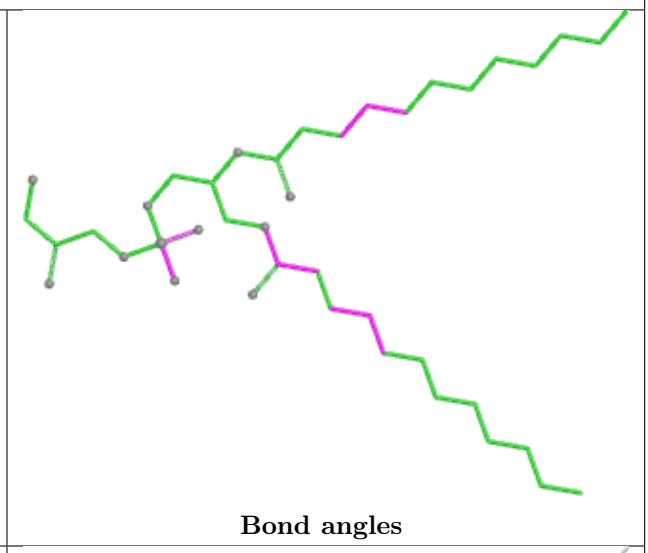


Rings

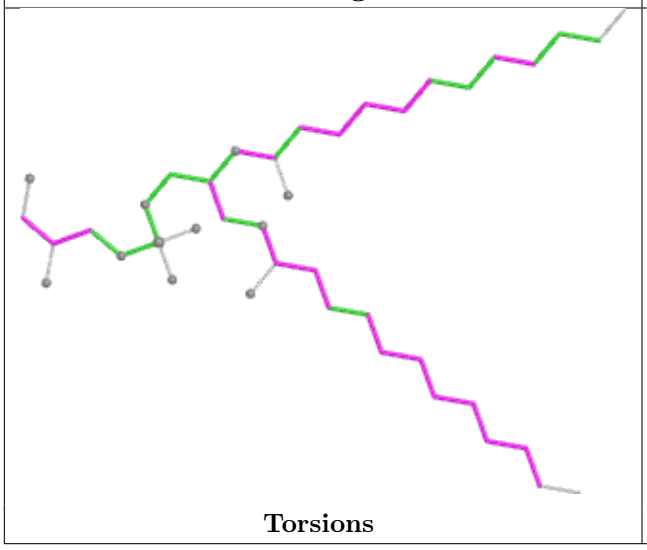
Ligand LHG L 5220



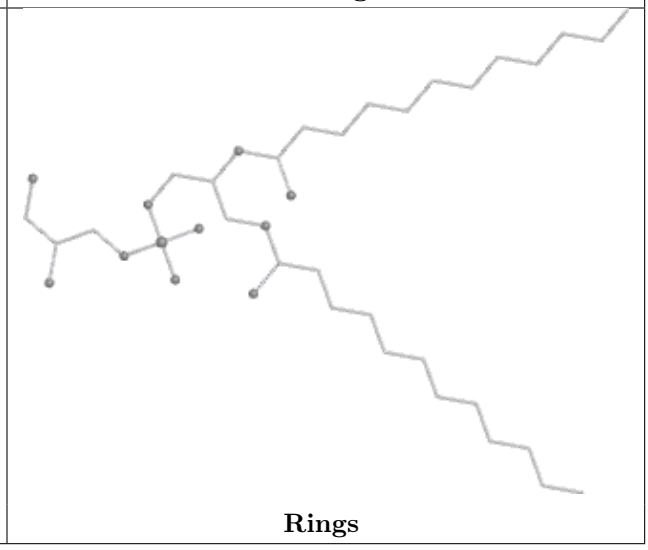
Bond lengths



Bond angles

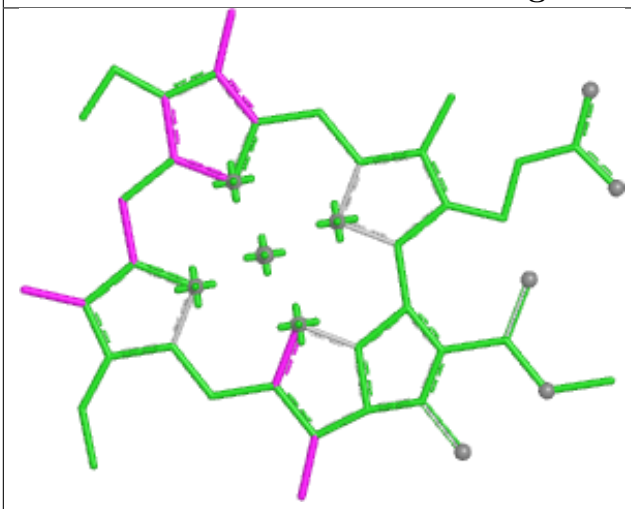


Torsions

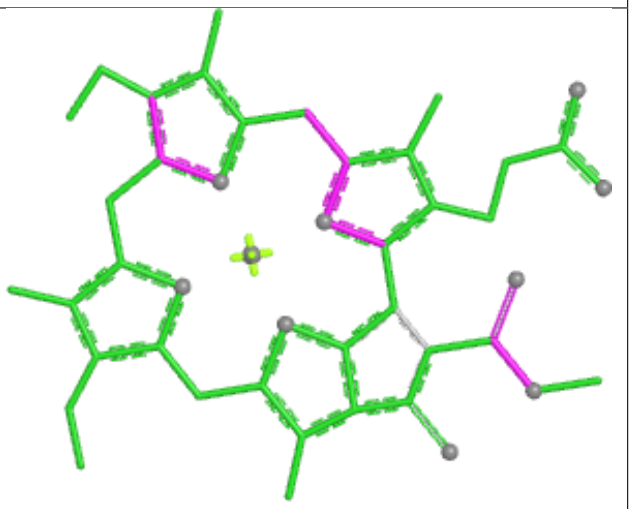


Rings

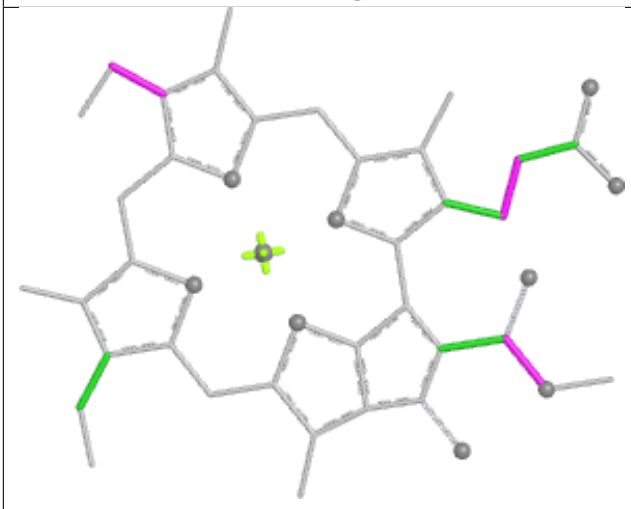
Ligand CLA 6 513



Bond lengths



Bond angles

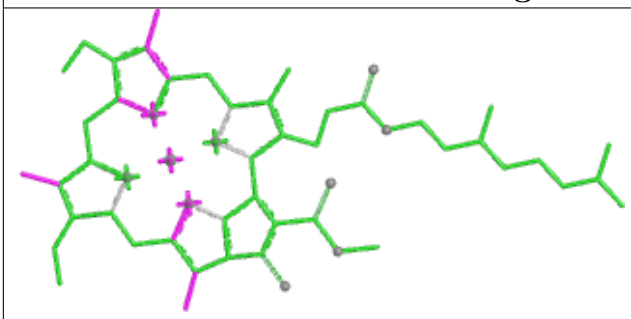


Torsions

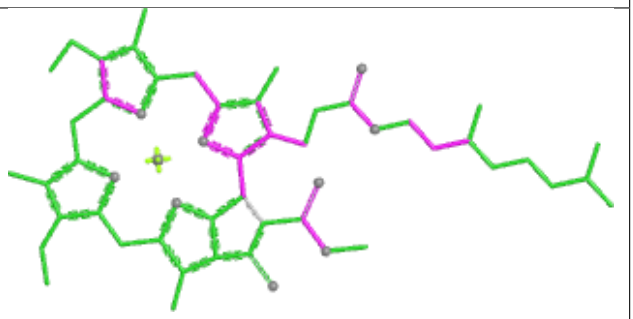


Rings

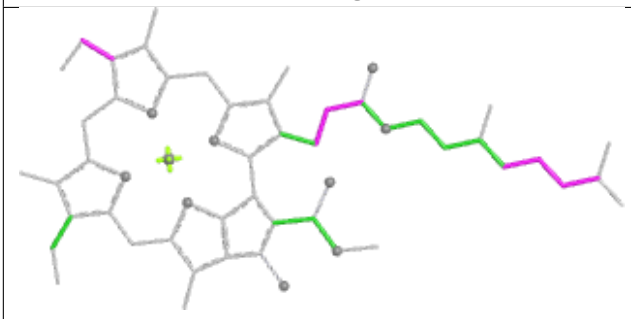
Ligand CLA G 1121



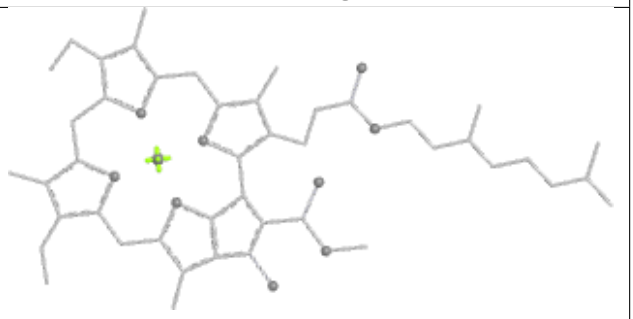
Bond lengths



Bond angles

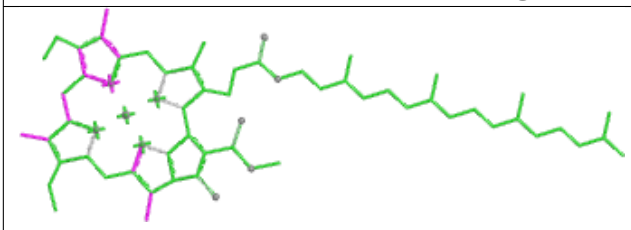


Torsions

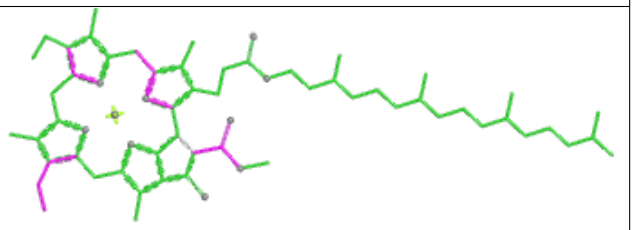


Rings

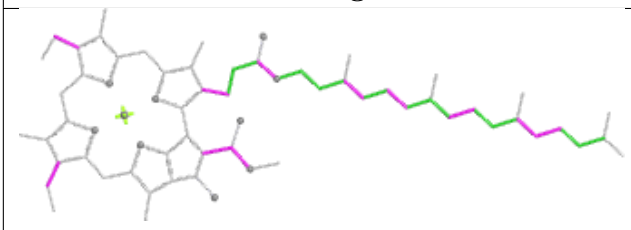
Ligand CLA G 1132



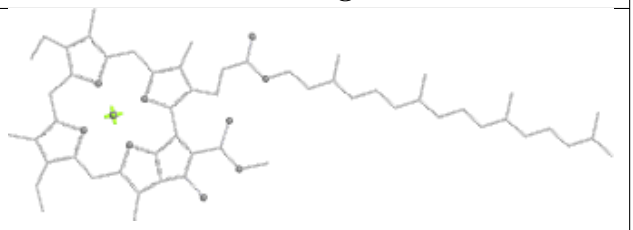
Bond lengths



Bond angles

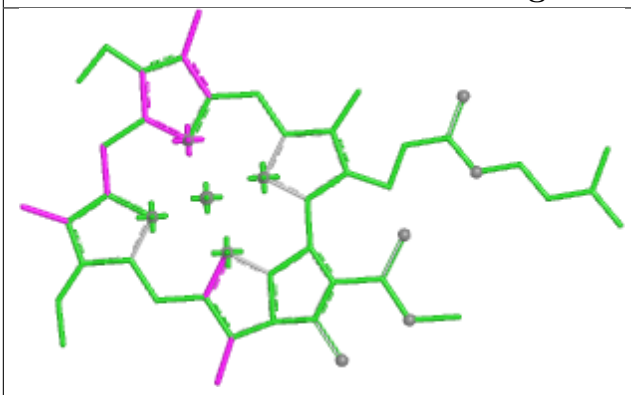


Torsions

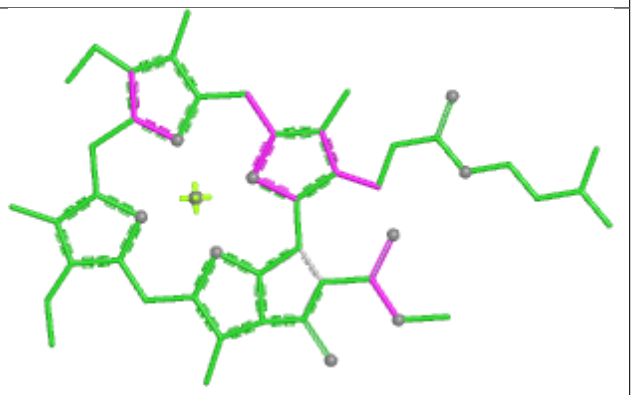


Rings

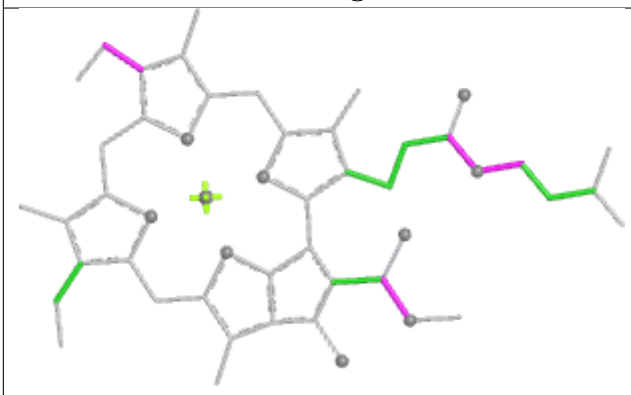
Ligand CLA 3 511



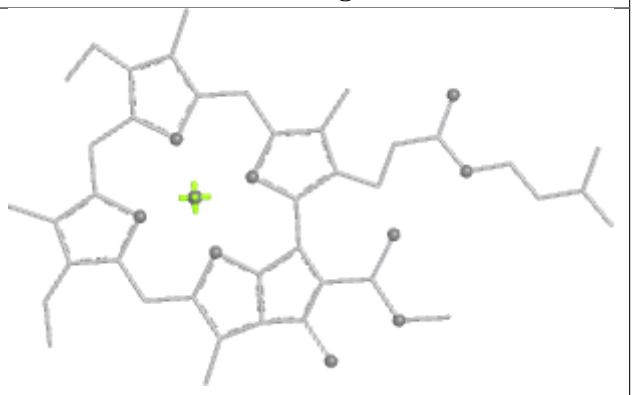
Bond lengths



Bond angles

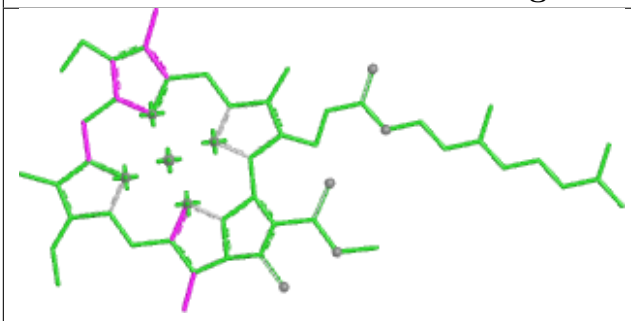


Torsions

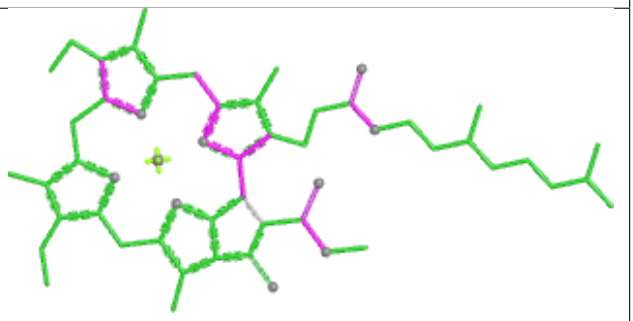


Rings

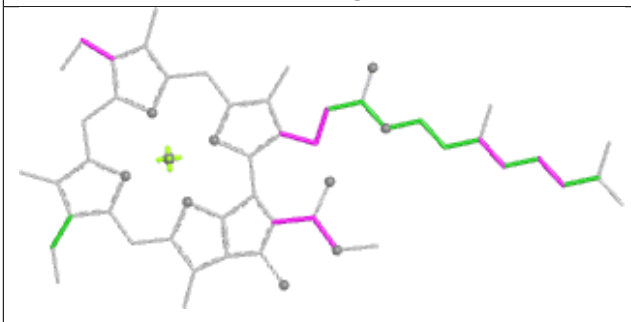
Ligand CLA c 503



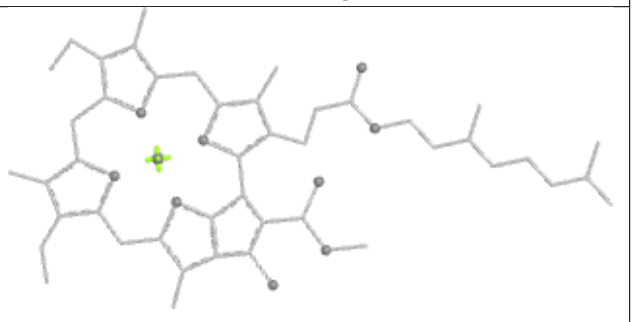
Bond lengths



Bond angles

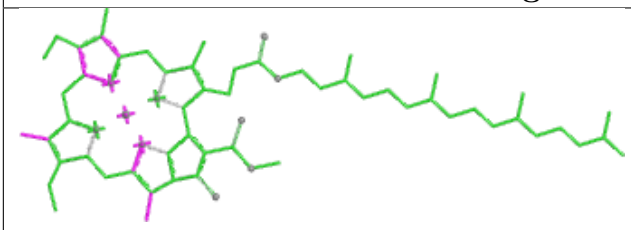


Torsions

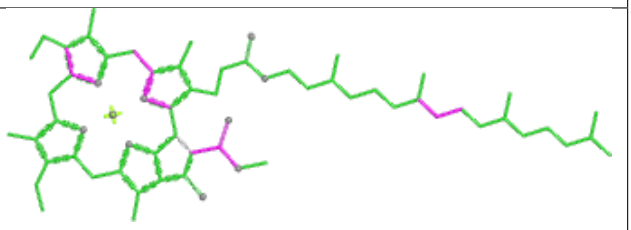


Rings

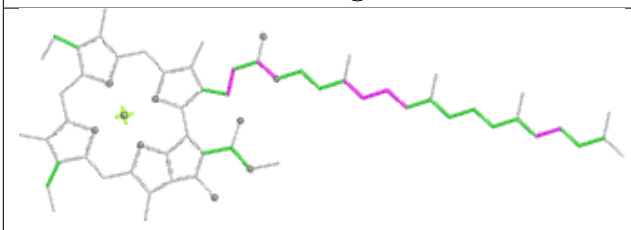
Ligand CLA f 1204



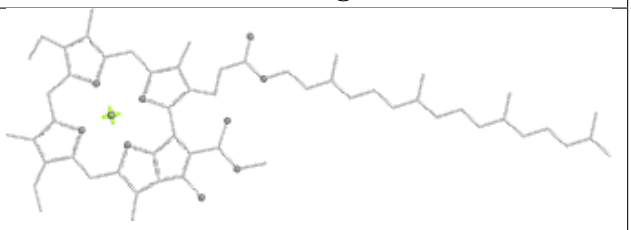
Bond lengths



Bond angles

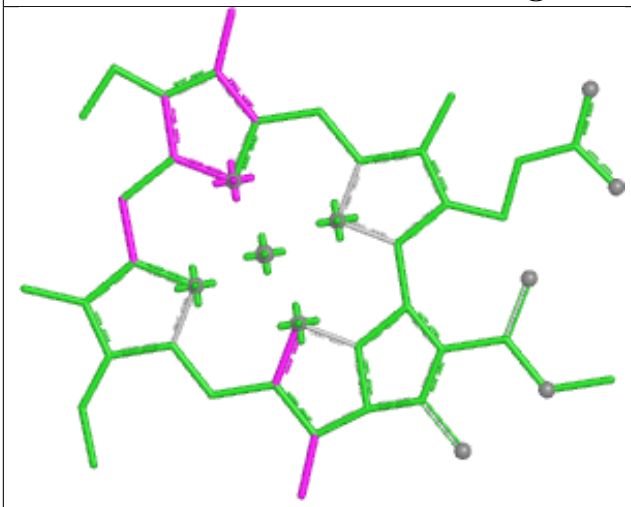


Torsions

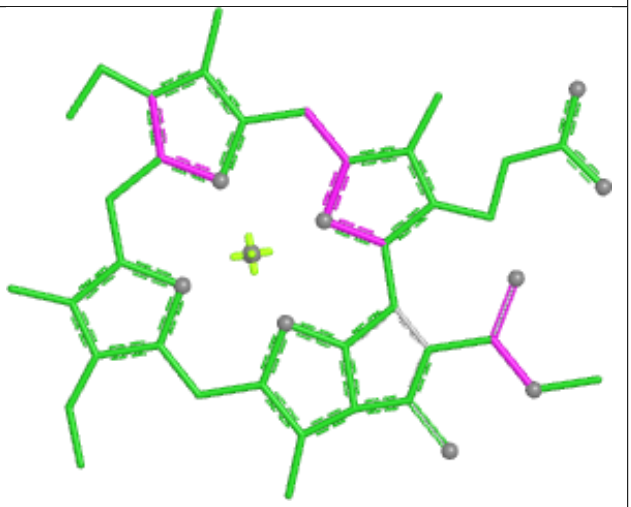


Rings

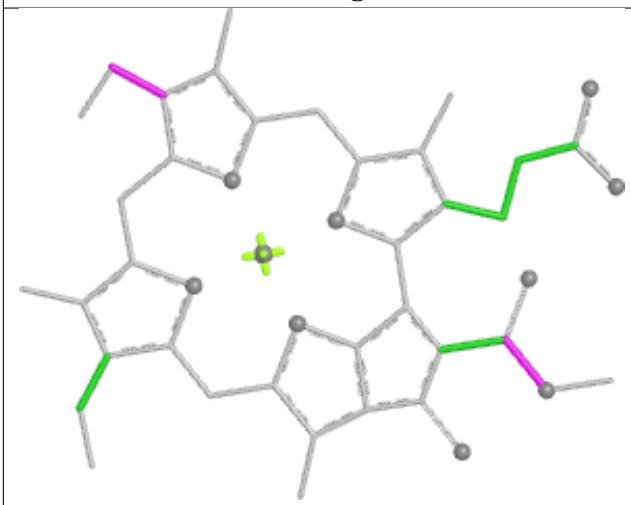
Ligand CLA u 504



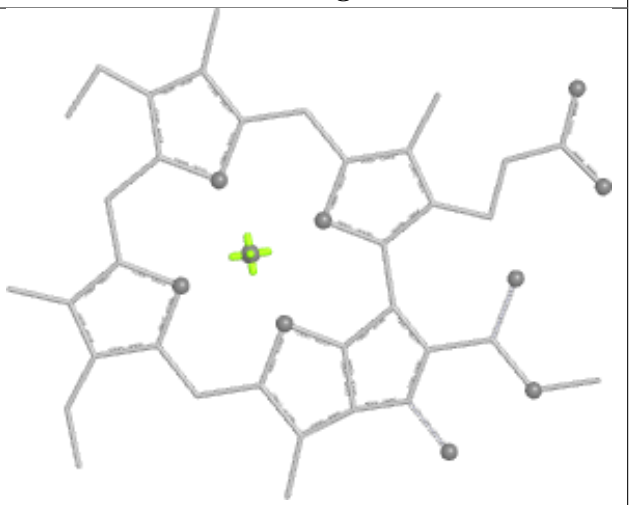
Bond lengths



Bond angles

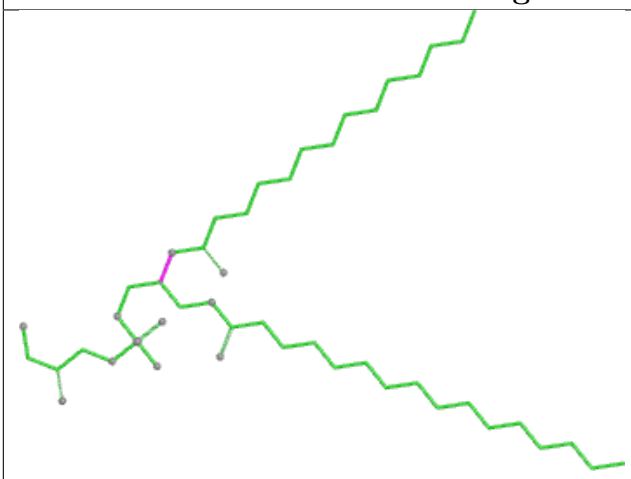


Torsions

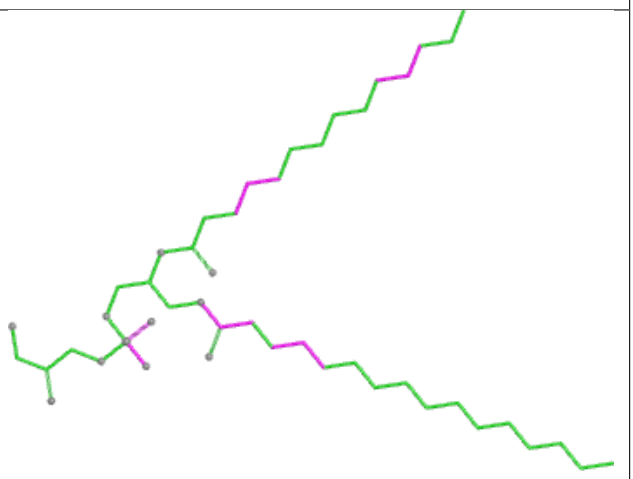


Rings

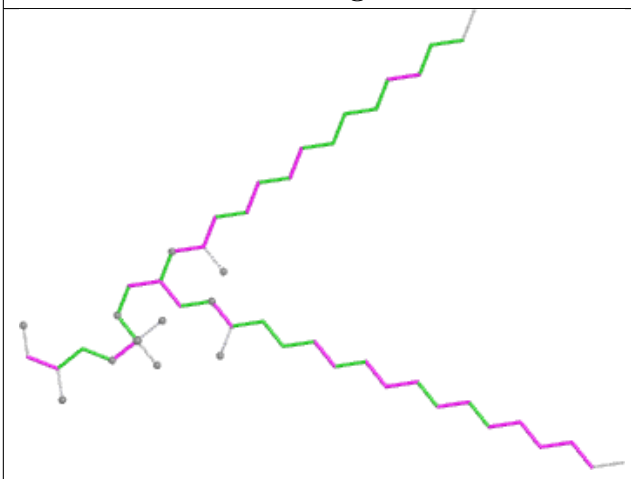
Ligand LHG G 5007



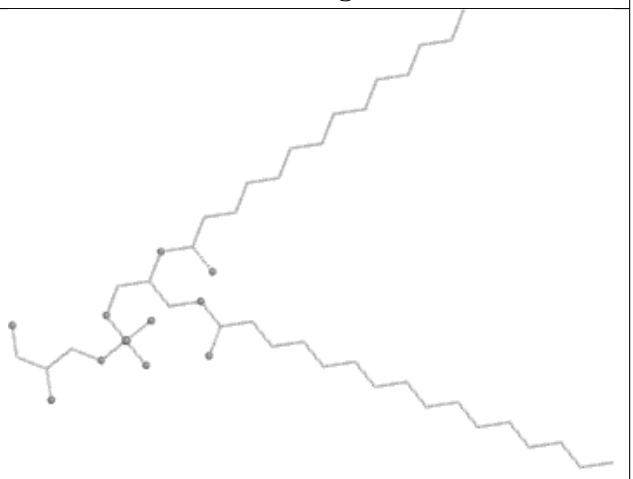
Bond lengths



Bond angles

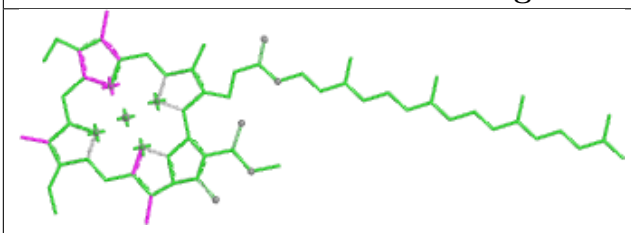


Torsions

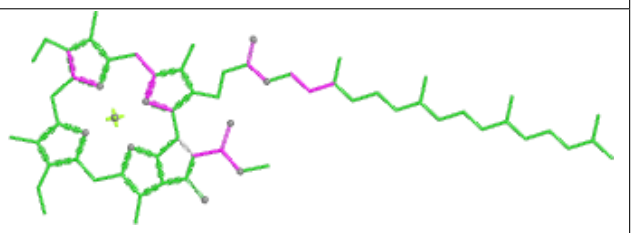


Rings

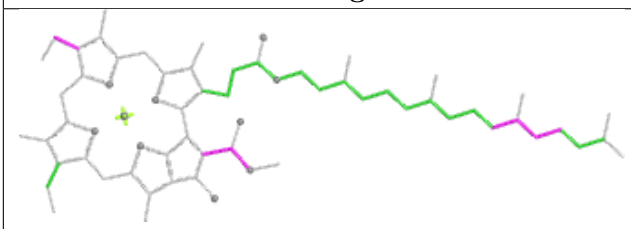
Ligand CLA G 1131



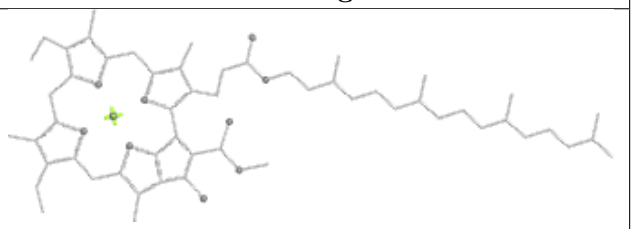
Bond lengths



Bond angles

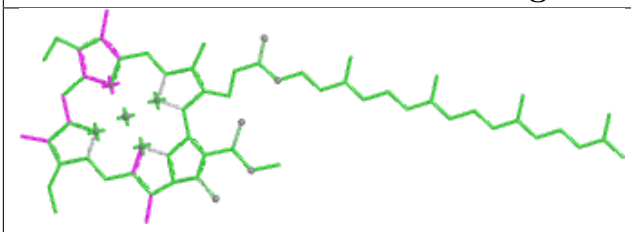


Torsions

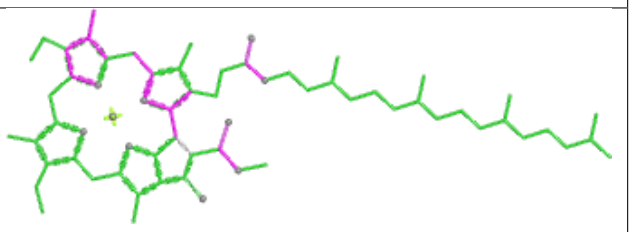


Rings

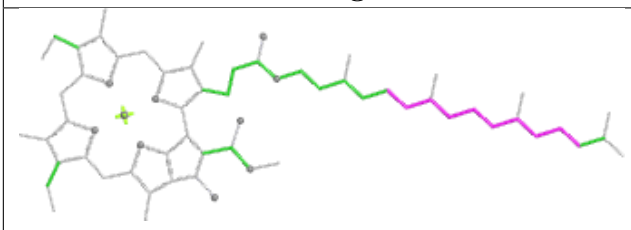
Ligand CLA c 509



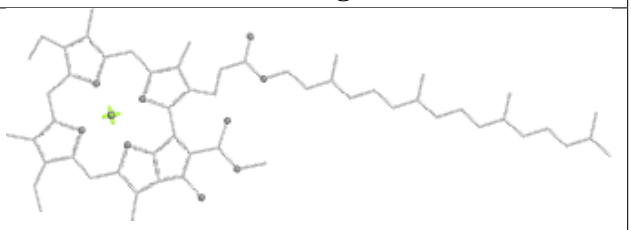
Bond lengths



Bond angles

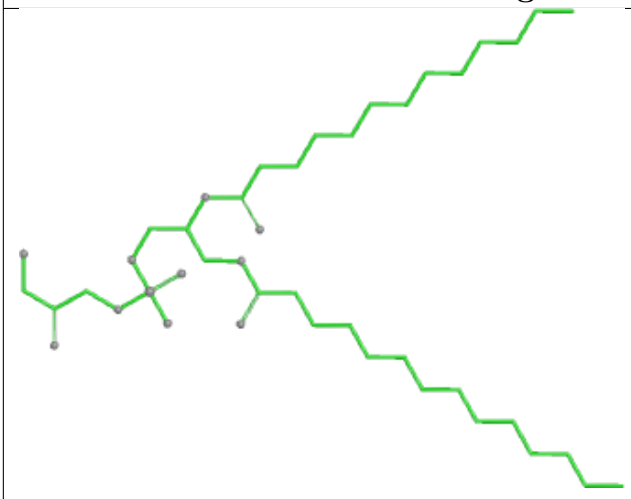


Torsions

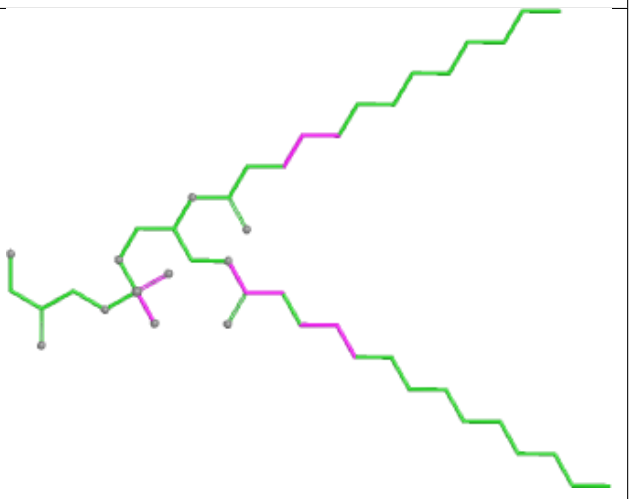


Rings

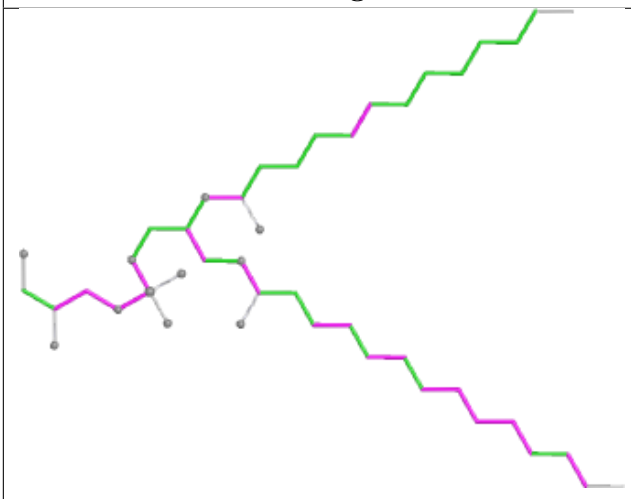
Ligand LHG k 5001



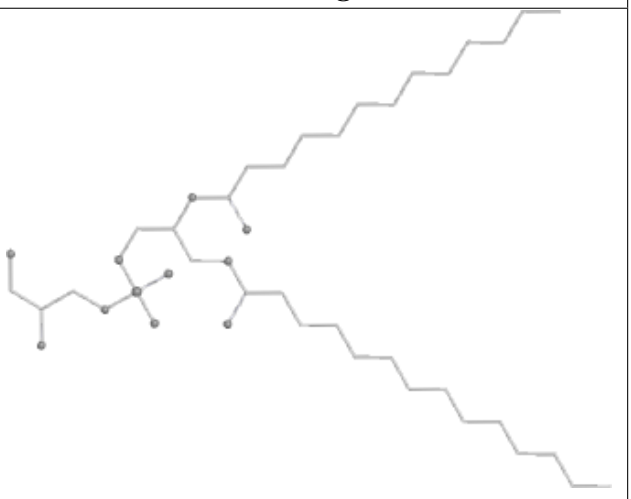
Bond lengths



Bond angles

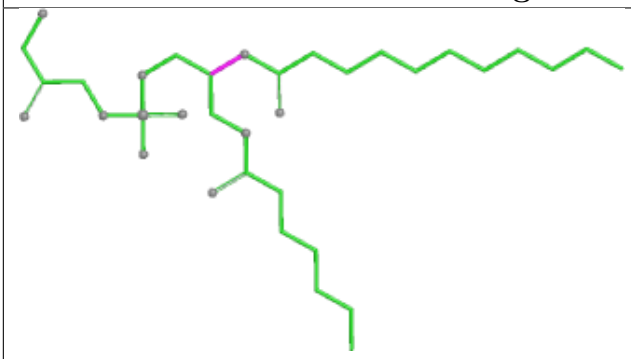


Torsions

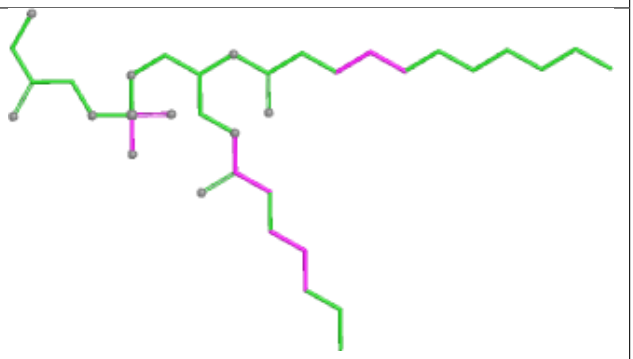


Rings

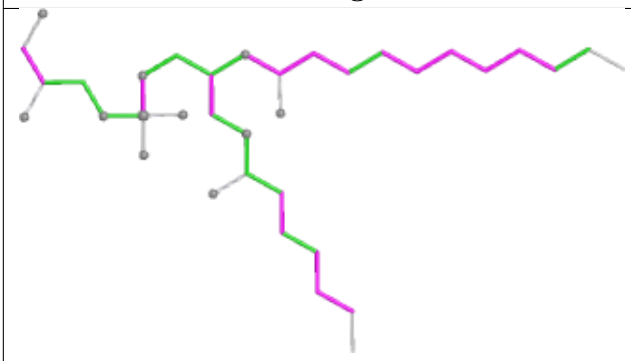
Ligand LHG A 5008



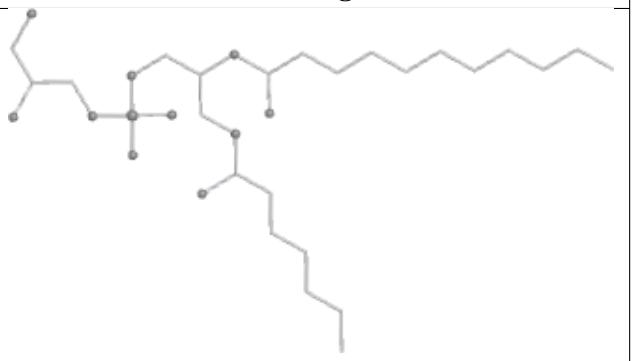
Bond lengths



Bond angles

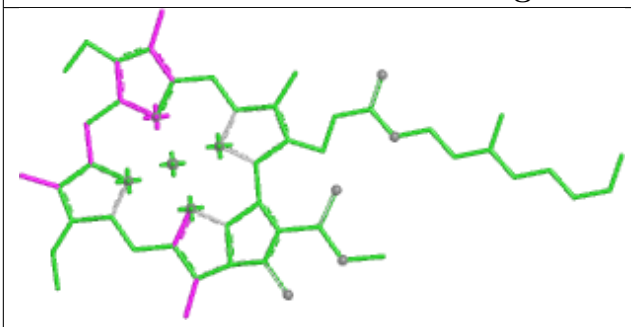


Torsions

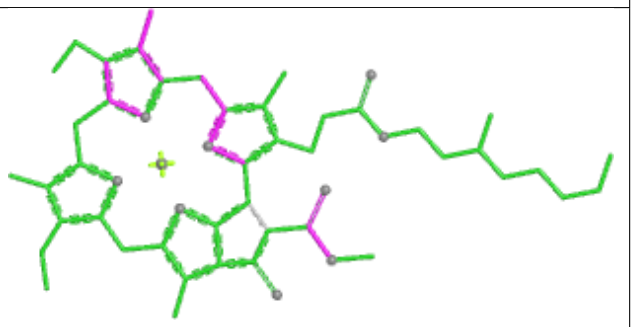


Rings

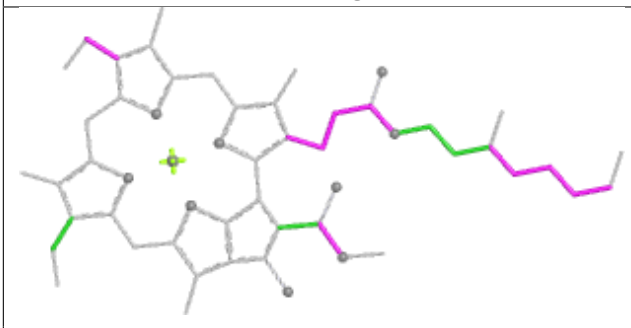
Ligand CLA G 1108



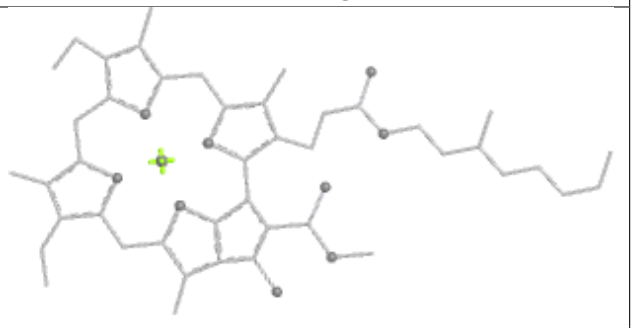
Bond lengths



Bond angles

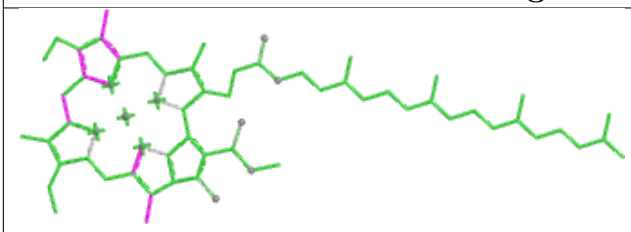


Torsions

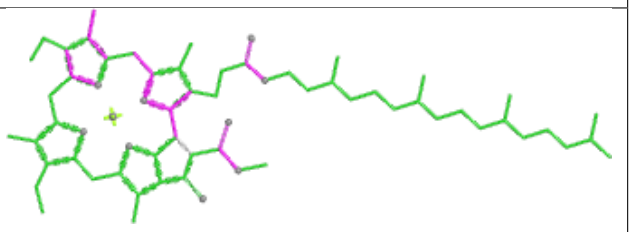


Rings

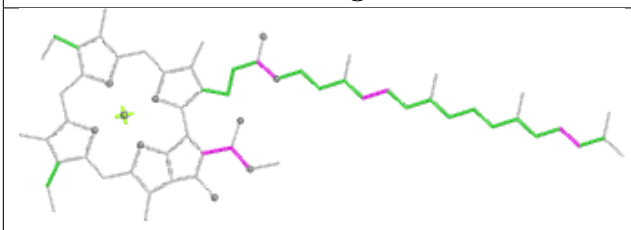
Ligand CLA b 509



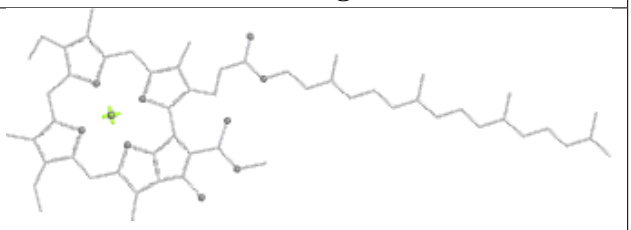
Bond lengths



Bond angles



Torsions

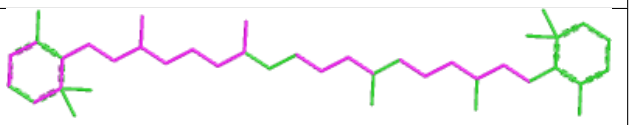


Rings

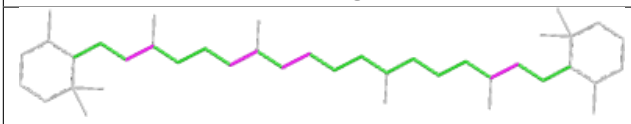
Ligand BCR e 4001



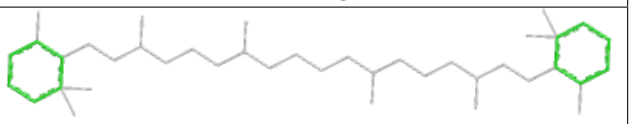
Bond lengths



Bond angles

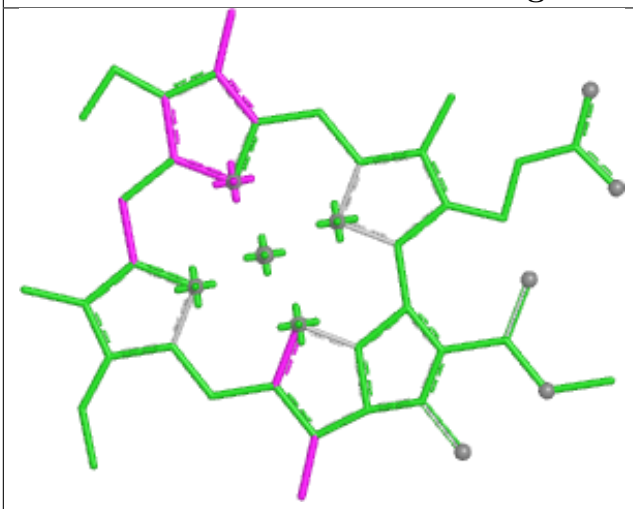


Torsions

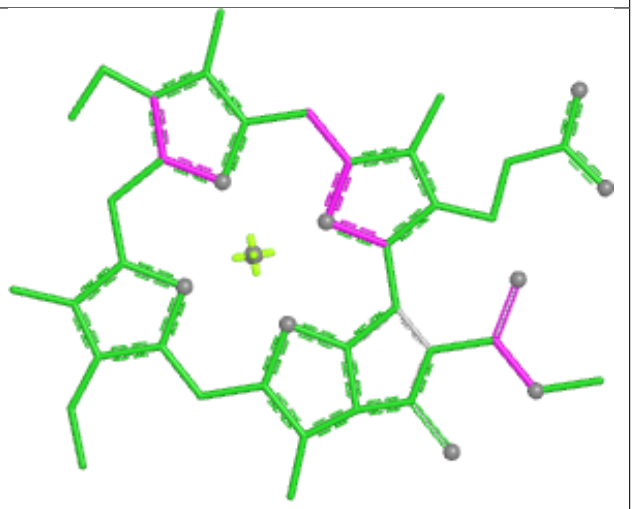


Rings

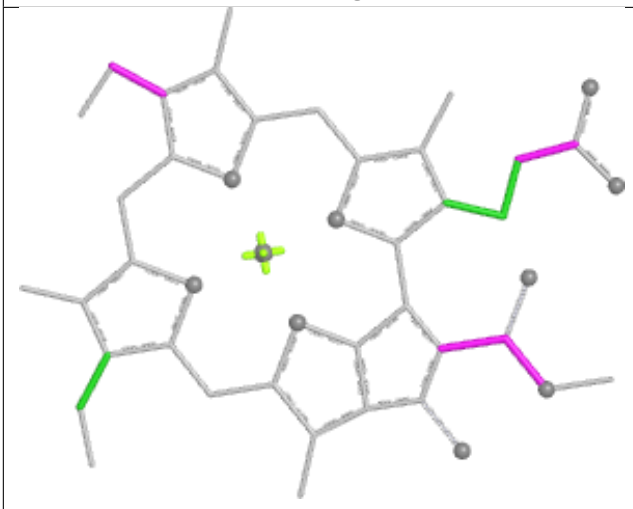
Ligand CLA u 510



Bond lengths



Bond angles

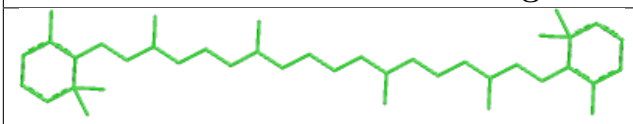


Torsions

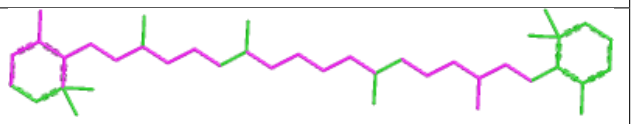


Rings

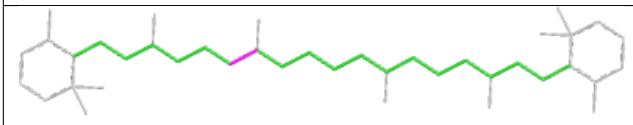
Ligand BCR Y 524



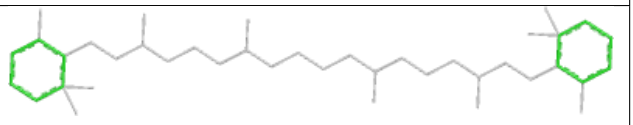
Bond lengths



Bond angles

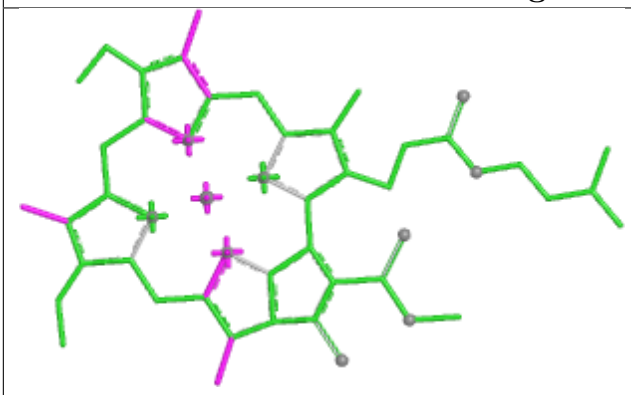


Torsions

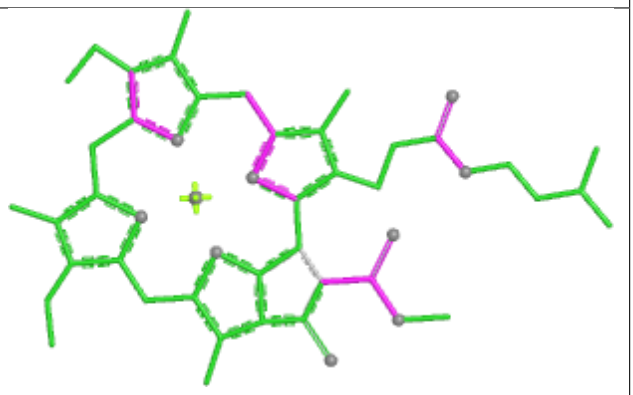


Rings

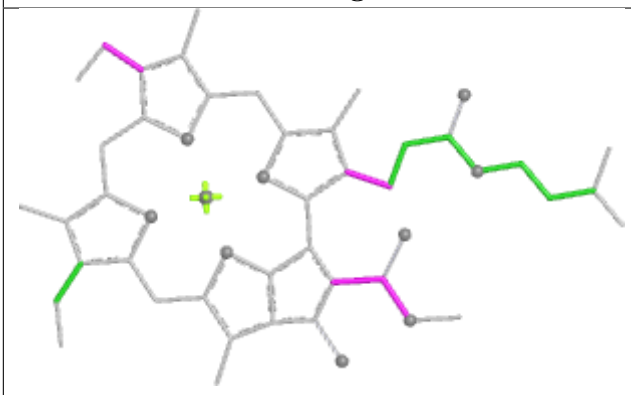
Ligand CLA 1 519



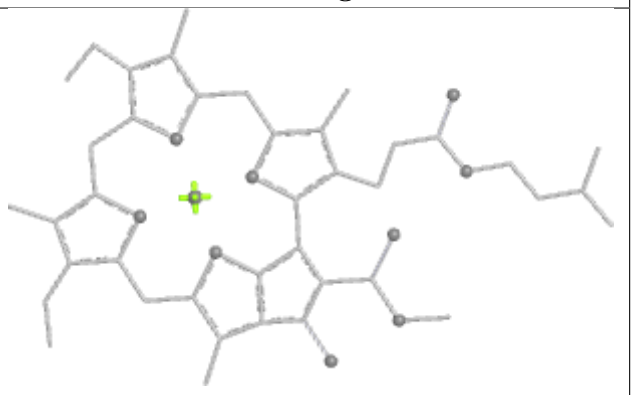
Bond lengths



Bond angles

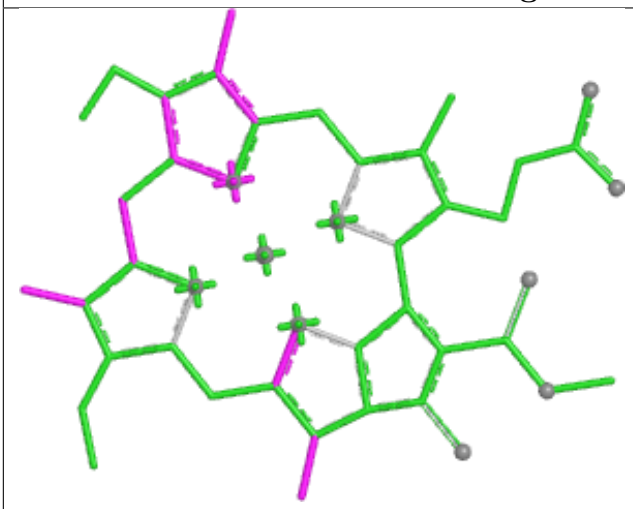


Torsions

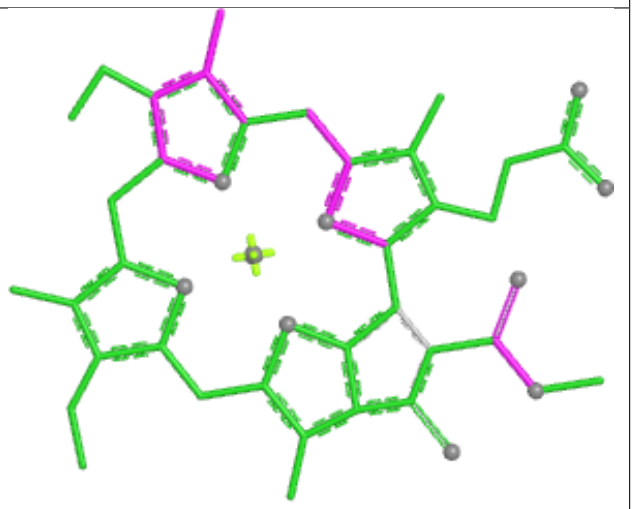


Rings

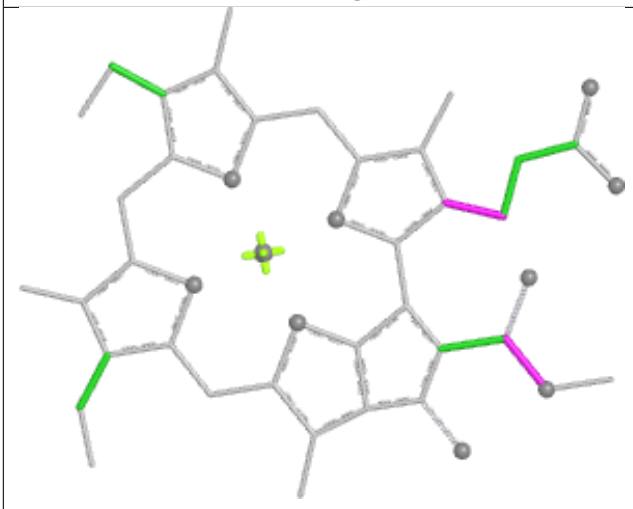
Ligand CLA e 1113



Bond lengths



Bond angles

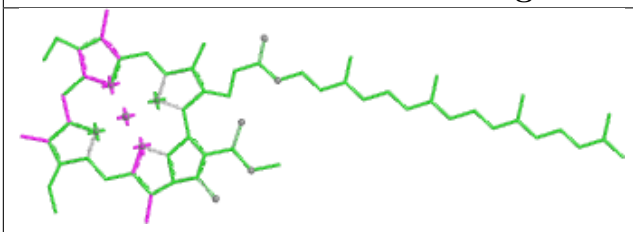


Torsions

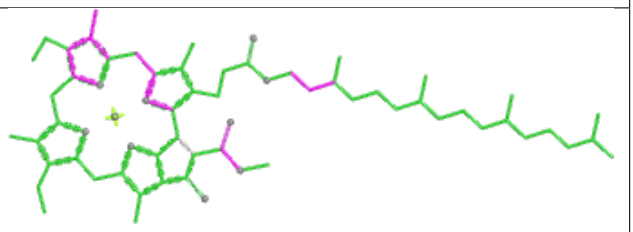


Rings

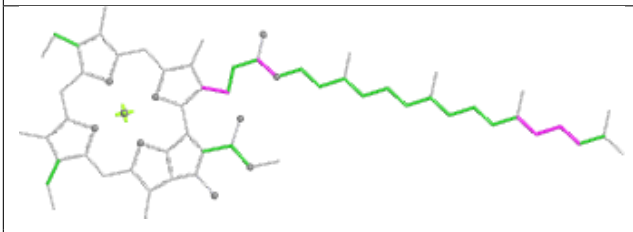
Ligand CLA B 1225



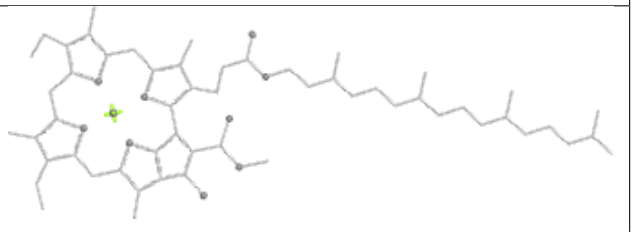
Bond lengths



Bond angles

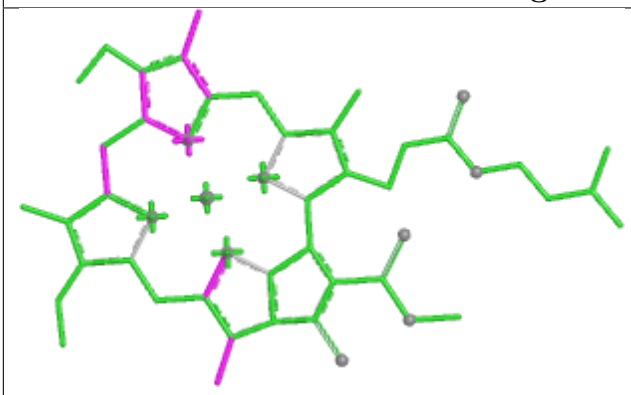


Torsions

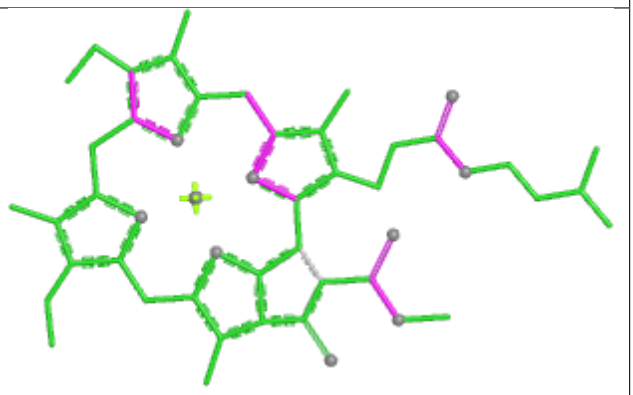


Rings

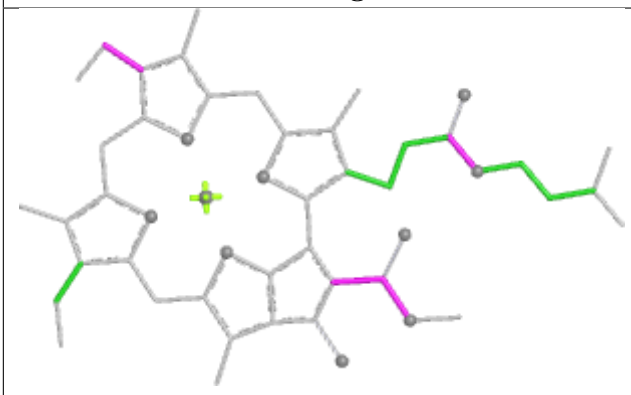
Ligand CLA t 510



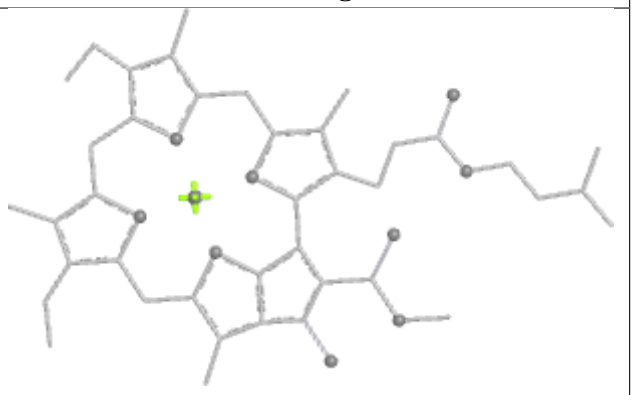
Bond lengths



Bond angles

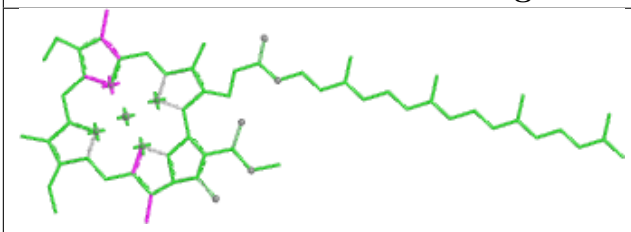


Torsions

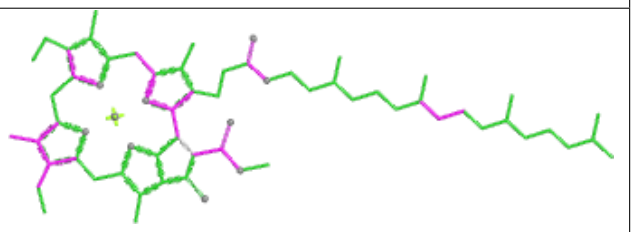


Rings

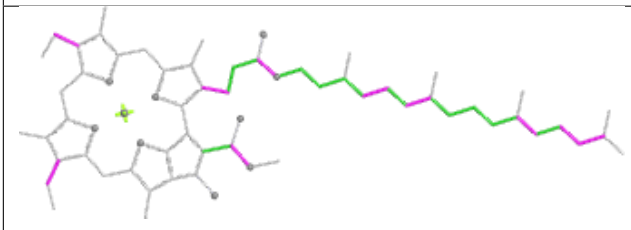
Ligand CLA H 1239



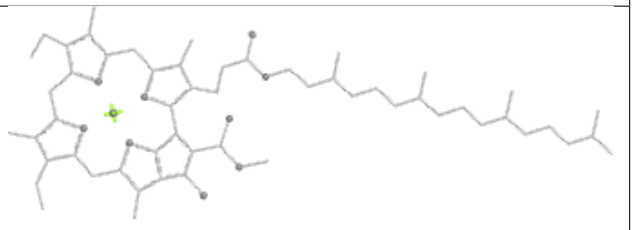
Bond lengths



Bond angles

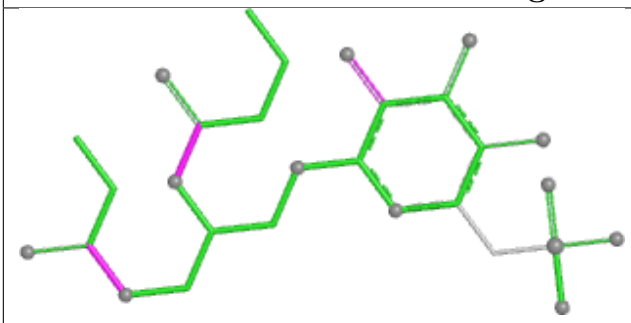


Torsions

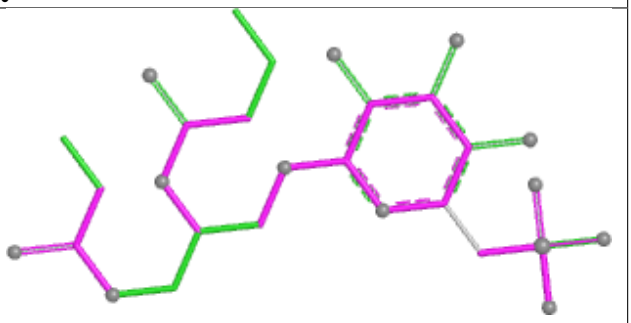


Rings

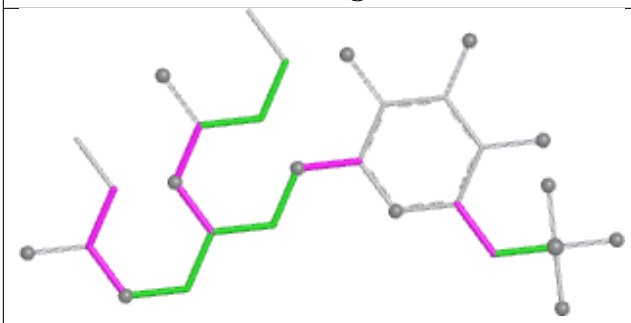
Ligand SQD 5 822



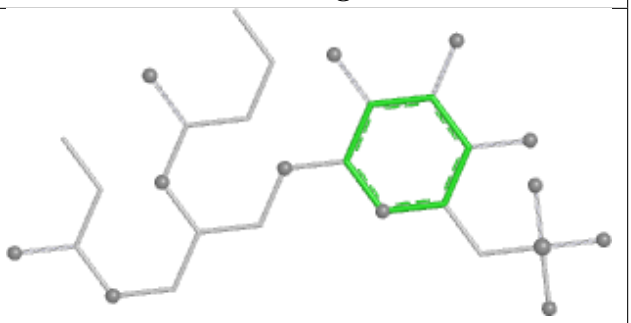
Bond lengths



Bond angles



Torsions

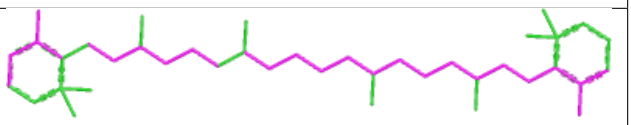


Rings

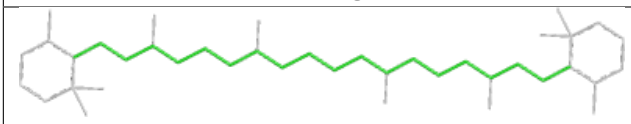
Ligand BCR A 4002



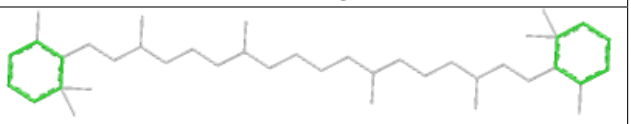
Bond lengths



Bond angles

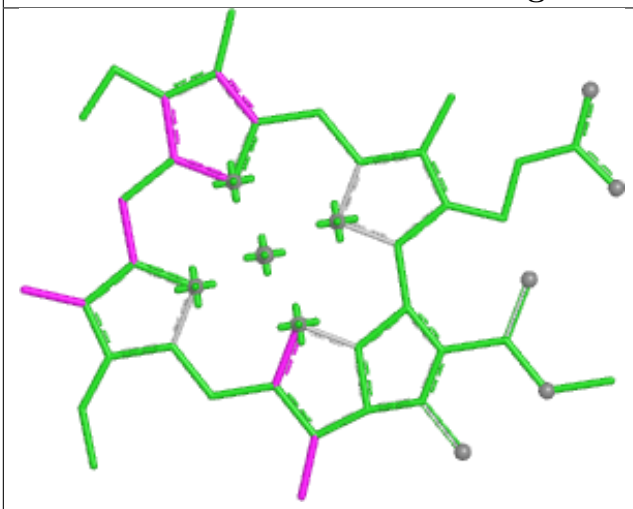


Torsions

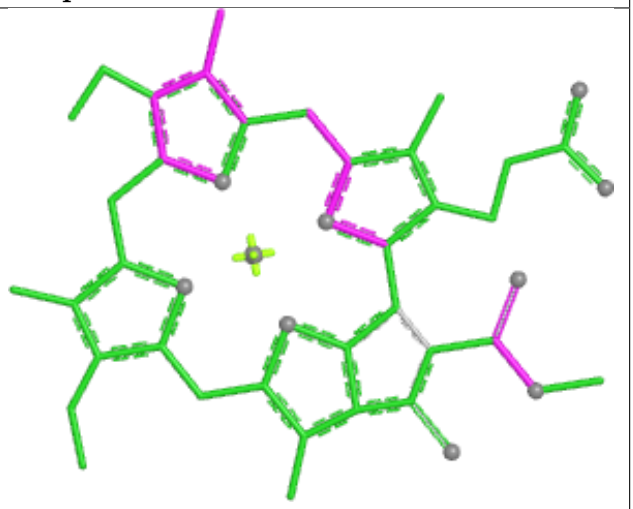


Rings

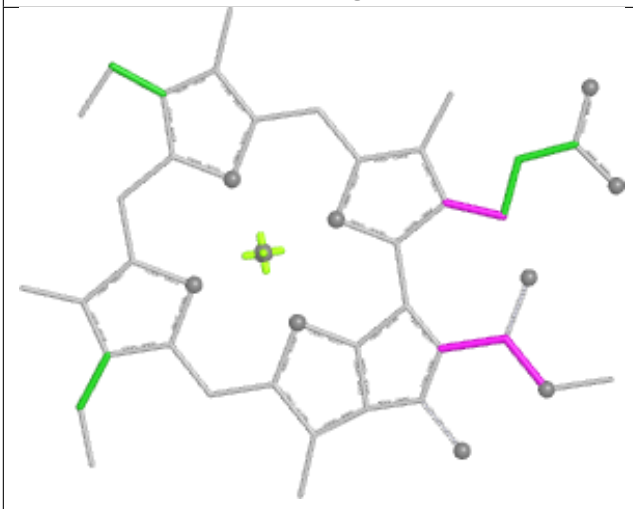
Ligand CLA q 506



Bond lengths



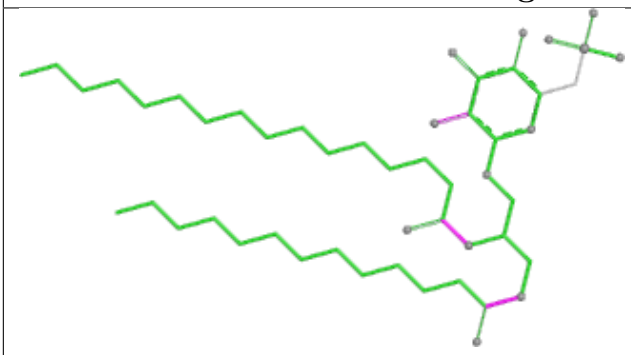
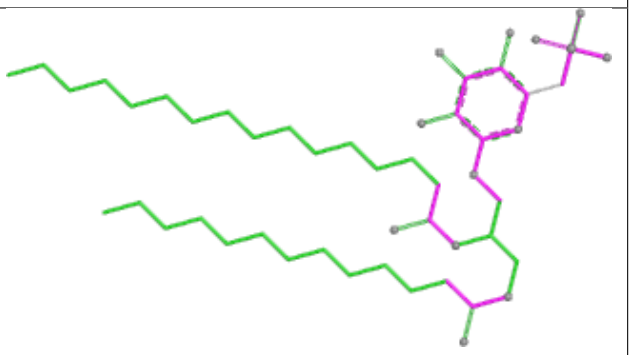
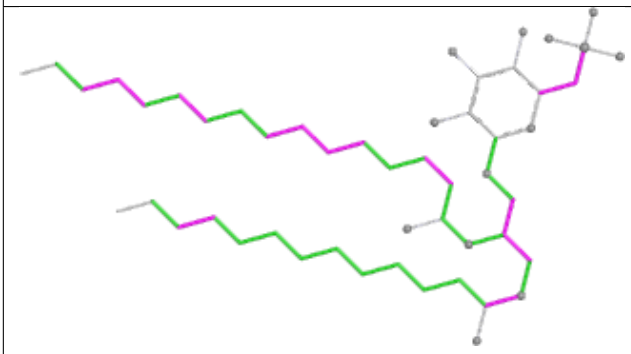
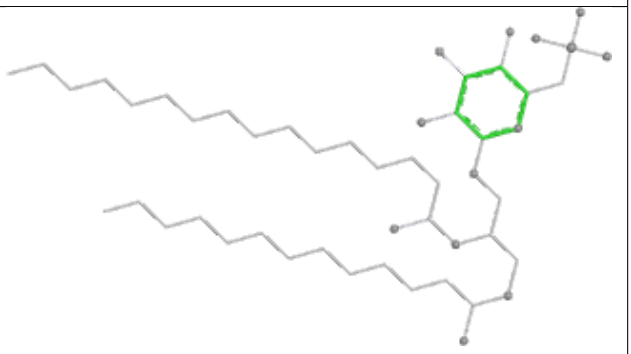
Bond angles

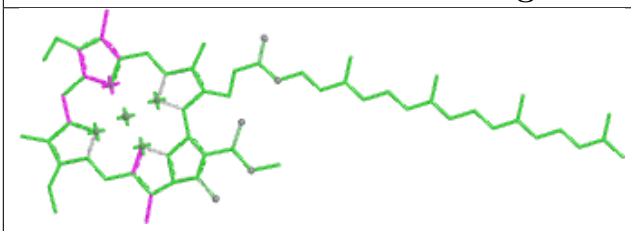
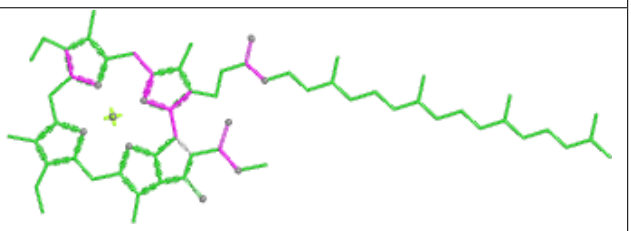
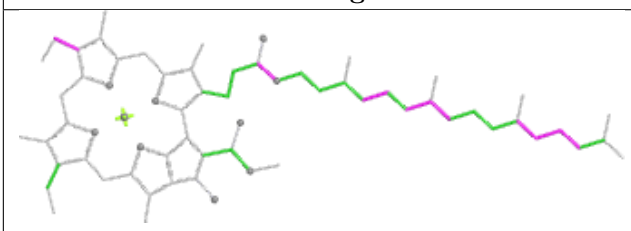
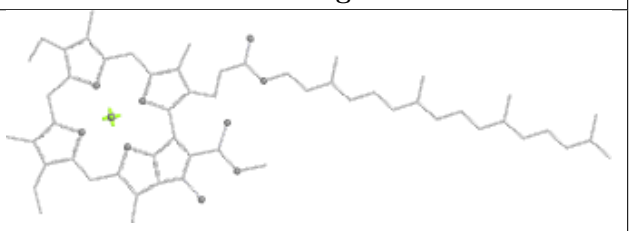


Torsions

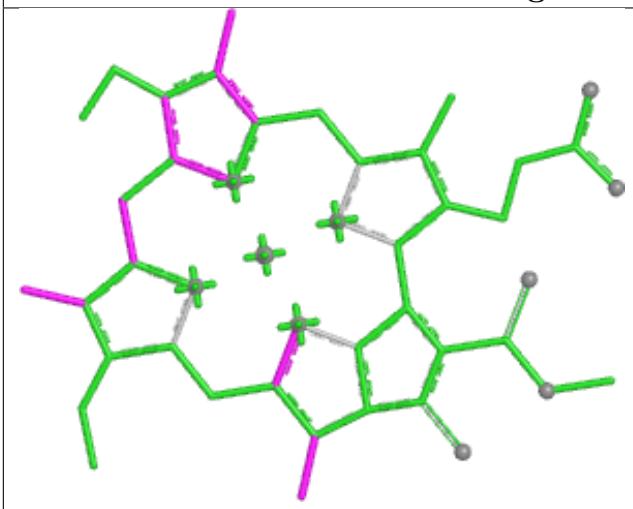


Rings

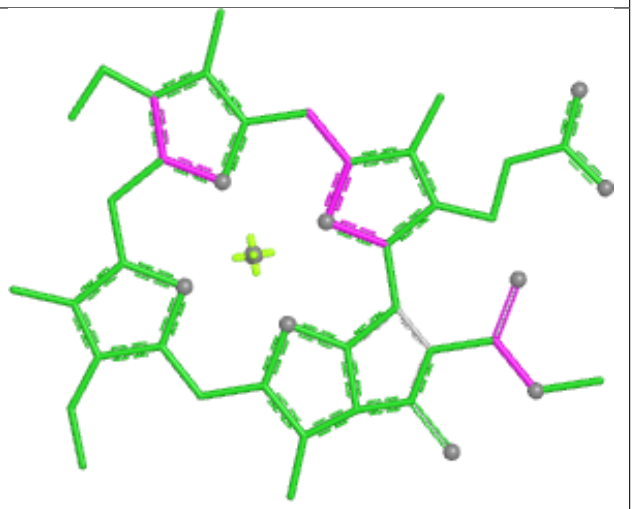
Ligand SQD L 5216	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

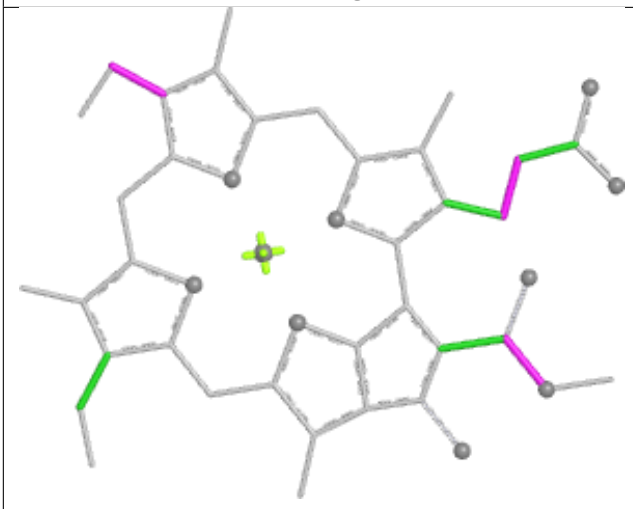
Ligand CLA v 513



Bond lengths



Bond angles

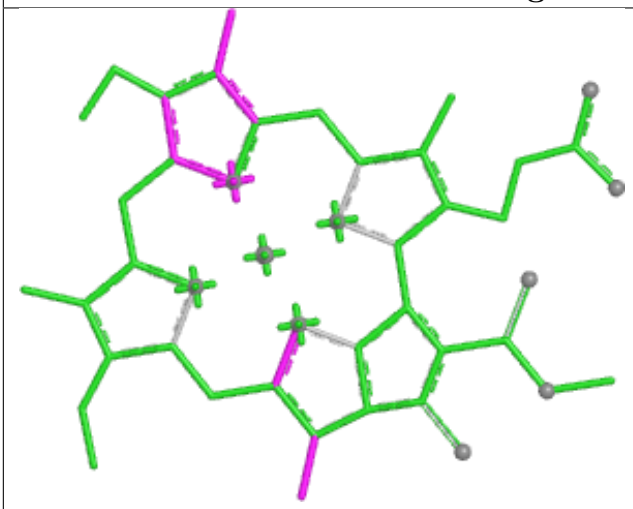


Torsions

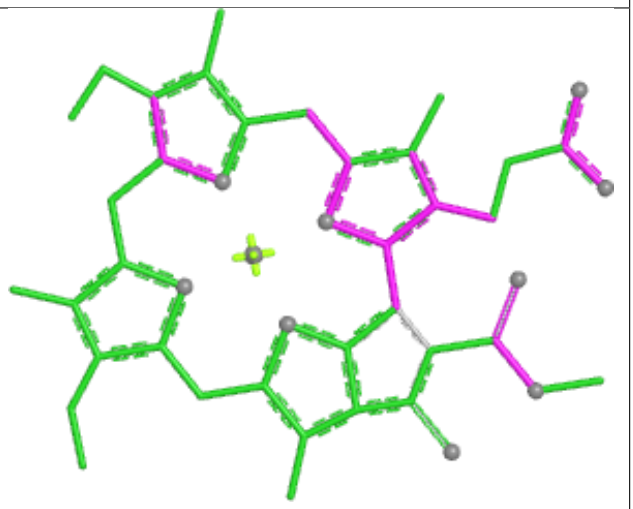


Rings

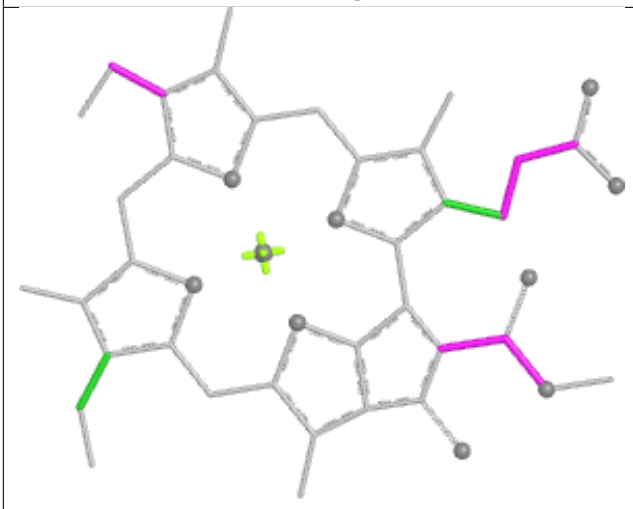
Ligand CLA u 507



Bond lengths



Bond angles

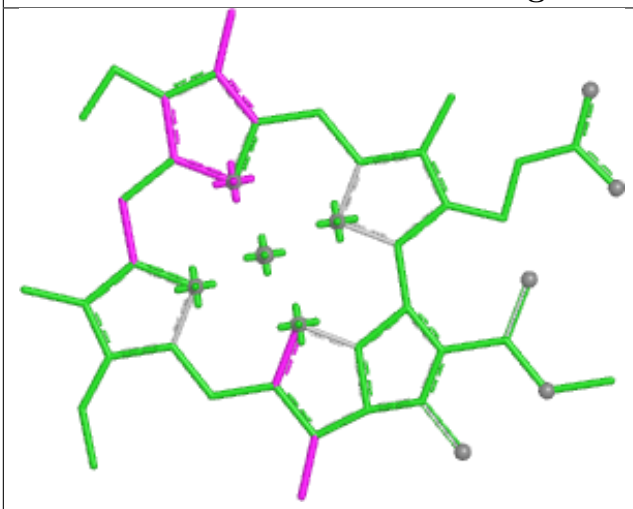


Torsions

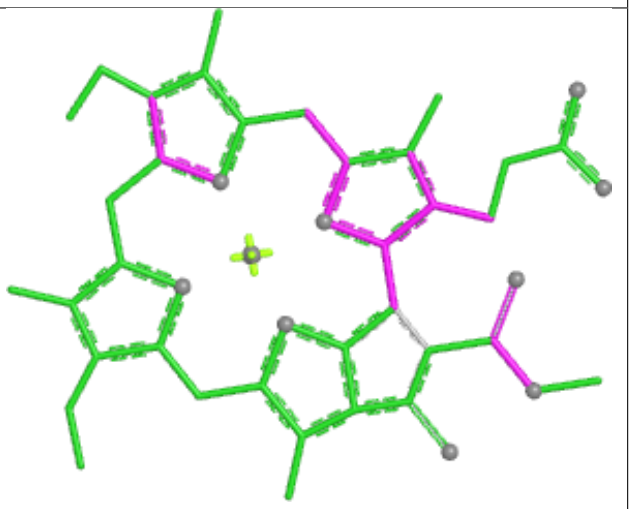


Rings

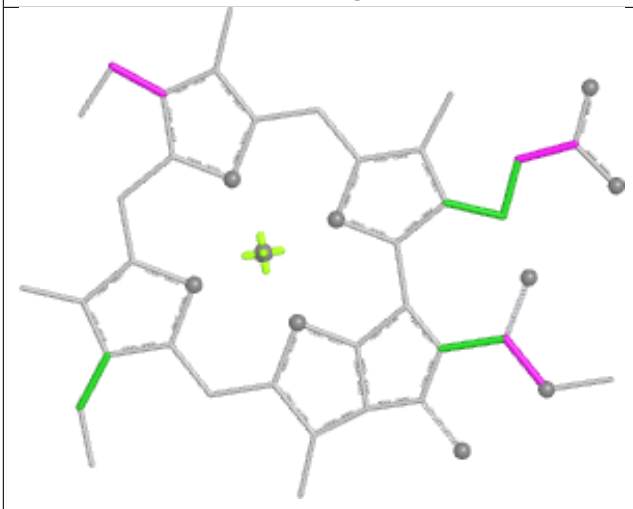
Ligand CLA v 507



Bond lengths



Bond angles

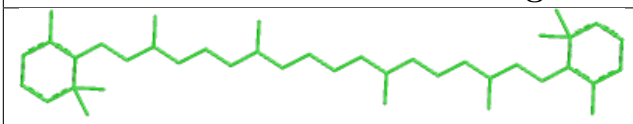


Torsions

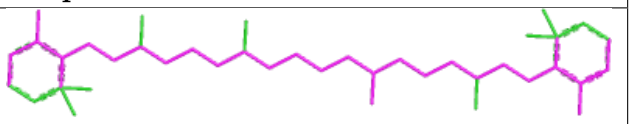


Rings

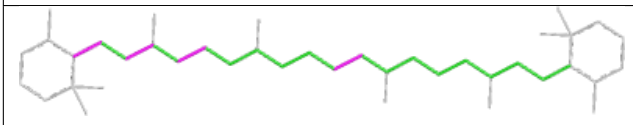
Ligand BCR q 522



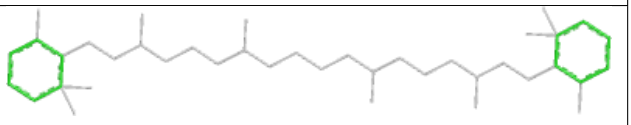
Bond lengths



Bond angles

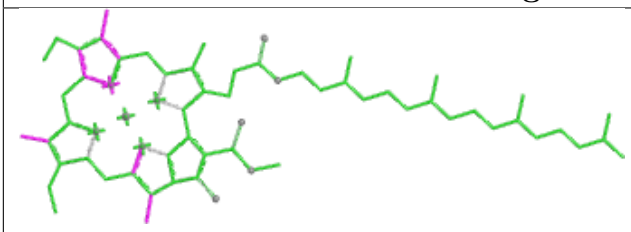


Torsions

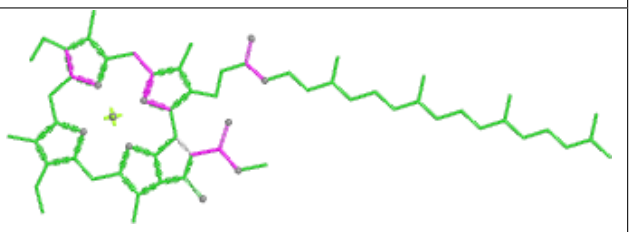


Rings

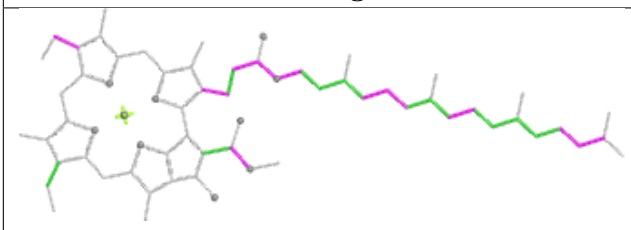
Ligand CLA f 1219



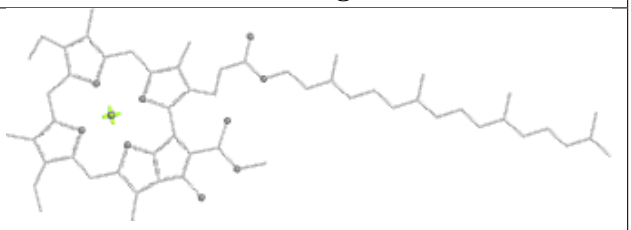
Bond lengths



Bond angles

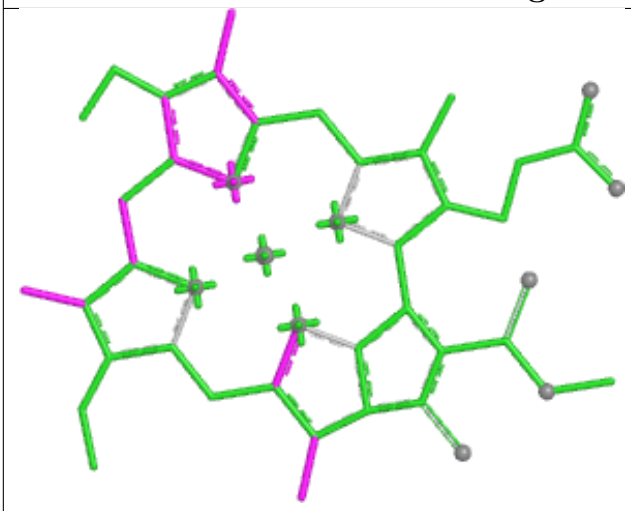


Torsions

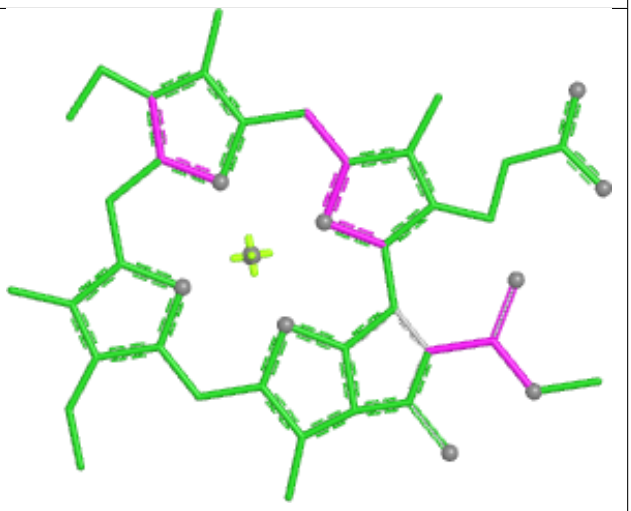


Rings

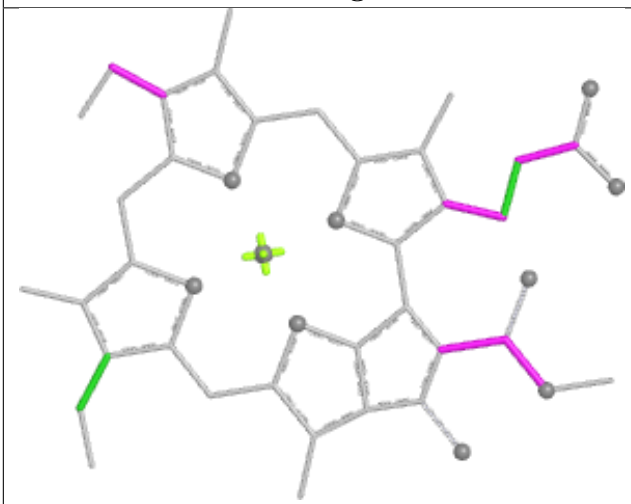
Ligand CLA 2 516



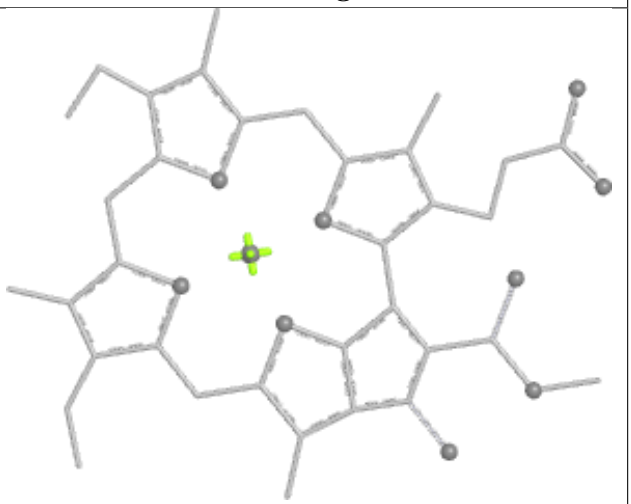
Bond lengths



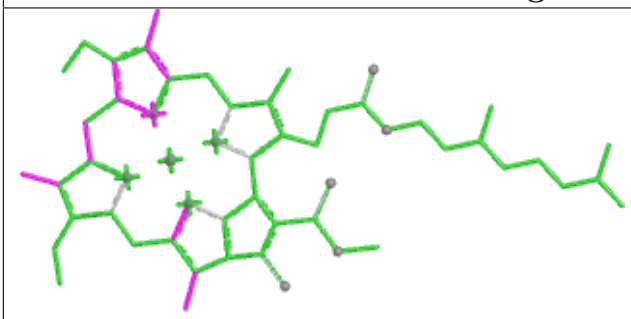
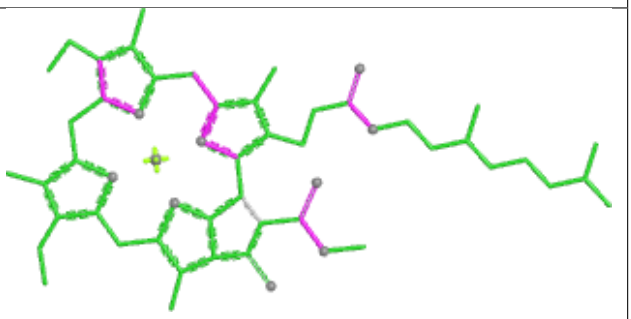
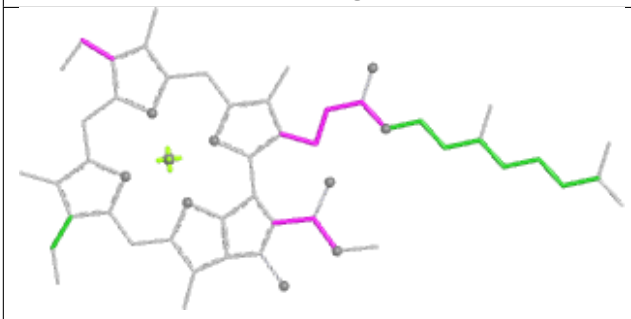
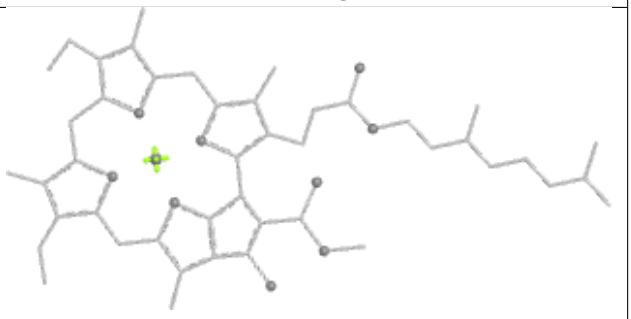
Bond angles

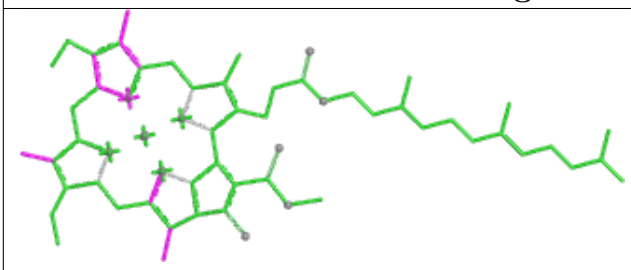
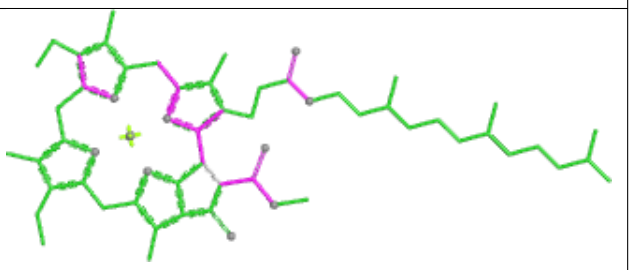
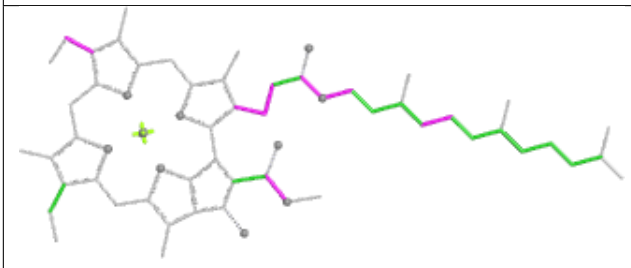
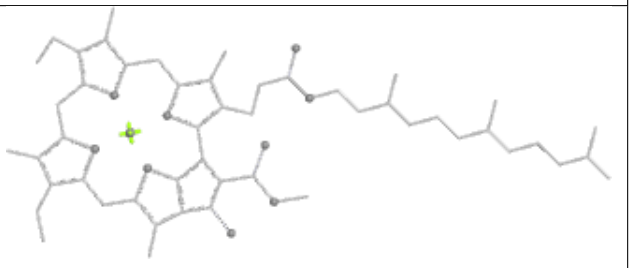


Torsions

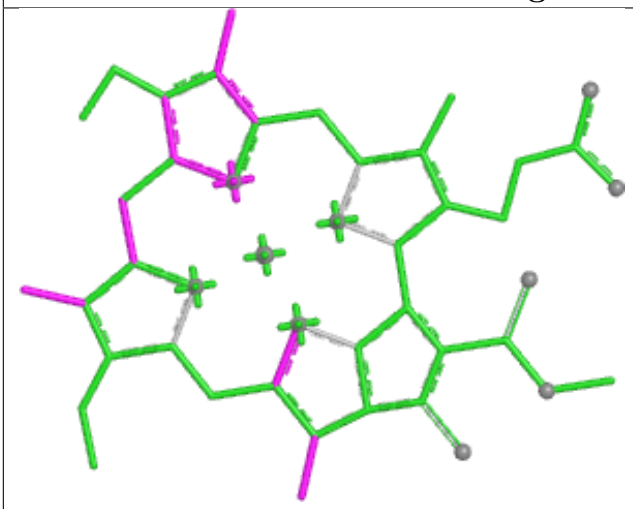


Rings

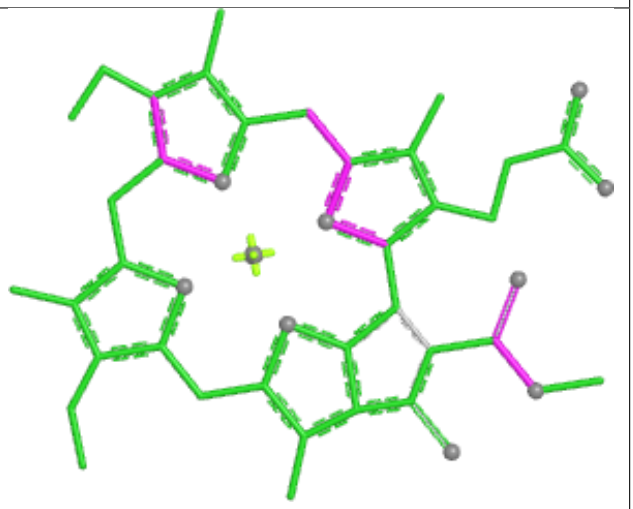
Ligand CLA d 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

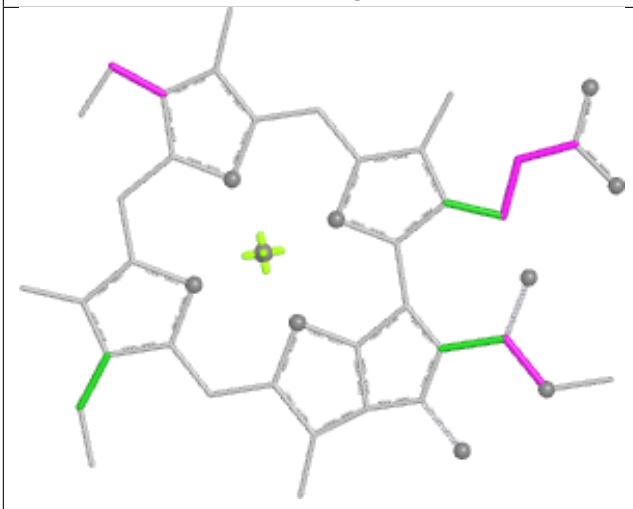
Ligand CLA 4 513



Bond lengths



Bond angles

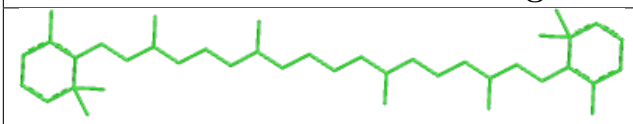


Torsions

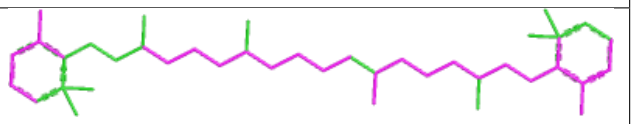


Rings

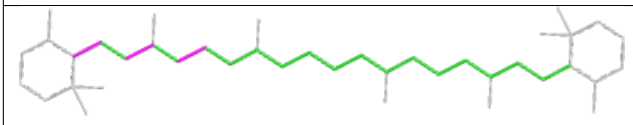
Ligand BCR 6 522



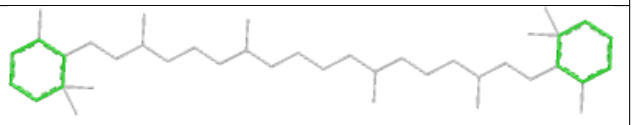
Bond lengths



Bond angles

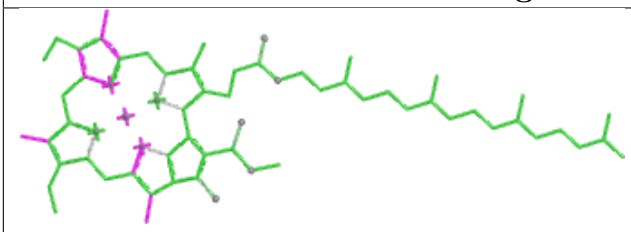


Torsions

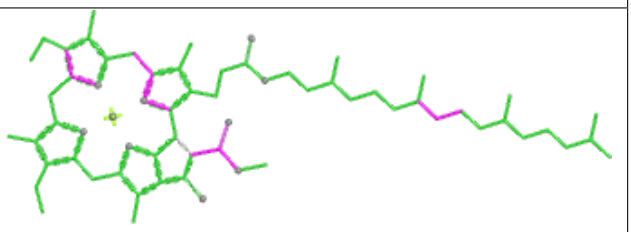


Rings

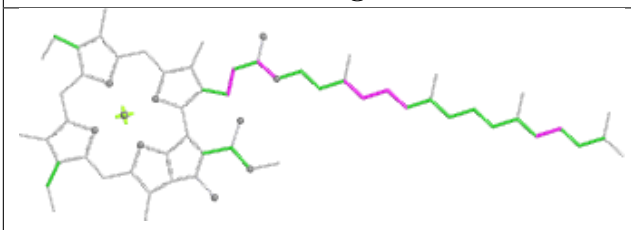
Ligand CLA B 1204



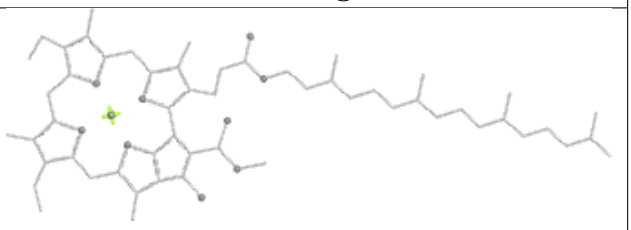
Bond lengths



Bond angles

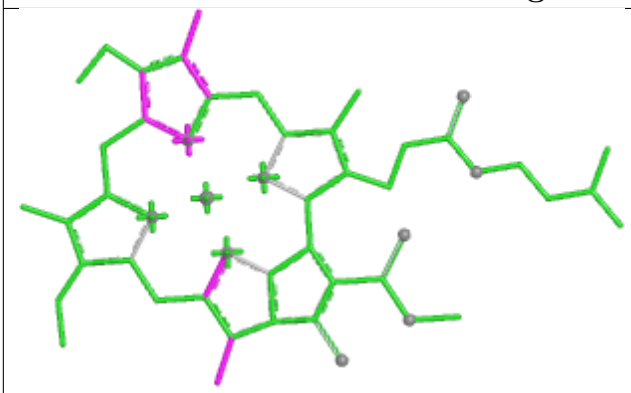


Torsions

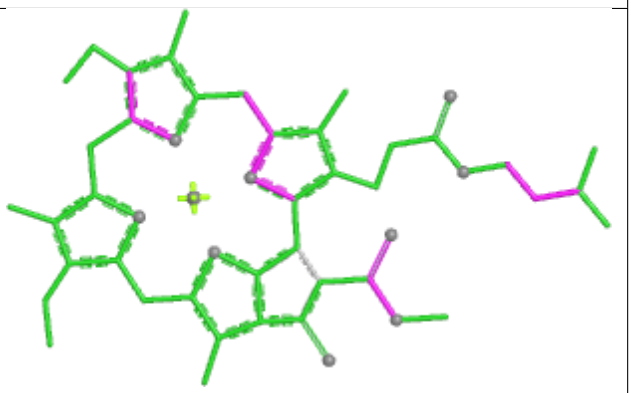


Rings

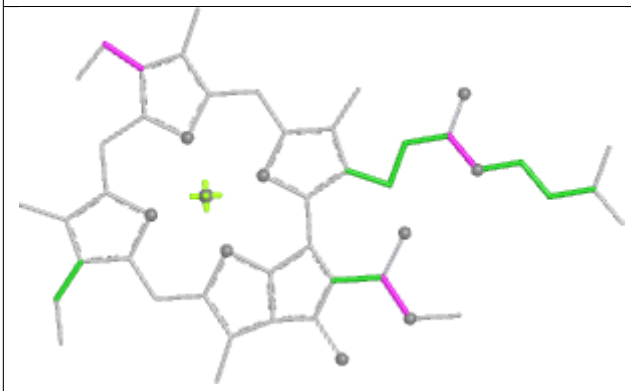
Ligand CLA d 502



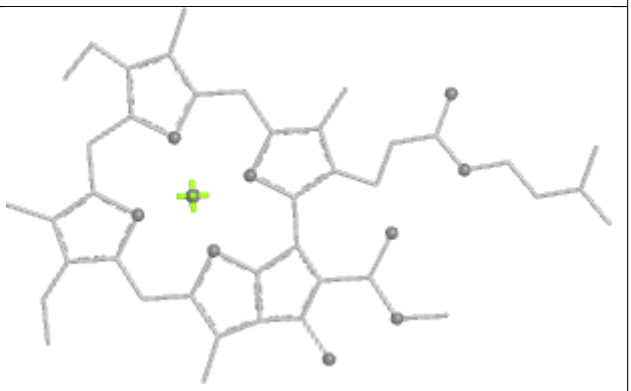
Bond lengths



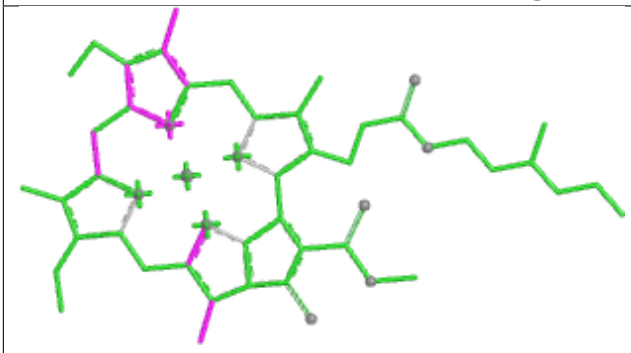
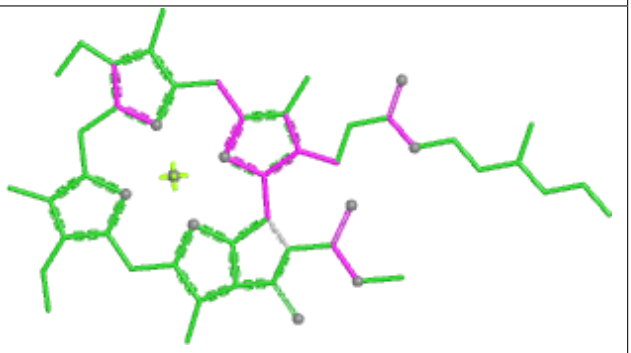
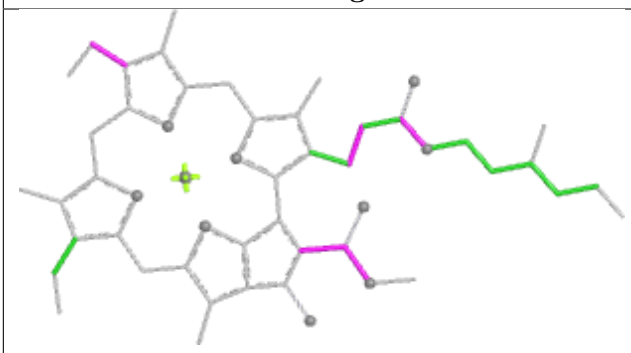
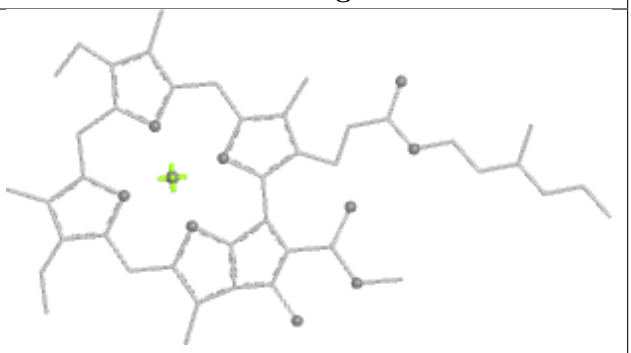
Bond angles

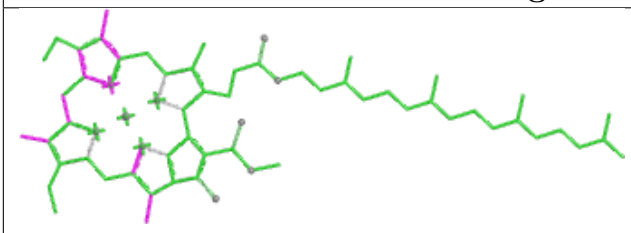
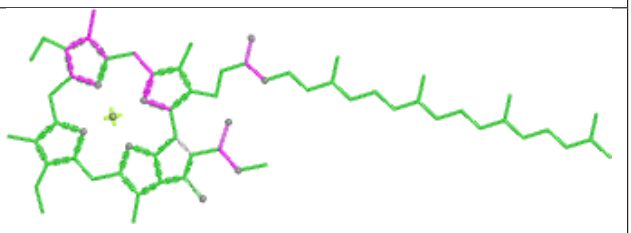
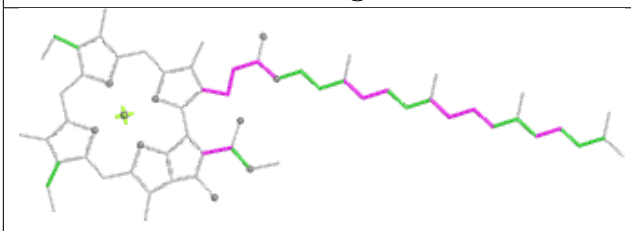
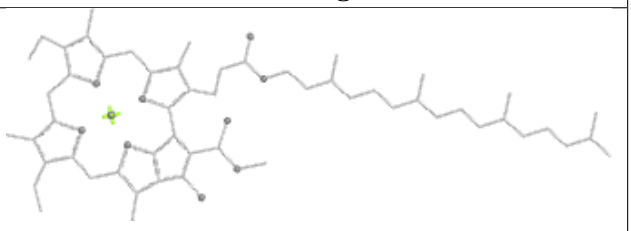


Torsions

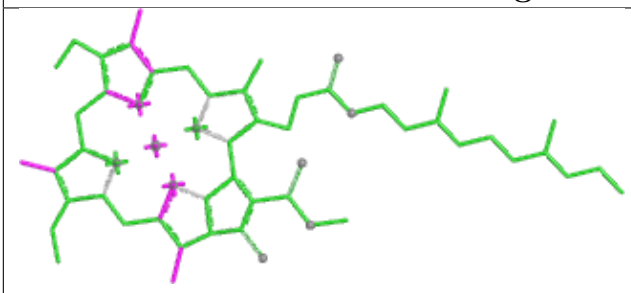


Rings

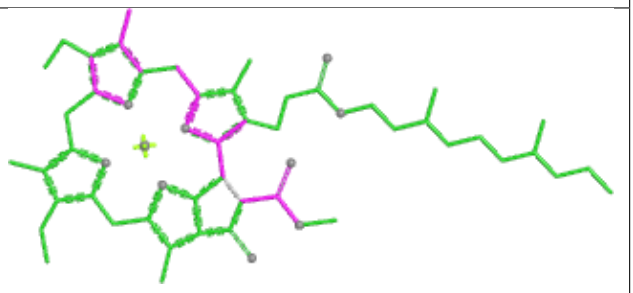
Ligand CLA 6 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

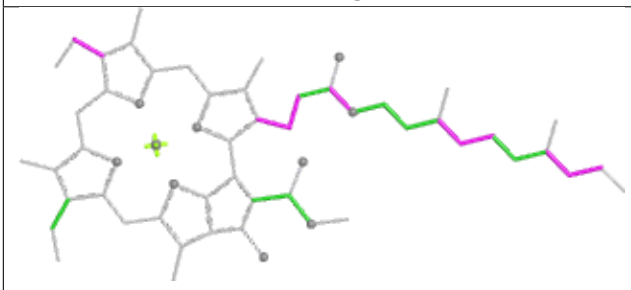
Ligand CLA H 1217



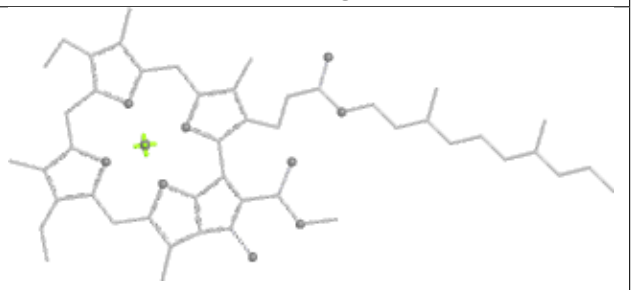
Bond lengths



Bond angles

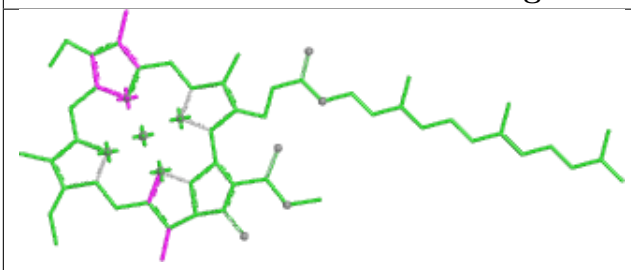


Torsions

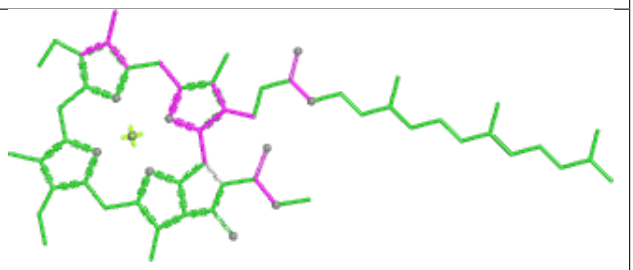


Rings

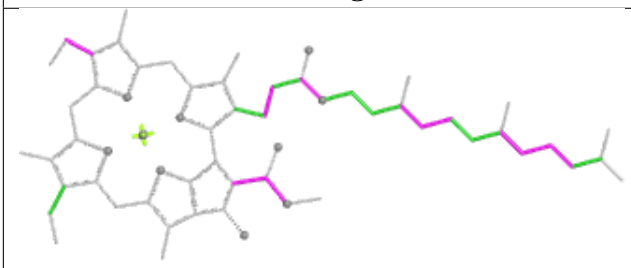
Ligand CLA Y 507



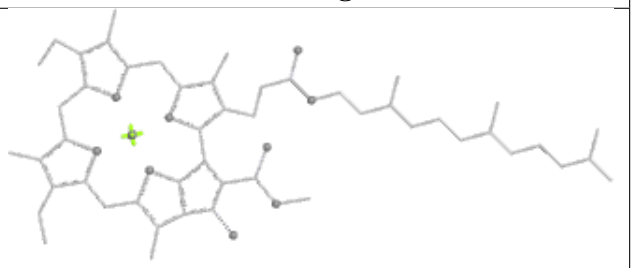
Bond lengths



Bond angles

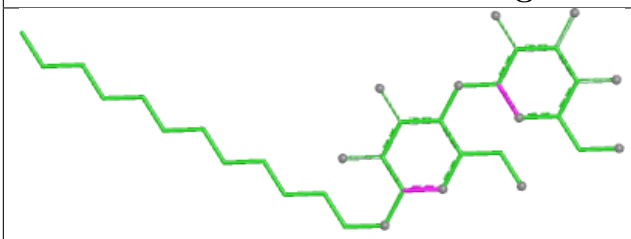


Torsions

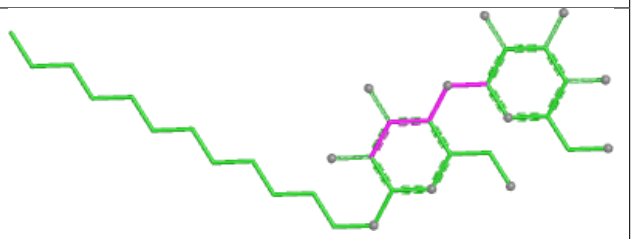


Rings

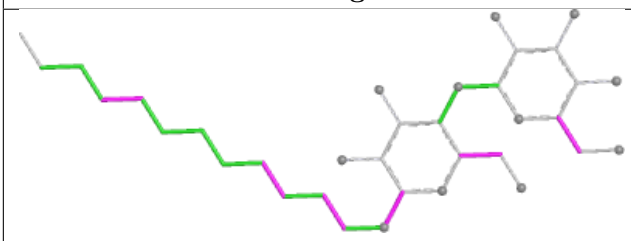
Ligand LMU e 1848



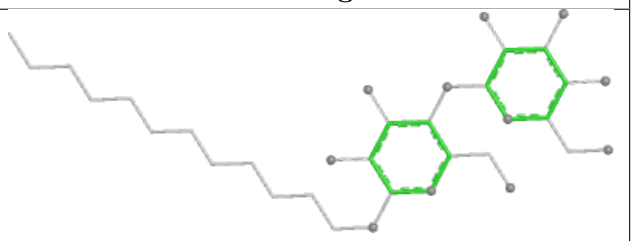
Bond lengths



Bond angles

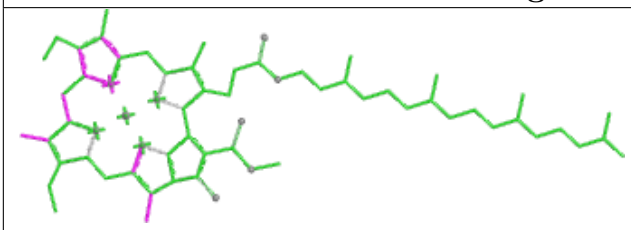


Torsions

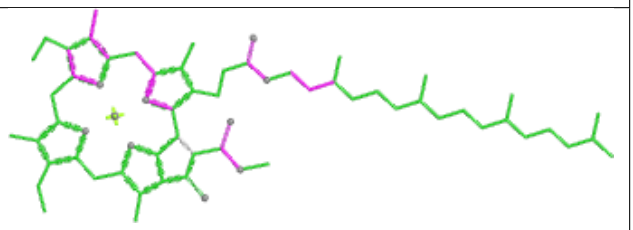


Rings

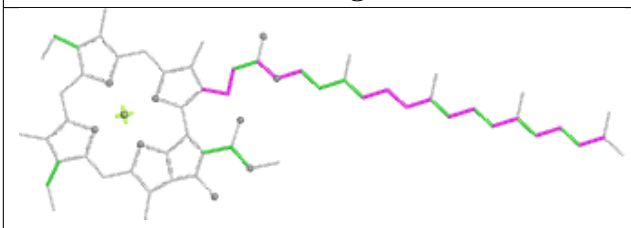
Ligand CLA d 505



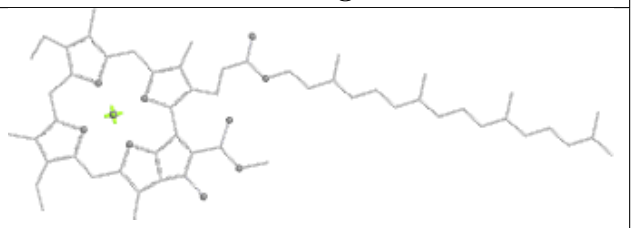
Bond lengths



Bond angles

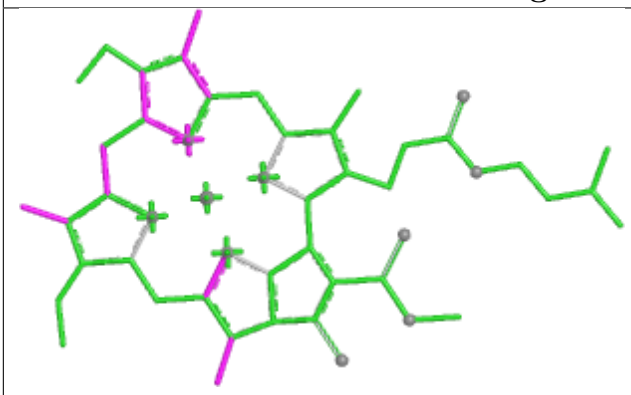


Torsions

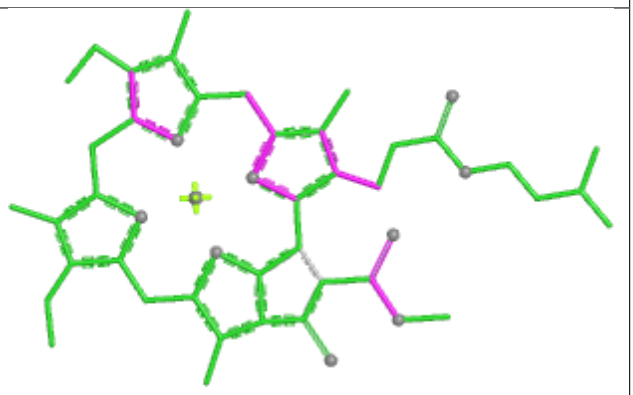


Rings

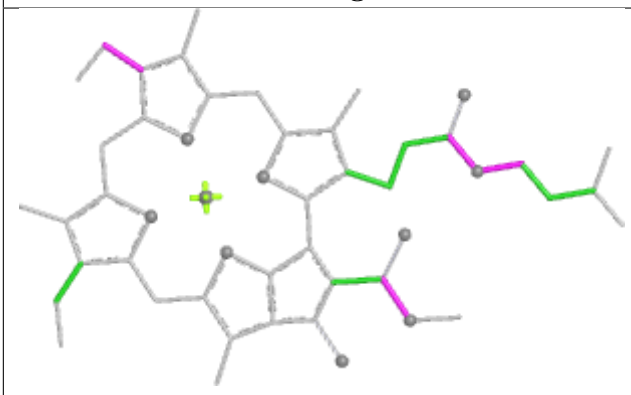
Ligand CLA s 511



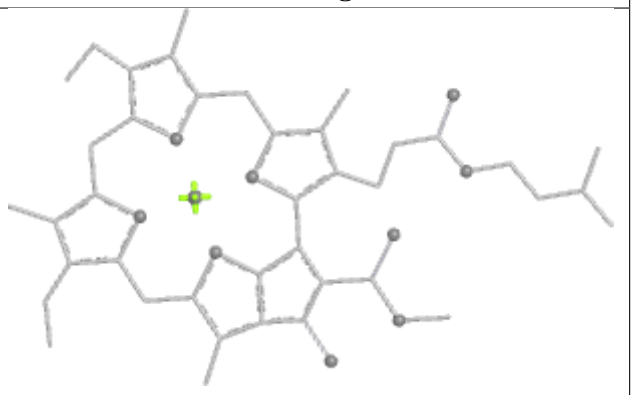
Bond lengths



Bond angles

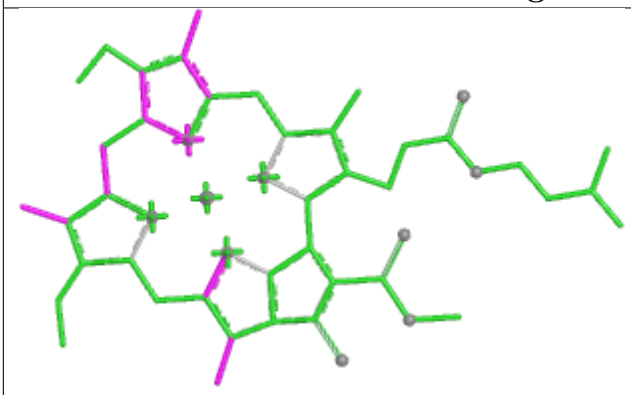


Torsions

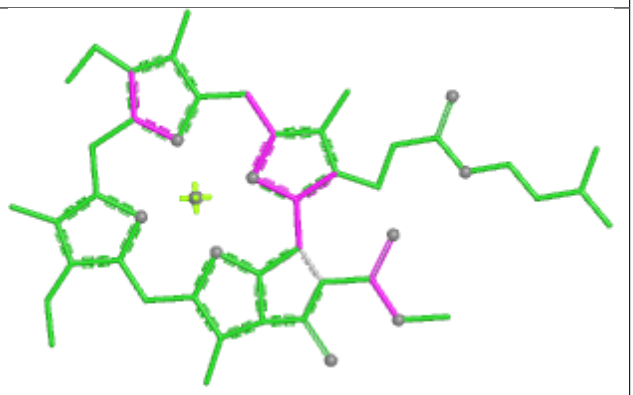


Rings

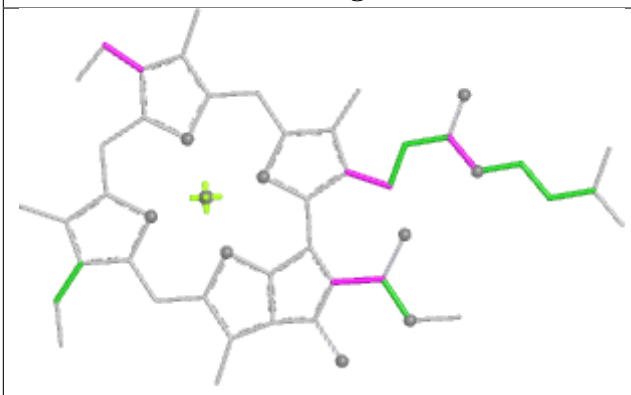
Ligand CLA b 502



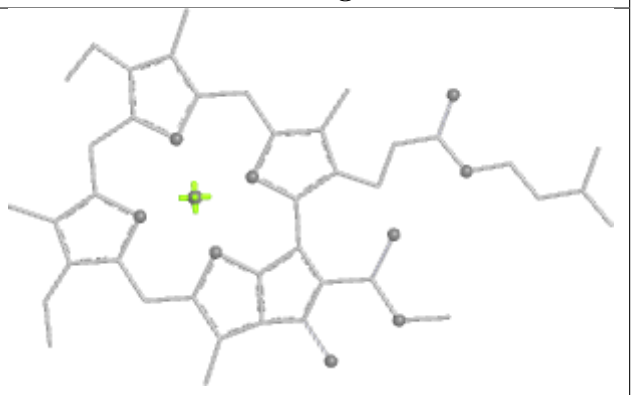
Bond lengths



Bond angles

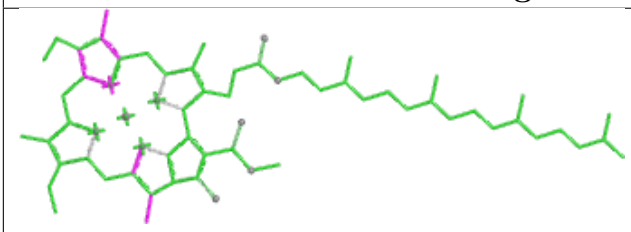


Torsions

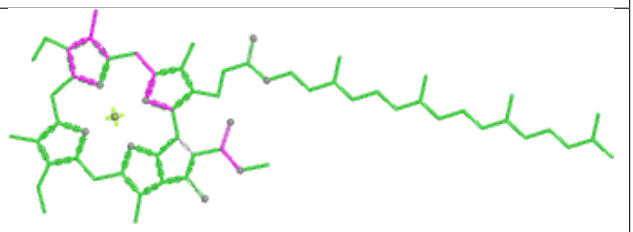


Rings

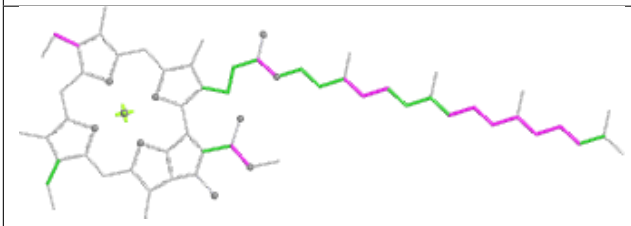
Ligand CLA G 1133



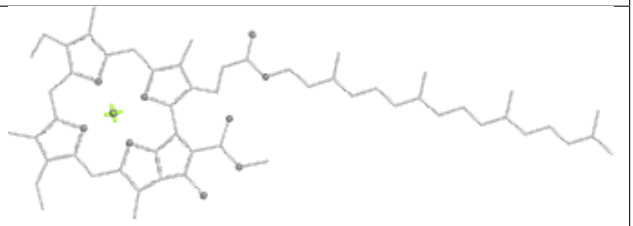
Bond lengths



Bond angles

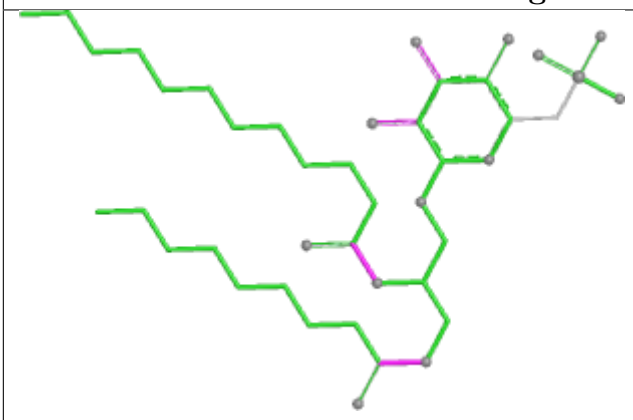


Torsions

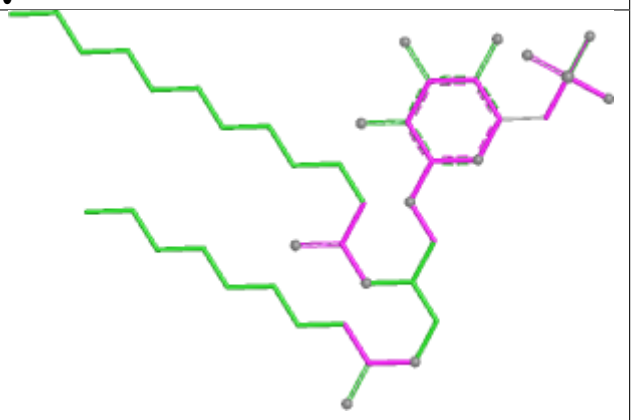


Rings

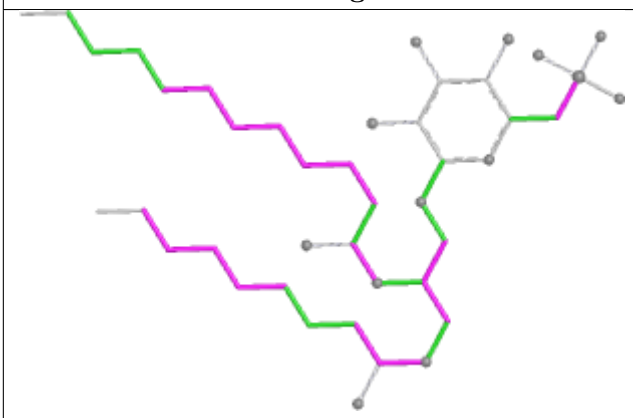
Ligand SQD a 822



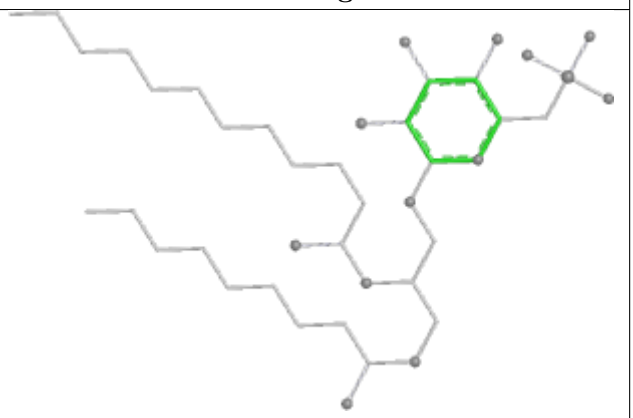
Bond lengths



Bond angles

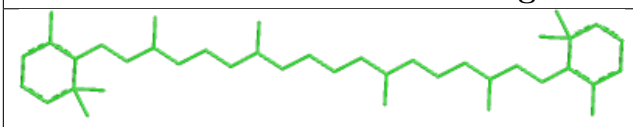


Torsions

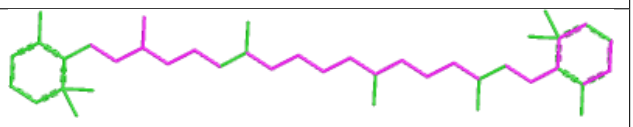


Rings

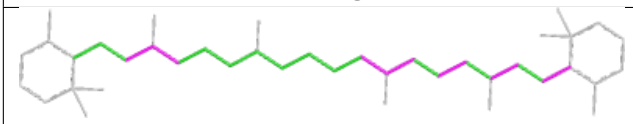
Ligand BCR e 4011



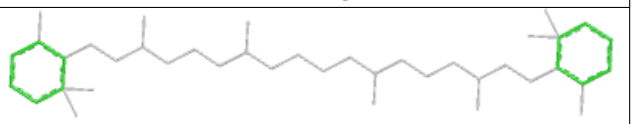
Bond lengths



Bond angles

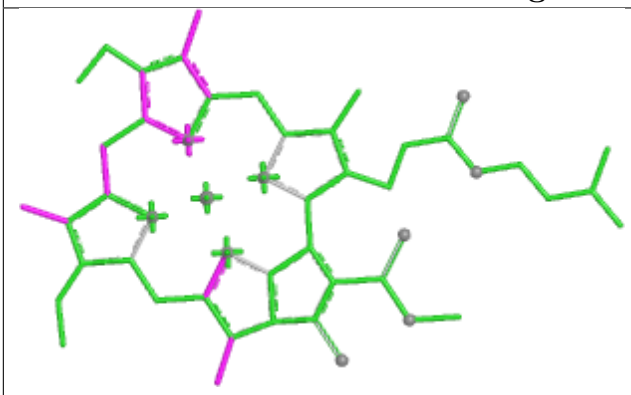


Torsions

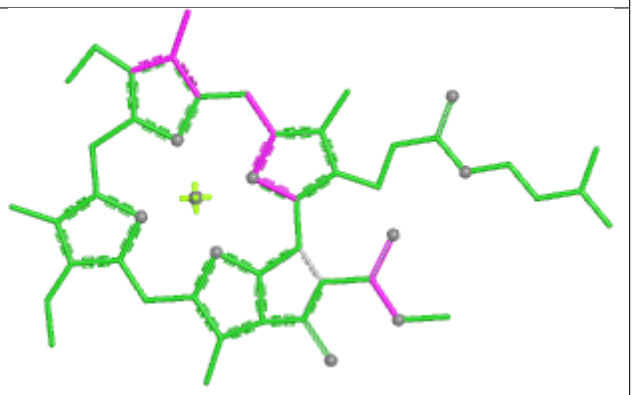


Rings

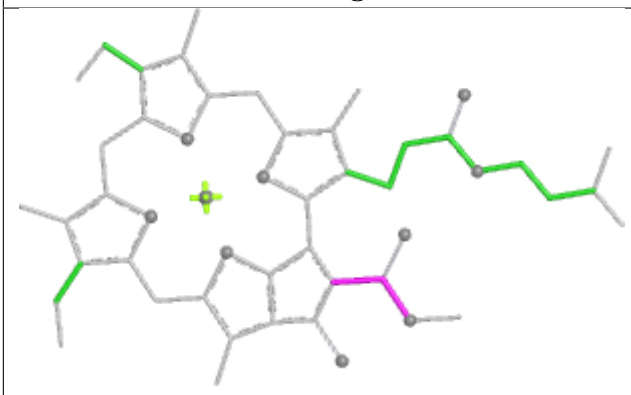
Ligand CLA a 506



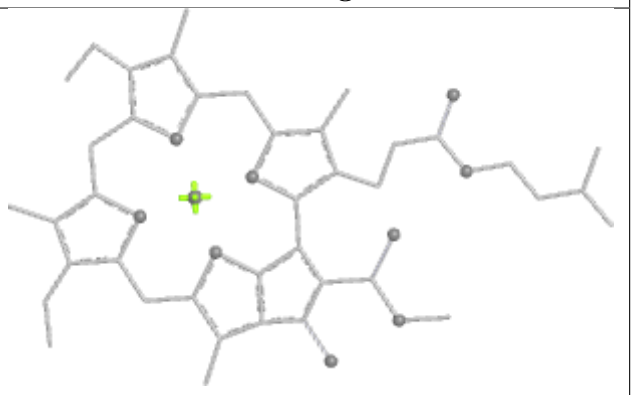
Bond lengths



Bond angles



Torsions

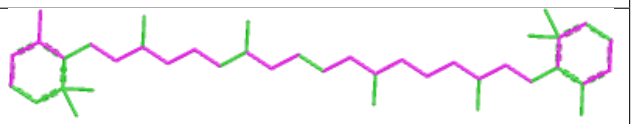


Rings

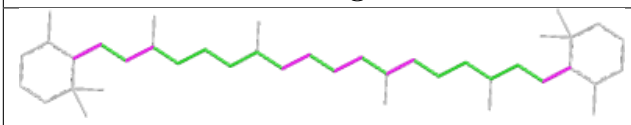
Ligand BCR 4 521



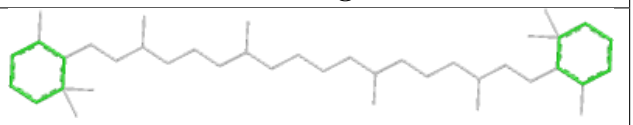
Bond lengths



Bond angles

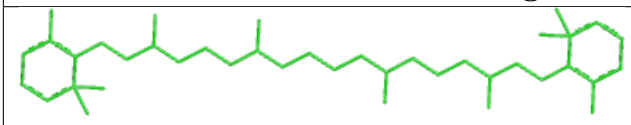


Torsions

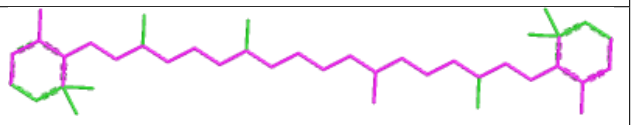


Rings

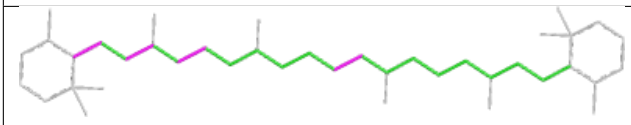
Ligand BCR Y 522



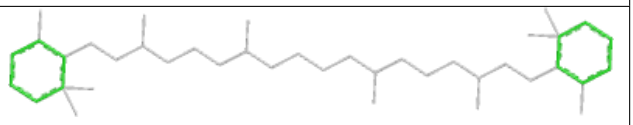
Bond lengths



Bond angles

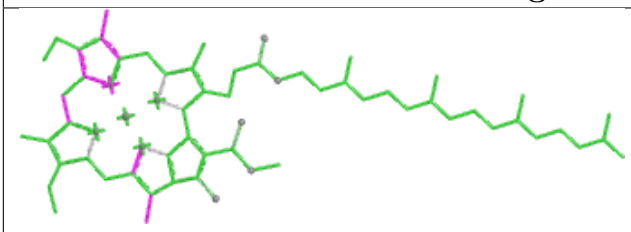


Torsions

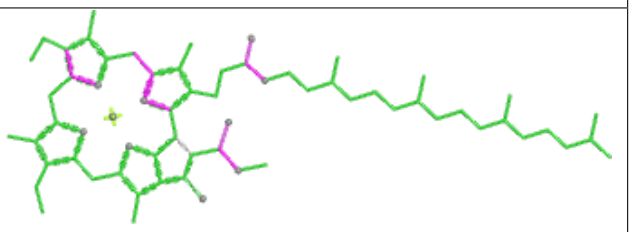


Rings

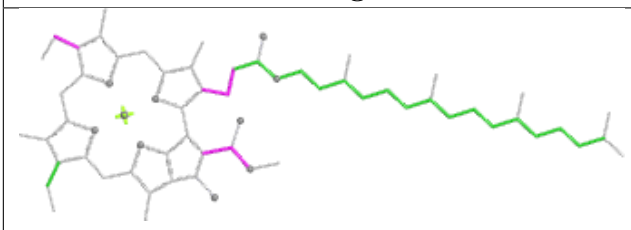
Ligand CLA a 503



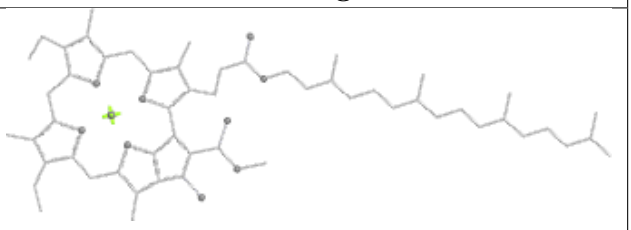
Bond lengths



Bond angles

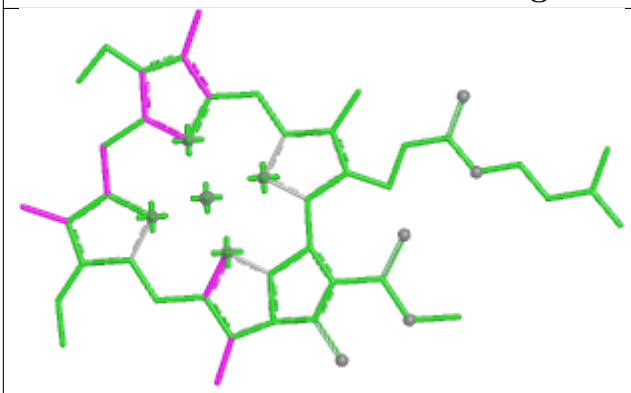


Torsions

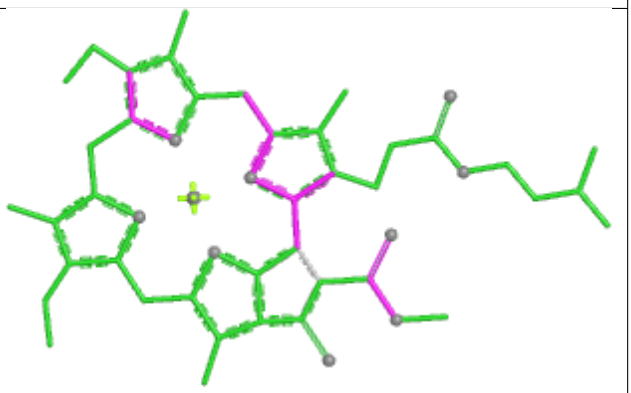


Rings

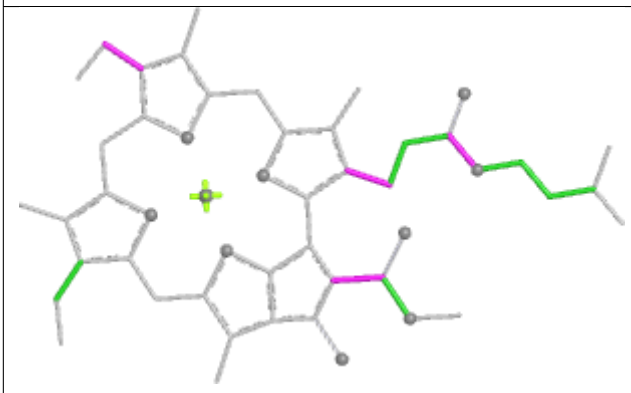
Ligand CLA t 502



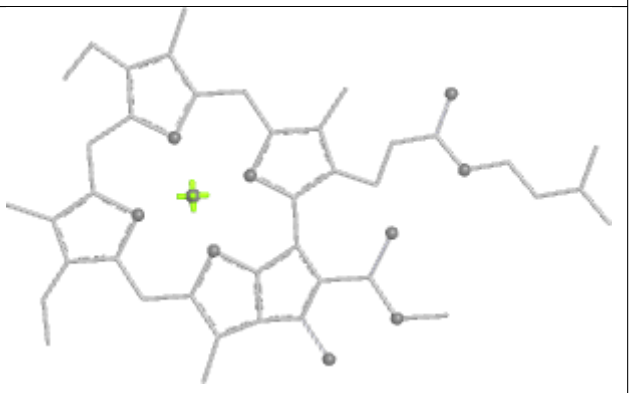
Bond lengths



Bond angles

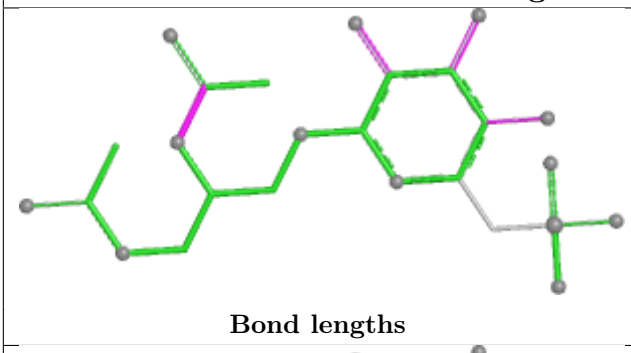


Torsions

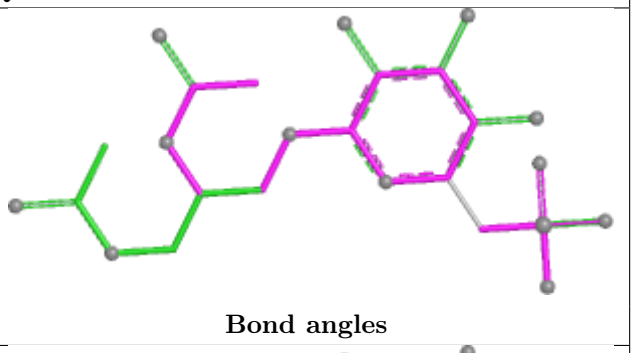


Rings

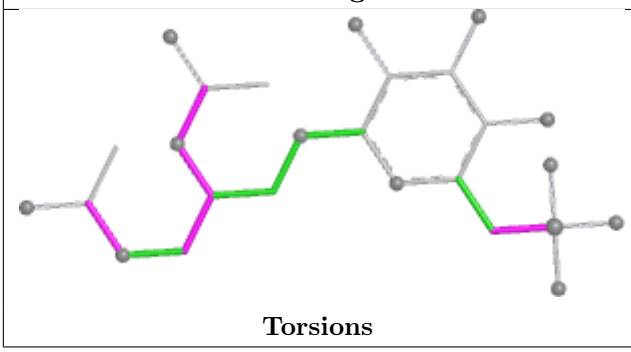
Ligand SQD 4 822



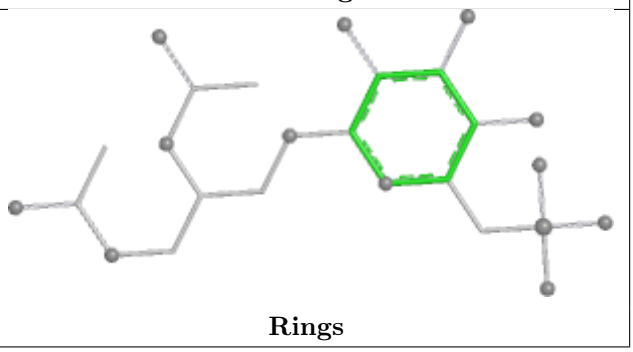
Bond lengths



Bond angles

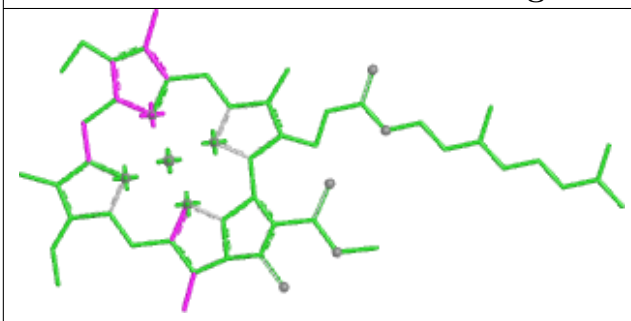


Torsions

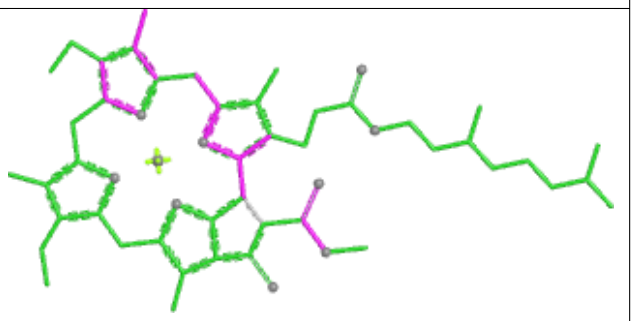


Rings

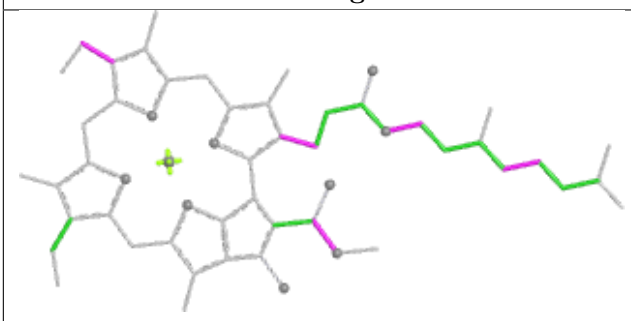
Ligand CLA u 511



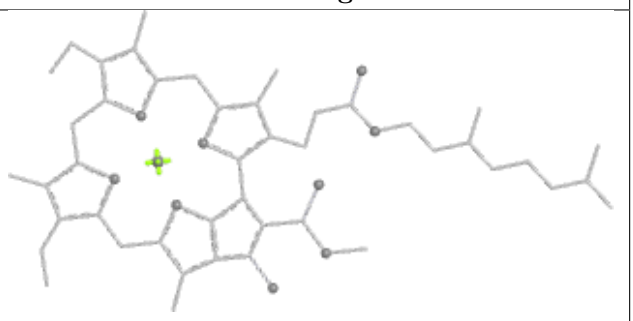
Bond lengths



Bond angles

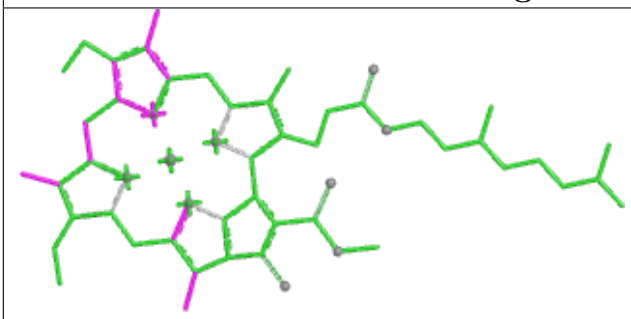


Torsions

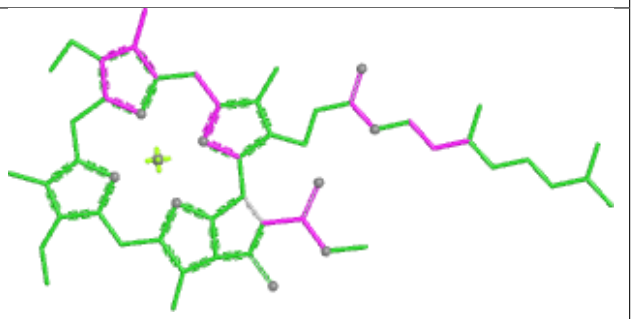


Rings

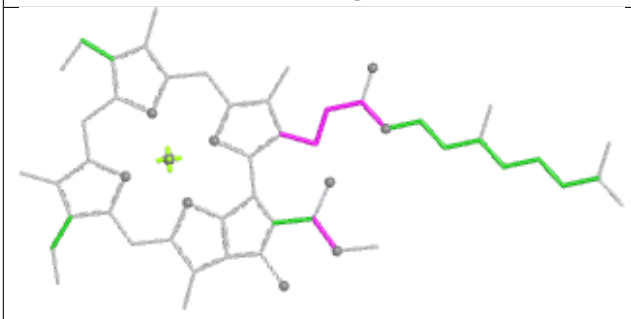
Ligand CLA H 1228



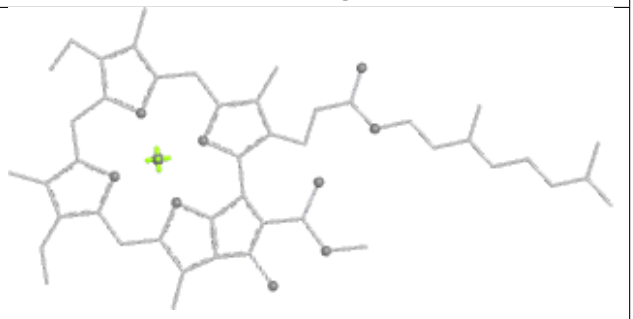
Bond lengths



Bond angles

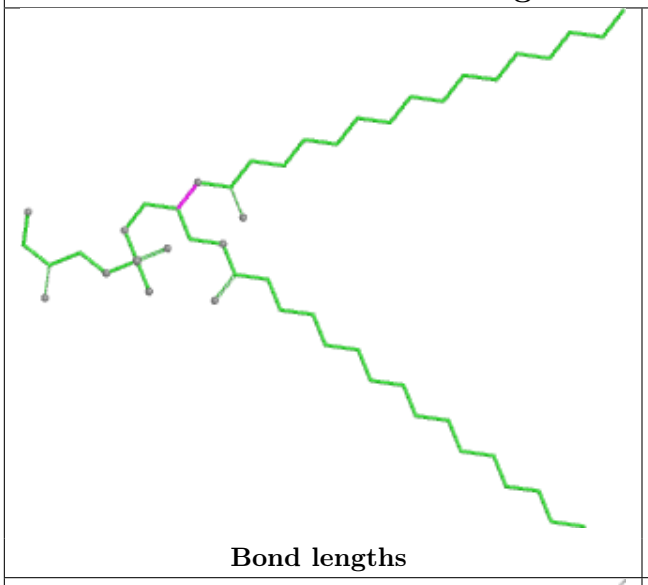


Torsions

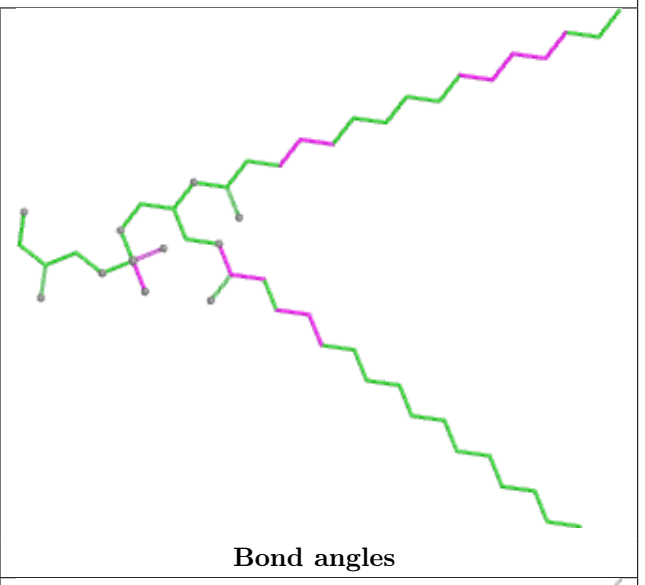


Rings

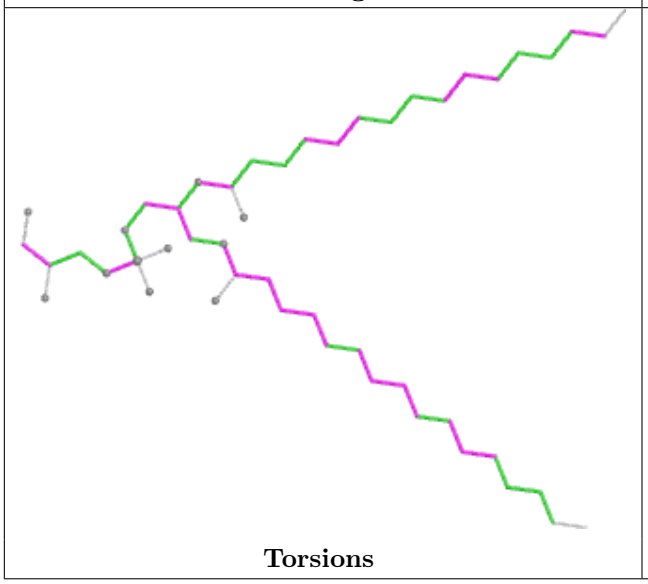
Ligand LHG A 5001



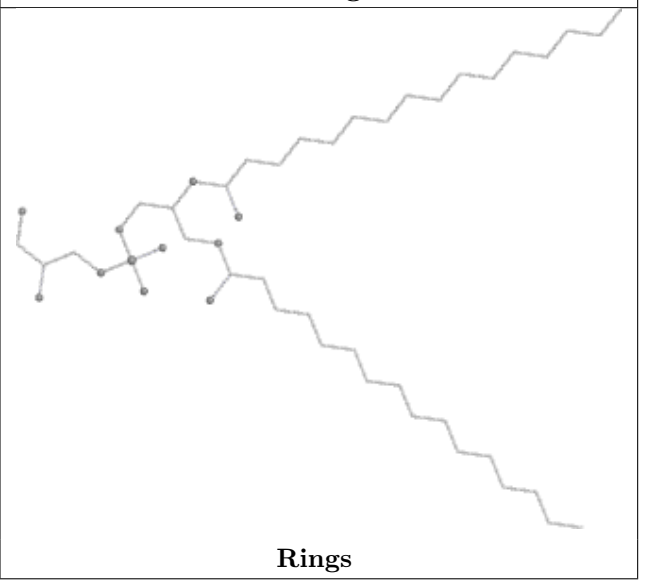
Bond lengths



Bond angles

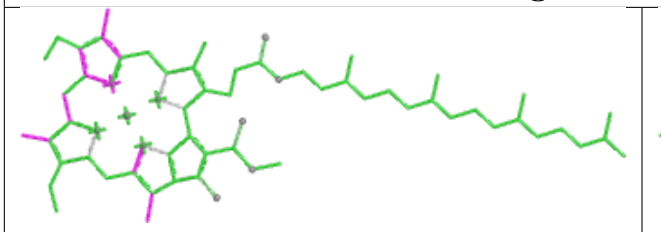


Torsions

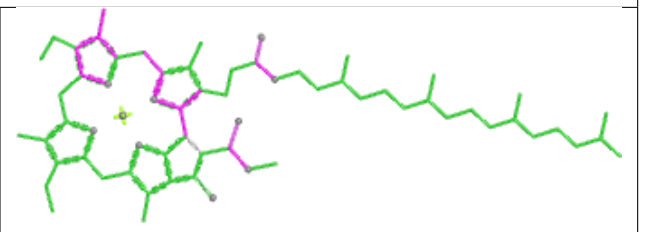


Rings

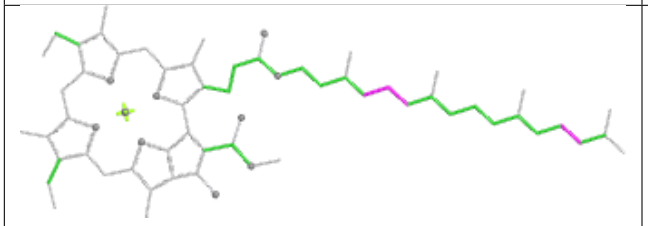
Ligand CLA 3 509



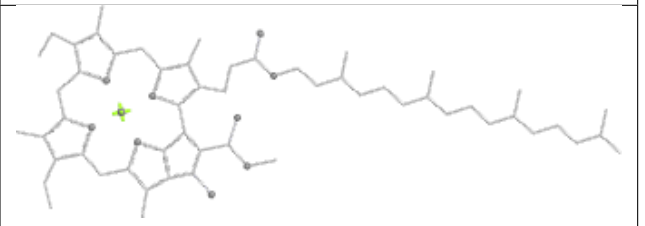
Bond lengths



Bond angles

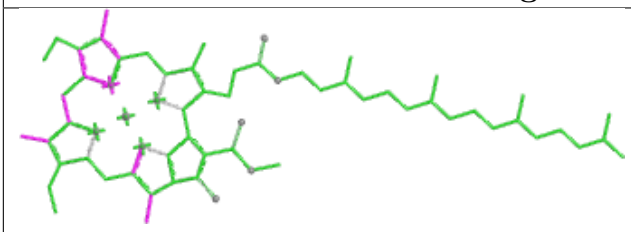


Torsions

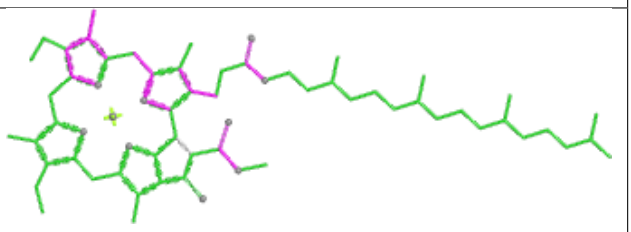


Rings

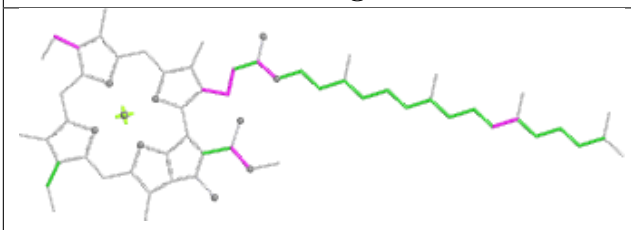
Ligand CLA e 1111



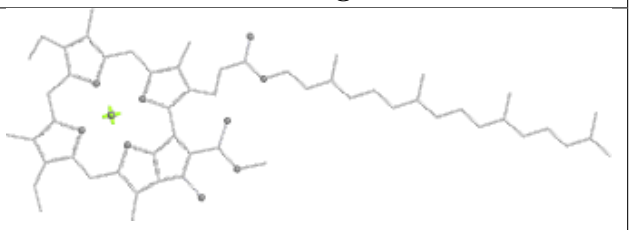
Bond lengths



Bond angles

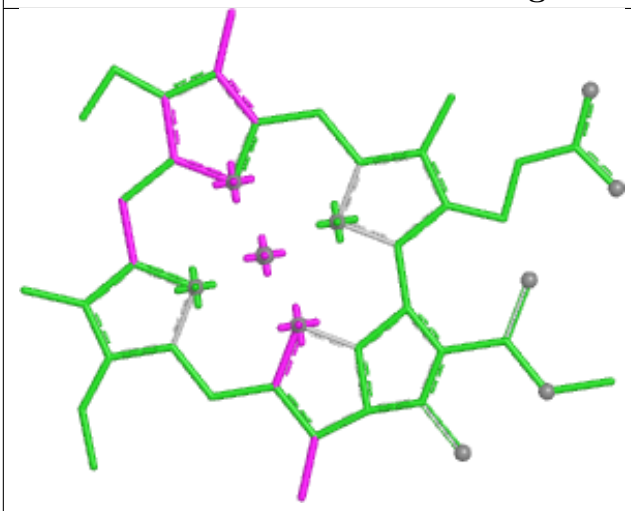


Torsions

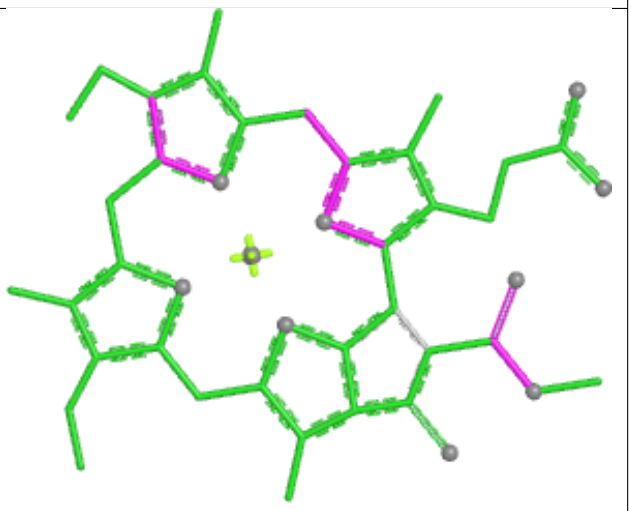


Rings

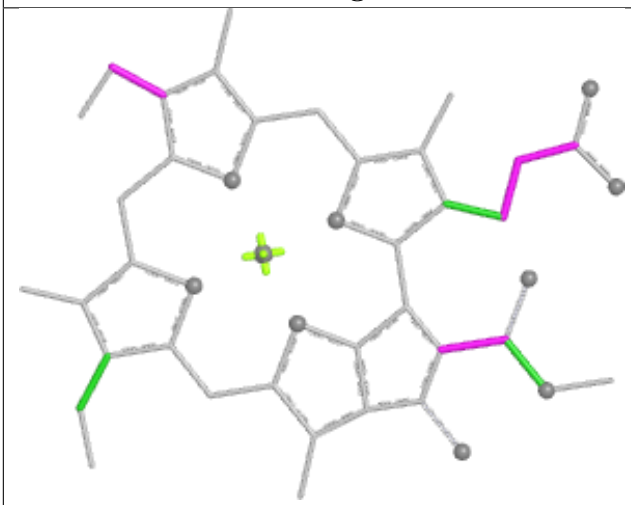
Ligand CLA 3 512



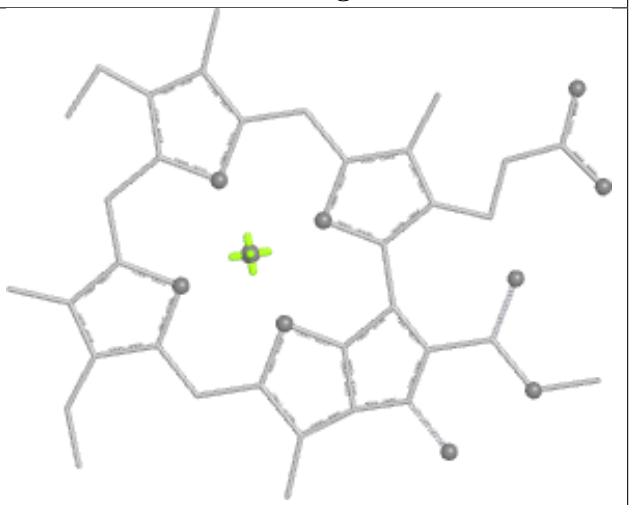
Bond lengths



Bond angles

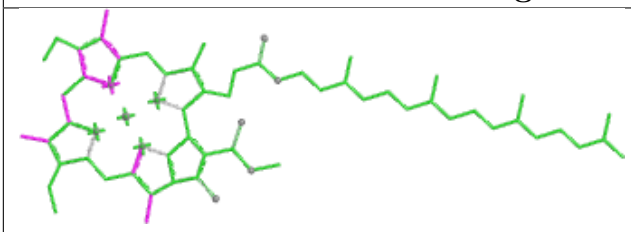


Torsions

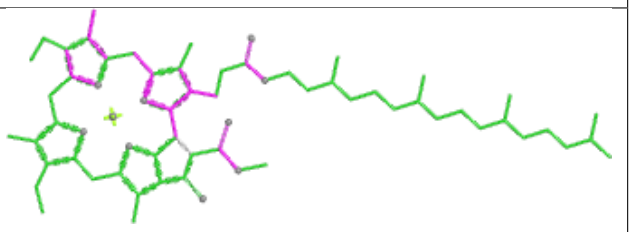


Rings

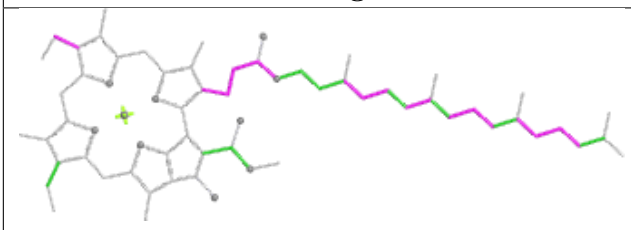
Ligand CLA V 1501



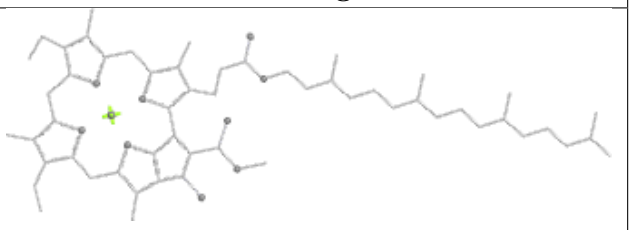
Bond lengths



Bond angles

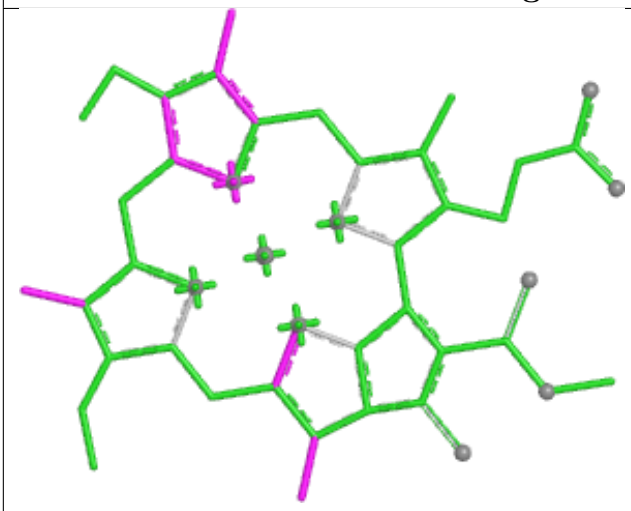


Torsions

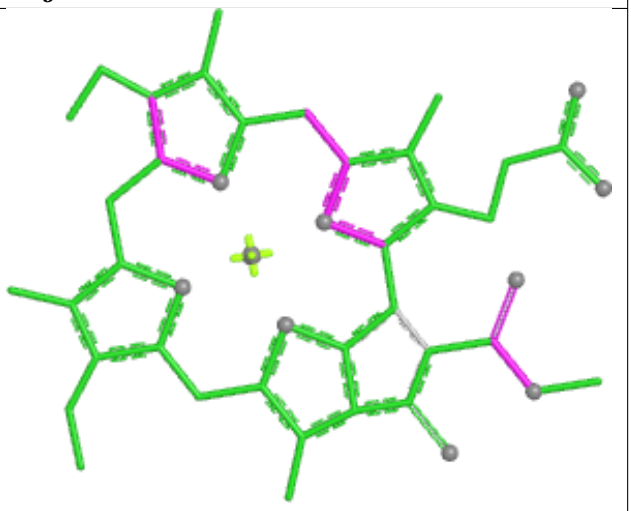


Rings

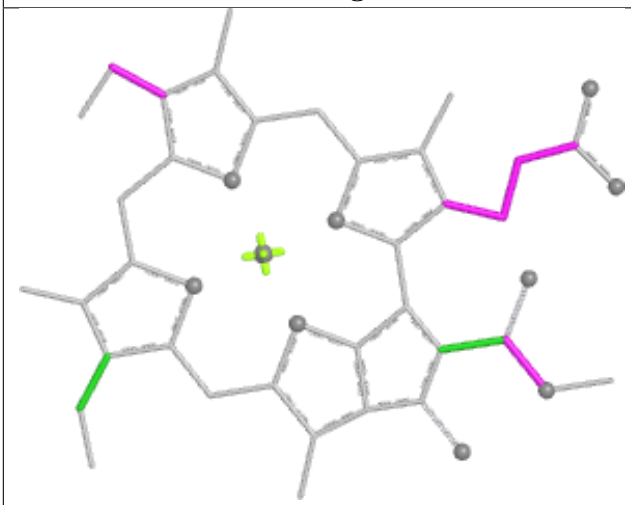
Ligand CLA j 1302



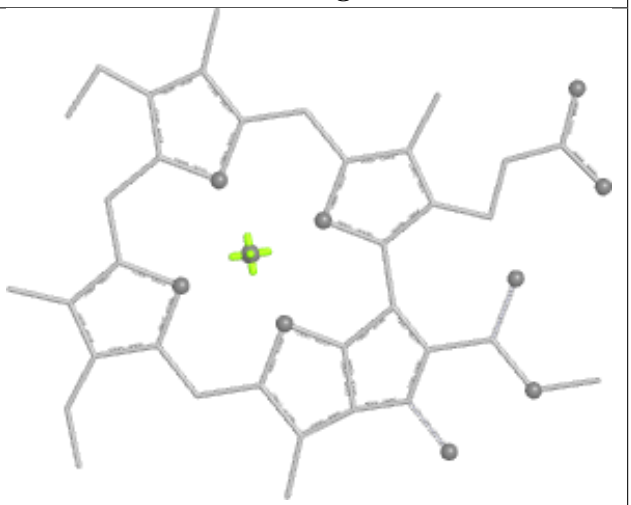
Bond lengths



Bond angles

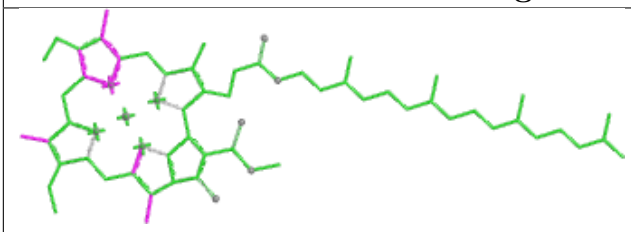


Torsions

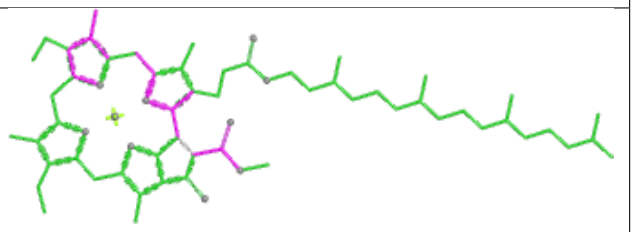


Rings

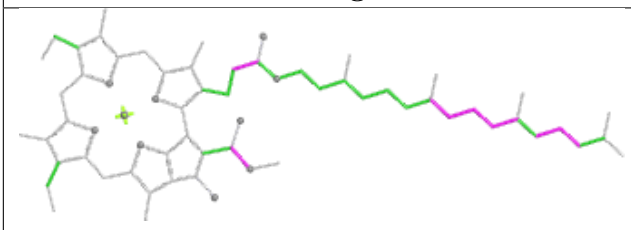
Ligand CLA A 1123



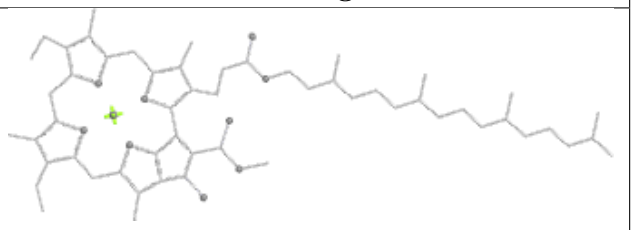
Bond lengths



Bond angles

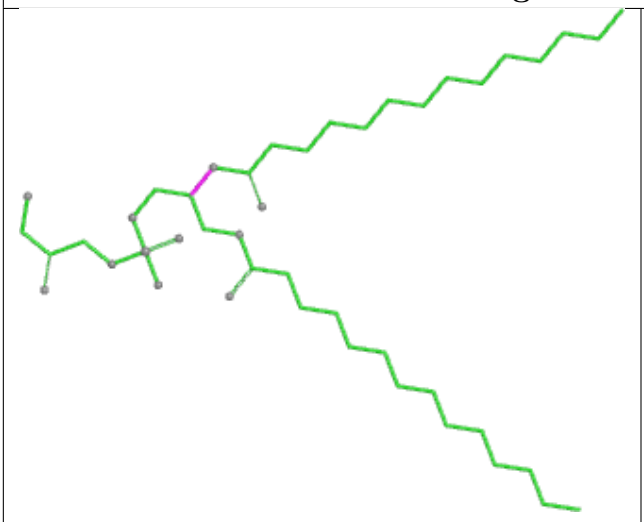


Torsions

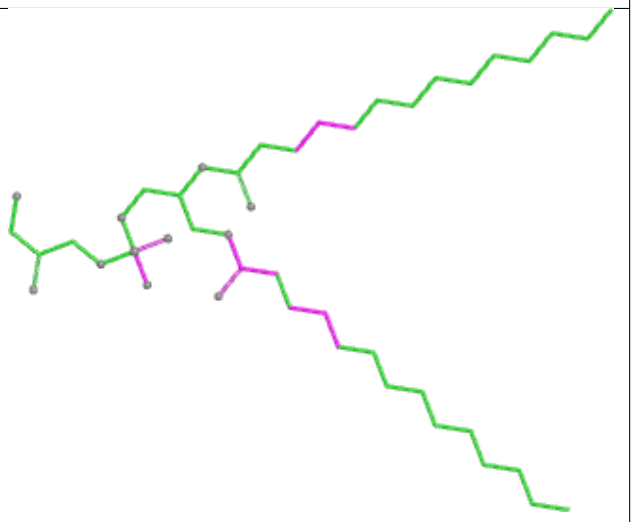


Rings

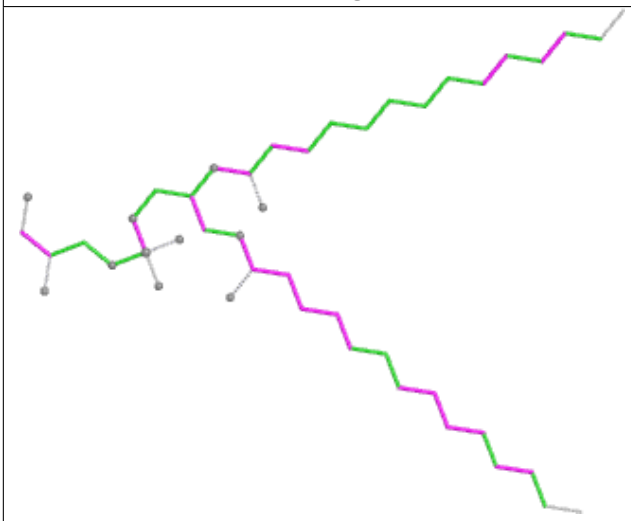
Ligand LHG G 5006



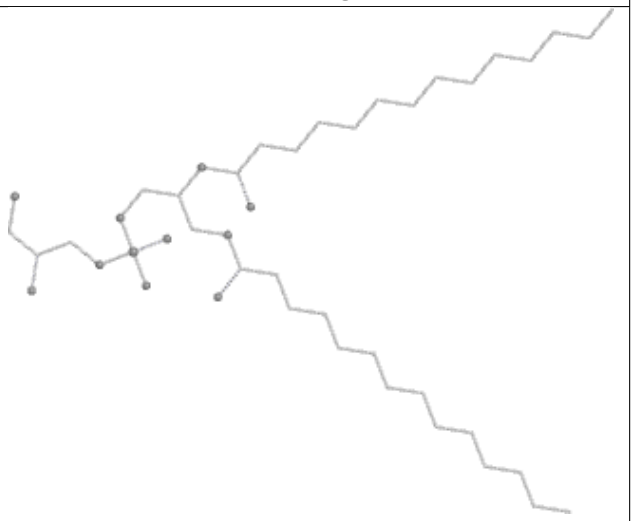
Bond lengths



Bond angles

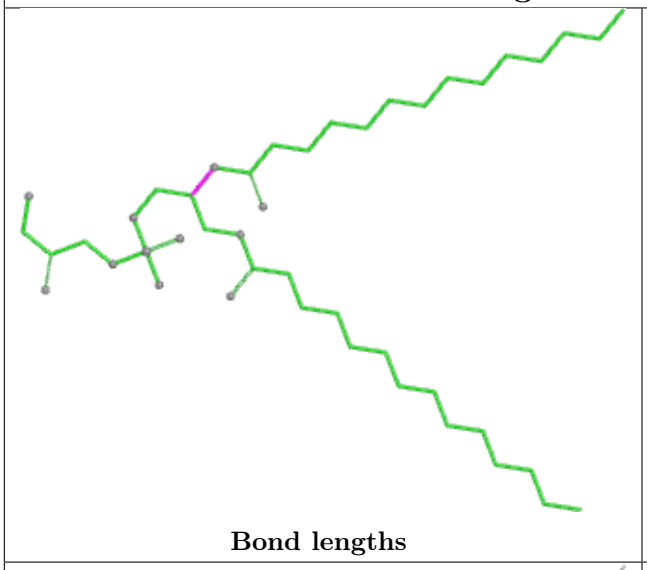


Torsions

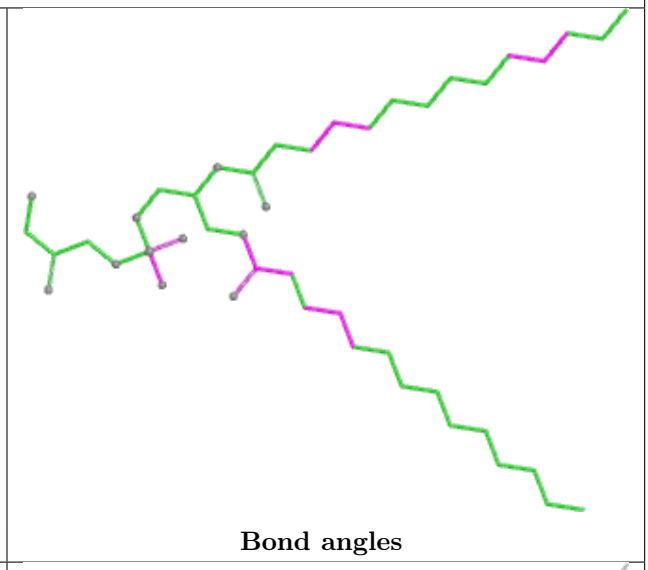


Rings

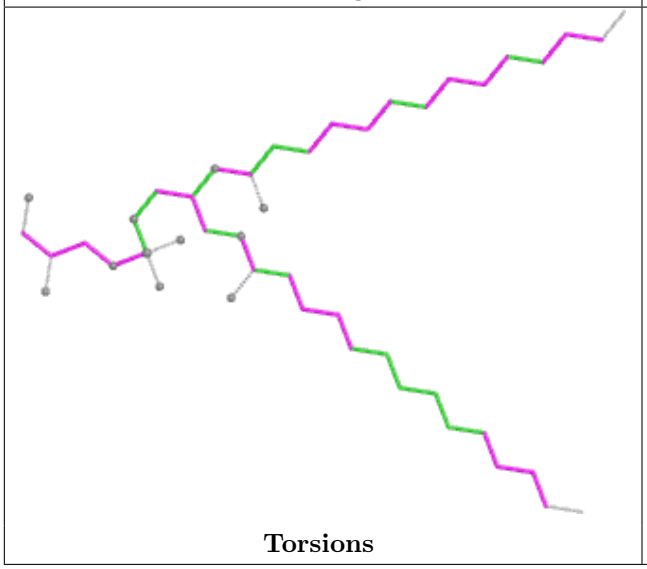
Ligand LHG A 5005



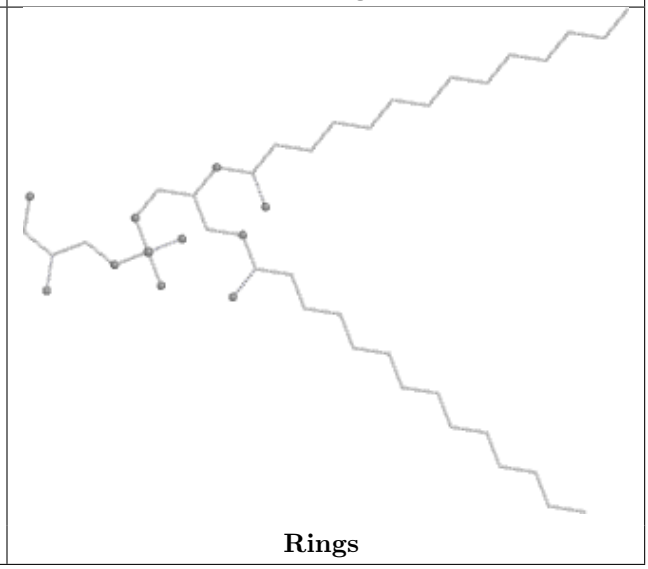
Bond lengths



Bond angles

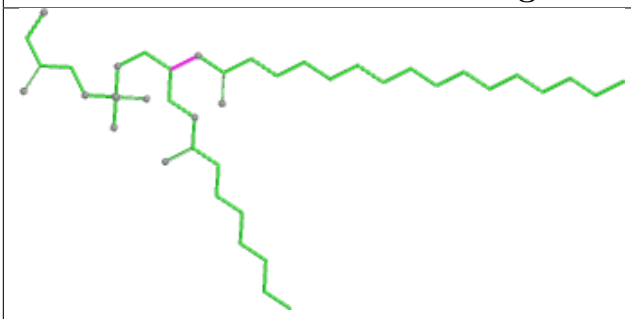


Torsions

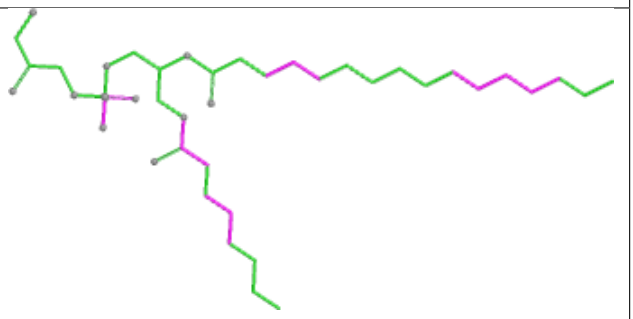


Rings

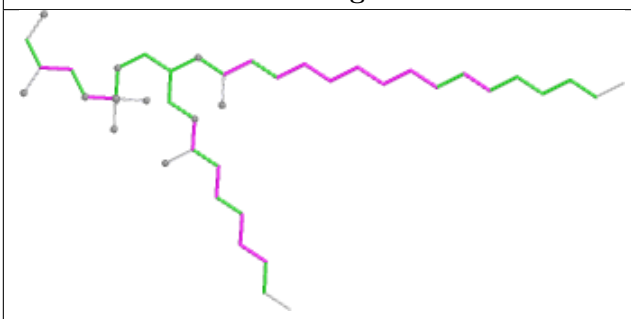
Ligand LHG e 5003



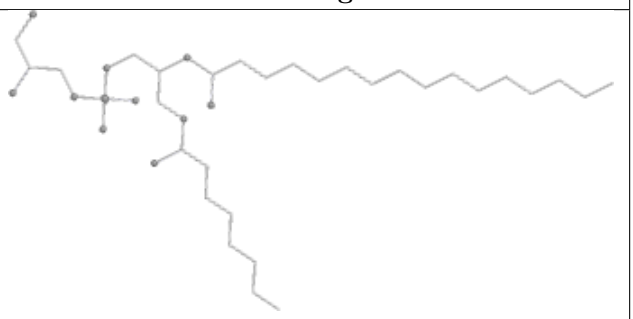
Bond lengths



Bond angles

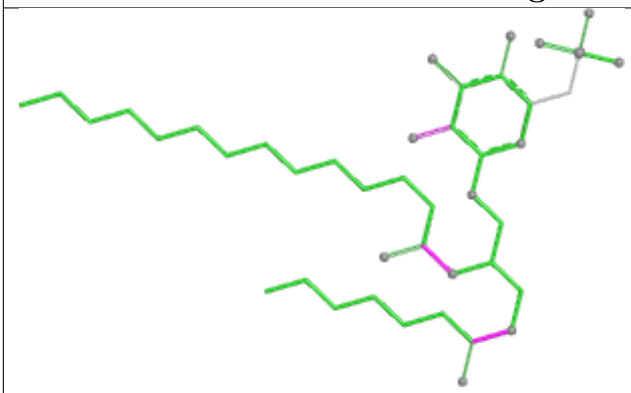


Torsions

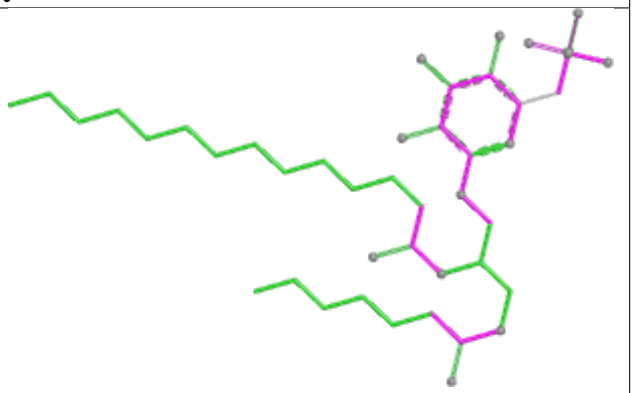


Rings

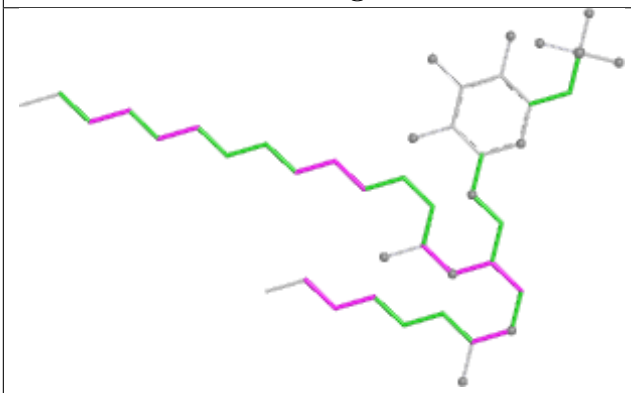
Ligand SQD 2 822



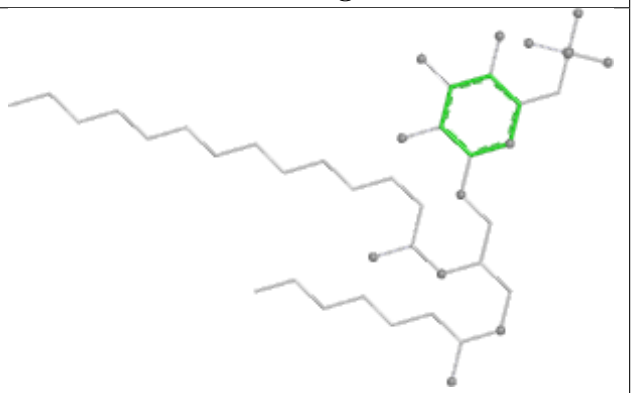
Bond lengths



Bond angles

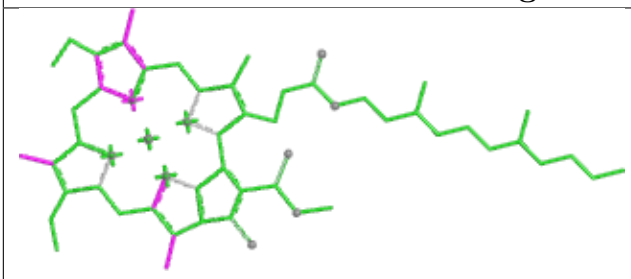


Torsions

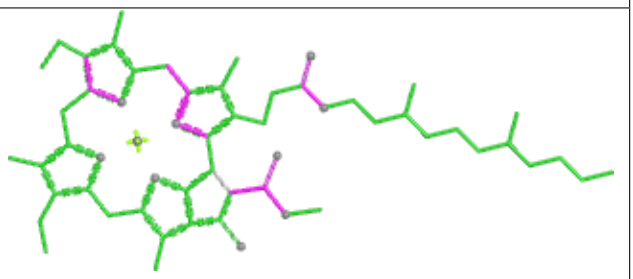


Rings

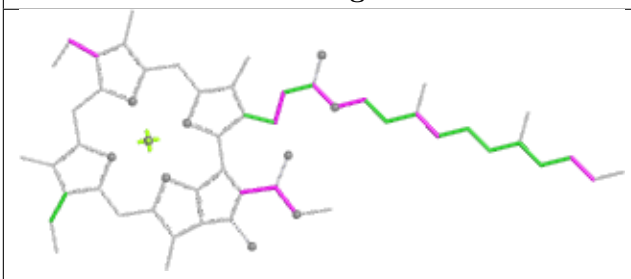
Ligand CLA J 1302



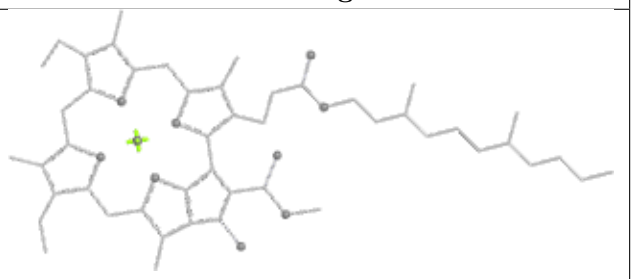
Bond lengths



Bond angles



Torsions

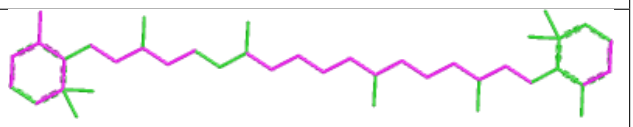


Rings

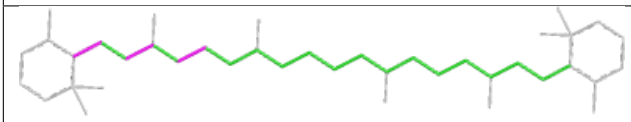
Ligand BCR 6 521



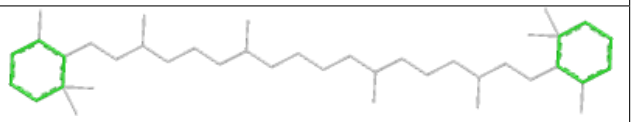
Bond lengths



Bond angles

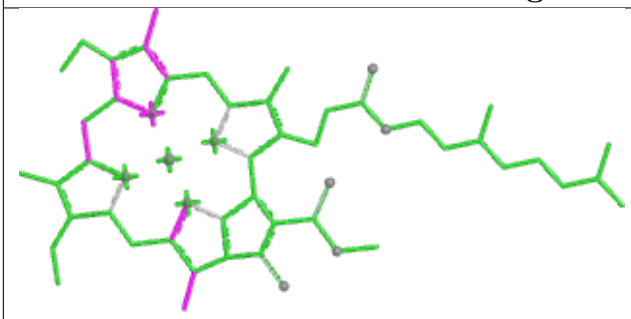


Torsions

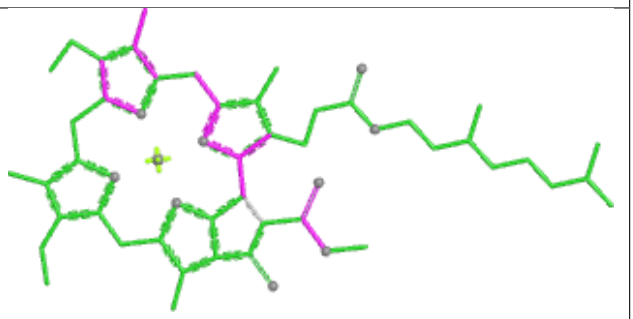


Rings

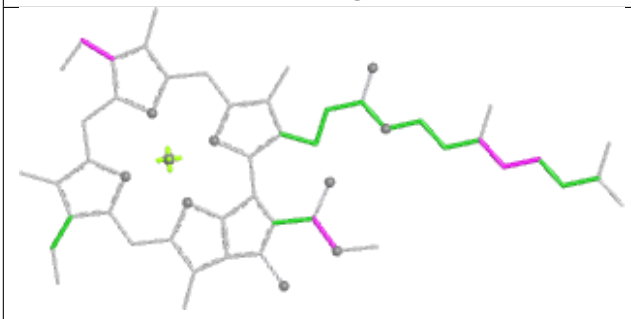
Ligand CLA Z 511



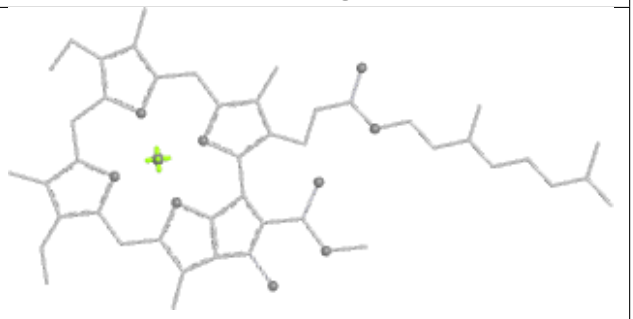
Bond lengths



Bond angles

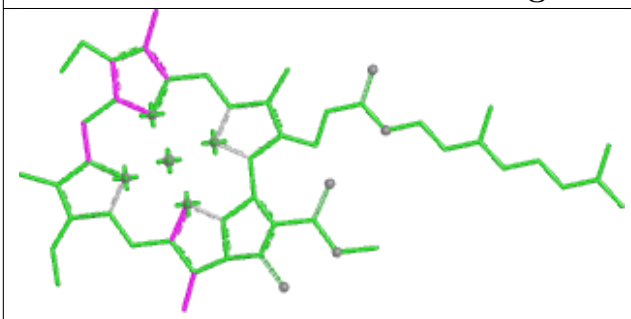


Torsions

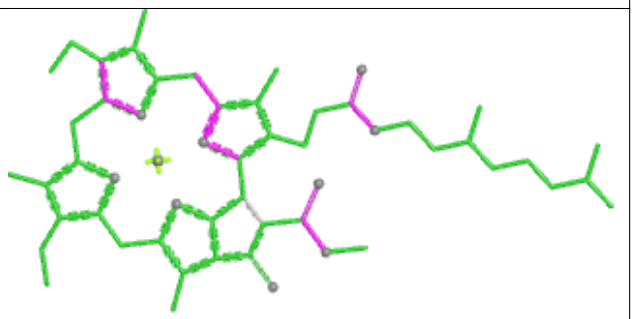


Rings

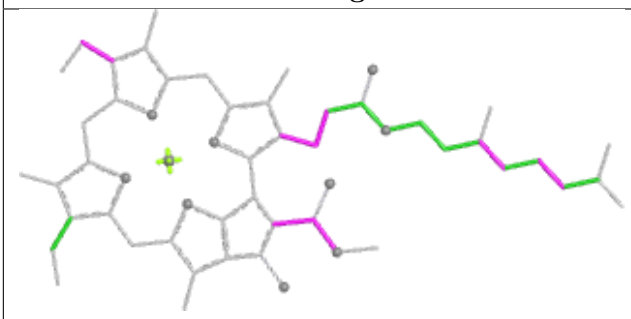
Ligand CLA 5 503



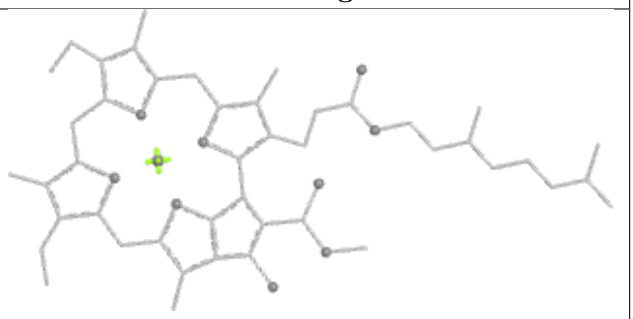
Bond lengths



Bond angles

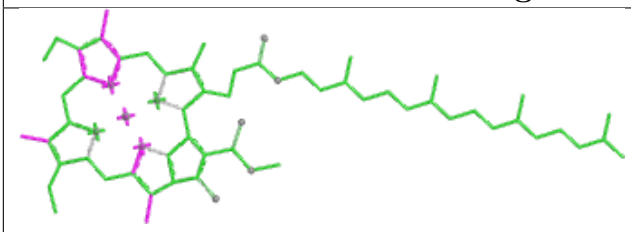


Torsions

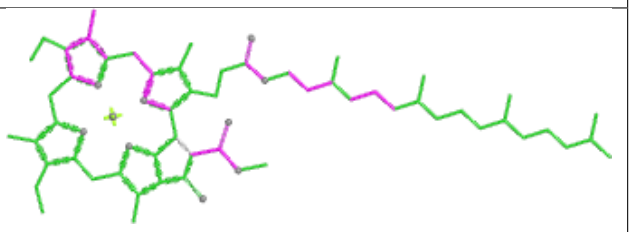


Rings

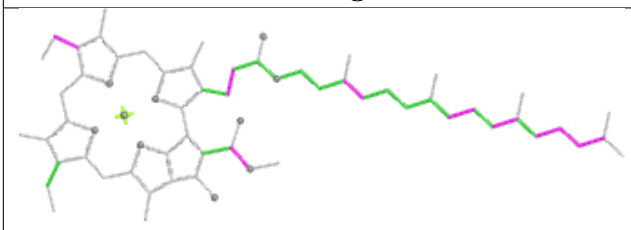
Ligand CLA A 1117



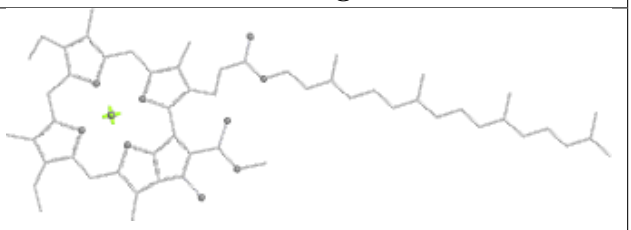
Bond lengths



Bond angles

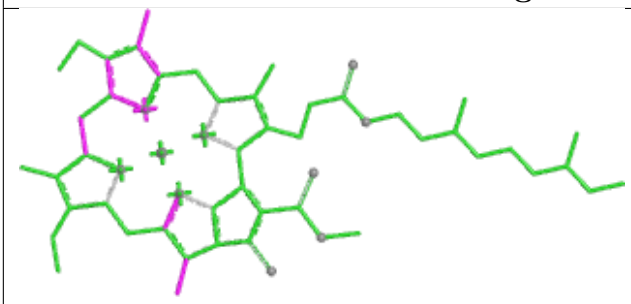


Torsions

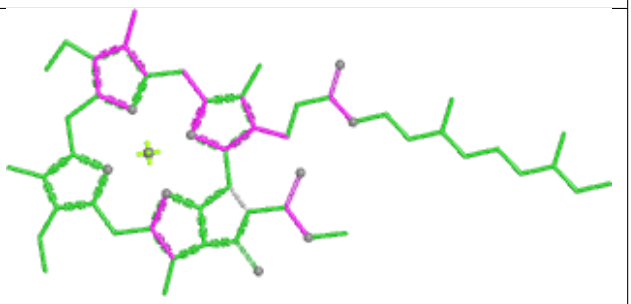


Rings

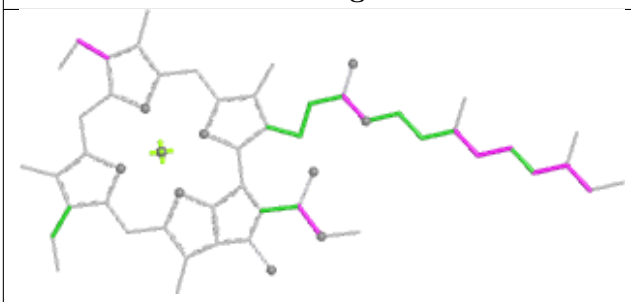
Ligand CLA A 1124



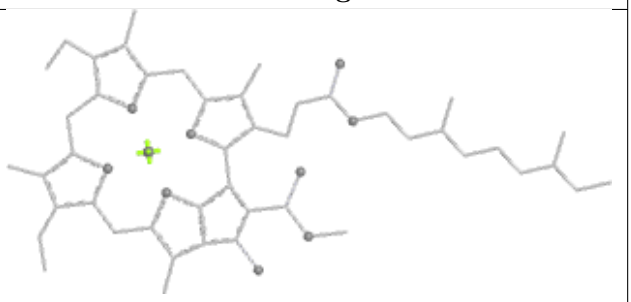
Bond lengths



Bond angles



Torsions

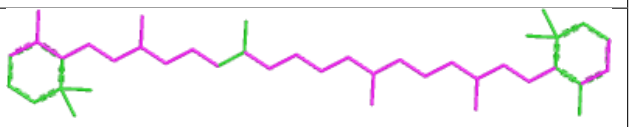


Rings

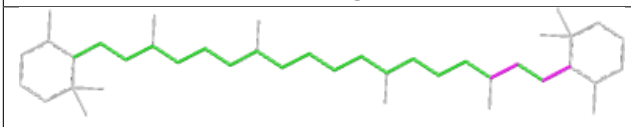
Ligand BCR 5 523



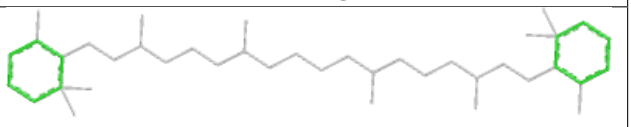
Bond lengths



Bond angles

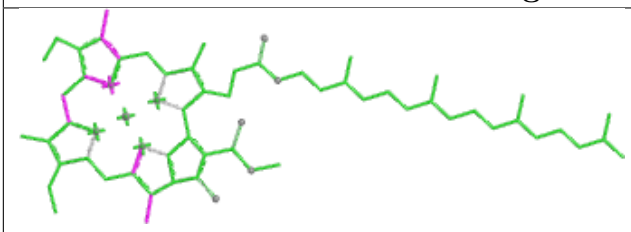


Torsions

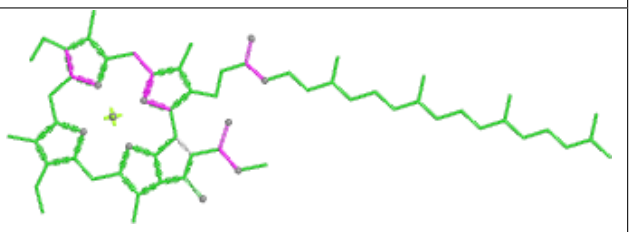


Rings

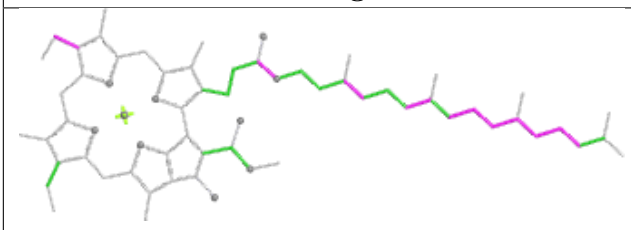
Ligand CLA f 1208



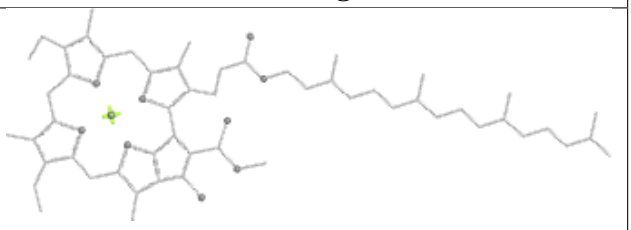
Bond lengths



Bond angles



Torsions

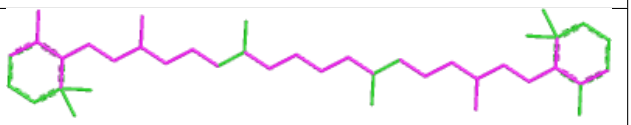


Rings

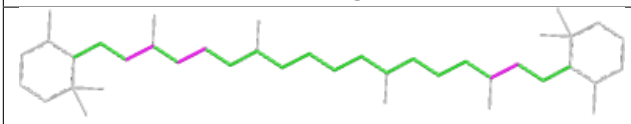
Ligand BCR 3 524



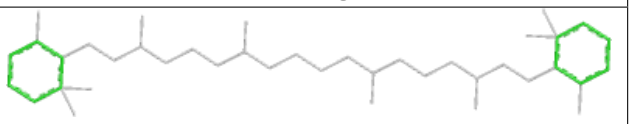
Bond lengths



Bond angles

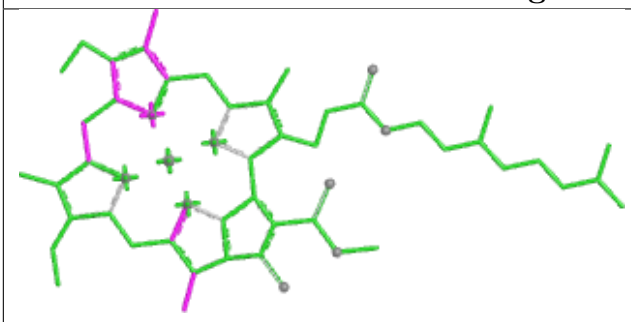


Torsions

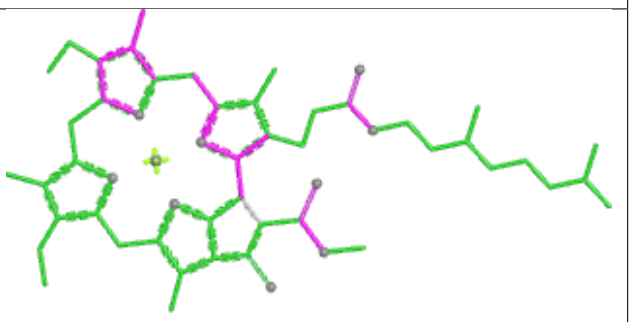


Rings

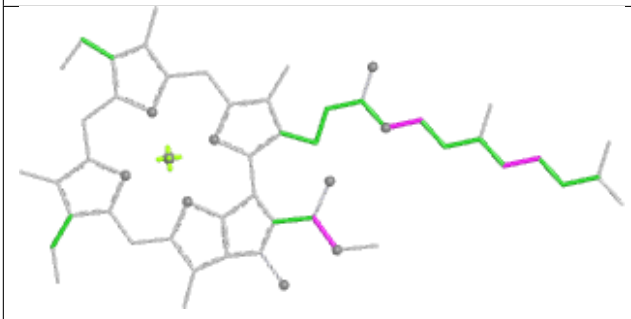
Ligand CLA 1 511



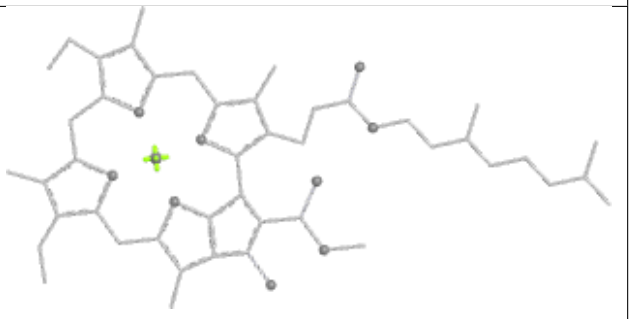
Bond lengths



Bond angles

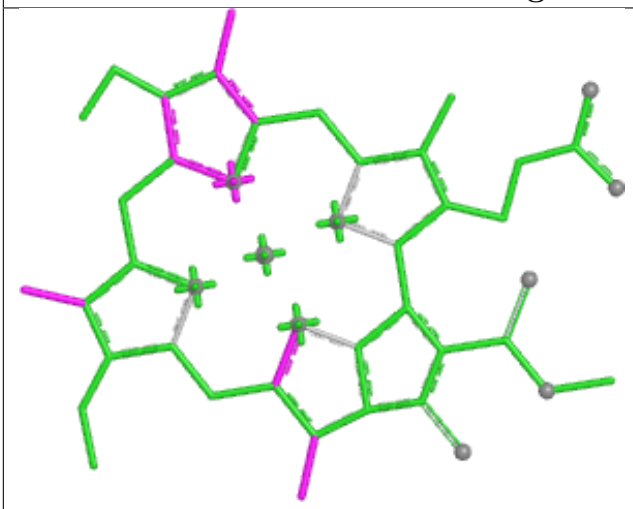


Torsions

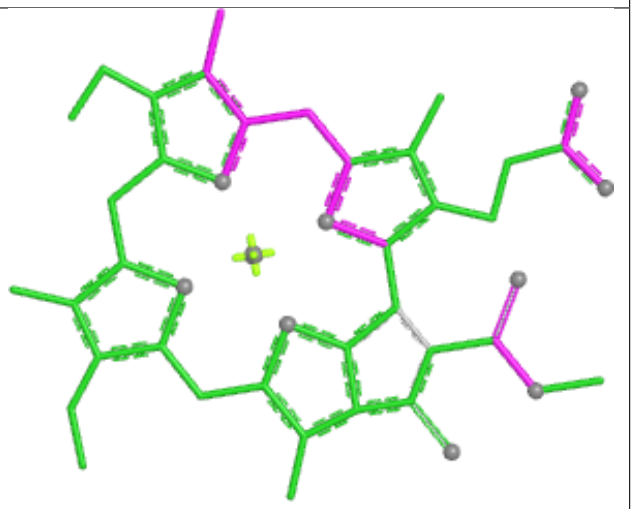


Rings

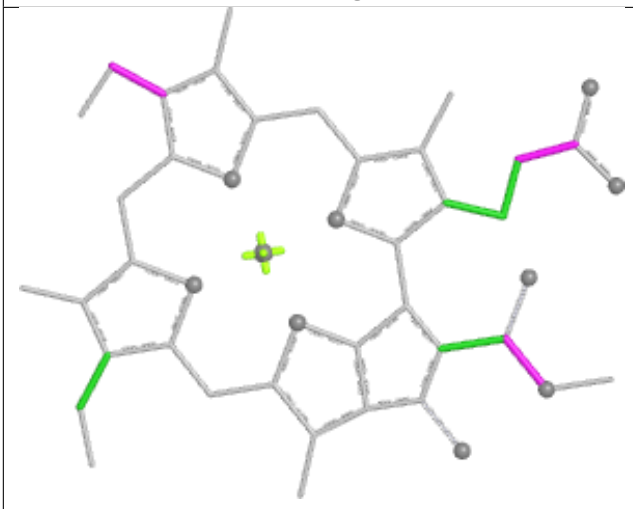
Ligand CLA b 508



Bond lengths



Bond angles

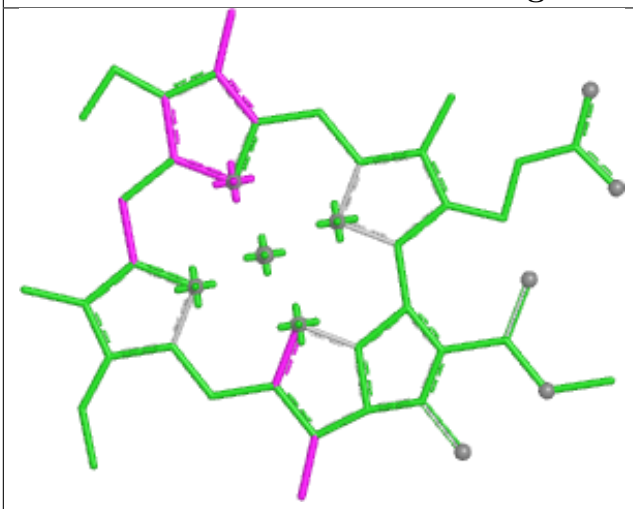


Torsions

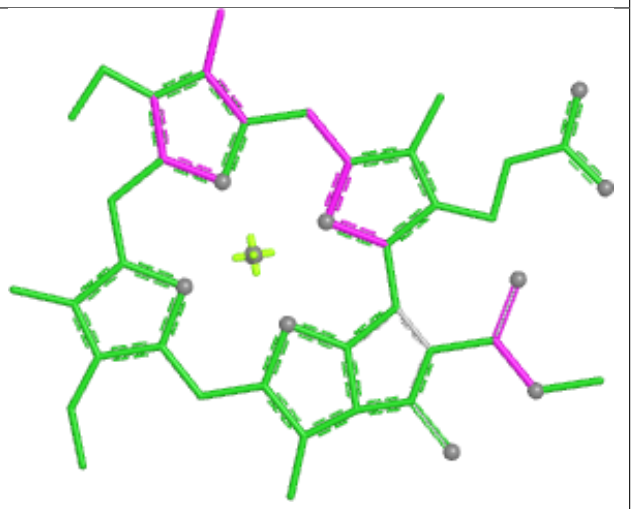


Rings

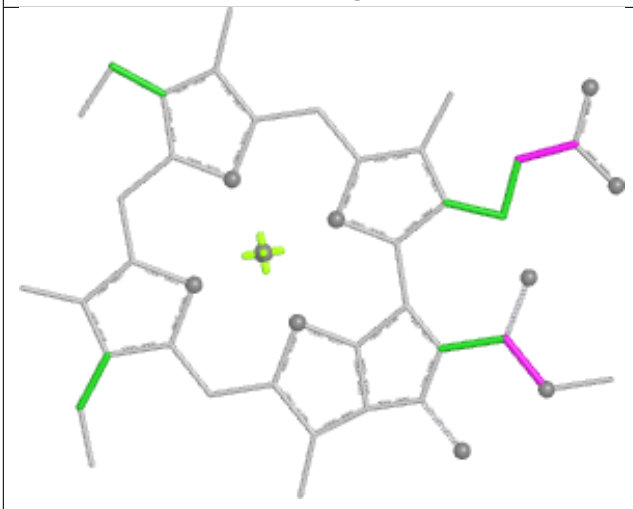
Ligand CLA d 509



Bond lengths



Bond angles

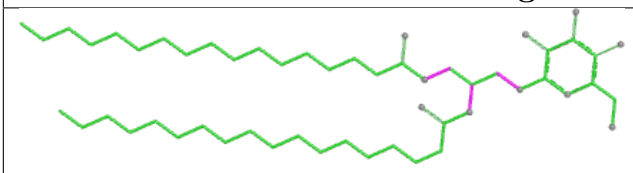


Torsions

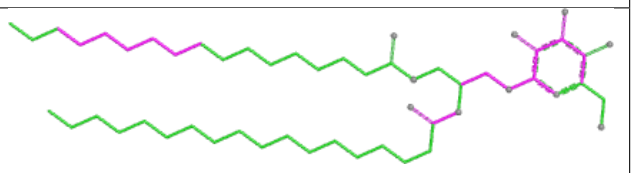


Rings

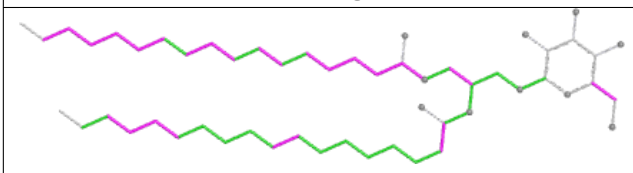
Ligand LMG f 5002



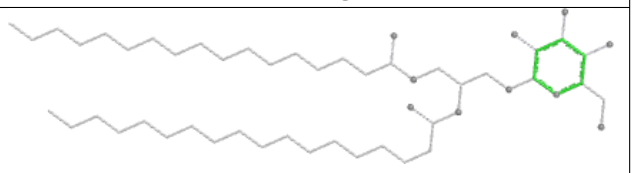
Bond lengths



Bond angles

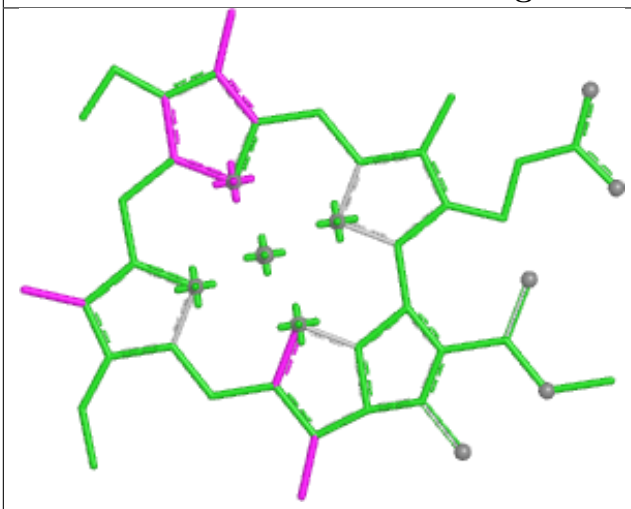


Torsions

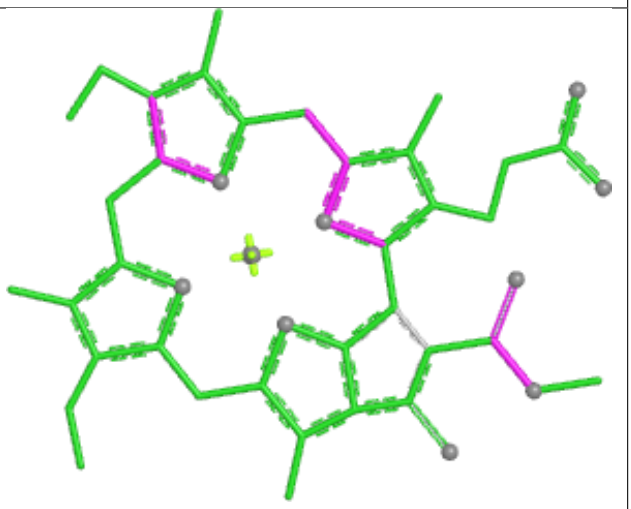


Rings

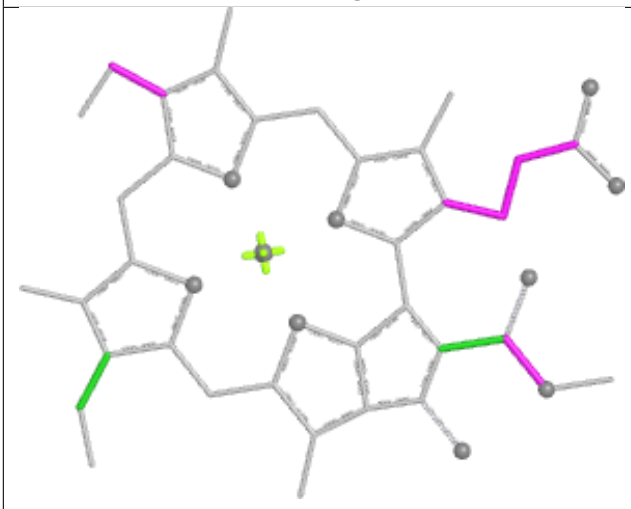
Ligand CLA R 1302



Bond lengths



Bond angles

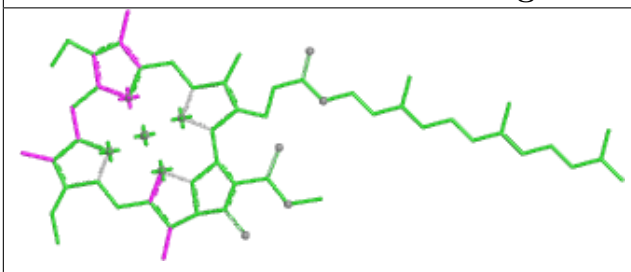


Torsions

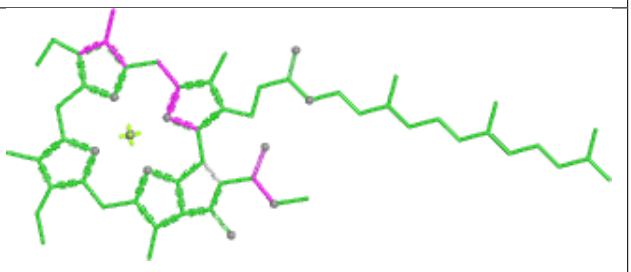


Rings

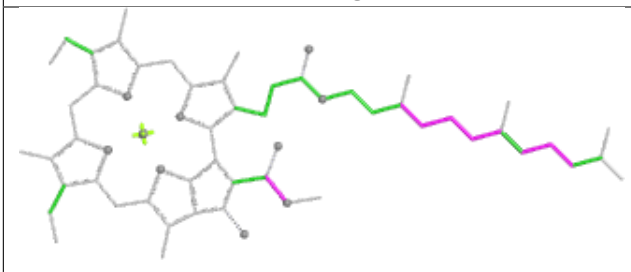
Ligand CLA L 1503



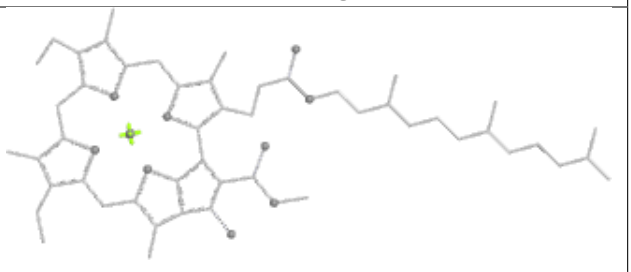
Bond lengths



Bond angles

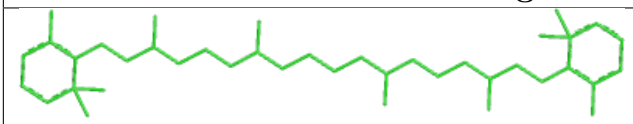


Torsions

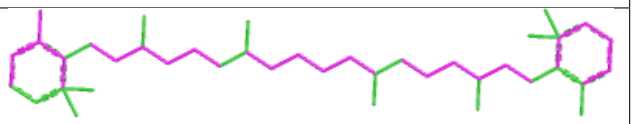


Rings

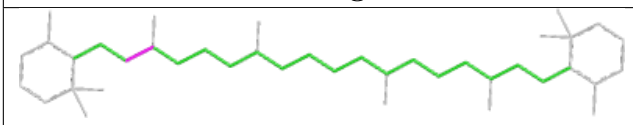
Ligand BCR n 4022



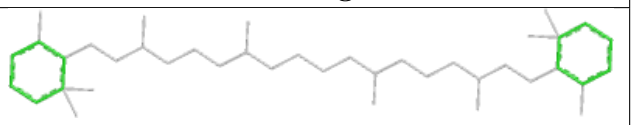
Bond lengths



Bond angles

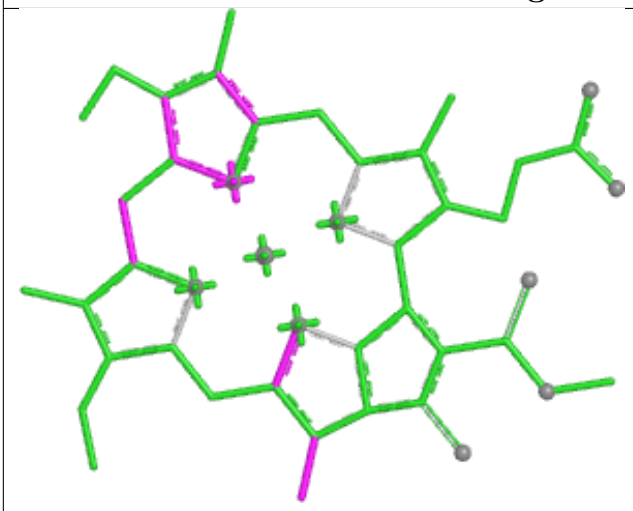


Torsions

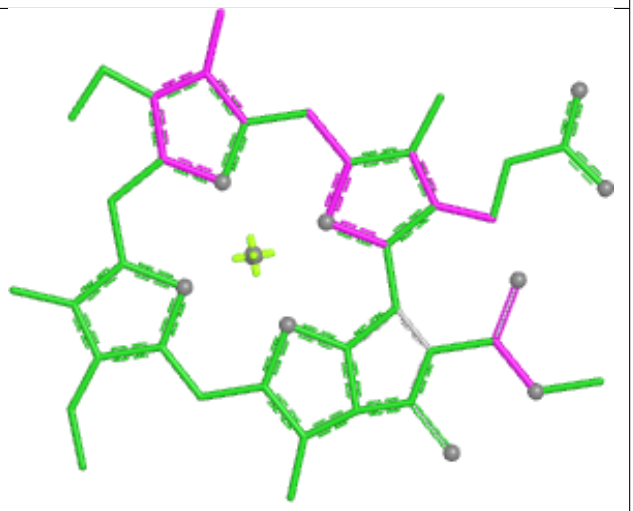


Rings

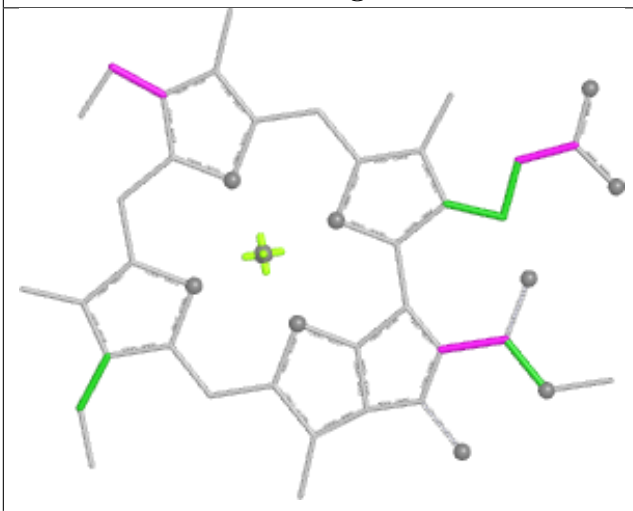
Ligand CLA v 504



Bond lengths



Bond angles

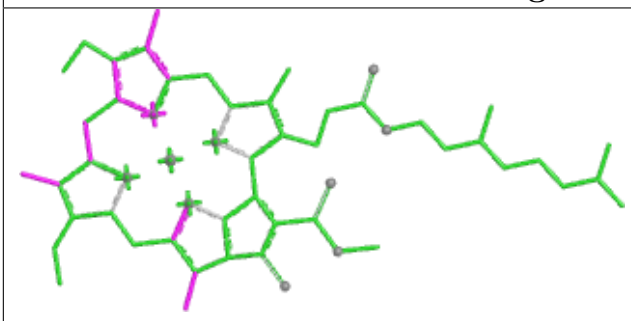


Torsions

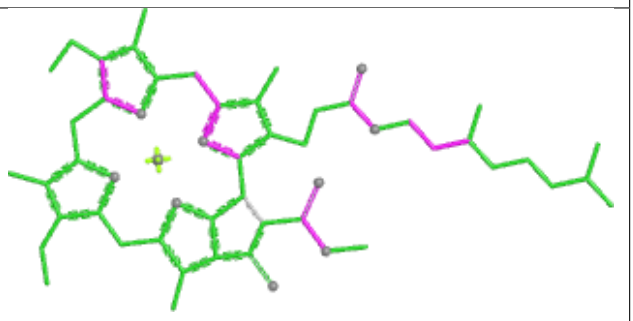


Rings

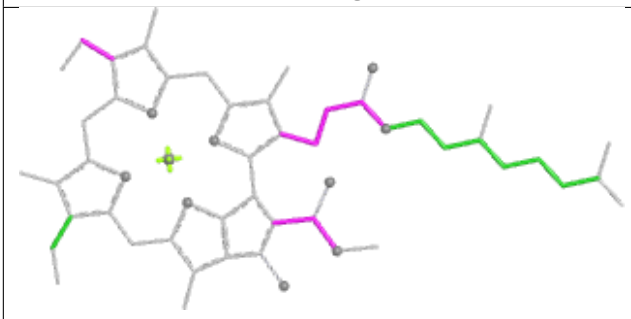
Ligand CLA a 518



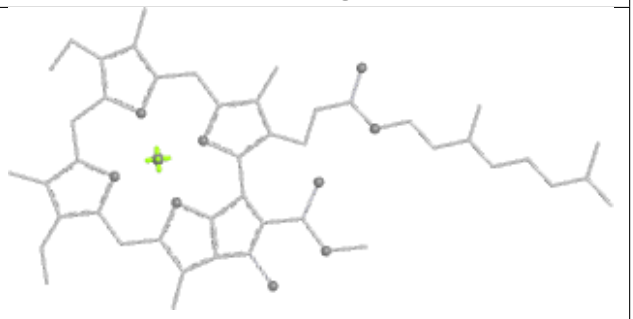
Bond lengths



Bond angles

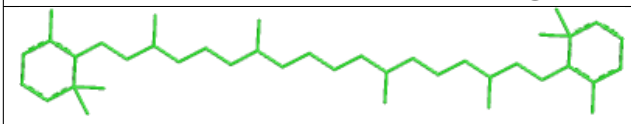


Torsions



Rings

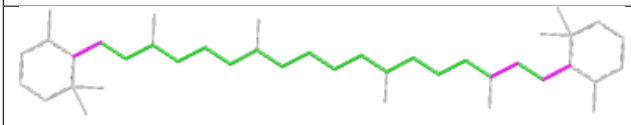
Ligand BCR 1 523



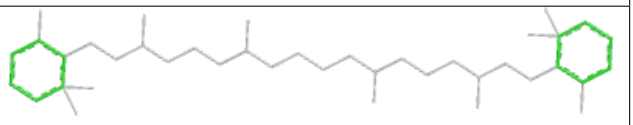
Bond lengths



Bond angles

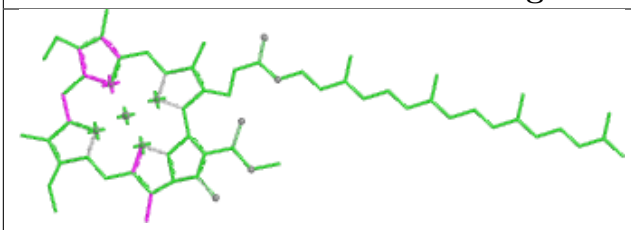


Torsions

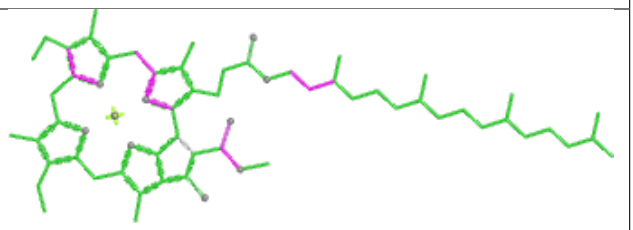


Rings

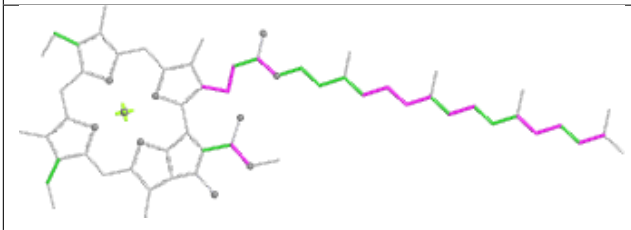
Ligand CLA Z 505



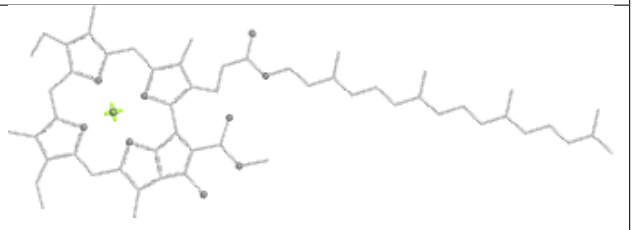
Bond lengths



Bond angles

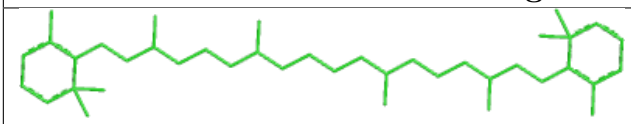


Torsions

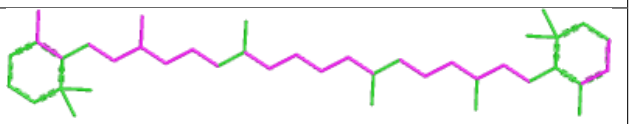


Rings

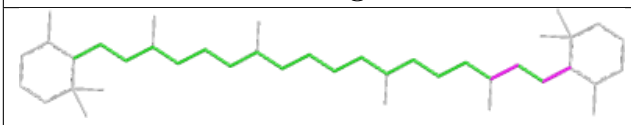
Ligand BCR b 523



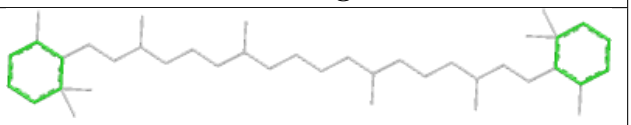
Bond lengths



Bond angles

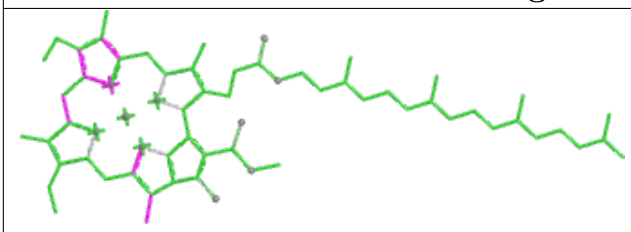


Torsions

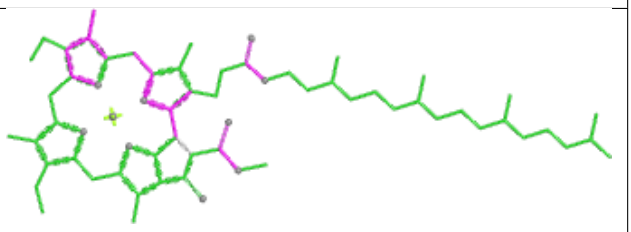


Rings

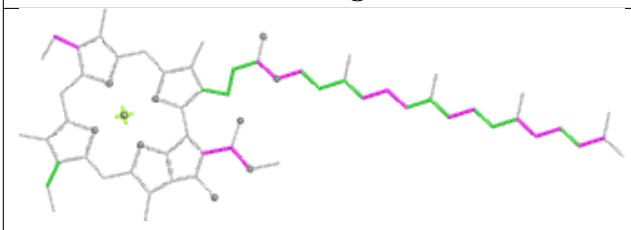
Ligand CLA a 510



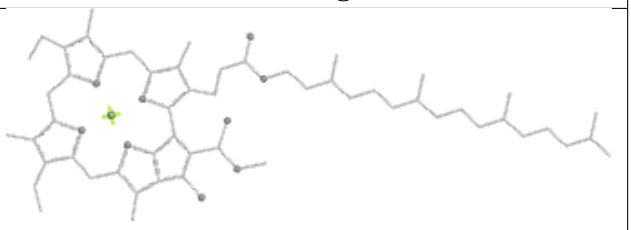
Bond lengths



Bond angles

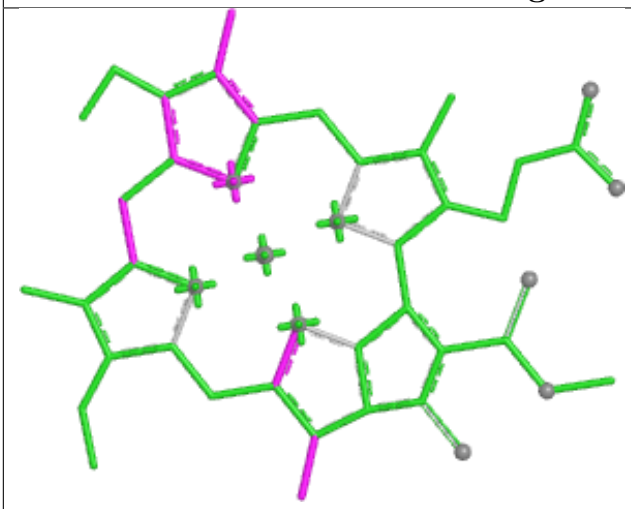


Torsions

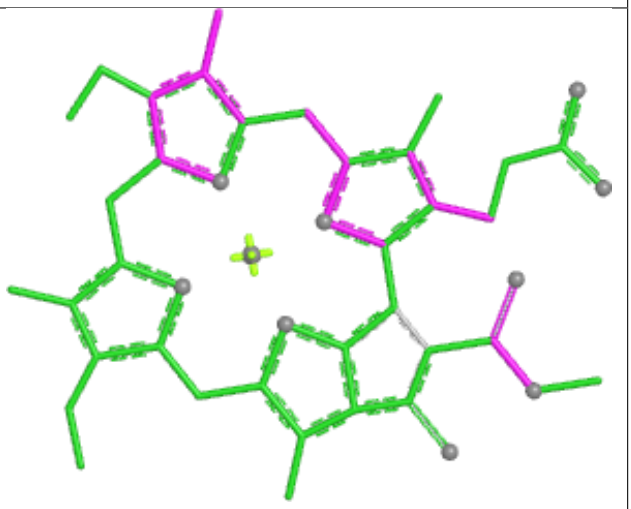


Rings

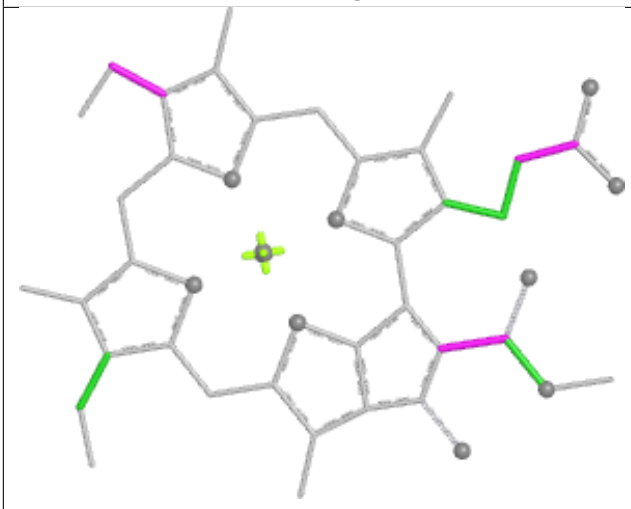
Ligand CLA 6 504



Bond lengths



Bond angles

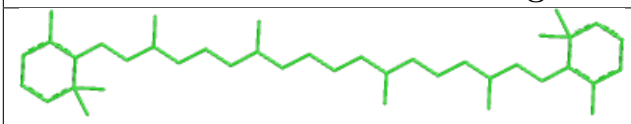


Torsions

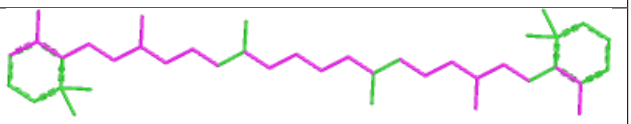


Rings

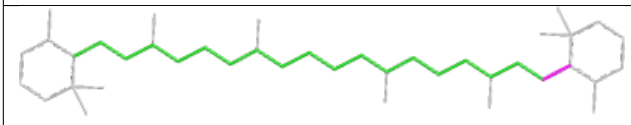
Ligand BCR c 524



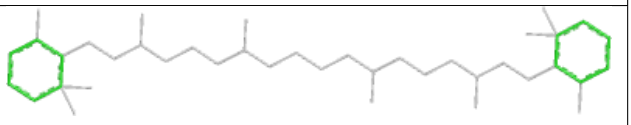
Bond lengths



Bond angles

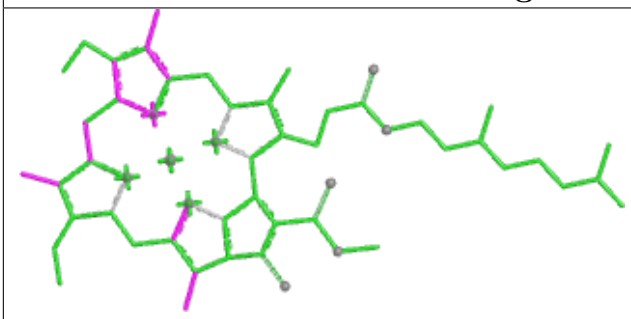


Torsions

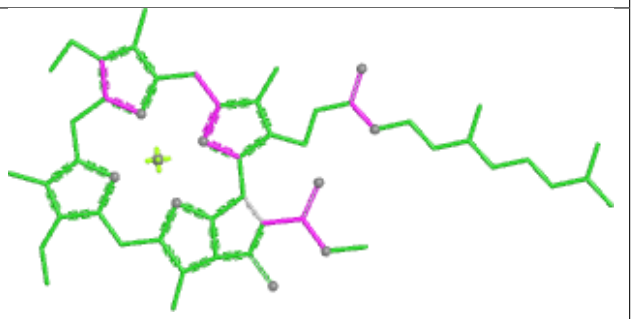


Rings

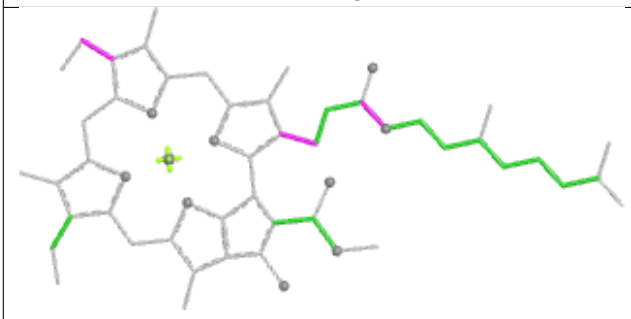
Ligand CLA B 1236



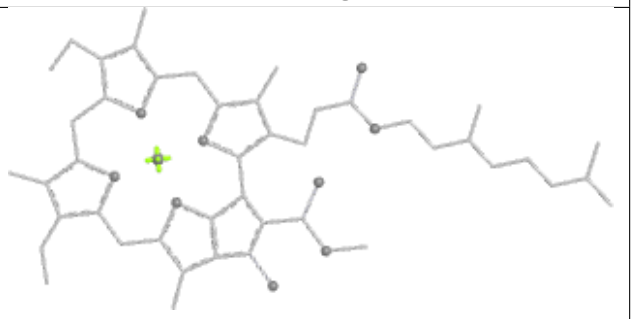
Bond lengths



Bond angles

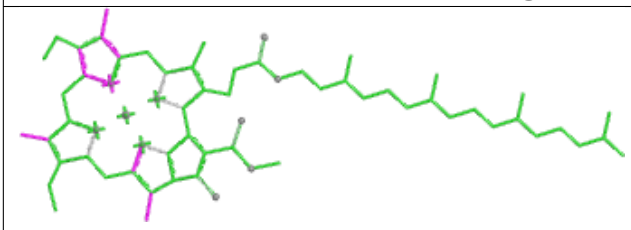


Torsions

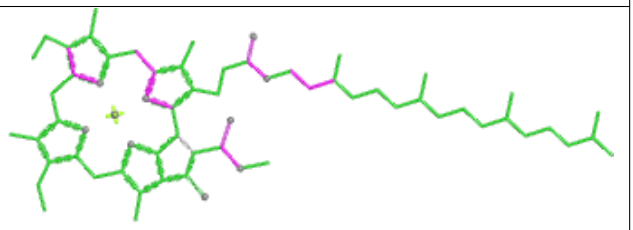


Rings

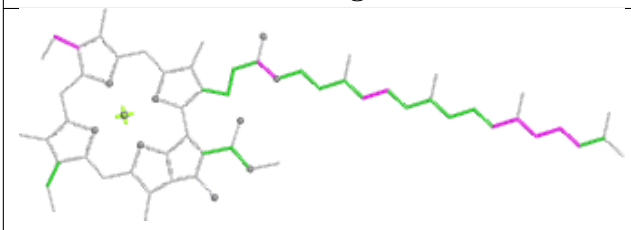
Ligand CLA e 1109



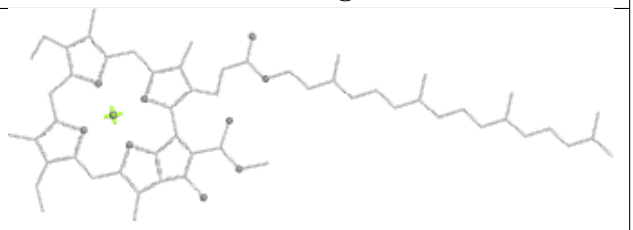
Bond lengths



Bond angles

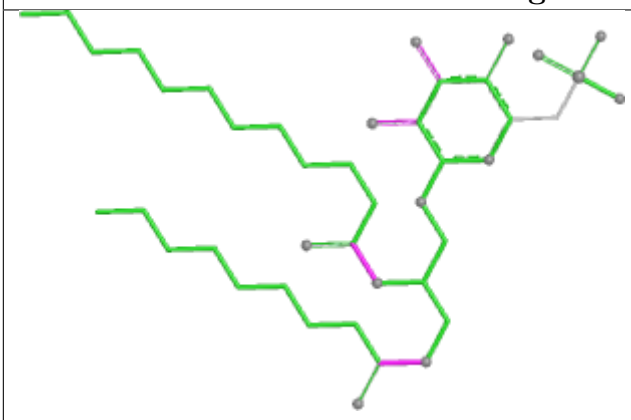


Torsions

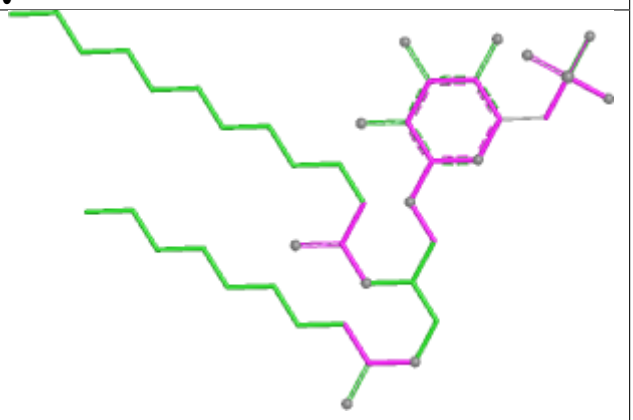


Rings

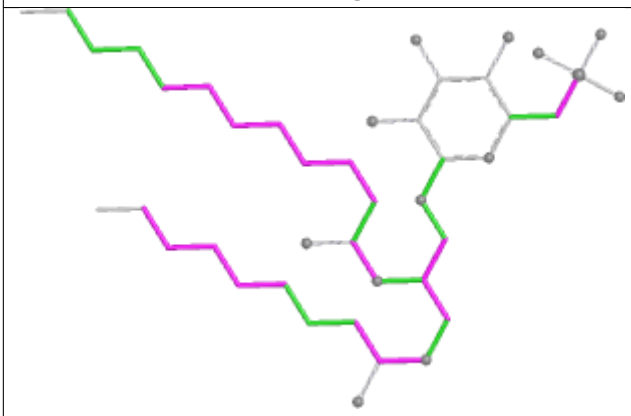
Ligand SQD 3 822



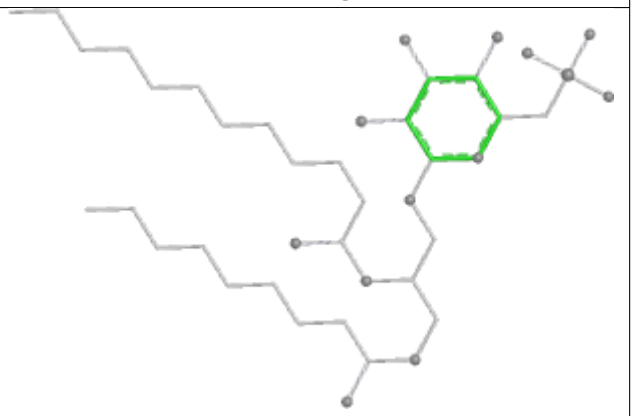
Bond lengths



Bond angles

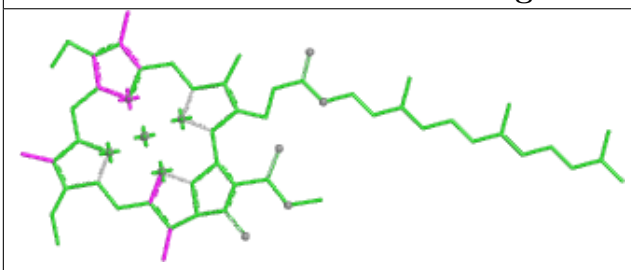


Torsions

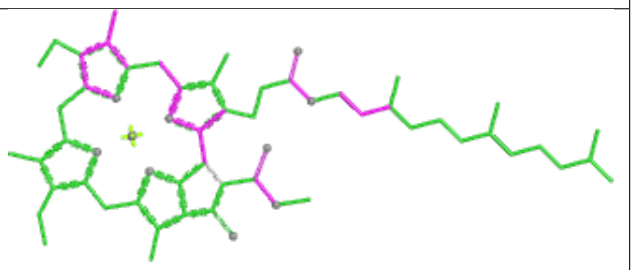


Rings

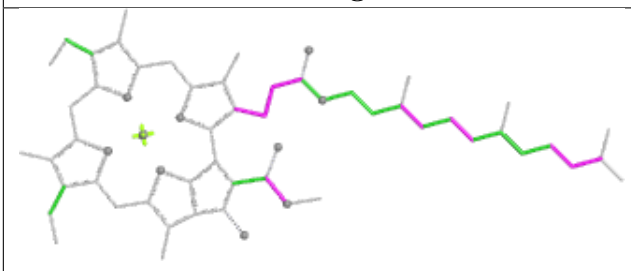
Ligand CLA B 1224



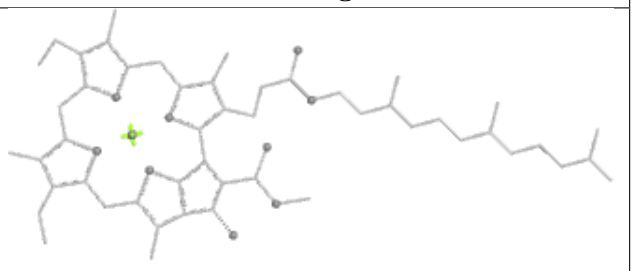
Bond lengths



Bond angles

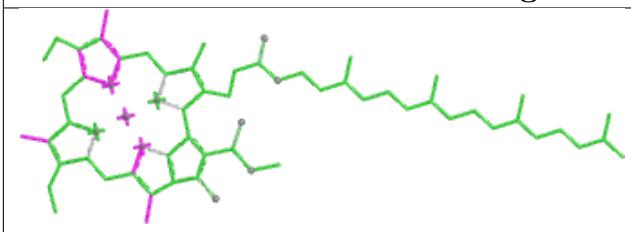


Torsions

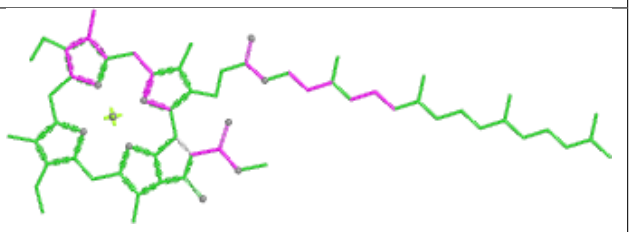


Rings

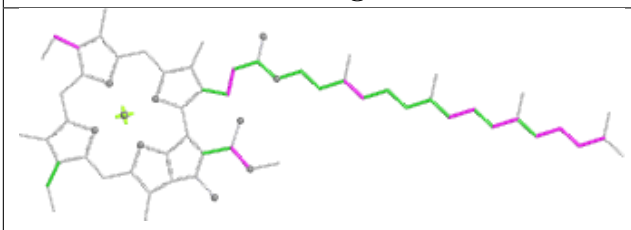
Ligand CLA e 1117



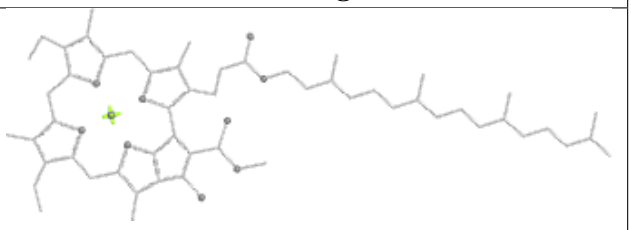
Bond lengths



Bond angles

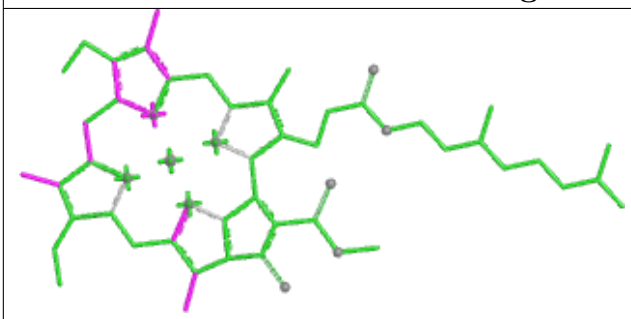


Torsions

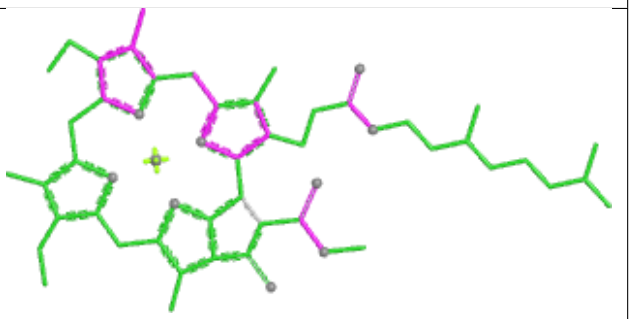


Rings

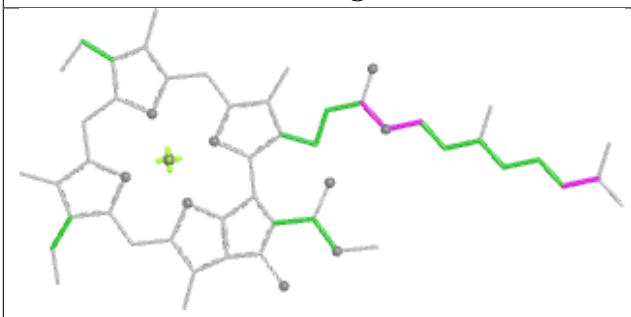
Ligand CLA e 1105



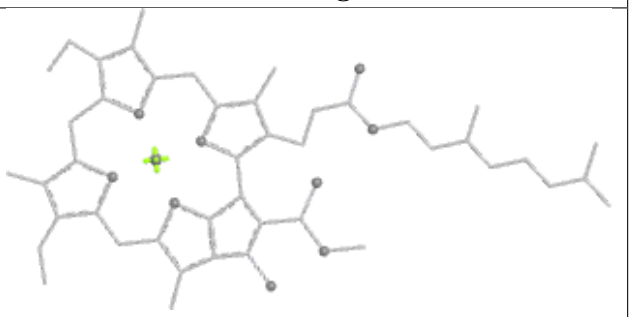
Bond lengths



Bond angles

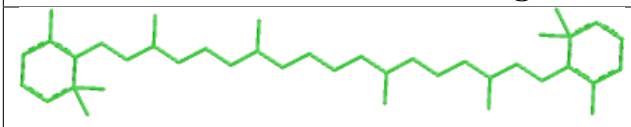


Torsions

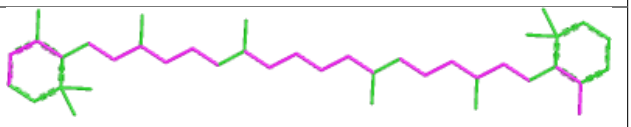


Rings

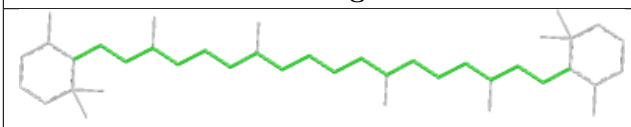
Ligand BCR A 4003



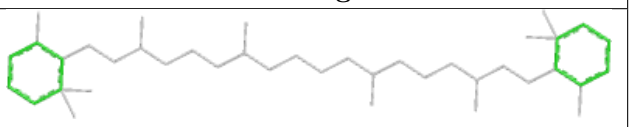
Bond lengths



Bond angles

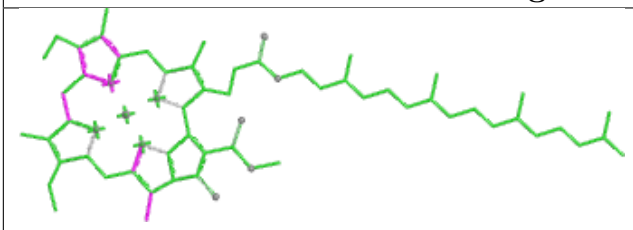


Torsions

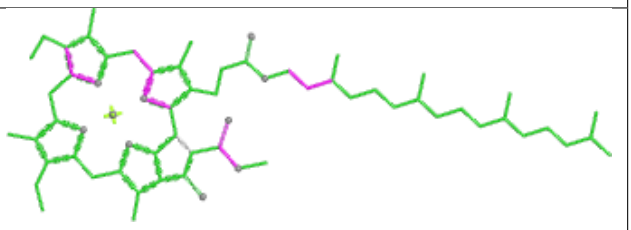


Rings

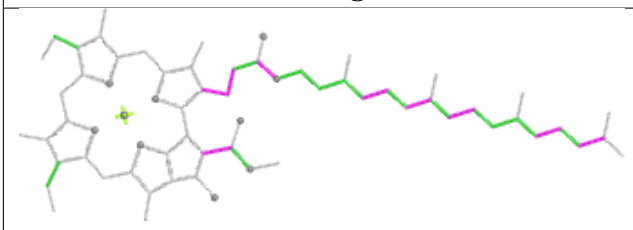
Ligand CLA 1 505



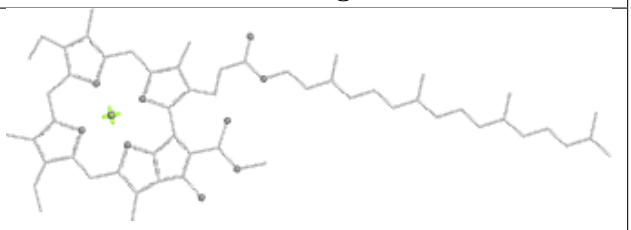
Bond lengths



Bond angles

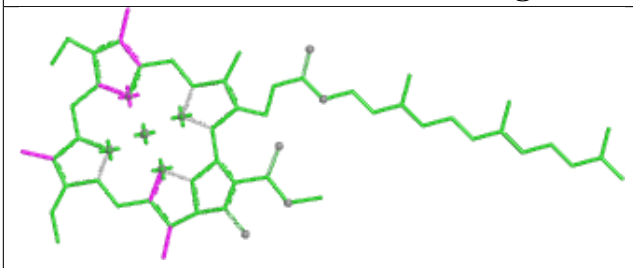


Torsions

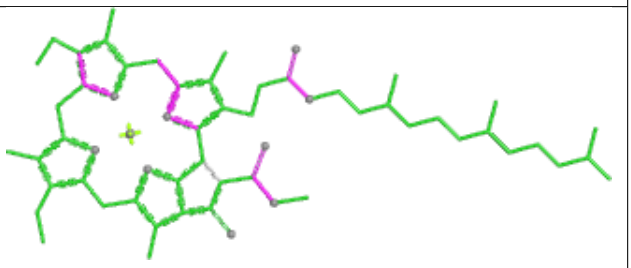


Rings

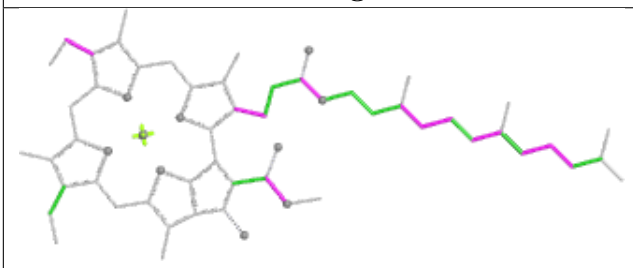
Ligand CLA G 1122



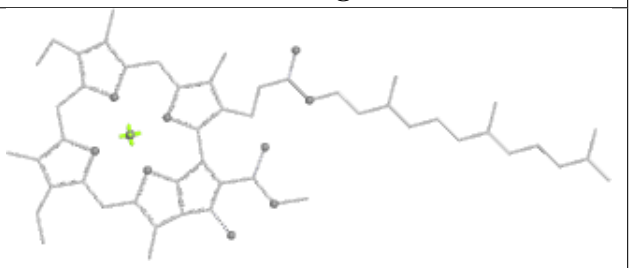
Bond lengths



Bond angles



Torsions



Rings

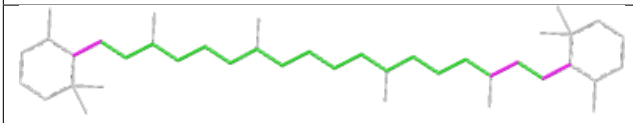
Ligand BCR Y 523



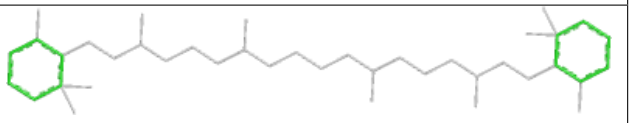
Bond lengths



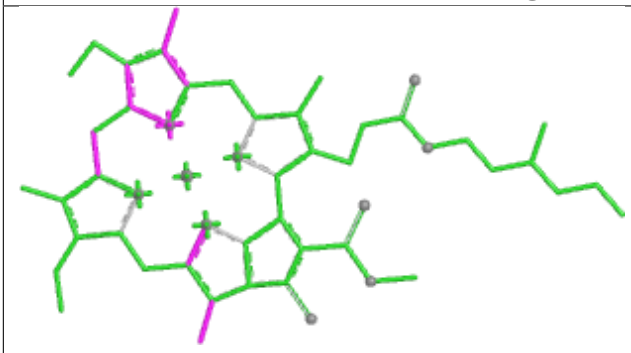
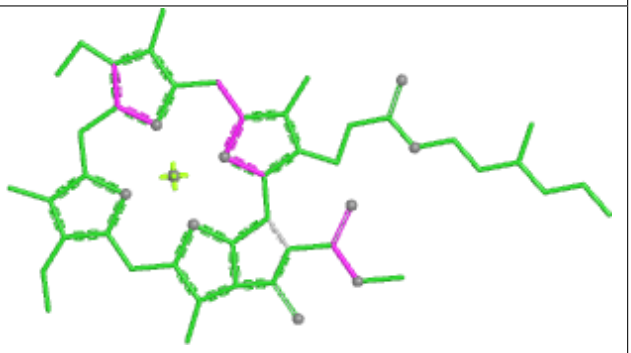
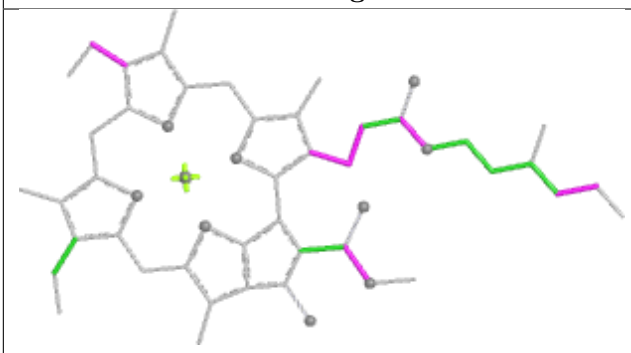
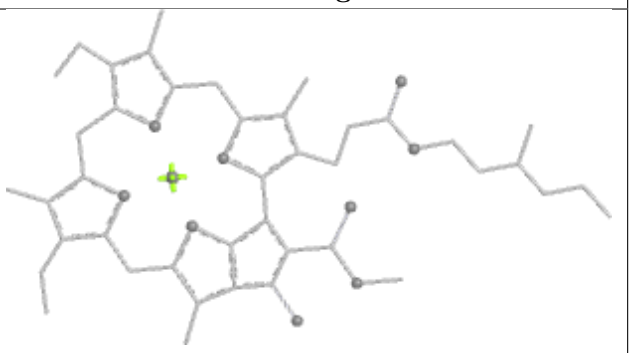
Bond angles

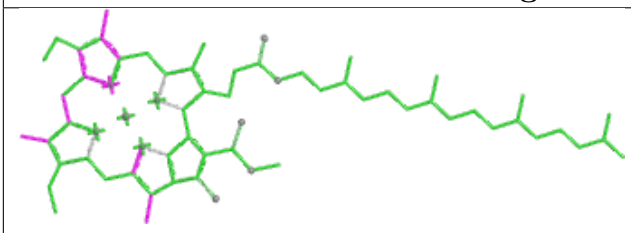
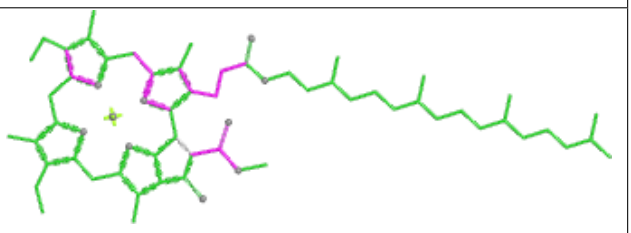
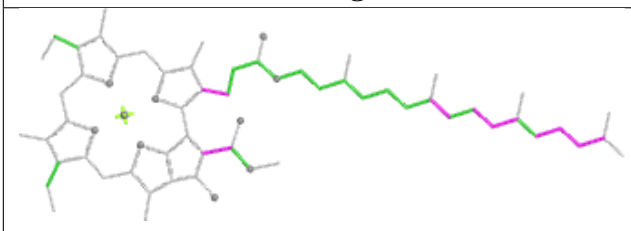
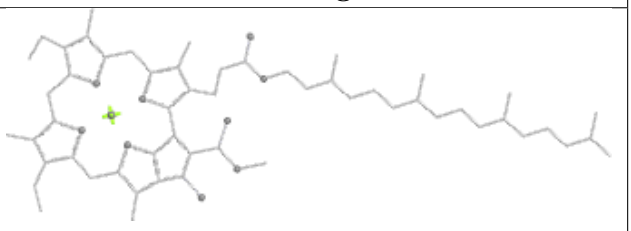


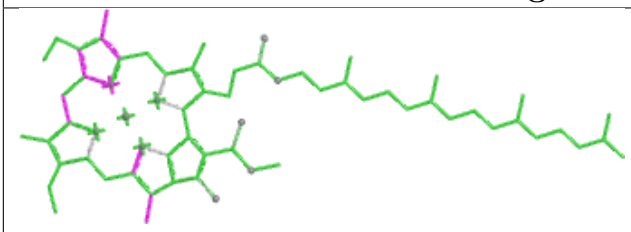
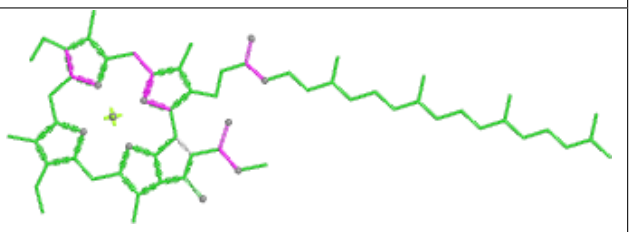
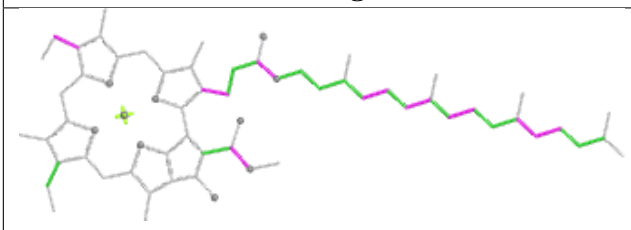
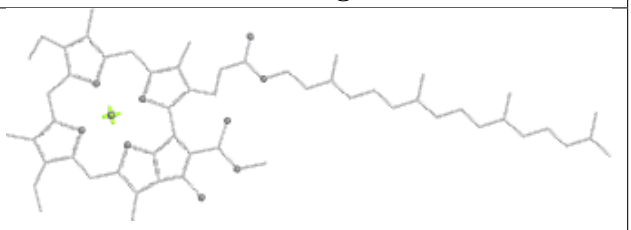
Torsions

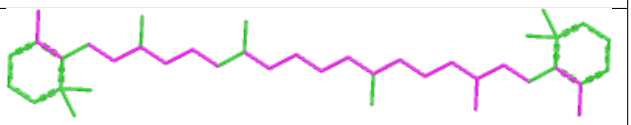
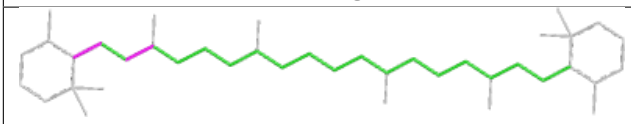
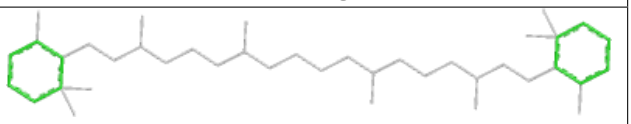


Rings

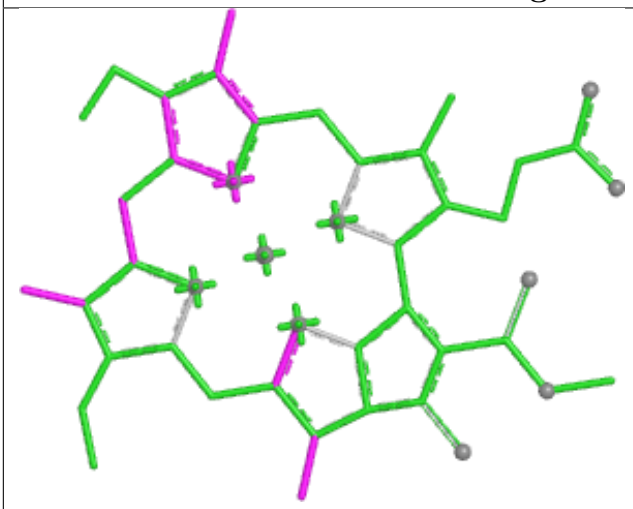
Ligand CLA Y 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 1101	
	
Bond lengths	Bond angles
	
Torsions	Rings

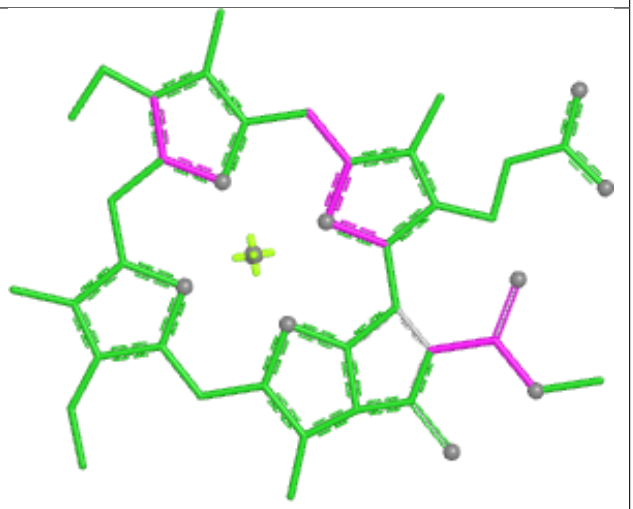
Ligand CLA 3 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR d 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

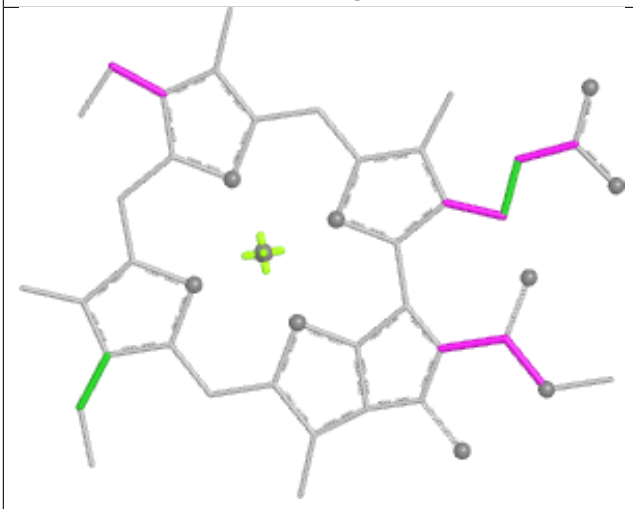
Ligand CLA r 516



Bond lengths



Bond angles

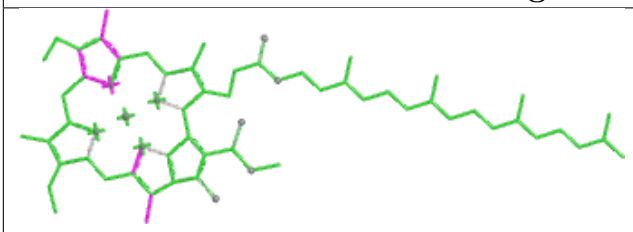


Torsions

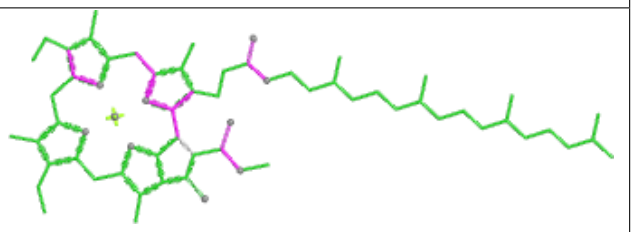


Rings

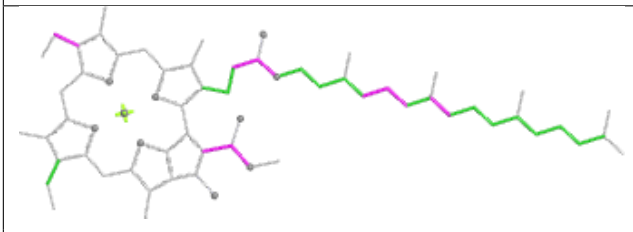
Ligand CLA a 507



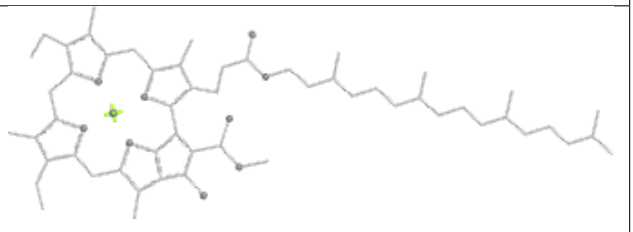
Bond lengths



Bond angles

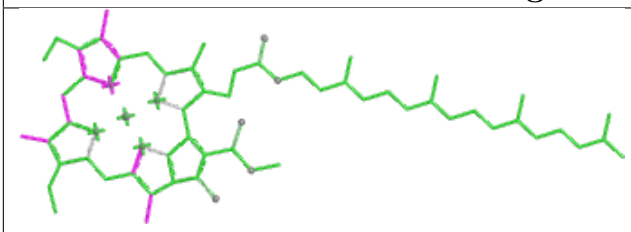


Torsions

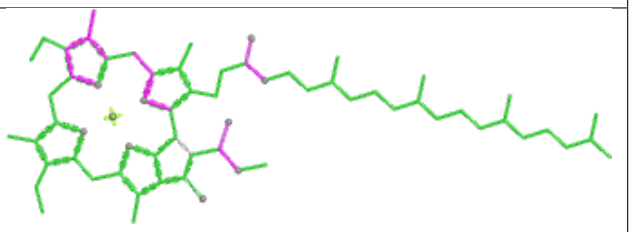


Rings

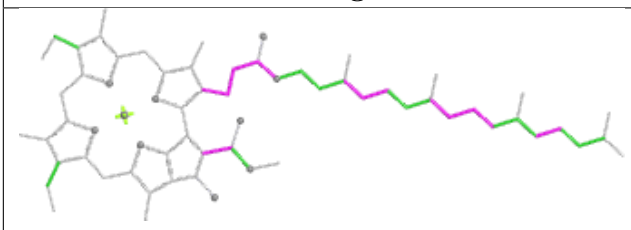
Ligand CLA Z 518



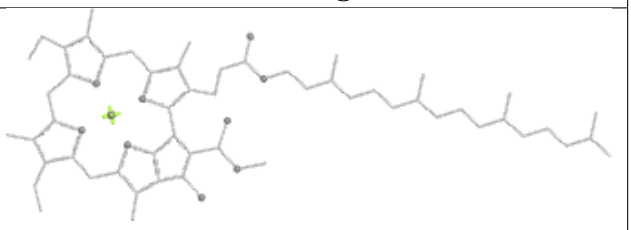
Bond lengths



Bond angles

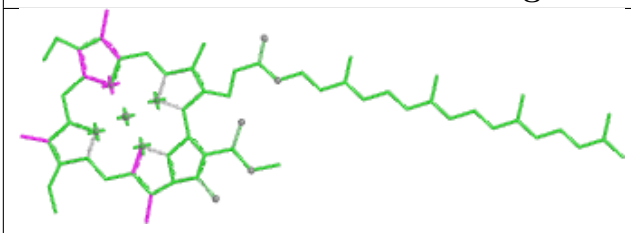


Torsions

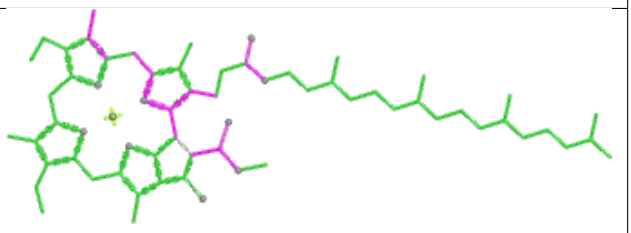


Rings

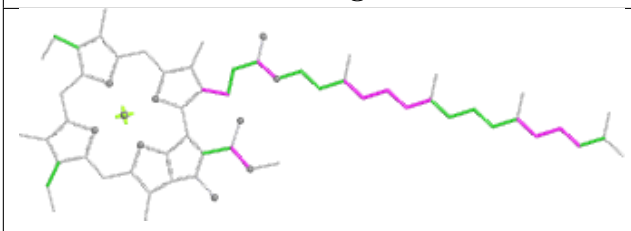
Ligand CLA l 1303



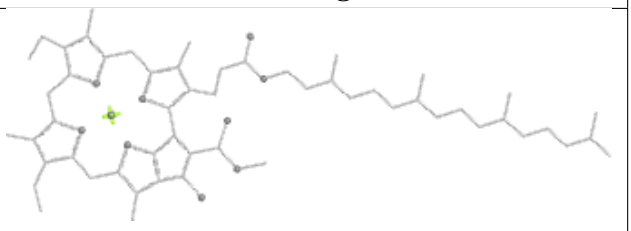
Bond lengths



Bond angles

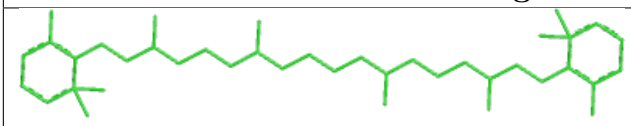


Torsions

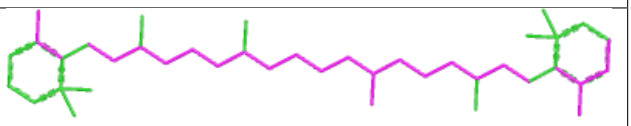


Rings

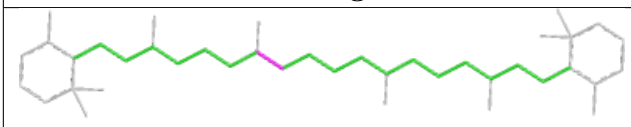
Ligand BCR R 4016



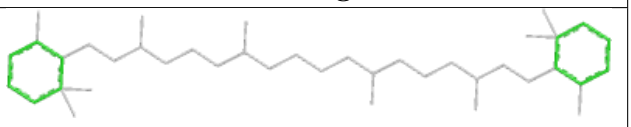
Bond lengths



Bond angles

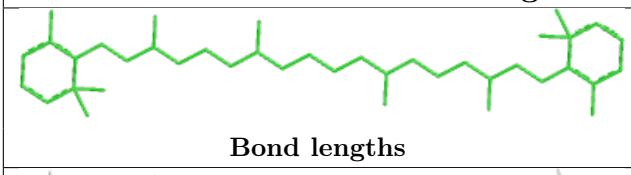


Torsions

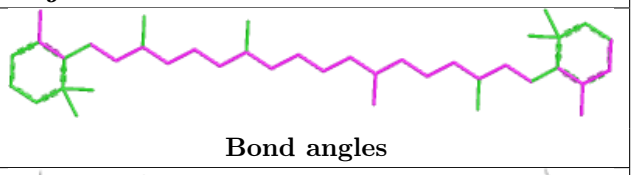


Rings

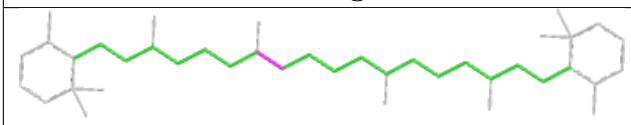
Ligand BCR j 4016



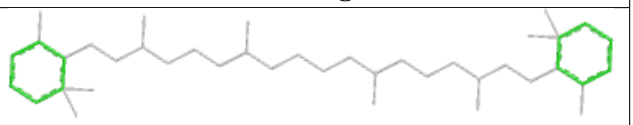
Bond lengths



Bond angles

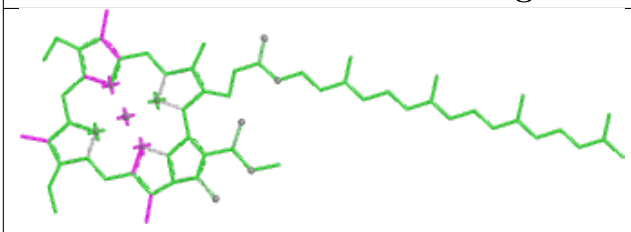


Torsions

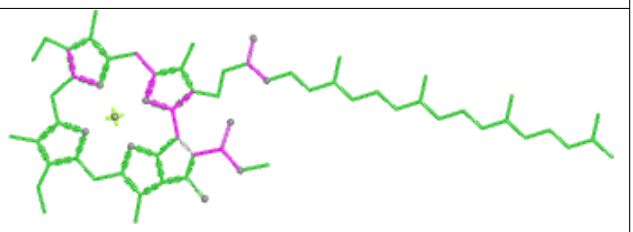


Rings

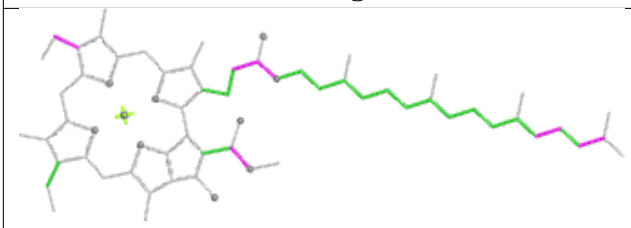
Ligand CLA B 1021



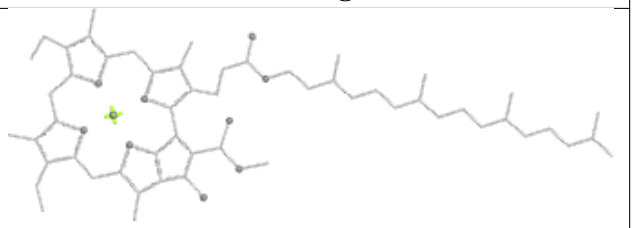
Bond lengths



Bond angles

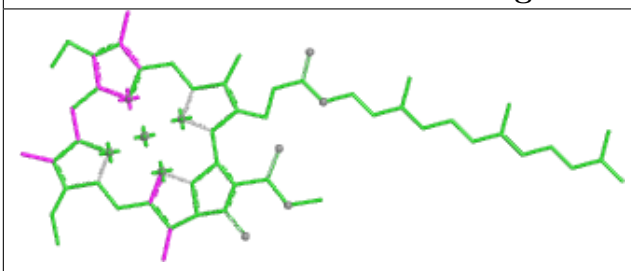


Torsions

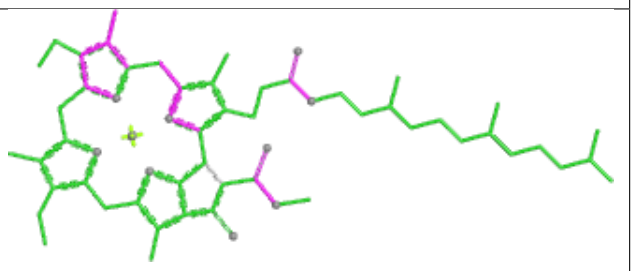


Rings

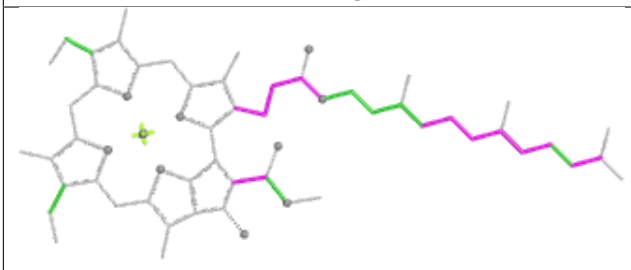
Ligand CLA A 1116



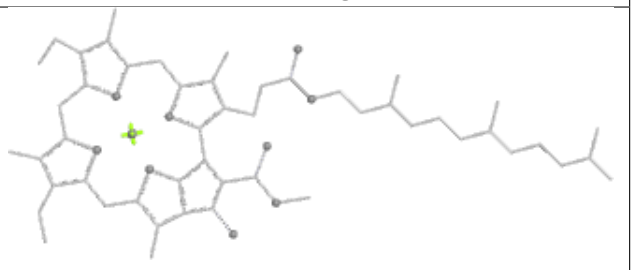
Bond lengths



Bond angles

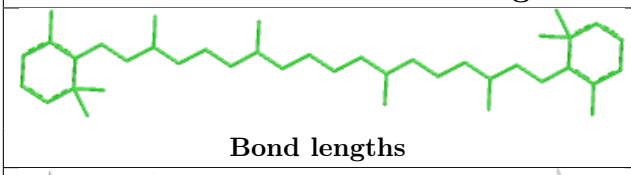


Torsions

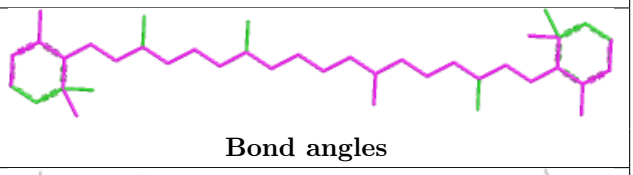


Rings

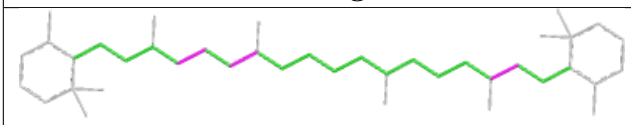
Ligand BCR H 4010



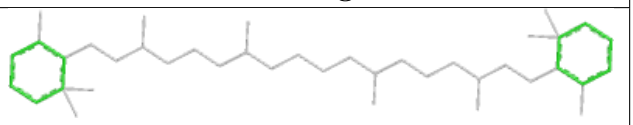
Bond lengths



Bond angles

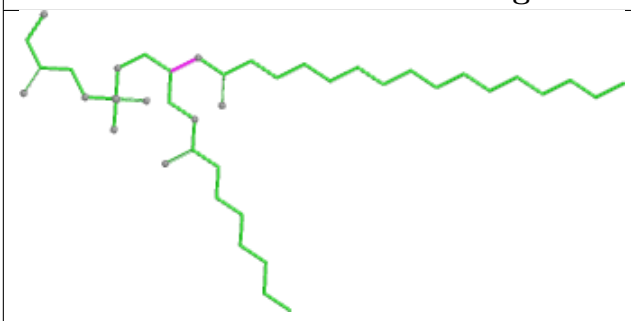


Torsions

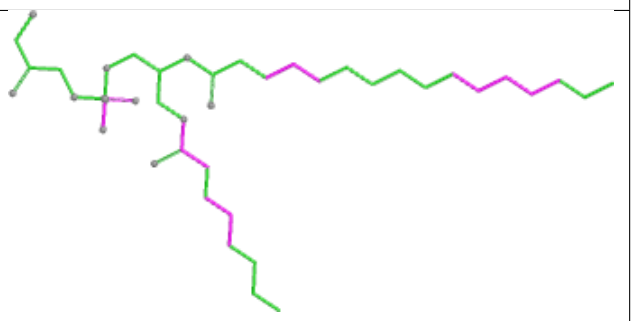


Rings

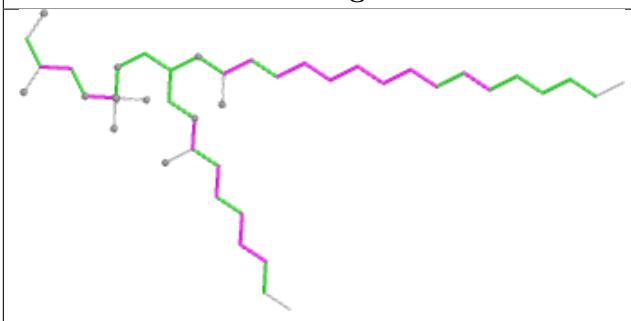
Ligand LHG G 5003



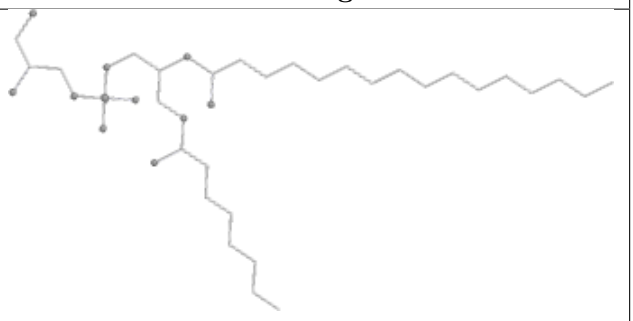
Bond lengths



Bond angles

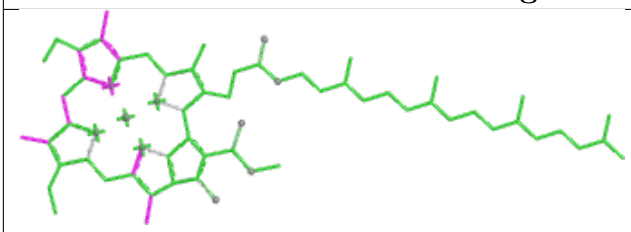


Torsions

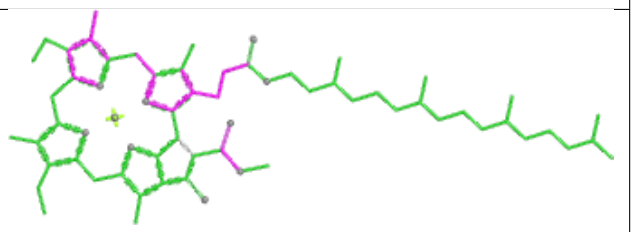


Rings

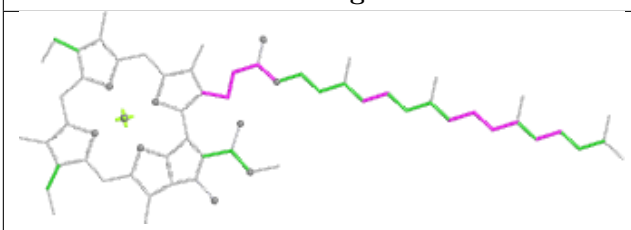
Ligand CLA e 1125



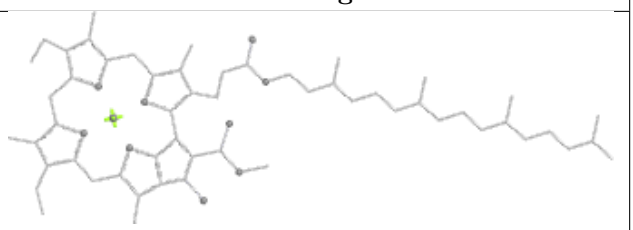
Bond lengths



Bond angles

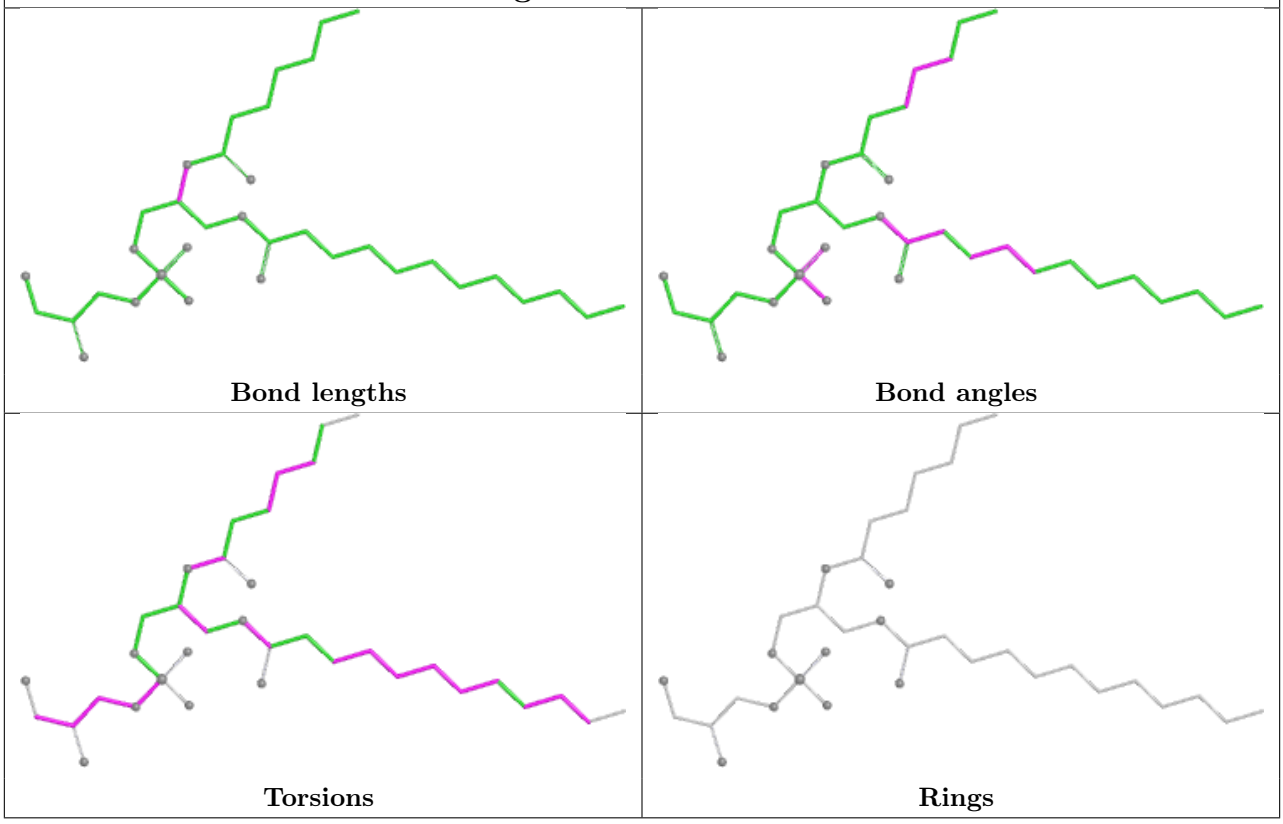


Torsions

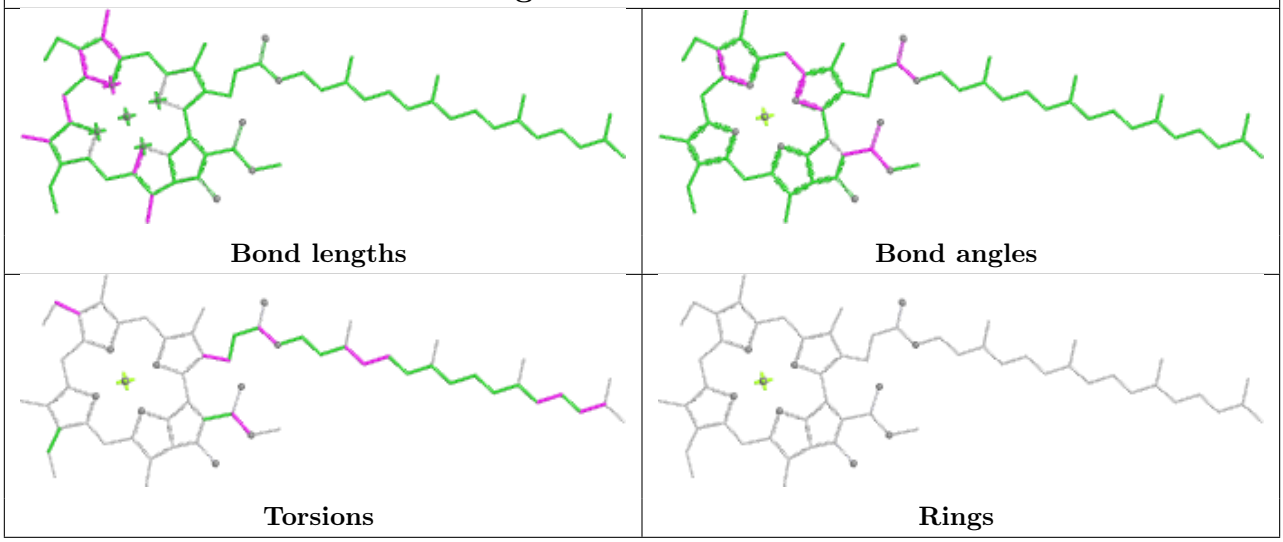


Rings

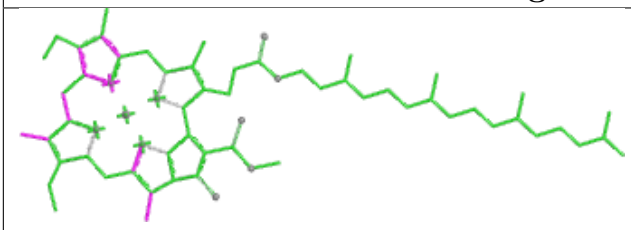
Ligand LHG A 5004



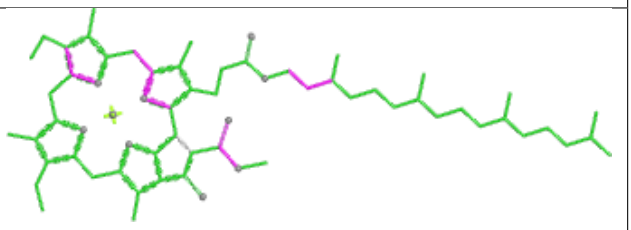
Ligand CLA H 1227



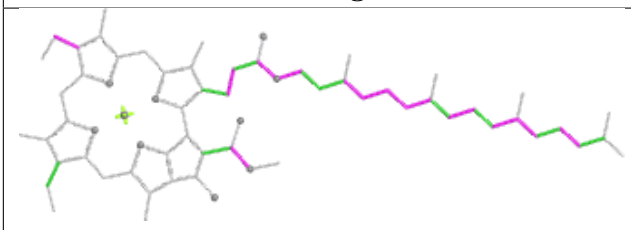
Ligand CLA a 505



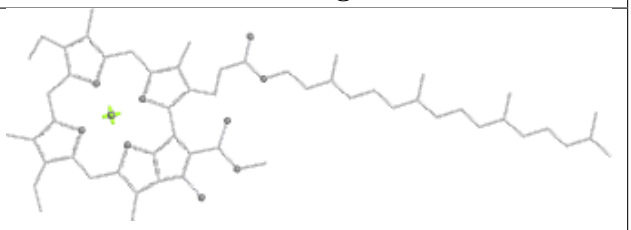
Bond lengths



Bond angles

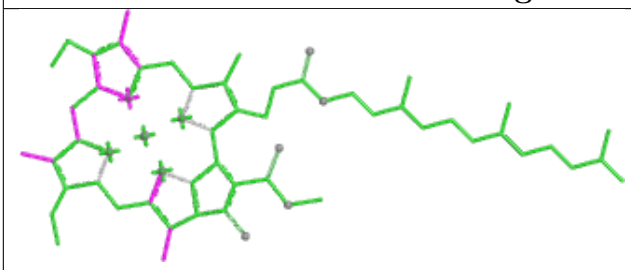


Torsions

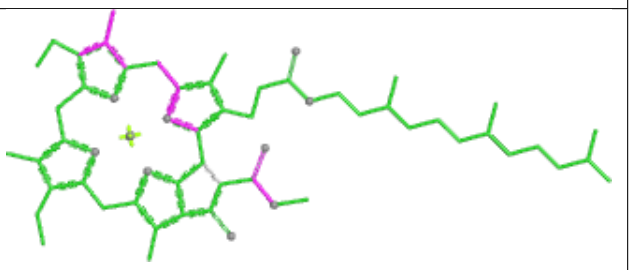


Rings

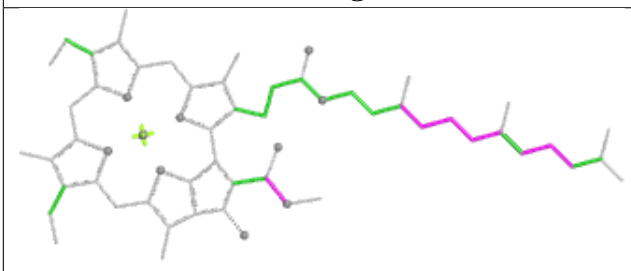
Ligand CLA V 1503



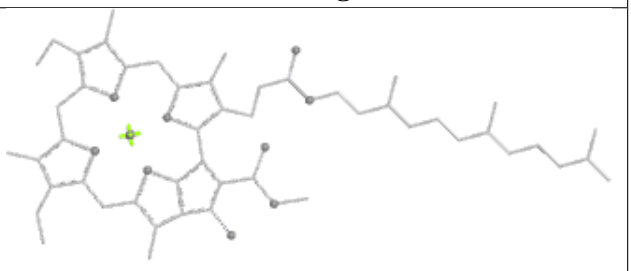
Bond lengths



Bond angles

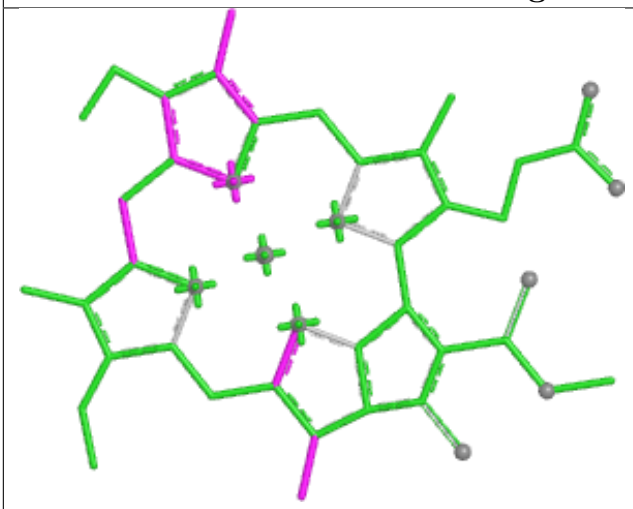


Torsions

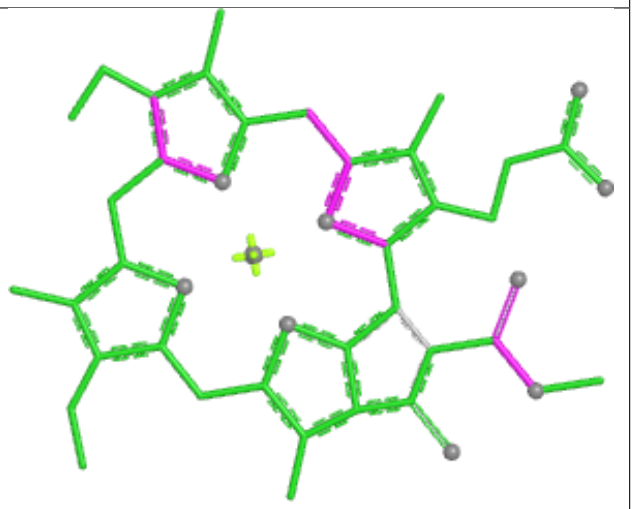


Rings

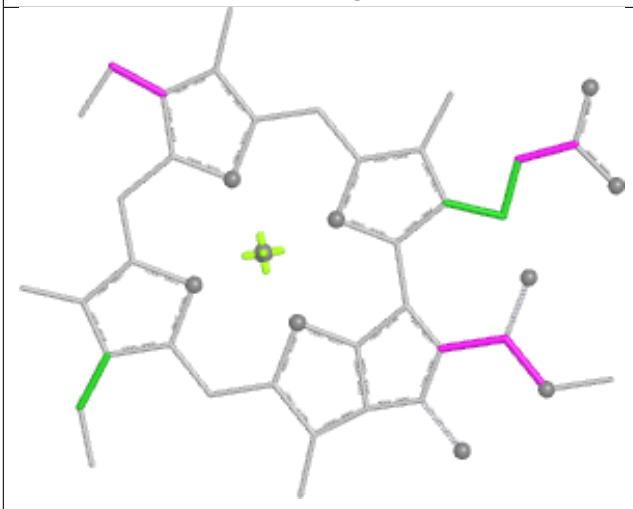
Ligand CLA 5 510



Bond lengths



Bond angles

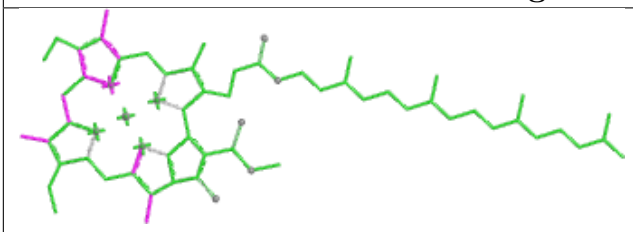


Torsions

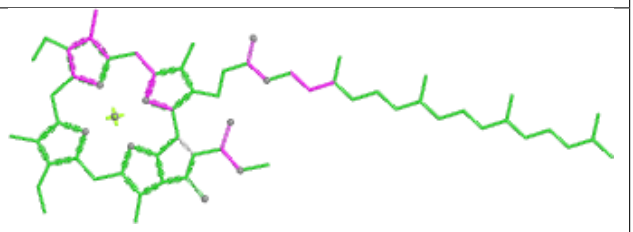


Rings

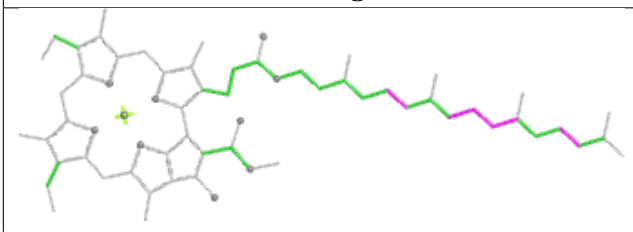
Ligand CLA 1 509



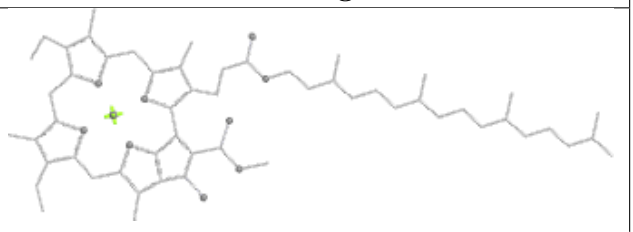
Bond lengths



Bond angles

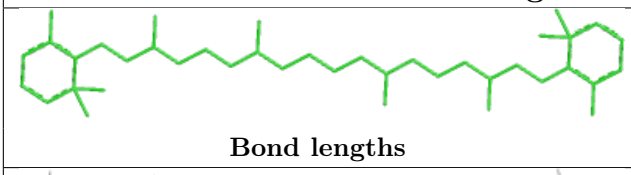


Torsions

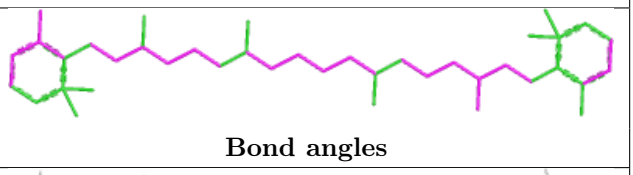


Rings

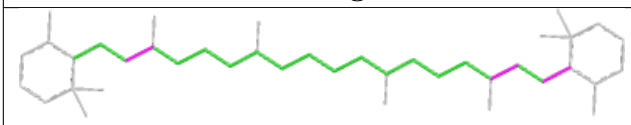
Ligand BCR 2 523



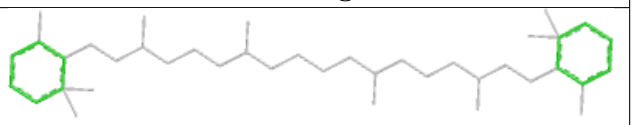
Bond lengths



Bond angles

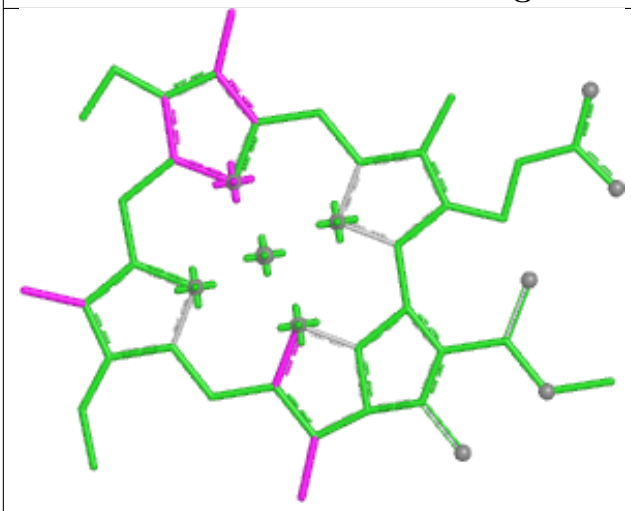


Torsions

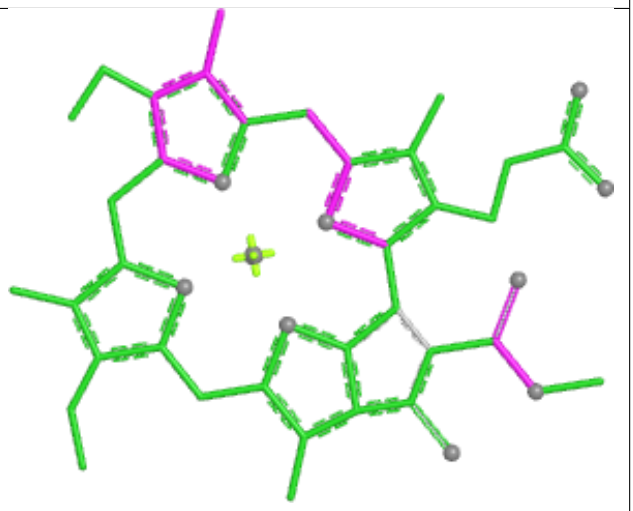


Rings

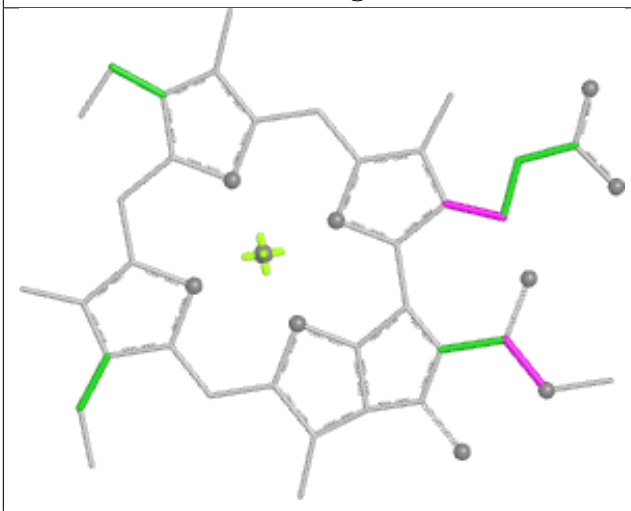
Ligand CLA G 1113



Bond lengths



Bond angles

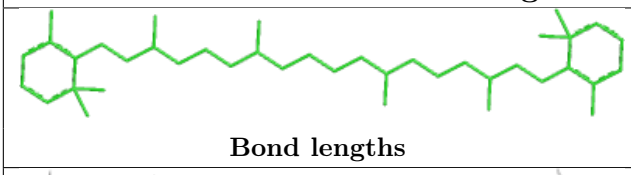


Torsions

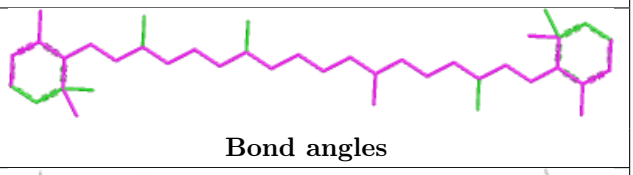


Rings

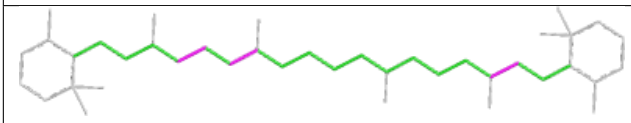
Ligand BCR f 4010



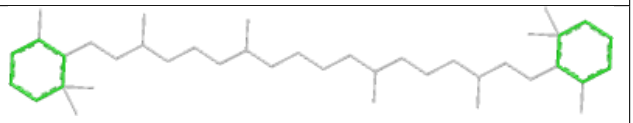
Bond lengths



Bond angles

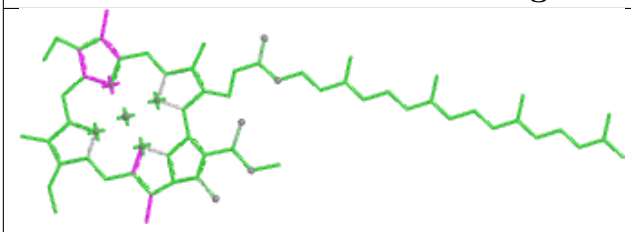


Torsions

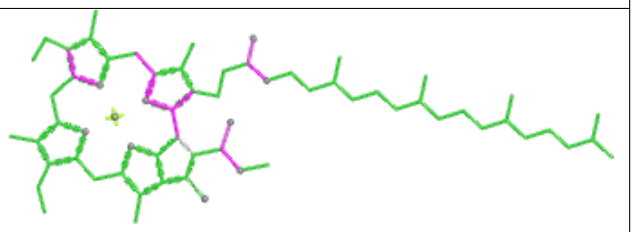


Rings

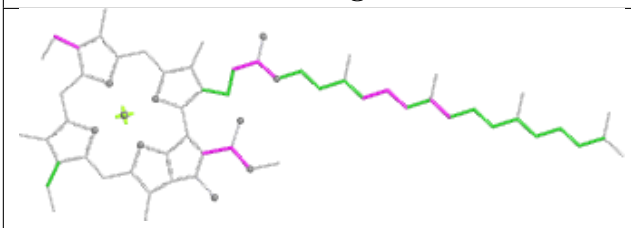
Ligand CLA s 507



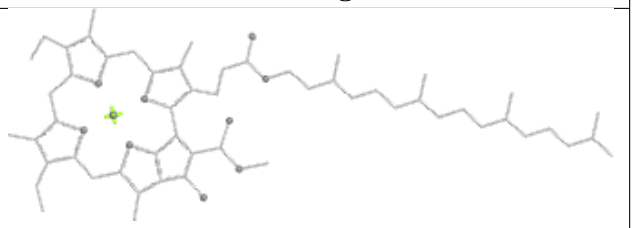
Bond lengths



Bond angles

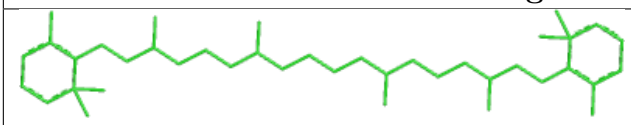


Torsions

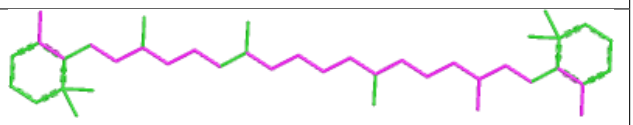


Rings

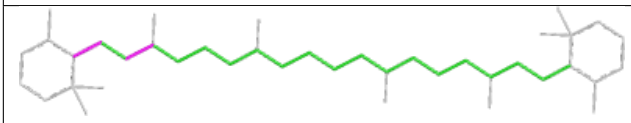
Ligand BCR v 524



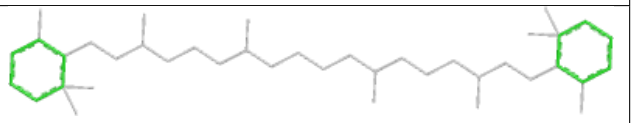
Bond lengths



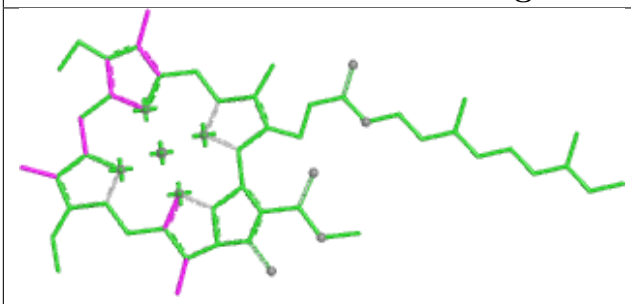
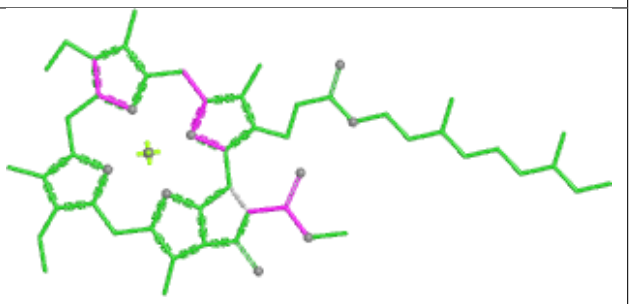
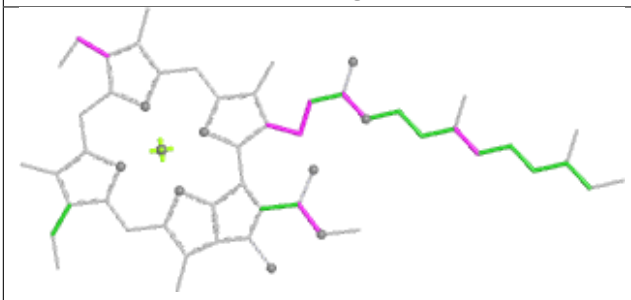
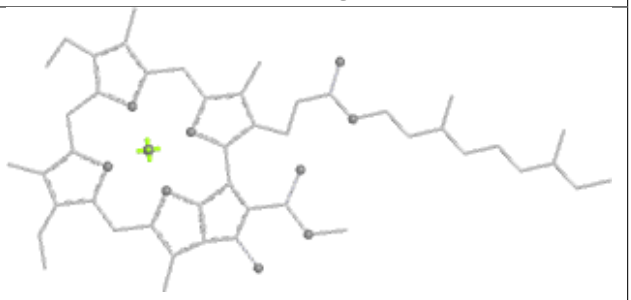
Bond angles

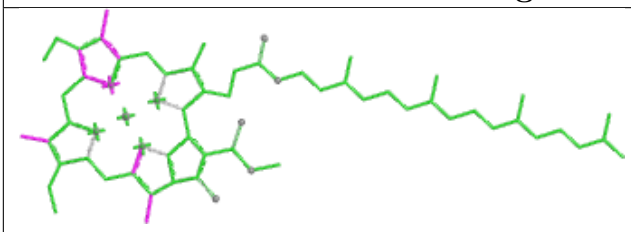
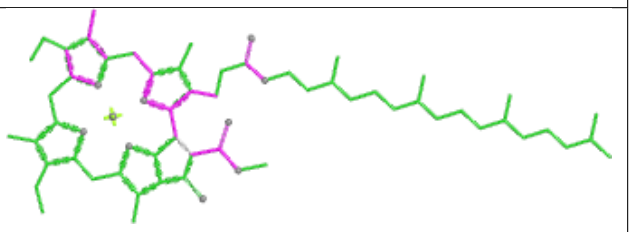
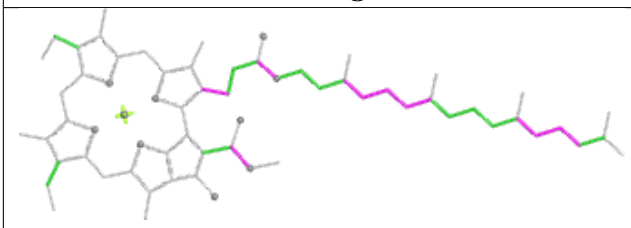
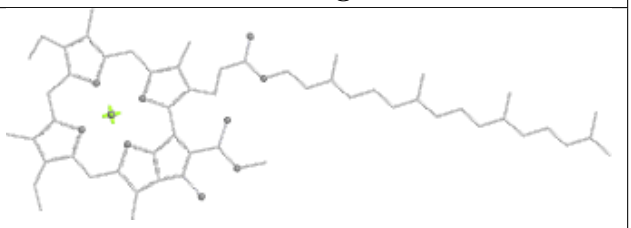


Torsions

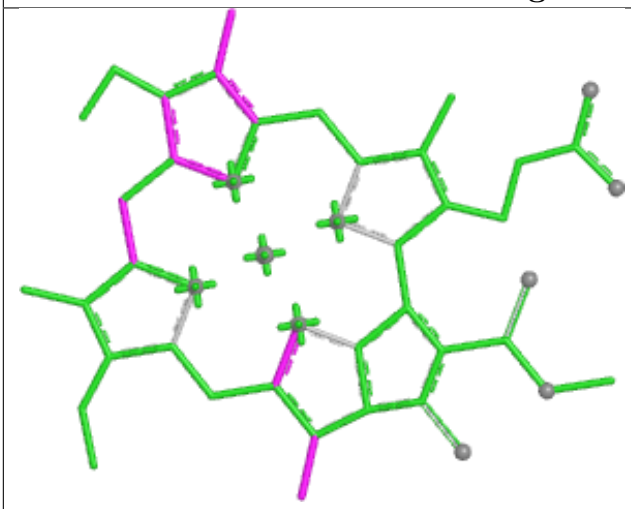


Rings

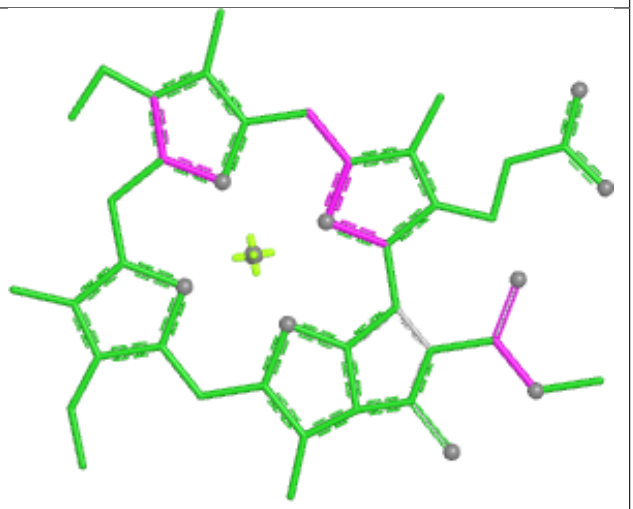
Ligand CLA A 1134	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA T 1303	
	
Bond lengths	Bond angles
	
Torsions	Rings

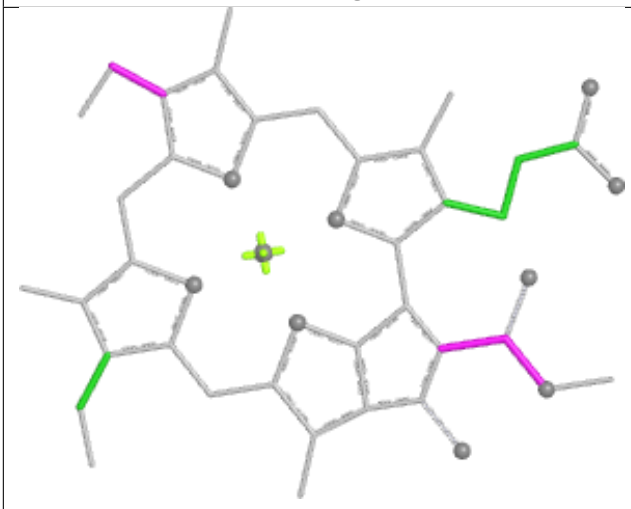
Ligand CLA 4 504



Bond lengths



Bond angles

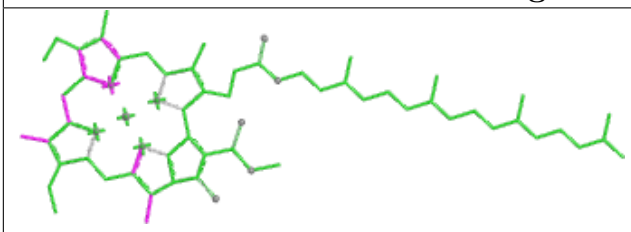


Torsions

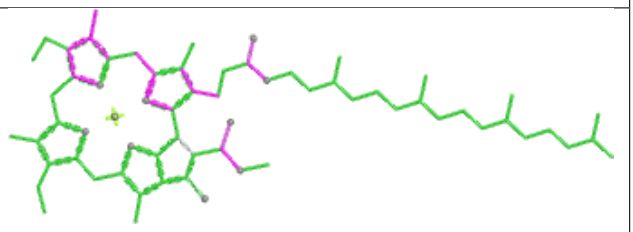


Rings

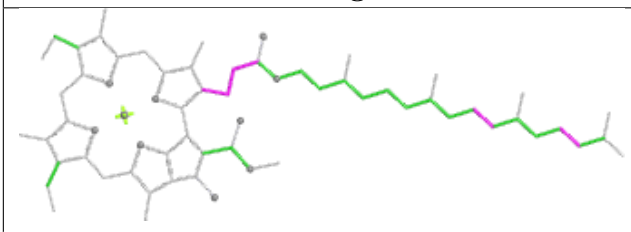
Ligand CLA a 501



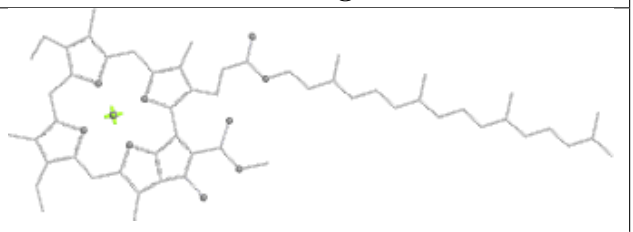
Bond lengths



Bond angles

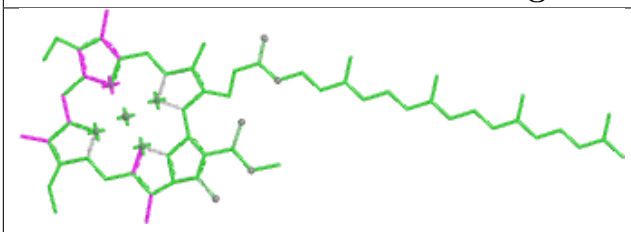


Torsions

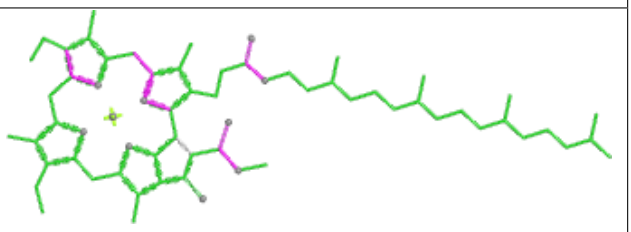


Rings

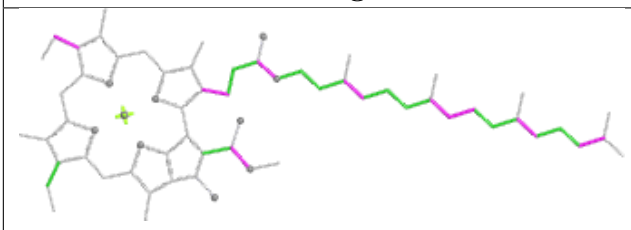
Ligand CLA 2 513



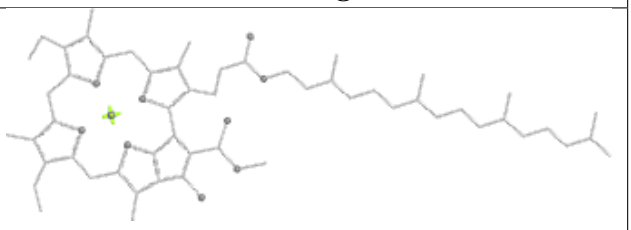
Bond lengths



Bond angles

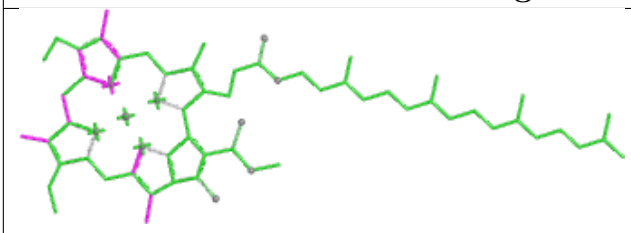


Torsions

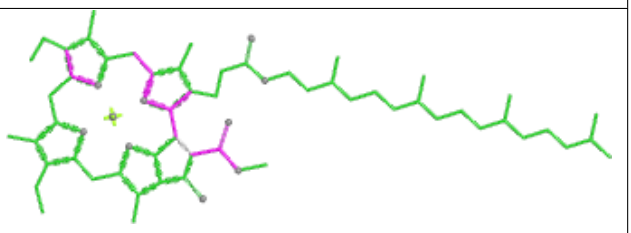


Rings

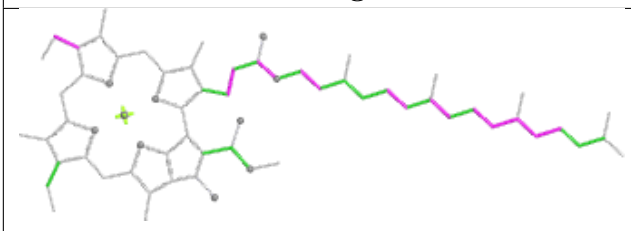
Ligand CLA H 1214



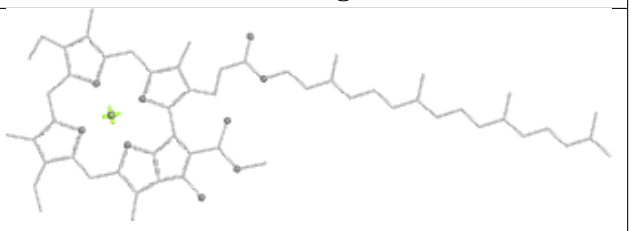
Bond lengths



Bond angles

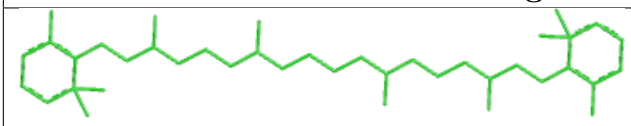


Torsions

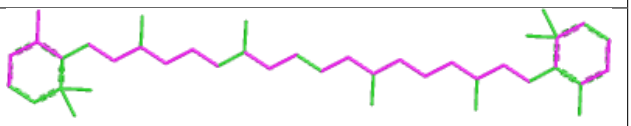


Rings

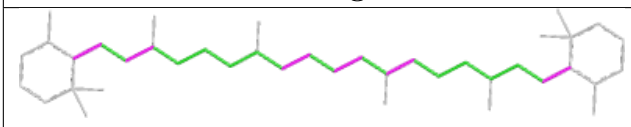
Ligand BCR b 521



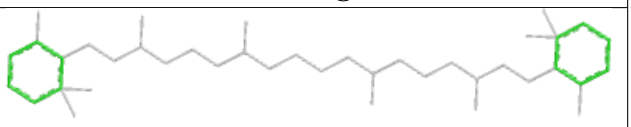
Bond lengths



Bond angles

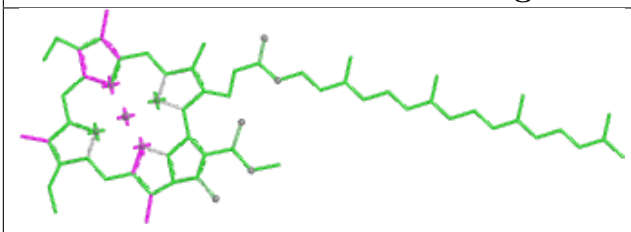


Torsions

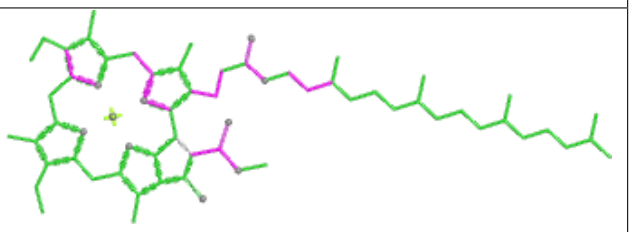


Rings

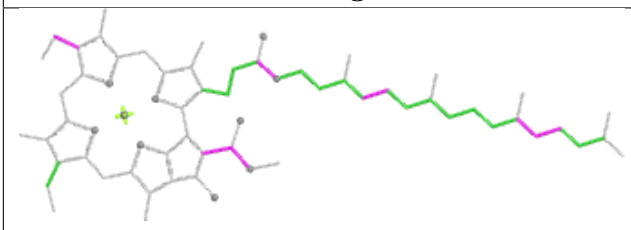
Ligand CLA H 1205



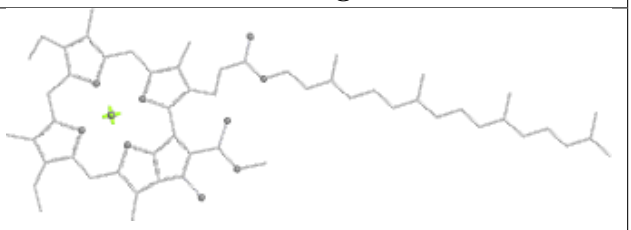
Bond lengths



Bond angles



Torsions

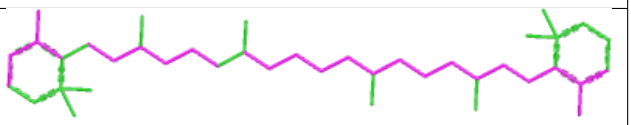


Rings

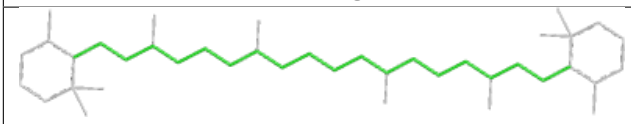
Ligand BCR G 4002



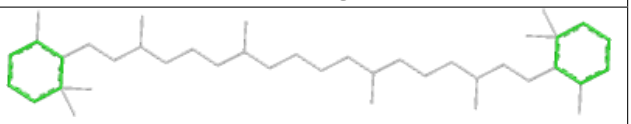
Bond lengths



Bond angles

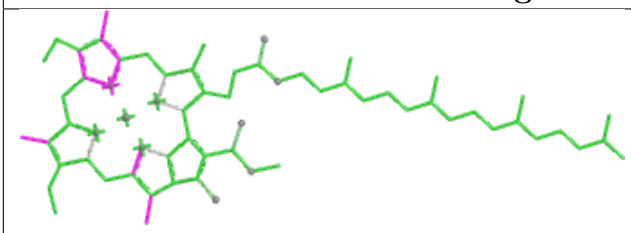


Torsions

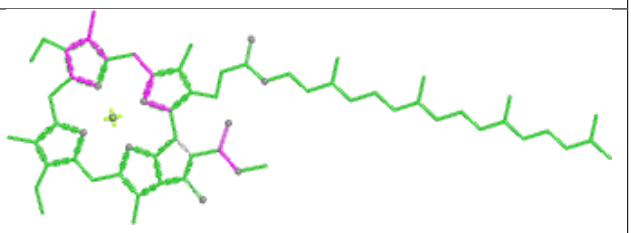


Rings

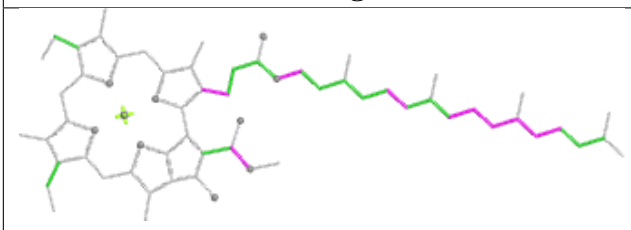
Ligand CLA H 1223



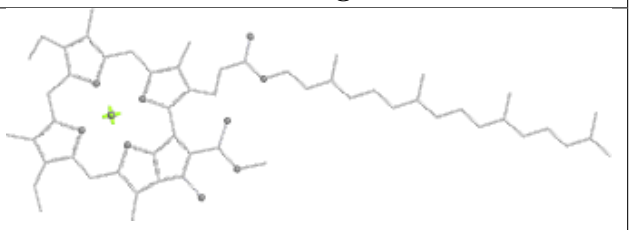
Bond lengths



Bond angles

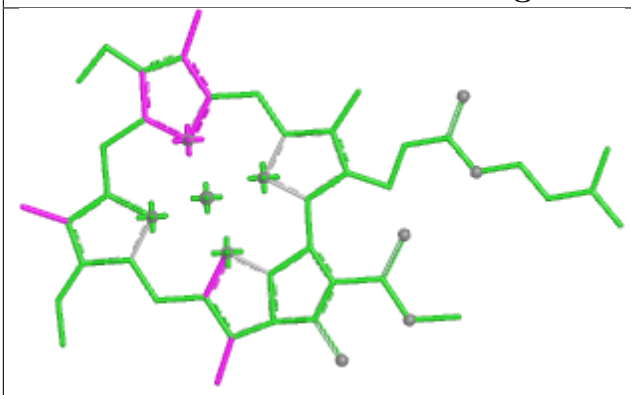


Torsions

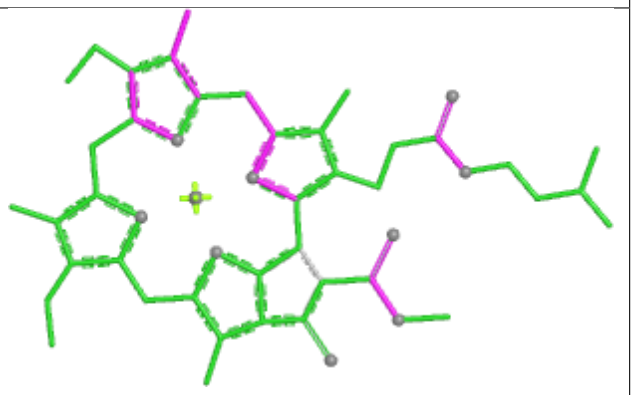


Rings

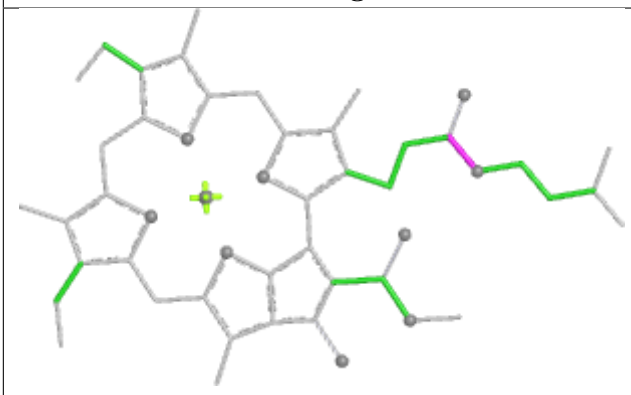
Ligand CLA G 1114



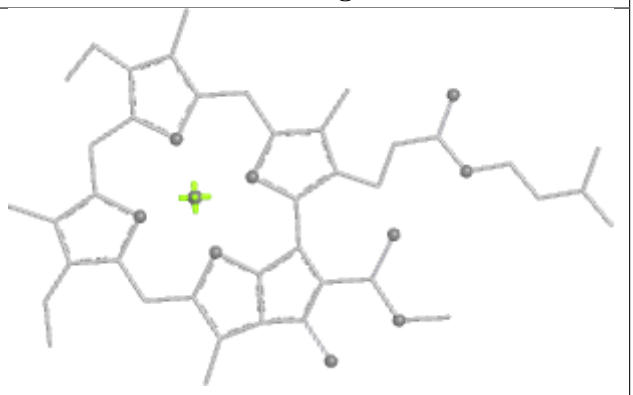
Bond lengths



Bond angles



Torsions

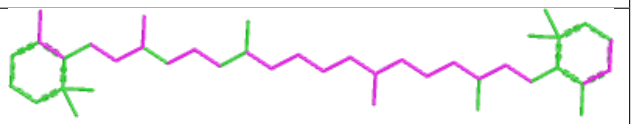


Rings

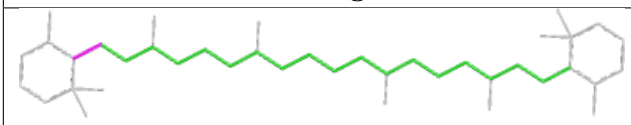
Ligand BCR V 4219



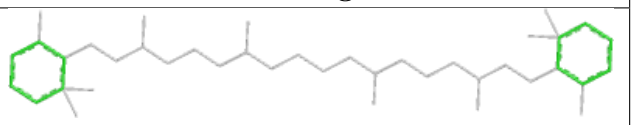
Bond lengths



Bond angles

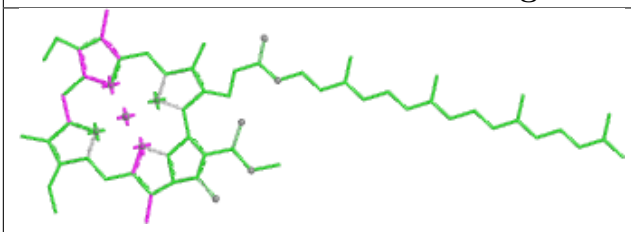


Torsions

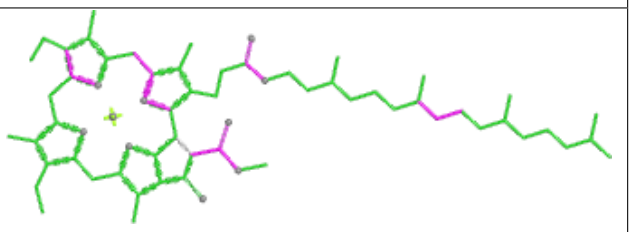


Rings

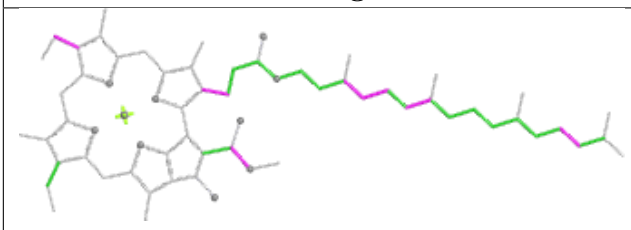
Ligand CLA e 1139



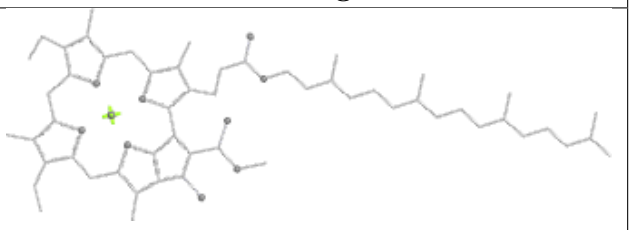
Bond lengths



Bond angles

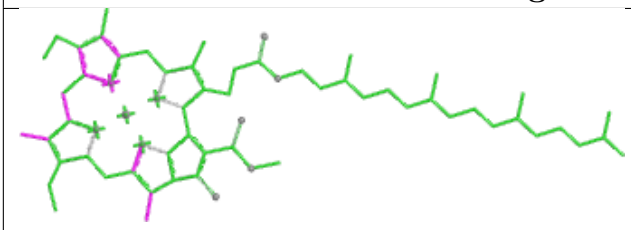


Torsions

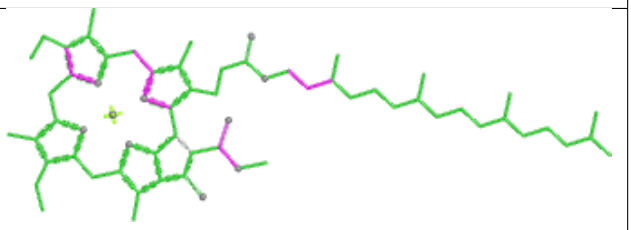


Rings

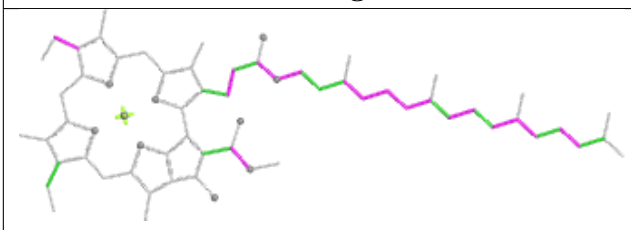
Ligand CLA 3 505



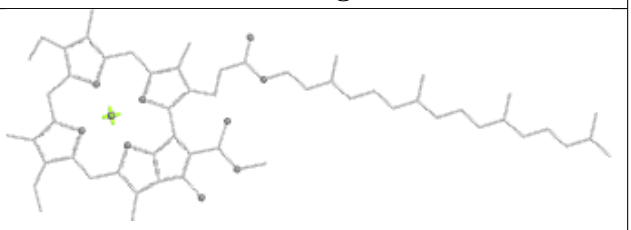
Bond lengths



Bond angles

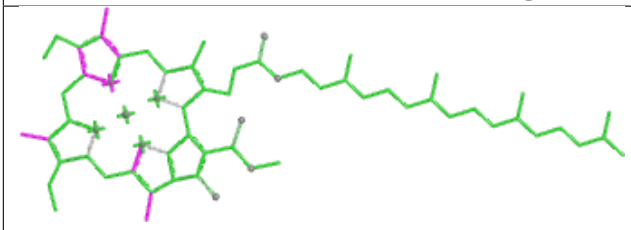


Torsions

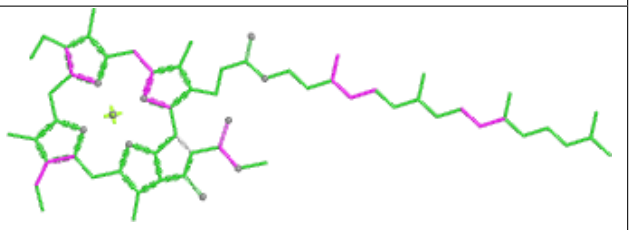


Rings

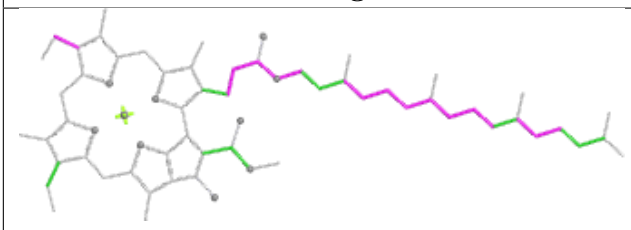
Ligand CLA e 1237



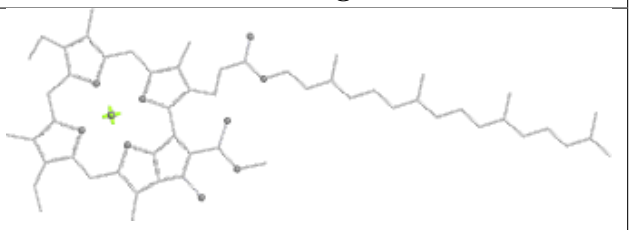
Bond lengths



Bond angles

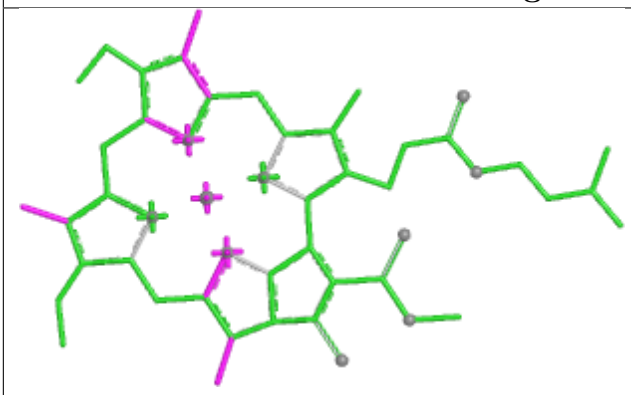


Torsions

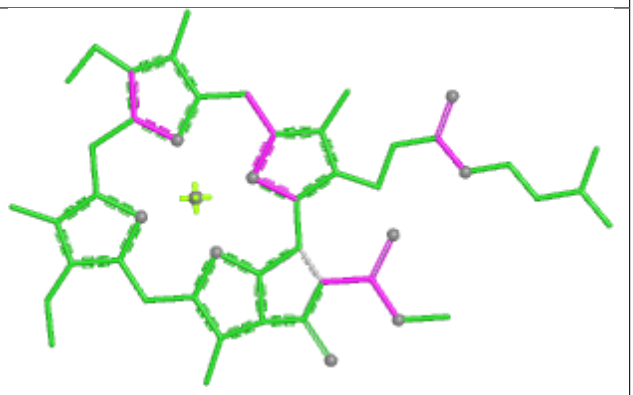


Rings

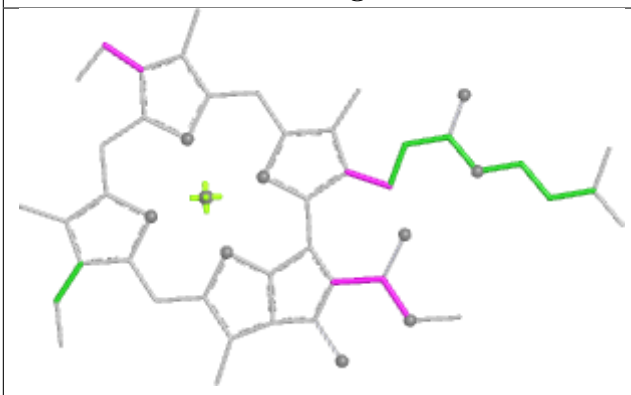
Ligand CLA Y 519



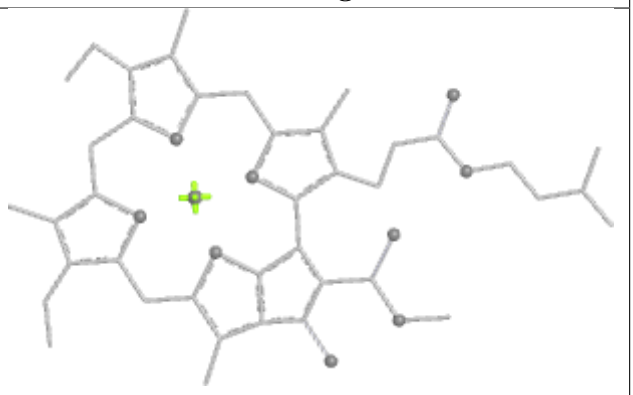
Bond lengths



Bond angles

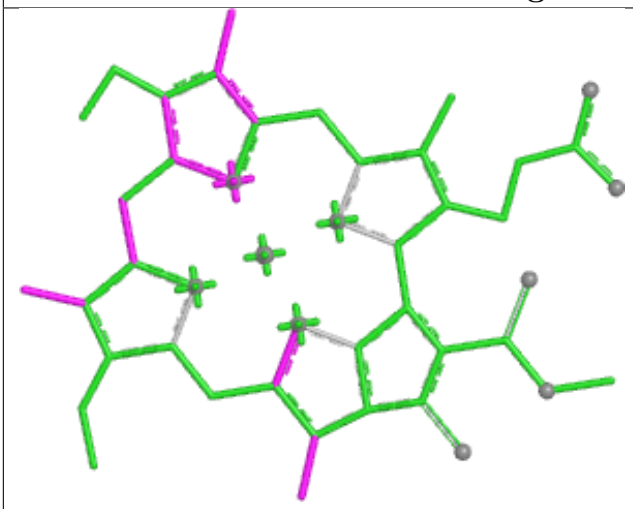


Torsions

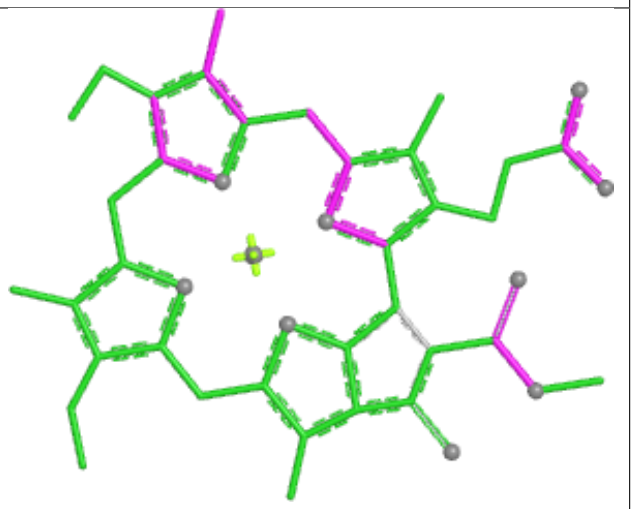


Rings

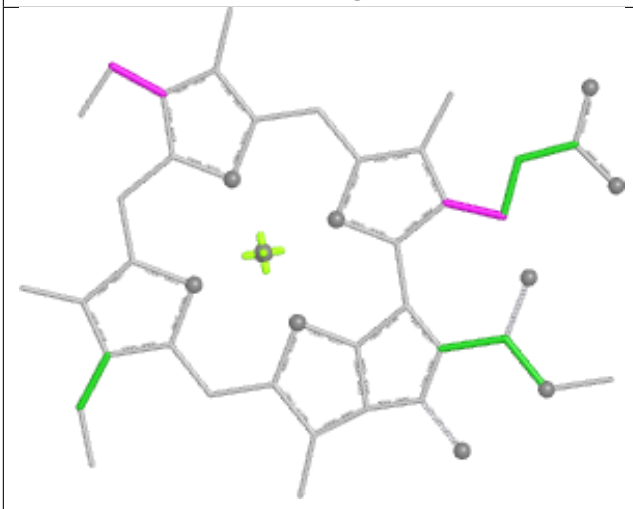
Ligand CLA d 508



Bond lengths



Bond angles

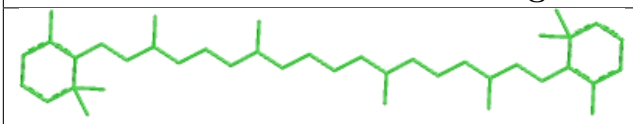


Torsions

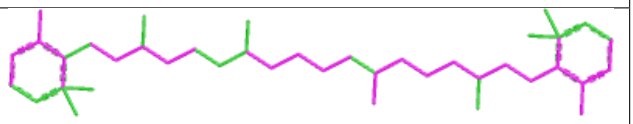


Rings

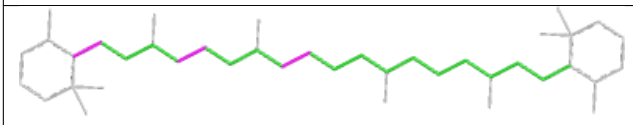
Ligand BCR t 522



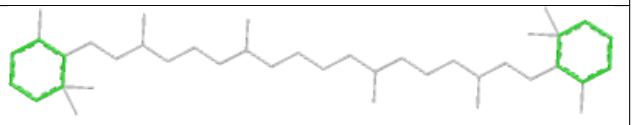
Bond lengths



Bond angles

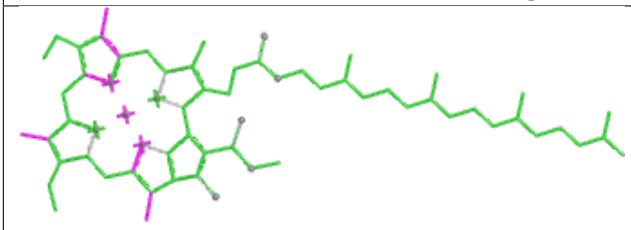


Torsions

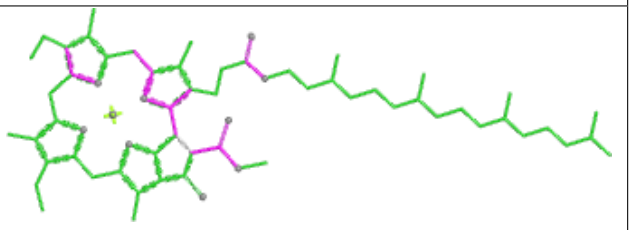


Rings

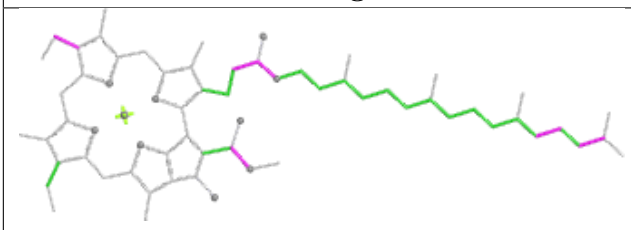
Ligand CLA f 1021



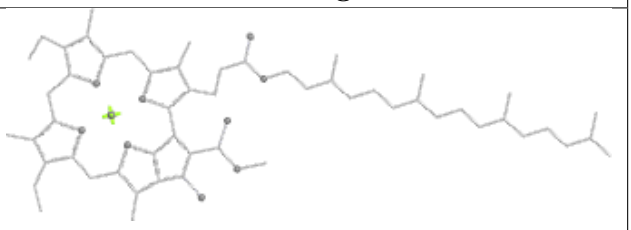
Bond lengths



Bond angles

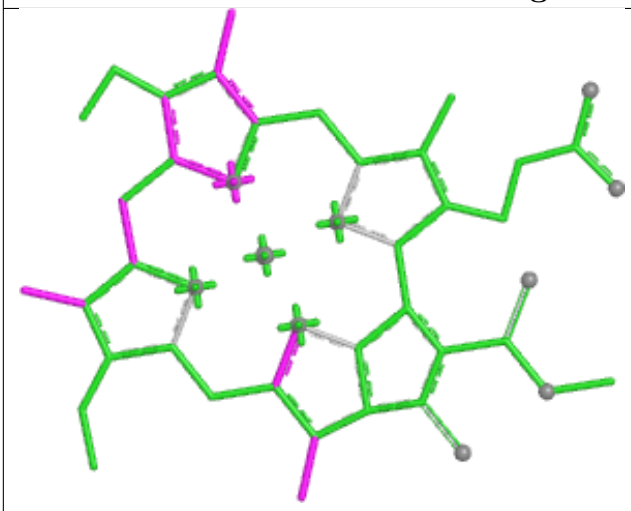


Torsions

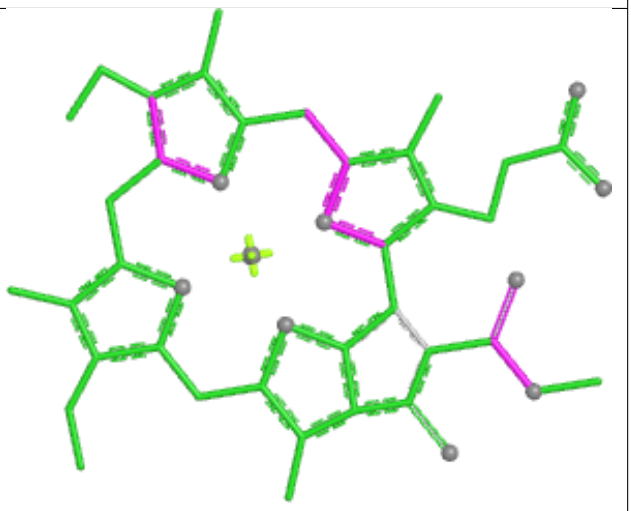


Rings

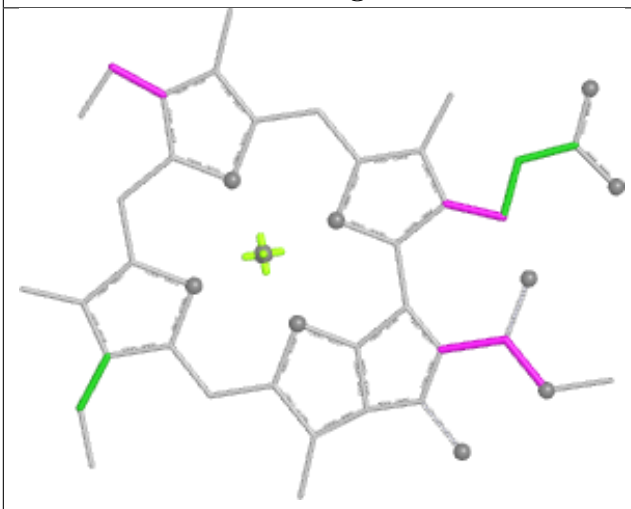
Ligand CLA s 517



Bond lengths



Bond angles

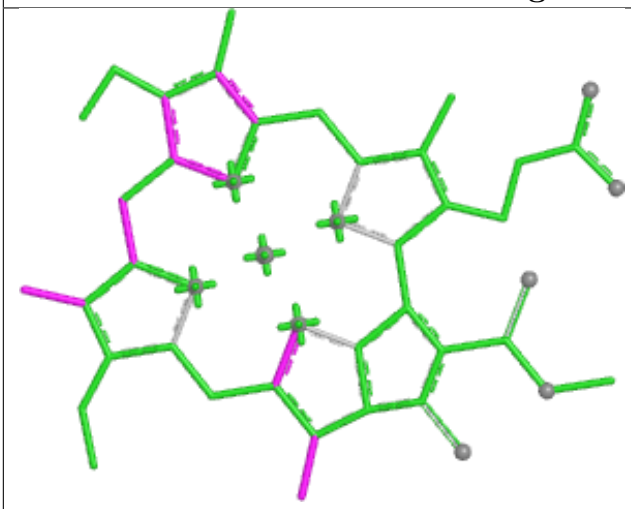


Torsions

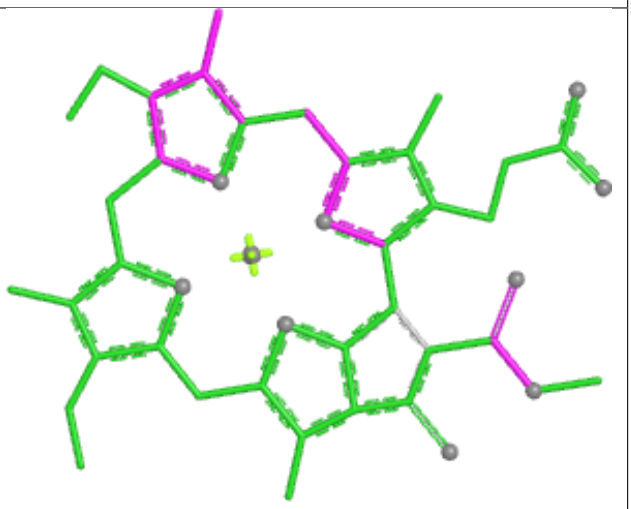


Rings

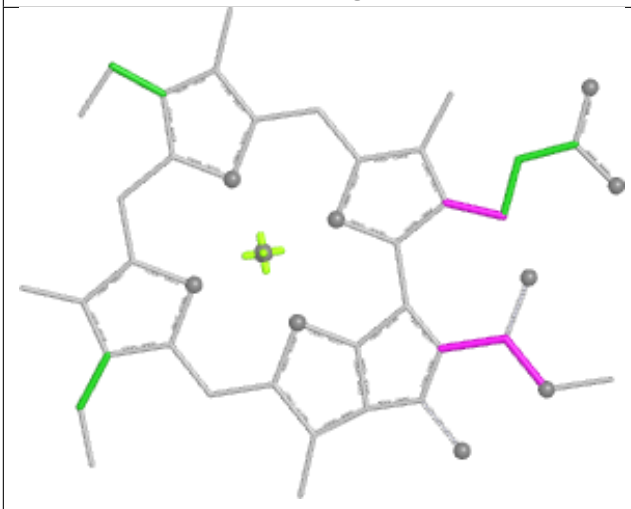
Ligand CLA 1 506



Bond lengths



Bond angles

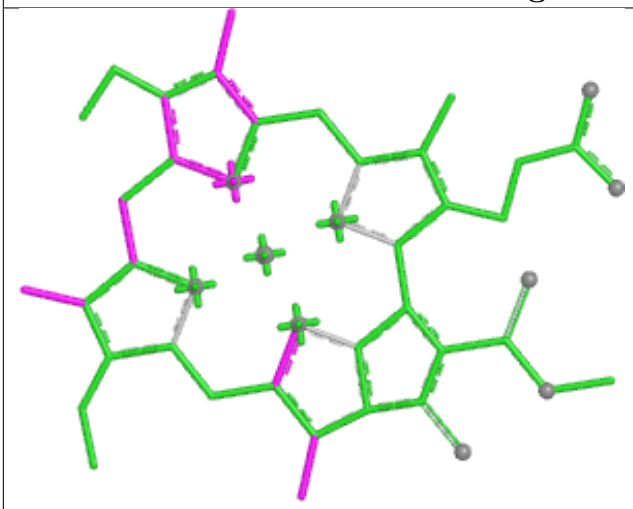


Torsions

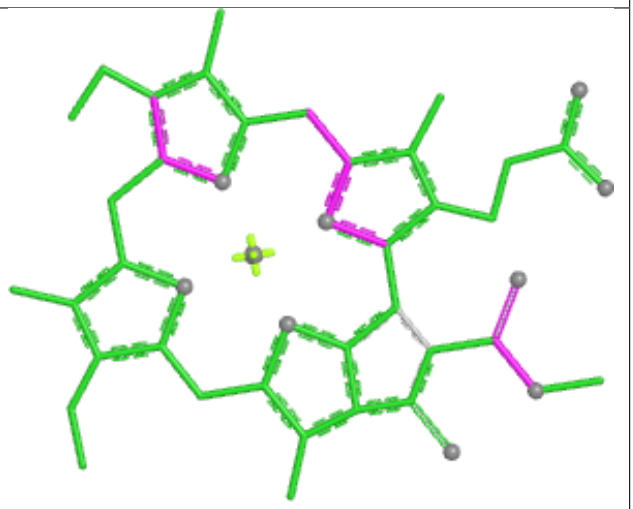


Rings

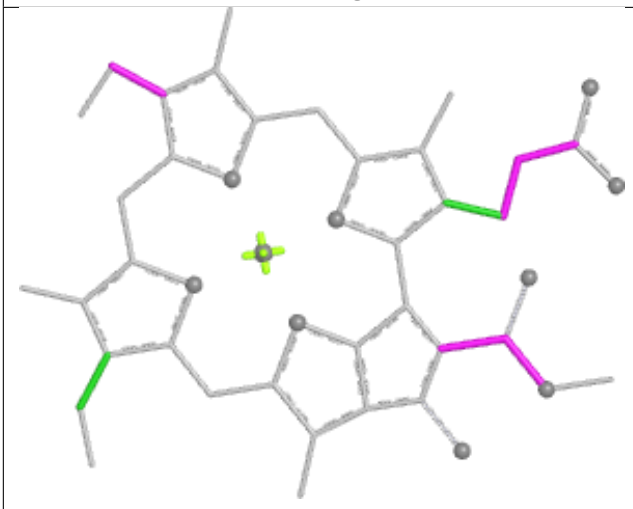
Ligand CLA 5 517



Bond lengths



Bond angles

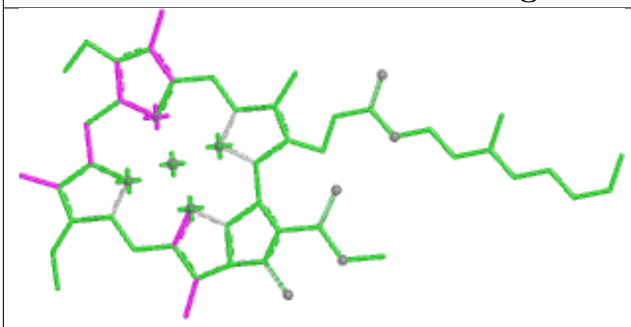


Torsions

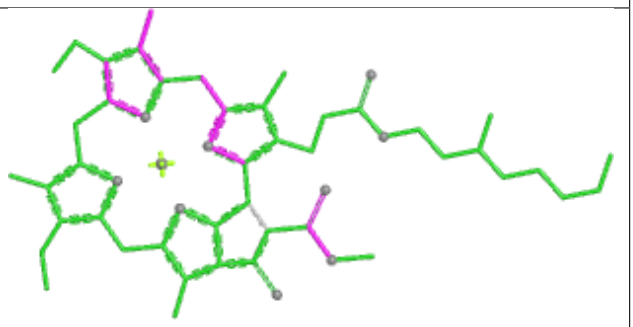


Rings

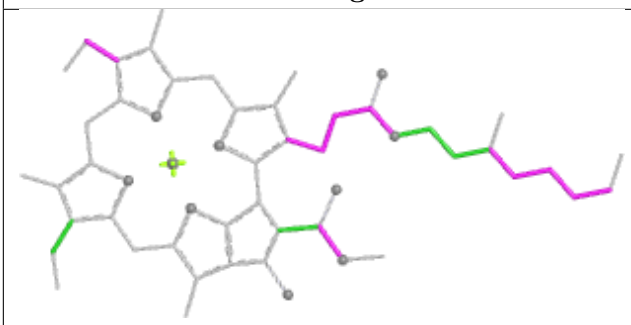
Ligand CLA e 1108



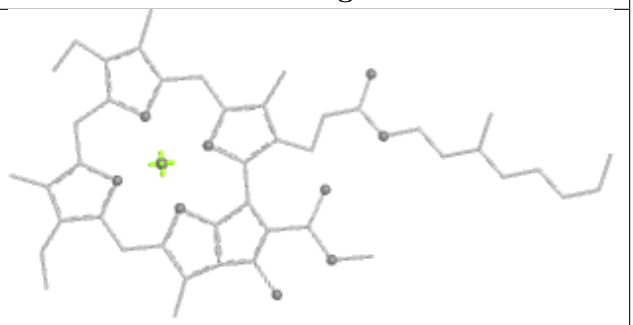
Bond lengths



Bond angles

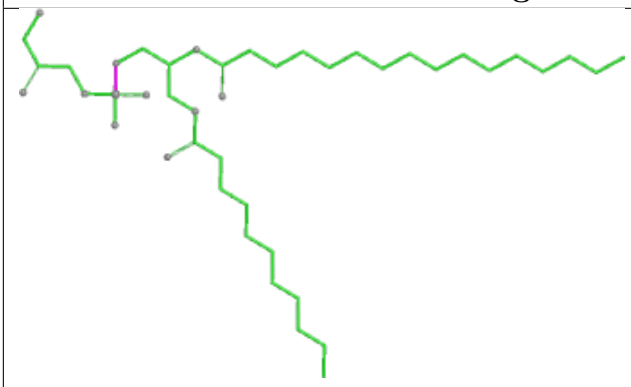


Torsions

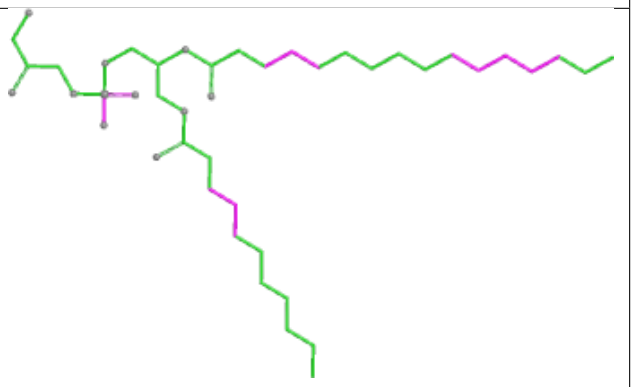


Rings

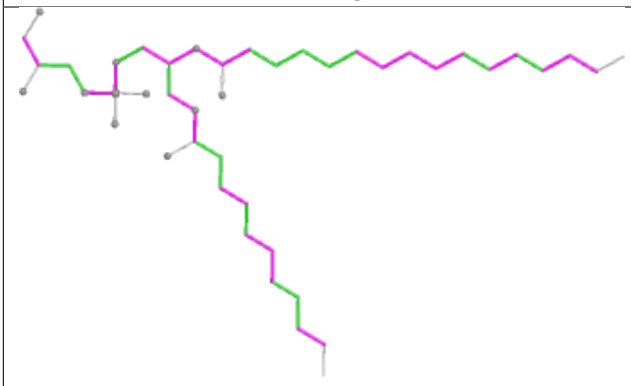
Ligand LHG H 1855



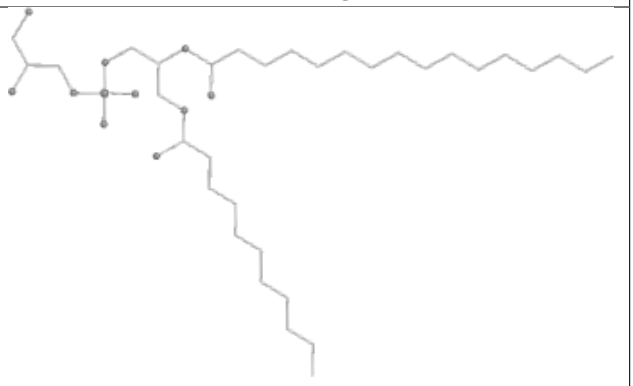
Bond lengths



Bond angles

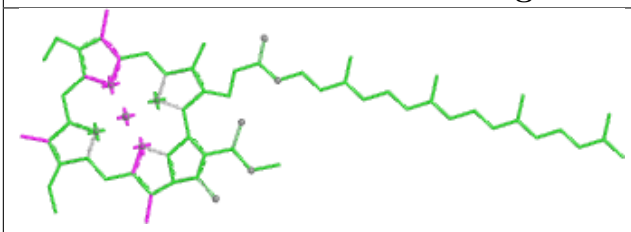


Torsions

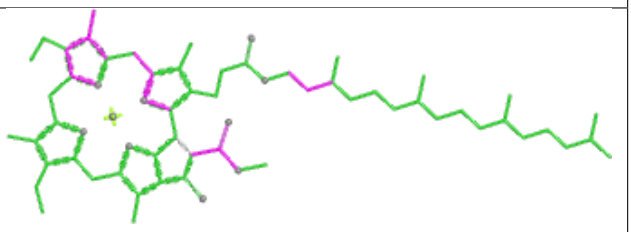


Rings

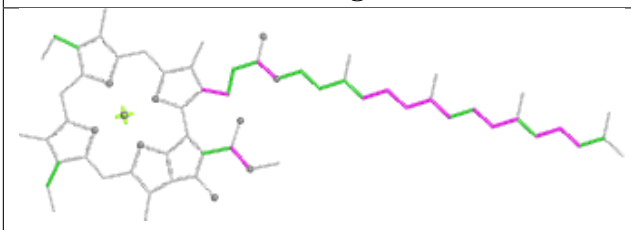
Ligand CLA B 1215



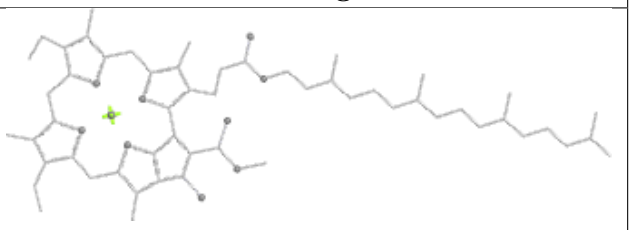
Bond lengths



Bond angles

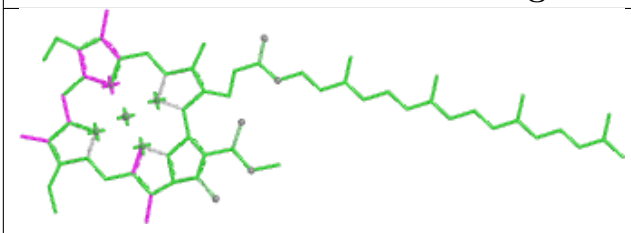


Torsions

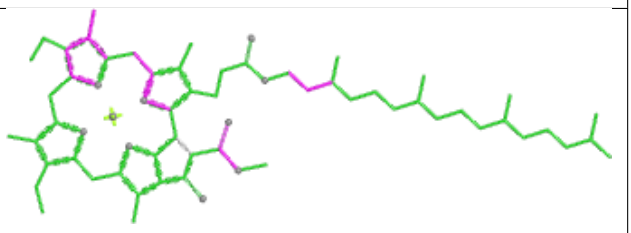


Rings

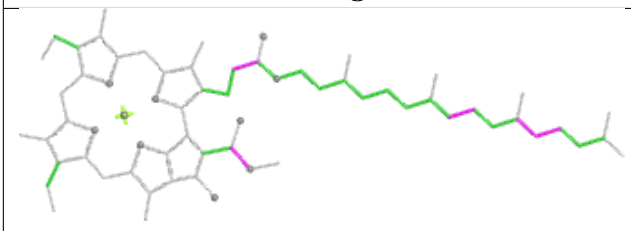
Ligand CLA 2 510



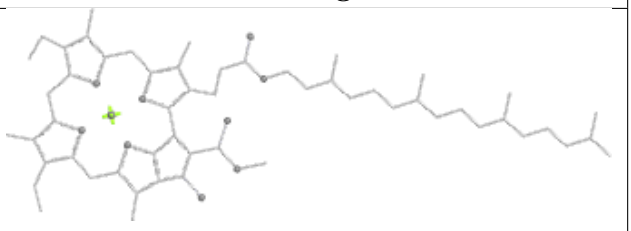
Bond lengths



Bond angles

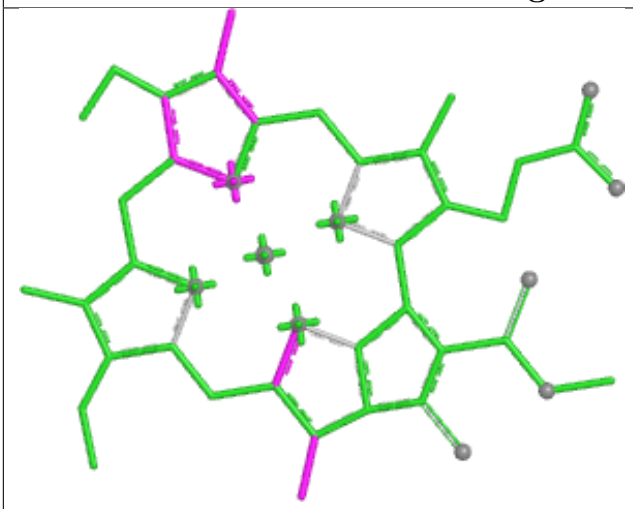


Torsions

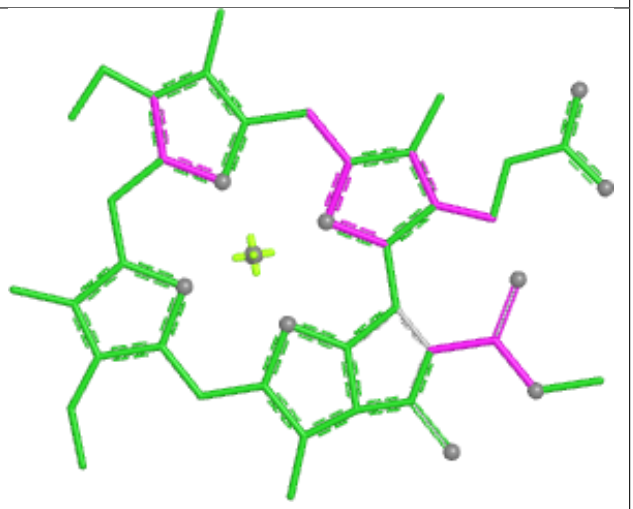


Rings

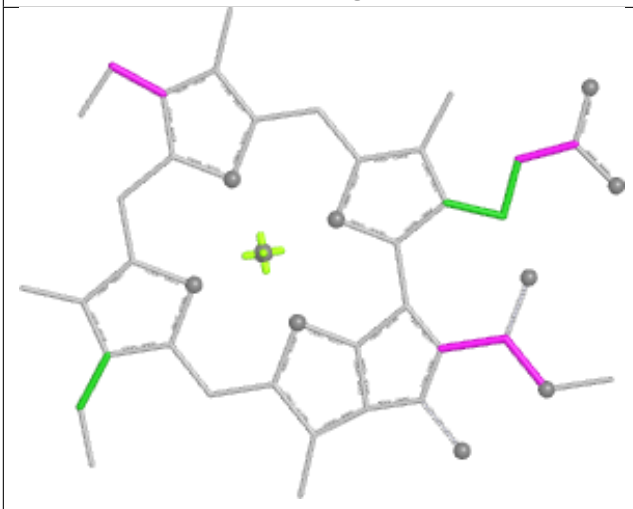
Ligand CLA 4 507



Bond lengths



Bond angles

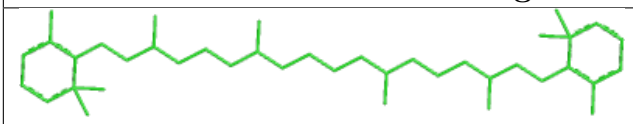


Torsions

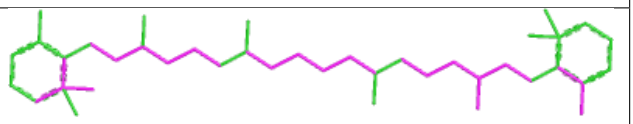


Rings

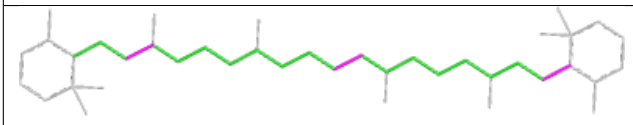
Ligand BCR T 4015



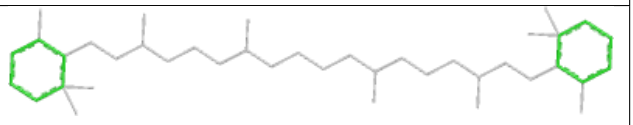
Bond lengths



Bond angles

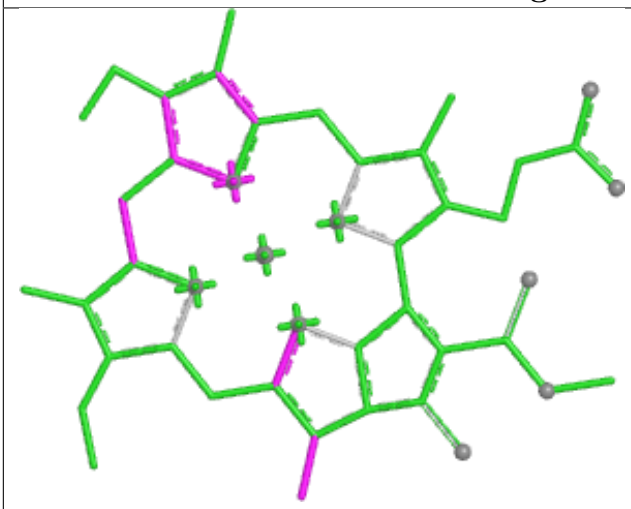


Torsions

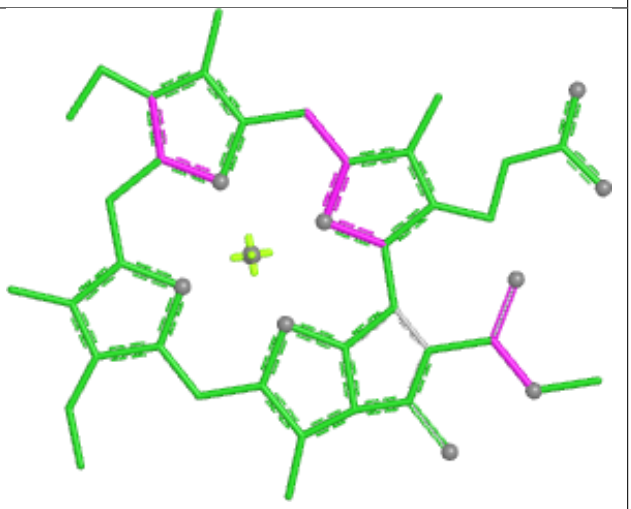


Rings

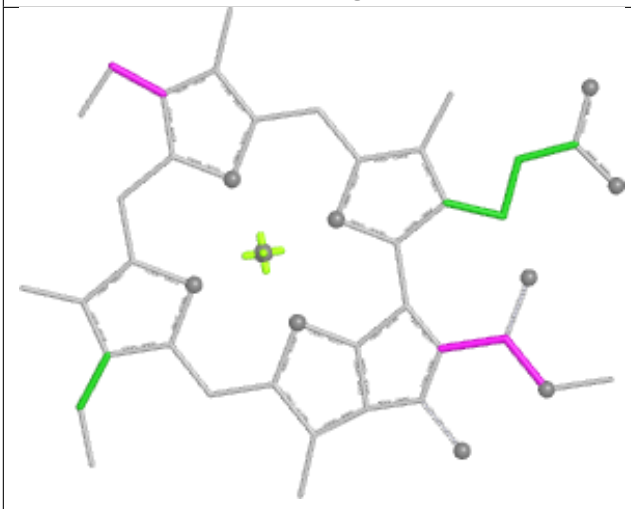
Ligand CLA t 504



Bond lengths



Bond angles

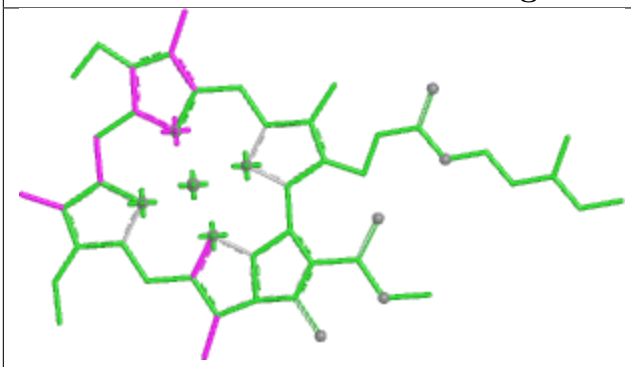


Torsions

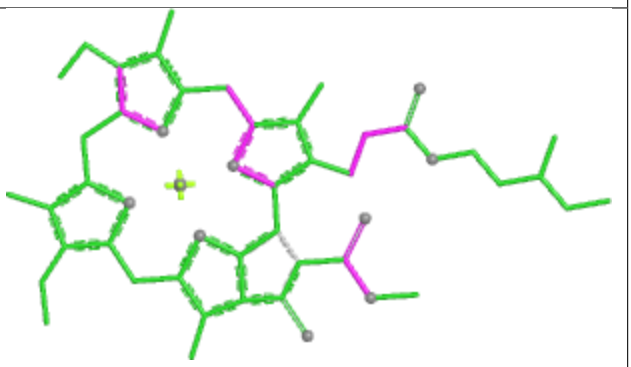


Rings

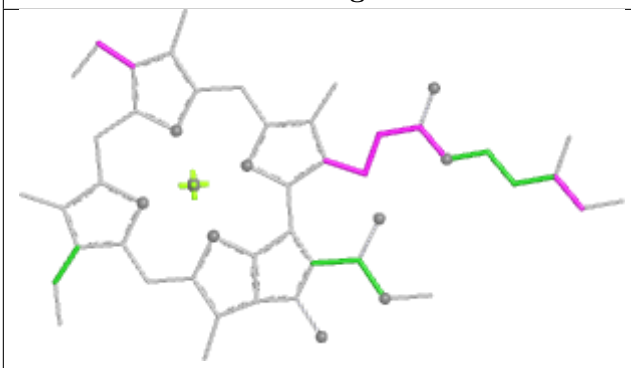
Ligand CLA e 1110



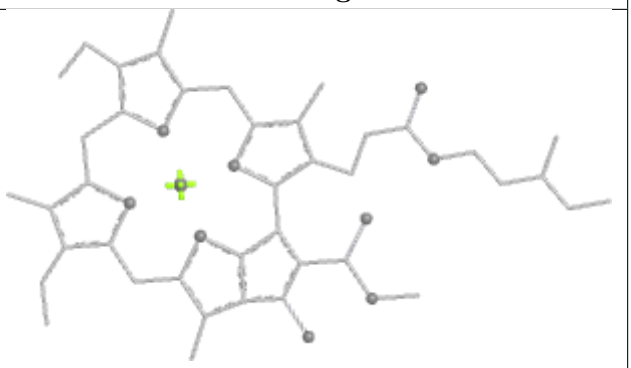
Bond lengths



Bond angles

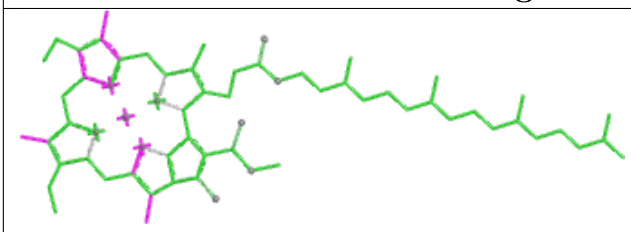


Torsions

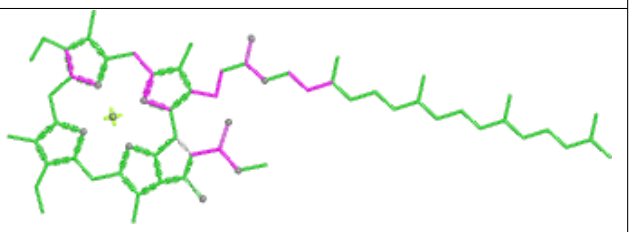


Rings

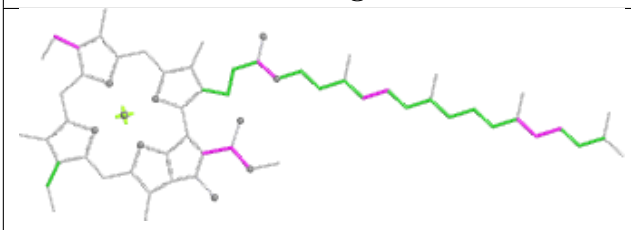
Ligand CLA B 1205



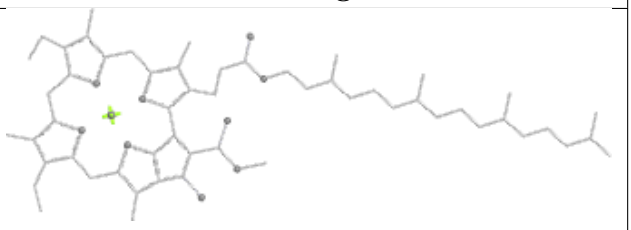
Bond lengths



Bond angles

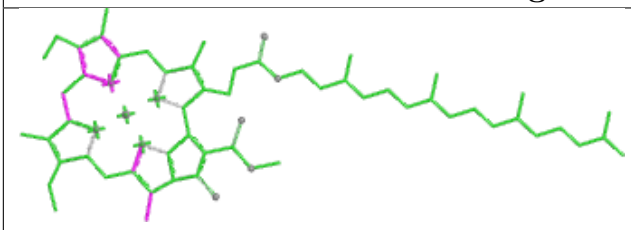


Torsions

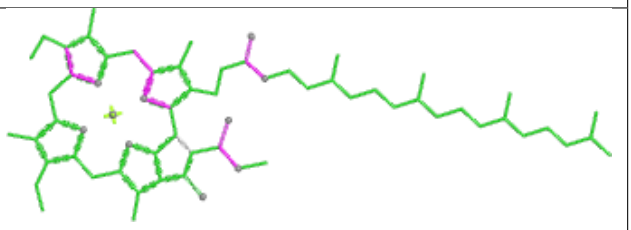


Rings

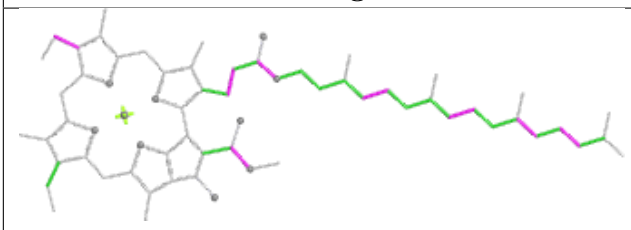
Ligand CLA 4 505



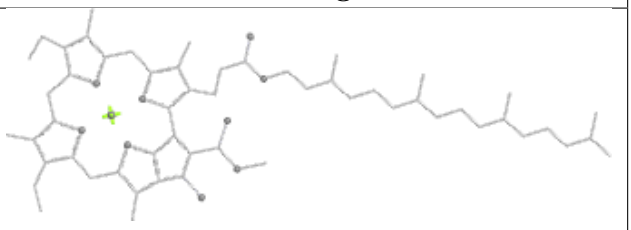
Bond lengths



Bond angles

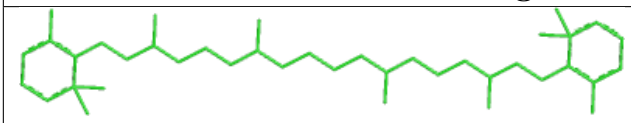


Torsions

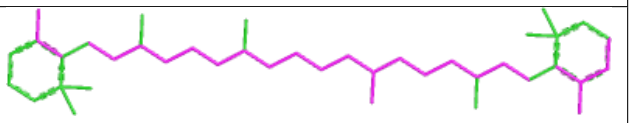


Rings

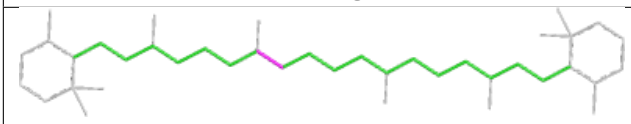
Ligand BCR F 4016



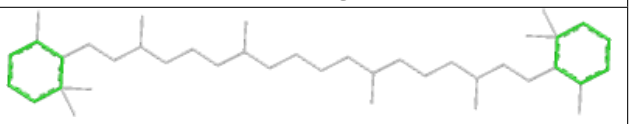
Bond lengths



Bond angles

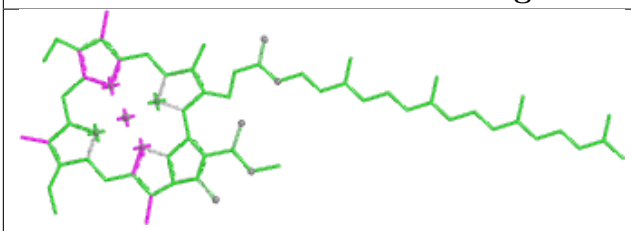


Torsions

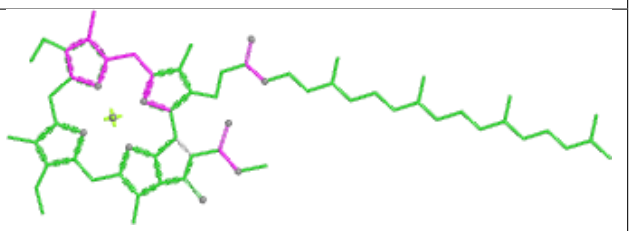


Rings

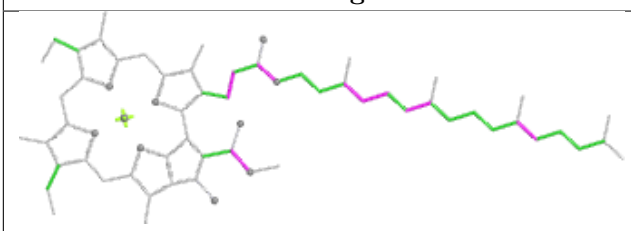
Ligand CLA G 1119



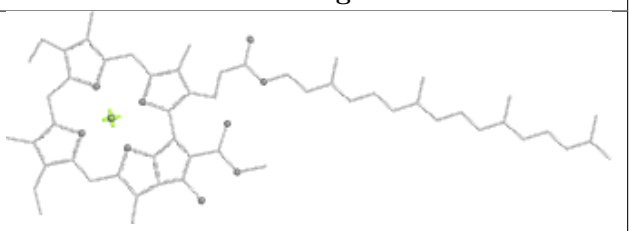
Bond lengths



Bond angles

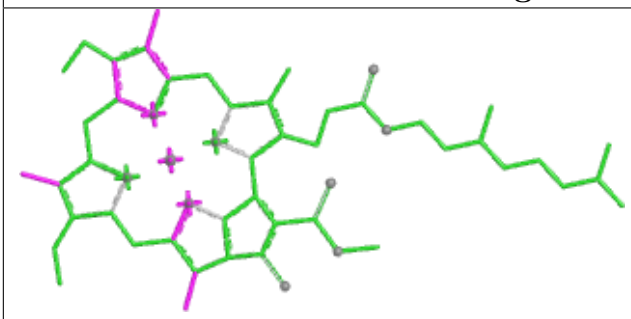


Torsions

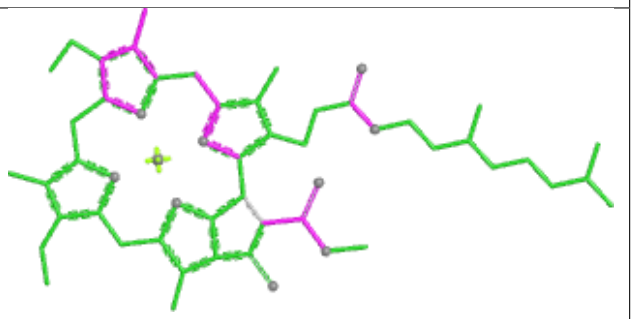


Rings

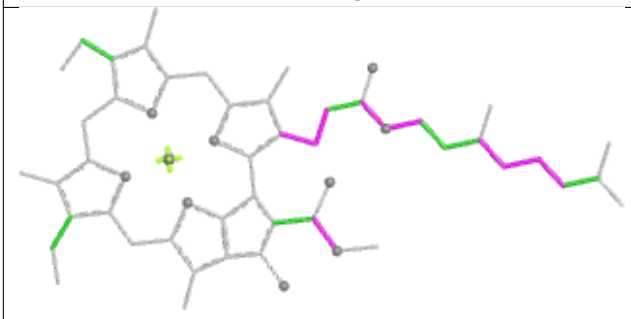
Ligand CLA H 1212



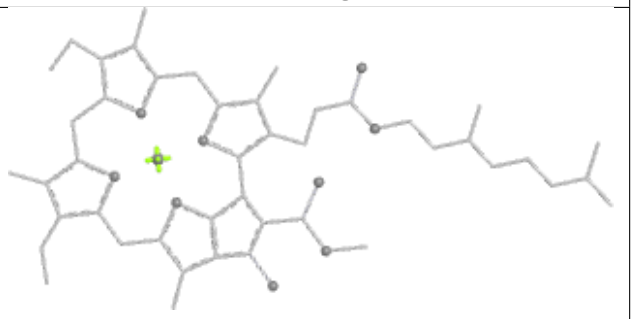
Bond lengths



Bond angles

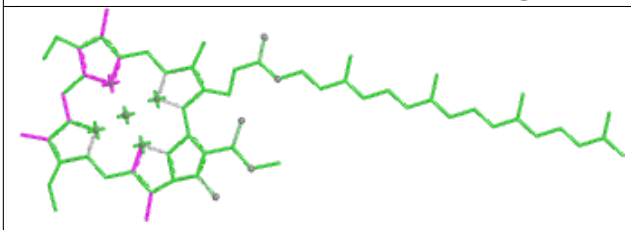


Torsions

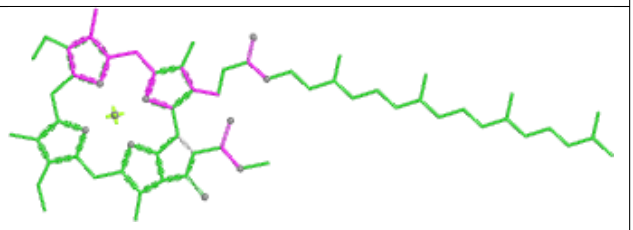


Rings

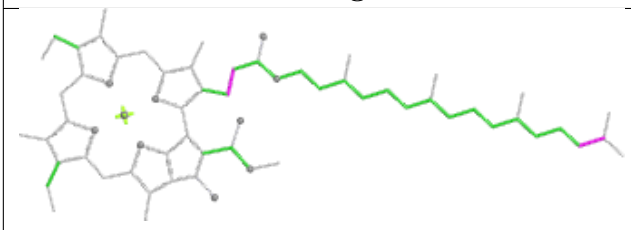
Ligand CLA B 1238



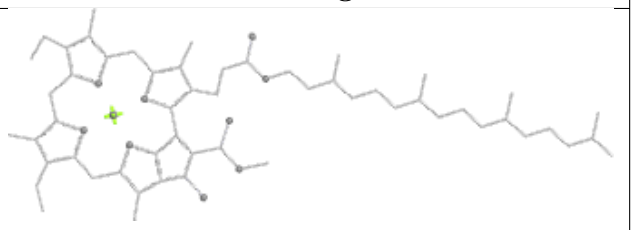
Bond lengths



Bond angles

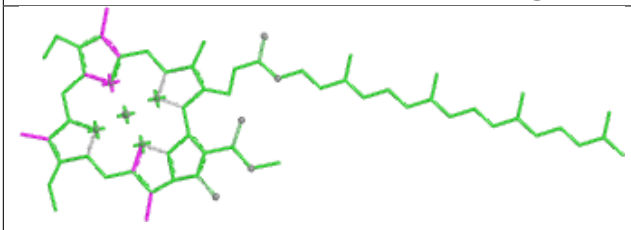


Torsions

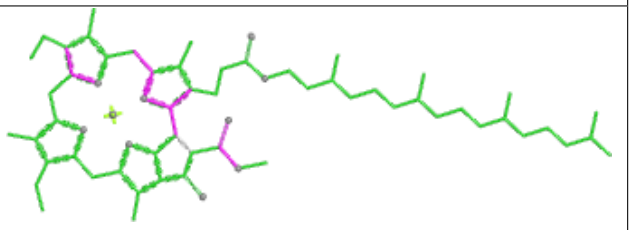


Rings

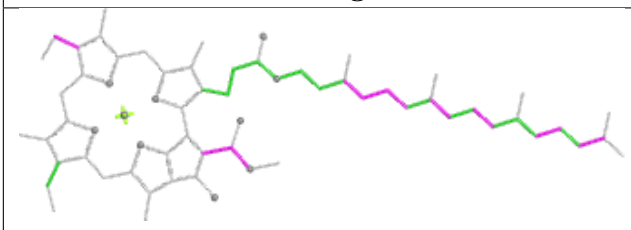
Ligand CLA 2 507



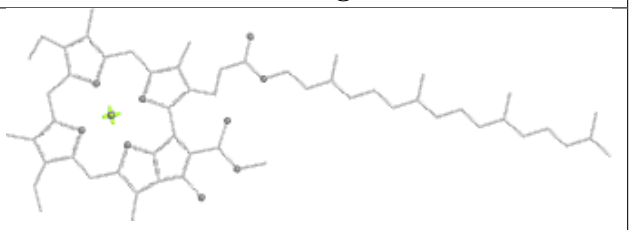
Bond lengths



Bond angles

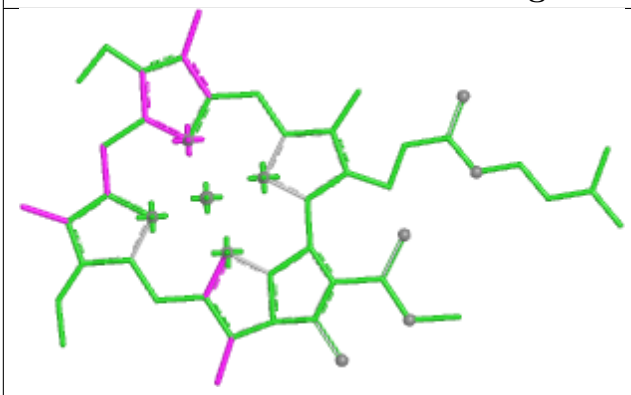


Torsions

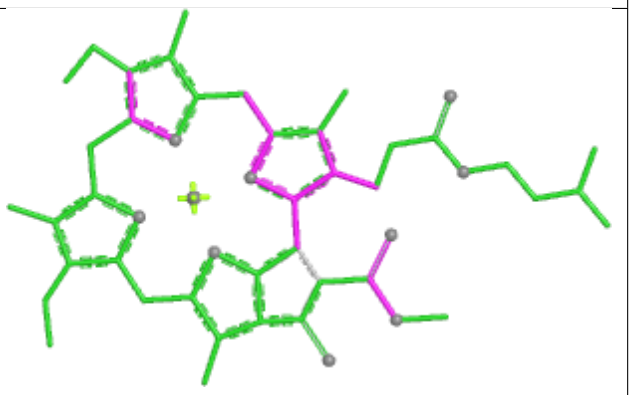


Rings

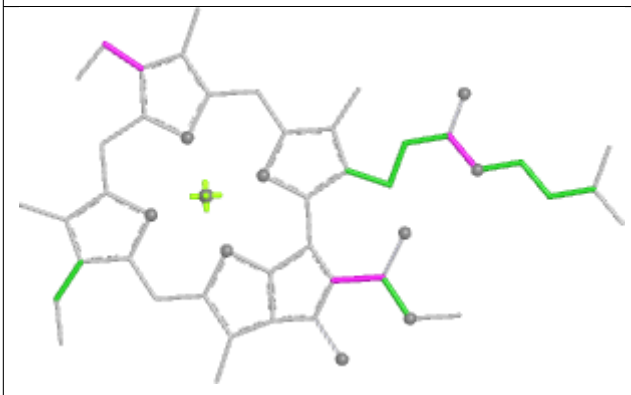
Ligand CLA 3 502



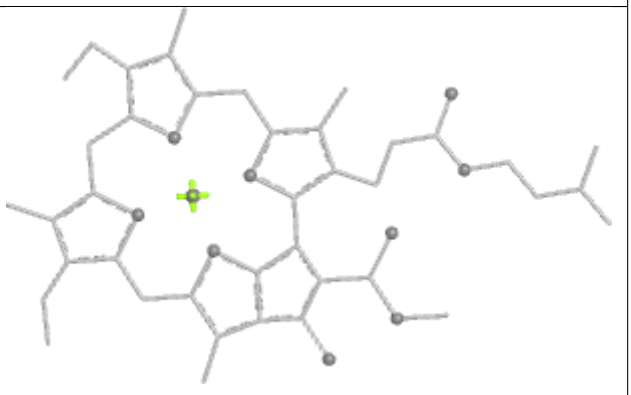
Bond lengths



Bond angles

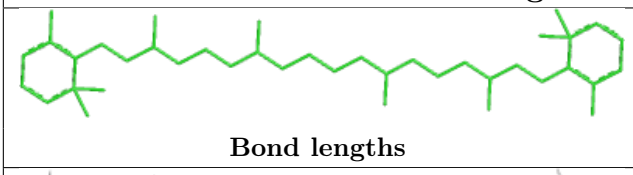


Torsions

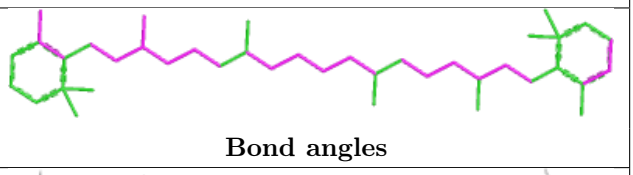


Rings

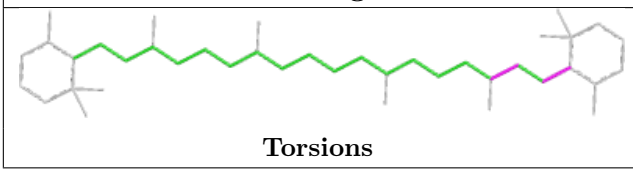
Ligand BCR 4 523



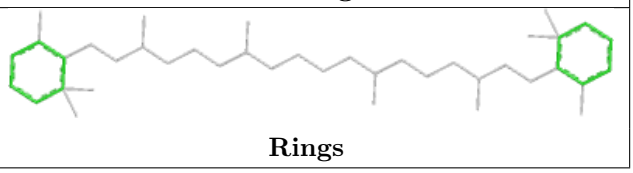
Bond lengths



Bond angles

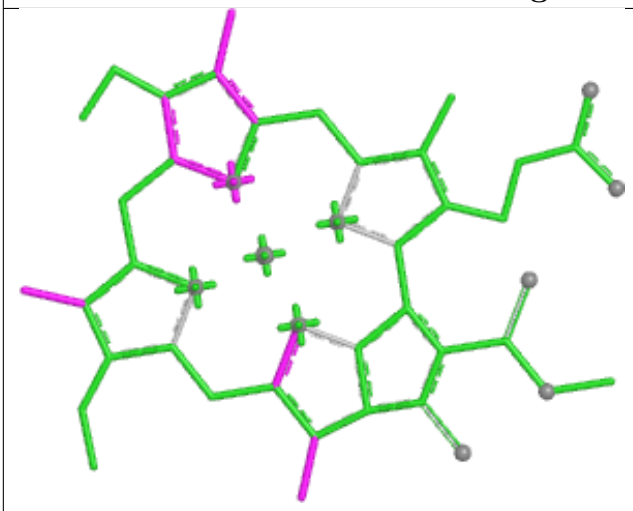


Torsions

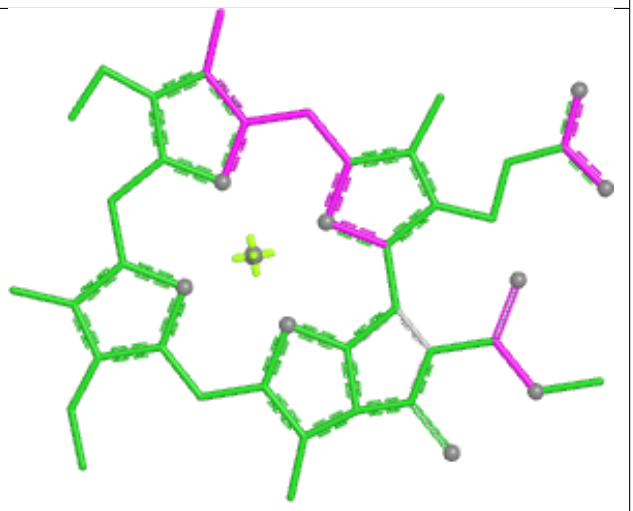


Rings

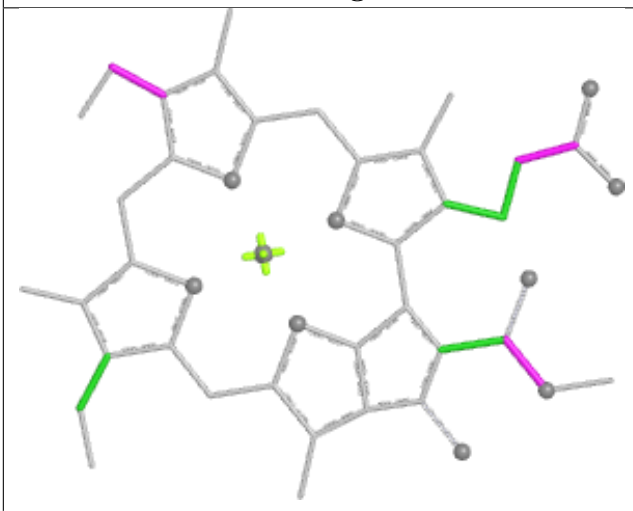
Ligand CLA t 508



Bond lengths



Bond angles

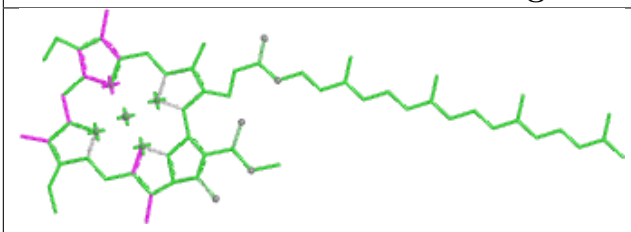


Torsions

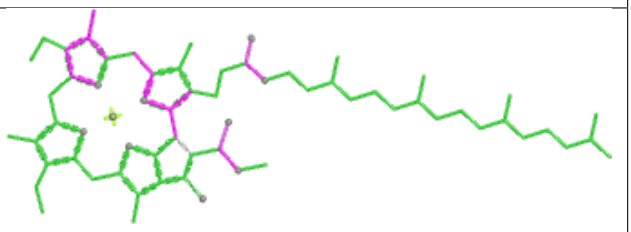


Rings

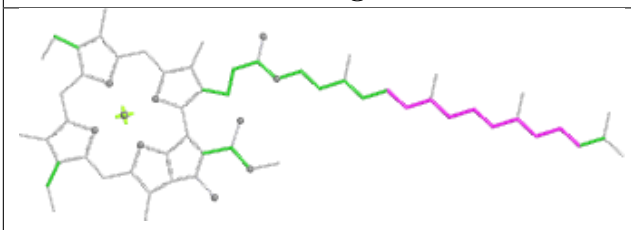
Ligand CLA u 509



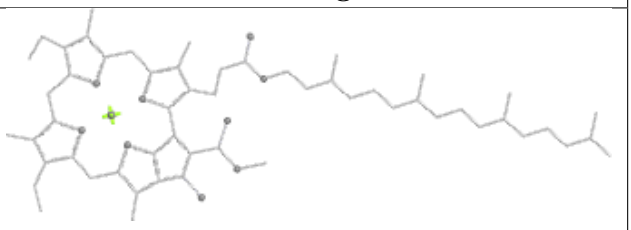
Bond lengths



Bond angles

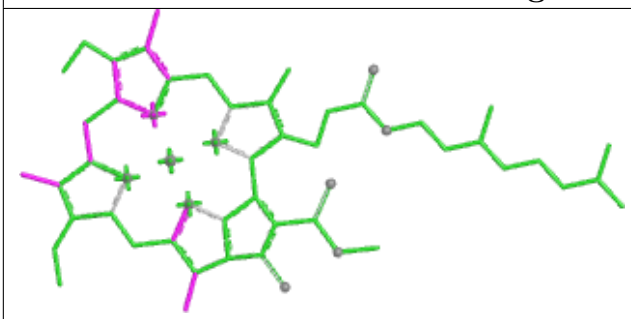


Torsions

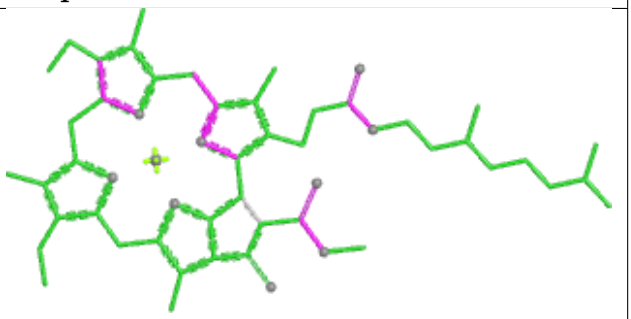


Rings

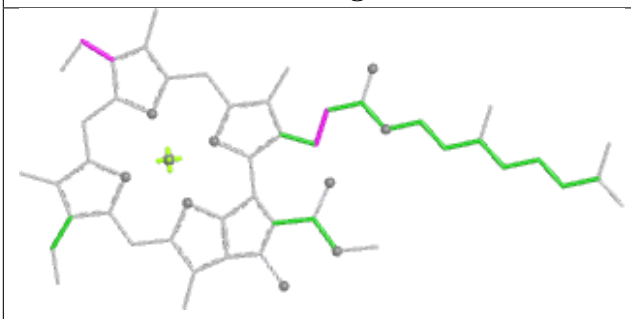
Ligand CLA q 513



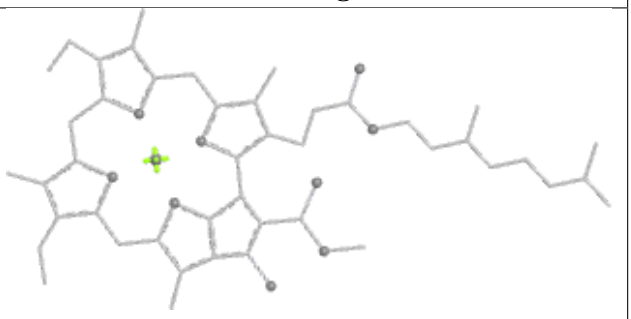
Bond lengths



Bond angles

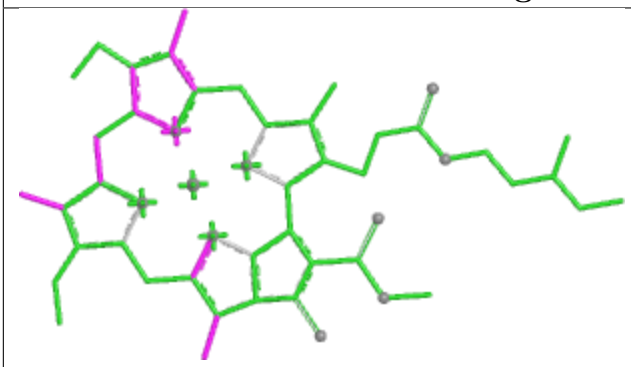


Torsions

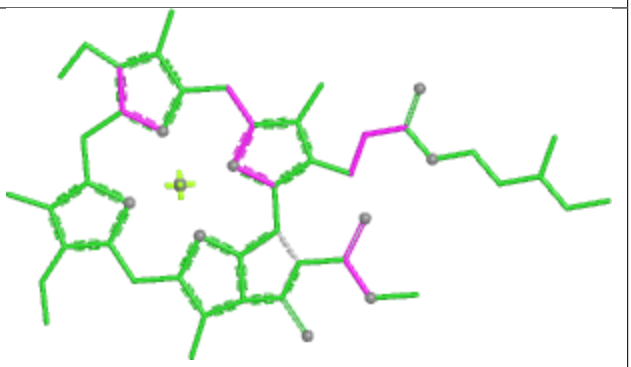


Rings

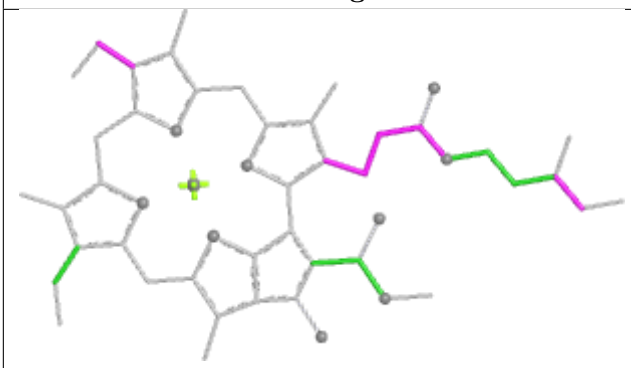
Ligand CLA A 1110



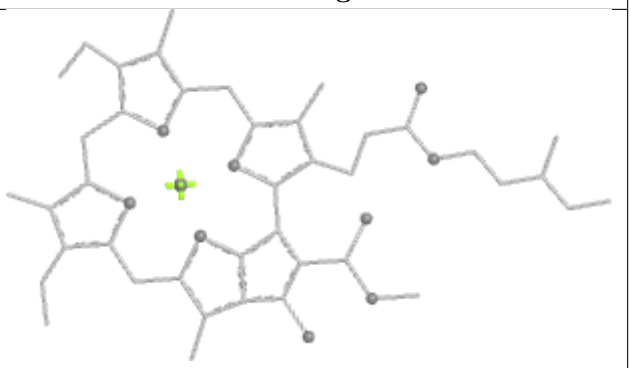
Bond lengths



Bond angles

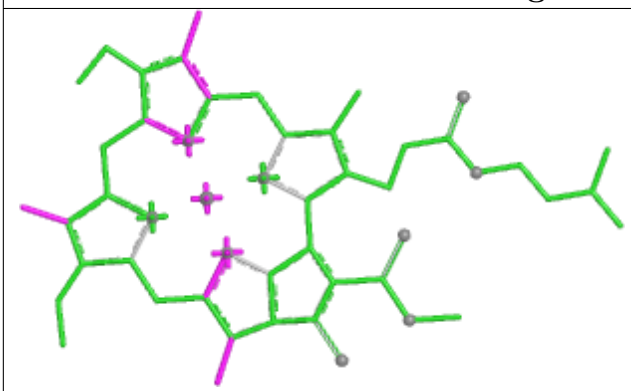


Torsions

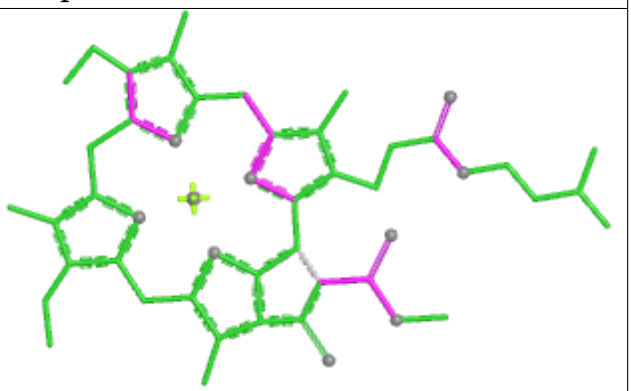


Rings

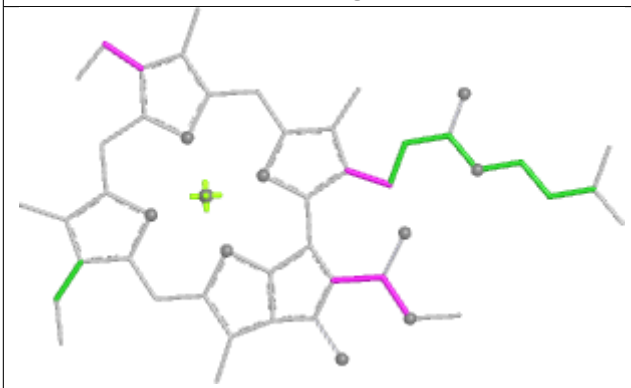
Ligand CLA q 519



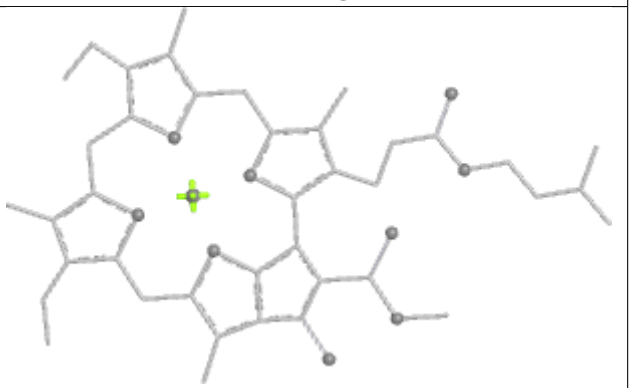
Bond lengths



Bond angles

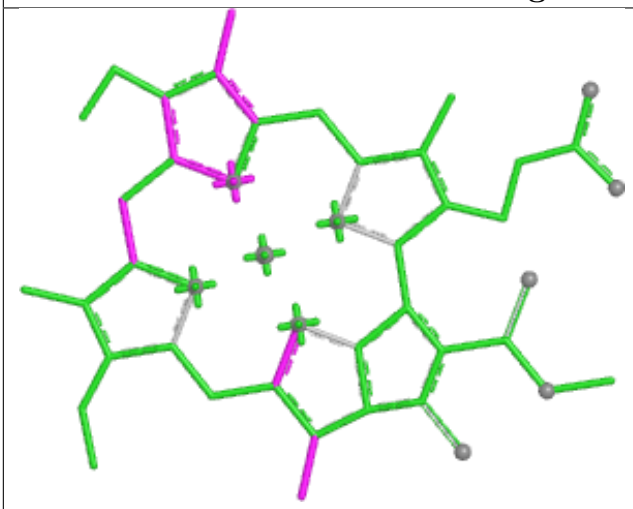


Torsions

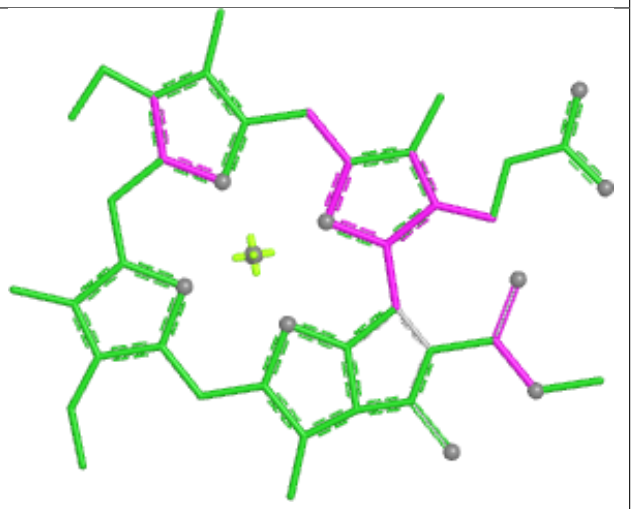


Rings

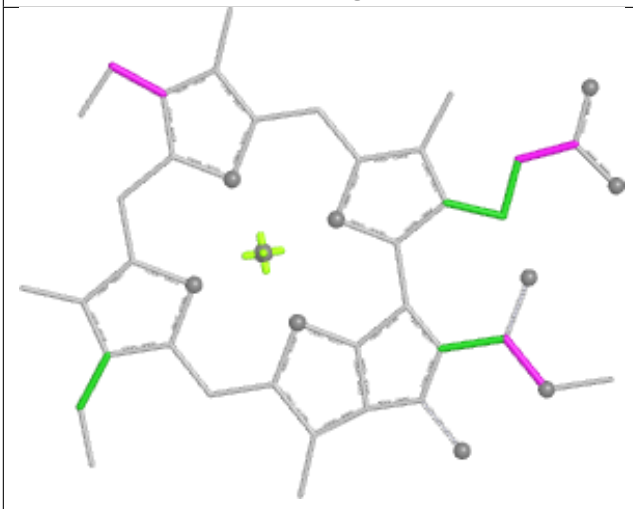
Ligand CLA 6 507



Bond lengths



Bond angles

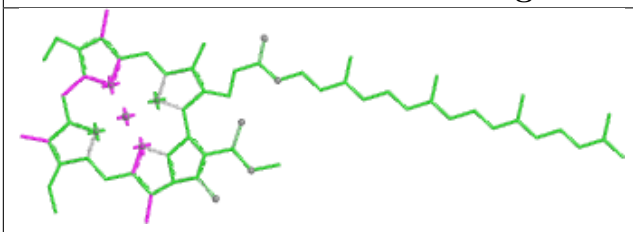


Torsions

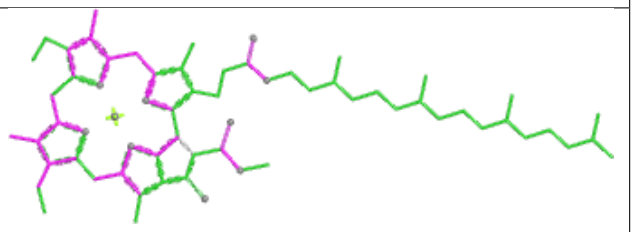


Rings

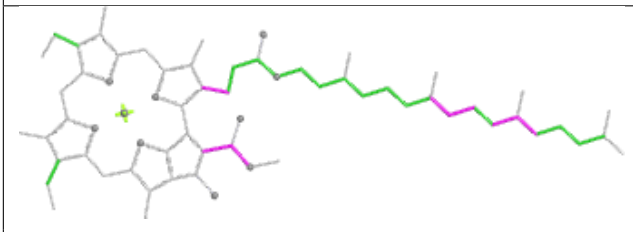
Ligand CLA B 1226



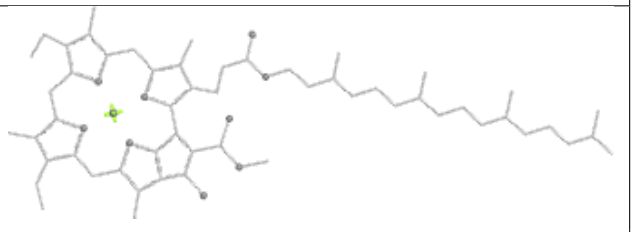
Bond lengths



Bond angles

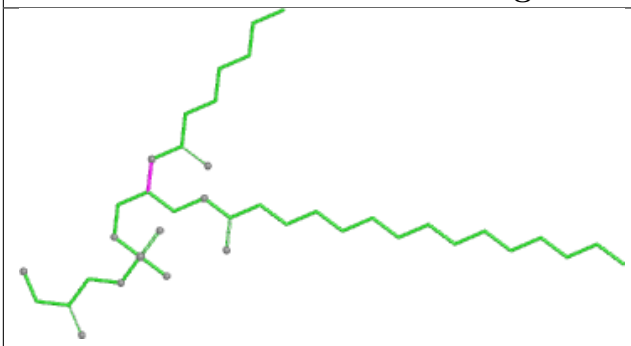


Torsions

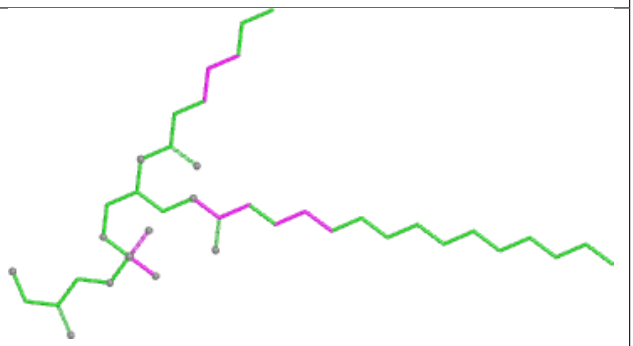


Rings

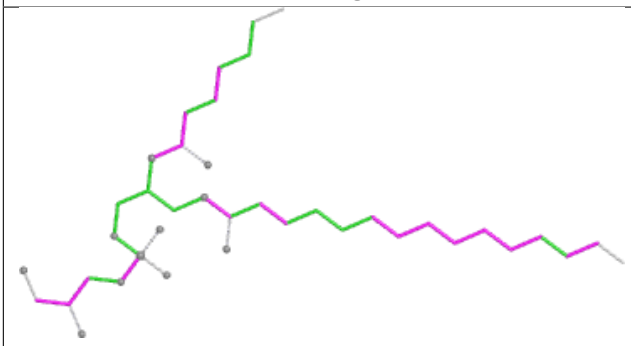
Ligand LHG B 1842



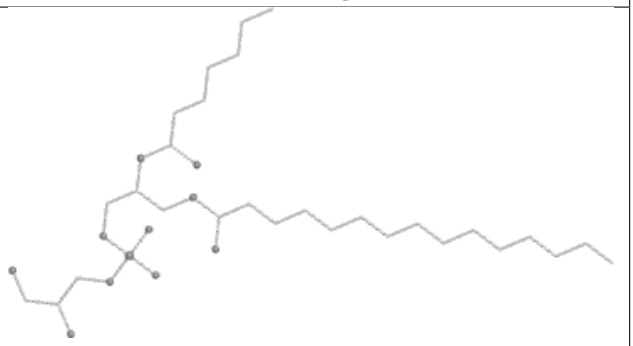
Bond lengths



Bond angles

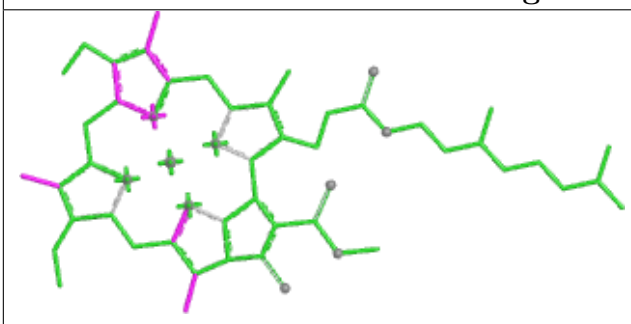


Torsions

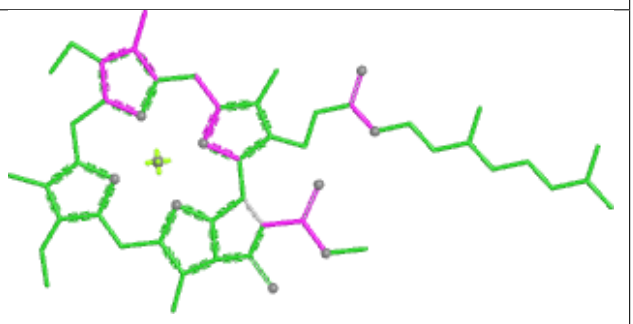


Rings

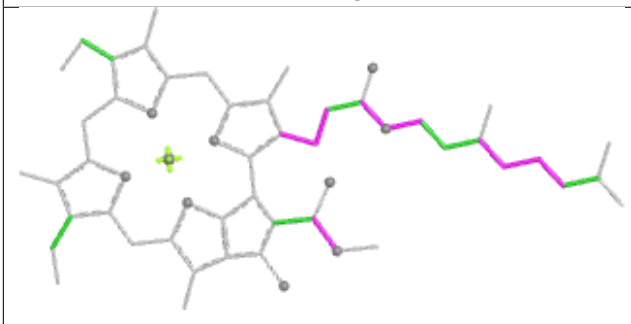
Ligand CLA f 1212



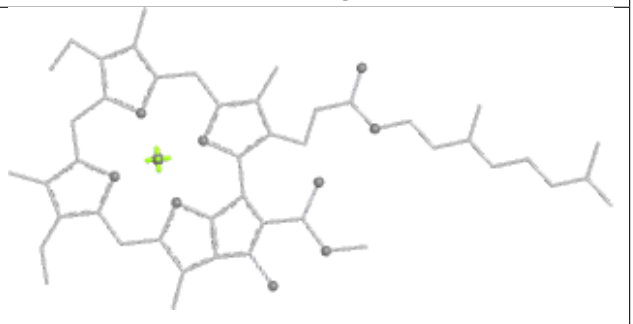
Bond lengths



Bond angles

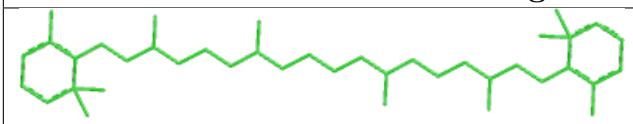


Torsions

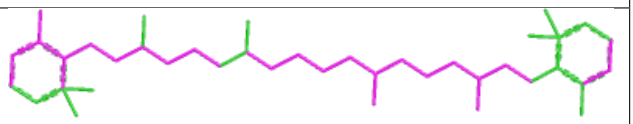


Rings

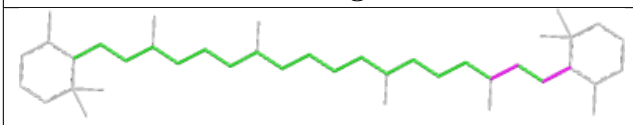
Ligand BCR s 523



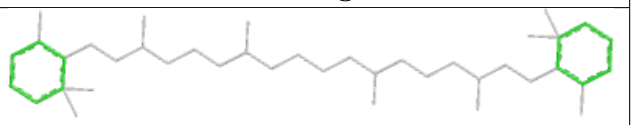
Bond lengths



Bond angles

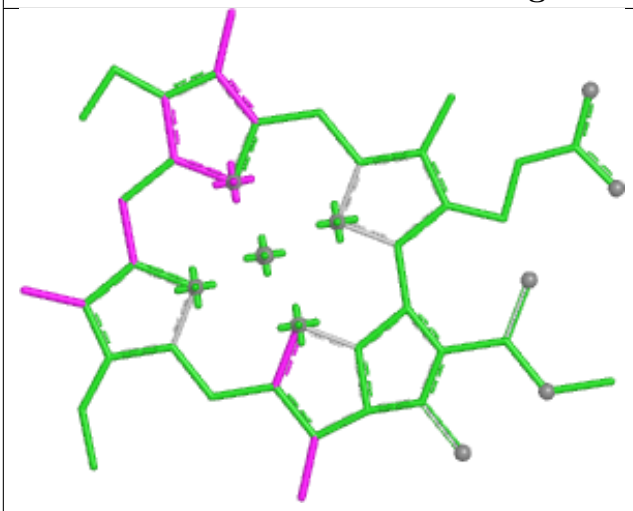


Torsions

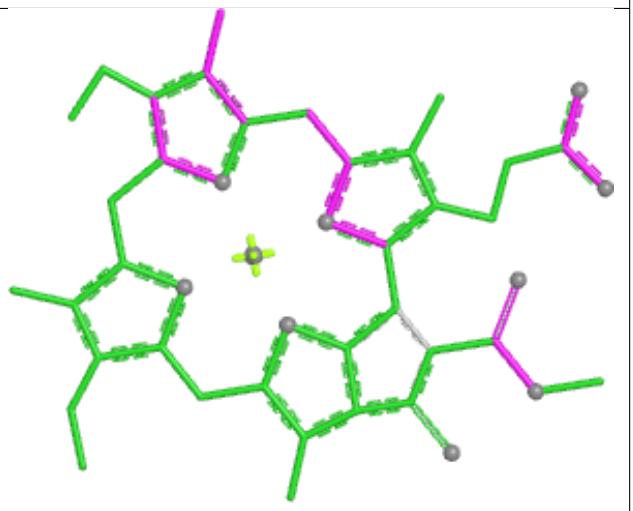


Rings

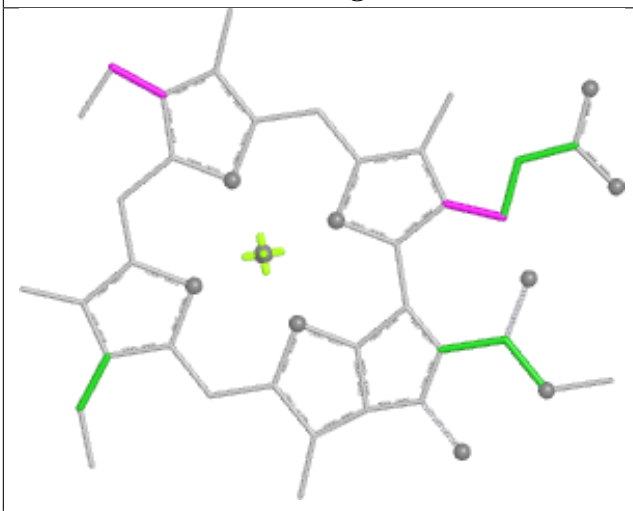
Ligand CLA 6 508



Bond lengths



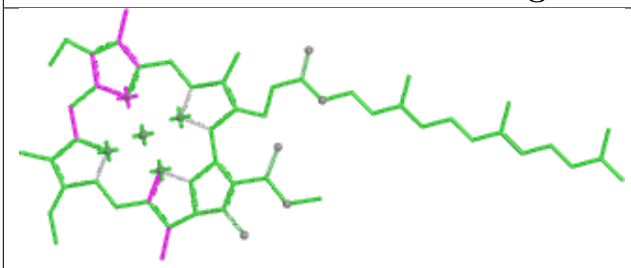
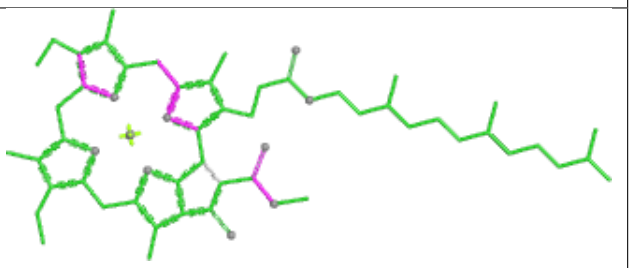
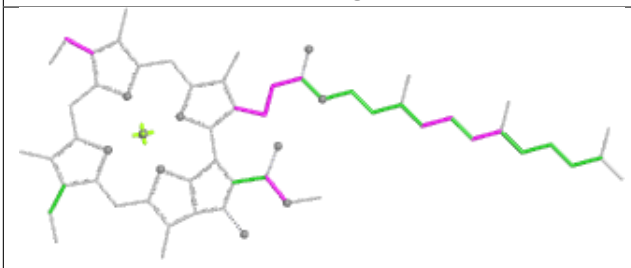
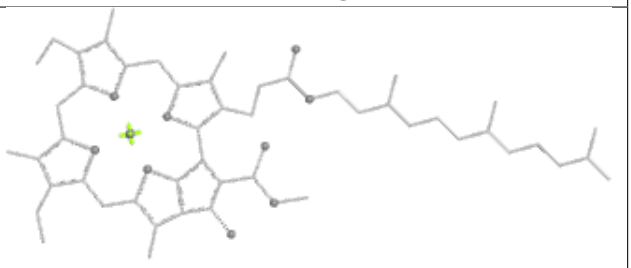
Bond angles

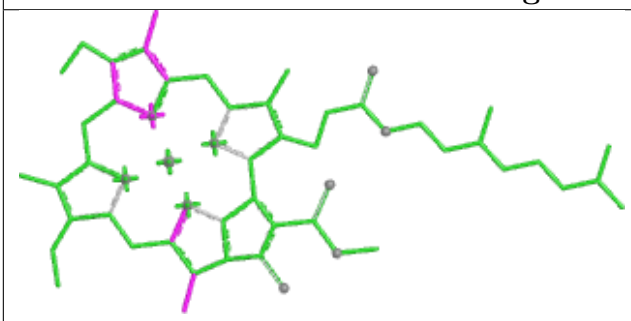
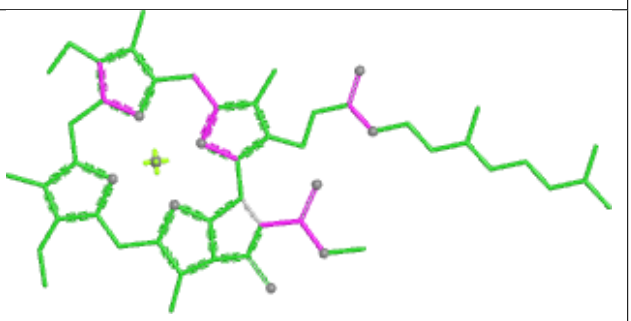
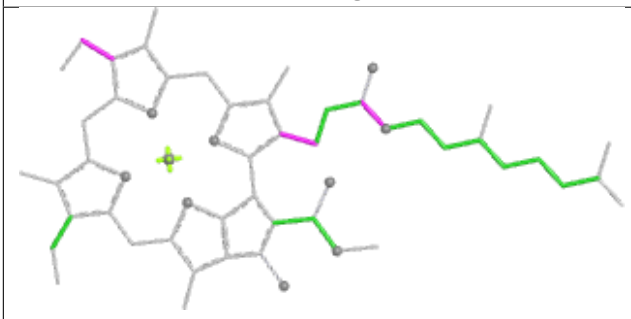
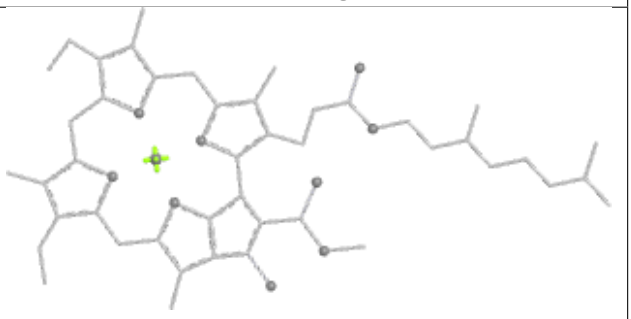


Torsions

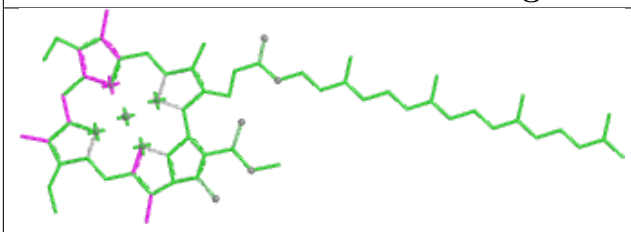


Rings

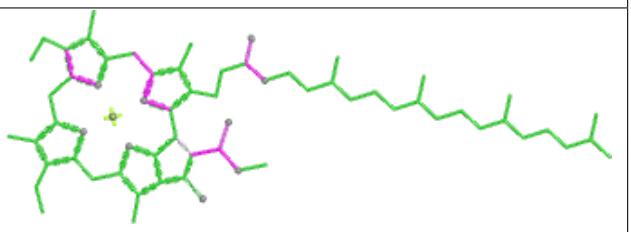
Ligand CLA 4 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 1236	
	
Bond lengths	Bond angles
	
Torsions	Rings

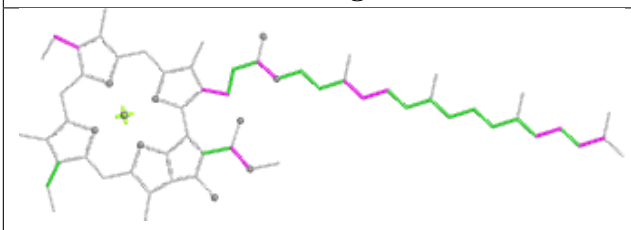
Ligand CLA f 1227



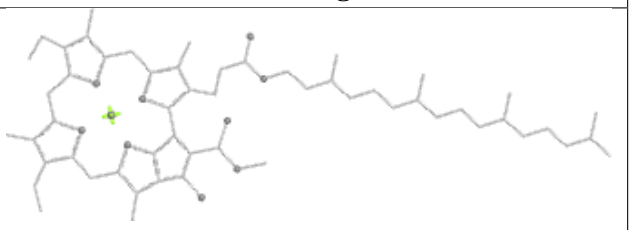
Bond lengths



Bond angles

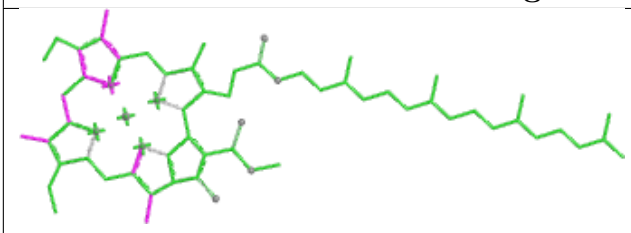


Torsions

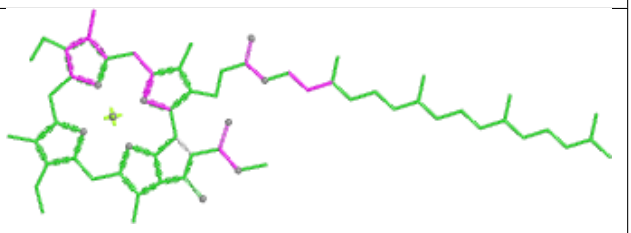


Rings

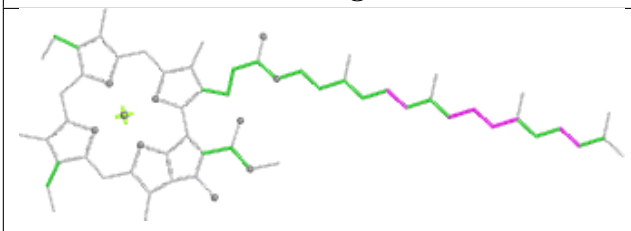
Ligand CLA Y 509



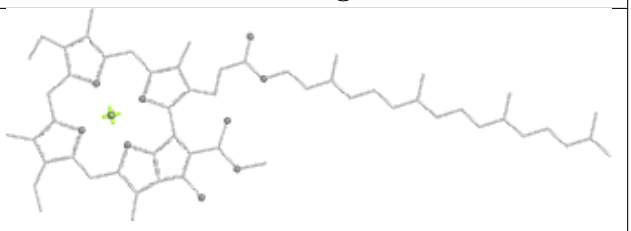
Bond lengths



Bond angles

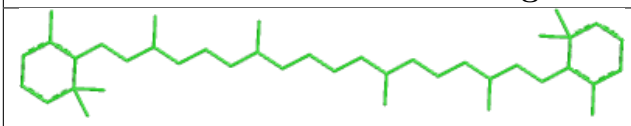


Torsions

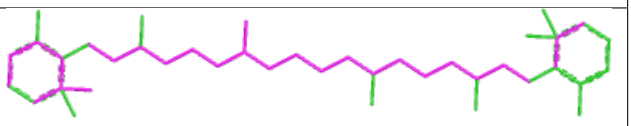


Rings

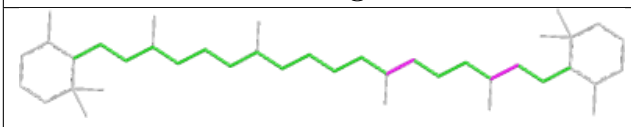
Ligand BCR l 4013



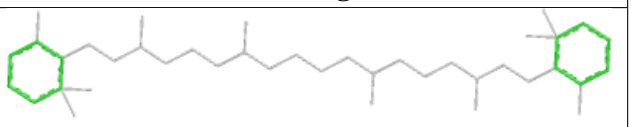
Bond lengths



Bond angles

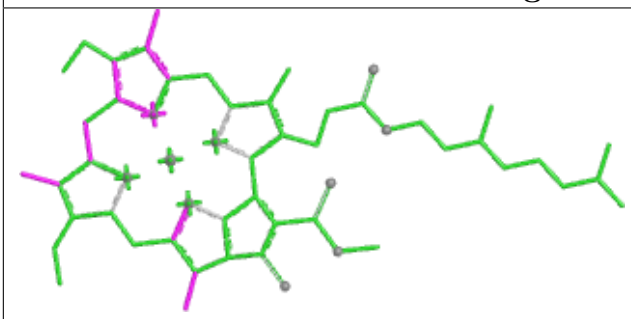


Torsions

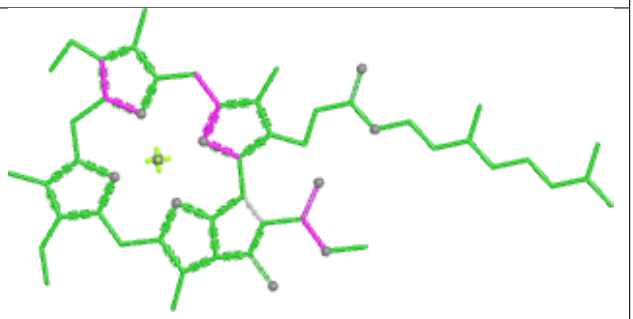


Rings

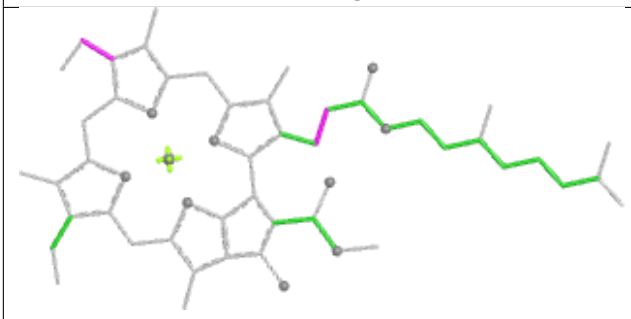
Ligand CLA Y 513



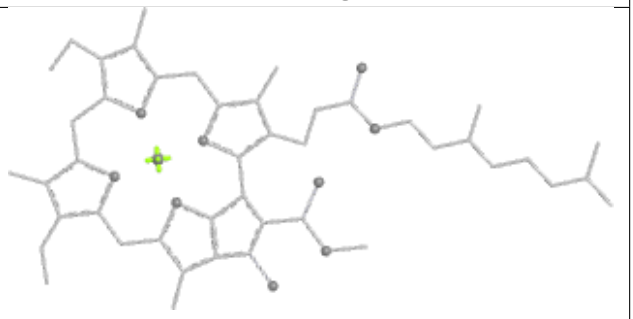
Bond lengths



Bond angles

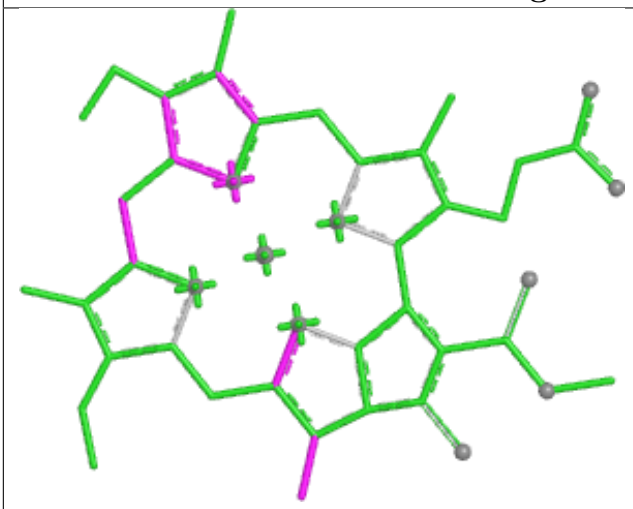


Torsions

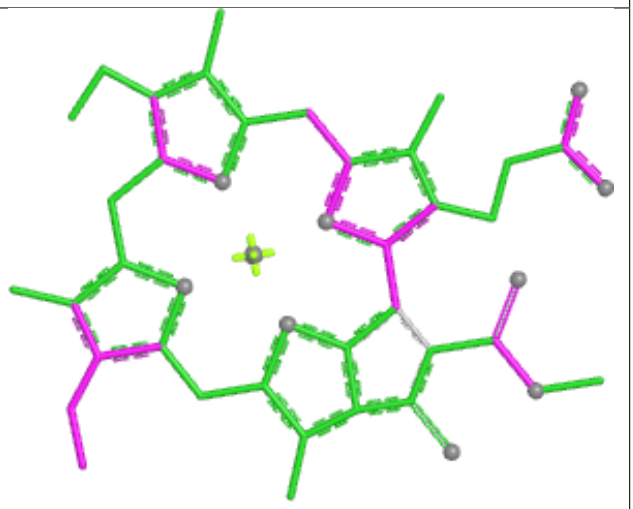


Rings

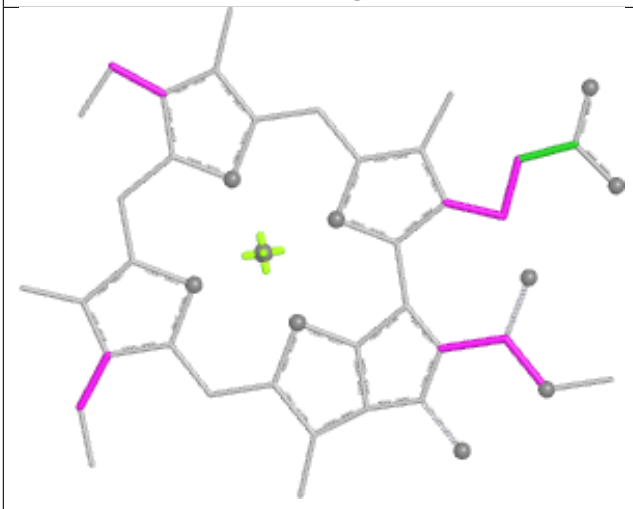
Ligand CLA s 516



Bond lengths



Bond angles

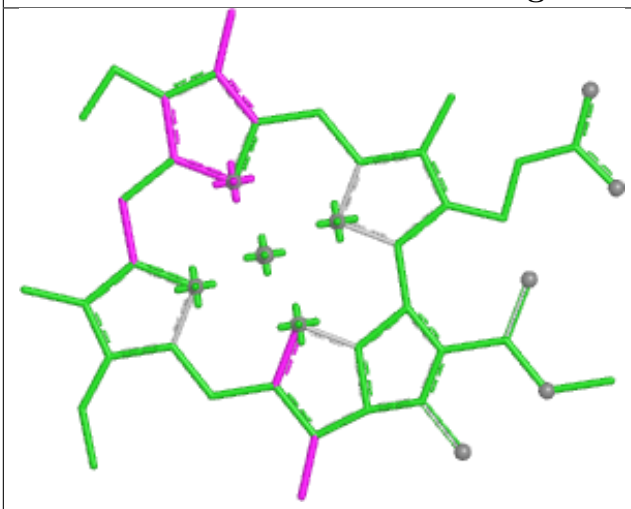


Torsions

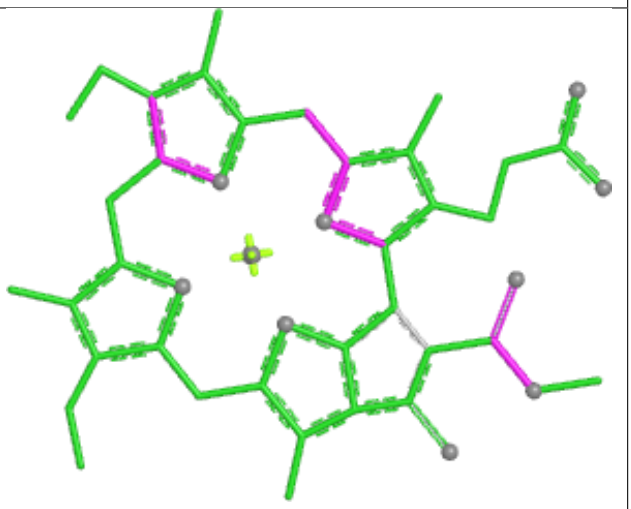


Rings

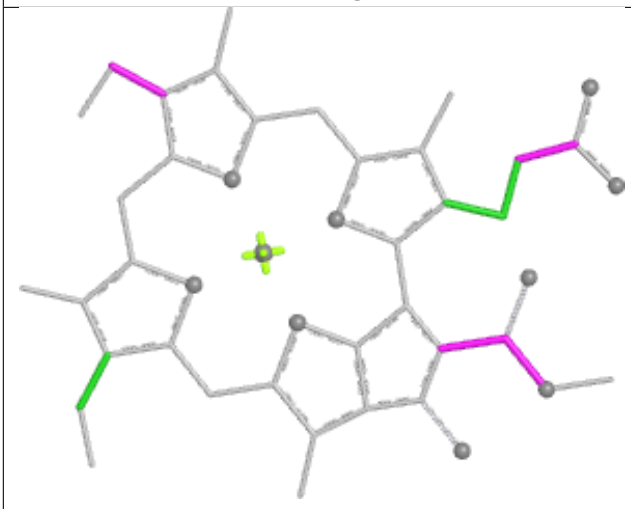
Ligand CLA u 512



Bond lengths



Bond angles

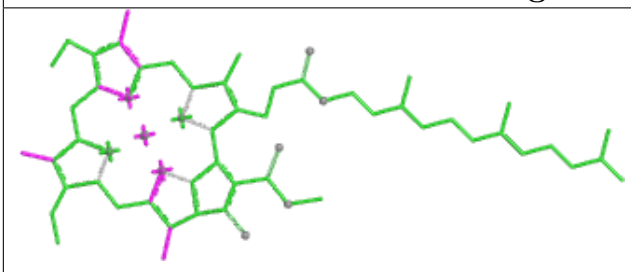


Torsions

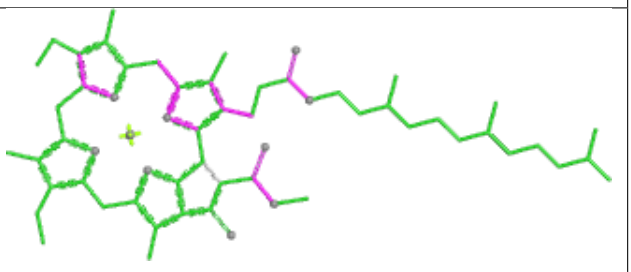


Rings

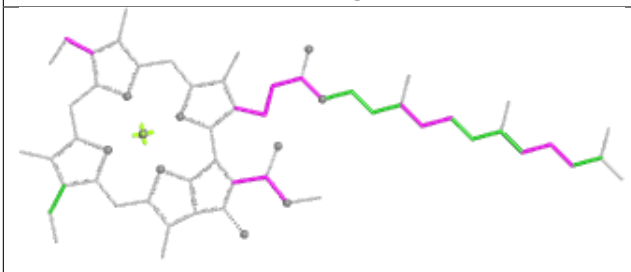
Ligand CLA 1 518



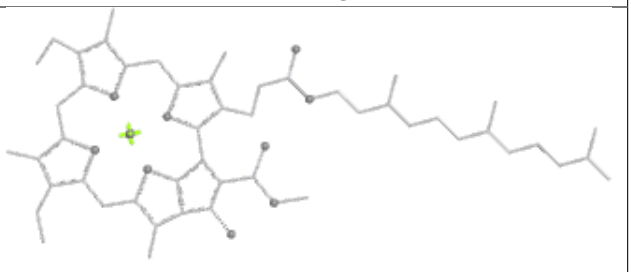
Bond lengths



Bond angles

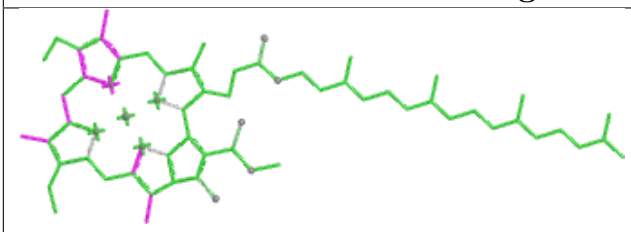


Torsions

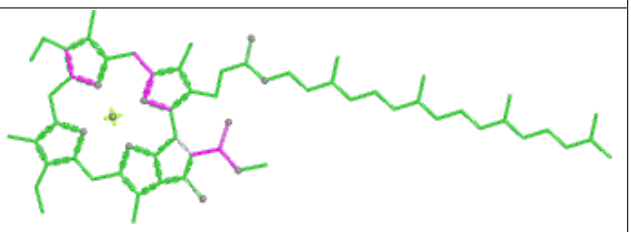


Rings

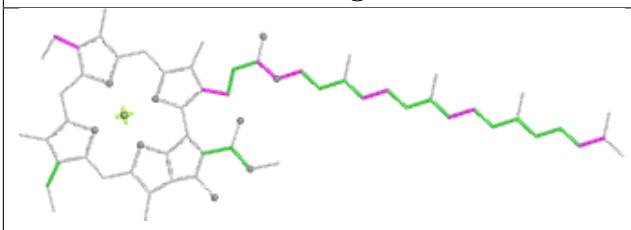
Ligand CLA n 1502



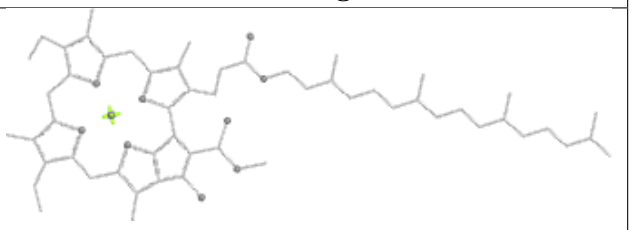
Bond lengths



Bond angles

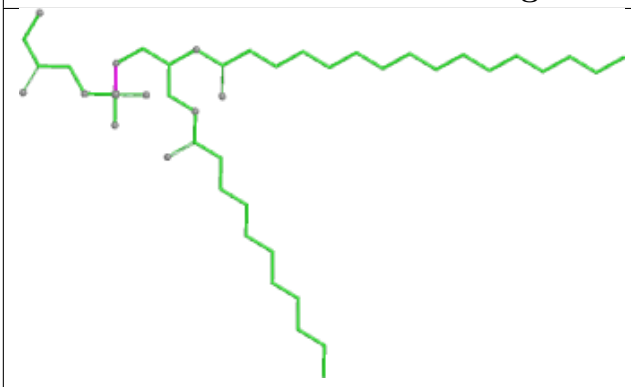


Torsions

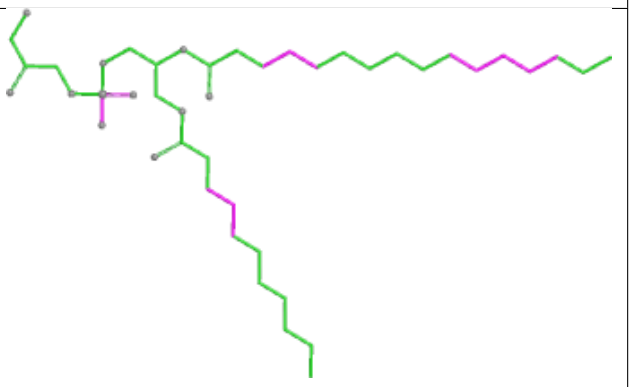


Rings

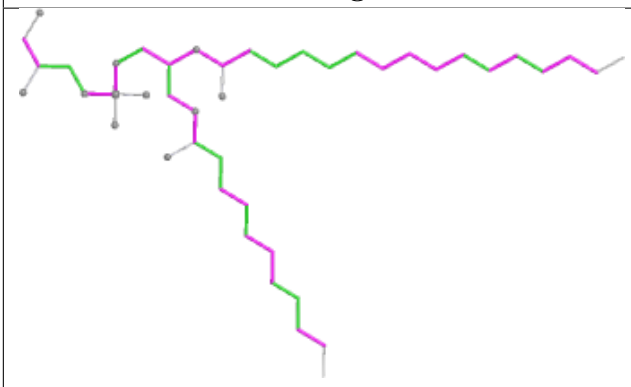
Ligand LHG f 1855



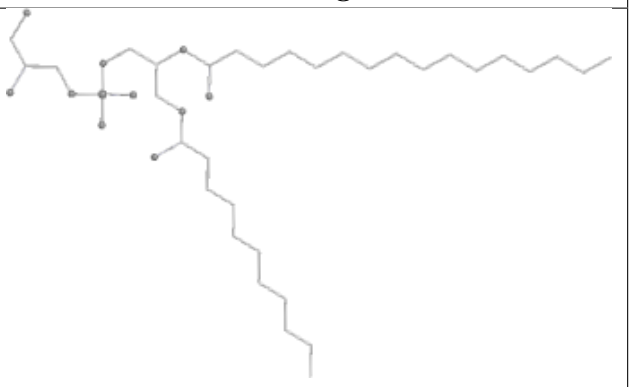
Bond lengths



Bond angles

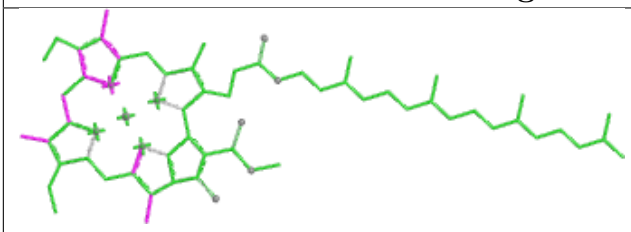


Torsions

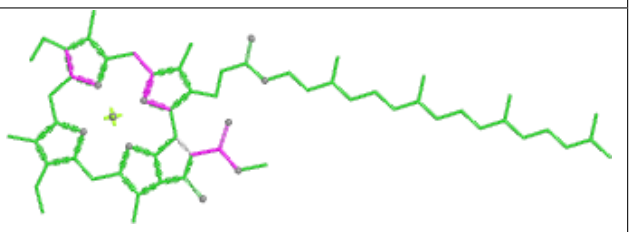


Rings

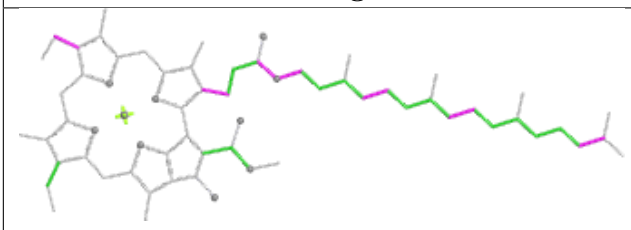
Ligand CLA L 1502



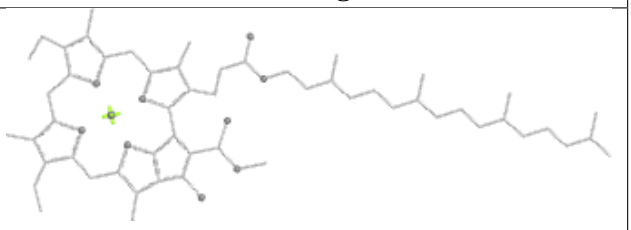
Bond lengths



Bond angles



Torsions

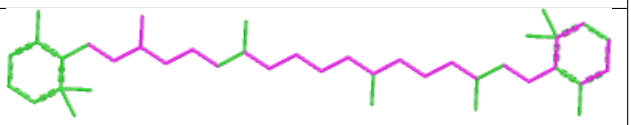


Rings

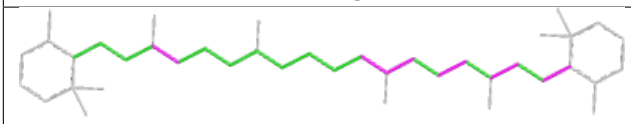
Ligand BCR G 4011



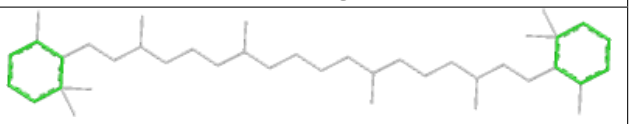
Bond lengths



Bond angles

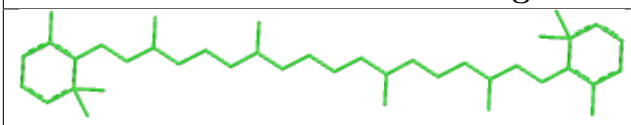


Torsions

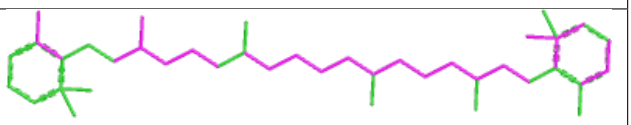


Rings

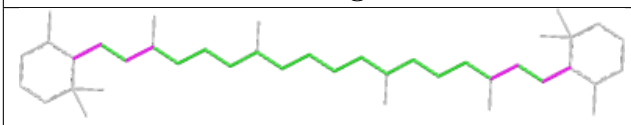
Ligand BCR H 4004



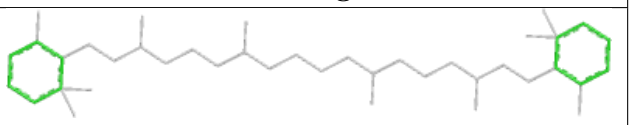
Bond lengths



Bond angles

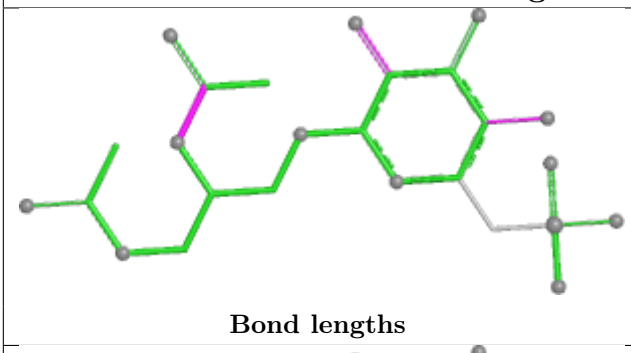


Torsions

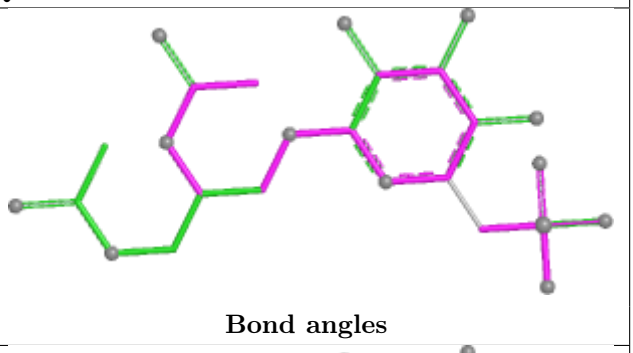


Rings

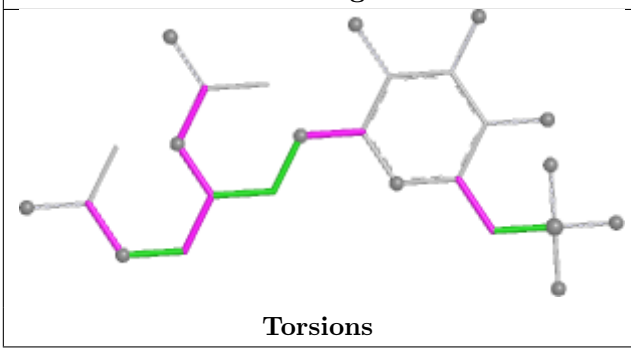
Ligand SQD 6 822



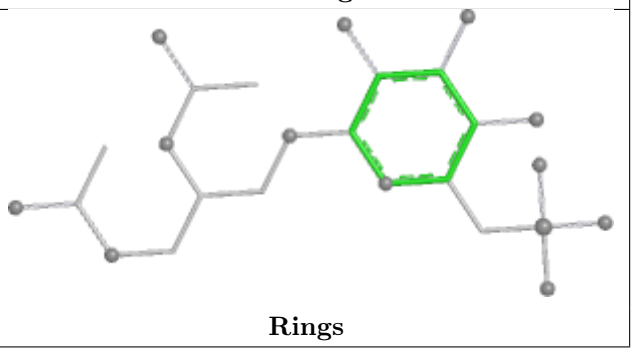
Bond lengths



Bond angles

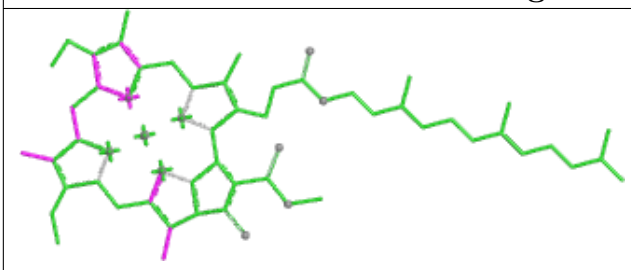


Torsions

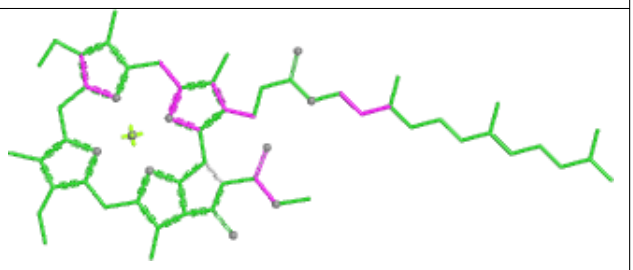


Rings

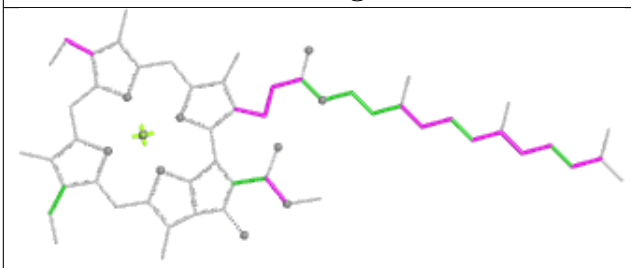
Ligand CLA v 501



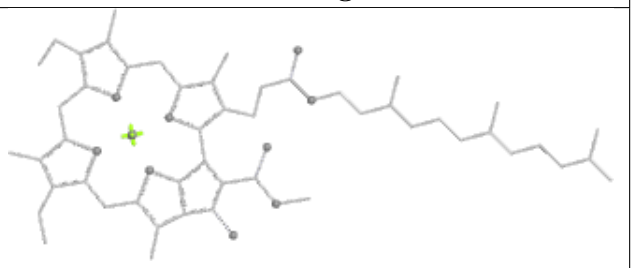
Bond lengths



Bond angles



Torsions

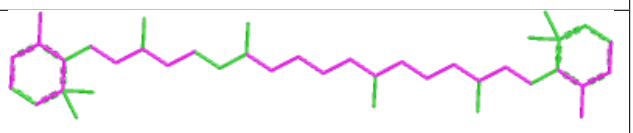


Rings

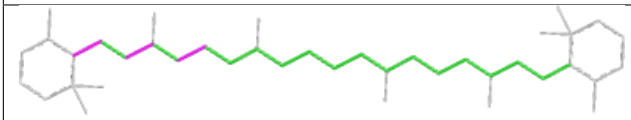
Ligand BCR d 521



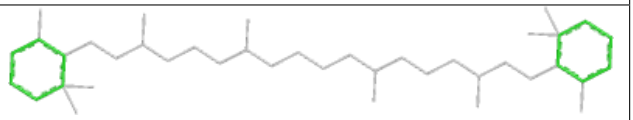
Bond lengths



Bond angles

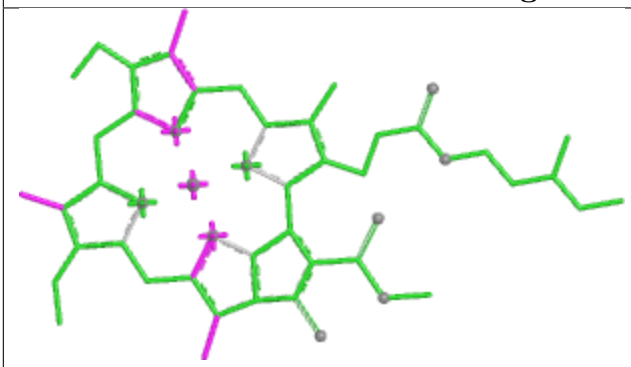


Torsions

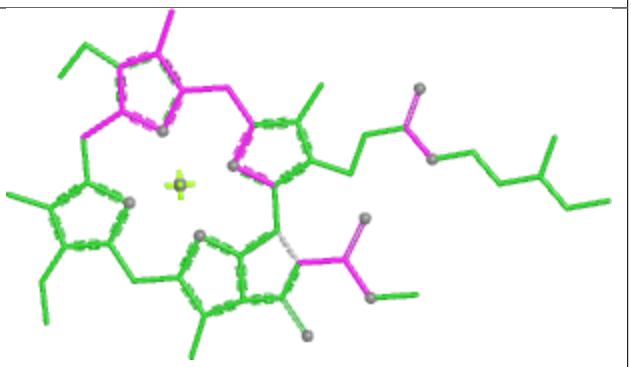


Rings

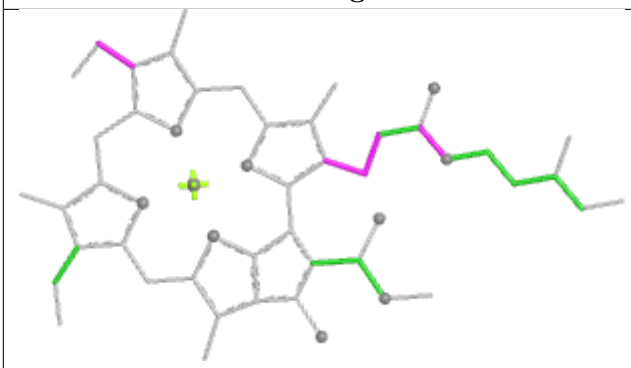
Ligand CLA e 1129



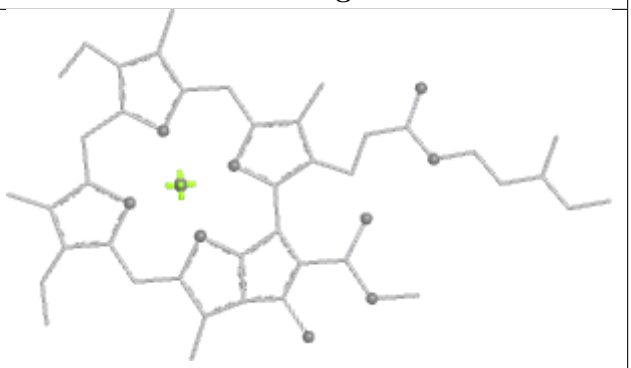
Bond lengths



Bond angles

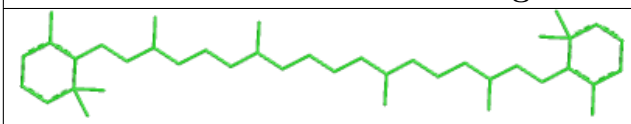


Torsions

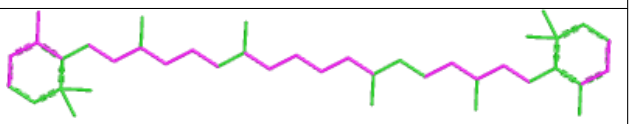


Rings

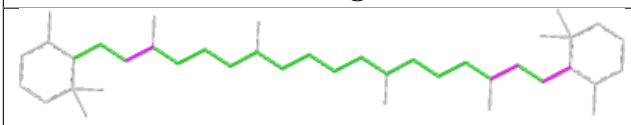
Ligand BCR H 4005



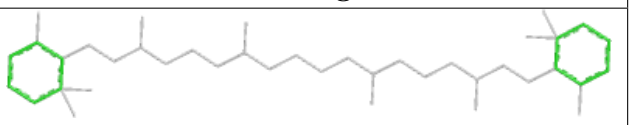
Bond lengths



Bond angles

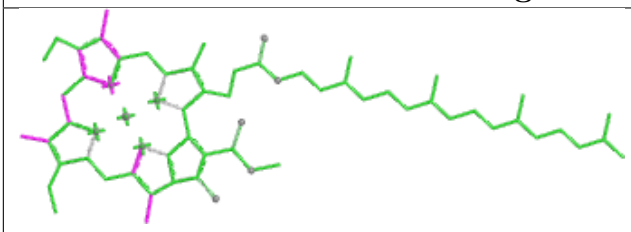


Torsions

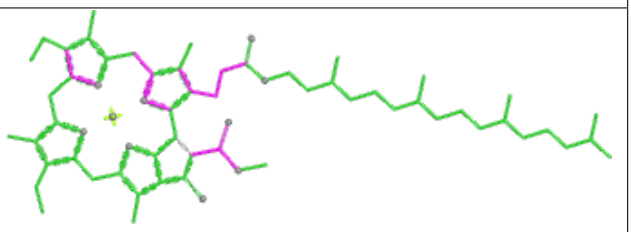


Rings

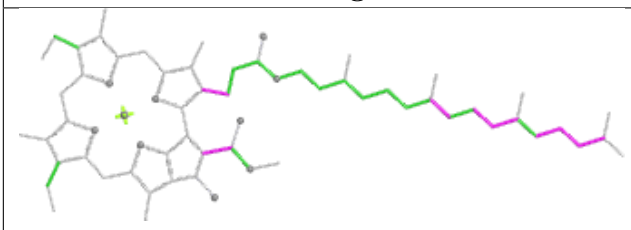
Ligand CLA A 1101



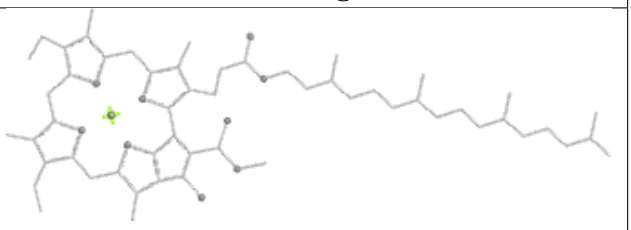
Bond lengths



Bond angles

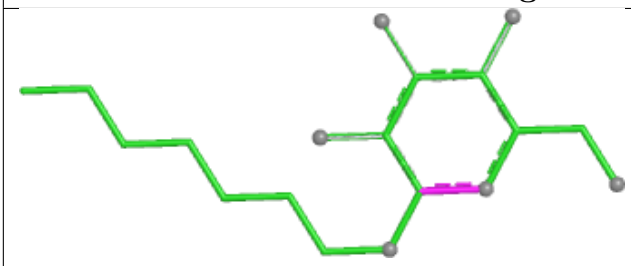


Torsions

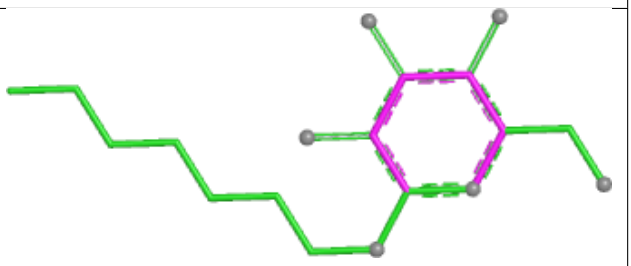


Rings

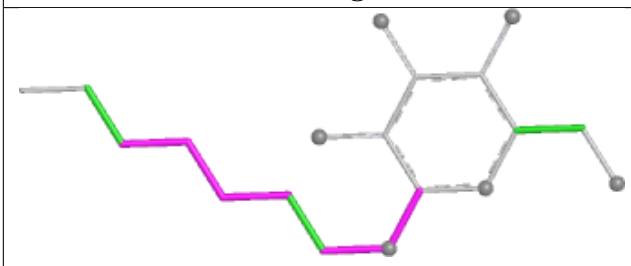
Ligand LMU Y 902



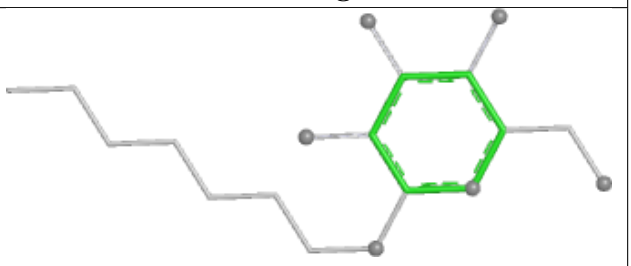
Bond lengths



Bond angles

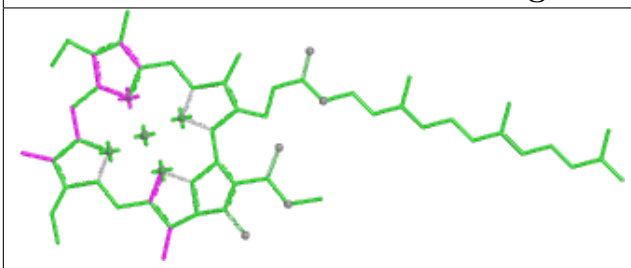


Torsions

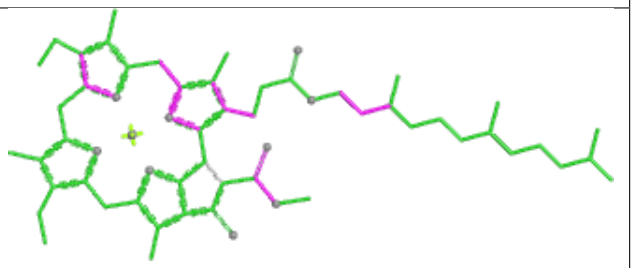


Rings

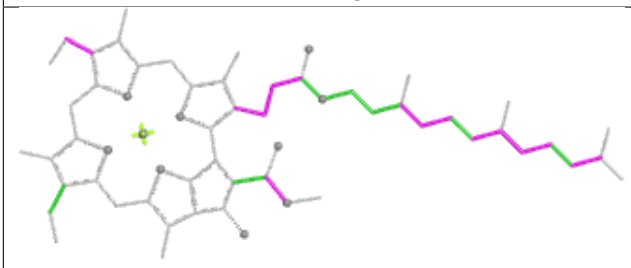
Ligand CLA 6 501



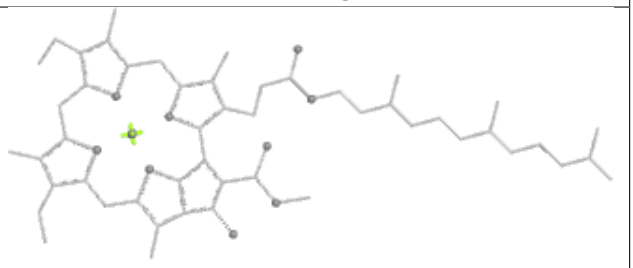
Bond lengths



Bond angles

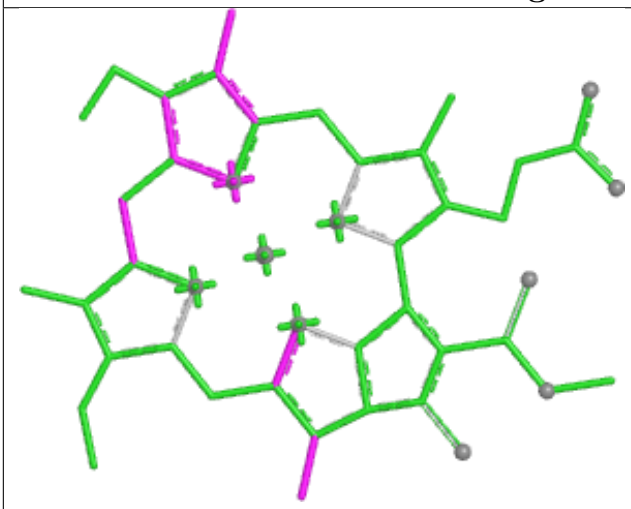


Torsions

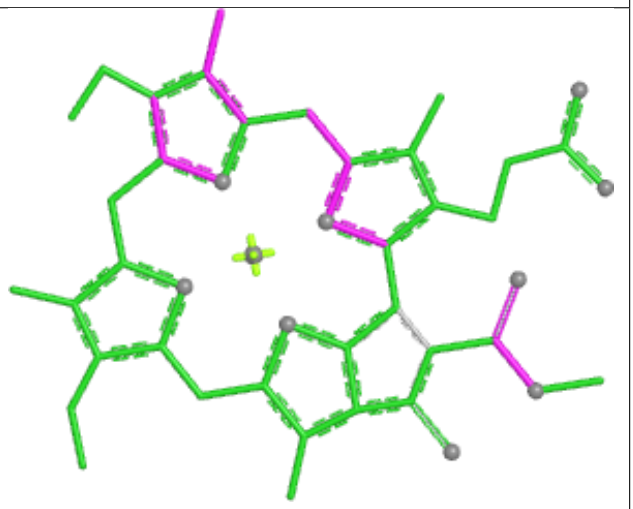


Rings

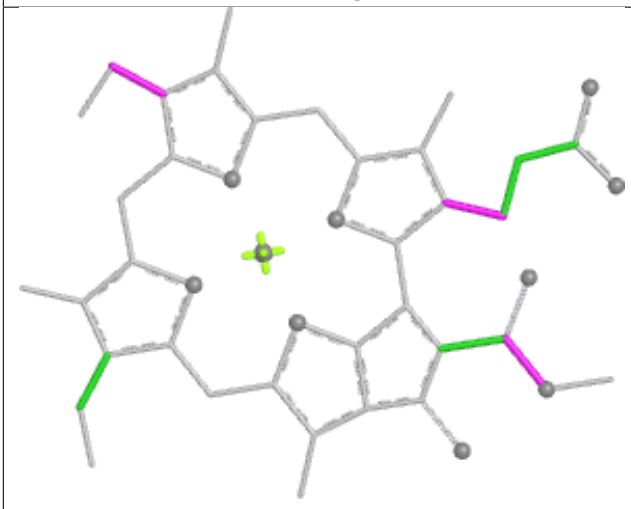
Ligand CLA 4 511



Bond lengths



Bond angles

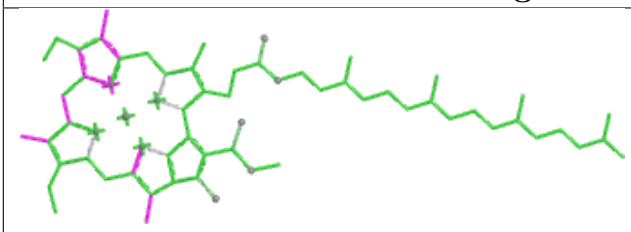


Torsions

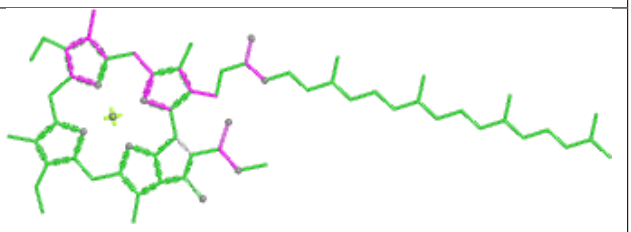


Rings

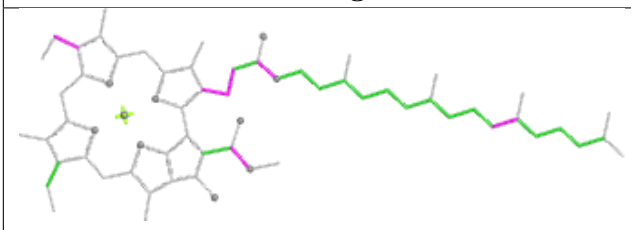
Ligand CLA G 1111



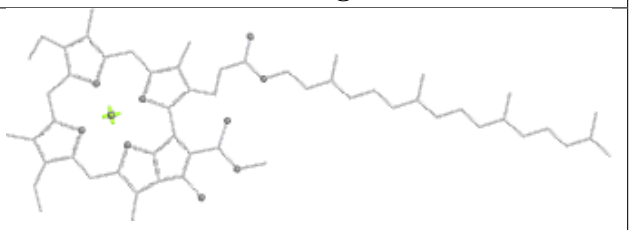
Bond lengths



Bond angles

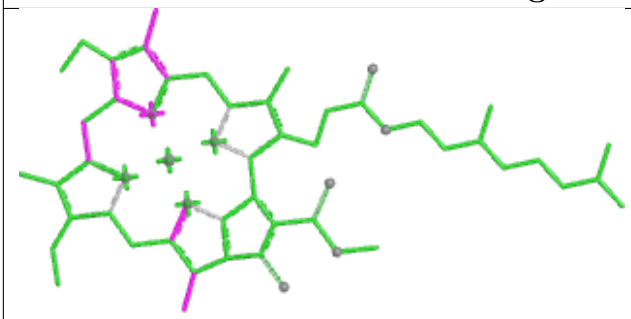


Torsions

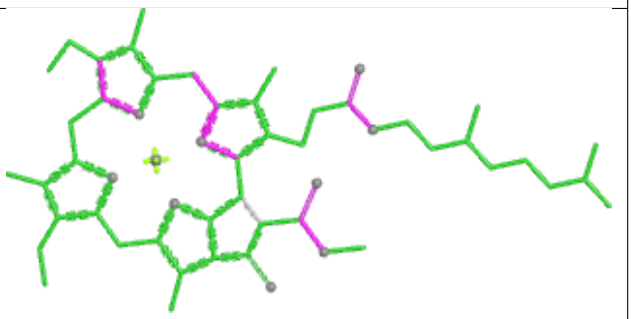


Rings

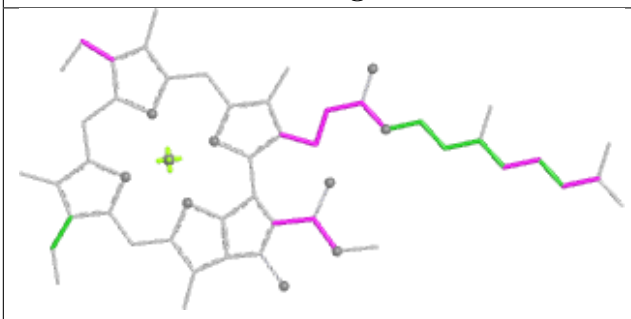
Ligand CLA 5 518



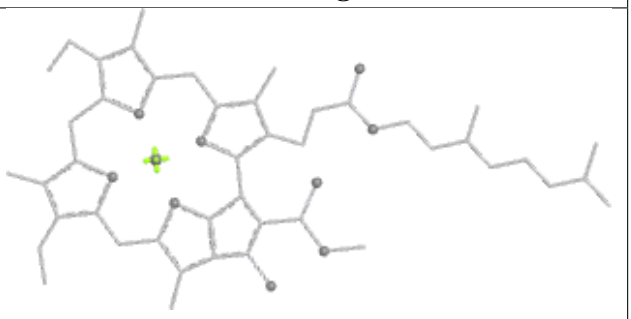
Bond lengths



Bond angles

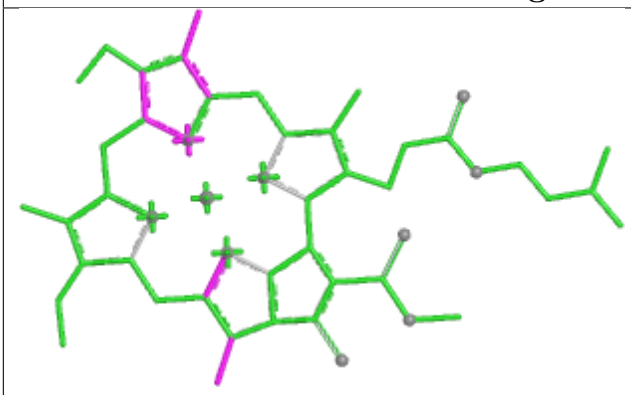


Torsions

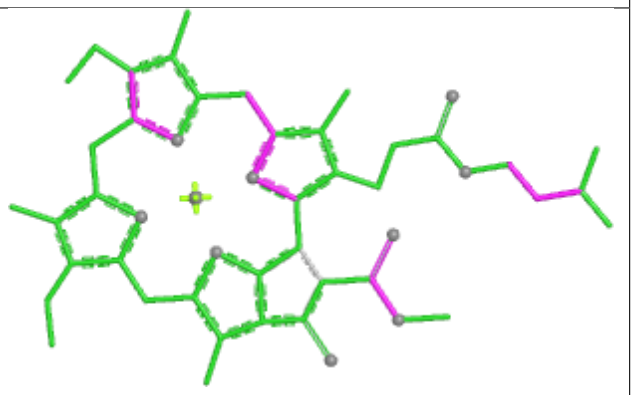


Rings

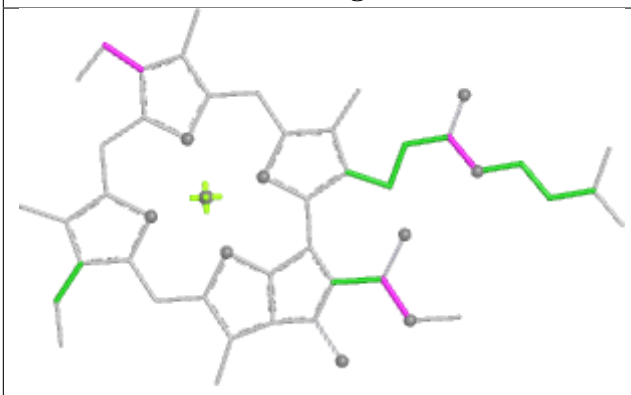
Ligand CLA 6 502



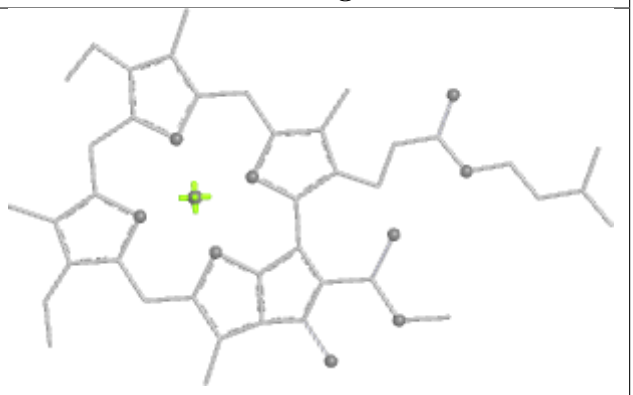
Bond lengths



Bond angles

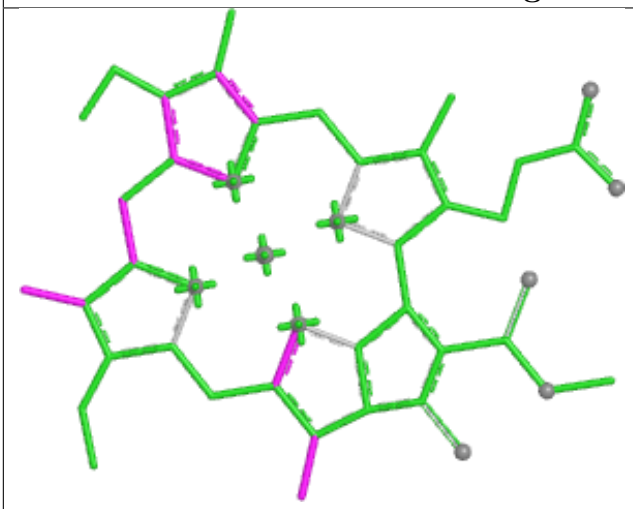


Torsions

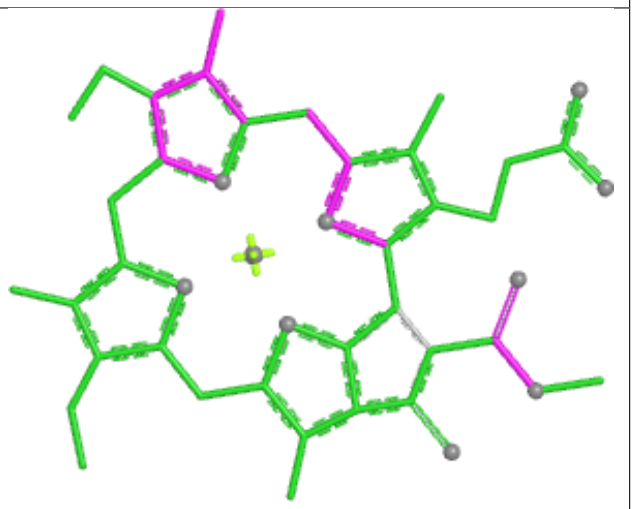


Rings

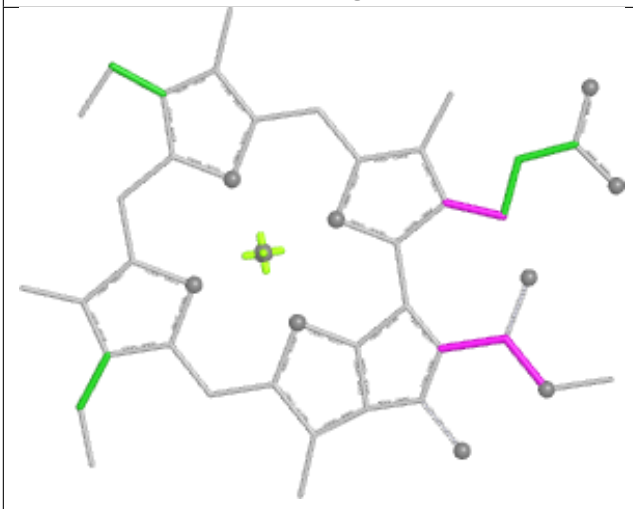
Ligand CLA Y 506



Bond lengths



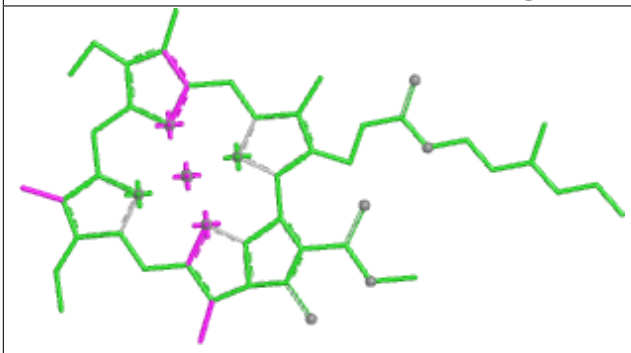
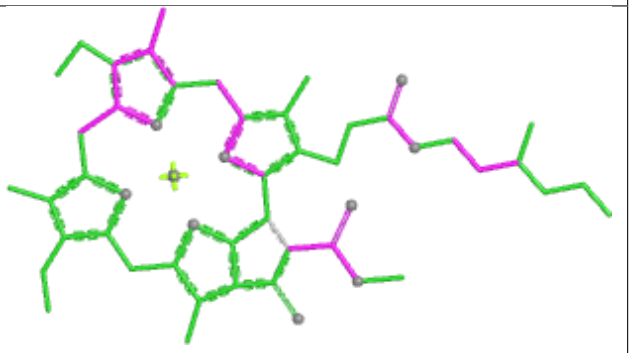
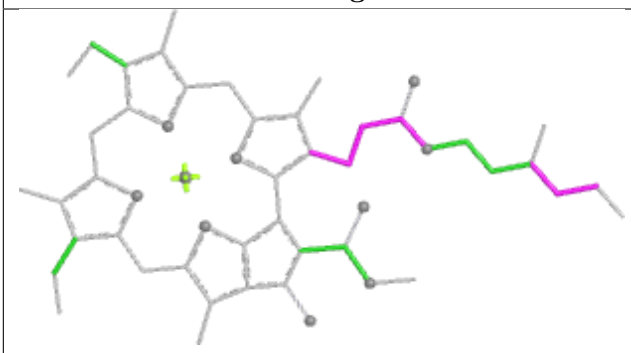
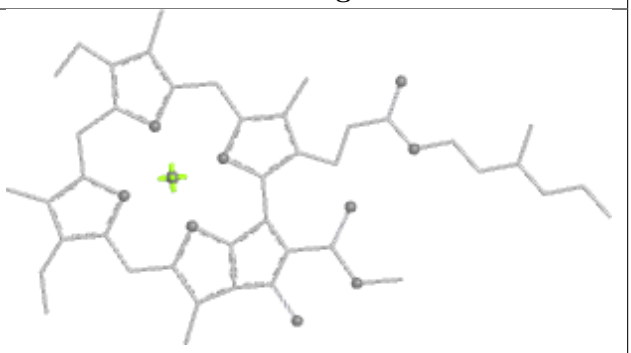
Bond angles

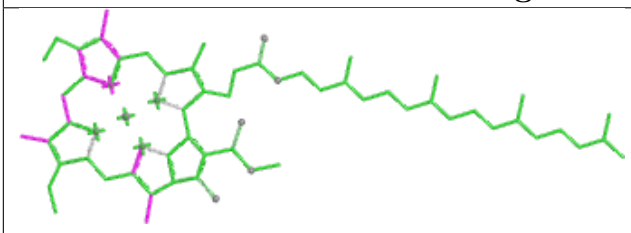
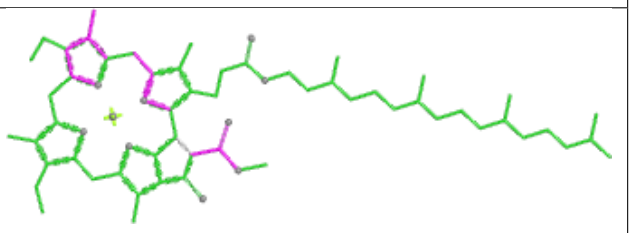
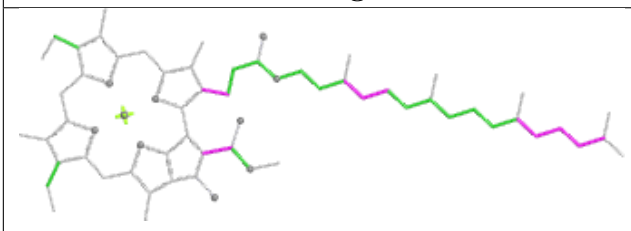
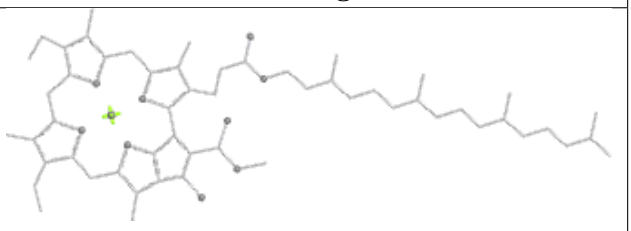


Torsions

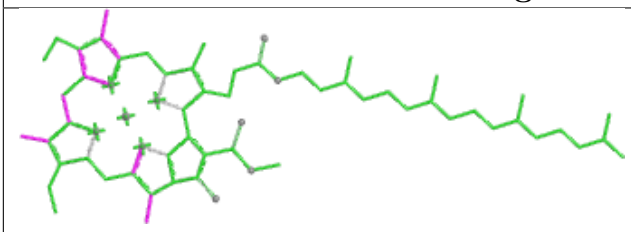


Rings

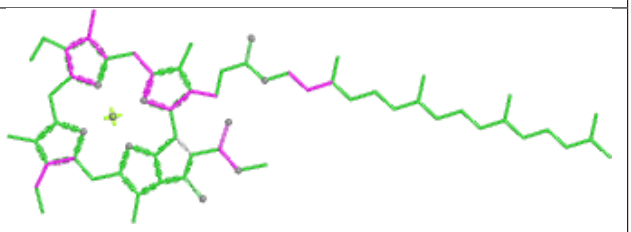
Ligand CLA e 1135	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

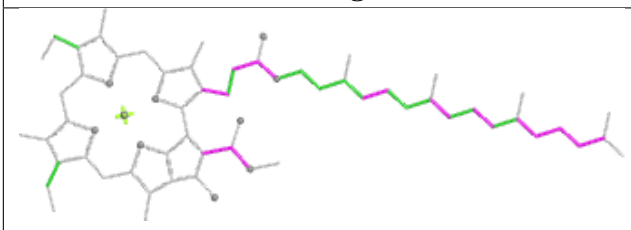
Ligand CLA A 1103



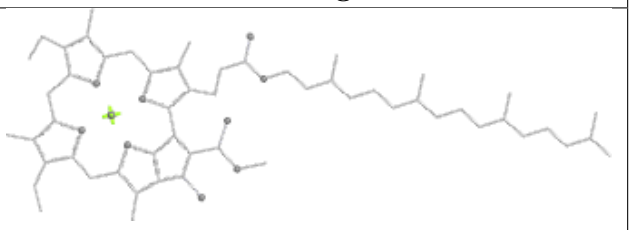
Bond lengths



Bond angles

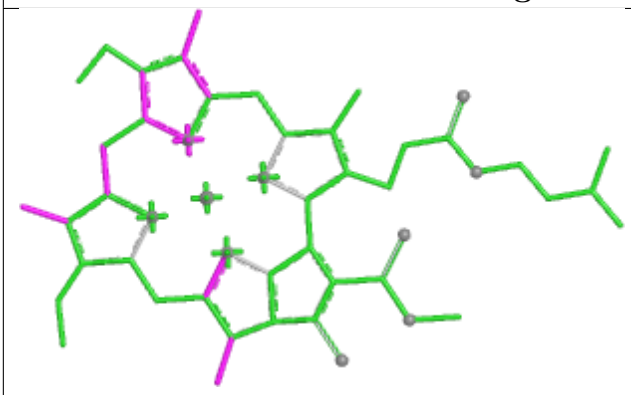


Torsions

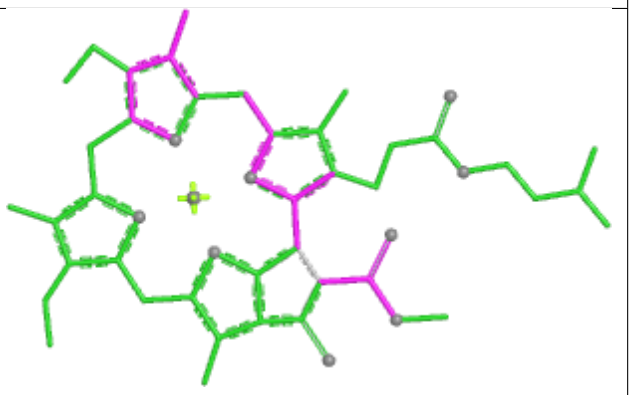


Rings

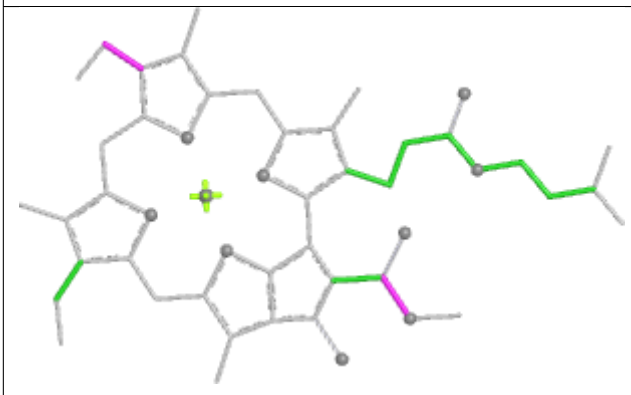
Ligand CLA G 1112



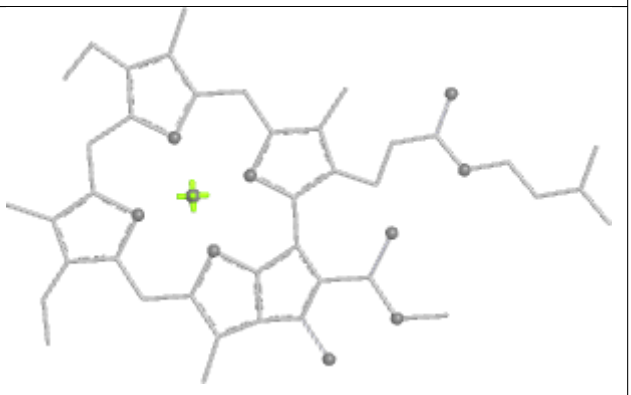
Bond lengths



Bond angles

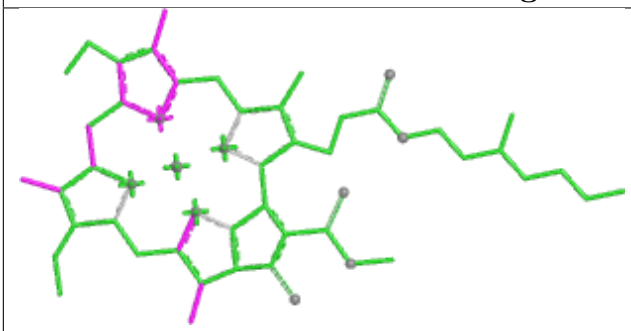


Torsions

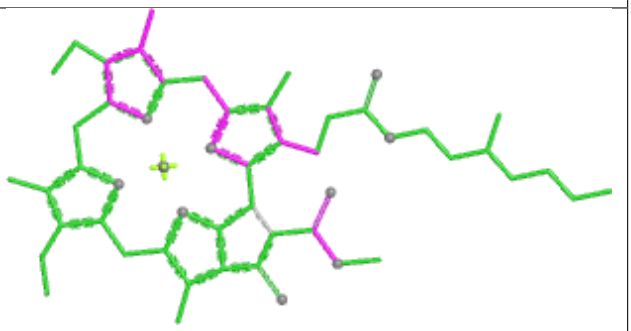


Rings

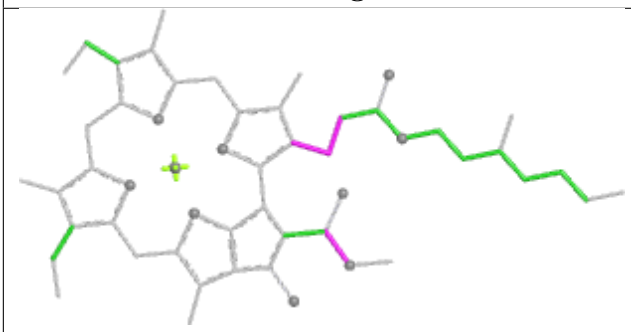
Ligand CLA e 1120



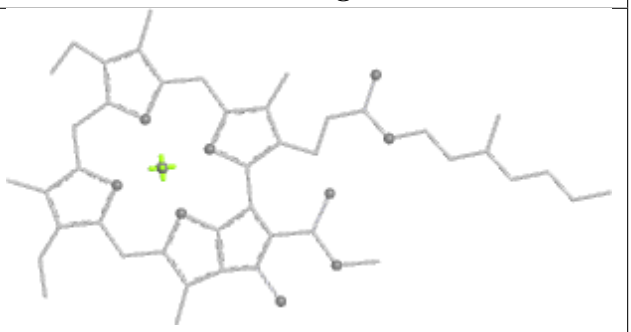
Bond lengths



Bond angles

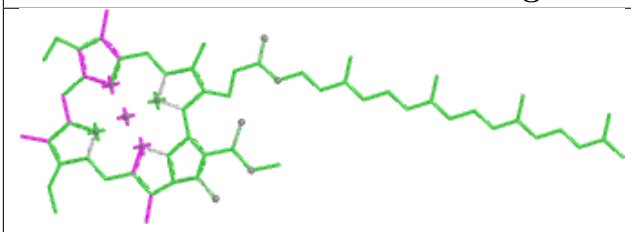


Torsions

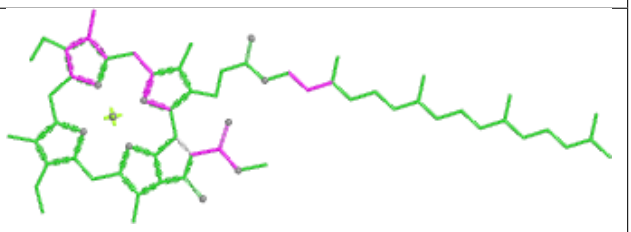


Rings

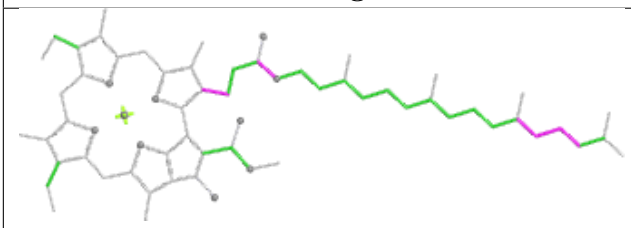
Ligand CLA f 1225



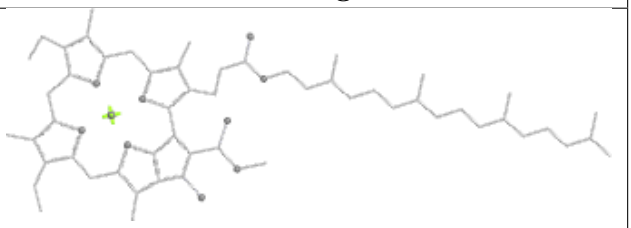
Bond lengths



Bond angles

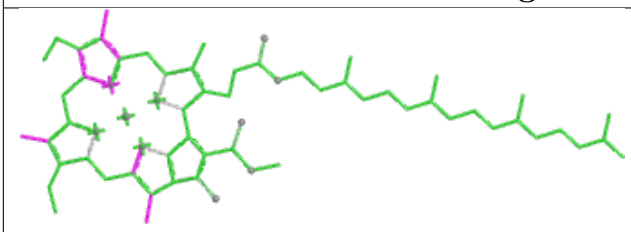


Torsions

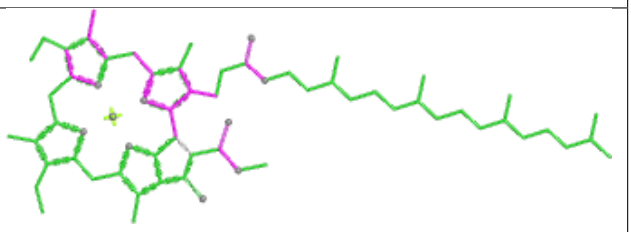


Rings

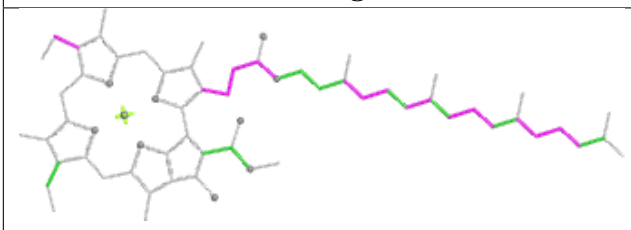
Ligand CLA n 1501



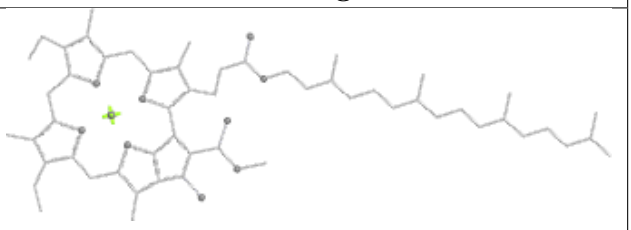
Bond lengths



Bond angles

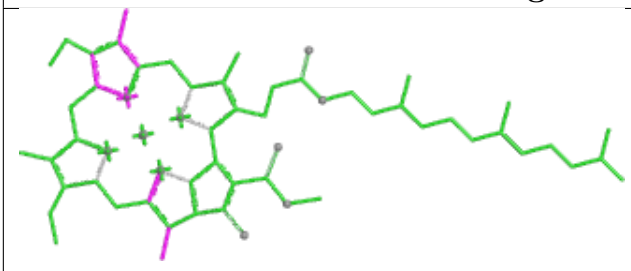


Torsions

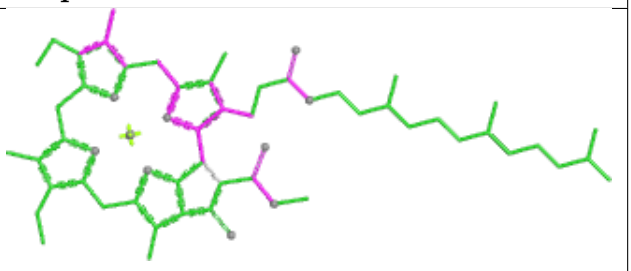


Rings

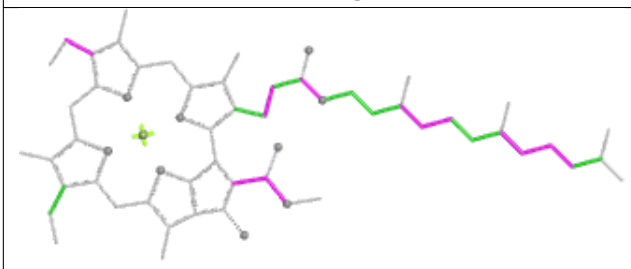
Ligand CLA q 507



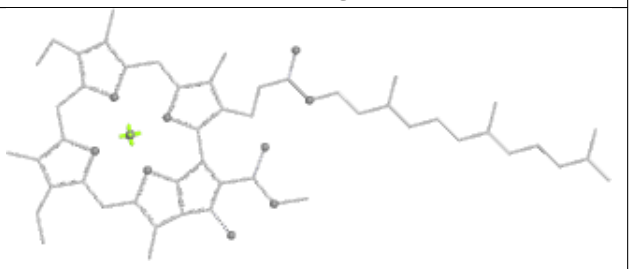
Bond lengths



Bond angles

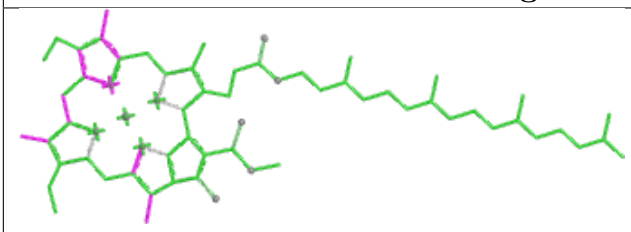


Torsions

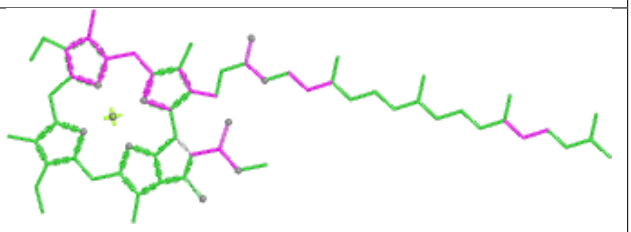


Rings

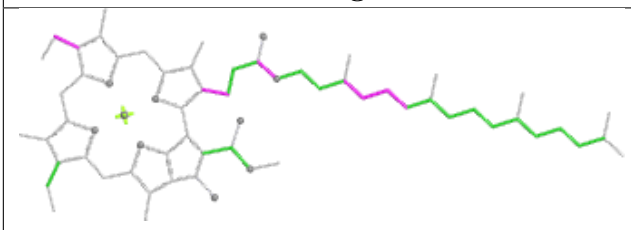
Ligand CLA e 1130



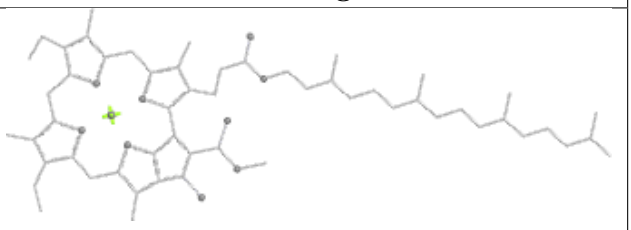
Bond lengths



Bond angles

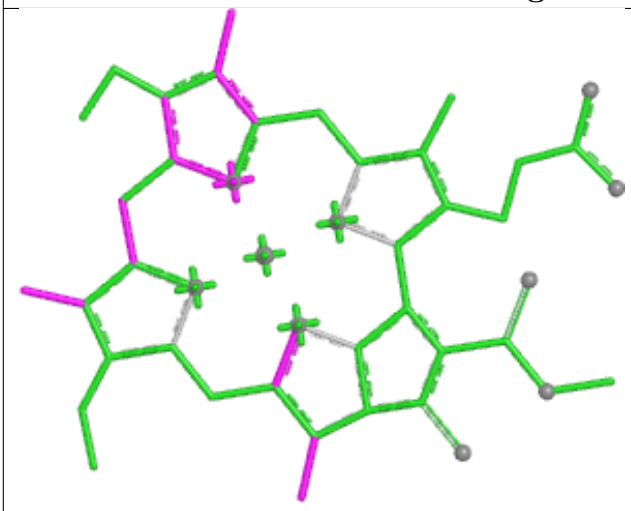


Torsions

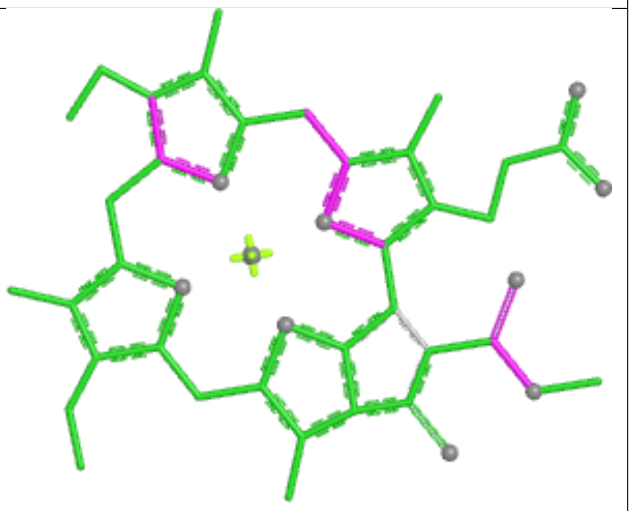


Rings

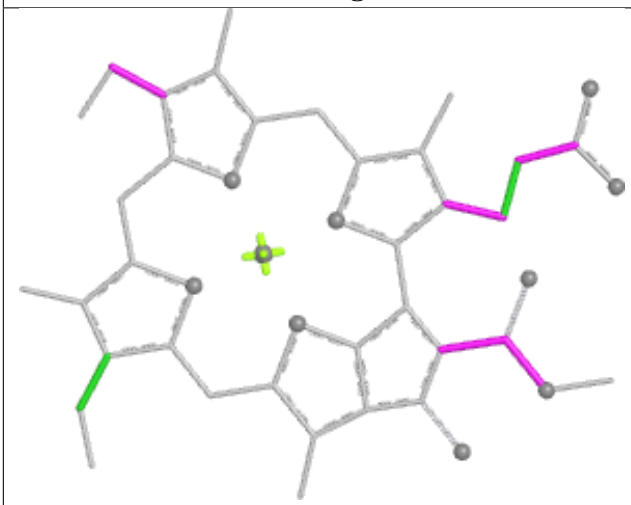
Ligand CLA d 512



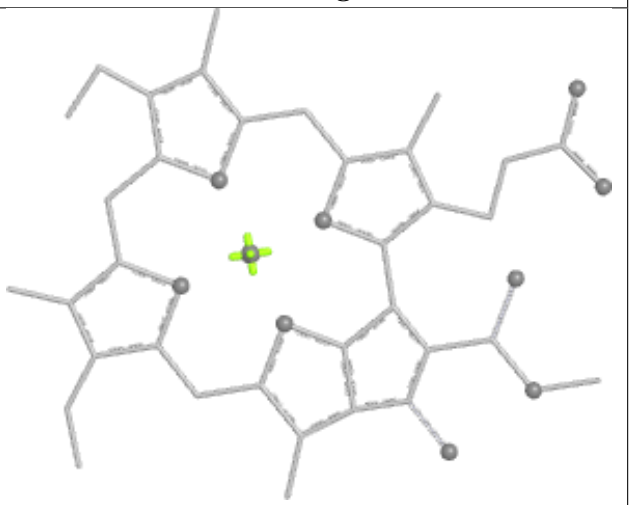
Bond lengths



Bond angles

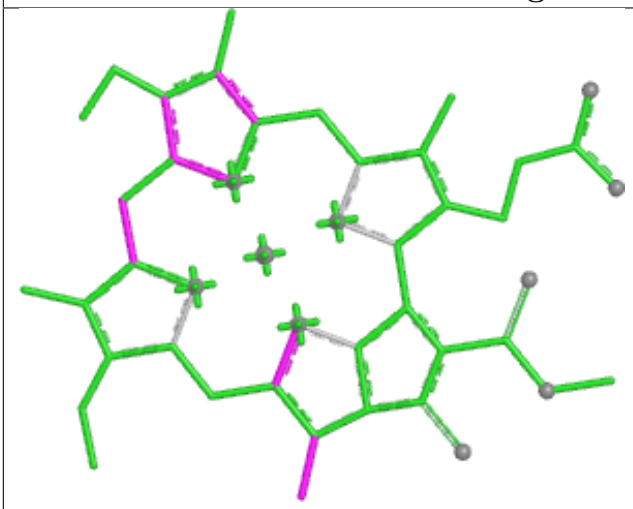


Torsions

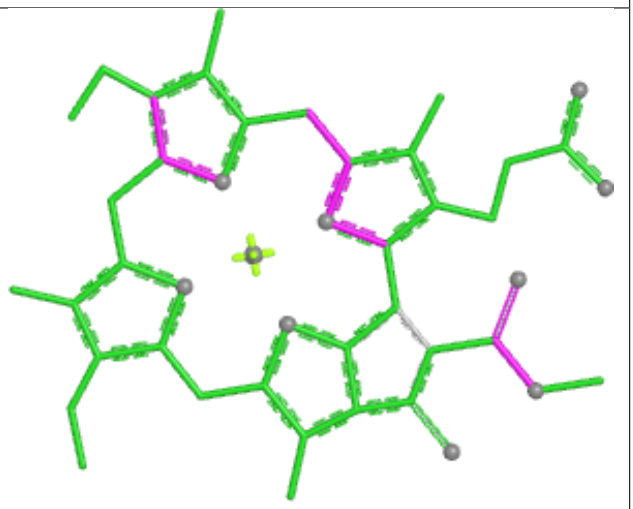


Rings

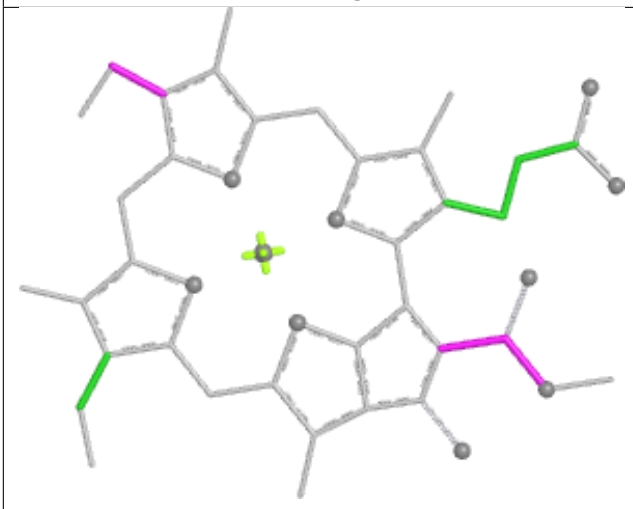
Ligand CLA b 504



Bond lengths



Bond angles

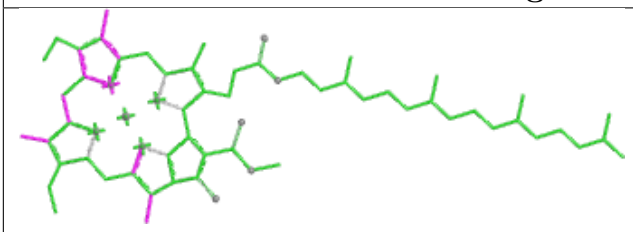


Torsions

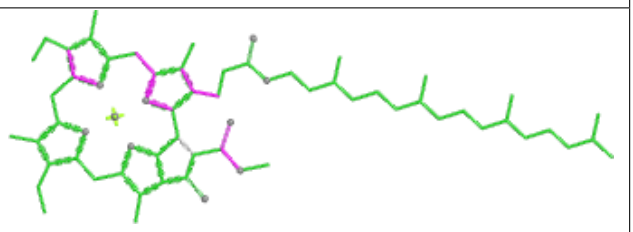


Rings

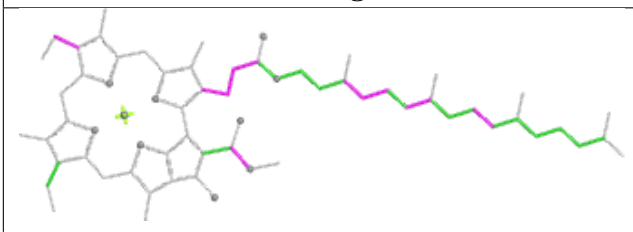
Ligand CLA Z 501



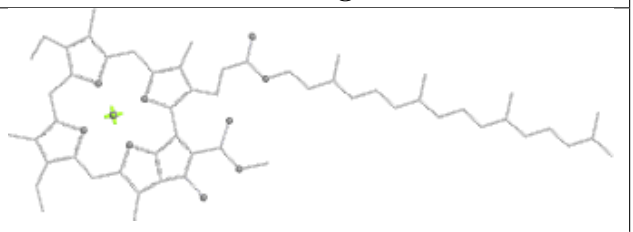
Bond lengths



Bond angles

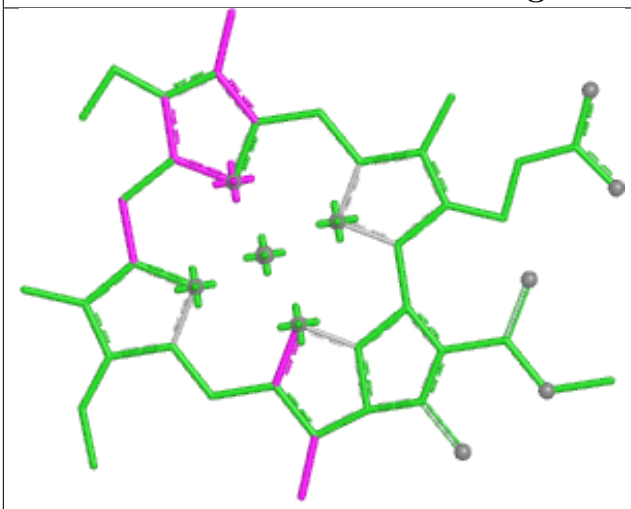


Torsions

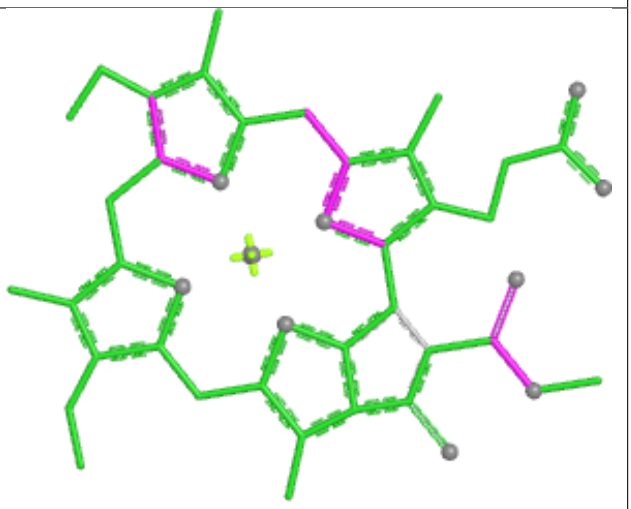


Rings

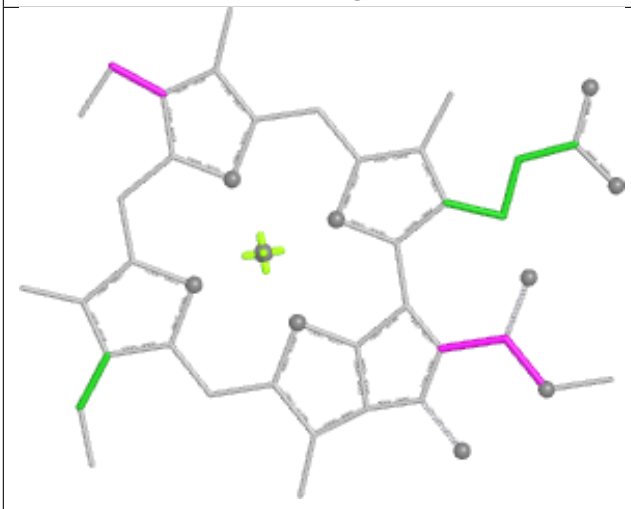
Ligand CLA b 506



Bond lengths



Bond angles

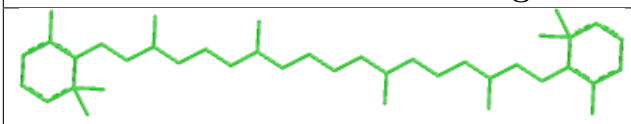


Torsions

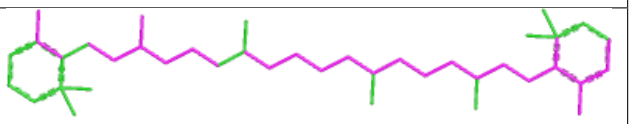


Rings

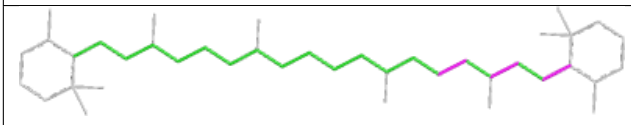
Ligand BCR G 4008



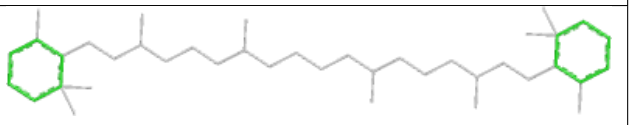
Bond lengths



Bond angles

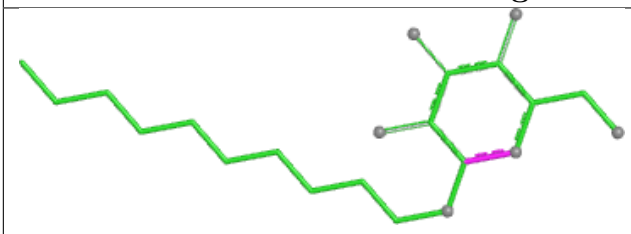


Torsions

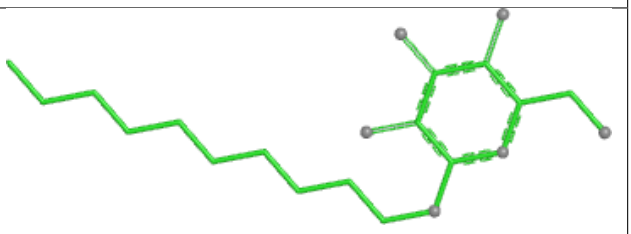


Rings

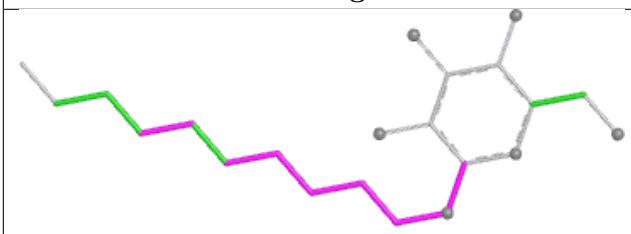
Ligand LMU T 5105



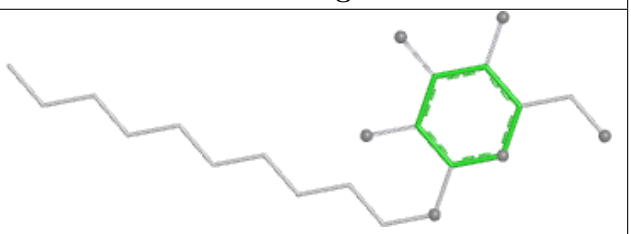
Bond lengths



Bond angles

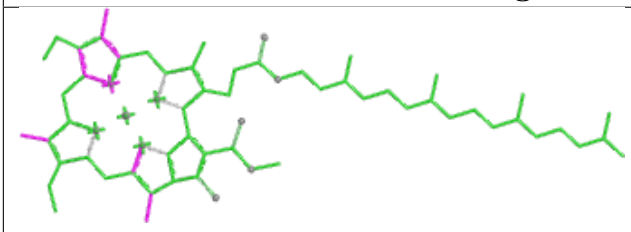


Torsions

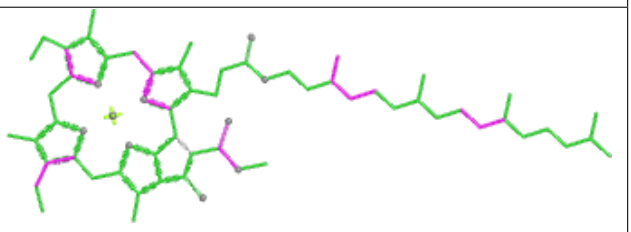


Rings

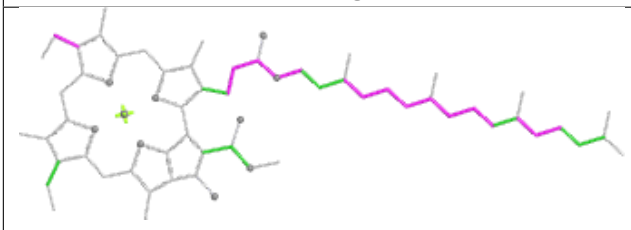
Ligand CLA G 1237



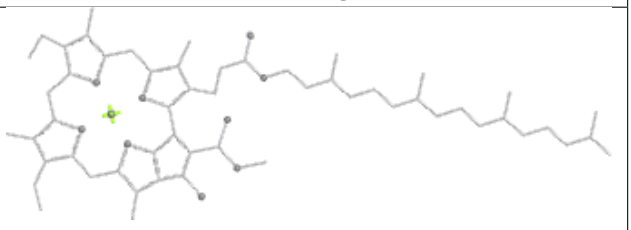
Bond lengths



Bond angles

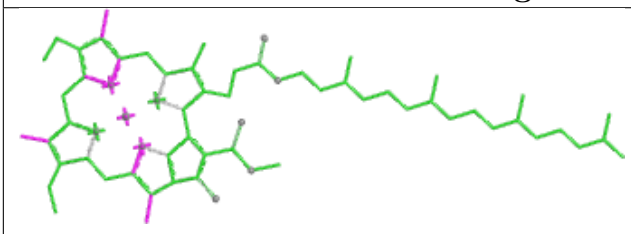


Torsions

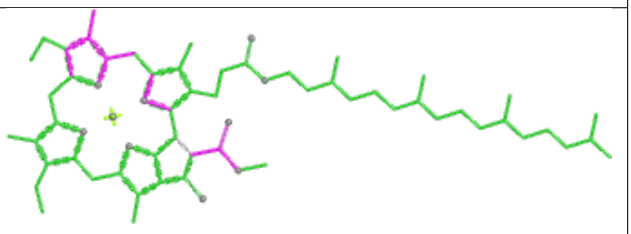


Rings

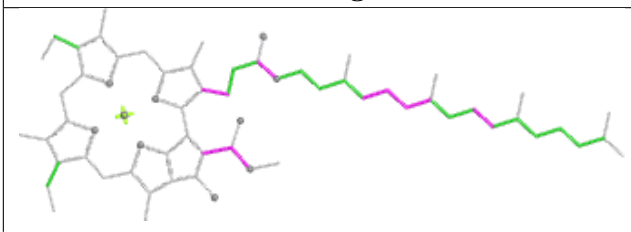
Ligand CLA G 1128



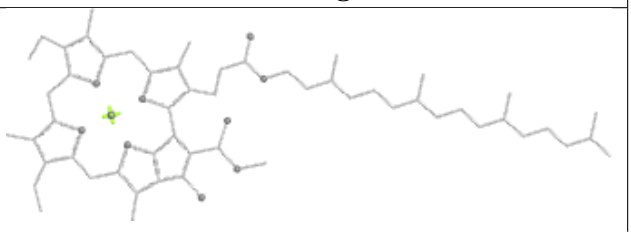
Bond lengths



Bond angles

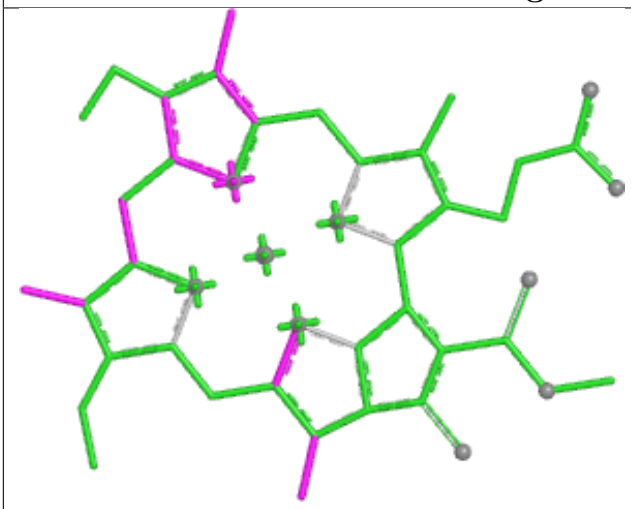


Torsions

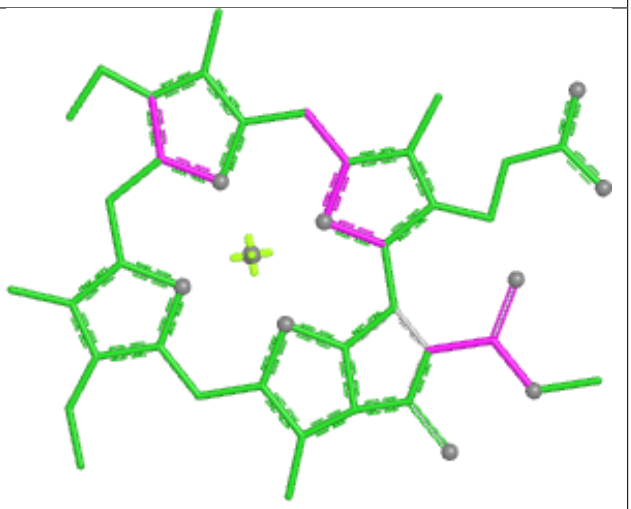


Rings

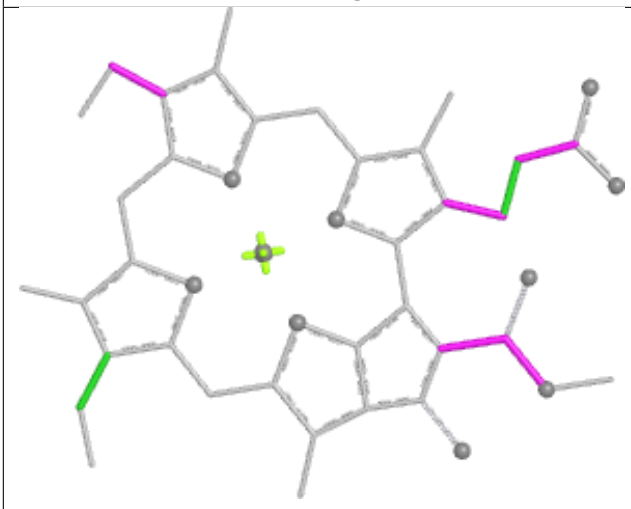
Ligand CLA Z 516



Bond lengths



Bond angles

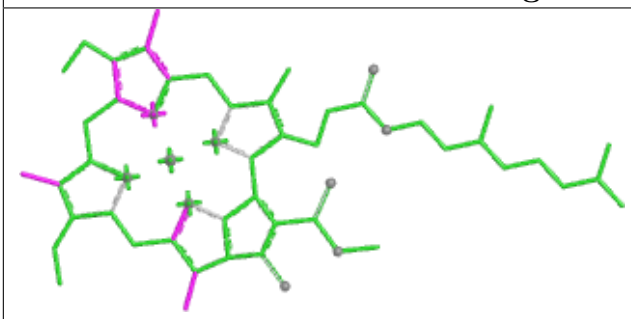


Torsions

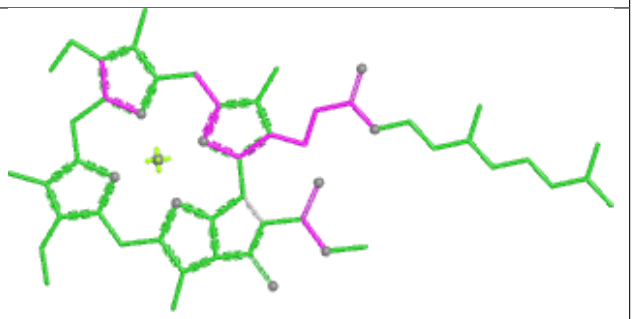


Rings

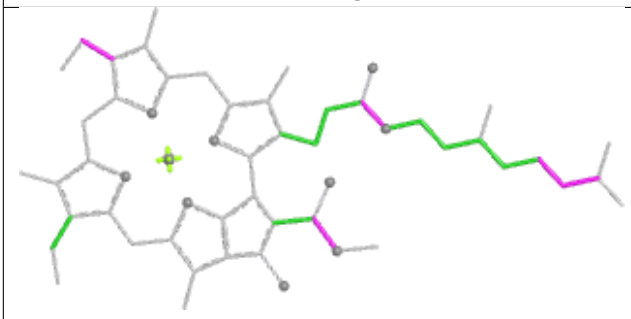
Ligand CLA f 1220



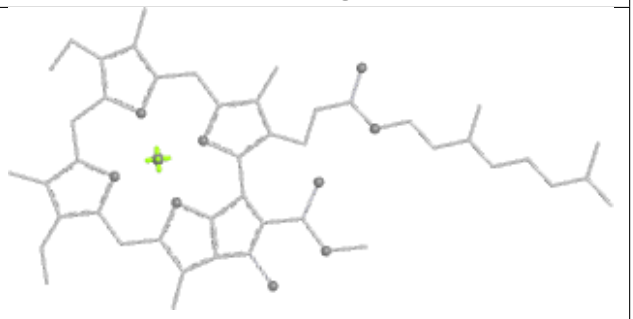
Bond lengths



Bond angles

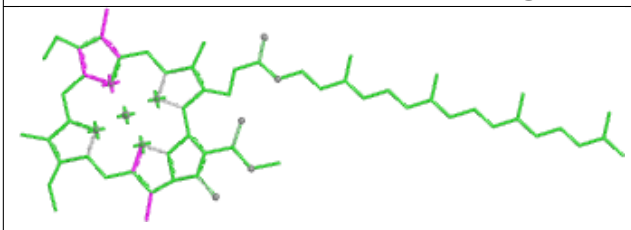


Torsions

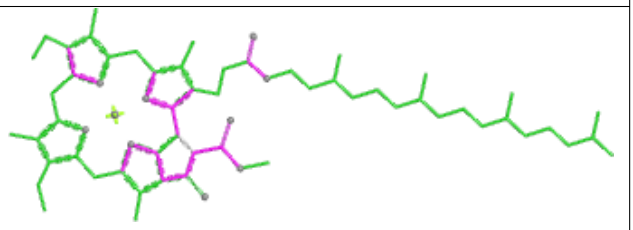


Rings

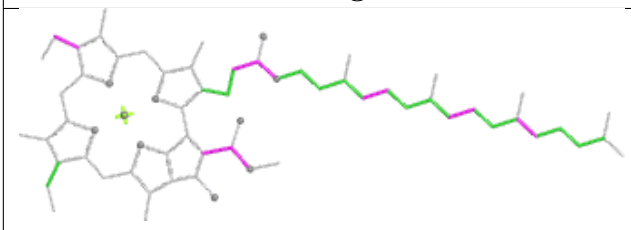
Ligand CLA e 1011



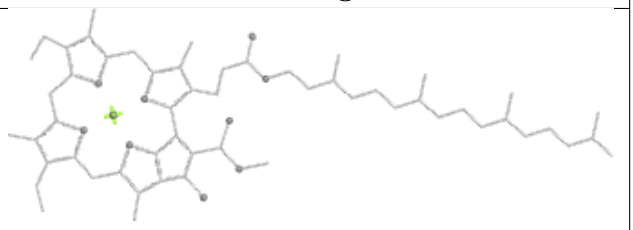
Bond lengths



Bond angles

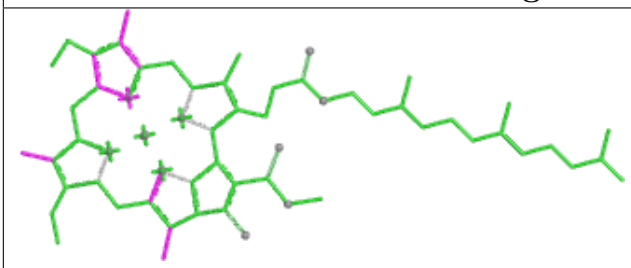


Torsions

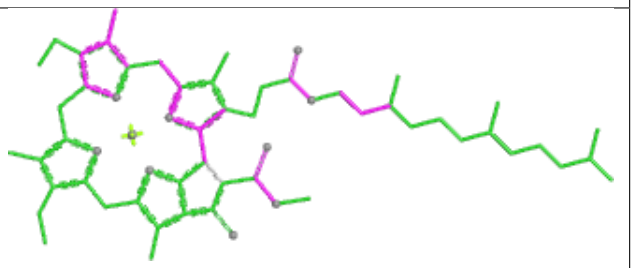


Rings

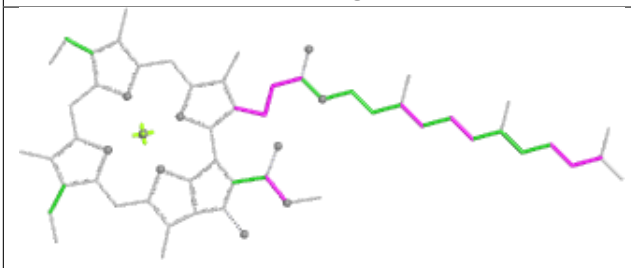
Ligand CLA f 1224



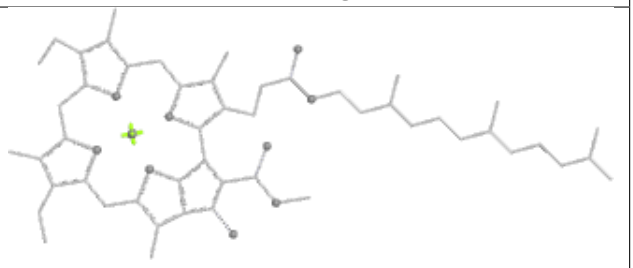
Bond lengths



Bond angles

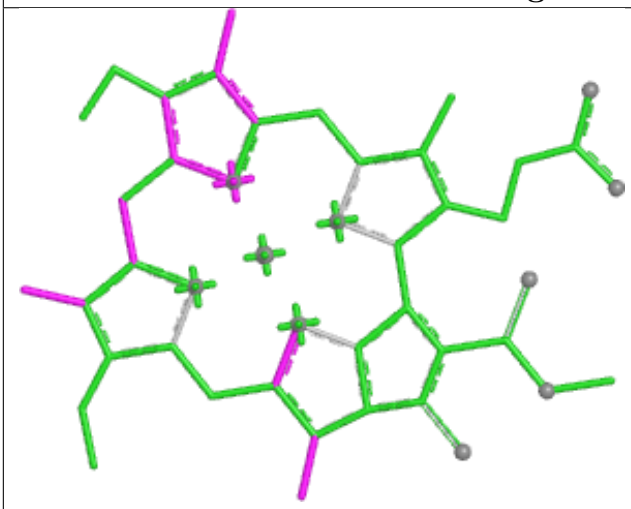


Torsions

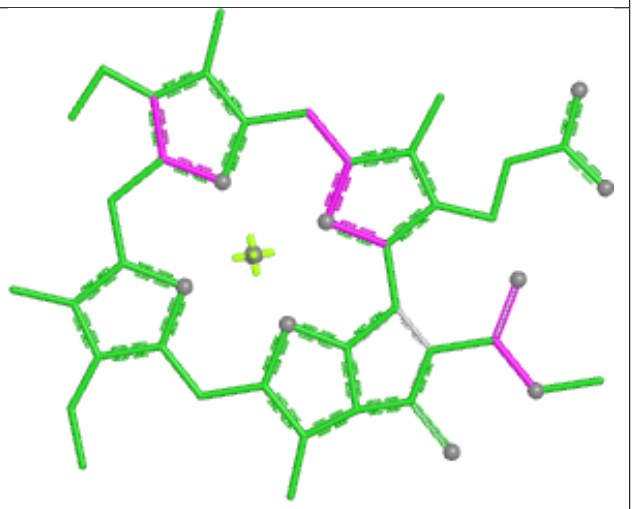


Rings

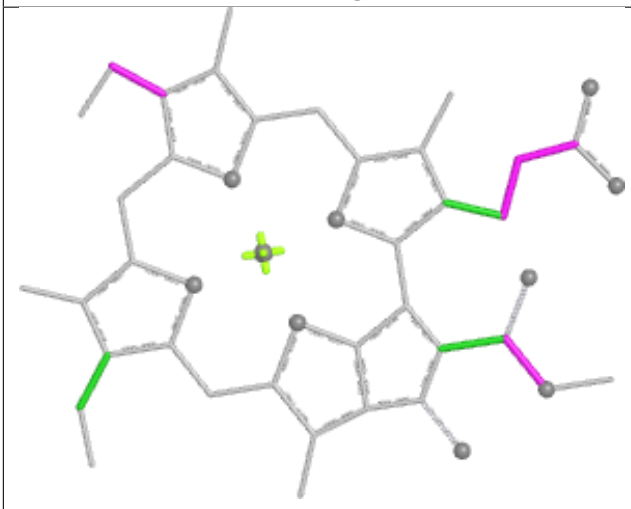
Ligand CLA b 513



Bond lengths



Bond angles

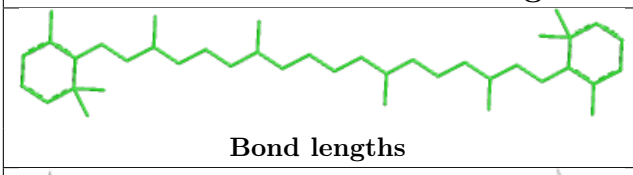


Torsions

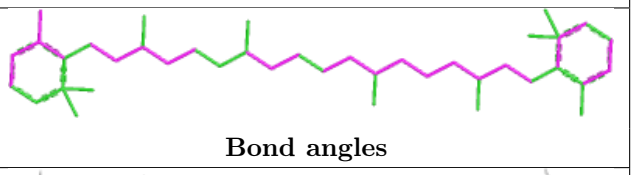


Rings

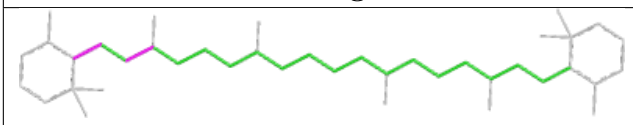
Ligand BCR Z 521



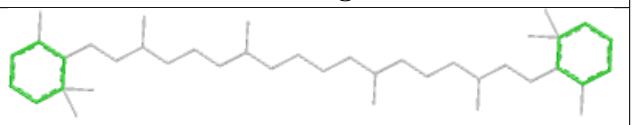
Bond lengths



Bond angles

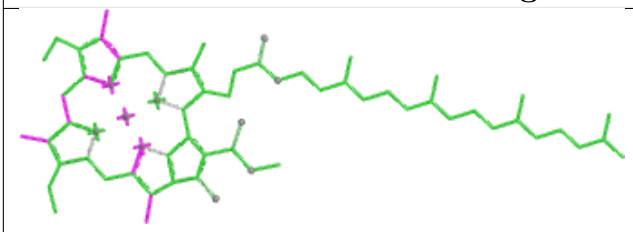


Torsions

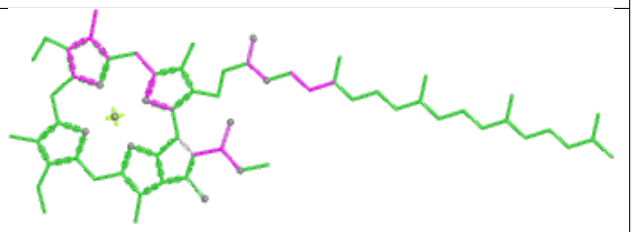


Rings

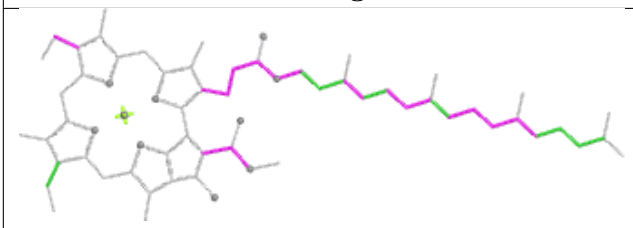
Ligand CLA e 1106



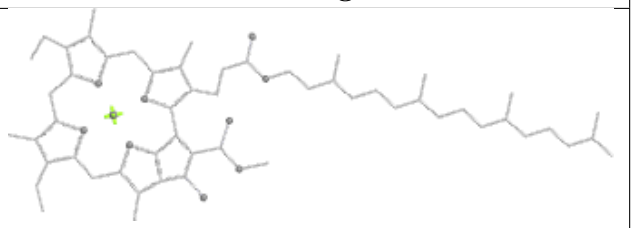
Bond lengths



Bond angles

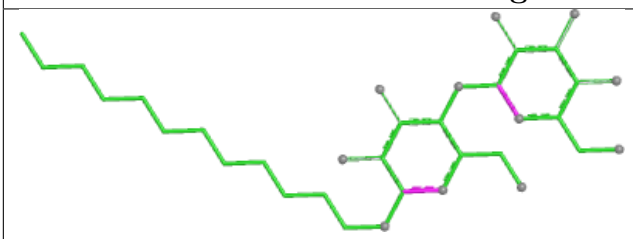


Torsions

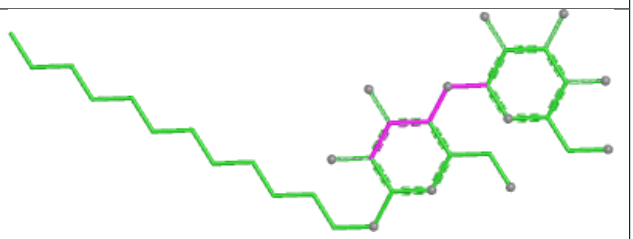


Rings

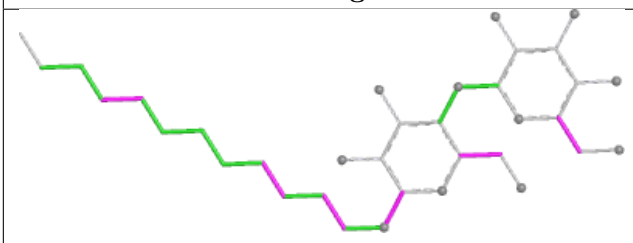
Ligand LMU G 1848



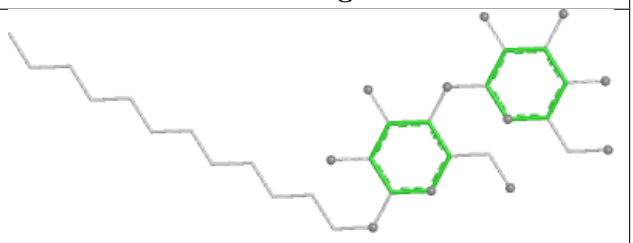
Bond lengths



Bond angles

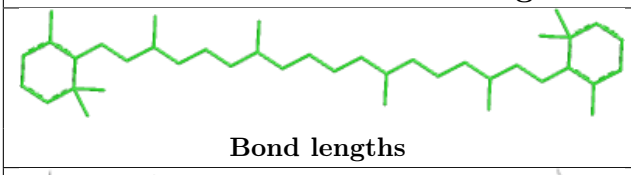


Torsions

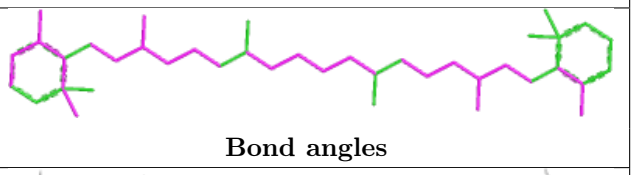


Rings

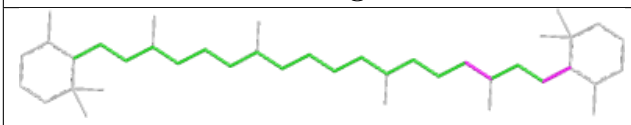
Ligand BCR L 4020



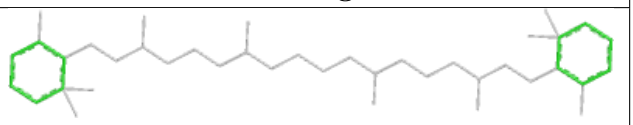
Bond lengths



Bond angles

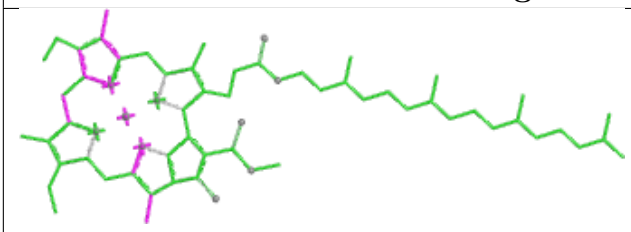


Torsions

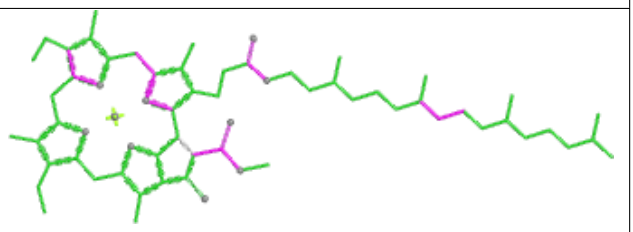


Rings

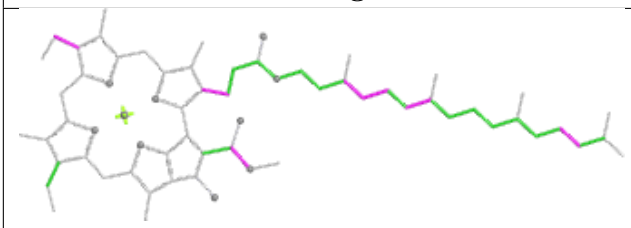
Ligand CLA G 1139



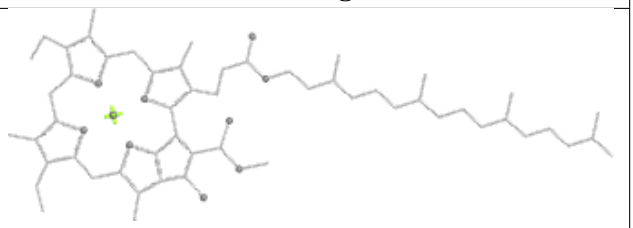
Bond lengths



Bond angles

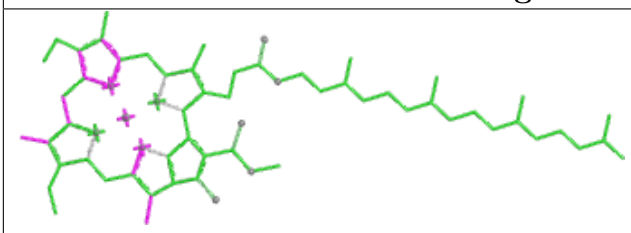


Torsions

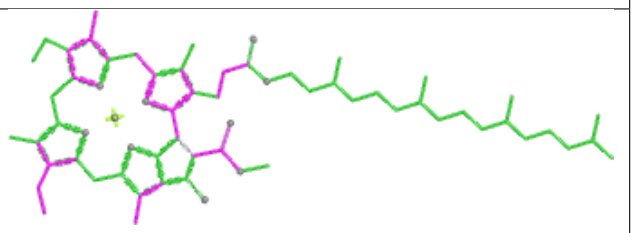


Rings

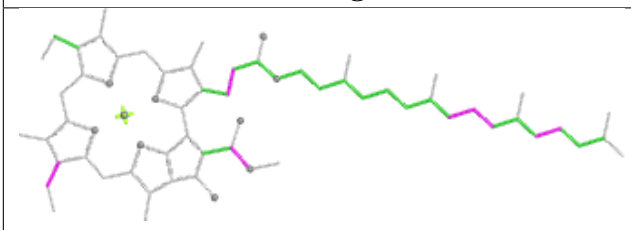
Ligand CLA H 1023



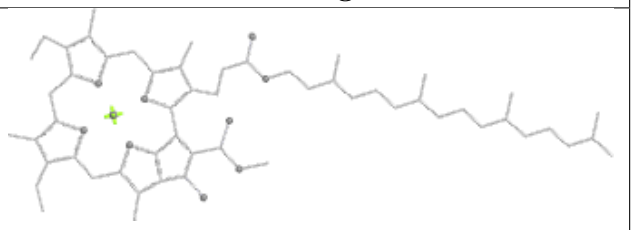
Bond lengths



Bond angles

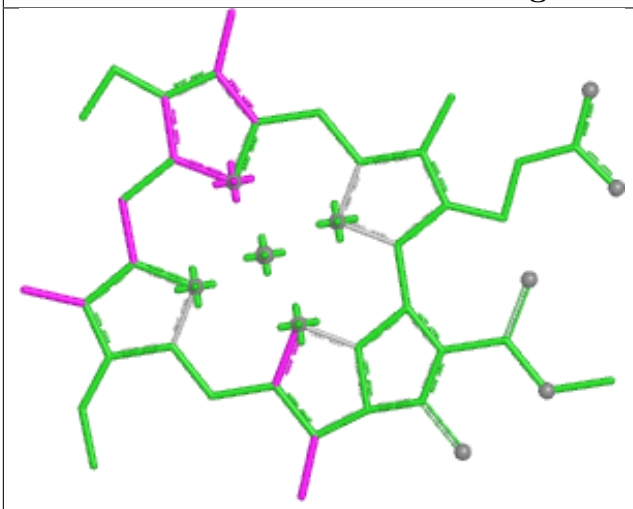


Torsions

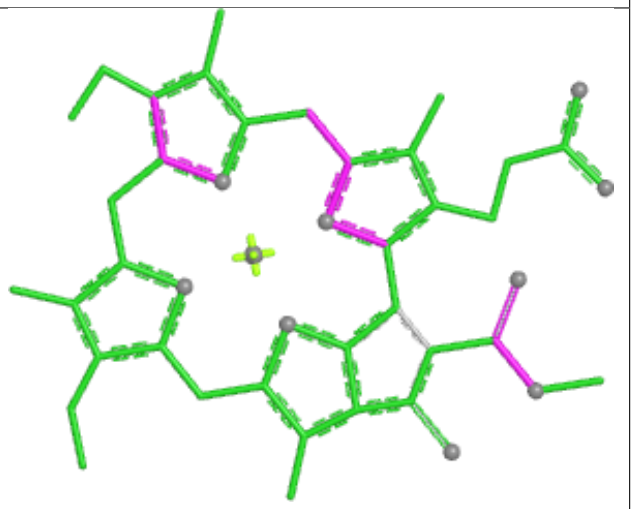


Rings

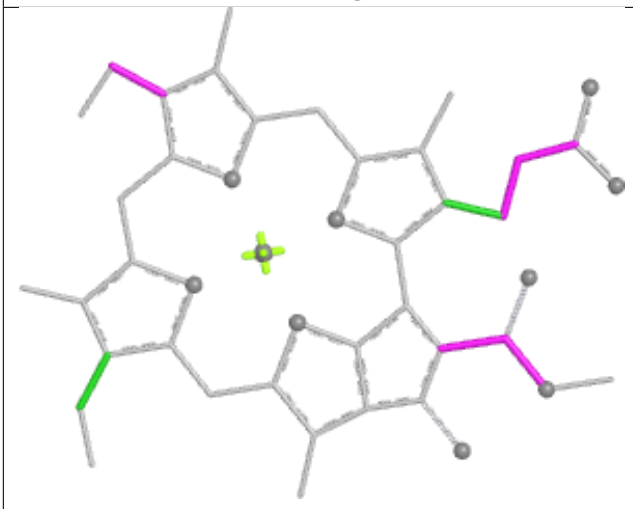
Ligand CLA c 517



Bond lengths



Bond angles

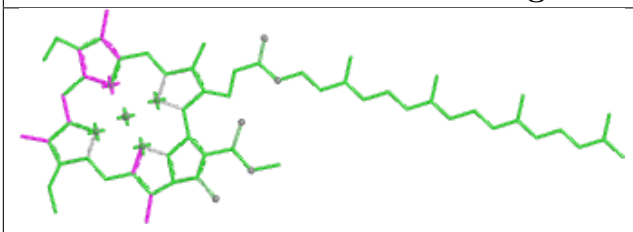


Torsions

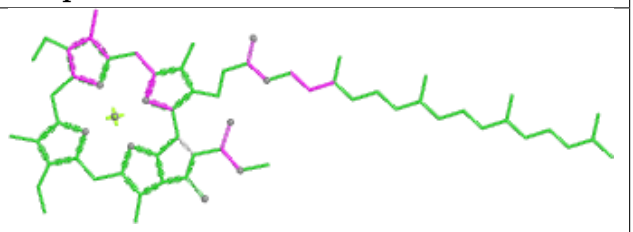


Rings

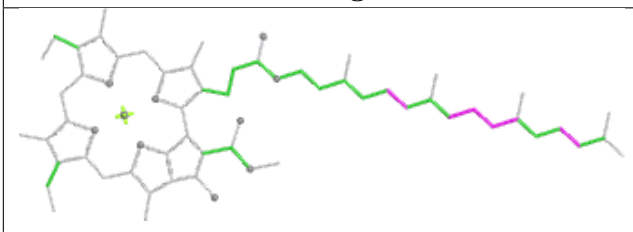
Ligand CLA q 509



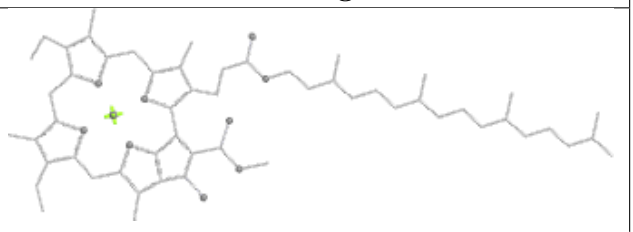
Bond lengths



Bond angles

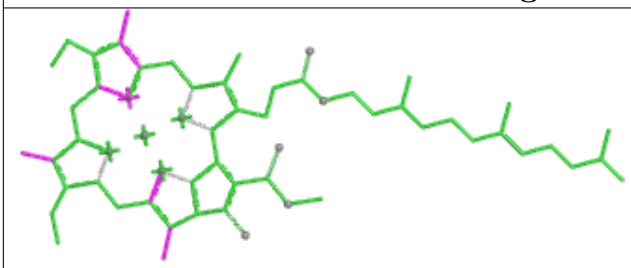


Torsions

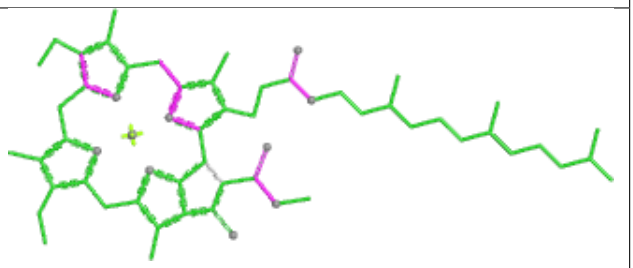


Rings

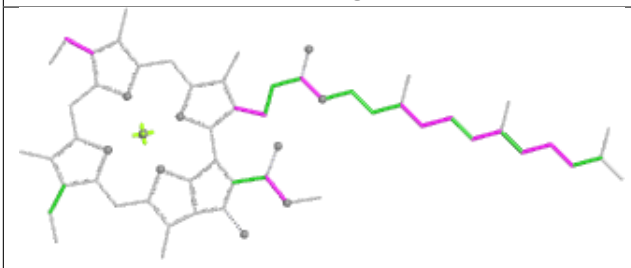
Ligand CLA e 1122



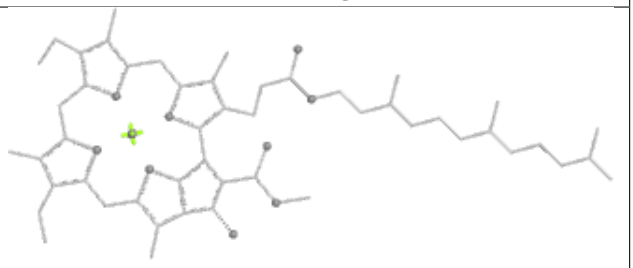
Bond lengths



Bond angles

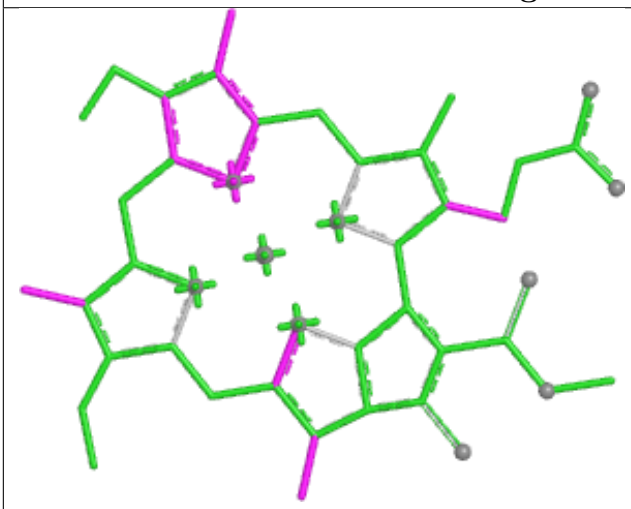


Torsions

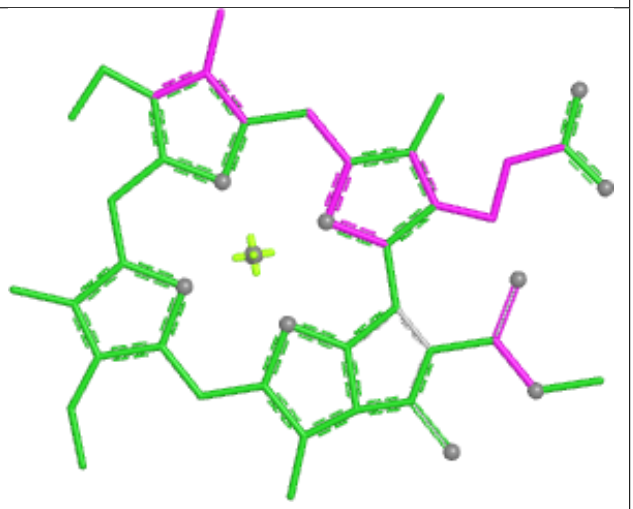


Rings

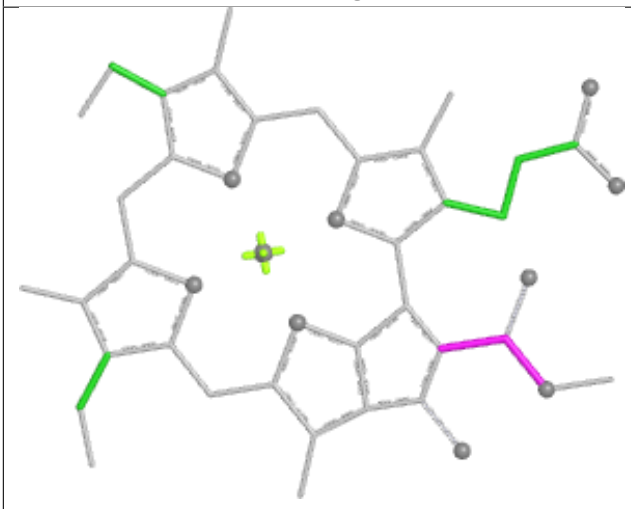
Ligand CLA e 1801



Bond lengths



Bond angles

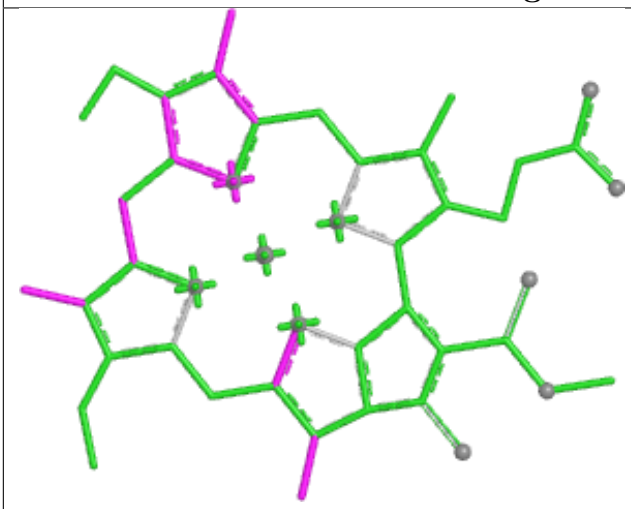


Torsions

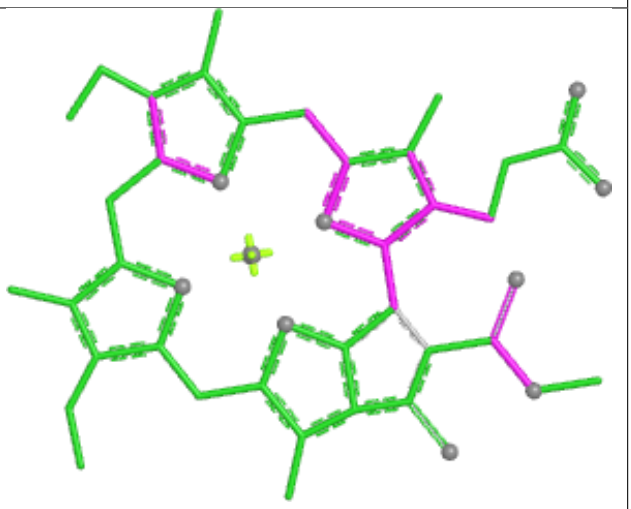


Rings

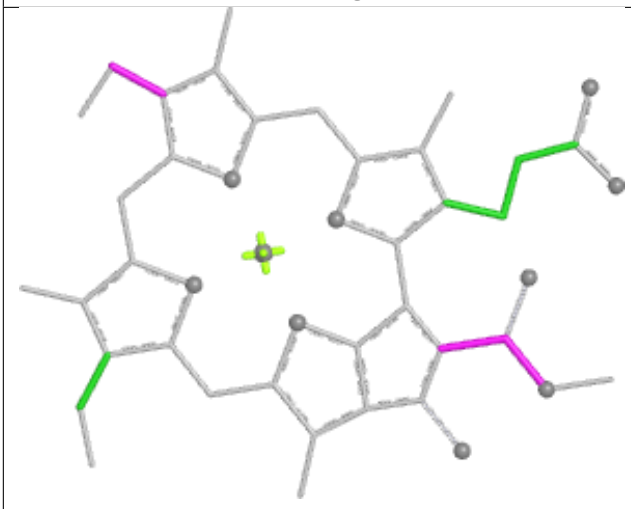
Ligand CLA Y 504



Bond lengths



Bond angles

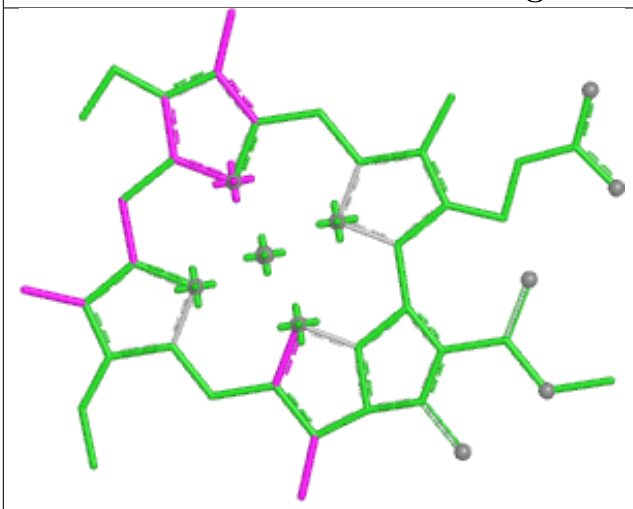


Torsions

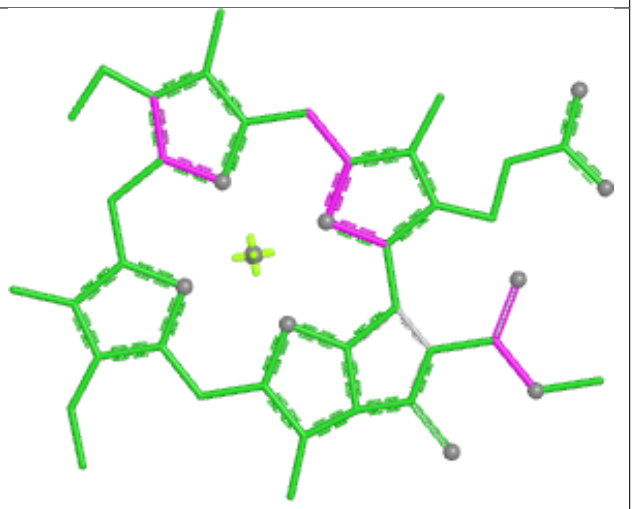


Rings

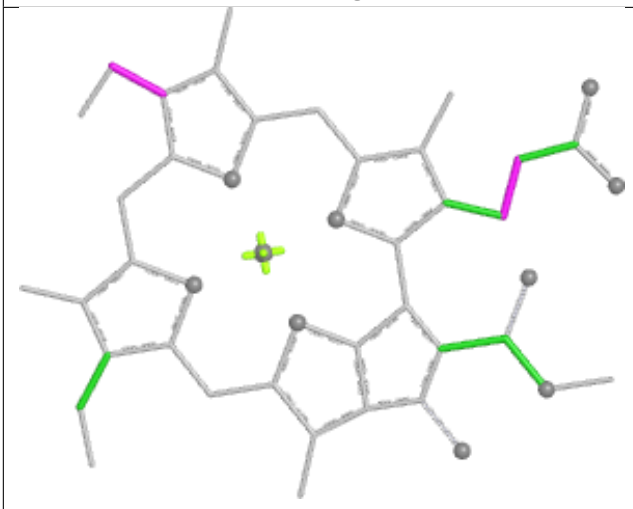
Ligand CLA Z 517



Bond lengths



Bond angles

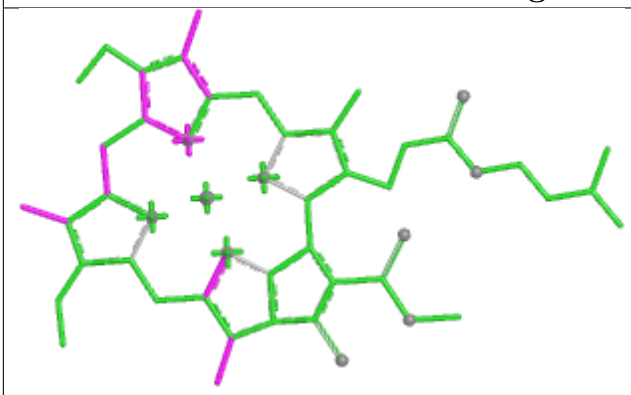


Torsions

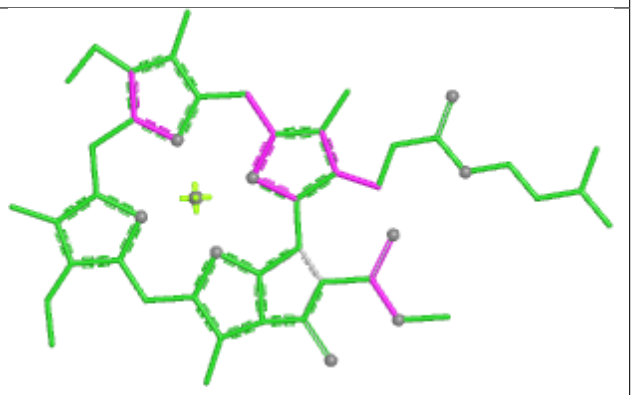


Rings

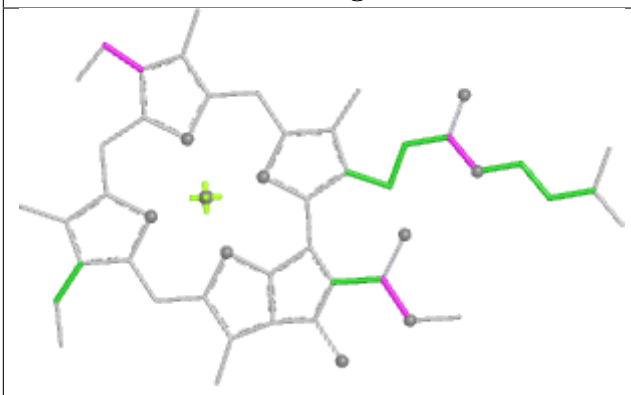
Ligand CLA 5 502



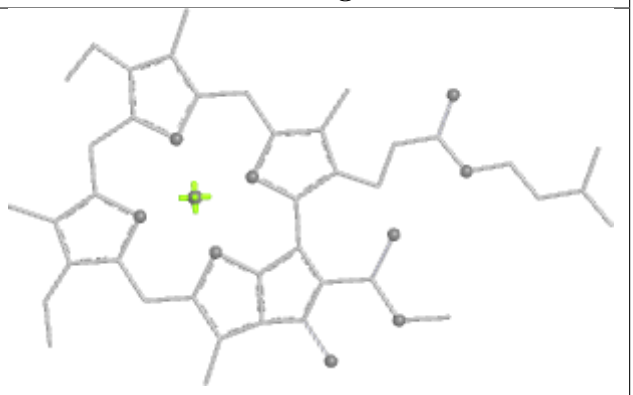
Bond lengths



Bond angles

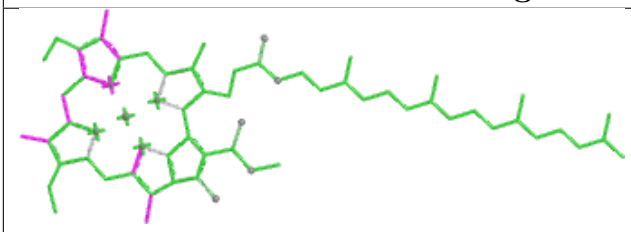


Torsions

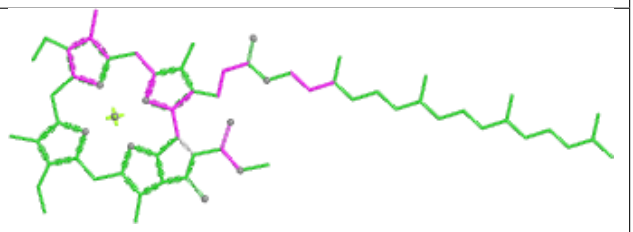


Rings

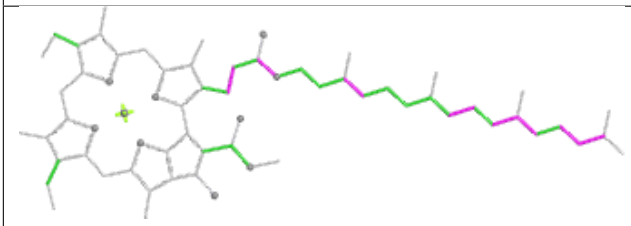
Ligand CLA G 1127



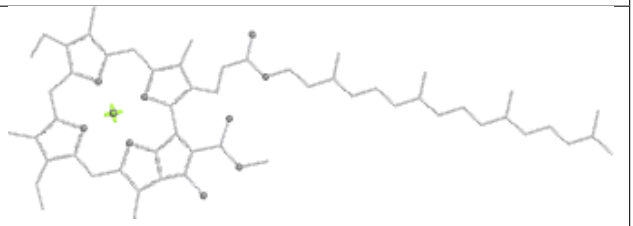
Bond lengths



Bond angles

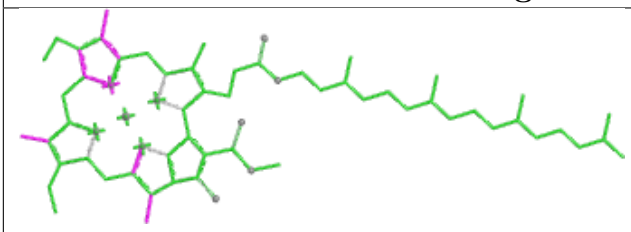


Torsions

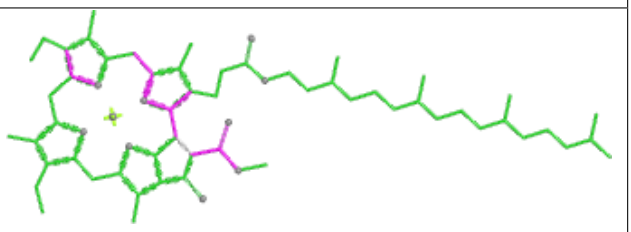


Rings

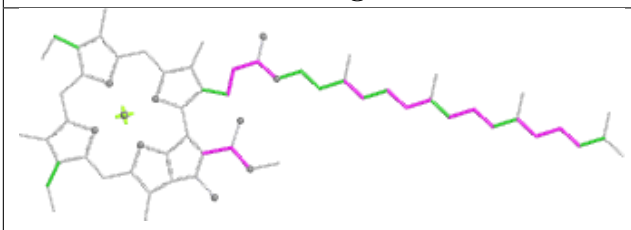
Ligand CLA A 1137



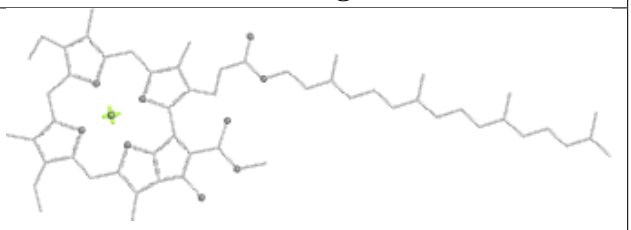
Bond lengths



Bond angles

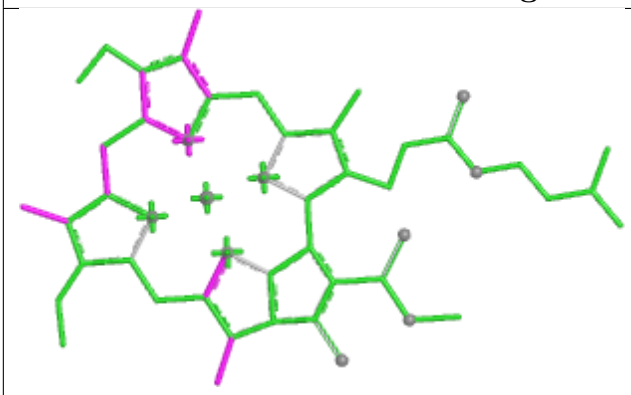


Torsions

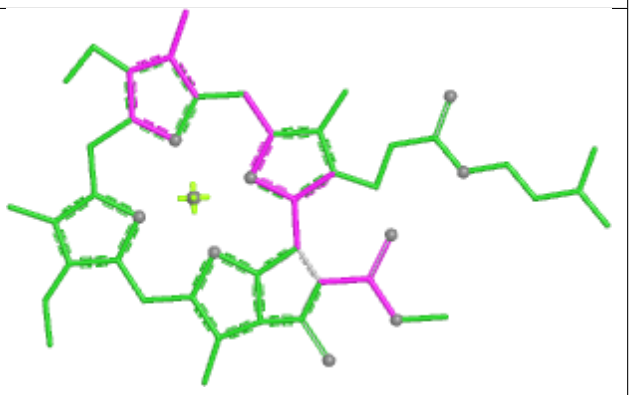


Rings

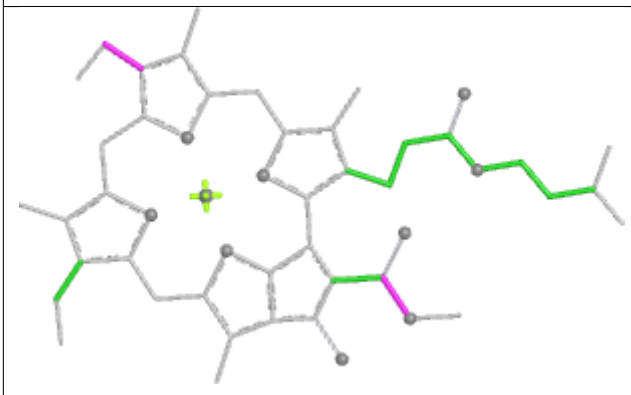
Ligand CLA e 1112



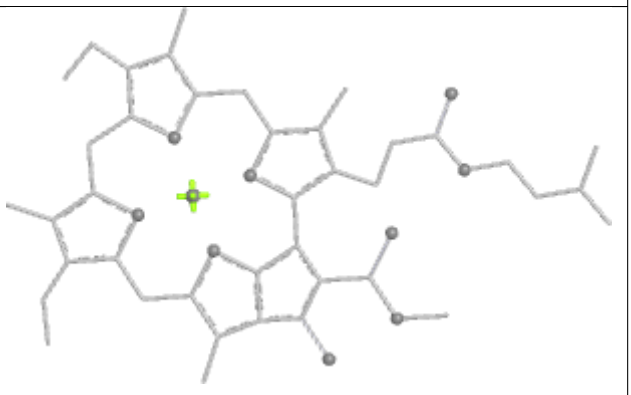
Bond lengths



Bond angles

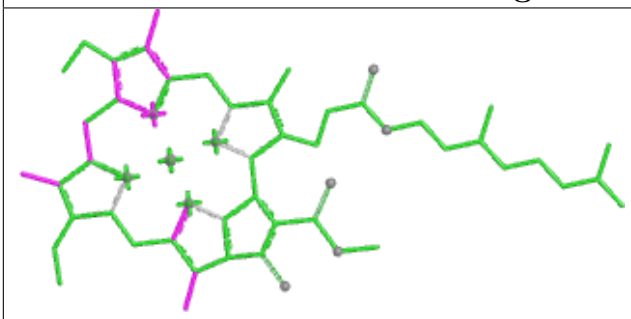


Torsions

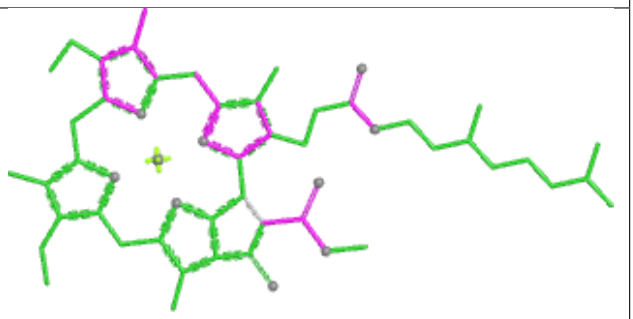


Rings

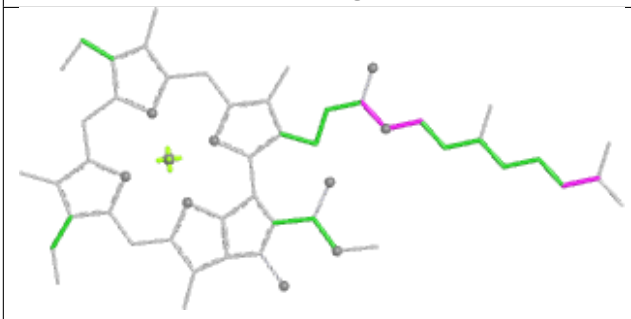
Ligand CLA G 1105



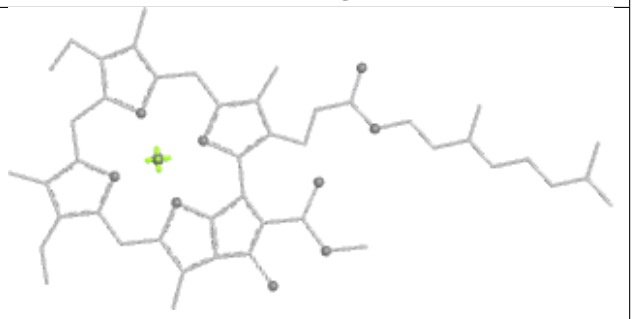
Bond lengths



Bond angles

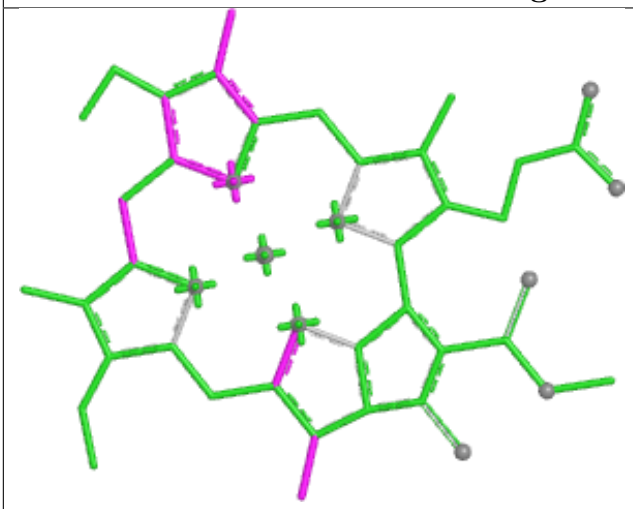


Torsions

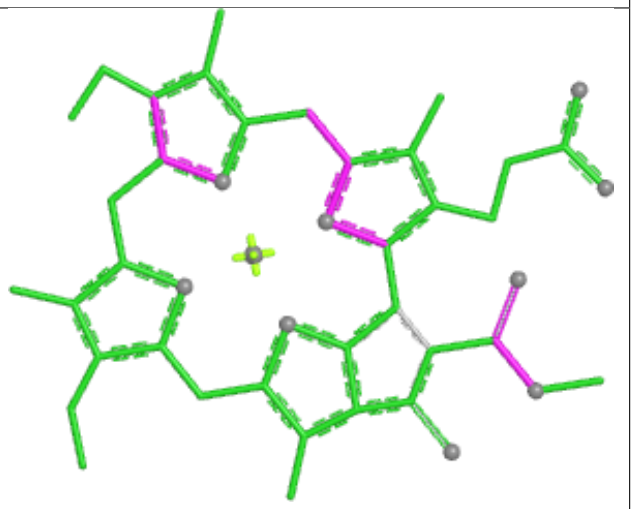


Rings

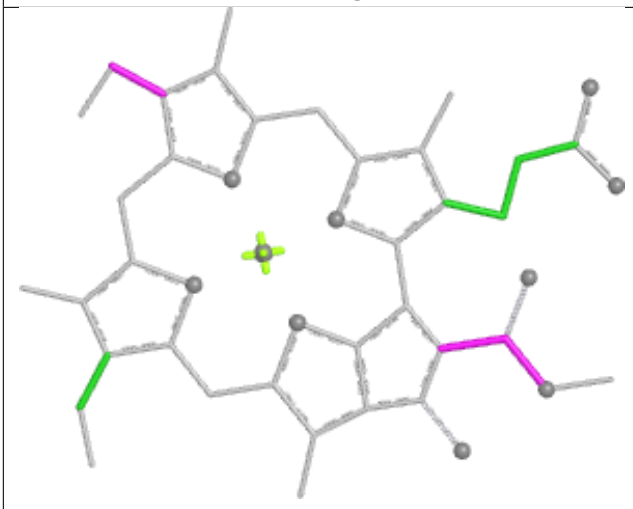
Ligand CLA t 506



Bond lengths



Bond angles

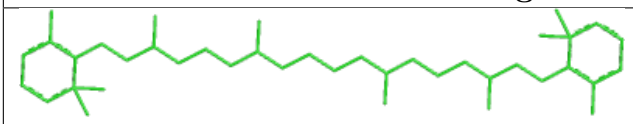


Torsions

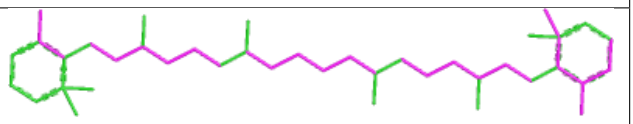


Rings

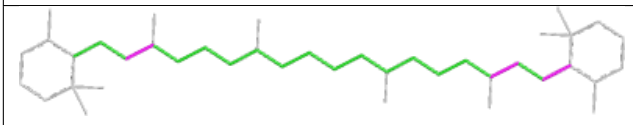
Ligand BCR L 4019



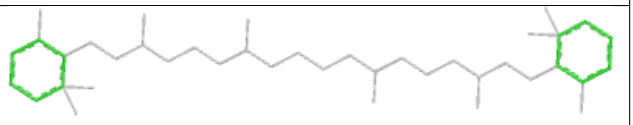
Bond lengths



Bond angles

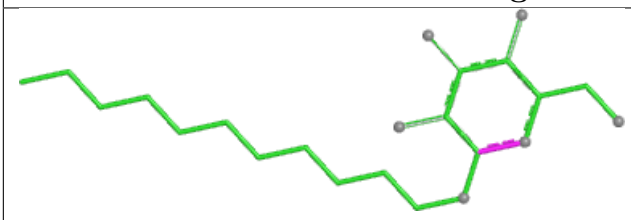


Torsions

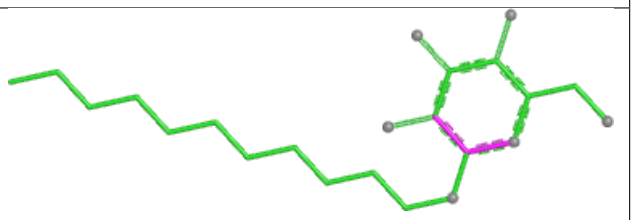


Rings

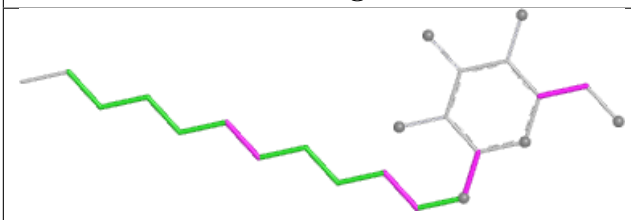
Ligand LMU G 1849



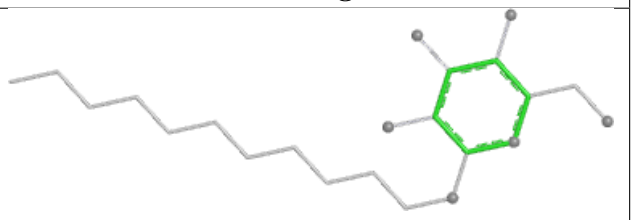
Bond lengths



Bond angles

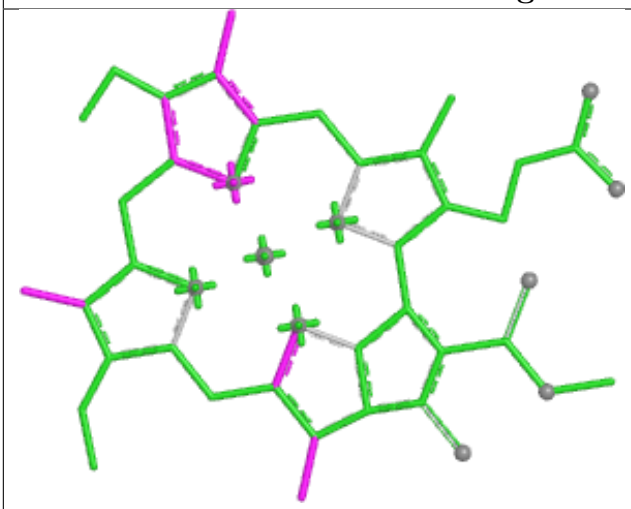


Torsions

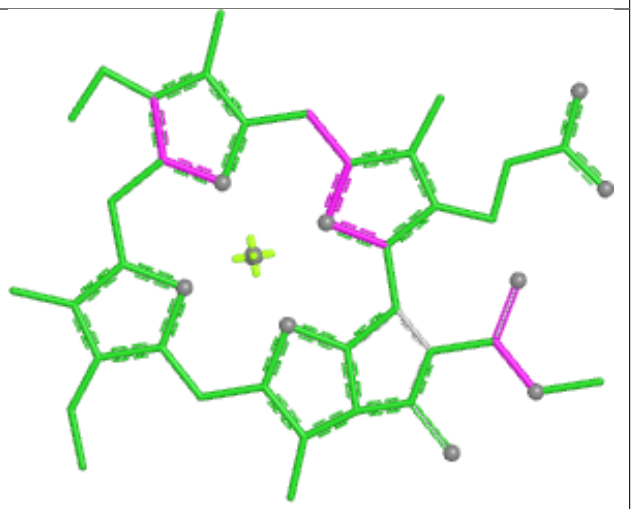


Rings

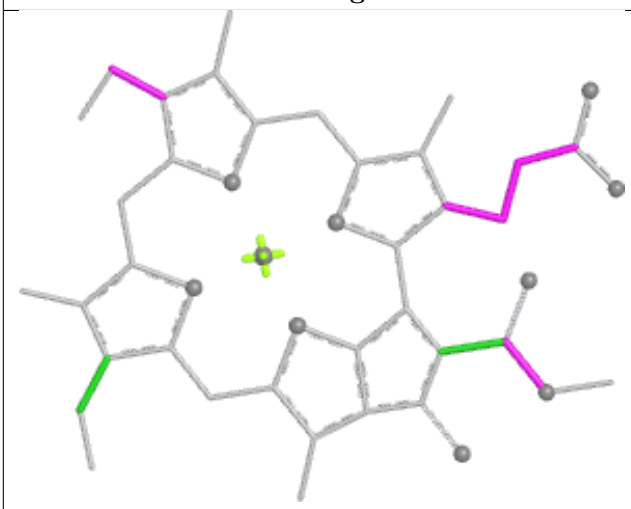
Ligand CLA F 1302



Bond lengths



Bond angles

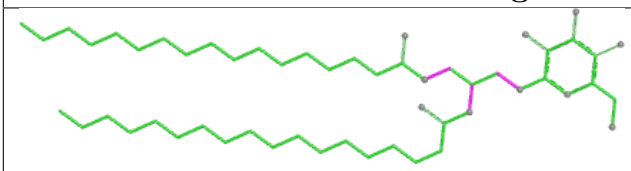


Torsions

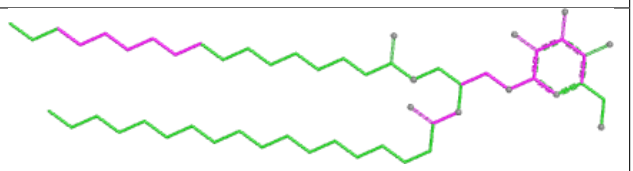


Rings

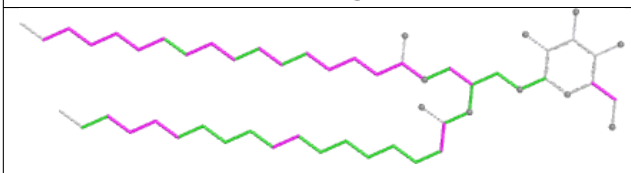
Ligand LMG B 5002



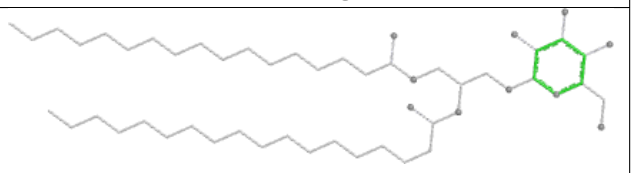
Bond lengths



Bond angles

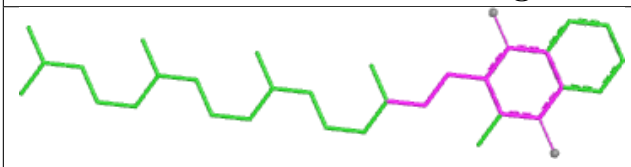


Torsions

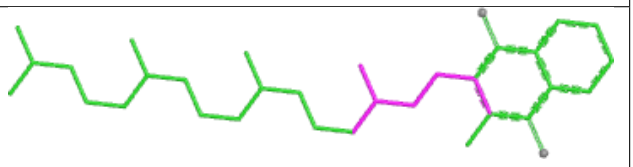


Rings

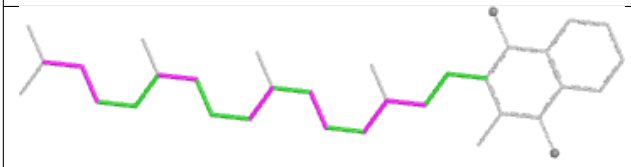
Ligand PQN B 2002



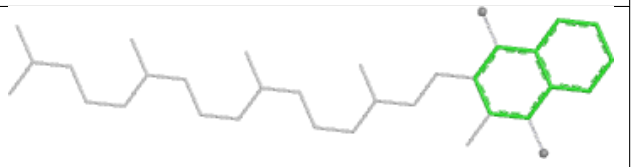
Bond lengths



Bond angles

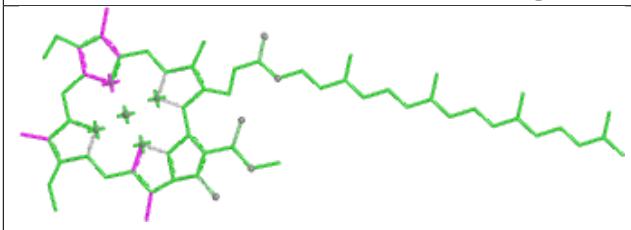


Torsions

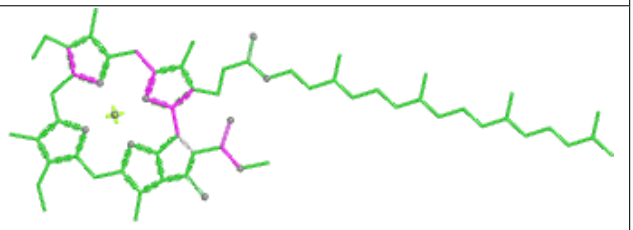


Rings

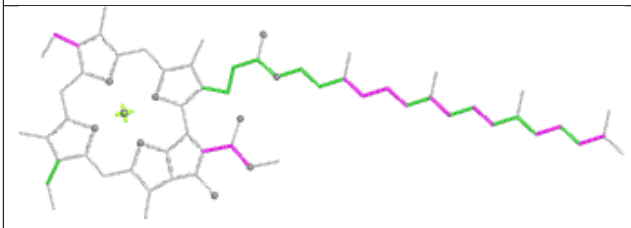
Ligand CLA r 507



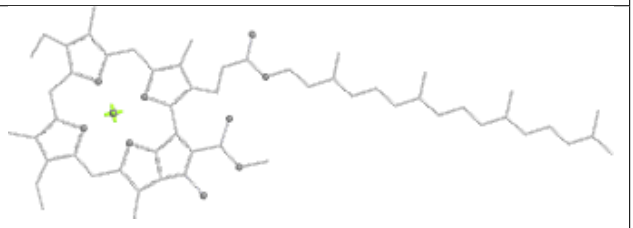
Bond lengths



Bond angles

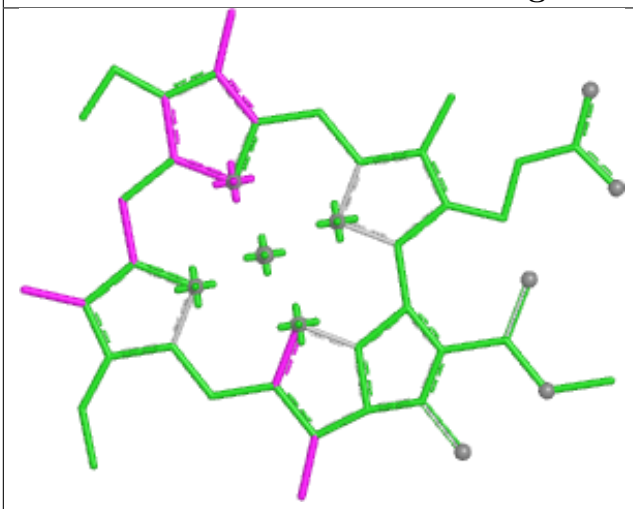


Torsions

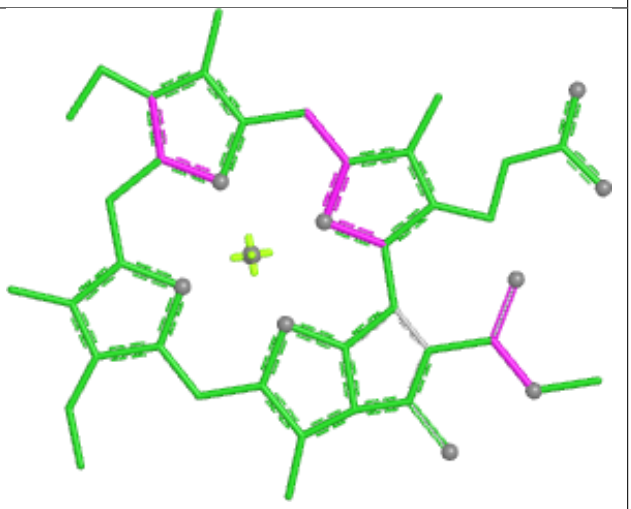


Rings

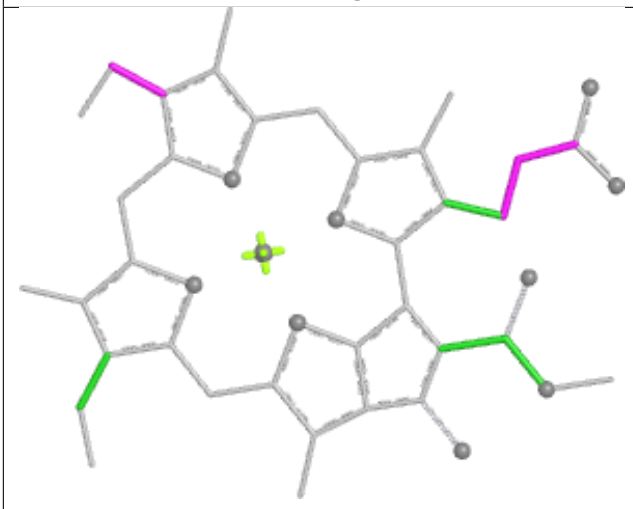
Ligand CLA 1 517



Bond lengths



Bond angles

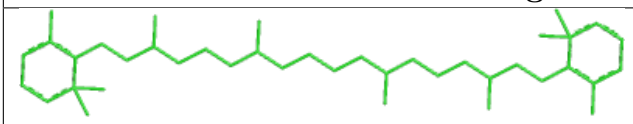


Torsions

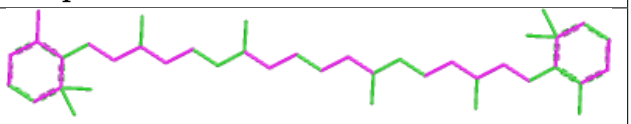


Rings

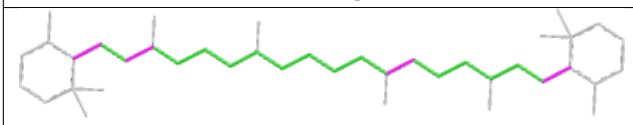
Ligand BCR q 521



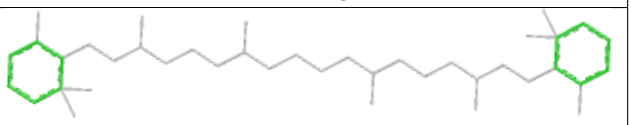
Bond lengths



Bond angles

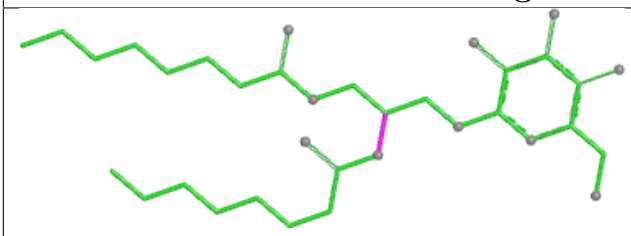


Torsions

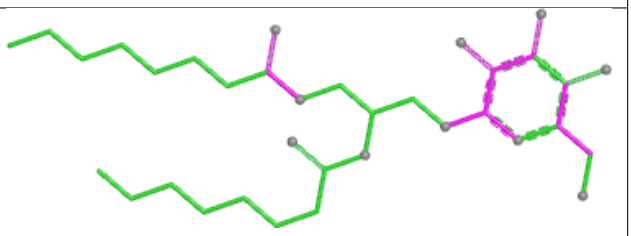


Rings

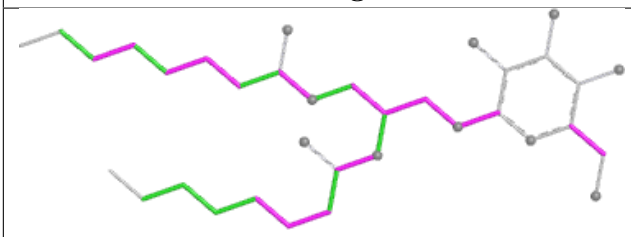
Ligand LMG J 5104



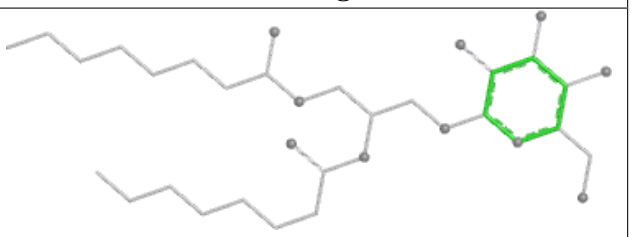
Bond lengths



Bond angles

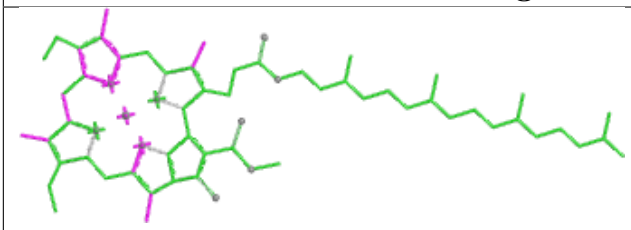


Torsions

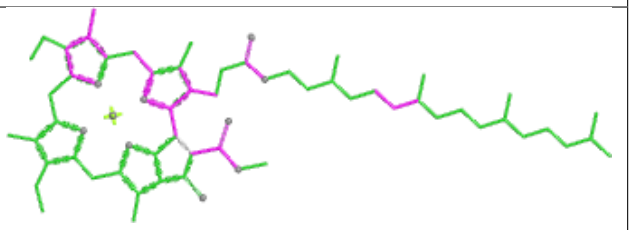


Rings

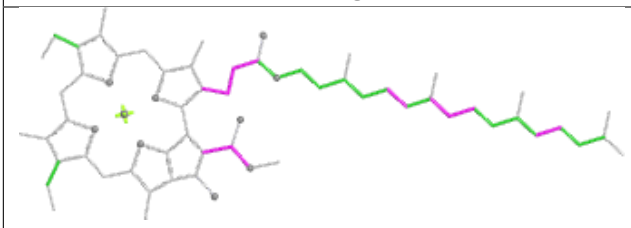
Ligand CLA B 1221



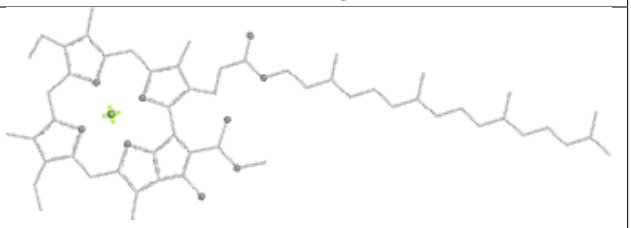
Bond lengths



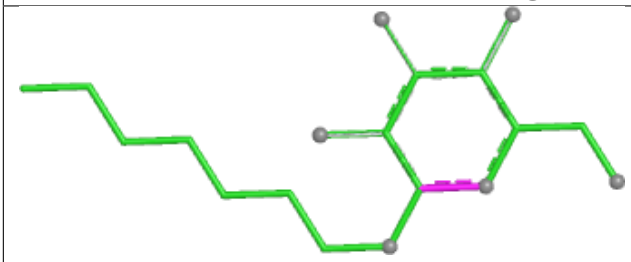
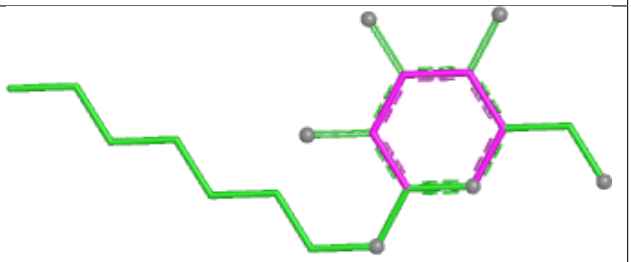
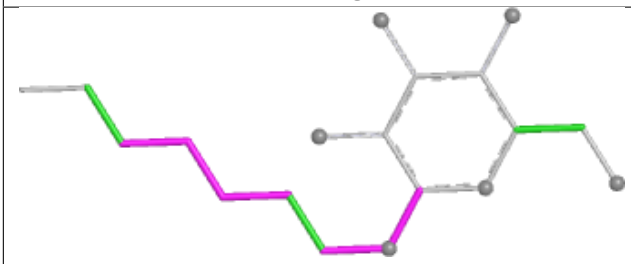
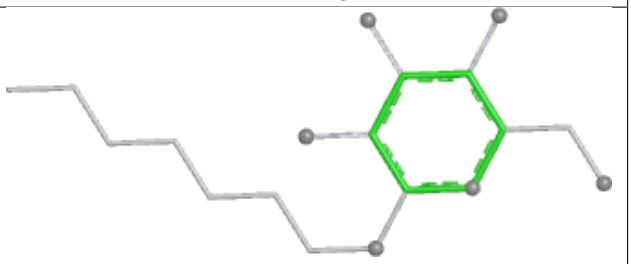
Bond angles

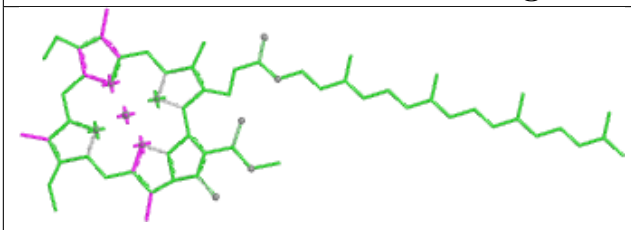
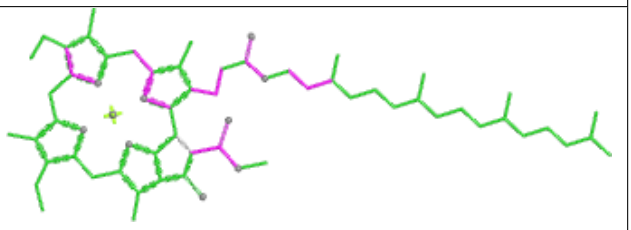
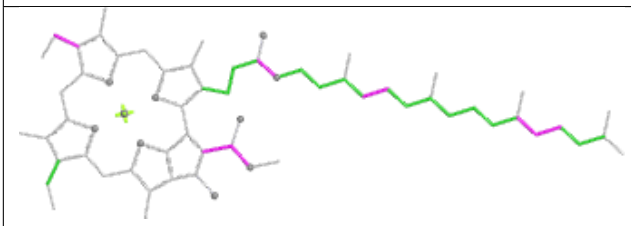
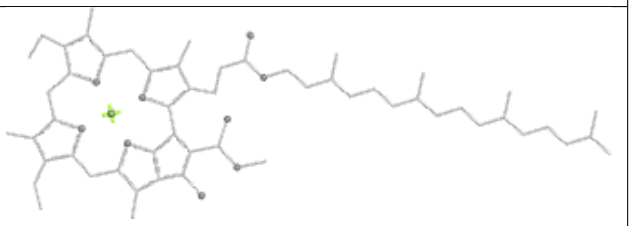


Torsions

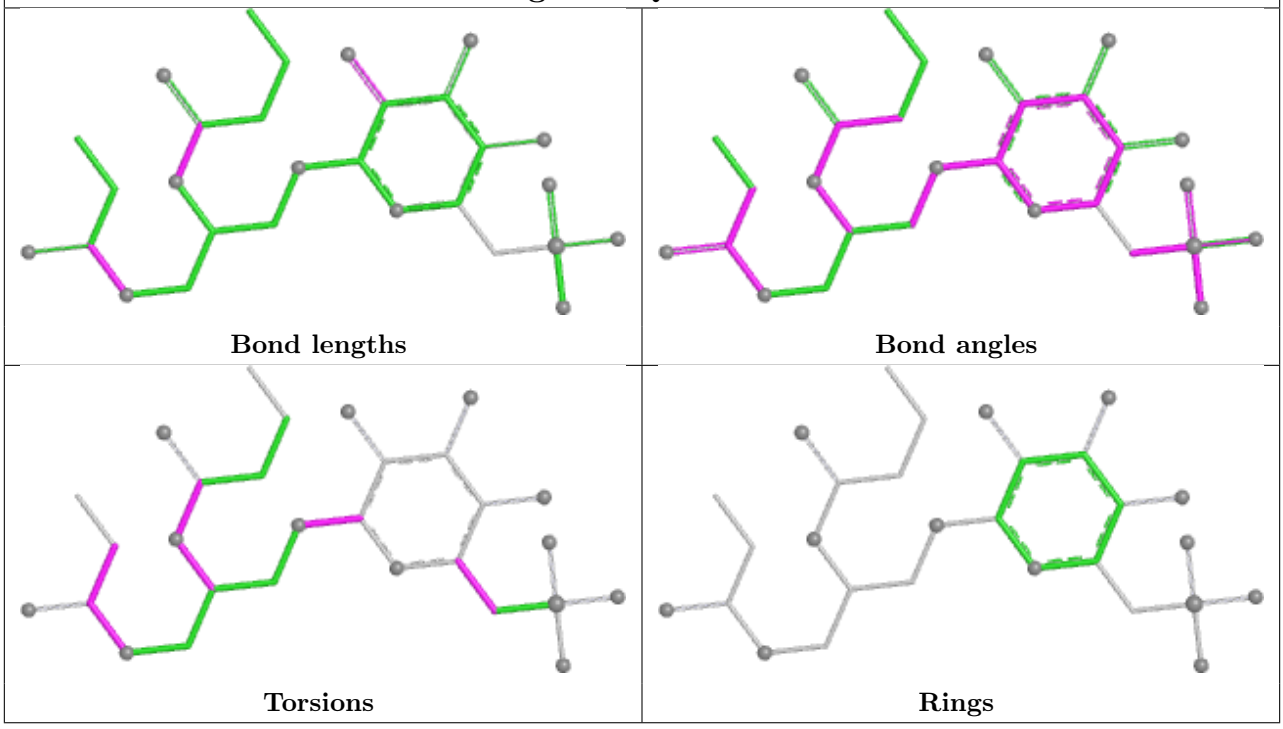


Rings

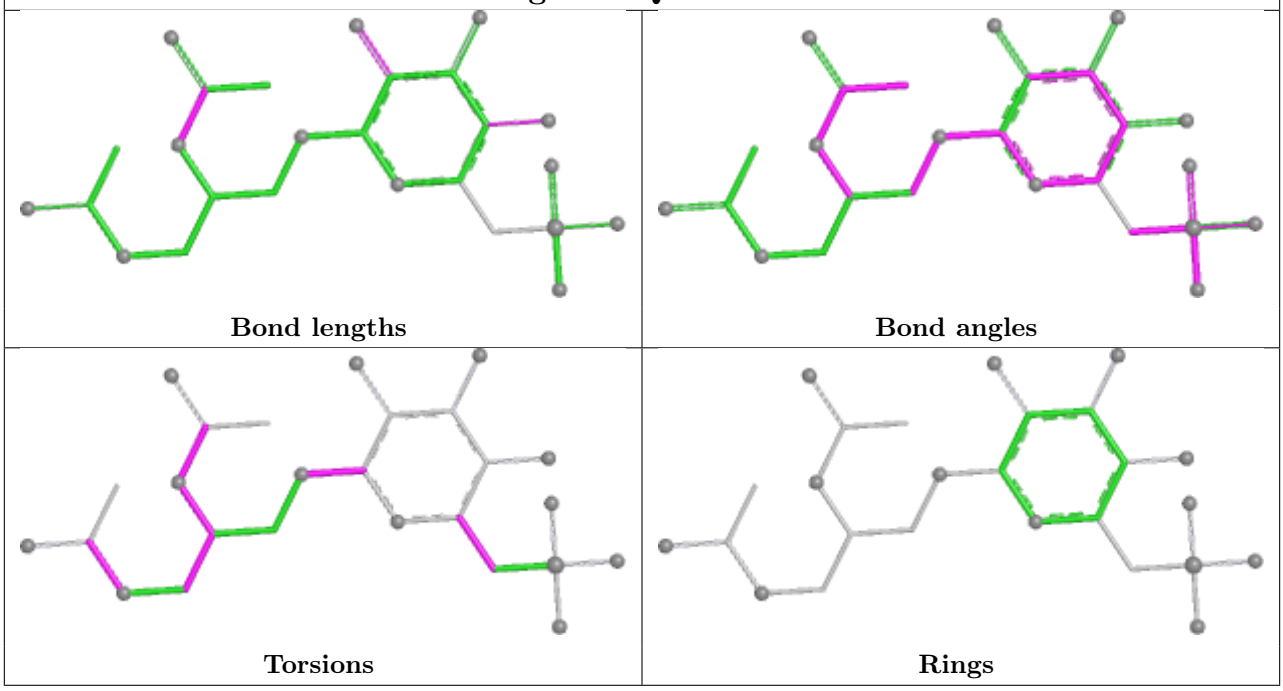
Ligand LMU 1 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings

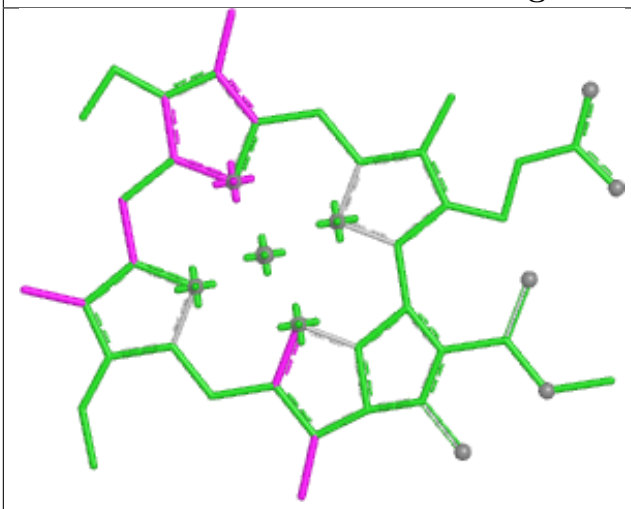
Ligand SQD u 822



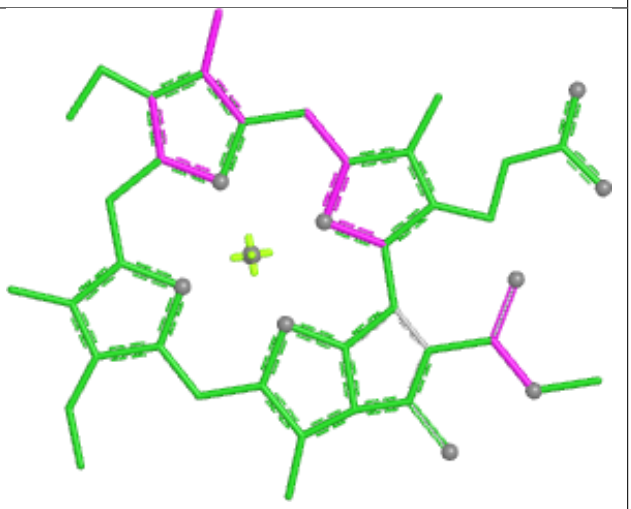
Ligand SQD v 822



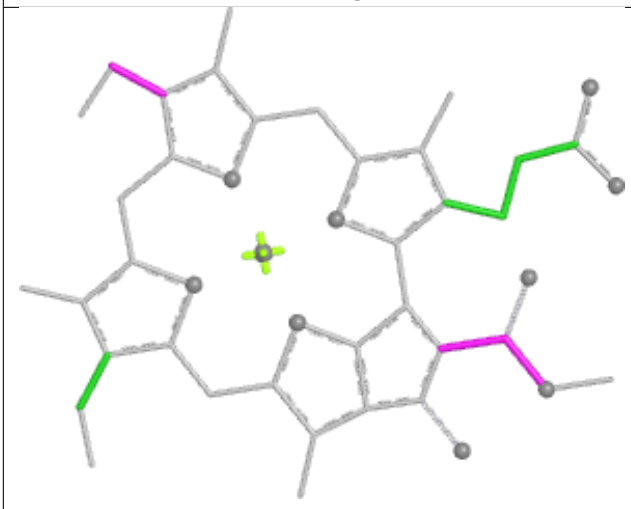
Ligand CLA 6 506



Bond lengths



Bond angles

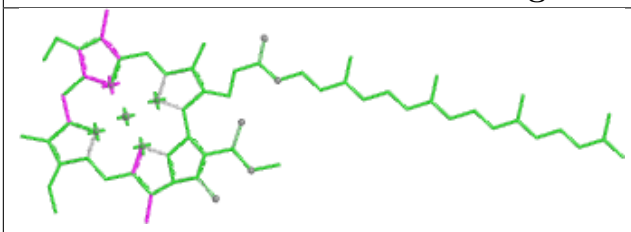


Torsions

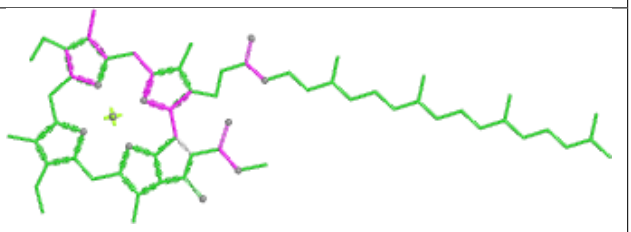


Rings

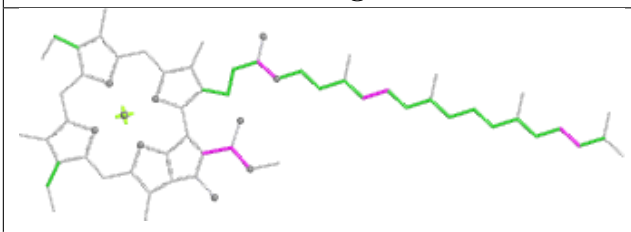
Ligand CLA 4 509



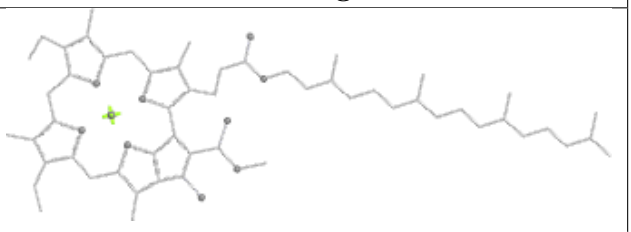
Bond lengths



Bond angles

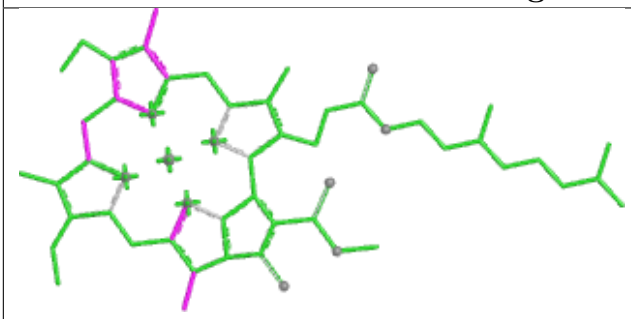


Torsions

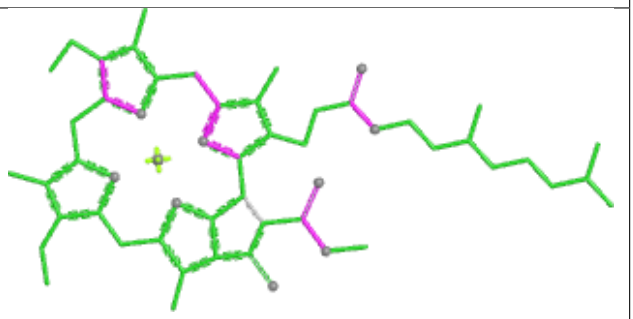


Rings

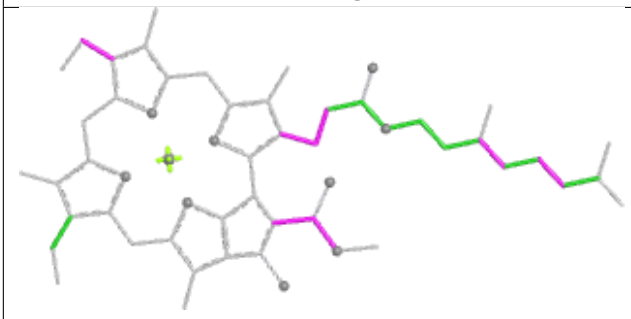
Ligand CLA u 503



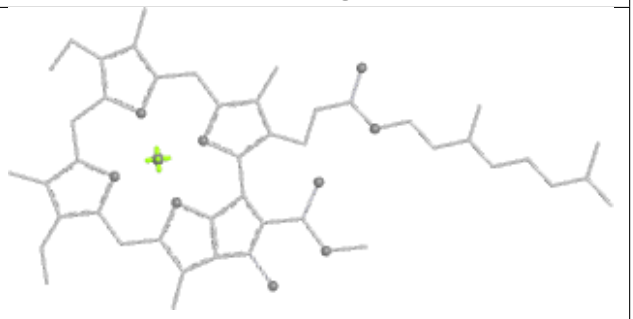
Bond lengths



Bond angles

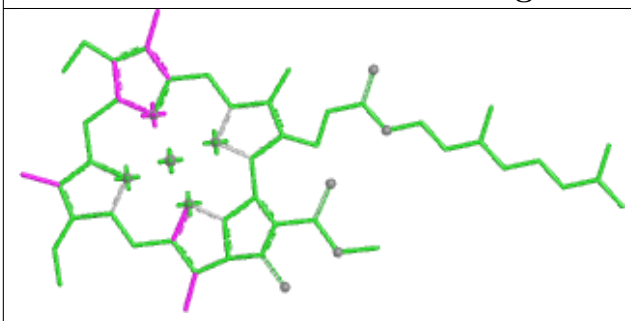


Torsions

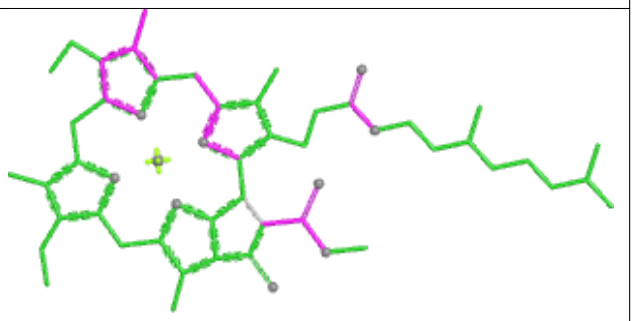


Rings

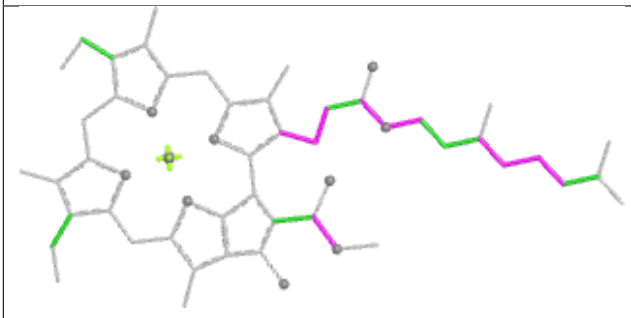
Ligand CLA B 1212



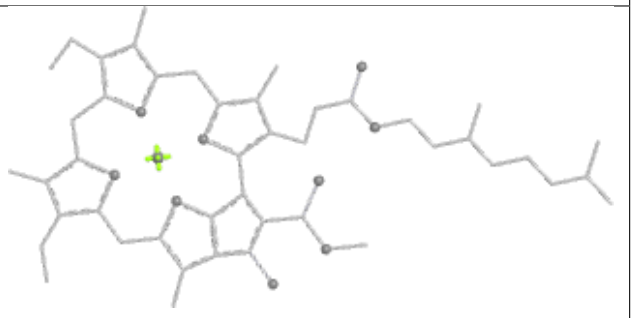
Bond lengths



Bond angles

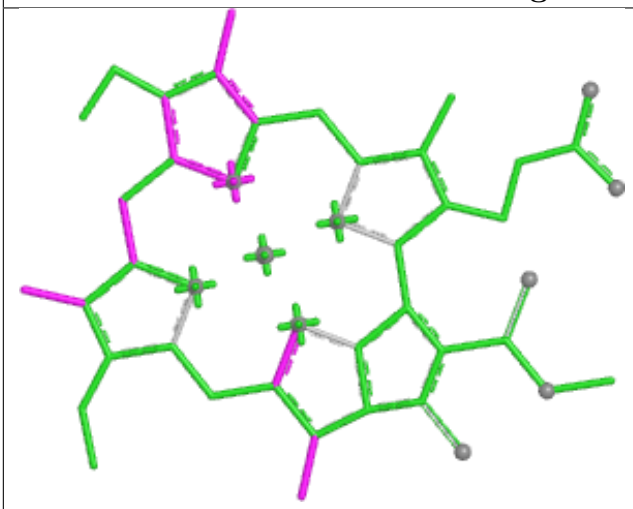


Torsions

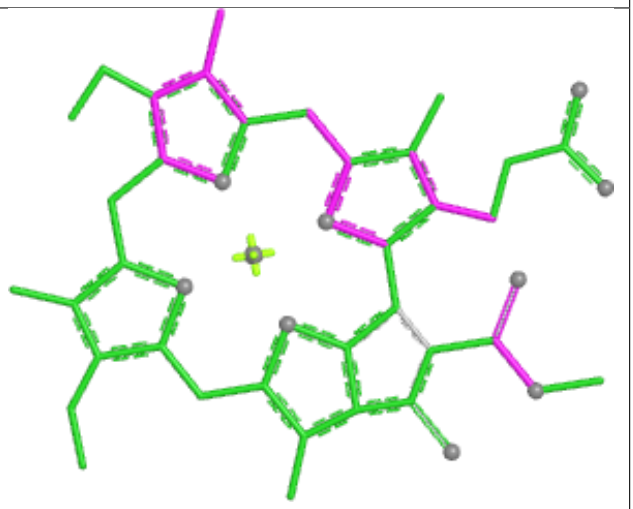


Rings

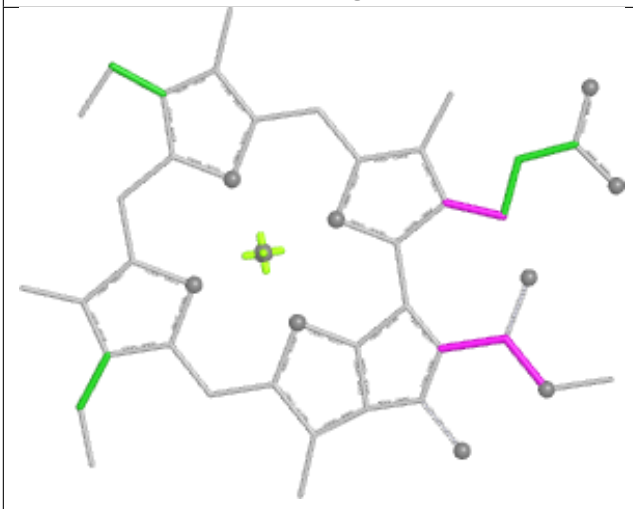
Ligand CLA s 504



Bond lengths



Bond angles

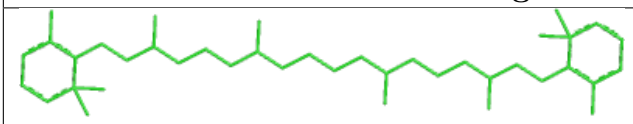


Torsions

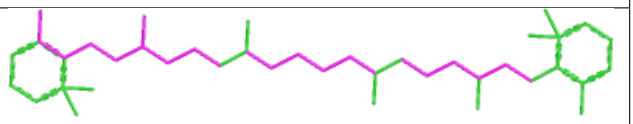


Rings

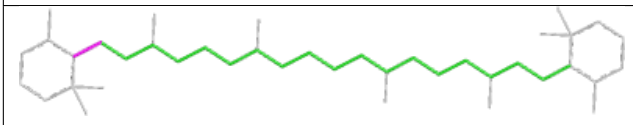
Ligand BCR H 4017



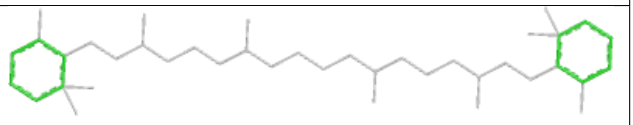
Bond lengths



Bond angles

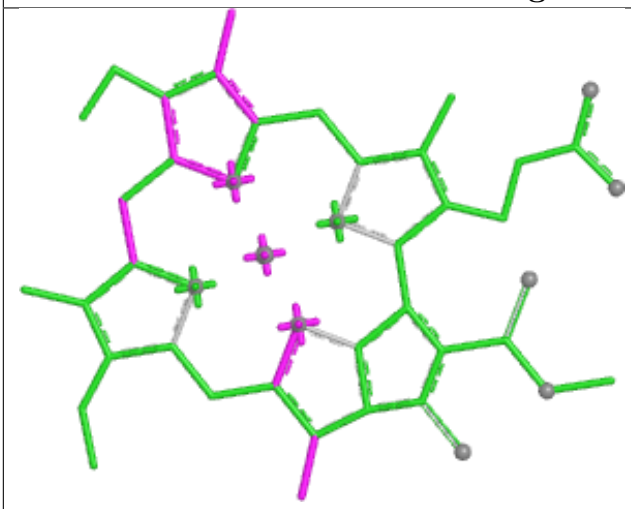


Torsions

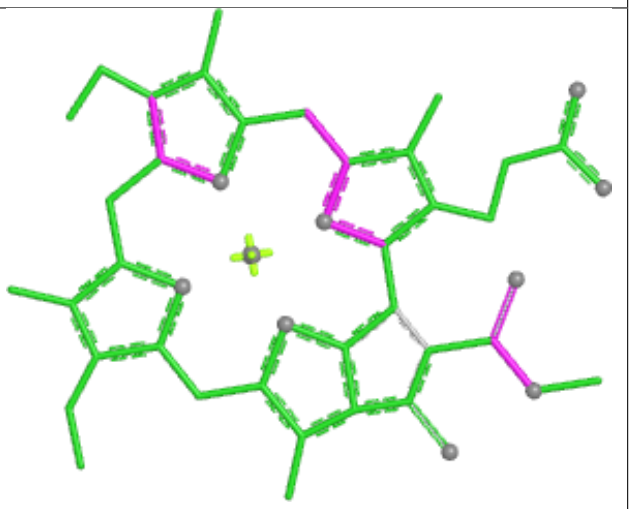


Rings

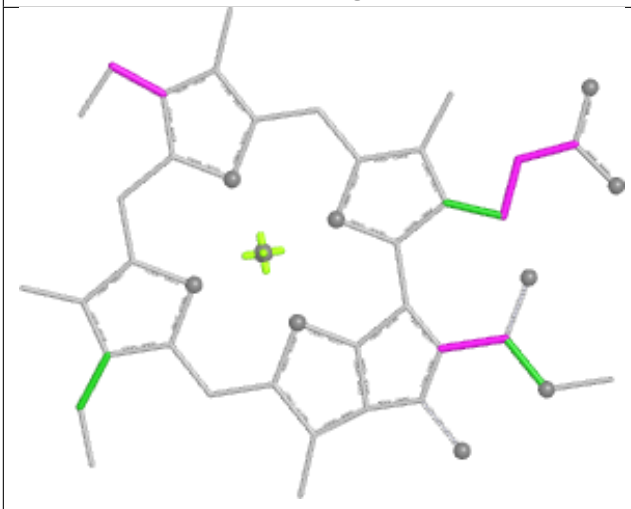
Ligand CLA a 512



Bond lengths



Bond angles

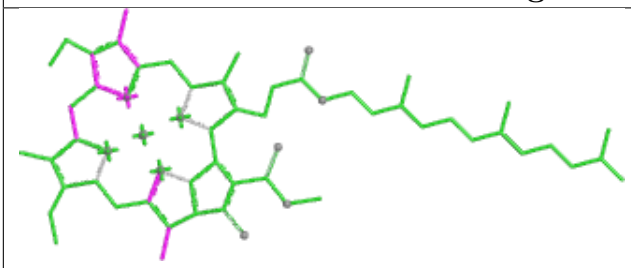


Torsions

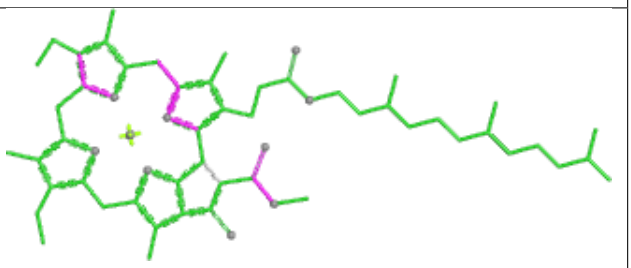


Rings

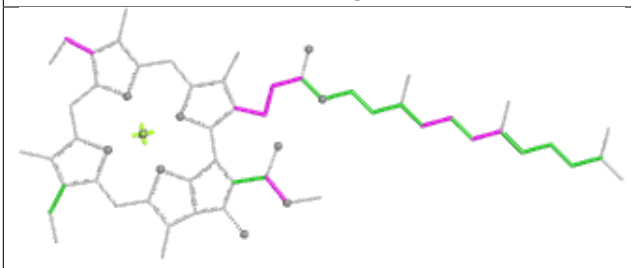
Ligand CLA b 501



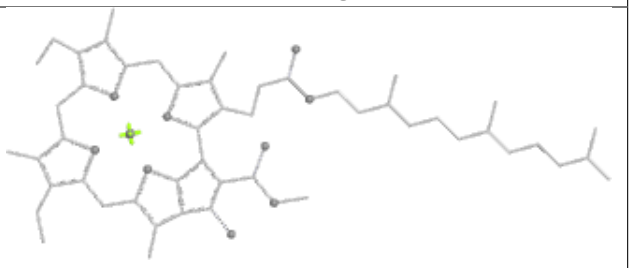
Bond lengths



Bond angles

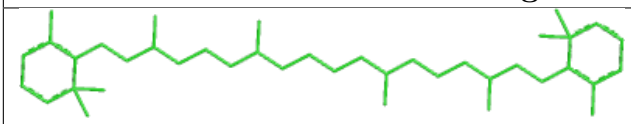


Torsions

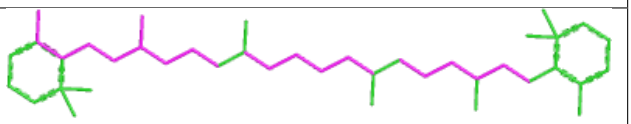


Rings

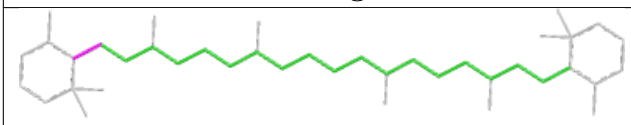
Ligand BCR f 4017



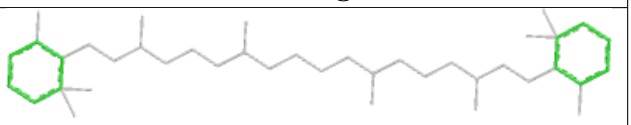
Bond lengths



Bond angles

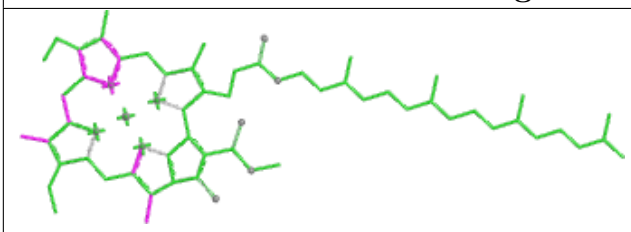


Torsions

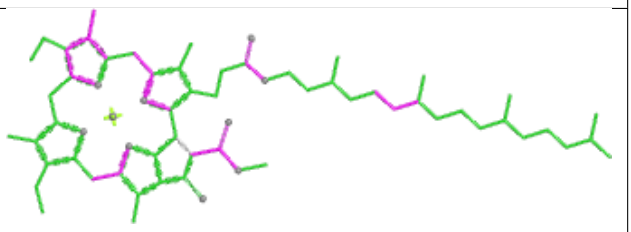


Rings

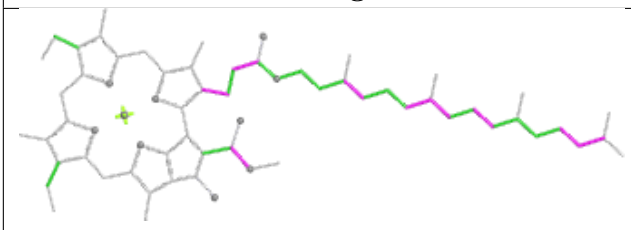
Ligand CLA H 1229



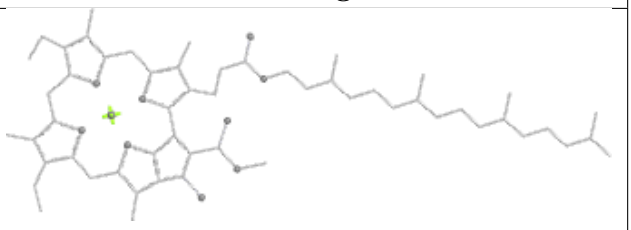
Bond lengths



Bond angles

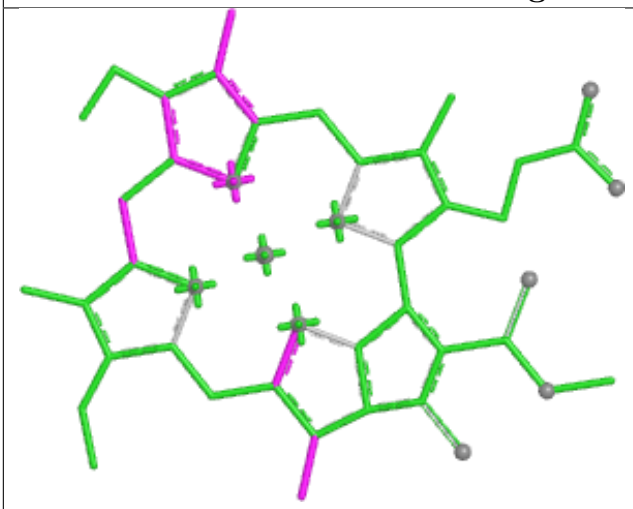


Torsions

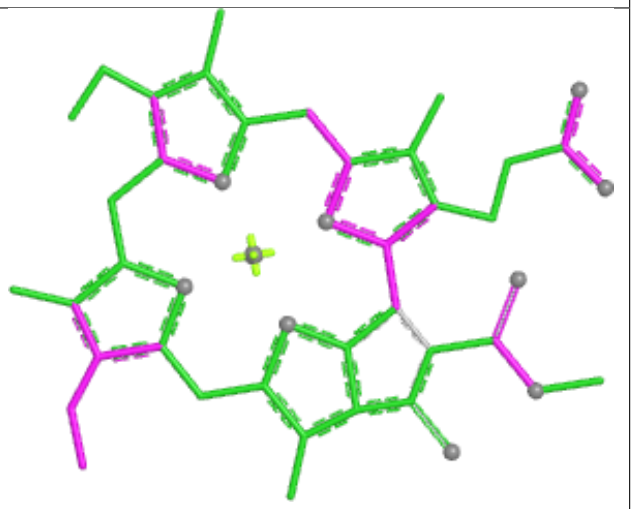


Rings

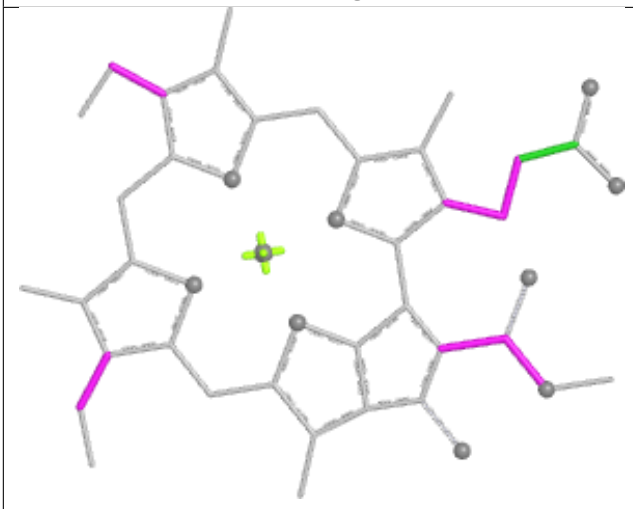
Ligand CLA 3 516



Bond lengths



Bond angles

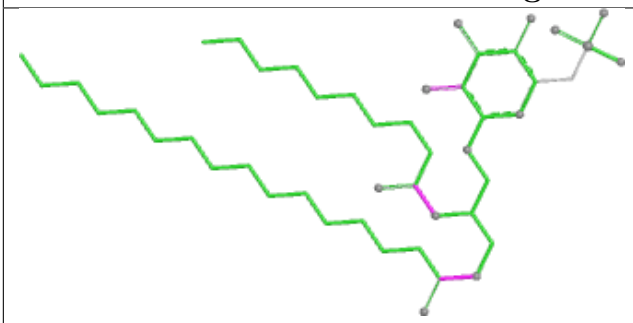


Torsions

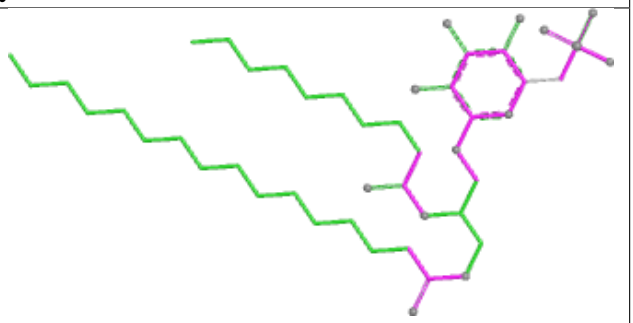


Rings

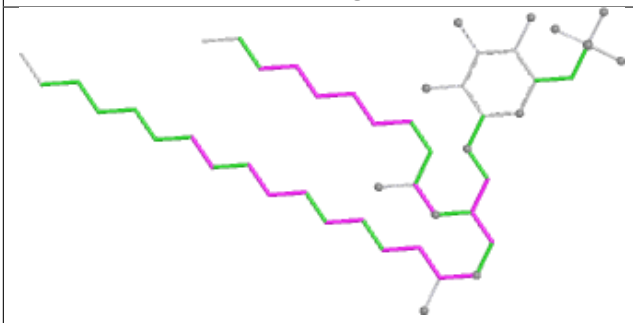
Ligand SQD Y 822



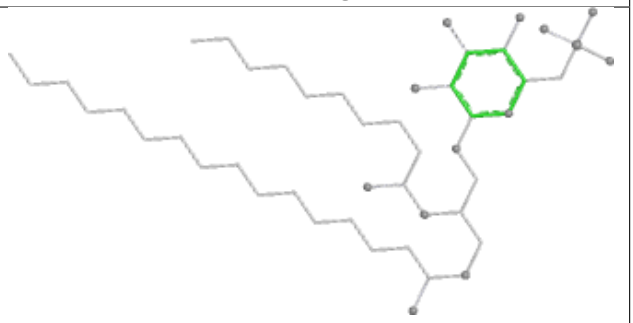
Bond lengths



Bond angles

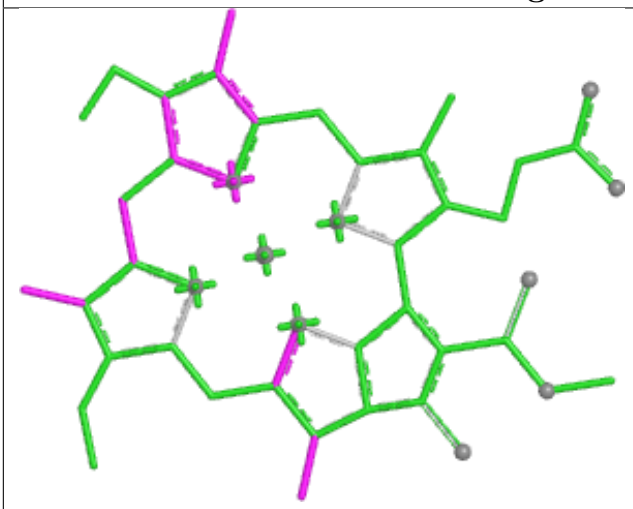


Torsions

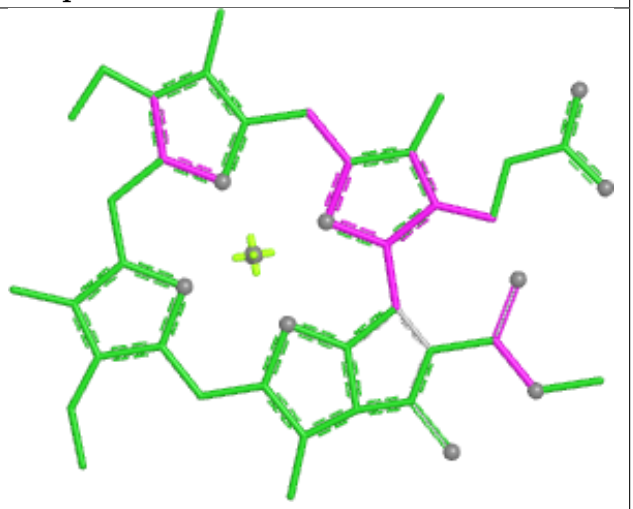


Rings

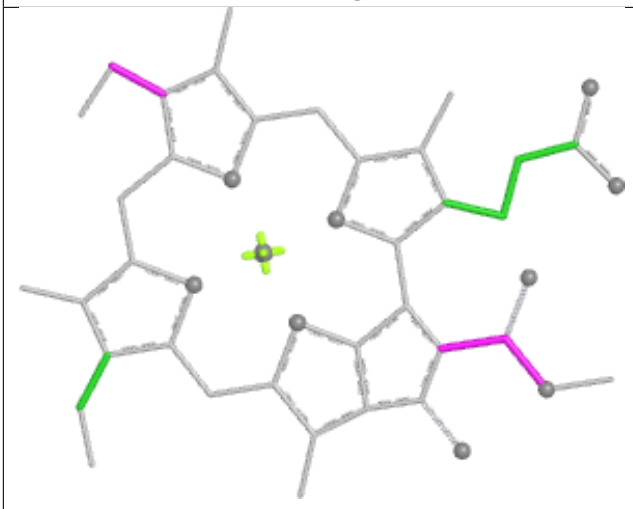
Ligand CLA q 504



Bond lengths



Bond angles

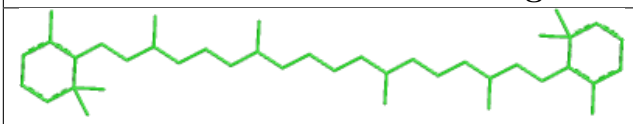


Torsions

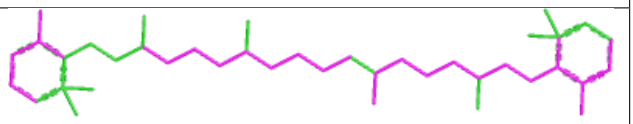


Rings

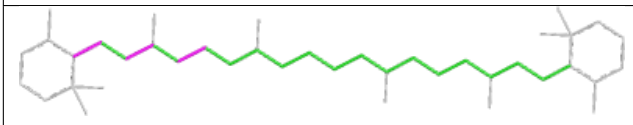
Ligand BCR d 522



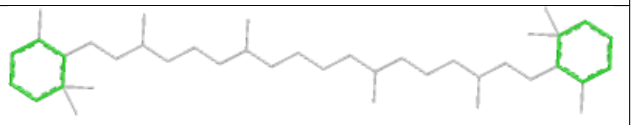
Bond lengths



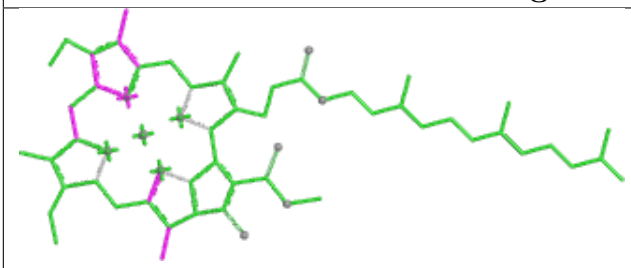
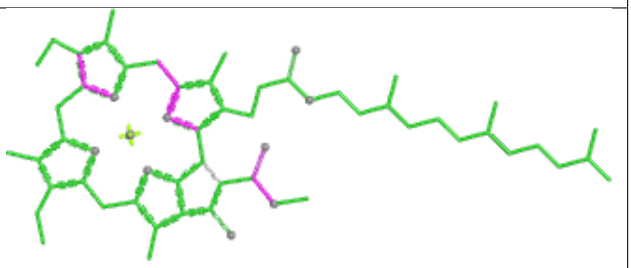
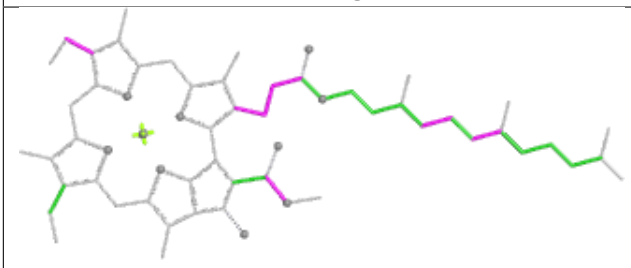
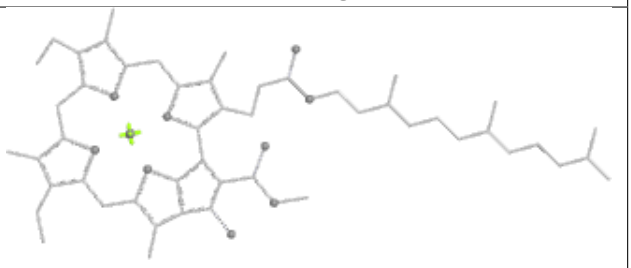
Bond angles

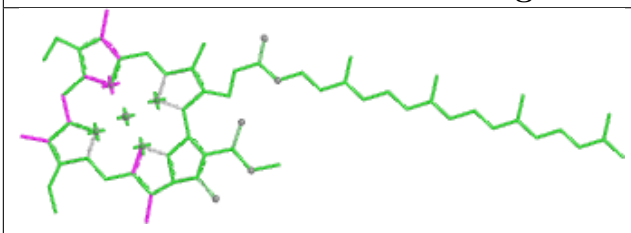
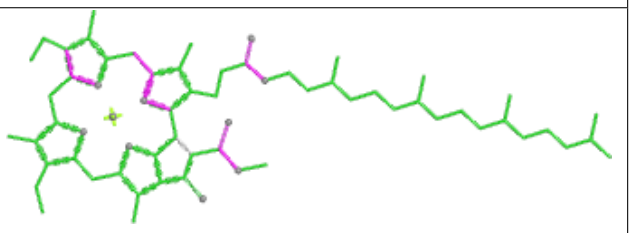
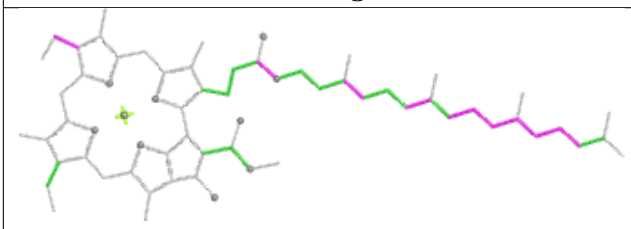
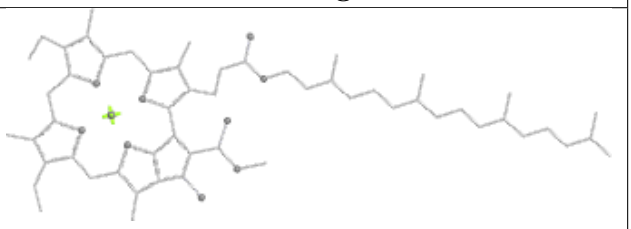


Torsions

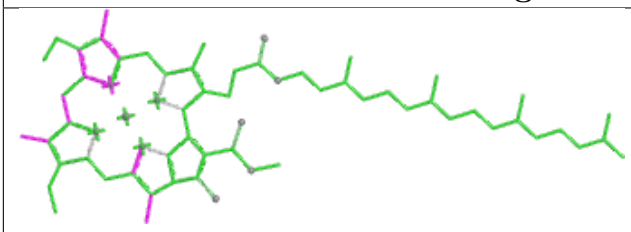


Rings

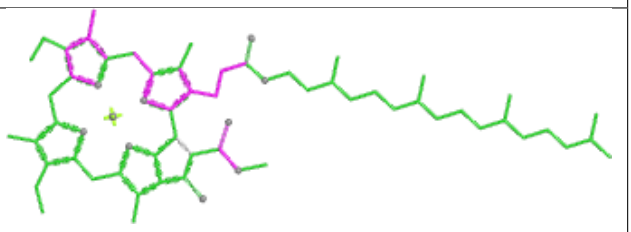
Ligand CLA t 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1208	
	
Bond lengths	Bond angles
	
Torsions	Rings

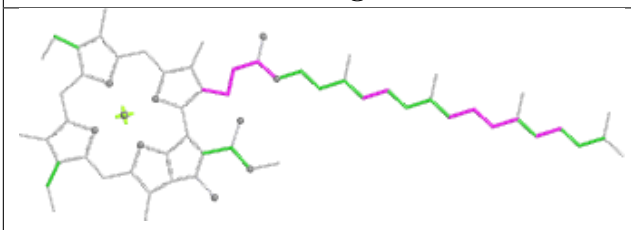
Ligand CLA A 1125



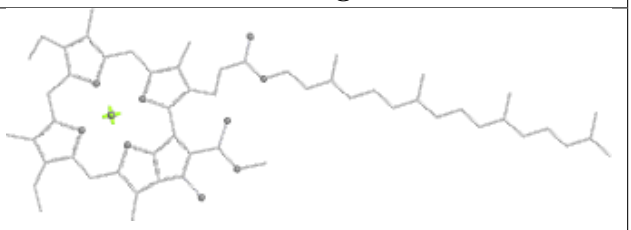
Bond lengths



Bond angles



Torsions

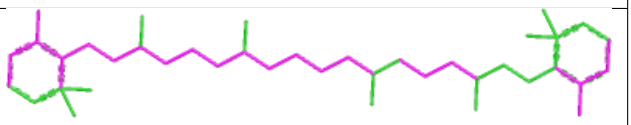


Rings

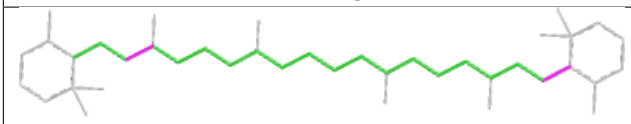
Ligand BCR 4 524



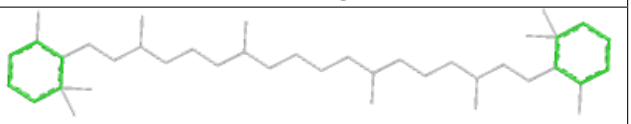
Bond lengths



Bond angles

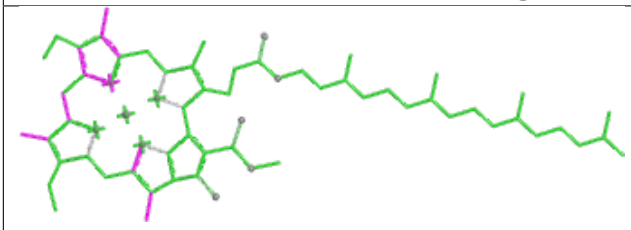


Torsions

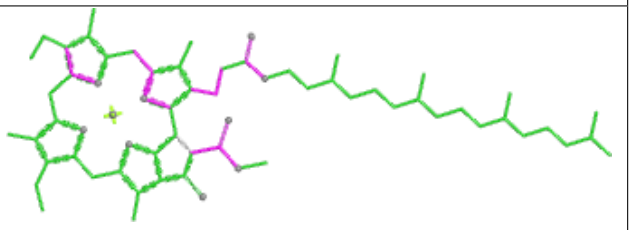


Rings

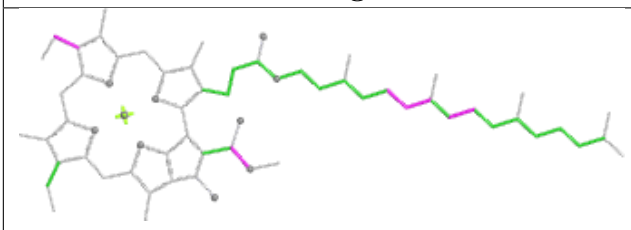
Ligand CLA H 1235



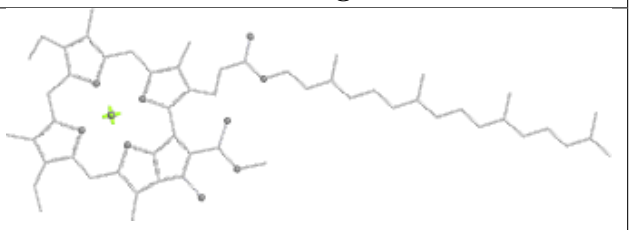
Bond lengths



Bond angles

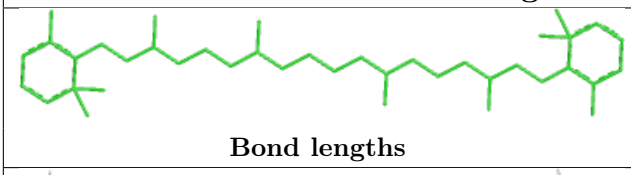


Torsions

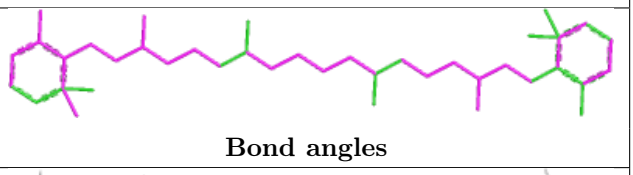


Rings

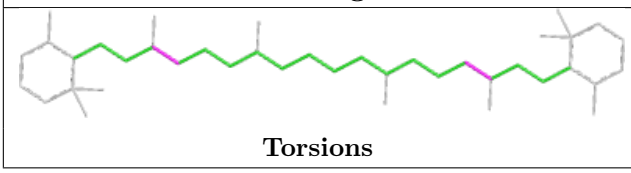
Ligand BCR f 4006



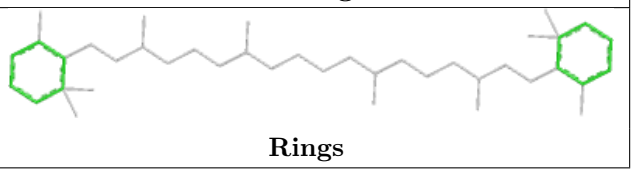
Bond lengths



Bond angles

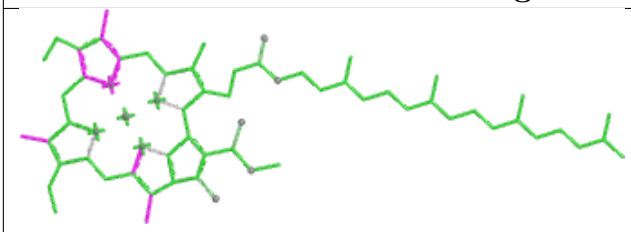


Torsions

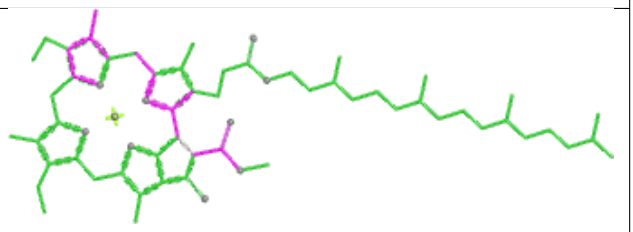


Rings

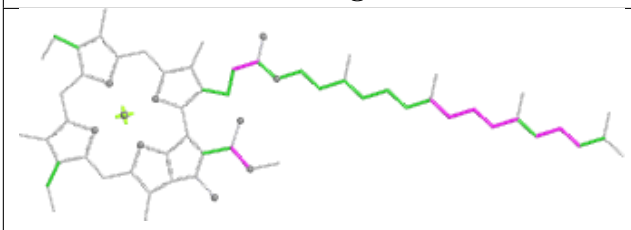
Ligand CLA G 1123



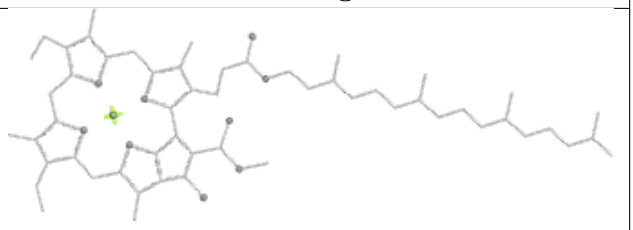
Bond lengths



Bond angles

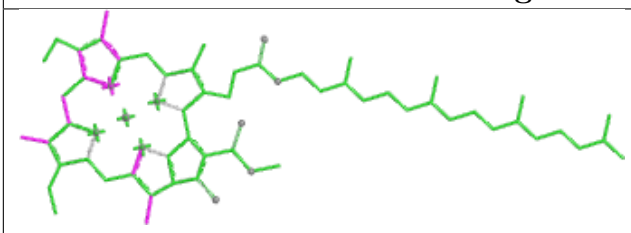


Torsions

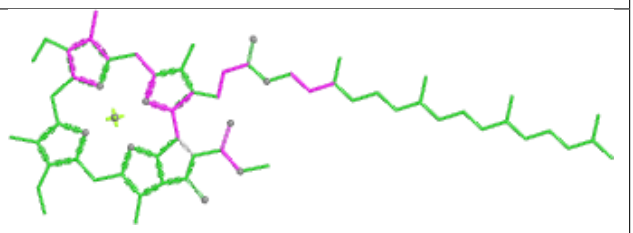


Rings

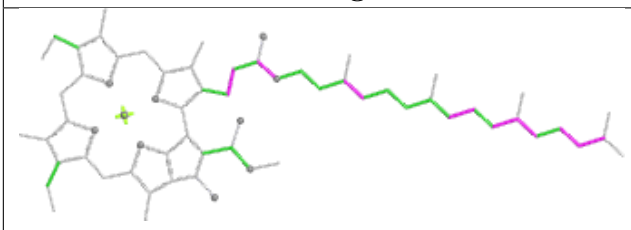
Ligand CLA A 1127



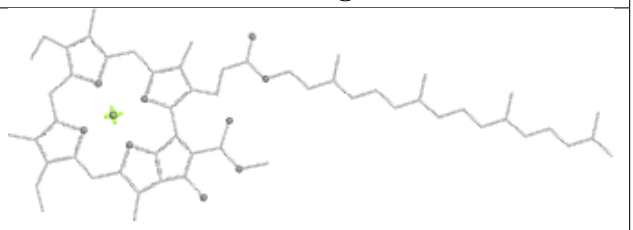
Bond lengths



Bond angles

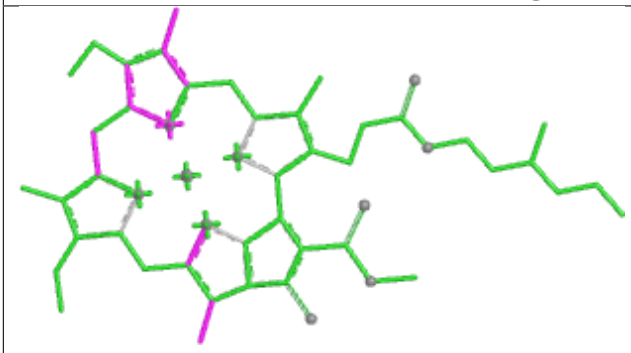


Torsions

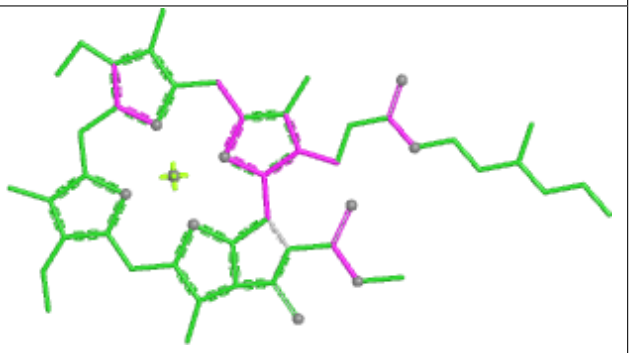


Rings

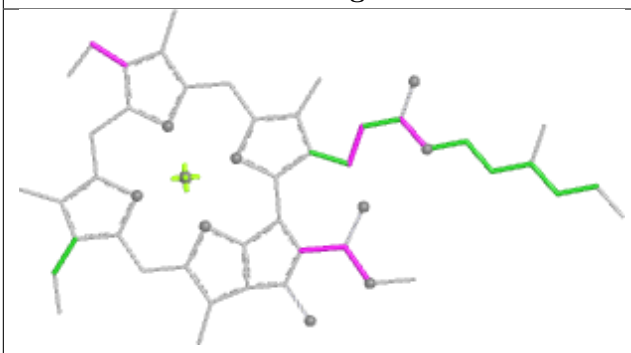
Ligand CLA d 503



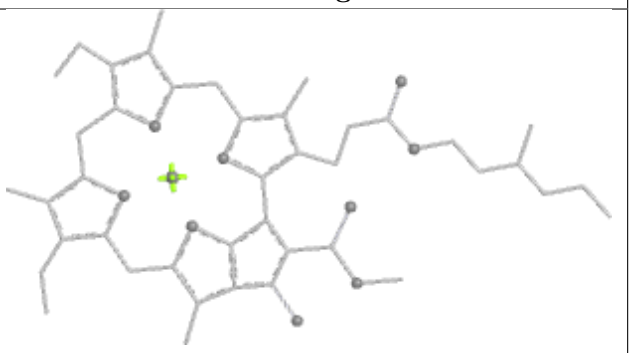
Bond lengths



Bond angles

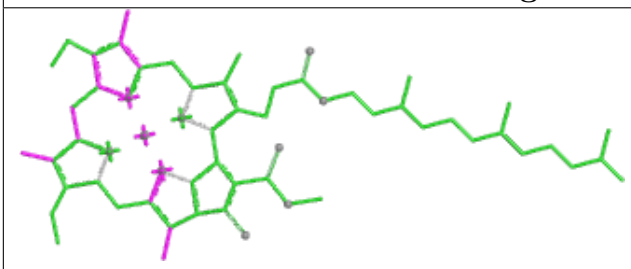


Torsions

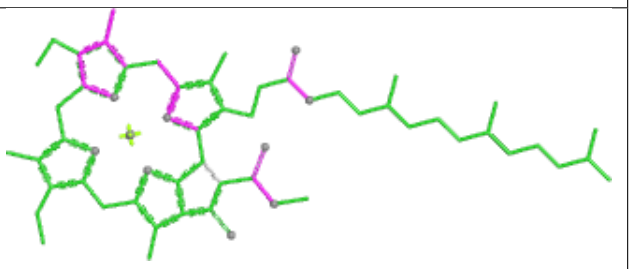


Rings

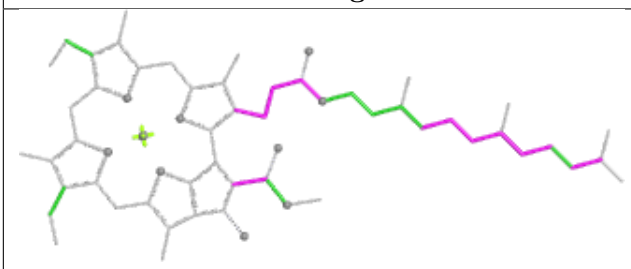
Ligand CLA e 1116



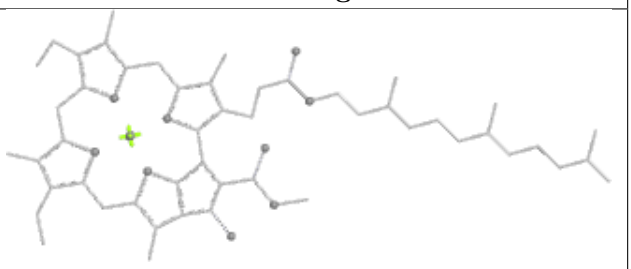
Bond lengths



Bond angles

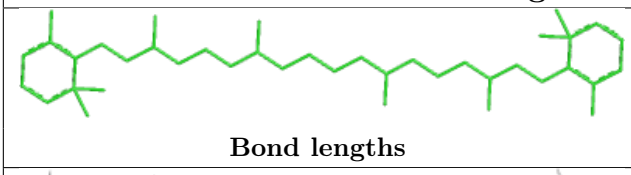


Torsions

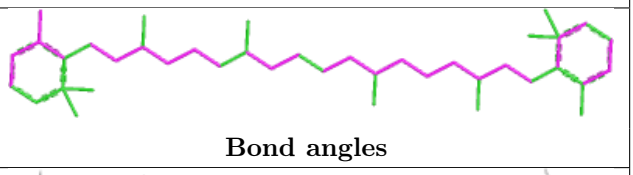


Rings

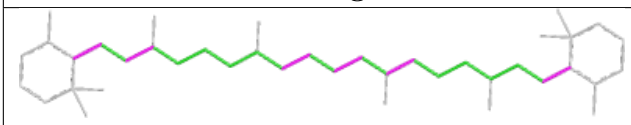
Ligand BCR t 521



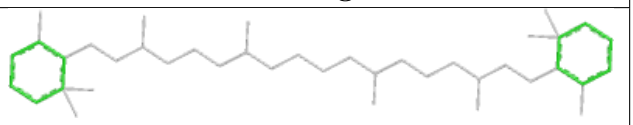
Bond lengths



Bond angles

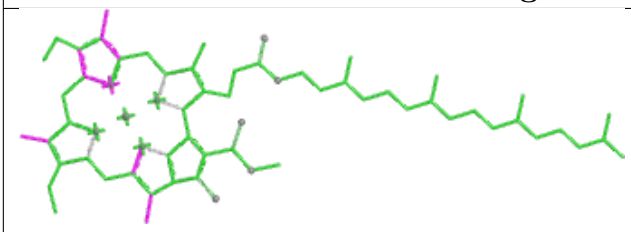


Torsions

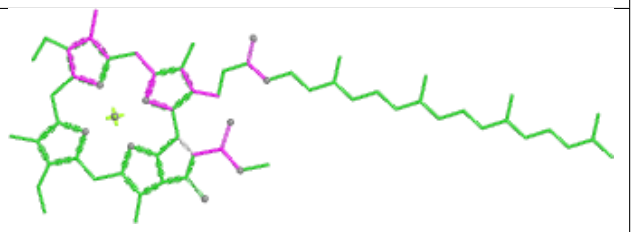


Rings

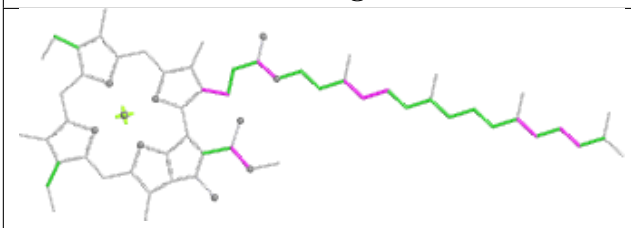
Ligand CLA e 1104



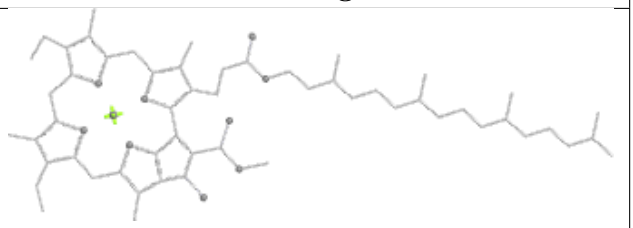
Bond lengths



Bond angles

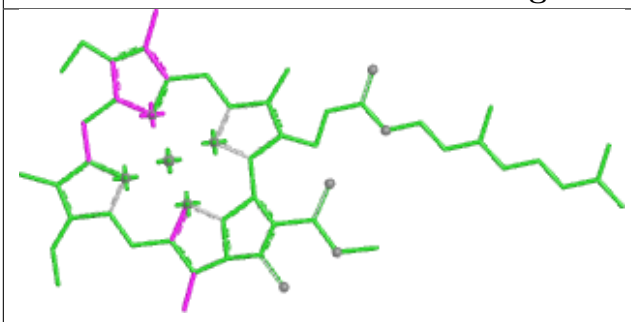


Torsions

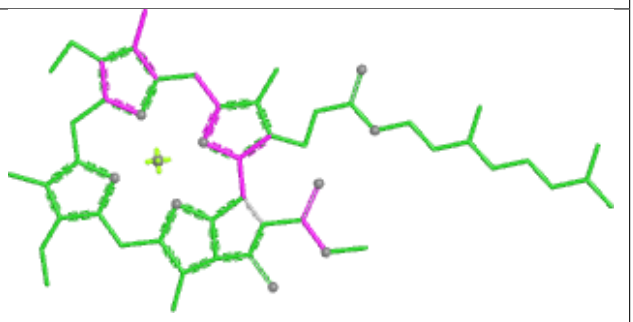


Rings

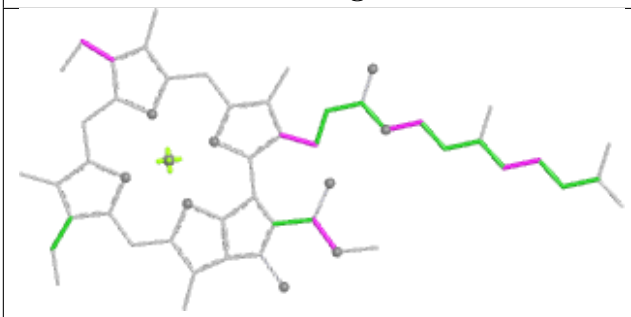
Ligand CLA c 511



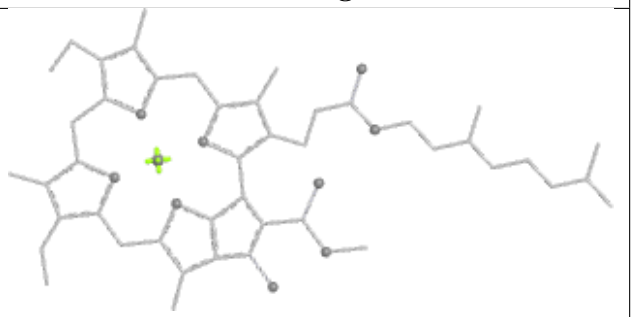
Bond lengths



Bond angles

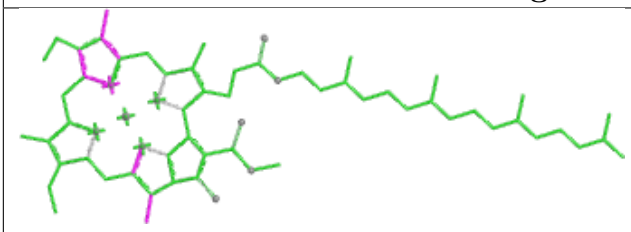


Torsions

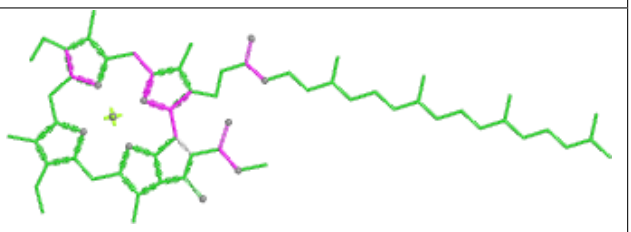


Rings

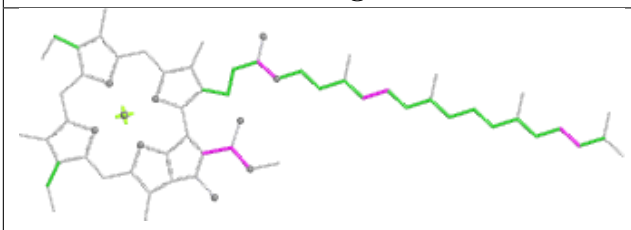
Ligand CLA t 509



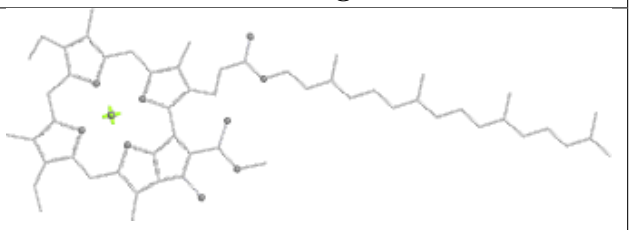
Bond lengths



Bond angles

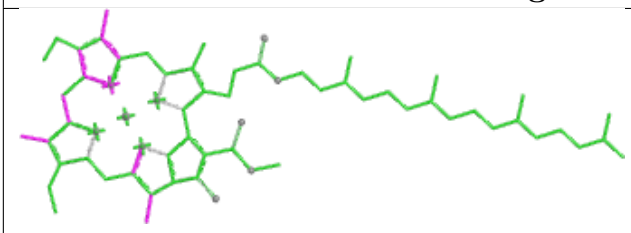


Torsions

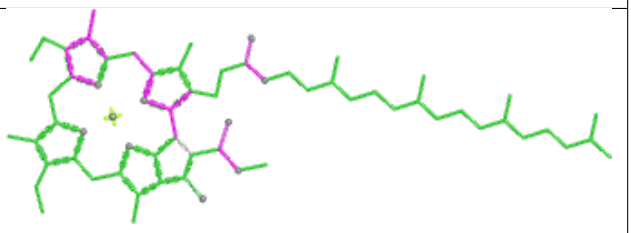


Rings

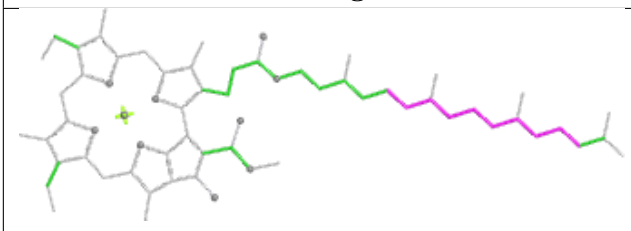
Ligand CLA 5 509



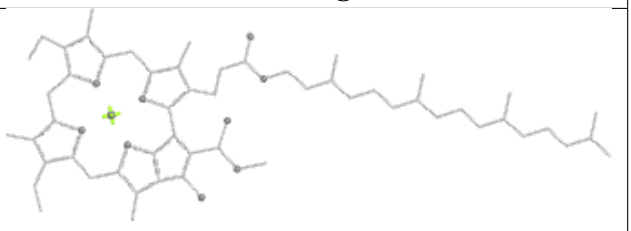
Bond lengths



Bond angles

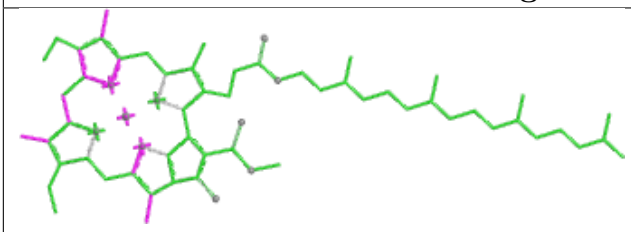


Torsions

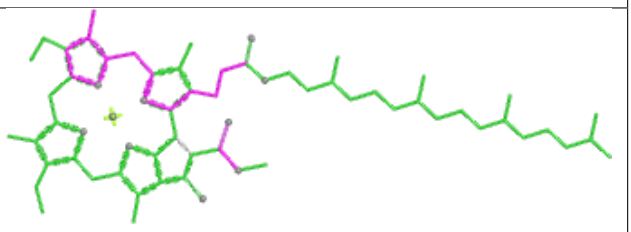


Rings

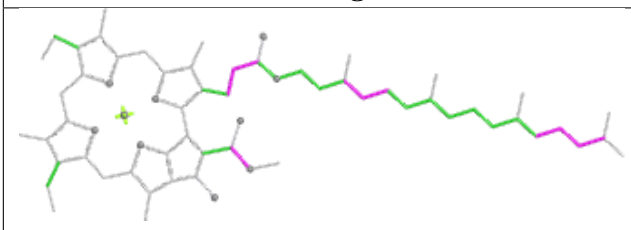
Ligand CLA e 1013



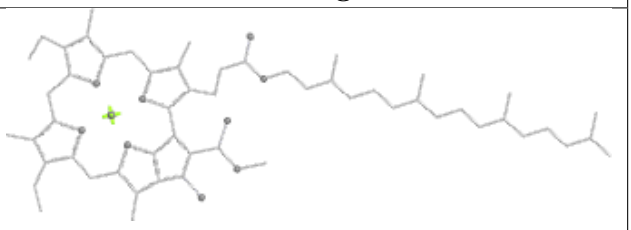
Bond lengths



Bond angles

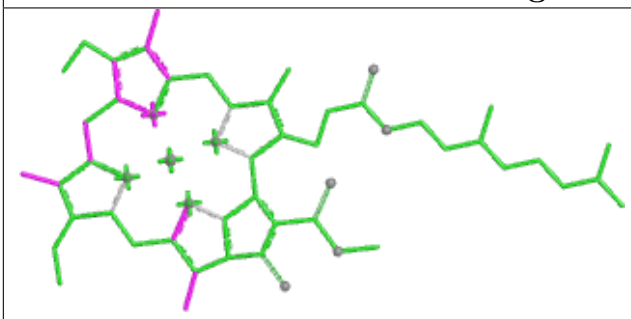


Torsions

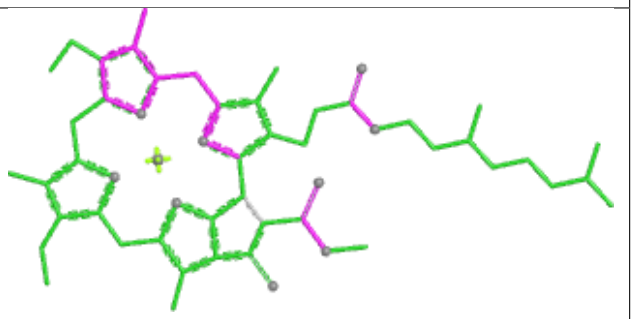


Rings

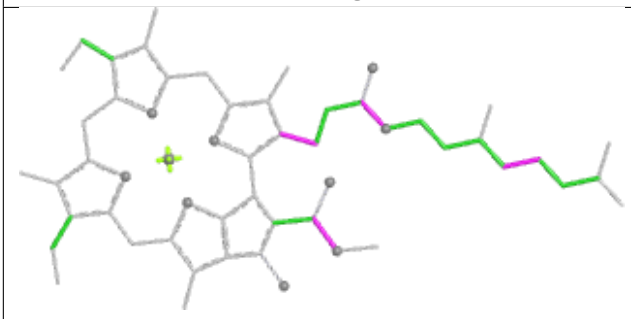
Ligand CLA 3 508



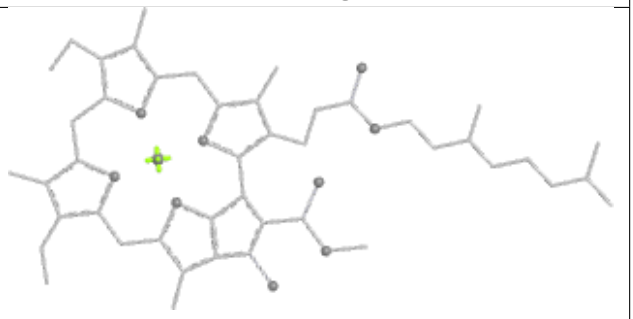
Bond lengths



Bond angles

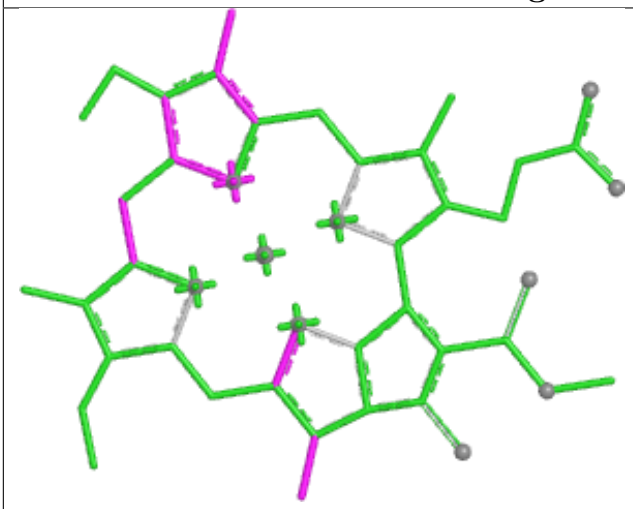


Torsions

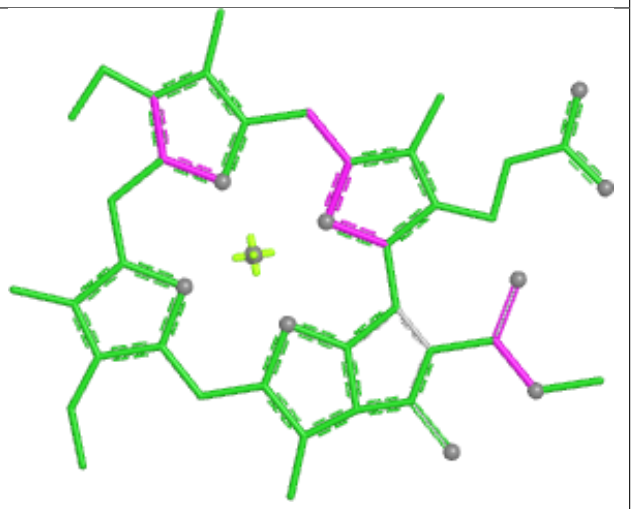


Rings

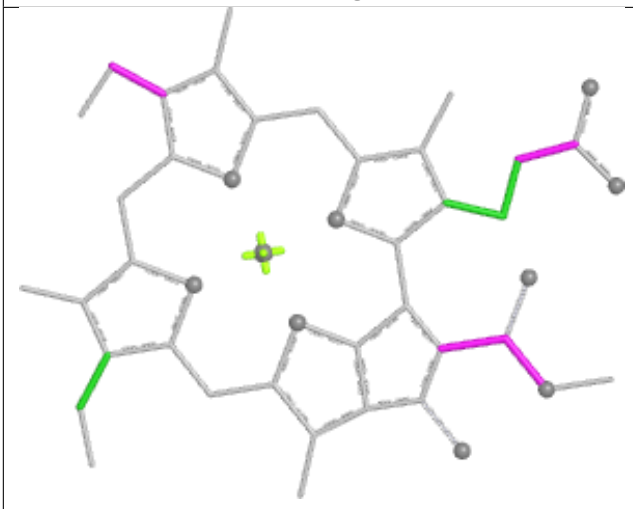
Ligand CLA 5 512



Bond lengths



Bond angles

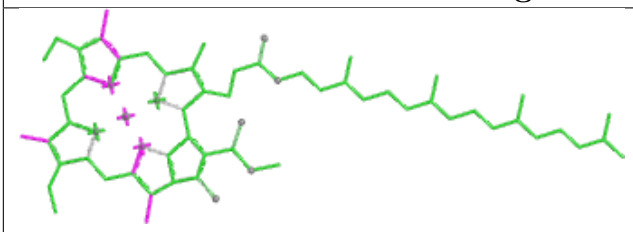


Torsions

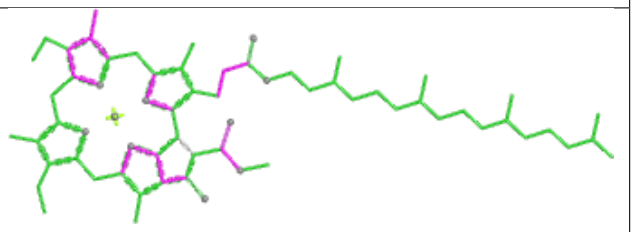


Rings

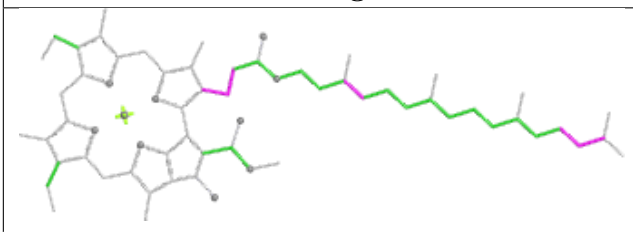
Ligand CLA A 1022



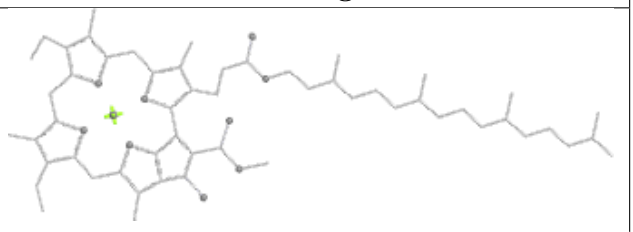
Bond lengths



Bond angles

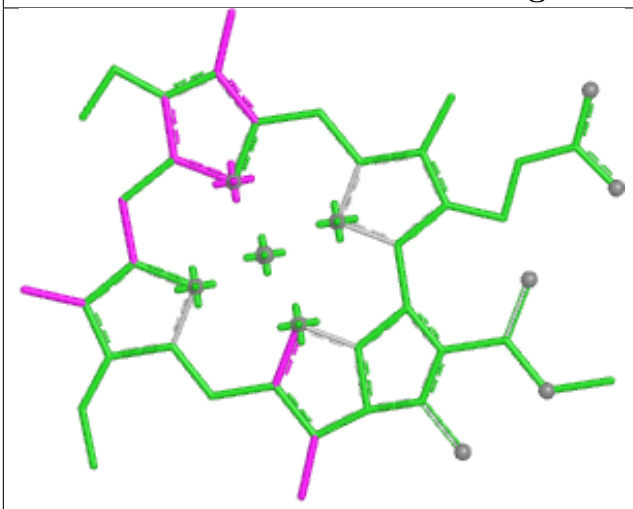


Torsions

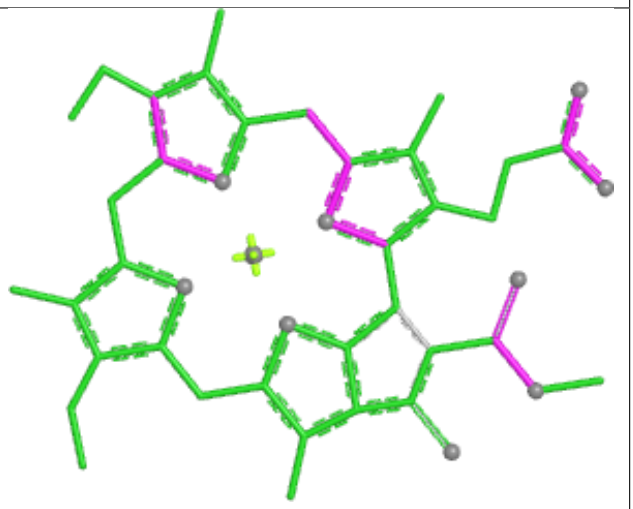


Rings

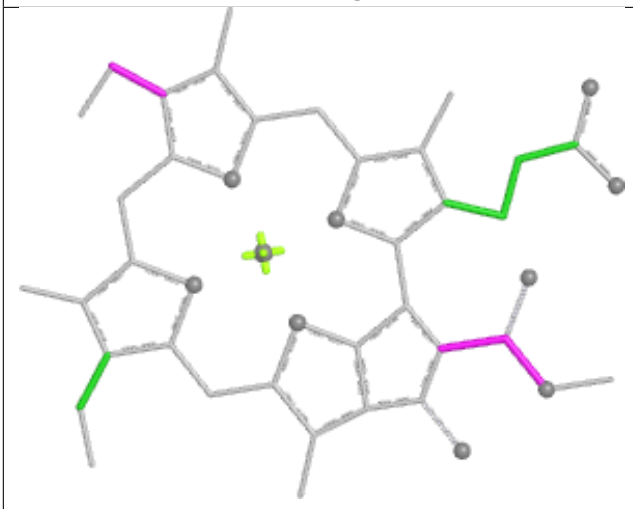
Ligand CLA 5 506



Bond lengths



Bond angles

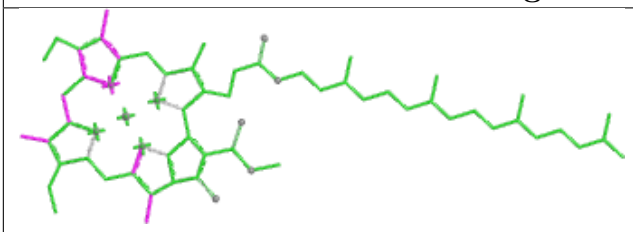


Torsions

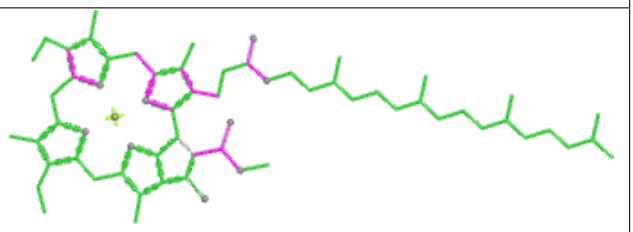


Rings

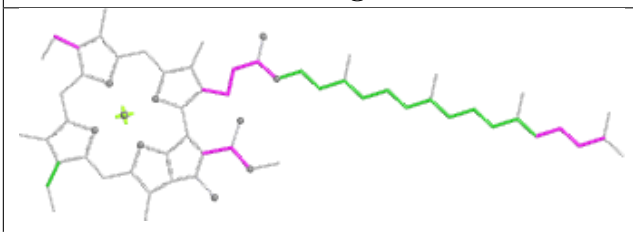
Ligand CLA Y 501



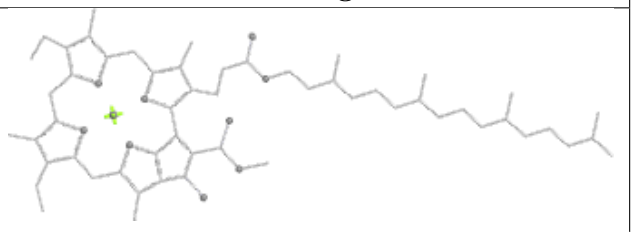
Bond lengths



Bond angles

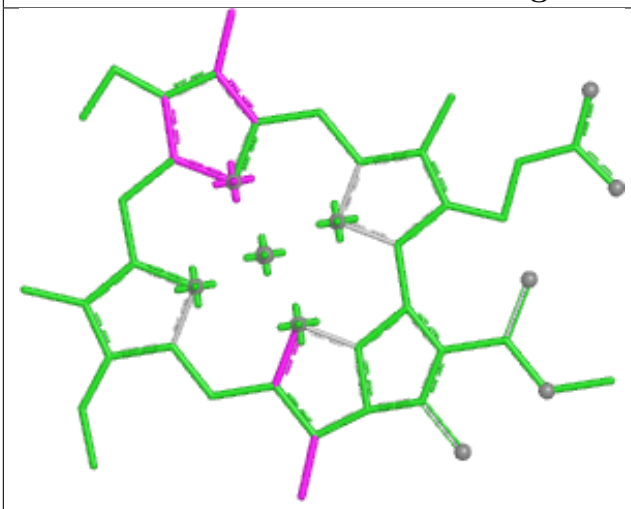


Torsions

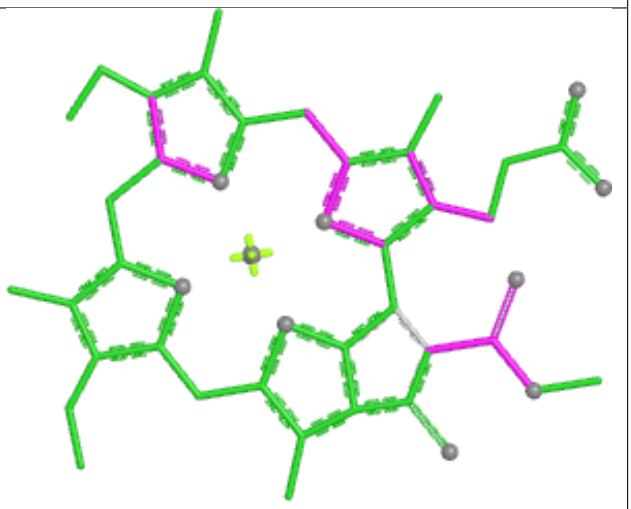


Rings

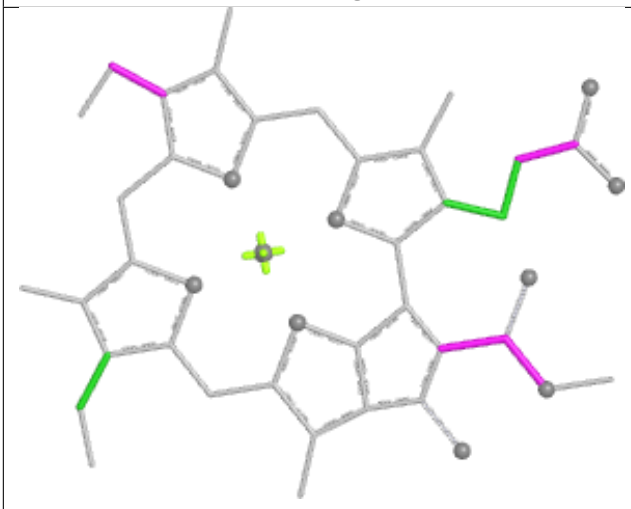
Ligand CLA t 507



Bond lengths



Bond angles

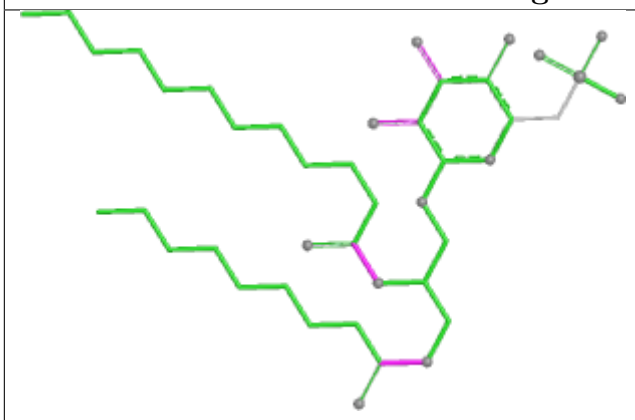


Torsions

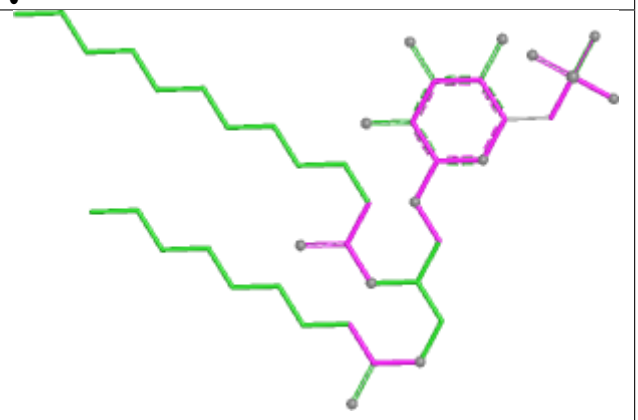


Rings

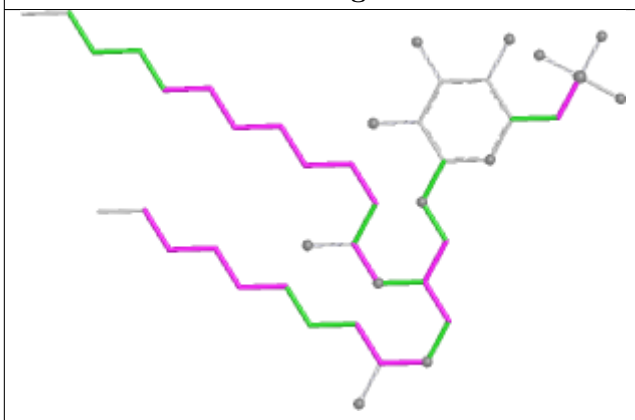
Ligand SQD s 822



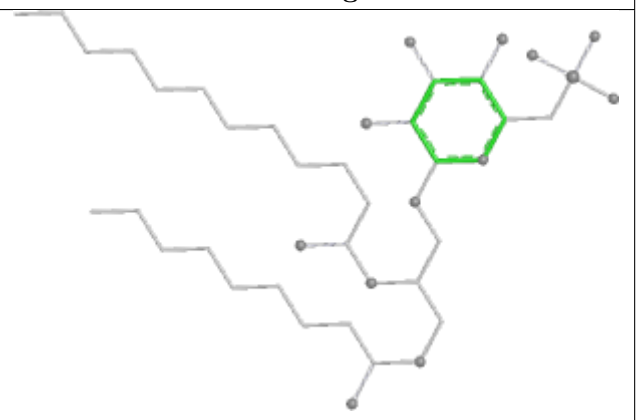
Bond lengths



Bond angles

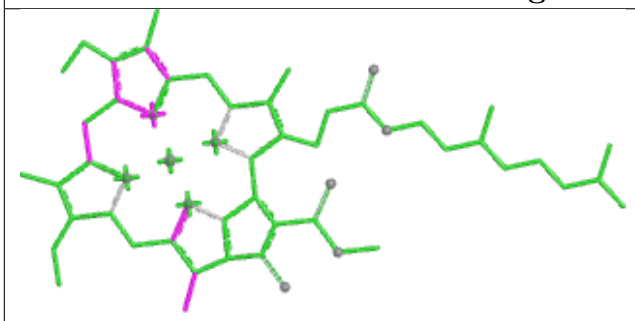


Torsions

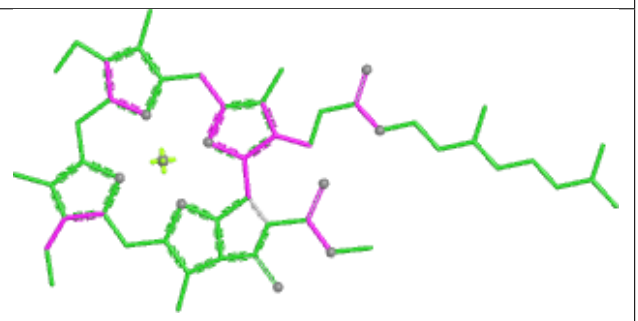


Rings

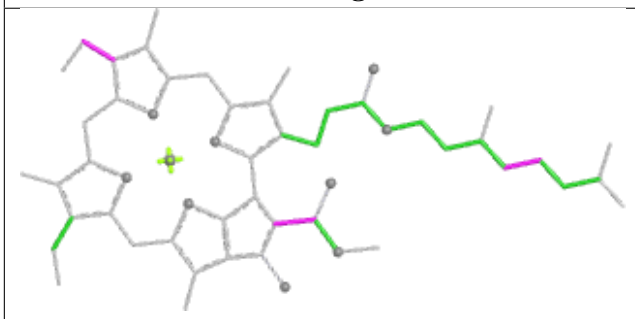
Ligand CLA b 503



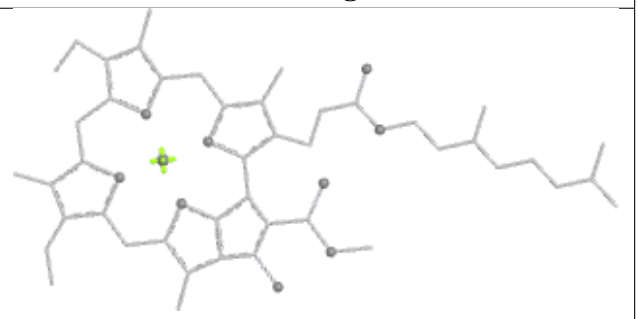
Bond lengths



Bond angles

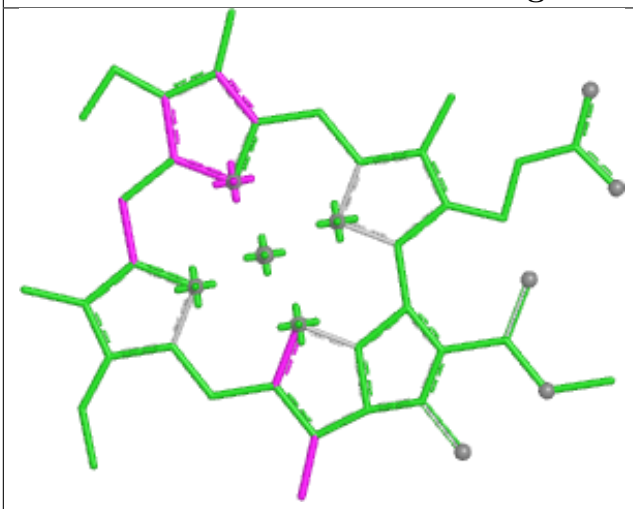


Torsions

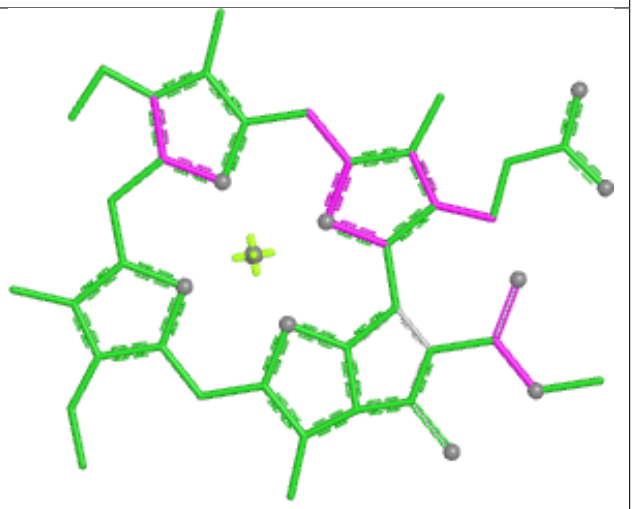


Rings

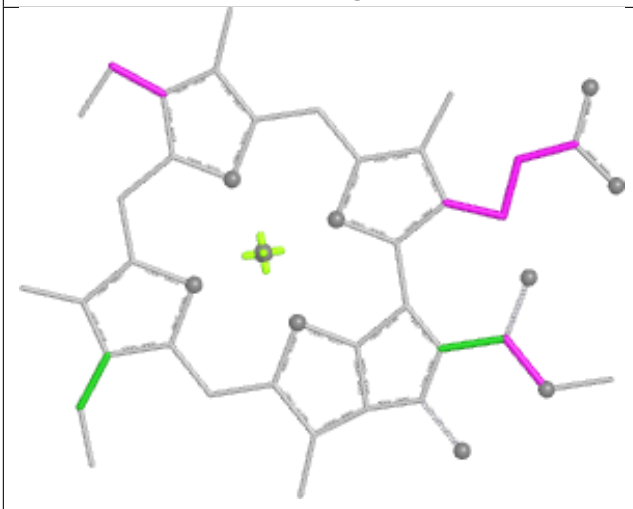
Ligand CLA d 516



Bond lengths



Bond angles

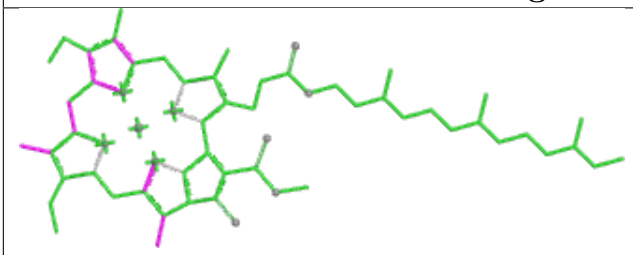


Torsions

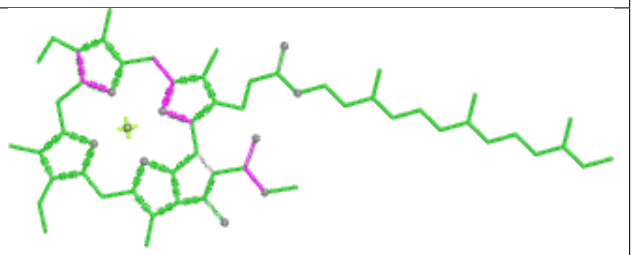


Rings

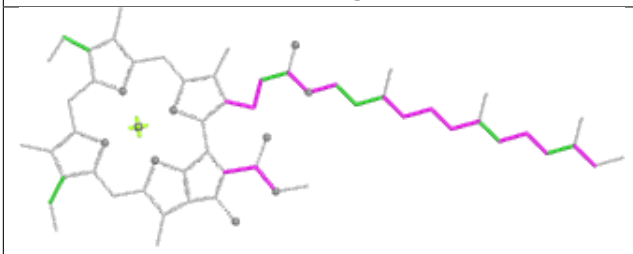
Ligand CLA 5 505



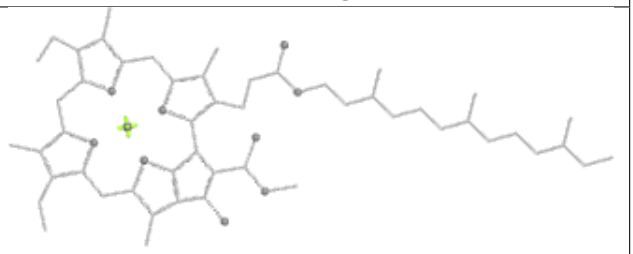
Bond lengths



Bond angles

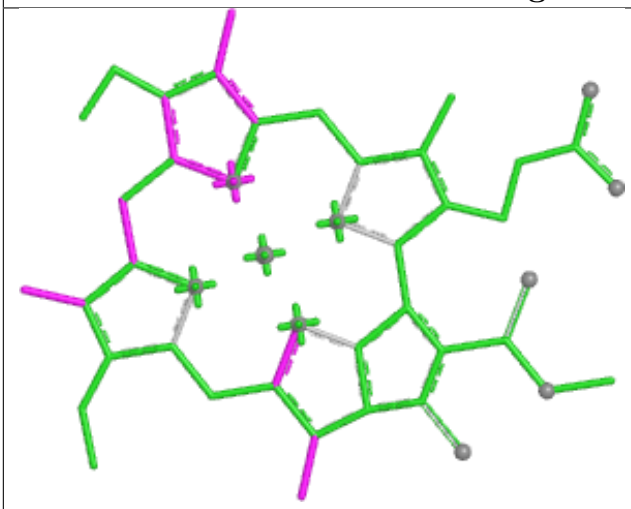


Torsions

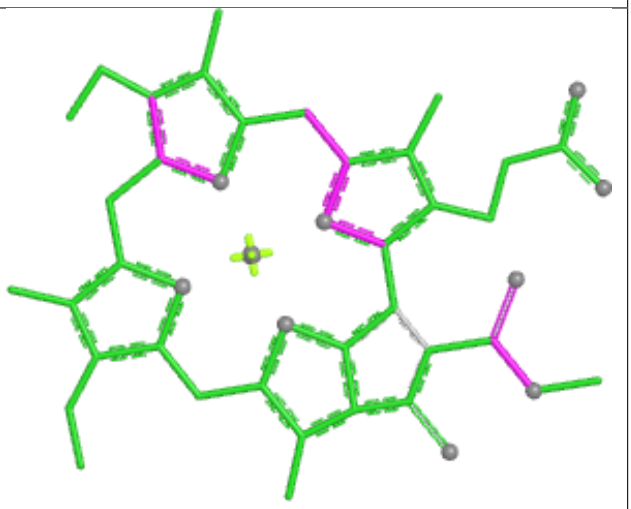


Rings

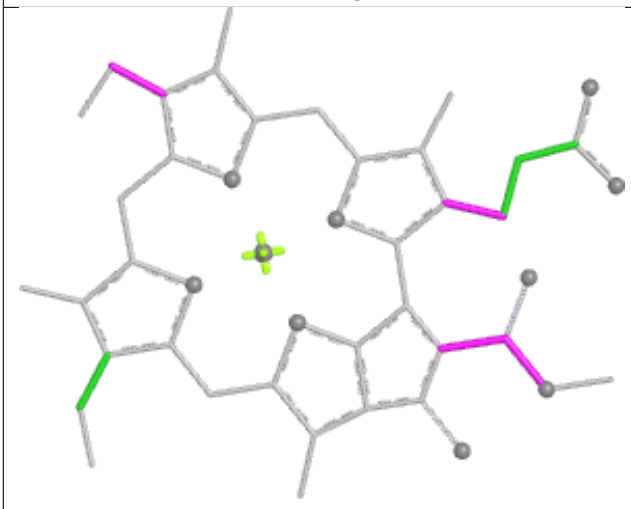
Ligand CLA 3 517



Bond lengths



Bond angles

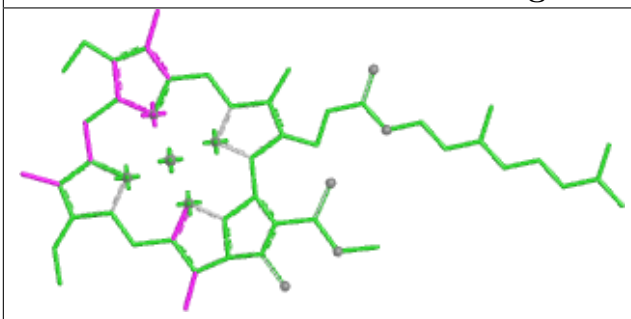


Torsions

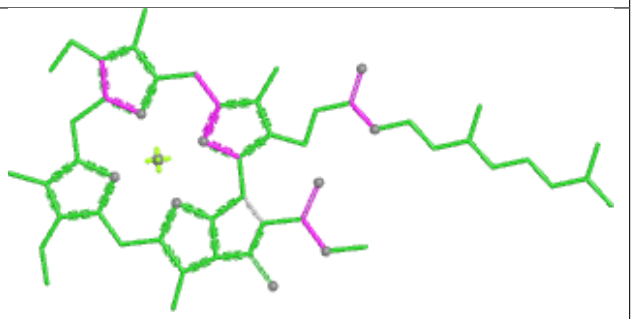


Rings

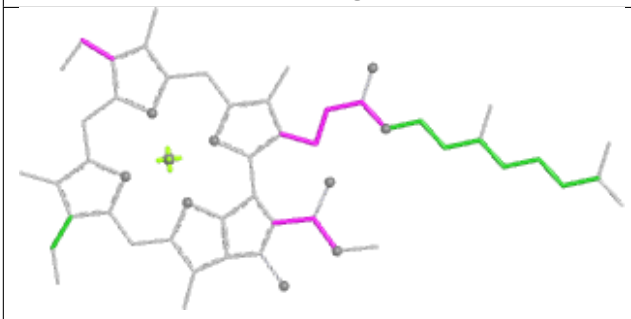
Ligand CLA 6 518



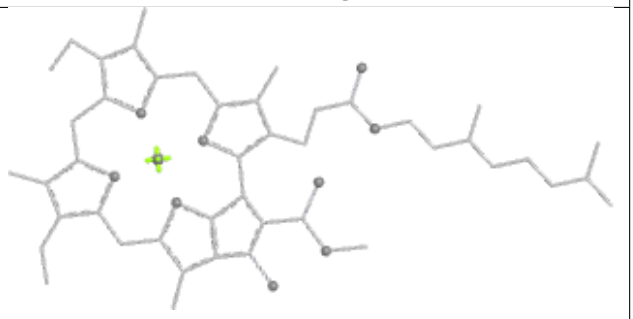
Bond lengths



Bond angles

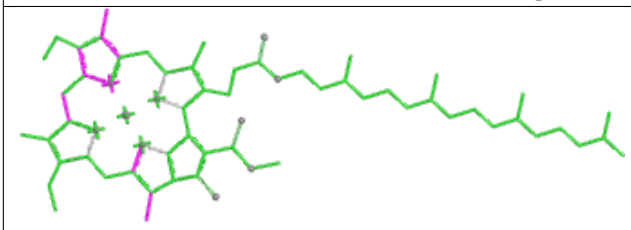


Torsions

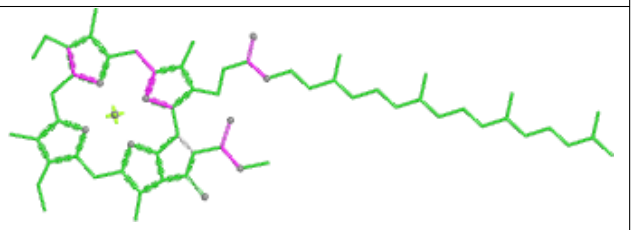


Rings

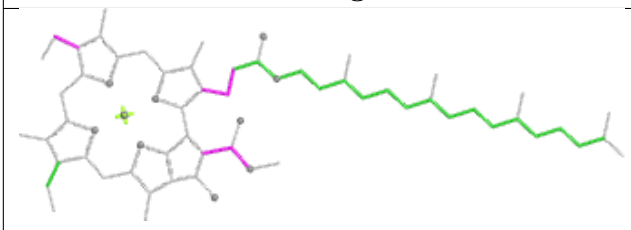
Ligand CLA s 503



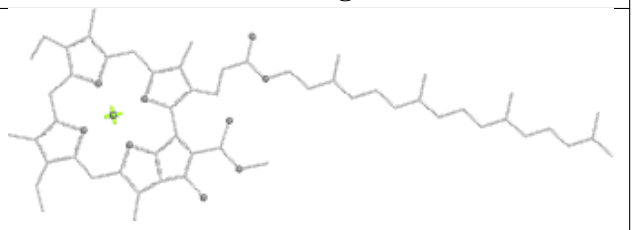
Bond lengths



Bond angles

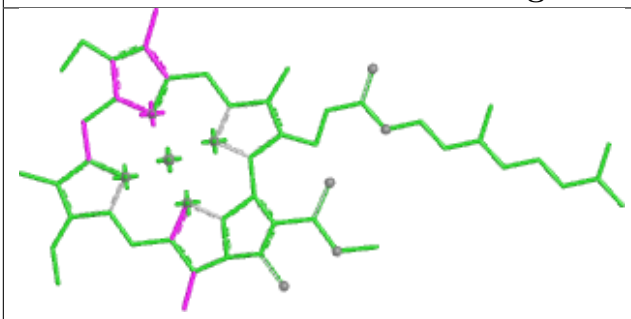


Torsions

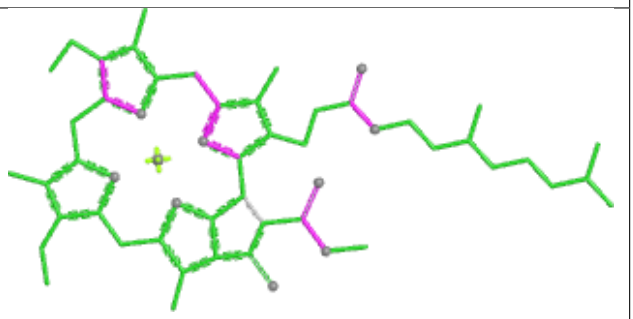


Rings

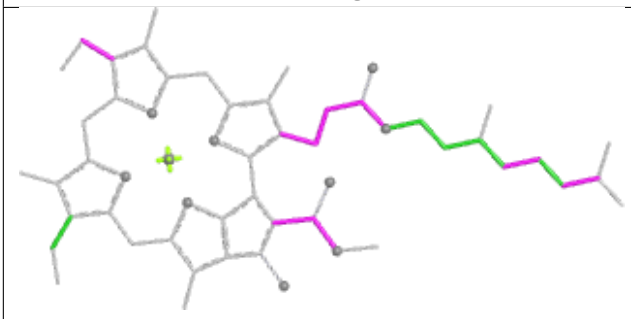
Ligand CLA u 518



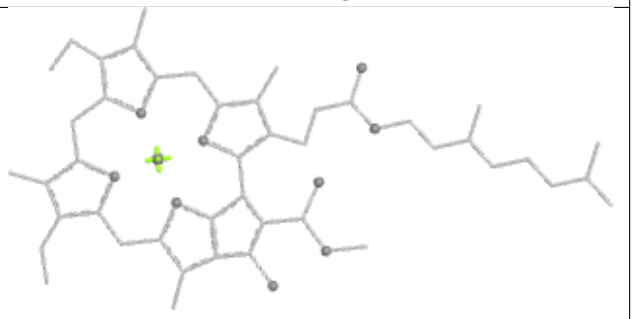
Bond lengths



Bond angles

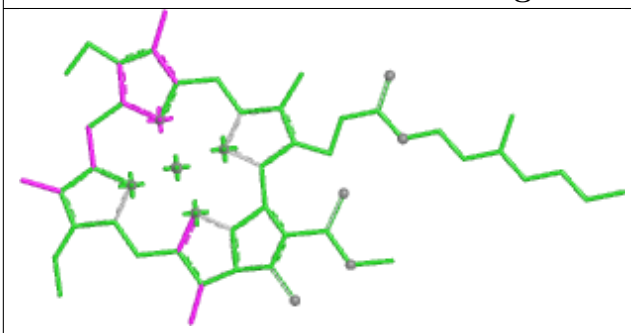


Torsions

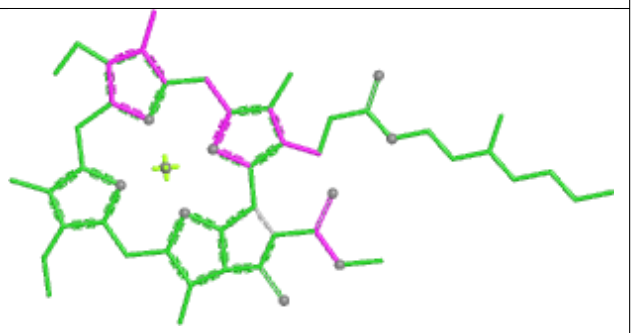


Rings

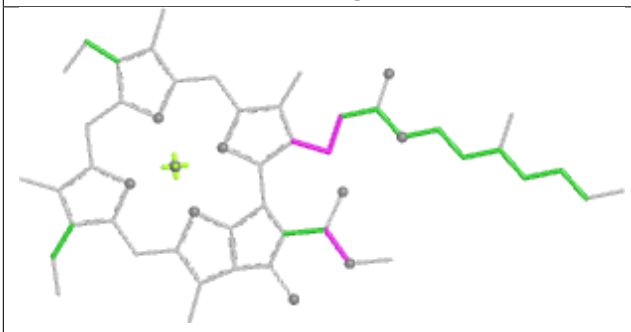
Ligand CLA G 1120



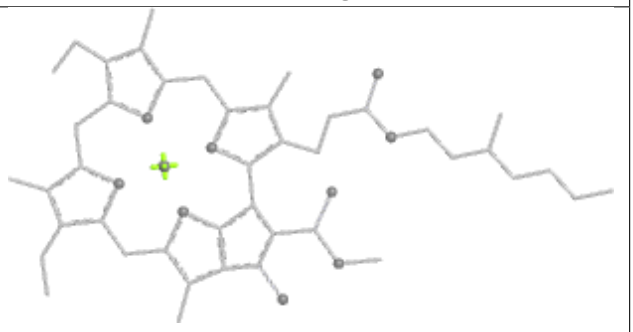
Bond lengths



Bond angles

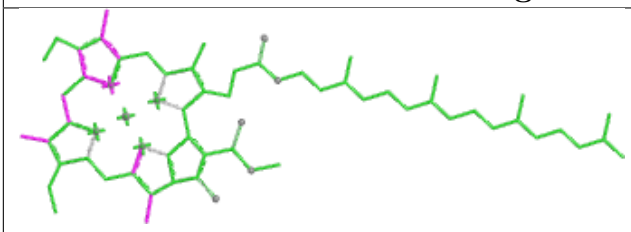


Torsions

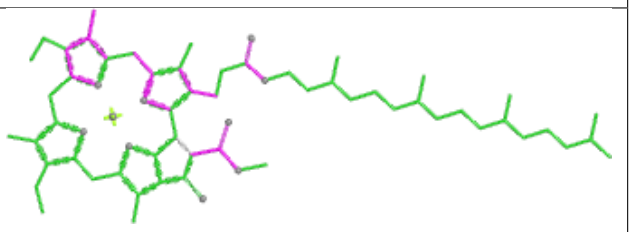


Rings

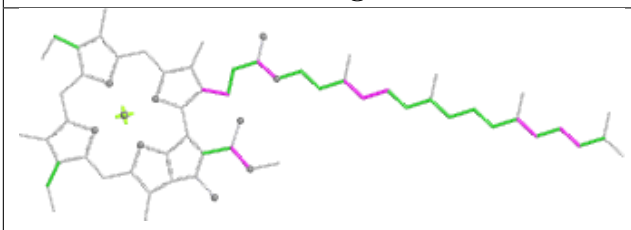
Ligand CLA A 1104



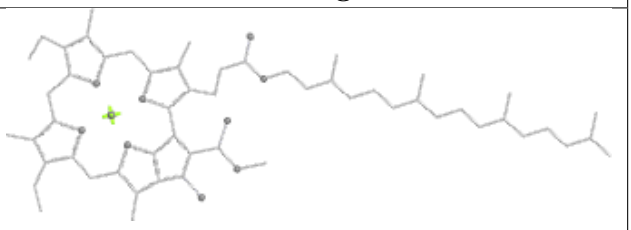
Bond lengths



Bond angles

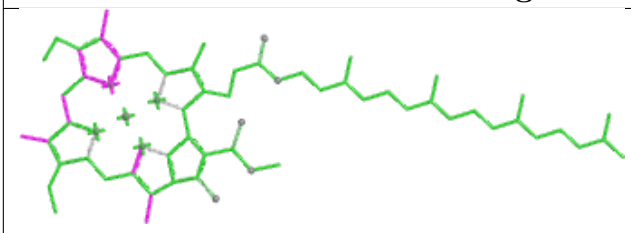


Torsions

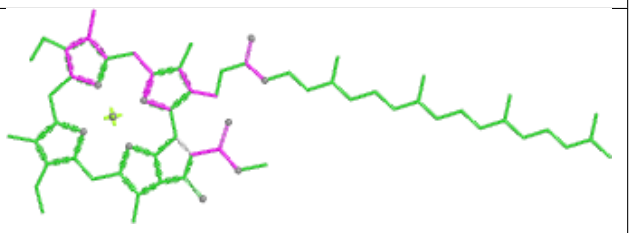


Rings

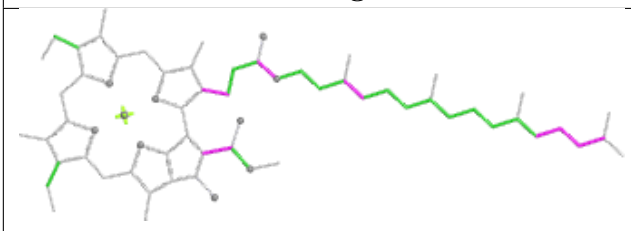
Ligand CLA B 1202



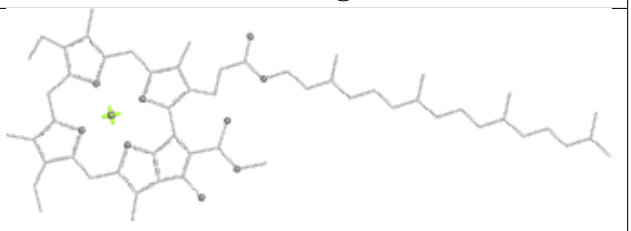
Bond lengths



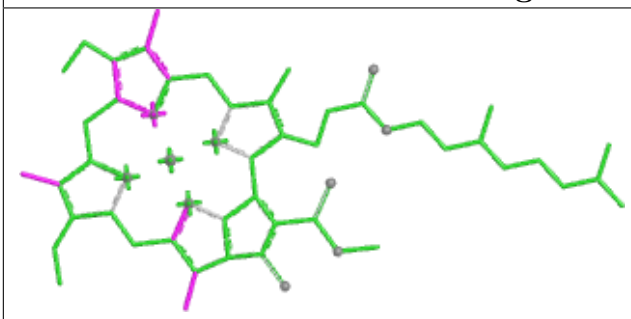
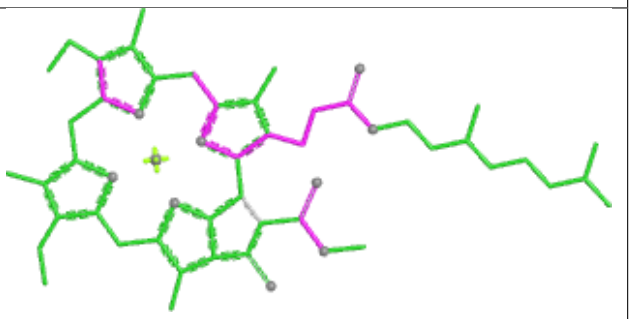
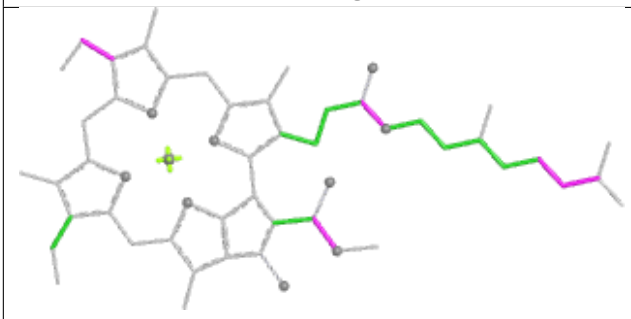
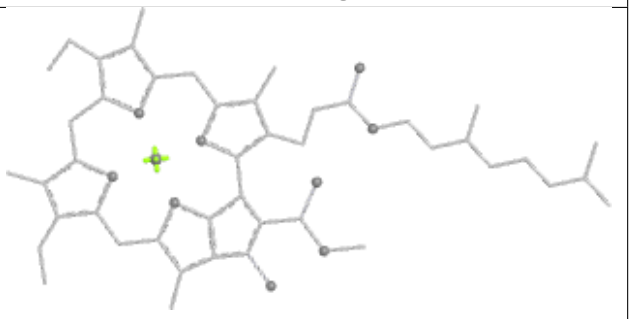
Bond angles

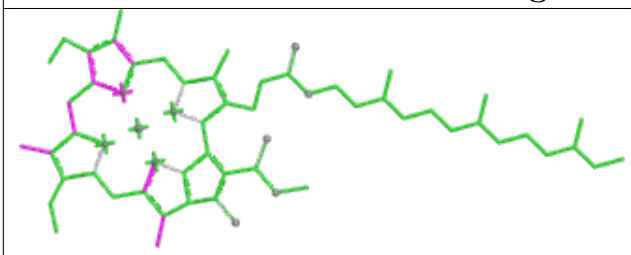
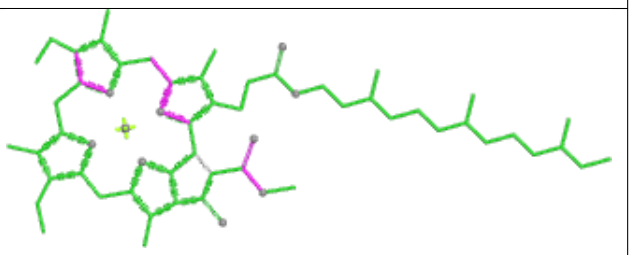
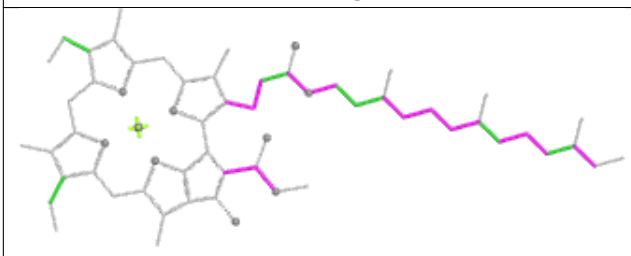
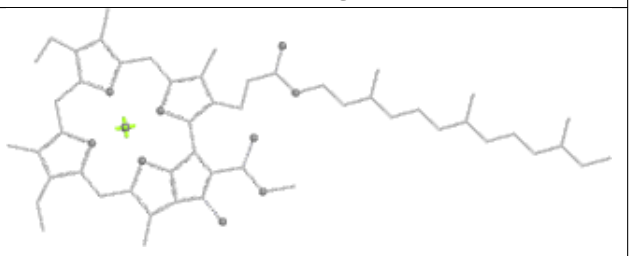


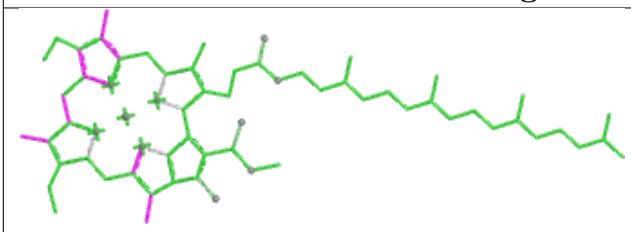
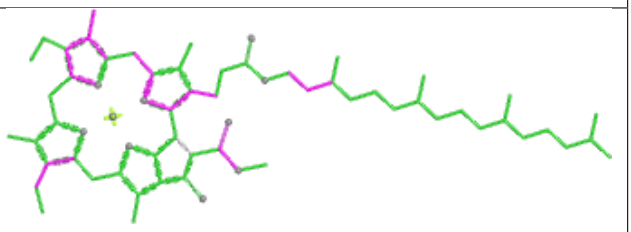
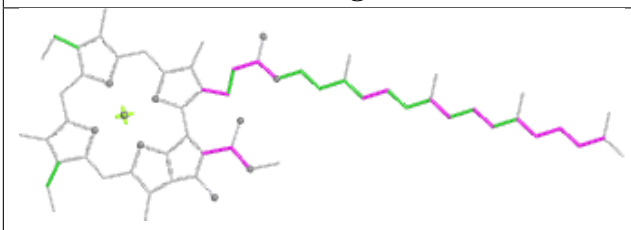
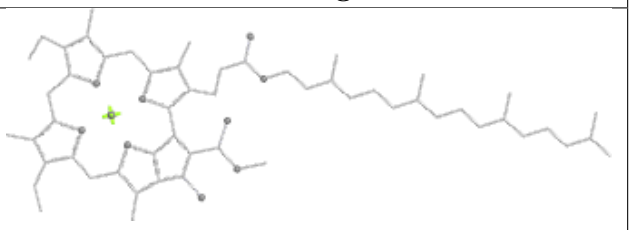
Torsions

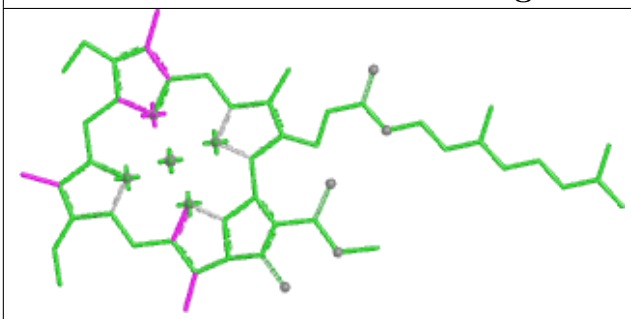
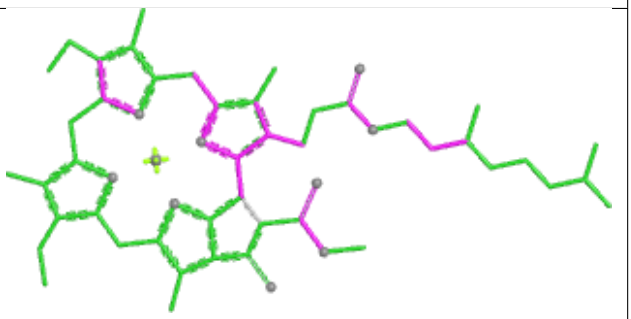
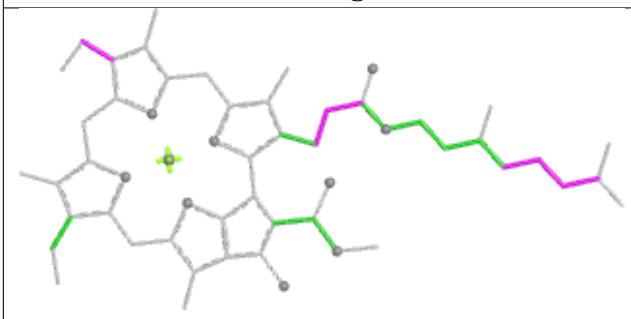
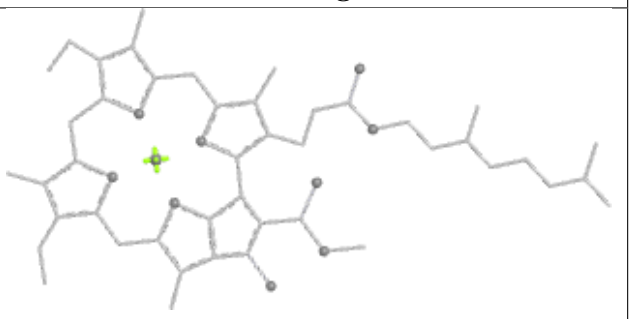


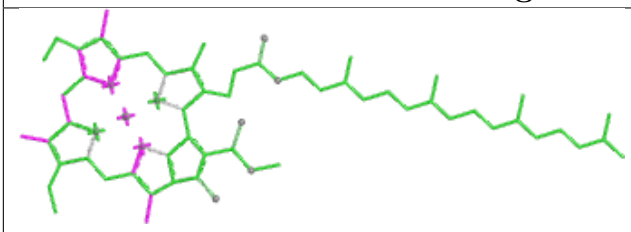
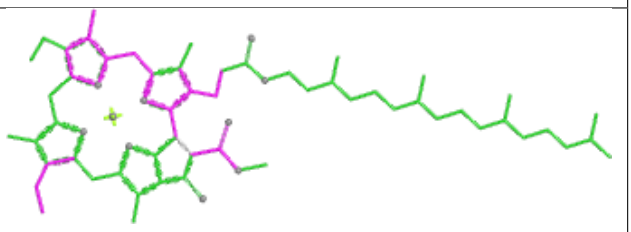
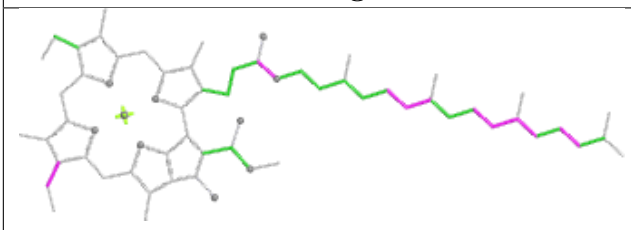
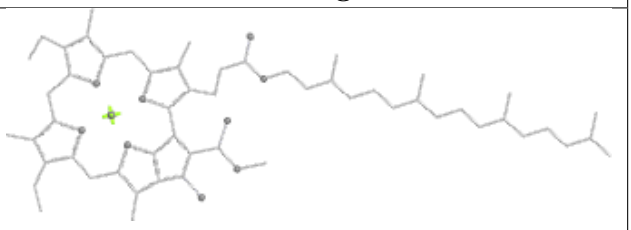
Rings

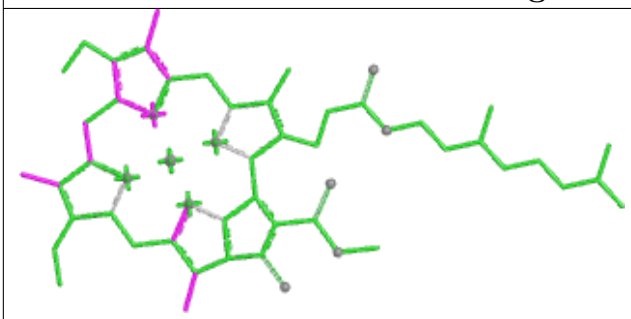
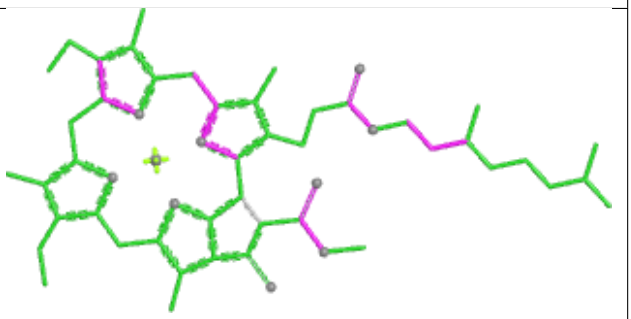
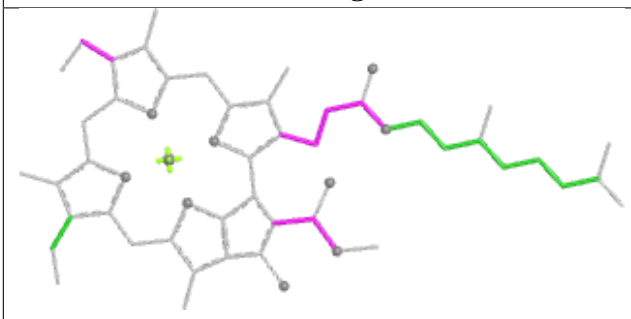
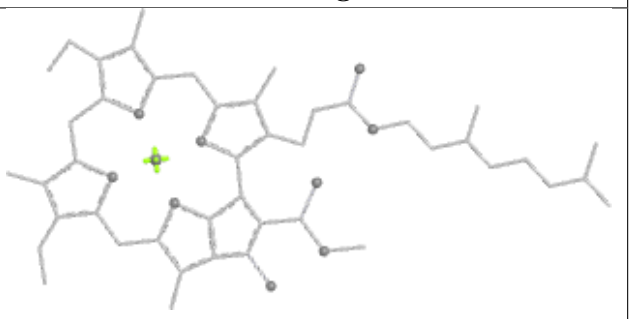
Ligand CLA B 1220	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

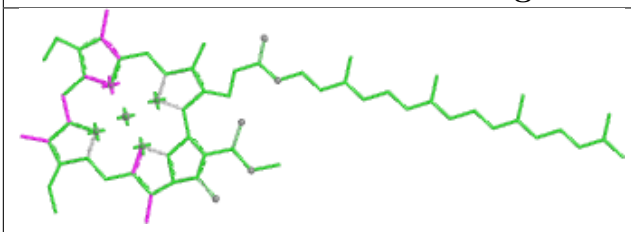
Ligand CLA e 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1121	
 Bond lengths	 Bond angles
 Torsions	 Rings

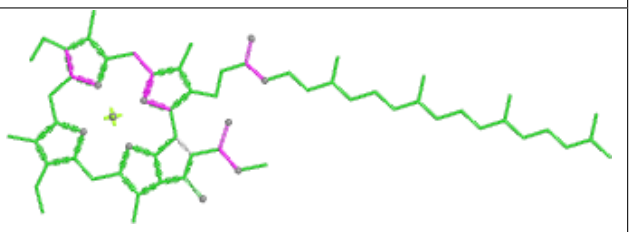
Ligand CLA B 1234	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

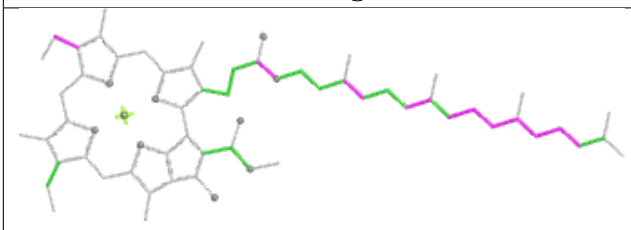
Ligand CLA H 1208



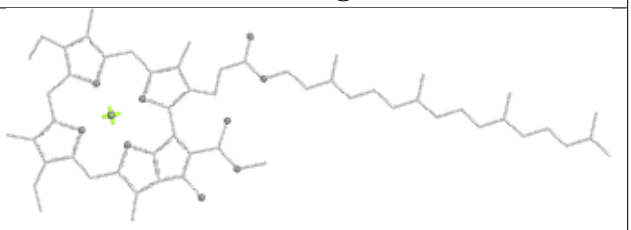
Bond lengths



Bond angles

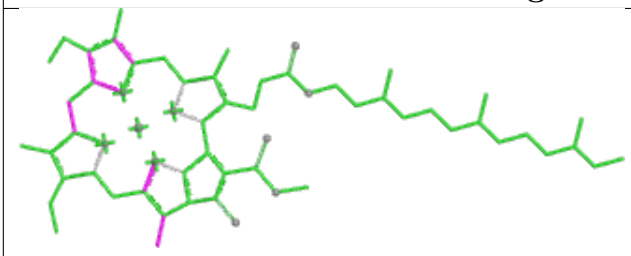


Torsions

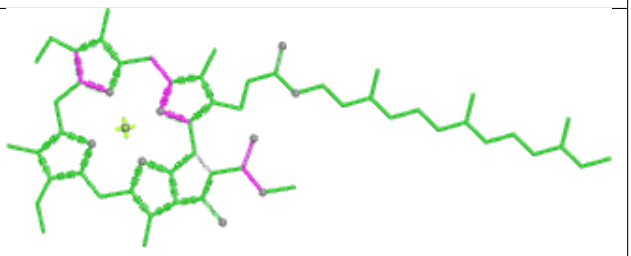


Rings

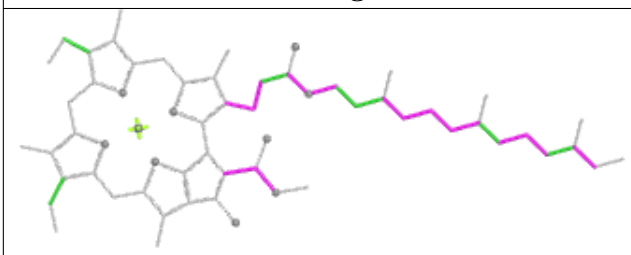
Ligand CLA u 505



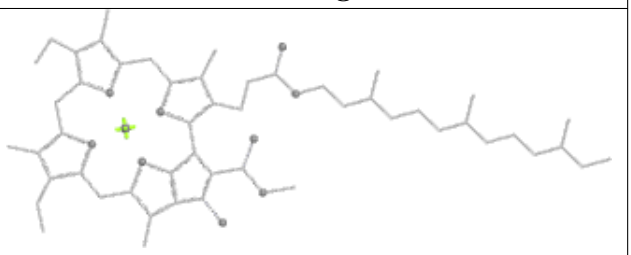
Bond lengths



Bond angles

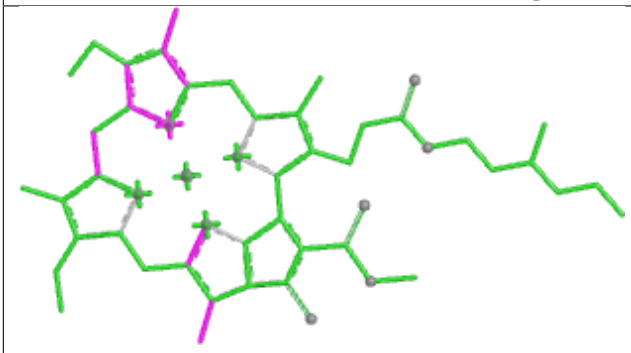


Torsions

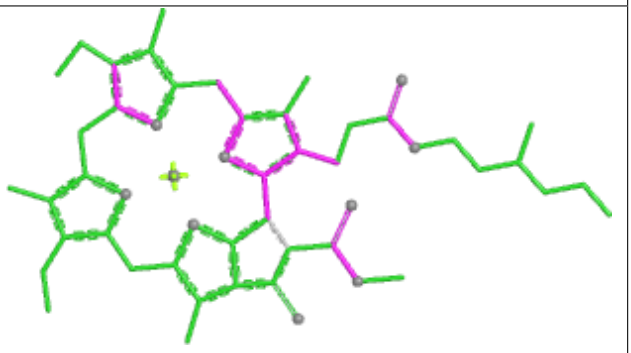


Rings

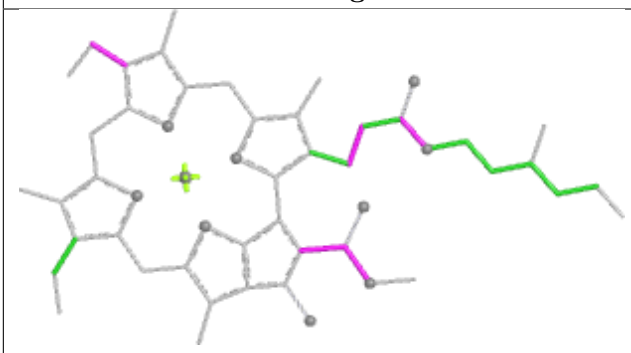
Ligand CLA v 503



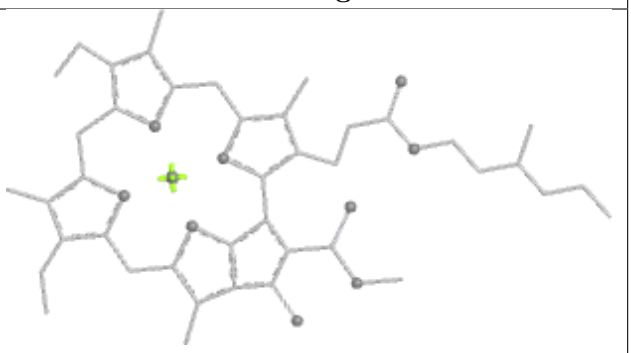
Bond lengths



Bond angles

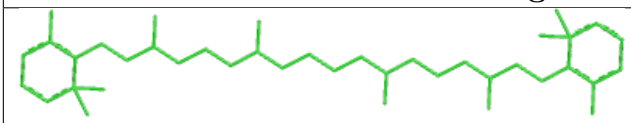


Torsions

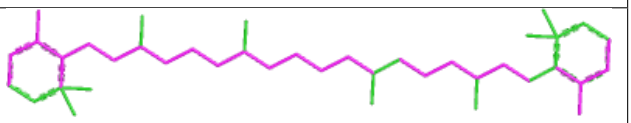


Rings

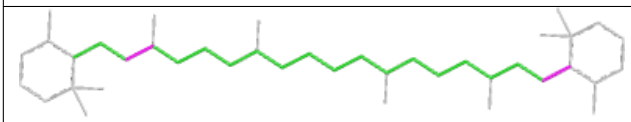
Ligand BCR t 524



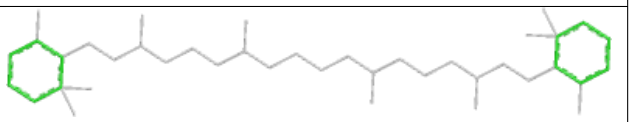
Bond lengths



Bond angles

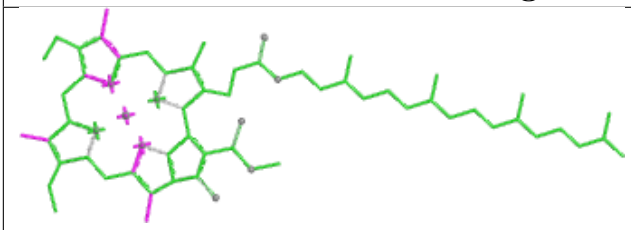


Torsions

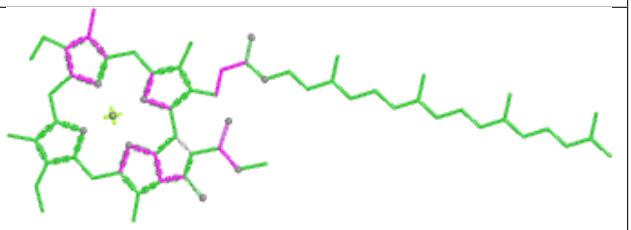


Rings

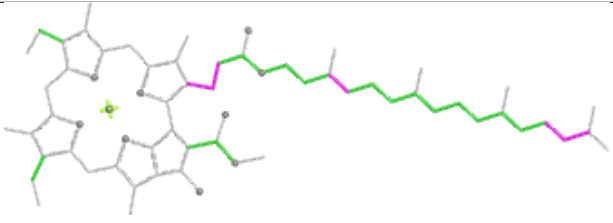
Ligand CLA e 1022



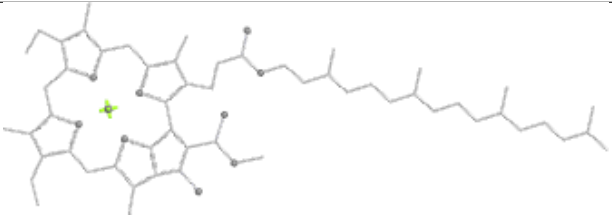
Bond lengths



Bond angles

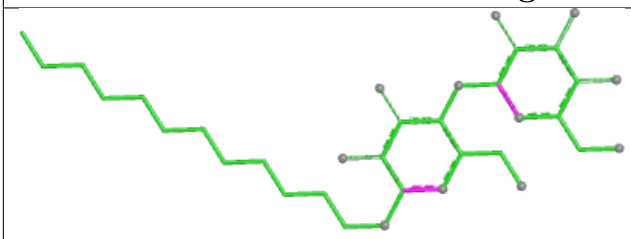


Torsions

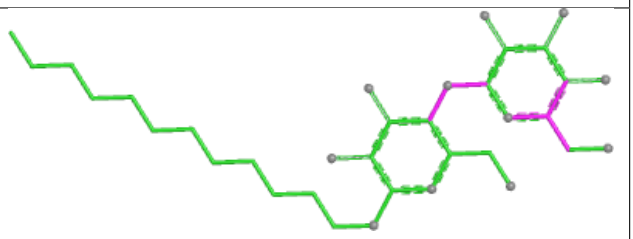


Rings

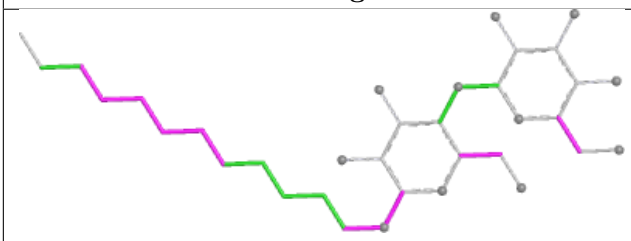
Ligand LMU f 1843



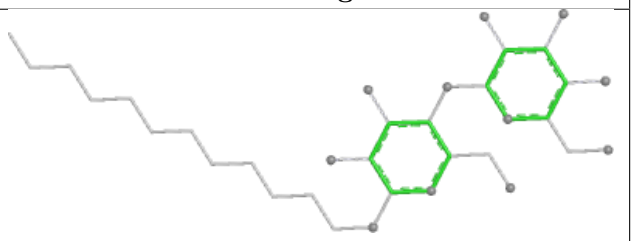
Bond lengths



Bond angles

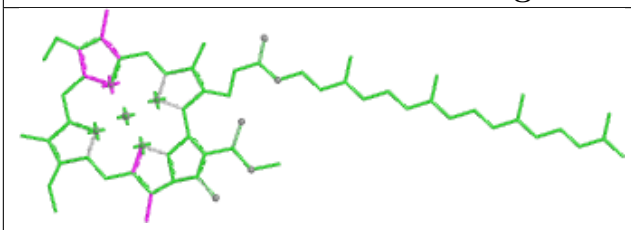


Torsions

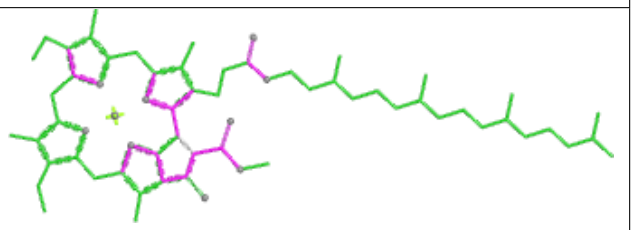


Rings

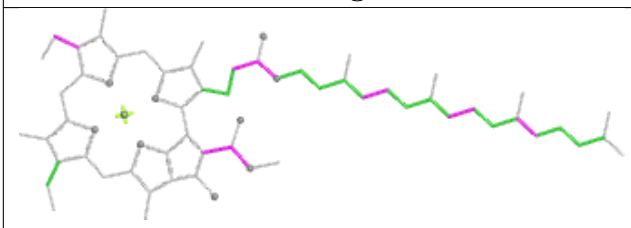
Ligand CLA G 1011



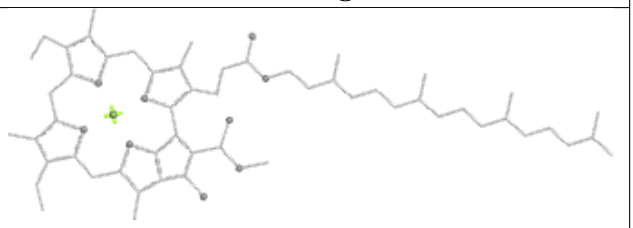
Bond lengths



Bond angles

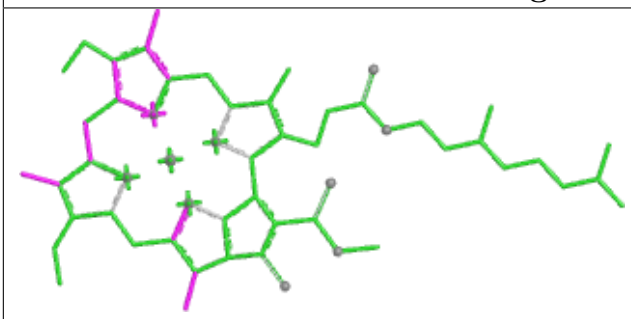


Torsions

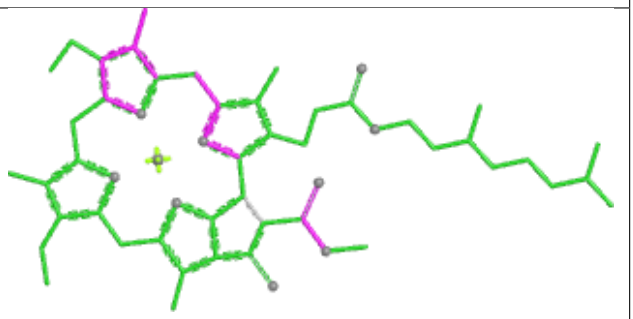


Rings

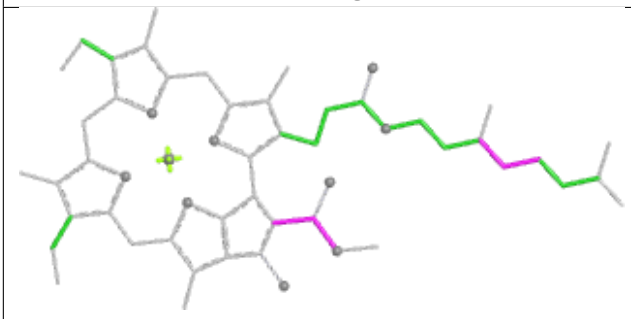
Ligand CLA r 506



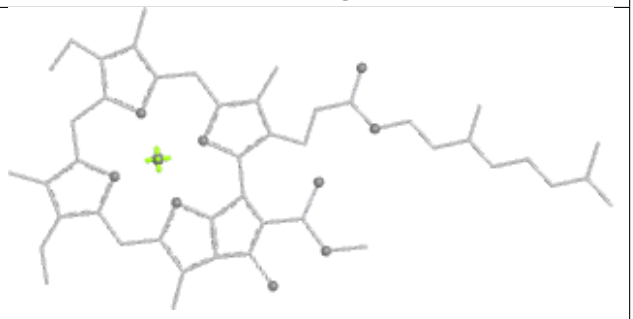
Bond lengths



Bond angles

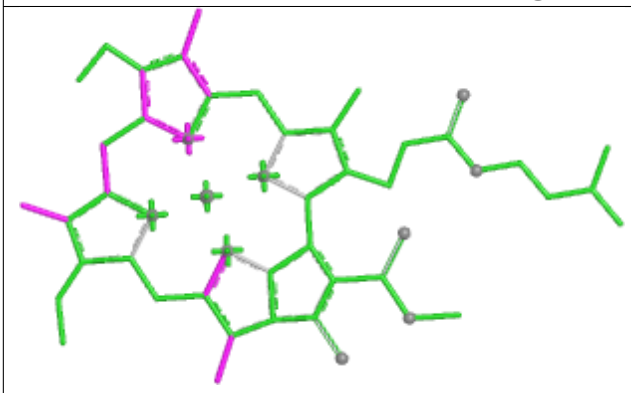


Torsions

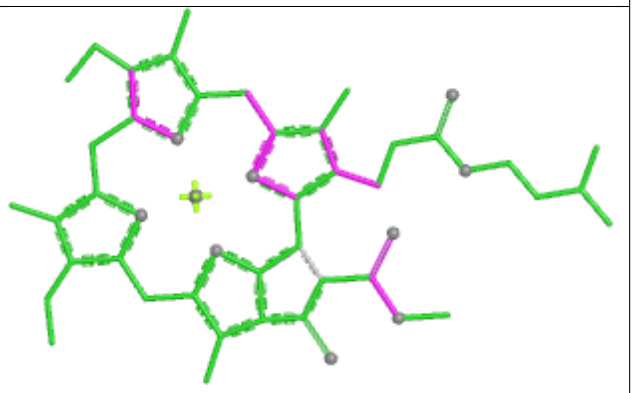


Rings

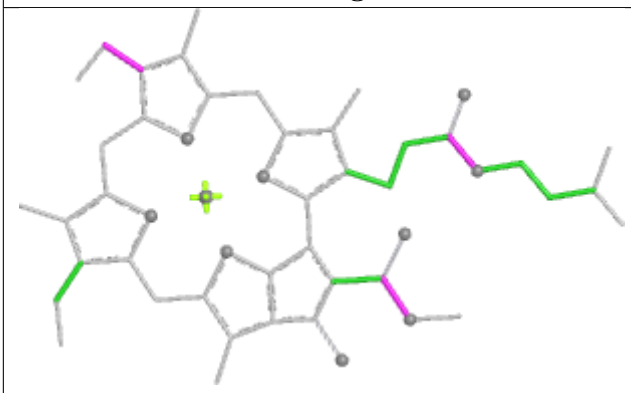
Ligand CLA c 502



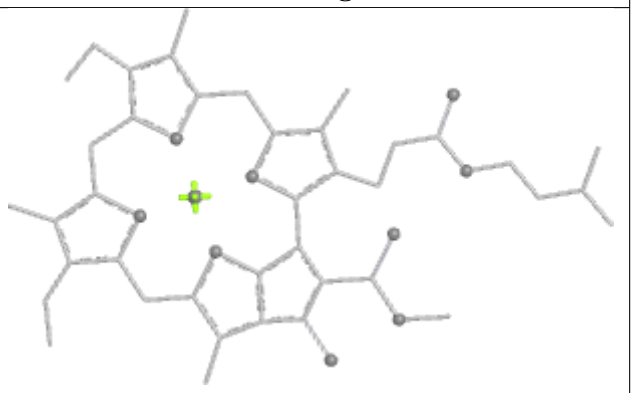
Bond lengths



Bond angles

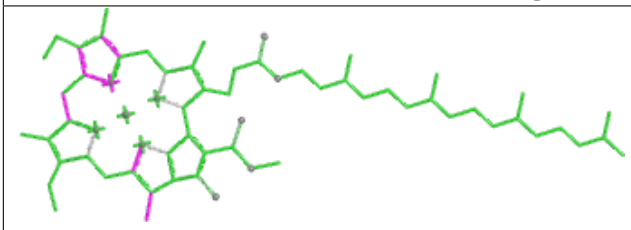


Torsions

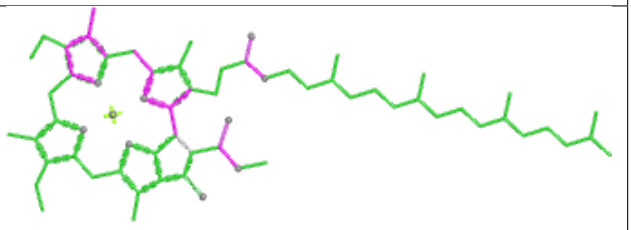


Rings

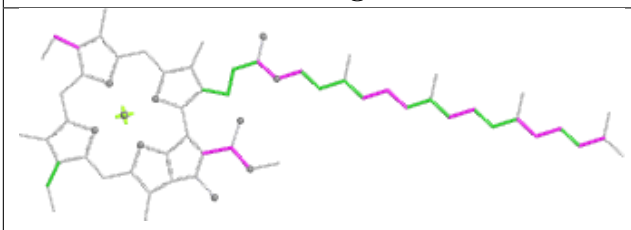
Ligand CLA 3 510



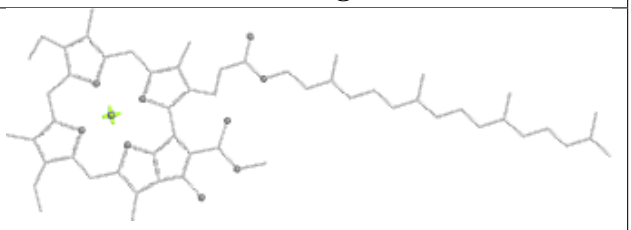
Bond lengths



Bond angles

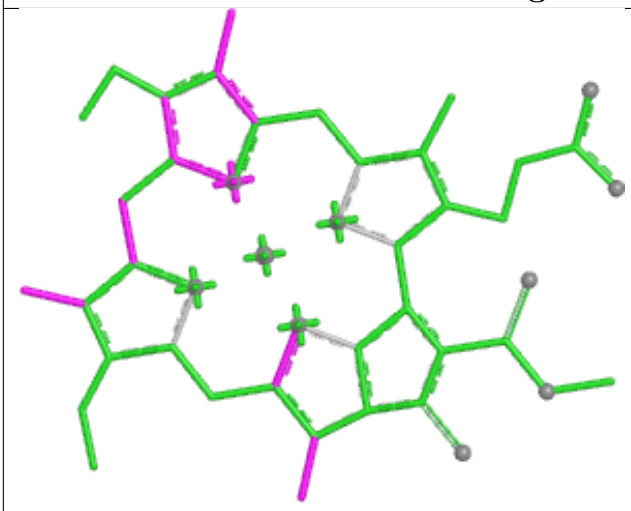


Torsions

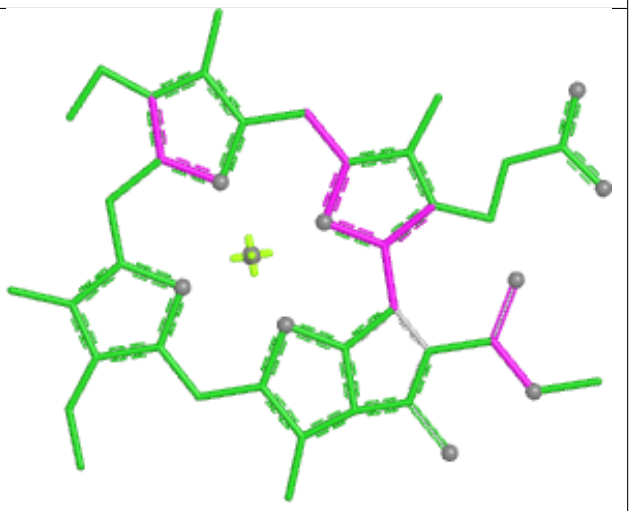


Rings

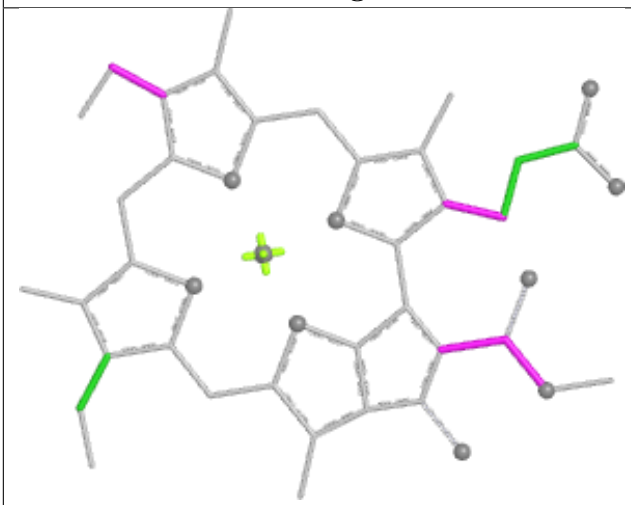
Ligand CLA 4 517



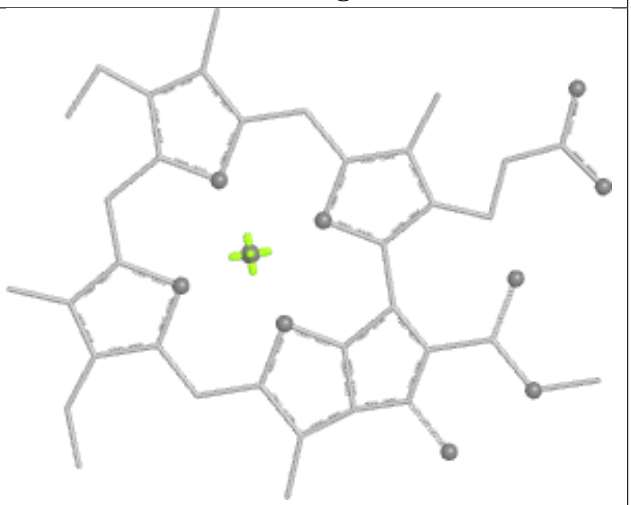
Bond lengths



Bond angles

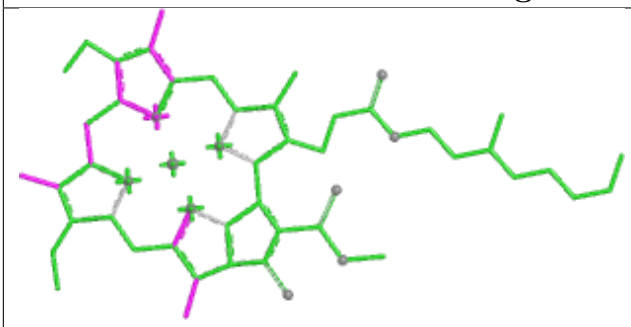


Torsions

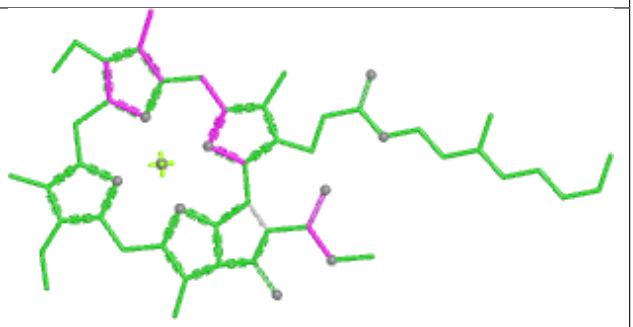


Rings

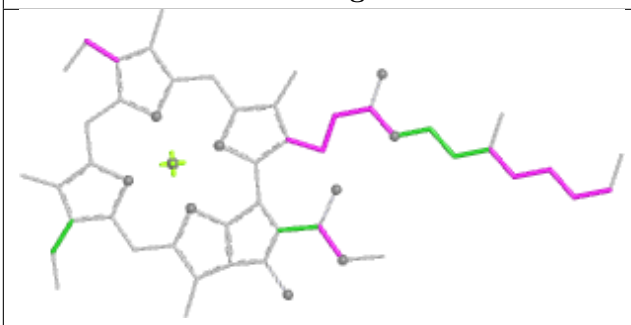
Ligand CLA A 1108



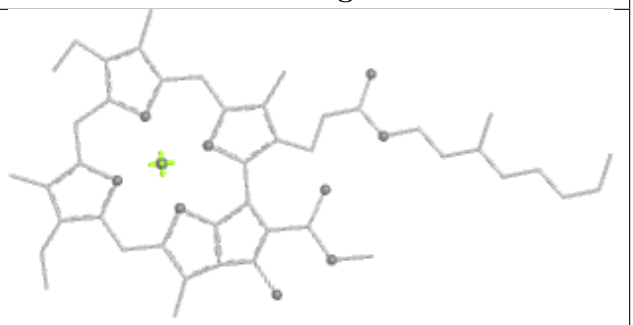
Bond lengths



Bond angles

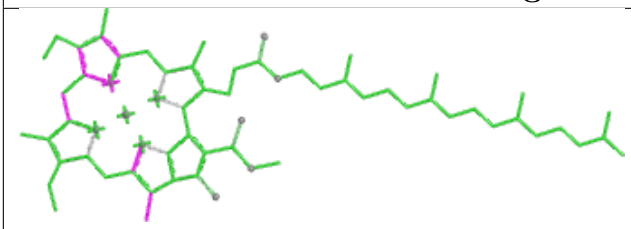


Torsions

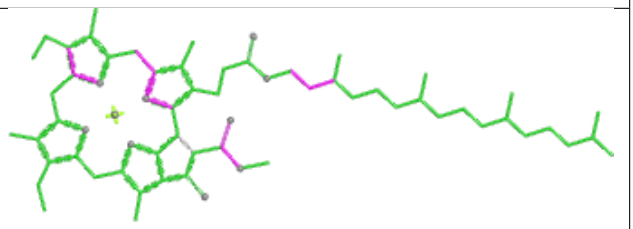


Rings

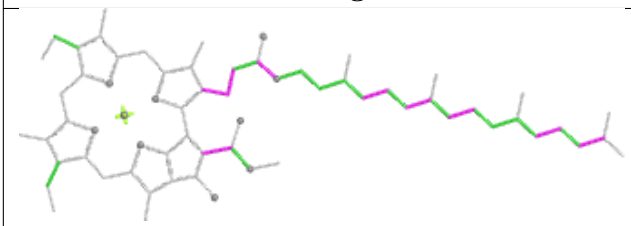
Ligand CLA Y 505



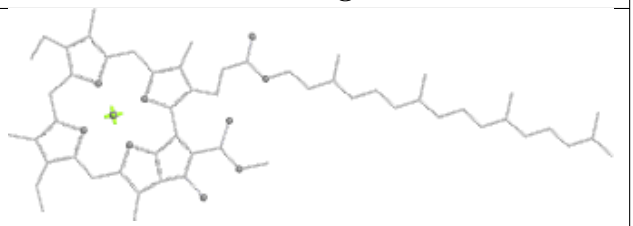
Bond lengths



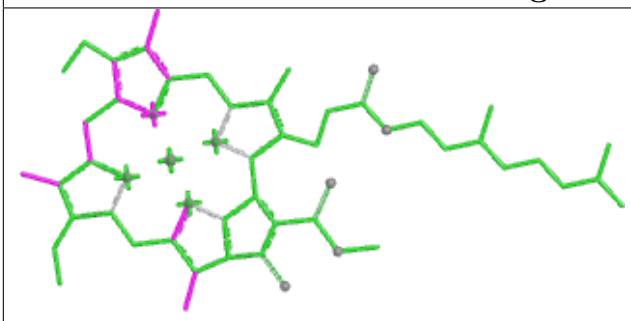
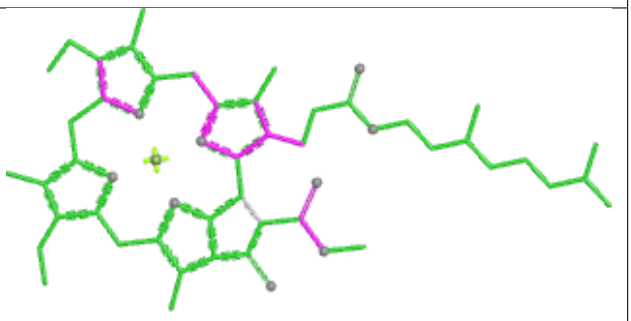
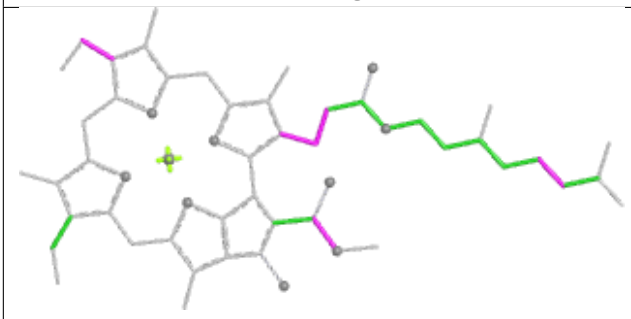
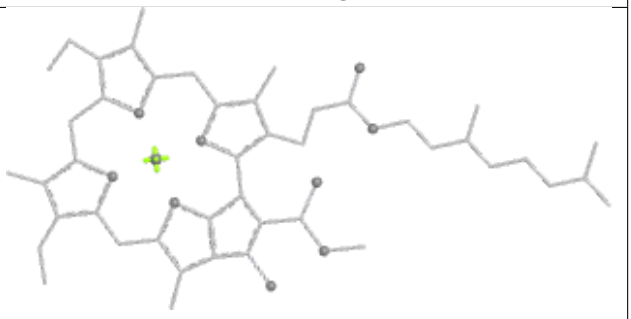
Bond angles

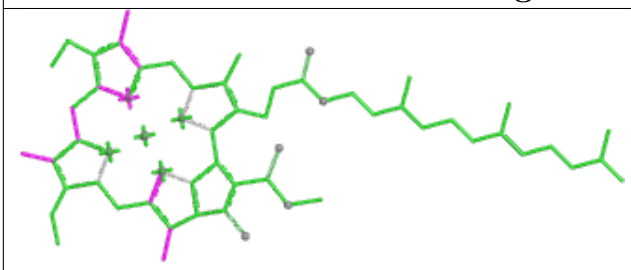
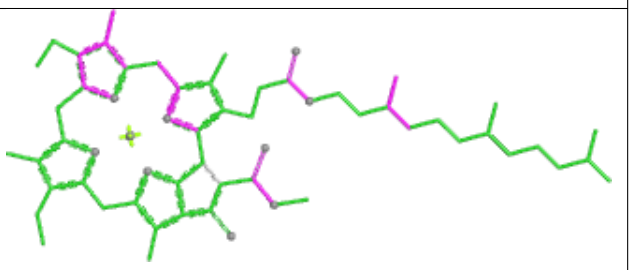
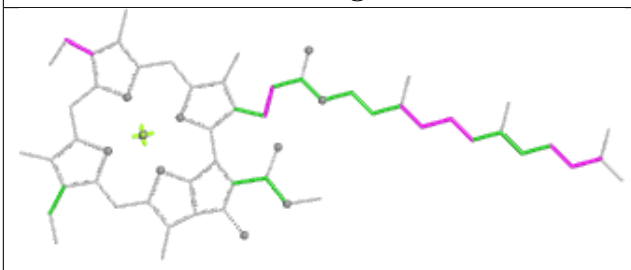
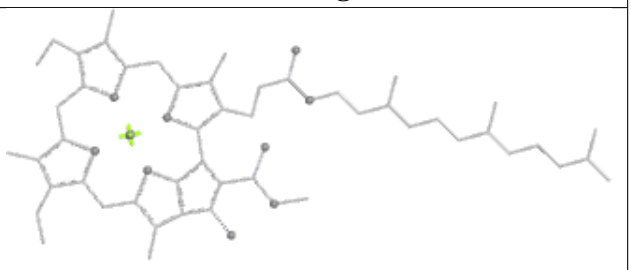


Torsions

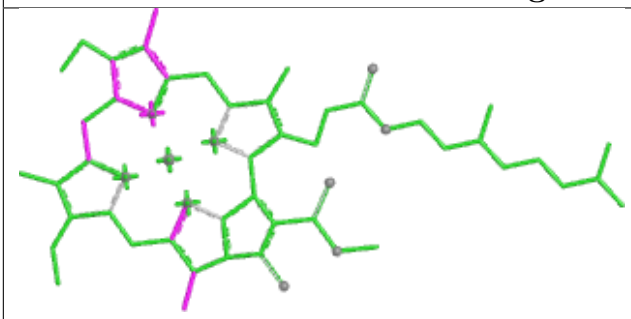


Rings

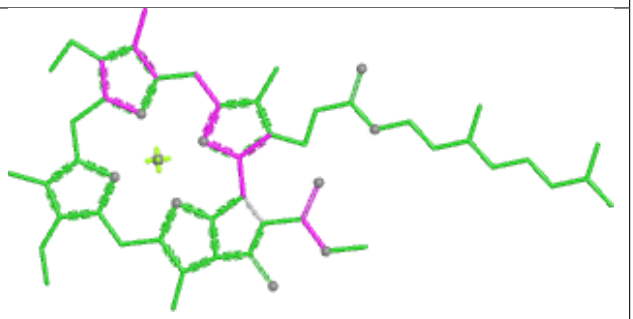
Ligand CLA r 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1115	
 Bond lengths	 Bond angles
 Torsions	 Rings

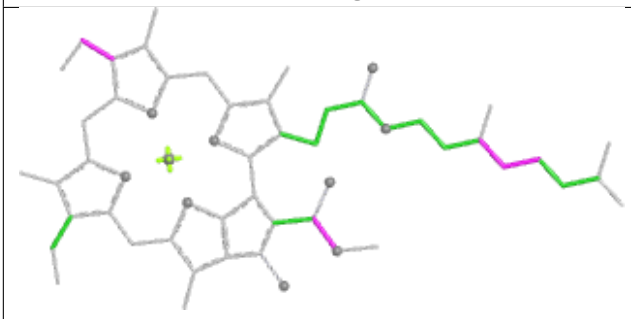
Ligand CLA 2 511



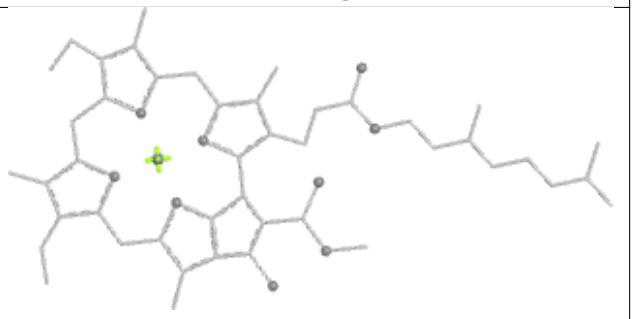
Bond lengths



Bond angles

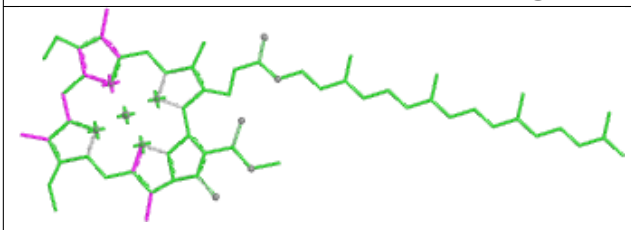


Torsions

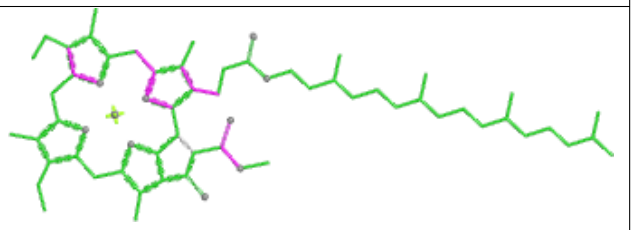


Rings

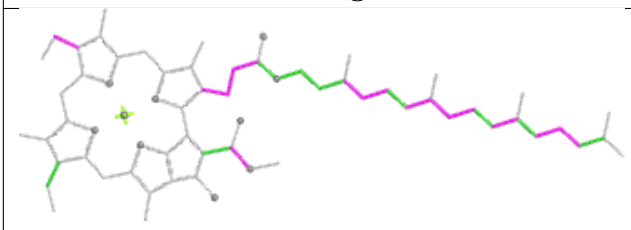
Ligand CLA c 501



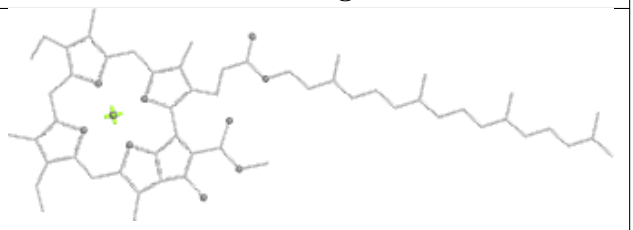
Bond lengths



Bond angles

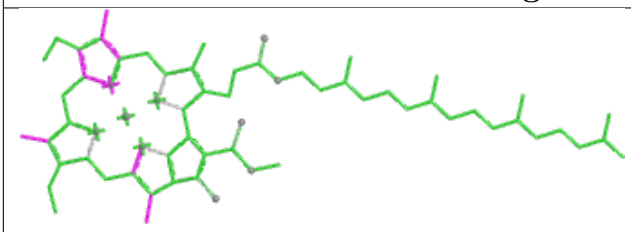


Torsions

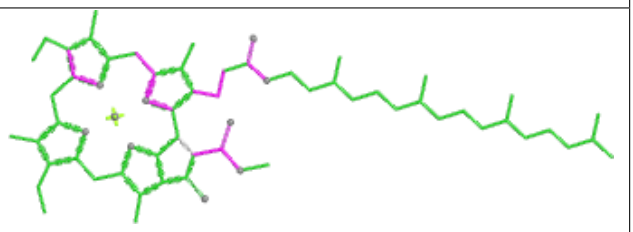


Rings

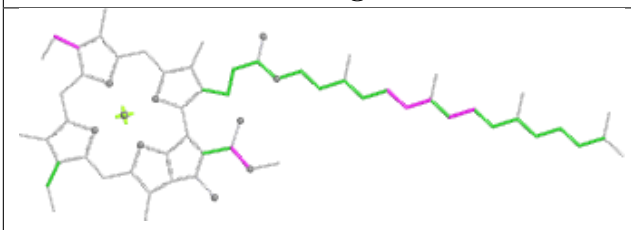
Ligand CLA f 1235



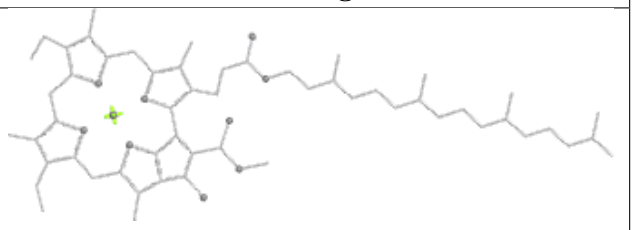
Bond lengths



Bond angles



Torsions

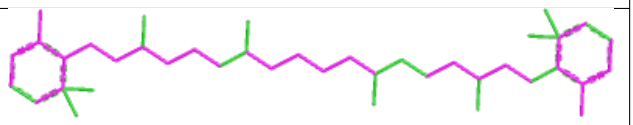


Rings

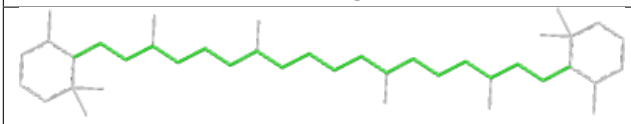
Ligand BCR A 4007



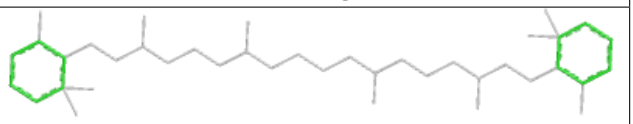
Bond lengths



Bond angles

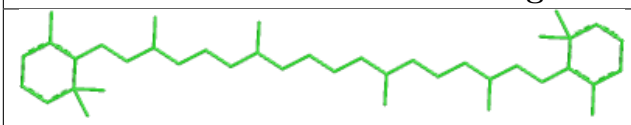


Torsions

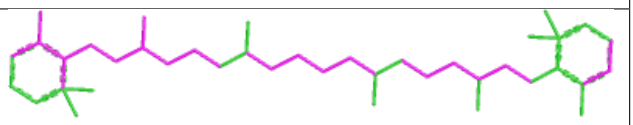


Rings

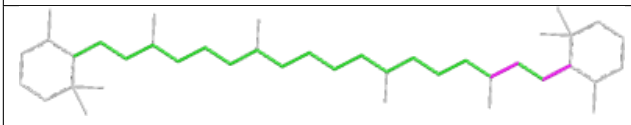
Ligand BCR 6 523



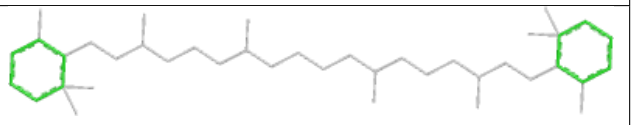
Bond lengths



Bond angles

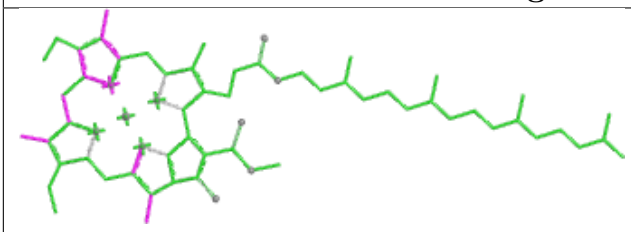


Torsions

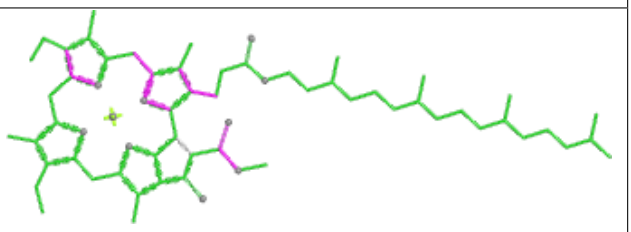


Rings

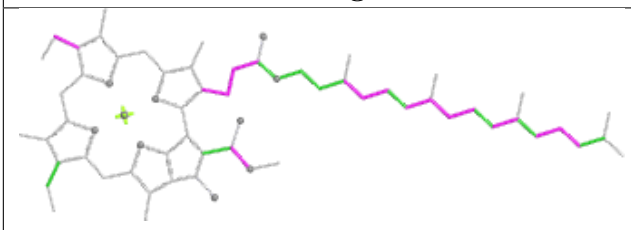
Ligand CLA u 501



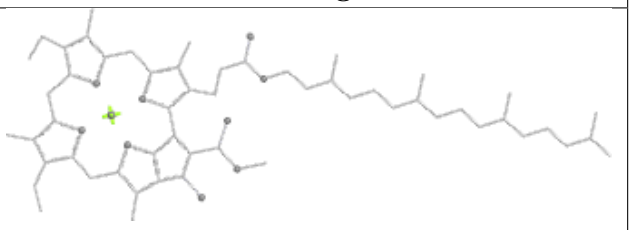
Bond lengths



Bond angles



Torsions

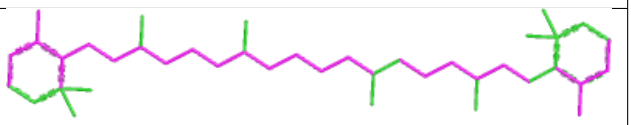


Rings

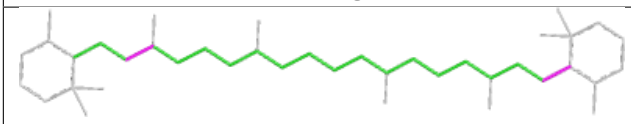
Ligand BCR b 524



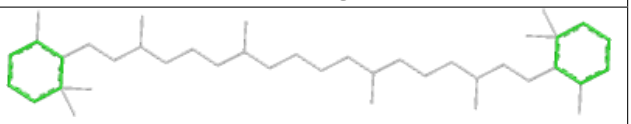
Bond lengths



Bond angles

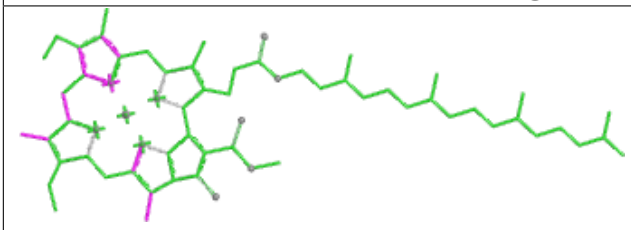


Torsions

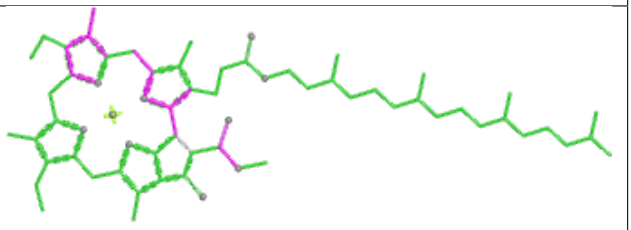


Rings

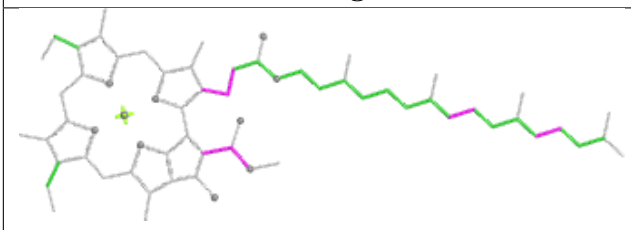
Ligand CLA Z 503



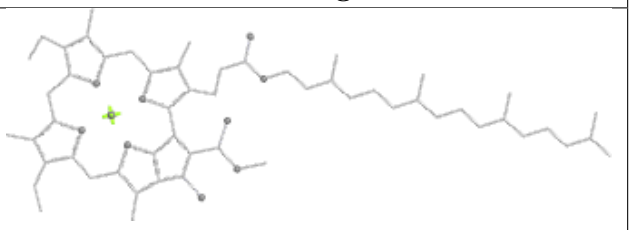
Bond lengths



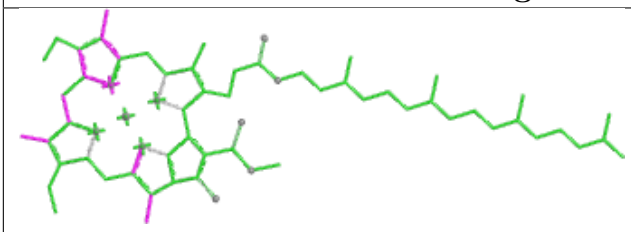
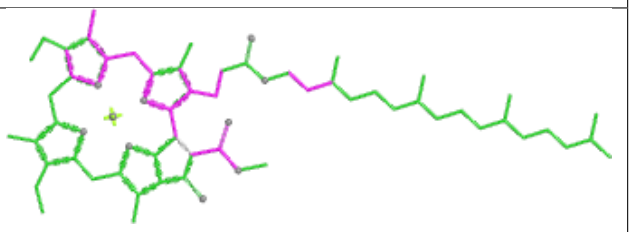
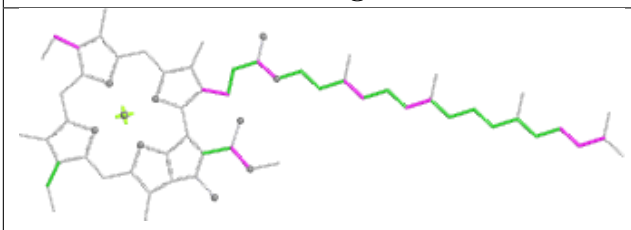
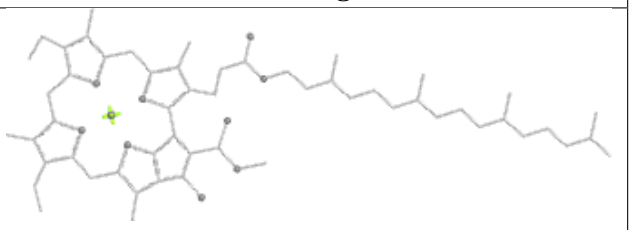
Bond angles

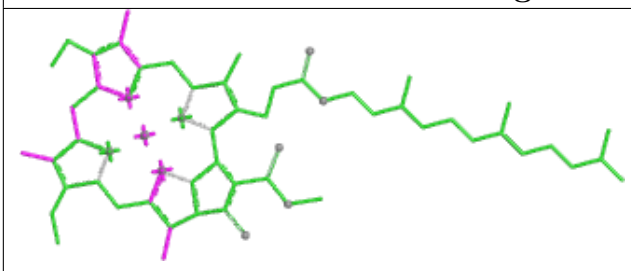
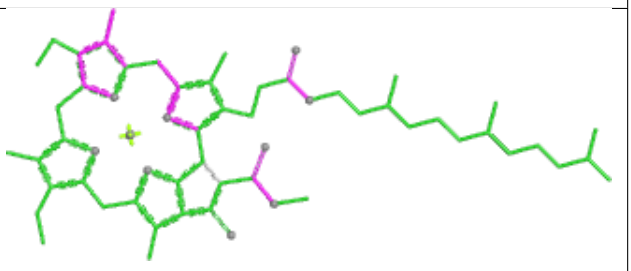
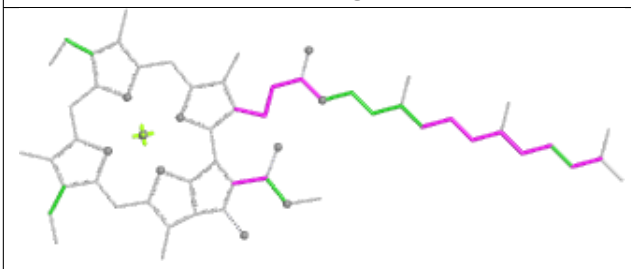
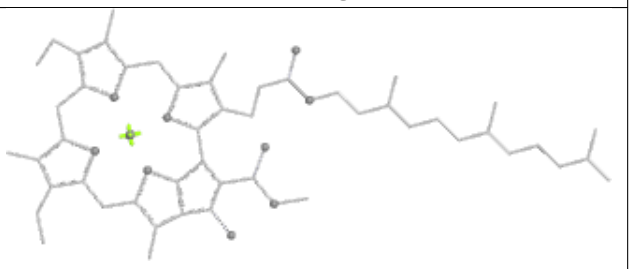


Torsions

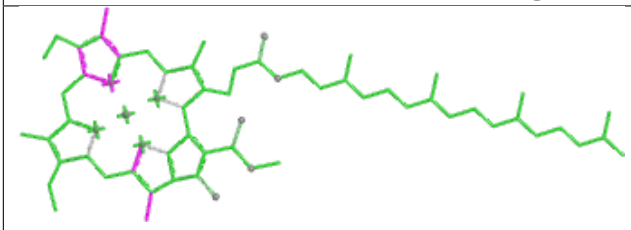


Rings

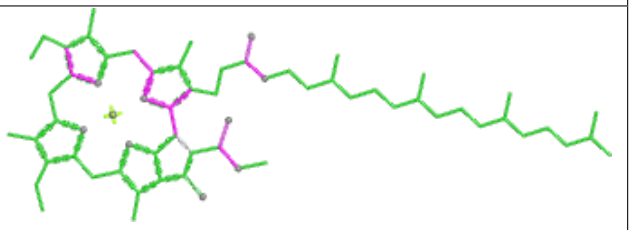
Ligand CLA G 1140	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1116	
 Bond lengths	 Bond angles
 Torsions	 Rings

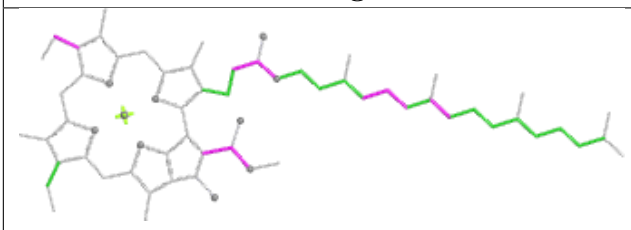
Ligand CLA 3 507



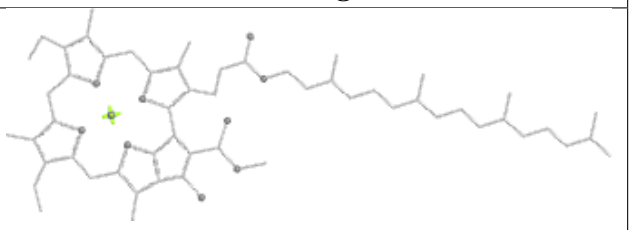
Bond lengths



Bond angles

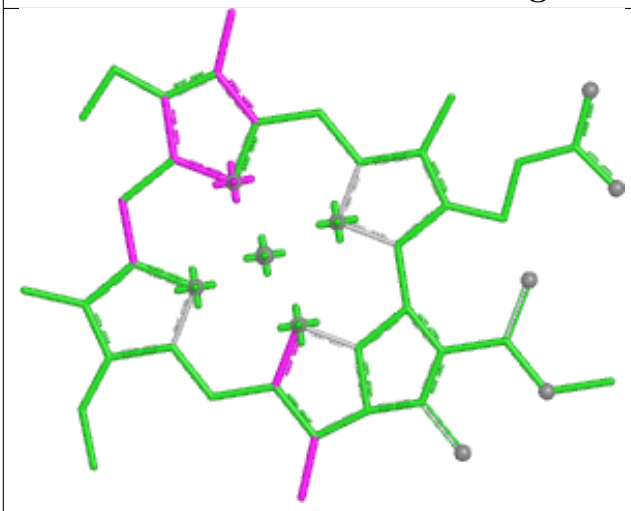


Torsions

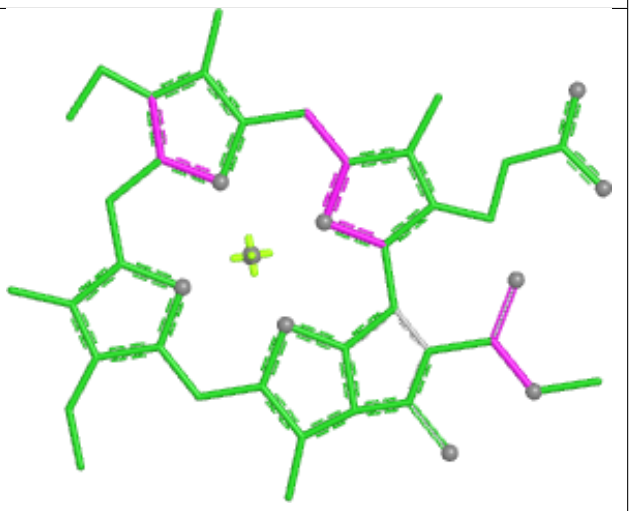


Rings

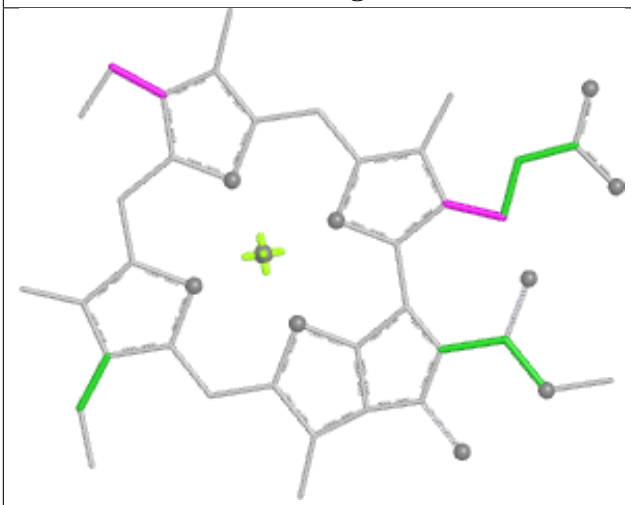
Ligand CLA c 516



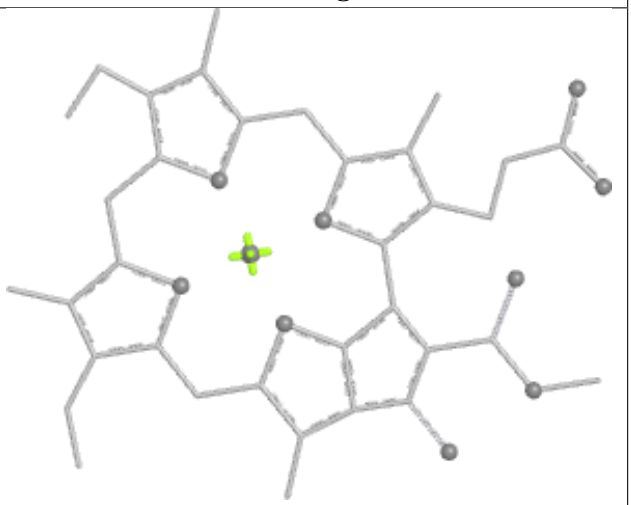
Bond lengths



Bond angles

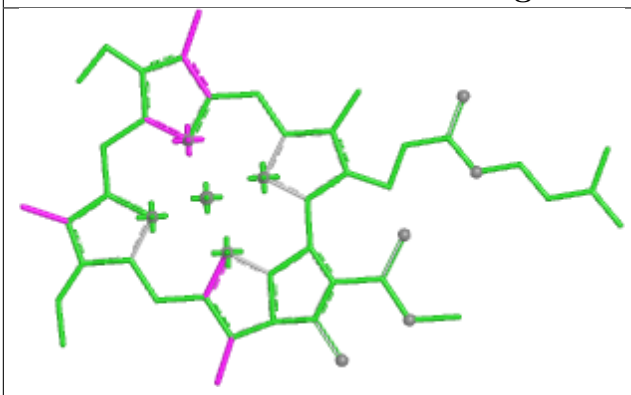


Torsions

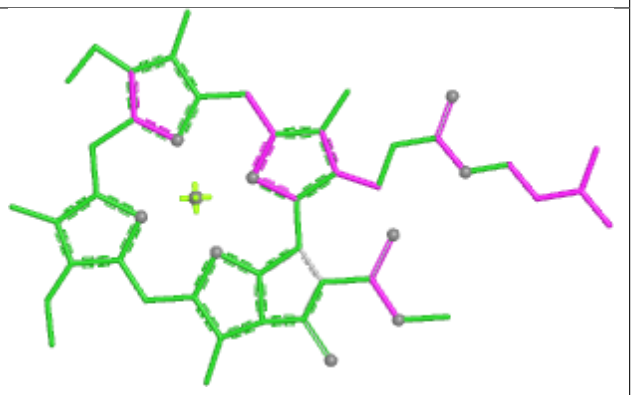


Rings

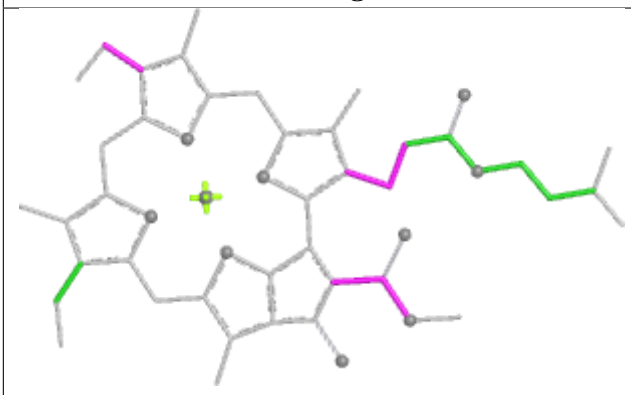
Ligand CLA K 1103



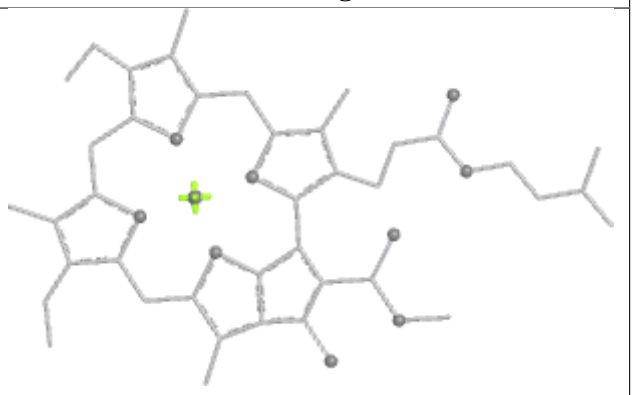
Bond lengths



Bond angles

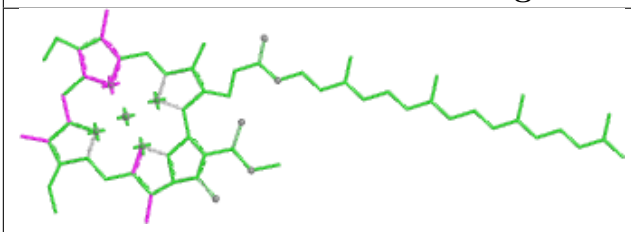


Torsions

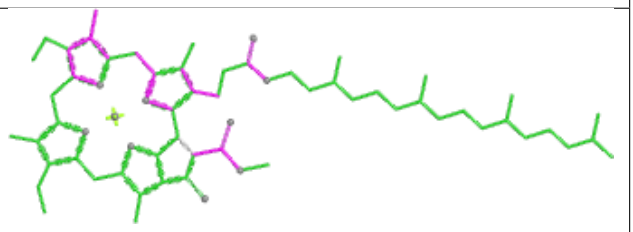


Rings

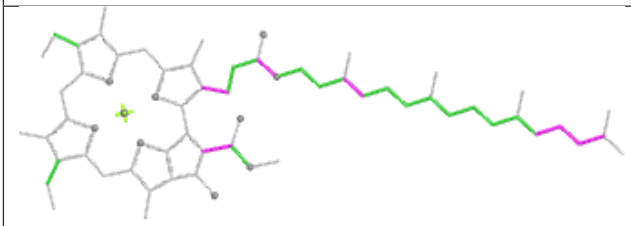
Ligand CLA H 1202



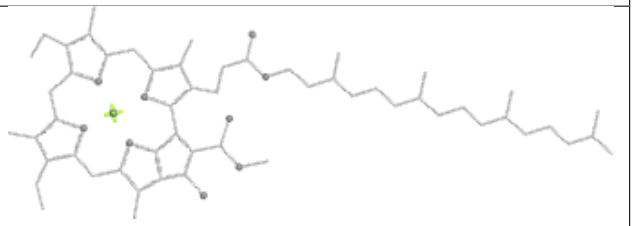
Bond lengths



Bond angles

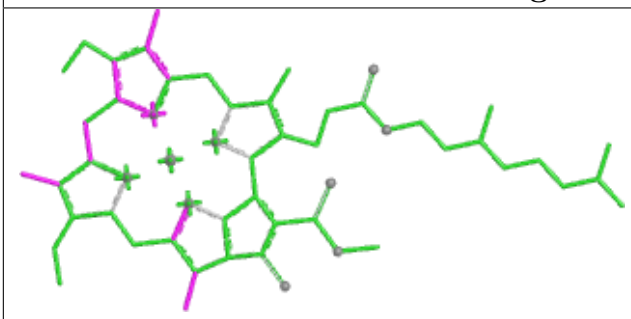


Torsions

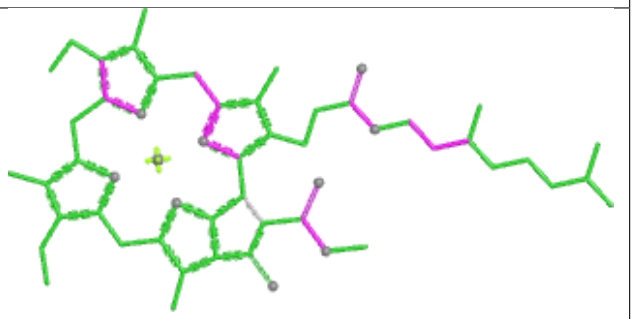


Rings

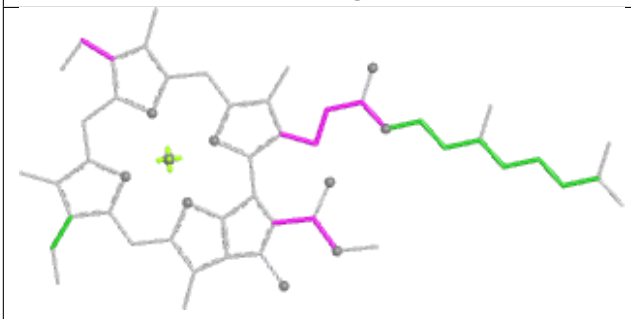
Ligand CLA s 518



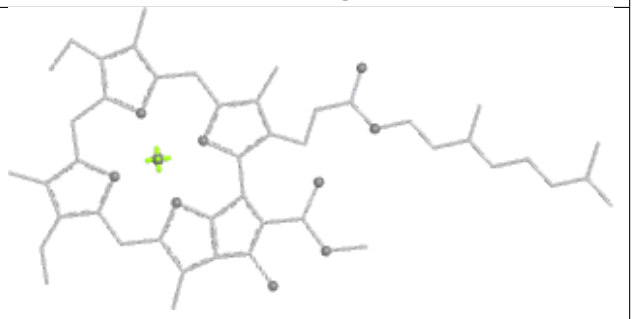
Bond lengths



Bond angles

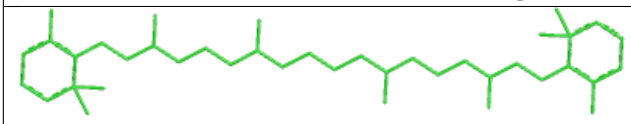


Torsions

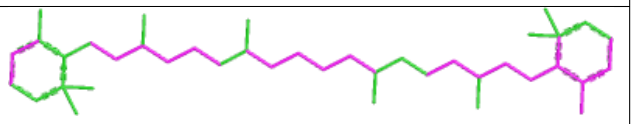


Rings

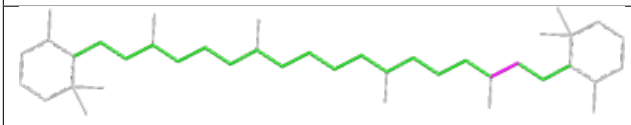
Ligand BCR m 4104



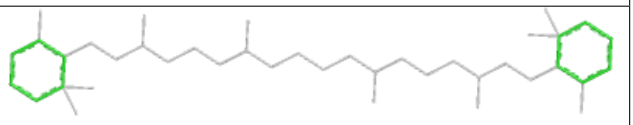
Bond lengths



Bond angles

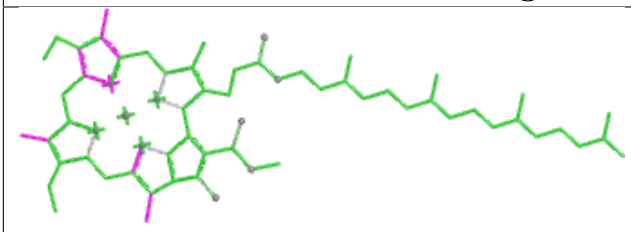


Torsions

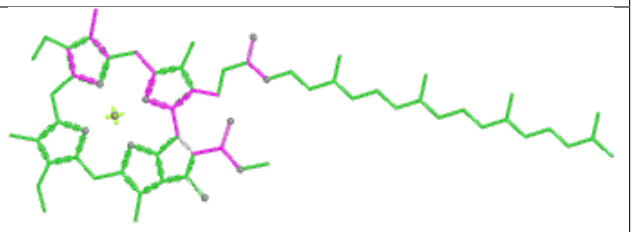


Rings

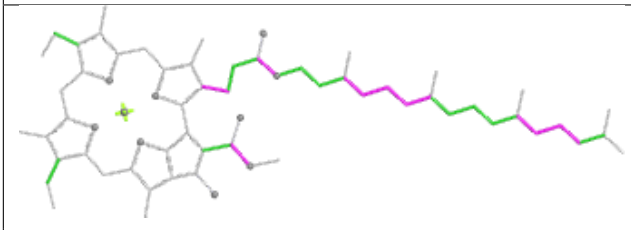
Ligand CLA J 1303



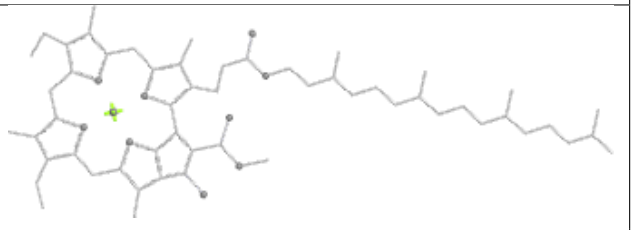
Bond lengths



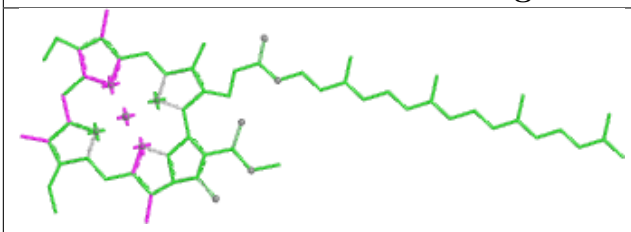
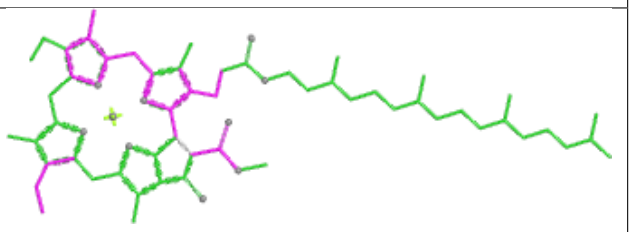
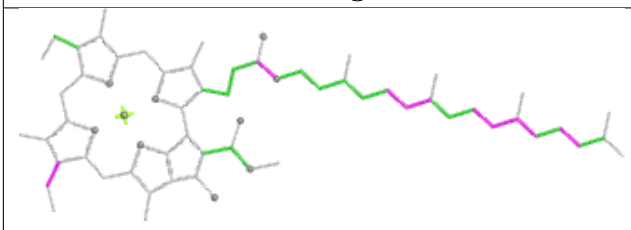
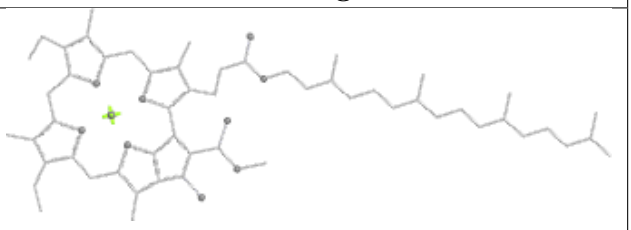
Bond angles

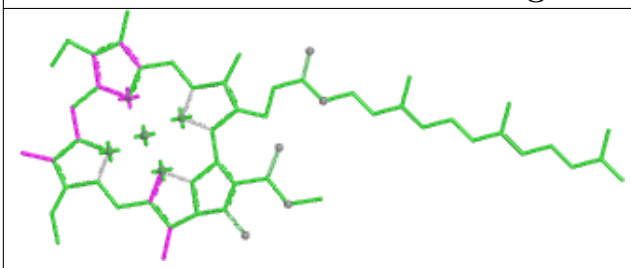
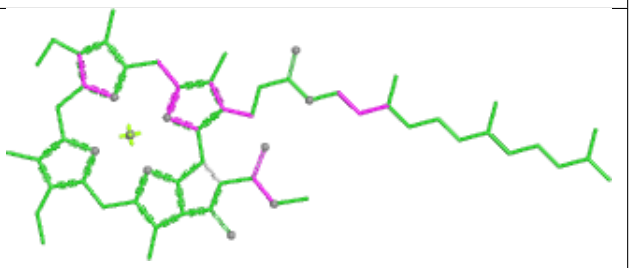
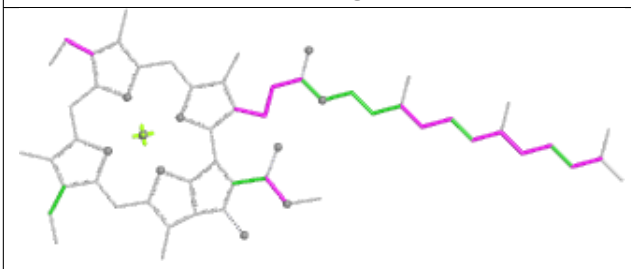
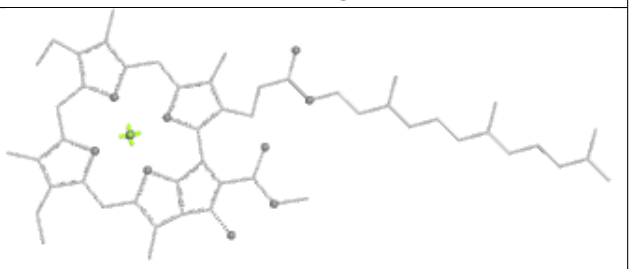


Torsions

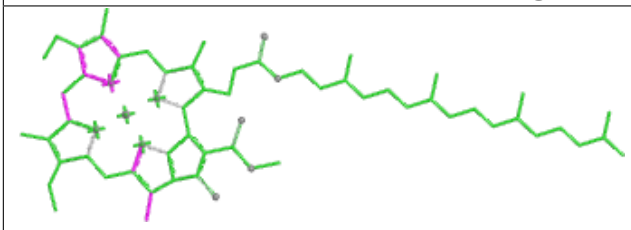


Rings

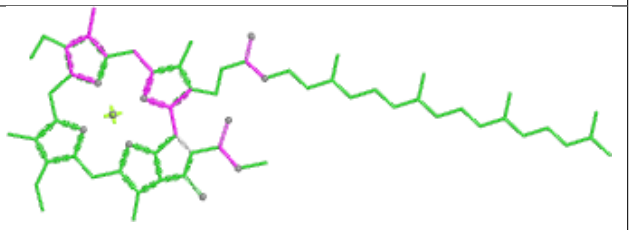
Ligand CLA H 1234	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

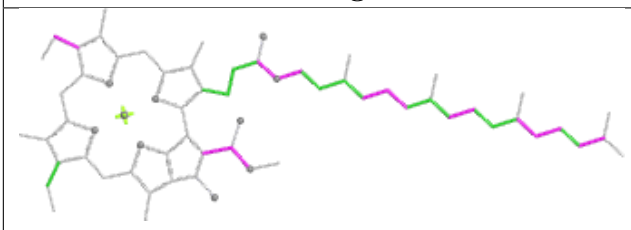
Ligand CLA s 510



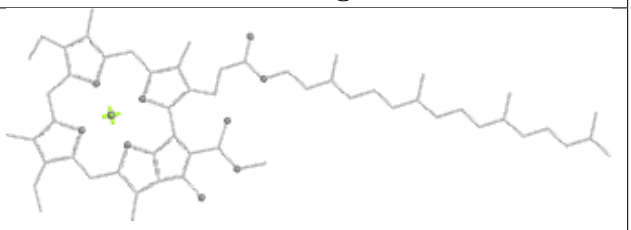
Bond lengths



Bond angles



Torsions

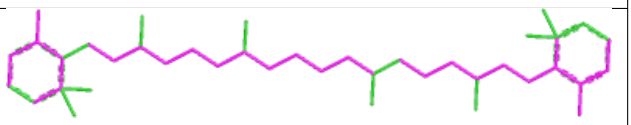


Rings

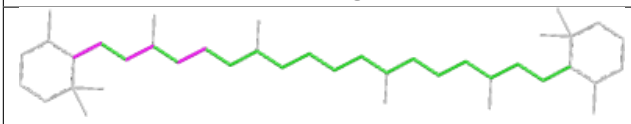
Ligand BCR a 522



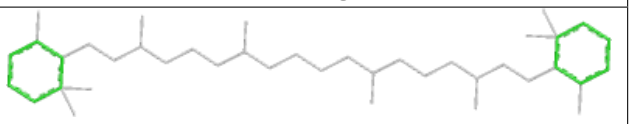
Bond lengths



Bond angles

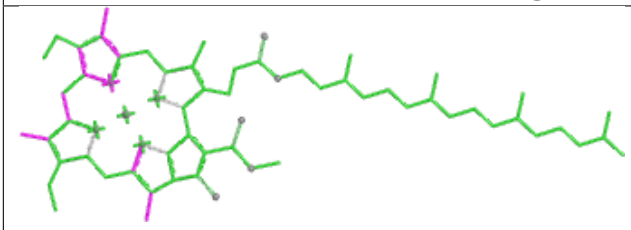


Torsions

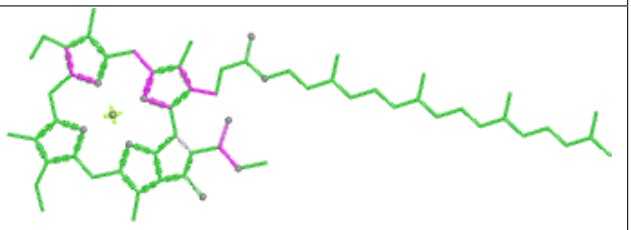


Rings

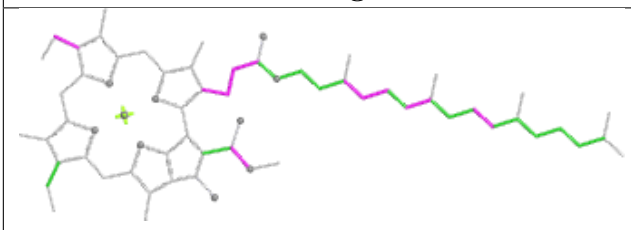
Ligand CLA 2 501



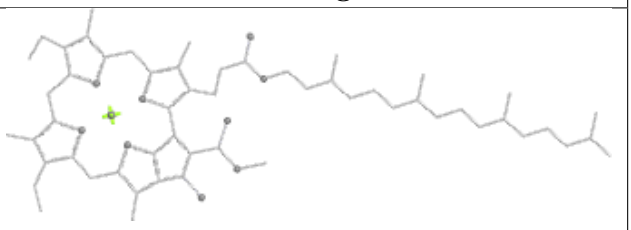
Bond lengths



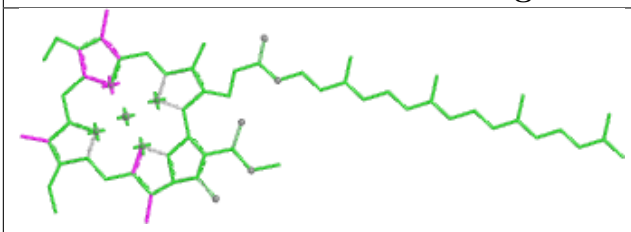
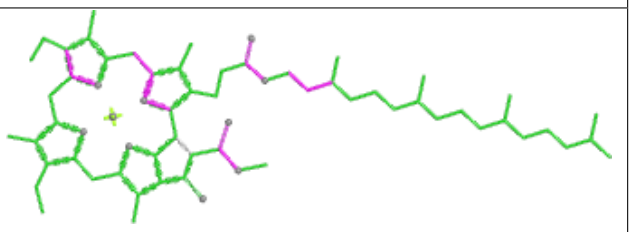
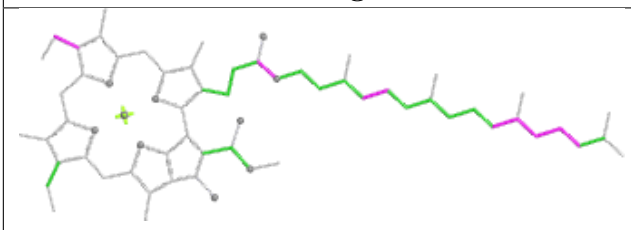
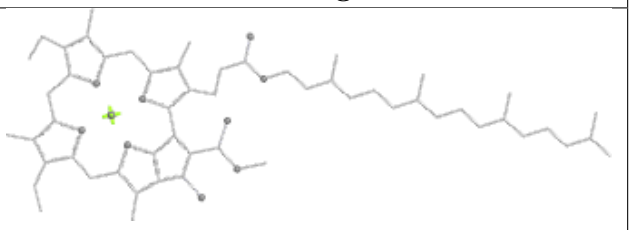
Bond angles

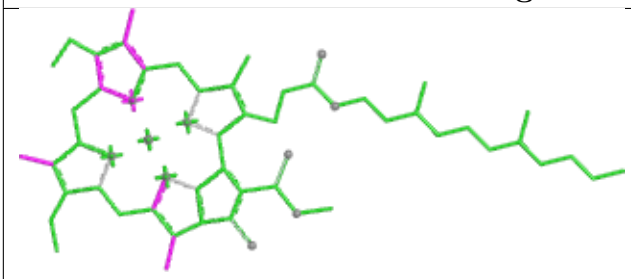
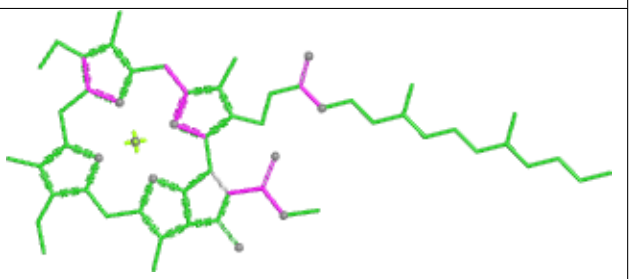
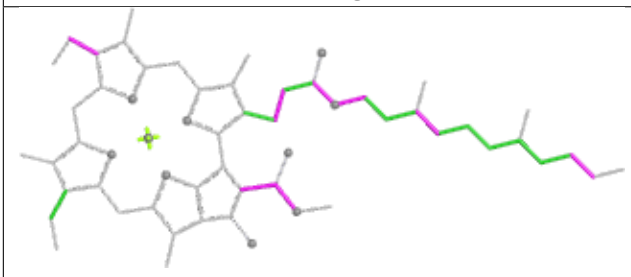
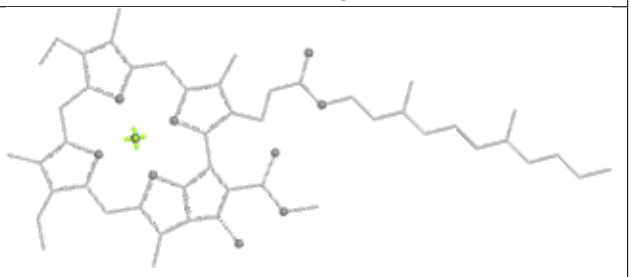


Torsions

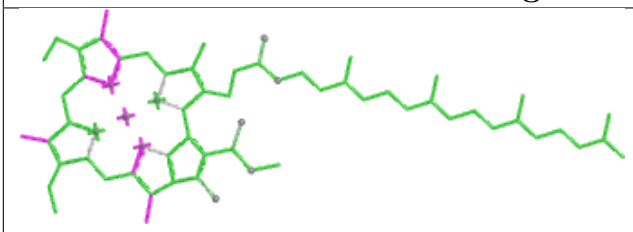


Rings

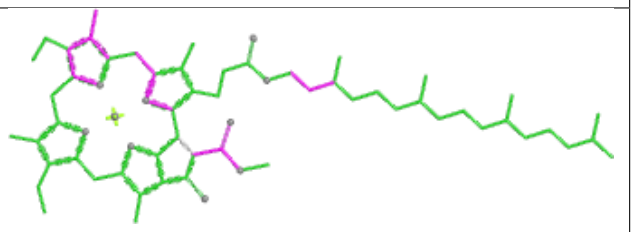
Ligand CLA A 1109	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA T 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

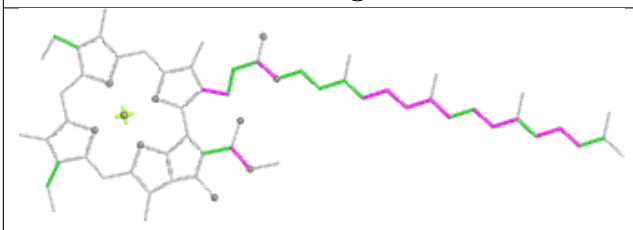
Ligand CLA f 1215



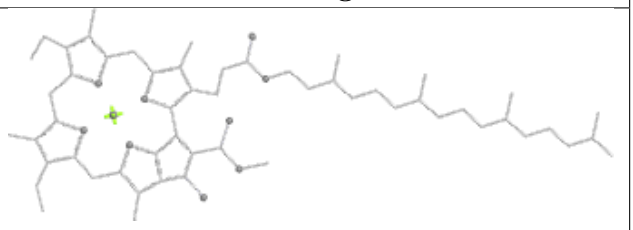
Bond lengths



Bond angles



Torsions

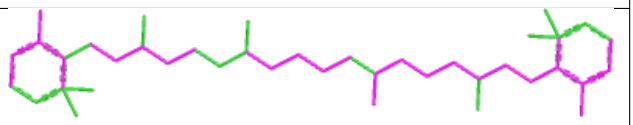


Rings

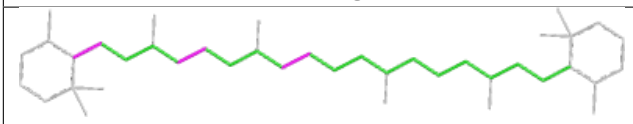
Ligand BCR 4 522



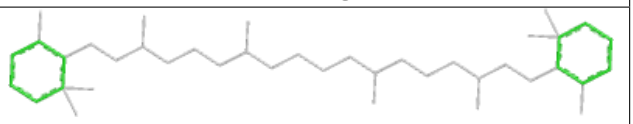
Bond lengths



Bond angles

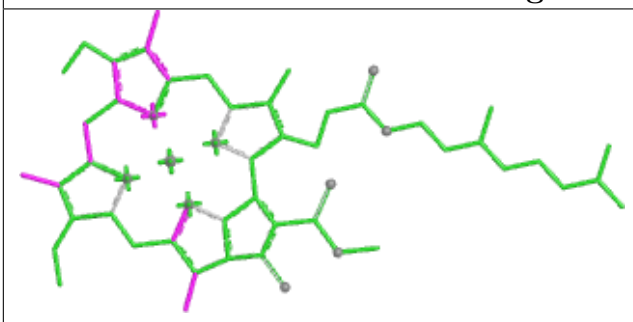


Torsions

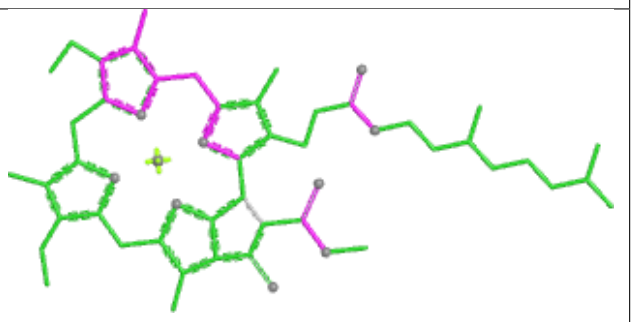


Rings

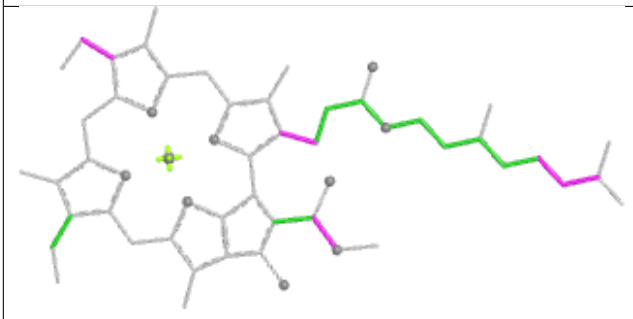
Ligand CLA Z 508



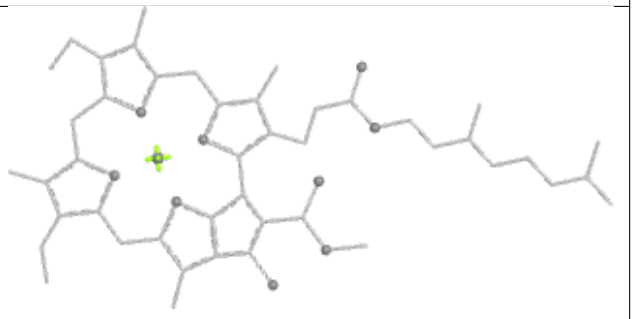
Bond lengths



Bond angles

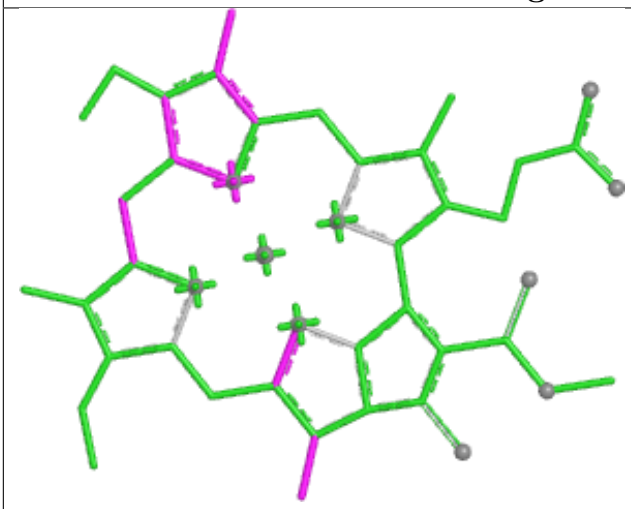


Torsions

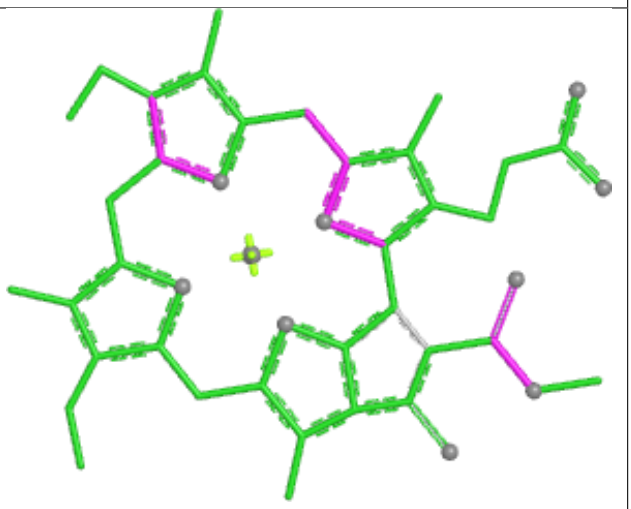


Rings

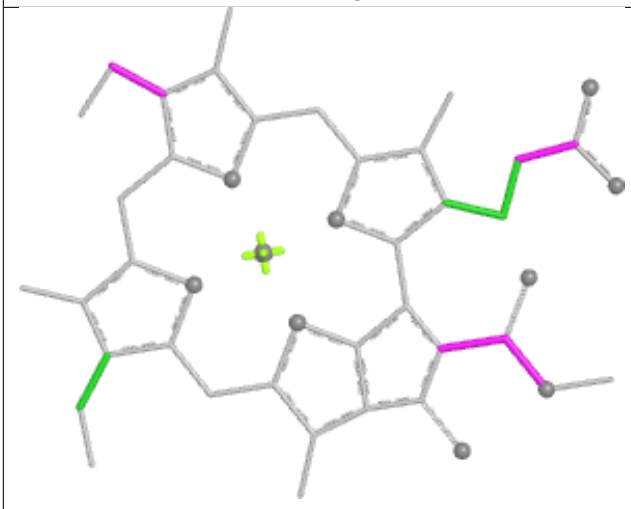
Ligand CLA v 510



Bond lengths



Bond angles

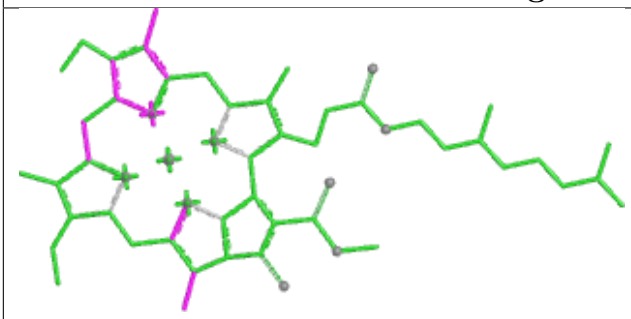


Torsions

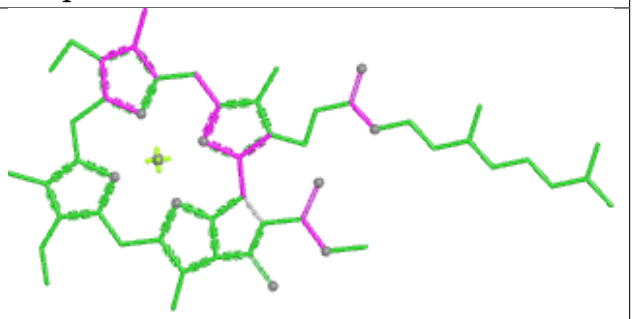


Rings

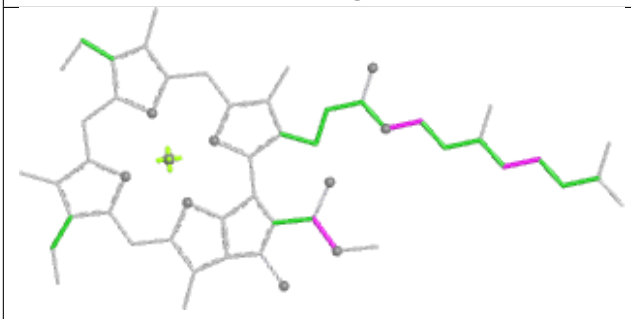
Ligand CLA q 511



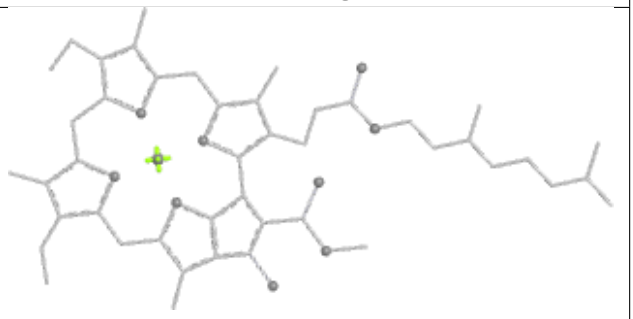
Bond lengths



Bond angles

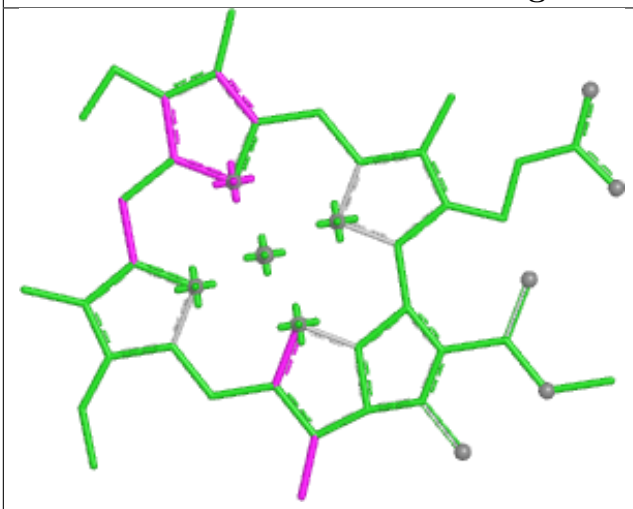


Torsions

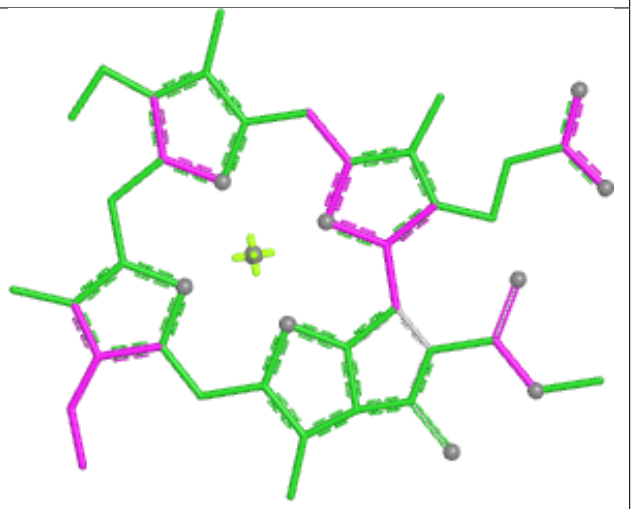


Rings

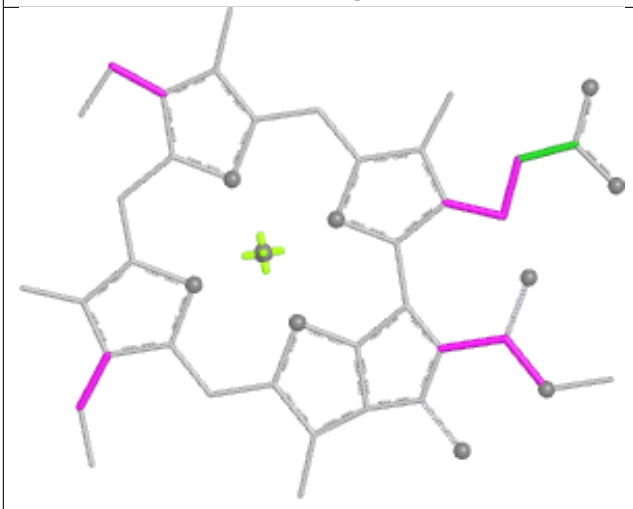
Ligand CLA a 516



Bond lengths



Bond angles

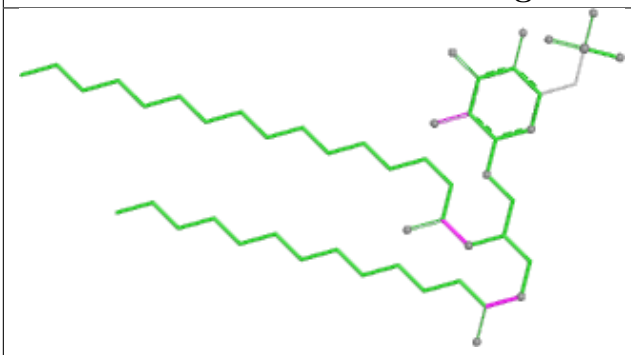


Torsions

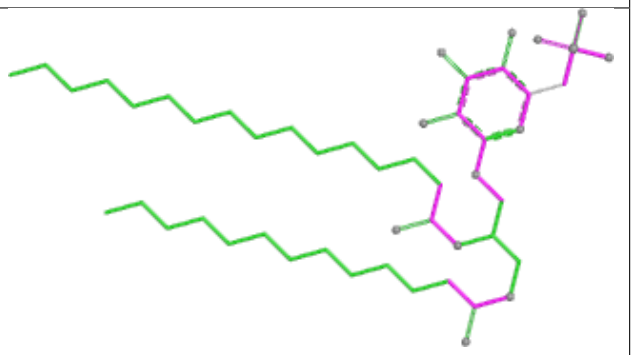


Rings

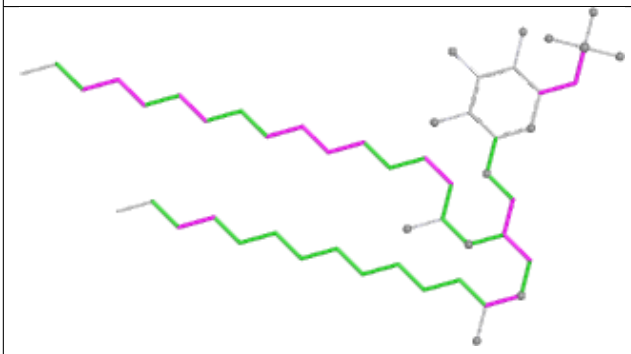
Ligand SQD V 5216



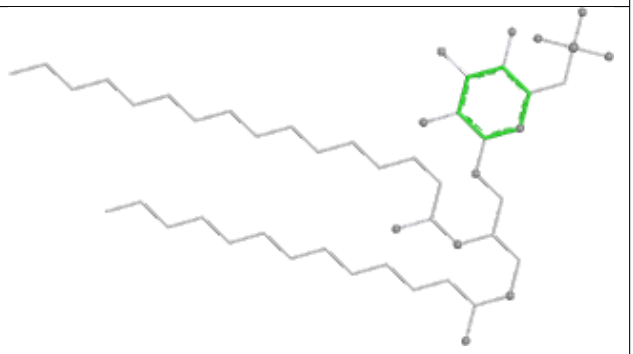
Bond lengths



Bond angles

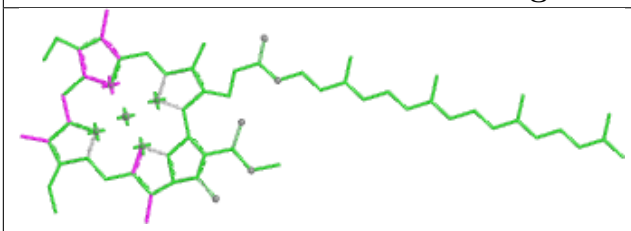


Torsions

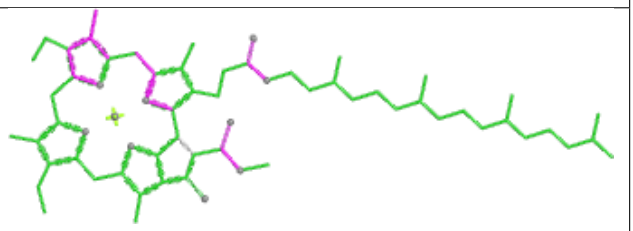


Rings

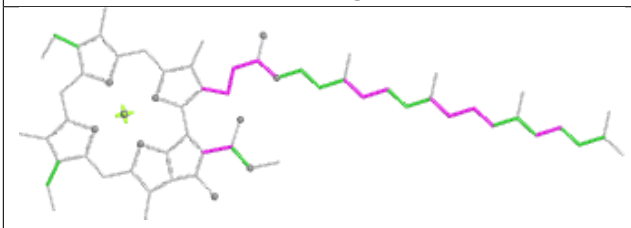
Ligand CLA r 518



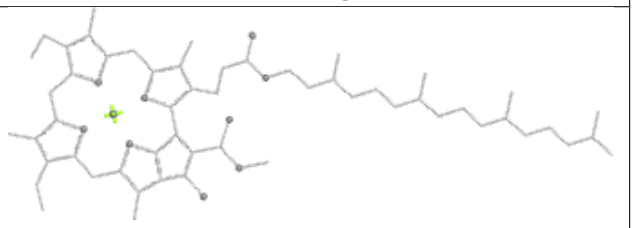
Bond lengths



Bond angles



Torsions

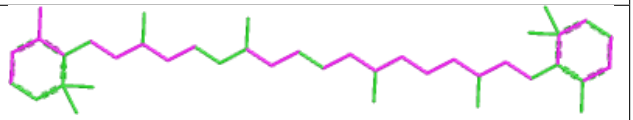


Rings

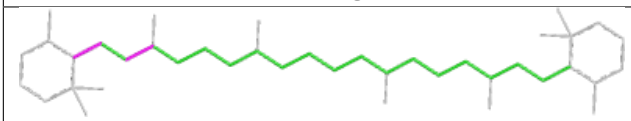
Ligand BCR 2 521



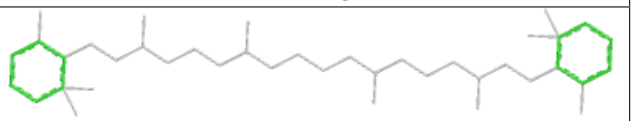
Bond lengths



Bond angles

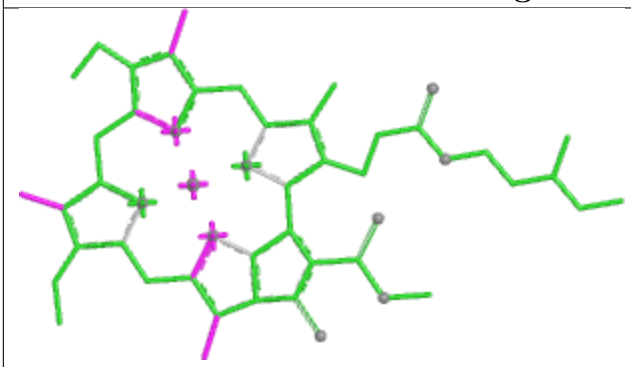


Torsions

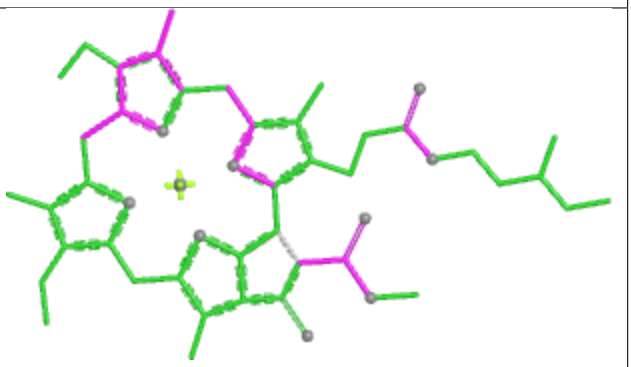


Rings

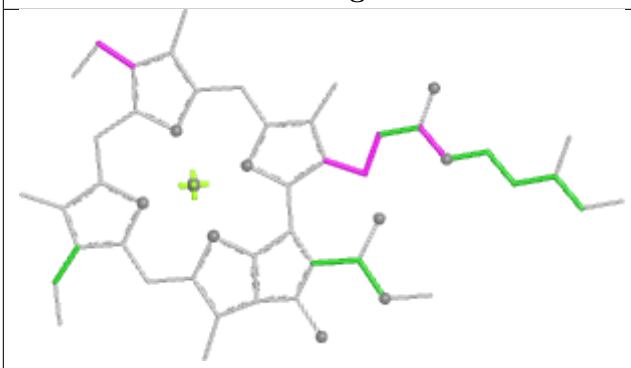
Ligand CLA G 1129



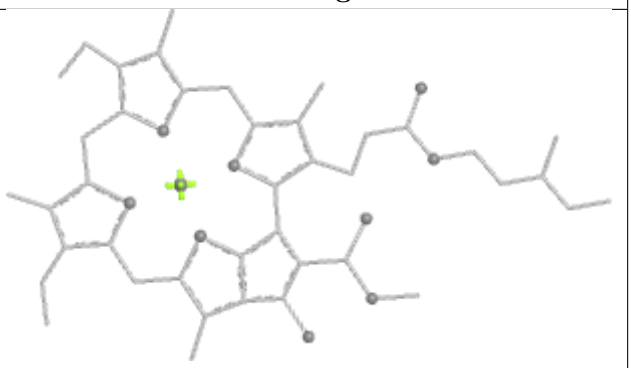
Bond lengths



Bond angles

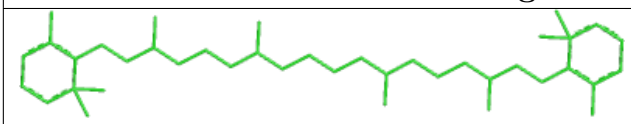


Torsions

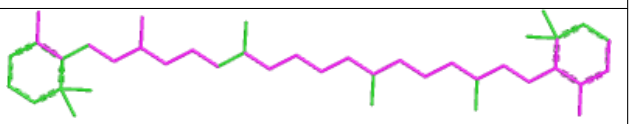


Rings

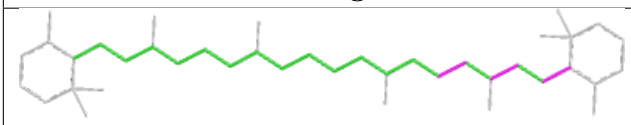
Ligand BCR e 4008



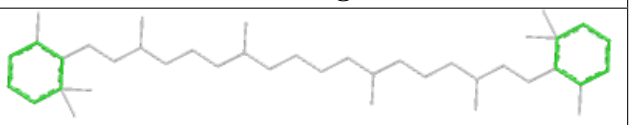
Bond lengths



Bond angles

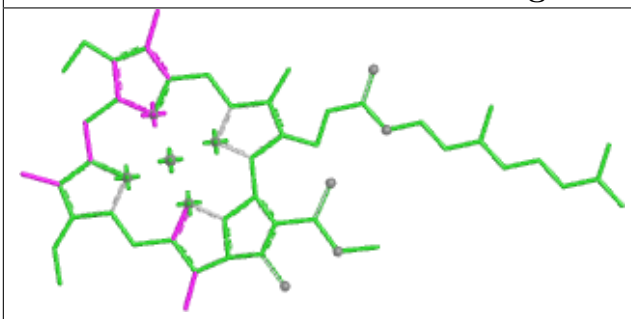


Torsions

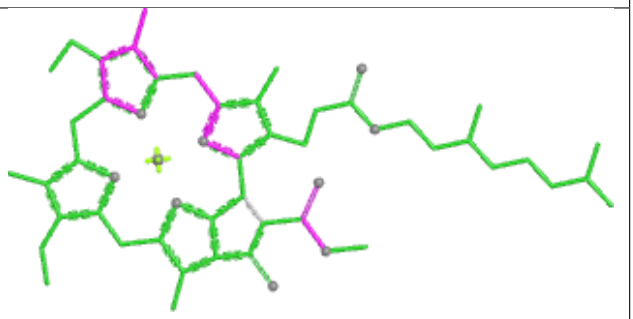


Rings

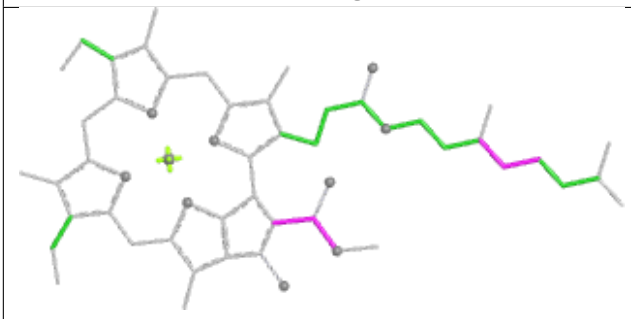
Ligand CLA 2 506



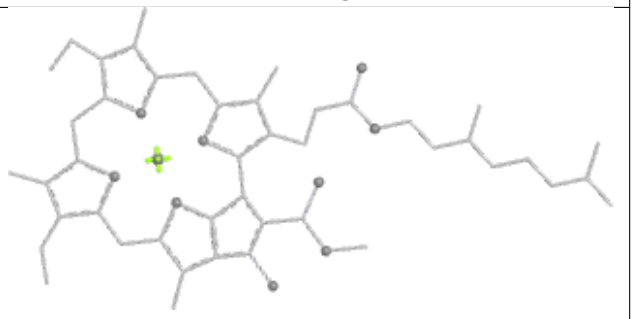
Bond lengths



Bond angles

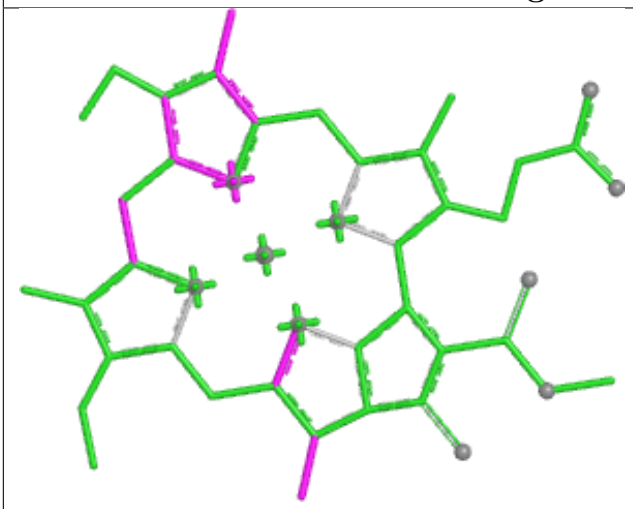


Torsions

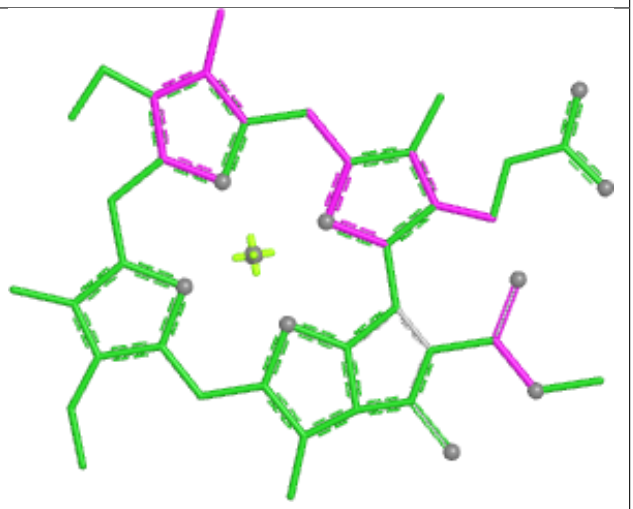


Rings

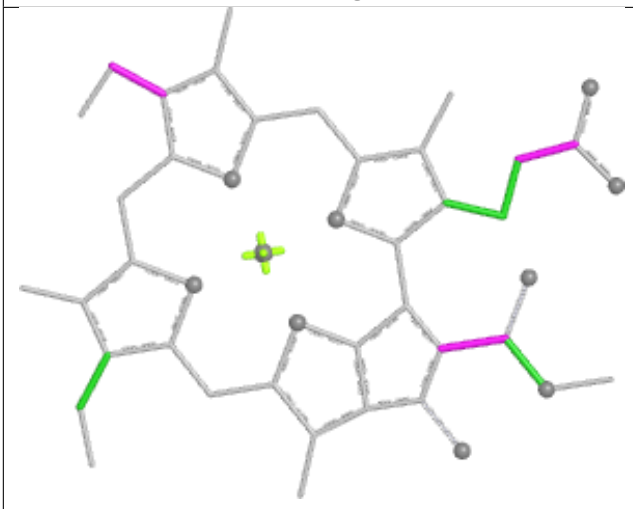
Ligand CLA d 504



Bond lengths



Bond angles

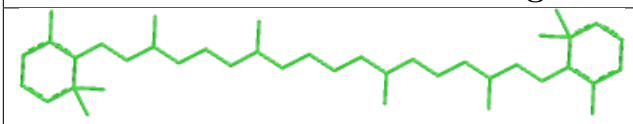


Torsions

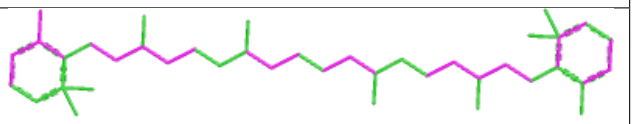


Rings

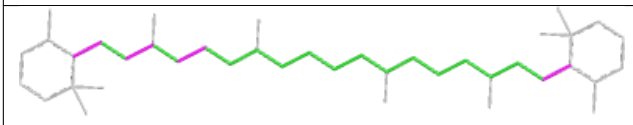
Ligand BCR a 521



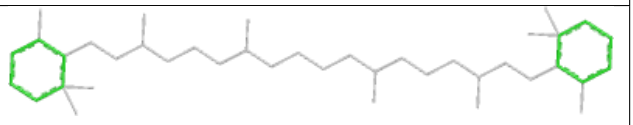
Bond lengths



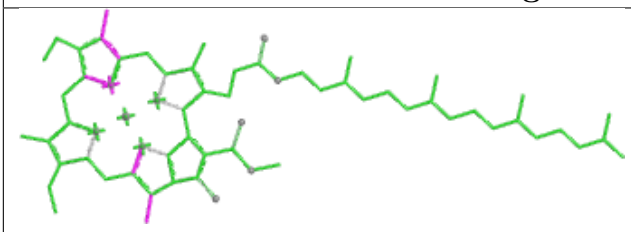
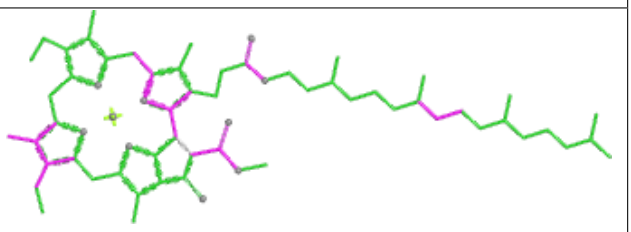
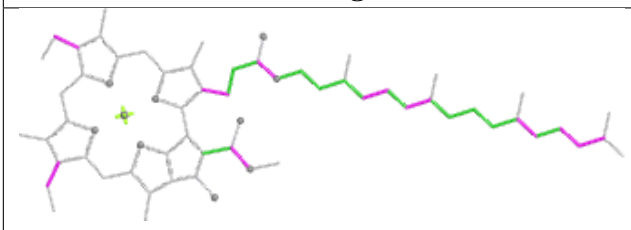
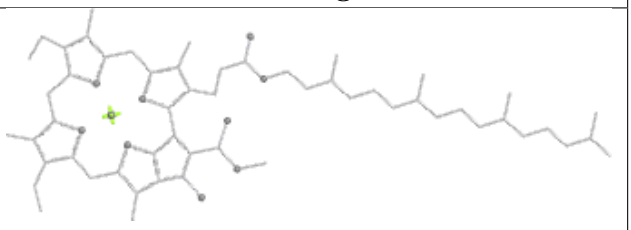
Bond angles

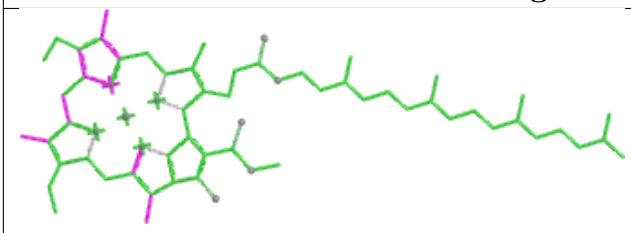
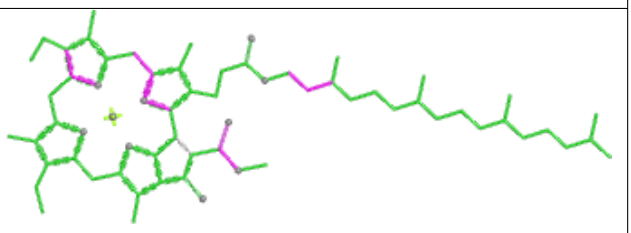
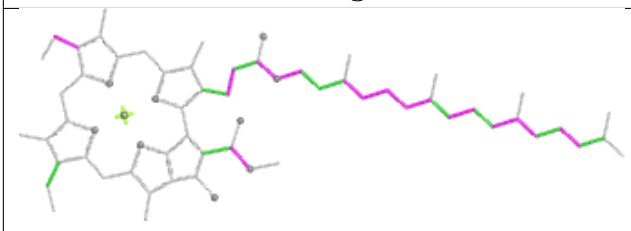
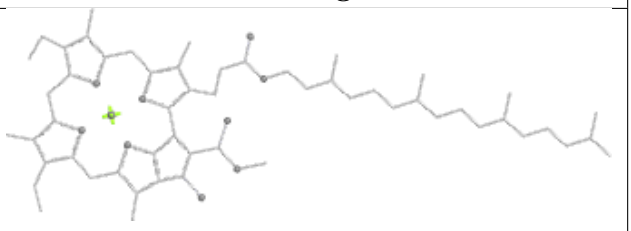


Torsions

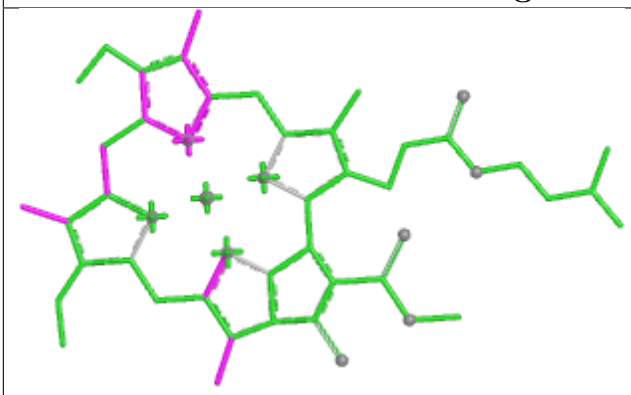


Rings

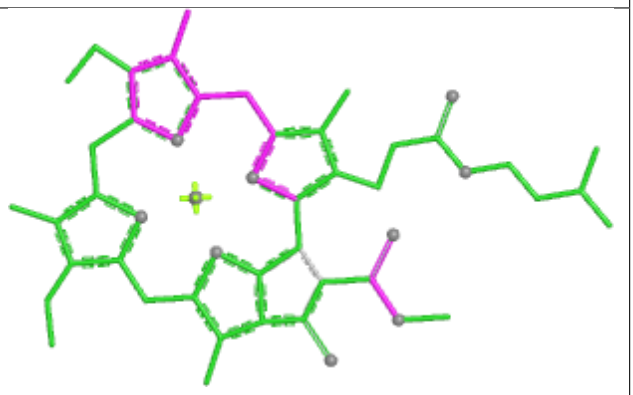
Ligand CLA f 1239	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

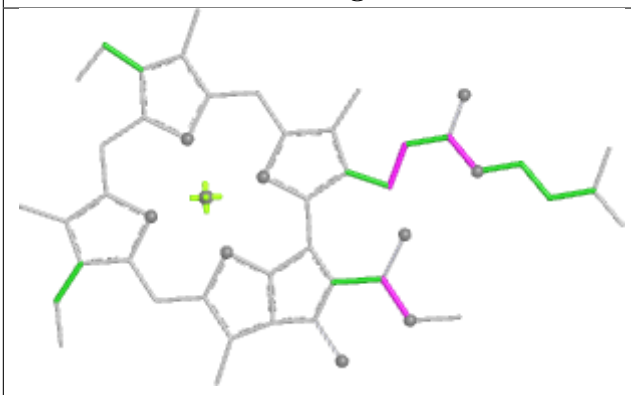
Ligand CLA H 1232



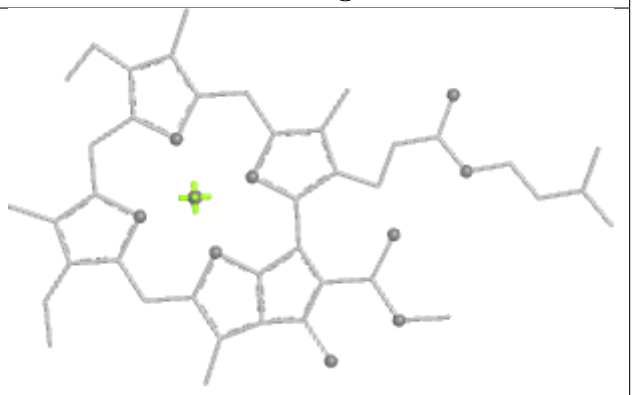
Bond lengths



Bond angles



Torsions

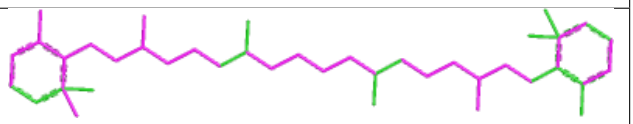


Rings

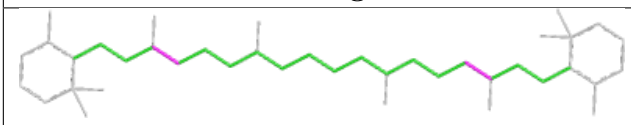
Ligand BCR B 4006



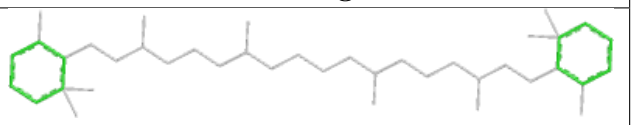
Bond lengths



Bond angles

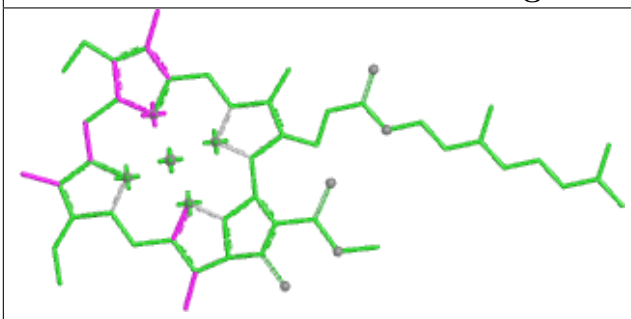


Torsions

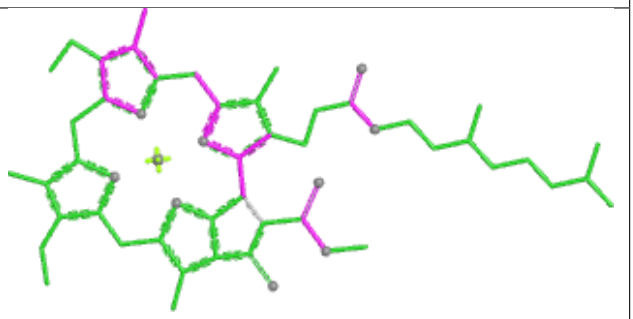


Rings

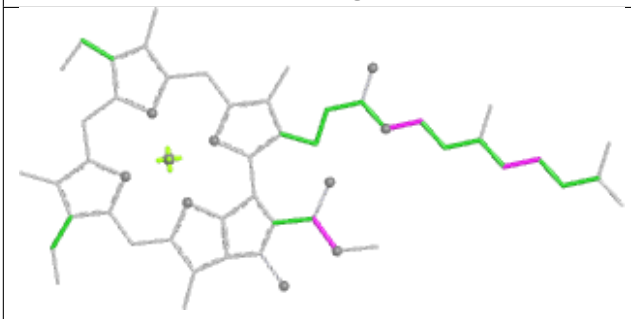
Ligand CLA Y 511



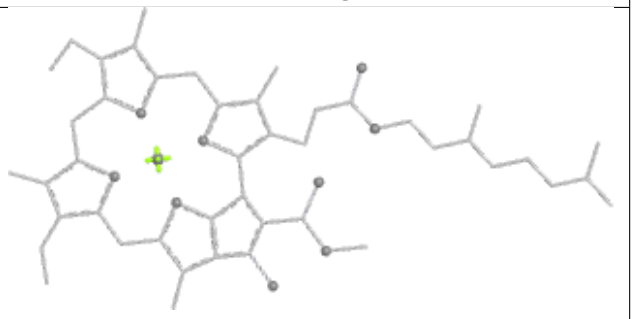
Bond lengths



Bond angles

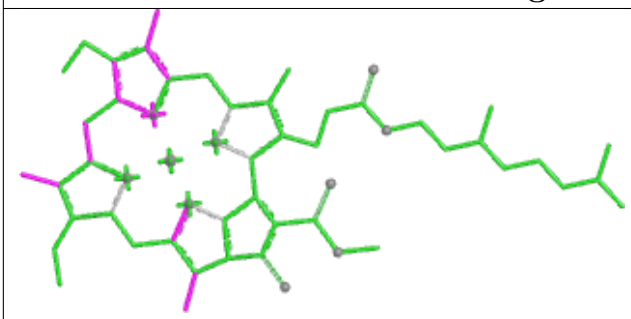


Torsions

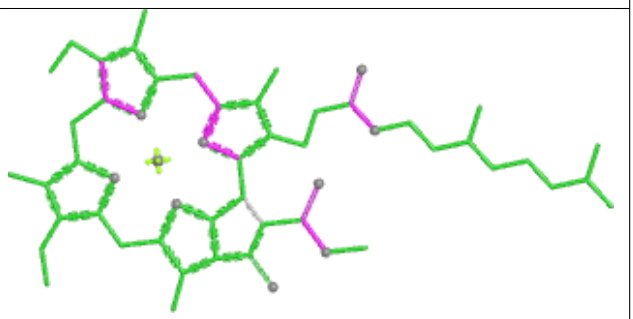


Rings

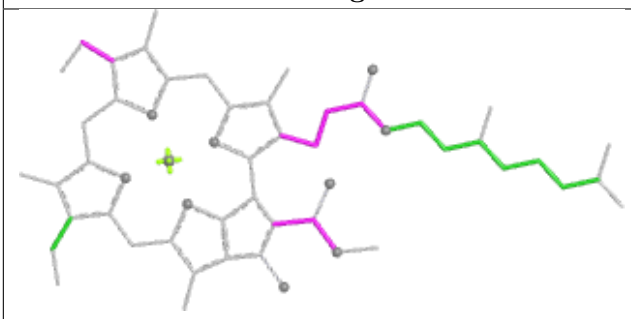
Ligand CLA 4 518



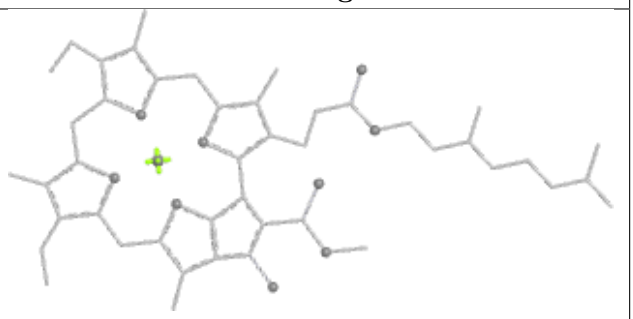
Bond lengths



Bond angles

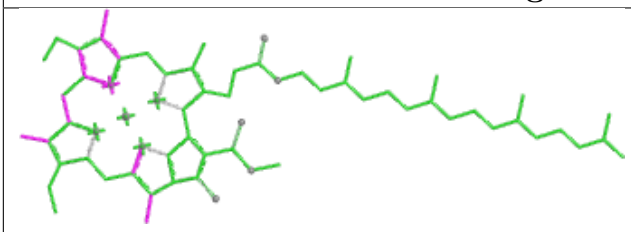


Torsions

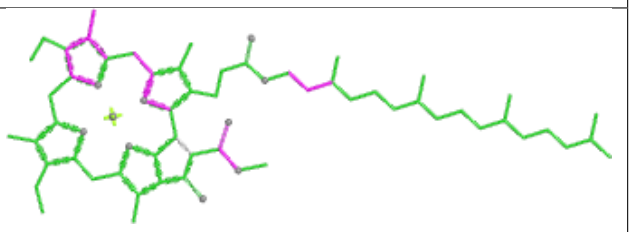


Rings

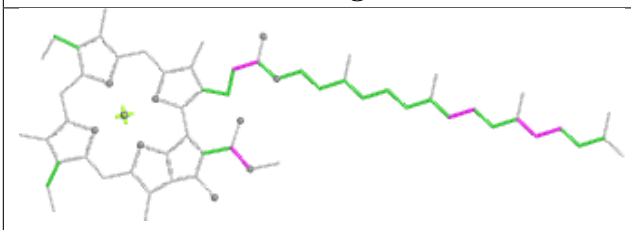
Ligand CLA Z 510



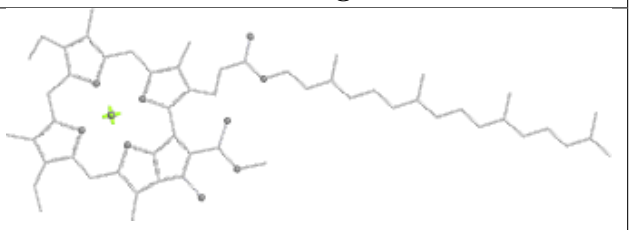
Bond lengths



Bond angles

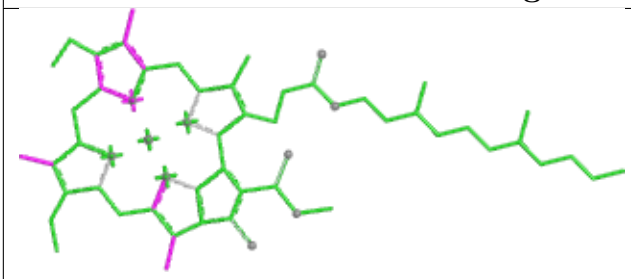


Torsions

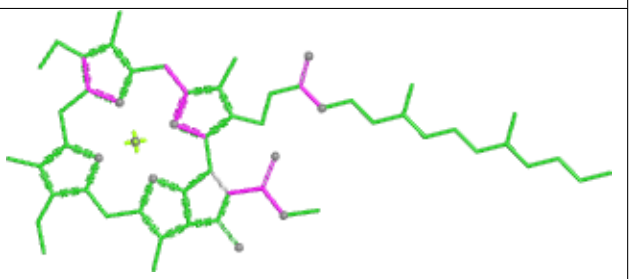


Rings

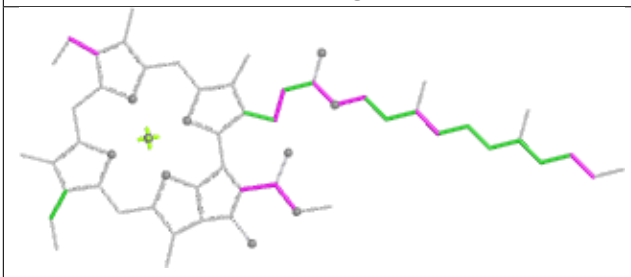
Ligand CLA l 1302



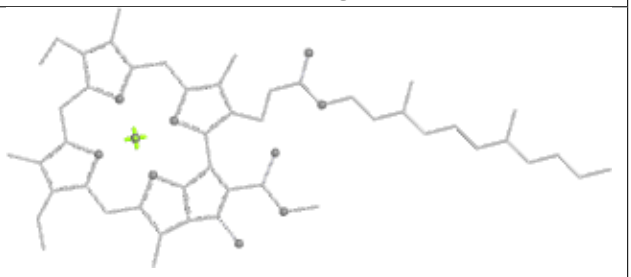
Bond lengths



Bond angles

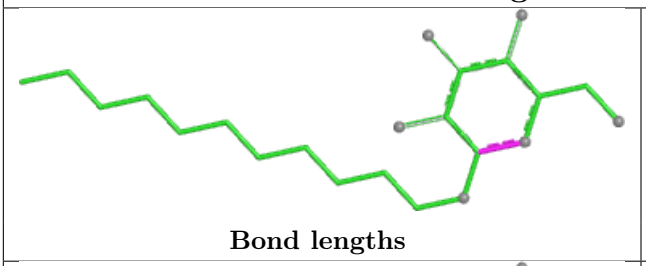


Torsions

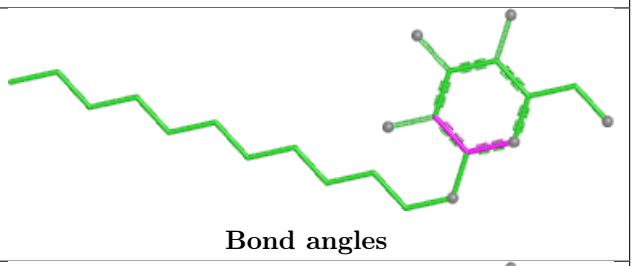


Rings

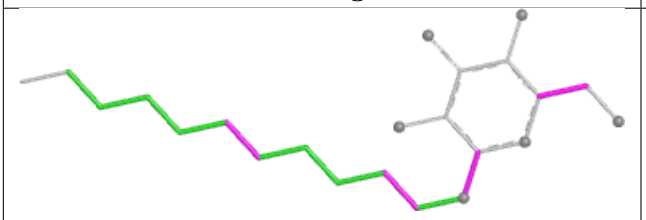
Ligand LMU A 1849



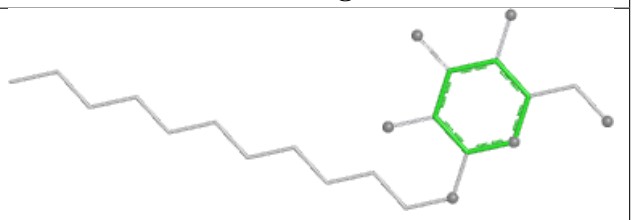
Bond lengths



Bond angles

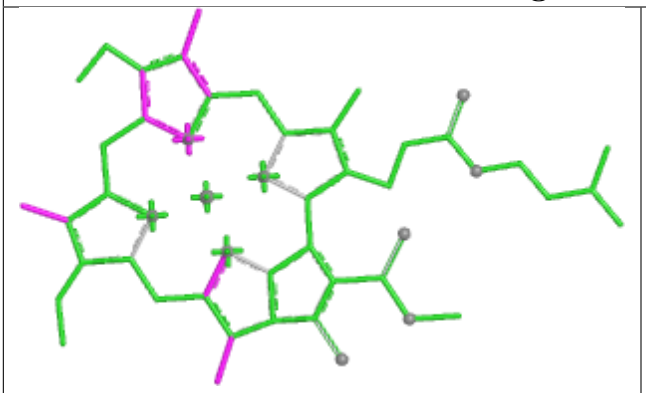


Torsions

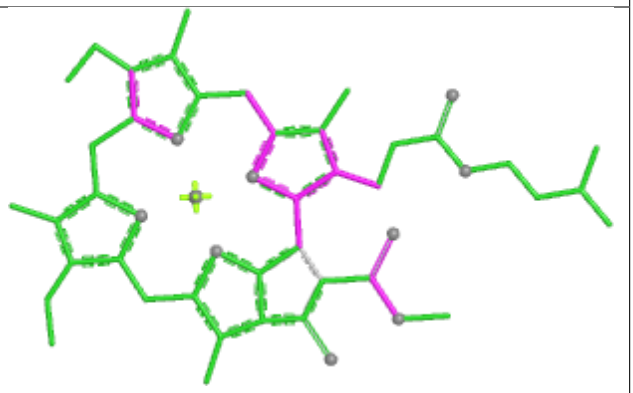


Rings

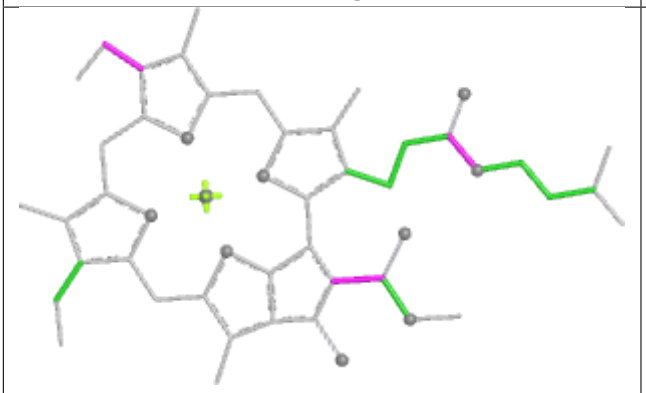
Ligand CLA s 502



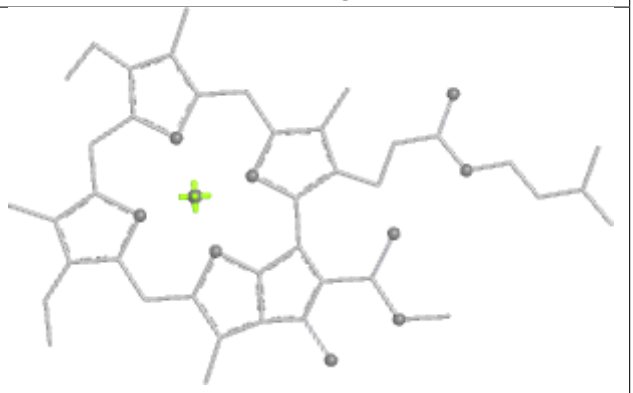
Bond lengths



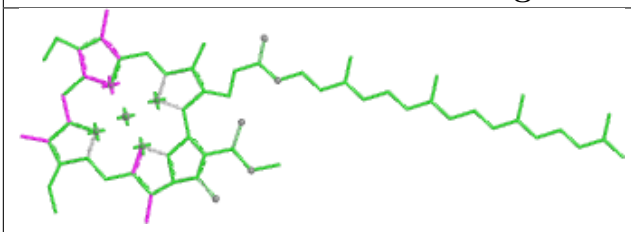
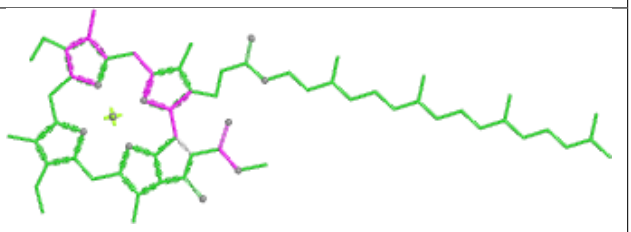
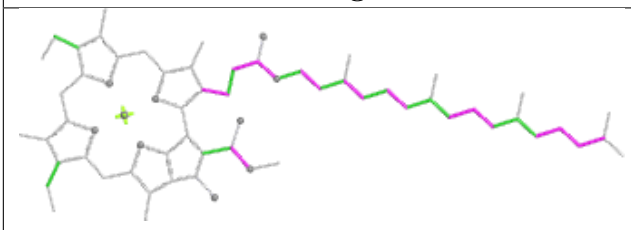
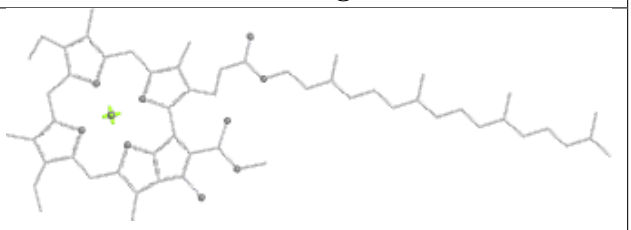
Bond angles

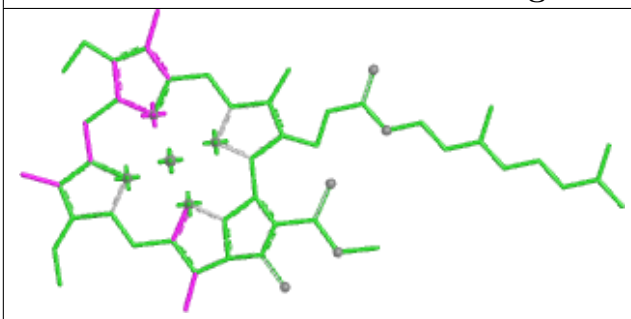
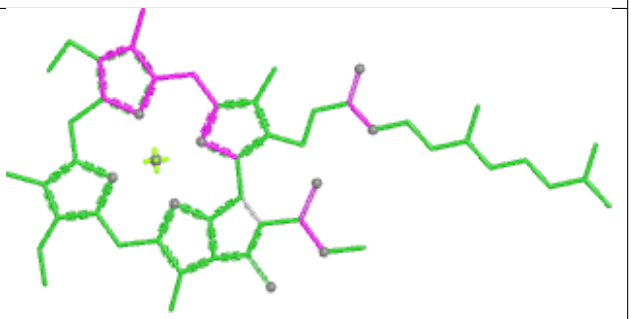
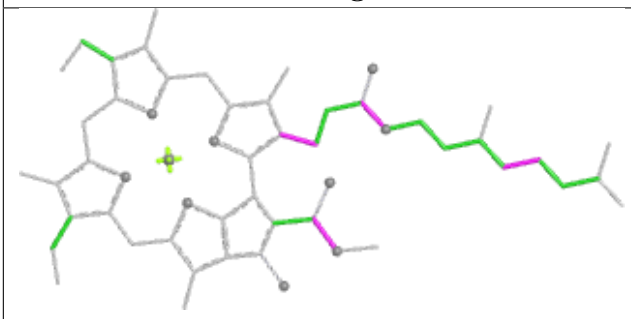
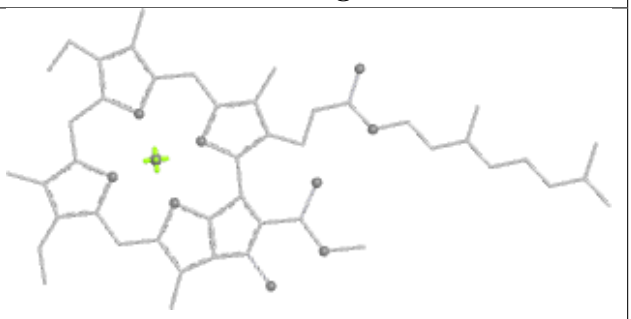


Torsions

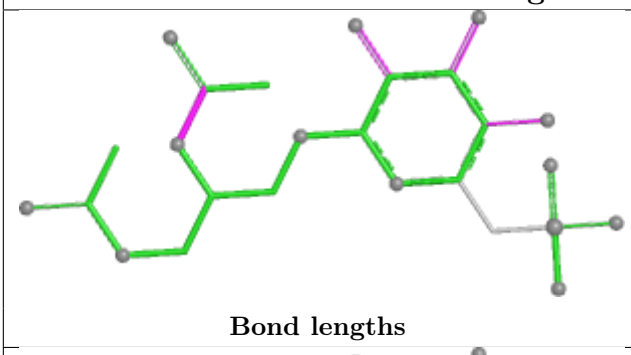


Rings

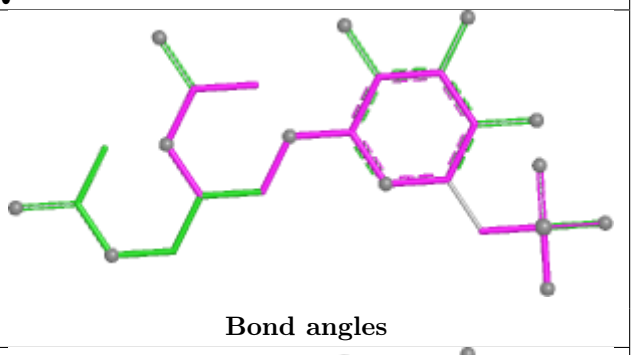
Ligand CLA G 1126	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

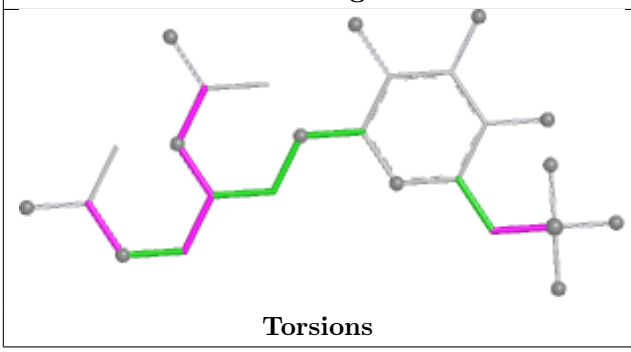
Ligand SQD b 822



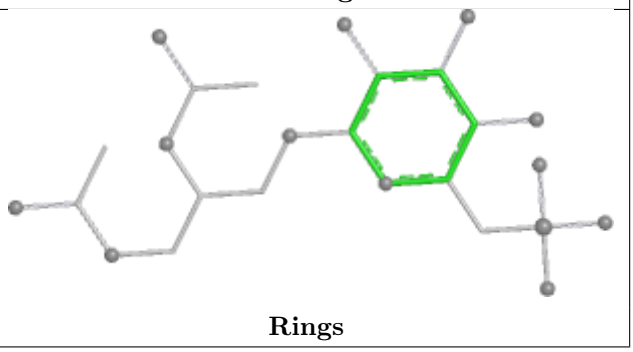
Bond lengths



Bond angles

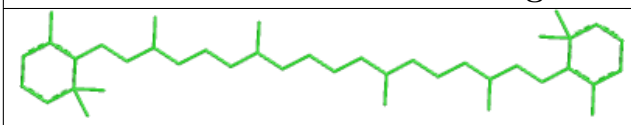


Torsions

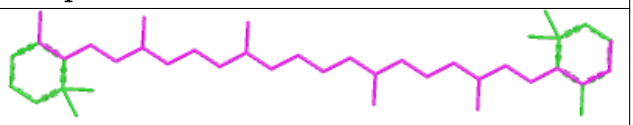


Rings

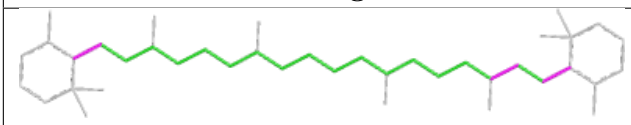
Ligand BCR q 523



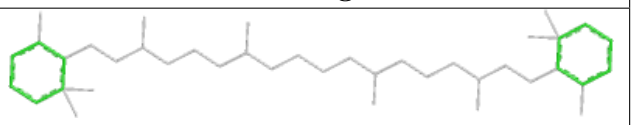
Bond lengths



Bond angles

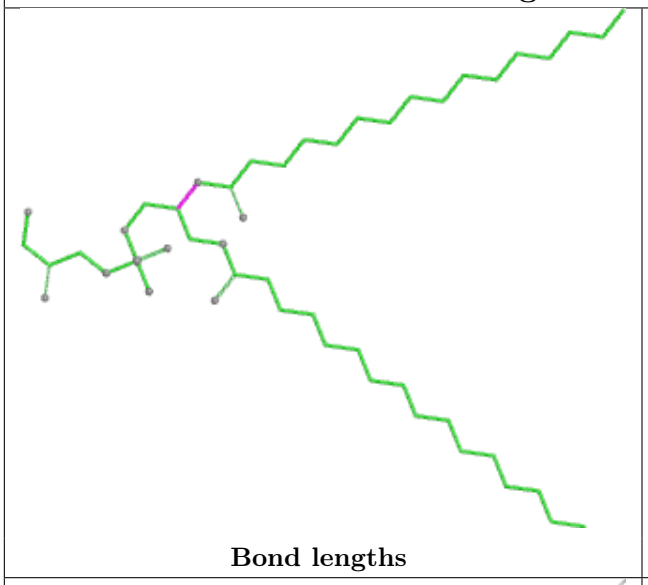


Torsions

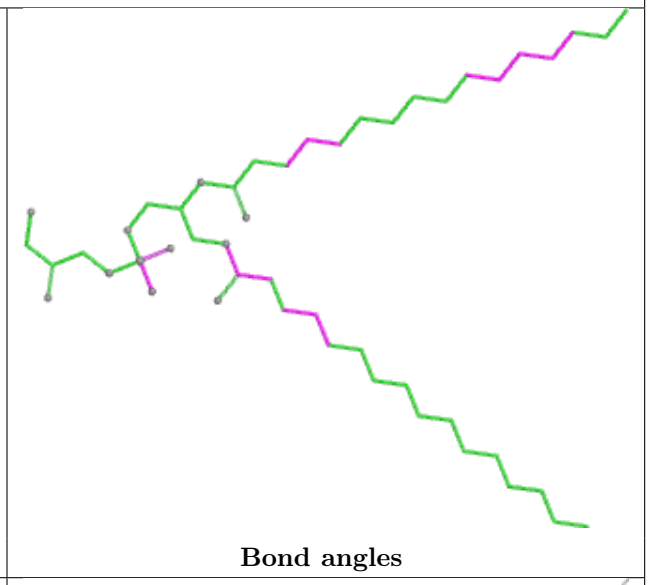


Rings

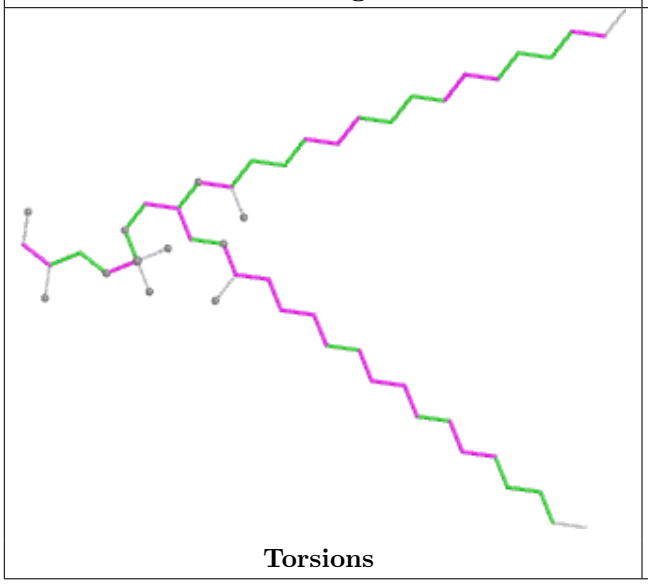
Ligand LHG e 5001



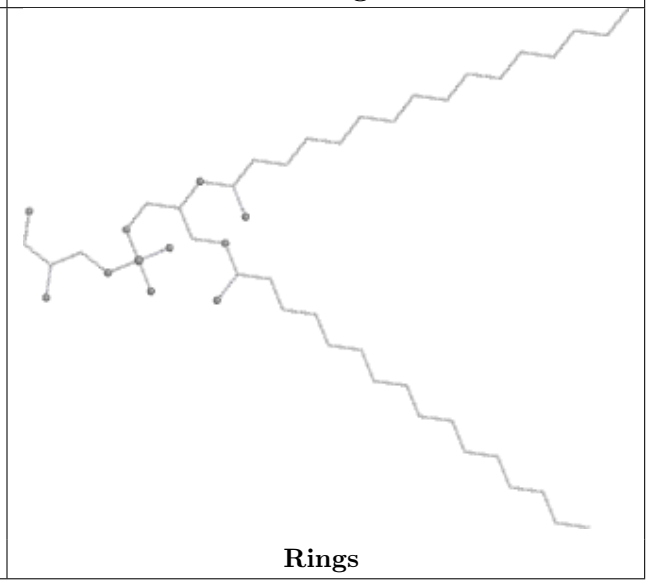
Bond lengths



Bond angles

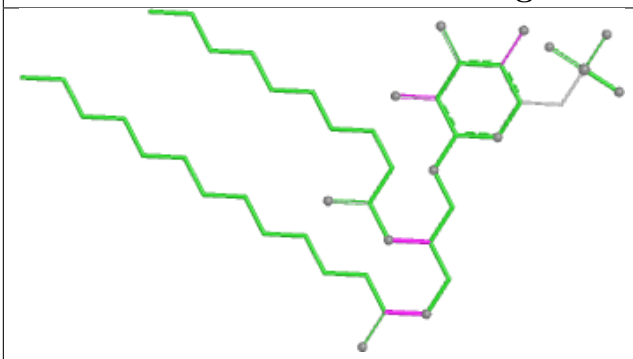


Torsions

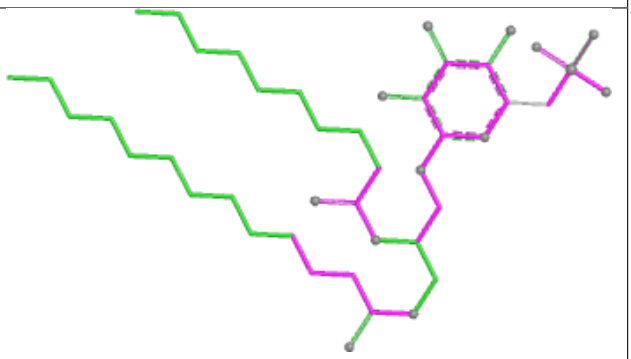


Rings

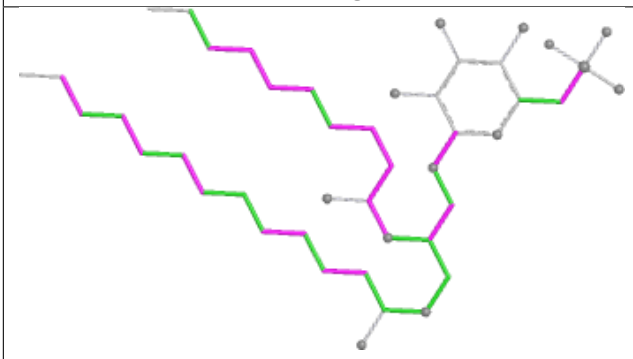
Ligand SQD B 1852



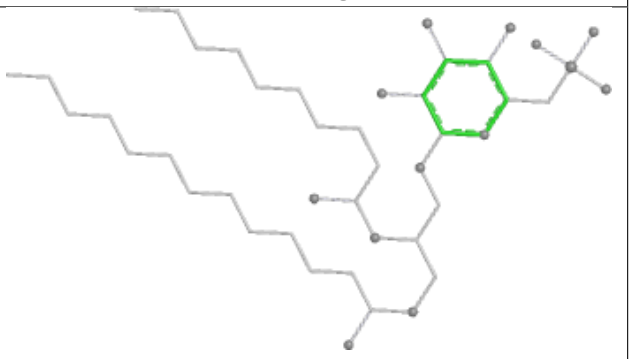
Bond lengths



Bond angles

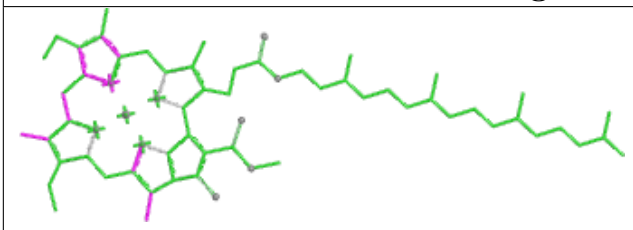


Torsions

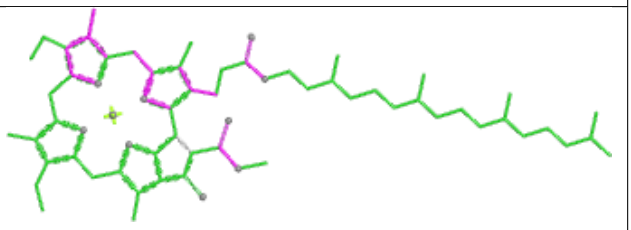


Rings

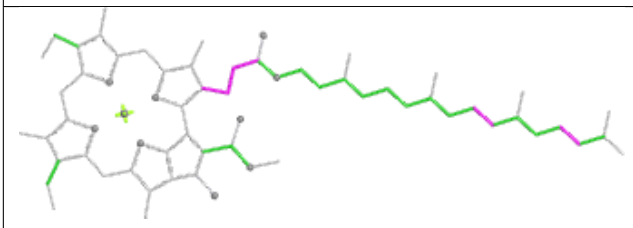
Ligand CLA s 501



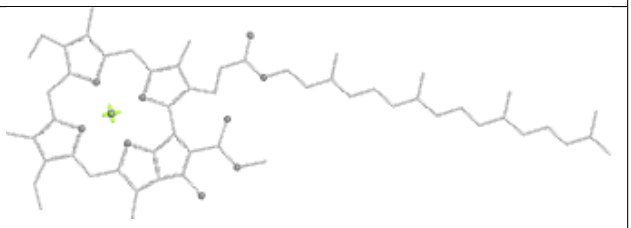
Bond lengths



Bond angles

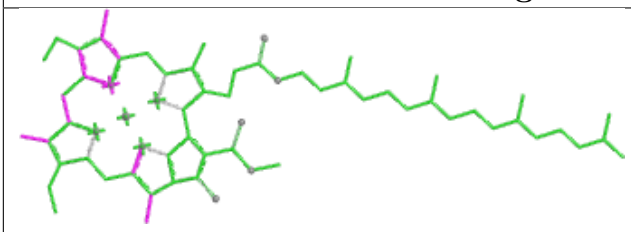


Torsions

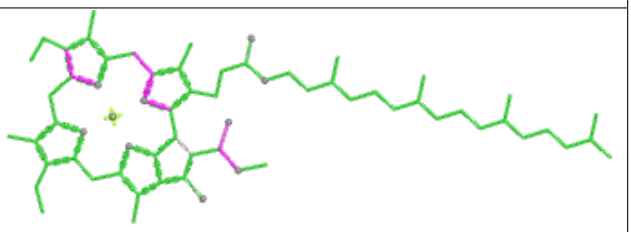


Rings

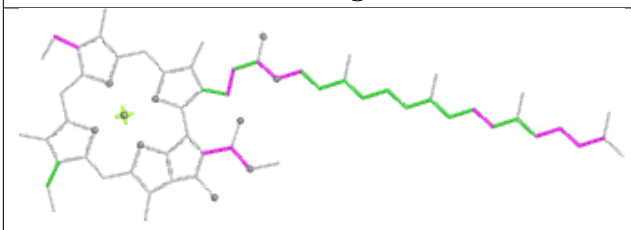
Ligand CLA B 1207



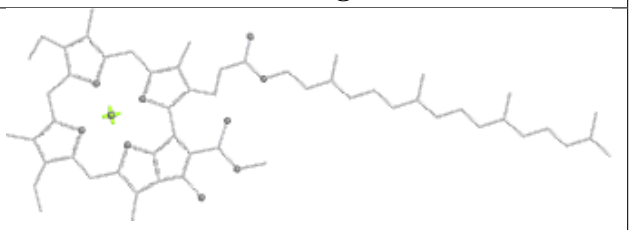
Bond lengths



Bond angles

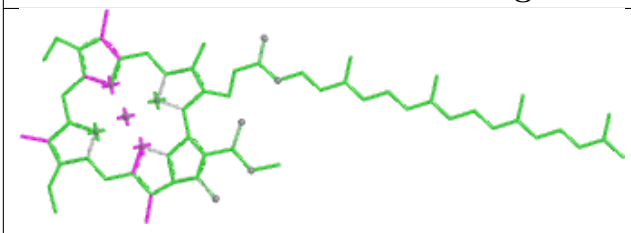


Torsions

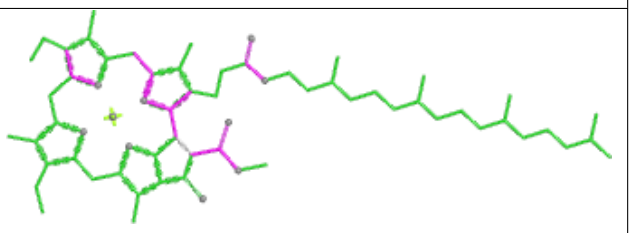


Rings

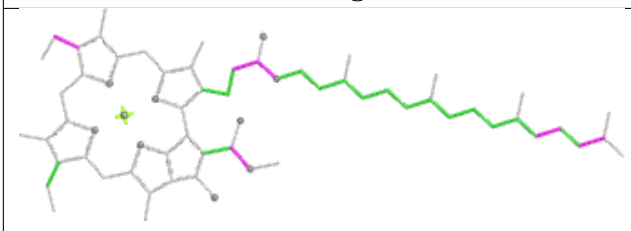
Ligand CLA H 1021



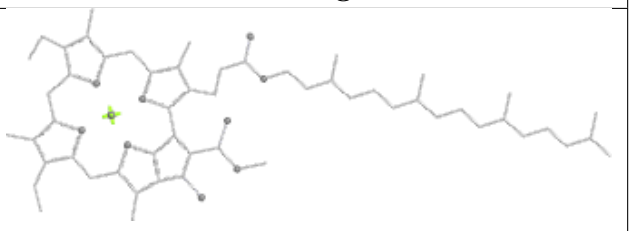
Bond lengths



Bond angles

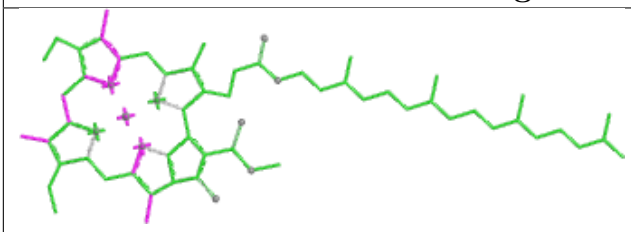


Torsions

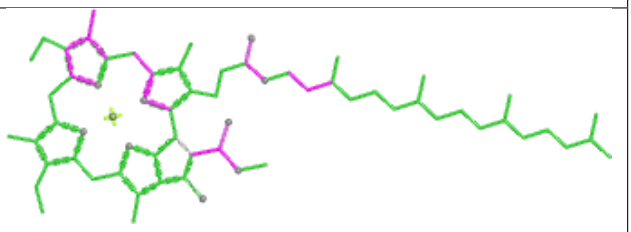


Rings

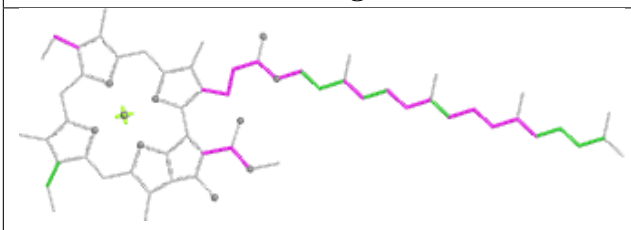
Ligand CLA G 1106



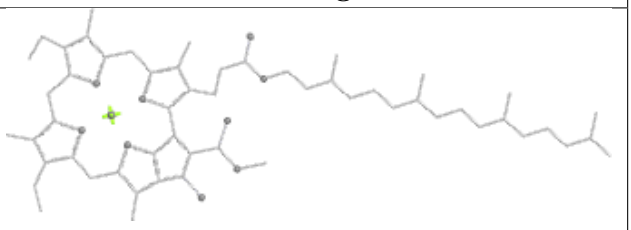
Bond lengths



Bond angles

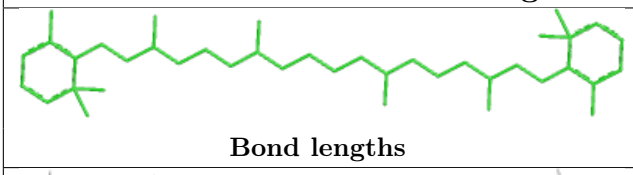


Torsions

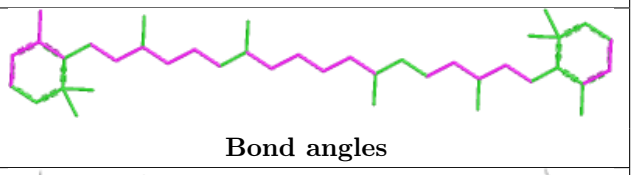


Rings

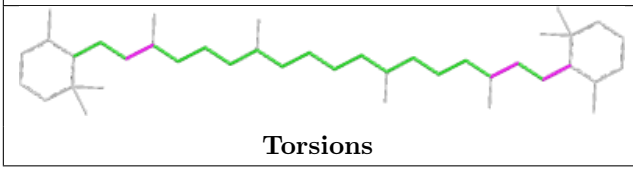
Ligand BCR f 4005



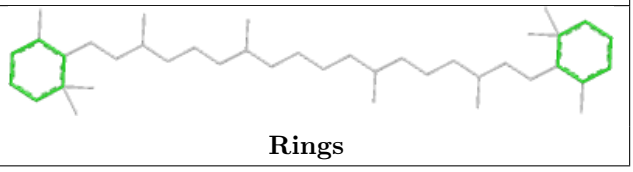
Bond lengths



Bond angles

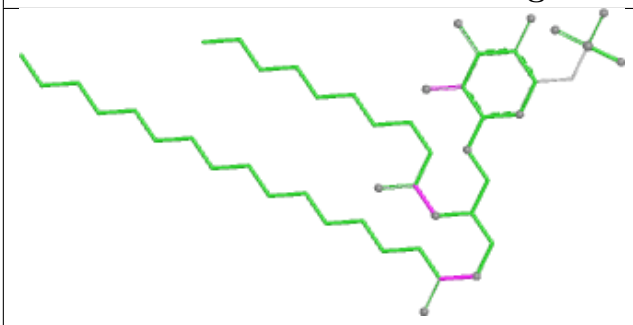


Torsions

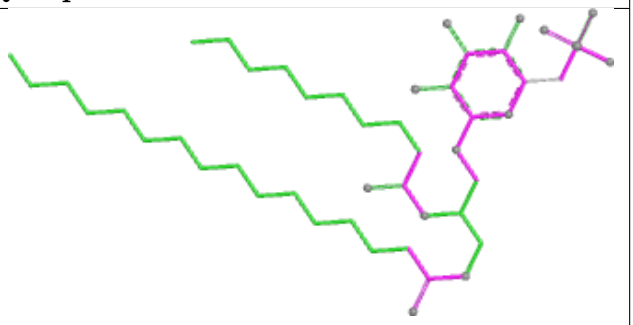


Rings

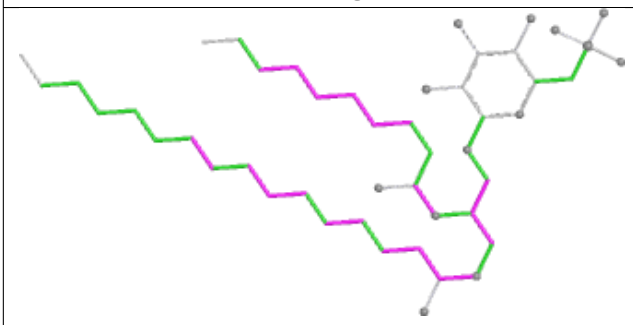
Ligand SQD q 822



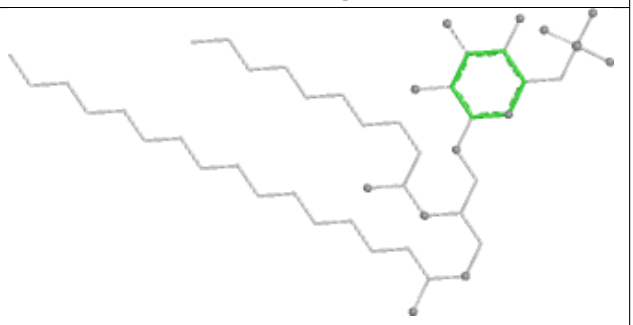
Bond lengths



Bond angles

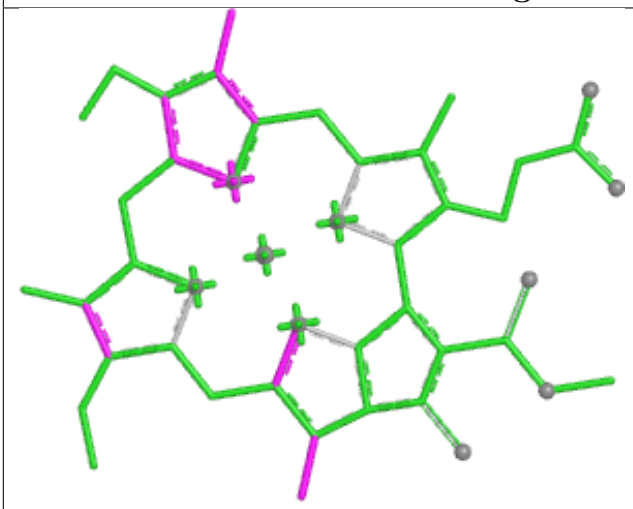


Torsions

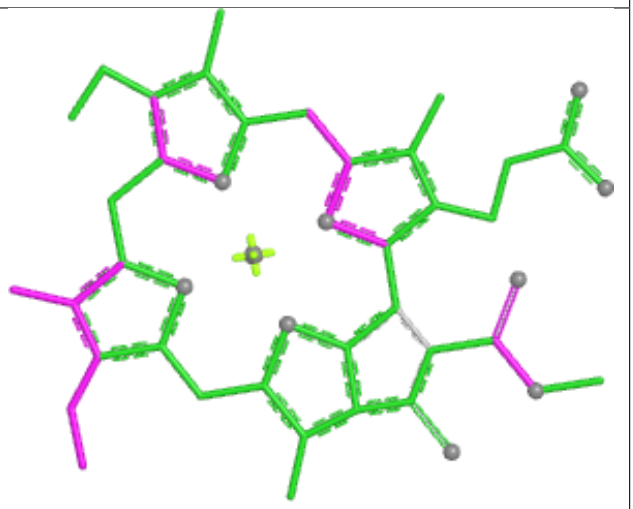


Rings

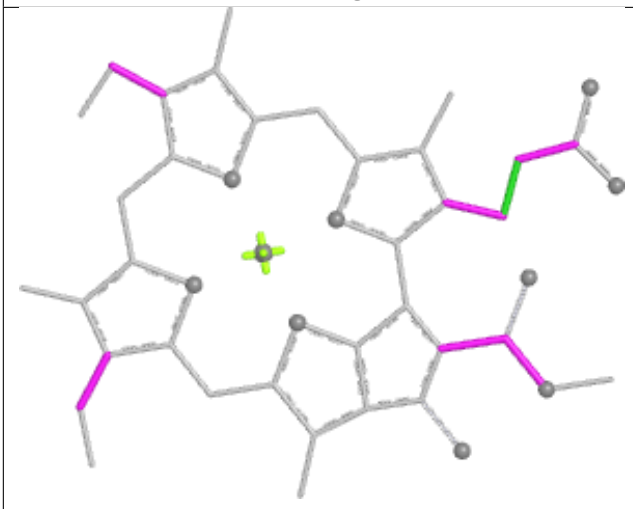
Ligand CLA m 1105



Bond lengths



Bond angles

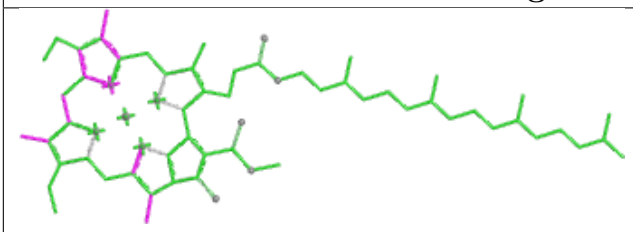


Torsions

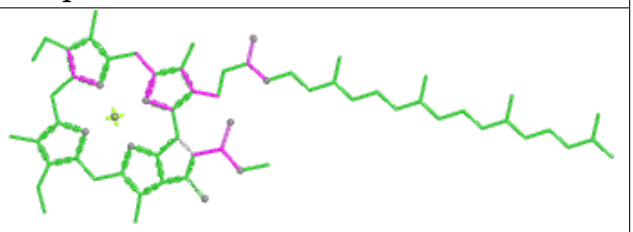


Rings

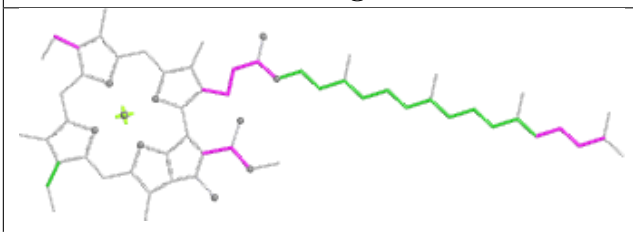
Ligand CLA q 501



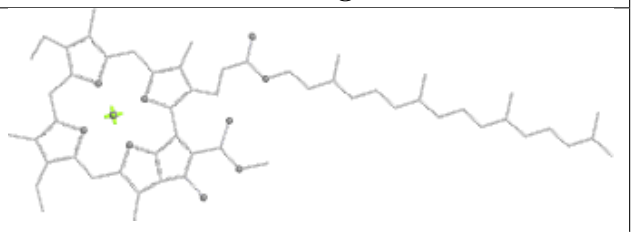
Bond lengths



Bond angles

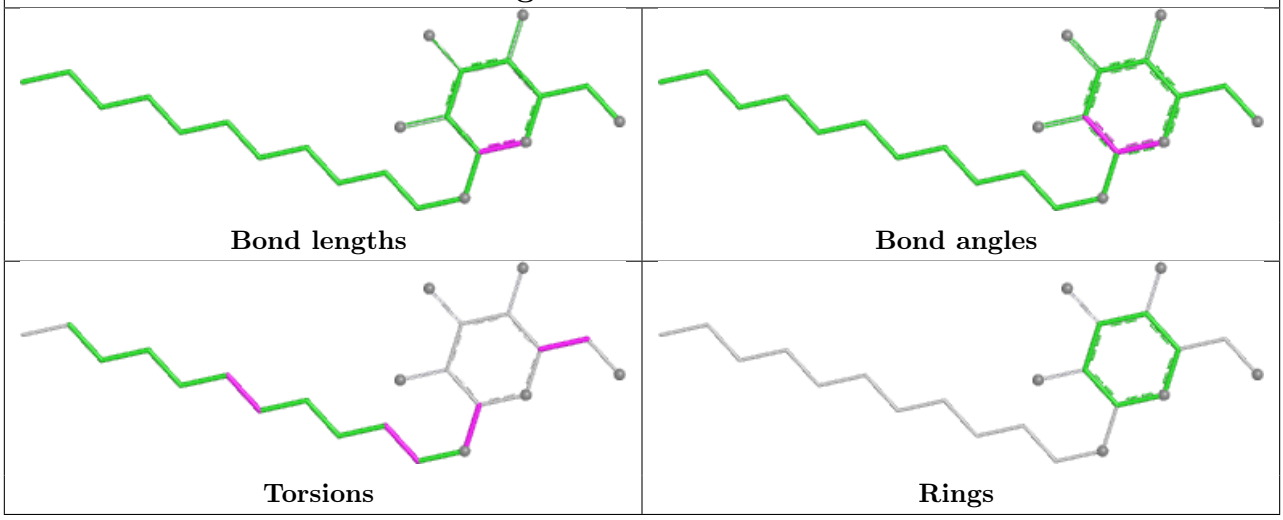


Torsions

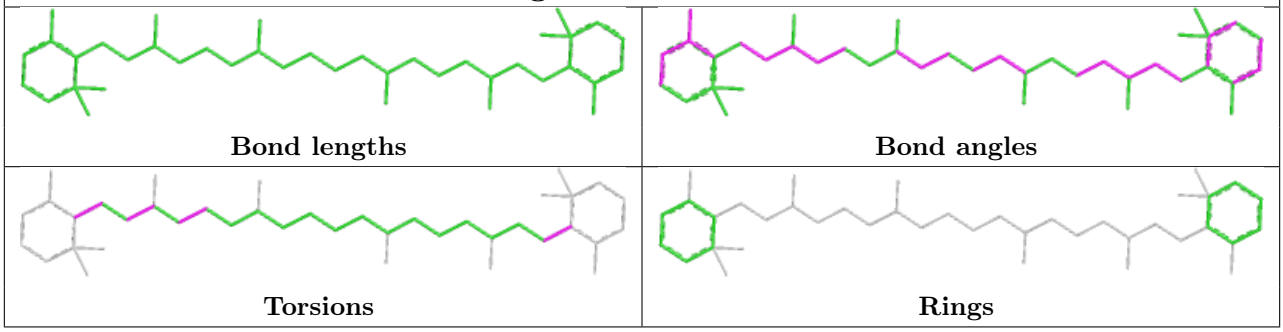


Rings

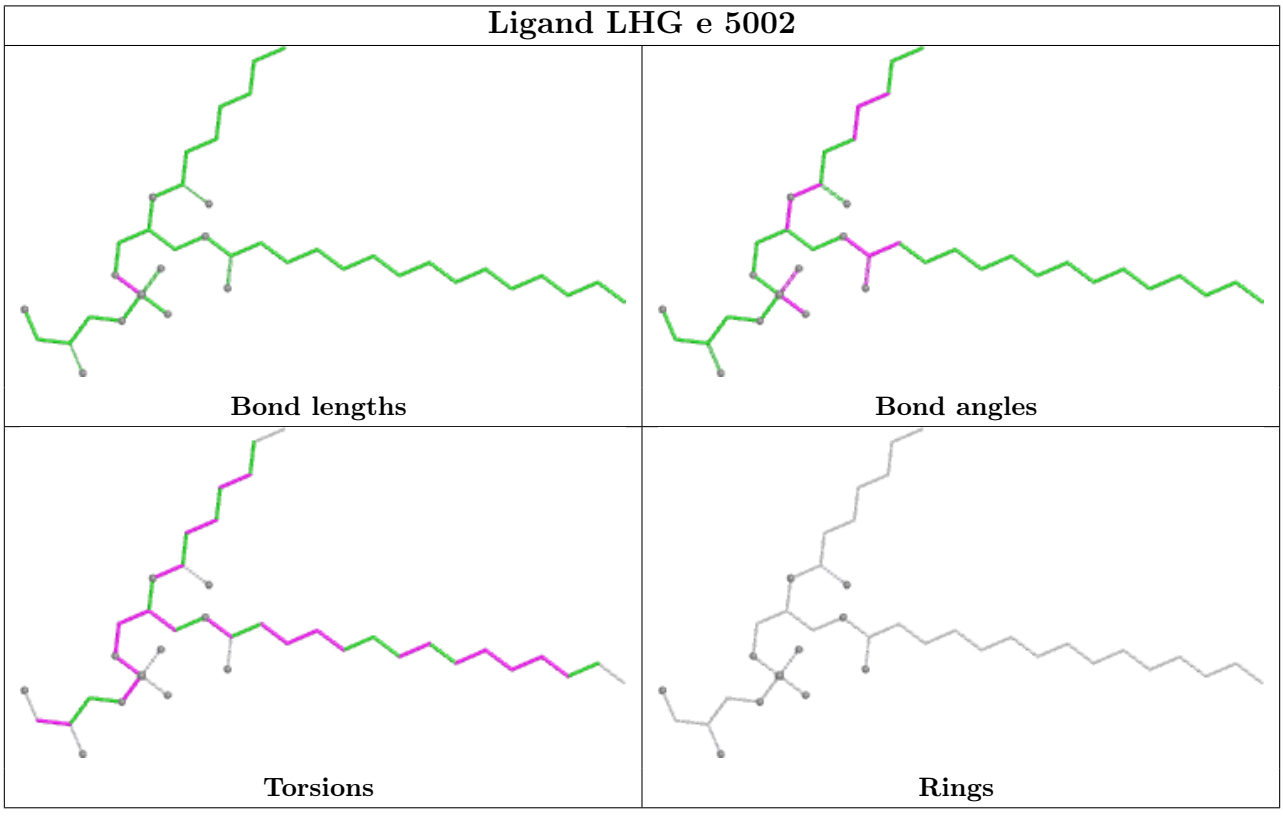
Ligand LMU e 1849



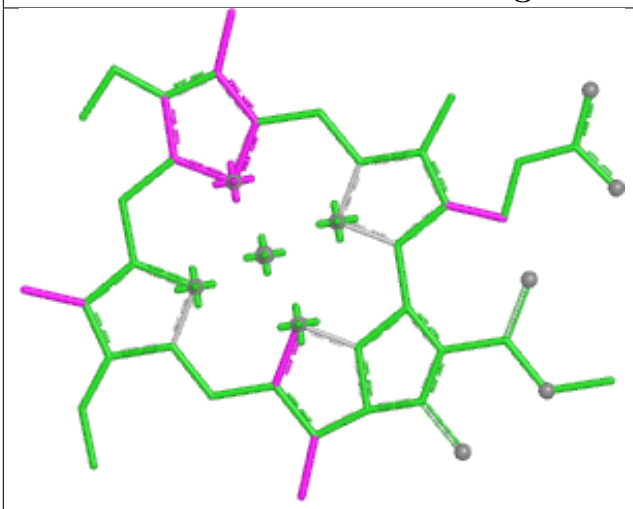
Ligand BCR s 521



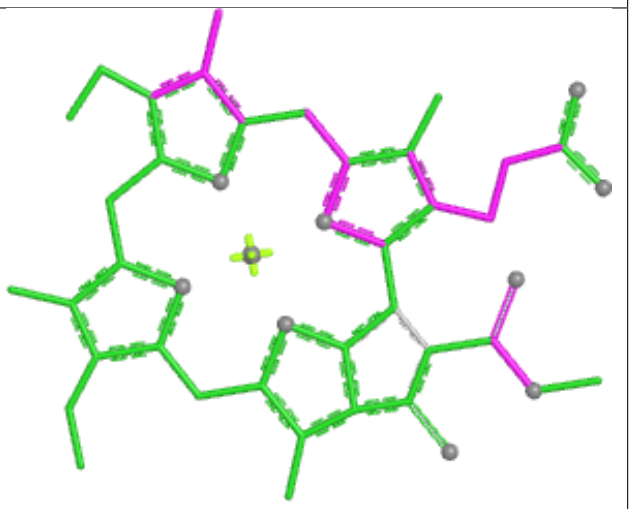
Ligand LHG e 5002



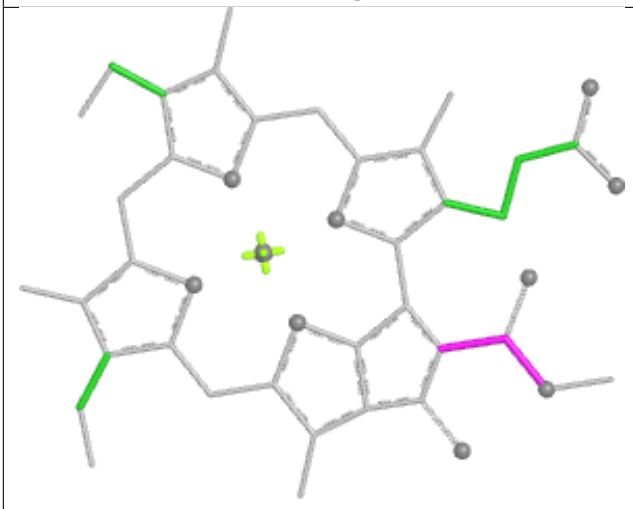
Ligand CLA G 1801



Bond lengths



Bond angles

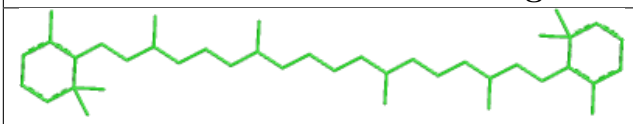


Torsions

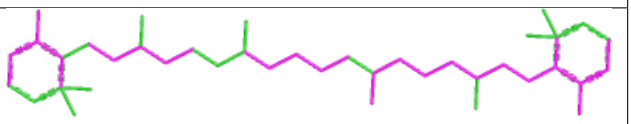


Rings

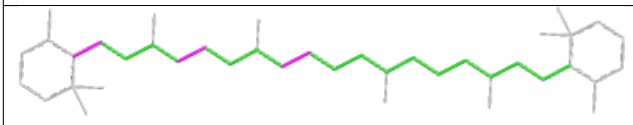
Ligand BCR b 522



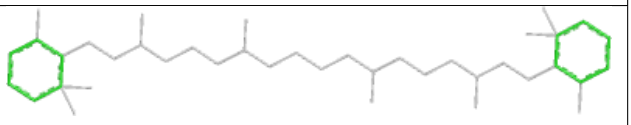
Bond lengths



Bond angles

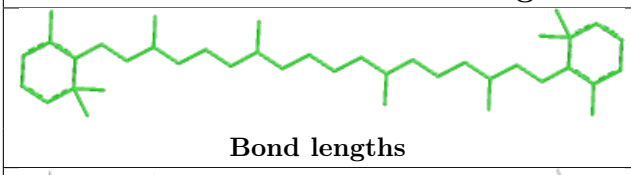


Torsions

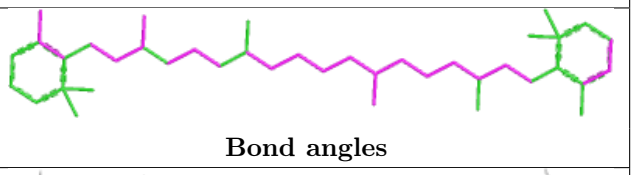


Rings

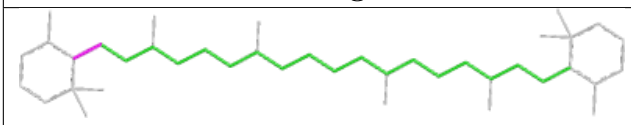
Ligand BCR n 4219



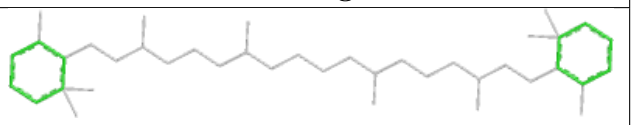
Bond lengths



Bond angles

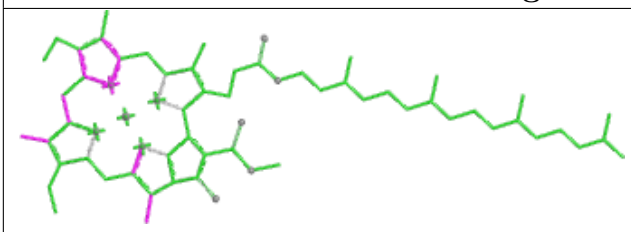


Torsions

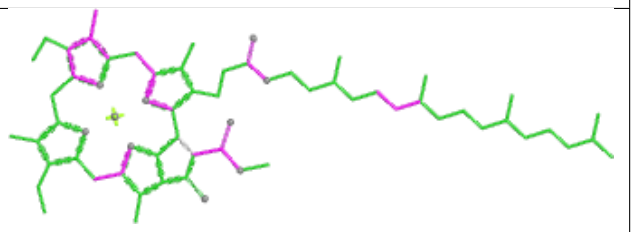


Rings

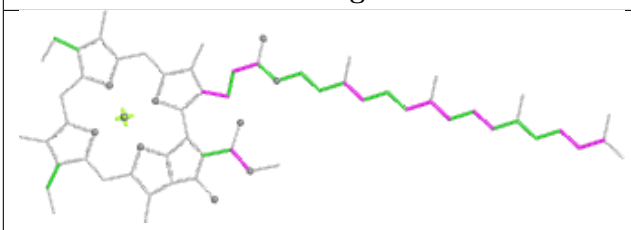
Ligand CLA f 1229



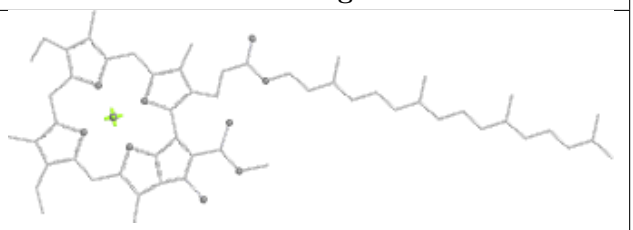
Bond lengths



Bond angles

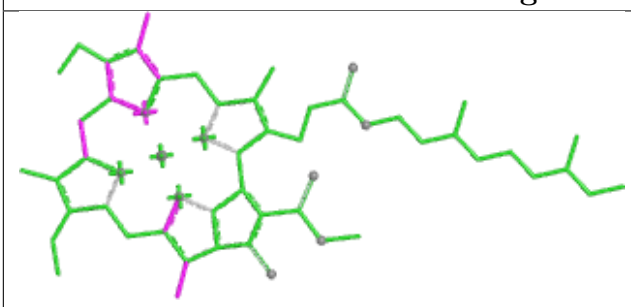


Torsions

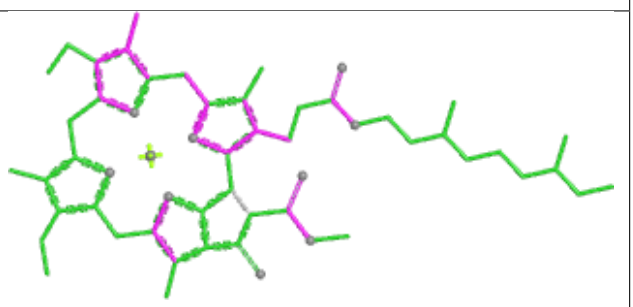


Rings

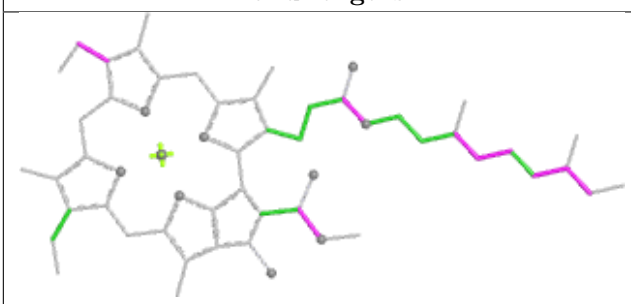
Ligand CLA e 1124



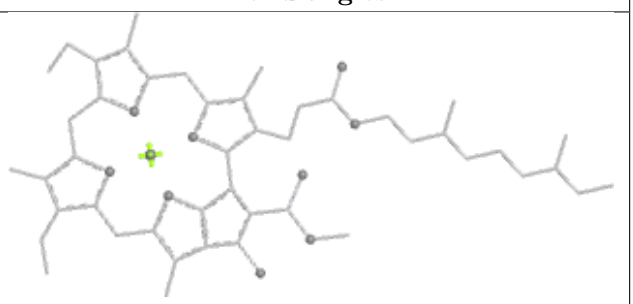
Bond lengths



Bond angles

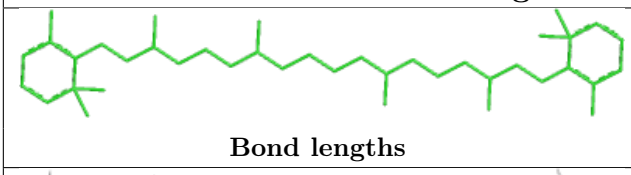


Torsions

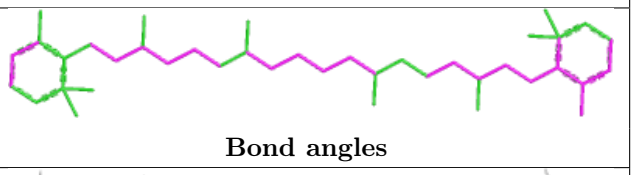


Rings

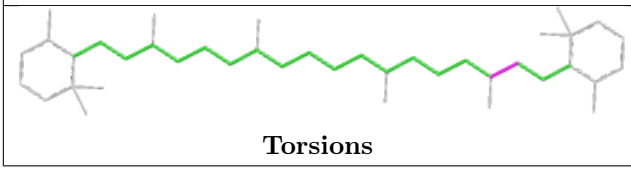
Ligand BCR K 4104



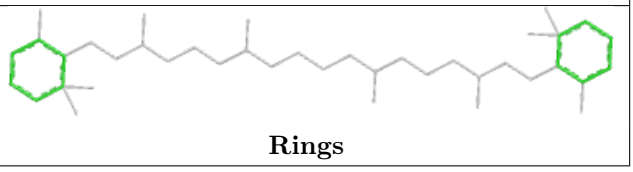
Bond lengths



Bond angles

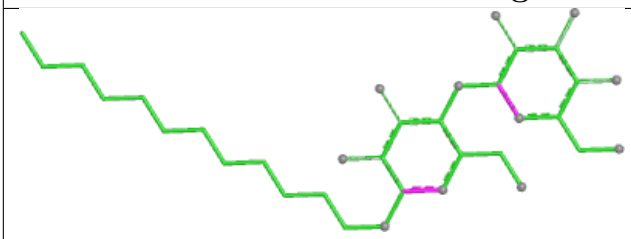


Torsions

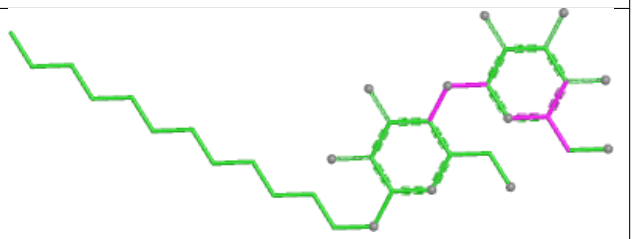


Rings

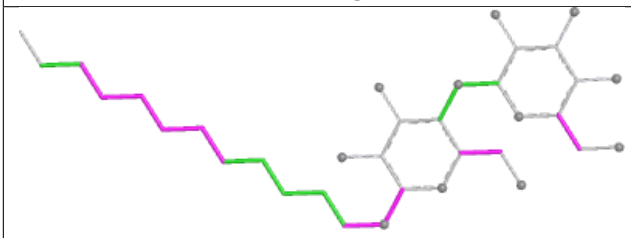
Ligand LMU B 1843



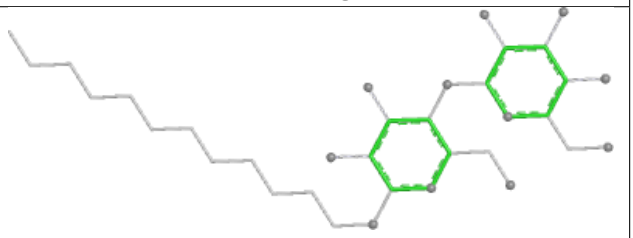
Bond lengths



Bond angles

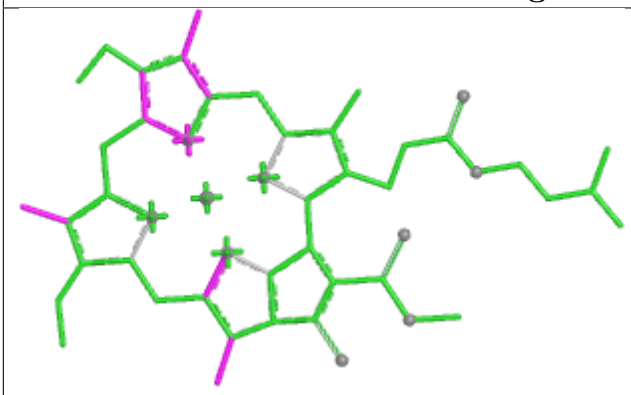


Torsions

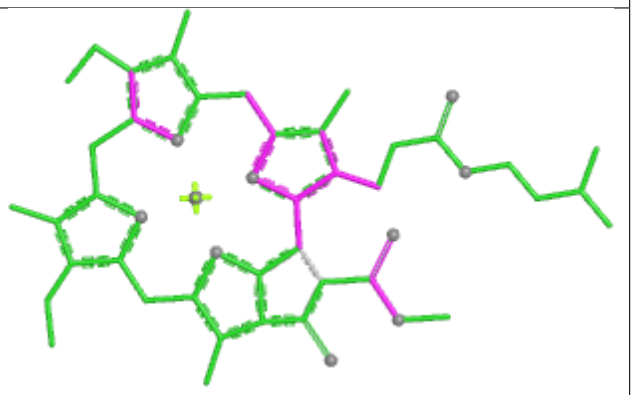


Rings

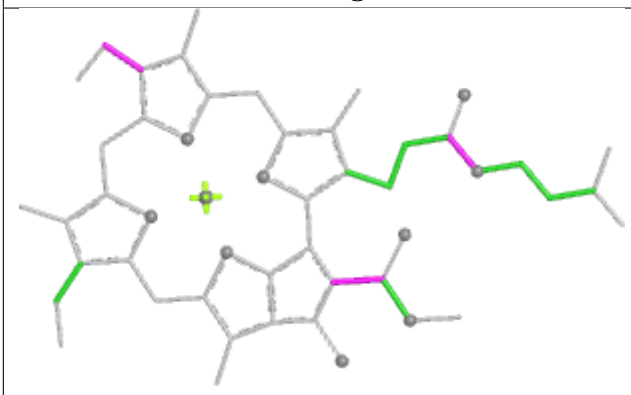
Ligand CLA a 502



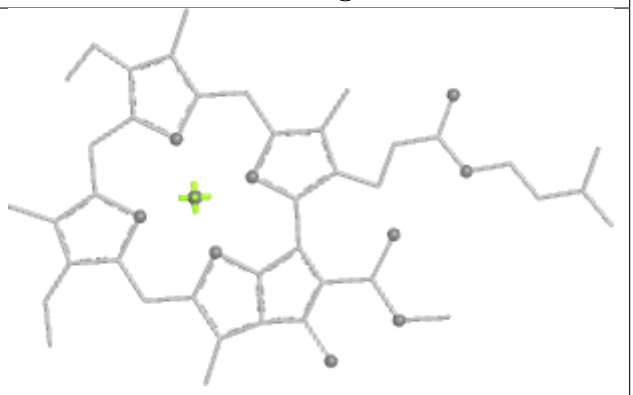
Bond lengths



Bond angles



Torsions

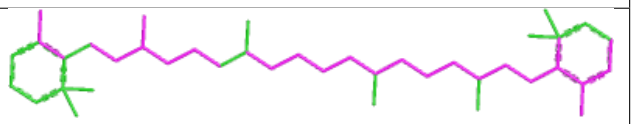


Rings

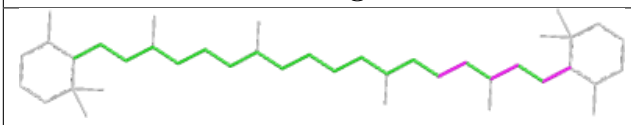
Ligand BCR A 4008



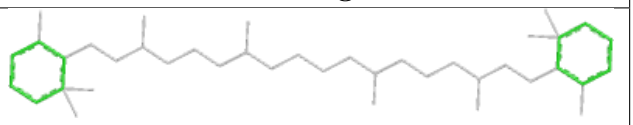
Bond lengths



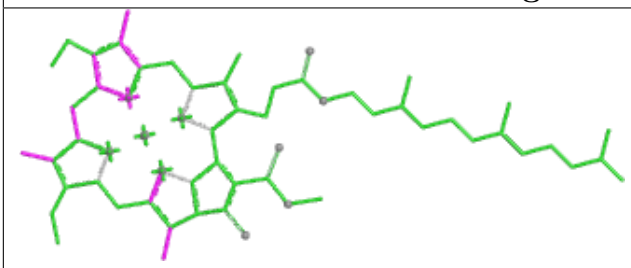
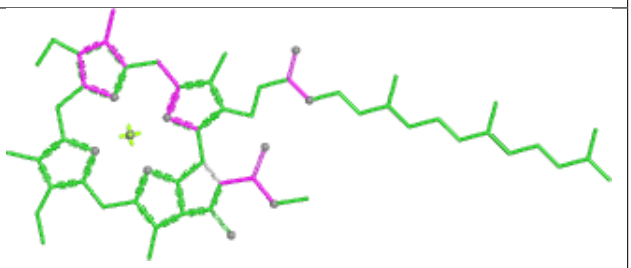
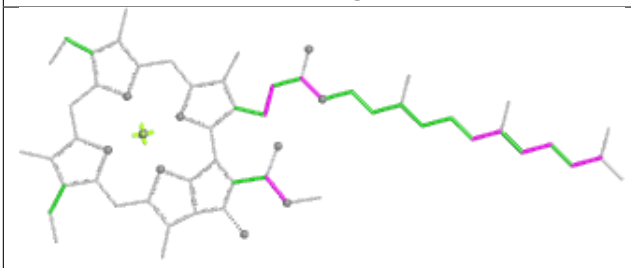
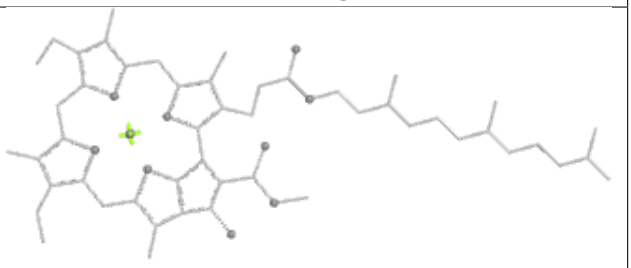
Bond angles

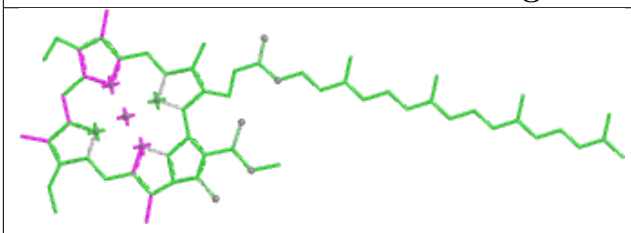
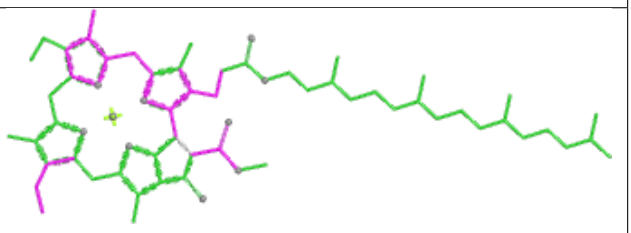
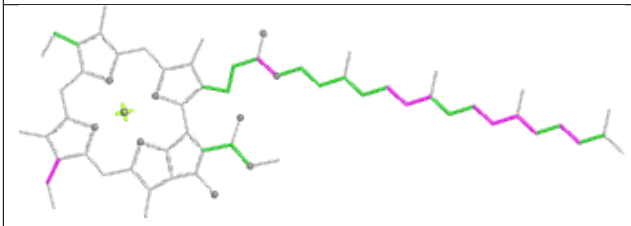
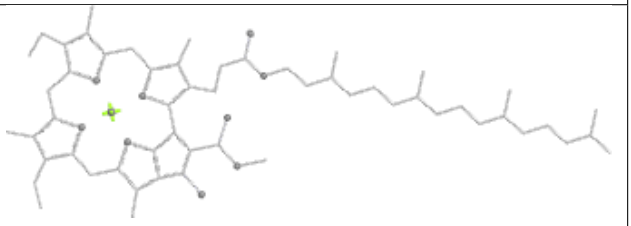


Torsions

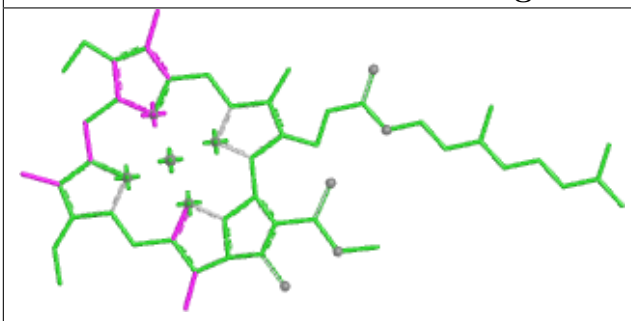


Rings

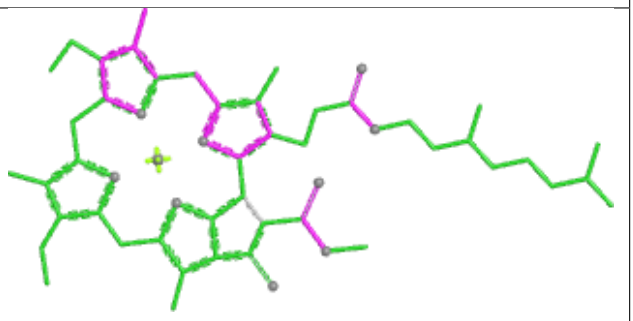
Ligand CLA f 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 1234	
 Bond lengths	 Bond angles
 Torsions	 Rings

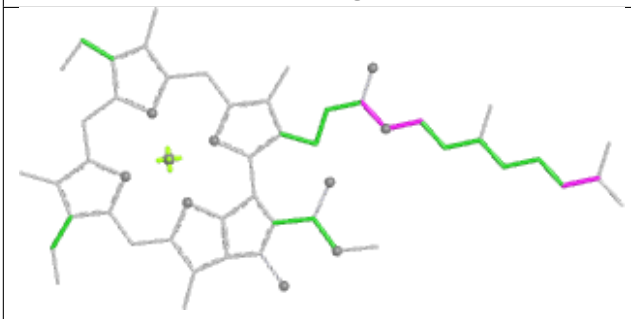
Ligand CLA A 1105



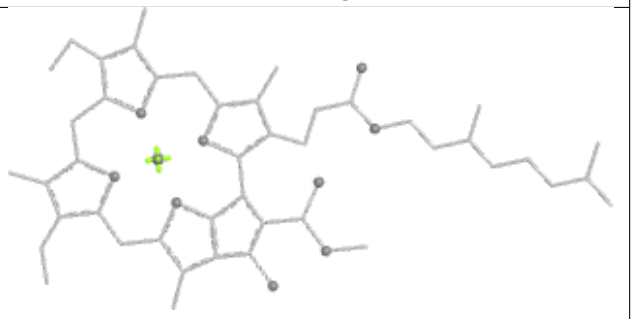
Bond lengths



Bond angles

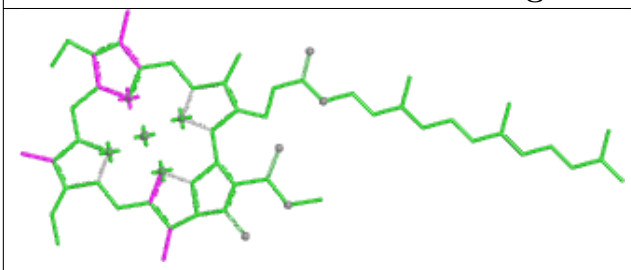


Torsions

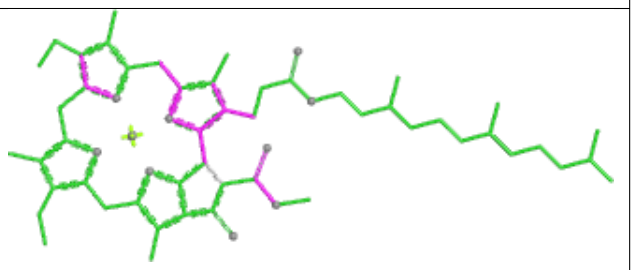


Rings

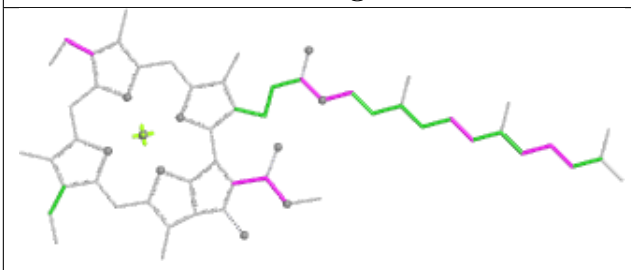
Ligand CLA Z 502



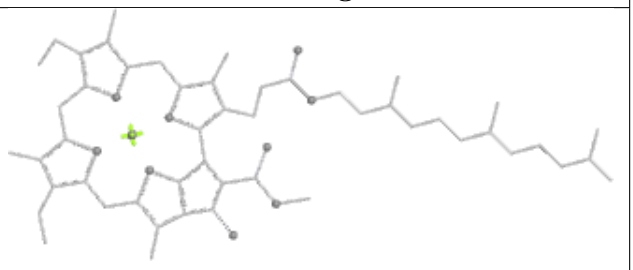
Bond lengths



Bond angles



Torsions

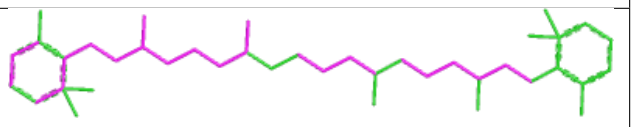


Rings

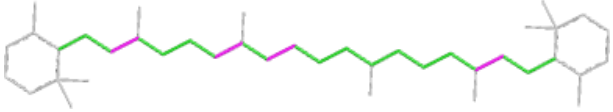
Ligand BCR G 4001



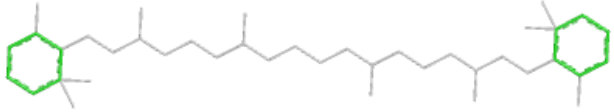
Bond lengths



Bond angles

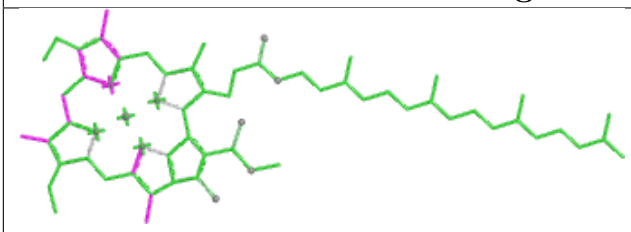


Torsions

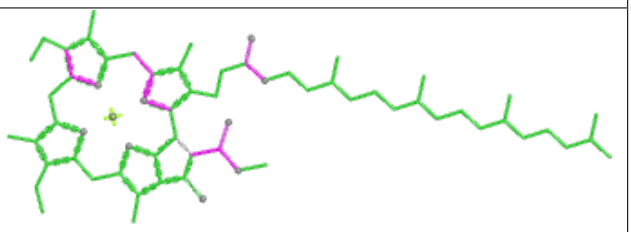


Rings

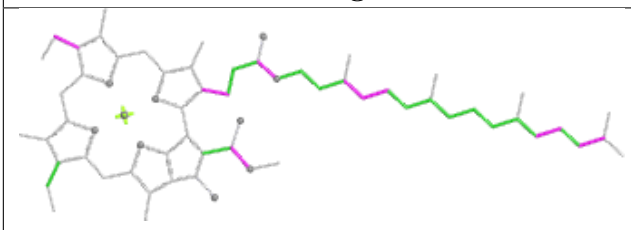
Ligand CLA B 1227



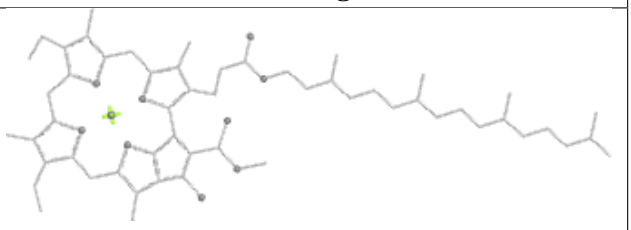
Bond lengths



Bond angles

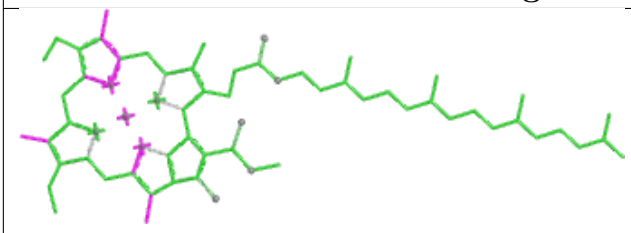


Torsions

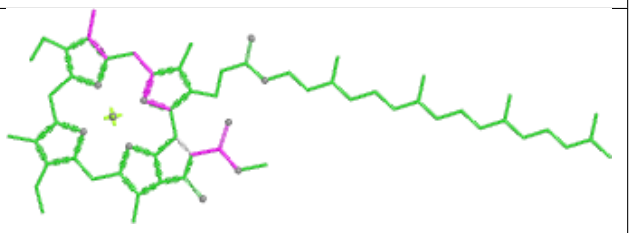


Rings

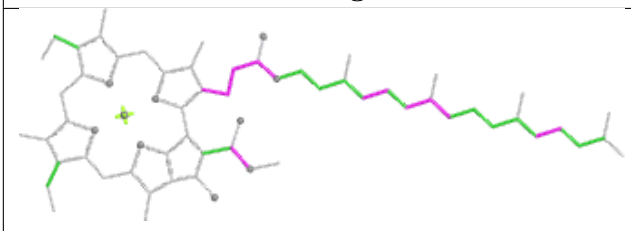
Ligand CLA f 1206



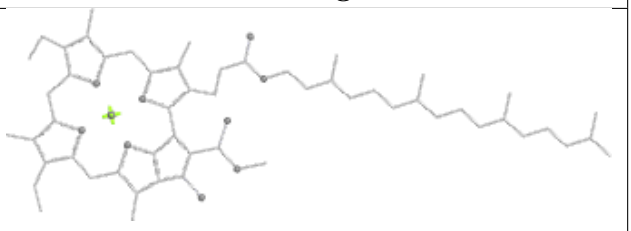
Bond lengths



Bond angles

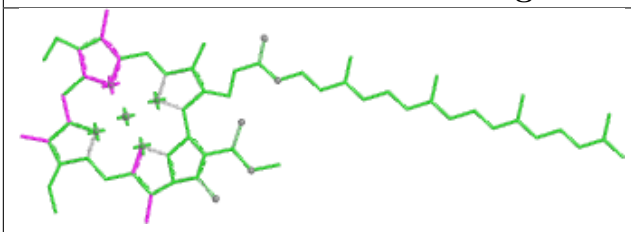


Torsions

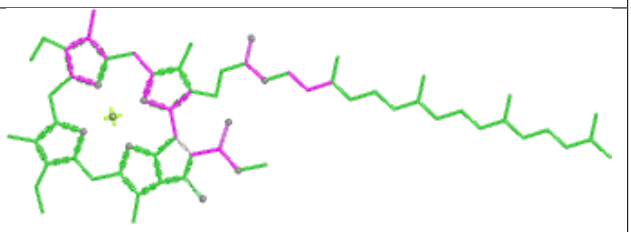


Rings

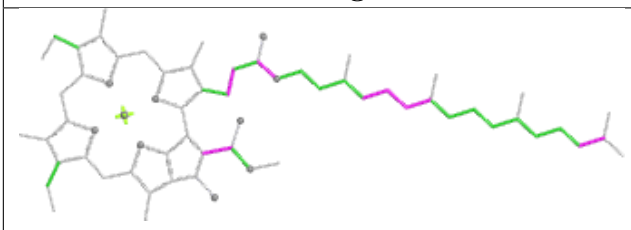
Ligand CLA B 1213



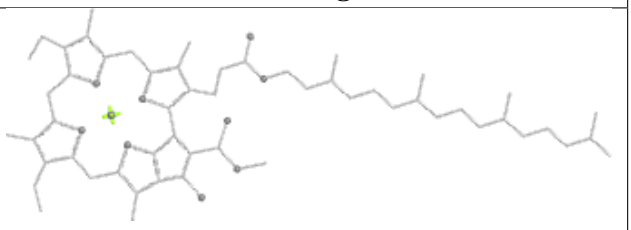
Bond lengths



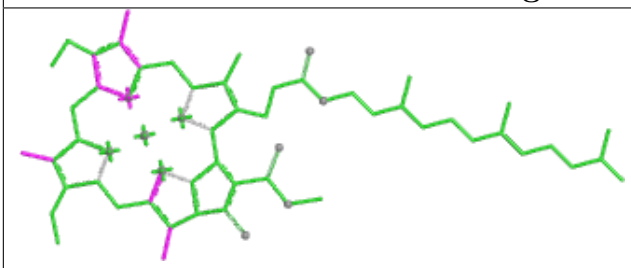
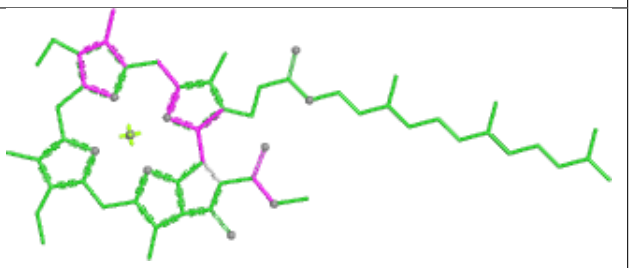
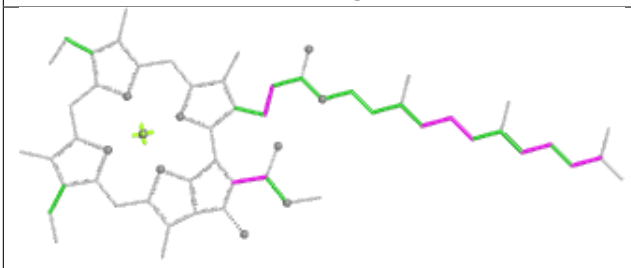
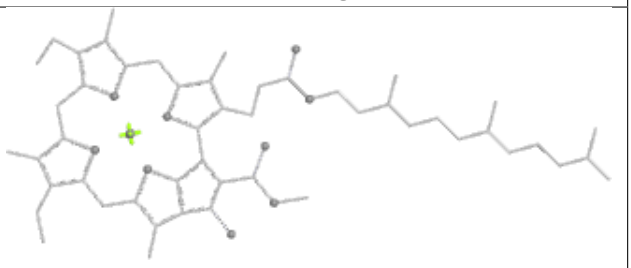
Bond angles

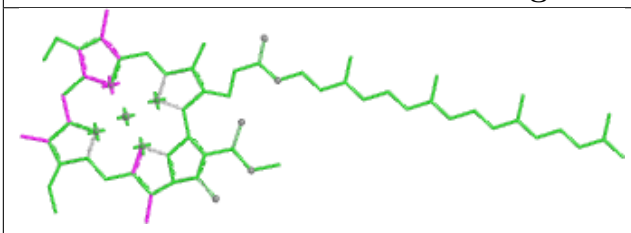
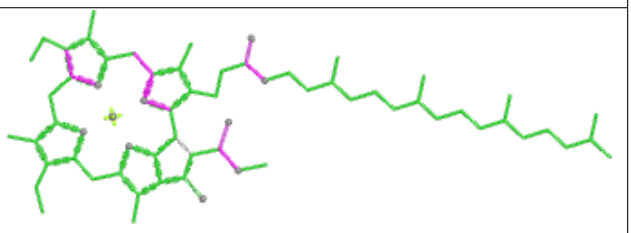
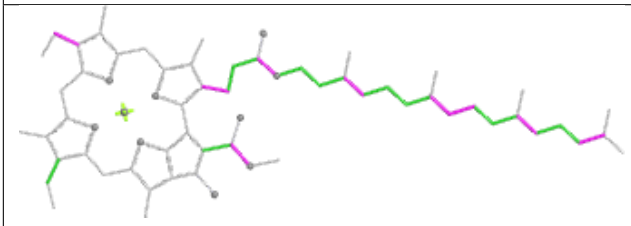
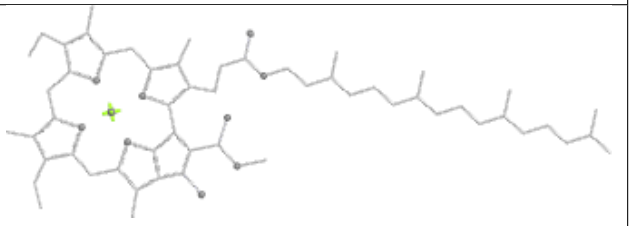


Torsions

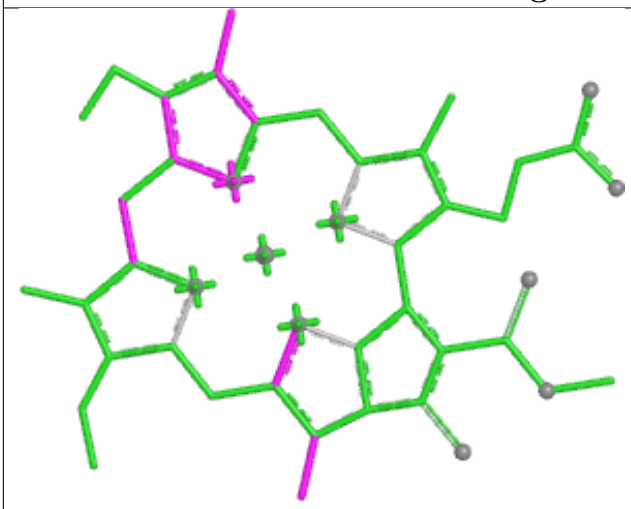


Rings

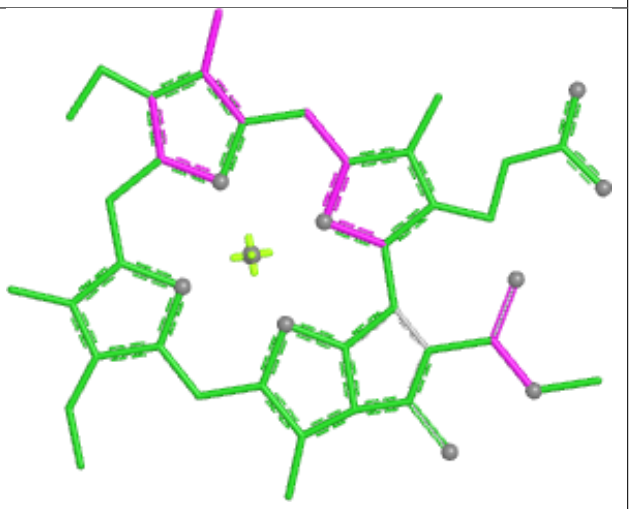
Ligand CLA f 1218	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

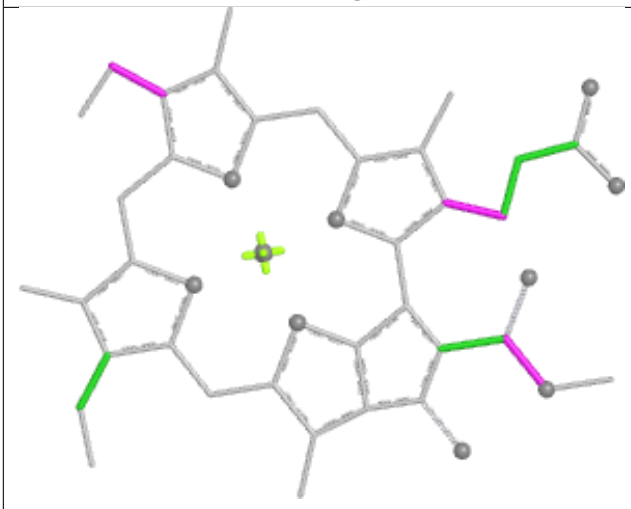
Ligand CLA t 511



Bond lengths



Bond angles

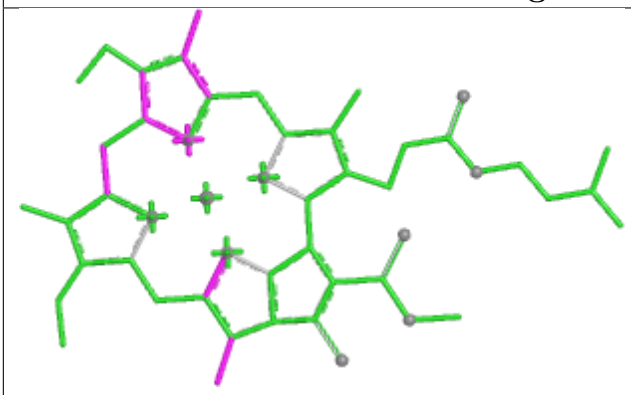


Torsions

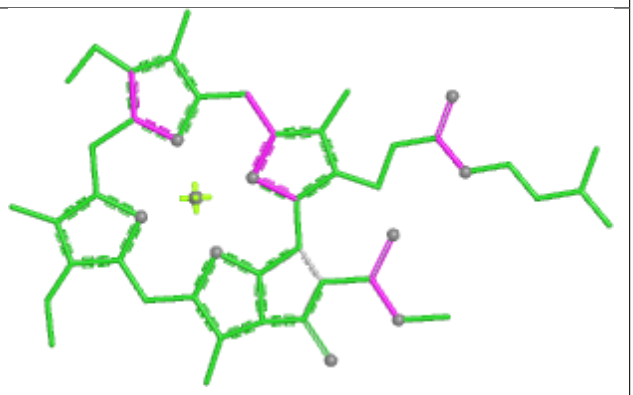


Rings

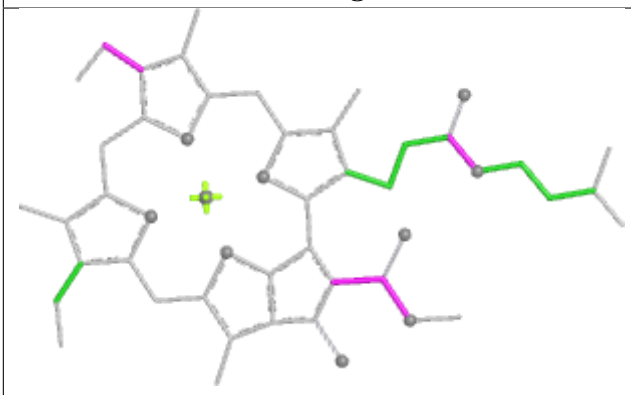
Ligand CLA 4 510



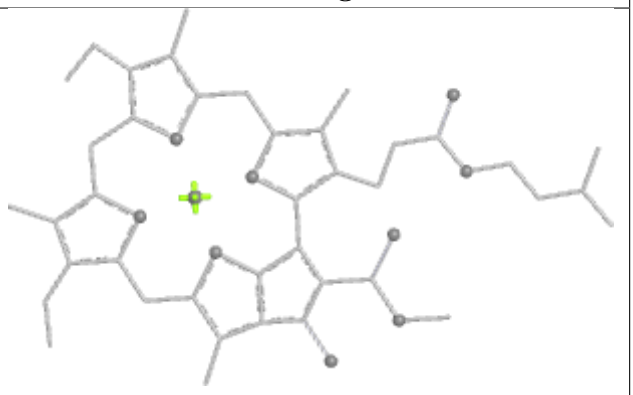
Bond lengths



Bond angles

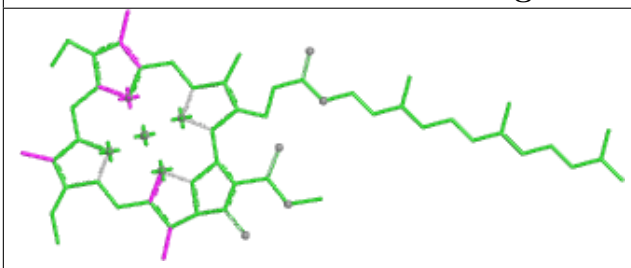


Torsions

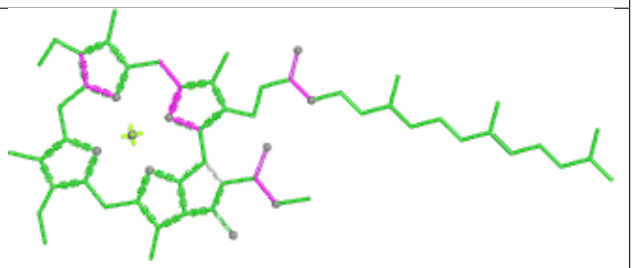


Rings

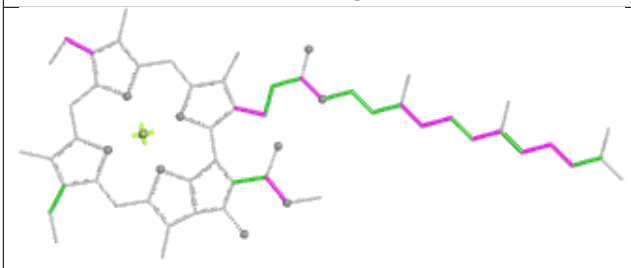
Ligand CLA A 1122



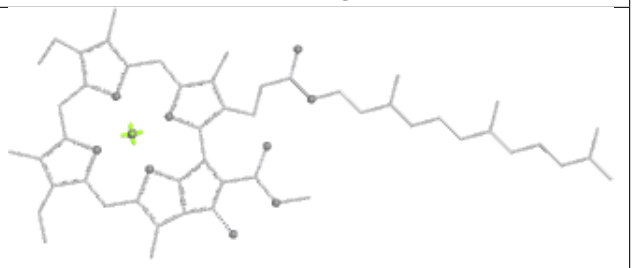
Bond lengths



Bond angles

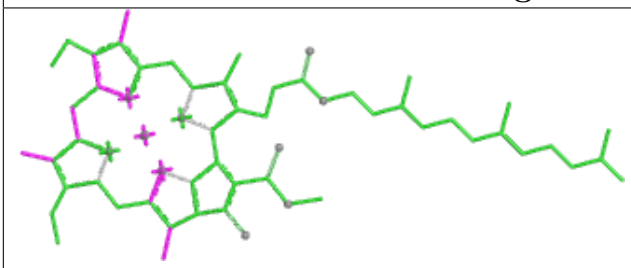


Torsions

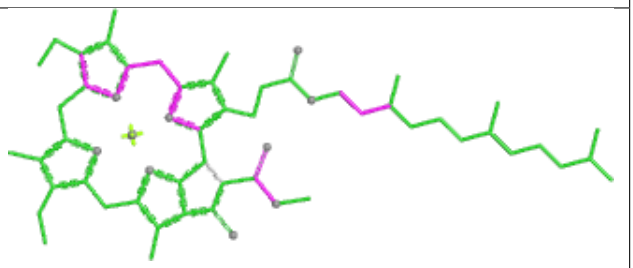


Rings

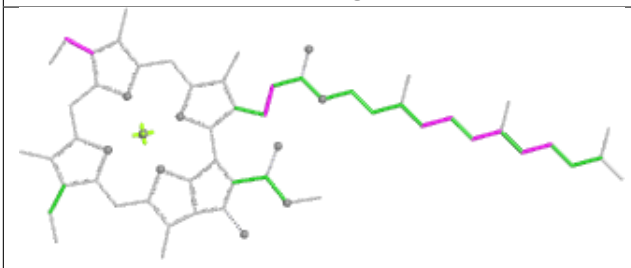
Ligand CLA H 1216



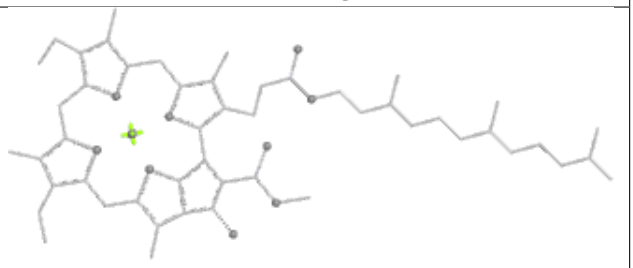
Bond lengths



Bond angles

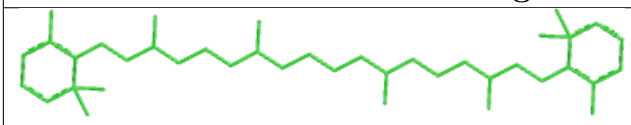


Torsions

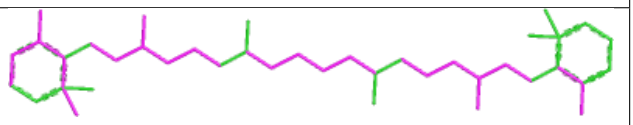


Rings

Ligand BCR V 4020



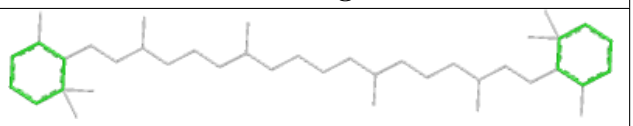
Bond lengths



Bond angles

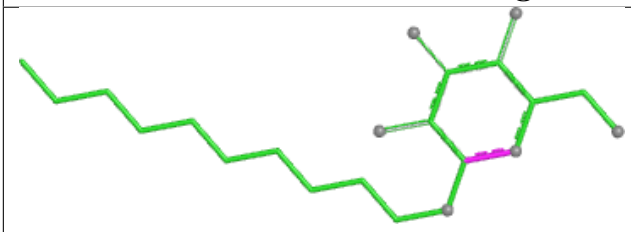


Torsions

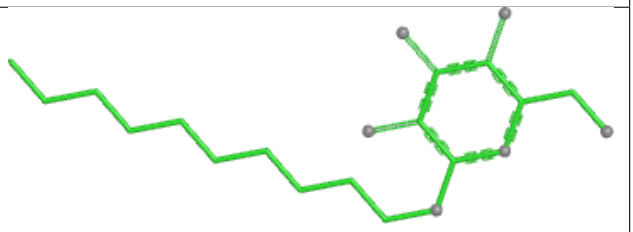


Rings

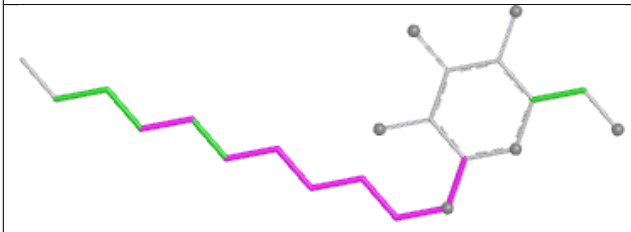
Ligand LMU J 5105



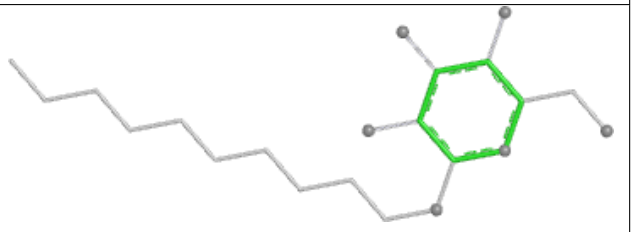
Bond lengths



Bond angles

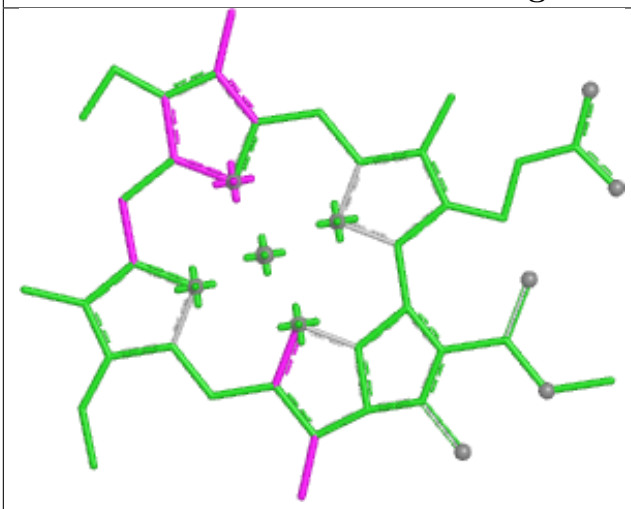


Torsions

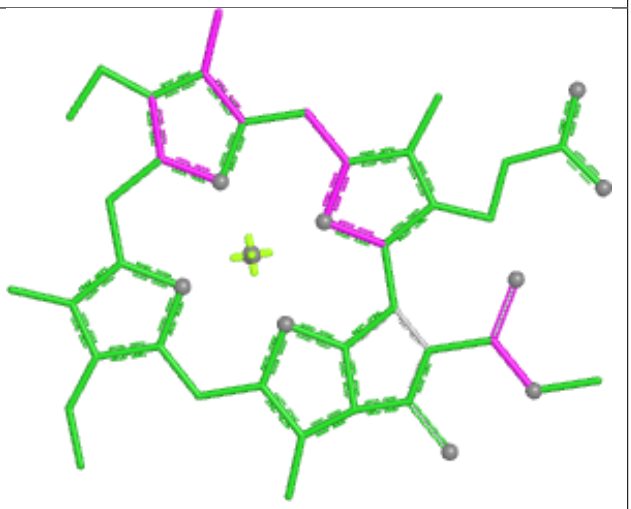


Rings

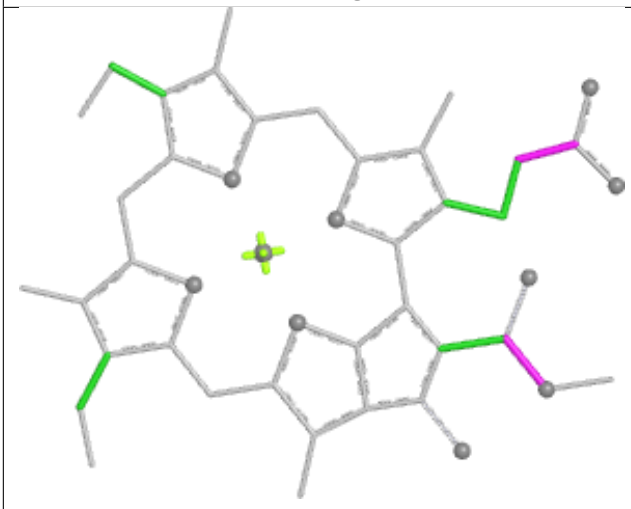
Ligand CLA 6 509



Bond lengths



Bond angles

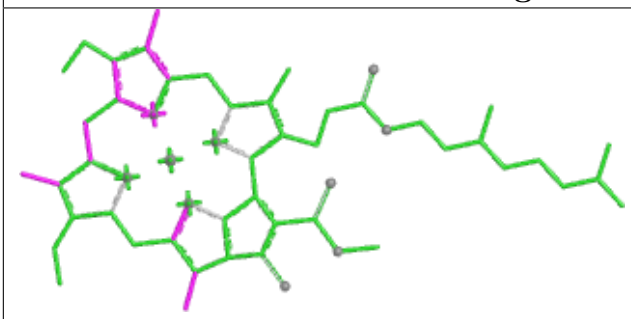


Torsions

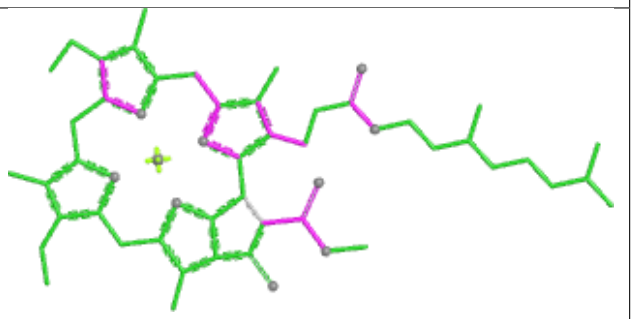


Rings

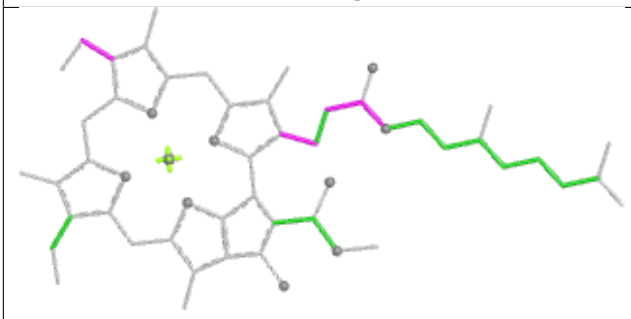
Ligand CLA K 1401



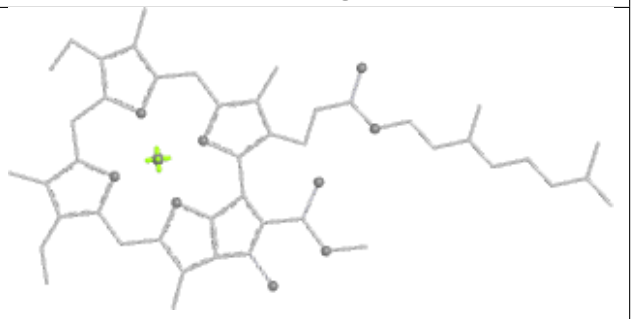
Bond lengths



Bond angles

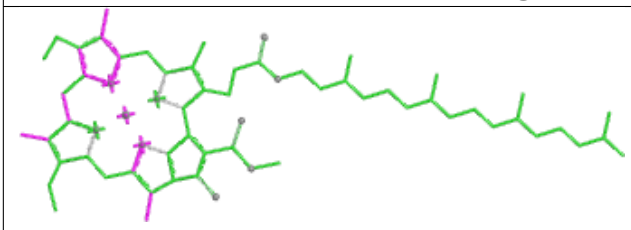


Torsions

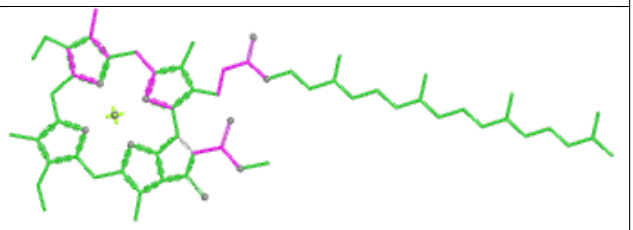


Rings

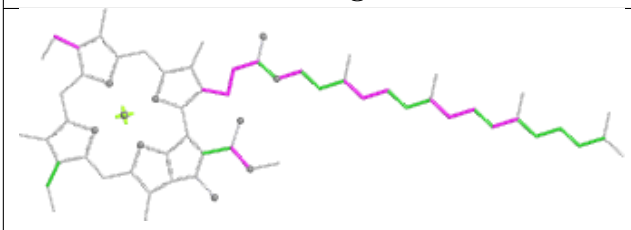
Ligand CLA A 1107



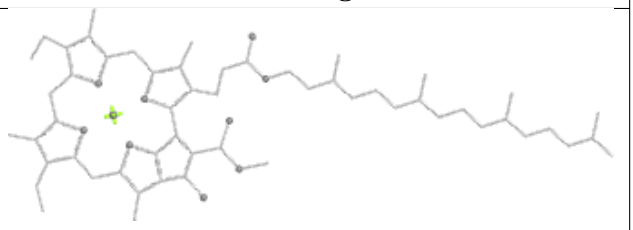
Bond lengths



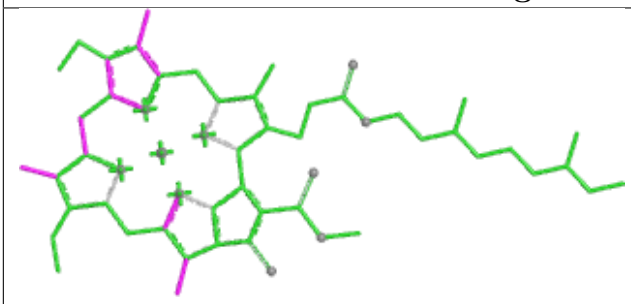
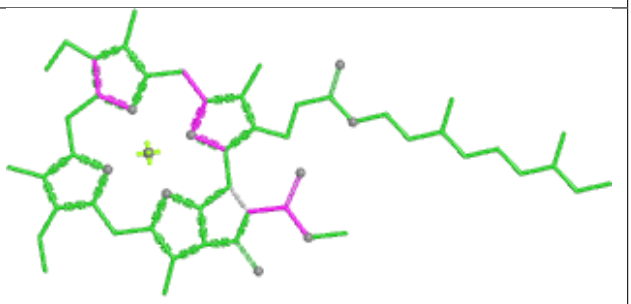
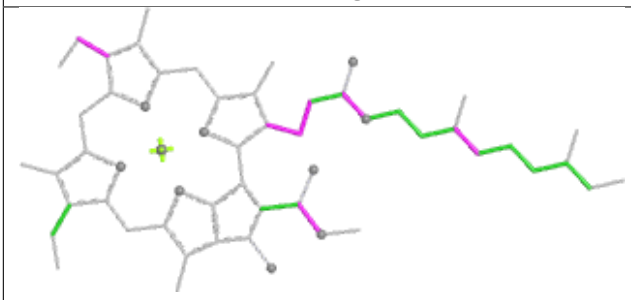
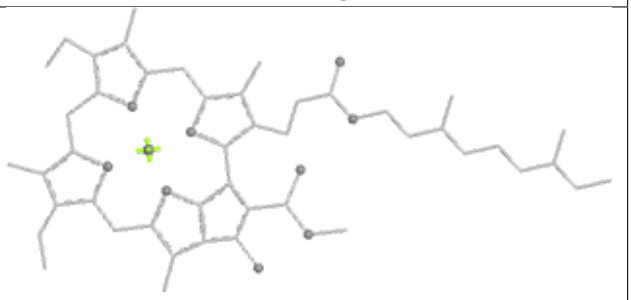
Bond angles

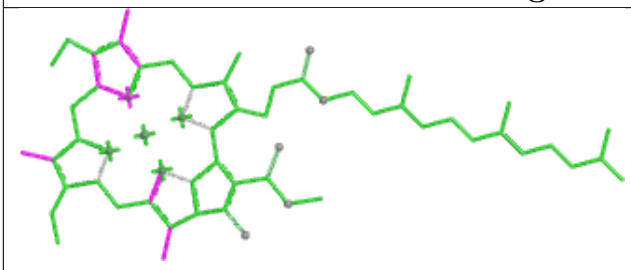
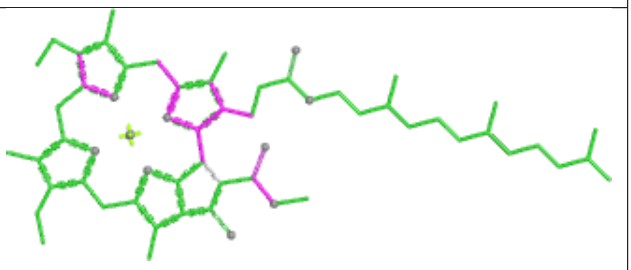
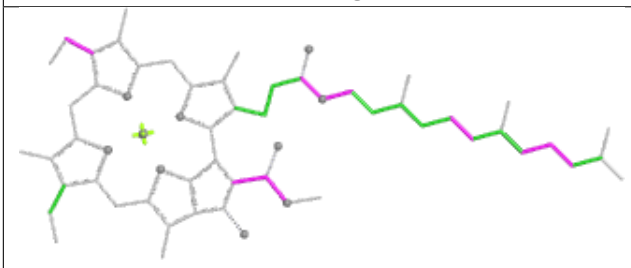
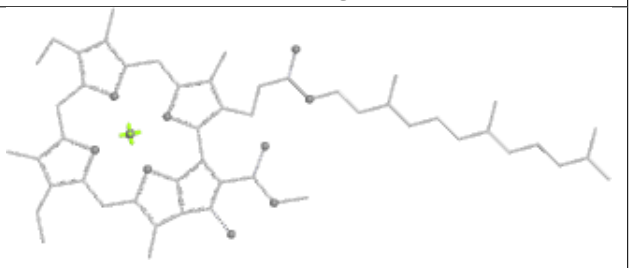


Torsions

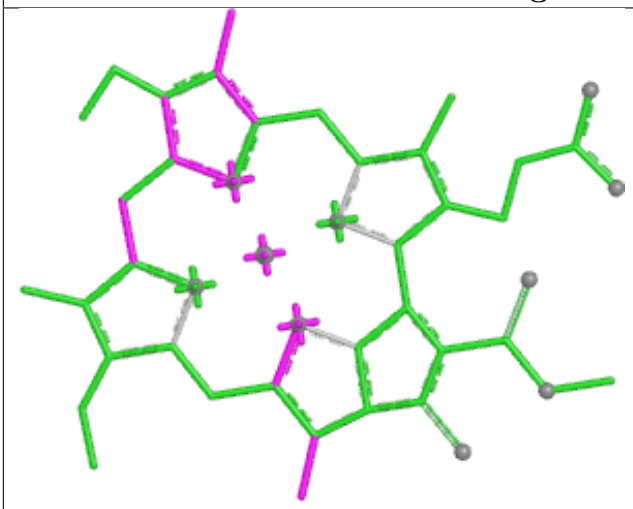


Rings

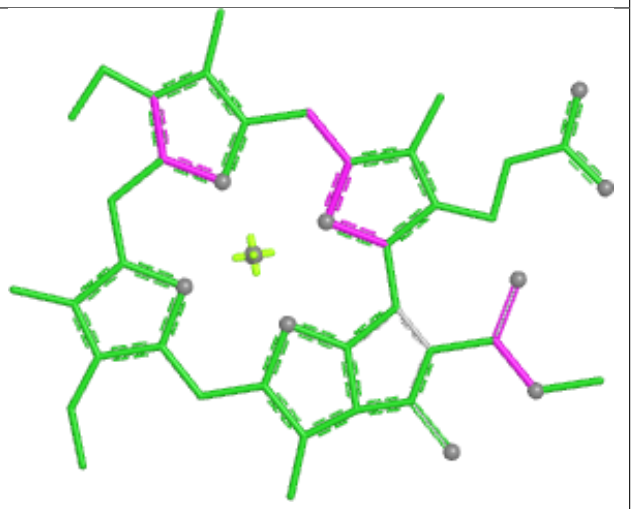
Ligand CLA G 1134	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

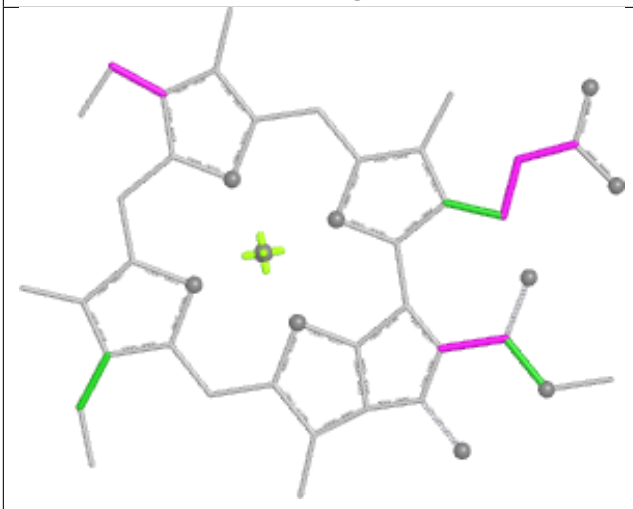
Ligand CLA s 512



Bond lengths



Bond angles

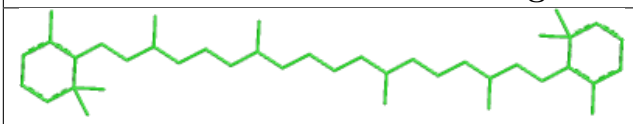


Torsions

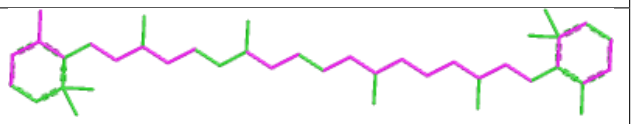


Rings

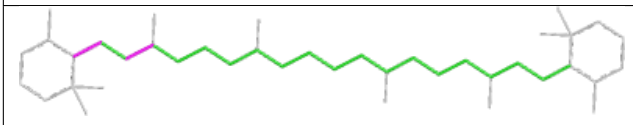
Ligand BCR r 521



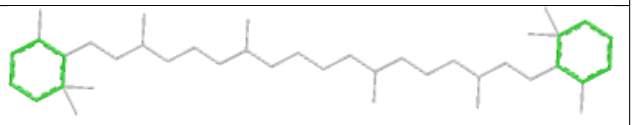
Bond lengths



Bond angles

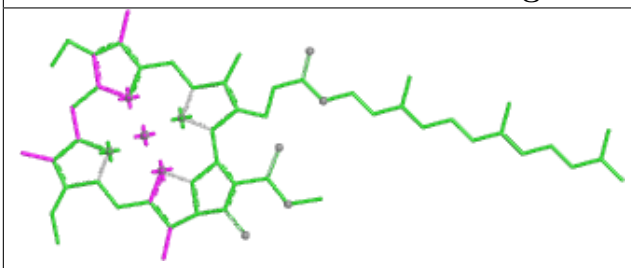


Torsions

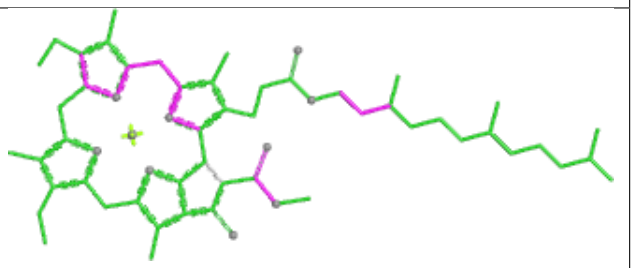


Rings

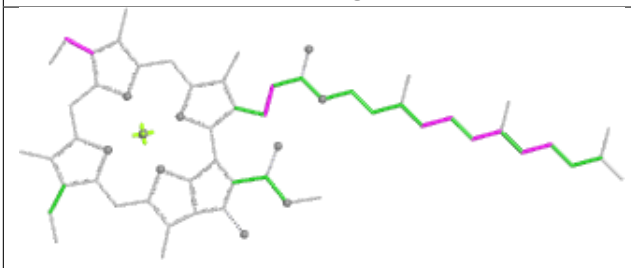
Ligand CLA f 1216



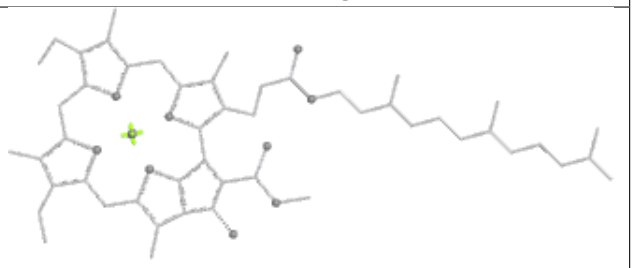
Bond lengths



Bond angles

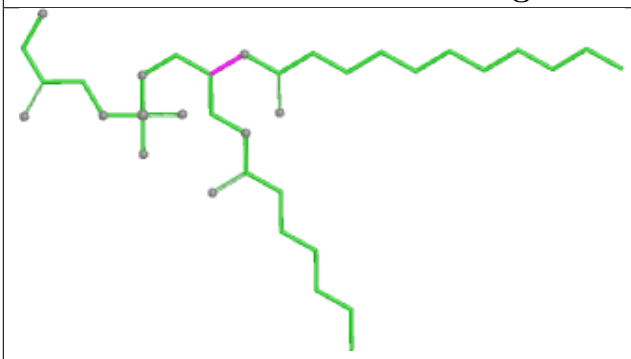


Torsions

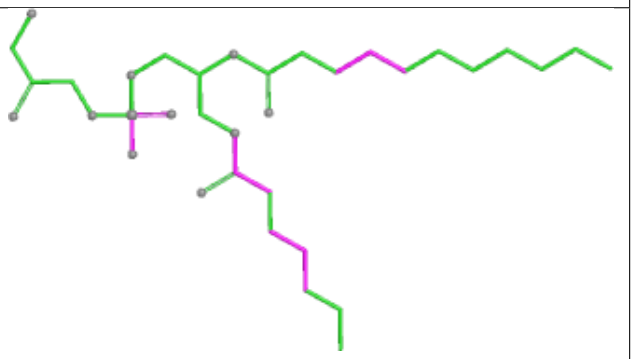


Rings

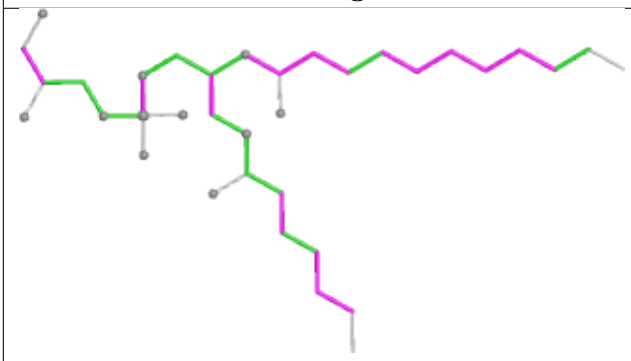
Ligand LHG G 5008



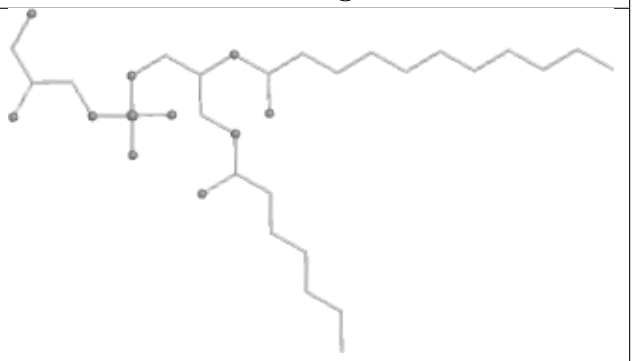
Bond lengths



Bond angles

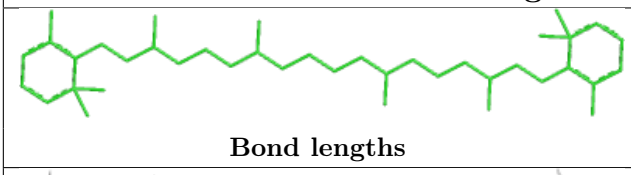


Torsions

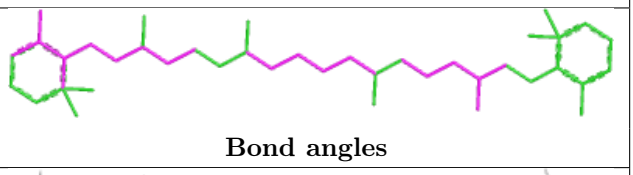


Rings

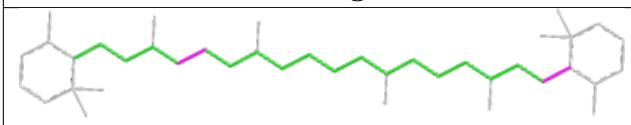
Ligand BCR Z 524



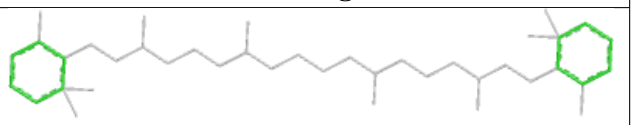
Bond lengths



Bond angles

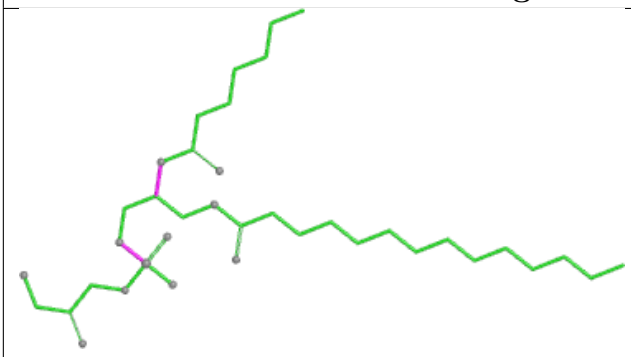


Torsions

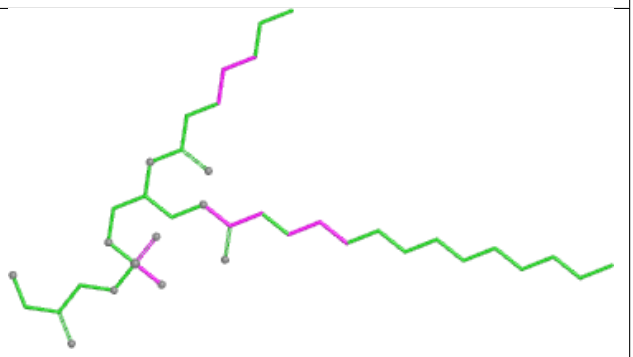


Rings

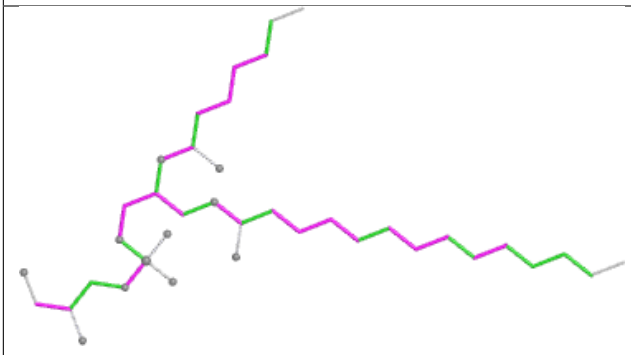
Ligand LHG V 5218



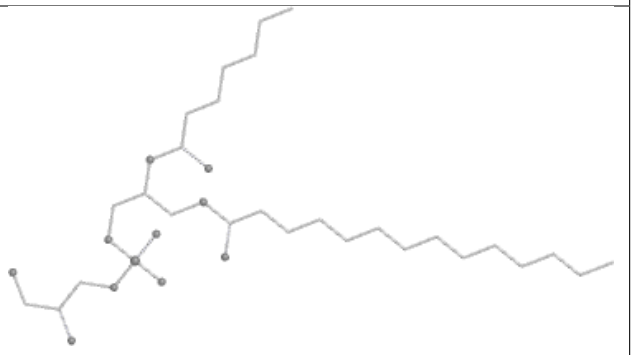
Bond lengths



Bond angles

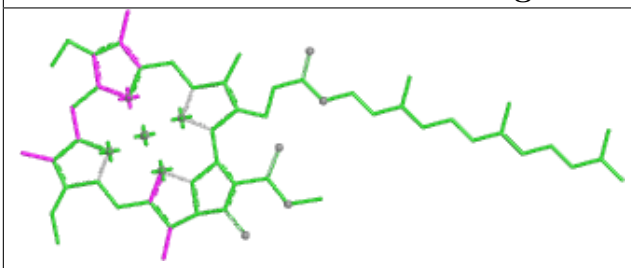


Torsions

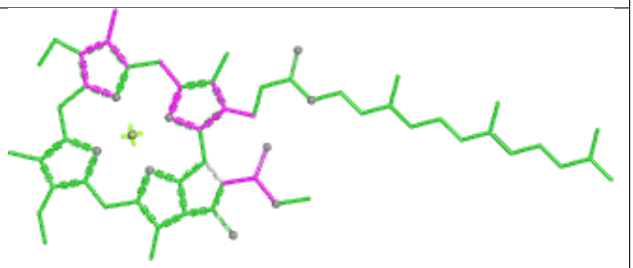


Rings

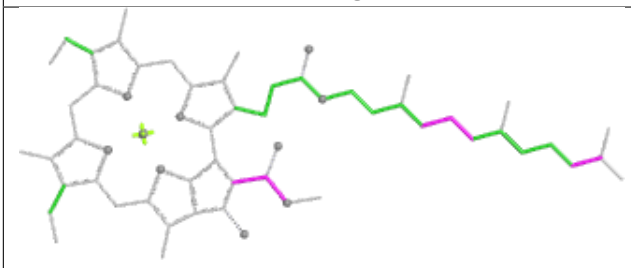
Ligand CLA H 1222



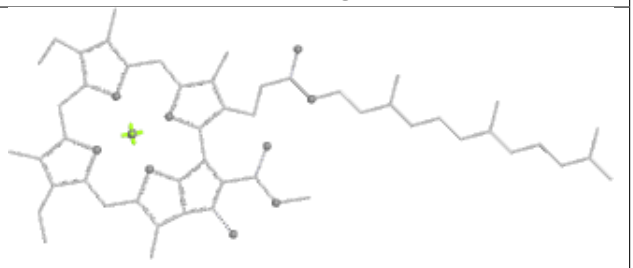
Bond lengths



Bond angles

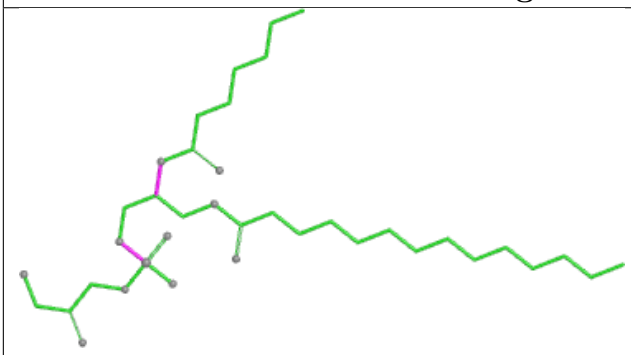


Torsions

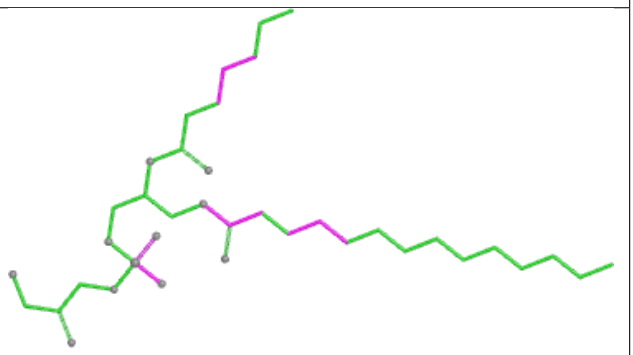


Rings

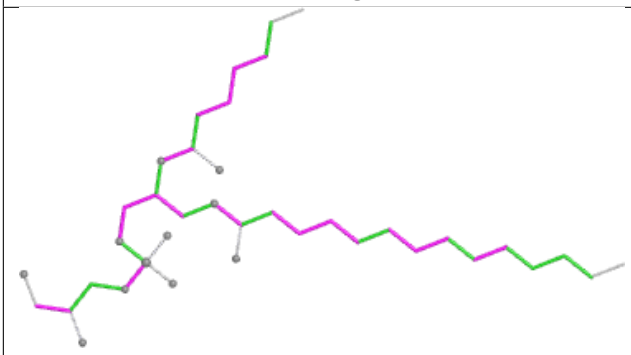
Ligand LHG L 5218



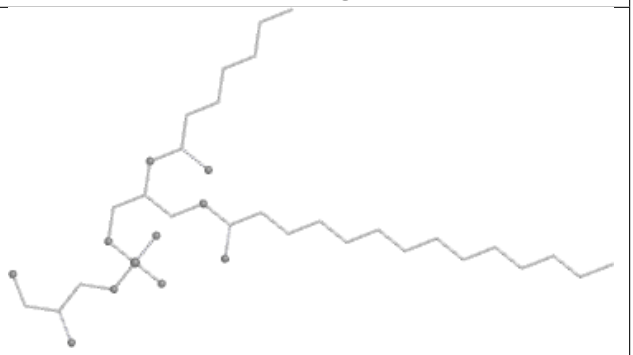
Bond lengths



Bond angles

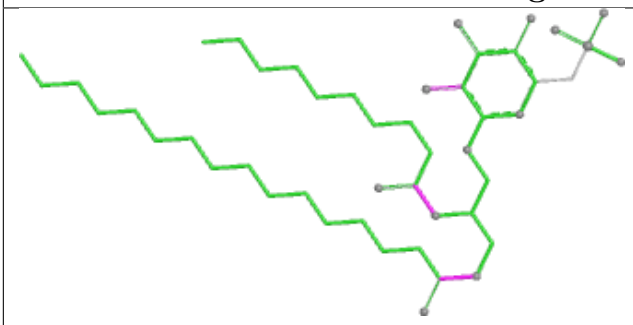


Torsions

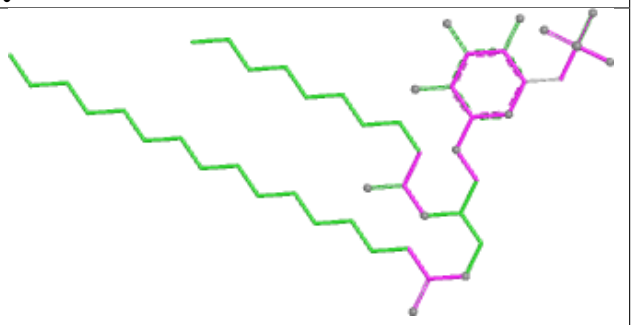


Rings

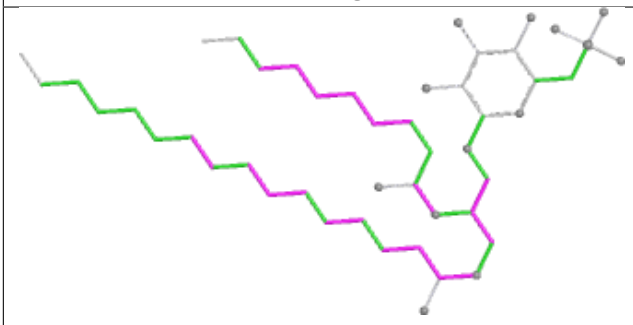
Ligand SQD 1 822



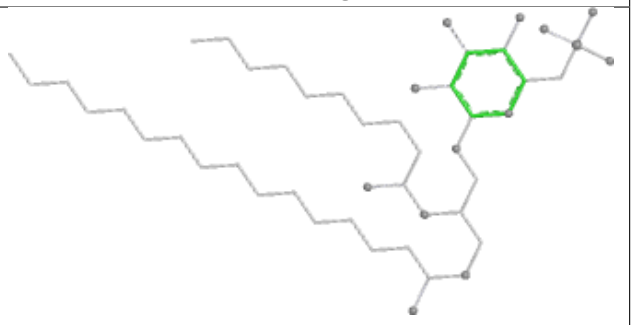
Bond lengths



Bond angles

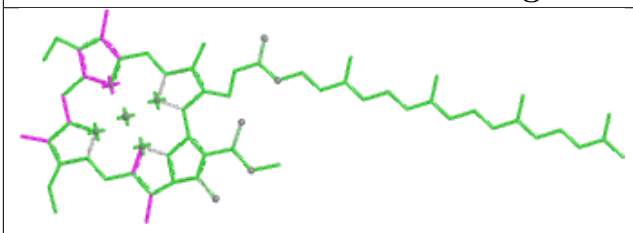


Torsions

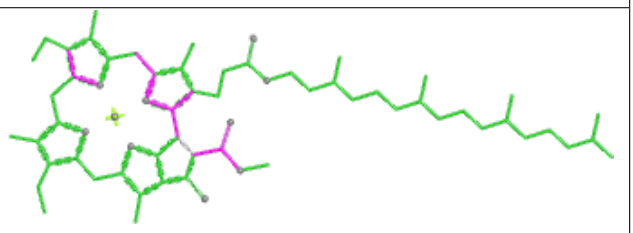


Rings

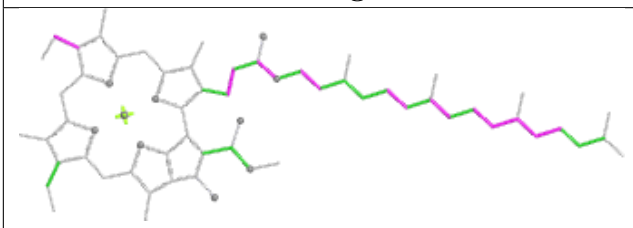
Ligand CLA f 1214



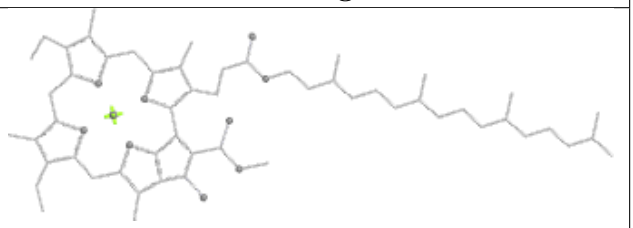
Bond lengths



Bond angles

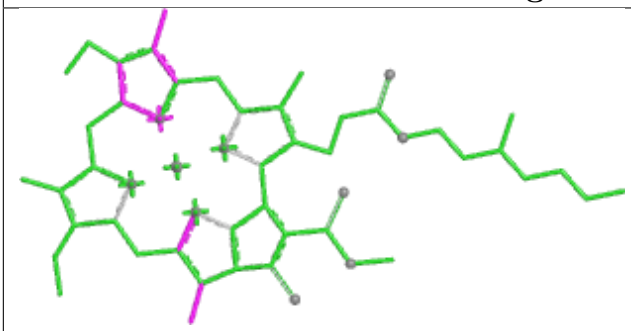


Torsions

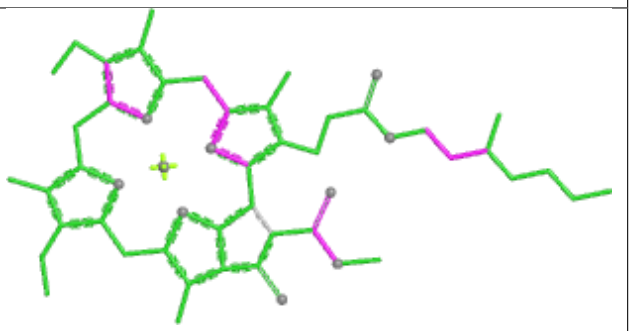


Rings

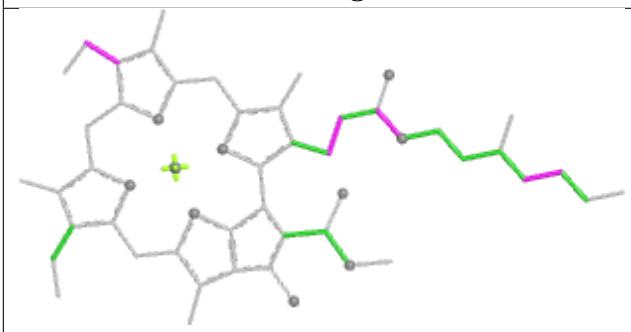
Ligand CLA Z 512



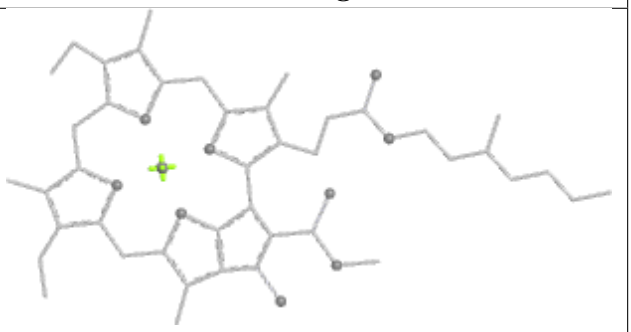
Bond lengths



Bond angles



Torsions

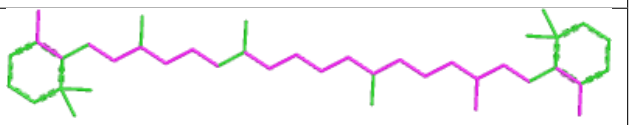


Rings

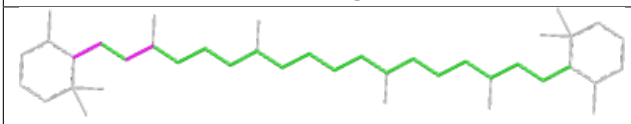
Ligand BCR 6 524



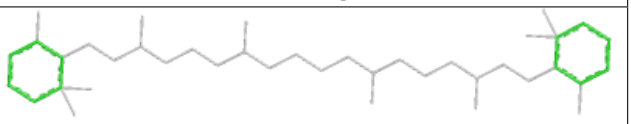
Bond lengths



Bond angles

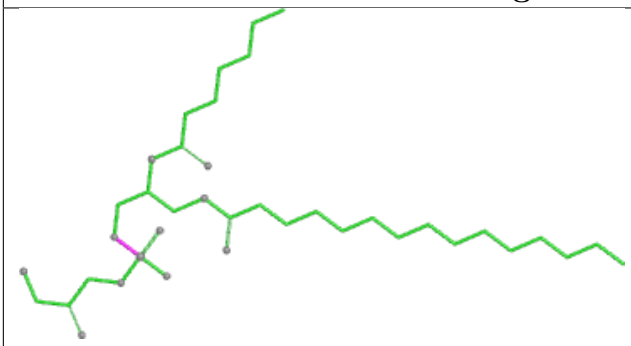


Torsions

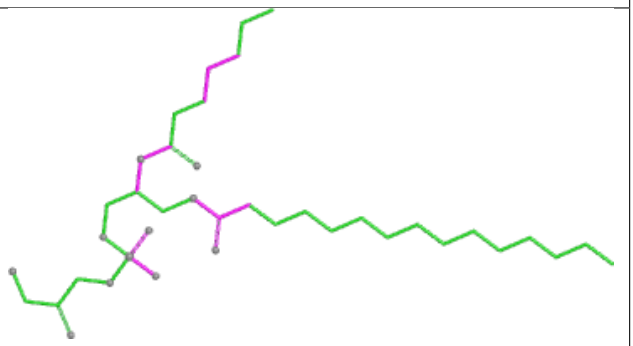


Rings

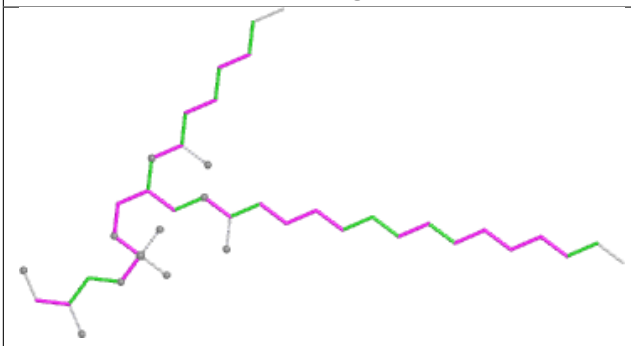
Ligand LHG A 5002



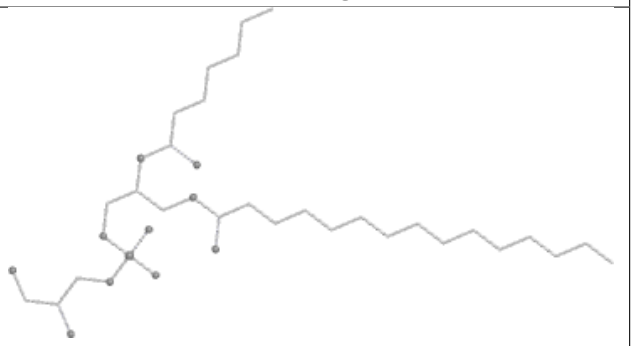
Bond lengths



Bond angles

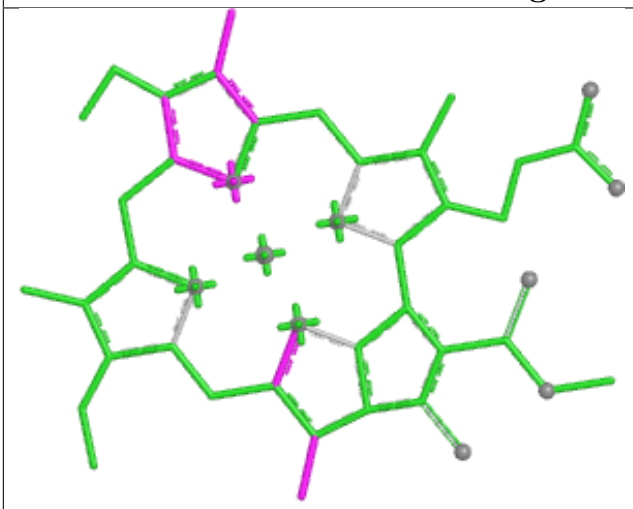


Torsions

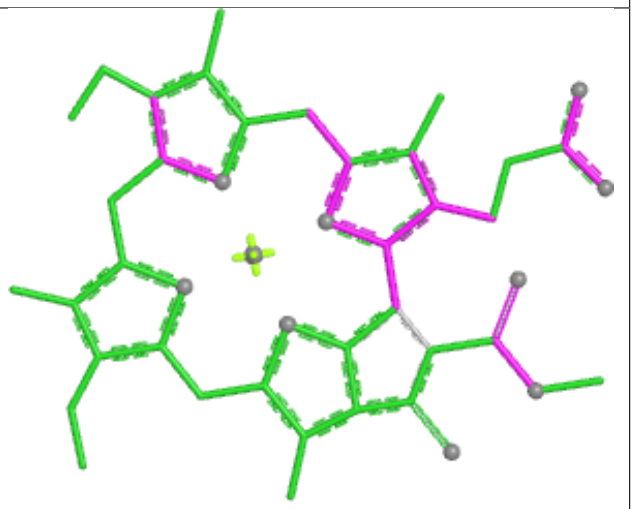


Rings

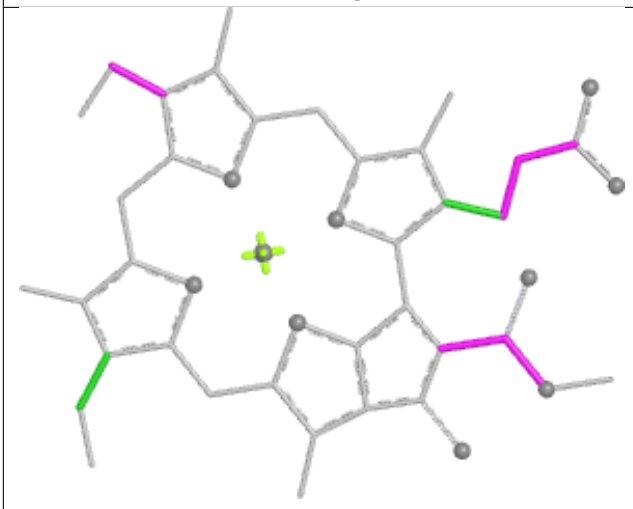
Ligand CLA c 507



Bond lengths



Bond angles

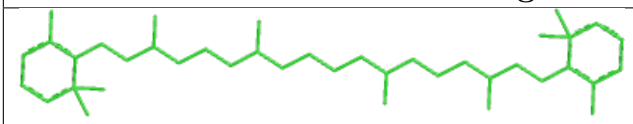


Torsions

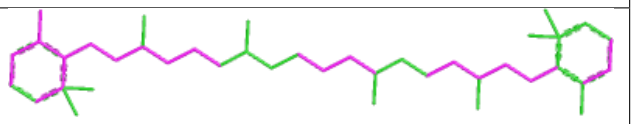


Rings

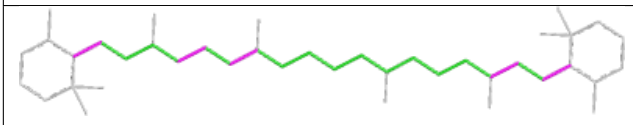
Ligand BCR J 4012



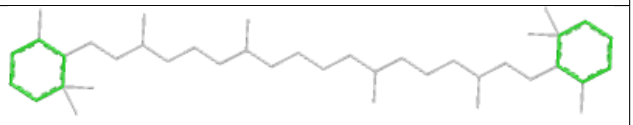
Bond lengths



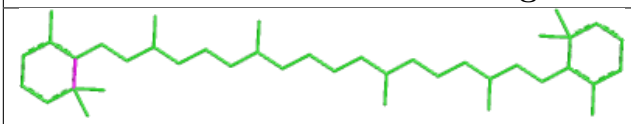
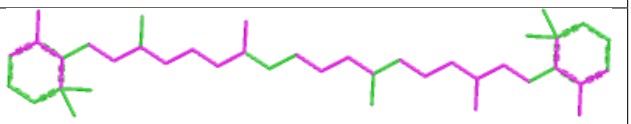
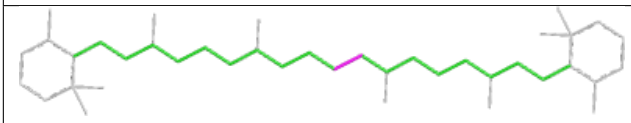
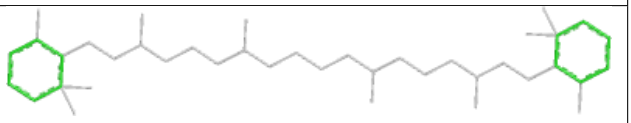
Bond angles

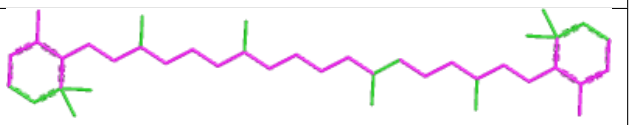
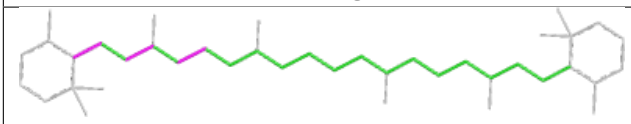
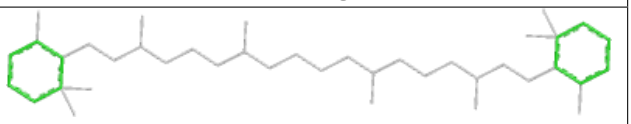


Torsions

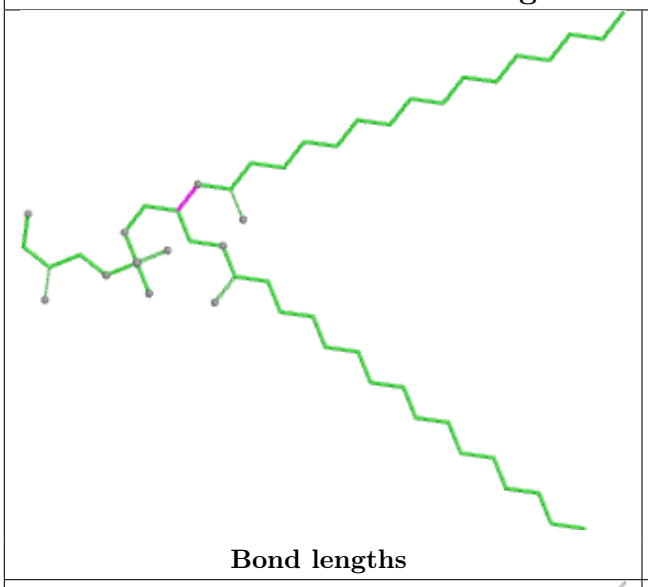


Rings

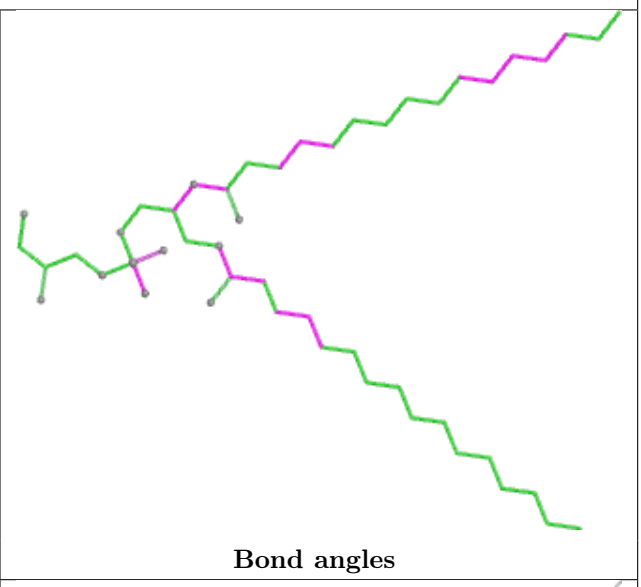
Ligand BCR I 4018	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR u 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

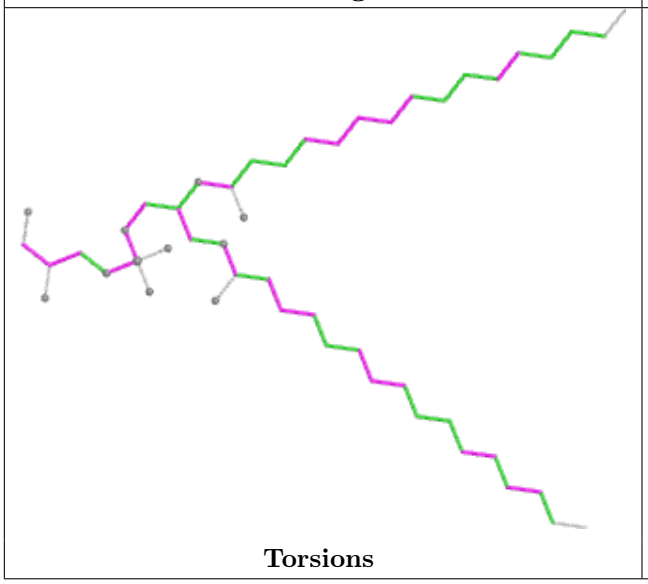
Ligand LHG e 5009



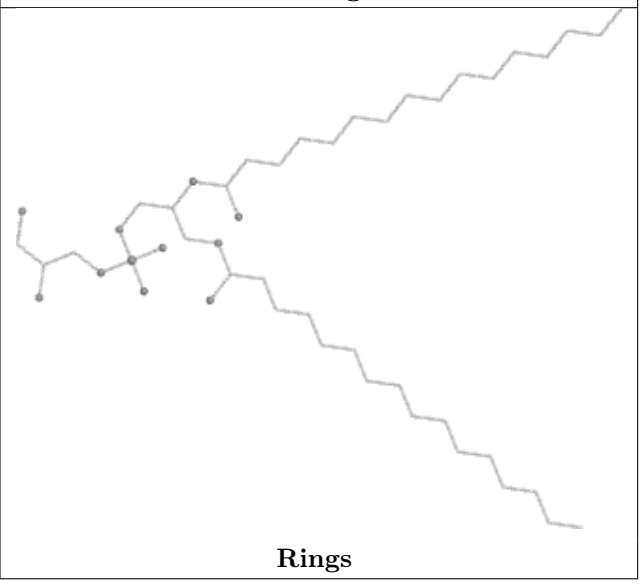
Bond lengths



Bond angles



Torsions

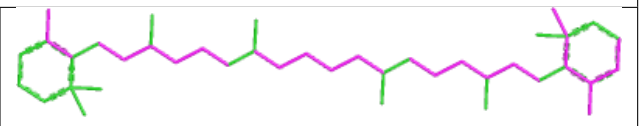


Rings

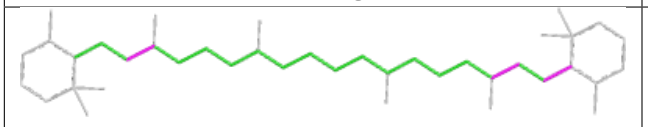
Ligand BCR n 4019



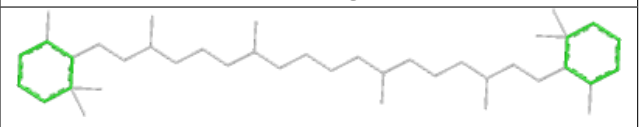
Bond lengths



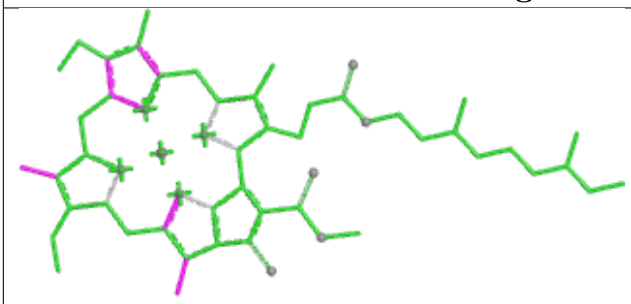
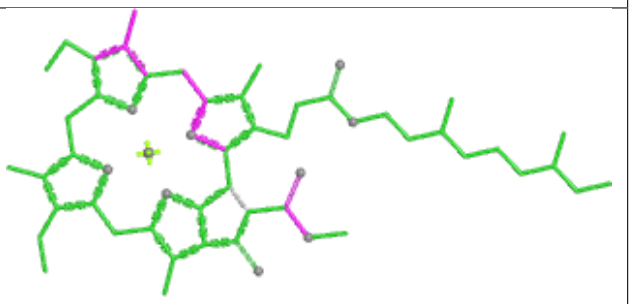
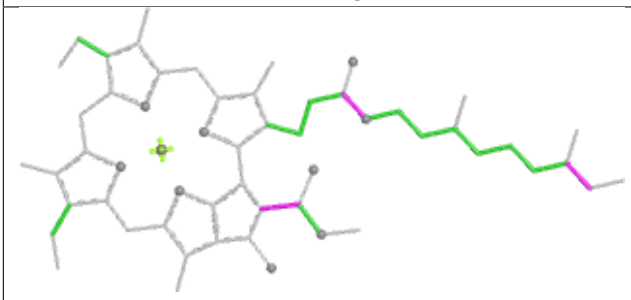
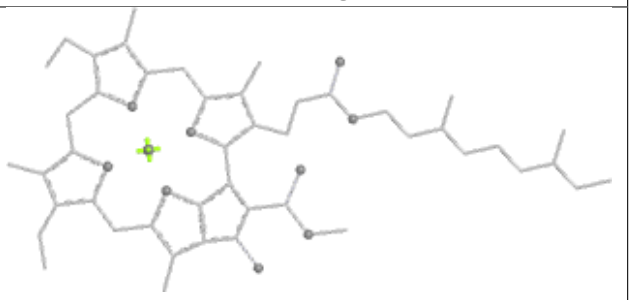
Bond angles

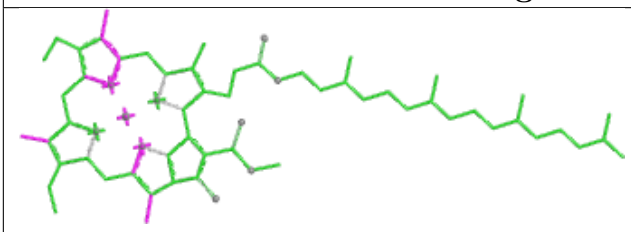
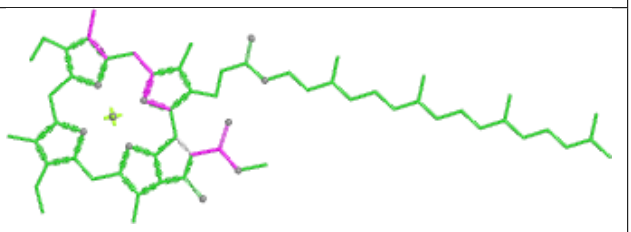
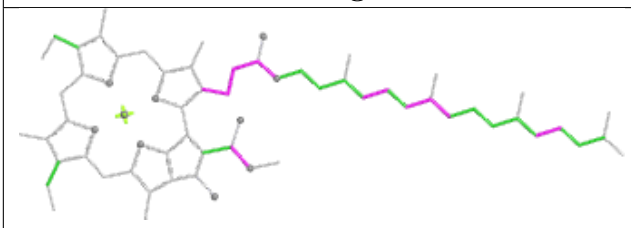
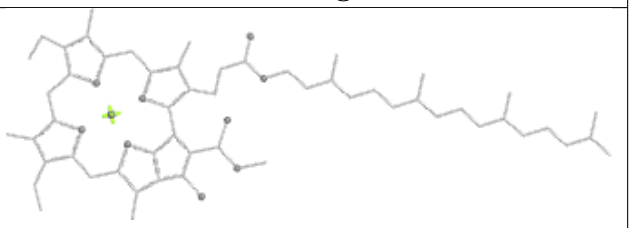


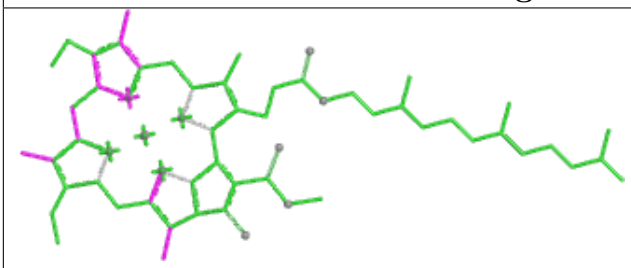
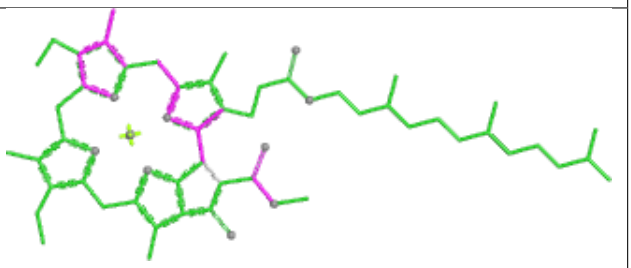
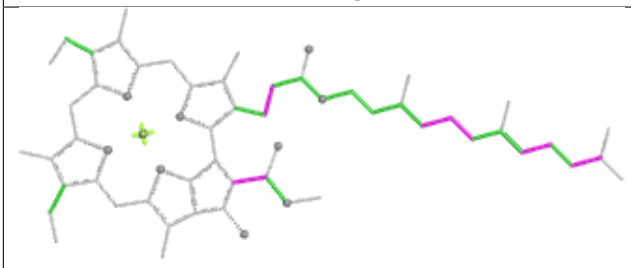
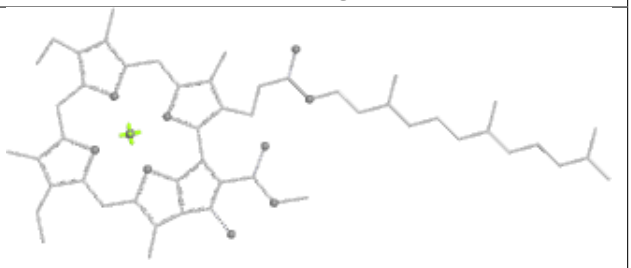
Torsions

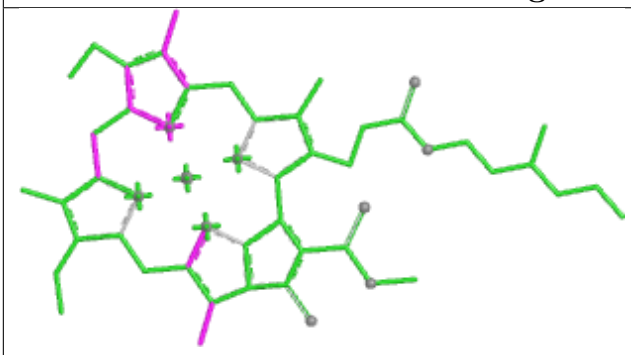
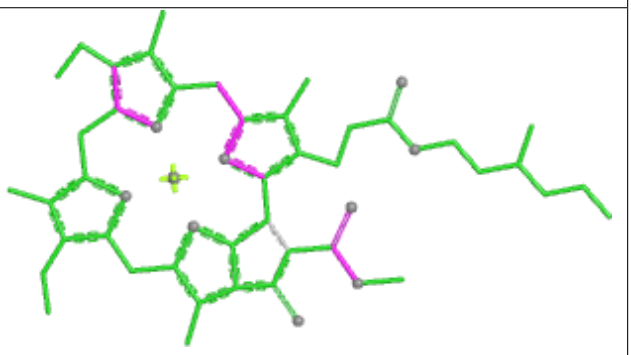
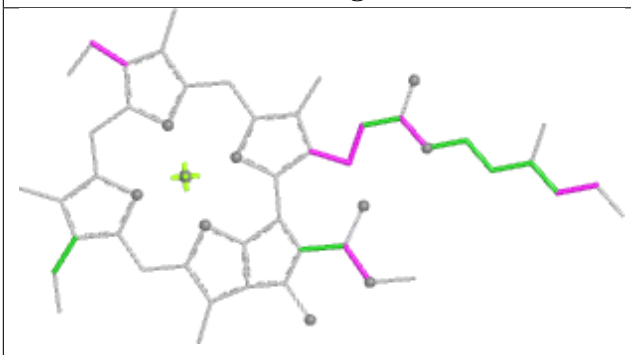
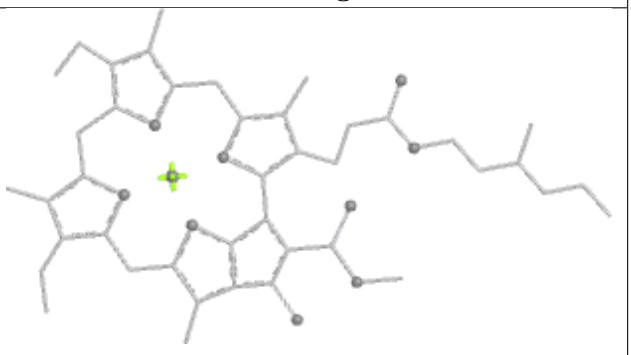


Rings

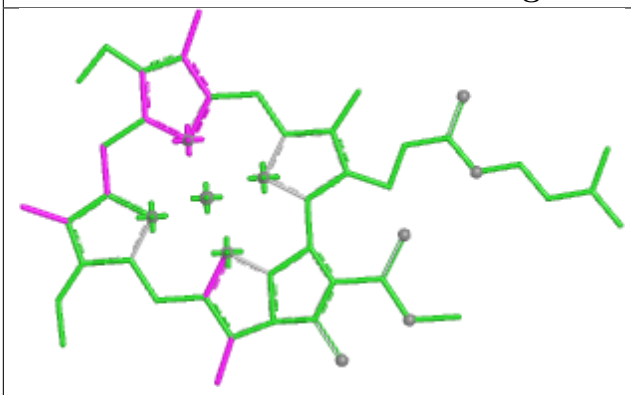
Ligand CLA B 1211	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1206	
	
Bond lengths	Bond angles
	
Torsions	Rings

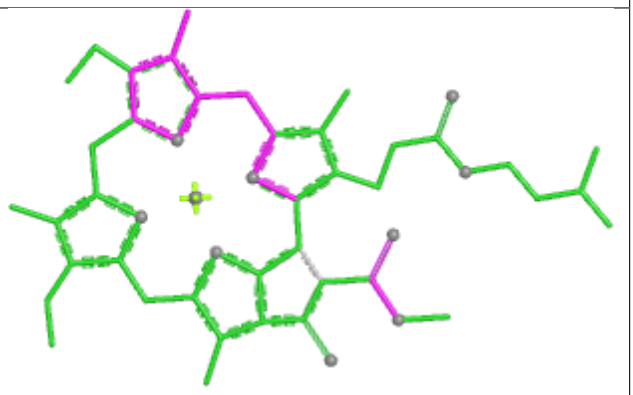
Ligand CLA B 1218	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

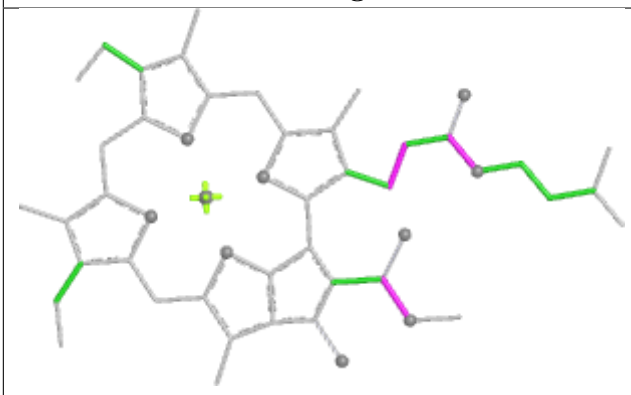
Ligand CLA f 1232



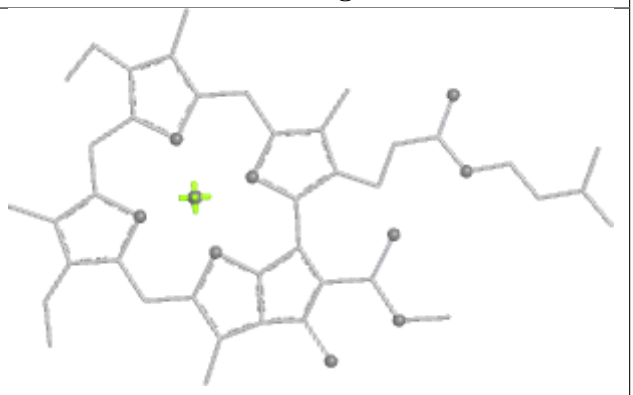
Bond lengths



Bond angles



Torsions

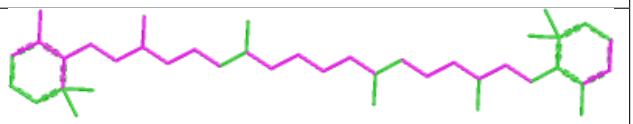


Rings

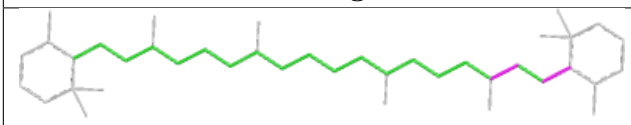
Ligand BCR v 523



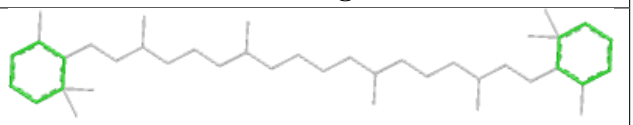
Bond lengths



Bond angles

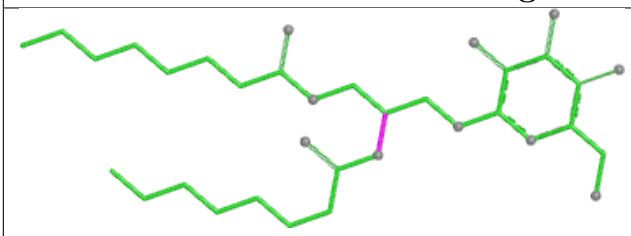


Torsions

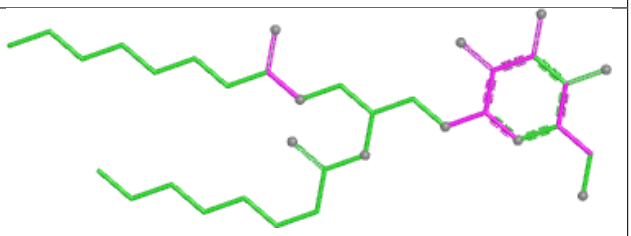


Rings

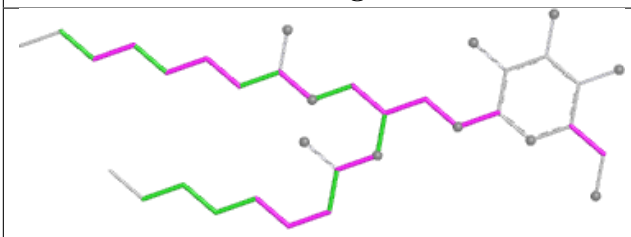
Ligand LMG l 5104



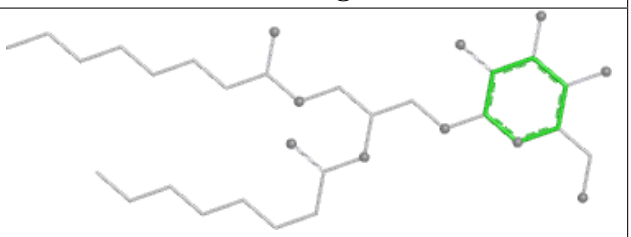
Bond lengths



Bond angles

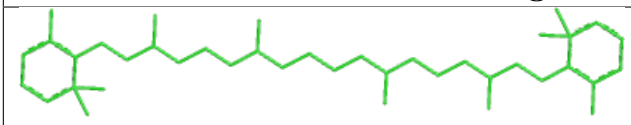


Torsions

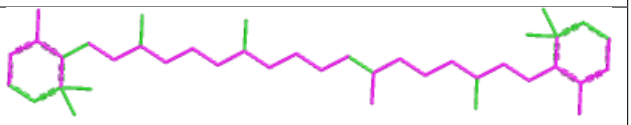


Rings

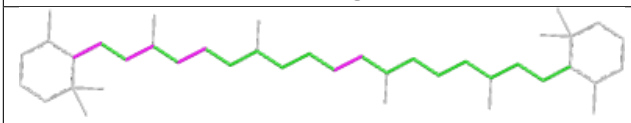
Ligand BCR r 522



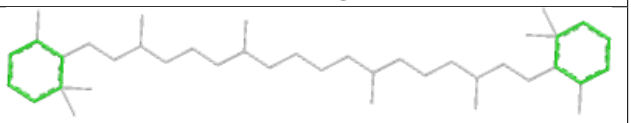
Bond lengths



Bond angles

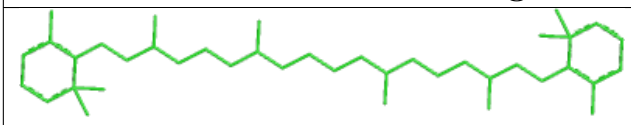


Torsions

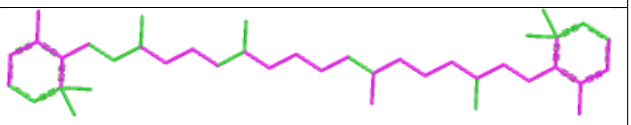


Rings

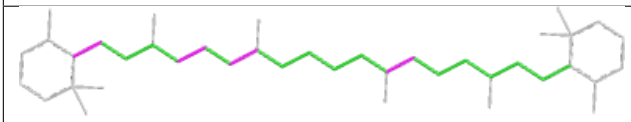
Ligand BCR W 4021



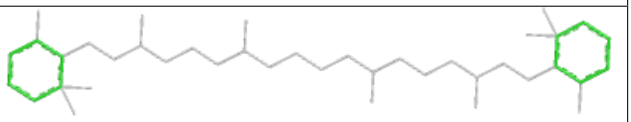
Bond lengths



Bond angles

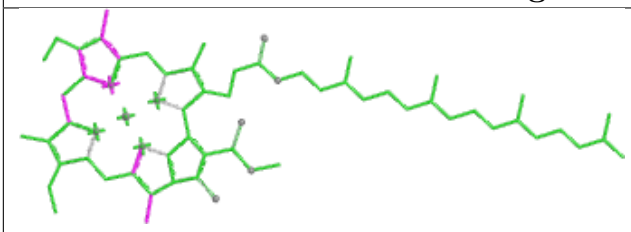


Torsions

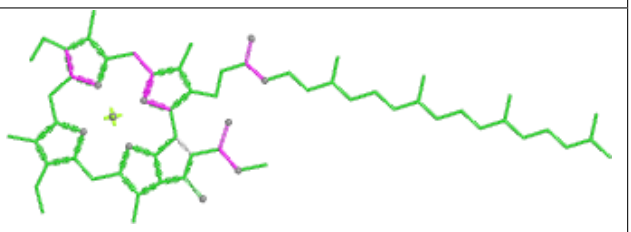


Rings

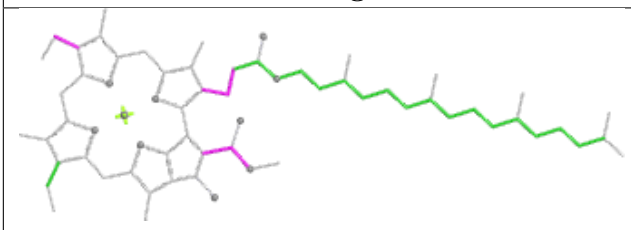
Ligand CLA 3 503



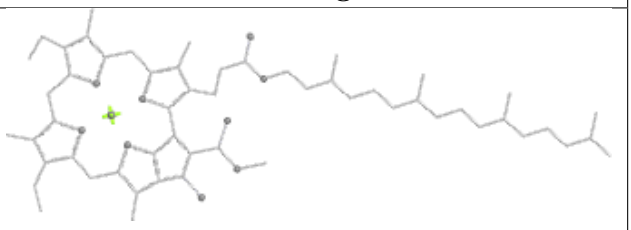
Bond lengths



Bond angles



Torsions

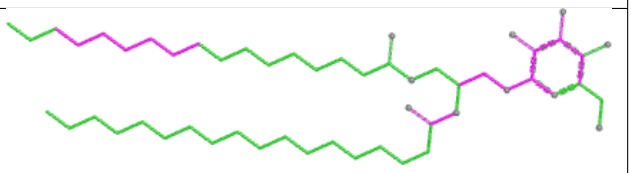


Rings

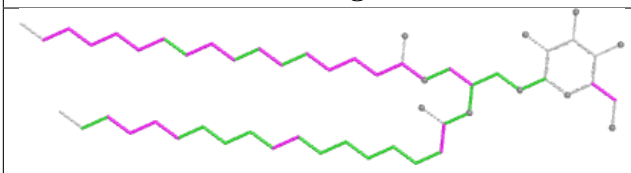
Ligand LMG H 5002



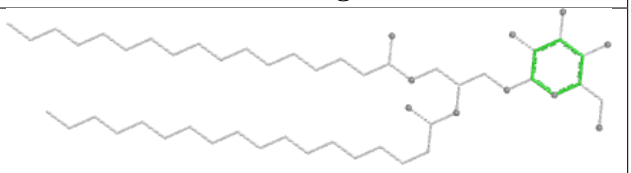
Bond lengths



Bond angles

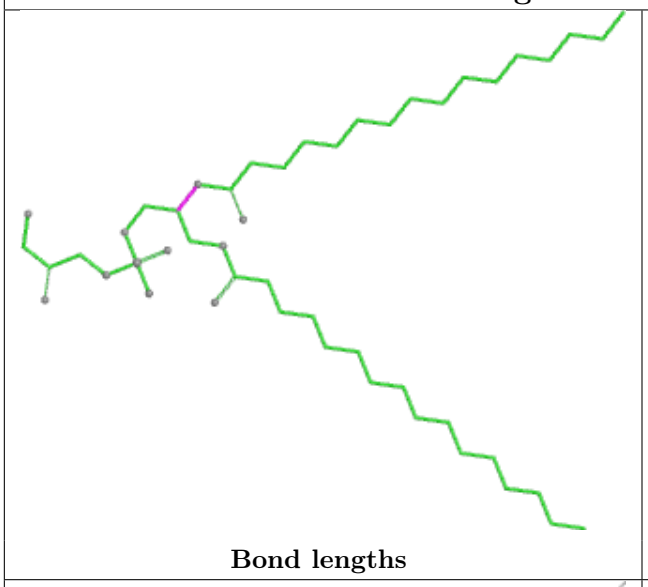


Torsions

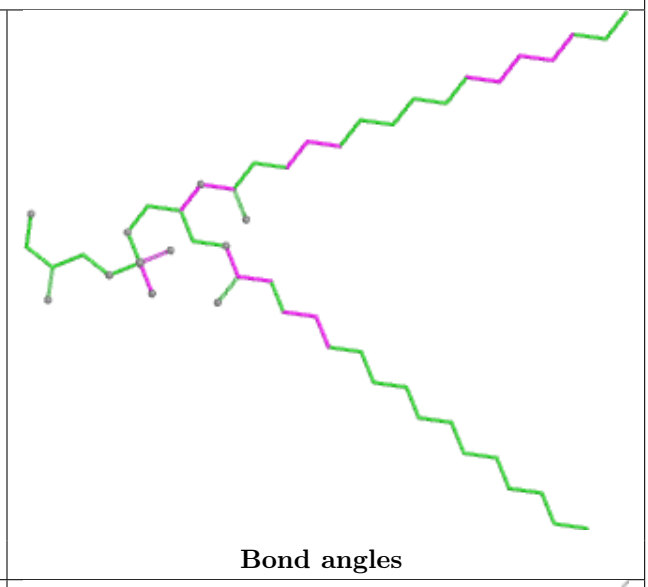


Rings

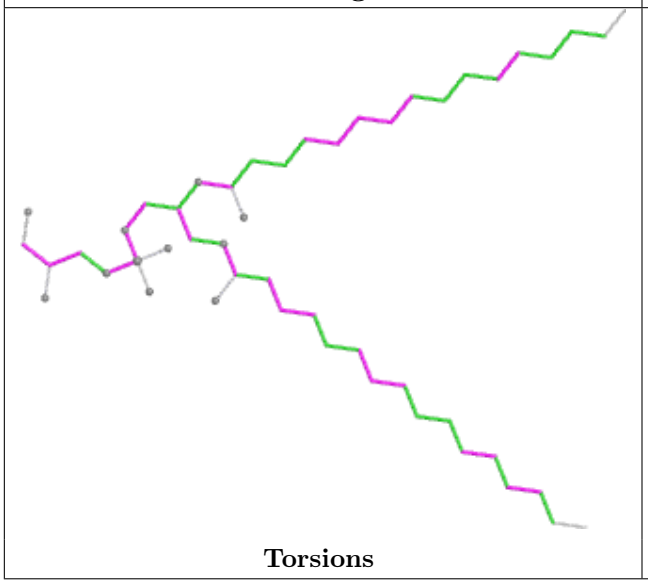
Ligand LHG A 5009



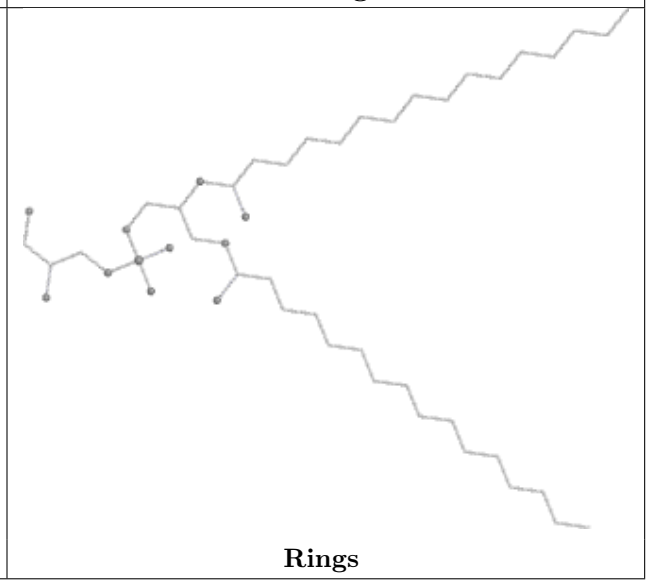
Bond lengths



Bond angles

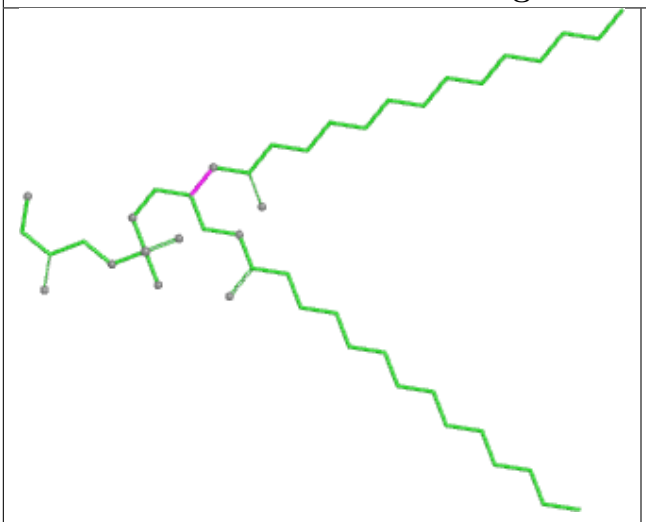


Torsions

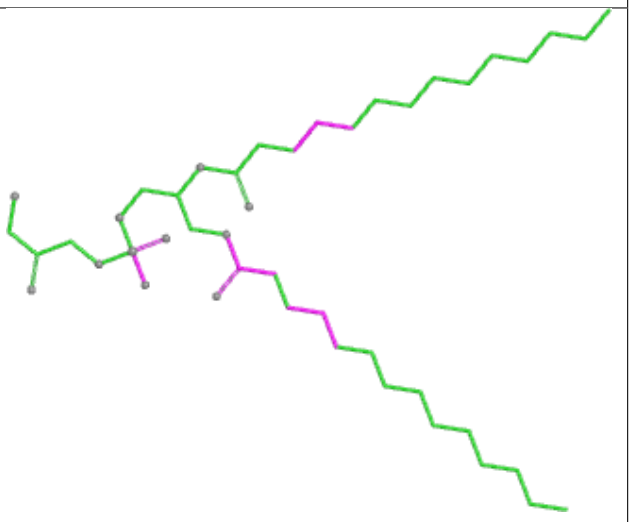


Rings

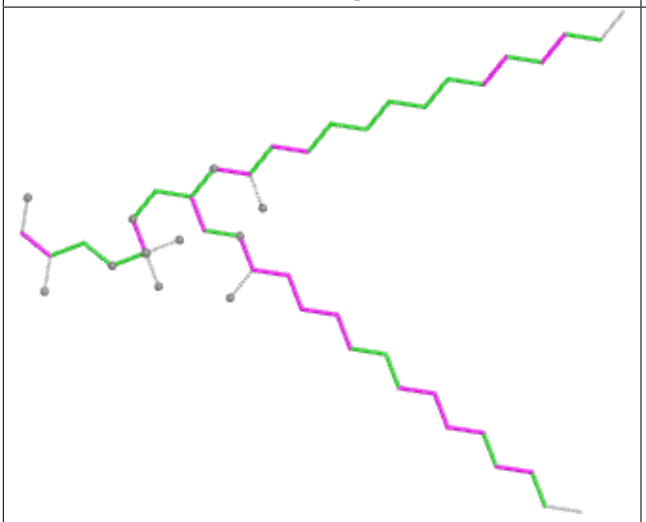
Ligand LHG A 5006



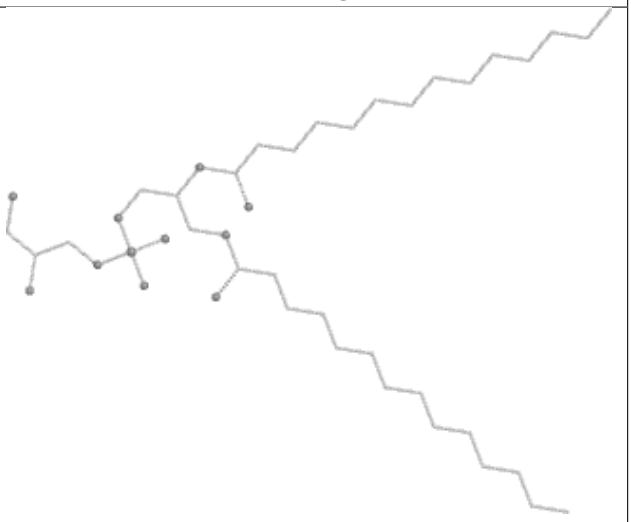
Bond lengths



Bond angles

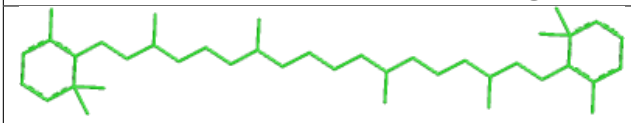


Torsions

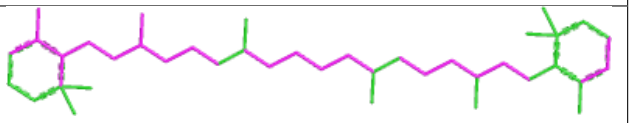


Rings

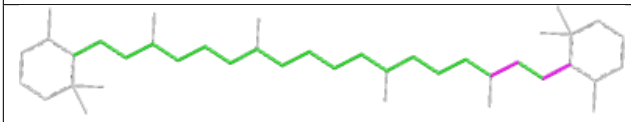
Ligand BCR d 523



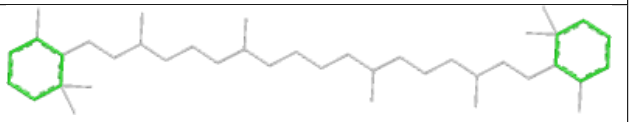
Bond lengths



Bond angles

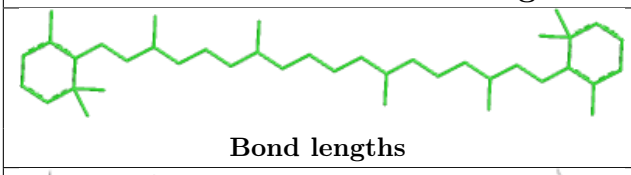


Torsions

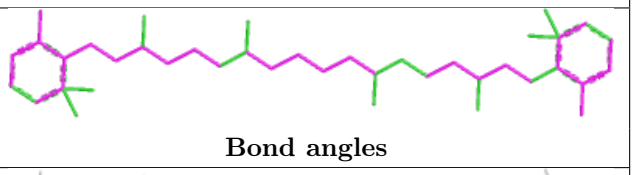


Rings

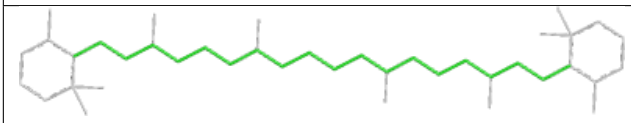
Ligand BCR e 4007



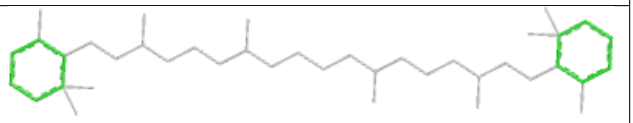
Bond lengths



Bond angles

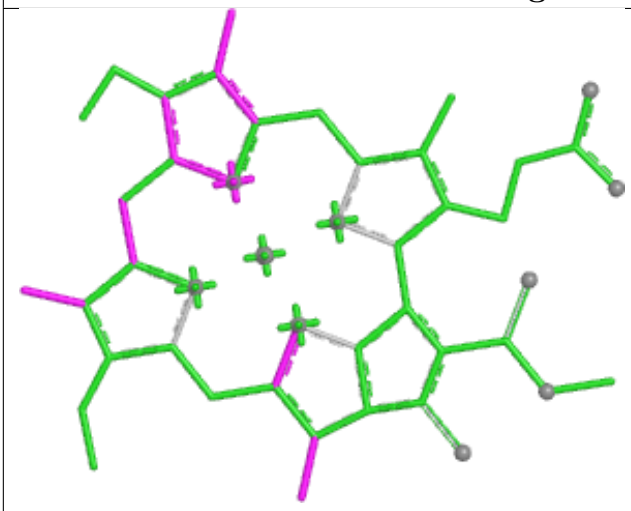


Torsions

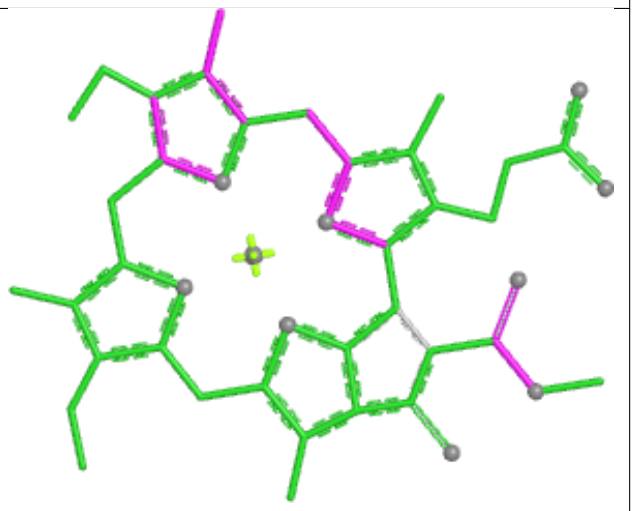


Rings

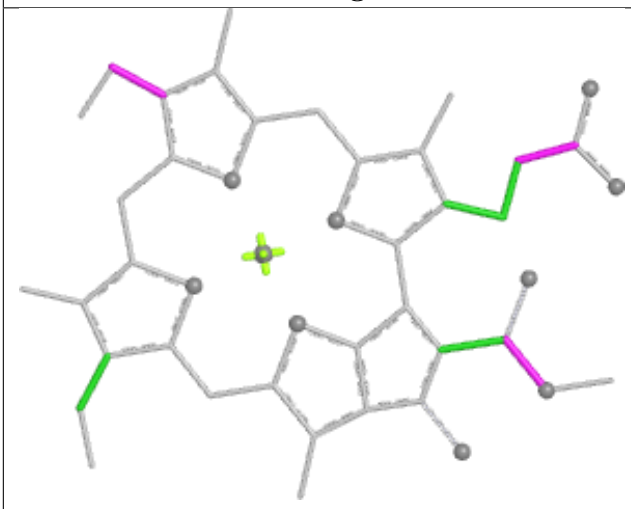
Ligand CLA 6 511



Bond lengths



Bond angles

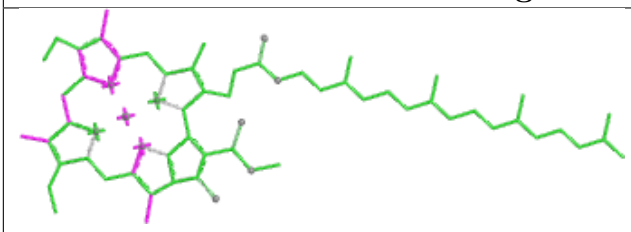


Torsions

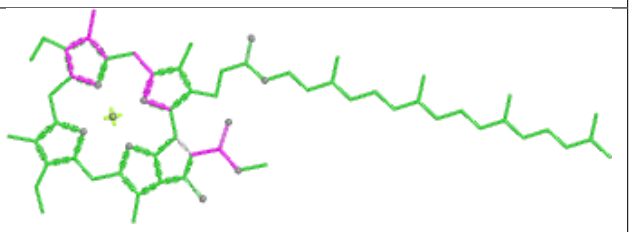


Rings

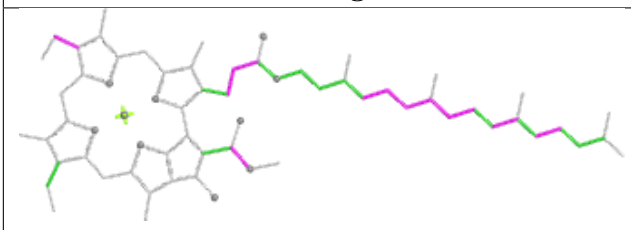
Ligand CLA B 1203



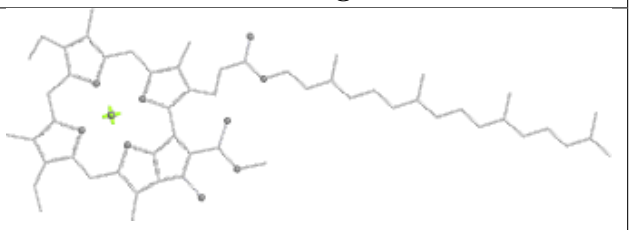
Bond lengths



Bond angles

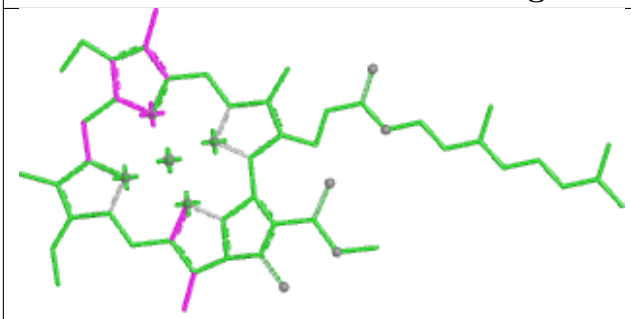


Torsions

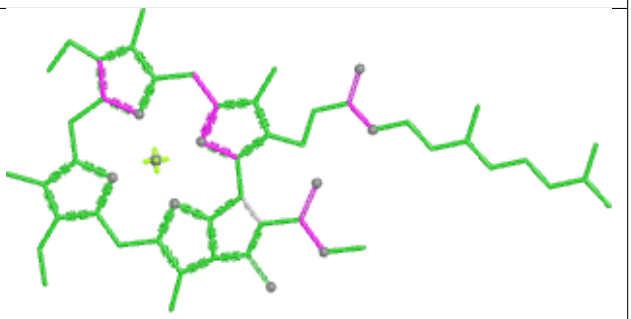


Rings

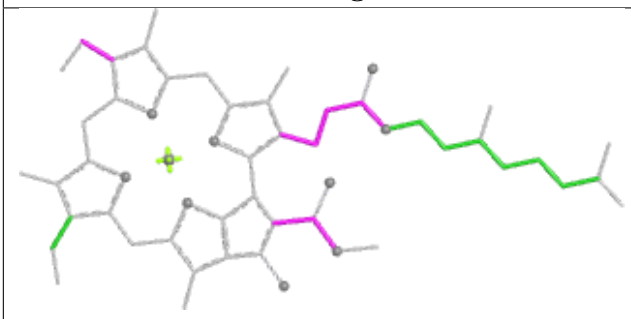
Ligand CLA v 518



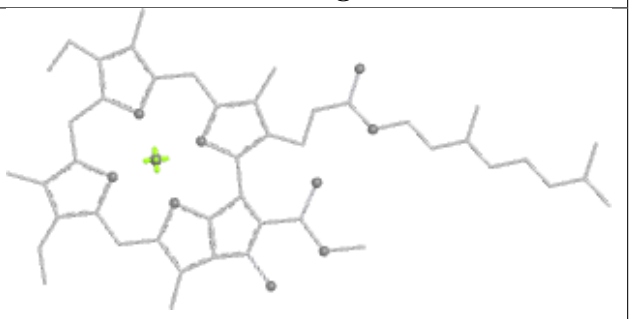
Bond lengths



Bond angles

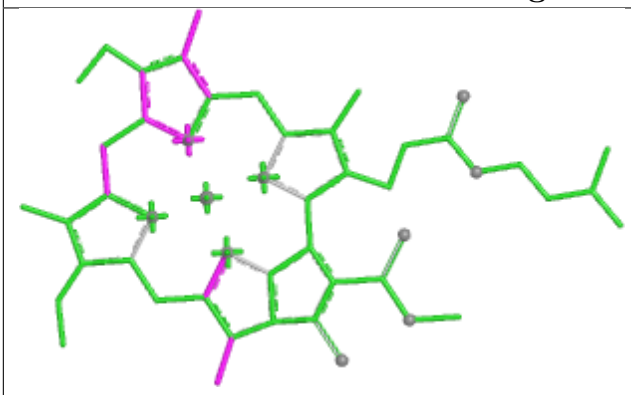


Torsions

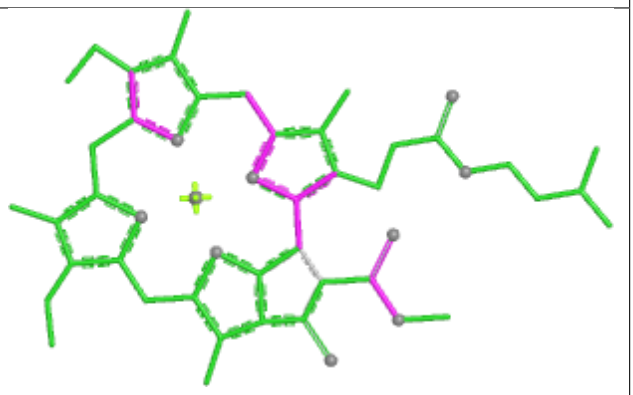


Rings

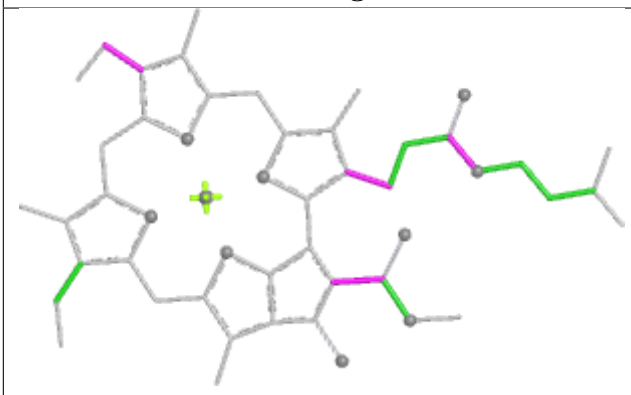
Ligand CLA 4 502



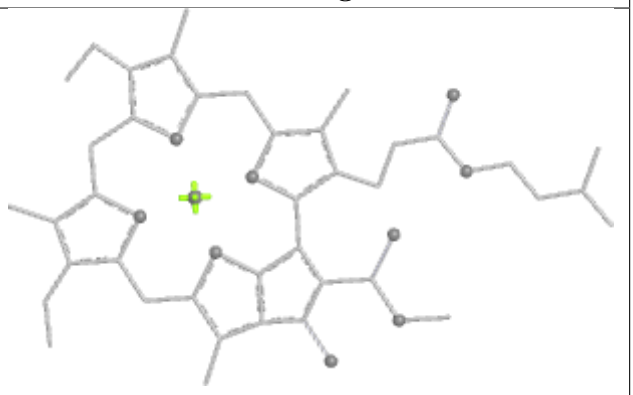
Bond lengths



Bond angles

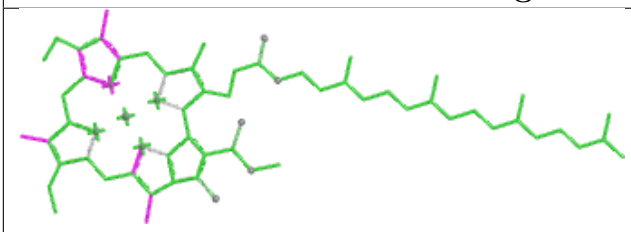


Torsions

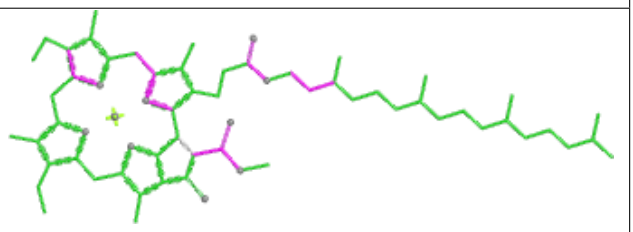


Rings

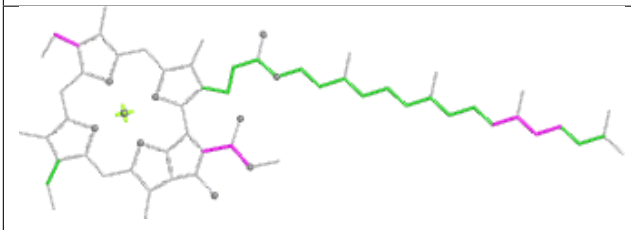
Ligand CLA A 1131



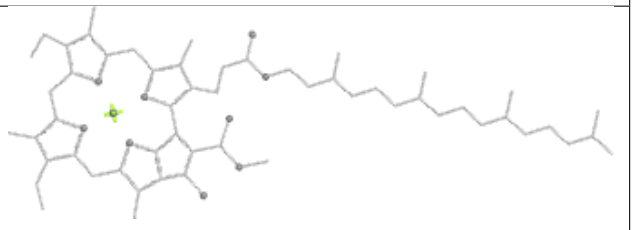
Bond lengths



Bond angles

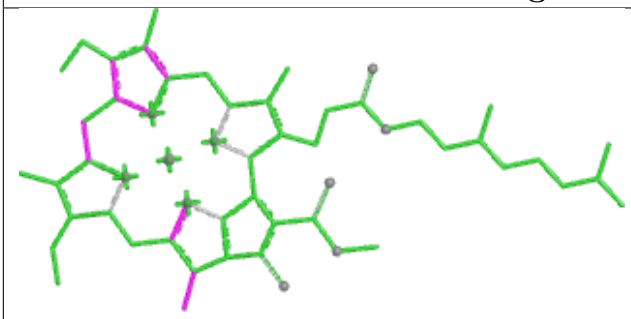


Torsions

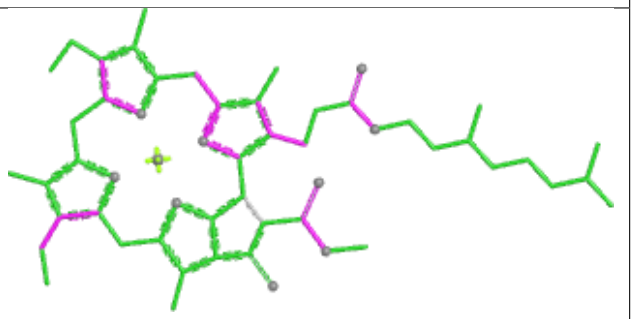


Rings

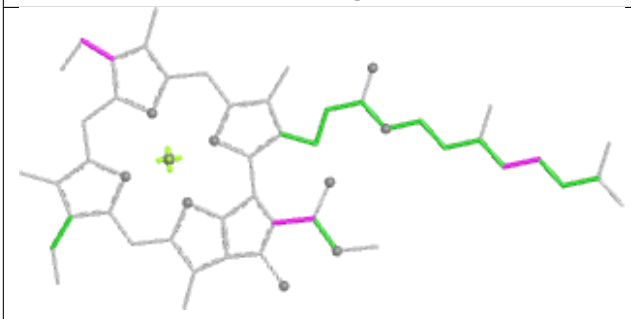
Ligand CLA 4 503



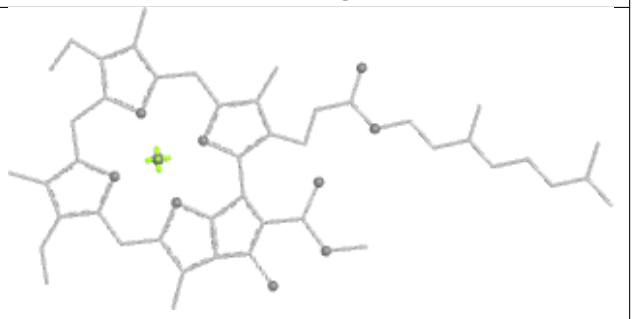
Bond lengths



Bond angles

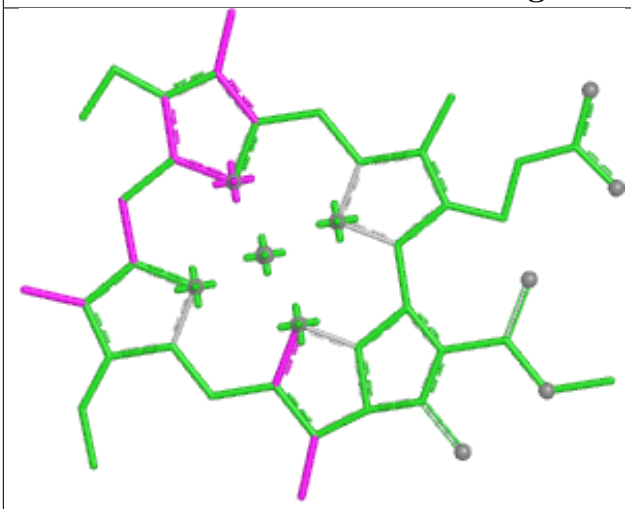


Torsions

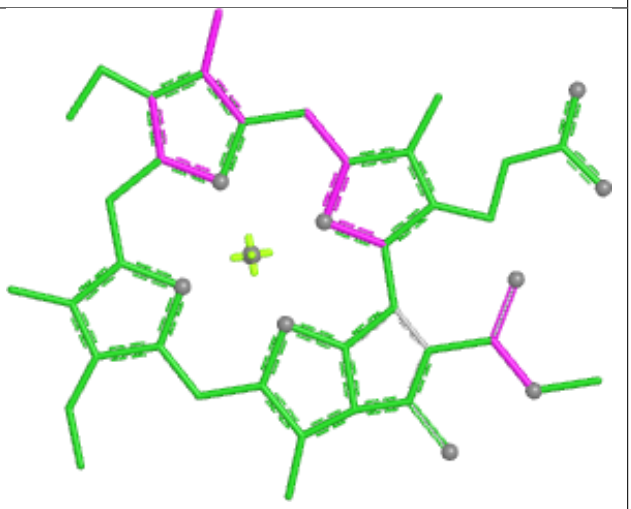


Rings

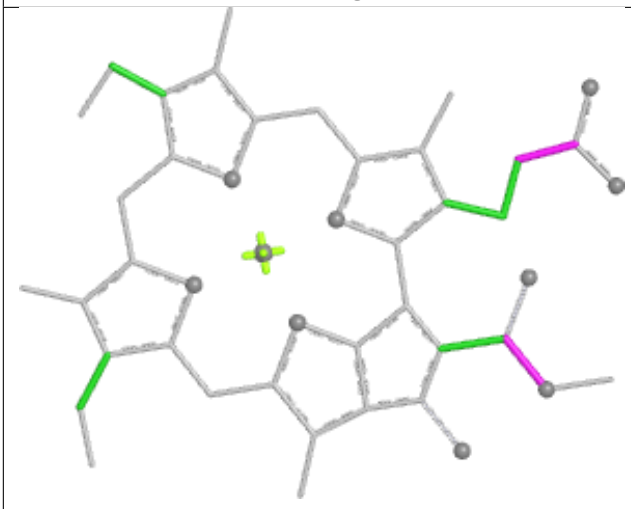
Ligand CLA v 509



Bond lengths



Bond angles

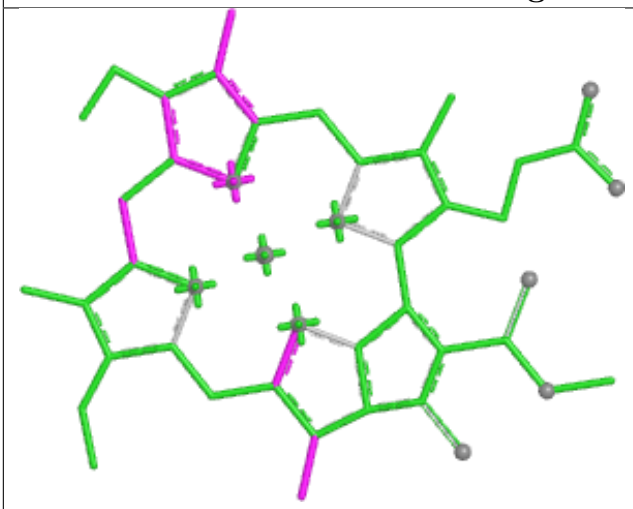


Torsions

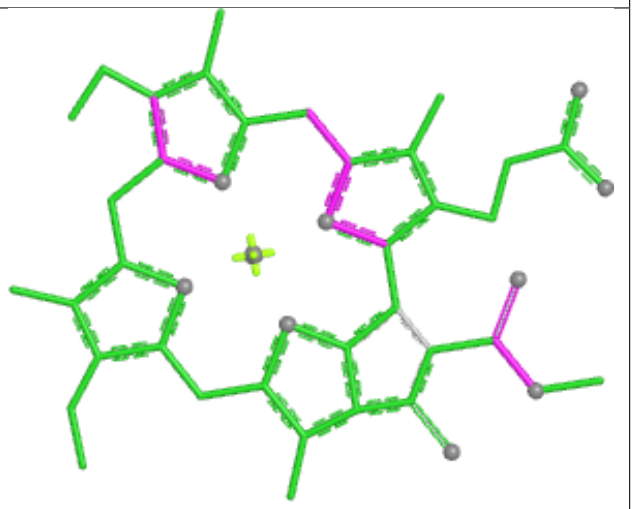


Rings

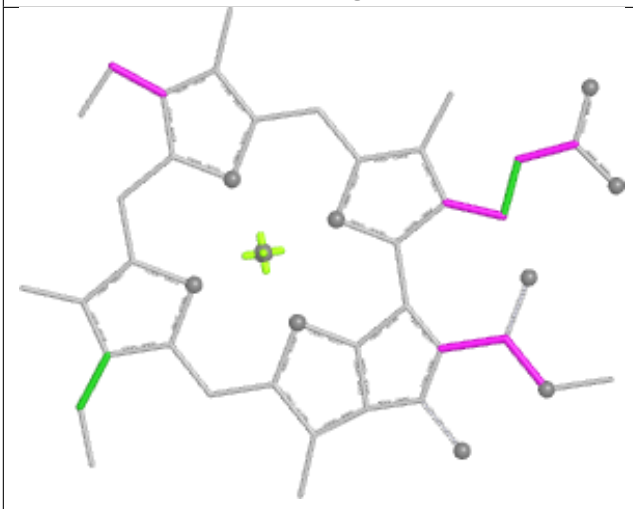
Ligand CLA v 512



Bond lengths



Bond angles

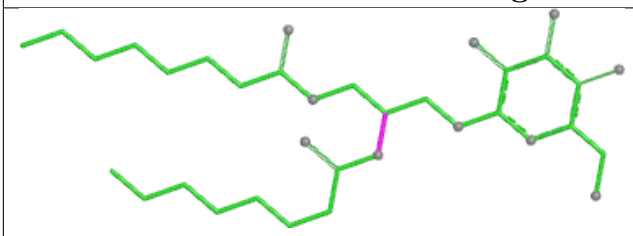


Torsions

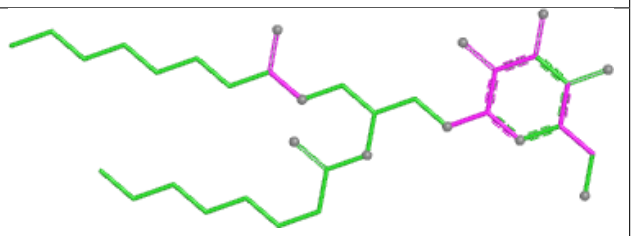


Rings

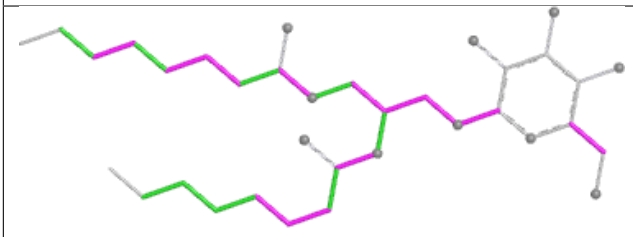
Ligand LMG T 5104



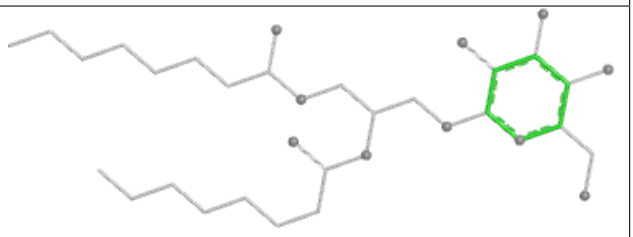
Bond lengths



Bond angles

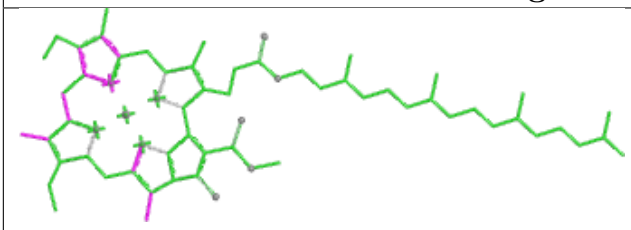


Torsions

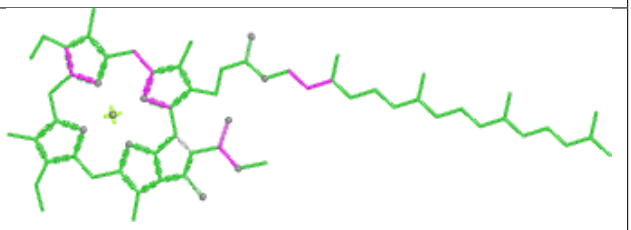


Rings

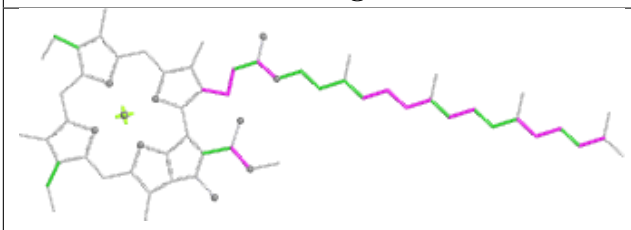
Ligand CLA 2 505



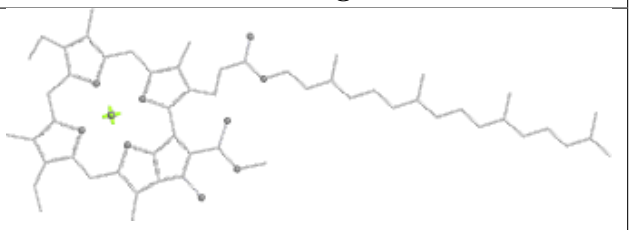
Bond lengths



Bond angles

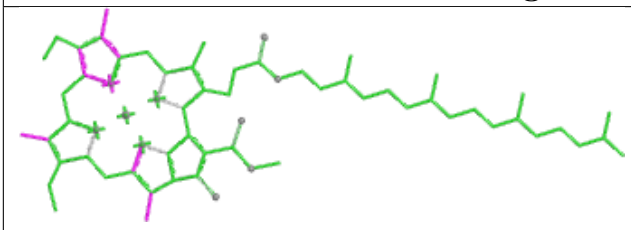


Torsions

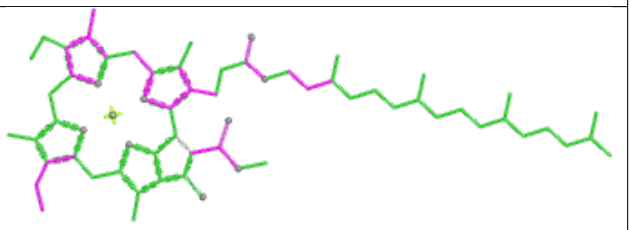


Rings

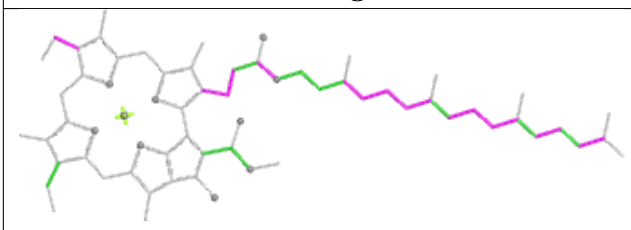
Ligand CLA f 1210



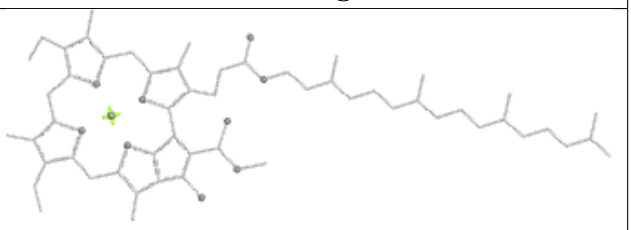
Bond lengths



Bond angles

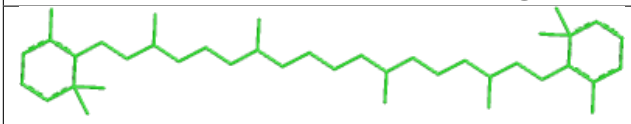


Torsions

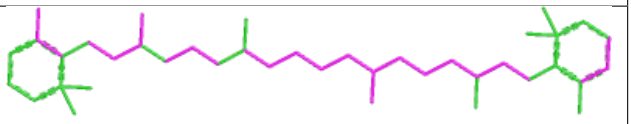


Rings

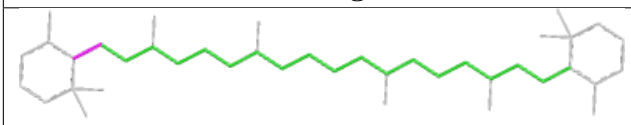
Ligand BCR L 4219



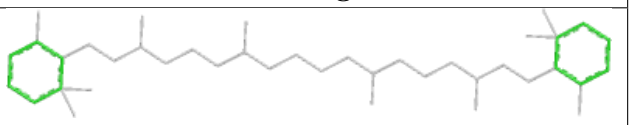
Bond lengths



Bond angles

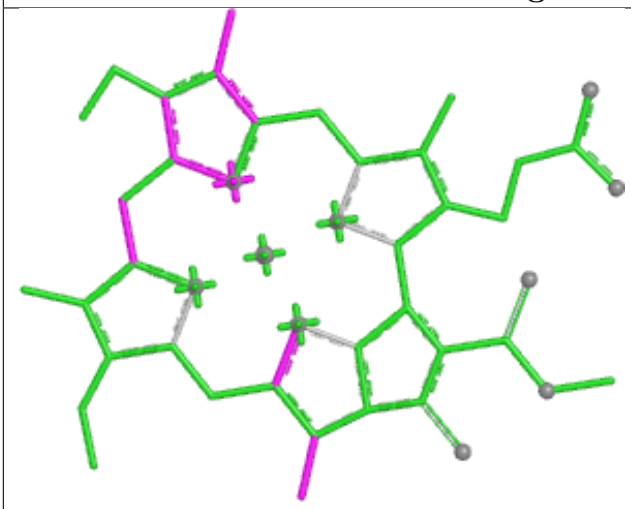


Torsions

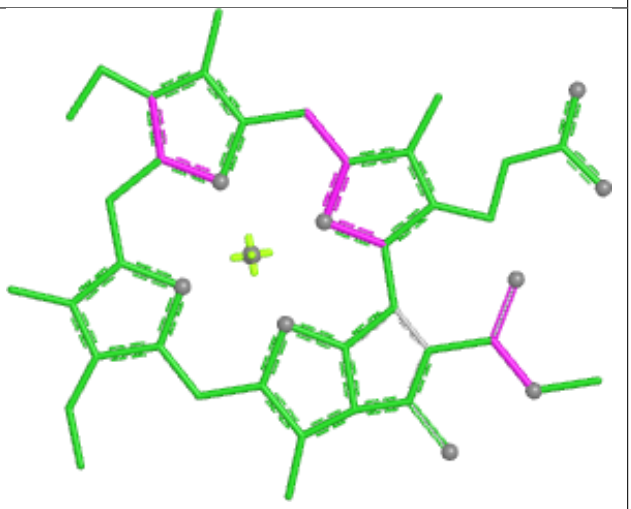


Rings

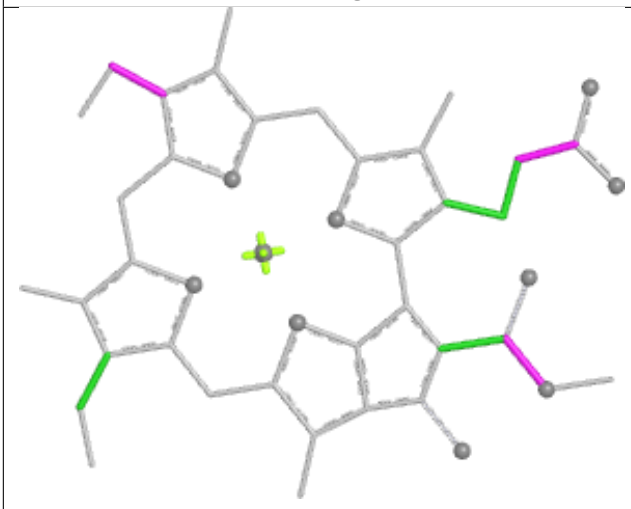
Ligand CLA v 511



Bond lengths



Bond angles

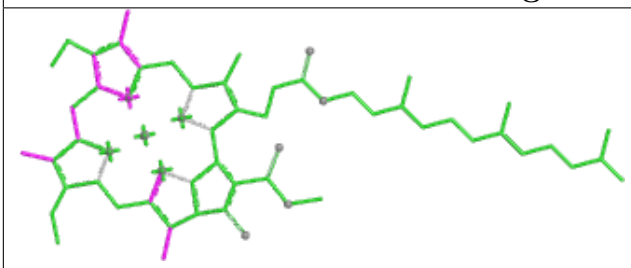


Torsions

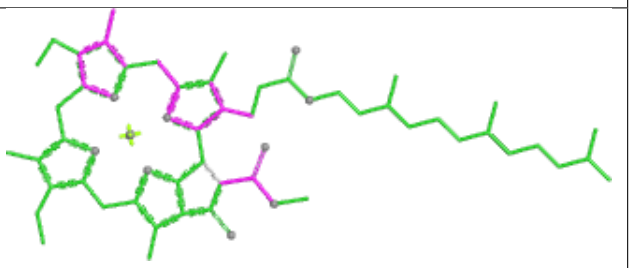


Rings

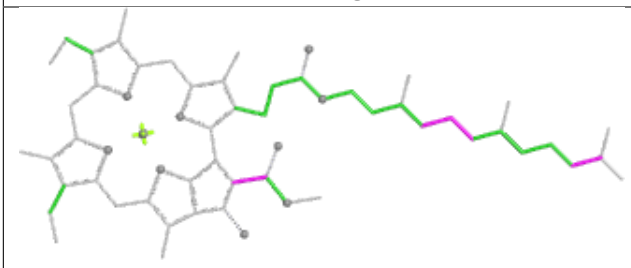
Ligand CLA f 1222



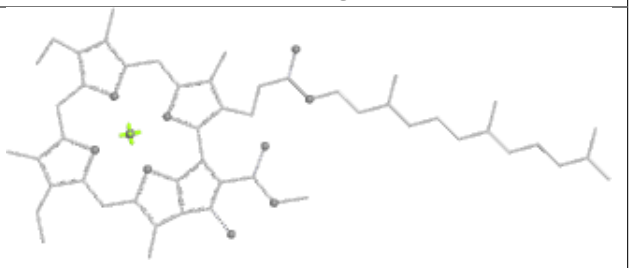
Bond lengths



Bond angles

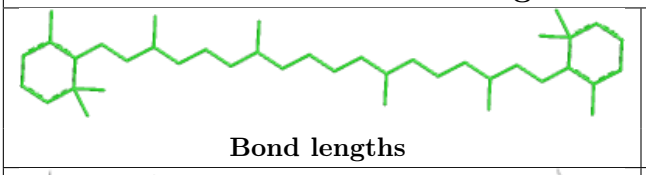


Torsions

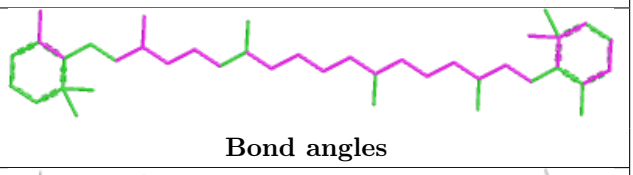


Rings

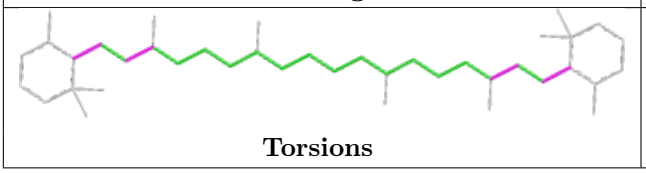
Ligand BCR B 4004



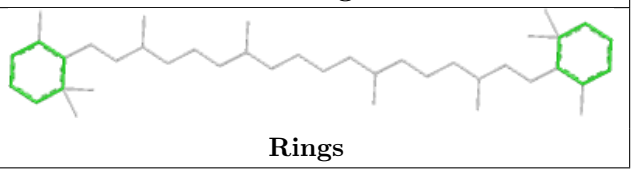
Bond lengths



Bond angles

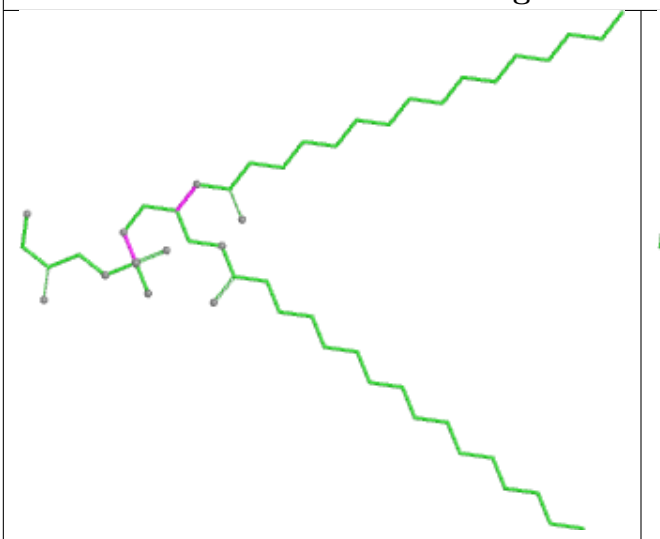


Torsions

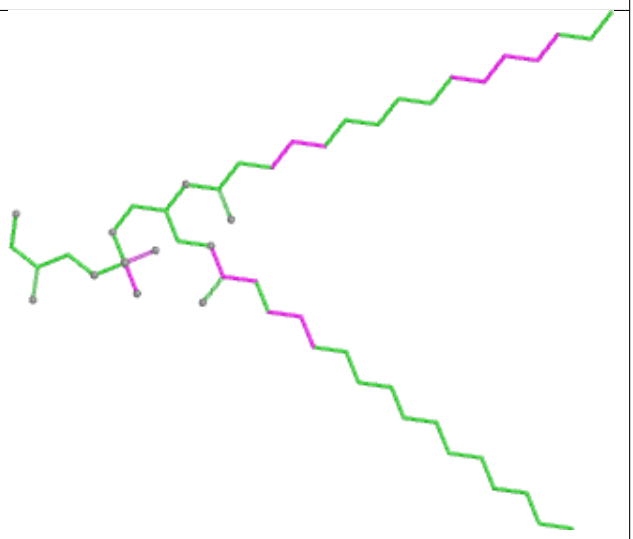


Rings

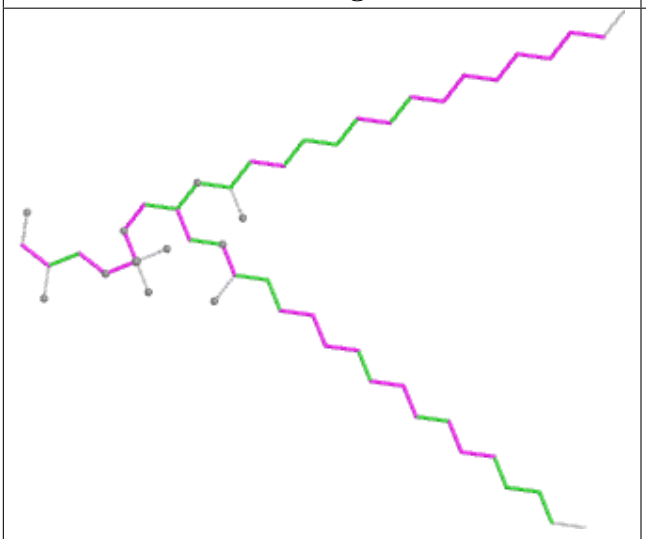
Ligand LHG V 5221



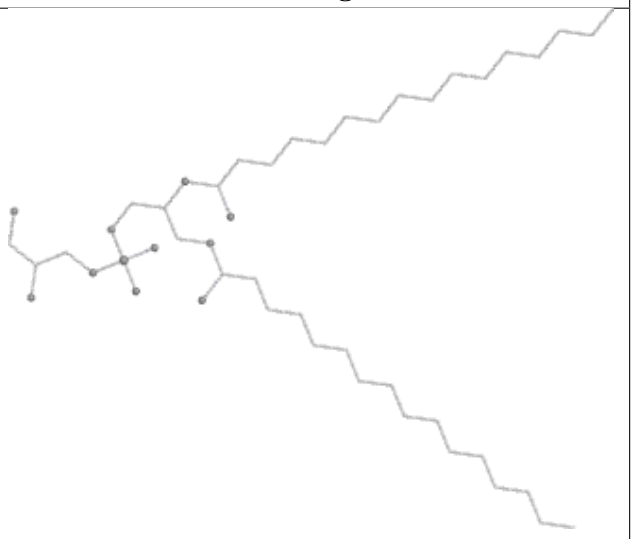
Bond lengths



Bond angles

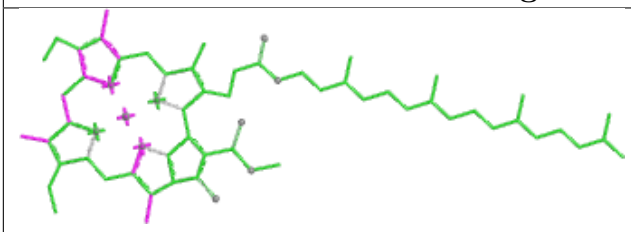


Torsions

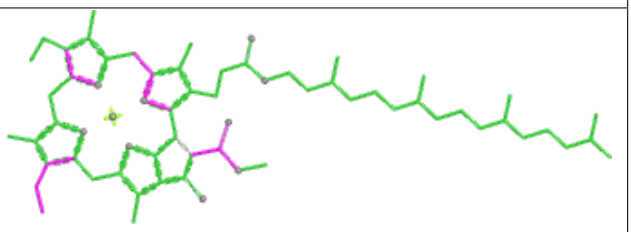


Rings

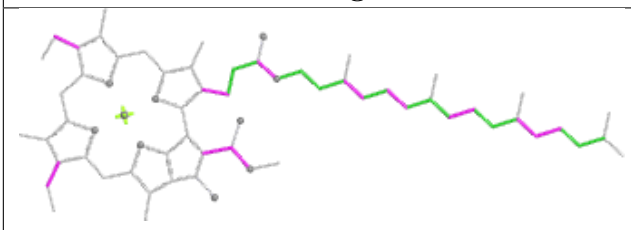
Ligand CLA e 1132



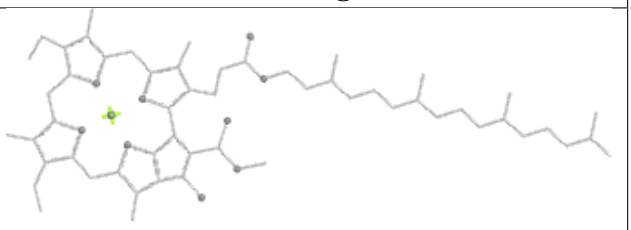
Bond lengths



Bond angles

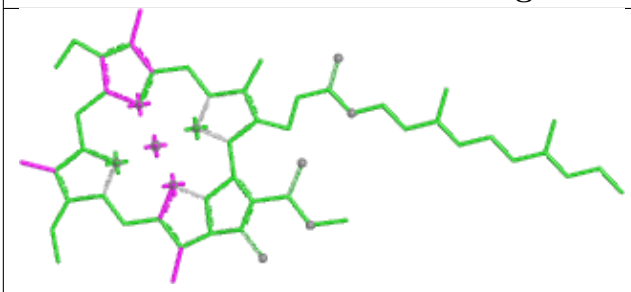


Torsions

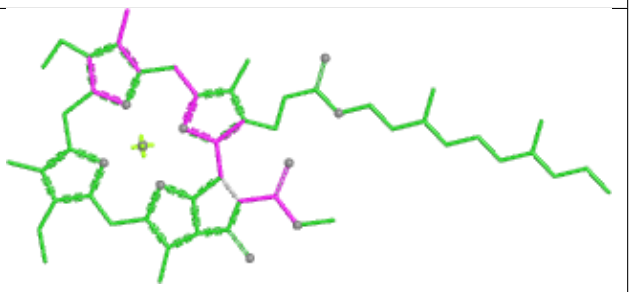


Rings

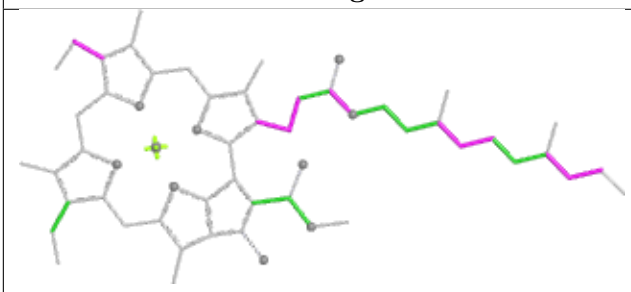
Ligand CLA B 1217



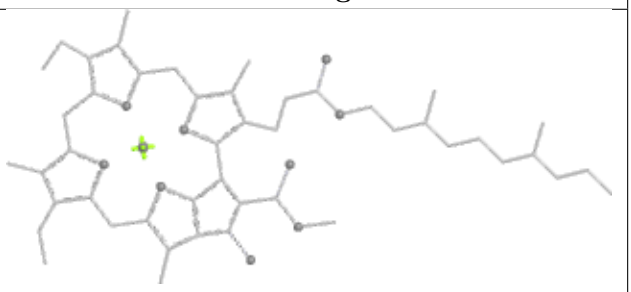
Bond lengths



Bond angles

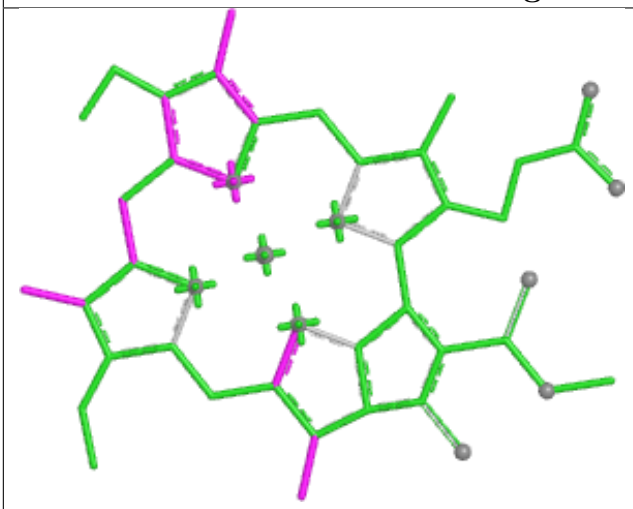


Torsions

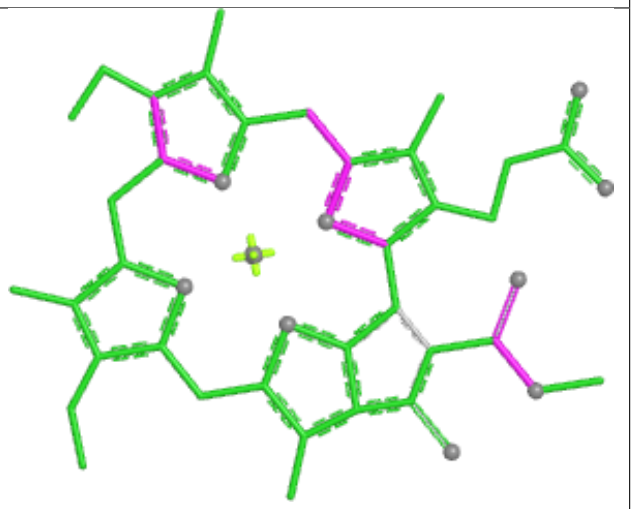


Rings

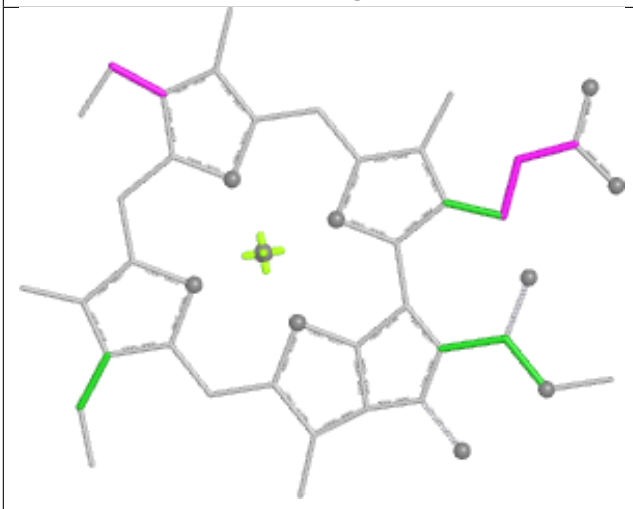
Ligand CLA Y 517



Bond lengths



Bond angles

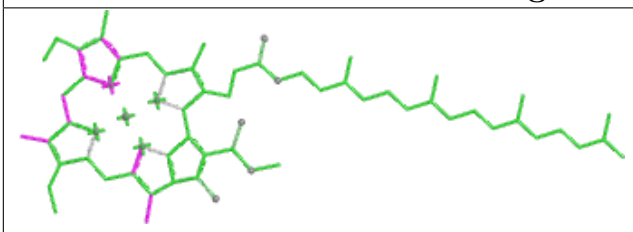


Torsions

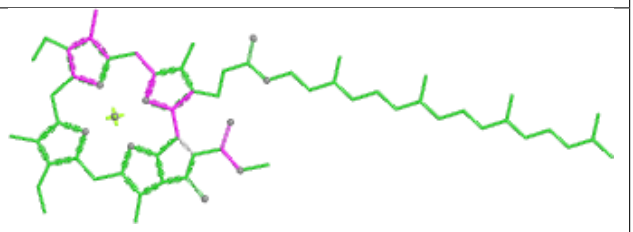


Rings

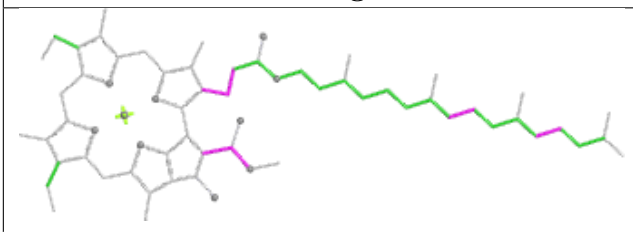
Ligand CLA 2 503



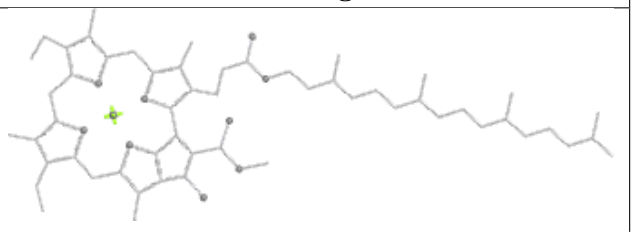
Bond lengths



Bond angles

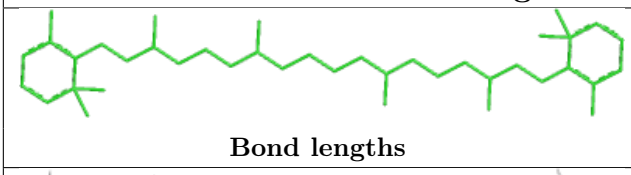


Torsions

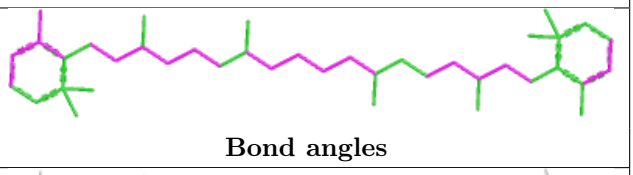


Rings

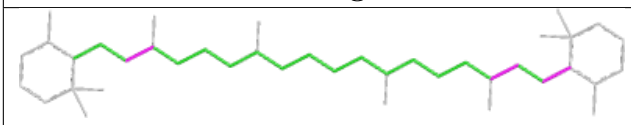
Ligand BCR B 4005



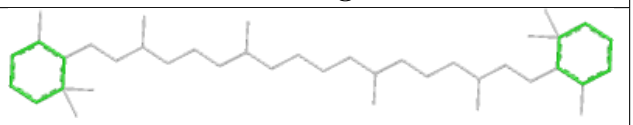
Bond lengths



Bond angles

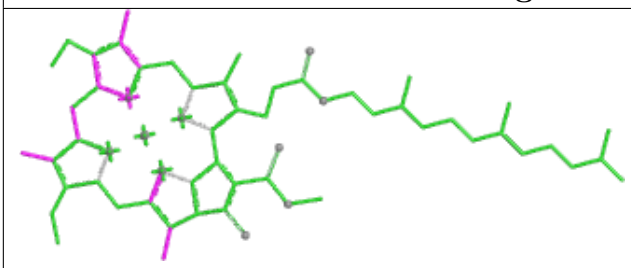


Torsions

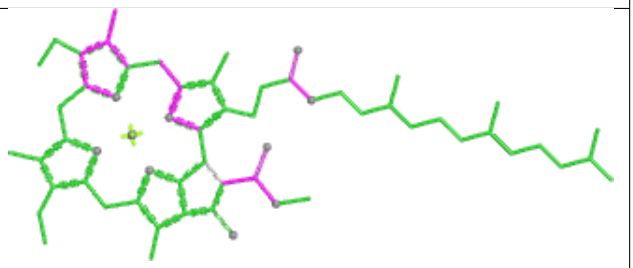


Rings

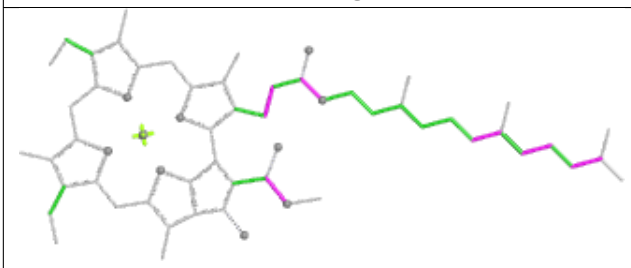
Ligand CLA B 1201



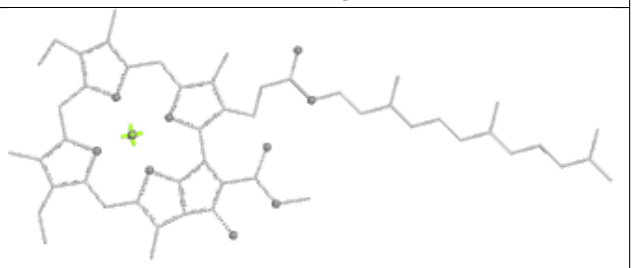
Bond lengths



Bond angles

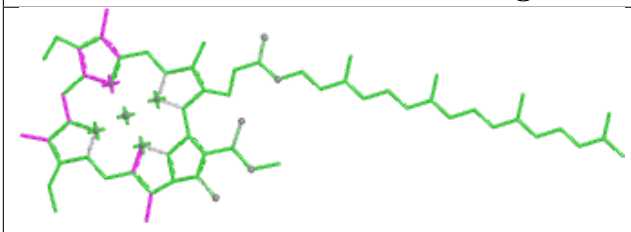


Torsions

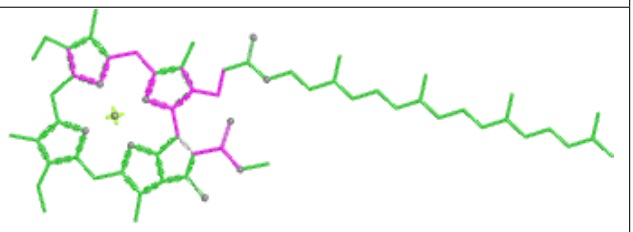


Rings

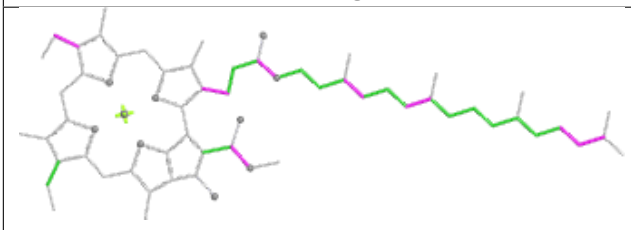
Ligand CLA A 1140



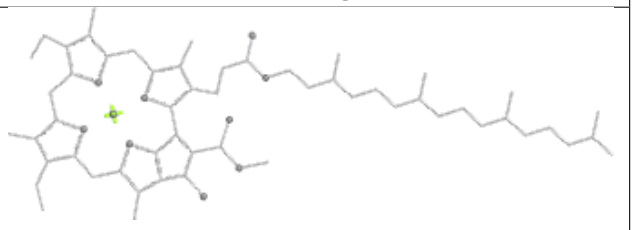
Bond lengths



Bond angles

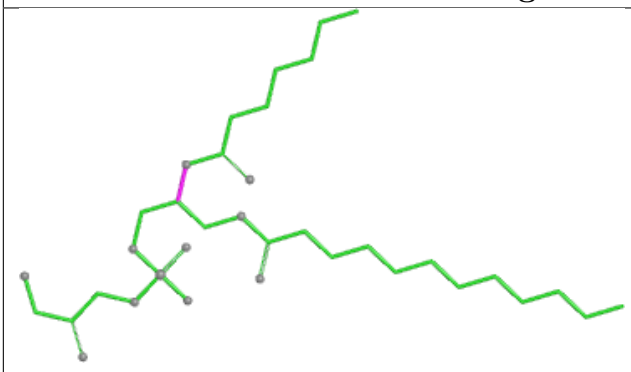


Torsions

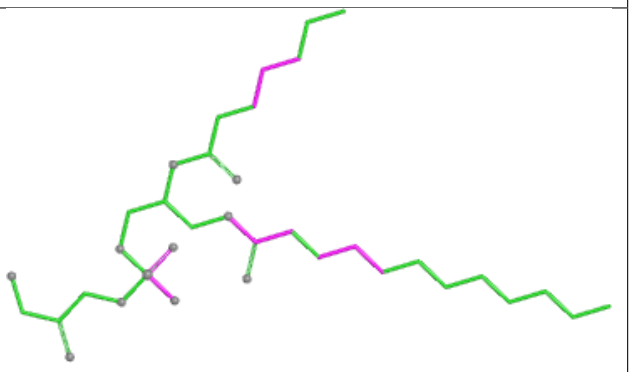


Rings

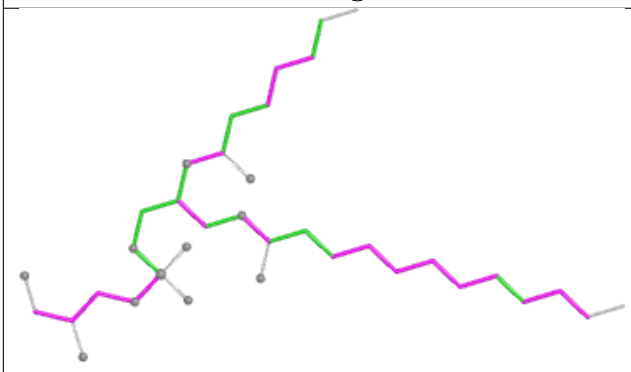
Ligand LHG e 5004



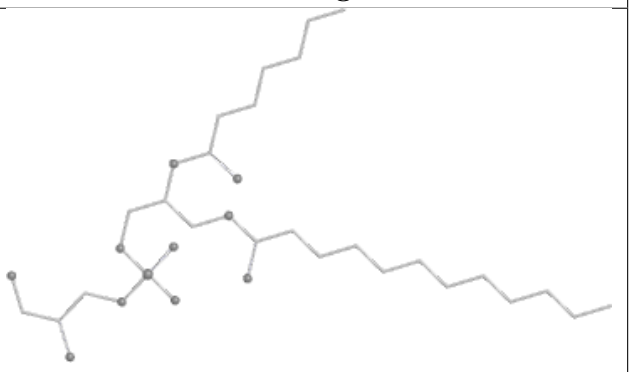
Bond lengths



Bond angles



Torsions

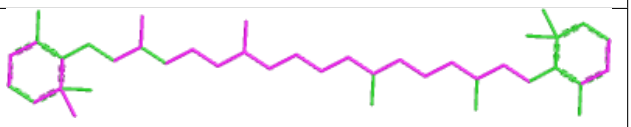


Rings

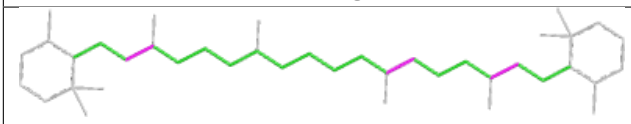
Ligand BCR f 4014



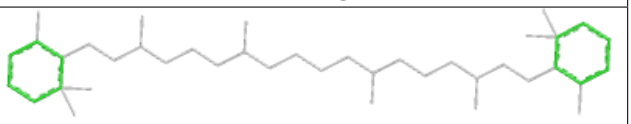
Bond lengths



Bond angles

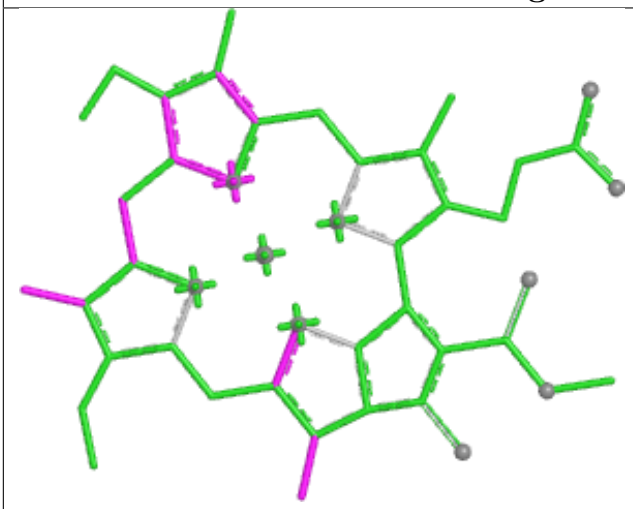


Torsions

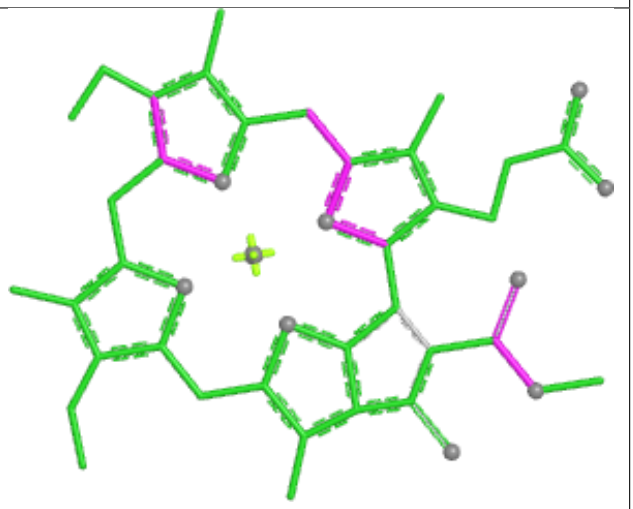


Rings

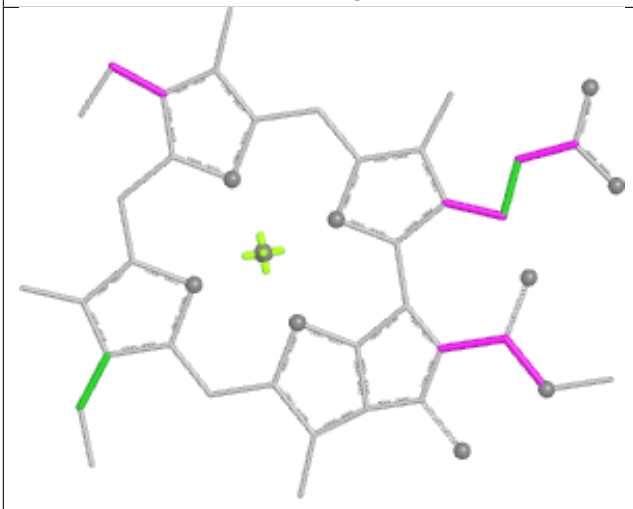
Ligand CLA 6 517



Bond lengths



Bond angles

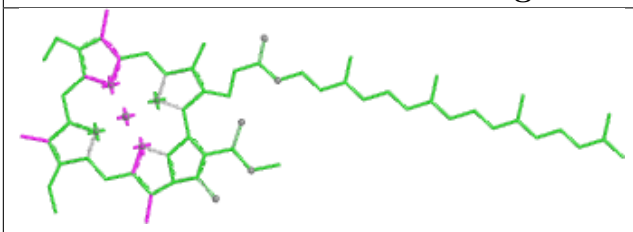


Torsions

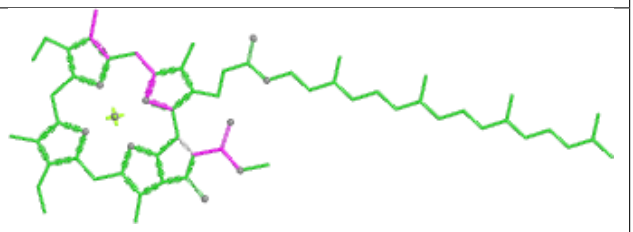


Rings

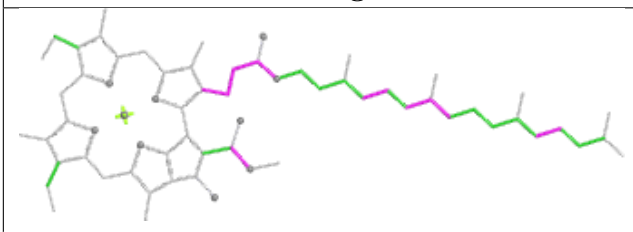
Ligand CLA H 1206



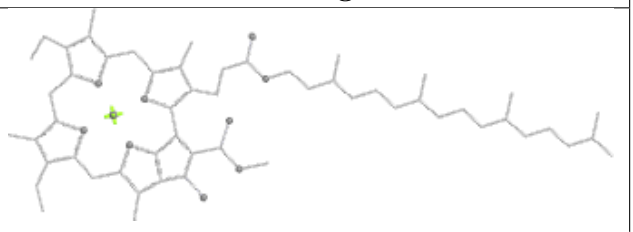
Bond lengths



Bond angles

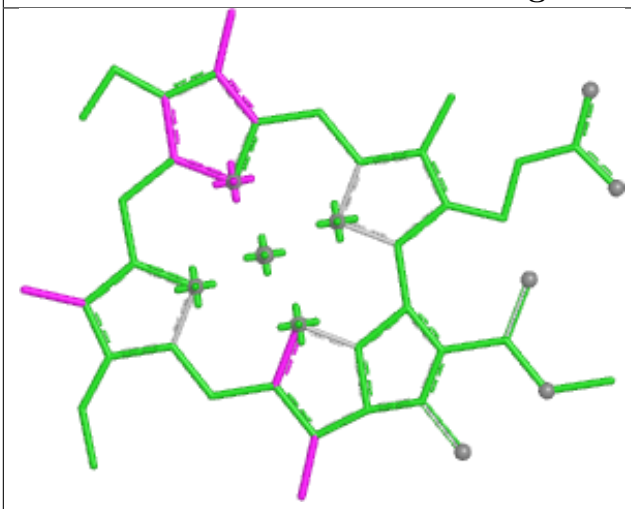


Torsions

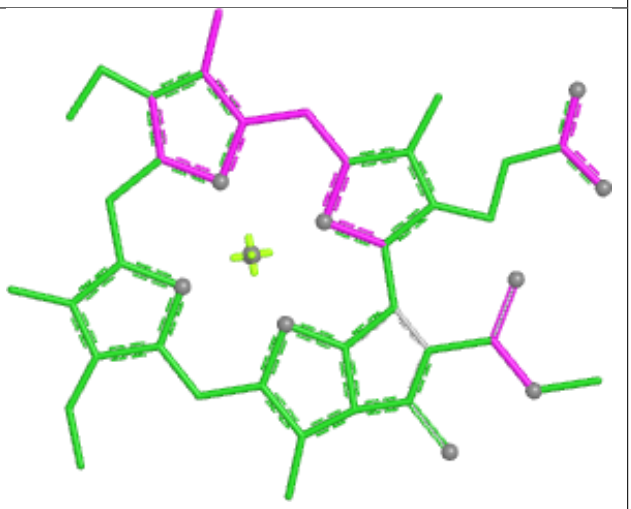


Rings

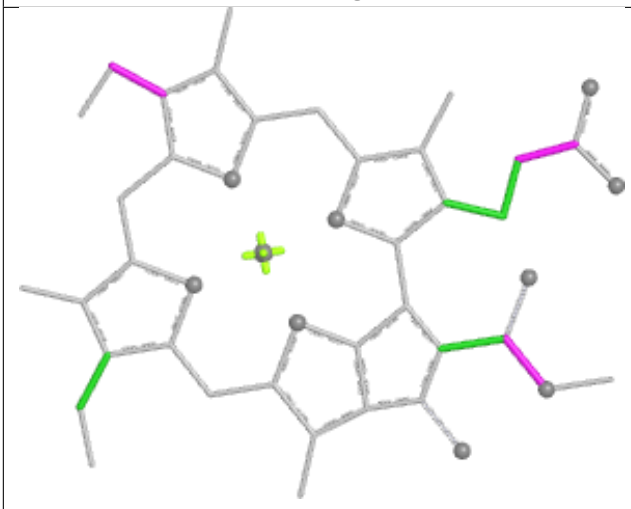
Ligand CLA 4 508



Bond lengths



Bond angles

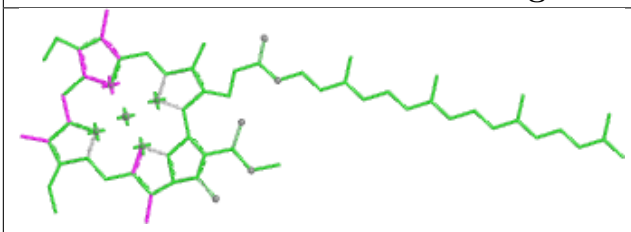


Torsions

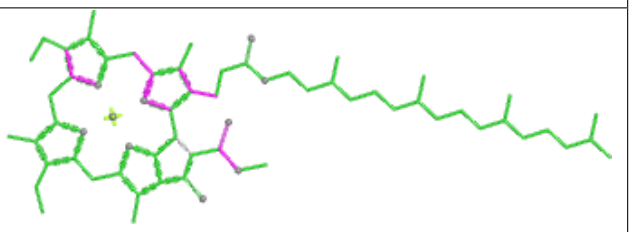


Rings

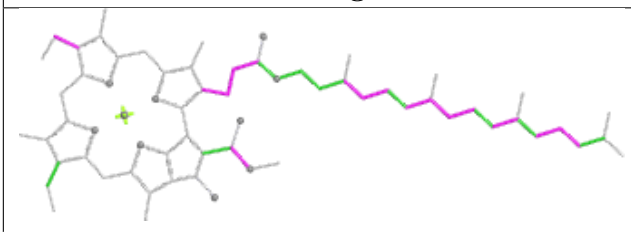
Ligand CLA 5 501



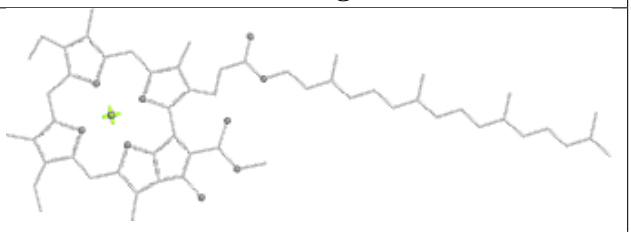
Bond lengths



Bond angles

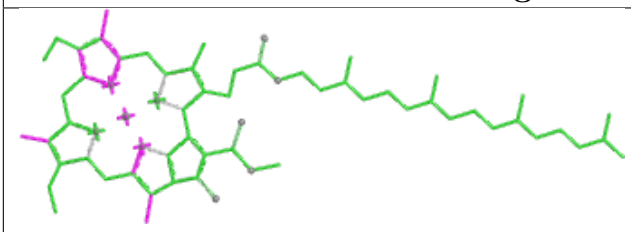


Torsions

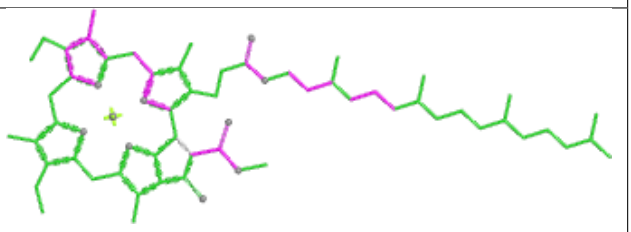


Rings

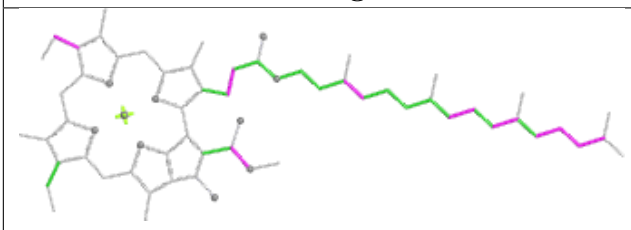
Ligand CLA G 1117



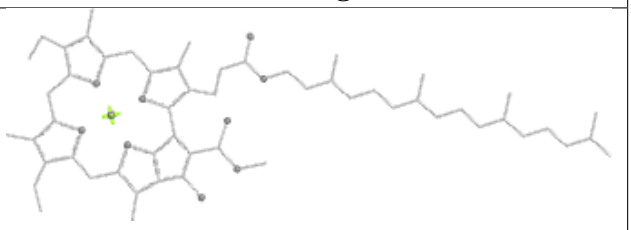
Bond lengths



Bond angles

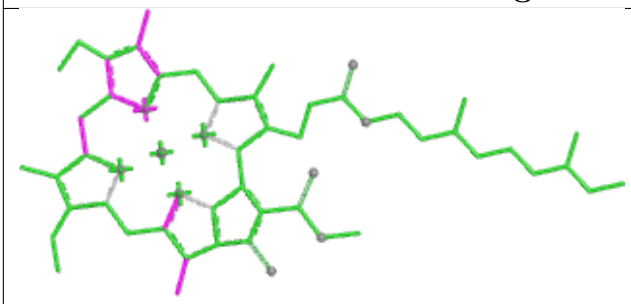


Torsions

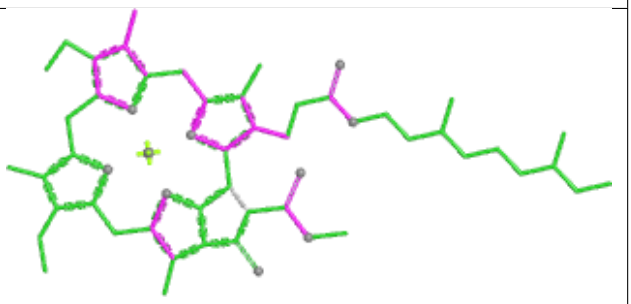


Rings

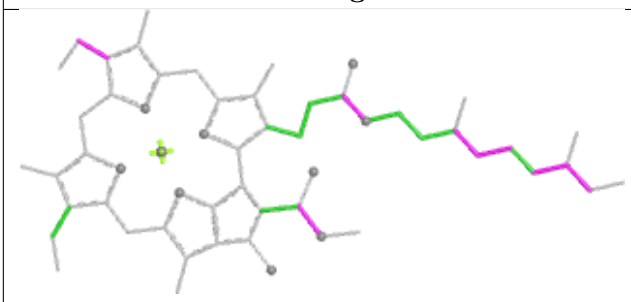
Ligand CLA G 1124



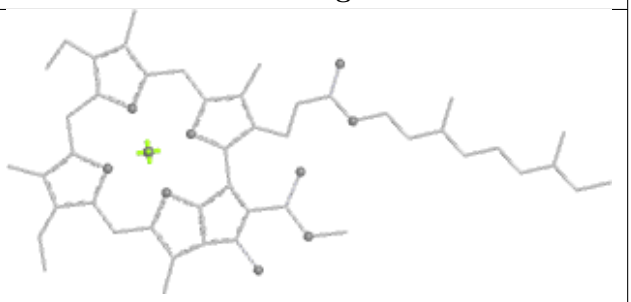
Bond lengths



Bond angles

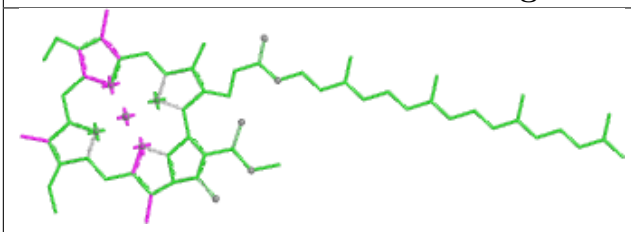


Torsions

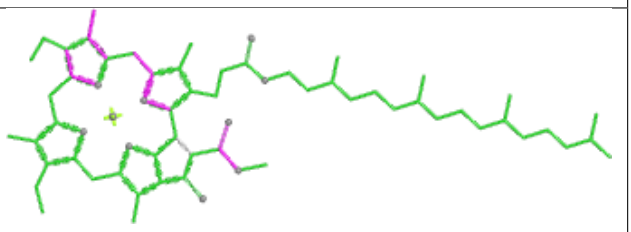


Rings

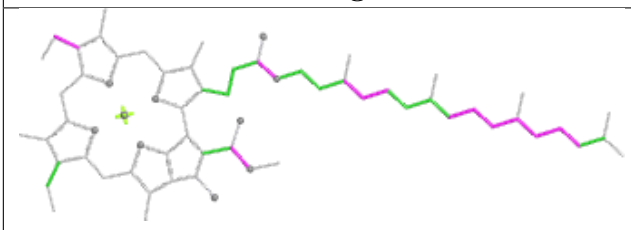
Ligand CLA e 1133



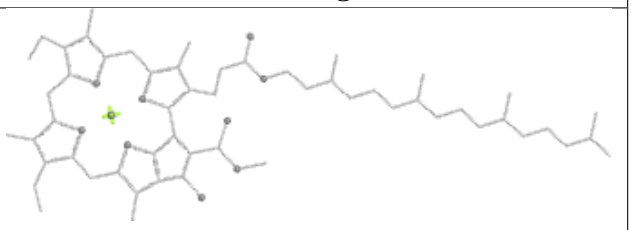
Bond lengths



Bond angles

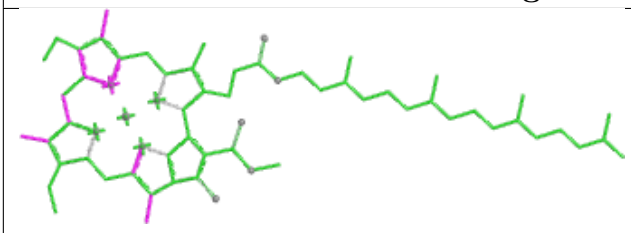


Torsions

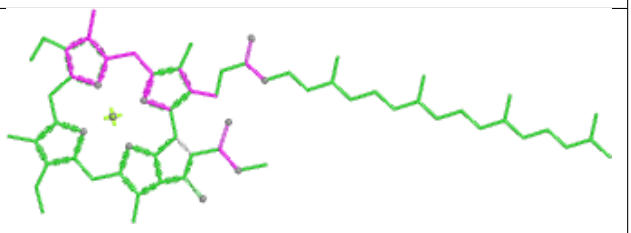


Rings

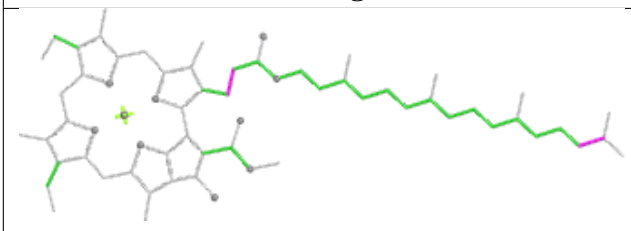
Ligand CLA f 1238



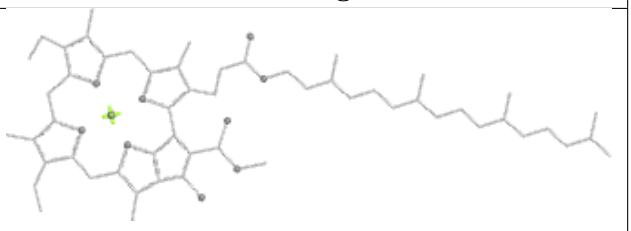
Bond lengths



Bond angles

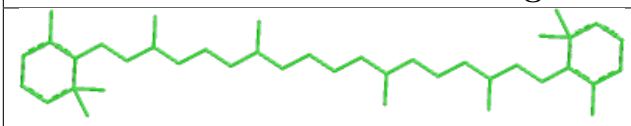


Torsions

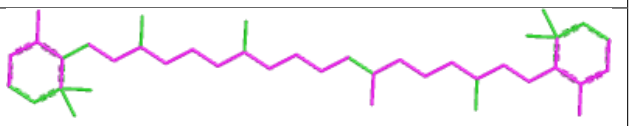


Rings

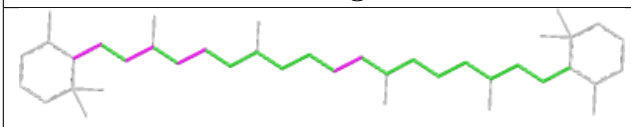
Ligand BCR Z 522



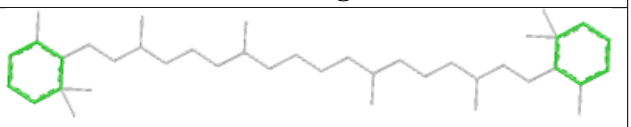
Bond lengths



Bond angles

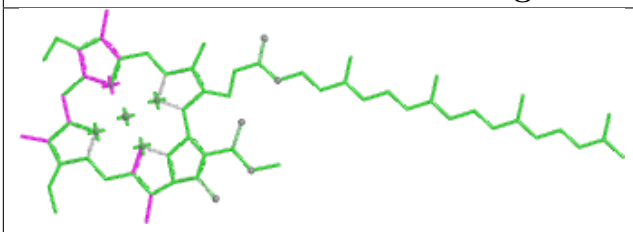


Torsions

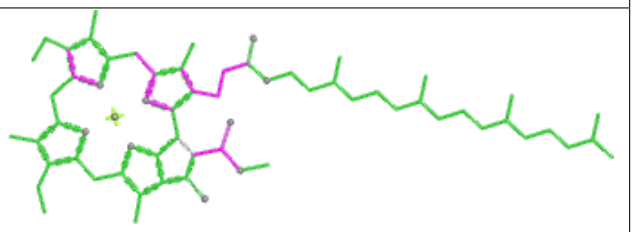


Rings

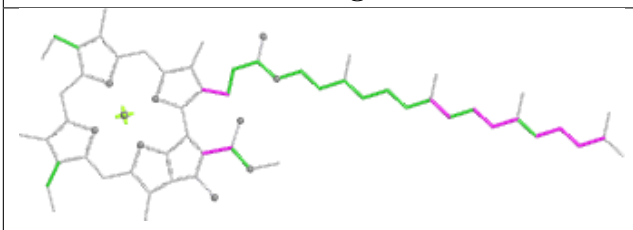
Ligand CLA G 1101



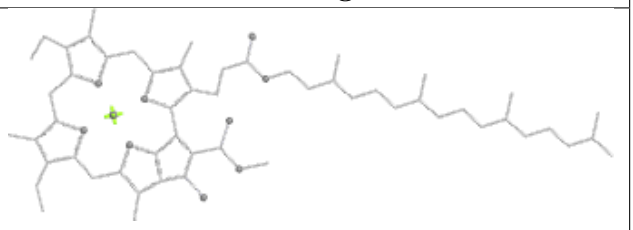
Bond lengths



Bond angles



Torsions

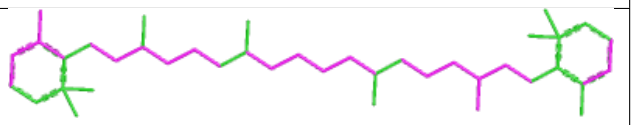


Rings

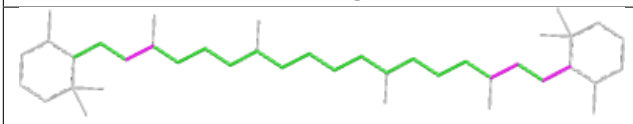
Ligand BCR r 523



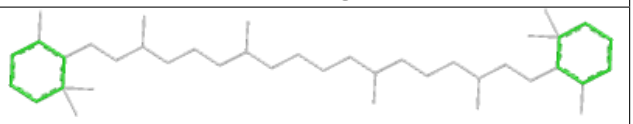
Bond lengths



Bond angles

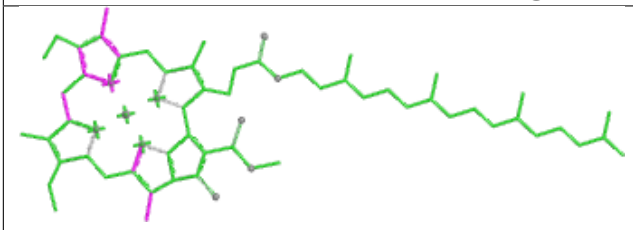


Torsions

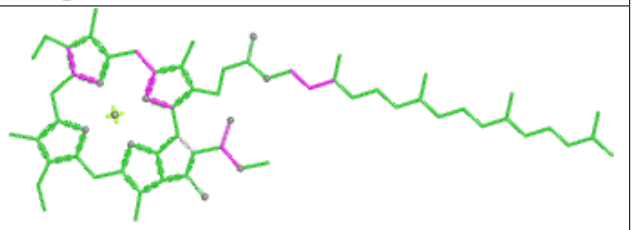


Rings

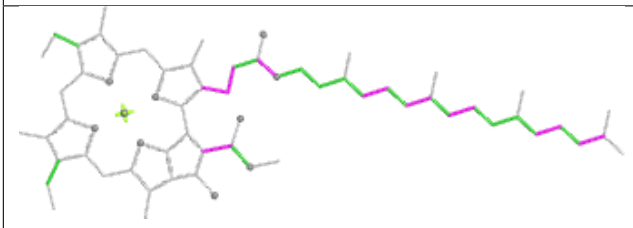
Ligand CLA q 505



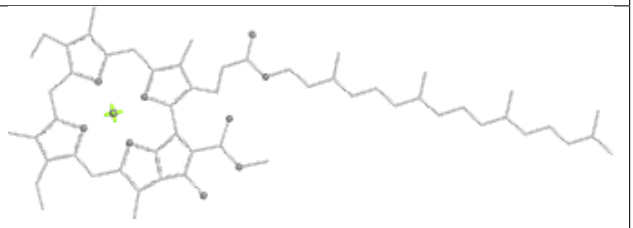
Bond lengths



Bond angles

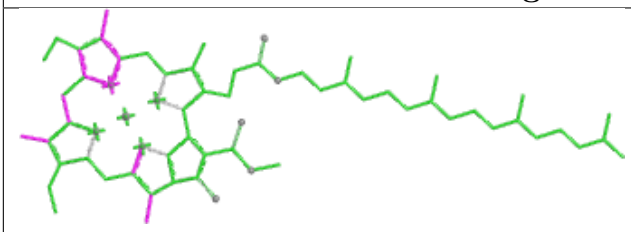


Torsions

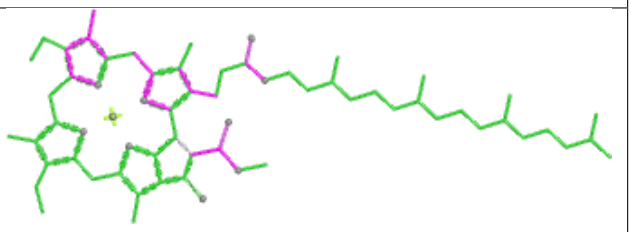


Rings

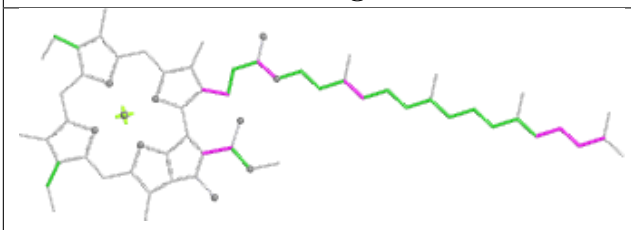
Ligand CLA f 1202



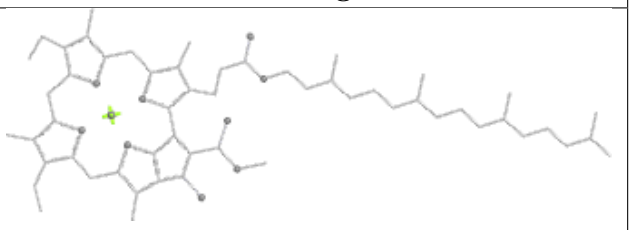
Bond lengths



Bond angles



Torsions



Rings

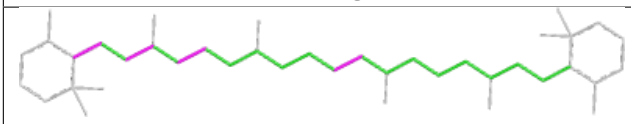
Ligand BCR 1 522



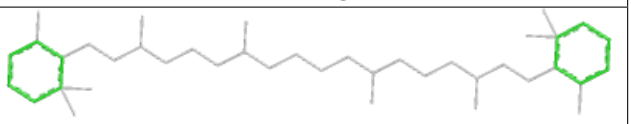
Bond lengths



Bond angles

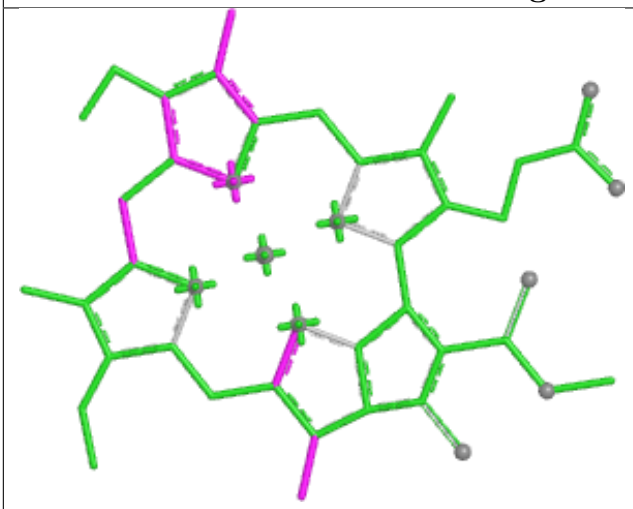


Torsions

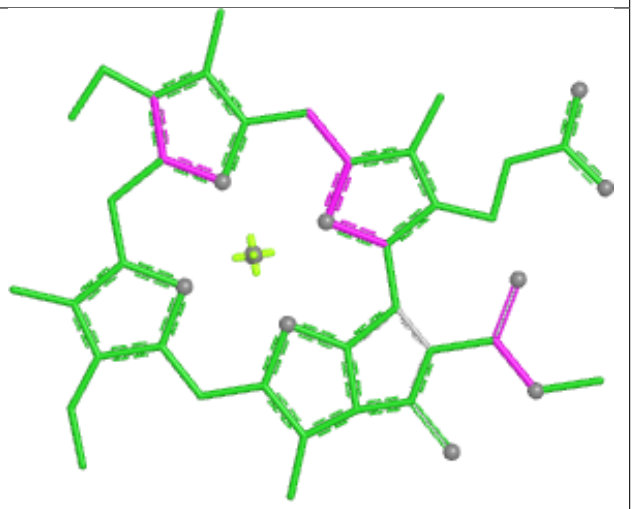


Rings

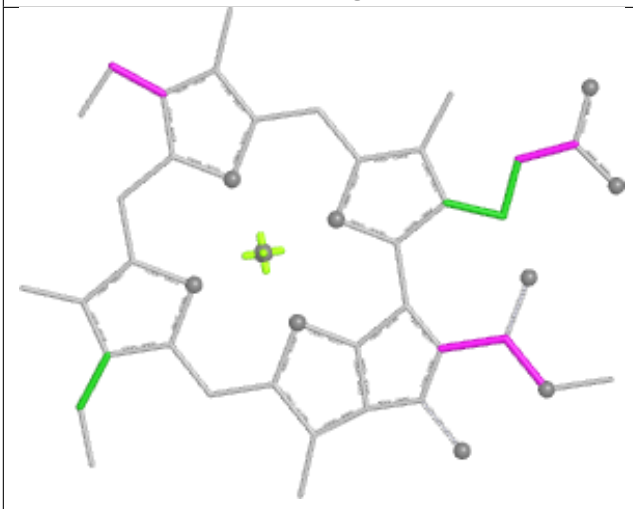
Ligand CLA c 512



Bond lengths



Bond angles

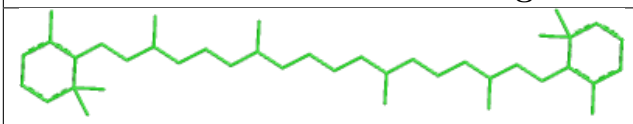


Torsions

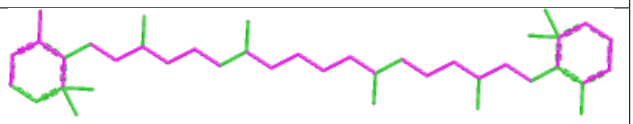


Rings

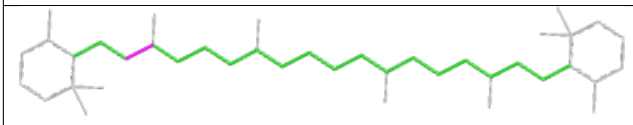
Ligand BCR L 4022



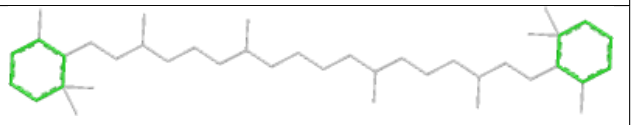
Bond lengths



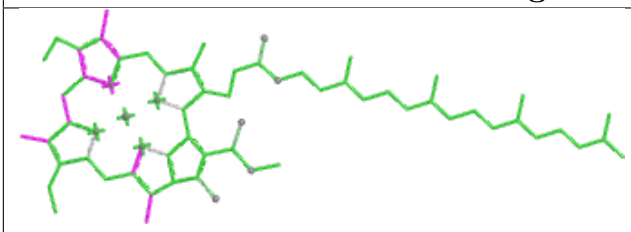
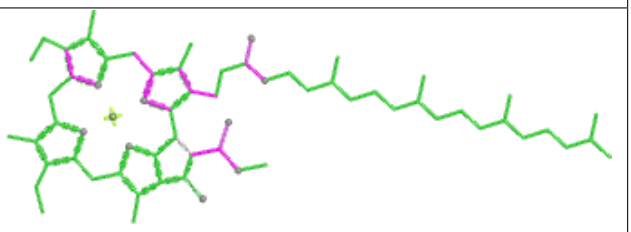
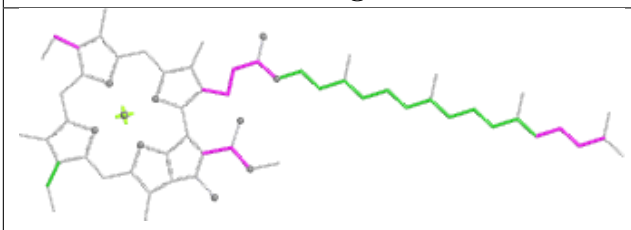
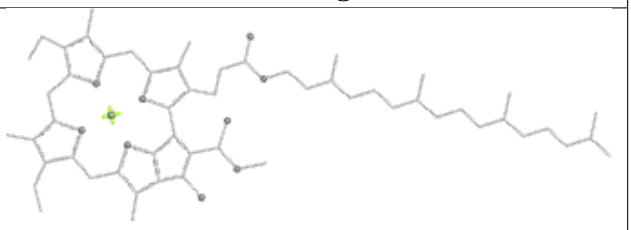
Bond angles

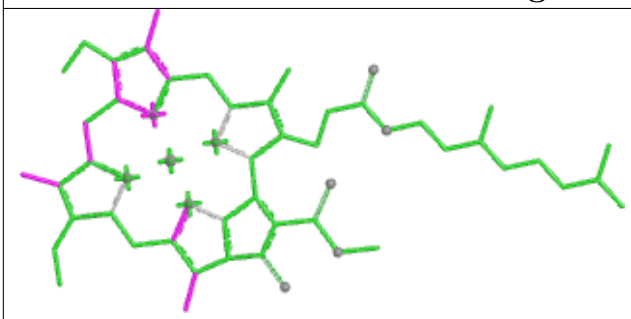
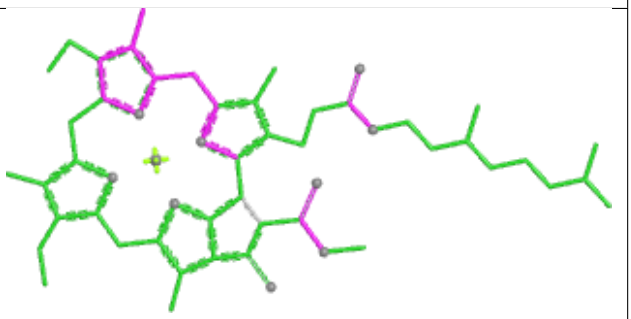
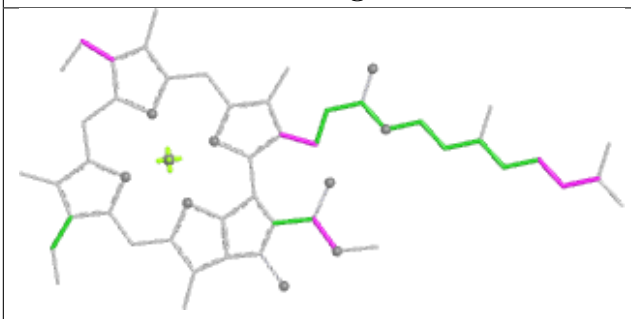
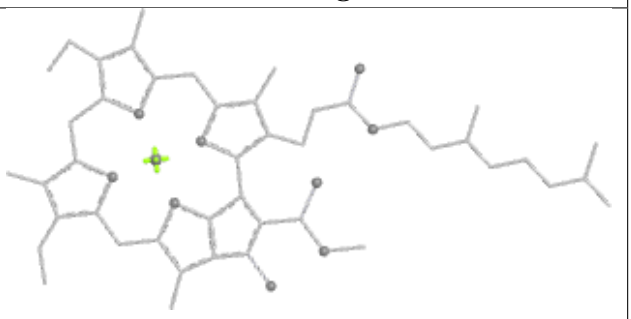


Torsions

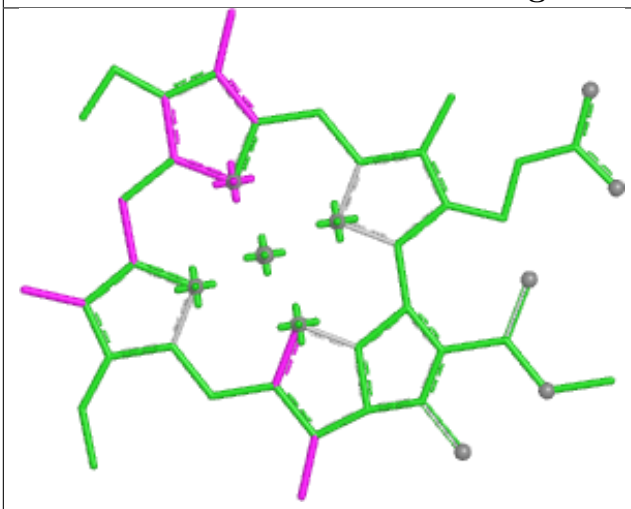


Rings

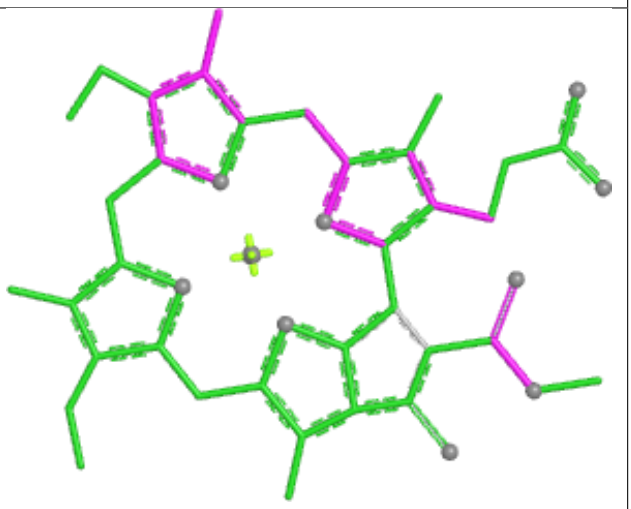
Ligand CLA 1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

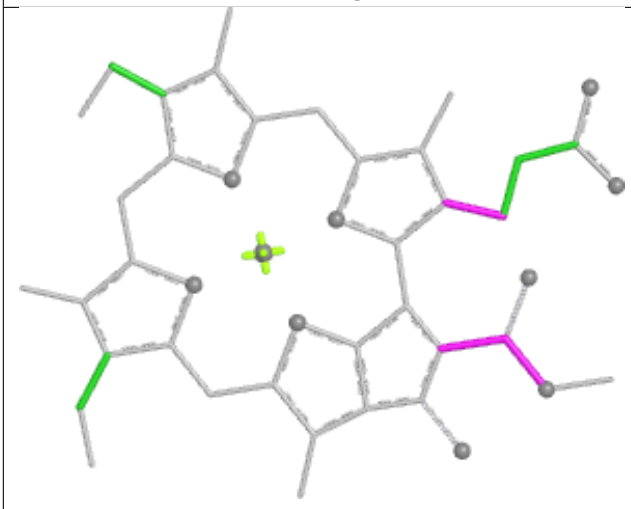
Ligand CLA 3 504



Bond lengths



Bond angles

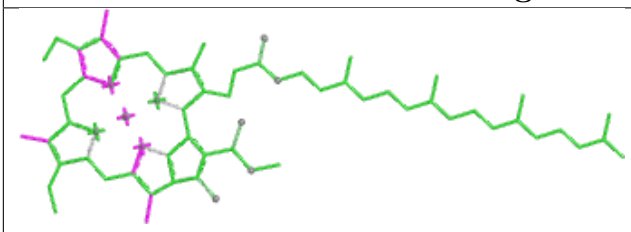


Torsions

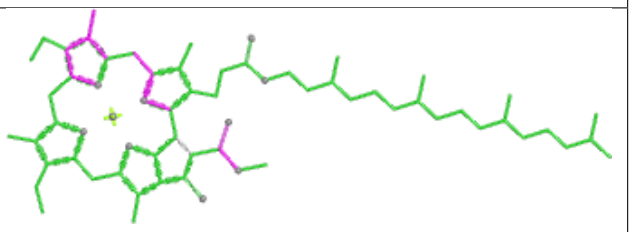


Rings

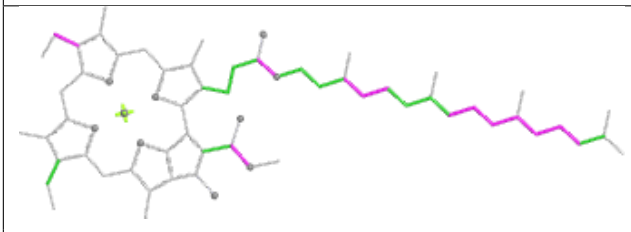
Ligand CLA A 1133



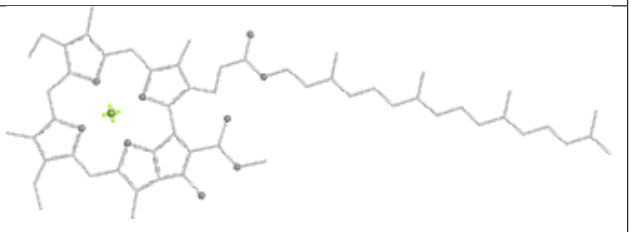
Bond lengths



Bond angles

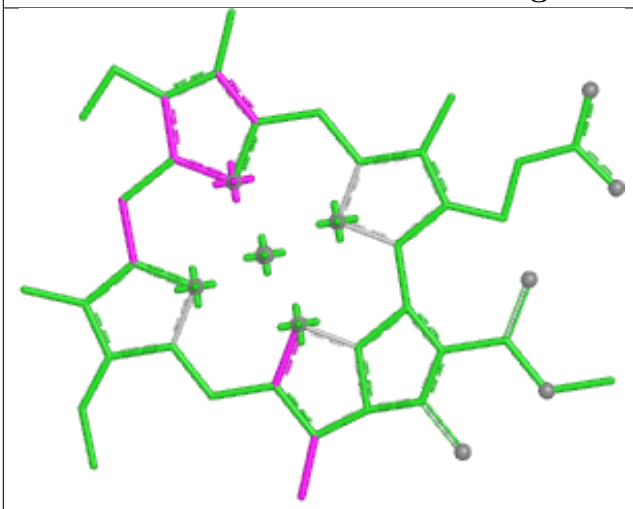


Torsions

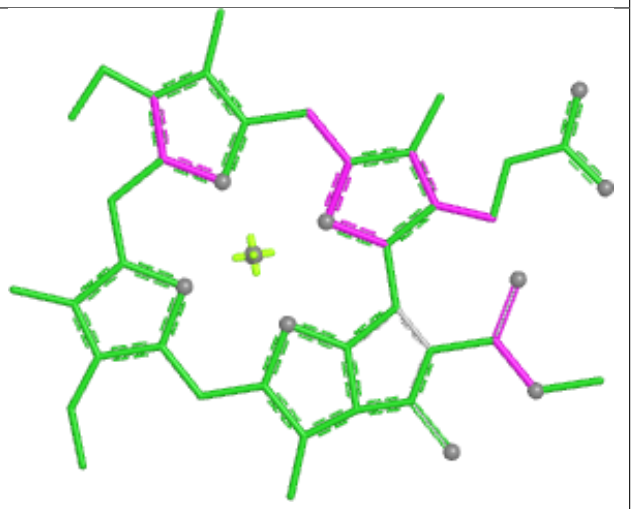


Rings

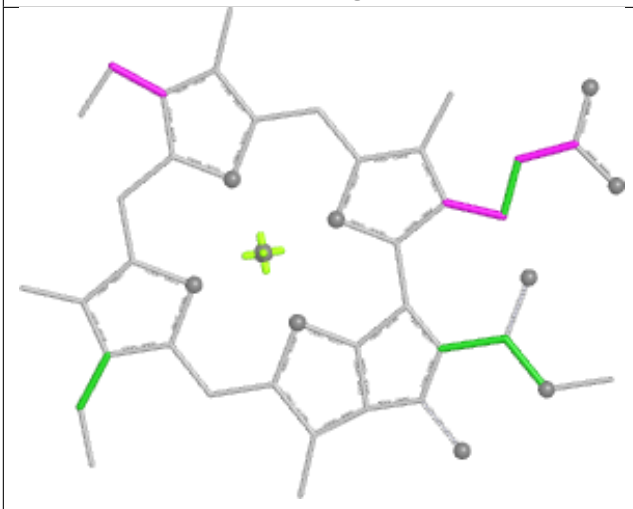
Ligand CLA t 516



Bond lengths



Bond angles

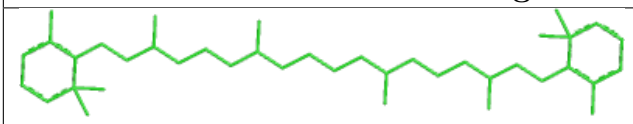


Torsions

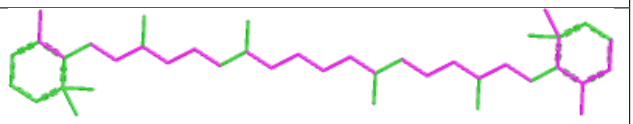


Rings

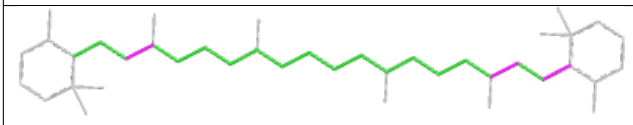
Ligand BCR V 4019



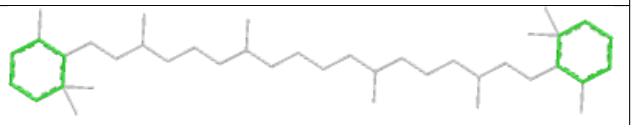
Bond lengths



Bond angles

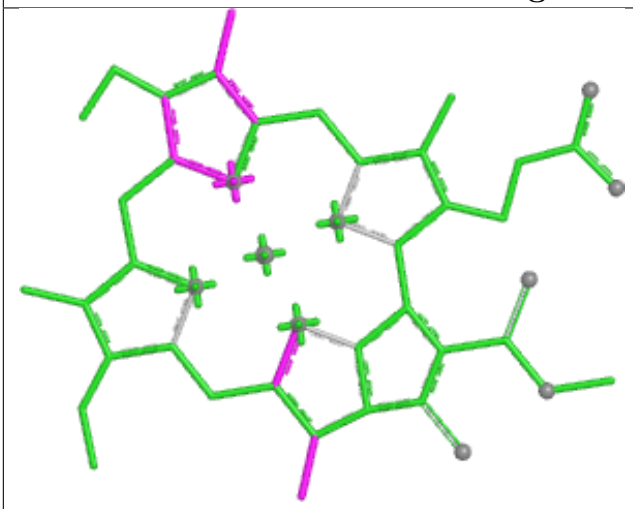


Torsions

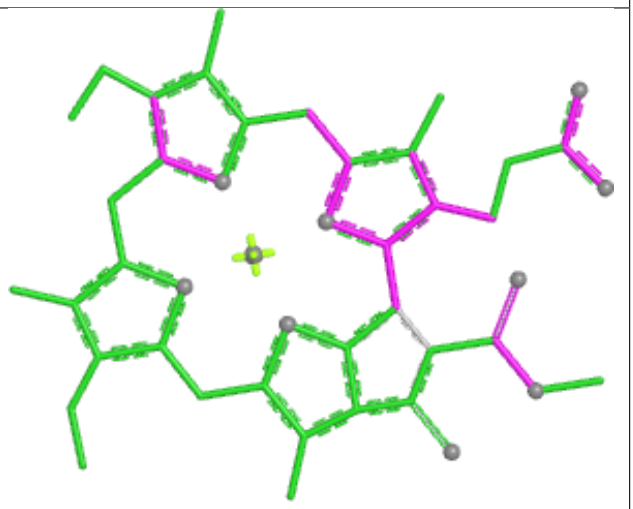


Rings

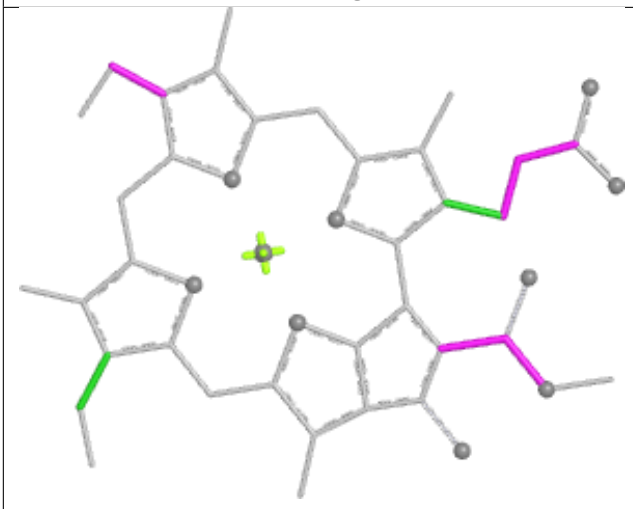
Ligand CLA 5 507



Bond lengths



Bond angles

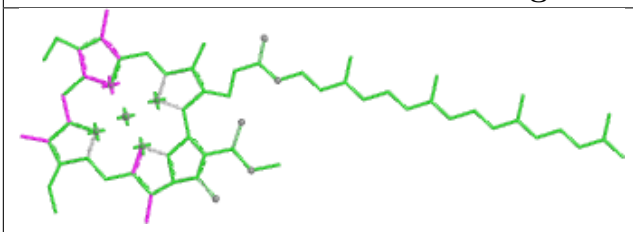


Torsions

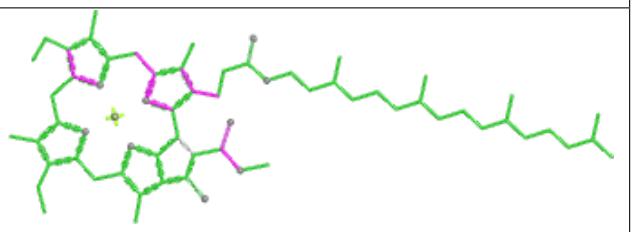


Rings

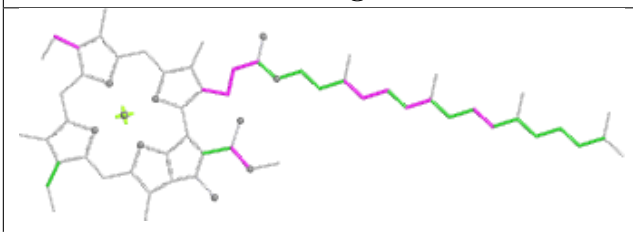
Ligand CLA r 501



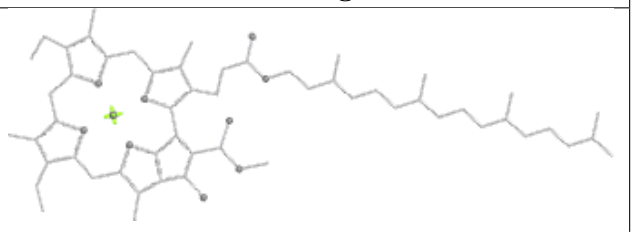
Bond lengths



Bond angles

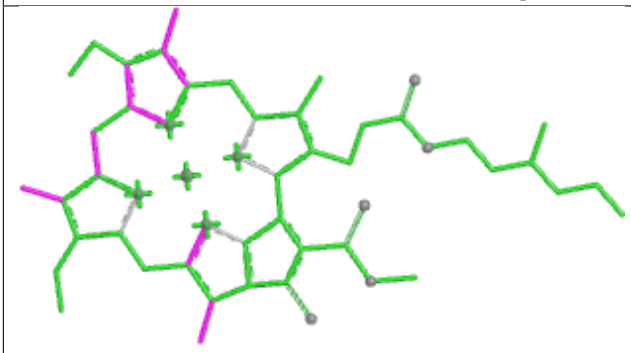


Torsions

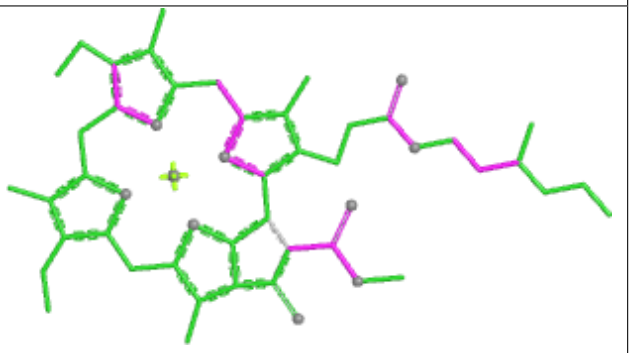


Rings

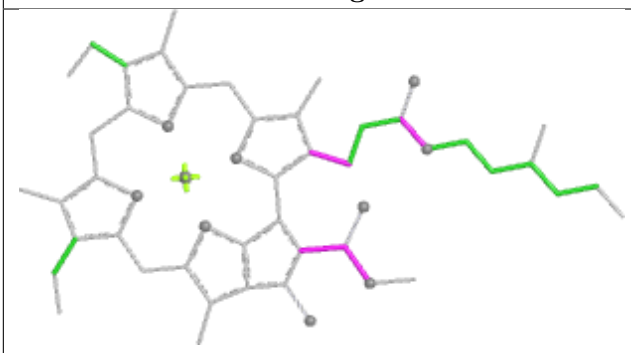
Ligand CLA H 1209



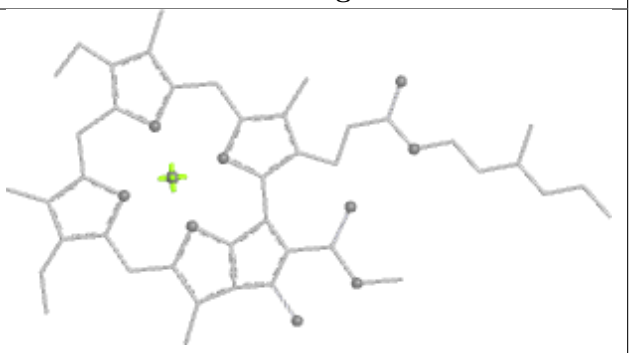
Bond lengths



Bond angles

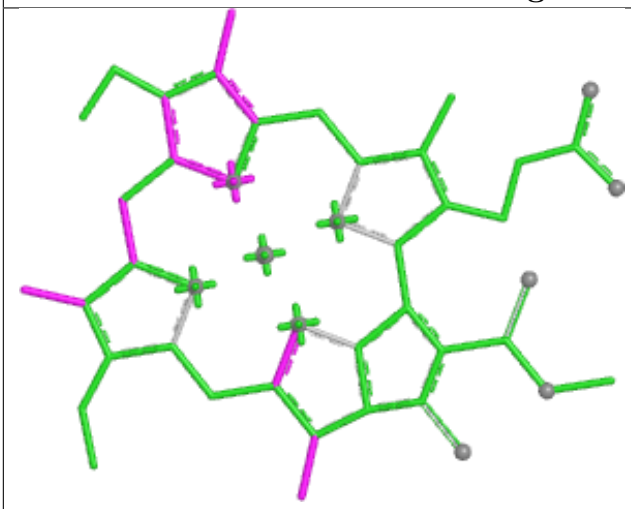


Torsions

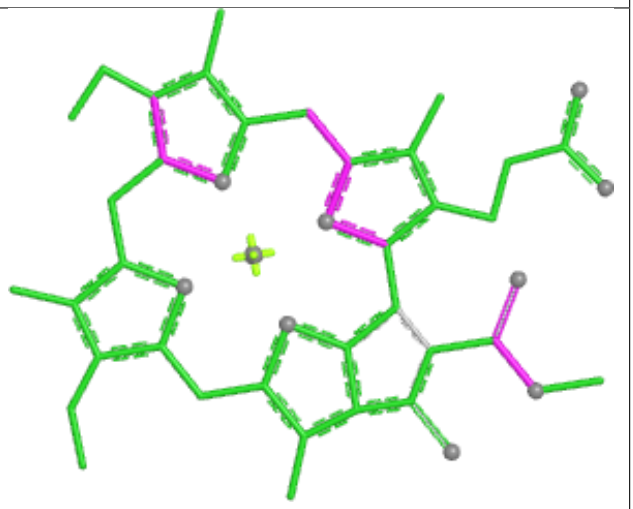


Rings

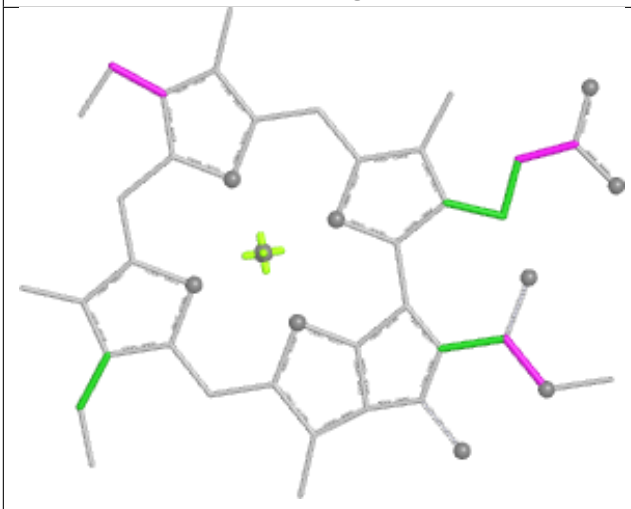
Ligand CLA u 513



Bond lengths



Bond angles

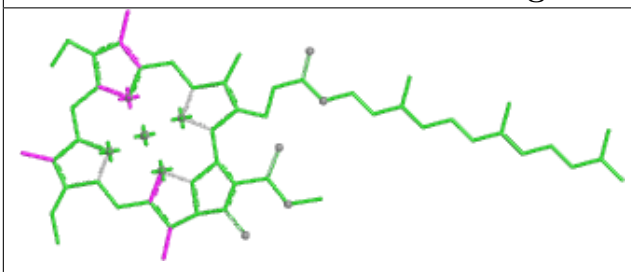


Torsions

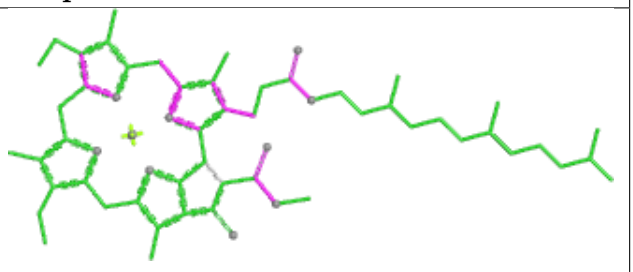


Rings

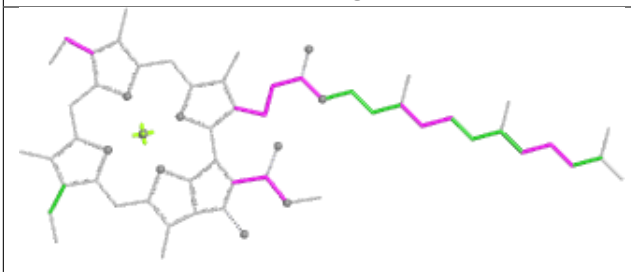
Ligand CLA q 518



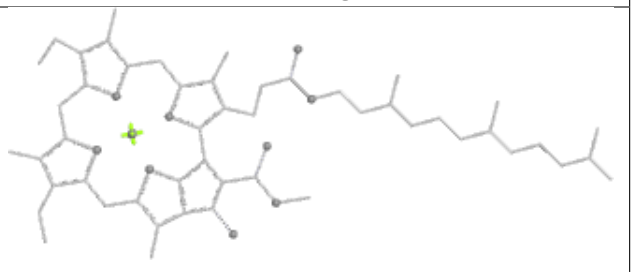
Bond lengths



Bond angles

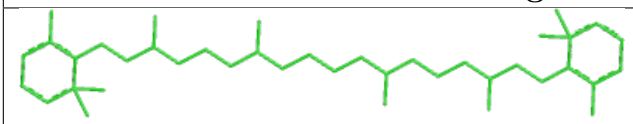


Torsions

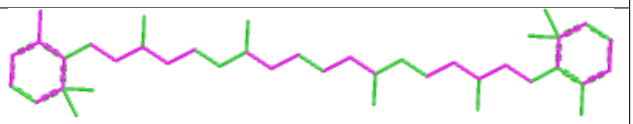


Rings

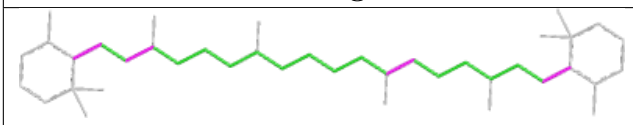
Ligand BCR 1 521



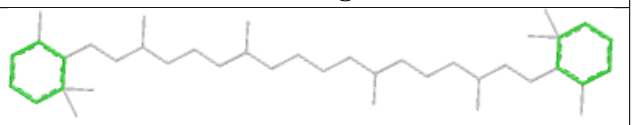
Bond lengths



Bond angles

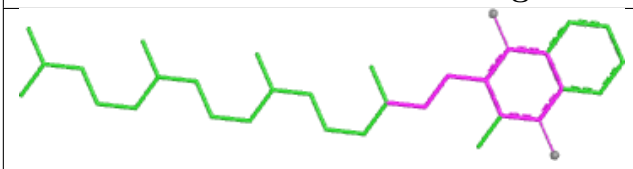


Torsions

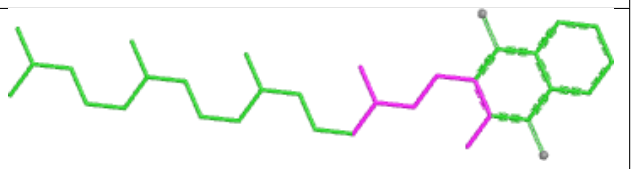


Rings

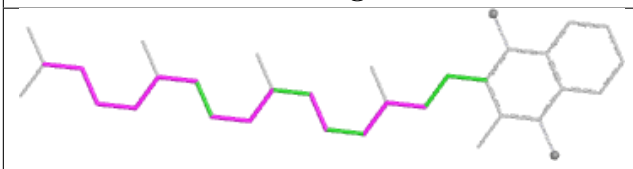
Ligand PQN G 2001



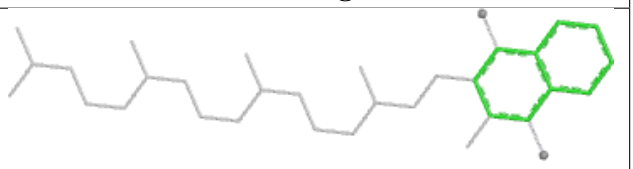
Bond lengths



Bond angles

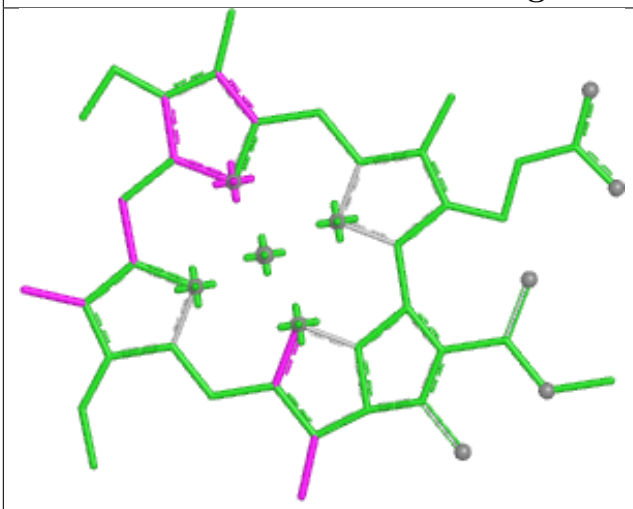


Torsions

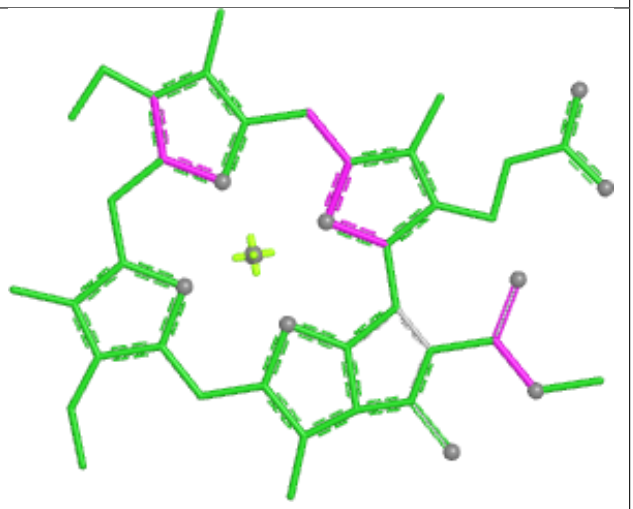


Rings

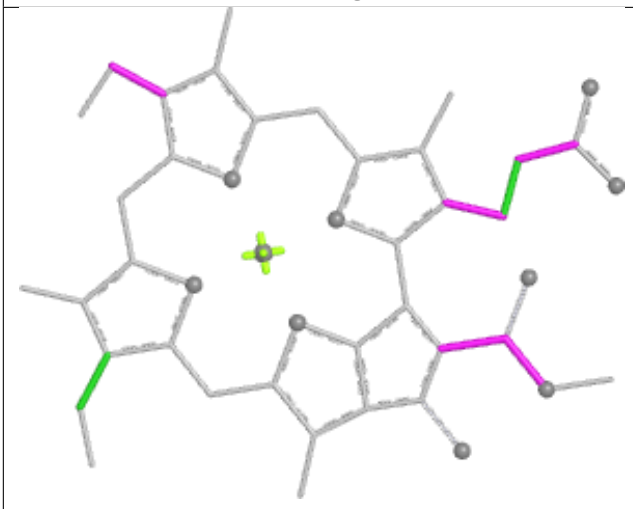
Ligand CLA v 517



Bond lengths



Bond angles

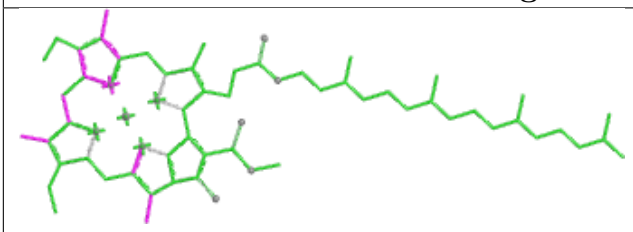


Torsions

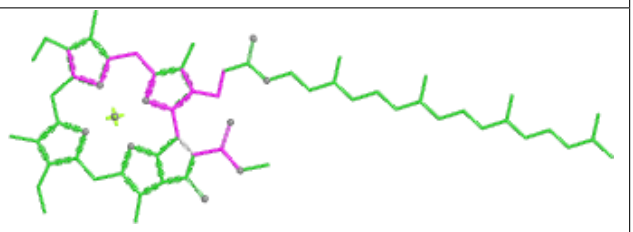


Rings

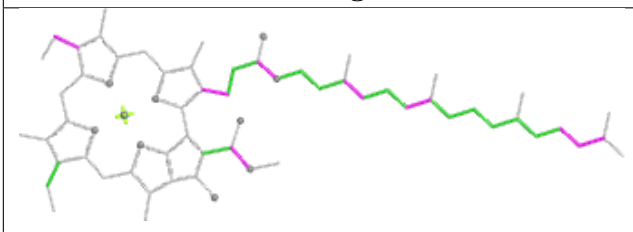
Ligand CLA e 1140



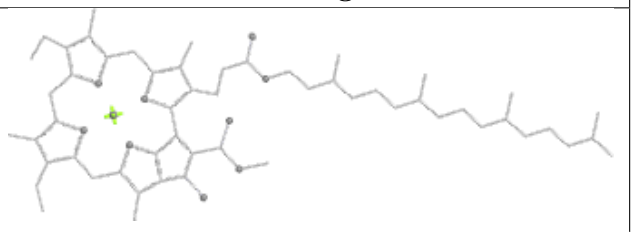
Bond lengths



Bond angles

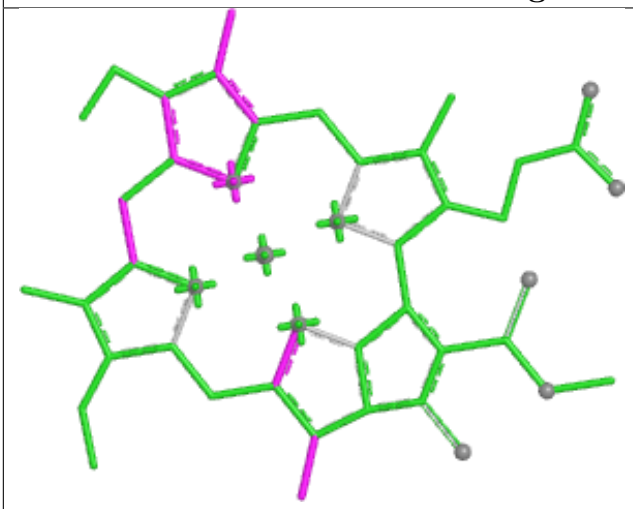


Torsions

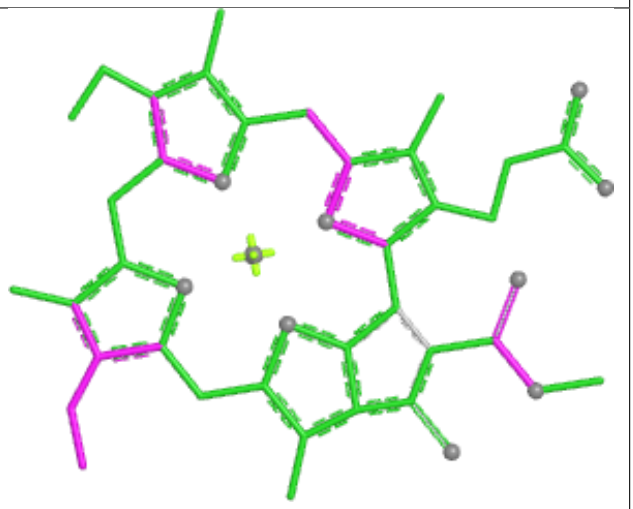


Rings

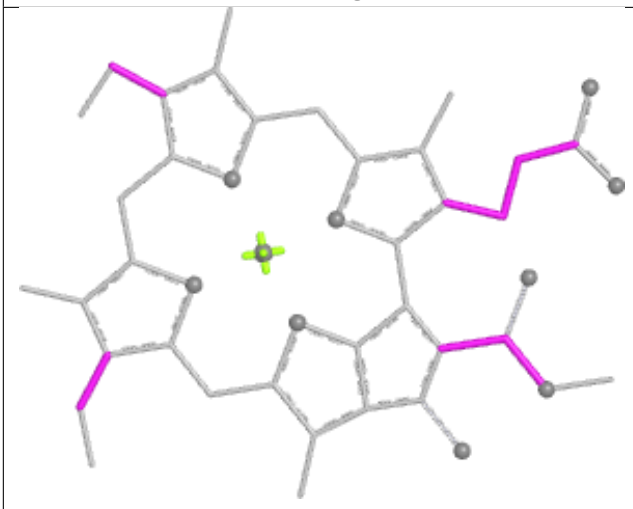
Ligand CLA 1 516



Bond lengths



Bond angles

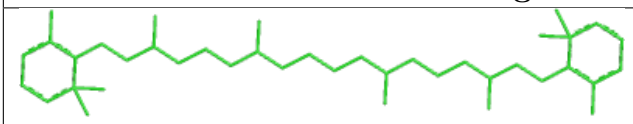


Torsions

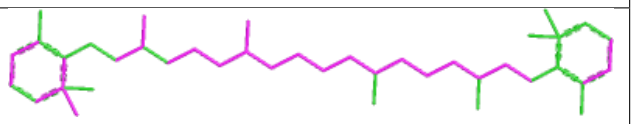


Rings

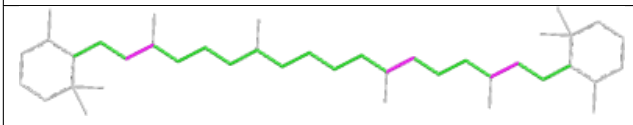
Ligand BCR B 4014



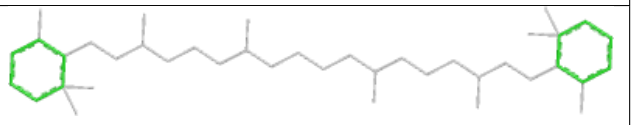
Bond lengths



Bond angles

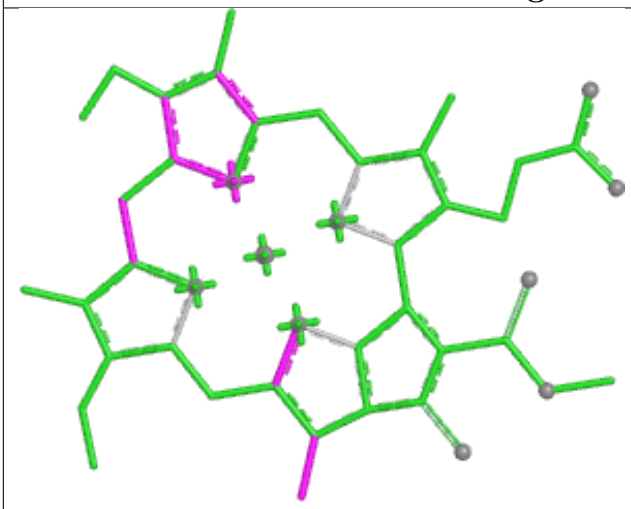


Torsions

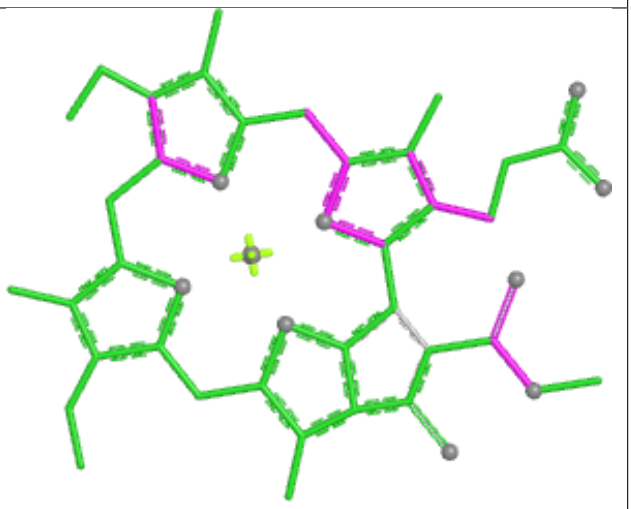


Rings

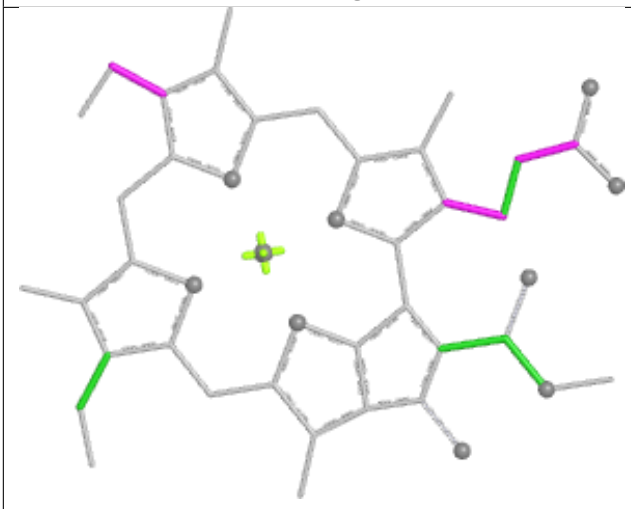
Ligand CLA b 516



Bond lengths



Bond angles

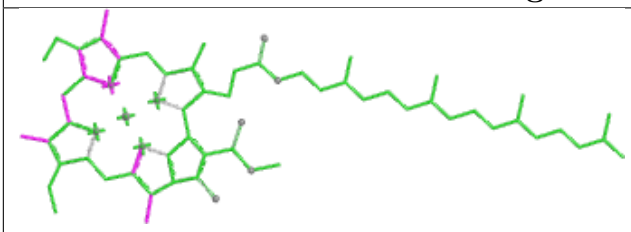


Torsions

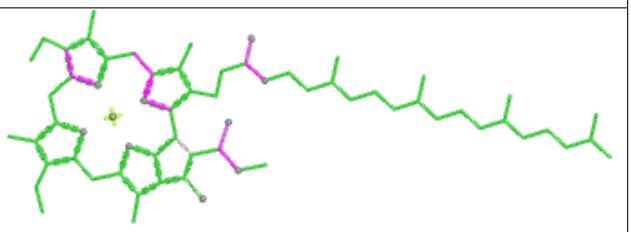


Rings

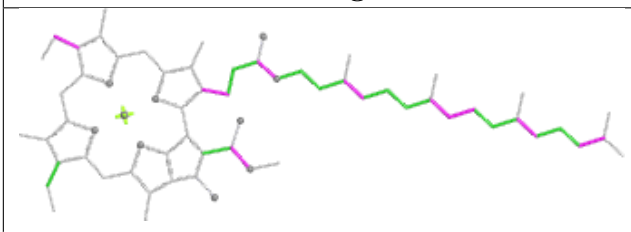
Ligand CLA Z 513



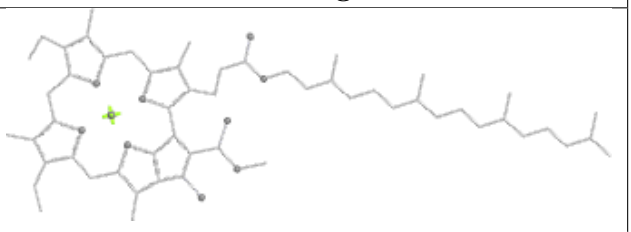
Bond lengths



Bond angles

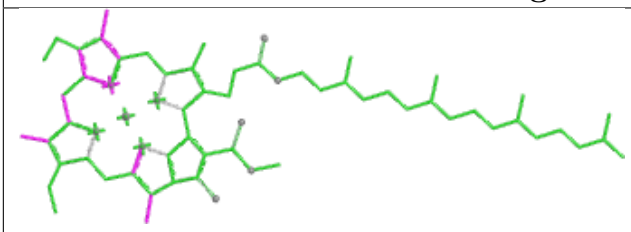


Torsions

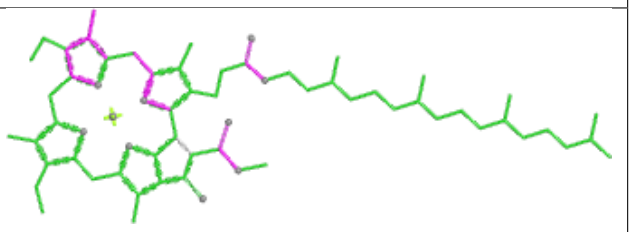


Rings

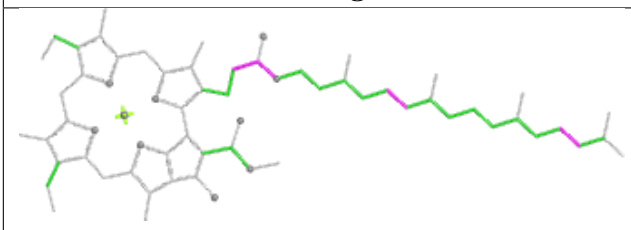
Ligand CLA r 509



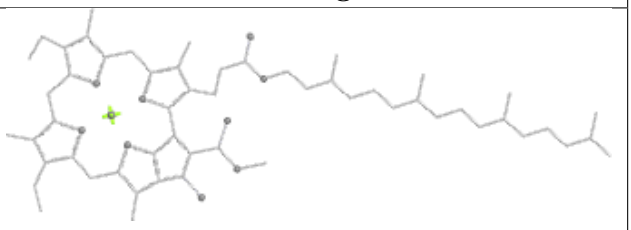
Bond lengths



Bond angles

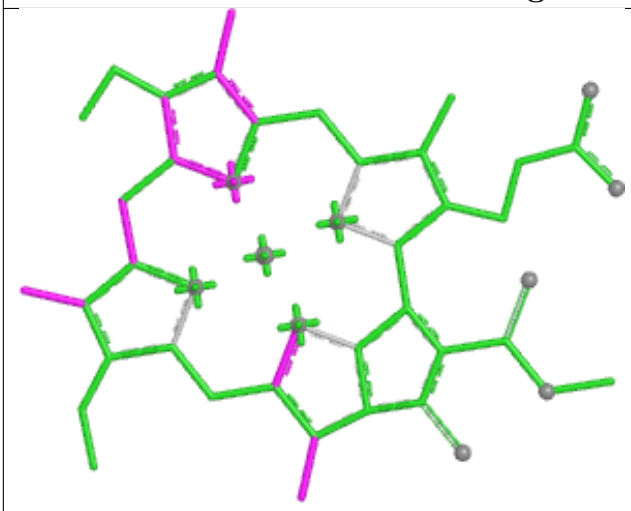


Torsions

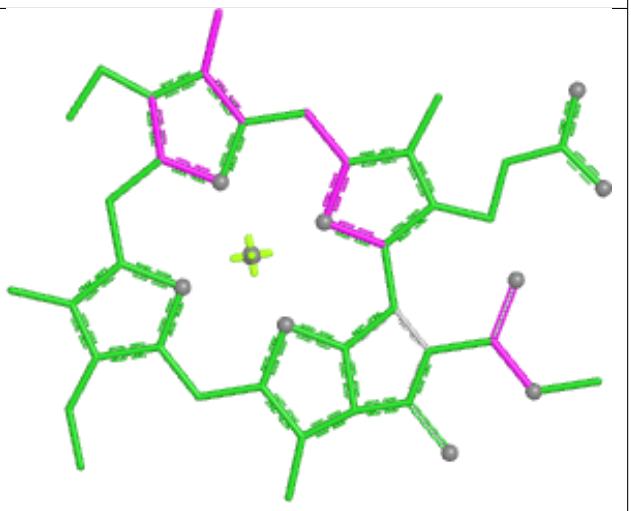


Rings

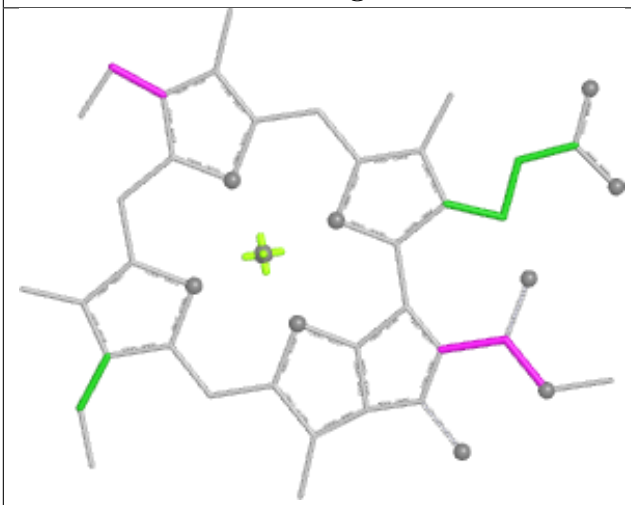
Ligand CLA d 506



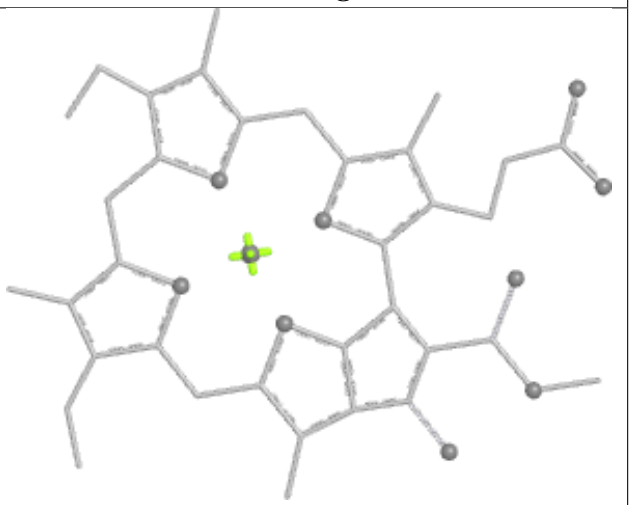
Bond lengths



Bond angles

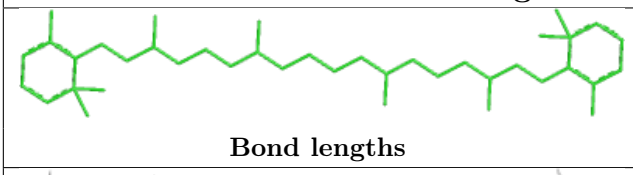


Torsions

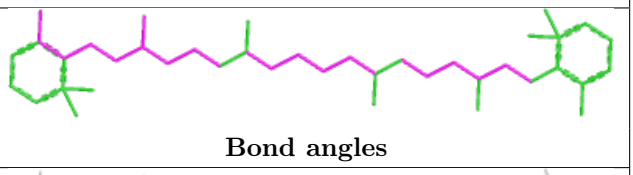


Rings

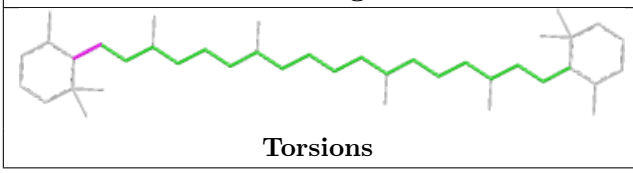
Ligand BCR B 4017



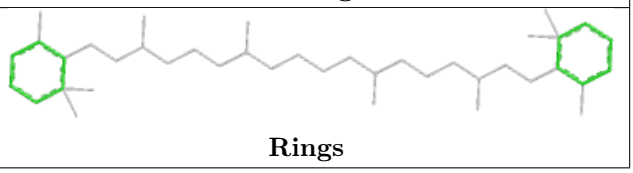
Bond lengths



Bond angles

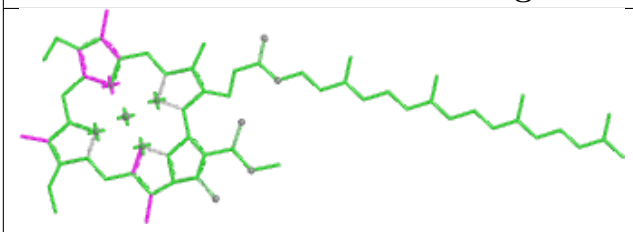


Torsions

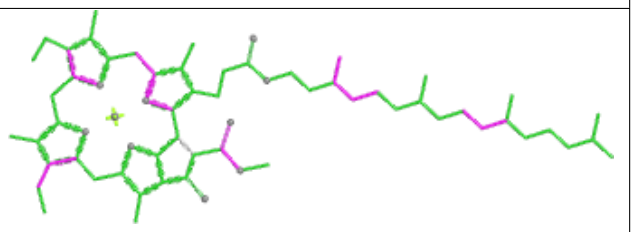


Rings

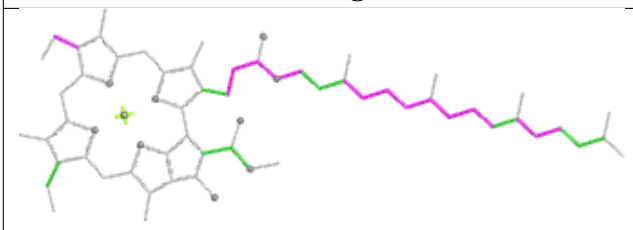
Ligand CLA A 1237



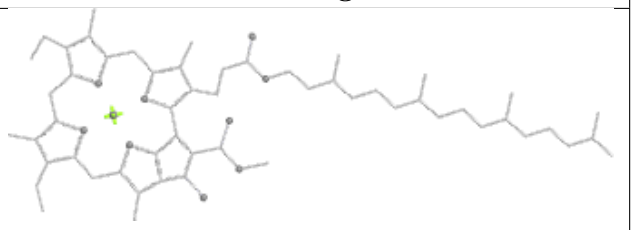
Bond lengths



Bond angles

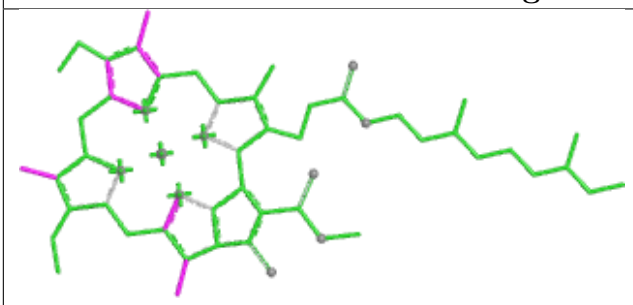


Torsions

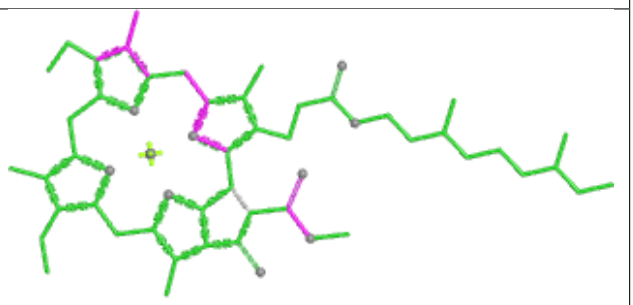


Rings

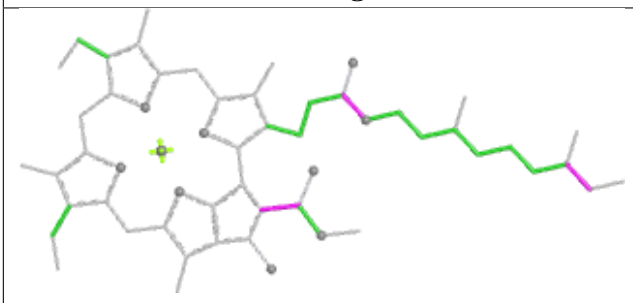
Ligand CLA f 1211



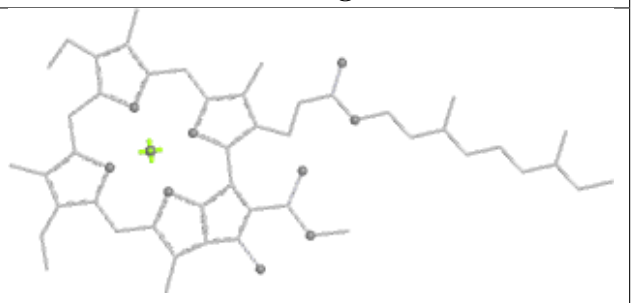
Bond lengths



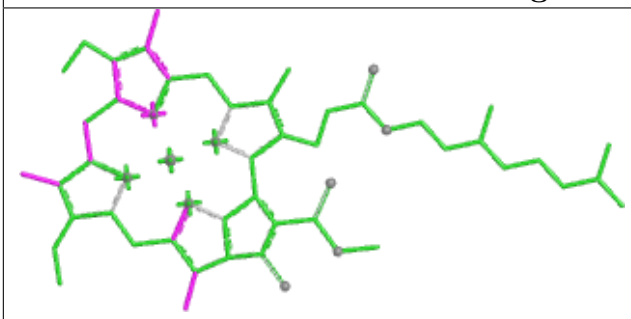
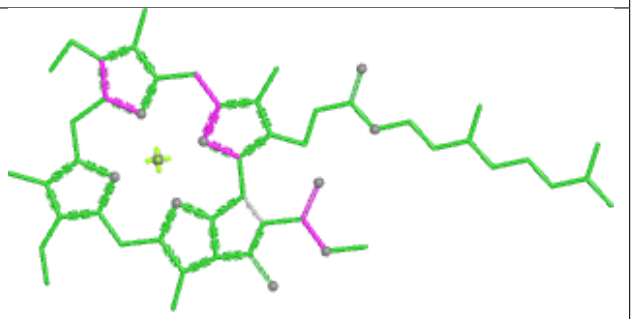
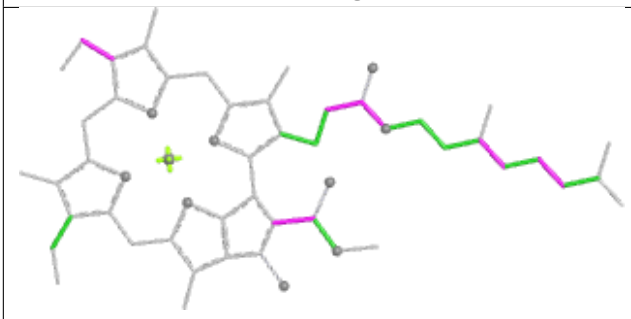
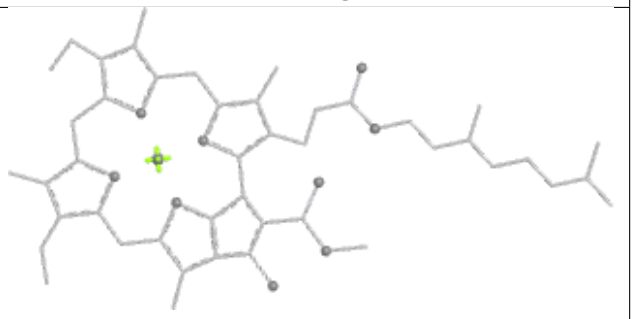
Bond angles



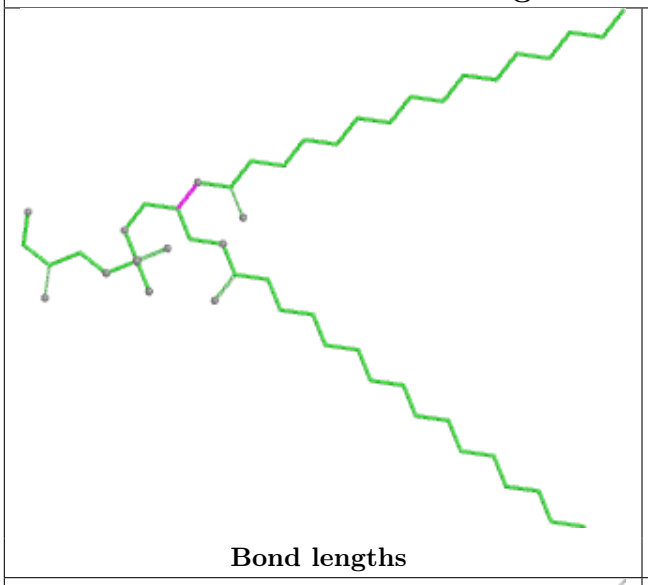
Torsions



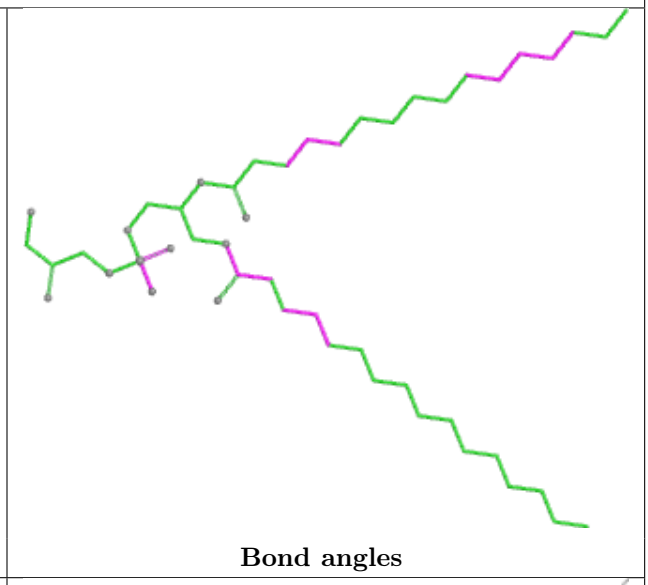
Rings

Ligand CLA t 519	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

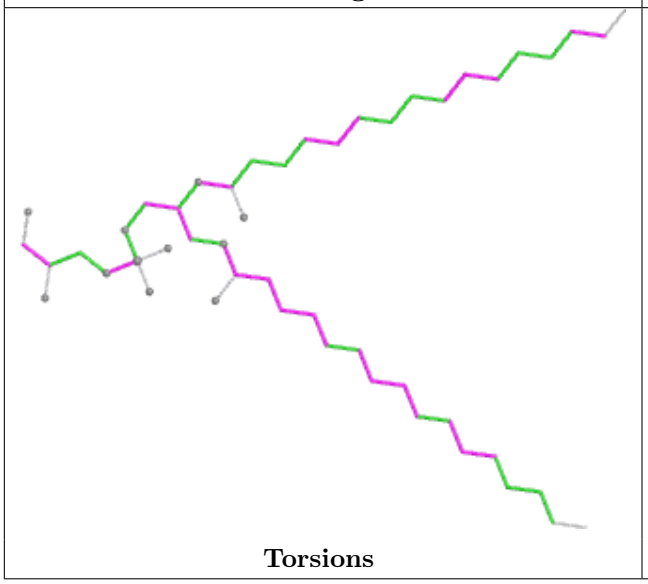
Ligand LHG G 5001



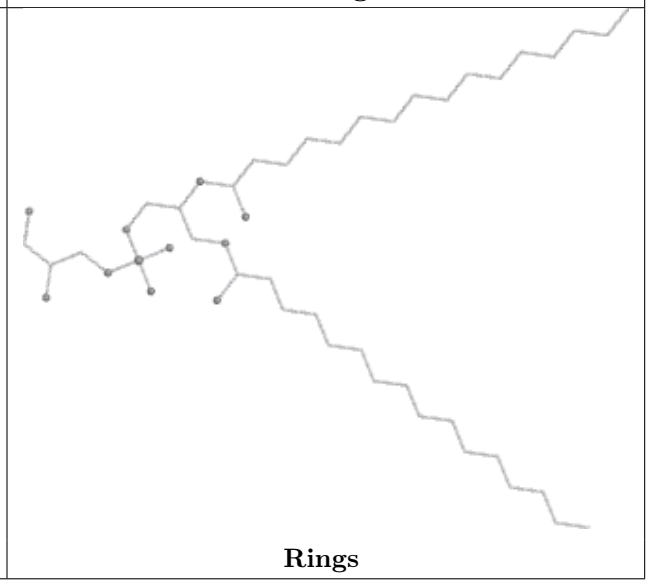
Bond lengths



Bond angles



Torsions

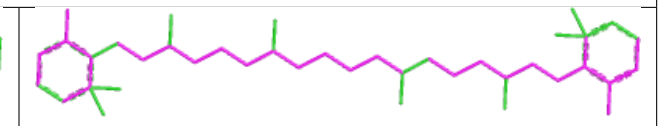


Rings

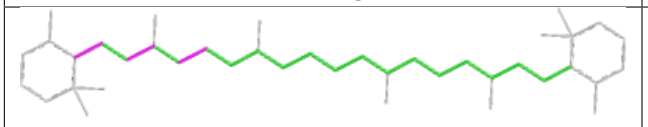
Ligand BCR s 522



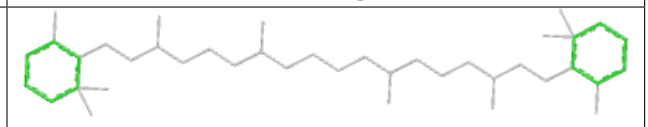
Bond lengths



Bond angles

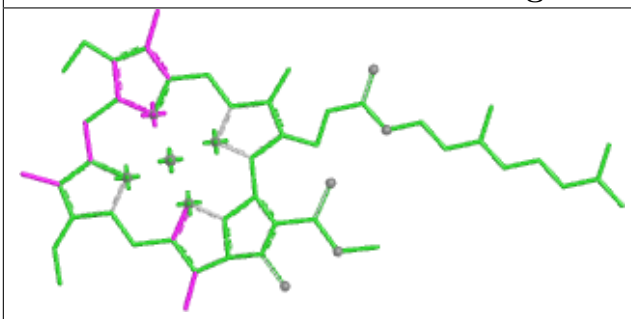


Torsions

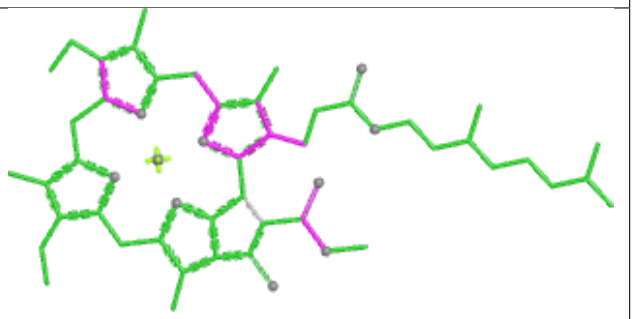


Rings

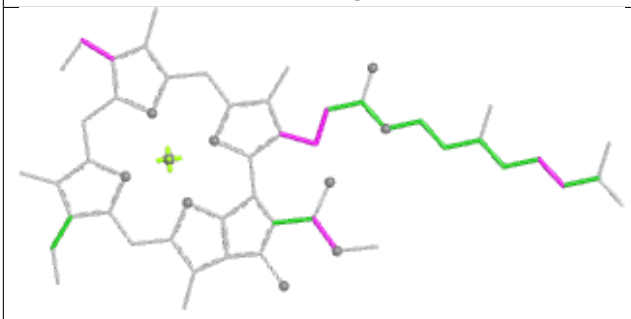
Ligand CLA Z 519



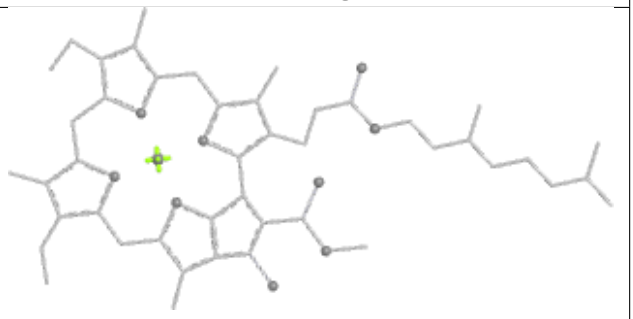
Bond lengths



Bond angles

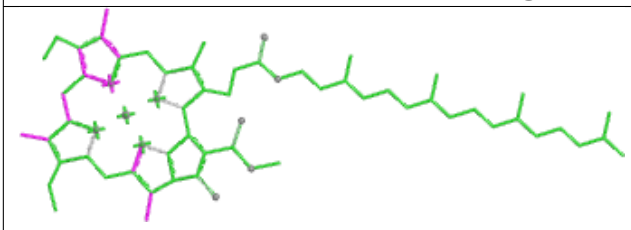


Torsions

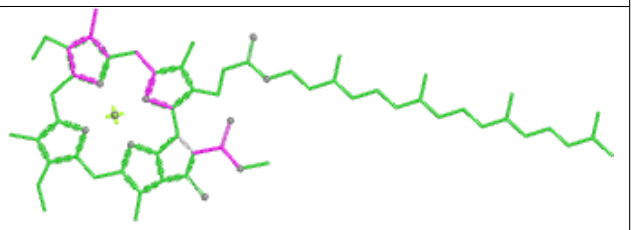


Rings

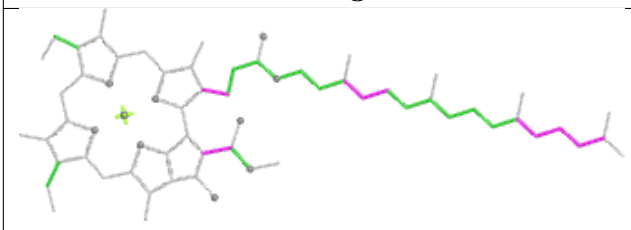
Ligand CLA e 1102



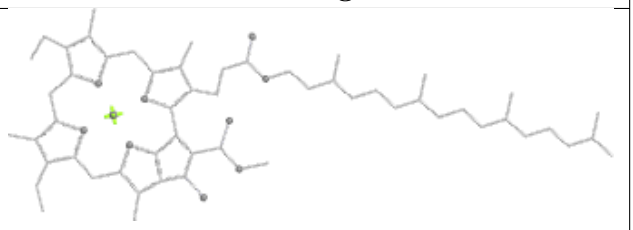
Bond lengths



Bond angles

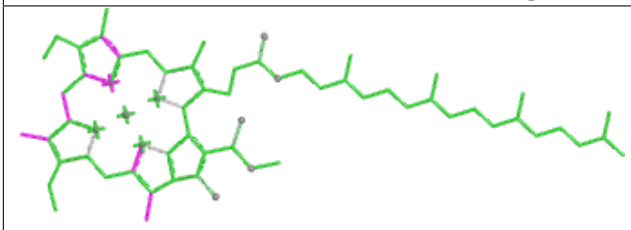


Torsions

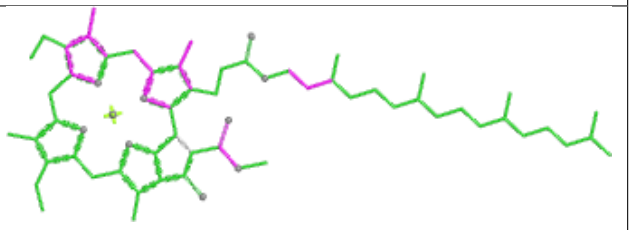


Rings

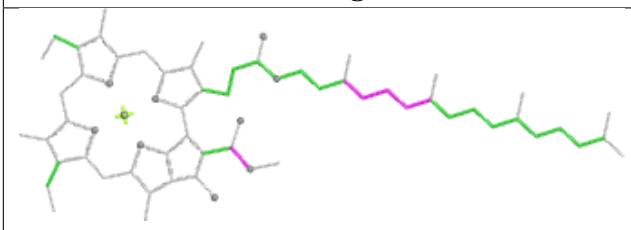
Ligand CLA f 1231



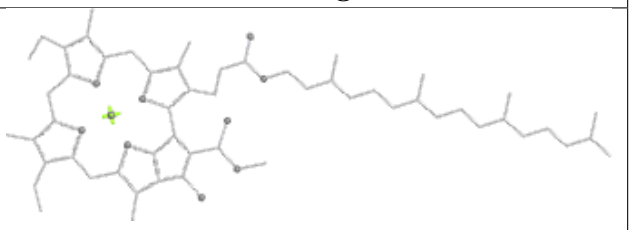
Bond lengths



Bond angles

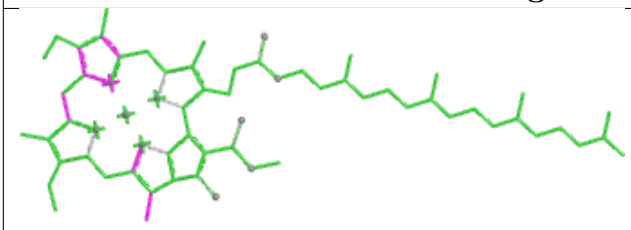


Torsions

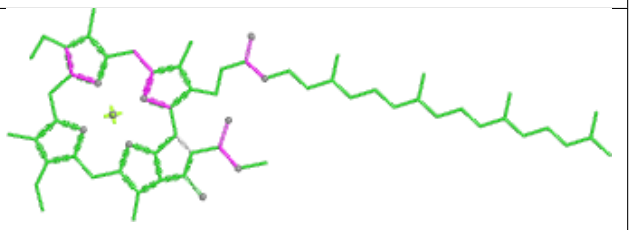


Rings

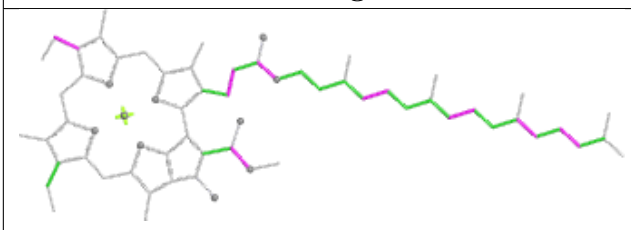
Ligand CLA b 505



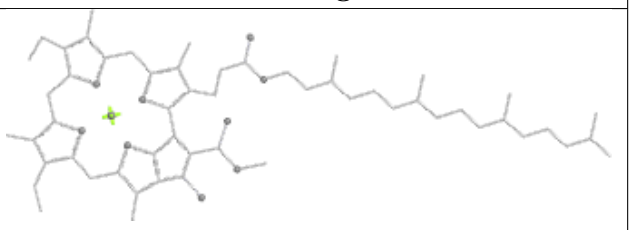
Bond lengths



Bond angles

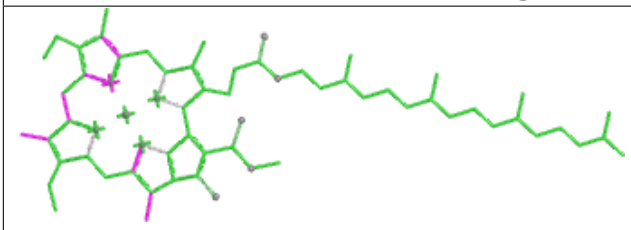


Torsions

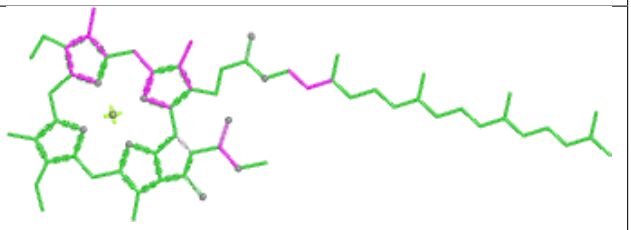


Rings

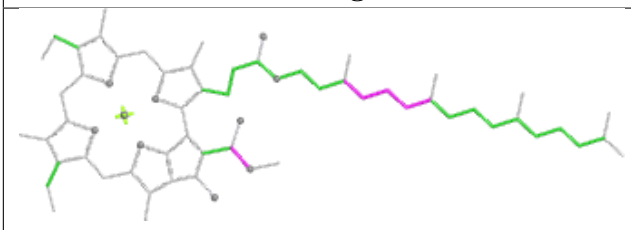
Ligand CLA H 1231



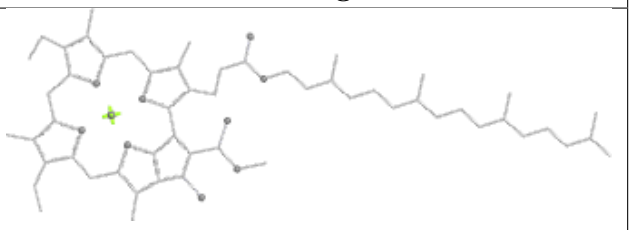
Bond lengths



Bond angles

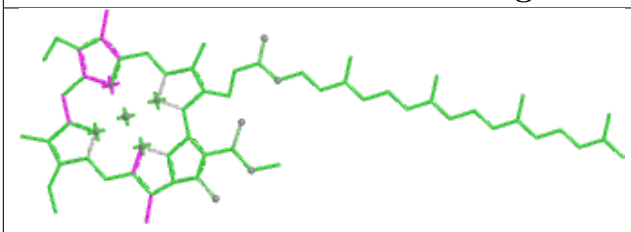


Torsions

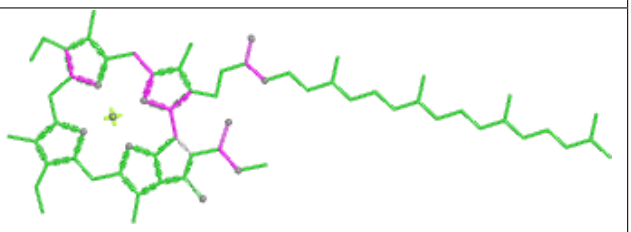


Rings

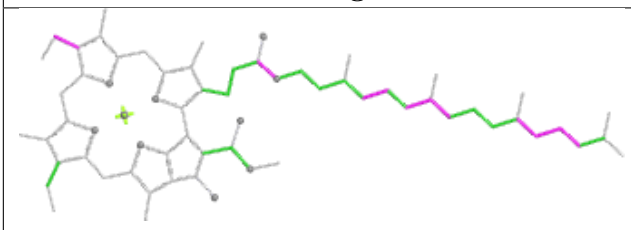
Ligand CLA R 1301



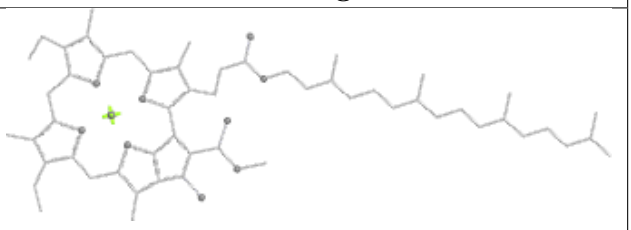
Bond lengths



Bond angles

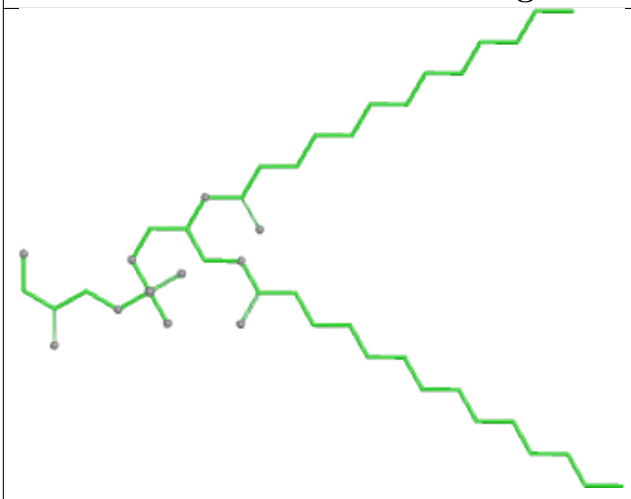


Torsions

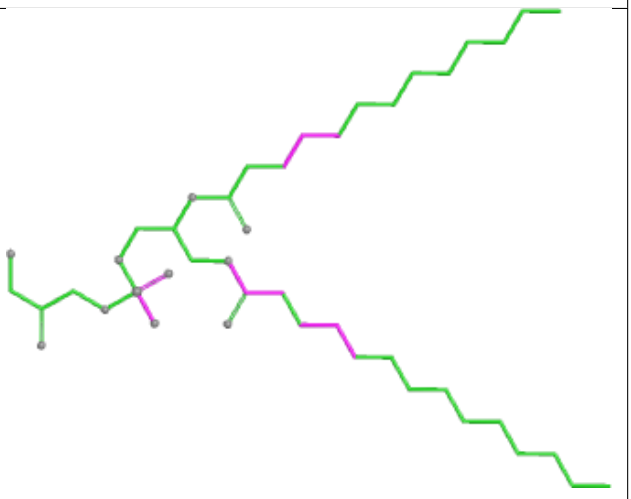


Rings

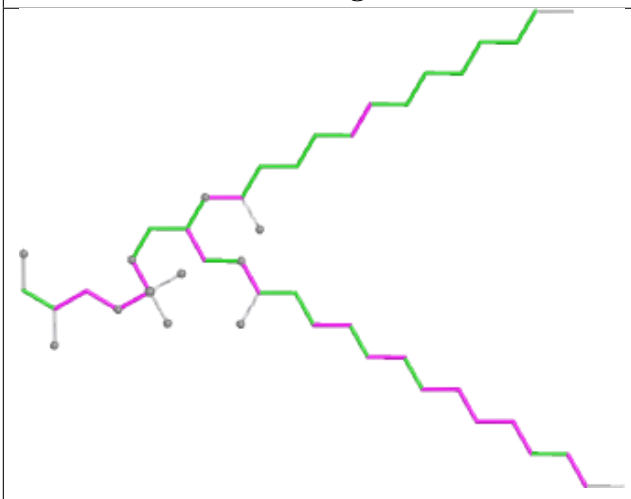
Ligand LHG S 5001



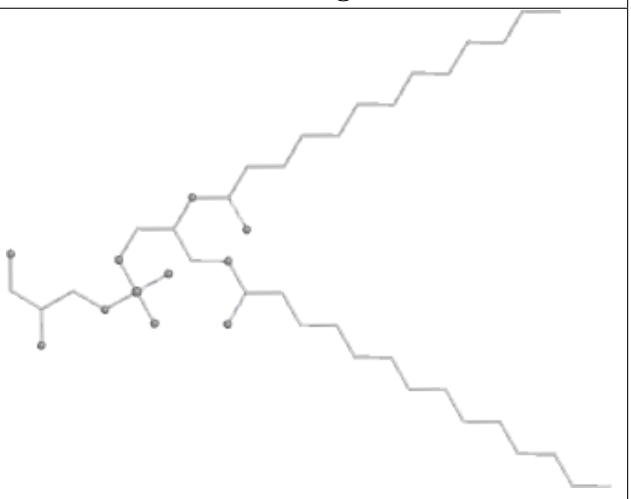
Bond lengths



Bond angles

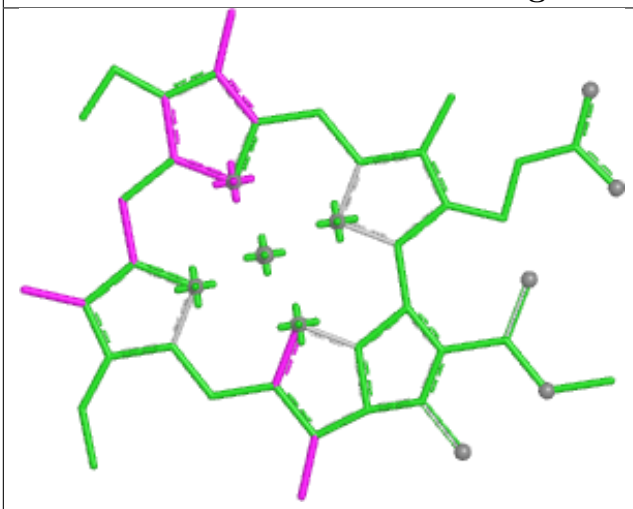


Torsions

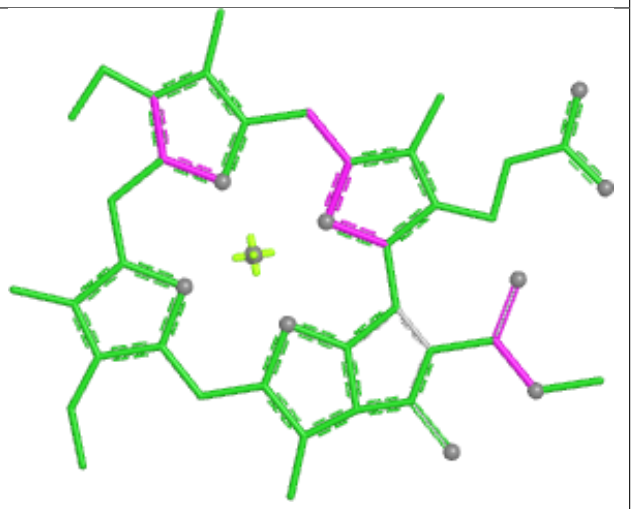


Rings

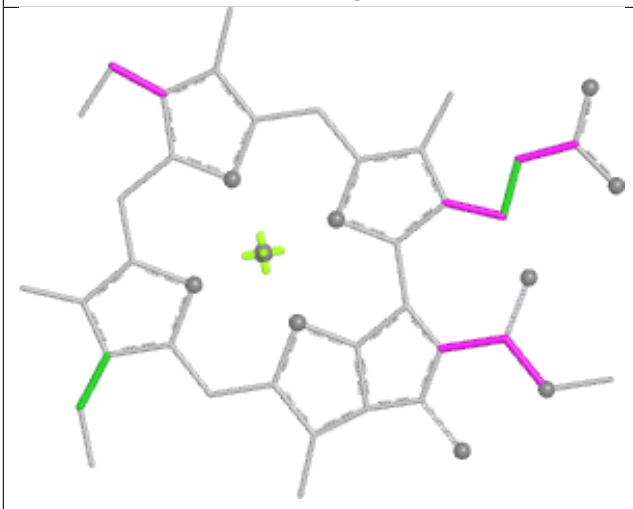
Ligand CLA 6 512



Bond lengths



Bond angles

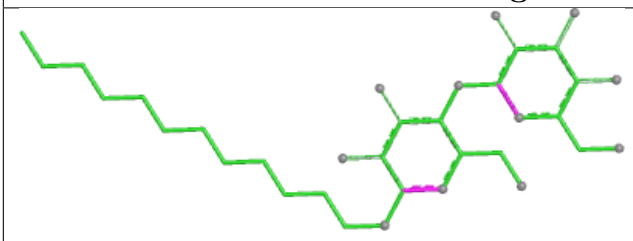


Torsions

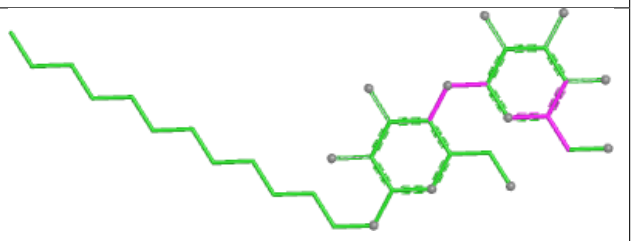


Rings

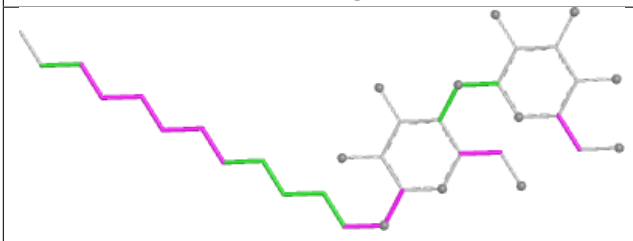
Ligand LMU H 1843



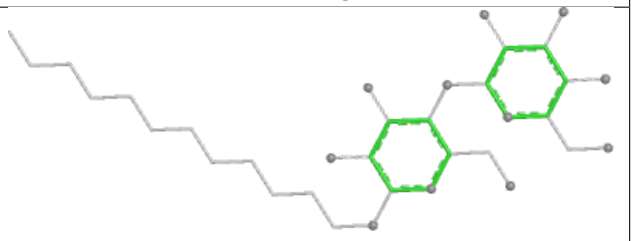
Bond lengths



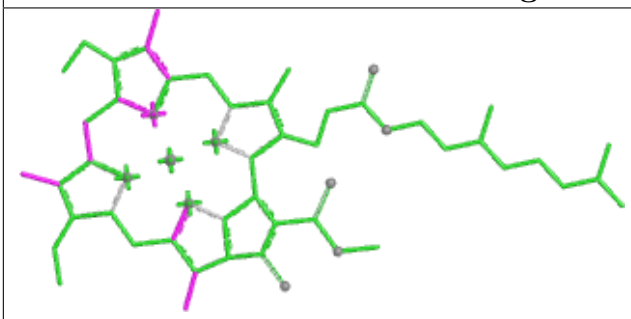
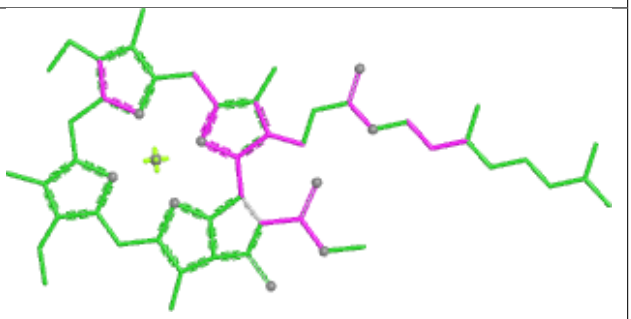
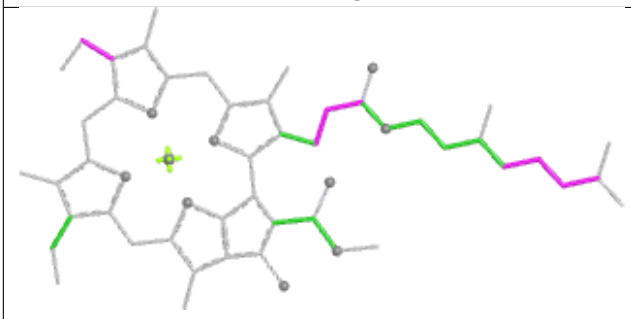
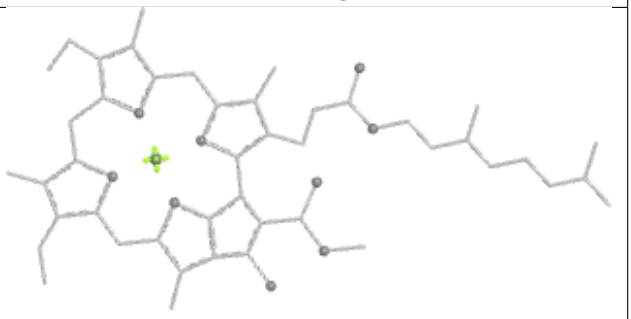
Bond angles

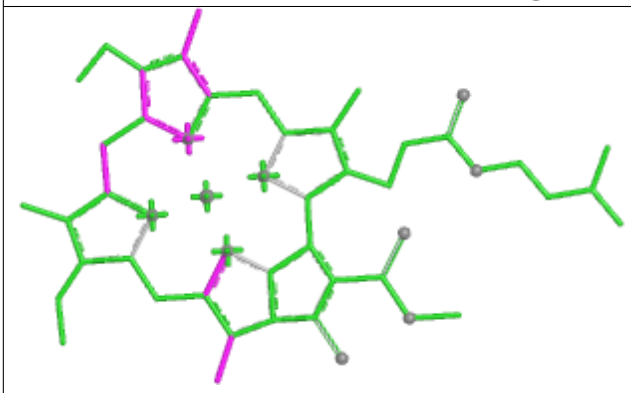
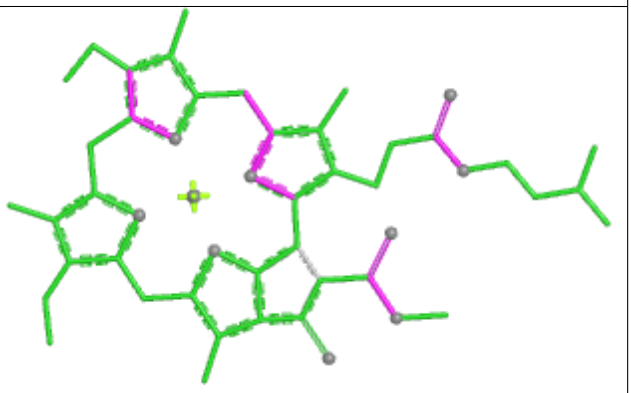
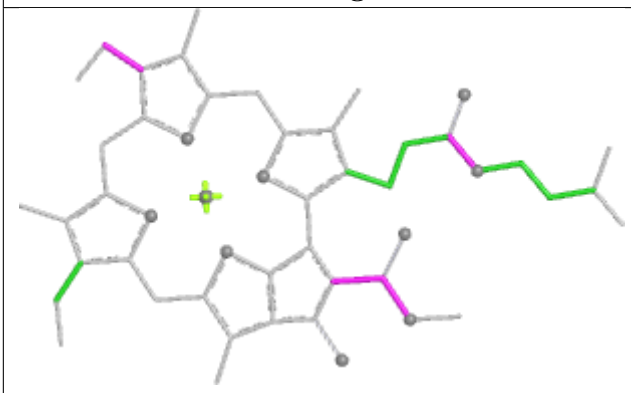
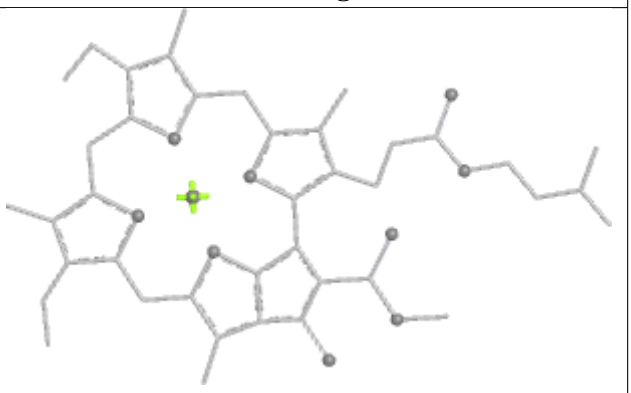


Torsions

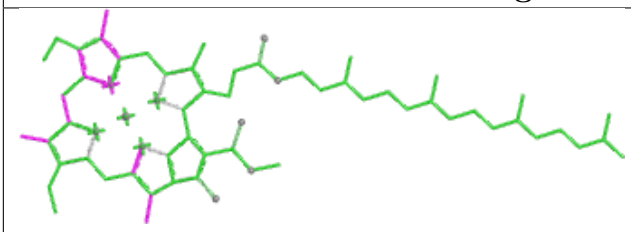


Rings

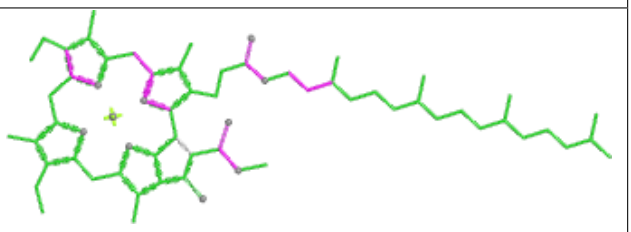
Ligand CLA e 1121	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

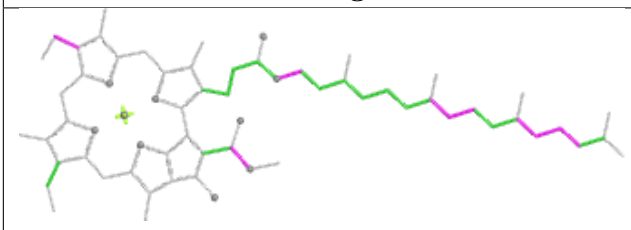
Ligand CLA A 1138



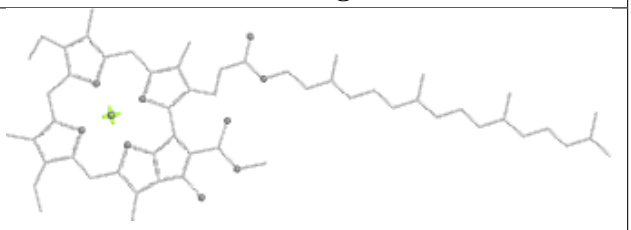
Bond lengths



Bond angles

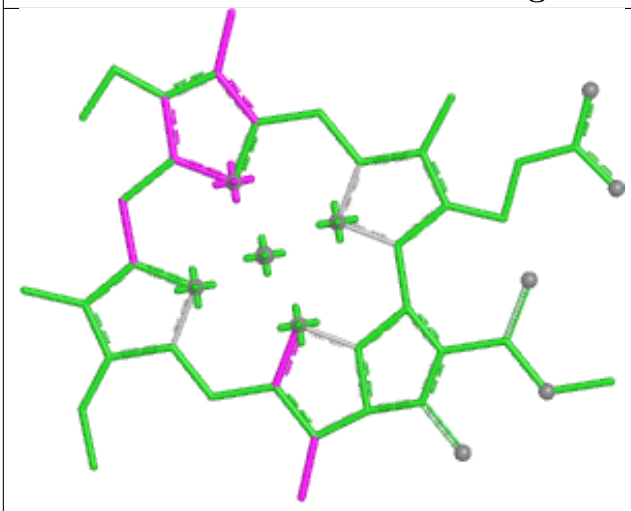


Torsions

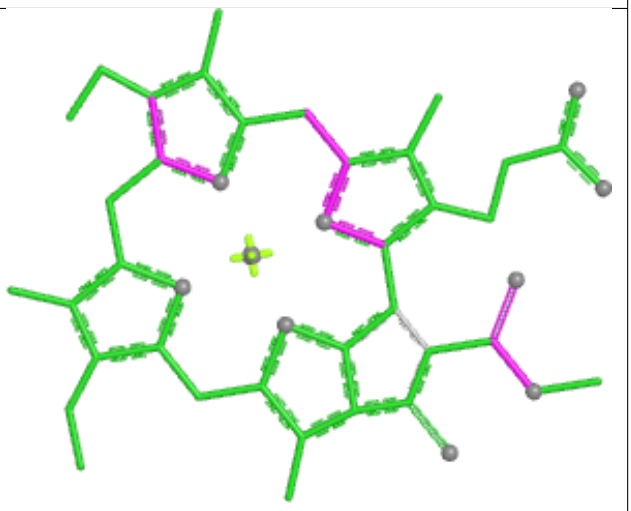


Rings

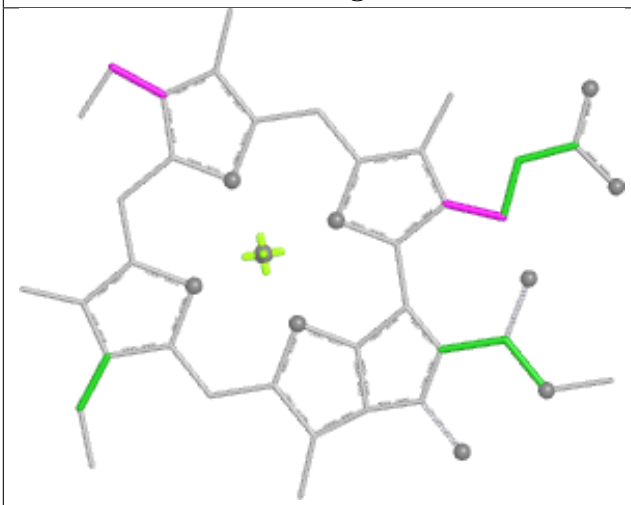
Ligand CLA 5 516



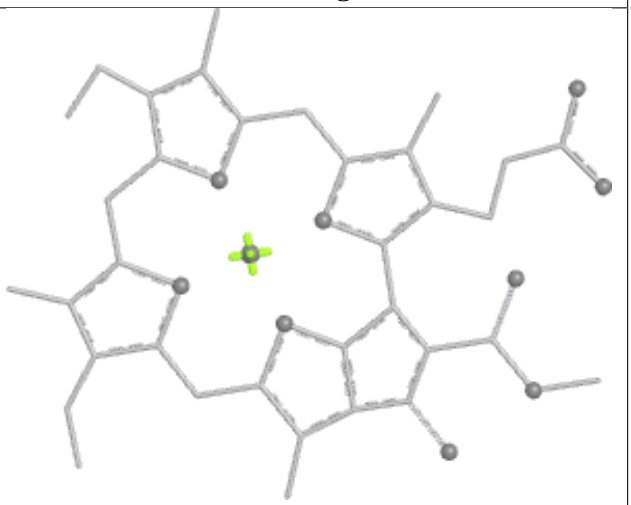
Bond lengths



Bond angles

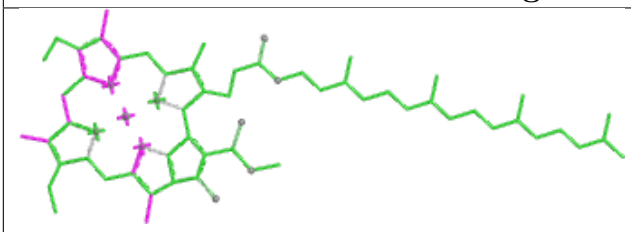


Torsions

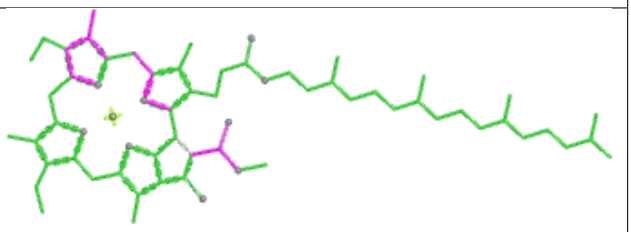


Rings

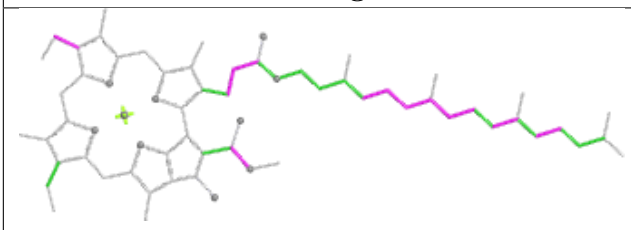
Ligand CLA f 1203



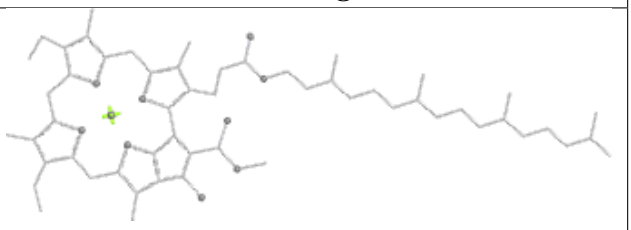
Bond lengths



Bond angles

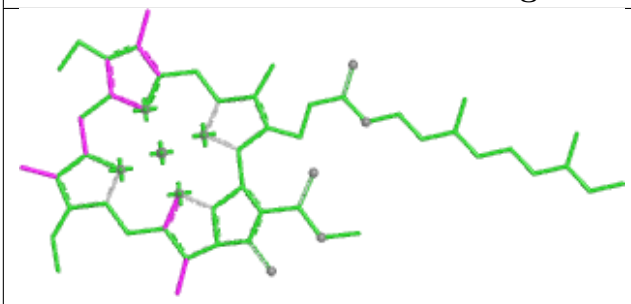


Torsions

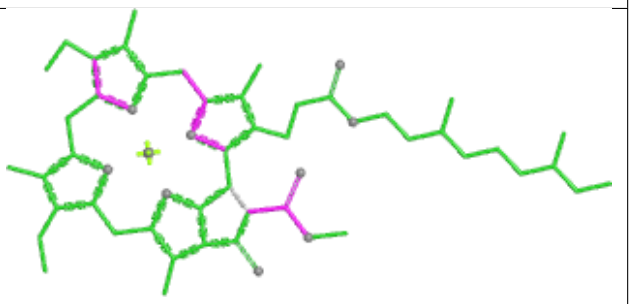


Rings

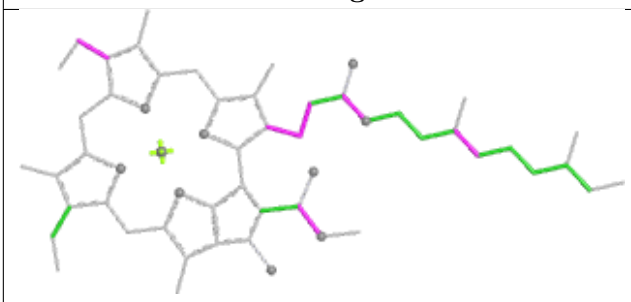
Ligand CLA e 1134



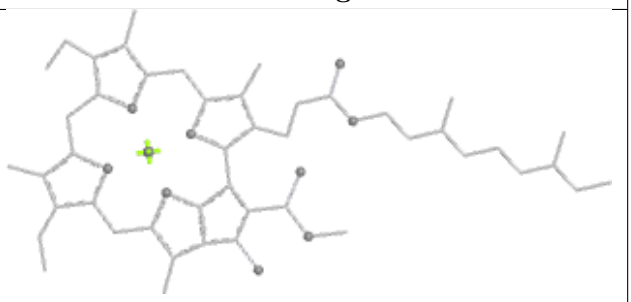
Bond lengths



Bond angles

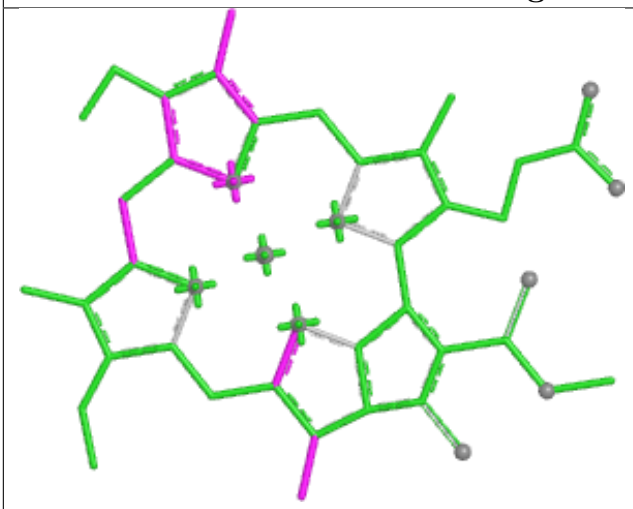


Torsions

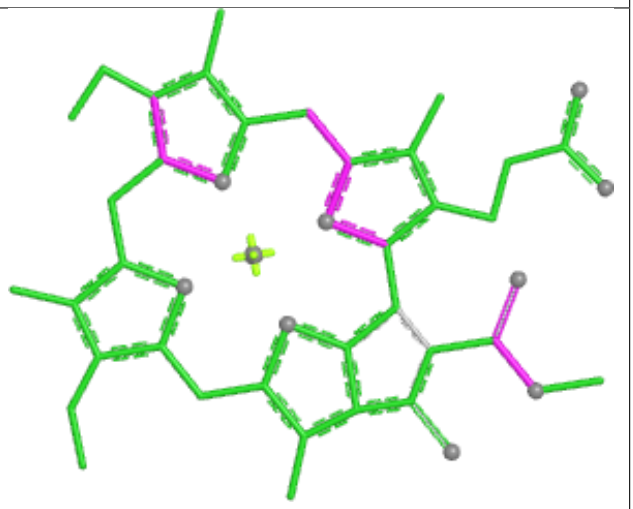


Rings

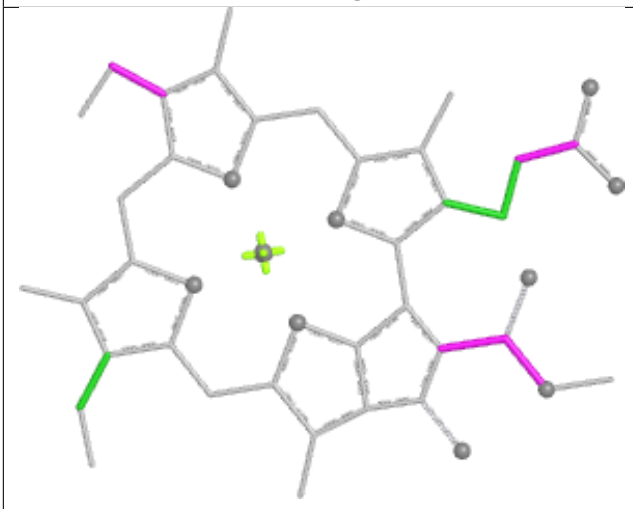
Ligand CLA d 510



Bond lengths



Bond angles

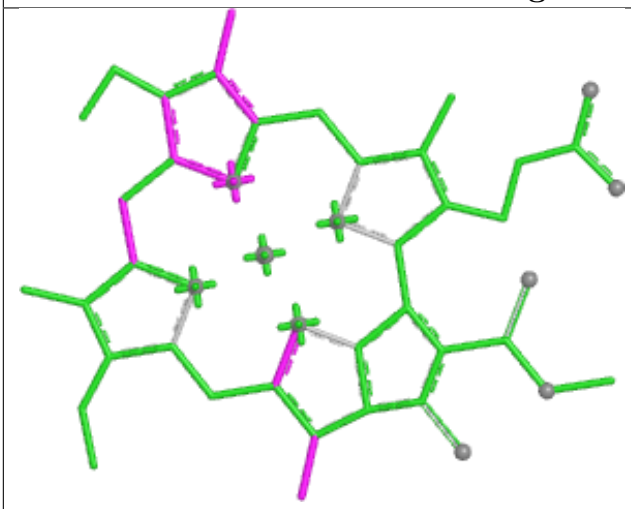


Torsions

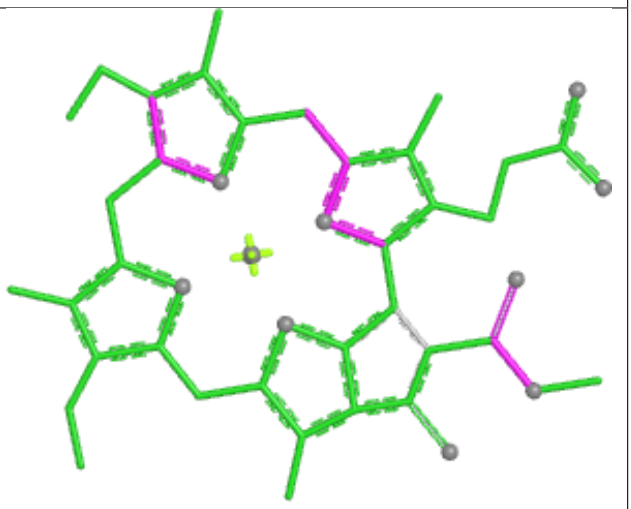


Rings

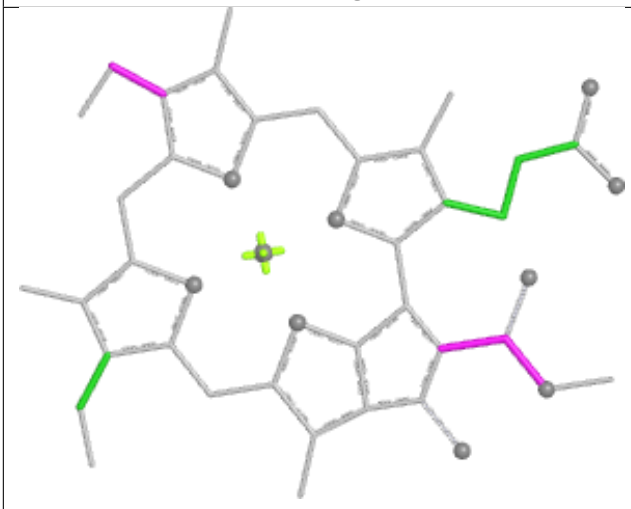
Ligand CLA 4 506



Bond lengths



Bond angles

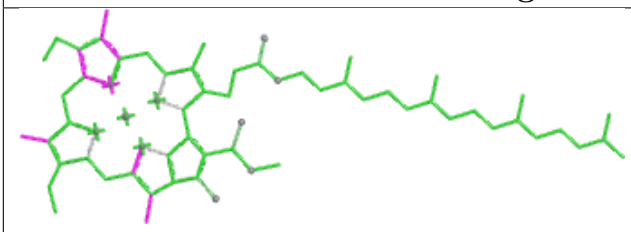


Torsions

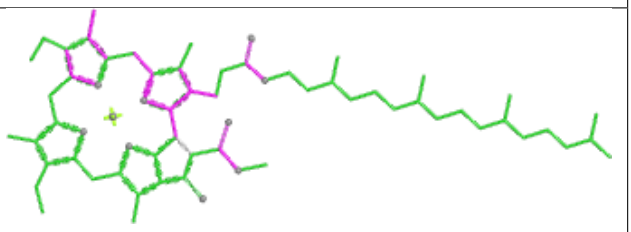


Rings

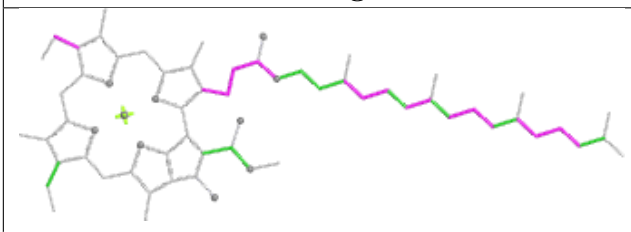
Ligand CLA L 1501



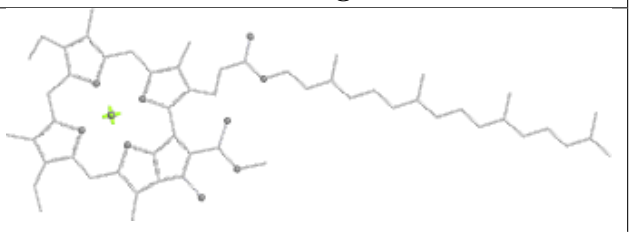
Bond lengths



Bond angles

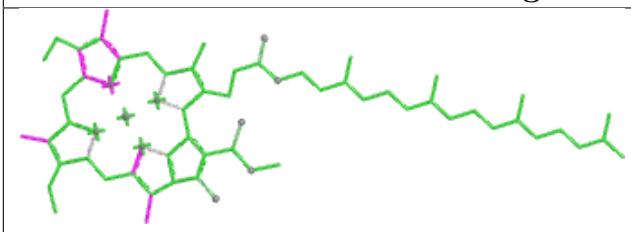


Torsions

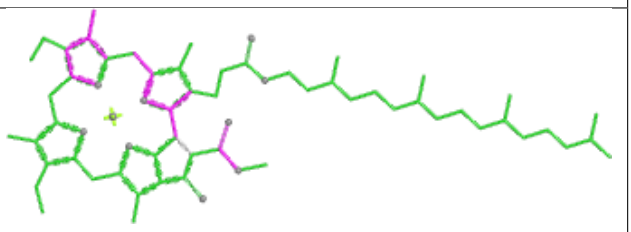


Rings

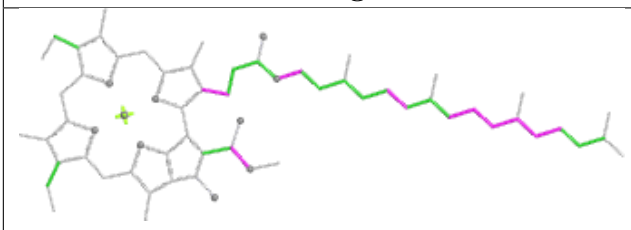
Ligand CLA f 1223



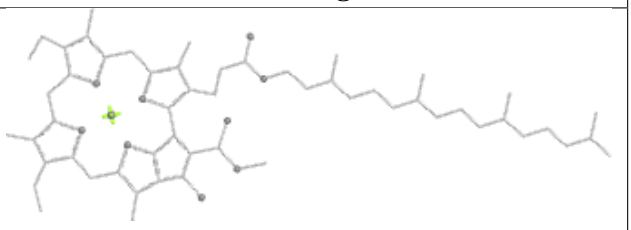
Bond lengths



Bond angles



Torsions



Rings

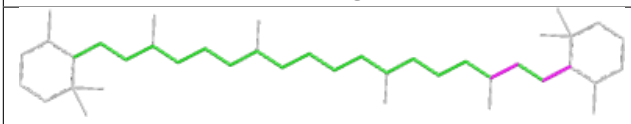
Ligand BCR 3 523



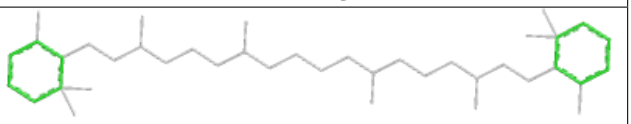
Bond lengths



Bond angles

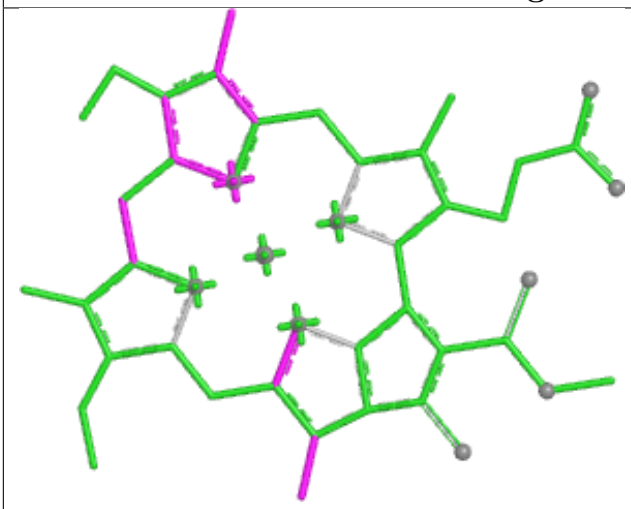


Torsions

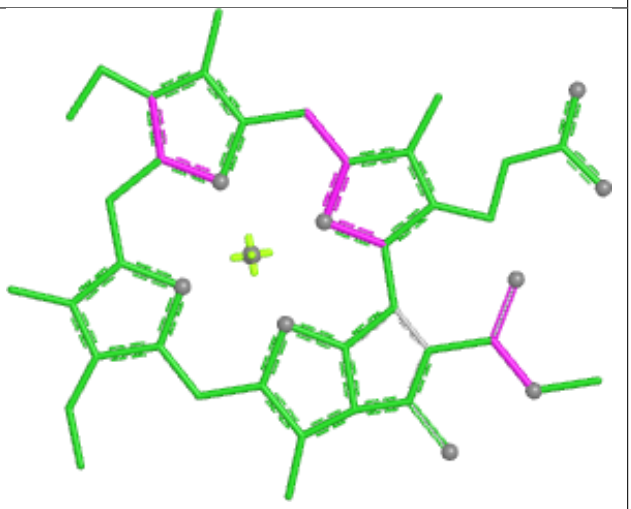


Rings

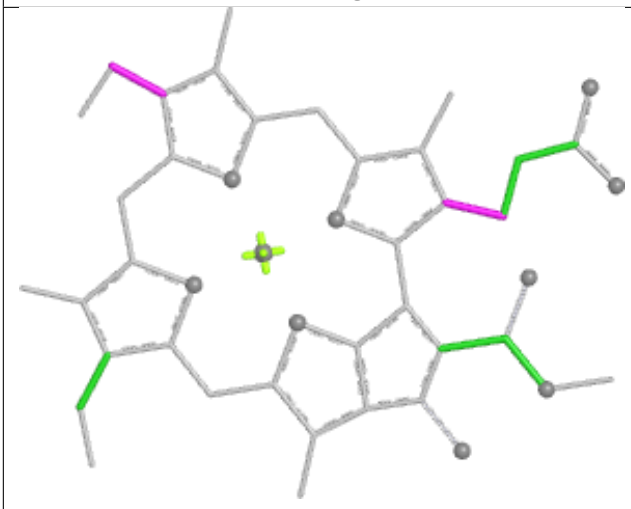
Ligand CLA u 516



Bond lengths



Bond angles

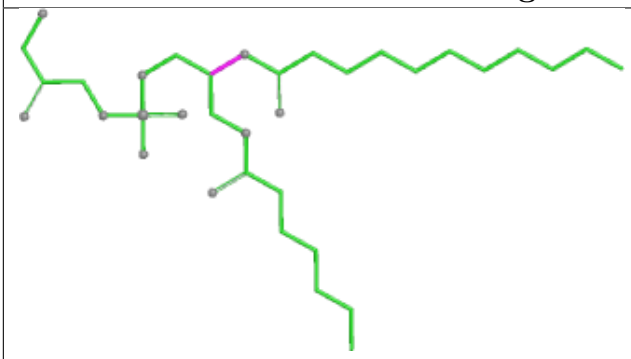


Torsions

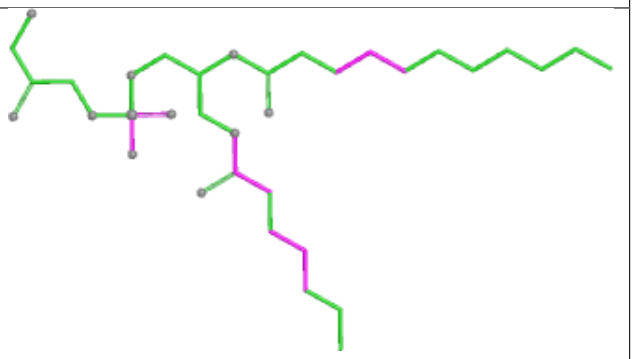


Rings

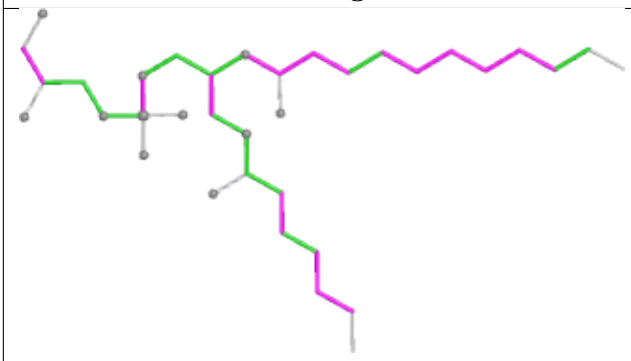
Ligand LHG e 5008



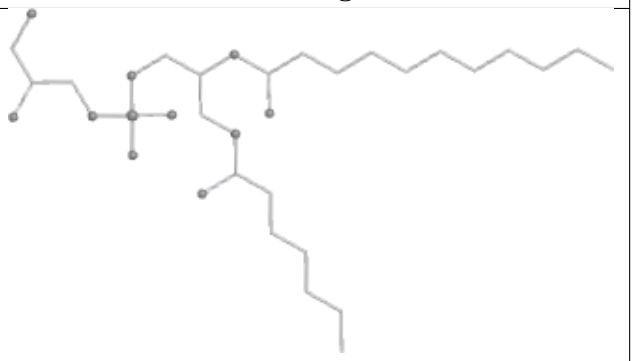
Bond lengths



Bond angles

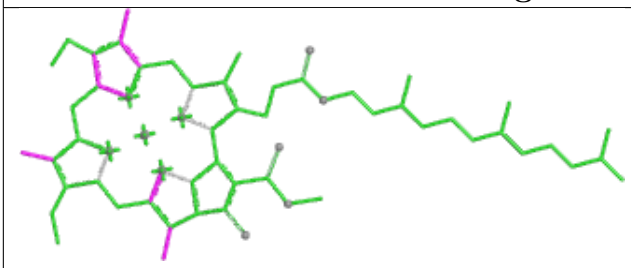


Torsions

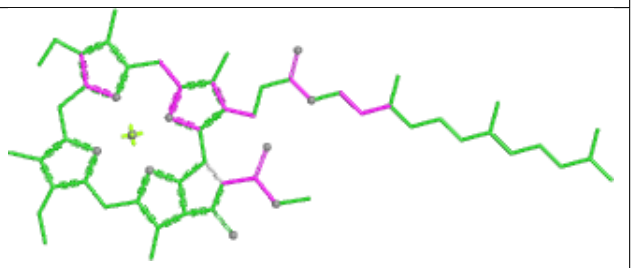


Rings

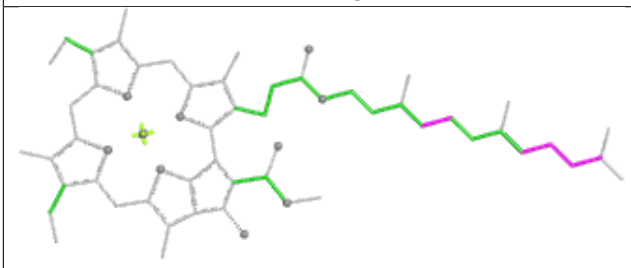
Ligand CLA A 1136



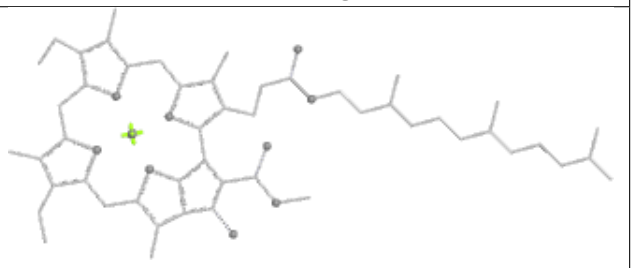
Bond lengths



Bond angles

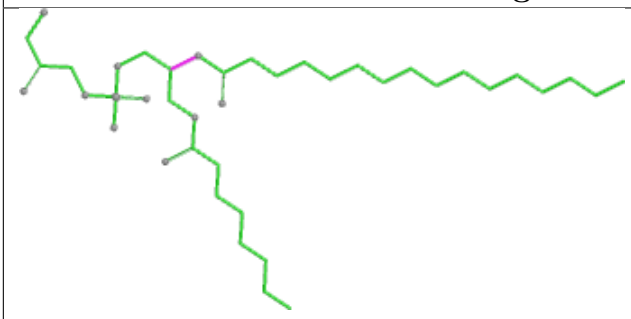


Torsions

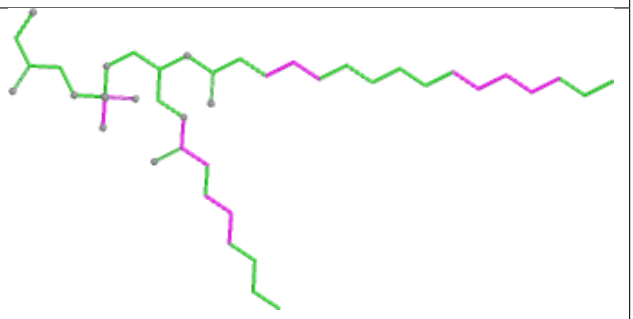


Rings

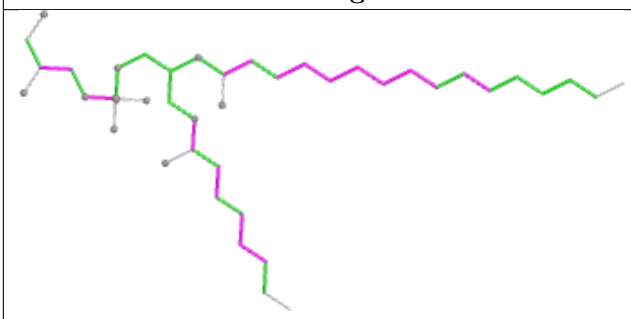
Ligand LHG A 5003



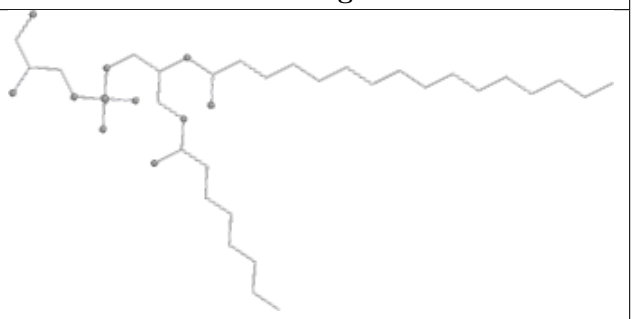
Bond lengths



Bond angles

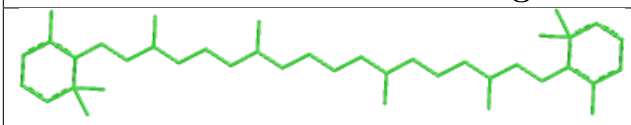


Torsions

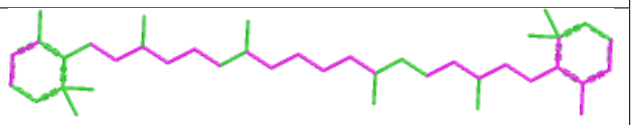


Rings

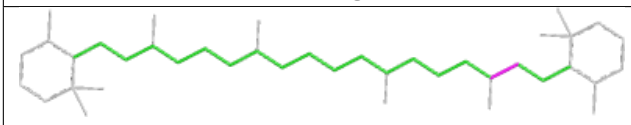
Ligand BCR U 4104



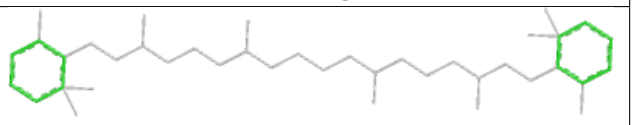
Bond lengths



Bond angles

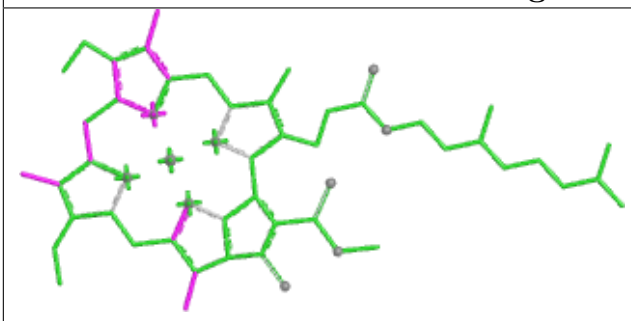


Torsions

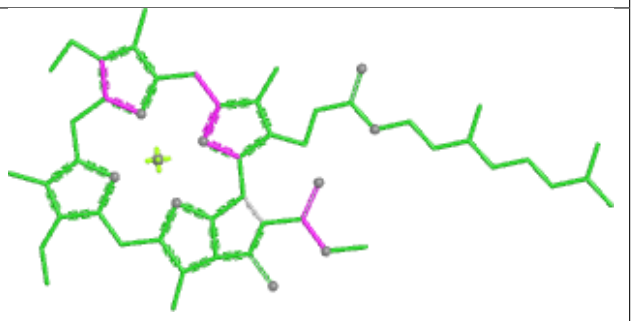


Rings

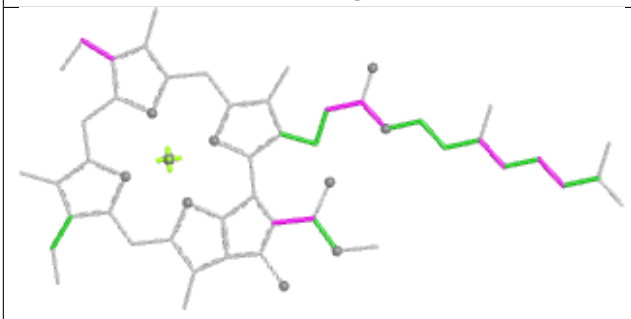
Ligand CLA 4 519



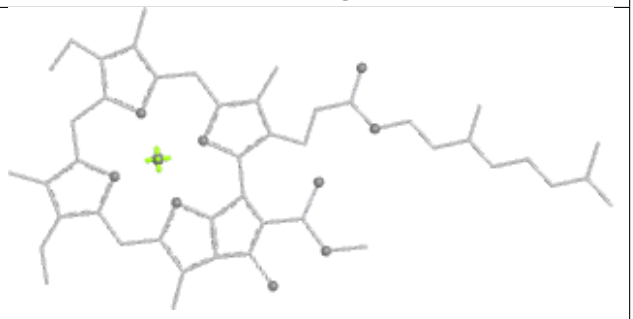
Bond lengths



Bond angles

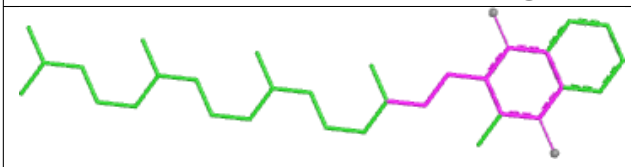


Torsions

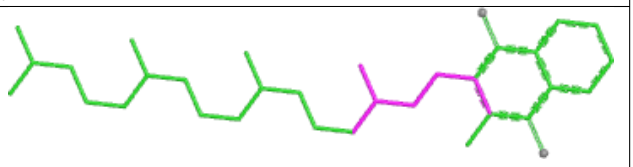


Rings

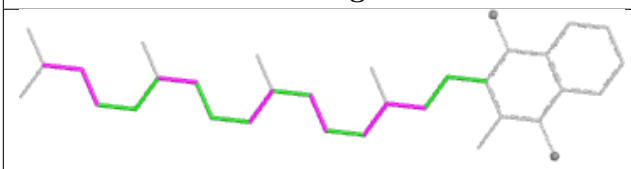
Ligand PQN f 2002



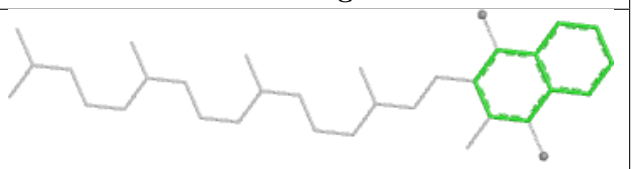
Bond lengths



Bond angles

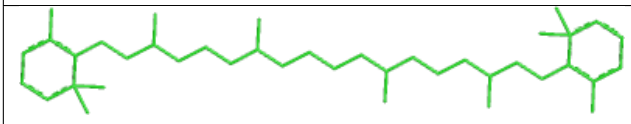


Torsions

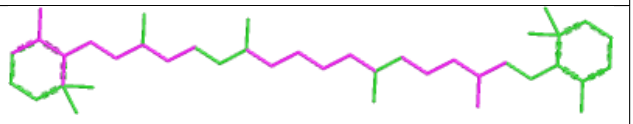


Rings

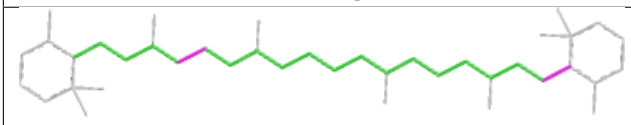
Ligand BCR 2 524



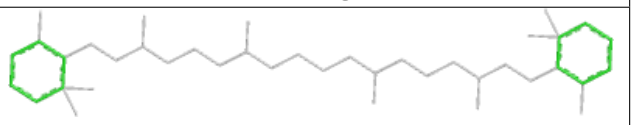
Bond lengths



Bond angles

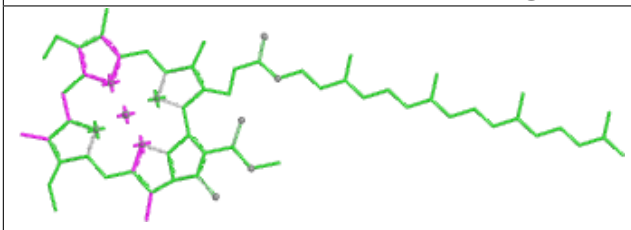


Torsions

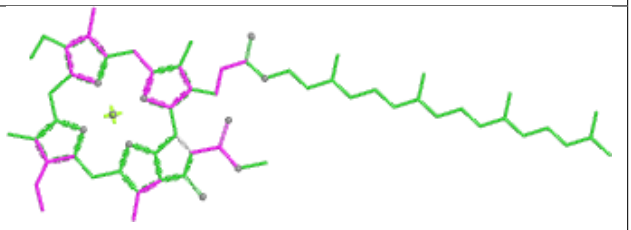


Rings

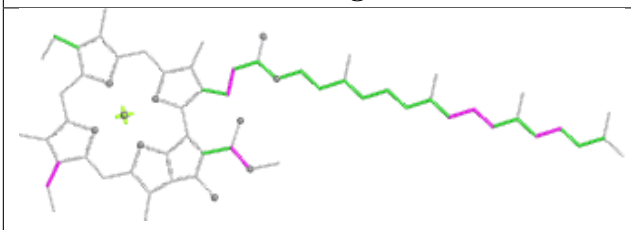
Ligand CLA f 1023



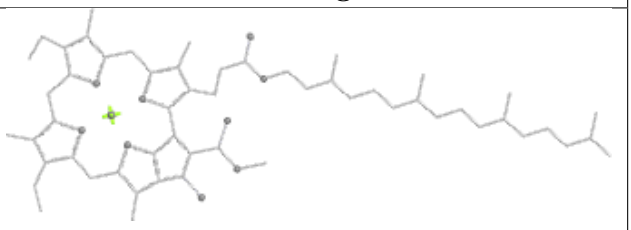
Bond lengths



Bond angles

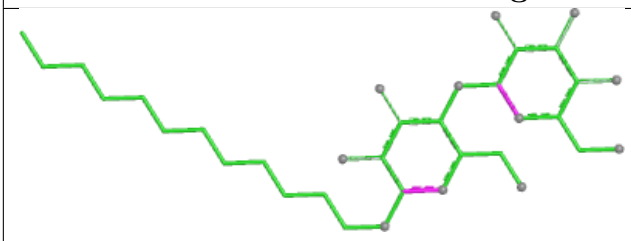


Torsions

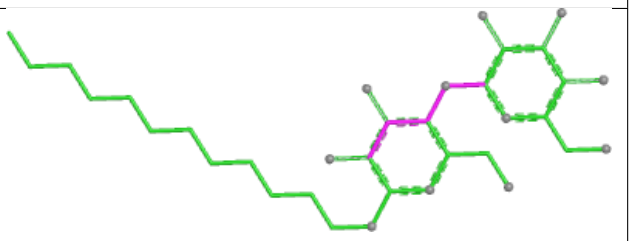


Rings

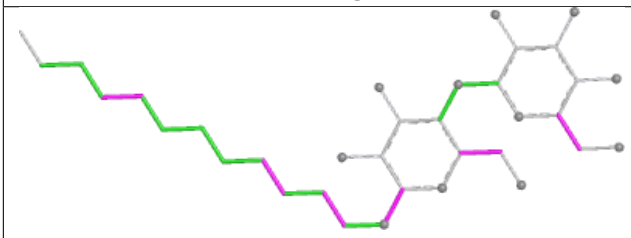
Ligand LMU A 1848



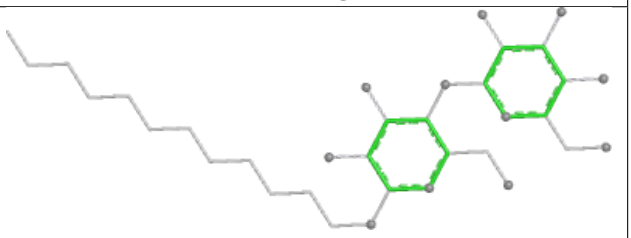
Bond lengths



Bond angles

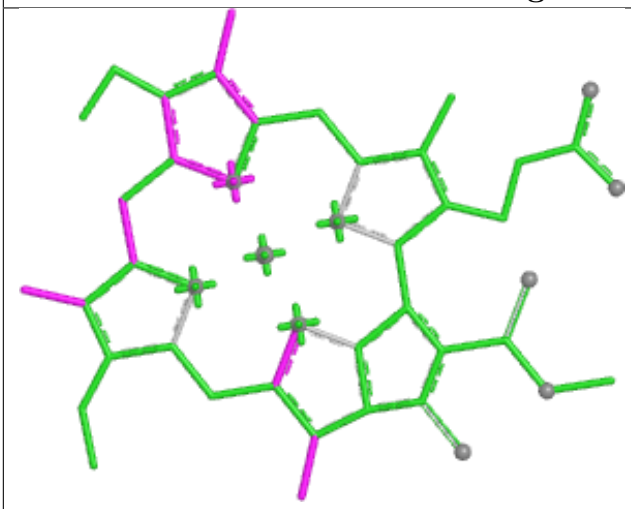


Torsions

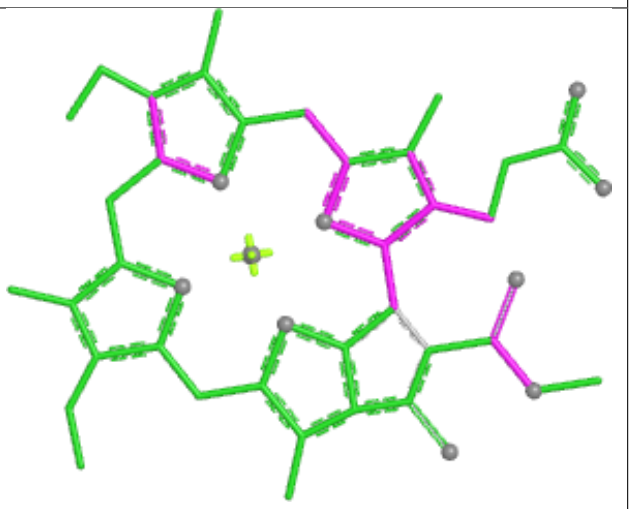


Rings

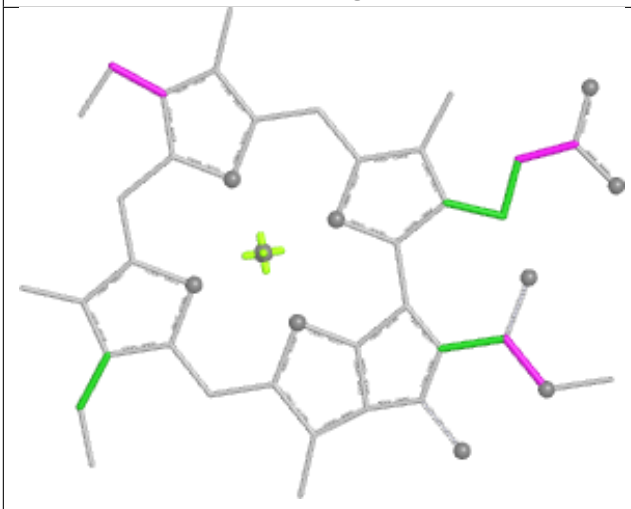
Ligand CLA d 507



Bond lengths



Bond angles

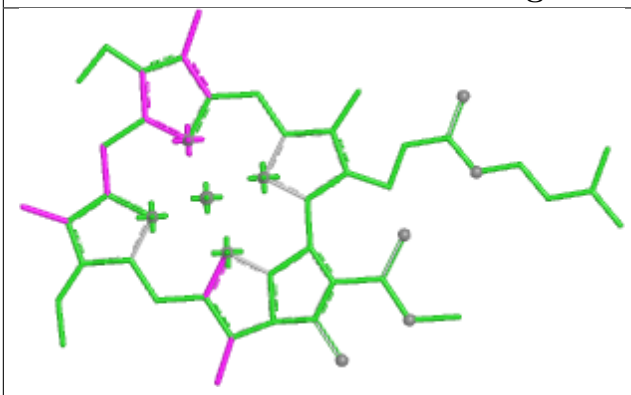


Torsions

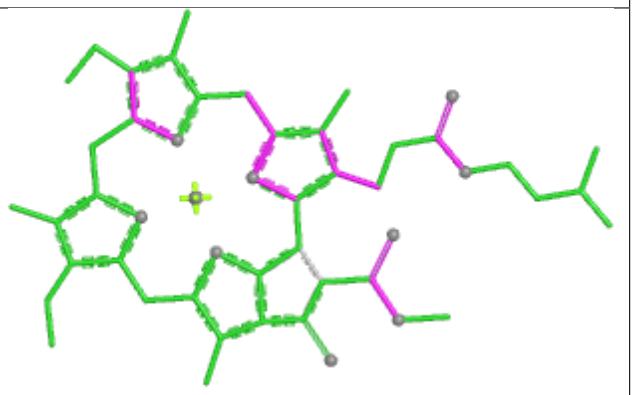


Rings

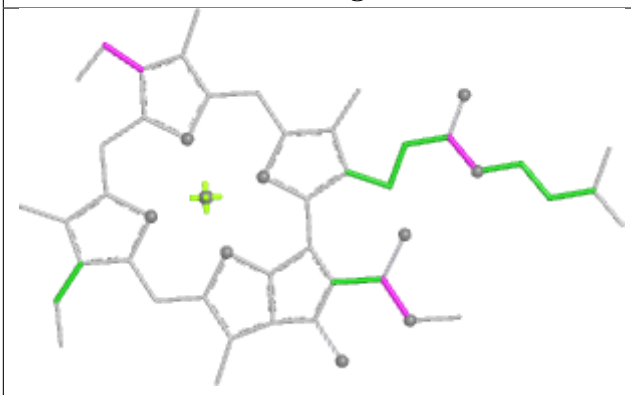
Ligand CLA Z 504



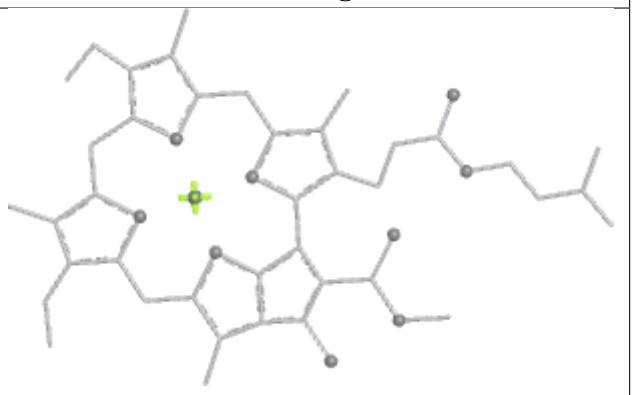
Bond lengths



Bond angles

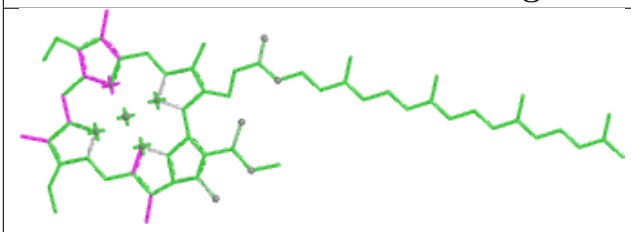


Torsions

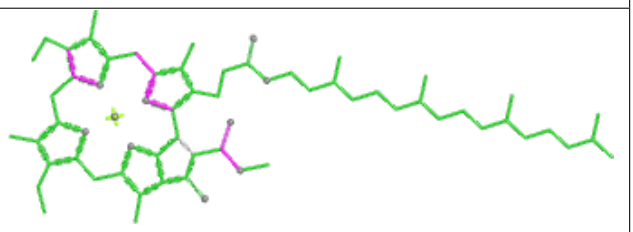


Rings

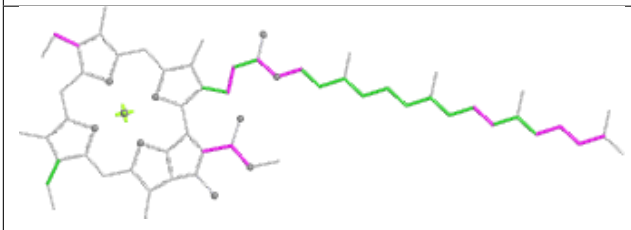
Ligand CLA f 1207



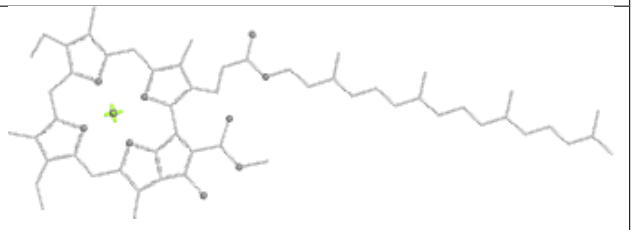
Bond lengths



Bond angles

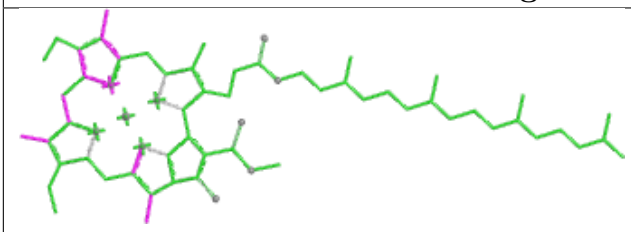


Torsions

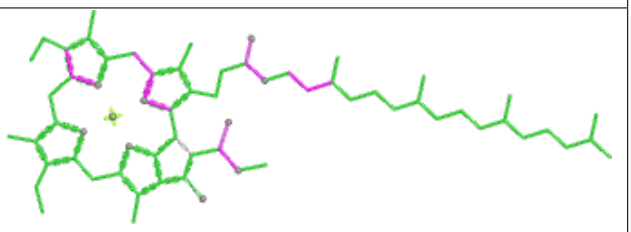


Rings

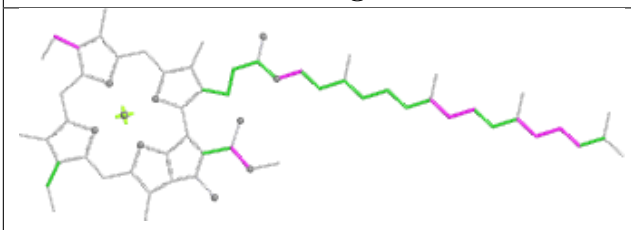
Ligand CLA e 1138



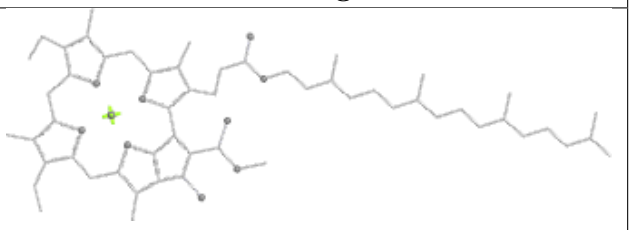
Bond lengths



Bond angles

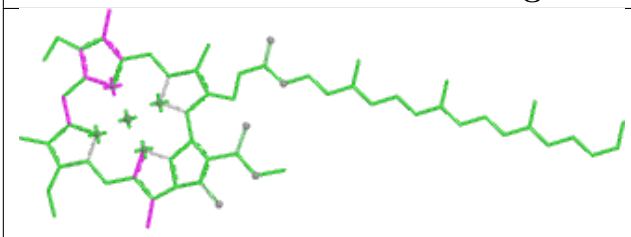


Torsions

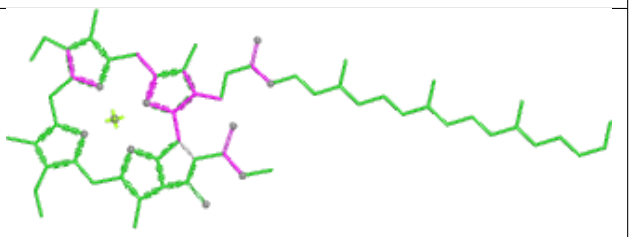


Rings

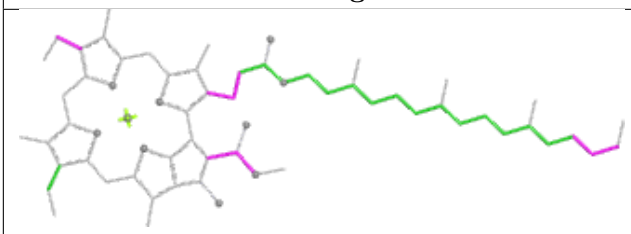
Ligand CLA Y 503



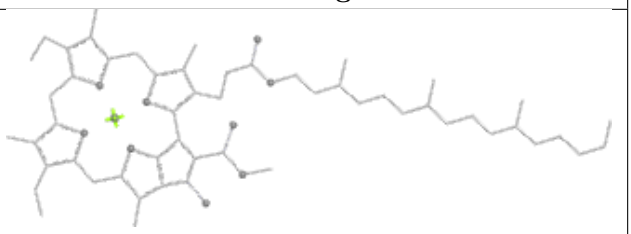
Bond lengths



Bond angles

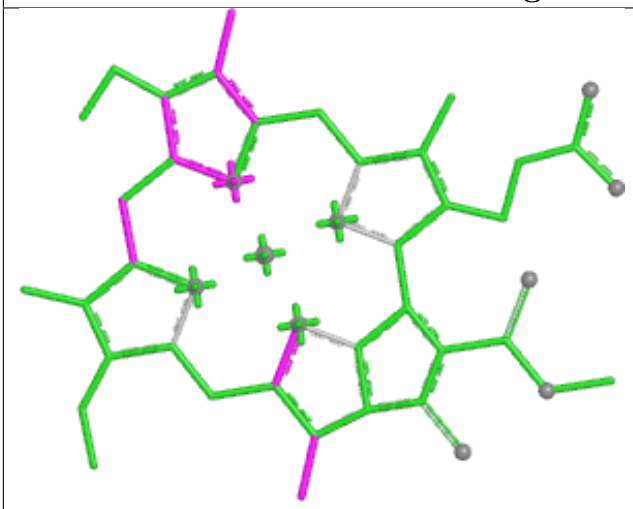


Torsions

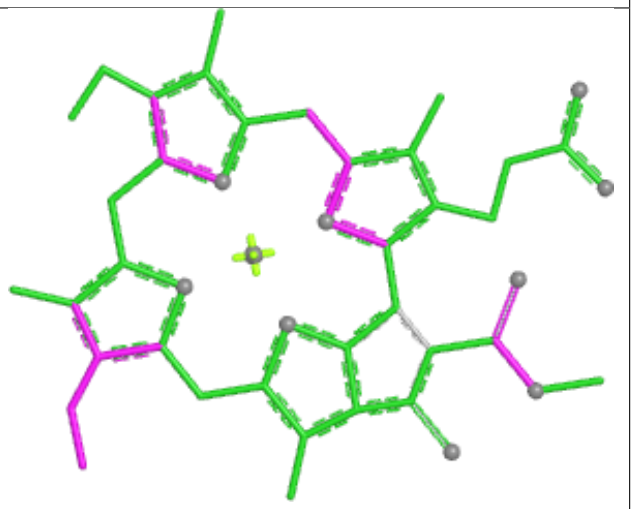


Rings

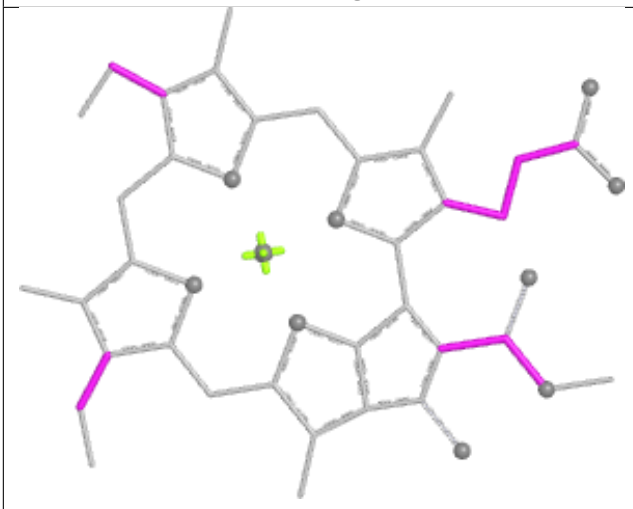
Ligand CLA Y 516



Bond lengths



Bond angles

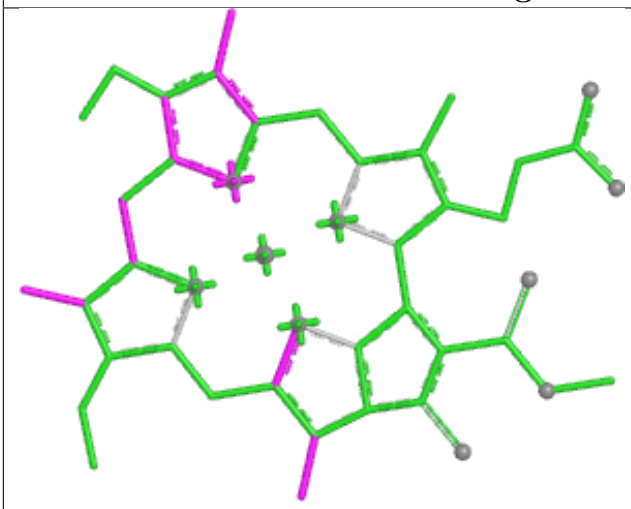


Torsions

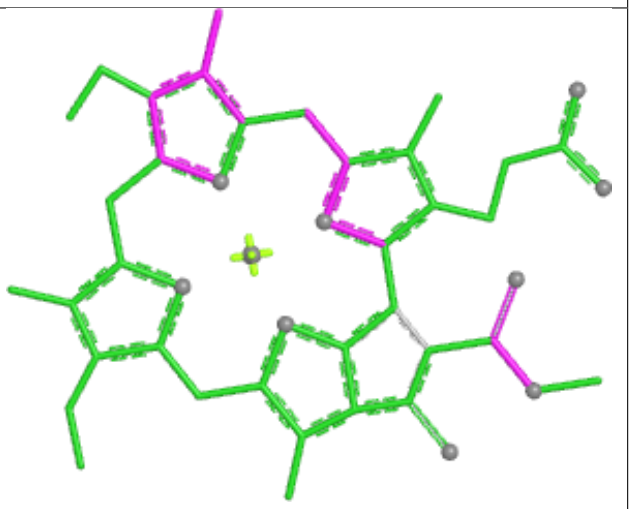


Rings

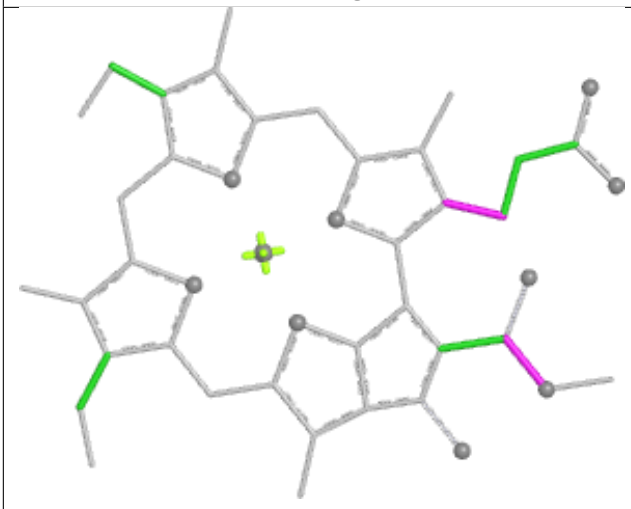
Ligand CLA A 1113



Bond lengths



Bond angles

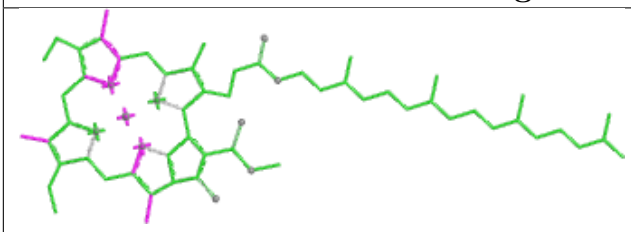


Torsions

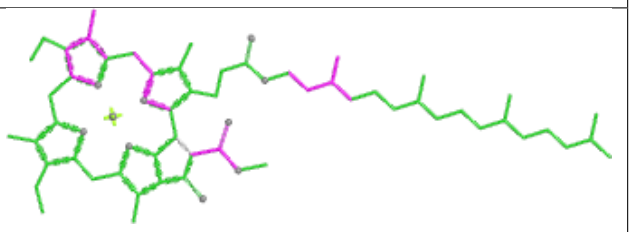


Rings

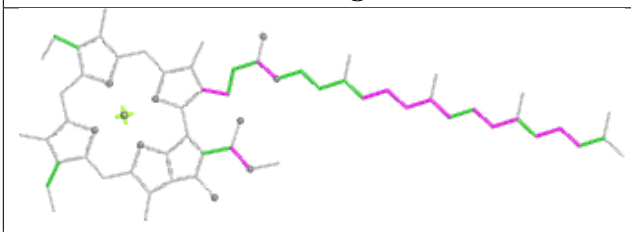
Ligand CLA H 1215



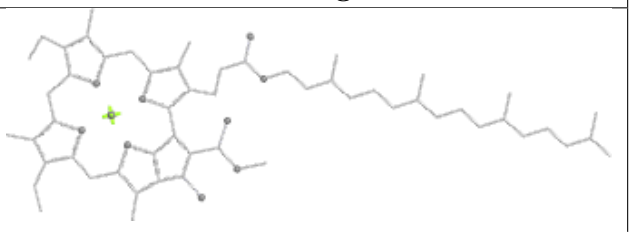
Bond lengths



Bond angles

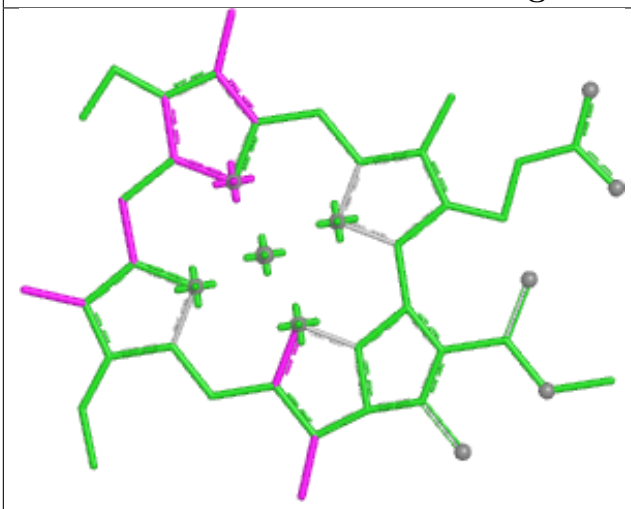


Torsions

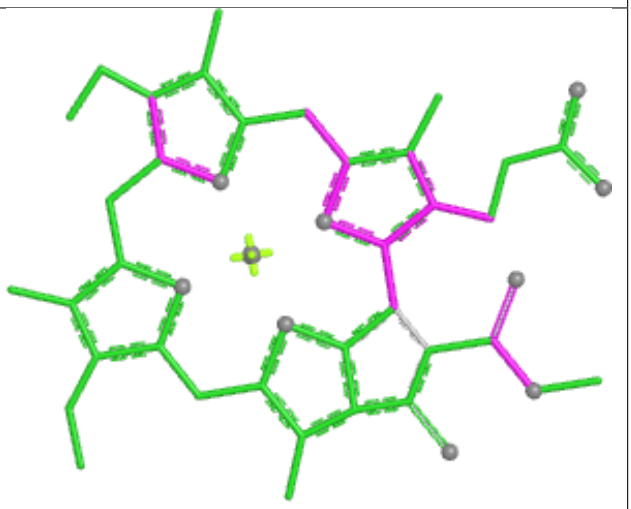


Rings

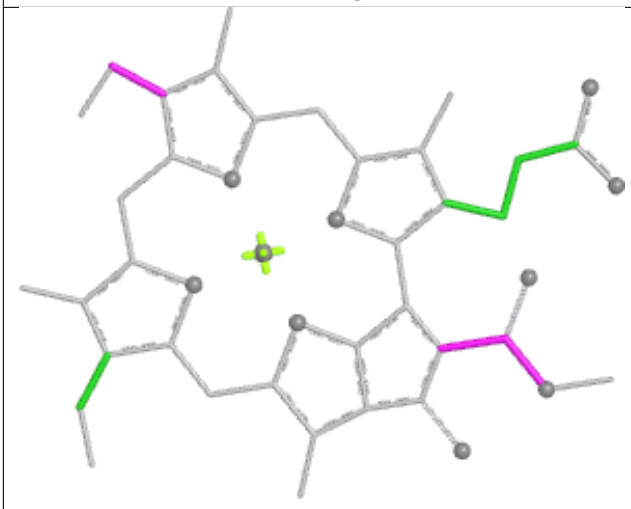
Ligand CLA 1 504



Bond lengths



Bond angles

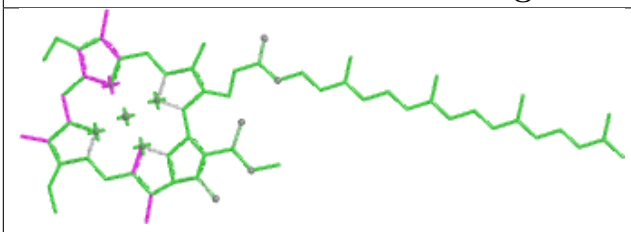


Torsions

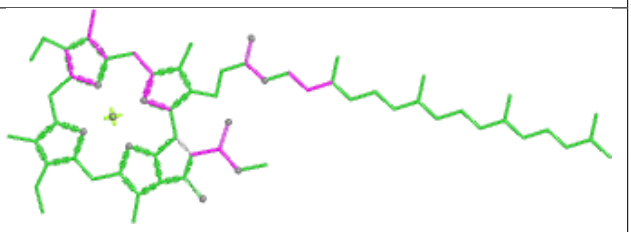


Rings

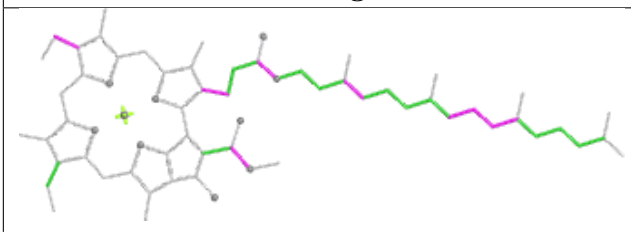
Ligand CLA H 1240



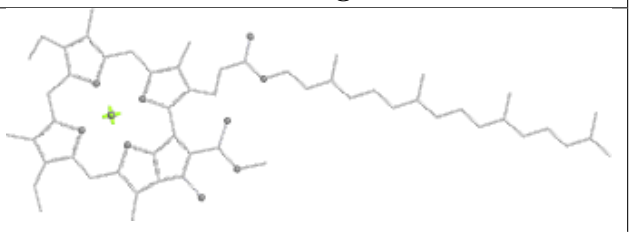
Bond lengths



Bond angles

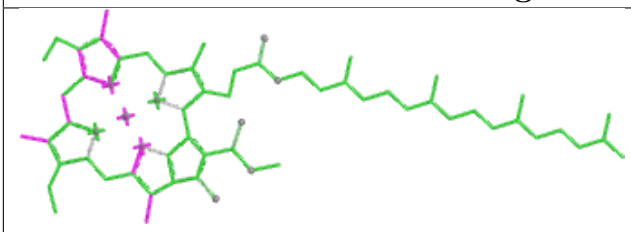


Torsions

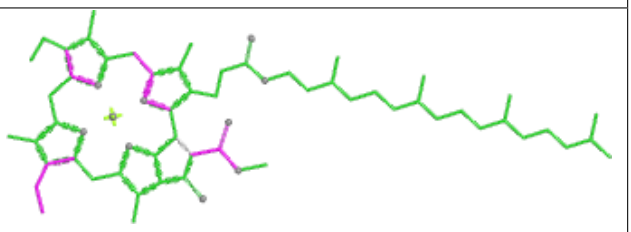


Rings

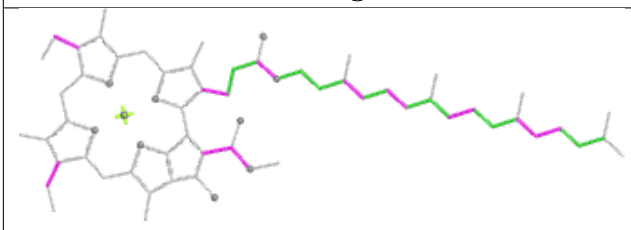
Ligand CLA A 1132



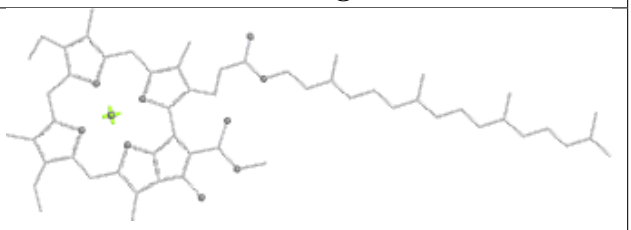
Bond lengths



Bond angles

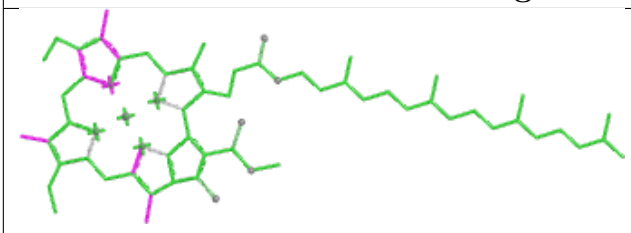


Torsions

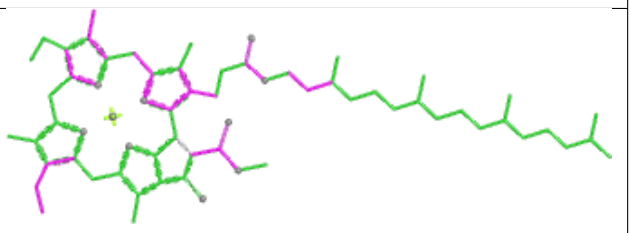


Rings

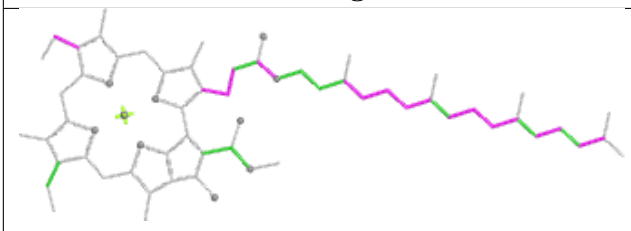
Ligand CLA H 1210



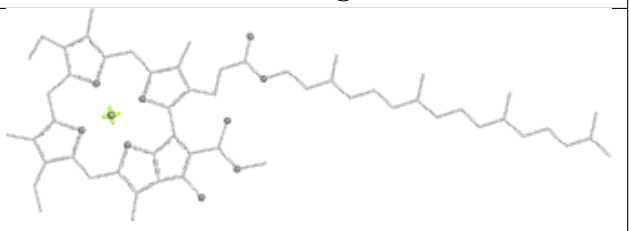
Bond lengths



Bond angles

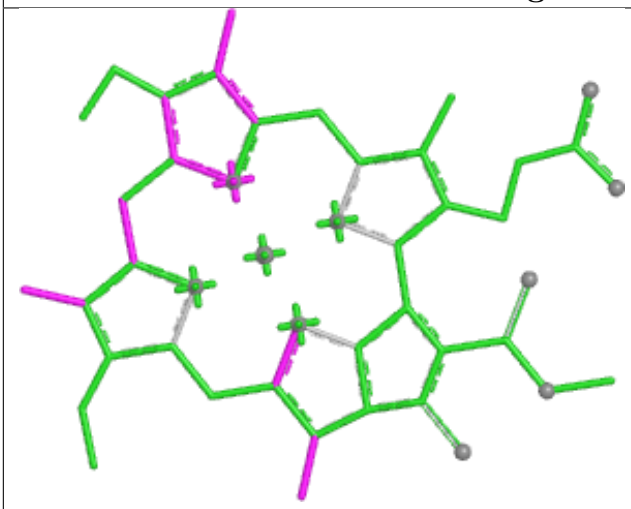


Torsions

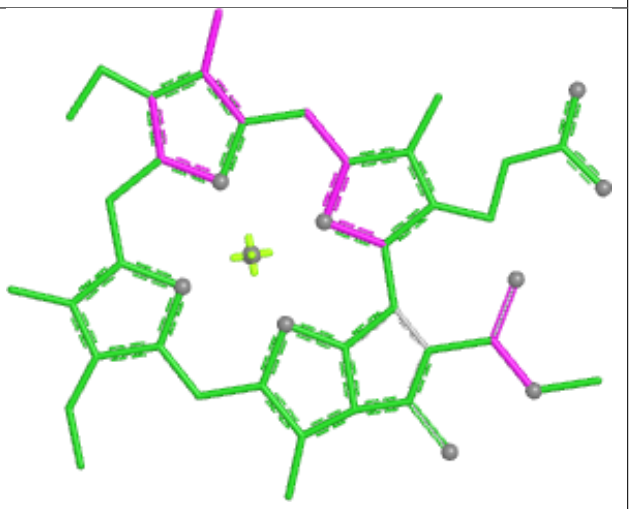


Rings

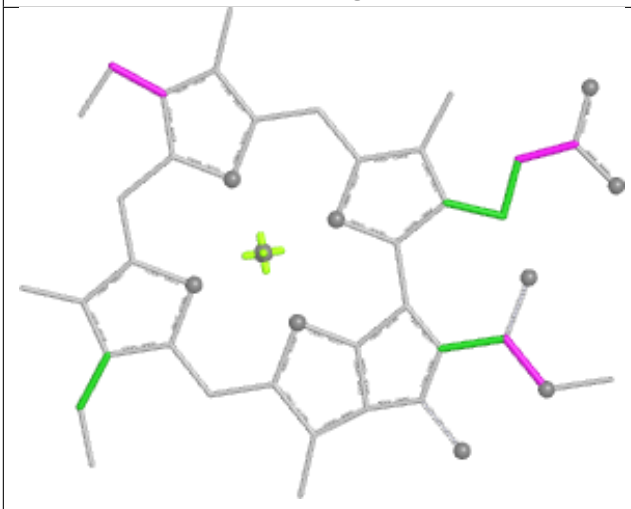
Ligand CLA u 508



Bond lengths



Bond angles

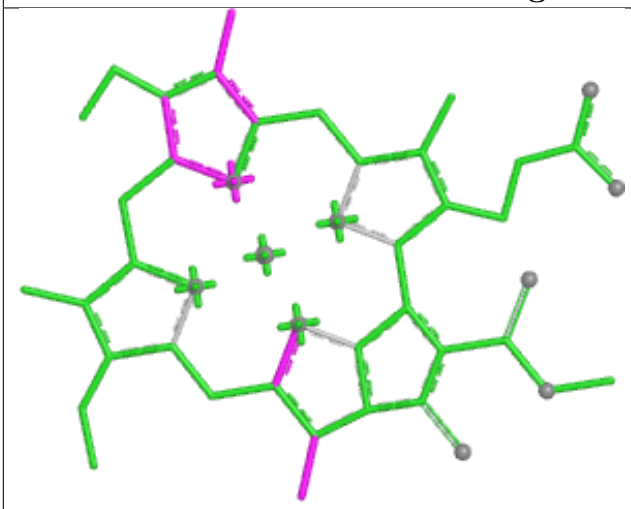


Torsions

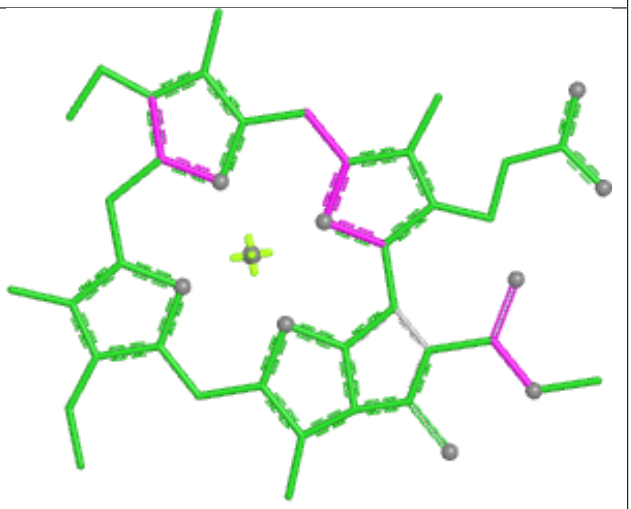


Rings

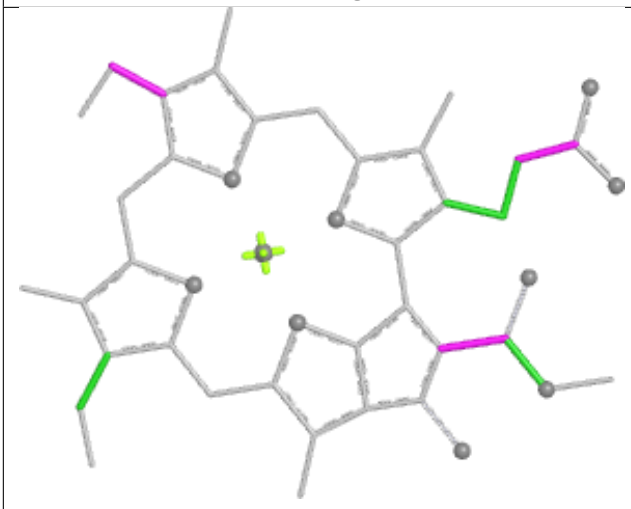
Ligand CLA 4 512



Bond lengths



Bond angles

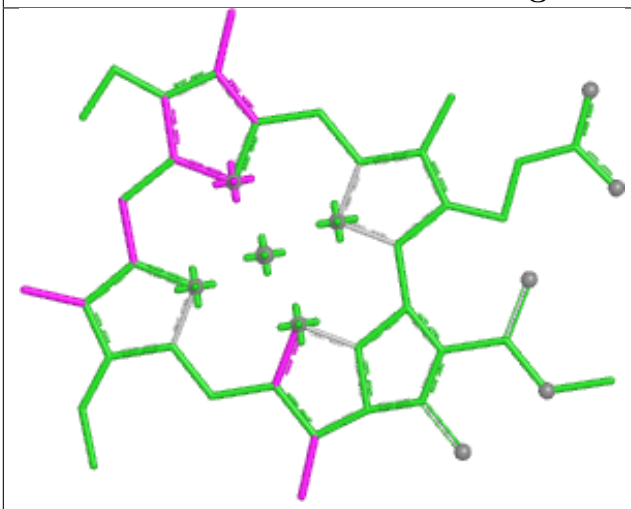


Torsions

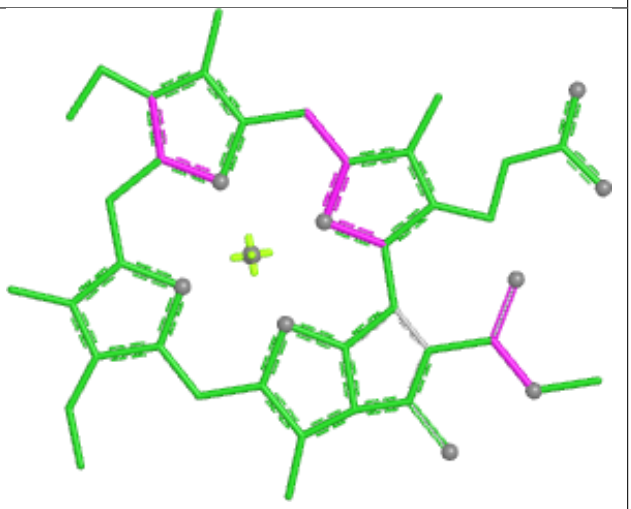


Rings

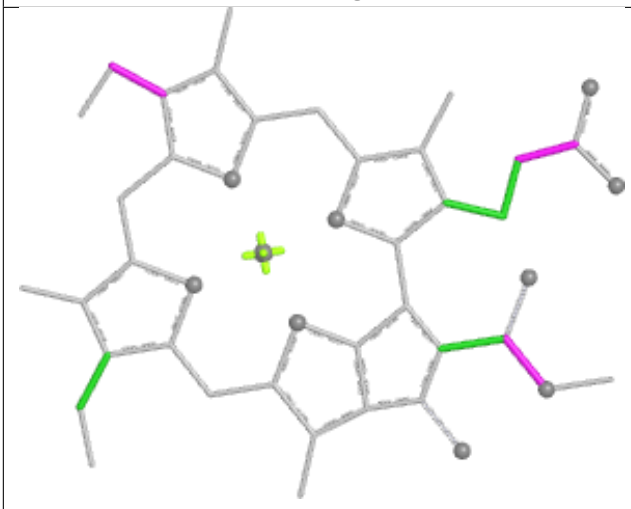
Ligand CLA c 513



Bond lengths



Bond angles

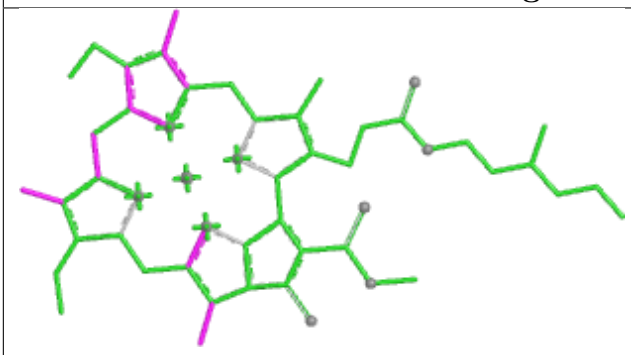


Torsions

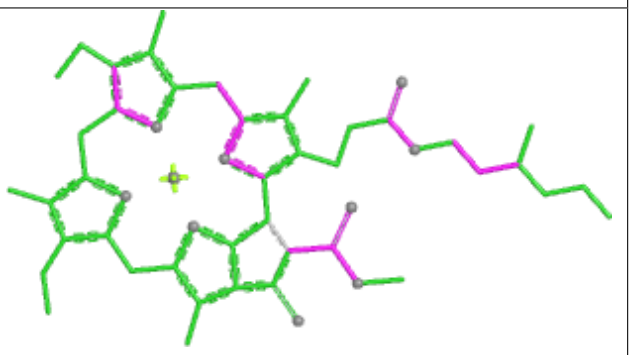


Rings

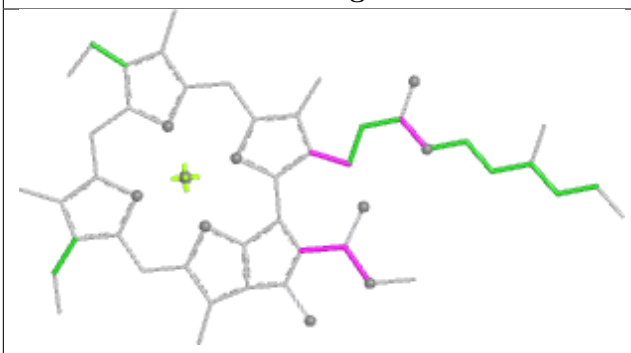
Ligand CLA f 1209



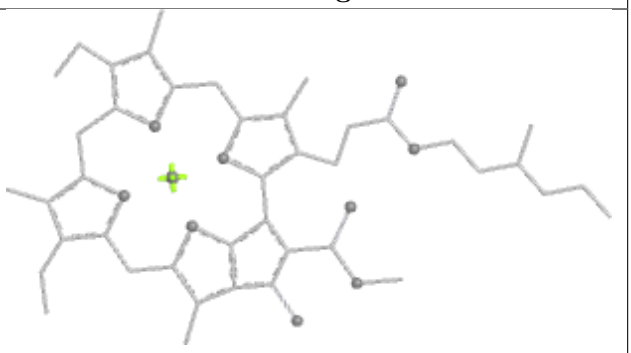
Bond lengths



Bond angles

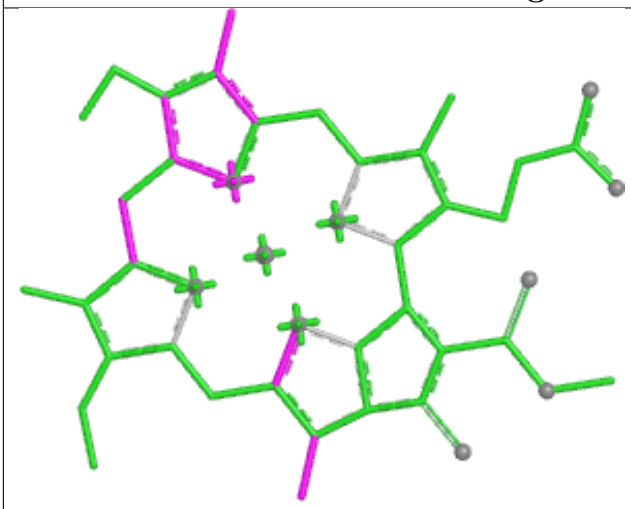


Torsions

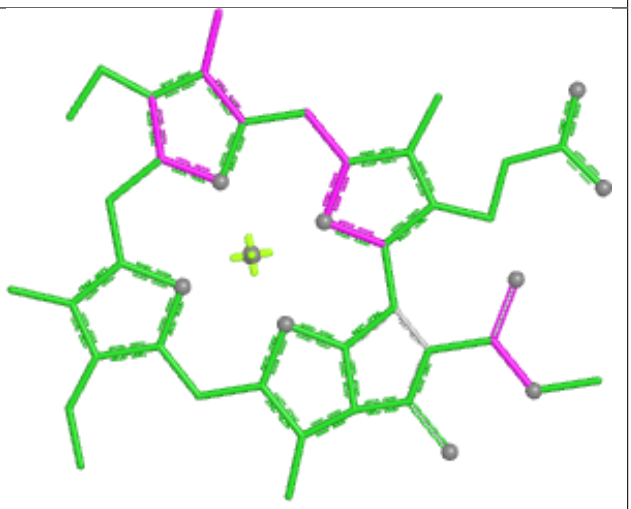


Rings

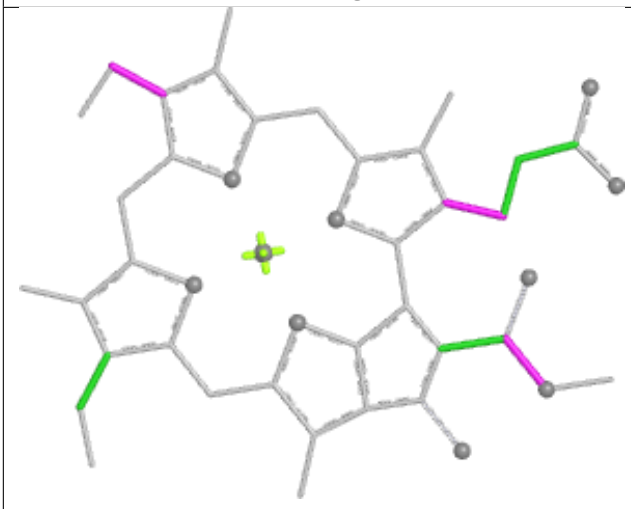
Ligand CLA b 511



Bond lengths



Bond angles

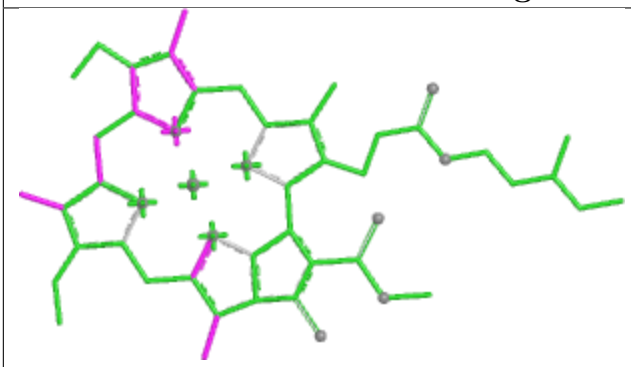


Torsions

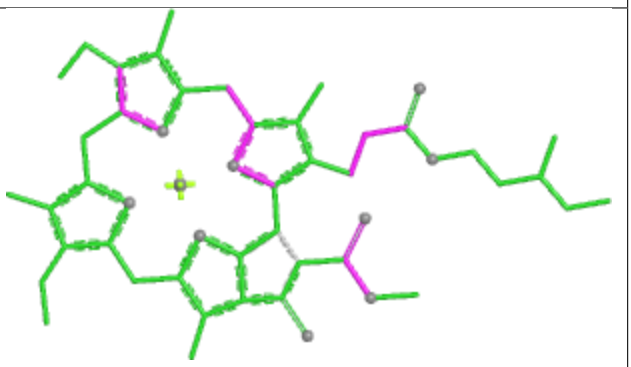


Rings

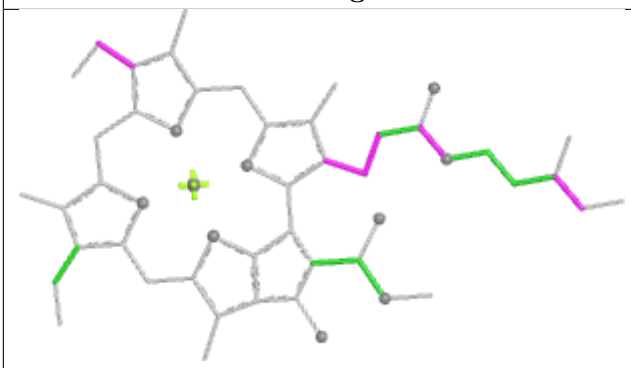
Ligand CLA G 1110



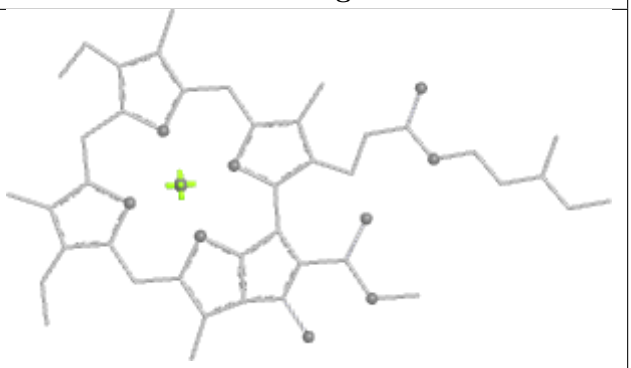
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9995. These allow visual inspection of the internal detail of the map and identification of artifacts.

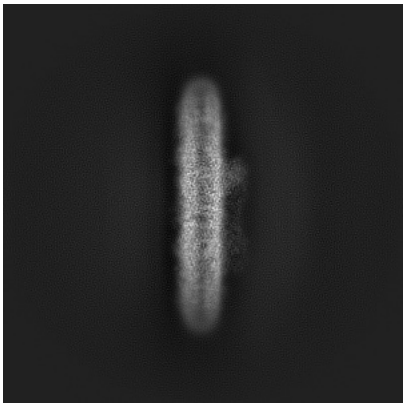
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

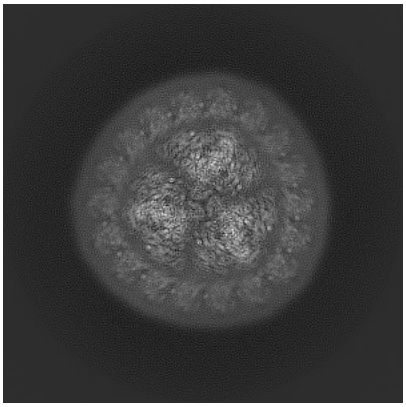
6.1.1 Primary map



X



Y

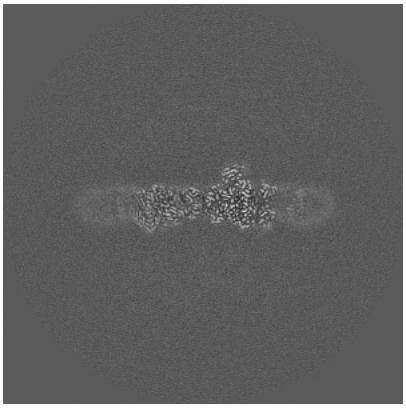


Z

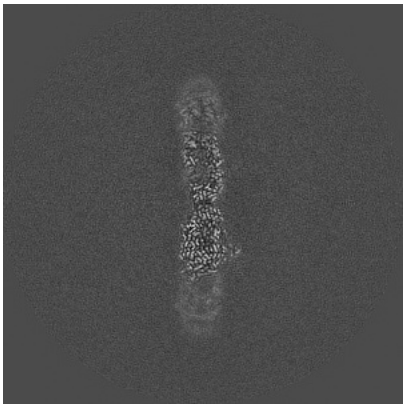
The images above show the map projected in three orthogonal directions.

6.2 Central slices

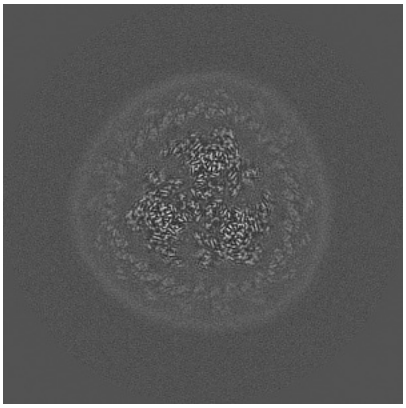
6.2.1 Primary map



X Index: 240



Y Index: 240

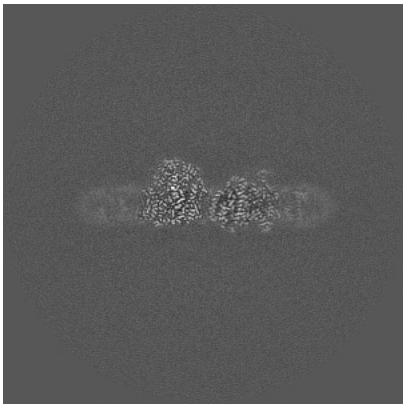


Z Index: 240

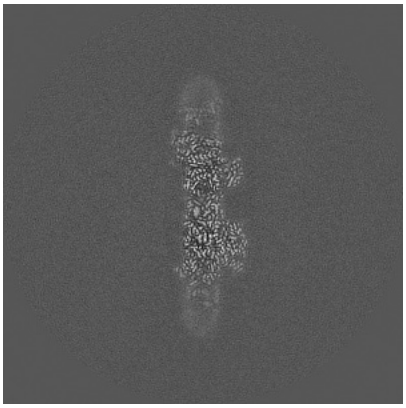
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

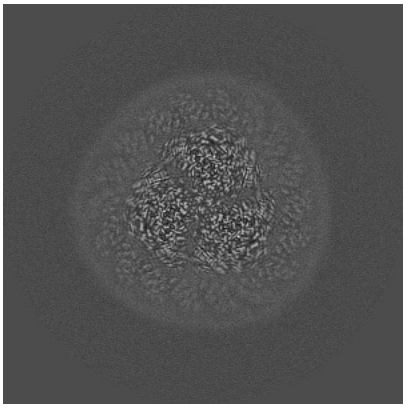
6.3.1 Primary map



X Index: 276



Y Index: 224

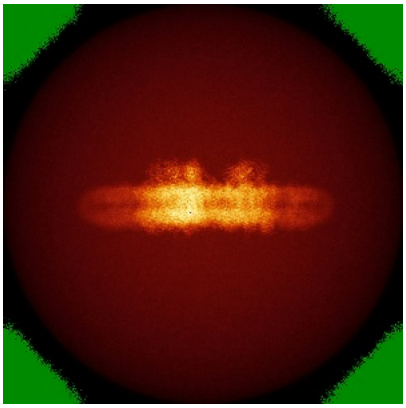


Z Index: 229

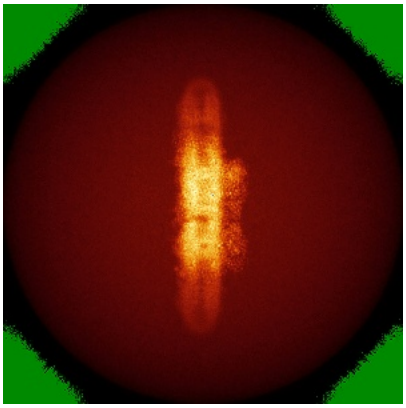
The images above show the largest variance slices of the map in three orthogonal directions.

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

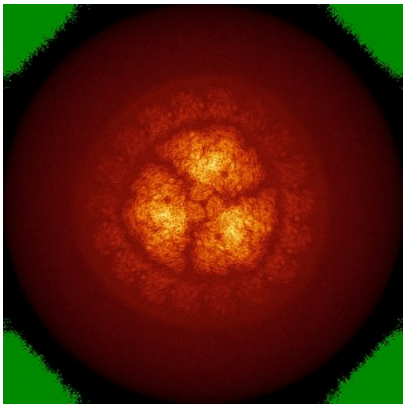
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

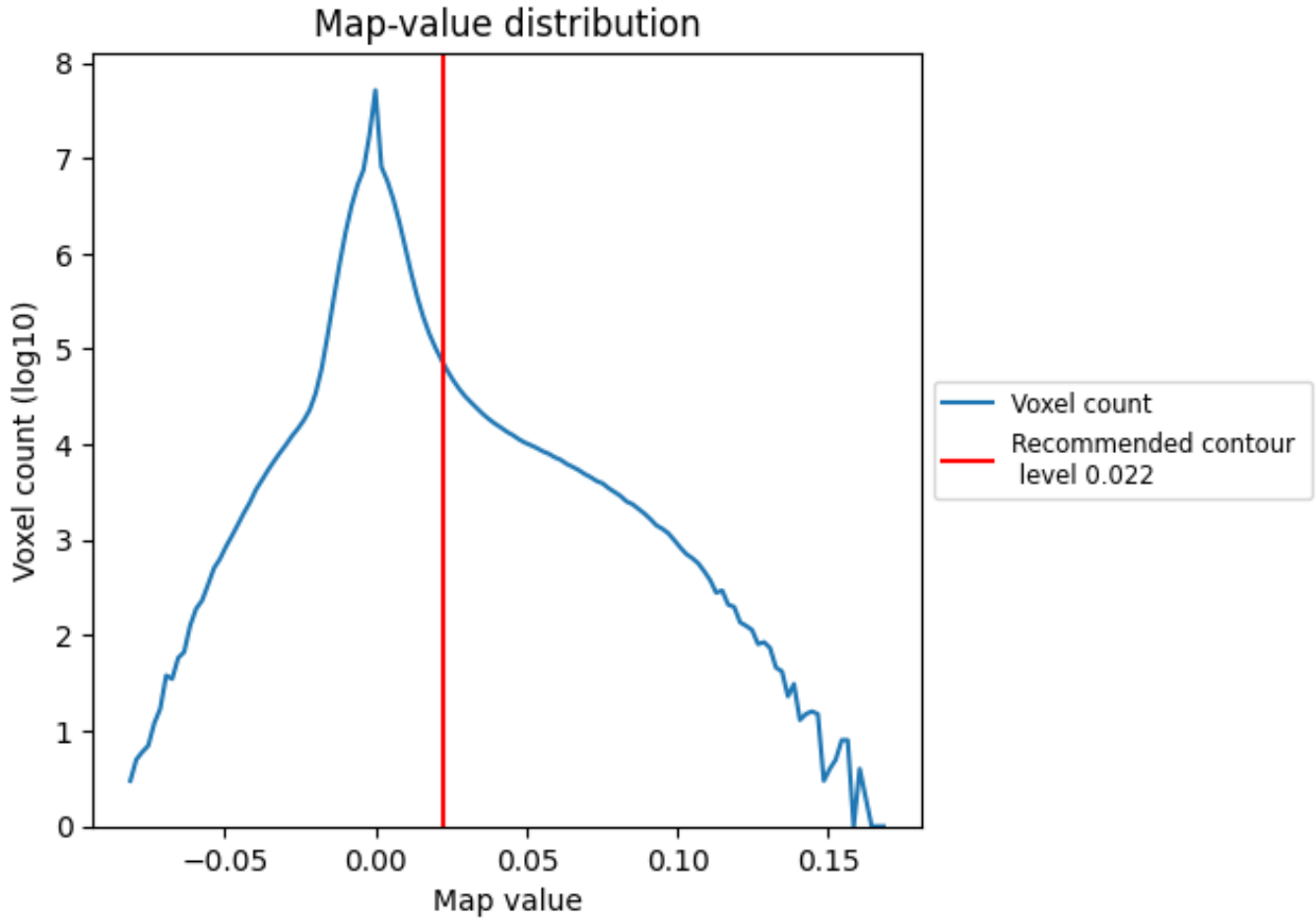
6.6 Mask visualisation (i)

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

7 Map analysis

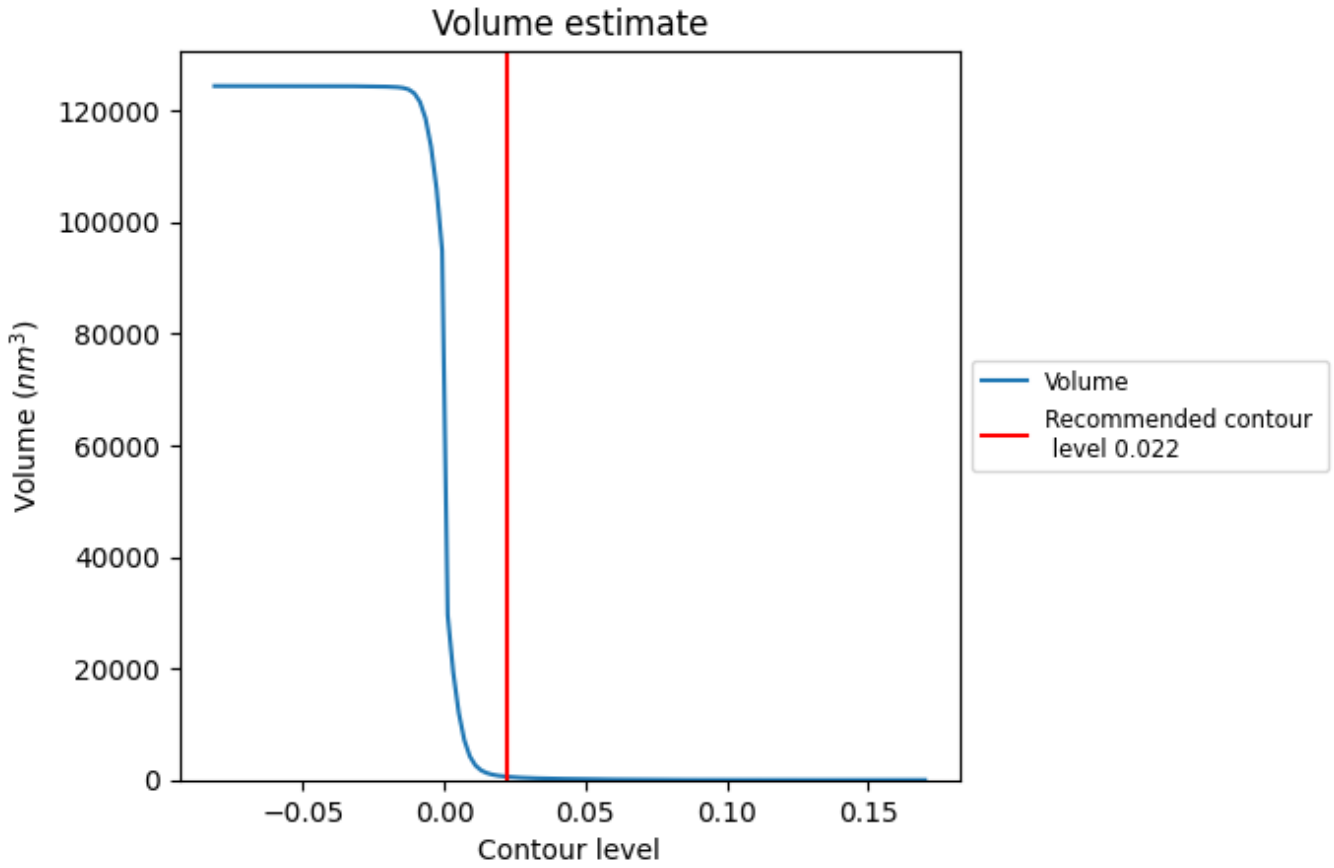
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

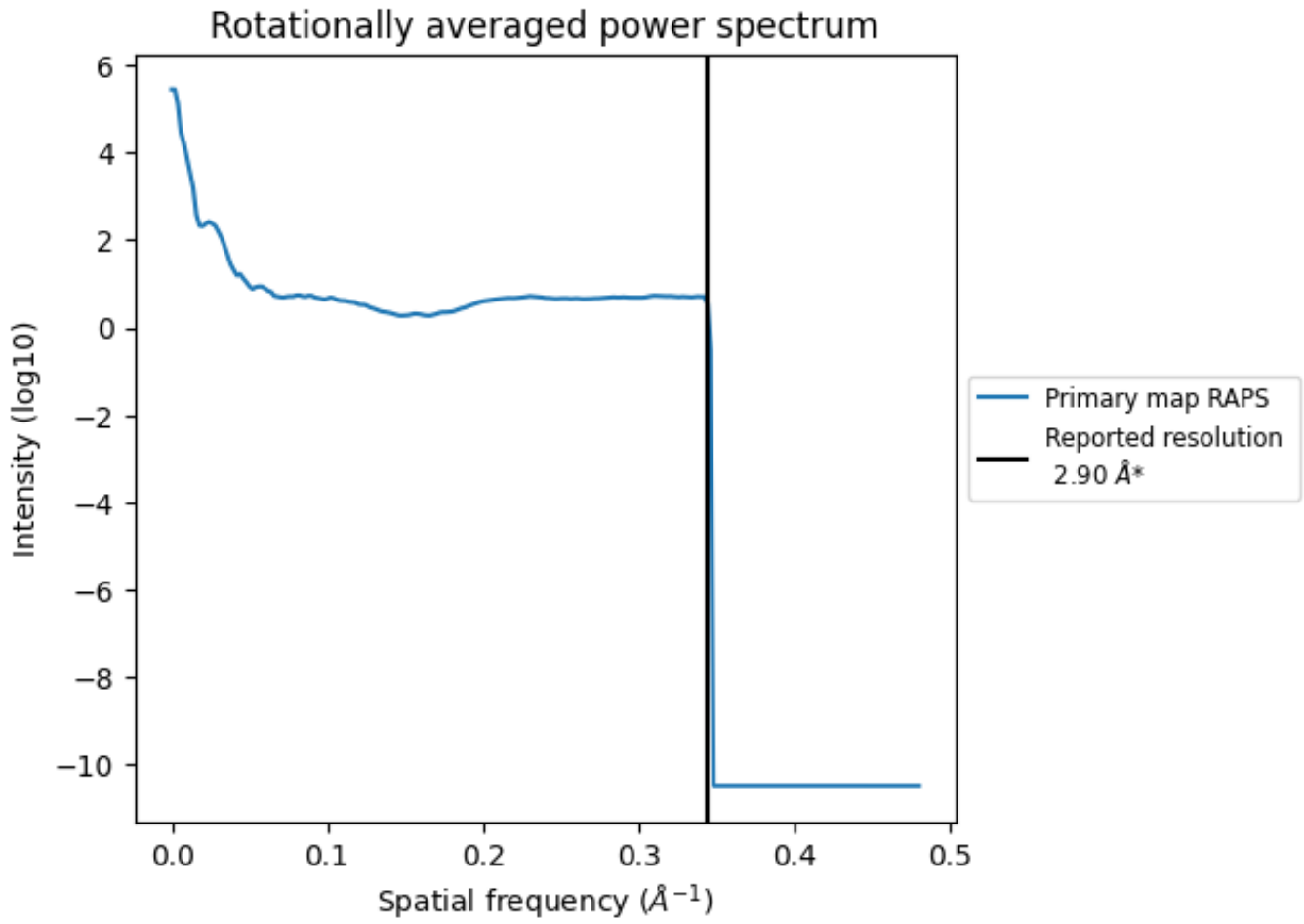
7.2 Volume estimate



The volume at the recommended contour level is 595 nm^3; this corresponds to an approximate mass of 538 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

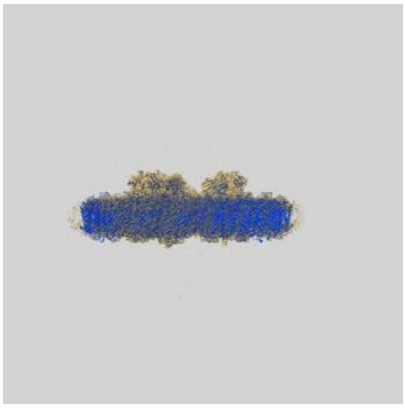
8 Fourier-Shell correlation (i)

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

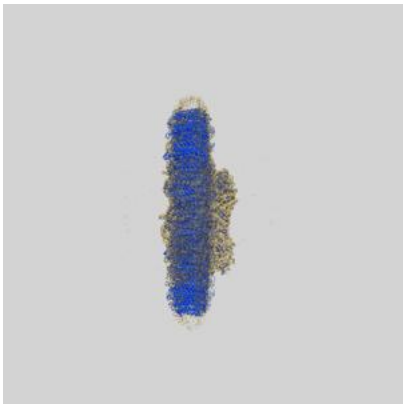
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9995 and PDB model 6KIG. Per-residue inclusion information can be found in section 3 on page 69.

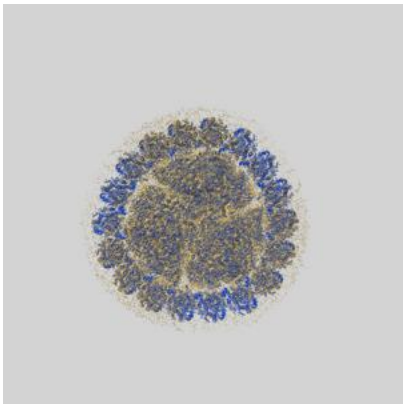
9.1 Map-model overlay



X



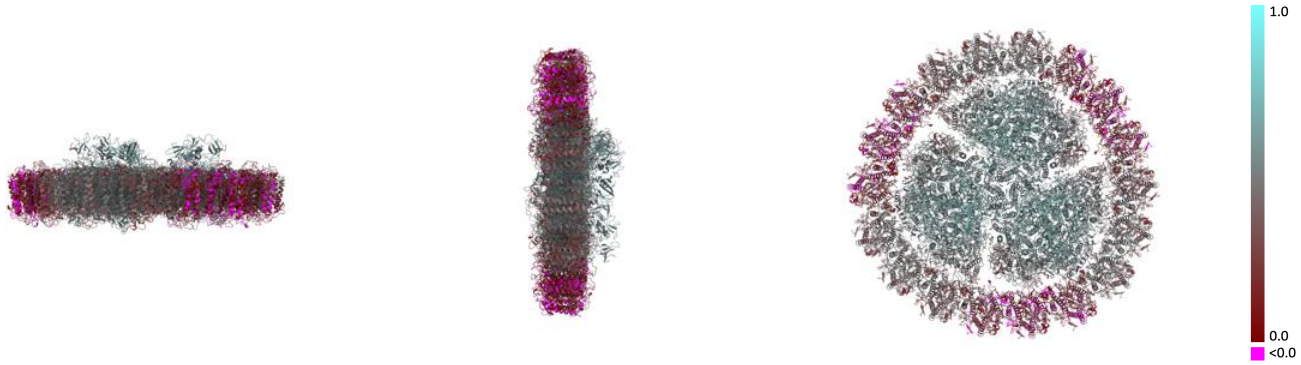
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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)



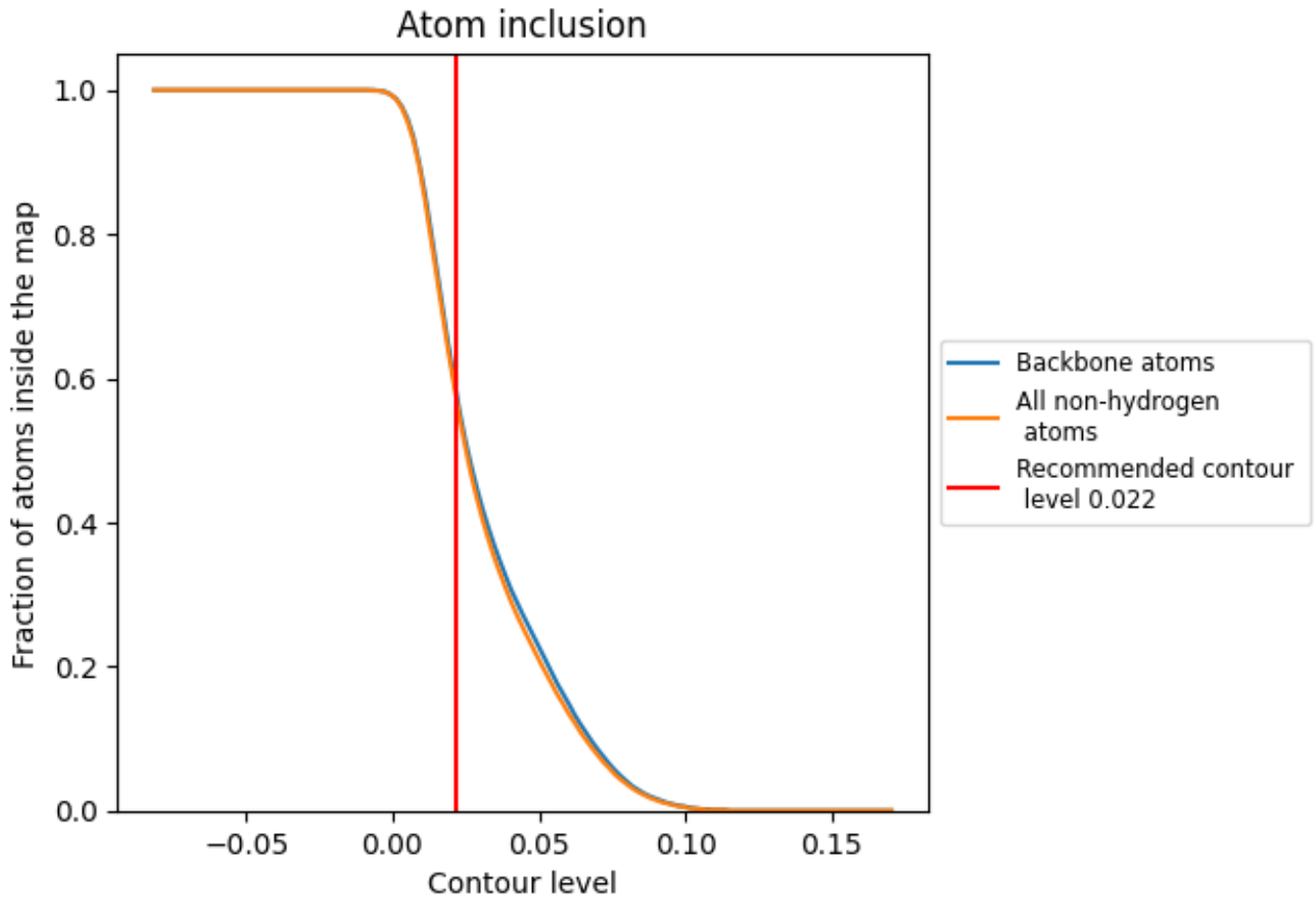
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 56% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5650	0.4190
1	0.4070	0.3640
2	0.4700	0.4180
3	0.3900	0.3830
4	0.1070	0.1410
5	0.0560	0.0860
6	0.1520	0.1850
A	0.8490	0.5780
B	0.8270	0.5450
C	0.9420	0.6070
D	0.8580	0.5770
E	0.7870	0.5410
F	0.7470	0.5290
G	0.8450	0.5770
H	0.8160	0.5370
I	0.8330	0.5720
J	0.7550	0.5460
K	0.5870	0.3890
L	0.8650	0.5930
M	0.7980	0.5290
N	0.9450	0.6070
O	0.8590	0.5780
Q	0.7810	0.5500
R	0.7440	0.5230
S	0.8250	0.5780
T	0.7360	0.5460
U	0.5810	0.3860
V	0.8690	0.5940
W	0.7790	0.5320
Y	0.4060	0.3660
Z	0.4670	0.4160
a	0.3870	0.3780
b	0.1040	0.1380
c	0.0530	0.0780
d	0.1450	0.1710



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.8420	0.5750
f	0.8210	0.5420
g	0.9420	0.6070
h	0.8690	0.5800
i	0.7950	0.5480
j	0.7500	0.5280
k	0.8410	0.5750
l	0.7470	0.5450
m	0.5790	0.3770
n	0.8670	0.5940
o	0.7820	0.5290
q	0.3920	0.3580
r	0.4580	0.4140
s	0.3910	0.3860
t	0.1100	0.1390
u	0.0560	0.0810
v	0.1540	0.1840